

Supporting Information

Assessment of the fragment docking program SEED

*Kenneth Goossens,^a Berthold Wroblowski,^b Cassiano Langini,^c Herman van Vlijmen,^b Amedeo Caflisch^c
and Hans De Winter^a*

^aDepartment of Pharmaceutical Sciences, Laboratory of Medicinal Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk, Belgium

^bJanssen Research and Development, Turnhoutseweg 30, 2340 Beerse, Belgium

^cDepartment of Biochemistry, University of Zurich, Winterthurerstrasse 190, Zurich, CH-8057, Switzerland

Table S1. Summary of the 15 datasets included in this study.

Protein name	Number of fragments in the full library	Number of fragments with <3 rotatable bonds	Comments
BACE	1,210	87	-
BLAC	1,284	734	X-ray structures reveal at least two distinct binding sites for fragment hits.
BTK	3,521	2,467	Fifteen in-house crystallized fragments were added to the initial library.
EPHA4	1,284	743	-
FALZ	395	92	Library was not filtered on the number of rotatable bonds.
HPK1	1,855	1,271	-
HSP90	1,257	724	-
NUDT5	694	279	Library was not filtered on the number of rotatable bonds.
NUDT7	792	228	Flexible binding site with both a hydrophobic and a hydrophilic pocket. Library was not filtered on the number of rotatable bonds.
OGA	1,007	751	350 was screened as a dimer. It is unclear if fragments bind at the dimer interface or not.
PARP14	645	162	Screened as a dimer. Library was not filtered on the number of rotatable bonds.
PCAF	958	534	-
PIM1	1,008	587	While X-ray structures of several protein-fragment complexes exist for this dataset, we had no access to this.
NhDMX	1,319	736	NhDMX interacts with peptides at the binding site, making it a difficult target for FBDD.
KHK	1,072	380	Ten in-house crystallized fragments were added to the initial library.

Table S2. Conformational difference between structure 1 and structure 2 for each target.

Protein name	PDB id: structure 1 / structure 2	RMSD structure 1 / structure 2 ^{a,b}	Number of residues with RMSD >1 Å ^b	Number of residues with RMSD >2 Å ^b
BACE	5HDZ / 2QP8	1.2	19	6
BLAC	4KZ4 / 4KZ5	0.3	1	0
BTK	in-house only	0.7	5	0
EPHA4	2XYU / 2Y6O	0.8	9	1
FALZ	FALZA-x0177 / FALZA-x0309	0.5	2	1
HPK1	in-house only	2.5	27	12
HSP90	3K98 / 2YEC	2.1	7	5
NUDT5	5QJ4 / 5QJA	0.6	2	1
NUDT7	5QGP / 5QGY	1.4	9	3
OGA	5UN9 / in-house	0.8	5	2
PARP14	5QHV / 5QI3	0.6	1	0
PCAF	5FE8 / 5FE9	1.2	8	1
PIM1	1XWS / 3R04	0.9	11	0
NhDMX	in-house only	-	-	-
KHK	in-house only	0.5	3	0

^aBackbone RMSD is considered. ^bOnly residues that were defined as part of the active site by MOE were considered.

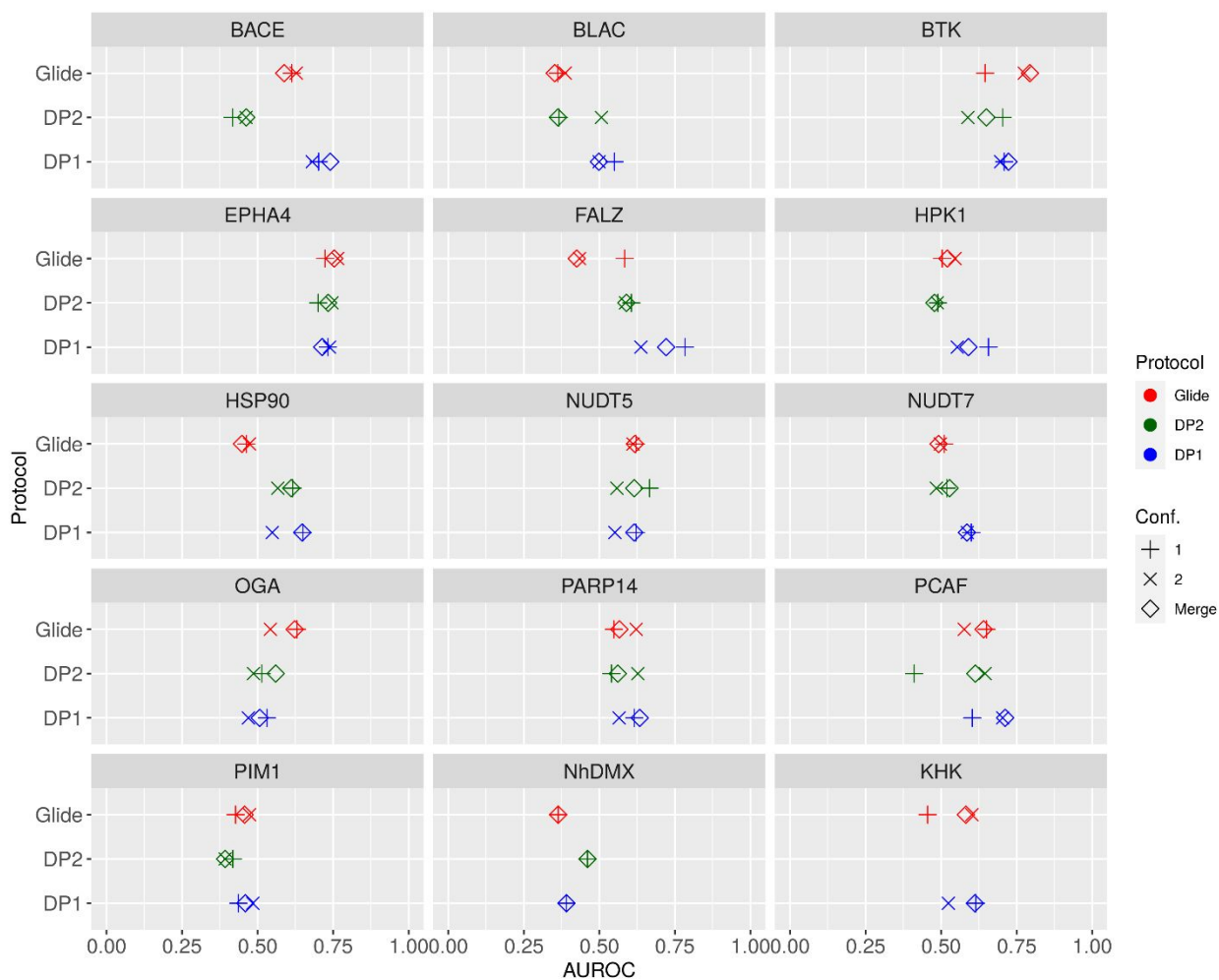


Figure S1. AUROC values for DP1 (blue), DP2 (green) and Glide (red) protocols from screening on all targets. The AUROC for each individual protein conformation is given (pluses and crosses), while the AUROC of a mixed approach is also given (diamonds). In the mixed approach, the output for both protein conformations is merged and the highest score for any given fragment is used to calculate the AUROC, regardless of the protein conformation.

SGC Dataset – FALZA (csv format)

CrystalName,CompoundSMILES,CompoundCode,MountingResult,DataCollectionOutcome,DataProcessingSpaceGroup,DataProcessingUnitCell,DataProcessingResolutionHigh,DataProcessingRmergeLow,DataProcessingIsigLow,DataProcessingIsigHigh,DataProcessingCompletenessOverall,DataProcessingCompletenessLow,DataProcessingCompletenessHigh,DimpleRcryst,DimpleRfree,RefinementRcryst,RefinementRfree,RefinementSpaceGroup,RefinementOutcome,Deposition_PDB_ID

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

,,,Fail_Melted,,,,,,,,,,,,,

FALZA-x0044,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.13,0.021,54.3,1.4,91.4,95.9,48.9,0.17847,0.19422,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0045,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.07,0.019,52.6,1.3,81.0,96.0,17.5,0.17204,0.18210,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0046,,,Mounted_Clear,success,C 1 2 1,110 27 38 90 96
90,1.51,62.697,0.5,0.7,98.9,97.1,97.7,,,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0047,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.09,0.029,38.4,2.2,76.7,95.2,22.8,0.16735,0.17976,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0048,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.06,0.017,66.9,1.7,77.9,97.6,13.1,0.16793,0.18344,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0049,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.14,0.020,45.1,2.0,92.3,94.3,55.5,0.16707,0.18083,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0050,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0051,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.73,0.046,21.8,1.2,98.9,96.6,99.3,0.18637,0.22349,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0052,,,Mounted_Clear,success,C 1 2 1,111 27 38 90 96
90,1.05,0.032,35.4,1.2,75.6,97.4,9.2,0.16915,0.17776, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0053,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.08,0.024,51.6,1.1,81.0,95.7,22.3,0.17216,0.18694, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0054,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.32,0.040,26.8,1.4,99.0,93.3,97.1,0.17739,0.19745, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0055,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.08,0.057,20.1,2.2,81.3,99.0,30.8,0.16948,0.18445, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0056,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.11,0.018,56.2,2.2,88.4,97.7,43.5,0.16645,0.18177, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0057,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.17,0.042,27.2,2.3,95.7,99.4,77.2,0.16934,0.18655, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0058,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.14,0.037,33.3,2.2,88.7,97.5,54.3,0.16920,0.18417, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0059,,,Mounted_Clear,success,C 1 2 1,232 55 72 90 98 90,6.22,-5.559,-
0.1,0.1,98.7,53.3,99.3,,, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0060,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0061,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.33,0.046,23.9,1.3,91.4,96.4,87.0,0.21189,0.23359, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0062,,,Mounted_Clear,success,C 1 2 1,111 27 38 90 96
90,1.15,0.031,43.4,1.3,89.2,92.6,49.7,0.17385,0.19310, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0063,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.18,0.024,41.6,2.2,91.3,95.2,71.6,0.15742,0.16954, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0064,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.24,0.033,37.8,1.2,98.2,93.6,92.1,0.17380,0.19020, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0065,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,2.73,0.129,10.7,3.4,99.3,92.9,99.6,0.23765,0.29884, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0066,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.12,0.036,29.2,2.2,83.8,95.6,39.3,0.16317,0.17923, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0067,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0068,,,Mounted_Clear,success,C 1 2 1,111 27 38 90 96
90,1.10,0.020,56.0,2.2,86.6,98.8,38.5,0.16232,0.17678, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0069,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.14,0.034,36.5,1.7,92.9,95.8,57.1,0.16884,0.18427, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0070,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0071,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.05,0.024,57.2,1.2,78.9,91.7,10.0,0.16581,0.17881, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0072,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.13,0.016,59.9,2.2,91.5,98.7,58.4,0.16184,0.17354, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0073,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.08,0.038,32.6,2.5,83.7,97.3,22.7,0.16491,0.17715, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0074,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.16,0.021,47.6,2.2,94.0,98.5,73.3,0.16239,0.17896, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0075,,,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.14,0.027,39.3,2.2,93.0,97.9,61.2,0.18449,0.19611, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0076,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0077,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0078,,,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,,,,-1 - Data Collection Failed,

FALZA-x0079,CCNC(=O)Oclccc(cc1)c2csnn2,FMOPL000621a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.25,0.014,60.6,2.2,92.0,95.5,84.2,0.17749,0.20187,0.18506,0.20799,C 1 2 1,5
- Deposition ready, None

FALZA-x0080,CCOC(=O)c1c(nc(s1)C)C(F)(F)F,FMSOA000791b,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.13,0.014,72.8,2.3,87.8,96.5,51.1,0.17164,0.18614, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0081,CC(C)COc1ccc(cc1)[C@@H]2C(=O)NC(=O)N2,FMOPL000301a,Mounted_Clear,success,C
1 2 1,112 27 38 90 96 90,1.16,0.019,53.2,2.2,94.9,97.1,72.1,0.17187,0.18903, None, None, C
1 2 1,1 - Analysis Pending, None

FALZA-x0082,CC(C)CNC(=O)c1ccc2ccccc2c1,FMOPL000732a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.22,0.034,31.3,2.1,93.6,97.3,84.3,0.17760,0.19617, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0083,c1ccc(cc1)c2ccccc2NNC(=S)N,FMOPL000624a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.20,0.016,59.9,2.2,97.7,98.1,91.7,0.18076,0.19974, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0084,C[NH+]1CCN(CC1)c2nc3ccccc3s2,FMOPL000478a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.23,0.021,52.7,1.3,94.4,96.3,83.4,0.17843,0.19496, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0085,CC(=O)NCCc1c[nH]c2c1cc(cc2)F,FMOPL000287a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.18,0.016,57.4,2.3,93.3,98.0,76.0,0.17998,0.19590,0.19000,0.20497,C 1 2
1,5 - Deposition ready, None

FALZA-x0086,c1c(cnccl1Br)C(=O)ON,FMOPL000692a,Mounted_Clear,success,C 1 2 1,112 27 38 90
96 90,1.27,0.042,28.0,2.2,98.3,97.7,94.7,0.17985,0.20415, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0087,CC(C)(C)c1ccc(cc1)NNC(=S)N,FMOPL000620a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.17,0.018,58.8,2.2,93.1,97.2,74.6,0.17935,0.19876,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0088,C[NH+](C)CCN1C(=O)c2ccccc2C1=O,FMOPL000477a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.26,0.018,53.8,1.1,95.2,97.3,87.8,0.19186,0.21830,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0089,c1cnc1CCNC(=O)NC2CCCCC2,FMOPL000299a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.17,0.016,62.2,2.2,96.1,97.1,81.8,0.17273,0.18885,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0090,c1cc(oc1)C(=O)OCc2ccc(cc2)Cl,FMOPL000714a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.020,48.3,2.2,90.9,96.0,60.5,0.18037,0.20189,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0091,COC(=O)[C@@H]1C[C@H](CN1C(=O)c2ccco2)O,FMOPL000622a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.18,0.019,53.3,2.2,96.6,96.3,84.4,0.17604,0.18760,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0092,CC(C)(C)NC(=O)Cn1ccc(n1)C(F)(F)F,FMOPL000482a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.23,0.023,51.1,1.2,95.7,87.8,93.9,0.19711,0.21898,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0093,Cc1cc(=O)oc2c1ccc(c2C[NH+](C)C)O,FMOPL000294a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.69,0.033,30.2,2.2,98.6,98.5,98.4,0.17934,0.21650,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0094,Cc1cc(no1)NC(=O)CCC2CCCCC2,FMOPL000741a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.38,0.077,17.6,1.7,86.2,90.8,83.6,0.21140,0.25128,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0095,COC(=O)[C@@H]1C[C@H](CN1C(=O)c2ccco2)O,FMOPL000622a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.23,0.030,32.4,1.3,94.5,97.4,85.0,0.18966,0.20982,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0096,C[C@]1(C(=O)NC(=O)N1)CCc2ccc(cc2)OC,FMOPL000497a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.34,0.017,49.7,1.2,96.1,95.0,93.7,0.18387,0.21042,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0097,c1cc(oc1)CNC(=O)NC2CCCCC2,FMOPL000286a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.13,0.025,43.3,2.4,85.2,95.6,43.5,0.17679,0.19740,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0098,COc1ccc(cc1)CC(=O)Nc2nncs2,FMOPL000738a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.11,0.025,40.5,2.2,86.6,96.8,45.1,0.18092,0.20063,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0099,CC(=O)NCc1cc(no1)c2ccc(cc2)OC,FMOPL000625a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.65,0.027,32.4,10.3,99.7,99.7,99.5,0.20581,0.24708,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0100,CC(C)C(=O)Nc1nnc(s1)COC,FMOPL000282a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.27,0.025,37.0,2.2,98.6,94.4,97.2,0.18282,0.21303,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0101,c1c(nns1)C(=O)NO,SDOOA000892b,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.20,0.018,48.7,2.1,98.3,96.8,95.8,0.18057,0.20554,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0102,CC(C)CC(=O)Nc1ccc(cc1)C(=O)NN,FMOP000483a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.17,0.022,40.4,1.1,96.0,96.0,69.8,0.18799,0.20728, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0103,c1ccc2c(c1)c(c[nH]2)C[NH+]3CCCCC3,FMOP000291a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.16,0.017,53.2,2.2,88.6,97.4,60.9,0.17438,0.19163, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0104,c1cc(ccc1NC(=O)C[NH+]2CCCC2)F,FMOP000715a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.24,0.031,34.1,2.2,98.5,95.4,96.3,0.17496,0.19639, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0105,C#Cc1ccc(cc1)OCc2ccccc2,FMOP000390b,Mounted_Clear,success,C 1 2 1,112 27 38
90 96 90,1.27,0.030,35.5,1.2,98.9,96.9,97.1,0.17843,0.19356, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0106,CC(C)[NH2+]Cc1ccc(cc1)N(C)C,FMOP000463a,Mounted_Clear,success,C 1 2 1,110
27 38 90 95 90,1.20,0.023,37.1,1.3,90.9,96.8,71.7,0.18644,0.20960, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0107,Cc1cccc(c1)C(=O)N2CCC(CC2)C(=O)N,FMOP000307a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.27,0.017,53.2,2.2,97.4,97.6,93.0,0.17633,0.20173, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0108,CCC(=O)Nc1ccc(cc1)N2CCC(CC2)C,FMOP000748a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.14,0.014,64.1,1.0,91.7,97.4,54.9,0.18793,0.20886, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0109,c1ccn(c1)CCNC(=O)C(F)(F)Cl,FMOP000616a,Mounted_Clear,success,C 1 2 1,111 27
38 90 96 90,1.15,0.017,55.8,2.2,94.3,96.6,68.3,0.17560,0.19156, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0110,c1cc(oc1)C(=O)N[C@@H]2CCCCNC2=O,FMOP000472a,Mounted_Clear,success,C 1 2
1,110 27 38 90 95 90,1.57,0.055,22.1,2.1,99.3,92.2,99.5,0.19187,0.23422, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0111,CNC(=O)[C@@H]1CC(=O)N(C1)c2ccc(cc2)OC,FMOP000304a,Mounted_Clear,success,C
1 2 1,111 27 37 90 95 90,1.13,0.022,45.1,2.2,91.2,96.7,54.0,0.18179,0.20196, None, None, C
1 2 1,1 - Analysis Pending, None

FALZA-x0112,C[C@@H](C[NH2+]Cc1ccc2c(c1)OCO2)O,FMOP000709a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.16,0.023,43.1,1.3,95.1,94.2,62.8,0.18212,0.20119, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0113,CC(=O)NCCc1cccc2c1cc(cc2)OC,BDOA011525c,Mounted_Clear,success,C 1 2 1,111
27 38 90 93 90,1.81,0.315,3.2,0.6,99.6,99.2,98.8,0.44531,0.47318, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0114,c1ccc(cc1)C[NH+]2CCC(CC2)n3cccc3,FMOP000492a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.29,0.022,39.2,1.1,95.2,95.7,89.8,0.19435,0.22673, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-
x0115,CC1([C@H]2CC=C([C@@H]1C2)C[NH+]3CCC[C@@H]3CO)C,FMOP000351a,Mounted_Clear,success
,C 1 2 1,111 27 38 90 95
90,1.55,0.063,18.6,2.1,97.9,99.3,96.7,0.19359,0.23209, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-
x0116,C[C@H]1CC[C@H](C1)[NH+]2CCN(CC2)c3cccc3,FMOP000376a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.40,0.046,26.3,1.0,97.4,92.1,95.5,0.19743,0.22930, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0117, c1cc(ccc1C[NH+]2CC[C@H](C2)O)Cl, FMOPL000314a, Mounted_Clear, success, C 1 2
1,111 27 38 90 96 90,1.26,0.037,31.3,1.3,97.7,96.2,91.8,0.17675,0.19751, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0118, Cc1ccsc1C[NH+]2CCC[C@H]2CO, FMOPL000320a, Mounted_Clear, success, C 1 2 1,111
27 38 90 96 90,1.22,0.013,68.9,2.1,95.4,96.3,87.6,0.17195,0.19139, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0119, C[C@H]1CCCC[NH+]1Cc2ccc(cc2)C(=O)OC, FMOPL000375a, Mounted_Clear, success, C 1
2 1,111 27 38 90 96 90,1.28,0.018,50.1,1.2,94.2,97.6,85.9,0.18212,0.21037, None, None, C 1
2 1,1 - Analysis Pending, None

FALZA-x0120, Cc1cc(c(cc1OC)C)C[NH+]2CC[C@H](C2)O, FMOPL000359a, Mounted_Clear, success, C 1
2 1,112 27 38 90 96 90,1.15,0.025,43.5,2.2,93.6,97.1,64.8,0.17492,0.18834, None, None, C 1
2 1,1 - Analysis Pending, None

FALZA-x0121, c1ccc2c(c1)CC[NH+](C2)Cc3ccccc3O, FMOPL000367a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.17,0.031,35.7,1.6,96.1,98.0,72.8,0.18938,0.20762, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0122, CCC1CCC(CC1)[NH+]2CCOCC2, FMOPL000315a, Mounted_Clear, success, C 1 2 1,112 27
38 90 96 90,1.20,0.014,60.9,2.1,91.4,96.4,78.2,0.17730,0.19793, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0123, CCC1CCC(CC1)[NH2+]C[C@H]2CCCO2, FMOPL000326a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.18,0.018,50.9,1.2,97.0,94.7,75.5,0.18198,0.20128, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0124, CC(=O)N1CC[NH+](CC1)CCCc2ccccc2, FMOPL000370a, Mounted_Clear, success, C 1 2
1,111 27 38 90 96 90,1.16,0.016,67.1,2.2,94.6,96.0,77.4,0.17611,0.19316, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0125, Cc1c(nc[nH]1)C[NH+]2CCc3ccccc3C2, FMOPL000358a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.27,0.024,45.8,1.2,96.0,92.9,88.7,0.18466,0.20561, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0126, Cc1c(n2ccccc2n1)C(=O)NCC(C)C, FMOPL000347a, Mounted_Clear, success, C 1 2 1,112
27 38 90 96 90,1.16,0.018,57.5,2.3,95.1,98.1,72.7,0.17297,0.18961, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0127, COC(=O)C1CC[NH+](CC1)CC(=O)N, FMOPL000077a, Mounted_Clear, success, C 1 2 1,112
27 38 90 96 90,1.13,0.023,43.4,1.1,91.1,96.0,45.3,0.18055,0.19553, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0128, C1CCN(CC1)C(=O)N2CCCC2, FMOPL000010a, Mounted_Clear, success, C 1 2 1,112 27 38
90 96 90,1.34,0.026,40.8,1.3,99.4,97.6,99.4,0.18027,0.19982, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0129, c1cc(ccc1C[NH2+]C[C@H]2CCCO2)F, FMOPL000166a, Mounted_Clear, success, C 1 2
1,111 27 38 90 95 90,1.44,0.083,17.6,1.0,99.2,98.0,99.2,0.19052,0.22478, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0130, CCOC(=O)C1CCN(CC1)c2cnccn2, FMOPL000218a, Mounted_Clear, Failed - low
resolution, C 1 2 1,138 32 46 90 95
90,4.03,0.197,2.5,0.5,98.9,94.7,96.1,, None, None, None, 1 - Analysis Pending, None

FALZA-x0131, c1ccnc(c1)NS(=O)(=O)c2ccc(cc2)N, FMOPL000078a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.19,0.086,19.5,1.7,94.6,90.8,80.3,0.19036,0.20789, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0132, c1ccc(c(c1)C(=O)[O-])OC(F)(F)F, FMOPL000013a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.16,0.023,45.2,2.2,91.1,98.9,65.8,0.17817,0.20026, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0133,C1CCCC(CC1)NC(=O)[C@H]2CCCO2,FMOPL000167a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.19,0.014,70.6,2.2,94.9,98.4,81.9,0.17910,0.19549,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0134,c1ccc2c(c1)ncn2Cc3ccc(cc3)C#N,FMOPL000219a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.15,0.013,78.4,2.2,88.3,97.1,55.6,0.17524,0.18894,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0135,CCOc1ccc2c(c1)sc(n2)C,FMOPL000079a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.16,0.021,50.9,2.2,95.2,97.6,72.8,0.17612,0.19331,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0136,COc1cc(cc(c1OC)OC)C[NH3+],FMOPL000011a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.18,0.019,44.7,1.1,96.7,95.8,75.4,0.18296,0.20260,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0137,C1CCC(CC1)NC(=O)NC[C@H]2CCCO2,FMOPL000168a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.41,0.028,35.8,1.4,97.3,97.5,94.8,0.18809,0.21918,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0138,Cn1c(cc(n1)c2cccs2)N,XST00000599c,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.017,60.2,2.2,95.5,97.6,76.0,0.17323,0.18909,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0139,c1ccc(cc1)COc2ccccc2N,FMOPL000014a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.40,0.034,29.0,1.3,99.5,95.3,99.6,0.19667,0.22802,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0140,COc1ccc(cc1)[C@@H](c2ccccc2)[NH3+],FMOPL000169a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.16,0.028,38.2,1.1,89.5,95.4,50.6,0.17826,0.19627,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0141,COCc1nnc(s1)N,FMOPL000544a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.28,0.017,51.2,2.2,96.0,98.2,90.7,0.17798,0.20211,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0142,CCc1cccc1NNC(=S)N,FMOPL000081a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.17,0.058,26.8,2.2,86.5,95.0,61.9,0.18874,0.21156,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0143,c1ccc(cc1)c2ccc(cc2)CC(=O)[O-],FMOPL000015a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.27,0.025,39.9,1.1,96.2,96.9,88.9,0.18420,0.20760,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0144,CCOC(=O)Nc1nc2ccc(cc2s1)C,FMOPL000170a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.26,0.021,42.9,2.1,95.9,97.8,91.0,0.17999,0.20093,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0145,c1cnc([nH]1)c2[nH]ccn2,FMOPL000545a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.33,0.023,40.8,1.5,96.8,91.2,92.9,0.18017,0.21123,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0146,c1cc(sc1)c2ccc(cc2)C[NH3+],FMOPL000080a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.10,0.030,44.1,1.9,86.4,91.7,31.2,0.17917,0.19988,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0147,c1ccc(cc1)C[NH2+]Cc2ccc(cc2)F,FMOPL000016a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.028,35.9,2.2,95.5,98.8,75.8,0.17779,0.20313,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0148,C[C@H]([C@H](c1cccc1)O)[NH2+]C,FMOPL000548a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.021,51.6,2.3,92.4,98.5,63.3,0.17410,0.18757,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0149,CNC(=O)NCc1c(cccc1Cl)F,FMOPL000084a,Mounted_Clear,success,C 1 2 1,112 27 38
90 96 90,1.18,0.014,66.6,2.2,96.6,98.0,85.2,0.17547,0.19389,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0150,C[NH2+]Cclccncc1,FMOPL000017a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.23,0.071,17.3,1.1,98.9,98.4,95.4,0.21031,0.23168,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0151,c1cc(cc(c1)F)NC(=O)c2cnccn2,FMOPL000172a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.27,0.025,32.6,1.1,95.3,96.3,87.6,0.18885,0.21328,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0152,c1ccc2c(c1)[nH]c(n2)NC#N,FMOPL000546a,Mounted_Clear,success,C 1 2 1,110 27
38 90 95 90,1.55,0.017,48.9,1.5,93.3,94.1,82.7,0.18039,0.21672,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0153,c1cn[nH]c1c2cc(cc(c2O)F)F,FMOPL000085a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.17,0.016,53.3,1.1,88.7,94.3,51.7,0.18165,0.19921,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0154,CC(=O)N1CCC(CC1)[NH2+]C2CC2,FMOPL000018a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.14,0.019,55.5,2.2,93.5,97.6,64.5,0.17311,0.18889,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0155,CC(C)[NH+]1CCN(CC1)C(=O)c2cccs2,FMOPL000173a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.25,0.019,46.1,2.1,98.8,97.8,96.3,0.17907,0.19864,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0156,C[NH+](C)CC#Cc1cccc1,FMOPL000549a,Mounted_Clear,success,C 1 2 1,111 27 38
90 96 90,1.31,0.014,63.0,1.3,98.9,96.2,96.7,0.17528,0.20063,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0157,CCc1nc(no1)c2ccc(cc2)Cl,FMOPL000083a,Mounted_Clear,success,C 1 2 1,111 27 38
90 96 90,1.43,0.026,40.3,1.4,99.3,90.8,98.7,0.17352,0.20412,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0158,CN(c1ccc(cn1)C(F)(F)F)N,FMSOA000815b,Mounted_Clear,success,C 1 2 1,112 27 38
90 96 90,1.20,0.014,69.1,2.1,94.2,97.4,83.5,0.18178,0.20287,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0159,Cc1ccc(cc1C)C(=O)Nc2nc[nH]n2,FMOPL000174a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.26,0.052,23.5,2.3,93.8,94.9,86.1,0.17942,0.19676,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0160,Cc1ccc(o1)c2ccccc2N,FMOPL000550a,Mounted_Clear,Failed -
unknown,None,None,None,None,None,None,None,None,None,,None,None,None,-1 - Data
Collection Failed,None

FALZA-x0161,Cc1ccc(o1)c2cccc(c2)N,FMOPL000020a,Mounted_Clear,success,C 1 2 1,112 27 38
90 96 90,1.25,0.023,41.5,1.5,97.6,97.4,92.0,0.18227,0.20265,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0162,c1c(c(=O)[nH]c(=O)[nH]1)N2CCOCC2,FMOPL000552a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.17,0.024,38.9,1.2,95.3,94.6,73.4,0.18492,0.20110,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0163,COc1ccc(cc1)C(=O)NCC(=O)N,FMOPL000090a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.20,0.026,40.6,1.1,96.0,95.9,84.4,0.18389,0.19959,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0164,CS(=O)(=O)Nc1ccc(cc1)C[NH3+],FMOPL000019a,Mounted_Clear,success,C 1 2 1,111
27 38 90 96 90,1.20,0.022,45.1,2.2,96.4,96.7,87.3,0.17344,0.19420,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0165, c1ccc(cc1)C2CC[NH+] (CC2)CC(=O) [O-], FMOPL000176a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.27, 0.014, 58.7, 1.2, 97.0, 93.4, 90.7, 0.18129, 0.20671, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0166, c1cc(ccc1c2cncnc2N)Cl, FMOPL000557a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.14, 0.025, 39.9, 1.1, 92.0, 92.7, 50.5, 0.18601, 0.20987, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0167, COC(=O) c1c(cc(s1) c2cccs2)N, FMOPL000088a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.26, 0.020, 49.0, 2.2, 98.8, 98.2, 96.8, 0.17170, 0.19020, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0168, c1cc(cc(c1)OC(C(F)F)(F)F)N, FMOPL000021a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.38, 0.045, 25.9, 1.2, 99.5, 94.2, 99.5, 0.17984, 0.20270, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0169, C[C@H]1CCCC[NH+]1Cc2ccccc2C#N, FMOPL000177a, Mounted_Precipitate, Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, -1 - Data Collection Failed, None

FALZA-x0170, COc1ccc(c(c1)O)c2cc[nH]n2, FMOPL000554a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.15, 0.026, 39.1, 2.3, 94.4, 97.2, 68.6, 0.17695, 0.19037, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0171, CNC(=O) c1cccc1NC(=O) c2ccco2, FMOPL000751a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.12, 0.031, 37.6, 1.1, 88.3, 97.8, 42.0, 0.18354, 0.20326, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0172, CC(=O)Nc1ccc(cc1)C(=O)Nn2cncnc2, FMOPL000443a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.28, 0.034, 29.4, 1.0, 98.7, 94.4, 97.2, 0.19316, 0.21494, 0.21125, 0.23261, C 1 2 1, 5 - Deposition ready, None

FALZA-x0173, c1cc(cnc1)Cnc2ccc(cc2C(=O) [O-])N, FMOPL000298a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.24, 0.021, 50.6, 1.1, 96.2, 97.1, 88.0, 0.17833, 0.19924, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0174, Cc1c(cccc1Cl)NC(=O) [C@@H]2CCCO2, FMOPL000722a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.27, 0.014, 63.5, 2.2, 95.0, 97.8, 89.3, 0.18174, 0.20687, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0175, C[C@H]1CCCCN1C(=O)N2CCOCC2, FMOPL000392a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.33, 0.024, 44.2, 1.4, 96.6, 96.8, 92.8, 0.18801, 0.21177, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0176, c1ccc(cc1)CC(=O)N2CCc3c2ccccc3, FMOPL000491a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.20, 0.023, 44.5, 1.3, 98.2, 98.1, 89.5, 0.18743, 0.20782, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0177, C1CCN(CC1) c2c(non2)N, FMOPL000280a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.39, 0.025, 43.2, 1.2, 97.0, 97.3, 94.7, 0.19044, 0.22594, 0.20283, 0.24088, C 1 2 1, 5 - Deposition ready, None

FALZA-x0178, CC[C@@H](C)NC(=O) c1cc(on1) c2ccccc2, FMOPL000750a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.12, 0.030, 37.9, 2.3, 89.7, 96.9, 49.8, 0.17902, 0.19752, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0179, CC(C) c1ccc(cc1)NC(=O)N2CCOCC2, FMOPL000442a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.26, 0.017, 56.6, 1.2, 98.2, 93.9, 93.8, 0.18481, 0.20503, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0180,c1cc(ccc1C[NH2+]C2CCCC2)O,FMOPL000467a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.46,0.024,39.2,2.2,97.6,98.1,96.5,0.17139,0.19267,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0181,CC[C@H](C)c1ccc(c(c1)O)NC(=O)C,FMOPL000285a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.22,0.021,44.0,1.3,94.6,90.2,84.2,0.17930,0.19867,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0182,c1cc(ccc1NC(=O)CC#N)OC(F)(F)F,FMOPL000725a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.48,0.034,26.7,1.5,98.9,90.1,99.0,0.18656,0.21648,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0183,Cc1c(c(n[nH]1)C)CCOc2ccc(cc2)F,FMOPL000488a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.016,65.5,2.3,92.0,98.0,70.0,0.17527,0.18796,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0184,Cc1ccc(c(c1)C)OCC(=O)N2CCOCC2,FMOPL000306a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.15,0.030,44.6,1.1,93.6,95.9,63.0,0.17832,0.18936,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0185,c1cc(ccc1C(=O)N)NC(=O)c2cncnc2,FMOPL000758a,Mounted_Clear,success,C 1 2 1,105 26 36 90 95 90,2.52,0.051,11.1,1.0,92.8,87.8,50.3,0.33163,0.41217,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0186,CCn1ccc(n1)C[NH2+]C,FMOPL000384a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.22,0.017,58.6,1.5,95.0,96.8,85.2,0.18009,0.20191,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0187,Cc1ccc(o1)C[NH+] (C)Cc2ccccc2,FMOPL000479a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.14,0.019,54.8,2.3,93.2,96.9,66.4,0.17266,0.19001,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0188,CCOC(=O)c1c(nc(s1)N(C)C(=O)C)C,FMOPL000288a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.29,0.026,40.8,1.3,98.7,94.1,94.3,0.18115,0.20763,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0189,c1ccc(cc1)Nc2nnc3n2nc(cc3)Cl,FMOPL000745a,Mounted_BadDispense,success,C 1 2 1,112 27 38 90 96 90,1.36,0.036,31.6,1.2,99.1,90.2,99.2,0.17991,0.20122,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0190,c1cc2c(cc1C(=O)N3CCCCC3)OCO2,FMOPL000435a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.23,0.017,59.1,2.1,99.0,96.2,97.6,0.17414,0.19214,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0191,COc1ccc(cc1)C(=O)Nc2ccccc2F,FMOPL000496a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.17,0.013,70.4,2.4,95.5,96.8,82.5,0.17386,0.19237,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0192,Cn1nc(nn1)NC(=O)c2ccc(cc2)Cl,FMOPL000290a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.22,0.019,56.6,1.3,98.0,95.6,92.1,0.18474,0.20652,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0193,CC(=O)Nc1ccc(cc1)C#N,FMSOA000445b,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.19,0.018,54.7,2.2,91.7,96.3,74.3,0.17665,0.19540,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0194,Cn1c(c(cn1)NC(=O)c2ccccc2)C(=O)N,FMOPL000456a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.11,0.022,49.4,2.2,87.9,97.9,43.7,0.17744,0.19449,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0195,C1CCC(CC1)C(=O)N2CCC(CC2)C(=O)N,FMOPL000480a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.015,64.0,2.2,89.9,95.2,61.3,0.18053,0.20076,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0196,Cn1nc (nn1)NC(=O)c2cc3ccccc3o2, FMOPL000309a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.20,0.012,72.9,2.1,97.9,98.1,93.7,0.18062,0.20193, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0197, c1cc (cnc1)C[NH2+]C[C@H]2CCC=CC2, FMOPL000760a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.27,0.028,35.6,2.3,98.7,94.6,97.2,0.17337,0.19088, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0198, CC(C)COc1ccc (cc1) [C@H]2C(=O)NC(=O)N2, FMOPL000441a, Mounted_Clear, success, C
1 2 1,112 27 38 90 96 90,1.27,0.035,34.2,1.5,98.1,93.7,95.8,0.19558,0.21864, None, None, C
1 2 1,1 - Analysis Pending, None

FALZA-x0199, C[C@H] (c1cccc1)NC(=O)COC, FMOPL000465a, Mounted_Clear, success, C 1 2 1,112 27
38 90 96 90,1.41,0.021,40.9,2.2,99.4,98.4,99.5,0.17187,0.19111, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0200, CCc1ccc (cc1)C(=O)Nc2nnn (n2)CC, FMOPL000303a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.35,0.029,33.0,1.3,99.2,89.6,99.3,0.18391,0.21361, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0201, CNC(=O)OCc1nccn1C, FMOPL000759a, Mounted_Clear, success, C 1 2 1,111 27 38 90 95
90,1.34,0.031,40.1,1.6,99.0,96.3,98.6,0.20029,0.23043, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0202, COc1ccc (cc1)CNC(=O)CC#N, FMOPL000389a, Mounted_Clear, success, C 1 2 1,112 27 38
90 96 90,1.27,0.019,51.3,2.3,95.0,96.3,87.9,0.17355,0.19434, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0203, COCC(=O)Nc1ccc (cc1)O, FMOPL000462a, Mounted_Clear, success, C 1 2 1,112 27 38 90
96 90,1.19,0.016,55.3,2.2,97.9,98.3,90.1,0.17519,0.19163, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0204, COc1ccc (cc1)C(=O)Nc2nnn (n2)C, FMOPL000302a, Mounted_Clear, success, C 1 2
1,111 27 37 90 95 90,1.25,0.016,58.7,2.1,94.3,98.4,86.7,0.18532,0.21129, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0205, c1ccc (c(c1)C(=O)N)Nc2cccc (c2)Cl, FMOPL000761a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.22,0.019,49.1,2.1,96.7,98.0,90.1,0.17648,0.19493, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0206, Cc1cc (no1)NC(=O)CSc2ccccc2, FMOPL000428a, Mounted_Clear, success, C 1 2 1,111 27
38 90 95 90,1.28,0.015,64.6,2.3,98.2,98.2,94.4,0.17642,0.20351, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0207, Cc1ccc (cc1)OCC(=O)Nc2cc (on2)C, FMOPL000498a, Mounted_Clear, Failed -
unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, -1 - Data
Collection Failed, None

FALZA-
x0208, c1cc (oc1)C(=O)Nc2ccc3c (c2) [nH]c(=O) [nH]3, FMOPL000310a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.23,0.020,45.9,2.2,98.8,96.3,96.5,0.18156,0.20465, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0209, Cc1cccc (c1)C(=O)Nc2ccc (cc2O)C, FMOPL000499a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.58,0.024,30.4,1.3,87.5,94.3,65.3,0.19468,0.24052, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0210, Cc1ccc (cc1)C[NH2+]Cc2ccncc2, FMOPL000289a, Mounted_Clear, success, C 1 2 1,111
27 38 90 96 90,1.23,0.015,53.9,1.2,98.3,93.8,93.0,0.17995,0.20004, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0211,COC(=O)c1ccc(o1)C[NH+]2CCCC2,FMOPL000562a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.17,0.017,58.4,2.3,88.4,94.7,62.1,0.17779,0.19855, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0212,C1CCC(CC1)NC(=O)CC#N,FMOPL000385a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.16,0.019,50.2,1.1,94.3,96.8,66.4,0.18358,0.20732, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0213,c1cc(oc1)CNC(=O)NCc2ccco2,FMOPL000471a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.25,0.024,46.2,2.2,98.7,99.0,94.9,0.17945,0.19881, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0214,c1cc(ccc1C[NH+]2CCC(CC2)C(=O)N)F,FMOPL000346a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.25,0.015,62.5,2.2,97.6,97.0,93.3,0.17700,0.19866, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0215,c1c(nc[nH]1)CC[NH2+]C2CCCCC2,FMOPL000322a,Mounted_Clear,success,C 1 2 1,110 27 38 90 95 90,1.19,0.016,60.3,2.2,95.0,98.1,81.6,0.18099,0.20485, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0216,c1cc(cc(c1)O)C[NH+]2CCSCC2,FMOPL000313a,Mounted_Precipitate,Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, -1 - Data Collection Failed, None

FALZA-x0217,CC(C)c1ccc(cc1)C[NH+]2CCC(CC2)O,FMOPL000348a,Mounted_Precipitate,Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, -1 - Data Collection Failed, None

FALZA-x0218,CCOc1ccc(cc1)C[NH+]2CCSCC2,FMOPL000336a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.46,0.025,31.4,1.1,99.3,96.8,99.8,0.18877,0.22577, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0219,C[NH+](C)CC(=O)c1ccc(cc1)c2ccccc2,FMOPL000377a,Mounted_BadDispense,success,C 1 2 1,112 27 38 90 96 90,1.21,0.020,47.4,1.3,98.0,97.8,90.9,0.17981,0.20241, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0220,Cc1ccc(cc1)C(=O)N[C@@H]2C[C@H]3CC[C@@H]2C3,FMOPL000360a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.018,54.1,2.2,86.2,97.0,51.3,0.18752,0.21111, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0221,Cc1c(non1)NC(=O)N2CCCC2,FMOPL000330a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.34,0.015,61.6,2.2,98.3,99.1,96.5,0.18383,0.21177, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0222,CCN1c2ccccc2nc1NC(=O)CC,FMOPL000352a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.26,0.031,32.2,2.2,99.2,98.9,97.8,0.18173,0.20257, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0223,COc1ccc(cc1OC)C[NH+]2CCOCC2,FMOPL000357a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.20,0.019,50.0,1.3,98.3,97.7,91.4,0.18494,0.20809, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0224,c1cnc(cn1)c2ncc(c(n2)N)C#N,FMOPL000086a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.34,0.021,46.8,2.1,97.6,98.9,95.3,0.19315,0.22105, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0225,c1ccnc(c1)c2ccc(s2)C(=S)N,FMOPL000022a,Mounted_Clear,success,C 1 2 1,110 27 38 90 95 90,2.02,0.056,14.2,1.4,98.8,95.0,97.9,0.20985,0.25752, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0226, c1cc(ccc1c2ccc(o2)CO)N, FMOPL000551a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.28, 0.016, 55.7, 2.2, 98.6, 98.4, 97.3, 0.18719, 0.21210, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0227, CC(C)NC(=O)N[C@@H]1CCCCNC1=O, FMOPL000087a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.28, 0.020, 49.6, 2.2, 99.1, 98.1, 97.2, 0.19233, 0.21105, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0228, c1cc(cnc1)C[NH2+][C@H]2CS(=O)(=O)C[C@@H]2O, FMOPL000179a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.43, 0.018, 45.3, 1.3, 99.3, 91.9, 99.5, 0.18421, 0.21860, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0229, COC(=O)c1cccc(c1)NS(=O)(=O)C, FMOPL000089a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.17, 0.043, 27.7, 2.3, 90.5, 95.7, 66.0, 0.17883, 0.19559, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0230, c1ccc(cc1)COC2CCCC(C2)N, FMOPL000023a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.31, 0.021, 41.8, 2.1, 98.9, 96.8, 98.0, 0.18112, 0.20790, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0231, C[NH+]1CCC(CC1)[NH+]2CCC[C@H](C2)C(=O)[O-], FMOPL000180a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.34, 0.022, 43.4, 2.2, 99.1, 98.2, 98.6, 0.18373, 0.20925, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0232, C[C@@H](C[NH2+])Cc1c(ccc1C1)ClO, FMOPL000555a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.12, 0.032, 36.0, 2.2, 90.4, 98.2, 51.7, 0.19446, 0.21258, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0233, c1csc(c1NC(=O)C(F)(F)F)C(=O)N, FMOPL000092a, Mounted_Clear, success, C 1 2 1, 111 27 37 90 95 90, 1.30, 0.022, 46.5, 1.4, 99.1, 95.9, 98.2, 0.19463, 0.22355, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0234, c1ccc(cc1)C[NH+]2CCO[C@H](C2)CO, FMOPL000024a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.13, 0.070, 23.0, 2.0, 89.3, 98.8, 49.7, 0.19439, 0.21201, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0235, C[NH+]1CCN(CC1)C(=O)c2ccc(c(c2)F)F, FMOPL000181a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 2.19, 0.063, 18.4, 2.1, 99.8, 98.9, 99.8, 0.19562, 0.28364, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0236, c1cc(sc1)c2ccc(s2)c3ccn[nH]3, FMOPL000091a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.13, 0.056, 21.5, 2.2, 92.7, 99.3, 63.0, 0.18118, 0.19836, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0237, CC(C)(C)OC(=O)N1CCC(CC1)[NH2+]C2CC2, FMOPL000025a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.41, 0.023, 40.0, 2.1, 98.5, 97.8, 99.0, 0.17791, 0.21550, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0238, c1ccc(cc1)COCc2c[nH]c(=O)[nH]c2=O, FMOPL000182a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.31, 0.028, 39.0, 1.3, 99.3, 96.7, 98.4, 0.19371, 0.22100, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0239, Cc1ccc2c(c1)c3c([NH2])[C@H](CCC3)[NH3+], FMOPL000564a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.25, 0.019, 49.3, 2.2, 99.2, 98.6, 97.6, 0.18665, 0.20712, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0240, COC(=O)NNc1cc(ccn1)C(F)(F)F, FMOPL000096a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.24, 0.031, 34.9, 1.2, 98.8, 97.0, 97.0, 0.18494, 0.20359, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0241, c1ccc(c(c1)CNC2ccc(cc2)F)CO, FMOPL000183a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.28, 0.020, 51.3, 2.2, 98.3, 98.7, 93.8, 0.17408, 0.19063, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0242, c1ccc(cc1)C[NH+]2CC(=O)NC(=O)C2, FMOPL000558a, Mounted_Clear, success, C 1 2 1, 110 27 38 90 95 90, 1.79, 0.038, 22.7, 1.9, 97.4, 97.2, 99.4, 0.17508, 0.21415, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0243, COc1cccc(c1)c2nc(c(o2)N)C#N, FMOPL000097a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.40, 0.032, 33.0, 1.1, 99.1, 97.8, 99.3, 0.19687, 0.23280, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0244, c1cc(ccc1NNC(=S)N)F, FMOPL000055a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.11, 0.020, 56.4, 2.2, 86.0, 98.2, 43.6, 0.18523, 0.20350, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0245, c1cc(ccc1CC(=O)NC2CCCC2)F, FMOPL000184a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.08, 0.028, 41.0, 2.2, 84.2, 97.9, 32.2, 0.18781, 0.20839, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0246, COc1cccc(c1)c2nnc(s2)N, FMOPL000560a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.17, 0.021, 48.6, 2.1, 96.5, 97.1, 83.2, 0.17752, 0.19459, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0247, c1cc(cc(c1)Cl)N2CC[NH+](CC2)CC#N, FMOPL000094a, Mounted_Clear, success, C 1 2 1, 112 27 37 90 96 90, 1.19, 0.016, 58.8, 2.2, 96.6, 98.6, 87.2, 0.18875, 0.21280, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0248, c1cc(ccc1NC(=O)CC#N)Cl, FMOPL000056a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.15, 0.026, 41.0, 2.2, 87.8, 96.3, 53.8, 0.18064, 0.20194, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0249, CC(C)CC(=O)NCc1ccc2c(c1)OCO2, FMOPL000185a, Mounted_Clear, success, C 1 2 1, 111 27 37 90 95 90, 1.15, 0.020, 52.2, 2.2, 94.1, 98.0, 66.6, 0.18933, 0.21206, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0250, c1ccc(cc1)C#CC[NH+]2CCCC2, FMOPL000559a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.16, 0.019, 51.5, 2.2, 94.7, 97.2, 70.2, 0.18192, 0.20268, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0251, Cc1c(c(c([nH]1)C)C(=O)OC)c2cc[nH]n2, FMOPL000098a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.12, 0.044, 31.3, 2.3, 81.6, 96.3, 34.8, 0.20231, 0.22368, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0252, c1ccc(cc1)c2cc(on2)C[NH3+], FMOPL000057a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.24, 0.028, 35.1, 1.3, 98.9, 95.4, 96.7, 0.18733, 0.20563, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0253, CC(=O)Nc1ccc(cc1)Nc2cccc2, FMOPL000186a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.18, 0.032, 33.5, 2.2, 96.8, 99.3, 84.7, 0.19535, 0.22018, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0254, c1cc(cc(c1)Cl)NC(=O)C[NH+]2CCCC2, FMOPL000567a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.20, 0.024, 45.6, 2.1, 98.2, 97.6, 94.8, 0.17848, 0.19626, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0255, CC(=O)c1ccc(o1)c2ccc(cc2F)F, FMOPL000095a, Mounted_Clear, success, C 1 2 1, 111 27 37 90 95 90, 1.19, 0.020, 52.9, 2.1, 94.3, 98.4, 80.0, 0.18849, 0.21231, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0256, c1cc(ccc1n2cc(nn2)CO)Cl, FMOPL000058a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.49, 0.027, 31.3, 1.1, 98.9, 93.1, 98.3, 0.18155, 0.21692, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0257,CC(=O)Nc1cc(ccc1O)c2ccccc2,FMOPL000187a,Mounted_Clear,success,C 1 2 1,111 27
38 90 95 90,1.20,0.021,47.2,1.3,98.2,95.1,90.1,0.19053,0.21369,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0258,CC(=O)Nc1ccc(cc1)c2csc(n2)N,FMOPL000568a,Mounted_Clear,success,C 1 2 1,110
27 38 90 95 90,1.08,0.020,53.2,2.1,85.0,98.7,33.6,0.18924,0.21153,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0259,c1cc(sc1)c2nc(no2)N3CCCC3,FMOPL000093a,Mounted_Clear,success,C 1 2 1,112 27
37 90 96 90,1.27,0.013,62.1,2.2,99.0,98.8,97.3,0.19038,0.21826,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0260,CC(=O)Nc1ccc(cc1)OCC(=O)[O-],FMOPL000059a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.13,0.015,61.0,2.2,91.5,96.8,58.9,0.18828,0.20717,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0261,Cc1nc(c(s1)NC(=O)OC)c2ccccc2,FMOPL000188a,Mounted_Clear,success,C 1 2 1,111
27 37 90 96 90,1.25,0.033,33.9,1.3,97.3,95.4,91.5,0.19482,0.22506,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0262,Cc1cc(nn1c2ccccc2)NC(=O)OC,FMOPL000105a,Mounted_Clear,success,C 1 2 1,111 27
38 90 95 90,1.21,0.014,67.2,2.1,97.2,98.4,89.1,0.18453,0.20872,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0263,c1cc(oc1)CNC(=O)Nc2ccc(cc2)F,FMOPL000189a,Mounted_Clear,success,C 1 2 1,111
27 38 90 95 90,1.37,0.016,54.5,2.2,99.8,98.7,99.8,0.18053,0.21019,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0264,Cc1ccc2c(c1)c3c([nH]2)[C@@H](CCC3)C#N,FMOPL000572a,Mounted_Clear,success,C
1 2 1,111 27 38 90 95 90,1.49,0.032,28.8,1.1,99.2,94.6,98.6,0.18809,0.22707,None,None,C
1 2 1,1 - Analysis Pending,None

FALZA-x0265,c1cc2c(cc1C[NH2+]C[C@@H]3CCC=CC3)OCO2,FMOPL000300a,Mounted_Clear,success,C
1 2 1,111 27 38 90 95 90,1.49,0.031,29.3,1.3,99.4,88.1,98.9,0.18194,0.22104,None,None,C
1 2 1,1 - Analysis Pending,None

FALZA-x0266,c1ccc2c(c1)[nH]c(n2)NCc3ccco3,FMOPL000565a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.34,0.027,31.6,1.1,99.0,94.6,98.5,0.19421,0.22538,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0267,CC(=O)N[C@@H](Cc1ccc(cc1)O)C(=O)NN,FMOPL000484a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.51,0.045,22.4,2.2,99.3,99.1,99.2,0.21050,0.24928,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0268,c1ccnc(c1)C[NH2+]Cc2ccc3c(c2)OCO3,FMOPL000297a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.39,0.018,48.3,2.1,99.3,97.8,99.6,0.17779,0.20982,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0269,c1ccc(cc1)CCnc2[nH]c3ccccc3n2,FMOPL000586a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.22,0.022,39.3,2.1,97.2,95.5,92.1,0.18429,0.20723,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0270,C[C@@H](CNC(=O)Nc1cccc1)O,FMOPL000464a,Mounted_Clear,success,C 1 2 1,111 27
38 90 95 90,1.23,0.045,32.1,1.4,96.5,96.2,91.2,0.21986,0.24281,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0271,CC(C)(C)NC(=O)N1CCC(CC1)C(=O)OC,FMOPL000292a,Mounted_Clear,success,C 1 2
1,111 27 38 90
90,1.18,0.022,40.4,2.1,96.1,96.3,82.9,0.19096,0.21345,0.20877,0.22536,C 1 2 1,5 -
Deposition ready,None

FALZA-x0272, c1ccc(cc1)CCNC(=O)c2ccc(=O)oc2, FMOPL000585a, Mounted_Clear, success, C 1 2
1,112 27 37 90 96 90,1.15,0.021,47.6,2.2,91.0,97.0,62.5,0.18488,0.20534, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0273, Cc1cc(nol)C(=O)NCC(=O)OC, FMOPL000387a, Mounted_Clear, success, C 1 2 1,111 27
38 90 95 90,1.43,0.029,35.7,1.2,98.8,90.9,97.9,0.18646,0.22527, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0274, c1cc(cc(c1)O)NC(=O)Nc2ccc(cc2)F, FMOPL000500a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.22,0.020,40.1,1.2,91.4,92.5,80.1,0.19504,0.22176, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0275, CCc1nnc(s1)NC(=O)C[NH+](C)C, FMOPL000283a, Mounted_Clear, success, C 1 2 1,111
27 37 90 95 90,1.29,0.019,48.9,2.2,99.2,98.9,96.3,0.18921,0.22017, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0276, CC1(C[C@H](CCO1)C(=O)Nc2ccccc2)C, FMOPL000592a, Mounted_Clear, success, C 1 2
1,111 27 38 90 95 90,1.47,0.032,31.7,2.3,99.4,99.7,99.0,0.18310,0.22127, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0277, Cn1ccc(n1)C(=O)Nc2cccc(c2)C(=O)[O-], FMOPL000457a, Mounted_Clear, success, C 1
2 1,110 27 38 90 95 90,1.45,0.018,46.9,2.3,99.1,97.2,99.7,0.17296,0.20056, None, None, C 1
2 1,1 - Analysis Pending, None

FALZA-x0278, c1ccc(cc1)OCC(=O)Nc2ccccc2O, FMOPL000490a, Mounted_Clear, success, C 1 2 1,110
27 38 90 95 90,1.31,0.031,34.1,2.1,97.7,93.0,96.4,0.18609,0.21179, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0279, c1cc(ccc1C[NH2+])Cc2ccc(cc2)F)C#N, FMOPL000296a, Mounted_Clear, success, C 1 2
1,112 27 38 90 96 90,1.32,0.022,44.1,2.1,99.5,98.9,99.0,0.18901,0.21476, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0280, CC(C)C(=O)Nc1nnn(n1)C, FMOPL000547a, Mounted_Clear, success, C 1 2 1,111 27 38
90 96 90,1.25,0.046,29.1,1.2,98.6,91.2,97.3,0.19169,0.21882, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0281, c1ccc(cc1)NS(=O)(=O)c2ccc(cc2)N, FMOPL000432a, Mounted_Clear, success, C 1 2
1,111 27 38 90 95 90,1.20,0.018,51.5,1.2,97.7,96.7,89.8,0.18517,0.20661, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0282, CC[C@H](CO)NC(=O)Nc1ccc(cc1)Cl, FMOPL000476a, Mounted_Clear, success, C 1 2
1,111 27 38 90 95 90,1.25,0.031,37.7,1.2,97.9,90.2,92.9,0.18233,0.20499, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0283, COc1cccc(c1)C[NH+]2CCC(CC2)C(=O)N, FMOPL000305a, Mounted_Clear, success, C 1 2
1,110 27 38 90 95 90,1.40,0.026,38.7,1.1,97.5,94.3,95.8,0.18266,0.21282, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0284, c1ccc(cc1)Coc2ccccc2C(=O)NN, FMOPL000587a, Mounted_Clear, success, C 1 2 1,111
27 38 90 95 90,1.15,0.015,62.0,2.2,93.6,96.1,67.5,0.17720,0.19392, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0285, c1c(c(=O)[nH]c(=O)[nH]1)NC2CCCC2, FMOPL000388a, Mounted_Clear, success, C 1 2
1,111 27 38 90 95 90,1.37,0.031,33.3,1.0,95.2,98.0,93.2,0.20067,0.22525, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0286, C[C@H](C[NH2+])C1CCCC1O, FMOPL000461a, Mounted_Clear, success, C 1 2 1,111 27
38 90 95 90,1.40,0.025,40.5,2.1,98.7,97.9,99.4,0.16957,0.19861, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0287, c1c(nns1)C(=O)N2CCOCC2, FMOPL000281a, Mounted_Clear, success, C 1 2 1,110 27 37
90 95 90,1.33,0.027,35.9,2.1,98.7,97.1,97.7,0.19585,0.22428, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0288,C[C@@H](C(=O)OC)NC(=O)N1CCOCC1,FMOPL000563a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.38,0.052,22.5,2.1,99.6,97.9,99.6,0.18384,0.21440,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0289,c1ccc(cc1)[C@@H]2C[C@H]2C(=O)Nc3nccs3,FMOPL000417a,Mounted_Clear,success,C
1 2 1,112 27 38 90 96 90,1.10,0.044,30.5,2.9,78.6,98.3,33.9,0.19719,0.21619,None,None,C
1 2 1,1 - Analysis Pending,None

FALZA-x0290,c1cc(c(cc1C(F)(F)F)N)N2CCCCC2,FMOPL000263a,Mounted_BadDispense,success,C 1
2 1,111 27 38 90 95 90,1.36,0.019,45.8,2.2,99.4,97.7,99.5,0.17894,0.21156,None,None,C 1
2 1,1 - Analysis Pending,None

FALZA-x0291,COc1cc(cc(c1)OC)C(=O)Nn2cnnc2,FMOPL000451a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.44,0.047,24.5,2.1,98.8,99.3,97.7,0.21438,0.24167,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0292,c1ccnc(c1)NC(=O)c2cnccn2,FMOPL000469a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.25,0.021,47.1,2.2,99.4,98.8,97.5,0.18955,0.21530,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0293,COC(=O)c1cccc2c1-c3cccc3C2=O,FMOPL000264a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.40,0.029,32.0,2.1,98.5,95.7,97.3,0.17865,0.20971,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0294,c1cc(cc(c1)F)NCC2ccc3c(c2)OCO3,FMOPL000650a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.14,0.023,45.2,2.3,93.2,97.7,63.9,0.17848,0.19647,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0295,Cc1c(sc(n1)NC(=O)OC)C(=O)N(C)C,FMOPL000409a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.29,0.030,47.7,1.5,98.0,95.8,94.5,0.19710,0.22146,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0296,COc1ccc2c(c1)sc(n2)NC(=O)C3CC3,FMOPL000487a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.19,0.017,55.0,2.2,97.6,98.4,89.3,0.18862,0.21160,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0297,CCOC(=O)Nc1cccc(c1)Cl,FMOPL000260a,Mounted_Clear,success,C 1 2 1,112 27 38
90 96 90,1.35,0.061,19.2,2.2,97.9,98.0,97.2,0.19675,0.22289,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0298,c1cc(cnc1)Nc2nnc(s2)C(F)(F)F,FMOPL000643a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.36,0.040,38.5,1.6,98.6,97.5,99.1,0.21137,0.23702,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0299,CC(C)C(=O)N1CCC(CC1)Cc2ccccc2,FMOPL000438a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.23,0.037,31.2,2.2,96.8,98.2,89.6,0.17972,0.19587,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0300,CC(C)NC(=O)c1ccc2ccccc2n1,FMOPL000474a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.26,0.027,40.4,2.2,99.0,98.8,95.4,0.18257,0.20292,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0301,Cc1ccc(o1)C[NH+] (C)C,FMOPL000259a,Mounted_Clear,success,C 1 2 1,112 27 38 90
96 90,1.14,0.021,44.2,2.2,92.9,97.5,60.8,0.18262,0.20381,None,None,C 1 2 1,1 - Analysis
Pending,None

FALZA-x0302,CN(C)C(=O)Nc1cnccc1C(F)(F)F,FMOPL000641a,Mounted_Clear,success,C 1 2 1,111
27 38 90 96 90,1.42,0.020,42.8,1.3,97.9,96.0,96.1,0.19288,0.22917,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0303,C[NH+]1CCN(CC1)C(=O)Nc2ccccc2,FMOPL000408a,Mounted_Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, -1 - Data
Collection Failed, None

FALZA-x0304,CCC(=O)Nc1ccc2c(c1)[nH]c(=O)[nH]2,FMOPL000468a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.17,0.025,43.8,2.2,92.0,98.0,68.3,0.18635,0.20590,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0305,C1CC[NH+](C1)C[C@H](CO)O,FMOPL000258a,Mounted_Clear,success,C 1 2 1,111 27
38 90 96 90,1.20,0.024,41.1,2.2,98.5,98.6,93.6,0.17978,0.20026,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0306,COCc1nnc(s1)NC(=O)c2ccccc2,FMOPL000424a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.18,0.031,35.2,2.2,97.4,98.7,87.9,0.18423,0.20395,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0307,CC(C)C(=O)NCc1[nH]c2ccccc2n1,FMOPL000473a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.33,0.026,39.0,1.3,98.8,97.1,97.0,0.20400,0.23051,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0308,c1cc(cc(c1)C1)C[NH+]2CCOCC2,FMOPL000312a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.28,0.029,50.0,1.8,98.9,97.6,96.4,0.19556,0.22053,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0309,CC(=O)Nc1ccc(cc1)C[NH+]2CCOCC2,FMOPL000349a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.13,0.016,55.7,1.5,91.1,95.2,46.0,0.17658,0.19324,0.19287,0.20909,C 1 2 1,5 -
Deposition ready,None

FALZA-x0310,Cc1cccc(c1)C[NH+]2CCOCC2,FMOPL000319a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.19,0.023,45.4,2.1,97.8,99.2,90.8,0.18819,0.20939,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0311,CC(C)(C)C1CCC(CC1)[NH2+]Cc2ccncc2,FMOPL000368a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.13,0.024,44.8,2.2,88.7,96.0,53.6,0.17224,0.18850,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0312,Cc1cc(cc(c1NC)C)[N+](C)(C)C,FMOPL000318a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.13,0.027,42.2,2.2,92.7,98.8,62.2,0.18499,0.20524,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0313,c1cc(ccc1OCC(=O)N2CCCC2)F,FMOPL000332a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.17,0.033,33.2,2.2,96.1,97.3,79.9,0.17990,0.19359,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0314,COCC(=O)Nc1nc(cs1)c2ccccc2,FMOPL000355a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.33,0.019,49.5,2.2,99.6,99.3,98.5,0.19126,0.21798,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0315,c1ccc(cc1)CCC(=O)Nc2ccc(cc2)O,FMOPL000363a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.19,0.048,24.2,1.2,96.0,91.5,80.1,0.19036,0.21152,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0316,c1ccc2c(c1)OC[C@H](O2)C(=O)N3CCOCC3,FMOPL000366a,Mounted_Clear,success,C 1
2 1,112 27 38 90 96 90,1.33,0.045,25.3,2.1,99.4,97.3,98.6,0.19257,0.21937,None,None,C 1
2 1,1 - Analysis Pending,None

FALZA-x0317,c1ccc(cc1)CNc2ccc(cc2)C(=O)[O-],FMOPL000343a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.24,0.031,33.5,1.1,97.7,96.8,91.5,0.17730,0.19719,None,None,C 1 2
1,1 - Analysis Pending,None

FALZA-x0318,c1ccc(cc1)SCC(=O)NC2CCCC2,FMOPL000344a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.18,0.019,55.7,2.2,97.2,98.5,85.3,0.17877,0.19558,None,None,C 1 2 1,1 -
Analysis Pending,None

FALZA-x0319, COCC(=O)Nc1cccc1C(=O)N, FMOPL000329a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.17, 0.023, 42.5, 2.1, 88.7, 96.2, 65.0, 0.18974, 0.20929, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0320, c1ccc(cc1)Coc2ccc(cc2)C(=O)N, FMOPL000099a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.11, 0.025, 44.3, 2.1, 89.4, 98.2, 48.7, 0.19252, 0.21569, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0321, CCOc1ccc(cc1)NC(=O)NC(C)(C)C, FMOPL000041a, Mounted_Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, -1 - Data Collection Failed, None

FALZA-x0322, CC[NH+]1CCN(CC1)C(=O)NC2CCCC2, FMOPL000190a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.09, 0.019, 50.8, 2.3, 82.2, 95.8, 31.6, 0.18822, 0.20924, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0323, COc1ccc2cc(ccc2c1)c3cc[nH]n3, FMOPL000102a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.14, 0.019, 53.5, 2.2, 92.9, 98.3, 66.1, 0.19157, 0.21249, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0324, CC1(CC(=CC(=O)C1)Nc2cccc(c2)O)C, FMOPL000040a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.24, 0.018, 56.4, 2.2, 98.6, 97.4, 97.5, 0.18964, 0.21566, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0325, c1cnc1c2nc(on2)C3CCCC3, FMOPL000191a, Mounted_Clear, success, C 1 2 1, 111 27 37 90 95 90, 1.28, 0.028, 39.1, 1.3, 96.5, 97.4, 89.6, 0.19687, 0.22806, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0326, CCCn1c(nnn1)NC(=O)c2cccs2, FMOPL000569a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.19, 0.026, 41.1, 1.3, 97.6, 97.8, 80.9, 0.17987, 0.19858, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0327, Cn1c(c(c(n1)C(F)(F)F)c2ccccc2)N, XST00000908c, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.19, 0.022, 43.5, 1.3, 97.2, 93.0, 84.2, 0.18796, 0.20863, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0328, C[C@H]1CC[C@H](C1)[NH2+]Cc2ccc3c(c2)OCO3, FMOPL000043a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.13, 0.021, 49.9, 2.3, 91.5, 96.7, 55.9, 0.17562, 0.19121, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0329, c1ccn(c1)c2ccc(cc2)N3CCOCC3, FMOPL000192a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.18, 0.017, 59.0, 2.1, 96.3, 98.1, 83.9, 0.18835, 0.21258, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0330, COc1cccc1N2CC[NH+](CC2)CC#N, FMOPL000103a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.27, 0.039, 29.9, 1.3, 98.9, 96.4, 96.9, 0.18297, 0.20580, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0331, CC1CCN(CC1)c2ccc(cc2N)C(=O)[O-], FMOPL000193a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.29, 0.031, 33.2, 1.3, 98.6, 94.6, 95.5, 0.18733, 0.21637, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0332, Cc1cc(no1)c2nc(on2)c3ccccc3, FMOPL000106a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.17, 0.022, 42.5, 1.2, 96.4, 95.6, 71.3, 0.18769, 0.21330, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0333, Cc1ccc(cc1)C(=O)n2cnc3c2ccccc3, FMOPL000194a, Mounted_Clear, success, C 1 2 1, 110 27 37 90 94 90, 1.67, 0.021, 35.9, 1.2, 99.2, 96.5, 99.7, 0.18307, 0.21726, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0334,Cc1cc(no1)C(=O)NNc2ccccc2F,FMOP000104a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.51,0.022,32.9,1.3,98.4,94.9,98.8,0.17777,0.21516,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0335,c1ccc2c(c1)ccc(c2O)C[NH+]3CCOCC3,FMOP000195a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.20,0.018,55.5,2.2,97.3,98.8,90.3,0.19084,0.21342,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0336,c1cc(ccc1C(=O)[O-])Oc2ccc(cc2)N,FMOP000584a,Mounted_Clear,success,C 1 2 1,110 27 38 90 94 90,1.77,0.024,34.0,1.5,99.3,96.3,99.6,0.18434,0.22768,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0337,c1cc2c(cc1NC(=O)NCC3CC3)CCO2,FMOP000100a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.12,0.040,32.6,1.1,89.9,95.2,42.1,0.19391,0.22090,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0338,CC(C)(C)NC(=O)Nc1ccccc1C(=O)N,FMOP000039a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.58,0.033,29.2,2.1,97.0,97.6,95.1,0.19247,0.23449,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0339,c1cc2c(cc1C[NH2+])Cc3ccncc3)OCO2,FMOP000196a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.10,0.028,41.8,2.2,86.7,97.8,38.3,0.17451,0.19031,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0340,CC1CC[NH+] (CC1)Cc2c[nH]c3c2ccccc3,FMOP000576a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.17,0.022,48.5,1.5,95.1,96.8,73.8,0.19281,0.21777,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0341,COc1ccc(cn1)NC(=O)Nc2cccs2,FMOP000101a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.28,0.019,47.4,1.3,99.2,95.9,97.3,0.17754,0.20101,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0342,c1cc(ccc1N2C(=O)CCC2=O)OCC(=O)[O-],FMOP000045a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.63,0.022,39.8,2.1,99.4,99.0,98.5,0.16925,0.20678,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0343,Cc1ccccc1OCC(=O)Nc2ccncc2,FMOP000197a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.20,0.022,41.0,1.2,98.3,96.4,90.0,0.18911,0.21400,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0344,c1ccc2c(c1)ncn2Cc3ccc(cc3)F,FMOP000574a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.30,0.017,54.4,2.2,99.1,98.2,96.9,0.18017,0.20424,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0345,Cc1nccc(n1)c2ccccc2)NC(=O)NC,FMOP000110a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.29,0.019,52.7,2.2,97.2,99.0,92.2,0.18690,0.21309,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0346,c1ccc(cc1)CCNC(=O)NC2CCCC2,FMOP000046a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.13,0.025,41.3,2.2,92.1,97.9,56.8,0.18498,0.20265,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0347,Cc1cccc(c1)NC(=O)C[NH+]2CCOCC2,FMOP000198a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.019,56.4,2.2,92.8,97.2,59.7,0.17545,0.19488,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0348,CCOC(=O)c1cc(no1)c2ccc(cc2)C,FMOP000579a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.020,42.0,1.4,92.2,95.6,50.0,0.19056,0.21245,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0349,c1cc(ccc1CNC(=O)N2CCOCC2)C#N,FMOP000108a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.42,0.025,36.7,1.7,99.3,96.2,98.7,0.18113,0.20993,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0350,CC[C@@H](C)[NH+]1CCN(CC1)C(=O)c2ccncc2,FMOPL000199a,Mounted_Clear,success,C 1 2 1,110 27 38 90 95 90,1.37,0.026,35.5,2.1,97.0,97.2,95.5,0.17432,0.20021, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0351,CCOC(=O)c1cc(no1)c2ccc(cc2)F,FMOPL000580a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.18,0.015,67.0,2.3,96.4,98.6,83.8,0.18906,0.20907, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0352,c1c(cncc1C(=O)[O-])C#CCC2CCCCC2,FMOPL000109a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.014,64.9,2.4,92.5,97.5,69.2,0.18485,0.20663, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0353,c1ccc(cc1)NC(=O)N2CCC(CC2)C(=O)N,FMOPL000200a,Mounted_Clear,success,C 1 2 1,111 27 37 90 96 90,1.22,0.014,64.9,2.1,98.9,97.7,96.5,0.18669,0.20854, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0354,CC(C)COc1ccc(cc1)c2csc(n2)N,FMOPL000575a,Mounted_Clear,success,C 1 2 1,112 27 37 90 96 90,1.17,0.030,35.1,1.4,93.3,90.7,64.8,0.19331,0.21763, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0355,c1ccc(cc1)[C@@H](CNC(=O)c2ccccc2)O,FMOPL000107a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.30,0.023,42.5,2.2,99.5,98.5,98.8,0.17945,0.20531, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0356,CC1(CC(=CC(=O)C1)Nc2ccccc2C#N)C,FMOPL000049a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.21,0.017,59.9,1.1,97.9,97.0,89.9,0.18606,0.20720, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0357,c1cc(cnc1)CNC2ccc(cc2N)C(=O)[O-],FMOPL000201a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.018,52.3,1.3,93.2,95.0,57.0,0.17546,0.19100, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0358,CCC(=O)Nc1c2ccccc2oc1C(=O)N,FMOPL000577a,Mounted_Clear,success,C 1 2 1,111 27 37 90 96 90,1.19,0.021,47.1,1.2,96.3,96.3,82.1,0.19682,0.22390, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0359,c1cc(cc(c1)c2ccc(cc2)O)C#N,FMOPL000261a,Mounted_Clear,success,C 1 2 1,110 27 37 90 95 90,1.37,0.023,41.4,1.3,99.4,91.8,99.3,0.18968,0.22114, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0360,Cc1cc(nc(c1)NC(=O)Nc2ccccc2)C,FMOPL000454a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.21,0.012,73.0,2.1,96.9,98.2,89.2,0.18172,0.20416, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0361,CCN1c(nnn1)NC(=O)c2ccco2,FMOPL000475a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.32,0.019,45.5,2.1,99.1,97.4,99.1,0.18465,0.21851, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0362,c1cc(cc(c1)c2cccc(c2)O)C#N,FMOPL000262a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.15,0.025,42.0,2.2,92.8,97.8,62.2,0.18183,0.20280,0.18079,0.20054, C 1 2 1,3 - In Refinement, None

FALZA-x0363,CCOC(=O)c1c(nc(s1)c2cnccn2)C,FMOPL000647a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.43,0.018,47.3,1.2,96.9,96.1,96.8,0.18726,0.22564, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0364,CC(C)Oc1ccc(cc1)[C@@H]2CC(=O)NC2,FMOPL000402a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.18,0.018,47.9,1.2,96.3,97.7,72.7,0.18738,0.20925, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0365,CC(=O)Nc1ccc(cc1)OC(=O)N2CCCC2,FMOPL000494a,Mounted_Clear,success,C 1 2 1,112 27 37 90 96 90,1.36,0.026,40.3,1.4,98.9,98.7,98.9,0.19727,0.22576, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0366,C[NH+] (C)Cclc[nH]c2c1cc(cc2)OC,FMOPL000690a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.73,0.023,33.8,2.1,99.4,99.5,99.4,0.18155,0.23216, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0367,C1COCC[NH+]1Cc2c(snn2)Cl,FMOPL000627a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.20,0.042,35.9,1.3,97.2,93.3,88.2,0.18224,0.19650, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0368,CCc1nnc(s1)NC(=O)c2cnccn2,FMOPL000404a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.27,0.023,41.9,2.3,98.7,98.6,94.5,0.18103,0.19941, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0369,c1ccc(cc1)CC[NH+]2CCC(CC2)C(=O)N,FMOPL000481a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.17,0.018,54.2,2.2,96.1,98.3,80.3,0.17766,0.19507, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0370,CC(=O)c1ccc(cc1)OCC(=O)[O-],FMOPL000688a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.52,0.053,20.9,1.6,98.6,93.1,98.7,0.18992,0.22530,0.20383,0.23609, C 1 2
1,3 - In Refinement, None

FALZA-x0371,CC(=O)Nc1nc2ccc(cc2s1)C(=O)NC,FMOPL000419a,Mounted_Clear,success,C 1 2
1,111 27 38 90 96 90,1.18,0.014,67.4,2.1,97.0,98.3,85.1,0.18065,0.19879, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0372,Cc1c(sc2c1c(ncn2)N(C)C)C,FMOPL000466a,Mounted_Clear,success,C 1 2 1,111 27
38 90 96 90,1.18,0.027,36.0,1.2,95.7,95.8,78.3,0.18610,0.20228, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0373,COc1ccc2c(c1)non2,FMOPL000686a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96
90,1.16,0.028,41.3,2.2,91.0,98.0,64.4,0.17682,0.19356, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-
x0374,c1ccc(cc1)[C@@H](C[NH+]2CCC(CC2)C(=O)N)O,FMOPL000653a,Mounted_Clear,success,C 1 2
1,111 27 38 90 95 90,1.19,0.022,38.3,1.2,97.5,97.3,86.9,0.18420,0.20650, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0375,c1cc(oc1)C(=O)NCCc2ccc(cc2)F,FMOPL000411a,Mounted_Clear,success,C 1 2 1,112
27 38 90 96 90,1.36,0.026,33.4,1.4,99.5,95.1,99.6,0.17713,0.19736, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0376,CC(C)c1ccc(cc1)C(=O)NC[C@@H]2CCCO2,FMOPL000493a,Mounted_Clear,success,C 1 2
1,112 27 38 90 96 90,1.26,0.024,41.3,2.2,98.8,97.5,96.7,0.17827,0.19411, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0377,c1ccc(cc1)COC(=O)NO,SDOOA000888b,Mounted_Clear,success,C 1 2 1,112 27 38 90
96 90,1.13,0.025,42.0,2.2,91.5,98.4,55.3,0.17943,0.19366, None, None, C 1 2 1,1 - Analysis
Pending, None

FALZA-x0378,COC(=O)c1ccc(s1)c2cccn2,FMOPL000638a,Mounted_Clear,success,C 1 2 1,110 27
37 90 95 90,1.54,0.061,17.4,1.1,97.9,96.4,96.1,0.21194,0.25569, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0379,CCn1cc(cn1)CNC(=O)c2cccn2,FMOPL000422a,Mounted_Clear,success,C 1 2 1,112 27
38 90 96 90,1.19,0.026,39.8,1.2,97.1,92.2,82.8,0.18213,0.19898, None, None, C 1 2 1,1 -
Analysis Pending, None

FALZA-x0380,CC(=O)c1ccc(cc1)N2CCC(CC2)C(=O)N,FMOPL000495a,Mounted_Clear,success,C 1 2
1,111 27 37 90 96 90,1.43,0.086,21.0,1.1,92.5,95.3,40.0,0.30029,0.36020, None, None, C 1 2
1,1 - Analysis Pending, None

FALZA-x0381,CCN(CCO)c1ccc(c(c1)C)N,FMOPL000689a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.05,0.039,40.5,1.9,78.4,96.8,8.7,0.17558,0.19263,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0382,c1ccc(cc1)[C@@H](C[NH2+][C@@H]2CCCCNC2=O)O,FMOPL000651a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.30,0.039,26.2,1.1,98.6,97.6,96.3,0.20067,0.22785,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0383,c1cc(oc1)C(=O)NC(=S)N2CCOCC2,FMOPL000401a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.23,0.023,41.8,2.2,98.7,99.1,98.0,0.18231,0.20605,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0384,CC(=O)Nc1ccc(cc1)Oc2ncccn2,FMOPL000485a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.24,0.019,40.1,1.3,98.4,96.7,96.9,0.18719,0.21286,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0385,c1ccc(cc1)COC(=O)N2CCC[C@H]2CO,FMOPL000691a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.12,0.022,49.0,2.2,88.5,97.1,49.8,0.18298,0.20411,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0386,Cc1ccc(cc1)C(=O)O[C@@H]2C[NH+]3CCC2CC3,FMOPL000661a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.025,43.0,2.3,92.8,97.7,61.4,0.18160,0.19534,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0387,Cc1ccc(cc1)CNC(=O)c2c(ccs2)C,FMOPL000429a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.25,0.031,32.6,2.2,98.9,95.3,97.7,0.19318,0.22126,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0388,COc1cc2cccnc2c(c1)N,FMOPL000687a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.38,0.035,40.0,1.3,98.1,95.8,98.4,0.20809,0.24328,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0389,C[C@H]1CN(C[C@H](O1)C)c2ccc(cc2C(=O)[O-])N,FMOPL000658a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.17,0.026,40.8,1.1,95.7,92.1,74.0,0.17676,0.19082,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0390,C[C@H]1C[C@H]1C(=O)NCCc2ccc(cc2)Cl,FMOPL000407a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.37,0.020,46.1,2.1,99.8,98.8,99.9,0.18688,0.22129,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0391,c1ccc(cc1)CCCC(=O)N2CCOCC2,FMOPL000501a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.26,0.026,37.1,1.2,97.2,96.9,89.7,0.18844,0.21549,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0392,COc1ccc(cc1N)N,FMOPL000685a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.15,0.016,64.5,2.2,94.0,98.7,66.2,0.18684,0.20636,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0393,Cc1c(c(n(n1)C)C)NC(=O)CC#N,FMOPL000633a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.29,0.023,48.4,1.3,96.8,97.3,91.4,0.18751,0.22053,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0394,COCC(=O)Nc1cccc1,FMOPL000504a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.40,0.033,30.0,1.3,96.8,97.2,94.0,0.19999,0.23589,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0395,c1ccc(cc1)NO,FMOPL000684a,Mounted_Clear,success,C 1 2 1,109 26 41 90 95 90,1.63,0.080,7.0,0.9,94.8,95.3,96.9,0.44560,0.50820,None,None,C 1 2 1,1 - Analysis Pending, None

FALZA-x0396, c1cc(oc1)C[NH+]2CCS(=O)(=O)CC2, FMOPL000629a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.16, 0.018, 59.3, 2.2, 94.8, 97.4, 73.9, 0.17546, 0.19388, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0397, COc1ccc(cc1)Nc2ccccc2O, FMOPL000426a, Mounted_Clear, success, C 1 2 1, 110 27 38 90 95 90, 1.38, 0.056, 21.3, 1.1, 95.0, 91.5, 92.7, 0.19928, 0.23081, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0398, c1ccc(c(c1)NC(=S)N)OC(F)(F)F, FMOPL000512a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.44, 0.025, 35.3, 1.1, 99.3, 98.0, 99.2, 0.18830, 0.22063, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0399, Cc1ccc(cc1)CNC(=O)Cc2cccs2, FMOPL000743a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.17, 0.033, 38.8, 2.2, 92.4, 98.0, 72.7, 0.19030, 0.21009, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0400, CC(=O)Nc1cccc1C(=O)NN, FMOPL000631a, Mounted_Clear, success, C 1 2 1, 110 27 38 90 95 90, 1.29, 0.019, 45.6, 2.1, 98.6, 98.7, 96.4, 0.18400, 0.21246, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0401, CCOC1ccc(cc1)NC(=O)c2cnccn2, FMOPL000446a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.53, 0.051, 26.0, 1.8, 98.0, 91.6, 97.4, 0.20501, 0.24752, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0402, CC(=O)NCCc1ccc(cc1)S(=O)(=O)N, FMOPL000513a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.11, 0.024, 44.3, 2.2, 87.7, 97.6, 42.0, 0.18329, 0.20040, 0.21541, 0.22740, C 1 2 1, 5 - Deposition ready, None

FALZA-x0403, CC(C)(C)NC(=O)N1CCC(CC1)C(=O)N, FMOPL000334a, Mounted_Clear, success, C 1 2 1, 112 27 37 90 96 90, 1.21, 0.026, 40.4, 2.1, 99.1, 99.6, 97.6, 0.18912, 0.21128, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0404, c1ccc(c(c1)C(=O)NCCc2ccncc2)F, FMOPL000361a, Mounted_Clear, success, C 1 2 1, 110 27 38 90 95 90, 1.49, 0.041, 25.2, 2.2, 98.7, 95.2, 99.5, 0.18727, 0.22376, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0405, CC(=O)N1CCNC(=O)[C@@H]1CC(=O)OC, FMOPL000325a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.36, 0.021, 41.5, 1.5, 98.8, 97.3, 98.7, 0.17913, 0.20789, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0406, CCCC(=O)Nc1nnn(n1)CC, FMOPL000311a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.30, 0.039, 27.7, 2.2, 99.4, 98.5, 98.4, 0.18761, 0.20817, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0407, CCNC(=O)c1ccc(cc1)NS(=O)(=O)C, FMOPL000335a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.18, 0.025, 45.4, 1.2, 96.0, 94.9, 77.0, 0.18667, 0.21135, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0408, c1cc(cc(c1)NC(=O)CCC2CCC2)C#N, FMOPL000364a, Mounted_Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, -1 - Data Collection Failed, None

FALZA-x0409, CN(C)C(=O)Oc1ccc(cc1)c2nnco2, FMOPL000354a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.32, 0.023, 36.9, 1.3, 99.4, 97.2, 96.2, 0.18799, 0.21236, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0410, CC1CCN(CC1)C(=O)c2cc3ccccc3o2, FMOPL000372a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.37, 0.026, 40.2, 2.1, 96.6, 97.2, 95.1, 0.17777, 0.21272, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0411,CC(C)(CO)NC(=O)c1cccc(c1)C1,FMOPL000324a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.29,0.014,65.3,2.2,96.4,98.2,91.2,0.18486,0.21147,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0412,Cc1c(nc[nH]1)C[NH+]2CCCCC2,FMOPL000317a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.32,0.017,49.8,2.1,99.3,98.5,97.6,0.17318,0.19320,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0413,CC[NH+]1CCC(CC1)Nc2ccccc2F,FMOPL000339a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.10,0.020,52.2,2.3,85.3,97.1,40.9,0.17257,0.18805,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0414,c1ccc(cc1)C#Cc2ccc(cc2)c3ccn[nH]3,FMOPL000111a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.53,0.040,25.8,1.6,99.5,96.0,99.5,0.20582,0.25143,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0415,Cc1ccc(cc1)OCC(=O)N2CC[NH+](CC2)C,FMOPL000202a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.23,0.023,40.4,1.1,98.6,94.6,97.0,0.18056,0.20001,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0416,Cc1cccc1c2nc(c(o2)N(C)C)C#N,FMOPL000583a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.23,0.026,45.2,1.2,97.6,96.7,89.4,0.18919,0.21310,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0417,CC(=O)N1CCC(CC1)C#N,XST00000907b,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.30,0.025,39.7,2.2,99.1,97.7,97.3,0.18275,0.20336,0.20501,0.21982,C 1 2 1,4 - CompChem ready,None

FALZA-x0418,CC(=O)Nc1cccc1OCc2ccccc2,FMOPL000047a,Mounted_Clear,success,C 1 2 1,112 27 37 90 96 90,1.39,0.017,52.6,2.0,99.2,99.6,98.5,0.19315,0.22253,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0419,CCc1ccc(cc1)OCC(=O)N2CCCC2,FMOPL000203a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.28,0.036,26.2,1.0,95.3,98.0,88.8,0.19432,0.21697,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0420,Cc1ccc(s1)Cnc2cccc(c2)C(=O)[O-],FMOPL000582a,Mounted_Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, -1 - Data Collection Failed, None

FALZA-x0421,C[NH2+]Cc1ccc(cc1)C(F)(F)F,FMOPL000112a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.27,0.028,36.3,2.2,99.4,99.0,97.5,0.17999,0.20409,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0422,COc1ccc2c(c1)cc([nH]2)C[NH3+],FMOPL000053a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.27,0.012,74.2,2.3,96.4,97.3,90.3,0.17559,0.19469,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0423,CCOc1ccc(c1)C(=O)Nc2nnn(n2)C,FMOPL000204a,Mounted_Clear,success,C 1 2 1,112 27 37 90 96 90,1.18,0.041,28.6,2.1,97.5,99.5,88.0,0.19665,0.22118,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0424,CCNC(=O)N1CCNC(=O)[C@H]1CC(=O)OC,FMOPL000578a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.17,0.021,56.6,1.5,94.0,92.3,69.1,0.17846,0.19787,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0425,c1ccc(cc1)CONC(=O)N,XST00001145b,Mounted_Clear,success,C 1 2 1,112 27 38 90 95 90,1.35,0.028,35.8,2.1,97.4,92.8,96.6,0.17551,0.20202,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0426,COc1ccc(cc1)C#CC(=O)[O-],FMOPL000052a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,2.04,0.089,13.5,9.8,96.4,94.1,94.0,0.18317,0.23977,None,None,C 1 2 1,1 - Analysis Pending,None

FALZA-x0427,CCOc1ccc(cc1)[C@@H](C)[NH3+],FMOPL000205a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.28,0.049,20.1,2.2,98.3,98.7,94.5,0.18091,0.20001, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0428,COc1cccc(c1)Nc2c3c([nH]cn3)ncn2,FMOPL000596a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.26,0.023,41.1,1.3,98.9,96.8,96.5,0.19700,0.22314, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0429,c1ccc(cc1)Nc2nncs2,FMOPL000113a,Mounted_Clear,success,C 1 2 1,110 27 37 90 95 90,1.29,0.023,42.0,2.2,95.4,95.9,88.2,0.18424,0.21290, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0430,c1cc2c(ccc(c2nc1)O)C[NH+]3CCOCC3,FMOPL000054a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.05,0.026,45.3,2.7,77.8,97.4,15.3,0.18566,0.20675, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0431,c1cc2c(cc1c[NH2+]C[C@H]3CCCO3)OCO2,FMOPL000206a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.027,43.4,2.2,89.9,98.3,56.3,0.17617,0.19603, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0432,c1ccc(cc1)NC(=O)NCCN2CCCC2=O,FMOPL000589a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.14,0.028,42.0,2.3,93.3,97.6,62.6,0.18293,0.20486, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0433,c1ccc(c(c1)N)Nc2ccccn2,FMOPL000114a,Mounted_Clear,success,C 1 2 1,111 27 38 90 96 90,1.22,0.016,53.9,1.1,93.0,96.9,81.1,0.18638,0.21129, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0434,COC(=O)C#Cc1ccc(cc1)Cl,FMOPL000060a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.16,0.023,39.5,1.2,95.2,93.8,63.1,0.19710,0.21803, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0435,CCn1c(ccn1)C[NH2+]C,FMOPL000221a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.15,0.034,33.7,2.3,92.9,98.8,68.0,0.18028,0.19664, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0436,Cc1ccc(cc1N)c2cnc3cccc3n2,FMOPL000598a,Mounted_Clear,success,C 1 2 1,111 27 37 90 95 90,1.19,0.042,27.9,2.2,98.0,99.1,92.8,0.20243,0.22312, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0437,C1C[C@@H](OC1)CNC(=O)N2CCOCC2,FMOPL000116a,Mounted_Clear,success,C 1 2 1,110 27 38 90 95 90,1.25,0.022,40.9,1.2,95.7,92.6,87.9,0.19112,0.21896, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0438,CCNC(=O)N1CCN(CC1)C(=O)C,FMOPL000061a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.28,0.036,40.4,1.3,97.3,97.4,96.1,0.22082,0.25304,0.21715,0.25731, C 1 2 1,5 - Deposition ready, None

FALZA-x0439,CS(=O)(=O)NC1CCCC1,FMOPL000222a,Mounted_Clear,success,C 1 2 1,111 27 38 90 95 90,1.28,0.016,60.7,2.2,99.1,97.8,96.1,0.18032,0.20337, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0440,CN(C)c1ccc(cc1)c2cc(on2)C(=O)OC,FMOPL000595a,Mounted_Clear,success,C 1 2 1,112 27 38 90 96 90,1.15,0.014,68.6,2.4,92.9,97.4,63.5,0.18773,0.20669, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0441,c1cc(cc(c1)F)Nc2[nH]c(=O)ccn2,FMOPL000115a,Mounted_Clear,success,C 1 2 1,111 27 37 90 96 90,1.35,0.017,48.7,1.6,99.5,92.6,99.6,0.19217,0.22239, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0442,CC(=O)c1ccc(cc1)OC(F)F,FMOPL000223a,Mounted_Clear,success,C 1 2 1,110 27 38 90 95 90,1.36,0.019,36.4,1.0,98.6,93.9,98.3,0.18819,0.21880, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0443, c1ccc2c(c1)[nH]c(n2)CNC(=O)c3ccco3, FMOPL000588a, Mounted_Clear, success, C 1 2 1,111 27 38 90 95 90,1.39,0.019,40.2,1.2,99.2,94.8,99.5,0.17728,0.20844, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0444, c1cc(ccc1c2ccc(o2)C(=O)NN)Cl, FMOPL000118a, Mounted_Clear, success, C 1 2 1,111 27 37 90 95 90,1.37,0.038,40.3,1.0,94.9,91.1,92.3,0.20444,0.23475, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0445, c1ccc(cc1)c2cnc(c(n2)C(=O)N)N, FMOPL000063a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.18,0.018,50.1,1.3,96.8,96.1,74.9,0.19413,0.21672, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0446, Cc1c(nc(=O)[nH]n1)Nc2cccc(c2)O, FMOPL000117a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.36,0.022,37.5,1.2,99.3,96.6,99.4,0.19755,0.22606, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0447, c1cc(ccc1CO)c2ccc(cc2)CO, FMOPL000064a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.21,0.028,39.5,1.2,98.2,93.7,95.3,0.20004,0.22321, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0448, COc1cccc1OCC(=O)NN, FMOPL000225a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.22,0.019,56.2,2.1,95.2,98.7,86.2,0.18018,0.19789, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0449, CC(=O)c1ccc(cc1)NC(=O)C[NH+]2CCCC2, FMOPL000591a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.22,0.022,46.4,2.1,98.8,98.9,96.7,0.18805,0.20608, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0450, CS(=O)(=O)Nc1ccc(cc1)c2cccc2, FMOPL000121a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.13,0.024,42.7,1.1,91.7,94.7,50.4,0.18710,0.20487, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0451, CS(=O)(=O)Nc1ccc(cc1)C(=O)N, FMOPL000226a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.35,0.018,45.6,1.4,99.0,98.4,97.4,0.18337,0.21415, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0452, CC1(C[C@H](CCO1)C(=O)NC2CCCC2)C, FMOPL000592a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.20,0.026,35.4,1.4,97.9,96.5,90.9,0.18063,0.20106, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0453, CCCc1nnc(s1)NC(=O)c2ccccn2, FMOPL000119a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.22,0.025,43.3,2.1,97.7,98.1,91.5,0.17192,0.18915, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0454, CCc1nnc(s1)NC(=O)C(F)(F)F, FMOPL000227a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.59,0.026,28.2,1.4,97.8,89.6,98.9,0.19047,0.21372, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0455, Cc1cc(n2c(n1)ncn2)Nc3ccc(cc3)O, FMOPL000597a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.25,0.018,54.3,2.3,99.2,98.4,97.2,0.17802,0.19716,0.20561,0.21964, C 1 2 1,3 - In Refinement, None

FALZA-x0456, CCC[C@H](C)C(=O)Nc1c(ccc1C)C, FMOPL000720a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.15,0.042,28.0,2.2,93.8,99.1,68.1,0.18969,0.20947, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0457, CCOC(=O)NCc1cccc1, FMOPL000628a, Mounted_Clear, success, C 1 2 1,112 27 38 90 96 90,1.17,0.023,37.5,1.1,93.0,93.7,64.3,0.18094,0.20045, None, None, C 1 2 1,1 - Analysis Pending, None

FALZA-x0458, COc1ccc(cc1)CNC(=O)c2cnccn2, FMOPL000452a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.16, 0.027, 40.6, 2.3, 94.5, 93.7, 70.8, 0.18407, 0.20808, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0459, c1cscclC[NH+]2CCC(CC2)O, FMOPL000505a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.24, 0.049, 25.5, 3.1, 87.5, 91.8, 86.4, 0.19076, 0.21540, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0460, CC(C)CC(=O)Nc1ccc(cc1)NC(=O)C, FMOPL000731a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.16, 0.016, 53.4, 1.1, 95.0, 98.4, 67.2, 0.19381, 0.21518, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0461, CC(C)c1ccc(cc1)NNC(=O)c2ccno2, FMOPL000654a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 95 90, 1.33, 0.050, 23.0, 2.1, 98.9, 98.3, 99.0, 0.20181, 0.23157, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0462, c1cnc(cn1)C(=O)NCCC2=CCCC2, FMOPL000415a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.15, 0.023, 45.7, 2.1, 94.0, 98.7, 66.0, 0.18884, 0.21036, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0463, Cc1ccc(cc1)CNC(=O)COC, FMOPL000511a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.48, 0.052, 29.4, 1.4, 98.6, 97.4, 98.7, 0.21004, 0.23672, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0464, CC(C)c1ccc(cc1)NNC(=O)C2CCC2, FMOPL000646a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.11, 0.019, 55.5, 2.2, 88.9, 97.2, 46.2, 0.18400, 0.20798, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0465, c1ccc(cc1)CCC(=O)NN2CCOCC2, FMOPL000413a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.10, 0.025, 44.7, 2.2, 85.4, 97.9, 40.2, 0.18711, 0.20969, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0466, COCC(=O)NCc1ccccc1, FMOPL000507a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.18, 0.014, 66.6, 2.2, 92.9, 97.8, 75.9, 0.18119, 0.19726, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0467, c1cc(c(c(c1)F)C(=O)N2CCCCC2)F, FMOPL000729a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.23, 0.033, 36.7, 1.2, 97.1, 90.1, 90.0, 0.18838, 0.21217, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0468, CCc1ccccc1NNC(=O)c2ccccc2, FMOPL000657a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.27, 0.029, 37.0, 2.2, 98.4, 99.4, 93.8, 0.19259, 0.21570, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0469, CC(C)C(=O)Nc1ccc(cc1)N2CCCC2, FMOPL000439a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.15, 0.021, 51.9, 2.2, 92.1, 97.7, 66.2, 0.18656, 0.20568, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0470, CCOC(=O)N1CCOCC1, FMOPL000502a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.07, 0.022, 50.1, 2.3, 82.1, 96.4, 26.1, 0.17700, 0.19355, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0471, Cc1ccc(cc1)CNC(=O)c2ccc(cc2)C, FMOPL000754a, Mounted_Clear, success, C 1 2 1, 112 27 38 90 96 90, 1.16, 0.049, 25.6, 1.2, 95.3, 95.5, 63.6, 0.19760, 0.21927, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0472, c1cc(cc(c1)NC(=O)c2ccno2)C(=O)[O-], FMOPL000648a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.33, 0.034, 30.0, 1.4, 98.8, 95.6, 97.6, 0.17916, 0.20696, None, None, C 1 2 1, 1 - Analysis Pending, None

FALZA-x0473, C1CCC(CC1)CCC(=O)N2CCOCC2, FMOPL000400a, Mounted_Clear, success, C 1 2 1, 111 27 38 90 96 90, 1.24, 0.016, 59.1, 2.2, 98.9, 98.3, 97.4, 0.17655, 0.19550, None, None, C 1 2 1, 1 - Analysis Pending, None

SGC Dataset – NUDT5A (csv format)

CrystalName,CompoundSMILES,CompoundCode,MountingResult,DataCollectionOutcome,DataProcessingSpaceGroup,DataProcessingUnitCell,DataProcessingResolutionHigh,DataProcessingRmergeLow,DataProcessingIsigLow,DataProcessingIsigHigh,DataProcessingCompletenessOverall,DataProcessingCompletenessLow,DataProcessingCompletenessHigh,DimpleRcryst,DimpleRfree,RefinementRcryst,RefinementRfree,RefinementSpaceGroup,RefinementOutcome,Deposition_PDB_ID

```
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
,,,FAIL: Melted,,,,,,,,,,,,,,,,,,,,,,,,,
```


,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,,,,,,,,,,,,,,,,,,,,,
,CNC=1N=CC=CN1,Z54628578,,,,,,,,,,,,,,,,,,,,,
,CC(=O)NC1=CC(C)=NN1,Z239136710,,,,,,,,,,,,,,,,,,,,,
,CCNC(=O)N1CCN(CC1)C(=O)C,Z44590919,,,,,,,,,,,,,,,,,,,,,
,CCNC=1C=CC(C)=NN1,Z1267773786,,,,,,,,,,,,,,,,,,,,,
,CC=1C=CC(C(=O)N)=C(F)C1,Z1343633025,,,,,,,,,,,,,,,,,,,,,
,CN1C=C(OC=2N=CN=CC2C1)C=N1,Z1918536193,,,,,,,,,,,,,,,,,,,,,
,CCNCC1=CN(C)N=N1,Z1271660837,,,,,,,,,,,,,,,,,,,,,
,COC=1C=CC=2C=NNC(=O)C2C1OC,Z102895082,,,,,,,,,,,,,,,,,,,,,
,CN1C=C(C(=O)N)C(=N1)C2CCCNC2,Z2377835233,,,,,,,,,,,,,,,,,,,,,
,CC1CCOC1C(=O)NC2=CN=NS2,Z1827602749,,,,,,,,,,,,,,,,,,,,,
,COC(=O)[C@@H]1C[C@@H](O)CN1C(=O)C2=CC=CO2,Z1614545742,,,,,,,,,,,,,,,,,,,,,
,O=C(C1CC1)N2CCN(CC2)C(=O)C3=CC=CO3,Z32327641,,,,,,,,,,,,,,,,,,,,,
,CN1CCN(CC1)C(=O)C=2C=CC(F)=C(F)C2,Z2856434829,,,,,,,,,,,,,,,,,,,,,
,CC1CN(C(C)CO1)C(=O)C=2C=NSN2,Z768399682,,,,,,,,,,,,,,,,,,,,,
,CC1=NC(C(=O)N2CCCC2)=C(C)S1,Z1497321453,,,,,,,,,,,,,,,,,,,,,
,CN(CC1CCOC1)C=2N=CN=CC2C1,Z1787627869,,,,,,,,,,,,,,,,,,,,,

NUDT5A-x0001, None, None, OK: Mounted Clear, success, P 1, 48 59 80 79 82
76, 1.60, 0.037, 17.7, 1.1, 95.8, 97.2, 93.9, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0002, None, None, OK: Mounted Clear, Failed -
unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0003, None, None, OK: Mounted Clear, success, P 1, 45 56 76 82 86
78, 2.74, 0.012, 47.5, 1.2, 86.9, 93.9, 96.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0004, None, None, OK: Mounted Clear, Failed - low resolution, P 1, 48 61 84 89 92
81, 5.83, 0.265, 0.8, 0.1, 95.9, 72.4, 95.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0005, None, None, OK: Mounted Clear, success, P 1, 48 59 80 79 82
76, 2.59, 0.027, 13.4, 0.9, 86.9, 86.5, 82.0, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0006, None, None, OK: Mounted Clear, Failed -
unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0007, None, None, OK: Mounted Clear, success, P 1, 46 58 76 81 85
 77, 2.38, 0.017, 32.6, 0.5, 79.0, 91.7, 77.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0008, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
 75, 1.56, 0.039, 15.8, 0.5, 94.0, 92.4, 89.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0009, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
 75, 1.76, 0.021, 27.8, 0.7, 94.3, 94.8, 95.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0010, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.64, 0.024, 20.5, 0.5, 93.9, 92.5, 94.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0011, None, None, OK: Crystalline, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0012, None, None, OK: Crystalline, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0013, None, None, OK: Mounted Clear, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0014, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 82
 75, 1.69, 0.028, 20.2, 1.1, 95.0, 96.4, 92.6, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0015, None, None, OK: Crystalline, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0016, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.92, 0.050, 19.2, 1.1, 96.9, 98.0, 95.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0017, None, None, OK: Mounted Clear, success, P 1, 48 59 79 80 82
 76, 1.89, 0.021, 28.2, 0.9, 79.5, 96.1, 44.1, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0018, None, None, OK: Mounted Clear, success, P 1, 49 59 80 80 82
 76, 3.07, 0.128, 8.7, 6.7, 23.5, 18.2, 26.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0019, None, None, OK: Mounted Clear, success, P 1, 47 58 79 80 83
 76, 1.99, 0.013, 41.8, 0.5, 84.6, 94.4, 72.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0020, None, None, OK: Mounted Clear, Failed - low resolution, P 1, 46 59 77 81 86
 77, 4.92, 0.098, 4.7, 0.6, 97.4, 92.5, 97.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0021, None, None, OK: Mounted Clear, success, P 1, 46 58 77 81 85
 77, 2.75, 0.012, 17.7, 1.2, 84.0, 95.7, 89.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0022, None, None, OK: Mounted Clear, success, P 1, 45 57 76 82 86
 78, 2.83, 0.010, 18.6, 1.0, 83.3, 94.2, 84.9, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0023, None, None, OK: Crystalline, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0024, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.68, 0.042, 16.7, 0.6, 95.2, 94.0, 94.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0025, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
 75, 2.11, 0.038, 18.4, 4.2, 97.2, 98.4, 95.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0026, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 2.35, 0.087, 6.6, 2.0, 51.6, 49.8, 52.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0027, None, None, OK: Mounted Clear, success, P 1, 45 56 76 83 87
79, 2.76, 0.026, 22.5, 0.0, 93.1, 97.7, 96.6, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0028, None, None, OK: Mounted Clear, success, P 1, 46 57 76 82 86
78, 2.78, 0.020, 24.6, 0.1, 96.3, 97.3, 97.1, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0029, None, None, OK: Crystalline, Failed - low resolution, P 1, 46 58 77 81 85
77, 4.04, 0.016, 13.4, 4.1, 91.1, 92.8, 86.9, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0030, None, None, OK: Mounted Clear, Failed - low resolution, P 1, 47 62 79 77 84
79, 4.13, 0.018, 1.7, 0.3, 77.1, 73.1, 82.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0031, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
75, 1.86, 0.020, 24.3, 1.3, 95.1, 98.3, 91.6, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0032, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
75, 1.95, 0.036, 14.7, 0.9, 95.0, 95.3, 95.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0033, None, None, OK: Crystalline, success, P 1, 49 60 80 79 81
75, 2.32, 0.024, 14.2, 0.3, 91.0, 88.9, 93.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0034, None, None, OK: Crystalline, success, P 1, 47 58 78 80 83
76, 3.03, 0.056, 13.0, 0.1, 95.3, 97.3, 97.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0035, None, None, OK: Crystalline, success, P 1, 49 60 79 79 81
75, 1.85, 0.053, 13.2, 0.6, 94.5, 93.1, 94.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0036, None, None, OK: Mounted Clear, success, P 1, 47 58 78 81 82
77, 2.28, 0.117, 7.3, 0.9, 96.1, 97.6, 94.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0037, None, None, OK: Mounted Clear, success, P 1, 46 58 78 81 83
78, 2.37, 0.017, 18.1, 0.3, 84.7, 94.1, 96.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0038, None, None, OK: Mounted Clear, success, P 1, 58 96 115 98 94
104, 1.97, 0.015, 19.9, 0.4, 94.2, 92.3, 95.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0039, None, None, OK: Mounted Clear, success, P 1, 48 59 79 80 82
76, 1.68, 0.010, 44.3, 1.2, 95.7, 98.9, 93.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0040, None, None, OK: Mounted Clear, success, P 1, 48 59 79 79 82
76, 1.69, 0.012, 42.0, 1.2, 95.6, 98.0, 93.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0041, None, None, OK: Mounted Clear, success, P 1, 50 61 82 79 82
75, 2.67, 0.048, 5.3, 0.4, 95.5, 92.3, 95.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0042, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
75, 1.77, 0.013, 48.6, 1.0, 95.1, 98.3, 92.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0043, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
75, 1.63, 0.028, 22.9, 0.5, 95.0, 94.8, 94.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0044, None, None, OK: Mounted Clear, success, P 1, 48 59 79 80 82
76, 1.65, 0.012, 46.3, 0.9, 95.6, 98.2, 93.6, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0045, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
75, 1.65, 0.013, 34.3, 0.6, 89.3, 93.2, 94.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0046, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
75, 1.69, 0.012, 44.0, 0.9, 95.6, 97.9, 93.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0047, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
75, 1.81, 0.021, 27.9, 1.4, 96.1, 98.4, 95.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0048, None, None, OK: Crystalline, success, P 1, 49 59 80 79 81
 75, 1.92, 0.011, 34.7, 1.2, 95.8, 99.5, 94.6, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0049, None, None, OK: Precipitated, success, P 1, 49 59 79 79 81
 75, 1.83, 0.017, 33.5, 0.6, 95.2, 94.5, 95.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0050, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.73, 0.020, 29.8, 0.9, 96.3, 98.8, 94.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0051, None, None, OK: Precipitated, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0052, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.55, 0.011, 45.6, 0.4, 93.3, 92.9, 88.0, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0053, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.65, 0.020, 33.8, 1.0, 96.0, 98.5, 94.1, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0054, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.79, 0.026, 22.8, 1.2, 96.1, 98.5, 94.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0055, None, None, OK: Precipitated, success, P 1, 49 59 79 79 81
 75, 2.02, 0.015, 39.9, 0.4, 84.3, 93.6, 78.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0056, None, None, OK: Crystalline, success, P 1, 49 59 80 79 81
 75, 1.68, 0.020, 33.0, 0.6, 81.8, 94.7, 78.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0057, None, None, OK: Mounted Clear, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0058, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
 75, 1.85, 0.032, 18.8, 0.4, 80.1, 89.0, 54.7, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0059, None, None, OK: Mounted Clear, success, P 1, 49 60 80 79 81
 75, 1.66, 0.019, 28.1, 0.6, 94.8, 91.8, 94.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0060, None, None, OK: Mounted Clear, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0061, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
 75, 1.77, 0.020, 19.3, 0.8, 93.8, 92.6, 95.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0062, None, None, OK: Crystalline, Failed -
 unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0063, None, None, OK: Crystalline, success, P 1, 49 59 80 79 81
 75, 1.73, 0.020, 33.3, 0.6, 76.2, 92.3, 94.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0064, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.72, 0.012, 49.0, 0.7, 78.7, 93.9, 94.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0065, None, None, OK: Crystalline, success, P 1, 49 59 80 79 81
 75, 1.60, 0.025, 26.4, 1.0, 95.6, 98.9, 93.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0066, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
 75, 2.12, 0.027, 22.2, 0.5, 91.1, 91.2, 91.0, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0067, None, None, OK: Mounted Clear, success, P 1, 53 64 84 79 86
 84, 1.58, 5.700, 0.0, 0.0, 70.6, 84.7, 31.3, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0068, None, None, OK: Crystalline, success, P 1, 49 59 80 79 81
 75, 1.83, 0.016, 26.5, 0.7, 94.7, 93.3, 95.2, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0069, None, None, OK: Mounted Clear, success, P 1, 49 60 79 79 81
 75, 1.64, 0.012, 43.4, 0.9, 95.6, 98.4, 93.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0070, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
 75, 1.75, 0.016, 36.0, 0.9, 95.5, 98.3, 93.5, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0071, None, None, OK: Mounted Clear, success, P 1, 49 59 79 79 81
 75, 1.68, 0.012, 51.5, 1.1, 95.8, 98.3, 93.4, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0072, None, None, OK: Mounted Clear, success, P 1, 49 59 80 79 81
 75, 1.67, 0.015, 37.3, 1.0, 95.6, 97.9, 93.1, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0073, None, None, OK: Mounted Clear, Failed -
 unknown, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
 Pending, None

NUDT5A-x0074, None, None, OK: Crystalline, success, P 1, 49 60 79 79 80
 75, 1.55, 0.019, 28.5, 0.5, 93.8, 94.0, 88.0, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0075, None, None, OK: Crystalline, success, P 1, 49 59 79 79 81
 75, 1.79, 0.015, 26.8, 0.7, 93.3, 94.4, 94.9, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0076, None, None, OK: Crystalline, success, P 1, 49 60 79 79 80
 75, 1.72, 0.017, 37.9, 0.5, 81.4, 92.4, 94.8, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0077, ClC=1C=CC=C (NC (=O) CN2CCCC2) C1, Z2735692823, OK: Mounted Clear, success, P 1, 49
 59 79 79 81 75, 1.50, 0.017, 31.8, 0.3, 94.5, 93.9, 93.7, 0.24134, 0.27661, 0.24134, 0.27661, P 1, 1
 - Analysis Pending, None

NUDT5A-x0078, FC=1C=CC=C (CNCC2=CC=CO2) C1, Z2737076969, OK: Precipitated, success, P 1, 49 59
 80 79 81 75, 1.61, 0.037, 18.1, 0.6, 95.1, 95.1, 94.5, 0.22182, 0.24653, 0.22182, 0.24653, P 1, 1 -
 Analysis Pending, None

NUDT5A-x0079, FC=1C=CC=C (NC (=O) COC=2C=CC=CC2) C1, Z19735192, OK: Mounted Clear, success, P
 1, 48 59 79 80 81
 76, 2.10, 0.016, 17.5, 1.6, 97.0, 96.0, 96.2, 0.21835, 0.26211, 0.21835, 0.26211, P 1, 1 - Analysis
 Pending, None

NUDT5A-x0080, CCN1C=C (NC (=O) C2CCC2) C=N1, Z373768900, OK: Precipitated, success, P 1, 48 59 79
 80 81 76, 2.81, 0.037, 9.3, 0.5, 94.9, 92.6, 97.0, 0.23190, 0.29147, 0.23190, 0.29147, P 1, 1 -
 Analysis Pending, None

NUDT5A-x0081, CN1CCN (CC1) C (=O) COC=2C=CC (C) =CC2, Z2856434836, OK: Mounted Clear, success, P
 1, 49 59 79 79 81
 75, 1.72, 0.020, 29.0, 0.6, 85.9, 94.9, 95.1, 0.22607, 0.26489, 0.22607, 0.26489, P 1, 1 - Analysis
 Pending, None

NUDT5A-x0082, CC (NC (=O) C=1C=CC=C (C) N1) C2CC2, Z287256168, OK: Mounted Clear, success, P 1, 48
 59 79 79 81 75, 2.53, 0.021, 18.6, 1.0, 97.6, 98.1, 96.7, 0.21051, 0.27093, 0.21051, 0.27093, P 1, 1
 - Analysis Pending, None

NUDT5A-x0083, CC1=CSC (CNC (=O) C=2C=CCN2) =N1, Z466628048, OK: Mounted Clear, success, P 1, 48
 59 79 80 82 76, 2.11, 0.010, 45.0, 1.3, 95.7, 98.9, 95.7, 0.23028, 0.27346, 0.23028, 0.27346, P 1, 1
 - Analysis Pending, None

NUDT5A-x0084, CC1=NOC (C) =C1C (=O) NCCC2=CCCC2, Z69092635, OK: Mounted Clear, success, P 1, 48
 59 80 79 81 76, 2.21, 0.023, 24.1, 1.1, 90.5, 92.9, 93.8, 0.27187, 0.32105, 0.27187, 0.32105, P 1, 1
 - Analysis Pending, None

NUDT5A-x0085,C(NC1=NC=2C=CC=CC2N1)C3=CC=CO3,Z57299526,OK: Mounted Clear,success,P 1,48
59 79 79 81 75,1.77,0.024,30.3,1.1,96.2,99.0,94.6,0.23028,0.26594,0.23028,0.26594,P 1,1
- Analysis Pending,None

NUDT5A-x0086,CCC=1C=CC=CC1NC(=O)C=2SN=NC2C,Z89385775,OK: Mounted Clear,success,P 1,48
59 79 79 81 76,1.98,0.024,24.3,0.7,88.4,88.2,81.6,0.24733,0.29133,0.24733,0.29133,P 1,1
- Analysis Pending,None

NUDT5A-x0087,C(NCC=1C=CN=CC1)C2=CC=CS2,Z2856434816,OK: Mounted Clear,success,P 1,48 59
79 80 82 76,1.86,0.016,39.2,1.1,96.5,99.0,95.3,0.22075,0.25707,0.22056,0.26056,P 1,3 -
In Refinement,None

NUDT5A-x0088,CC=1C=CC(NC(=O)C2CCCO2)=NC1,Z71580604,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.82,0.023,26.8,0.7,93.5,94.0,92.1,0.23858,0.27931,0.23858,0.27931,P 1,1 -
Analysis Pending,None

NUDT5A-x0089,O=C(NC1=NC=CS1)[C@H]2C[C@H]2C=3C=CC=CC3,Z2064107709,OK: Mounted
Clear,success,P 1,49 59 79 79 81
75,2.17,0.039,11.1,0.7,95.6,97.8,94.3,0.30744,0.35539,0.30744,0.35539,P 1,1 - Analysis
Pending,None

NUDT5A-x0090,COC=1C=CC=2N=C(NC(=O)C3CC3)SC2C1,Z27678561,OK: Mounted Clear,success,P
1,49 59 79 79 81 75,2.14,0.062,8.1,1.5,97.2,97.7,96.8,0.24048,0.27905,0.24048,0.27905,P
1,1 - Analysis Pending,None

NUDT5A-x0091,CCC1=CC=C(S1)C(=O)NCC=2C=NN(C)C2,Z804566442,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0092,COC=1C=CC(CNC(=O)C2=CSN=N2)=CC1,Z741218268,OK: Mounted Clear,success,P
1,48 59 79 79 82 76,1.62,0.021,31.0,1.0,95.3,98.8,93.1,0.22089,0.24496,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0093,CC1=CSC(NC(=O)NC=2C=CC=C(C)C2)=N1,Z44602971,OK: Mounted Clear,success,P
1,48 59 79 79 82 76,1.69,0.016,32.4,0.5,94.3,92.9,95.1,0.22070,0.25414,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0094,C1C=1C=CC=C(C1)C(=O)NC=2C=CON2,Z86622311,OK: Mounted Clear,success,P 1,48
59 79 80 82 76,1.77,0.016,30.1,0.7,95.3,94.2,95.1,0.21933,0.25453,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0095,COC=1C=CC=C(C1)C(=O)NC=2C=CC=CC2F,Z28290384,OK: Mounted Clear,success,P
1,48 59 79 79 81 76,1.76,0.012,42.3,1.2,95.5,98.8,94.6,0.22102,0.25064,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0096,COC=1C=CC(NCC=2C=CC(F)=CC2)=CC1,Z57328997,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.92,0.030,11.3,0.7,92.9,92.3,94.5,0.24128,0.27958,0.24128,0.27958,P 1,1
- Analysis Pending,None

NUDT5A-x0097,OC=1C=CC=C(CN2CCSCC2)C1,Z2856434857,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.96,0.066,11.5,1.7,96.4,98.1,94.6,0.24180,0.27748,0.24180,0.27748,P 1,1 -
Analysis Pending,None

NUDT5A-x0098,O=C(NC=1C=CC=NC1)C=2C=NN3C=CC=NC23,Z296054478,OK: Mounted Clear,success,P
1,48 59 79 79 81
75,1.85,0.021,29.1,1.0,96.5,99.1,95.5,0.22872,0.26670,0.22872,0.26670,P 1,1 - Analysis
Pending,None

NUDT5A-x0099,CCN1C=C(C=N1)C(=O)NCC=2C=CC(F)=CC2,Z1203107138,OK: Mounted Clear,success,P
1,48 59 79 80 81
76,2.09,0.032,22.5,1.4,97.3,97.2,96.9,0.22549,0.27106,0.22549,0.27106,P 1,1 - Analysis
Pending,None

NUDT5A-x0100,CCC1CCC(CC1)NC[C@H]2CCCO2,Z2856434866,OK: Mounted Clear,success,P 1,48 59
79 80 81 76,1.80,0.014,32.9,0.5,94.4,94.0,95.0,0.22667,0.26469,0.22667,0.26469,P 1,1 -
Analysis Pending,None

NUDT5A-x0101,O=C(N1CCCCC1)C=2C=CC=3OCOC3C2,Z31432226,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.78,0.023,25.3,0.7,95.2,95.4,94.7,0.24622,0.29100,0.24622,0.29100,P 1,1
- Analysis Pending,None

NUDT5A-x0102,CC1CCN(CC2=CNC=3C=CC=CC23)CC1,Z2856434912,OK: Mounted Clear,success,P 1,48
59 79 79 82 76,1.60,0.021,26.8,1.0,95.7,99.0,93.3,0.21909,0.24435,0.21909,0.24435,P 1,1
- Analysis Pending,None

NUDT5A-x0103,CC(C)(C)C1CCN(CC1)C(=O)C=2C=CC=CC2,Z1217741507,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,2.07,0.044,19.8,1.1,96.8,98.7,96.0,0.24910,0.30248,0.24910,0.30248,P 1,1 - Analysis
Pending,None

NUDT5A-x0104,CC=1C=CC=CC1OCC(=O)NC=2C=CC=CC2,Z19733979,OK: Crystalline,success,P 1,48
59 79 79 81 76,2.02,0.016,36.6,0.6,92.9,91.7,93.6,0.24356,0.29098,0.24356,0.29098,P 1,1
- Analysis Pending,None

NUDT5A-x0105,O=C(NCCC=1C=CC=CC1)NC2CCCCC2,Z44585920,OK: Mounted Clear,success,P 1,48 59
79 80 82 76,1.77,0.041,32.4,1.1,96.6,97.3,95.7,0.22564,0.25533,0.22564,0.25533,P 1,1 -
Analysis Pending,None

NUDT5A-x0106,CC=1C=CC=C(NC(=O)CN2CCOCC2)C1C,Z2856434834,OK: Mounted Clear,success,P
1,49 60 79 79 80
75,1.71,0.010,52.4,0.9,96.1,98.7,95.2,0.24417,0.28031,0.24417,0.28031,P 1,1 - Analysis
Pending,None

NUDT5A-x0107,CC=1C=CC=C(NC(=O)[C@H]2CCCN2)N1,Z1267881672,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,1.67,0.019,31.6,1.0,96.3,99.0,94.8,0.23558,0.26827,0.23558,0.26827,P 1,1 - Analysis
Pending,None

NUDT5A-x0108,N#CC=1C=CC(=CN1)N2CCCOCC2,Z1348371854,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.98,0.016,32.2,1.1,96.8,99.4,94.7,0.22162,0.26149,0.22162,0.26149,P 1,1 -
Analysis Pending,None

NUDT5A-x0109,CC=1C(C1)=CC=CC1NC(=O)[C@H]2CCCO2,Z1545312521,OK: Mounted Clear,success,P
1,49 60 80 79 81
75,2.04,0.023,20.6,1.5,96.2,99.2,94.3,0.23893,0.28520,0.23893,0.28520,P 1,1 - Analysis
Pending,None

NUDT5A-x0110,CC=1OC=CC1C(=O)NC=2C=CN=CC2,Z136583524,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,2.00,0.029,19.4,0.7,93.1,92.7,93.0,0.23797,0.28239,0.23797,0.28239,P 1,1 -
Analysis Pending,None

NUDT5A-x0111,C1CC2(CCN(C2)C=3C=NC=CN3)CO1,Z1401276297,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0112,FC=1C=CC=CC1C(=O)NCCC=2C=CN=CC2,Z1310876699,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,1.58,0.016,37.8,0.5,94.9,93.7,94.2,0.25795,0.29968,0.25795,0.29968,P 1,1 - Analysis
Pending,None

NUDT5A-x0113,OC=1C=CC(NC(=O)CCC=2C=CC=CC2)=CC1,Z69118333,OK: Precipitated,Failed -
unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0114,CC1CCOC1C(=O)NC2=CN=NS2,Z1827602749,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.89,0.027,25.1,1.0,96.4,98.2,95.4,0.22262,0.26212,0.21502,0.25335,P 1,5 -
Deposition ready,5QJ4

NUDT5A-x0115,CN1CCN(CC1=O)C=2N=CC=CC2F,Z1373445602,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.66,0.021,29.6,0.5,95.5,95.4,95.0,0.24299,0.27847,0.24299,0.27847,P 1,1 -
Analysis Pending,None

NUDT5A-x0116,CC=1C=CC(=CC1C)C(=O)NC2=NN=CN2,Z2856434827,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,1.82,0.015,33.2,0.6,93.9,94.9,95.1,0.22327,0.25671,0.22327,0.25671,P 1,1 - Analysis
Pending,None

NUDT5A-x0117,CC1CCC(CC1)NC2CCC(O)CC2,Z2241963319,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.53,0.017,35.1,0.3,94.7,94.7,94.0,0.25678,0.29886,0.25678,0.29886,P 1,1 -
Analysis Pending,None

NUDT5A-x0118,C(N1CCC(CC1)N2C=CC=C2)C=3C=CC=CC3,Z2856434898,OK: Mounted Clear,success,P
1,48 59 79 79 81
75,1.55,0.031,22.9,1.1,95.9,98.8,93.9,0.22077,0.24373,0.22077,0.24373,P 1,1 - Analysis
Pending,None

NUDT5A-x0119,CN1C(CNC2CCCC2)=NC=3C=CC=CC13,Z2856434855,OK: Mounted Clear,success,P
1,48 59 80 79 81
76,1.92,0.020,23.7,0.6,93.3,94.6,94.5,0.23358,0.27879,0.23358,0.27879,P 1,1 - Analysis
Pending,None

NUDT5A-x0120,COC=1C=CC=C(CN2CCC(CC2)C(=O)N)C1,Z2856434854,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,2.07,0.042,17.4,1.3,97.2,95.6,96.1,0.22060,0.26165,0.22060,0.26165,P 1,1 - Analysis
Pending,None

NUDT5A-x0121,CN1N=CC=C1C(=O)NCC2=CC=CS2,Z915492990,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.79,0.018,30.2,0.6,88.5,95.2,95.1,0.22603,0.26124,0.22603,0.26124,P 1,1 -
Analysis Pending,None

NUDT5A-x0122,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.72,0.023,30.6,0.8,96.5,98.6,95.6,0.22244,0.25296,0.21632,0.25267,P 1,5
- Deposition ready,5QJ5

NUDT5A-x0123,C1CCN(CC1)C2=NOC(=N2)C3=CC=CS3,Z1623890017,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0124,FC=1C=CC(CNCC=2C=CC=CC2)=CC1,Z2856434783,OK: Mounted Clear,success,P 1,49
90 149 89 87 88,1.92,0.017,11.2,1.1,96.4,98.8,94.8,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0125,COC(=O)[C@@H]1C[C@@H](O)CN1C(=O)C2=CC=CO2,Z1614545742,OK: Mounted
Clear,success,P 1,49 59 80 79 81
75,1.65,0.038,27.8,1.0,96.3,97.6,94.8,0.22035,0.25336,0.21352,0.24900,P 1,6 -
Deposited,5QJ6

NUDT5A-x0126,C1CCC(CC1)C2=NC(=NO2)C=3C=CN=CC3,Z57715447,OK: Bad Dispense,success,P 1,49
59 80 79 81 75,1.97,0.022,20.2,0.6,85.3,93.1,80.4,0.24497,0.28828,0.24497,0.28828,P 1,1
- Analysis Pending,None

NUDT5A-x0127,CC(=O)C=1C=CC=C(NC(=O)C(F)(F)F)C1,Z57111868,OK: Precipitated,success,P
1,49 59 80 79 81
75,2.03,0.029,22.4,1.9,96.5,94.8,92.3,0.23697,0.27689,0.23697,0.27689,P 1,1 - Analysis
Pending,None

NUDT5A-x0128,O=C(NC=1C=CC(=CC1)N2CCOCC2)C3CC3,Z30485868,OK: Mounted Clear,success,P
 1,49 59 80 79 81
 75,1.65,0.016,30.2,1.1,95.9,98.2,93.7,0.22373,0.25294,0.22373,0.25294,P 1,1 - Analysis
 Pending,None

NUDT5A-x0129,CC=1C=NC=C(NCC=2C=CN=CC2)C1,Z1478435544,OK: Mounted Clear,success,P 1,47
 59 80 80 84 77,1.70,0.016,32.3,1.2,95.7,98.5,94.3,0.30147,0.34541,0.30147,0.34541,P 1,1
 - Analysis Pending,None

NUDT5A-x0130,FC=1C=CC(NC(=O)CN2CCCC2)=CC1,Z2856434942,OK: Mounted Clear,success,P 1,49
 60 79 79 81 75,1.66,0.017,32.7,0.6,94.8,94.8,94.6,0.25100,0.29458,0.25100,0.29458,P 1,1
 - Analysis Pending,None

NUDT5A-x0131,O=C(C1CC1)N2CCN(CC2)C(=O)C3=CC=CO3,Z32327641,OK: Mounted Clear,success,P
 1,49 59 79 79 81
 75,1.56,0.020,32.2,0.8,94.9,95.8,94.0,0.24866,0.28051,0.23879,0.27376,P 1,6 -
 Deposited,5QJ7

NUDT5A-x0132,CC(C)N1CCN(CC1)C(=O)C2=CC=CS2,Z2856434826,OK: Mounted Clear,success,P 1,49
 60 79 79 80 75,1.81,0.034,19.6,1.0,96.8,98.3,95.4,0.24689,0.28824,0.24689,0.28824,P 1,1
 - Analysis Pending,None

NUDT5A-x0133,CC(C)N(C)S(=O)(=O)N1CCOC(C)C1,Z416341642,OK: Mounted Clear,success,P 1,49
 59 79 79 81 75,1.62,0.014,39.8,0.5,94.9,94.2,94.4,0.23632,0.26926,0.23632,0.26926,P 1,1
 - Analysis Pending,None

NUDT5A-x0134,FC=1C=CC(CCNC(=O)C2=CC=CO2)=CC1,Z26769872,OK: Mounted Clear,success,P 1,49
 59 80 79 81 75,1.65,0.025,27.8,1.0,96.4,99.2,94.5,0.23108,0.25952,0.23108,0.25952,P 1,1
 - Analysis Pending,None

NUDT5A-x0135,CC=1C=CC=CC1CNC2=NN=NN2C,Z57778470,OK: Precipitated,success,P 1,49 59 79
 79 81 75,1.78,0.018,28.7,0.6,94.8,93.9,95.0,0.23536,0.26988,0.23536,0.26988,P 1,1 -
 Analysis Pending,None

NUDT5A-x0136,COC(=O)CNC(=O)C1CCCC1,Z18618496,OK: Mounted Clear,success,P 1,49 90 149
 89 87 88,1.74,0.031,14.3,0.9,96.3,97.3,95.7,,None,None,None,1 - Analysis Pending,None

NUDT5A-x0137,CC[C@H](CO)NC(=O)NC=1C=CC(C1)=CC1,Z1593306637,OK: Mounted Clear,Failed -
 unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
 Pending,None

NUDT5A-x0138,C1CCCC(CC1)NC=2N=CC=CN2,Z31244728,OK: Crystalline,Failed -
 unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
 Pending,None

NUDT5A-x0139,N#CC=1C=CC(CN2C=NC=3C=CC=CC23)=CC1,Z26333434,OK: Mounted Clear,success,P
 1,49 59 80 79 81
 75,1.66,0.024,24.1,0.6,94.9,94.5,95.0,0.22972,0.26006,0.22972,0.26006,P 1,1 - Analysis
 Pending,None

NUDT5A-x0140,O=C(NC1=NN=C(S1)C2=CC=CO2)C3CC3,Z165141116,OK: Mounted Clear,success,P
 1,48 59 79 79 82
 75,1.79,0.024,22.4,1.1,96.8,97.3,95.5,0.21557,0.25014,0.21557,0.25014,P 1,1 - Analysis
 Pending,None

NUDT5A-x0141,O=C(NC=1C=CC(C#N)=CC1)C2=CC=CS2,Z30612387,OK: Mounted Clear,success,P 1,49
 59 79 79 81 75,1.79,0.009,54.3,1.1,95.4,98.5,94.0,0.22632,0.25862,0.22632,0.25862,P 1,1
 - Analysis Pending,None

NUDT5A-x0142,CC=1C=CC=C(C1)C(=O)NC=2C=CC(C)=CC2O,Z33452549,OK: Mounted Clear,success,P
 1,49 59 79 79 81

75,1.79,0.024,29.8,1.1,96.8,97.8,95.7,0.22929,0.26612,0.22929,0.26612,P 1,1 - Analysis Pending, None

NUDT5A-x0143, N[C@H]1CCN(C1)S(=O)(=O)C=2C=CC=CC2, Z2443429438, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0144, FC=1C=CC(=CC1)N2CCN(CC2)C(=O)C3CC3, Z30620520, OK: Mounted Clear, success, P 1,49 59 79 79 81
75,1.70,0.025,25.7,0.5,95.0,94.9,95.2,0.22887,0.25963,0.22887,0.25963,P 1,1 - Analysis Pending, None

NUDT5A-x0145, CCOC(=O)NCC=1C=CC=CC1, Z31478129, OK: Mounted Clear, success, P 1,49 60 80 79 81
75,1.97,0.023,19.9,0.7,95.0,95.6,92.8,0.24597,0.28351,0.24597,0.28351,P 1,1 - Analysis Pending, None

NUDT5A-x0146, C[1C@H]1CC[1C@@H](O1)C(=O)N2CCC=C(F)C2, Z2272040604, OK: Mounted Clear, success, P 1,49 59 79 79 81
75,1.69,0.026,22.8,0.7,93.6,89.1,93.2,0.24046,0.27235,0.24046,0.27235,P 1,1 - Analysis Pending, None

NUDT5A-x0147, CC(=O)N1CCC(CC1)NCCC=2C=CC=CC2, Z2856434883, OK: Mounted Clear, success, P 1,49 59 79 79 81
75,1.76,0.014,34.3,0.9,95.9,98.3,95.1,0.24172,0.28184,0.24172,0.28184,P 1,1 - Analysis Pending, None

NUDT5A-x0148, FC=1C=CC=C(F)C1C(=O)N2CCCC2, Z54226006, OK: Mounted Clear, success, P 1,49 60 79 79 81
75,2.07,0.023,8.5,0.6,92.6,89.8,94.8,0.25701,0.30831,0.25701,0.30831,P 1,1 - Analysis Pending, None

NUDT5A-x0149, OC=1C=CC=CC1NC(=O)COC=2C=CC=CC2, Z68195082, OK: Mounted Clear, success, P 1,49 59 80 79 81
75,1.81,0.021,23.3,0.8,94.3,92.1,95.2,0.22836,0.26619,0.22836,0.26619,P 1,1 - Analysis Pending, None

NUDT5A-x0150, FC=1C=CC(CNC(=O)NC=2C=CC=CC2)=CC1, Z44609285, OK: Mounted Clear, success, P 1,48 59 80 79 82
76,1.64,0.013,38.2,1.0,95.5,98.6,93.4,0.22317,0.24834,0.22317,0.24834,P 1,1 - Analysis Pending, None

NUDT5A-x0151, NC(=O)C=1C=CC(NC(=O)[C@H]2CCCCO2)=CC1, Z1545313172, OK: Crystalline, success, P 1,49 59 79 79 81
75,1.64,0.018,37.8,1.0,95.7,97.2,93.4,0.23323,0.26252,0.23323,0.26252,P 1,1 - Analysis Pending, None

NUDT5A-x0152, FC=1C=CC=CC1NCC=2C=CCN2, Z1545196403, OK: Mounted Clear, success, P 1,49 60 79 79 81
75,1.77,0.017,30.5,0.5,95.3,95.4,95.1,0.24364,0.28606,0.24364,0.28606,P 1,1 - Analysis Pending, None

NUDT5A-x0153, CC(=O)N1CCN(CCCC=2C=CC=CC2)CC1, Z2856434884, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0154, CC(C)C=1C=CC(=CC1)C(=O)NC=2C=CC=CN2, Z85525355, OK: Crystalline, success, P 1,49 59 79 79 81
75,1.78,0.011,50.0,1.0,96.0,98.6,94.4,0.23150,0.26745,0.23150,0.26745,P 1,1 - Analysis Pending, None

NUDT5A-x0155, CN1C=CC(=N1)C(=O)NC[C@H]2CCCCO2, Z2643472210, OK: Precipitated, success, P 1,49 59 79 79 81
75,1.66,0.018,28.8,0.6,94.6,93.5,94.9,0.23774,0.27308,0.23774,0.27308,P 1,1 - Analysis Pending, None

NUDT5A-x0156,FC=1C=CC=NC1NCC2CCOCC2,Z1373430305,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.66,0.014,34.7,0.5,94.5,93.7,94.5,0.25517,0.30008,0.25517,0.30008,P 1,1 - Analysis Pending,None

NUDT5A-x0157,FC=1C=CC(CN2C=NC=3C=CC=CC23)=CC1,Z26333448,OK: Precipitated,success,P 1,49 59 79 79 81 75,1.74,0.018,28.0,0.7,94.4,94.3,95.2,0.22954,0.26621,0.22954,0.26621,P 1,1 - Analysis Pending,None

NUDT5A-x0158,CN1CCN(CC1)C(=O)C=2C=CC(F)=C(F)C2,Z2856434829,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.76,0.032,25.3,1.0,96.8,97.7,96.0,0.23762,0.27444,0.23670,0.27771,P 1,6 - Deposited,5QJ8

NUDT5A-x0159,CN(CC(=O)O)C(=O)C=1C=CC=CN1,Z1171978788,OK: Crystalline,success,P 1,46 58 79 81 84 78,1.73,0.010,40.7,0.7,94.4,94.1,94.8,0.34241,0.38674,0.34241,0.38674,P 1,1 - Analysis Pending,None

NUDT5A-x0160,CC=1C=C(C)N=C(NC=2C=CC=CC2)N1,Z285675722,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,2.06,0.031,22.1,1.2,95.7,96.0,94.9,0.23309,0.27606,0.23309,0.27606,P 1,1 - Analysis Pending,None

NUDT5A-x0161,CCC(=O)NC=1C=CC(=CC1)N2CCC(C)CC2,Z57344995,OK: Mounted Clear,success,P 1,48 59 79 79 81 75,1.64,0.014,33.3,0.5,94.9,95.8,94.7,0.22473,0.25650,0.22473,0.25650,P 1,1 - Analysis Pending,None

NUDT5A-x0162,OC=1C=CC=C(NC(=O)NC=2C=CC(F)=CC2)C1,Z55290386,OK: Mounted Clear,success,P 1,48 59 79 79 81 76,1.88,0.016,28.9,0.5,90.0,91.4,94.4,0.23086,0.27498,0.23086,0.27498,P 1,1 - Analysis Pending,None

NUDT5A-x0163,CN(C(=O)[C@H]1CC1(C)C)C=2C=CC=NC2,Z1506050651,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.88,0.013,33.2,1.4,95.6,98.5,94.3,0.23610,0.27702,0.23610,0.27702,P 1,1 - Analysis Pending,None

NUDT5A-x0164,CC(=O)C=1C=CC(=CC1)N2CCC(CC2)C(=O)N,Z126933926,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.65,0.032,21.9,1.0,96.3,98.9,94.6,0.23422,0.26649,0.23422,0.26649,P 1,1 - Analysis Pending,None

NUDT5A-x0165,COC=1C=CC(NC=2N=CN=C3NC=NC23)=CC1,Z276545932,OK: Mounted Clear,success,P 1,48 59 80 79 81 75,1.58,0.020,28.6,0.6,94.8,94.8,94.2,0.22419,0.25380,0.22419,0.25380,P 1,1 - Analysis Pending,None

NUDT5A-x0166,CCN(CC)S(=O)(=O)C=1C=CC(C)=CC1,Z45516134,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.77,0.017,38.6,1.0,95.7,98.8,94.8,0.22798,0.25780,0.22798,0.25780,P 1,1 - Analysis Pending,None

NUDT5A-x0167,CC(N)CN1CCOCC1,Z818732104,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,2.29,0.103,7.1,1.7,97.0,98.2,96.5,0.24199,0.28630,0.24199,0.28630,P 1,1 - Analysis Pending,None

NUDT5A-x0168,CC(C)NC(=O)N(C)C1CCS(=O)(=O)C1,Z445856640,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.70,0.017,39.3,1.1,96.0,98.4,95.0,0.23210,0.26272,0.23210,0.26272,P 1,1 - Analysis Pending,None

NUDT5A-x0169,CC1CN(C(C)CO1)C(=O)C=2C=NSN2,Z768399682,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.85,0.023,22.7,0.9,96.5,99.0,95.4,0.24904,0.28711,0.24416,0.28836,P 1,5 - Deposition ready,5QJ9

NUDT5A-x0170,FC=1C=CC=C(C1)C(=O)NCC=2C=CC=CC2,Z27749656,OK: Mounted Clear,success,P
 1,49 59 80 79 81
 75,1.83,0.036,18.5,0.6,79.3,91.3,47.8,0.24231,0.28420,0.24231,0.28420,P 1,1 - Analysis
 Pending,None

NUDT5A-x0171,CC1=NC(C(=O)N2CCCC2)=C(C)S1,Z1497321453,OK: Mounted Clear,success,P 1,49
 59 80 79 81 75,1.64,0.012,47.6,1.1,95.9,98.6,93.8,0.23664,0.26480,0.22696,0.25714,P 1,6
 - Deposited,5QJA

NUDT5A-x0172,CC=1C=CC=C(C1)C(=O)NCC(=O)O,Z56827661,OK: Mounted Clear,success,P 1,46 58
 80 80 84 78,1.51,0.010,46.4,1.2,95.0,98.5,92.1,0.34669,0.38666,0.27294,0.31210,P 1,3 -
 In Refinement,None

NUDT5A-x0173,COC(=O)NC1=NC=2C(C)=CC=CC2S1,Z192981502,OK: Precipitated,success,P 1,49 59
 79 79 81 75,1.71,0.023,25.2,0.5,82.3,95.6,94.4,0.23207,0.26691,0.23207,0.26691,P 1,1 -
 Analysis Pending,None

NUDT5A-x0174,O=C(NC[C@H]1CCCC1)N2CCOCC2,Z2064898127,OK: Mounted Clear,success,P 1,49 60
 79 79 81 75,1.77,0.027,25.3,0.9,96.2,98.8,95.1,0.23353,0.27009,0.23353,0.27009,P 1,1 -
 Analysis Pending,None

NUDT5A-x0175,CC(=O)NC=1C=CC(CN2CCOCC2)=CC1,Z2856434875,OK: Crystalline,success,P 1,49
 59 80 79 81 75,1.80,0.013,36.1,0.6,80.6,95.1,67.6,0.22480,0.26608,0.22480,0.26608,P 1,1
 - Analysis Pending,None

NUDT5A-x0176,CN(CC1CCOC1)C=2N=CN=CC2C1,Z1787627869,OK: Mounted Clear,success,P 1,49 60
 79 79 80 75,1.66,0.024,29.6,1.1,96.0,97.8,94.0,0.25339,0.28881,0.25245,0.29152,P 1,6 -
 Deposited,5QJB

NUDT5A-x0177,CCNC(=O)C1=CN=N1,Z755044716,OK: Crystalline,success,P 1,49 59 80 79 81
 75,1.47,0.020,29.7,0.6,93.6,93.3,88.3,0.23551,0.26192,0.22231,0.25416,P 1,6 -
 Deposited,5QJC

NUDT5A-x0178,CCOC(=O)C=1C=CC(F)=CC1F,Z53836105,OK: Crystalline,success,P 1,48 59 80 79
 82 76,1.89,0.044,16.4,0.7,90.5,91.5,92.0,0.23848,0.28095,0.23848,0.28095,P 1,1 -
 Analysis Pending,None

NUDT5A-x0179,OC=1N=CC(NCCC=2C=CC=CC2)=C(O)N1,Z57744604,OK: Precipitated,success,P 1,49
 60 80 79 81 75,1.74,0.012,41.5,1.0,96.2,98.8,95.2,0.23255,0.26409,0.23191,0.26529,P 1,3
 - In Refinement,None

NUDT5A-x0180,CCNC(=O)C=1C=CC(N(C)C)=C(F)C1,Z907784200,OK: Mounted Clear,success,P 1,49
 60 80 79 81 75,1.79,0.014,37.5,0.6,94.2,94.4,94.6,0.23142,0.26723,0.23142,0.26723,P 1,1
 - Analysis Pending,None

NUDT5A-x0181,CCC(=O)NC=1C=CC(=CC1)S(=O)(=O)N,Z27682767,OK: Mounted Clear,success,P 1,49
 60 80 79 81 75,1.74,0.015,45.1,1.1,96.0,98.6,94.6,0.22955,0.26241,0.22955,0.26241,P 1,1
 - Analysis Pending,None

NUDT5A-x0182,C(NC1CCCC1)C2CCCC2,Z90504169,OK: Mounted Clear,success,P 1,49 59 80 79 81
 75,1.74,0.012,41.6,1.0,96.0,98.8,95.0,0.22476,0.25749,0.22476,0.25749,P 1,1 - Analysis
 Pending,None

NUDT5A-x0183,COC(=O)C=1SC=CC1NC(=O)C2CC2,Z109092588,OK: Mounted Clear,success,P 1,49 59
 80 79 81 75,1.79,0.019,25.2,1.1,96.5,97.4,95.3,0.23227,0.26892,0.23126,0.27081,P 1,1 -
 Analysis Pending,None

NUDT5A-x0184,CCNC=1C=CC(C)=NN1,Z1267773786,OK: Crystalline,success,P 1,49 60 80 79 81
 75,1.80,0.022,30.0,0.6,78.3,94.7,61.3,0.23344,0.27725,0.23344,0.27725,P 1,1 - Analysis
 Pending,None

NUDT5A-x0185,O=C(CCC1CCCC1)NC=2C=CC=C(C#N)C2,Z26548228,OK: Mounted Clear,success,P 1,48
60 80 79 82 76,2.36,0.069,8.6,1.4,52.5,68.1,48.9,0.33856,0.34133,0.33856,0.34133,P 1,1
- Analysis Pending,None

NUDT5A-x0186,O=C(CCC1CCCC1)N2CCOCC2,Z31721798,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.94,0.068,21.0,1.3,97.0,98.5,95.4,0.22184,0.25672,0.22253,0.25738,P 1,3 - In
Refinement,None

NUDT5A-x0187,O=C(NCCN1CCCC1=O)NC=2C=CC=CC2,Z2472938267,OK: Mounted Clear,success,P 1,48
59 80 79 82 76,1.73,0.026,22.1,1.0,96.0,96.7,94.8,0.22460,0.26184,0.22460,0.26184,P 1,1
- Analysis Pending,None

NUDT5A-x0188,C1C=1C=CC(CC(=O)NC=2N=CC=CN2)=CC1,Z203581214,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,1.66,0.013,34.6,0.6,81.5,92.9,80.5,0.26618,0.31112,0.26618,0.31112,P 1,1 - Analysis
Pending,None

NUDT5A-x0189,C(N1CCOCC1)C2=NC(=NO2)C3CC3,Z295848548,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0190,OC=1C=CC(CN2CCC=3C=CC=CC3C2)=CC1,Z2856434812,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0191,CN1C=CC(NCC=2C=CC=CC2)=N1,Z1401333862,OK: Mounted Clear,success,P 1,48 59
79 79 81 76,1.71,0.012,52.4,0.9,96.0,99.2,94.7,0.22003,0.24932,0.22003,0.24932,P 1,1 -
Analysis Pending,None

NUDT5A-x0192,CC1=CC(=NS1)C(=O)NCC2CCCO2,Z1881545321,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.66,0.020,32.2,1.1,96.0,99.0,94.1,0.24524,0.28019,0.24524,0.28019,P 1,1 -
Analysis Pending,None

NUDT5A-x0193,CC=1C=CC(CN2CCS(=O)(=O)CC2)=CC1,Z2856434929,OK: Mounted Clear,success,P
1,48 59 79 79 81
75,1.69,0.020,25.7,1.0,96.4,97.8,95.1,0.22278,0.25133,0.22278,0.25133,P 1,1 - Analysis
Pending,None

NUDT5A-x0194,OC1CCN(CC=2C=CSC2)CC1,Z2856434899,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.85,0.020,13.4,1.4,96.6,98.9,95.4,0.24234,0.28588,0.24234,0.28588,P 1,1 -
Analysis Pending,None

NUDT5A-x0195,CC=1C=C(ON1)C(=O)NC=2C=CN(C)N2,Z240297434,OK: Mounted Clear,success,P 1,48
59 80 79 82 76,1.61,0.022,29.8,0.8,95.3,98.6,92.8,0.22628,0.25361,0.21130,0.23693,P 1,6
- Deposited,5QJD

NUDT5A-x0196,OC=1C=CC=CC1C2=NC(=NO2)C=3C=CC=CC3,Z276351322,OK: Bad Dispense,success,P
1,48 59 79 79 82
76,1.62,0.013,45.2,0.9,95.6,98.8,93.2,0.21656,0.24120,0.21656,0.24120,P 1,1 - Analysis
Pending,None

NUDT5A-x0197,CCN1C=C(CNC(=O)C=2C=CC=NC2)C=N1,Z275181224,OK: Mounted Clear,success,P
1,48 59 79 79 81
76,1.75,0.015,37.6,1.2,95.6,98.7,94.9,0.22166,0.25282,0.21175,0.24553,P 1,6 -
Deposited,5QJE

NUDT5A-x0198,OC=1C=CC=CC1CNC2=NC=3C=CC=CC3N2,Z1587220559,OK: Mounted Clear,success,P
1,48 59 79 80 82
76,2.20,0.027,16.6,1.2,97.2,91.9,96.5,0.21278,0.26027,0.21278,0.26027,P 1,1 - Analysis
Pending,None

NUDT5A-x0199,CC=1NC=NC1CN2CCC=3C=CC=CC3C2,Z2856434879,OK: Mounted Clear,Failed - unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis Pending,None

NUDT5A-x0200,CCOC(=O)C1CCN(CC1)C=2C=NC=CN2,Z31217395,OK: Bad Dispense,success,P 1,48 59 79 80 82 76,2.09,0.023,23.4,0.8,88.1,93.1,95.2,0.23785,0.28405,0.23785,0.28405,P 1,1 - Analysis Pending,None

NUDT5A-x0201,CC1=NC=C(CN2CCNCC2)S1,Z1171217421,OK: Mounted Clear,success,P 1,49 59 79 80 81 76,1.76,0.021,28.7,1.1,96.8,98.5,95.5,0.25626,0.30238,0.25626,0.30238,P 1,1 - Analysis Pending,None

NUDT5A-x0202,CC1=NN=C(CN2CCC=C(F)C2)S1,Z1619978933,OK: Mounted Clear,success,P 1,48 59 79 80 81 76,1.93,0.022,23.3,0.7,89.1,93.5,80.7,0.24084,0.28760,0.24084,0.28760,P 1,1 - Analysis Pending,None

NUDT5A-x0203,CN(C1CC(O)C1)C=2C=C(C)N=C(C)N2,Z1675346324,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,2.17,0.034,8.8,0.8,92.1,93.0,81.3,0.23333,0.27573,0.23333,0.27573,P 1,1 - Analysis Pending,None

NUDT5A-x0204,CN(CC=1C=C(C)ON1)C(=O)NC2CC2,Z369936976,OK: Mounted Clear,success,P 1,48 59 79 79 81 76,1.60,0.023,28.3,0.5,94.9,95.7,94.1,0.24140,0.27602,0.24140,0.27602,P 1,1 - Analysis Pending,None

NUDT5A-x0205,C(CN1CCOCC1)SC=2C=CC=CC2,Z2856434865,OK: Crystalline,success,P 1,48 59 79 79 81 76,1.67,0.017,31.2,0.5,88.1,94.8,95.0,0.22257,0.25668,0.22257,0.25668,P 1,1 - Analysis Pending,None

NUDT5A-x0206,CC1=NN=C(S1)N2CCCC2,Z1251207602,OK: Mounted Clear,success,P 1,48 59 79 79 81 76,1.87,0.009,49.4,1.2,95.7,98.9,94.6,0.22365,0.26037,0.22365,0.26037,P 1,1 - Analysis Pending,None

NUDT5A-x0207,CC1CN(C)CCC1NC=2C=NN(C)C2,Z1694504496,OK: Mounted Clear,success,P 1,49 59 79 80 81 76,1.73,0.013,42.0,1.0,95.8,98.5,95.0,0.23700,0.27003,0.23700,0.27003,P 1,1 - Analysis Pending,None

NUDT5A-x0208,OC=1C=CC(CCNC(=O)C=2C=CC=CN2)=CC1,Z730649594,OK: Mounted Clear,success,P 1,49 59 79 80 81 75,1.77,0.027,28.7,1.0,96.5,99.1,95.3,0.25312,0.29474,0.25312,0.29474,P 1,1 - Analysis Pending,None

NUDT5A-x0209,CC=1OC=CC1C(=O)NC=2C=C(ON2)C(C)(C)C,Z1086293874,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.86,0.069,4.6,1.1,96.8,98.1,95.3,0.22485,0.25574,0.22485,0.25574,P 1,1 - Analysis Pending,None

NUDT5A-x0210,CCCC1=NN=C(NC(=O)C=2C=CC=CN2)S1,Z52425517,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.63,0.016,35.0,0.5,91.1,95.5,94.6,0.22277,0.25489,0.21587,0.24931,P 1,6 - Deposited,5QJF

NUDT5A-x0211,CC1=NC=C(CNC=2C=NC=C(F)C2)S1,Z1983897532,OK: Mounted Clear,success,P 1,48 59 79 80 81 76,1.92,0.013,41.6,1.1,96.3,98.6,94.7,0.22186,0.26187,0.22186,0.26187,P 1,1 - Analysis Pending,None

NUDT5A-x0212,CC=1C=CC(OCC(=O)N2CCOCC2)=C(C)C1,Z17497990,OK: Mounted Clear,success,P 1,48 59 79 79 81 76,1.71,0.016,38.5,1.0,96.1,98.6,94.9,0.23097,0.26060,0.23097,0.26060,P 1,1 - Analysis Pending,None

NUDT5A-x0213,CN1C=C(C1)C(=N1)C(=O)NC2CCCC2,Z275151340,OK: Mounted Clear,success,P 1,48 59 79 80 81 76,1.65,0.012,41.4,0.5,94.8,94.3,94.8,0.23705,0.27442,0.23705,0.27442,P 1,1 - Analysis Pending,None

NUDT5A-x0214, CC1=CC (=NO1) C (=O) NCC2=CC=CS2, Z29692148, OK: Precipitated, success, P 1, 49 59 79 79 81 75, 1.79, 0.043, 19.0, 1.3, 96.6, 98.2, 95.5, 0.23035, 0.26759, 0.23035, 0.26759, P 1, 1 - Analysis Pending, None

NUDT5A-x0215, CC1=C (C=NN1C) C (=O) NCC2CCC2, Z396380540, OK: Mounted Clear, success, P 1, 48 59 79 80 81 76, 1.81, 0.017, 30.0, 0.5, 76.0, 93.9, 59.1, 0.23048, 0.27706, 0.23048, 0.27706, P 1, 1 - Analysis Pending, None

NUDT5A-x0216, COC=1C=CC (NC (=O) NC2=CC=CS2) =CN1, Z1152242726, OK: Mounted Clear, success, P 1, 48 59 79 79 81 75, 1.86, 0.020, 21.4, 1.2, 96.6, 99.2, 95.6, 0.21793, 0.25116, 0.21793, 0.25116, P 1, 1 - Analysis Pending, None

NUDT5A-x0217, CCN1CCN (CC1) C (=O) NC2CCCC2, Z2856434830, OK: Mounted Clear, success, P 1, 48 59 79 79 81 75, 1.79, 0.020, 24.4, 0.6, 84.9, 93.5, 80.4, 0.23313, 0.27082, 0.23313, 0.27082, P 1, 1 - Analysis Pending, None

NUDT5A-x0218, CC1CN (CCO1) C (=O) CN2C=CC=N2, Z217038356, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 2.03, 0.039, 19.3, 1.5, 96.7, 95.7, 93.6, 0.22337, 0.26115, 0.22352, 0.26457, P 1, 3 - In Refinement, None

NUDT5A-x0219, COC (=O) C=1C=CC (NC (=O) C2CCCC2) =CC1, Z28226359, OK: Mounted Clear, success, P 1, 48 59 79 80 82 76, 1.76, 0.053, 23.9, 1.1, 96.5, 97.2, 95.4, 0.21949, 0.25424, 0.21949, 0.25424, P 1, 1 - Analysis Pending, None

NUDT5A-x0220, O=S1 (=O) CCN (CC2=CC=CO2) CC1, Z2856434926, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.95, 0.045, 11.0, 1.0, 96.1, 98.7, 94.8, 0.24161, 0.27300, 0.24161, 0.27300, P 1, 1 - Analysis Pending, None

NUDT5A-x0221, O=C (COC=1C=CC=CC1) N2CCNC (=O) C2, Z31602870, OK: Mounted Clear, success, P 1, 48 59 79 79 82 76, 2.06, 0.022, 13.3, 0.5, 95.0, 95.9, 95.7, 0.22628, 0.27233, 0.22628, 0.27233, P 1, 1 - Analysis Pending, None

NUDT5A-x0222, CC=1C=CC=CC1OCC (=O) NC=2N=CC=CN2, Z53834613, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0223, FC=1C=CC (CNC [C@H] 2CCCO2) =CC1, Z2856434824, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0224, CC1=CSC (NC (=O) C2CCOCC2) =N1, Z73240835, OK: Precipitated, success, P 1, 48 59 79 79 81 76, 1.75, 0.013, 41.7, 1.0, 96.1, 98.8, 95.1, 0.22482, 0.25900, 0.22482, 0.25900, P 1, 1 - Analysis Pending, None

NUDT5A-x0225, CC1=CC (NC (=O) CSC=2C=CC=CC2) =NO1, Z19750454, OK: Precipitated, Failed - unknown, None, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0226, COC=1C=CC (NC (=O) NC=2C=CN=CC2) =CC1, Z321318226, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.72, 0.026, 23.3, 0.6, 95.3, 96.5, 95.2, 0.23187, 0.26685, 0.23187, 0.26685, P 1, 1 - Analysis Pending, None

NUDT5A-x0227, COC=1C=CC (NCC=2C=CC=CC2O) =CC1, Z56943440, OK: Mounted Clear, success, P 1, 48 59 79 79 81 76, 1.80, 0.020, 30.1, 0.7, 87.5, 94.2, 94.2, 0.22396, 0.25916, 0.22396, 0.25916, P 1, 1 - Analysis Pending, None

NUDT5A-x0228, O=C (CCCC=1C=CC=CC1) N2CCOCC2, Z419995480, OK: Mounted Clear, success, P 1, 48 59 79 79 81 75, 1.73, 0.025, 39.9, 1.0, 96.2, 99.1, 95.3, 0.22145, 0.25294, 0.22145, 0.25294, P 1, 1 - Analysis Pending, None

NUDT5A-x0229,CC=1N=CSC1C(=O)N2CCCNCC2,Z803153598,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,2.04,0.021,22.8,1.0,96.4,99.2,94.7,0.23300,0.27867,0.23300,0.27867,P 1,1 -
Analysis Pending,None

NUDT5A-x0230,CN1C=C(CNC(=O)C2=CC=CO2)C=N1,Z275179758,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.71,0.031,35.5,1.3,96.7,98.8,95.5,0.23198,0.26280,0.23198,0.26280,P 1,1
- Analysis Pending,None

NUDT5A-x0231,FC=1C=CC(NC(=O)NCC2=CC=CO2)=CC1,Z44584202,OK: Mounted Clear,success,P 1,48
59 79 79 81 76,1.59,0.047,26.3,1.2,96.5,99.2,93.9,0.21710,0.23942,0.21710,0.23942,P 1,1
- Analysis Pending,None

NUDT5A-x0232,CCOC=1C=CC(NC(=O)NC(C)(C)C)=CC1,Z44586802,OK: Mounted Clear,success,P 1,48
59 79 79 82 76,1.64,0.021,41.8,1.0,96.1,99.0,93.6,0.21970,0.24602,0.21970,0.24602,P 1,1
- Analysis Pending,None

NUDT5A-x0233,CCC=1C=CC(OCC(=O)N2CCCC2)=CC1,Z18839017,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.94,0.027,17.2,1.2,96.9,96.5,95.7,0.22386,0.26302,0.22386,0.26302,P 1,1
- Analysis Pending,None

NUDT5A-x0234,CC=1C=CC(CNC(=O)C2CCC2)=CN1,Z437516460,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.91,0.016,20.7,0.5,94.9,94.9,94.8,0.23145,0.27336,0.23145,0.27336,P 1,1 -
Analysis Pending,None

NUDT5A-x0235,COC(=O)C1CCN(CC1)C(=O)NC(C)(C)C,Z44567722,OK: Mounted Clear,success,P 1,48
59 80 79 82 76,1.57,0.037,30.8,1.2,96.5,99.3,93.9,0.22146,0.24407,0.20695,0.23279,P 1,2
- PANDDA model,5QJG

NUDT5A-x0236,CC1(C)CN(CC1O)C=2N=CC=CC2F,Z1929757385,OK: Mounted Clear,success,P 1,48 59
79 79 82 76,1.56,0.022,46.1,1.5,96.3,98.9,94.6,0.21777,0.24287,0.21777,0.24287,P 1,1 -
Analysis Pending,None

NUDT5A-x0237,CC1=CC(=NO1)C(=O)NC=2C=CC=3NC=CC3C2,Z1190787729,OK: Precipitated,success,P
1,48 59 79 79 81
76,1.66,0.018,31.3,0.5,95.1,93.7,94.6,0.22148,0.25555,0.22148,0.25555,P 1,1 - Analysis
Pending,None

NUDT5A-x0238,O=C(COC=1C=CC=CC1)NC2CCCC2,Z19735904,OK: Mounted Clear,success,P 1,48 59
79 80 82 76,1.61,0.024,40.7,1.2,96.2,99.0,93.3,0.21826,0.24290,0.21826,0.24290,P 1,1 -
Analysis Pending,None

NUDT5A-x0239,CC1=NC(CN2CCC(CN)CC2)=CS1,Z1259335913,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.74,0.017,35.6,0.6,94.8,92.6,95.1,0.23544,0.27732,0.23544,0.27732,P 1,1 -
Analysis Pending,None

NUDT5A-x0240,CCOC(=O)CN1CCS(=O)(=O)CC1,Z2856434920,OK: Mounted Clear,success,P 1,48 59
79 79 82 76,1.69,0.037,30.2,1.0,96.6,99.0,94.7,0.22110,0.25071,0.22110,0.25071,P 1,1 -
Analysis Pending,None

NUDT5A-x0241,C(CC=1C=CC=CC1)NC2=NC=3C=CC=CC3N2,Z57299529,OK: Mounted Clear,success,P
1,48 59 79 79 82
76,1.76,0.037,22.3,1.3,96.2,96.4,95.5,0.21996,0.25177,0.21996,0.25177,P 1,1 - Analysis
Pending,None

NUDT5A-x0242,CC1C(O)CCCN1CC=2C=CC=CC2,Z2217052426,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,2.09,0.096,24.7,1.4,97.4,98.1,95.1,0.21870,0.26413,0.21870,0.26413,P 1,1 -
Analysis Pending,None

NUDT5A-x0243,OC=1C=CC(NC(=O)C=2C=CC(C1)=CC2)=CC1,Z56346825,OK: Crystalline,success,P
1,48 59 79 79 82
76,1.72,0.016,30.5,1.0,95.9,99.1,95.0,0.21726,0.24567,0.21726,0.24567,P 1,1 - Analysis
Pending,None

NUDT5A-x0244,COC(=O)CNC(=O)C=1C=C(C)ON1,Z375990520,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,2.03,0.026,19.6,1.3,96.2,97.6,94.8,0.22784,0.26932,0.22613,0.27266,P 1,6 - Deposited,5QJH

NUDT5A-x0245,CC(C)N1CCN(CC1)C(=O)C(C)C,Z106307058,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.75,0.029,23.9,0.6,95.5,96.0,95.3,0.23629,0.27876,0.23629,0.27876,P 1,1 - Analysis Pending,None

NUDT5A-x0246,CC(=O)NCCN1CCCCC1,Z169226638,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.48,0.018,31.8,0.4,93.8,94.6,88.3,0.27269,0.31291,0.27269,0.31291,P 1,1 - Analysis Pending,None

NUDT5A-x0247,CN(C)C=1C=CC(CNN2C=NN=C2)=CC1,Z57258487,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.70,0.032,14.3,0.7,94.3,92.9,94.7,0.23658,0.26648,0.23658,0.26648,P 1,1 - Analysis Pending,None

NUDT5A-x0248,CC1=NC(CN2C[C@@H](F)C[C@H]2CN)=CS1,Z2444997446,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.64,0.063,27.5,1.0,97.0,98.4,94.8,0.21781,0.24125,0.21781,0.24125,P 1,1 - Analysis Pending,None

NUDT5A-x0249,CC(N1CCNCC1)C=2C=CC=CC2F,Z2466069494,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.84,0.014,40.1,0.5,81.3,92.9,45.7,0.23098,0.27139,0.23098,0.27139,P 1,1 - Analysis Pending,None

NUDT5A-x0250,NC(=O)C=1C=CC=CC1NC(=O)C=2C=CN=CC2,Z91797745,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.55,0.020,41.8,1.1,96.7,99.3,93.1,0.21830,0.23998,0.21830,0.23998,P 1,1 - Analysis Pending,None

NUDT5A-x0251,CC1=NN(CC=2C(C)=NOC2C)C(=O)S1,Z1899842917,OK: Mounted Clear,success,P 1,48 59 79 79 81 75,1.69,0.040,53.5,0.7,97.1,98.4,95.5,0.25799,0.29761,0.25884,0.30070,P 1,6 - Deposited,5QJI

NUDT5A-x0252,FC=1C=CC(CC(=O)NC=2C=CC(F)=CC2)=CC1,Z27805986,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.78,0.019,26.7,1.0,95.7,99.3,94.8,0.22163,0.25061,0.22163,0.25061,P 1,1 - Analysis Pending,None

NUDT5A-x0253,CC(C)N(C)S(=O)(=O)N1CCNC(=O)C1,Z431807512,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.66,0.061,46.1,0.7,97.1,98.4,95.2,0.21294,0.23795,0.21294,0.23795,P 1,1 - Analysis Pending,None

NUDT5A-x0254,O=C(NCC=1C=CC(C#N)=CC1)N2CCOCC2,Z509756472,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.66,0.030,19.5,0.6,95.2,95.1,95.2,0.22594,0.25660,0.22594,0.25660,P 1,1 - Analysis Pending,None

NUDT5A-x0255,C(NC1CCNC1)C=2C=CC=CC2,Z1827898537,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.60,0.024,26.1,0.4,94.9,95.0,94.4,0.22202,0.25403,0.22202,0.25403,P 1,1 - Analysis Pending,None

NUDT5A-x0256,COC(=O)C=1C=CC=C(NS(=O)(=O)C)C1,Z24758179,OK: Mounted Clear,success,P 1,48 59 79 79 81 76,1.71,0.018,86.6,0.2,96.0,98.8,94.9,0.22310,0.25534,0.21616,0.24722,P 1,6 - Deposited,5QJJ

NUDT5A-x0257,CCNC(=O)C=1C=CC(NS(=O)(=O)C)=CC1,Z57614330,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.97,0.015,35.7,0.7,84.8,93.5,74.7,0.22414,0.27059,0.22414,0.27059,P 1,1 - Analysis Pending,None

NUDT5A-x0258,C(NC=1C=CC=CN1)C2CCNC2,Z1262327505,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.59,0.043,28.6,0.3,87.2,96.0,94.1,0.23449,0.27379,0.23500,0.27645,P 1,3 - In
Refinement,None

NUDT5A-x0259,CN(C)C(=O)CNC=1C=CC=CC1,Z104584152,OK: Mounted Clear,success,P 1,48 59 79
79 81 76,1.71,0.031,30.3,1.3,97.4,99.4,95.9,0.21775,0.24411,0.21775,0.24411,P 1,1 -
Analysis Pending,None

NUDT5A-x0260,COCC(=O)NC1=NN=C(C)S1,Z263785508,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.78,0.053,20.7,1.1,96.6,97.4,94.6,0.23112,0.26539,0.23112,0.26539,P 1,1 -
Analysis Pending,None

NUDT5A-x0261,FC=1C=CC=C(CN2CCOCC2)C1,Z2856434791,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.55,0.032,39.7,1.1,96.9,98.4,94.3,0.24181,0.27187,0.24181,0.27187,P 1,1 -
Analysis Pending,None

NUDT5A-x0262,C1CN(C1)C=2N=CN=C3N=CNC23,Z373221060,OK: Mounted Clear,success,P 1,48 59
80 79 81 75,1.65,0.034,30.2,1.4,96.7,98.9,94.6,0.22381,0.25500,0.20821,0.23729,P 1,6 -
Deposited,5QJK

NUDT5A-x0263,CC1(C)CN(C(=O)NCC2CC2)C1(C)C,Z1328078283,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.79,0.029,30.7,1.5,97.2,99.4,96.0,0.23995,0.28011,0.23995,0.28011,P 1,1
- Analysis Pending,None

NUDT5A-x0264,C1C=1C=CC(COC(=O)C=2C=CC=NC2)=CC1,Z57515803,OK: Precipitated,success,P
1,49 59 79 79 81
75,1.69,0.019,28.0,0.6,93.9,90.8,95.1,0.23999,0.27250,0.23999,0.27250,P 1,1 - Analysis
Pending,None

NUDT5A-x0265,COCC(=O)NCC=1C=CC(C)=CC1,Z33297786,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.66,0.056,23.3,0.8,97.0,98.8,95.2,0.23320,0.26602,0.23320,0.26602,P 1,1 -
Analysis Pending,None

NUDT5A-x0266,CC1CCCN1CCN,Z1245580425,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.86,0.011,47.0,1.1,96.0,98.8,95.1,0.23000,0.26659,0.23000,0.26659,P 1,1 - Analysis
Pending,None

NUDT5A-x0267,CC(C)NC(=O)C1=CC(C)=NO1,Z135394292,OK: Mounted Clear,success,P 1,48 59 79
79 81 76,1.66,0.019,30.3,0.6,92.6,94.3,95.0,0.25590,0.29910,0.25590,0.29910,P 1,1 -
Analysis Pending,None

NUDT5A-x0268,CC=1N=CC=C(N1)N2CCC(N)CC2,Z1333043417,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.65,0.028,40.7,1.4,96.2,98.8,94.4,0.24696,0.28106,0.24696,0.28106,P 1,1 -
Analysis Pending,None

NUDT5A-x0269,CCOC=1C=CC=C(C1)C(=O)NC=2N=NN(C)N2,Z57292400,OK: Mounted Clear,success,P
1,48 59 79 80 82
76,1.68,0.026,39.4,1.0,97.3,98.5,95.0,0.21721,0.24182,0.21721,0.24182,P 1,1 - Analysis
Pending,None

NUDT5A-x0270,COC=1C=CC(C)=CC1NC(=O)NN2C=NN=C2,Z2234920345,OK: Precipitated,success,P
1,49 59 79 79 81
75,1.86,0.052,34.7,1.4,97.5,97.0,96.3,0.22886,0.26413,0.22886,0.26413,P 1,1 - Analysis
Pending,None

NUDT5A-x0271,CC(C)(O)CN1CC[C@H](N)C1,Z2429435052,OK: Mounted Clear,success,P 1,48 59 79
79 81 75,1.70,0.026,22.2,0.6,95.2,94.3,94.5,0.22274,0.25401,0.22274,0.25401,P 1,1 -
Analysis Pending,None

NUDT5A-x0272,CC=1C=CC=C(CN2CCOCC2)C1,Z2856434862,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.65,0.038,28.4,1.1,96.6,99.1,93.8,0.22295,0.25081,0.22295,0.25081,P 1,1 -
Analysis Pending,None

NUDT5A-x0273,NC(=O)C=1C=CC(NC(=O)C=2C=NC=CN2)=CC1,Z30242120,OK: Mounted Clear,success,P
1,48 59 80 79 81
76,2.09,0.038,27.8,1.0,97.0,98.3,95.9,0.21417,0.25458,0.21417,0.25458,P 1,1 - Analysis
Pending,None

NUDT5A-x0274,OC=1C=CC(CNC2CCCCC2)=CC1,Z2241127906,OK: Mounted Clear,success,P 1,49 59
79 80 81 75,2.34,0.025,16.1,0.9,96.3,97.8,97.6,0.25534,0.31992,0.25534,0.31992,P 1,1 -
Analysis Pending,None

NUDT5A-x0275,CC=1OC=CC1C(=O)N2CCC=3C=CC=CC23,Z89307993,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,2.42,0.075,6.0,0.7,96.6,97.9,95.5,0.29357,0.34730,0.29357,0.34730,P 1,1
- Analysis Pending,None

NUDT5A-x0276,CC1CCCN(CC1)C(=O)C2=CSC=N2,Z1101755952,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0277,C(C1CCNCC1)C2=NC(=NO2)C3CC3,Z2442270563,OK: Mounted Clear,success,P 1,48
59 79 79 82 76,1.65,0.032,16.5,1.1,96.6,97.9,95.0,0.21778,0.24467,0.21778,0.24467,P 1,1
- Analysis Pending,None

NUDT5A-x0278,CC1CN(CC1)C=2C=CC=C(C)N2,Z1267885772,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.69,0.019,28.4,0.6,95.0,94.9,95.0,0.23097,0.26839,0.23097,0.26839,P 1,1 -
Analysis Pending,None

NUDT5A-x0279,CCN1CCC(CC1)NC=2C=CC=CC2F,Z2856434868,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.73,0.048,15.6,1.0,96.9,98.2,96.1,0.23852,0.27557,0.23889,0.27811,P 1,3 -
In Refinement,None

NUDT5A-x0280,CC(C)NC(=O)C=1C=CC=2C=CC=CC2N1,Z31385861,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.71,0.016,39.0,1.0,96.2,99.2,95.1,0.22687,0.25961,0.22687,0.25961,P 1,1
- Analysis Pending,None

NUDT5A-x0281,FC(F)(F)C=1C=CC(CN2CCOCC2)=CC1,Z2856434871,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,1.63,0.042,26.9,0.9,96.4,98.3,94.5,0.23253,0.26599,0.23253,0.26599,P 1,1 - Analysis
Pending,None

NUDT5A-x0282,O=C(NCCC=1C=CN=CC1)NC2CCCCC2,Z111507846,OK: Mounted Clear,success,P 1,49
59 79 79 80 75,1.81,0.020,15.1,0.5,94.0,92.5,93.8,0.24406,0.28649,0.24406,0.28649,P 1,1
- Analysis Pending,None

NUDT5A-x0283,FC(F)(F)C(=O)NC=1C=CC=C(C1)C1,Z111810692,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.76,0.015,31.1,0.7,78.5,95.0,95.0,0.22213,0.26423,0.22213,0.26423,P 1,1
- Analysis Pending,None

NUDT5A-x0284,FC(F)N1C=CN=C1CN2CCNCC2,Z2444672448,OK: Crystalline,success,P 1,46 58 77
82 86 79,1.77,0.011,56.3,0.8,77.7,93.7,94.8,0.36533,0.40716,0.36533,0.40716,P 1,1 -
Analysis Pending,None

NUDT5A-x0285,CCC1=NN=C(NC(=O)C(F)(F)F)S1,Z275156196,OK: Mounted Clear,success,P 1,46 58
77 82 85 79,1.85,0.013,45.2,0.3,72.9,94.1,31.0,0.37442,0.42333,0.37442,0.42333,P 1,1 -
Analysis Pending,None

NUDT5A-x0286,CC=1C=CC=C(NC=2N=CN=C3N(C)N=CC23)C1,Z56983806,OK: Mounted Clear,success,P
1,48 59 79 79 82
76,1.66,0.038,26.2,1.0,96.6,98.4,95.1,0.22673,0.25654,0.20926,0.24081,P 1,6 -
Deposited,5QJL

NUDT5A-x0287,CN1CCC(OC=2C=CC=C(F)C2)C1=O,Z1217960891,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.62,0.022,36.6,1.0,95.8,97.1,93.6,0.23248,0.25986,0.23248,0.25986,P 1,1
- Analysis Pending,None

NUDT5A-x0288,C1C=1C=CC(=CC1)C(=O)N2CCSCC2,Z437584380,OK: Mounted Clear,success,P 1,48
59 79 79 82 76,1.63,0.016,37.3,0.7,93.5,93.7,93.9,0.22772,0.25962,0.22772,0.25962,P 1,1
- Analysis Pending,None

NUDT5A-x0289,CC1(C)CCCN1CCN,Z1741815708,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.78,0.024,25.7,0.9,96.2,98.7,94.7,0.22923,0.26643,0.22923,0.26643,P 1,1 - Analysis
Pending,None

NUDT5A-x0290,FC=1C=CC(OCC(=O)N2CCCC2)=CC1,Z19735067,OK: Mounted Clear,success,P 1,48 59
79 79 82 76,1.63,0.018,31.0,1.1,95.2,98.6,92.5,0.22540,0.25073,0.22540,0.25073,P 1,1 -
Analysis Pending,None

NUDT5A-x0291,CCCC(=O)NC=1C=CC=NC1C1,Z240654968,OK: Mounted Clear,success,P 1,48 59 79
79 81 76,1.74,0.019,28.7,0.6,95.3,95.7,95.0,0.23155,0.26754,0.23155,0.26754,P 1,1 -
Analysis Pending,None

NUDT5A-x0292,FC=1C=CC=CC1CNC2CCOCC2,Z823455846,OK: Mounted Clear,success,P 1,49 60 79
79 80 75,2.16,0.040,8.3,1.2,96.9,97.7,95.0,0.23188,0.28571,0.23188,0.28571,0.23188,0.28571,P 1,1 - Analysis
Pending,None

NUDT5A-x0293,CC=1C=CC(NC=2N=CN=C3NN=CC23)=CC1,Z57101343,OK: Crystalline,success,P 1,48
59 79 79 81 75,1.90,0.045,13.8,0.6,89.4,92.8,80.7,0.24109,0.28117,0.24109,0.28117,0.24109,0.28117,P 1,1 -
Analysis Pending,None

NUDT5A-x0294,CN(CCC=1C=CC=CN1)C(=O)C=2C=CC=CC2,Z68277692,OK: Precipitated,success,P
1,49 59 79 79 81 75,1.87,0.035,19.9,0.6,66.5,96.1,30.4,0.22722,0.27627,0.22722,0.27627,0.22722,0.27627,P 1,1
- Analysis Pending,None

NUDT5A-x0295,CS(=O)(=O)C1=NC=CN1CC2=CSC=N2,Z1328968520,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.85,0.023,20.1,0.6,93.3,92.5,94.7,0.23844,0.27789,0.23844,0.27789,0.23844,0.27789,P 1,1 -
Analysis Pending,None

NUDT5A-x0296,COC(=O)N1CCN(CC1)C=2C=CC(F)=CC2,Z192955056,OK: Mounted Clear,success,P
1,49 59 79 79 81 75,1.80,0.028,15.2,1.0,96.0,97.8,94.6,0.23915,0.27181,0.23915,0.27181,0.23915,0.27181,P 1,1
- Analysis Pending,None

NUDT5A-x0297,CC(C)NCC1=NC(=NO1)C=2C=CC(C)=CC2,Z2856434849,OK: Mounted Clear,success,P
1,49 59 79 79 81 75,2.10,0.020,16.4,0.9,96.5,98.6,95.5,0.23815,0.27956,0.23815,0.27956,0.23815,0.27956,P 1,1
- Analysis Pending,None

NUDT5A-x0298,C1C=1C=CC=C(C1)N2CCN(CC#N)CC2,Z2856434806,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.51,0.017,33.3,0.4,94.3,94.3,93.9,0.23134,0.26308,0.23134,0.26308,0.23134,0.26308,P 1,1 -
Analysis Pending,None

NUDT5A-x0299,CC(C)N(C)C=1N=CN=C2N(C)N=CC12,Z328695024,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.75,0.040,14.9,0.8,87.3,95.3,94.8,0.23298,0.27321,0.22492,0.27103,P 1,6
- Deposited,5QJM

NUDT5A-x0300,OCC1CN(CC=2C=CC=CC2)CCO1,Z1259086950,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.58,0.024,22.4,0.5,93.1,94.1,94.1,0.22943,0.26048,0.22943,0.26048,0.22943,0.26048,P 1,1 -
Analysis Pending,None

NUDT5A-x0301,OCC1CCN(CC1)C=2N=CC=CN2,Z645232558,OK: Mounted Clear,success,P 1,49 60 80
79 81 75,1.71,0.025,21.0,0.7,93.2,93.1,94.9,0.23925,0.27542,0.23925,0.27542,0.23925,0.27542,P 1,1 - Analysis
Pending,None

NUDT5A-x0302,CC1(CC1)S(=O)(=O)N2CCC=C(F)C2,Z2277255954,OK: Mounted Clear,success,P 1,49
60 80 79 81 75,1.83,0.013,34.2,1.4,94.8,97.9,93.6,0.22636,0.25876,0.22636,0.25876,0.22636,0.25876,P 1,1 -
Analysis Pending,None

NUDT5A-x0303,COCC(=O)NC=1C(C)=CC(C)=CC1C,Z57260516,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.68,0.022,32.4,1.1,95.6,95.8,93.8,0.23324,0.26451,0.23324,0.26451,0.23324,0.26451,P 1,1 -
Analysis Pending,None

NUDT5A-x0304,O=C(CSC=1C=CC=CC1)NC2CCCC2,Z19751622,OK: Precipitated,success,P 1,49 59
79 79 81 75,1.56,0.026,22.5,0.7,93.9,91.0,94.4,0.23487,0.26451, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0305,CCS(=O)(=O)NCC=1C=CC=2OCOC2C1,Z53860899,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.70,0.028,15.6,1.2,96.0,98.5,94.9,0.22962,0.26318, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0306,CC1=NC(CC(=O)N2CCOCC2)=CS1,Z31720228,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.62,0.023,31.6,0.9,95.8,98.0,93.2,0.23648,0.26865, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0307,OC=1C=CC=CC1CN2CCC=3C=CC=CC3C2,Z2856434881,OK: Mounted Clear,success,P
1,49 59 80 79 81 75,1.53,0.052,18.5,1.0,96.1,98.6,94.3,0.22618,0.24836, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0308,CS(=O)(=O)NC=1C=CC(=CC1)C=2C=CC=CC2,Z45641455,OK: Precipitated,success,P
1,49 59 79 79 81 75,1.68,0.028,20.1,0.9,95.9,98.4,94.3,0.23241,0.26452, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0309,CC(C)NC=1N=CC=CN1,Z31190928,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.59,0.029,21.8,0.7,94.5,92.6,94.3,0.23176,0.25953, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0310,CNCC(=O)NC=1C=C(C)C=CN1,Z927746322,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.78,0.033,20.9,0.9,95.9,98.0,95.3,0.23089,0.26520, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0311,C1C=1C=CC(NC(=O)CC#N)=CC1,Z56837087,OK: Precipitated,success,P 1,49 60 80
79 81 75,1.67,0.050,16.5,1.0,96.5,98.1,95.2,0.23492,0.26310, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0312,CCOC(=O)CN1CCCC1,Z2856434773,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.80,0.074,13.3,1.5,96.8,98.3,95.5,0.24160,0.27206, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0313,CC1CN(CC=2N=NSC2C1)C(C)CO1,Z354992234,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.70,0.023,20.9,0.6,93.1,93.5,94.6,0.23258,0.26796, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0314,FC(F)OCC(=O)N1CCCC2(CC2)C1,Z2074076908,OK: Mounted Clear,success,P 1,49 60
79 79 80 75,1.90,0.020,11.1,0.5,94.0,91.1,94.9,0.26388,0.31334,0.26401,0.31738,P 1,3 -
In Refinement, None

NUDT5A-x0315,CC(N)C=1C=CC(NC(=O)C2CC2)=CC1,Z1891773393,OK: Bad Dispense,success,P 1,49
59 79 79 81 75,1.60,0.029,20.1,0.6,94.2,92.5,94.6,0.22711,0.25666, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0316,C[C@H](O)CNCC=1C(C1)=CC=CC1C1,Z2856434909,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.57,0.019,27.8,0.5,92.2,93.0,94.3,0.22510,0.25580, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0317,CCNC=1C=CC(=CC1F)S(=O)(=O)C,Z2142244288,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.76,0.018,33.9,0.7,92.8,91.8,93.9,0.22393,0.26177, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0318,CCCC(=O)NCC1=NC=2C=CC=CC2N1,Z26781952,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.98,0.030,20.0,1.0,96.4,99.3,95.2,0.24455,0.28199, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0319,CC1OCCN(C1C)C2=NC(C)=NS2,Z1439422127,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.77,0.067,19.3,1.0,95.9,98.0,93.6,0.23662,0.27281,0.23105,0.27299,P 1,5 -
Deposition ready,5QJN

NUDT5A-x0320,CC(C)C(=O)NC=1N=NN(C)N1,Z57292369,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.98,0.029,16.1,2.2,96.6,98.7,94.6,0.22357,0.25771,0.21231,0.24877,P 1,6 -
Deposited,5QJO

NUDT5A-x0321,CC=1C=CC(NC(=O)C=2C=CC=C(F)C2)=CC1O,Z1430613393,OK: Mounted
Clear,success,P 1,49 59 79 79 81
75,1.66,0.081,13.4,1.1,96.7,96.5,95.1,0.24123,0.27581,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0322,FC=1C=CC(CNCC=2C=CC(C#N)=CC2)=CC1,Z2856434851,OK: Mounted Clear,success,P
1,49 60 79 79 81 75,1.45,0.018,32.5,0.4,91.7,89.6,85.0,0.24075,0.26919,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0323,CS(=O)(=O)NC1(CCCCC1)C(=O)O,Z133622412,OK: Mounted Clear,success,P 1,47 59
80 79 83 77,1.81,0.022,20.2,0.4,92.3,91.5,94.2,0.25434,0.29889,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0324,CCC(C)NC(=O)C=1C=CC=CC1N,Z56040660,OK: Mounted Clear,success,P 1,48 59 79
80 81 76,2.04,0.017,22.2,0.5,83.4,91.1,84.3,0.24193,0.28976,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0325,CN(C(=O)C1CCNC1)C=2C=CC=CC2,Z2447286438,OK: Mounted Clear,success,P 1,48
59 79 80 81 76,1.54,0.017,32.7,0.4,86.5,93.7,94.0,0.25815,0.30310,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0326,O=C(CC1CCCC1)NN2C=NN=C2,Z57261895,OK: Mounted Clear,success,P 1,48 59 79
80 81 75,1.62,0.037,17.6,0.8,88.8,94.1,94.9,0.25105,0.28967,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0327,CC1CCCN(C1)C(=O)CO,Z228585534,OK: Mounted Clear,success,P 1,49 59 79 79 80
75,1.49,0.030,16.1,0.5,79.5,82.7,89.8,0.25356,0.29524,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0328,CN1CCN(CC1)C(=O)C2CCCO2,Z31432964,OK: Mounted Clear,success,P 1,48 59 79
79 81 76,1.67,0.030,21.1,1.1,96.6,98.2,95.8,0.22416,0.25367,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0329,CC1=NN=C(NC(=O)N2CCOCC2)S1,Z410633222,OK: Mounted Clear,success,P 1,48 59
79 80 82 76,1.85,0.043,15.6,1.2,96.2,97.8,95.7,0.23540,0.26928,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0330,CN(C)C(=O)OCCN1C=CN=C1,Z1722836661,OK: Mounted Clear,success,P 1,48 59 79
79 81 76,1.86,0.043,15.7,1.4,96.0,98.7,95.0,0.23525,0.27494,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0331,CCC1=NN=C(NC(=O)C=2C=NC=CN2)S1,Z26824727,OK: Mounted Clear,success,P 1,48
59 79 80 81 76,1.66,0.026,28.0,1.0,96.5,98.8,95.1,0.22773,0.25709,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0332,CC=1C=CC(C)=C(OC(=O)C=2C=CN=CC2)C1,Z30891796,OK: Precipitated,success,P
1,49 59 79 79 81 75,2.15,0.092,5.2,0.8,96.8,99.2,95.7,0.30543,0.33993,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0333,CC1=NSC(=N1)N2CCCNCC2,Z1578665941,OK: Mounted Clear,success,P 1,49 59 79
79 81 76,1.50,0.028,21.2,0.5,88.0,92.9,93.8,0.23147,0.26169,0.22424,0.25543,P 1,6 -
Deposited,5QJP

NUDT5A-x0334,CN1CCN(CC1)C=2C=CC(C#N)=CC2,Z2856434840,OK: Mounted Clear,success,P 1,48
59 79 80 82 76,1.76,0.020,25.5,0.7,94.1,92.9,94.8,0.22565,0.26439,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0335, COC=1C=CC (CNC (=O) CC#N) =CC1, Z190662888, OK: Precipitated, success, P 1, 49 59 79 79 81 75, 1.48, 0.037, 16.0, 0.6, 91.5, 90.7, 88.7, 0.24752, 0.28001, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0336, CCC1=NOC (C) =C1C (=O) NC=2C=C (C) ON2, Z117233350, OK: Mounted Clear, success, P 1, 48 59 79 79 81 76, 1.66, 0.084, 13.7, 1.0, 96.6, 98.9, 95.3, 0.23657, 0.26990, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0337, CC1 (C) CN (CCO1) C (=O) CC (F) (F) F, Z394039592, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.63, 0.018, 31.6, 0.9, 93.2, 91.6, 94.7, 0.25011, 0.28803, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0338, COC (=O) C=1C=CC (NC (=O) C (F) (F) F) =CC1, Z56767614, OK: Mounted Clear, success, P 1, 48 59 79 79 81 76, 1.69, 0.046, 19.6, 1.1, 96.7, 98.5, 95.3, 0.23063, 0.25781, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0339, CCN (CC) C1=CC (C) =NC2=NC=NN12, Z56791867, OK: Mounted Clear, success, P 1, 48 59 79 79 82 76, 1.55, 0.019, 34.8, 1.1, 95.5, 97.0, 93.6, 0.22963, 0.25769, 0.21286, 0.23992, P 1, 6 - Deposited, 5QJQ

NUDT5A-x0340, CC (C) C (=O) NCC1CCCNC1, Z1262327459, OK: Mounted Clear, success, P 1, 49 59 79 80 81 75, 1.59, 0.025, 24.8, 0.6, 89.3, 95.2, 94.0, 0.25016, 0.28773, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0341, CC (NC1CC1) C=2C=CC=NC2, Z1263529721, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.60, 0.028, 19.5, 0.6, 94.6, 92.7, 94.3, 0.25004, 0.28722, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0342, CC1CCN (CC1) C (=O) C2=CC=3C=CC=CC3O2, Z32665176, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.64, 0.034, 25.1, 0.9, 96.4, 95.4, 94.8, 0.23494, 0.26797, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0343, COCC (=O) NC=1C=CC=CC1C (=O) N, Z57260539, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.65, 0.044, 19.6, 1.0, 96.6, 98.7, 94.9, 0.24337, 0.28065, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0344, CCNC (=O) NC=1C=C (C) ON1, Z56880342, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0345, OC=1C=CC=CC1CN2CCOCC2, Z2856434887, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.53, 0.023, 24.4, 0.4, 93.7, 94.0, 94.3, 0.24152, 0.27583, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0346, COC=1C=CC (NC (=O) CN) =CC1, Z1449748885, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.76, 0.031, 16.4, 0.6, 93.0, 93.5, 95.0, 0.23240, 0.27077, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0347, CC (C) (CO) NC (=O) NC=1C=CC (C1) =CC1, Z123970702, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.65, 0.055, 21.9, 1.1, 96.4, 98.5, 94.9, 0.22991, 0.25895, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0348, CNC (=O) CN (C) C1CCCCC1, Z204776284, OK: Mounted Clear, success, P 1, 49 59 79 80 80 75, 1.56, 0.047, 17.6, 0.9, 92.4, 92.6, 94.6, 0.25865, 0.29335, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0349, CS (=O) (=O) N1CCC (CC1) C (=O) NC2CC2, Z227998000, OK: Mounted Clear, success, P 1, 48 59 79 80 82 76, 1.70, 0.028, 22.5, 0.9, 95.7, 98.5, 94.3, 0.21926, 0.24772, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0350, CN (C) CC1=NC (=NO1) C2 (N) CCCC2, Z1259339735, OK: Mounted Clear, success, P 1, 48 59 79 80 81 76, 1.68, 0.052, 20.6, 1.1, 96.5, 95.4, 95.3, 0.22941, 0.25877, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0351,CC(C)NCC=1C=CC(=CC1)N(C)C,Z2856434894,OK: Mounted Clear,success,P 1,48 59
79 80 81 76,1.88,0.035,17.5,1.1,96.4,98.0,95.8,0.22879,0.26482, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0352,CC1=NN(C)C(C)=C1CN2CCNCC2,Z1263820300,OK: Mounted Clear,success,P 1,49 59
79 80 81 76,1.70,0.076,15.9,1.0,96.4,98.4,95.6,0.24404,0.28086, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0353,CC(C)(CO)NC(=O)C=1C=CC=C(C1)C1,Z68299550,OK: Bad Dispense,success,P 1,48
59 79 80 82 76,1.79,0.037,15.4,1.3,96.8,97.1,95.2,0.21087,0.24442, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0354,FC=1C=CC(NC2CCOCC2)=NC1,Z1172243962,OK: Mounted Clear,success,P 1,48 59 79
80 81 76,1.52,0.016,35.1,0.4,86.8,93.7,94.0,0.23749,0.27005, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0355,CN1CCN(CC1)C(=O)NC=2C=CC(F)=CC2,Z2856434944,OK: Mounted Clear,success,P
1,48 59 79 79 81 76,1.60,0.035,19.5,0.7,93.9,92.6,94.6,0.23789,0.27043, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0356,CC(CO)(CO)NC(=O)NC=1C=CC=CC1,Z57472297,OK: Mounted Clear,success,P 1,48 59
79 80 81 76,1.55,0.025,24.1,0.4,94.7,95.1,94.1,0.24363,0.27572, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0357,CC(C)NC(=O)CN1CCCNCC1,Z1262254278,OK: Mounted Clear,success,P 1,49 59 79
80 81 76,1.66,0.052,18.3,1.1,96.5,98.4,95.1,0.23682,0.26807, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0358,CCOC(=O)C=1C=NNC1,Z1124201124,OK: Mounted Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0359,CC(C)C(=O)NC=1C=CC=C(C#N)C1,Z26548083,OK: Mounted Clear,success,P 1,48 59
79 79 81 76,1.49,0.016,33.4,0.3,85.3,92.3,90.7,0.24300,0.27986, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0360,CC(N1CCN(CC1)S(=O)(=O)C)C(=O)N,Z134785326,OK: Mounted Clear,success,P 1,48
59 79 80 81 76,1.75,0.014,36.8,0.9,95.8,98.7,95.0,0.22386,0.25766, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0361,COCC1CN(CC01)C=2C=CC=CN2,Z1272480091,OK: Mounted Clear,success,P 1,49 60
79 79 81 75,1.71,0.022,28.1,0.6,87.5,93.9,94.9,0.23684,0.27573, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0362,O=C(CC1CCCC1)NC=2C=CC=NC2,Z31792168,OK: Mounted Clear,success,P 1,49 90
149 89 87 88,1.74,0.036,11.1,0.9,95.9,98.4,95.2, , , None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0363,COC=1C=CC(CC(=O)NC2=NN=CS2)=CC1,Z86416929,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.54,0.060,17.3,1.1,95.8,98.6,94.1,0.22294,0.24926, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0364,COCC(=O)NC=1C=CC=C(NC(=O)C)C1,Z31735562,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.67,0.036,18.7,0.6,94.3,94.1,94.3,0.23605,0.27376, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0365,CCCN1C(NC(=O)CC)=NC=2C=CC=CC12,Z29077827,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.49,0.041,16.9,0.5,94.2,93.6,90.1,0.23420,0.26113, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0366,COCC(=O)NCC=1C=CC=CC1,Z31478538,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.94,0.046,15.6,1.4,96.6,98.2,94.8,0.23456,0.27107, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0367,CC(=O)NC=1C=C2OCOC2=CC1C,Z1635496816,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.66,0.035,24.8,1.1,95.9,98.3,94.7,0.22352,0.24909,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0368,CN(C)C(=O)COC=1C=CC=CC1C,Z19733482,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.66,0.047,15.6,1.3,95.7,96.9,93.5,0.23090,0.25986,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0369,CN1CCN(CCN)CC1(C)C,Z1992316315,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.64,0.058,24.8,1.0,96.2,98.1,94.0,0.23868,0.27170,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0370,CC(=O)NC1CCC(N)CC1,Z1787158625,OK: Crystalline,success,P 1,49 59 79 79 81 75,1.67,0.042,15.3,1.1,95.8,98.0,94.0,0.23598,0.26607,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0371,CC(=O)N1CCCC2(C1)CCCCC2,Z1275599911,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.48,0.019,32.3,0.6,93.6,92.7,89.3,0.25678,0.29176,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0372,CNC(=O)C1=C(C)ON=C1C=2C=CC(F)=CC2,Z363104204,OK: Crystalline,success,P 1,49 60 80 79 81 75,1.95,0.041,13.8,1.1,96.1,98.2,94.7,0.24957,0.28476,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0373,CN(C)C(=O)C=1C=CC=C(C)C1C,Z32014663,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.69,0.030,17.7,1.1,96.0,98.2,94.7,0.23114,0.26017,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0374,C(NC1CC1)C2CCOC2,Z818727262,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.66,0.015,40.9,0.9,95.4,97.6,93.5,0.22534,0.25363,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0375,CC(=O)N1CCOC(CO)C1,Z1454840342,OK: Crystalline,success,P 1,49 59 80 79 81 75,1.61,0.048,22.7,1.1,96.2,97.8,93.9,0.22453,0.25345,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0376,C[C@H](O)CNC(=O)NC=1C=CC=CC1,Z1563512128,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.61,0.027,26.8,1.1,95.7,97.5,93.3,0.22379,0.25063,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0377,CC(=O)C=1C=CC(OC(F)F)=CC1,Z55671900,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.60,0.036,16.4,0.7,93.7,92.2,93.7,0.23863,0.27021,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0378,C1=NN=NN1C=2C=CC(=CC2)C=3C=CC=CC3,Z57479285,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.63,0.035,28.6,1.1,96.1,97.9,94.1,0.21981,0.24368,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0379,COC=1C=CC(C)=CC1NC(=O)CN,Z235341991,OK: Mounted Clear,success,P 1,48 59 80 79 81 75,1.69,0.018,29.3,0.6,85.5,92.4,94.2,0.21957,0.25669,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0380,CC1CCNC(C1)C(=O)N,Z1741785925,OK: Mounted Clear,success,P 1,49 60 79 79 80 75,1.61,0.045,21.9,1.0,96.3,98.0,93.9,0.25713,0.29476,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0381,CC(C)N1C=C(N=N1)C(=O)O,Z2510259379,OK: Mounted Clear,success,P 1,46 58 79 80 84 78,1.82,0.023,22.9,0.9,91.0,91.8,93.8,0.32500,0.36898,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0382,OC(=O)CC=1C=CC(=CC1)C=2C=CC=CC2,Z2856434779,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.75,0.032,16.6,0.7,86.7,93.3,95.1,0.22816,0.26579,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0383,CNC(=O)C=1C=CC=C(N1)C(=O)O,Z1816233707,OK: Crystalline,success,P 1,46 59 79 80 84 78,1.74,0.019,30.9,0.9,95.1,97.9,94.2,0.31906,0.36339, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0384,COC=1C=CC(CCC2(C)NC(=O)NC2=O)=CC1,Z56772132,OK: Crystalline,success,P 1,49 59 79 79 81 75,1.56,0.027,21.8,0.6,94.2,94.3,94.3,0.23810,0.27039, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0385,CCN1N=CC=C1CNC,Z2856434839,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.98,0.053,12.7,1.4,96.2,98.2,94.7,0.23259,0.26764, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0386,C[C@@H](CO)NC=1N=CC(C1)=CC1F,Z1432018343,OK: Mounted Clear,success,P 1,49 60 79 79 80 75,1.46,0.035,20.6,0.4,93.0,93.1,86.1,0.28309,0.32615, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0387,CN1C=C(C(=O)N)C(=N1)C(F)F,Z1515654336,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.95,0.028,20.7,1.0,91.8,93.2,86.3,0.22449,0.26115, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0388,CSC1=NSC(NC(=O)C)=N1,Z26804467,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.64,0.029,19.0,1.0,95.3,97.0,93.2,0.22208,0.24950, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0389,CC(=O)NC=1C=CC(=CC1)C2=CSC(N)=N2,Z48847594,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0390,CC(NC(=O)C)C1=NN=C2C=CC=CN12,Z131516158,OK: Crystalline,success,P 1,49 59 80 79 81 75,1.62,0.077,16.7,1.0,96.3,98.7,94.2,0.23177,0.26167, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0391,CC(=O)N1CCN(CC1)C=2C=CC(C1)=CC2,Z275165822,OK: Mounted Clear,success,P 1,48 59 80 79 81 75,1.70,0.027,25.1,0.8,96.0,98.5,95.0,0.21464,0.24341, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0392,CC(=O)N1CCCC(C1)C(=O)N,Z220816104,OK: Mounted Clear,success,P 1,49 60 79 79 81 75,1.62,0.049,23.6,0.9,96.3,98.5,94.5,0.24339,0.27505,0.24345,0.27664, P 1,6 - Deposited,5QJR

NUDT5A-x0393,CC1=CSC(CNC(=O)C2CCC2)=N1,Z212122838,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.67,0.024,29.6,1.0,96.0,98.5,94.6,0.23235,0.26666, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0394,CC(CC=1C(C)=NOC1C)C(=O)N(C)C,Z1246465616,OK: Mounted Clear,success,P 1,48 59 80 79 81 76,1.64,0.033,18.2,0.6,82.4,94.5,81.6,0.22085,0.25344, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0395,CC1CCN(CCN)CC1,Z1245580461,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.77,0.048,17.9,1.0,96.8,96.0,95.8,0.22617,0.26348, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0396,COC=1C=CC(NC2=NCCN2)=CC1,Z57186564,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.50,0.031,18.6,0.4,93.3,91.1,93.6,0.22637,0.25206, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0397,CC(=O)NC=1C=CN=CC1C,Z1148747945,OK: Bad Dispense,success,P 1,49 59 80 79 81 75,1.58,0.025,27.0,1.1,95.6,97.4,93.1,0.22095,0.25003, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0398,N[C@@H]1CCCN(C1)C(=O)CCC(F)(F)F,Z1818332938,OK: Mounted Clear,success,P 1,49 90 150 89 87 88,1.71,0.054,6.4,1.0,96.2,97.6,95.2,, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0399,C(N1CCNCC1)C=2C=CON2,Z1263714198,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.76,0.043,14.6,0.9,96.0,97.2,95.0,0.25768,0.29487,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0400,CC1=NC=CN1CC=2C=CC=C(C#N)C2,Z319545618,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.75,0.047,8.8,0.5,92.9,94.7,91.4,0.22829,0.26212,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0401,COC=1C=CC=CC1N2CCN(CC#N)CC2,Z2856434807,OK: Crystalline,success,P 1,49 59
79 79 81 75,1.57,0.020,28.9,0.6,87.2,92.1,93.8,0.22951,0.26501,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0402,CN1CCN(CC1)C(=O)C2CCCN2,Z241832786,OK: Mounted Clear,success,P 1,48 59 80
79 81 76,1.57,0.022,22.5,0.5,93.5,91.0,93.9,0.22341,0.25119,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0403,COC(=O)NC=1SC(C)=NC1C=2C=CC=CC2,Z979145504,OK: Mounted Clear,success,P
1,49 59 79 79 81
75,1.58,0.022,28.0,0.5,94.8,94.5,94.2,0.24022,0.27187,0.23649,0.27156,P 1,6 -
Deposited,5QJS

NUDT5A-x0404,CCC(=O)NC1CCNC1,Z1650040241,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.63,0.032,17.6,0.8,92.5,93.3,94.6,0.23229,0.26099,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0405,CNC(=O)C=1C=CC=C2C=CNC12,Z1273312153,OK: Mounted Clear,success,P 1,49 60
80 79 81 75,1.53,0.039,18.0,0.7,94.1,93.7,94.2,0.23099,0.25590,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0406,O[C@@H]1CCN(CC=2C=CC(C1)=CC2)C1,Z2856434858,OK: Mounted Clear,success,P
1,49 59 80 79 81
75,1.56,0.017,34.2,0.6,94.6,93.7,94.1,0.23074,0.26050,0.22925,0.26257,P 1,3 - In
Refinement,None

NUDT5A-x0407,CC1=CC(NC(=O)COC=2C=CC(C)=CC2)=NO1,Z19731563,OK: Mounted Clear,success,P
1,48 59 80 79 81 75,1.56,0.032,19.9,1.2,95.3,98.2,93.1,0.22113,0.24421,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0408,CC(N)C(=O)N1CCCC1C,Z927412236,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,2.16,0.046,8.3,2.2,87.9,87.7,89.9,0.25813,0.29423,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0409,COCC(=O)NC=1C=CC(O)=CC1,Z943693514,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.61,0.041,25.7,1.3,96.2,96.8,94.3,0.23239,0.25796,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0410,COC(=O)NC1=NN=C(CC2CCCC2)S1,Z1119505742,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.51,0.027,20.7,0.6,93.0,92.7,93.3,0.23663,0.25840,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0411,C(C1CCCC1)N2C=CN=N2,Z1891776952,OK: Crystalline,success,P 1,47 59 80 80
83 77,1.67,0.026,20.5,0.5,93.6,94.2,94.8,0.24238,0.27717,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0412,CNC(=O)C1=CN=C(C)S1,Z969560582,OK: Crystalline,success,P 1,49 59 80 79 81
75,1.62,0.024,27.5,0.8,94.8,94.3,94.6,0.22802,0.25579,0.22138,0.25098,P 1,6 -
Deposited,5QJT

NUDT5A-x0413,CCNCC=1C=CC=C2NC=CC12,Z1137725943,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.68,0.033,21.9,1.3,96.0,97.1,94.4,0.22640,0.25606,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0414,COC=1C=CC(CN2CCOCC2)=CC1OC,Z2856434878,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.79,0.032,20.8,0.8,94.9,93.5,94.9,0.22599,0.26013, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0415,CNS(=O)(=O)C=1C=CC=CC1C1,Z45527714,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.68,0.016,36.3,0.9,95.4,98.2,93.5,0.23072,0.25928, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0416,COC(=O)COC=1C=CC(C#N)=CC1,Z19234337,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.58,0.012,39.8,0.5,93.9,92.7,94.1,0.22903,0.26363, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0417,O=C(NCC1=NC=2C=CC=CC2N1)C3=CC=CO3,Z26781964,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.77,0.065,12.5,1.0,96.9,96.6,95.5,0.22335,0.25474, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0418,CCNC(=O)CN1CC(C)OCC1C,Z355728146,OK: Bad Dispense,success,P 1,48 59 79 79 82 76,1.47,0.022,21.5,0.6,92.5,90.7,88.0,0.22288,0.24437, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0419,C1C=1C=CC=C(CN2CCOCC2)C1,Z2856434856,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.89,0.044,15.8,1.0,96.4,98.3,95.6,0.23306,0.26965, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0420,CC(C)C(=O)N1CCC(CC=2C=CC=CC2)CC1,Z30162334,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.70,0.034,19.8,0.8,88.2,92.0,95.1,0.23533,0.26898, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0421,CCS(=O)(=O)N1CCC(CC1)C(=O)O,Z53825020,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.67,0.041,14.8,0.8,88.6,91.0,94.2,0.22141,0.25100, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0422,FC=1C=CC=C(CN2CCCS2(=O)=O)C1,Z729352906,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.83,0.036,23.6,1.7,96.3,98.0,95.2,0.22087,0.25136, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0423,COCC(=O)NCC1=NC=2C=CC=CC2N1,Z111529496,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.59,0.029,22.7,1.0,95.0,98.3,92.4,0.21897,0.24133, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0424,CC=1C(C1)=CC=CC1NC(=O)CN,Z85956652,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.56,0.071,16.2,1.1,96.2,98.4,94.4,0.22189,0.24771, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0425,CC(=O)NC1=CC=CC2=NON=C12,Z2027158783,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.75,0.025,23.0,0.9,93.3,93.3,93.8,0.23549,0.27283, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0426,CCC(CC)C(=O)NC1=NC=CS1,Z28173817,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.81,0.022,18.4,1.1,96.8,97.4,95.7,0.21783,0.25234, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0427,CC(=O)NCCC1=CNC=2C=CC(F)=CC12,Z1220452176,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.79,0.017,24.8,1.9,96.6,98.1,95.1,0.22031,0.25393,0.21933,0.25647, P 1,3 - In Refinement, None

NUDT5A-x0428,CC(C)(N)CN1CCCC1,Z1741966630,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.67,0.055,14.6,1.0,96.7,97.5,95.0,0.23216,0.26322, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0429,CC(=O)NC=1C=C(C=CC1F)C(=O)O,Z364328788,OK: Crystalline,success,P 1,47 59 80 80 83 77,1.82,0.025,21.1,0.5,93.8,94.0,94.9,0.25811,0.29748, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0430,CC(=O)NC=1C=NC=CC1C,Z1129283193,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,1.93,0.082,20.8,1.3,96.3,97.3,94.9,0.27734,0.30107,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0431,NC=1C=CC(=CC1)S(=O)(=O)NC=2C=CC=CN2,Z271004858,OK: Mounted Clear,success,P
1,49 59 80 79 81
75,1.62,0.032,23.2,1.0,95.9,97.7,93.8,0.22620,0.25342,0.22639,0.25647,P 1,3 - In
Refinement, None

NUDT5A-x0432,CC(=O)NCC=1C=NNC1,Z383325512,OK: Crystalline,success,P 1,49 59 80 79 81
75,1.66,0.042,14.9,0.6,94.6,93.5,95.4,0.23439,0.26732, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0433,FC=1C=CC=CC1CNC=2C=NNC2,Z1454310449,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.87,0.084,8.3,1.0,97.0,97.6,95.9,0.23639,0.27173, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0434,CN(CC=1C=CC=C(F)C1)S(=O)(=O)N,Z300245038,OK: Mounted Clear,success,P 1,49
60 80 79 81 75,1.70,0.031,18.3,0.7,93.9,93.6,94.4,0.22732,0.25895, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0435,CC1=NOC(NC(=O)CC2CCCC2)=N1,Z729726784,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.70,0.058,13.5,0.9,95.8,97.3,94.5,0.24541,0.28063, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0436,CC(OC=1C=CC=CC1F)C(=O)O,Z65532537,OK: Mounted Clear,success,P 1,48 59 80
79 82 76,1.77,0.023,17.6,0.9,95.8,98.6,94.8,0.24747,0.28523, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0437,CC(=O)NCC1(O)CCCC1,Z1203329531,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,2.25,0.072,9.4,1.3,97.2,99.6,95.2,0.23115,0.27982, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0438,CC(=O)N1CCC(N)CC1,Z90664455,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.99,0.056,13.6,1.4,96.3,96.5,94.0,0.23519,0.27542, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0439,COC=1C=C(CN)C=C(OC)C1OC,Z1741959530,OK: Mounted Clear,success,P 1,49 60 80
79 81 75,1.84,0.034,19.7,1.2,93.9,96.1,88.0,0.24121,0.27796, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0440,COCC1=CC(=NO1)C(=O)N,Z1273141646,OK: Bad Dispense,success,P 1,49 59 80 79
81 75,1.87,0.033,15.5,1.3,96.2,98.7,95.6,0.23282,0.26756, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0441,CC(C)C(=O)NCC1=NC=2C=CC=CC2N1,Z26781943,OK: Mounted Clear,success,P 1,49
60 79 79 81 75,1.54,0.032,19.9,0.5,93.6,91.5,94.2,0.24576,0.28170, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0442,CNC(C)C=1C=CC(F)=CC1,Z166605480,OK: Bad Dispense,success,P 1,49 59 80 79
81 75,1.67,0.047,18.7,1.0,96.5,98.4,95.4,0.23517,0.26504, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0443,NC=1C=CC=C(OCC=2C=CC=CC2)C1,Z933326822,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.75,0.026,25.6,0.9,90.5,93.2,95.1,0.23002,0.26413, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0444,CC=1N=CSC1C(=O)N2CCNC(=O)C2,Z422344882,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.62,0.077,14.6,1.0,96.4,98.4,94.4,0.23017,0.26320,0.22904,0.26698,P 1,3 -
In Refinement, None

NUDT5A-x0445,CS(=O)(=O)N1CCCC(C1)C(=O)O,Z133632670,OK: Bad Dispense,success,P 1,48 59
80 79 82 76,1.65,0.020,24.5,0.4,94.9,94.4,94.5,0.23129,0.26641, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0446,NC(=O)N1CCN(CC1)C=2C=CC(F)=CC2,Z198194394,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.71,0.042,24.1,1.0,96.6,98.2,95.9,0.24373,0.28316, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0447,O=C(CC#N)N1CCC(CC=2C=CC=CC2)CC1,Z1688493887,OK: Precipitated,success,P
1,49 59 79 79 81 75,1.53,0.027,22.8,0.5,94.7,92.8,94.3,0.23383,0.26267, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0448,OC(=O)C=1C=CC=C(NC(=O)C2=CC=NO2)C1,Z2856434931,OK: Precipitated,success,P
1,48 59 80 79 82 77,1.70,0.019,27.6,0.5,93.2,93.1,95.0,0.23957,0.27768, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0449,CCN1N=C(CC1=O)C(F)(F)F,Z1268152398,OK: Mounted Clear,success,P 1,47 59 80
79 83 77,1.54,0.055,16.5,1.1,95.7,97.9,93.8,0.29923,0.34220, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0450,CCC(CC)C(=O)NC=1C=CC=CC1O,Z1331830630,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.76,0.053,17.4,1.2,96.8,98.3,95.8,0.22507,0.25923, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0451,CNCC=1C=CN=CC1,Z2856434786,OK: Crystalline,success,P 1,49 60 80 79 81
75,1.72,0.048,18.0,1.1,96.7,98.4,95.9,0.23079,0.26655, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0452,CCC1=NC(=NO1)C2CCCN2,Z1350579414,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.74,0.022,25.7,1.0,96.0,98.3,95.2,0.22905,0.26303, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0453,CN1N=CC(C1)=C1C(=O)N2CCCC2,Z275179946,OK: Crystalline,success,P 1,49 60
79 79 81 75,1.64,0.020,23.6,1.0,96.0,98.3,94.0,0.24122,0.27556, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0454,COCCNC1CCN(CC1)C(=O)C,Z2856434813,OK: Crystalline,success,P 1,49 59 79 79
81 75,1.47,0.046,14.9,0.4,93.5,94.1,87.8,0.24298,0.26890, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0455,[O-]C(=O)COCC=1C=CC=CC1,Z2856434906,OK: Crystalline,success,P 1,46 58 79
80 84 78,1.58,0.015,34.9,0.6,91.5,94.0,94.0,0.33619,0.37772, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0456,COC(=O)C=1C=CN=CC1,Z19684186,OK: Mounted Clear,success,P 1,48 59 79 79 82
76,1.61,0.046,18.9,1.0,96.3,98.9,94.4,0.22057,0.25013,0.22042,0.25136,P 1,3 - In
Refinement, None

NUDT5A-x0457,C(C1CCOCC1)N2CCNCC2,Z1267773591,OK: Mounted Clear,success,P 1,48 59 79 80
81 76,1.72,0.058,20.4,1.1,96.6,94.9,95.6,0.23049,0.26330, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0458,CC1CCN(CC1)C=2C=CC(N)=CC2C1,Z57345491,OK: Mounted Clear,success,P 1,48 59
79 80 82 76,1.59,0.022,32.4,1.0,95.5,98.1,93.1,0.21874,0.24473, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0459,CC(=O)N1CCC(CC1)C#N,Z952656810,OK: Mounted Clear,success,P 1,48 59 79 79
82 76,1.66,0.017,30.9,1.0,95.9,96.9,94.2,0.21607,0.24828, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0460,CC1CCCC1NCCO,Z1396419547,OK: Mounted Clear,success,P 1,49 59 79 80 81
76,1.50,0.027,24.1,0.4,93.9,93.2,92.7,0.24961,0.28226, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0461,CNC=1C=CC=CC1S(=O)(=O)C,Z285782452,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,2.03,0.055,15.9,2.0,96.9,97.6,95.2,0.21503,0.25525, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0462,CC(=O)NC=1C=CC=CC1O,Z57040482,OK: Mounted Clear,success,P 1,48 59 79 79 81 76,1.96,0.035,14.2,1.5,96.5,98.0,95.4,0.21826,0.25613,0.21783,0.25796,P 1,3 - In Refinement, None

NUDT5A-x0463,CC(C)C=1N=CC(C1)=C(N1)C(=O)N,Z906021418,OK: Mounted Clear,success,P 1,48 59 80 79 81 76,1.77,0.031,19.9,0.9,95.1,96.5,94.5,0.22221,0.26203,0.21157,0.24793,P 1,6 - Deposited,5QJU

NUDT5A-x0464,NC=1C=CC=CC1OCC=2C=CC=CC2,Z336089202,OK: Precipitated,success,P 1,46 58 79 80 84 77,1.68,0.016,38.7,0.6,82.8,94.4,94.5,0.33563,0.38181, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0465,OCC1=CN(N=N1)C=2C=CC(C1)=CC2,Z1374778753,OK: Precipitated,success,P 1,48 59 79 80 82 76,1.76,0.028,24.7,1.1,95.9,98.5,94.6,0.22040,0.25296, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0466,CS(=O)(=O)CC(O)C=1C=CC=CC1,Z822382694,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.63,0.047,19.1,1.0,96.4,98.7,94.4,0.24627,0.28491, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0467,ONC(=O)C=1C=CC=2C=CC=CC2N1,Z59181945,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.67,0.020,26.0,0.6,93.0,94.0,94.7,0.21726,0.25107, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0468,CC(=O)NC=1C=CC=C(F)C1C(=O)O,Z1229798311,OK: Crystalline,success,P 1,48 59 80 79 82 76,1.66,0.019,29.3,0.5,94.0,93.8,94.9,0.24350,0.28096, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0469,CNC=1N=CC=C(OC)N1,Z281802060,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.61,0.035,17.5,1.0,96.0,97.7,93.4,0.22343,0.25395,0.21503,0.24671,P 1,6 - Deposited,5QJV

NUDT5A-x0470,CC=1C=C(N=C(C)N1)N2CCNCC2,Z274575916,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0471,CC(=O)NC=1C=CC=CC1CC(=O)O,Z1444783243,OK: Mounted Clear,success,P 1,46 58 79 81 84 78,1.94,0.019,32.2,0.8,91.2,95.3,93.2,0.34920,0.39101, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0472,COC=1C=CC(=CC1)C(=O)C2CCNCC2,Z1741973467,OK: Mounted Clear,success,P 1,49 59 79 80 81 76,1.66,0.027,23.3,1.0,95.8,98.1,93.8,0.22855,0.25952, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0473,CC=1C=CC=CC1CC(=O)N,Z52214433,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0474,NCC1=CC(=NO1)C=2C=CC=CC2,Z425449682,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.74,0.031,19.6,0.6,78.6,95.1,95.4,0.21321,0.25182, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0475,CCC(=O)NC=1C=CC=2NC(=O)NC2C1,Z26794351,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.52,0.020,27.0,0.5,91.2,93.8,93.9,0.22439,0.25424, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0476,CC1=NC=2C=CC=CC2N1CCC(=O)N,Z53116498,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.59,0.026,27.6,0.5,94.7,91.9,94.1,0.22194,0.25314,0.22142,0.25377,P 1,3 - In Refinement, None

NUDT5A-x0477,CC(=O)NC1=NC=C(CC=2C=CC=C(C)C2)S1,Z57080305,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.89,0.023,28.6,0.6,80.8,90.5,54.9,0.22519,0.26051, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0478,C1=CSC(=C1)C2=NC=CN2,Z744754722,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.75,0.027,21.9,0.7,94.5,92.6,95.0,0.23450,0.27018, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0479,CC(=O)NCC1CNCCO1,Z1269638430,OK: Mounted Clear,success,P 1,49 59 79 79 81 76,1.70,0.048,16.8,1.1,96.6,97.0,95.1,0.22769,0.25723, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0480,COC(C)C1=NC(=CS1)C=2C=NOC2C,Z1945710531,OK: Precipitated,success,P 1,48 59 79 79 81 76,1.65,0.020,37.6,0.9,95.9,97.5,93.8,0.22213,0.25114, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0481,CC(=O)N1CC(C1)C(=O)O,Z1868430535,OK: Mounted Clear,success,P 1,46 58 79 81 84 78,1.53,0.014,37.2,0.4,94.1,94.0,93.6,0.34328,0.37850, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0482,C[C@H](O)CNCC=1C=CC=2OCOC2C1,Z2856434941,OK: Mounted Clear,success,P 1,48 59 79 80 81 76,1.70,0.036,18.6,1.2,96.2,99.0,94.9,0.21959,0.24948, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0483,CNCCC1CCCCC1,Z2856434901,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.94,0.028,18.7,0.7,85.2,91.2,74.5,0.23602,0.27568, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0484,COC(=O)NC=1C=CC(CC=2C=CN=CC2)=CC1,Z57190020,OK: Mounted Clear,success,P 1,48 59 79 80 81 76,1.61,0.035,21.8,1.1,95.7,95.1,93.3,0.22148,0.24742, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0485,CC1CCN(CC1)C(=O)CC(F)(F)F,Z316425948,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.67,0.034,25.8,1.2,96.3,97.6,95.1,0.22471,0.25808, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0486,CC(C)C(N)C(=O)N1CCOCC1,Z927400026,OK: Mounted Clear,success,P 1,49 59 79 80 81 76,1.60,0.035,20.3,1.1,95.9,95.9,93.5,0.24868,0.28310, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0487,COC(=O)C=1C=CC(=CC1)S(=O)(=O)N,Z18197050,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.69,0.032,20.8,1.0,95.9,98.5,94.7,0.22034,0.25008, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0488,CCCN1N=CC=C1C=2C=CN=CC2,Z1381484542,OK: Mounted Clear,success,P 1,48 59 79 80 81 76,1.81,0.050,19.2,1.0,96.5,98.6,95.3,0.22599,0.26085, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0489,CC(NS(=O)(=O)C)C=1C=CC=CC1C1,Z133729708,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.60,0.019,27.0,0.5,93.5,94.8,94.2,0.22270,0.25271, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0490,CC(C)NC(=O)C=1C=CNN1,Z381729066,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.62,0.040,20.8,1.0,96.2,97.1,94.3,0.23001,0.25707, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0491,CS(=O)(=O)NCC1CCNCC1,Z1741966151,OK: Crystalline,success,P 1,49 59 79 79 81 75,1.50,0.033,17.9,0.5,93.2,89.2,91.9,0.23871,0.26549, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0492,CCN(C)C(=O)C=1C=CC=C(N)C1,Z2092370954,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.64,0.020,35.1,1.0,95.7,96.4,93.6,0.22449,0.25085, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0493,CNCC1COC=2C=CC=CC2O1,Z1891773476,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,1.67,0.025,24.8,0.6,92.2,93.7,94.4,0.23208,0.26485,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0494,NC(=S)NC=1C=CC=CC1OC(F)(F)F,Z291279160,OK: Precipitated,success,P 1,49 59
80 79 81 75,2.04,0.043,9.9,1.5,96.4,98.1,94.9,0.25149,0.29105,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0495,C1C=1SN=NC1CN2CCOCC2,Z2856434925,OK: Mounted Clear,success,P 1,49 60 80 79
81 75,1.87,0.040,13.3,1.6,96.1,98.0,95.2,0.23572,0.27017,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0496,CS(=O)(=O)NC1CCNCC1,Z212045094,OK: Mounted Clear,success,P 1,49 60 80 79
81 75,1.69,0.056,10.0,1.2,96.6,97.5,94.9,0.23020,0.26474,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0497,NC(=O)NC=1C=CC(=CC1)C=2C=CC=CC2,Z198195774,OK: Precipitated,success,P 1,49
59 80 79 81 75,1.48,0.028,24.1,0.5,93.8,94.7,89.1,0.23831,0.26949,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0498,CCC(=O)NC=1C=CC=C(N)C1C,Z235361315,OK: Mounted Clear,success,P 1,48 59 80
79 81 75,1.79,0.018,31.8,0.6,79.9,92.2,81.2,0.22402,0.26255,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0499,CNS(=O)(=O)CC1CCCC1,Z1003207278,OK: Mounted Clear,success,P 1,49 60 79 79
80 75,1.67,0.055,21.8,1.2,96.4,98.6,95.2,0.24493,0.28414,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0500,NC(=S)NC=1C=CC(OC(F)(F)F)=CC1,Z1741960769,OK: Precipitated,success,P 1,49
59 80 79 81 75,1.53,0.018,34.1,0.7,94.1,93.7,94.1,0.22581,0.25149,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0501,N#CCCN1CCOCC1,Z2856434767,OK: Mounted Clear,success,P 1,49 59 80 79 81
75,1.54,0.036,20.1,1.3,95.5,94.5,93.6,0.23399,0.25819,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0502,COC=1C=CC(=CC1)C(=O)NCC(=O)N,Z33546965,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.76,0.049,22.4,1.3,96.8,96.6,95.8,0.23402,0.26150,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0503,CCOC(=O)C=1C=COC1,Z293079056,OK: Mounted Clear,success,P 1,49 60 79 79 81
75,1.74,0.066,13.1,1.1,96.8,98.5,95.7,0.22837,0.26353,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0504,CC(O)COC=1C=CC=C(F)C1,Z1250132544,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.90,0.029,13.5,0.6,87.5,85.9,89.5,0.25992,0.30513,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0505,CC1COCCN1CCN,Z1263811695,OK: Mounted Clear,success,P 1,49 59 80 79 81
75,1.71,0.030,19.8,0.6,92.3,94.5,95.4,0.23165,0.26531,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0506,COC=1C=CC(=CC1)C(N)C(=O)O,Z56755722,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.58,0.024,31.2,1.1,95.5,94.1,93.3,0.22730,0.25518,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0507,CCOC=1C(F)=CC=CC1C(=O)N(C)C,Z1273312142,OK: Mounted Clear,success,P 1,48
59 80 79 82 76,1.79,0.017,25.1,0.6,91.8,92.4,94.1,0.22804,0.26695,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0508,CC1CNCCN1CCO,Z1741794237,OK: Mounted Clear,success,P 1,49 60 79 79 81
75,1.55,0.030,21.2,0.7,93.0,92.0,94.1,0.23032,0.25997,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0509,CC(=O)NC=1C=CC=C(NC(=O)N)C1,Z198195770,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.65,0.075,15.2,1.2,96.5,96.2,95.1,0.22989,0.25917, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0510,CCNC=1N=CC=CC1C,Z1992316287,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.74,0.015,38.3,0.8,95.2,98.7,94.3,0.22711,0.25963, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0511,O=C1NC=C(NCC=2C=CC=CC2)C(=O)N1,Z111666026,OK: Mounted Clear,success,P 1,48 59 80 79 81 76,1.56,0.052,19.6,1.2,96.1,99.0,94.4,0.22074,0.24248, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0512,CC(=O)N1CC=2C=CC(N)=CC2C1,Z1354416068,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.66,0.047,12.4,1.0,96.2,99.0,94.5,0.22591,0.25369, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0513,CN(C)C(=O)C=1C=CC(F)=CC1Br,Z100642432,OK: Mounted Clear,success,P 1,48 59 79 79 81 75,1.68,0.020,29.0,0.4,92.9,93.4,93.4,0.22528,0.25886, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0514,CC(N)C1=NC(CC=2C=CC=CC2)=NO1,Z2442288995,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.67,0.048,16.1,1.2,96.2,97.3,94.7,0.22615,0.25522, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0515,N(C1=NN=CS1)C=2C=CC=CC2,Z56347187,OK: Precipitated,success,P 1,49 59 80 79 81 75,1.75,0.017,33.8,1.2,96.0,98.2,95.0,0.22088,0.24980, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0516,CC(=O)NC=1C=CC(F)=C(C1)C(=O)O,Z364321922,OK: Crystalline,success,P 1,47 59 80 80 83 78,2.25,0.047,5.8,1.0,96.6,98.9,95.7,,, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0517,CCC(=O)NC1=NC(C)=CS1,Z30820160,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.54,0.022,23.6,0.4,93.5,91.0,94.1,0.24006,0.27287, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0518,CCS(=O)(=O)NC=1C=CC=CC1F,Z53825177,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.87,0.014,30.9,1.2,94.6,97.7,93.3,0.22636,0.25882, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0519,NC=1N=CN=CC1C=2C=CC(C1)=CC2,Z1262398388,OK: Mounted Clear,success,P 1,48 59 79 80 82 76,1.64,0.032,25.6,1.2,96.1,98.3,94.9,0.22479,0.24987, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0520,CS(=O)(=O)NC1CCCC1,Z53825479,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, ,, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0521,O=C(NC=1C=CC=2N=CC=CC2C1)C=3C=CC=CC3,Z453319206,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.94,0.076,12.0,2.2,94.5,97.2,88.8,0.23811,0.27345, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0522,CN(C(=O)C)C=1C=CC=CC1C(=O)O,Z223688272,OK: Mounted Clear,success,P 1,47 59 80 80 83 77,1.90,0.021,27.5,0.9,66.3,91.8,33.3,0.24294,0.28255, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0523,CNC1CCN(C1=O)C=2C=CC=CC2F,Z1186029914,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.58,0.019,28.5,0.6,93.8,91.1,94.5,0.22136,0.24708, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0524, CC(=O)N1CCC(CC1)C2=CNC=3C=CC=CC23, Z223388508, OK: Mounted Clear, success, P 1, 48 59 80 79 82 76, 1.63, 0.016, 31.9, 0.8, 94.6, 97.8, 91.4, 0.22616, 0.25094, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0525, NC(=O)N1CCN(CC1)C(=O)C2=CC=CO2, Z198194396, OK: Crystalline, success, P 1, 49 59 80 79 81 75, 1.57, 0.022, 29.3, 0.9, 94.7, 94.7, 94.0, 0.23940, 0.26822, 0.23356, 0.26710, P 1, 6 - Deposited, 5QJW

NUDT5A-x0526, [O-]C(=O)C=1C=CC=CC1OC(F)(F)F, Z2856434778, OK: Crystalline, success, P 1, 48 59 80 79 82 76, 1.73, 0.030, 22.3, 1.1, 96.4, 98.2, 95.8, 0.22506, 0.25431, 0.22221, 0.25644, P 1, 6 - Deposited, 5QJX

NUDT5A-x0527, NC(=O)C1=CNC(=N1)C2CC2, Z1407672867, OK: Mounted Clear, success, P 1, 48 59 80 79 81 75, 1.70, 0.019, 32.9, 0.5, 89.2, 90.1, 94.7, 0.22869, 0.26536, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0528, CN1N=C(C(=O)N)C=2C=CC=CC12, Z2697514548, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.62, 0.034, 26.3, 1.1, 96.0, 98.6, 94.3, 0.22745, 0.25532, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0529, CNC1CCCN(C1)C=2C=CC=NN2, Z1139246057, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.63, 0.012, 44.9, 0.9, 95.8, 97.5, 93.4, 0.23115, 0.26162, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0530, COC=1C=CC(=CC1)N2CC(CC2=O)C(=O)N, Z57324924, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.76, 0.051, 20.9, 1.1, 95.8, 96.0, 94.5, 0.23098, 0.26431, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0531, C(NC=1C=CN=CC1)C2CCCO2, Z1267882044, OK: Mounted Clear, success, P 1, 49 60 79 79 81 75, 1.65, 0.040, 17.3, 0.6, 94.6, 95.6, 94.9, 0.24645, 0.28293, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0532, CN(C)S(=O)(=O)N1CCN(C)CC1, Z2735592898, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.56, 0.023, 24.5, 0.6, 94.2, 93.0, 94.4, 0.22388, 0.25135, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0533, CN1CCC[C@H](C1)OC(=O)C2=CC=CO2, Z2940170964, OK: Mounted Clear, success, P 1, 49 60 79 79 81 75, 2.14, 0.038, 9.6, 0.7, 95.8, 97.8, 95.2, 0.25707, 0.30792, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0534, CS(=O)(=O)NCCC=1C=CC=CC1, Z45617795, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.71, 0.030, 22.5, 1.0, 96.3, 98.2, 95.3, 0.22074, 0.25242, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0535, OCC1=CN(N=N1)C=2C=CC(C1)=C(C1)C2, Z1891776064, OK: Precipitated, success, P 1, 49 60 80 79 81 75, 1.52, 0.030, 27.0, 1.2, 95.3, 92.4, 93.3, 0.22421, 0.24877, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0536, CCN1C=C(CCO)C=N1, Z1674937530, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.64, 0.025, 21.2, 0.5, 93.7, 90.8, 94.8, 0.22307, 0.25324, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0537, CCN1C=CC(CNC)=N1, Z2856434888, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.97, 0.032, 19.7, 0.5, 70.5, 95.6, 69.1, 0.26031, 0.31649, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0538, O=C1CN(CC=2C=CC=CC2)CC(=O)N1, Z2856434910, OK: Mounted Clear, success, P 1, 48 59 80 79 82 76, 1.57, 0.030, 23.3, 1.1, 95.4, 94.9, 93.3, 0.23076, 0.25521, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0539, CS(=O)(=O)N1CCC(O)CC1, Z1247413608, OK: Mounted Clear, success, P 1, 48 59 80 79 81 75, 1.68, 0.018, 34.5, 0.5, 79.7, 90.9, 94.6, 0.21739, 0.25348, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0540,CN(C)C=1C=CN=CC1,Z2856434762,OK: Bad Dispense,success,P 1,49 59 79 79 81
75,1.65,0.029,25.5,1.0,89.1,89.5,93.0,0.23439,0.27116,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0541,CC(CS(=O)(=O)N)C=1C=CC=CC1,Z1407673036,OK: Mounted Clear,success,P 1,48 59
80 79 82 76,1.56,0.019,27.6,0.5,87.8,93.1,94.0,0.22371,0.25701,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0542,CC(=O)N1CCN(CC1)C(=O)N,Z90122368,OK: Crystalline,success,P 1,49 60 80 79
81 75,1.56,0.020,25.6,0.6,94.2,93.6,94.2,0.22378,0.24948,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0543,CC(=O)NC(C)(C1CC1)C(=O)O,Z1259162160,OK: Crystalline,success,P 1,47 59 79
80 83 77,1.72,0.020,27.5,0.9,96.0,97.6,95.4,0.28808,0.32525,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0544,CC(OC=1C=CC(C1)=CC1)C(=O)N,Z19727416,OK: Precipitated,success,P 1,49 59 80
79 81 75,1.52,0.042,25.9,1.1,95.9,98.1,94.1,0.21947,0.24313,0.21834,0.24594,P 1,3 - In
Refinement,None

NUDT5A-x0545,CC(N)C1=CN(N=N1)C=2C=CC=CC2,Z2527301677,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.77,0.028,18.1,0.7,93.8,93.6,95.1,0.23312,0.27045,0.23279,0.27177,P 1,3
- In Refinement,None

NUDT5A-x0546,CS(=O)(=O)CC1=NC=2C=CC=CC2N1,Z126932614,OK: Bad Dispense,success,P 1,49 59
80 79 81 75,1.98,0.070,9.6,0.9,96.3,98.1,94.2,0.26048,0.29153,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0547,FC(F)(F)CC(=O)N1CCNCC1,Z1262246195,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.71,0.036,9.8,0.5,87.0,93.6,94.4,0.22979,0.26001,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0548,CC(C)N1C=NC(=C1)S(=O)(=O)N,Z1509882419,OK: Mounted Clear,success,P 1,48 59
80 79 82 76,1.77,0.023,21.4,2.1,96.4,99.2,95.4,0.22067,0.25005,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0549,CCOC=1C=CC=CC1N2CCNCC2,Z425387594,OK: Bad Dispense,success,P 1,48 59 79 79
82 76,1.73,0.037,22.3,1.0,96.5,98.4,95.8,0.21301,0.24526,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0550,CC(=O)NC=1C=CC(C)=C2NCCCC12,Z1650168321,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.61,0.016,41.1,0.8,95.4,97.0,93.0,0.22276,0.24938,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0551,O=C(CC=1C=CC=CC1)N2CCC=3C=CC=CC23,Z30624464,OK: Mounted Clear,success,P
1,48 59 80 79 82 76,1.65,0.029,24.8,1.4,95.5,97.4,93.2,0.21764,0.24383,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0552,CN(C)S(=O)(=O)C=1C(C)=NNC1C,Z94597856,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.77,0.014,32.2,0.7,74.5,94.4,92.6,0.21743,0.25553,0.21613,0.25916,P 1,6 -
Deposited,5QJY

NUDT5A-x0553,CC(N)C=1C=CC(=CC1)C=2C=NC=NC2,Z1696822287,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.52,0.012,42.4,0.4,94.1,92.5,94.2,0.23041,0.26204,0.22771,0.26261,P 1,6
- Deposited,5QJZ

NUDT5A-x0554,CC1=NNC(C)=C1C=2C=CC=CC2N,Z1270312110,OK: Mounted Clear,success,P 1,49 60
79 79 80 75,1.44,0.038,21.1,0.4,82.5,85.9,70.0,0.27304,0.31560,0.30767,0.33838,P 1,6 -
Deposited,5QK0

NUDT5A-x0555,NC(=O)C(O)C1CCOCC1,Z1312590981,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,2.21,0.044,8.4,1.0,95.9,94.8,94.6,0.33812,0.38697,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0556,CC=1C=CC(CC(=O)NC2=NC=CS2)=CC1,Z90713255,OK: Precipitated,success,P 1,49
59 79 79 81 75,1.63,0.019,25.2,0.5,77.5,91.3,87.4,0.22255,0.26053,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0557,CNC(=O)NCC=1C(F)=CC=CC1C1,Z933840894,OK: Mounted Clear,success,P 1,48 59
79 80 82 76,1.80,0.047,17.0,1.7,95.0,97.3,95.1,0.23296,0.26789,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0558,CC(C)NC(=O)N(C)CC=1C=NN(C)C1,Z183344018,OK: Bad Dispense,success,P 1,48 59
79 79 81 75,1.59,0.020,29.2,0.5,91.5,93.8,94.3,0.22159,0.25197,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0559,CC(C)(C)N1CC(O)C1,Z2856434900,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.58,0.030,26.1,1.0,95.6,95.4,93.4,0.23481,0.26527,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0560,CCC(=O)NC1=C(OC=2C=CC=CC12)C(=O)N,Z108545814,OK: Mounted Clear,success,P
1,48 59 80 79 82 76,1.71,0.040,8.5,0.5,94.9,95.4,95.2,0.22760,0.25695,0.22717,0.25879,P
1,3 - In Refinement,None

NUDT5A-x0561,NCC=1C=CC=CC1OC(F)(F)F,Z2856434776,OK: Crystalline,success,P 1,49 59 79 79
81 75,1.63,0.015,43.0,0.8,95.4,97.8,93.4,0.22691,0.25522,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0562,CC(C)C=1C=CC(CN2CCC(O)CC2)=CC1,Z2856434874,OK: Mounted Clear,success,P
1,49 59 79 79 81 75,1.77,0.044,23.4,1.3,96.0,97.8,95.6,0.23695,0.27423,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0563,CC(=O)NC=1C=CC(NC=2C=CC=CC2)=CC1,Z68404778,OK: Mounted Clear,success,P
1,49 59 80 79 81 75,1.58,0.031,18.2,1.1,95.6,97.3,93.2,0.23199,0.25573,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0564,CN1CCN(CC1)C(=O)NC=2C=CC=CC2,Z2856434890,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.64,0.026,22.4,0.6,93.1,94.4,94.5,0.22742,0.26032,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0565,CN(C)C(=O)N1CCOCC21CCOC2,Z1998104358,OK: Bad Dispense,success,P 1,49 60 80
79 81 75,1.51,0.035,18.6,0.4,92.5,92.7,93.2,0.24035,0.26975,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0566,CC1=NOC(CN2CCC(CO)CC2)=N1,Z416877194,OK: Crystalline,success,P 1,49 60 79
79 80 75,1.74,0.048,19.7,1.1,96.6,98.5,95.5,0.25457,0.29771,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0567,CC(C)NC1=NC=2C=CC=CC2N1,Z2467208649,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.93,0.032,11.8,0.6,80.2,89.8,74.1,0.23402,0.27467,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0568,CNC(=O)C=1C=CC(CS(=O)(=O)C)=CC1,Z30272045,OK: Mounted Clear,success,P 1,48
59 80 79 81 75,1.50,0.021,25.3,0.6,93.5,91.9,92.2,0.22608,0.24975,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0569,CN(C)S(=O)(=O)C=1C=NNC1,Z805551440,OK: Mounted Clear,success,P 1,49 60 80
79 81 75,1.59,0.043,15.4,1.0,95.9,96.2,93.5,0.23493,0.26196,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0570,CS(=O)(=O)NCCC=1C=CC(F)=CC1,Z45705015,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.51,0.021,27.7,0.4,94.0,93.5,94.0,0.23258,0.26354,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0571,NC=1C=CC=CC1N2CCOCC2,Z56785490,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,1.73,0.082,14.4,1.0,96.8,98.3,95.7,0.22865,0.26140,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0572,CC1=CSC(NCC2CCCO2)=N1,Z48852953,OK: Crystalline,success,P 1,49 60 79 79 81
75,1.89,0.049,15.5,1.3,96.8,97.9,94.4,0.22779,0.26699,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0573,O=C(CC#N)NC1CCCC1,Z56813508,OK: Precipitated,success,P 1,49 60 79 79 80
75,1.42,0.030,24.7,0.4,92.2,91.2,82.0,0.25879,0.29241,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0574,C1=CSC(=N1)C2=NN=CN2,Z2027049478,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,1.49,0.028,21.5,0.5,93.5,91.5,91.0,0.23324,0.26148,0.21990,0.25196,P 1,6 -
Deposited,5QK1

NUDT5A-x0575,COC=1C=CC(Br)=CC1CNC(=O)C,Z955369596,OK: Precipitated,success,P 1,49 59 80
79 81 75,1.59,0.037,24.6,1.0,95.5,95.5,93.2,0.23483,0.26237,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0576,CC=1SC(N)=NC1C=2C=CC(C)=C(C)C2,Z48847633,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.48,0.030,22.3,0.6,93.9,93.8,89.5,0.22458,0.24892,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0577,NC(=O)C1CCN(CC1)C(=O)NC=2C=CC=CC2,Z33545544,OK: Mounted Clear,success,P
1,49 59 80 79 81 75,1.72,0.040,19.5,1.0,95.3,98.3,95.1,0.23387,0.26289,None,None,P 1,1
- Analysis Pending, None

NUDT5A-x0578,CC=1C=CC=CC1N2C=C(N=N2)C(=O)O,Z2327226104,OK: Mounted Clear,success,P 1,48
59 80 79 82 75,1.70,0.020,27.9,0.5,93.1,94.0,94.7,0.23118,0.26204,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0579,CC(=O)NCCC=1C=CC(=CC1)S(=O)(=O)N,Z30857828,OK: Mounted Clear,success,P
1,49 59 80 79 81 75,1.64,0.063,13.9,1.1,96.5,97.5,94.8,0.23004,0.25862,None,None,P 1,1
- Analysis Pending, None

NUDT5A-x0580,OCC=1C=CC=CC1N2CCOCC2,Z235361235,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,2.04,0.036,14.0,0.4,76.0,93.2,69.7,0.29639,0.34881,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0581,NC=1N=CC=C(N1)C=2C=CC(C1)=CC2,Z363993198,OK: Precipitated,success,P 1,49
59 80 79 81 75,1.59,0.027,23.9,0.7,95.5,97.6,93.3,0.22912,0.25530,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0582,CC(=O)N1CCCC(O)(C1)C(=O)O,Z2293643386,OK: Mounted Clear,success,P 1,47 59
80 79 83 77,1.90,0.032,16.5,1.0,95.8,98.3,94.4,0.24845,0.28073,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0583,CCN1C(NC(=O)C)=NC=2C=CC=CC12,Z68639747,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,2.26,0.151,5.6,1.0,96.6,98.4,95.3,,None,None,1 - Analysis
Pending, None

NUDT5A-x0584,CCOC(=O)NC=1C=CC=C(C1)C1,Z31697001,OK: Precipitated,success,P 1,49 59 80
79 81 75,1.63,0.037,20.6,0.6,94.9,94.0,94.4,0.23324,0.26563,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0585,COC=1C=CC=2NC=C(CN(C)C)C2C1,Z2856434938,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.70,0.034,17.7,1.0,96.2,98.5,95.4,0.22588,0.25603,None,None,P 1,1 -
Analysis Pending, None

NUDT5A-x0586,CCOC(=O)N1CCOCC1,Z31721097,OK: Mounted Clear,success,P 1,49 60 80 79 81
75,2.02,0.085,8.7,1.1,90.9,94.8,90.6,0.25433,0.30410,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0587,CNC(C)C=1SC(C)=NC1C,Z1266823232,OK: Mounted Clear,success,P 1,49 59 80 79
81 75,1.53,0.021,30.2,0.7,92.9,87.6,94.4,0.23522,0.26344,None,None,P 1,1 - Analysis
Pending, None

NUDT5A-x0588,COCC=1C=CC(CN)=CC1OC,Z2856434917,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.56,0.041,24.0,1.3,96.0,97.1,93.8,0.23535,0.26305, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0589,CC(CO)N(C)C=1N=CC(C1)=CN1,Z1546887028,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.92,0.037,13.8,1.3,96.5,96.2,95.4,0.22466,0.26193, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0590,CC(=O)N1CCCNCC1,Z168883358,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.86,0.028,16.5,0.6,91.8,91.3,94.2,0.25695,0.29791, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0591,OCC=1C=CC(=CC1)N2C=NC=3C=CC=CC23,Z235449082,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.67,0.027,25.7,1.3,96.0,96.9,94.3,0.23147,0.26283, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0592,CNC=1N=CC(=CC1C1)C(F)(F)F,Z54628157,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.65,0.014,35.9,0.6,81.8,93.8,81.4,0.22119,0.25640, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0593,CC(=O)NC=1C=CC(OC=2N=CC=CN2)=CC1,Z54571979,OK: Precipitated,success,P 1,49 59 79 79 81 75,1.62,0.020,30.3,0.6,91.9,94.5,94.3,0.23096,0.26084, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0594,CN1CCCC=2C=CC(=CC12)S(=O)(=O)N,Z1367324110,OK: Bad Dispense,success,P 1,48 59 79 80 82 76,1.83,0.015,36.2,0.6,90.2,94.0,86.0,0.22189,0.26146, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0595,CC(N)C=1C=CC(=CC1)N2CCOCC2,Z1259341012,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0596,CC(=O)NC1CNC=2C=CC=CC2C1,Z1492796719,OK: Bad Dispense,success,P 1,48 59 79 79 82 76,1.72,0.059,22.4,1.2,95.6,94.9,95.3,0.24231,0.27326, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0597,CNC1(CCCC1)C(=O)N,Z1348559502,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.61,0.048,16.4,1.0,96.3,97.0,94.3,0.23409,0.26723, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0598,CN1CCN(CC1)C(=O)CO,Z228585842,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.83,0.041,18.6,0.4,75.1,91.5,45.0,0.25422,0.29795, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0599,CC=1C=C(ON1)C(=O)NCC2CCOC2,Z384361454,OK: Bad Dispense,success,P 1,48 59 80 79 82 76,1.56,0.042,20.5,1.1,96.0,98.5,94.3,0.22417,0.24963, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0600,CNC=1N=CC=CN1,Z54628578,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.65,0.027,24.4,0.4,75.2,92.8,68.7,0.23177,0.26870,0.22548,0.26719, P 1,6 - Deposited,5QK2

NUDT5A-x0601,NC(=O)C=1C=CC=2NCCC2C1,Z2434225559,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.72,0.052,16.3,0.9,96.4,98.4,95.4,0.22154,0.25027, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0602,CN(CC(=O)O)C(=O)C=1C=CC(F)=CC1,Z85895198,OK: Crystalline,success,P 1,46 58 79 81 85 78,1.89,0.016,38.6,0.7,81.7,93.7,57.6,0.33940,0.38617, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0603,CC(C)(C)NC(=O)CN1C=CC(=N1)C(F)(F)F,Z55009317,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.78,0.041,21.8,1.0,96.7,96.7,96.0,0.22173,0.25600, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0604,CC(CC=1C=CC(Br)=CC1)C(=O)N,Z1551999220,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.62,0.066,11.7,1.0,96.4,98.5,94.5,0.22599,0.25178,0.22386,0.25353,P 1,3 - In Refinement,None

NUDT5A-x0605,CC(=O)NC1=CC(C)=NN1,Z239136710,OK: Mounted Clear,success,P 1,49 60 80 79 81 75,1.71,0.083,10.9,1.1,96.8,97.2,95.9,0.23349,0.26395,0.22988,0.26624,P 1,6 - Deposited,5QK3

NUDT5A-x0606,CCC(=O)NC=1C=CC(C)=CC1O,Z33452106,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.59,0.047,22.4,1.0,96.3,98.8,94.3,0.22283,0.24977,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0607,CC(N)C(=O)NC1=CC(=NN1)C(F)(F)F,Z1622626423,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.74,0.026,21.4,0.8,95.0,95.0,94.7,0.21901,0.25210,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0608,COC=1C=CC=CC1NC(=O)C2=CC=C(C)S2,Z27797417,OK: Precipitated,success,P 1,49 59 79 79 81 75,1.59,0.040,17.8,0.5,84.5,94.4,94.4,0.22890,0.26608,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0609,CNC(C)C=1C=NN(C)C1,Z1437171658,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.48,0.054,13.1,0.7,94.0,95.0,89.3,0.23726,0.26334,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0610,CNC(=O)C1CNCCO1,Z1636723439,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.63,0.046,15.3,1.1,96.0,97.9,93.7,0.23674,0.26585,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0611,CC(O)CCN1C=CC=N1,Z1613492358,OK: Mounted Clear,Failed - unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis Pending,None

NUDT5A-x0612,C(N1CCNCC1)C2=CSC=N2,Z812517112,OK: Mounted Clear,Failed - unknown,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis Pending,None

NUDT5A-x0613,CC=1C=CC(NC(=O)C2=CC=CO2)=CC1O,Z1430613384,OK: Precipitated,success,P 1,49 60 80 79 81 75,1.80,0.030,10.3,0.4,93.9,89.7,94.4,0.24683,0.28788,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0614,O=C(COC=1C=CC=CC1)N2CCCC2,Z19735981,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.76,0.036,17.4,0.6,94.5,93.1,94.8,0.24183,0.27998,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0615,CC(C)NC(=O)C=1C=C(C)N(C)N1,Z733898630,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.61,0.017,31.3,0.5,86.8,93.8,94.6,0.22485,0.25680,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0616,C1OC=2C=CC(=CC2O1)C=3C=CNN3,Z2204875953,OK: Mounted Clear,success,P 1,49 60 80 79 81 75,1.85,0.013,28.0,1.4,96.0,98.3,94.7,0.22300,0.25677,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0617,CC(C)C=1C=CC(=CC1)C(=O)NC2=NN=CS2,Z86416893,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.68,0.062,17.8,1.1,96.3,97.9,94.4,0.22238,0.25210,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0618,CC1CCCCN1C(=O)C=2C=NC=CN2,Z32968340,OK: Mounted Clear,success,P 1,49 60 79 79 80 75,1.67,0.067,13.5,1.1,96.2,98.8,94.3,0.24556,0.28055,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0619,CC(=O)NC(C1CCOCC1)C(=O)O,Z1891772663,OK: Crystalline,success,P 1,46 58 79 80 84 78,1.68,0.015,30.0,0.8,95.7,98.6,94.1,0.30288,0.34544,None,None,P 1,1 - Analysis Pending,None

NUDT5A-x0620, COC=1C=C (C=C (OC) C1OC) C (=O) O, Z2734782702, OK: Crystalline, Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0621, CC (=O) NC=1C=CC=NC1C (=O) O, Z1815155460, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.61, 0.020, 29.3, 1.0, 95.4, 96.7, 93.1, 0.22931, 0.25807, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0622, CC (C) C1=NC=CN1CC (=O) O, Z2446040567, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 2.28, 0.048, 12.8, 6.0, 97.1, 97.1, 96.4, 0.21140, 0.24657, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0623, CCC1=CSC (=N1) C2=CNC=N2, Z1530301542, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.62, 0.086, 12.0, 1.0, 96.4, 98.5, 94.4, 0.22882, 0.25528, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0624, CC1CN (C (=O) C) C=2C=CC=C (F) C2O1, Z1730522163, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.98, 0.046, 18.2, 1.6, 94.8, 94.7, 93.7, 0.24688, 0.28766, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0625, CC (=O) NCC=1C=CC (=CC1) S (=O) (=O) N, Z30932204, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.61, 0.093, 16.9, 1.0, 96.3, 99.0, 93.5, 0.22407, 0.25144, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0626, CNC (=O) C1CCCC=2SC (C) =NC12, Z1904249627, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.98, 0.039, 3.7, 0.8, 90.3, 92.6, 91.4, 0.23450, 0.26300, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0627, CCNC (=O) N1CCN (CC1) C (=O) C, Z44590919, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.62, 0.053, 17.1, 0.8, 95.2, 95.3, 94.4, 0.23372, 0.26317, 0.22411, 0.25483, P 1, 6 - Deposited, 5QK4

NUDT5A-x0628, CCOC=1C=CC (CC (=O) O) =CC1, Z2856434918, OK: Mounted Clear, success, P 1, 47 59 80 79 83 77, 1.92, 0.034, 14.3, 0.6, 89.8, 94.5, 93.6, 0.27006, 0.31790, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0629, CC (=O) N1C [C@H] 2CC [C@H] 1C=3C=CC=CC23, Z2017861827, OK: Mounted Clear, success, P 1, 49 59 80 79 81 75, 1.65, 0.028, 22.8, 1.0, 95.7, 97.9, 93.8, 0.22654, 0.25439, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0630, CC1=NN (C) C (=O) C=C1CC (=O) N, Z287484230, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.70, 0.059, 13.0, 1.3, 95.8, 98.6, 93.3, 0.23076, 0.26203, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0631, CNCC=1C=NN (C1) C=2C=CC=CC2, Z102768020, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0632, CN1CCN (CC1) C=2C=CC (NC (=O) C) =CC2, Z2856434903, OK: Mounted Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0633, COC=1C=CC=C2NC=CC12, Z1429867185, OK: Mounted Clear, success, P 1, 49 59 79 79 81 75, 1.58, 0.019, 28.7, 0.5, 86.6, 93.8, 94.2, 0.22826, 0.26357, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0634, CC (NC (=O) C1CCCC1) C (=O) O, Z1238477790, OK: Crystalline, success, P 1, 46 58 79 80 84 78, 1.57, 0.023, 30.3, 1.0, 95.3, 97.1, 92.8, 0.31189, 0.35261, None, None, P 1, 1 - Analysis Pending, None

NUDT5A-x0635,C(NC1CCCC1)C2CCCO2,Z90504169,OK: Mounted Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0636,COC(=O)C=1SC=CC1NC(=O)C2CC2,Z109092588,OK: Mounted Clear,success,P 1,48 59
79 79 82 76,1.94,0.041,15.7,0.9,86.4,93.4,74.3,0.23622,0.27626, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0637,CCNC=1C=CC(C)=NN1,Z1267773786,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.63,0.057,13.4,1.1,96.3,98.5,94.0,0.24132,0.27212,0.23269,0.26563,P 1,6 -
Deposited,5QK5

NUDT5A-x0638,CN1C=CC(=N1)C(=O)NC=2C=CC=C(C2)C(=O)[O-],Z2856434892,OK: Mounted
Clear,success,P 1,48 59 80 79 82
76,1.56,0.045,15.2,0.6,94.6,94.3,94.2,0.22550,0.24877, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0639,CC1=NC(=NO1)C=2C=CC=CC2,Z57791725,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.69,0.045,16.3,1.1,96.5,99.3,95.2,0.22974,0.25757, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0640,CC=1C=C(F)C=C(C1)S(=O)(=O)N,Z1324080698,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.53,0.037,17.5,0.5,94.2,92.9,93.9,0.22945,0.25335,0.22703,0.25188,P 1,3
- In Refinement, None

NUDT5A-x0641,CC(O)CN1C=CN=C1C,Z1362754425,OK: Mounted Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0642,CC1=NOC(CC(N)C=2C=CC=CC2)=N1,Z2442269480,OK: Mounted Clear,success,P 1,49
59 80 79 81 75,1.64,0.068,15.7,1.1,96.3,98.5,94.6,0.22827,0.25855, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0643,CCC(NC)C=1C=CN=CC1,Z1250132788,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.74,0.029,20.5,0.9,96.3,98.6,95.5,0.23371,0.26718, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0644,CNCC=1C=CC=C(OC)N1,Z1603775714,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.57,0.036,16.5,0.7,94.3,93.5,94.0,0.23166,0.26130, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0645,CNC1(CO)CCOCC1,Z1169060901,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.65,0.024,29.5,0.9,95.8,98.1,93.8,0.23442,0.26602, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0646,C[C@@H](CO)N(C)C=1N=CC=CC1F,Z2017168803,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.63,0.053,14.7,1.0,96.5,98.6,94.6,0.25662,0.29262, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0647,CC1CCN(CC1)C(=O)CCCC=2C=CC=CC2,Z419884046,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,2.08,0.039,30.7,4.9,97.1,96.8,96.0,0.22201,0.26067, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0648,CS(=O)(=O)N1CCC[C@@H]1CN,Z1713595338,OK: Mounted Clear,success,P 1,49 60
79 79 81 75,1.55,0.065,16.5,0.8,96.2,98.8,94.3,0.24048,0.27177, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0649,COC=1C=CC=CC1C2=NN=CO2,Z1359419878,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.77,0.018,27.7,0.7,94.0,93.7,94.8,0.22485,0.25888, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0650,CC1=NN(C(=O)C1)C=2C=CC=CC2,Z50145861,OK: Mounted Clear,success,P 1,48 59
80 79 81 75,1.76,0.073,13.2,1.0,96.8,97.3,95.5,0.23233,0.26634, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0651,CC=1C=CC(C(=O)N)=C(F)C1,Z1343633025,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.51,0.062,21.4,1.0,95.8,98.2,93.6,0.23740,0.26158,0.22816,0.25488,P 1,6 -
Deposited,5QK6

NUDT5A-x0652,CNC(=O)CN1CCNCC1,Z85934875,OK: Mounted Clear,success,P 1,49 59 79 79 81
75,1.66,0.017,39.5,1.2,95.8,98.2,93.9,0.22471,0.25268, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0653,CC=1NNC(=O)C1CCO,Z1259155959,OK: Mounted Clear,success,P 1,48 59 79 79 82
76,1.57,0.033,16.2,1.2,95.8,98.0,93.5,0.21914,0.24337, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0654,CC(OC=1C=CC(=CC1)C=2C=CC=CC2)C(=O)O,Z111782404,OK: Precipitated,success,P
1,48 59 80 79 81 75,1.46,0.017,33.4,0.5,92.7,91.7,85.9,0.22650,0.25274, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0655,NC(=O)C1CCCN2C=CN=C12,Z1324853681,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.67,0.073,15.2,0.9,96.5,97.2,95.5,0.22984,0.26147, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0656,CCN(CC)C=1C=CC=C(O)C1,Z2856434814,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.71,0.017,34.3,0.7,95.8,98.4,94.9,0.22009,0.25043, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0657,COC=1C=C(NC(=O)C)C(OC)=CC1C1,Z26968795,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.73,0.027,25.1,0.9,96.0,98.4,95.1,0.22949,0.26344, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0658,COC=1C=CC=C2NC(=O)CCCC12,Z1507502062,OK: Mounted Clear,success,P 1,49 59
80 79 81 75,1.71,0.022,31.0,0.8,96.1,98.5,94.9,0.22125,0.25245, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0659,CCNC=1C=CC(C#N)=CN1,Z219104216,OK: Mounted Clear,success,P 1,49 59 79 79
81 75,1.63,0.038,26.1,1.1,96.2,96.3,94.7,0.23463,0.26577, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0660,CC(=O)NC=1C=CC=CC1OCC=2C=CC=CC2,Z26365442,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.49,0.029,19.7,0.4,93.5,91.2,91.0,0.23066,0.25908, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0661,CC1CN(CCO1)C(=O)C=2C=NC=CN2,Z212851096,OK: Crystalline,success,P 1,49 59
80 79 81 75,1.69,0.081,17.5,1.0,96.7,97.9,95.0,0.22832,0.25878, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0662,CS(=O)(=O)NC=1C=CC(CN)=CC1,Z426041412,OK: Crystalline,success,P 1,48 59 80
79 82 75,1.58,0.053,17.2,1.2,96.1,98.5,93.7,0.21459,0.24130, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0663,CNC1CCCN(C1=O)C=2C=CC=CC2,Z1212984951,OK: Bad Dispense,success,P 1,49 59
80 79 81 75,1.54,0.064,14.9,1.2,95.7,96.5,93.5,0.22776,0.25315, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0664,OC1CN(C1)C(C=2C=CC=CC2)C=3C=CC=CC3,Z1741964527,OK: Mounted Clear,success,P
1,49 59 79 79 81 75,1.71,0.024,23.3,0.5,94.6,95.4,94.9,0.22513,0.25815, None, None, P 1,1
- Analysis Pending, None

NUDT5A-x0665,CC(=O)C=1C=CC=C(NC(=O)N2CCOCC2)C1,Z274555794,OK: Mounted Clear,success,P
1,49 59 80 79 81 75,2.21,0.077,9.9,3.4,97.0,98.3,95.5,0.23251,0.27302, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0666,OC(=O)CCN1CCCC1,Z53115945,OK: Mounted Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0667,OCCN1CCOCC1,Z2856434843,OK: Mounted Clear,success,P 1,49 59 80 79 81
75,1.58,0.061,16.2,1.0,96.2,98.3,94.3,0.22887,0.25523, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0668,CN(C)CC=1C=CC(C#N)=CC1,Z2856434815,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.50,0.050,13.5,0.6,94.3,93.2,91.8,0.23336,0.25961, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0669,CNC1CCCC1S(=O)(=O)C,Z1259161657,OK: Mounted Clear,success,P 1,49 60 79 79
81 75,1.47,0.021,27.5,0.4,86.6,93.4,73.1,0.24633,0.28092, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0670,CC(=O)N1C[C@H](O)C[C@@H]1C(=O)O,Z1824511473,OK: Crystalline,success,P 1,47
59 80 80 83 78,1.77,0.030,18.7,0.7,93.0,93.0,94.4,0.29032,0.32422, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0671,C1CC1C2=NOC(=N2)C3CCNC3,Z2177153697,OK: Mounted Clear,success,P 1,49 60 79
79 80 75,1.62,0.027,27.1,1.1,95.8,95.1,93.5,0.26661,0.30935, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0672,COC=1C=CC=2SC(N)=NC2C1,Z1954800564,OK: Mounted Clear,success,P 1,49 59 80
79 81 75,1.61,0.042,17.8,1.1,95.8,97.3,93.5,0.22460,0.25333, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0673,CN1C=C(OC=2N=CN=CC2C1)C=N1,Z1918536193,OK: Mounted Clear,success,P 1,48 59
80 79 82 76,1.66,0.025,22.3,0.5,87.7,92.1,94.8,0.22838,0.26438,0.21860,0.25494, P 1,6 -
Deposited, 5QK7

NUDT5A-x0674,CN(CCC#N)S(=O)(=O)C=1C=CC(C)=CC1,Z45515569,OK: Precipitated,success,P 1,48
59 80 79 81 75,1.79,0.016,32.1,0.8,90.9,94.6,88.7,0.21778,0.25263, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0675,CCCC(=O)NC=1N=NN(CC)N1,Z57475877,OK: Bad Dispense,success,P 1,48 59 80 79
81 75,1.54,0.014,34.3,0.5,93.7,93.1,94.0,0.22507,0.25457, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0676,CC(=O)NCCC=1C=CC=CC1C,Z52314092,OK: Crystalline,success,P 1,49 59 80 79 81
75,1.80,0.025,21.4,0.7,87.2,91.8,94.1,0.24850,0.28925, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0677,CC(C)C(N)C1=NC(C)=NO1,Z1267773566,OK: Mounted Clear,success,P 1,49 59 79
79 81 75,1.77,0.040,17.2,0.9,94.4,93.3,94.2,0.23554,0.26586, None, None, P 1,1 - Analysis
Pending, None

NUDT5A-x0678,CCC1=NC=C(CNC)S1,Z1267773633,OK: Mounted Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0679,CC1CN(CCC1N)S(=O)(=O)C,Z1346370629,OK: Mounted Clear,Failed -
unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis
Pending, None

NUDT5A-x0680,OC(=O)CN1CCC(CC1)C=2C=CC=CC2,Z287148438,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.50,0.029,21.6,0.4,94.6,94.9,92.9,0.23481,0.26082, None, None, P 1,1 -
Analysis Pending, None

NUDT5A-x0681,CCNCC1=CN(C)N=N1,Z1271660837,OK: Mounted Clear,success,P 1,49 59 80 79 81
75,1.71,0.016,41.3,1.1,95.4,97.8,94.2,0.23159,0.26170,0.22690,0.25997, P 1,6 -
Deposited, 5QK8

NUDT5A-x0682,CCN(CCO)C=1C=CC(N)=CC1,Z752989138,OK: Precipitated,success,P 1,49 59 80 79 81 75,1.64,0.030,20.3,1.1,96.3,98.3,94.4,0.22656,0.25312, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0683,NC(=O)C=1C=NC(=NC1)C(F)(F)F,Z1745658474,OK: Crystalline,Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0684,NC(=O)C1CCC(F)(F)CC1,Z1526748660,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0685,COC=1C=CC=2C=NNC(=O)C2C1OC,Z102895082,OK: Precipitated,success,P 1,49 59 80 79 81 75,1.56,0.022,29.9,0.7,91.5,94.8,94.2,0.23017,0.26285,0.21635,0.25113,P 1,6 - Deposited,5QK9

NUDT5A-x0686,CC(=O)NC=1C=CC=C(C(=O)O)C1C,Z364368134,OK: Crystalline,success,P 1,47 59 80 80 83 77,1.53,0.017,31.6,0.5,93.0,92.6,93.6,0.23773,0.26887, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0687,CNC(=O)C=1C=CC(=CC1)S(=O)(=O)N,Z165170770,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, , , None, None, None, 1 - Analysis Pending, None

NUDT5A-x0688,NC(=O)C=1C=NN(CCO)C1,Z1562205518,OK: Crystalline,success,P 1,49 59 79 79 81 75,1.66,0.036,22.5,1.1,96.4,98.6,94.5,0.23018,0.25841, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0689,CC=1C=C(F)C=CC1CS(=O)(=O)N,Z1849009686,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.60,0.023,32.6,1.0,95.7,97.1,93.4,0.22620,0.25161,0.22627,0.25359,P 1,3 - In Refinement, None

NUDT5A-x0690,CNS(=O)(=O)C=1C=CC=C(C)C1F,Z1639162606,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.76,0.028,21.0,0.7,93.6,93.3,95.2,0.22959,0.26492, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0691,NC=1C=C(C=CC1N2CCCCC2)C(F)(F)F,Z56792776,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.47,0.022,24.8,0.6,92.4,89.3,87.7,0.22537,0.24778, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0692,CN1C=C(C(=O)N)C(=N1)C2CCCNC2,Z2377835233,OK: Mounted Clear,success,P 1,49 60 79 79 81 75,1.55,0.017,31.4,0.5,92.9,91.3,94.3,0.24738,0.28278,0.24754,0.28630,P 1,6 - Deposited,5QKA

NUDT5A-x0693,CC1=CN=C(S1)N2CCNCC2,Z1741975423,OK: Crystalline,success,P 1,49 59 79 79 81 75,1.46,0.036,17.7,0.5,93.1,94.0,86.3,0.23567,0.26511,0.23588,0.26615,P 1,3 - In Refinement, None

NUDT5A-x0694,CC=1C=CC(CS(=O)(=O)N)=CC1F,Z1703168683,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.61,0.056,13.4,1.1,96.1,98.5,93.9,0.21927,0.24598, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0695,CCCN1N=NN=C1NC(=O)C2=CC=CO2,Z57446103,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.64,0.059,14.6,1.1,96.6,98.1,95.0,0.22872,0.25645, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0696,CC(=O)NC=1C=CC(OC(=O)N2CCCC2)=CC1,Z274555566,OK: Bad Dispense,success,P 1,49 59 79 79 81 75,1.77,0.026,20.1,0.7,94.7,94.1,95.0,0.23079,0.26611, None, None, P 1,1 - Analysis Pending, None

NUDT5A-x0697,CNS(=O)(=O)CC=1C=C(C)ON1,Z763030030,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.59,0.071,21.8,1.1,96.4,98.7,94.8,0.23351,0.25936,0.23397,0.26097,P 1,3 - In Refinement, None

NUDT5A-x0698,CC1=CC(=NO1)C2CCCN2S(=O)(=O)C,Z319891284,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.90,0.017,24.8,0.6,77.3,95.1,57.7,0.22161,0.27020,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0699,CC1=NC(CN2C=CC(C)=CC2=O)=CS1,Z1134990241,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.49,0.018,32.2,0.5,93.8,94.0,91.3,0.22418,0.25052,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0700,CN(C1CCCCC1)S(=O)(=O)C,Z216450634,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.99,0.045,9.5,1.3,97.0,97.6,95.5,0.24522,0.28730,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0701,CC1=NN(C)C(C)=C1NC(=O)CC#N,Z1688504114,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0702,CC=1C=CC=C(C1)C(=O)N2CCC(CC2)C(=O)N,Z32400357,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.63,0.052,11.6,0.8,94.9,93.5,95.0,0.23287,0.26444,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0703,CN(C(=O)C)C=1C=CC=NC1,Z1203252645,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.72,0.025,30.1,0.7,96.1,98.3,95.3,0.22412,0.25725,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0704,COCC(=O)NC=1C=CC=CC1,Z31504642,OK: Mounted Clear,success,P 1,49 60 79 79 81 75,1.61,0.047,13.2,0.5,95.1,95.2,94.5,0.24974,0.28508,0.24748,0.28650,P 1,0 - All Datasets, None

NUDT5A-x0705,COCC(=O)NC1=NC(=CS1)C=2C=CC=CC2,Z62645406,OK: Precipitated,success,P 1,49 59 79 79 81 75,1.59,0.072,16.8,1.1,96.3,98.4,94.5,0.23749,0.27037,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0706,O=C(N1CCOCC1)C2=CSN=N2,Z741055844,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.63,0.044,16.8,1.1,96.0,98.2,94.0,0.22876,0.25809,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0707,CCNC1CCN(CC1)C=2C=CN=CC2,Z2065616520,OK: Mounted Clear,Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

NUDT5A-x0708,CN1C=C(C(=O)O)C(=N1)C=2C=CN=CC2,Z815264062,OK: Mounted Clear,success,P 1,48 59 80 79 82 76,1.60,0.046,18.2,1.1,95.7,98.3,94.3,0.22127,0.24488,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0709,COC=1C=CC=NC1C#N,Z1955122823,OK: Mounted Clear,success,P 1,48 59 79 79 82 76,1.49,0.042,15.1,0.4,85.2,92.7,91.3,0.22582,0.25799,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0710,CN(C)C(=O)C1(CC1)C(=O)O,Z1874937335,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.63,0.051,8.1,0.6,87.5,93.3,94.4,0.21952,0.24989,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0711,CC(=O)NCC1=NC=CN1,Z1203191681,OK: Mounted Clear,success,P 1,49 59 79 79 81 75,1.67,0.030,21.8,0.8,93.2,94.1,93.7,0.23635,0.27194,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0712,CN(C)CCN1C(=O)C=2C=CC=CC2C1=O,Z2856434895,OK: Mounted Clear,success,P 1,49 59 80 79 81 75,1.45,0.081,20.7,1.2,94.2,98.5,82.4,0.23461,0.25966,0.23341,0.26048,P 1,3 - In Refinement, None

NUDT5A-x0713,CC(O)C(=O)NCC=1C=CC=CN1,Z1551688335,OK: Mounted Clear,success,P 1,46 58 79 80 84 78,1.70,0.018,31.9,0.5,92.5,91.0,94.8,0.31231,0.35944,None,None,P 1,1 - Analysis Pending, None

NUDT5A-x0714,CCOC=1N=CC=CC1C(=O)N,Z272156568,OK: Mounted Clear,success,P 1,47 59 80 80
83 77,1.70,0.037,20.7,1.1,96.4,98.2,95.5,0.23100,0.26206,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0715,CN(C)CC1=CC=C(O)C(=O)O,Z359352902,OK: Crystalline,Failed -
unknown,None,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0716,CNC=1N=CC=NC1C#N,Z1896597864,OK: Crystalline,success,P 1,48 59 79 79 82
76,1.63,0.061,18.4,1.1,96.5,98.5,94.8,0.21956,0.24763,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0717,CCC(=O)NCC1=NN=C2CCCCN12,Z438067480,OK: Mounted Clear,success,P 1,48 59 80
79 82 76,1.62,0.015,36.8,0.8,94.1,97.0,90.2,0.22527,0.24973,None,None,P 1,1 - Analysis
Pending,None

NUDT5A-x0718,CC(=O)NCC1(COCC1)C=2C=CC=CC2,Z384468096,OK: Mounted Clear,success,P 1,49
59 79 79 81 75,1.45,0.059,15.4,0.3,93.2,94.2,84.7,0.23409,0.26179,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0719,CCC=1C=CC(=CC1)C=2N=C(N)SC2C,Z48847639,OK: Bad Dispense,success,P 1,48 59
79 80 82 76,1.58,0.063,17.3,1.1,96.1,97.1,94.3,0.22788,0.24710,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0720,NNC(=O)C=1C=CC(OCC=2C=CC=CC2)=CC1,Z58982727,OK: Precipitated,success,P
1,48 59 79 79 81 75,1.57,0.032,23.7,1.5,95.6,94.7,93.5,0.22497,0.25152,None,None,P 1,1
- Analysis Pending,None

NUDT5A-x0721,COC=1C=CC(=CC1)C(N)C=2C=CC=CC2,Z2574937229,OK: Mounted Clear,Failed -
unknown,None,None,None,None,None,None,None,None,None,,None,None,None,1 - Analysis
Pending,None

NUDT5A-x0722,CN(C)C=1N=CN=C2SC(C)=C(C)C12,Z31222641,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.56,0.042,23.4,0.3,94.3,94.3,93.6,0.23114,0.26442,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0723,OC=1N=CC(NC2CCCCC2)=C(O)N1,Z57283017,OK: Mounted Clear,success,P 1,49 59
79 79 81 75,1.75,0.099,15.1,0.9,96.1,96.4,94.6,0.25440,0.29469,None,None,P 1,1 -
Analysis Pending,None

NUDT5A-x0724,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Crystalline:No
comment,success,P 1,48 59 79 79 82
76,2.19,0.020,20.3,1.3,97.0,98.5,95.8,0.22814,0.26847,,,P 1,1 - Analysis Pending,

NUDT5A-x0725,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
76,1.84,0.025,20.0,1.2,95.5,19.8,95.3,0.23221,0.26321,,,P 1,1 - Analysis Pending,

NUDT5A-x0726,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,49 59 79 79 81 75,2.05,0.091,8.0,1.2,97.1,97.4,95.3,0.23312,0.27134,,,P 1,1 -
Analysis Pending,

NUDT5A-x0727,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P
1,49 59 79 79 81 75,1.90,0.074,11.5,1.1,96.5,95.9,95.4,0.23357,0.26379,,,P 1,1 -
Analysis Pending,

NUDT5A-x0728,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P
1,48 59 80 79 82 76,1.90,0.012,37.6,0.9,95.7,98.3,94.1,0.23117,0.26179,,,P 1,1 -
Analysis Pending,

NUDT5A-x0729,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P
1,49 59 79 79 81 76,1.80,0.010,39.3,1.1,96.0,77.8,94.9,0.22744,0.25483,,,P 1,1 -
Analysis Pending,

NUDT5A-x0730,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P 1,48 59 79 79 81 76,1.96,0.018,28.6,1.4,97.0,95.9,95.9,0.21546,0.24695,,,P 1,1 - Analysis Pending,

NUDT5A-x0731,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,48 59 79 80 82 76,2.09,0.014,32.7,0.9,96.2,98.8,95.0,0.23913,0.28597,,,P 1,1 - Analysis Pending,

NUDT5A-x0732,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,49 59 80 79 81 75,2.16,0.039,10.5,1.0,97.0,99.0,95.9,0.23959,0.27964,,,P 1,1 - Analysis Pending,

NUDT5A-x0733,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P 1,48 59 79 79 82 76,2.05,0.019,30.1,2.0,95.7,98.7,94.5,0.23348,0.26945,,,P 1,1 - Analysis Pending,

NUDT5A-x0734,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,48 59 79 79 82 76,1.88,0.010,70.6,1.1,96.0,98.2,94.8,0.22506,0.25302,,,P 1,1 - Analysis Pending,

NUDT5A-x0735,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,49 59 79 79 81 75,1.81,0.028,36.4,1.2,96.8,97.8,95.8,0.22753,0.25630,,,P 1,1 - Analysis Pending,

NUDT5A-x0736,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,48 59 80 79 82 76,2.38,0.010,21.7,1.0,95.3,97.7,95.2,0.24206,0.29263,,,P 1,1 - Analysis Pending,

NUDT5A-x0737,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,49 59 80 79 81 75,1.84,0.018,22.4,1.2,95.0,13.2,95.3,0.23661,0.27353,,,P 1,1 - Analysis Pending,

NUDT5A-x0738,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,49 60 80 73 75 75,2.14,0.094,1.6,0.8,96.7,97.2,96.0,0.67134,0.68142,,,P 1,1 - Analysis Pending,

NUDT5A-x0739,O=C (NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Normal,success,P 1,49 59 80 79 81 75,2.12,0.032,19.5,1.0,97.1,99.5,96.2,0.23732,0.27400,,,P 1,1 - Analysis Pending,

NUDT5A-x0740,CC1CCOC1C(=O)NC2=CN=NS2,Z1827602749,OK: No comment:Normal,success,P 1,48 59 79 80 82 77,1.89,0.035,27.4,1.2,96.6,99.1,95.6,0.22200,0.25082,,,P 1,1 - Analysis Pending,

NUDT5A-x0741,COC(=O)[C@@H]1C[C@@H](O)CN1C(=O)C2=CC=CO2,Z1614545742,OK: No comment:Cracked,success,P 1,48 59 79 80 81 76,1.98,0.037,15.7,1.2,96.8,98.9,95.1,0.23066,0.26420,,,P 1,1 - Analysis Pending,

NUDT5A-x0742,O=C(C1CC1)N2CCN(CC)C(=O)C3=CC=CO3,Z32327641,OK: No comment:Cracked,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT5A-x0743,CN1CCN(CC)C(=O)C=2C=CC(F)=C(F)C2,Z2856434829,OK: Bad Dispense:No comment,success,P 1,48 59 79 80 82 76,1.79,0.020,28.7,1.3,96.2,97.7,94.9,0.21882,0.24513,,,P 1,1 - Analysis Pending,

NUDT5A-x0744,CC1CN(C(C)CO1)C(=O)C=2C=NSN2,Z768399682,OK: No comment:Cracked,success,P 1,49 59 78 79 81 75,1.87,0.012,30.3,1.2,96.1,98.8,95.2,0.25971,0.29910,,,P 1,1 - Analysis Pending,

NUDT5A-x0745,CC1=NC(C(=O)N2CCCC2)=C(C)S1,Z1497321453,OK: Bad Dispense:No comment,success,P 1,48 59 79 80 81 76,1.96,0.093,14.2,1.0,96.3,93.3,95.0,0.28421,0.32832,,,P 1,1 - Analysis Pending,

NUDT5A-x0746,CN(CC1CCOC1)C=2N=CN=CC2C1,Z1787627869,OK: No comment:Normal,success,P 1,47
59 79 80 82 76,1.65,0.035,30.1,1.2,96.4,97.1,95.3,0.22227,0.24872,,,P 1,1 - Analysis
Pending,

NUDT5A-x0747,CCNC(=O)C1=CN=N1,Z755044716,OK: No comment:Cracked,success,P 1,48 59 79
80 82 76,1.77,0.016,26.8,1.0,96.4,97.2,95.3,0.22548,0.25637,,,P 1,1 - Analysis Pending,

NUDT5A-x0748,CC=1C=C(ON1)C(=O)NC=2C=CN(C)N2,Z240297434,OK: No comment:Normal,success,P
1,48 59 79 80 81 76,1.76,0.040,27.8,1.1,96.6,97.7,95.7,0.22571,0.25156,,,P 1,1 -
Analysis Pending,

NUDT5A-x0749,CCN1C=C(CNC(=O)C=2C=CC=NC2)C=N1,Z275181224,OK: No
comment:Cracked,success,P 1,48 59 79 80 82
76,1.88,0.060,25.2,1.2,96.7,97.6,95.9,0.22486,0.25802,,,P 1,1 - Analysis Pending,

NUDT5A-x0750,CCCC1=NN=C(NC(=O)C=2C=CC=CN2)S1,Z52425517,OK: No comment:Normal,success,P
1,48 59 79 80 82 76,1.63,0.025,29.5,1.0,95.9,94.7,93.2,0.22306,0.24564,,,P 1,1 -
Analysis Pending,

NUDT5A-x0751,COC(=O)CNC(=O)C=1C=C(C)ON1,Z375990520,OK: Precipitated:No
comment,success,P 1,48 59 79 80 81
76,1.73,0.013,50.6,1.0,96.3,98.1,95.3,0.22123,0.24695,,,P 1,1 - Analysis Pending,

NUDT5A-x0752,CC1=NN(CC=2C(C)=NOC2C)C(=O)S1,Z1899842917,OK: Precipitated:No
comment,success,P 1,51 61 83 79 81
76,3.04,0.053,6.6,0.6,97.3,97.6,97.3,0.30641,0.36368,,,P 1,1 - Analysis Pending,

NUDT5A-x0753,COC(=O)C=1C=CC=C(NS(=O)(=O)C)C1,Z24758179,OK: No comment:Normal,success,P
1,48 59 79 80 82 76,1.80,0.026,29.4,1.2,96.4,97.1,95.3,0.21770,0.25002,,,P 1,1 -
Analysis Pending,

NUDT5A-x0754,C1CN(C1)C=2N=CN=C3N=CNC23,Z373221060,OK: No comment:Normal,success,P 1,49
60 80 79 82 76,2.10,0.064,7.2,1.1,96.3,98.5,94.9,0.23165,0.26665,,,P 1,1 - Analysis
Pending,

NUDT5A-x0755,CC=1C=CC=C(NC=2N=CN=C3N(C)N=CC23)C1,Z56983806,OK: No
comment:Normal,success,P 1,48 59 79 80 82
77,1.85,0.024,23.3,1.1,95.7,98.9,95.0,0.21995,0.24870,,,P 1,1 - Analysis Pending,

NUDT5A-x0756,CC(C)N(C)C=1N=CN=C2N(C)N=CC12,Z328695024,OK: Bad Dispense:No
comment,success,P 1,48 59 79 80 82
77,1.89,0.039,22.4,1.4,96.0,97.5,92.2,0.22919,0.26071,,,P 1,1 - Analysis Pending,

NUDT5A-x0757,CC1OCCN(C1C)C2=NC(C)=NS2,Z1439422127,OK: Bad Dispense:No comment,success,P
1,48 59 79 80 82 76,1.74,0.043,23.9,0.9,96.2,97.1,95.8,0.22585,0.25543,,,P 1,1 -
Analysis Pending,

NUDT5A-x0758,CC(C)C(=O)NC=1N=NN(C)N1,Z57292369,OK: No comment:Normal,success,P 1,48 59
79 80 82 76,2.28,0.039,23.8,5.4,96.4,92.6,94.7,0.20729,0.25008,,,P 1,1 - Analysis
Pending,

NUDT5A-x0759,CC1=NSC(=N1)N2CCCNCC2,Z1578665941,OK: Precipitated:No comment,success,P
1,48 59 79 80 82 76,1.76,0.030,29.6,1.0,96.4,96.9,95.7,0.22304,0.25469,,,P 1,1 -
Analysis Pending,

NUDT5A-x0760,CCN(CC)C1=CC(C)=NC2=NC=NN12,Z56791867,OK: Bad Dispense:No
comment,success,P 1,48 59 79 80 82
76,1.65,0.016,45.0,1.0,95.9,97.5,94.0,0.22789,0.25855,,,P 1,1 - Analysis Pending,

NUDT5A-x0761,CC(=O)N1CCCC(C1)C(=O)N,Z220816104,OK: No comment:Normal,success,P 1,48 59
79 80 81 76,2.06,0.035,17.0,1.3,96.4,98.5,95.1,0.22368,0.26139,,,P 1,1 - Analysis
Pending,

NUDT5A-x0762, COC(=O)NC=1SC(C)=NC1C=2C=CC=CC2, Z979145504, OK: No comment:Normal, success, P 1,49 59 79 80 81 76,1.98,0.028,19.8,1.0,96.6,99.0,94.6,0.23134,0.26347,,,P 1,1 - Analysis Pending,

NUDT5A-x0763, CNC(=O)C1=CN=C(C)S1, Z969560582, OK: No comment:Normal, success, P 1,48 59 79 79 81 76,1.67,0.016,36.6,1.0,96.0,96.6,94.3,0.22703,0.25309,,,P 1,1 - Analysis Pending,

NUDT5A-x0764, CC(C)C=1N=CC(C1)=C(N1)C(=O)N, Z906021418, OK: No comment:Normal, success, P 1,48 59 80 79 81 76,2.06,0.052,16.2,1.0,96.8,98.2,95.8,0.26614,0.30504,,,P 1,1 - Analysis Pending,

NUDT5A-x0765, CNC=1N=CC=C(OC)N1, Z281802060, OK: Bad Dispense:No comment, success, P 1,48 59 79 80 81 76,1.92,0.028,23.5,1.1,96.2,98.9,94.6,0.23272,0.26224,,,P 1,1 - Analysis Pending,

NUDT5A-x0766, NC(=O)N1CCN(CC1)C(=O)C2=CC=CO2, Z198194396, OK: No comment:No comment, success, P 1,48 59 79 80 82 76,1.63,0.018,43.1,1.0,95.7,97.0,93.4,0.22738,0.25154,,,P 1,1 - Analysis Pending,

NUDT5A-x0767, [O-]C(=O)C=1C=CC=CC1OC(F)(F)F, Z2856434778, OK: No comment:Cracked, success, P 1,48 59 79 80 82 76,1.95,0.011,45.5,1.2,95.9,98.7,94.3,0.22829,0.26041,,,P 1,1 - Analysis Pending,

NUDT5A-x0768, CN(C)S(=O)(=O)C=1C(C)=NNC1C, Z94597856, OK: No comment:No comment, success, P 1,48 59 78 80 81 76,1.77,0.009,65.8,1.1,95.9,98.5,95.1,0.24150,0.27385,,,P 1,1 - Analysis Pending,

NUDT5A-x0769, CC(N)C=1C=CC(=CC1)C=2C=NC=NC2, Z1696822287, OK: No comment:No comment, success, P 1,48 59 79 80 82 76,1.79,0.013,40.2,1.1,95.8,98.1,94.6,0.22385,0.25322,,,P 1,1 - Analysis Pending,

NUDT5A-x0770, CC1=NNC(C)=C1C=2C=CC=CC2N, Z1270312110, OK: No comment:No comment, success, P 1,48 59 78 80 82 76,1.77,0.019,27.0,1.2,96.2,98.6,95.1,0.23276,0.26112,,,P 1,1 - Analysis Pending,

NUDT5A-x0771, C1=CSC(=N1)C2=NN=CN2, Z2027049478, OK: No comment:No comment, success, P 1,48 59 79 80 82 76,1.67,0.014,31.7,1.0,95.9,98.2,94.3,0.22187,0.24967,,,P 1,1 - Analysis Pending,

NUDT5A-x0772, O=C(NC=1C=CC=CC1)NC=2C=CC=NC2, Z44592329, OK: No comment:Normal, success, P 1,47 58 78 81 82 78,1.91,0.031,11.2,1.2,95.4,40.7,94.7,0.28660,0.32178,,,P 1,1 - Analysis Pending,

NUDT5A-x0773, O=C(NC=1C=CC=CC1)NC=2C=CC=NC2, Z44592329, OK: No comment:Normal, success, P 1,47 58 78 81 82 78,1.73,0.014,30.1,0.8,95.4,98.8,94.6,0.23523,0.26445,,,P 1,1 - Analysis Pending,

NUDT5A-x0774, O=C(NC=1C=CC=CC1)NC=2C=CC=NC2, Z44592329, OK: Bad Dispense:No comment, success, P 1,48 59 78 80 82 77,1.88,0.056,14.7,1.0,96.4,97.4,94.2,0.22144,0.25362,,,P 1,1 - Analysis Pending,

NUDT5A-x0775, O=C(NC=1C=CC=CC1)NC=2C=CC=NC2, Z44592329, OK: No comment:Cracked, success, P 1,48 59 79 80 81 76,1.71,0.029,28.8,1.1,96.5,98.0,95.5,0.24552,0.27414,,,P 1,1 - Analysis Pending,

NUDT5A-x0776, O=C(NC=1C=CC=CC1)NC=2C=CC=NC2, Z44592329, OK: No comment:No comment, success, P 1,48 59 79 80 82 77,1.75,0.030,24.3,1.1,96.7,97.7,95.8,0.22342,0.25002,,,P 1,1 - Analysis Pending,

NUDT5A-x0777, O=C(NC=1C=CC=CC1)NC=2C=CC=NC2, Z44592329, OK: No comment:Cracked, success, P 1,48 59 78 80 82 77,1.81,0.027,28.0,1.4,96.8,97.8,95.6,0.22377,0.25374,,,P 1,1 - Analysis Pending,

NUDT5A-x0778,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,48 59 78 80 82 76,2.10,0.081,5.9,1.1,97.2,99.1,96.4,0.30999,0.34230,,,P 1,1 -
Analysis Pending,

NUDT5A-x0779,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
77,2.09,0.017,15.4,1.1,95.8,98.4,94.3,0.23741,0.27546,,,P 1,1 - Analysis Pending,

NUDT5A-x0780,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,48 59 78 80 81 76,1.77,0.020,28.6,1.0,96.0,98.7,95.0,0.24773,0.27790,,,P 1,1 -
Analysis Pending,

NUDT5A-x0781,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 79 80 82
77,1.74,0.010,54.6,1.1,95.9,98.5,95.0,0.22139,0.25034,,,P 1,1 - Analysis Pending,

NUDT5A-x0782,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
76,1.63,0.016,44.0,1.0,95.8,96.7,93.5,0.22096,0.24844,,,P 1,1 - Analysis Pending,

NUDT5A-x0783,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,47 58 78 81 82
77,1.72,0.015,35.7,1.0,96.2,99.2,94.9,0.22010,0.24708,,,P 1,1 - Analysis Pending,

NUDT5A-x0784,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,48 59 79 80 81 76,2.11,0.034,13.1,1.0,96.4,98.3,95.7,0.24468,0.28550,,,P 1,1 -
Analysis Pending,

NUDT5A-x0785,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
77,1.76,0.044,17.0,1.0,96.4,97.6,95.8,0.22918,0.26293,,,P 1,1 - Analysis Pending,

NUDT5A-x0786,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 80 81
77,2.09,0.058,19.6,1.1,97.2,98.7,96.1,0.23659,0.26742,,,P 1,1 - Analysis Pending,

NUDT5A-x0787,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 80 82
77,1.95,0.018,28.2,1.1,96.7,98.2,96.0,0.22155,0.25220,,,P 1,1 - Analysis Pending,

NUDT5A-x0788,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
77,1.87,0.022,30.1,1.0,95.6,98.8,94.5,0.22258,0.25279,,,P 1,1 - Analysis Pending,

NUDT5A-x0789,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 79 80 82
77,1.79,0.021,20.8,1.1,95.9,99.0,94.6,0.22603,0.25512,,,P 1,1 - Analysis Pending,

NUDT5A-x0790,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
76,1.84,0.012,36.5,0.9,94.9,98.8,93.9,0.22983,0.25871,,,P 1,1 - Analysis Pending,

NUDT5A-x0791,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,47 58 78 81 82 78,2.23,0.076,6.3,1.6,97.3,96.9,95.6,0.23061,0.27135,,,P 1,1 -
Analysis Pending,

NUDT5A-x0792,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 79 80 82
76,2.00,0.033,16.6,1.3,96.5,98.1,95.1,0.22461,0.25770,,,P 1,1 - Analysis Pending,

NUDT5A-x0793,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 80 81
76,2.04,0.009,33.5,1.2,96.4,98.7,95.0,0.22120,0.25748,,,P 1,1 - Analysis Pending,

NUDT5A-x0794,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Precipitated:No
comment,success,P 1,48 59 79 80 82
76,1.82,0.018,30.8,1.1,96.5,95.9,95.3,0.22056,0.24840,,,P 1,1 - Analysis Pending,

NUDT5A-x0795,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
76,1.92,0.025,19.2,1.3,96.1,99.0,94.2,0.22328,0.25559,,,P 1,1 - Analysis Pending,

NUDT5A-x0796,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 81 82
77,1.60,0.034,27.5,1.2,96.1,94.8,94.4,0.21896,0.24494,,,P 1,1 - Analysis Pending,

NUDT5A-x0797,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 81 82
77,1.64,0.012,45.8,1.0,95.6,99.0,93.5,0.22250,0.24791,,,P 1,1 - Analysis Pending,

NUDT5A-x0798,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 81 82
77,1.60,0.018,28.4,0.9,95.6,82.8,93.3,0.22244,0.24723,,,P 1,1 - Analysis Pending,

NUDT5A-x0799,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,50 61 82 80 81 76,2.87,0.031,13.0,1.4,97.1,95.8,97.5,0.22943,0.30593,,,P 1,1 -
Analysis Pending,

NUDT5A-x0800,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:Cracked,success,P
1,48 59 79 80 82 76,1.77,0.014,30.8,0.9,96.1,98.3,95.3,0.21879,0.24820,,,P 1,1 -
Analysis Pending,

NUDT5A-x0801,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 78 80 82
76,1.77,0.010,56.6,1.1,95.6,98.7,94.6,0.22947,0.25780,,,P 1,1 - Analysis Pending,

NUDT5A-x0802,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: Bad Dispense:No
comment,success,P 1,48 59 78 80 82
77,1.76,0.038,27.9,1.2,96.5,97.5,95.8,0.22051,0.25032,,,P 1,1 - Analysis Pending,

NUDT5A-x0803,O=C(NC=1C=CC=CC1)NC=2C=CC=NC2,Z44592329,OK: No comment:No
comment,success,P 1,48 59 79 80 82
76,1.73,0.013,32.8,1.0,95.8,98.4,95.1,0.22126,0.25058,,,P 1,1 - Analysis Pending,

NUDT5A-x0804,CNC(=O)C1=CN=C(C)S1,Z969560582,OK: No comment:No comment,success,P 1,48 59
78 80 82 77,1.83,0.026,34.1,1.2,96.9,97.1,95.7,0.22184,0.25367,,,P 1,1 - Analysis
Pending,

NUDT5A-x0805,CC(C)C=1N=CC(C1)=C(N1)C(=O)N,Z906021418,OK: No comment:No
comment,success,P 1,47 58 78 81 82
78,1.71,0.040,14.9,0.8,96.2,93.1,95.5,0.23157,0.26137,,,P 1,1 - Analysis Pending,

NUDT5A-x0806,CNC=1N=CC=C(OC)N1,Z281802060,OK: No comment:No comment,success,P 1,48 59
79 80 82 77,2.08,0.021,23.6,1.2,96.2,98.5,94.6,0.24050,0.28379,,,P 1,1 - Analysis
Pending,

NUDT5A-x0807,NC(=O)N1CCN(CC1)C(=O)C2=CC=CO2,Z198194396,OK: No comment:Cracked,success,P
1,49 59 79 80 81 76,1.82,0.010,41.9,1.1,96.0,98.7,94.6,0.23435,0.26771,,,P 1,1 -
Analysis Pending,

NUDT5A-x0808,[O-]C(=O)C=1C=CC=CC1OC(F)(F)F,Z2856434778,OK: No comment:Jelly,success,P
1,48 58 78 81 82 77,1.62,0.014,37.2,1.0,95.4,97.8,93.0,0.22127,0.24996,,,P 1,1 -
Analysis Pending,

NUDT5A-x0809,CN(C)S(=O)(=O)C=1C(C)=NNC1C,Z94597856,OK: No comment:No comment,success,P
1,48 59 78 81 82 77,1.72,0.015,39.1,1.0,95.2,98.9,94.7,0.22049,0.24922,,,P 1,1 -
Analysis Pending,

NUDT5A-x0810,CC(N)C=1C=CC(=CC1)C=2C=NC=NC2,Z1696822287,OK: No comment:No comment,success,P 1,48 59 78 80 81 76,2.03,0.022,25.4,1.2,96.4,98.9,94.6,0.23921,0.27734,,,P 1,1 - Analysis Pending,

NUDT5A-x0811,CC1=NNC(C)=C1C=2C=CC=CC2N,Z1270312110,OK: No comment:No comment,success,P 1,48 58 78 81 82 77,1.61,0.015,40.3,0.9,95.6,96.8,93.1,0.22216,0.24712,,,P 1,1 - Analysis Pending,

NUDT5A-x0812,C1=CSC(=N1)C2=NN=CN2,Z2027049478,OK: No comment:No comment,success,P 1,47 58 78 81 82 78,1.60,0.014,47.3,0.9,95.8,97.8,93.9,0.22507,0.25349,,,P 1,1 - Analysis Pending,

NUDT5A-x0813,CNC=1N=CC=CN1,Z54628578,OK: No comment:No comment,success,P 1,48 59 78 80 82 77,1.66,0.030,32.0,1.1,96.3,96.7,95.3,0.22650,0.25013,,,P 1,1 - Analysis Pending,

NUDT5A-x0814,CC(=O)NC1=CC(C)=NN1,Z239136710,OK: No comment:No comment,success,P 1,48 59 78 80 81 76,2.05,0.042,10.4,1.6,96.8,97.8,95.6,0.24662,0.27928,,,P 1,1 - Analysis Pending,

NUDT5A-x0815,CCNC(=O)N1CCN(CC1)C(=O)C,Z44590919,OK: No comment:No comment,success,P 1,48 59 78 80 82 77,1.61,0.015,41.3,1.0,95.7,96.4,93.5,0.22619,0.25331,,,P 1,1 - Analysis Pending,

NUDT5A-x0816,CCNC=1C=CC(C)=NN1,Z1267773786,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.65,0.014,48.0,1.0,95.8,98.3,94.1,0.24554,0.26912,,,P 1,1 - Analysis Pending,

NUDT5A-x0817,CC=1C=CC(C(=O)N)=C(F)C1,Z1343633025,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.74,0.021,27.4,1.1,95.8,98.7,94.8,0.22213,0.24877,,,P 1,1 - Analysis Pending,

NUDT5A-x0818,CN1C=C(OC=2N=CN=CC2C1)C=N1,Z1918536193,OK: No comment:Jelly,success,P 1,48 59 78 80 82 77,1.82,0.025,16.4,1.1,96.6,98.6,95.4,0.22438,0.25640,,,P 1,1 - Analysis Pending,

NUDT5A-x0819,CCNCC1=CN(C)N=N1,Z1271660837,OK: No comment:No comment,success,P 1,48 58 78 81 82 78,1.56,0.016,44.9,1.0,95.4,98.3,93.3,0.22065,0.24281,,,P 1,1 - Analysis Pending,

NUDT5A-x0820,COC=1C=CC=2C=NNC(=O)C2C1OC,Z102895082,OK: No comment:No comment,success,P 1,48 58 78 81 82 78,1.55,0.015,41.0,1.1,95.5,98.5,93.3,0.22480,0.24646,,,P 1,1 - Analysis Pending,

NUDT5A-x0821,CN1C=C(C(=O)N)C(=N1)C2CCCNC2,Z2377835233,OK: No comment:No comment,success,P 1,48 58 78 81 82 77,1.62,0.013,47.1,1.1,95.7,98.9,93.1,0.22065,0.24391,,,P 1,1 - Analysis Pending,

NUDT5A-x0822,CC1CCOC1C(=O)NC2=CN=NS2,Z1827602749,OK: No comment:No comment,success,P 1,49 60 79 80 82 76,2.44,0.036,6.3,1.3,97.1,98.7,95.9,0.23837,0.29917,,,P 1,1 - Analysis Pending,

NUDT5A-x0823,COC(=O)[C@@H]1C[C@@H](O)CN1C(=O)C2=CC=CO2,Z1614545742,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.91,0.018,34.3,1.1,96.5,99.6,95.1,0.22388,0.25671,,,P 1,1 - Analysis Pending,

NUDT5A-x0824,O=C(C1CC1)N2CCN(CC2)C(=O)C3=CC=CO3,Z32327641,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.67,0.016,36.0,1.1,95.9,85.4,94.4,0.22906,0.25500,,,P 1,1 - Analysis Pending,

NUDT5A-x0825,CN1CCN(CC1)C(=O)C=2C=CC(F)=C(F)C2,Z2856434829,OK: No comment:No comment,Failed - low resolution,P 1,48 59 79 80 82 76,3.84,0.267,1.4,0.8,98.1,93.3,97.6,,,,,,

NUDT5A-x0826,CC1CN(C(C)CO1)C(=O)C=2C=NSN2,Z768399682,OK: No comment:Jelly,success,P 1,48 59 79 80 81 76,1.93,0.021,29.9,1.4,96.9,97.6,95.3,0.22564,0.26005,,,P 1,1 - Analysis Pending,

NUDT5A-x0827,CC1=NC(C(=O)N2CCCC2)=C(C)S1,Z1497321453,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.97,0.030,27.9,0.9,96.4,99.0,94.5,0.22838,0.26427,,,P 1,1 - Analysis Pending,

NUDT5A-x0828,CN(CC1CCOC1)C=2N=CN=CC2C1,Z1787627869,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.79,0.035,24.3,1.0,96.8,97.9,95.2,0.23393,0.26295,,,P 1,1 - Analysis Pending,

NUDT5A-x0829,CCNC(=O)C1=CNN=N1,Z755044716,OK: No comment:No comment,success,P 1,49 59 80 80 81 76,2.49,0.077,5.6,1.1,97.4,98.3,96.2,0.27275,0.32420,,,P 1,1 - Analysis Pending,

NUDT5A-x0830,CC=1C=C(ON1)C(=O)NC=2C=CN(C)N2,Z240297434,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.84,0.035,28.6,1.1,96.1,99.1,95.1,0.22502,0.25602,,,P 1,1 - Analysis Pending,

NUDT5A-x0831,CCN1C=C(CNC(=O)C=2C=CC=NC2)C=N1,Z275181224,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.96,0.011,46.4,1.1,96.4,98.7,94.7,0.22632,0.26057,,,P 1,1 - Analysis Pending,

NUDT5A-x0832,CCCC1=NN=C(NC(=O)C=2C=CC=CN2)S1,Z52425517,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.87,0.020,29.9,1.1,96.3,99.2,95.5,0.22883,0.26050,,,P 1,1 - Analysis Pending,

NUDT5A-x0833,COC(=O)CNC(=O)C=1C=C(C)ON1,Z375990520,OK: No comment:No comment,success,P 1,48 59 79 81 82 77,1.74,0.021,26.5,0.9,96.0,98.8,94.9,0.21860,0.24952,,,P 1,1 - Analysis Pending,

NUDT5A-x0834,CC1=NN(CC=2C(C)=NOC2C)C(=O)S1,Z1899842917,OK: No comment:No comment,success,P 1,47 58 78 81 82 78,1.65,0.026,17.3,1.1,95.9,98.9,93.9,0.23141,0.25711,,,P 1,1 - Analysis Pending,

NUDT5A-x0835,COC(=O)C=1C=CC=C(NS(=O)(=O)C)C1,Z24758179,OK: No comment:No comment,success,P 1,48 59 79 81 82 77,1.74,0.013,41.2,1.0,95.8,99.5,94.9,0.21938,0.24704,,,P 1,1 - Analysis Pending,

NUDT5A-x0836,C1CN(C1)C=2N=CN=C3N=CNC23,Z373221060,OK: No comment:Normal,success,P 1,48 59 79 80 82 76,1.83,0.011,27.7,1.1,96.3,98.8,95.1,0.21500,0.24703,,,P 1,1 - Analysis Pending,

NUDT5A-x0837,CC=1C=CC=C(NC=2N=CN=C3N(C)N=CC23)C1,Z56983806,OK: No comment:No comment,success,P 1,48 59 78 81 82 77,1.81,0.028,26.3,1.1,96.3,97.4,95.2,0.22159,0.25178,,,P 1,1 - Analysis Pending,

NUDT5A-x0838,CC(C)N(C)C=1N=CN=C2N(C)N=CC12,Z328695024,OK: No comment:Cracked,success,P 1,48 59 78 81 82 77,2.01,0.033,19.1,1.3,96.5,99.0,94.4,0.24356,0.28293,,,P 1,1 - Analysis Pending,

NUDT5A-x0839,CC1OCCN(C1C)C2=NC(C)=NS2,Z1439422127,OK: No comment:Cracked,success,P 1,48 59 79 80 82 76,1.92,0.017,39.5,1.1,96.0,98.6,94.2,0.22576,0.26011,,,P 1,1 - Analysis Pending,

NUDT5A-x0840,CC(C)C(=O)NC=1N=NN(C)N1,Z57292369,OK: No comment:Cracked,success,P 1,48 59 79 80 82 76,1.78,0.017,40.5,1.2,96.4,98.5,95.0,0.22336,0.25375,,,P 1,1 - Analysis Pending,

NUDT5A-x0841,CC1=NSC(=N1)N2CCCNCC2,Z1578665941,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.72,0.026,39.8,1.2,96.6,98.2,95.8,0.22280,0.24852,,,P 1,1 - Analysis Pending,

NUDT5A-x0842,CCN(CC)C1=CC(C)=NC2=NC=NN12,Z56791867,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.80,0.013,51.0,1.1,95.8,99.1,94.7,0.22712,0.25411,,,P 1,1 - Analysis Pending,

NUDT5A-x0843,CC(=O)N1CCCC(C1)C(=O)N,Z220816104,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.82,0.016,36.2,1.3,96.1,98.9,94.1,0.22875,0.25459,,,P 1,1 - Analysis Pending,

NUDT5A-x0844,COC(=O)NC=1SC(C)=NC1C=2C=CC=CC2,Z979145504,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.91,0.025,27.8,1.2,96.4,98.5,94.7,0.21988,0.25128,,,P 1,1 - Analysis Pending,

NUDT5A-x0845,CNC(=O)C1=CN=C(C)S1,Z969560582,OK: No comment:Cracked,success,P 1,48 59 79 80 82 76,1.73,0.015,48.7,1.1,96.1,97.2,95.0,0.22637,0.25328,,,P 1,1 - Analysis Pending,

NUDT5A-x0846,CC(C)C=1N=CC(C1)=C(N1)C(=O)N,Z906021418,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.79,0.022,25.7,1.2,96.5,95.5,95.3,0.22533,0.25356,,,P 1,1 - Analysis Pending,

NUDT5A-x0847,CNC=1N=CC=C(OC)N1,Z281802060,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.92,0.017,27.7,1.5,96.8,97.8,95.4,0.22626,0.25959,,,P 1,1 - Analysis Pending,

NUDT5A-x0848,NC(=O)N1CCN(CC1)C(=O)C2=CC=CO2,Z198194396,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.83,0.014,41.3,1.1,95.6,98.9,94.5,0.23641,0.26920,,,P 1,1 - Analysis Pending,

NUDT5A-x0849,[O-]C(=O)C=1C=CC=CC1OC(F)(F)F,Z2856434778,OK: No comment:No comment,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT5A-x0850,CN(C)S(=O)(=O)C=1C(C)=NNC1C,Z94597856,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.77,0.012,50.9,1.2,96.2,98.8,94.5,0.22267,0.25096,,,P 1,1 - Analysis Pending,

NUDT5A-x0851,CC(N)C=1C=CC(=CC1)C=2C=NC=NC2,Z1696822287,OK: No comment:No comment,success,P 1,48 59 78 80 82 77,1.92,0.015,32.2,1.0,96.6,98.7,95.3,0.21910,0.25382,,,P 1,1 - Analysis Pending,

NUDT5A-x0852,CC1=NNC(C)=C1C=2C=CC=CC2N,Z1270312110,OK: No comment:No comment,success,P 1,48 59 78 80 82 77,2.09,0.015,25.6,1.0,96.2,98.9,95.3,0.22627,0.26396,,,P 1,1 - Analysis Pending,

NUDT5A-x0853,C1=CSC(=N1)C2=NN=CN2,Z2027049478,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.71,0.026,30.1,1.0,96.7,98.3,95.8,0.22334,0.25039,,,P 1,1 - Analysis Pending,

NUDT5A-x0854,CNC=1N=CC=CN1,Z54628578,OK: No comment:No comment,success,P 1,48 59 79 80 82 76,1.81,0.011,61.9,1.1,95.9,98.8,94.5,0.22778,0.25694,,,P 1,1 - Analysis Pending,

NUDT5A-x0855,CC(=O)NC1=CC(C)=NN1,Z239136710,OK: No comment:No comment,success,P 1,48 59 79 80 82 77,1.78,0.028,23.7,1.4,96.7,98.1,95.9,0.21783,0.24529,,,P 1,1 - Analysis Pending,

NUDT5A-x0856,CCNC(=O)N1CCN(CC1)C(=O)C,Z44590919,OK: No comment:Cracked,success,P 1,48 59 78 80 82 77,1.71,0.025,28.3,0.9,96.6,97.7,95.7,0.22625,0.25330,,,P 1,1 - Analysis Pending,

NUDT5A-x0857,CCNC=1C=CC(C)=NN1,Z1267773786,OK: No comment:No comment,success,P 1,48 59 79 80 81 76,1.69,0.015,46.9,1.1,95.9,97.5,94.3,0.23118,0.25633,,,P 1,1 - Analysis Pending,

NUDT5A-x0858,CC=1C=CC(C(=O)N)=C(F)C1,Z1343633025,OK: No comment:No comment,success,P
1,48 59 79 80 82 76,1.80,0.013,42.8,1.2,96.1,98.9,94.6,0.22539,0.25596,,,P 1,1 -
Analysis Pending,

NUDT5A-x0859,CN1C=C(OC=2N=CN=CC2C1)C=N1,Z1918536193,OK: No comment:No comment,success,P
1,49 60 80 79 81 76,2.14,0.014,27.0,0.9,96.6,98.6,95.6,0.21414,0.25921,,,P 1,1 -
Analysis Pending,

NUDT5A-x0860,CCNCC1=CN(C)N=N1,Z1271660837,OK: No comment:No comment,success,P 1,48 59
79 80 81 76,1.70,0.016,44.7,1.0,96.2,97.7,95.2,0.22320,0.25050,,,P 1,1 - Analysis
Pending,

NUDT5A-x0861,COC=1C=CC=2C=NNC(=O)C2C1OC,Z102895082,OK: No comment:No comment,success,P
1,48 59 79 80 82 76,1.94,0.013,32.8,1.1,96.2,98.7,94.5,0.22126,0.25717,,,P 1,1 -
Analysis Pending,

NUDT5A-x0862,CN1C=C(C(=O)N)C(=N1)C2CCCNC2,Z2377835233,OK: No comment:No
comment,success,P 1,49 59 79 79 81
76,1.92,0.034,32.2,0.8,96.7,98.4,95.7,0.24424,0.28113,,,P 1,1 - Analysis Pending,

SGC Dataset – NUDT7A (csv format)

CrystalName,CompoundSMILES,CompoundCode,MountingResult,DataCollectionOutcome,DataProcessingSpaceGroup,DataProcessingUnitCell,DataProcessingResolutionHigh,DataProcessingRmergeLow,DataProcessingIsigLow,DataProcessingIsigHigh,DataProcessingCompletenessOverall,DataProcessingCompletenessLow,DataProcessingCompletenessHigh,DimpleRcryst,DimpleRfree,RefinementRcryst,RefinementRfree,RefinementSpaceGroup,RefinementOutcome,Deposition_PDB_ID

NUDT7A-x0091, None, None, None, success, P 3 2 1,126 126 41 90 90
120,2.08,0.025,56.2,1.4,99.1,96.8,97.5,0.19833,0.23044,0.19833,0.23044,P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x0092, None, None, None, success, P 3 2 1,126 126 41 90 90
120,1.93,0.069,23.4,1.7,98.7,97.8,93.6,0.21438,0.24036,0.21438,0.24036,P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x0093, None, None, None, success, P 3 2 1,125 125 41 90 90
120,2.71,0.057,25.9,1.5,97.9,99.1,99.9,0.21709,0.28345, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0094, None, None, None, success, P 3 2 1,126 126 41 90 90
120,2.08,0.033,44.4,0.1,99.3,96.8,92,0.19159,0.22091, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0095, None, None, None, success, P 3 2 1,126 126 41 90 90
120,2.28,0.015,114,1.8,99.9,95.8,99.4,0.17532,0.21088, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0096, None, None, None, success, P 3 2 1,126 126 41 90 90
120,2,0.026,58.7,1.1,94.4,96.1,100,, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0097, None, None, None, success, P 3 2 1,126 126 41 90 90
120,2.4,0.041,47.7,3.1,99.9,99.7,100,0.19947,0.24665, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0098, None, None, None, success, P 3 2 1,126 126 41 90 90
120,2.04,0.017,86.8,1,96.2,96.7,99.7,0.20615,0.24865, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0099, None, None, None, success, P 3 2 1,126 126 41 90 90
120,1.95,0.022,85.9,2.6,99.8,97.3,98.3,0.18486,0.21472, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0100, None, None, None, success, P 3 2 1,125 125 41 90 90
120,2.44,0.064,34.3,2.6,99.8,94.8,97.7,0.18148,0.22484, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0101, None, None, None, success, P 3 2 1,125 125 41 90 90
120,1.71,0.023,60.6,1.3,98.8,98.3,100,0.20269,0.22901, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0102, None, None, None, success, P 3 2 1,126 126 41 90 90
120,1.95,0.023,81.8,2.6,99.9,97.4,98.4,0.18752,0.21793, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0103, None, None, None, success, P 3 2 1,125 125 41 90 90
120,2.47,0.034,53,2.4,99.7,94.6,97.3,0.17342,0.21688, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0104, None, None, None, success, P 3 2 1,127 127 41 90 90
120,1.94,0.026,62.6,2.5,99.5,96.9,94.4,0.19281,0.22239, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0105, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.17, 0.05, 35.5, 1.3, 100, 99.5, 100, 0.22254, 0.26849, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0107, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.18, 0.02, 83.6, 2.2, 99.8, 96.4, 98.1, 0.17914, 0.21349, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0108, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.96, 0.03, 63.1, 2.7, 99.9, 97.3, 99.1, 0.17524, 0.20172, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0109, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.62, 0.034, 65.5, 2.4, 99.9, 98.5, 98.9, 0.1875, 0.21051, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0110, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.81, 0.033, 52.7, 1.2, 100, 99.4, 100, 0.1865, 0.21251, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0111, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.44, 0.087, 15.2, 1.8, 100, 99.2, 100, 0.2086, 0.24951, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0112, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2, 0.018, 91.2, 2.1, 99.7, 97.2, 96.8, 0.18395, 0.21527, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0113, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.02, 0.032, 62.5, 2.3, 99.9, 96.7, 99.5, 0.17736, 0.20476, None, None, None, 2 - PANDDA
 model, None

NUDT7A-x0114, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.88, 0.039, 57.2, 2.4, 99.8, 97, 98.2, 0.18078, 0.2108, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0115, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.29, 0.023, 75.4, 1.9, 99.8, 95.5, 98.6, 0.17929, 0.21995, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0116, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.95, 0.027, 67.7, 2.6, 99.9, 97.3, 99.4, 0.17673, 0.20656, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0118, COC(=O)Nc1nnc(s1)CC2CCCC2, FMOPL000243a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.8, 0.023, 65, 1.5, 97.7, 97.9, 100, 0.20985, 0.23892, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0119, COc1cc(ccc1N)Nc2ccccc2, FMOPL000626a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.77, 0.02, 87.9, 2.4, 99.8, 98, 97.6, 0.18353, 0.21179, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0120, CCc1ccc(cc1)NC(=O)c2cnccn2, FMOPL000244a, None, success, P 3 2 1, 124 124 41 90
 90 120, 2.88, 0.027, 39.3, 1.8, 99.7, 98.7, 99.6, 0.16231, 0.22544, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0121, CCc1c(c(on1)C)C(=O)Nc2cc(on2)C, FMOPL000245a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.84, 0.026, 66.1, 1.5, 98.4, 95.7, 100, 0.20285, 0.22548, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0122, C[C@@H](Cc1ccc(cc1)O)[NH+](C)C, FMOPL000138a, None, success, P 3 2 1, 125 125 41
 90 90 120, 1.7, 0.029, 73.1, 2.4, 99.8, 98, 98.1, 0.18825, 0.21264, 0.18881, 0.19166, P 3 2 1, 3 - In
 Refinement, None

NUDT7A-x0123, Cc1ccc(s1)C(=O)Nc2ccccc2OC, FMOPL000247a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.46, 0.026, 57.1, 1.4, 99.9, 90.8, 100, 0.17002, 0.2125, 0.17002, 0.21250, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0124, c1cc(scl)C[NH2+]Cc2ccncc2, FMOPL000139a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.01, 0.012, 137.7, 2.4, 99.9, 96, 99, 0.18628, 0.21775, 0.18628, 0.21775, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0125, CC(=O)c1cccc(c1)NC(=O)N2CCOCC2, FMOPL000248a, None, success, P 3 2 1, 125 125 41
 90 90 120, 1.98, 0.015, 115.3, 2.2, 99.9, 96.8, 98.7, 0.17594, 0.20235, 0.18092, 0.18379, P 3 2 1, 3
 - In Refinement, None

NUDT7A-x0126, c1cc(c2c(c1)c3c([nH]2)CCCC3)C#N, FMOPL000140a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.28, 0.035, 46.4, 1.1, 99.9, 89.8, 100, 0.17709, 0.22017, 0.17709, 0.22017, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0127, c1cc(ccc1N2CCN(CC2)C(=O)C3CC3)F, FMOPL000249a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.01, 0.02, 89.2, 2.2, 99.9, 97.1, 99.4, 0.1739, 0.20525, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0128, Cc1cccc1Cnc2nnnn2C, FMOPL000143a, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.54, 0.025, 65.5, 2.6, 99.8, 94.4, 98.4, 0.16427, 0.20763, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0129, C[C@H](C(=O)[O-])Oc1ccc(cc1)c2ccccc2, FMOPL000250a, None, success, P 3 2 1, 125
 125 41 90 90 120, 2.45, 0.021, 77.1, 2, 99.9, 94.8, 99.2, 0.17086, 0.21515, 0.17775, 0.22737, P 3 2
 1, 3 - In Refinement, None

NUDT7A-x0130, CCC(=O)Nc1ccc(cc1)S(=O)(=O)N, FMOPL000141a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.87, 0.06, 30.1, 1.5, 100, 99.8, 100, 0.23747, 0.26861, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0131, c1ccc2c(c1)[nH]c(n2)NC(=O)C3CCCC3, FMOPL000251a, None, success, P 3 2 1, 125
 125 41 90 90 120, 2.55, 0.023, 77.4, 2.1, 99.7, 94, 96.8, 0.16082, 0.20176, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0132, c1ccc(cc1)OCC(=O)N2CCNC(=O)C2, FMOPL000730a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.82, 0.02, 103.2, 2.3, 99.9, 97.9, 99.4, 0.19375, 0.22009, 0.20057, 0.23315, P 3 2 1, 3
 - In Refinement, None

NUDT7A-x0133, c1c(c(=O)[nH]c(=O)[nH]1)N2CCCC2, FMOPL000665a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.98, 0.036, 53, 2.6, 99.9, 97.2, 98.6, 0.17769, 0.21037, 0.17769, 0.21037, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0135, Cc1ccc(cc1)CC(=O)NC[C@H]2CCCO2, FMOPL000530a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.34, 0.029, 46, 1.7, 98.4, 99, 99.8, 0.21112, 0.26033, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0136, C1CCC(C1)C(=O)N2CCNC(=O)C2, FMOPL000699a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.7, 0.036, 66.1, 2.5, 99.8, 98, 98, 0.18981, 0.21619, 0.18981, 0.21619, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0137, C[NH+]1CCC[C@H](C1)OC(=O)c2ccco2, FMOPL000668a, None, success, P 3 2 1, 125 125
 41 90 90 120, 1.94, 0.034, 61.4, 1.4, 100, 99.6, 100, 0.20123, 0.23144, 0.20123, 0.23144, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0138, COC(=O)NCc1cc2cc(ccc2[nH]1)C1, FMOPL000405a, None, success, P 3 2 1, 125 125 41
 90 90 120, 1.99, 0.017, 85.3, 1.4, 99.8, 99.8, 100, 0.18688, 0.21871, 0.18688, 0.21871, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0139, CCn1c2ccccc2nc1NC(=O)C, FMOPL000521a, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.43, 0.062, 28.8, 1.3, 99.9, 98.6, 100, 0.17233, 0.20952, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0140, Cc1ccc(C[NH2+]CC(C)O)s1, FMOPL000693a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.91, 0.034, 62.5, 2.4, 99.9, 97.6, 99.4, 0.18422, 0.2159, 0.19182, 0.22359, P 3 2 1, 6 -
 Deposited, 5QGG

NUDT7A-x0141, COCC(=O)NCc1[nH]c2ccccc2n1, FMOPL000672a, None, success, P 3 2 1, 124 124 41 90
 90 120, 2.6, 0.029, 59.8, 2.4, 99.9, 93.7, 99.4, 0.1578, 0.19981, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0142, CCOC(=O)Nc1c(ccs1)C(=O)N, FMOPL000386a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.91, 0.023, 75.5, 2.1, 99.9, 97.2, 98.6, 0.18033, 0.20832, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0143, COc1ccc(cc1)CNC(=O)c2csnn2, FMOPL000527a, None, success, P 3 2 1, 125 125 41 90
 90 120, 1.95, 0.02, 88.6, 2.4, 99.8, 97.3, 97.5, 0.17845, 0.20956, 0.17845, 0.20956, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0144, c1ccc(cc1)CNC(=O)c2cccc(c2)F, FMOPL000727a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.45, 0.025, 78.1, 2, 99.7, 94.8, 96.2, 0.17116, 0.21338, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0145, Cc1cccc2c1nc(s2)NC(=O)OC, FMOPL000395a, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.14, 0.032, 58.2, 2.5, 99.9, 96.6, 98.5, 0.17665, 0.2081, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0146, c1cc(sc1)CCNC(=O)C2CCCC2, FMOPL000523a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.17, 0.021, 81.6, 2, 99.9, 96.4, 99.4, 0.18123, 0.21168, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0147, CCC(CC)C(=O)Nc1nccs1, FMOPL000695a, None, success, P 3 2 1, 124 124 41 90 90
 120, 2.91, 0.026, 57.8, 2.3, 99.4, 91.2, 93.8, 0.15257, 0.20248, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0148, CC1(C[C@H](CCO1)[NH2+]Cc2ccc(cc2)O)C, FMOPL000676a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.97, 0.029, 48.7, 1.5, 95.5, 97, 94.6, 0.23779, 0.27081, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0149, CCC(C(=O)Nc1ccon1)c1ccccc1, FMOPL000420a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.82, 0.031, 71.9, 2.8, 99.9, 97.6, 99.1, 0.18147, 0.21158, 0.19267, 0.21668, P 3 2 1, 6 -
 Deposited, 5QGH

NUDT7A-x0150, C[NH+]1CCN(CC1)C(=O)c2ccc3cc[nH]c3c2, FMOPL000532a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.75, 0.028, 65.2, 2, 99.8, 97.9, 97.7, 0.19051, 0.21654, 0.19051, 0.21654, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0151, Cc1cc(c(c(c1)C)NC(=O)COC)C, FMOPL000710a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.95, 0.026, 86.5, 3.4, 99.8, 97.1, 98.4, 0.18646, 0.21539, 0.19332, 0.22358, P 3 2 1, 6 -
 Deposited, 5QGI

NUDT7A-x0152, c1cc(oc1)C(=O)N2CCN(CC2)C(=O)N, FMOPL000670a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.44, 0.033, 52.4, 2.4, 99.7, 94.8, 96.9, 0.16875, 0.21094, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0153, CCc1ccc(s1)C(=O)NCc2cnn(c2)C, FMOPL000421a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.06, 0.018, 92.4, 2.7, 99.9, 96.9, 99.2, 0.17232, 0.20372, 0.17232, 0.20372, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0154, CC(C)NC(=O)c1ccc(cc1)NC(=O)NC, FMOPL000525a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.75, 0.029, 74, 2.4, 99.8, 98.1, 97.9, 0.18832, 0.21576, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0155, CCCC(=O)Nc1cccnc1Cl, FMOPL000696a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.98, 0.028, 66.8, 2.4, 99.9, 97.3, 98.9, 0.17907, 0.21091, 0.17907, 0.21091, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0156,C1CCC2(CC1)OC[C@@H](O2)C[NH+]3CCCC3,FMOPL000674a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.79, 0.027, 70.4, 1.9, 99.7, 97.9, 96.5, 0.18672, 0.21396, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0157,CCC(=O)Nc1nnc(s1)c2ccncc2,FMOPL000403a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.85, 0.036, 64.5, 2.6, 99.9, 97.4, 98.8, 0.18828, 0.22159, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0158,C1C[C@H](CC=C1)C[NH+]2CCC(CC2)C(=O)N,FMOPL000333a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.96, 0.06, 39.6, 1.5, 99.9, 99.6, 100, 0.18953, 0.22163, 0.18953, 0.22163, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0159,CCC(CC)C(=O)Nc1cccc1O,FMOPL000706a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.95, 0.024, 76.2, 2.6, 99.7, 97, 96.5, 0.18528, 0.21879, 0.18734, 0.21436, P 3 2 1, 6 -
 Deposited, 5QGJ

NUDT7A-x0160,CC(=O)Nc1ccc2c(c1)nsn2,FMOPL000664a, None, success, P 3 2 1, 124 124 41 90 90
 120, 3.23, 0.088, 10.2, 1.5, 99.9, 93.9, 100, 0.18179, 0.24681, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0161,c1cc(cc(c1)Cl)C(=O)Nc2ccon2,FMOPL000399a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.88, 0.052, 30.7, 1.7, 99.8, 98.1, 100, 0.15864, 0.2041, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0162,CCOc1ccc(cc1)C[NH+]2CCC(CC2)O,FMOPL000353a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.46, 0.038, 56.6, 2.3, 99.9, 94.8, 99.9, 0.16668, 0.20765, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0163,COc1cccc1OC(=O)C2CCCC2,FMOPL000721a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.8, 0.016, 111.5, 2.9, 99.9, 97.8, 99.4, 0.18179, 0.20828, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0166,CSc1nnc(s1)NC(=O)c2ccco2,FMOPL000708a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.94, 0.026, 64.5, 2.4, 99.7, 97.3, 97, 0.19614, 0.22176, 0.19614, 0.22176, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0168,C[C@@H](c1ccc(cc1)N2CCOCC2)[NH3+],FMOPL000390a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.02, 0.021, 86.2, 2.7, 100, 97.1, 99.8, 0.17765, 0.20907, 0.17765, 0.20907, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0170,CCCC(=O)Nc1nnc(s1)SC,FMOPL000697a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.87, 0.021, 70.9, 1.6, 99.7, 97.3, 96.1, 0.18604, 0.21846, 0.18604, 0.21846, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0171,C[NH+]1CCC[C@H](C1)OC(=O)c2cccc(c2)F,FMOPL000678a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.02, 0.016, 106.3, 2.3, 99.8, 96.7, 98.1, 0.17697, 0.20831, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0172,c1cc2c(cc1CNC(=O)[C@@H]3CCCC3)OCO2,FMOPL000436a, None, success, P 3 2 1, 125
 125 41 90 90 120, 2.17, 0.016, 91.1, 1.8, 99.5, 95.7, 94.3, 0.17402, 0.20966, 0.17948, 0.17977, P 3
 2 1, 3 - In Refinement, None

NUDT7A-x0175,CN(C)c1ccc(cc1)CNn2cnnc2,BDILV000151b, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.92, 0.02, 100.8, 2.8, 99.8, 97, 98.3, 0.18125, 0.21583, 0.18125, 0.21583, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0177,Cc1c(nc(=O)[nH]n1)Nc2ccc(cc2)N(C)C,FMOPL000371a, None, success, P 3 2 1, 124
 124 41 90 90 120, 2.83, 0.022, 77.6, 1.9, 99.7, 91.5, 96.6, 0.15296, 0.21558, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0178,CN(c1ccc(cc1)C(=O)N)S(=O)(=O)C,FMOPL000142a, None, success, P 3 2 1, 124 124 41
 90 90 120, 2.47, 0.067, 16.7, 1.1, 100, 99.5, 100, 0.21447, 0.27681, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0179, CC(C)Sc1nnc(s1)NC(=O)C, FMOPL000027a, None, success, P 3 2 1, 126 126 41 90 90
120, 1.75, 0.027, 75.6, 2.2, 99.6, 97.8, 94.5, 0.18869, 0.21503, 0.18869, 0.21503, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0181, C[NH+] (C)Cc1ccc(cc1)C#N, FMOPL000137a, None, success, P 3 2 1, 124 124 41 90 90
120, 3.4, 0.038, 25.5, 1.7, 88.3, 98.8, 66.8, 0.17001, 0.26116, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0182, CC(C) [NH+]1CCN(CC1) c2ccc(cc2)O, FMOPL000145a, None, success, P 3 2 1, 126 126 41
90 90 120, 1.8, 0.019, 101.9, 2.6, 99.9, 97.9, 98.9, 0.18449, 0.21241, 0.18449, 0.21241, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0184, COC(=O) c1cccc1NC(=O)N2CCCC2, FMOPL000253a, None, success, P 3 2 1, 123 123 41
90 90 120, 3.29, 0.025, 58.2, 1.8, 99.6, 86.7, 96.6, 0.14766, 0.22704, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0185, CC(C)C(=O)Nc1nnc(s1) [C@@H]2CCCO2, FMOPL000144a, None, success, P 3 2 1, 125 125
41 90 90 120, 1.91, 0.023, 83.1, 2.3, 99.8, 97.2, 98, 0.18317, 0.21065, 0.18317, 0.21065, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0186, c1cc2c(cc1c3cc[nH]n3)OCO2, FMOPL000029a, None, success, P 3 2 1, 124 124 41 90
90 120, 2.38, 0.027, 75.9, 2.3, 99.5, 94.9, 94.4, 0.17577, 0.20899, 0.17577, 0.20899, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0187, CN(CCc1ccccn1)C(=O) c2cccc2, FMOPL000254a, None, success, P 3 2 1, 124 124 41 90
90 120, 2.99, 0.042, 44.2, 1.3, 99.4, 89, 93.6, 0.1595, 0.24192, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0189, CCN(CC)S(=O) (=O) c1ccc(cc1)C, FMOMB000142b, None, success, P 3 2 1, 126 126 41 90
90 120, 1.8, 0.024, 60.5, 1.4, 99.1, 98, 100, 0.19843, 0.22488, 0.19843, 0.22488, P 3 2 1, 2 - PANDDA
model, None

NUDT7A-x0191, COc1ccc(cc1) [C@@H] (C(=O) [O-]) [NH3+], FMOPL000076a, None, success, P 3 2 1, 125
125 41 90 90 120, 2.36, 0.029, 48.7, 1.1, 99.5, 99.3, 99.9, 0.19905, 0.25311, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0192, CNC(=O)Nc1nc2ccc(cc2s1)OC, FMO3D000631b, None, success, P 3 2 1, 125 125 41 90
90 120, 2.31, 0.026, 64.1, 1.6, 99.4, 94.9, 93.5, 0.18645, 0.22693, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0193, c1ccc(cc1)CC2CCN(CC2)C(=O)CC#N, FMOPL000256a, None, success, P 3 2 1, 126 126 41
90 90 120, 1.87, 0.025, 59.2, 1.1, 98.6, 97.5, 99.9, 0.20802, 0.24005, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0195, COC(=O) c1ccc(cc1)NC(=O)C(F)(F)F, FMOPL000149a, None, success, P 3 2 1, 124 124
41 90 90 120, 2.97, 0.047, 40.3, 1.5, 99.5, 90.4, 95.3, 0.1629, 0.21421, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0196, c1ccc(cc1)CC[NH+]2CCC(CC2)O, FMOPL000030a, None, success, P 3 2 1, 126 126 41 90
90 120, 2.28, 0.019, 89.3, 0, 99.5, 95.6, 94.1, 0.18102, 0.21927, 0.18102, 0.21927, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0197, c1ccc(cc1) c2ccc(cc2)NC(=O)N, FMOPL000257a, None, success, P 3 2 1, 126 126 41 90
90 120, 3.02, 0.074, 16.7, 1.8, 95.7, 91.6, 99.6, 0.27887, 0.32941, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0198, Cc1c(=O)n(c(nn1)Nc2cccc2OC)N, FMOPL000049a, None, success, P 3 2 1, 126 126 41
90 90 120, 2.01, 0.021, 81.5, 1.9, 99.7, 97.2, 96.7, 0.18495, 0.21576, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0199, Cc1c(nc2c(n1) c(nc(n2)N)OC(C)C)C, FMOPL000147a, None, success, P 3 2 1, 126 126
41 90 90 120, 2.15, 0.044, 34.1, 0.6, 98.9, 96.5, 86.2, 0.18946, 0.21964, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0200,CS(=O)(=O)N(CC(=O)N)C1CCCCC1,FMOPL000032a, None, success, P 3 2 1,126 126 41
90 90 120,1.97,0.02,86.7,2,99.8,96.9,97.2,0.18295,0.21376,0.18295,0.21376,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0201,CCC(=O)NC(=S)N1CCCC2c1cccc2,FMOPL000148a, None, success, P 3 2 1,126 126 41 90
90 120,1.83,0.018,101.6,2.3,99.9,97.8,99.1,0.19463,0.22689,0.19463,0.22689,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0202,CC(=O)Nc1cc(cc(c1)C(=O)N)C(=O)N,FMOPL000034a, None, success, P 3 2 1,125 125
41 90 90 120,2.55,0.024,54.7,1.4,99.8,98.4,100,0.16519,0.21282, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0203,c1ccc(cc1)N(CCC#N)CC,FMOPL000540a, None, success, P 3 2 1,127 127 41 90 90
120,2.44,0.032,41.4,1.3,99.7,96,100,0.18694,0.23144, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0205,CC(C)(CO)NC(=O)Nc1ccc(cc1)Cl,FMOPL000033a, None, success, P 3 2 1,126 126 41
90 90 120,1.94,0.022,68.7,1.2,99.7,96.9,96.8,0.18533,0.21923, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0206,c1cc(ccc1CCC(=O)[O-])c2ccc(cc2)O,FMOPL000151a, None, success, P 3 2 1,124 124
41 90 90 120,3.14,0.027,57.1,1.4,99.1,89,91.9,0.18152,0.24266, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0207,Cc1ccc(cc1)CC(=O)Nc2nccs2,FMOPL000037a, None, success, P 3 2 1,126 126 41 90
90 120,2.38,0.028,61.8,2.1,99.4,94.8,93.4,0.1815,0.21816, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0208,CC1([C@@H](SC(=S)N1C)NO)C,FMOPL000152a, None, success, P 3 2 1,126 126 41 90
90 120,2.02,0.024,84,2.8,99.9,97.1,98.9,0.18587,0.21577,0.18587,0.21577,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0209,c1ccc(cc1)c2ccsc2,FMOPL000153a, None, success, P 3 2 1,126 126 41 90 90
120,2.31,0.025,77.1,1.8,99.5,95.1,94.5,0.18237,0.22168, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0210,C[NH+](Cc1cccc1)Cc2cccc2,FMOPL000036a, None, success, P 3 2 1,126 126 41 90
90 120,1.97,0.018,94.5,2.4,99.8,97.3,97.6,0.18102,0.2135, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0211,Cc1ccc(cc1O)NC(=O)c2cccc(c2)F,FMOPL000756a, None, success, P 3 2 1,126 126 41
90 90 120,2.28,0.022,79.2,2.7,99.5,95.8,93.9,0.17043,0.20498,0.17043,0.20498,P 3 2 1,2
- PANDDA model, None

NUDT7A-x0212,CS(=O)(=O)N1CC[NH+](CC1)Cc2ccco2,FMOPL000340a, None, success, P 3 2 1,125 125
41 90 90 120,2.69,0.021,77.3,2.2,99.6,92.4,95.8,0.15843,0.2089, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0213,CN(C)c1ccc(cc1)NCc2ccccc2O,FMOPL000682a, None, success, P 3 2 1,126 126 41 90
90 120,2.62,0.043,31,0.9,97.1,98.3,94.8,0.27606,0.31785, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0214,c1ccc(c(c1)C(=O)N)NC(=O)C[NH+]2CCCC2,FMOPL000365a, None, success, P 3 2 1,125
125 41 90 90 120,2.7,0.078,26.3,1.9,99.6,93.2,97.9,0.20429,0.26175, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0215,c1cc(c(nc1)Cl)C(=O)Nc2nc[nH]n2,FMOPL000712a, None, success, P 3 2 1,126 126 41
90 90 120,1.96,0.032,50,1.4,97.2,99.3,99.8,0.21076,0.24475, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0216,Cn1nc(nn1)NC(=O)c2ccc(cc2)F,FMOPL000673a, None, success, P 3 2 1,124 124 41 90
90 120,3.66,0.048,33.4,2.9,98.9,80.4,93.2,, None, None, None,1 - Analysis Pending, None

NUDT7A-x0217, CC(C)COc1ccc(cc1)C(=O)N2CCCC2, FMOPL000440a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.95, 0.026, 84.6, 2.5, 99.9, 97, 99.1, 0.18842, 0.22033, 0.19619, 0.20007, P 3 2 1, 3 - In Refinement, None

NUDT7A-x0218, Cc1cccc1OCC(=O)Nc2cccc2, FMOPL000380a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.02, 0.021, 91.2, 2.3, 99.7, 97.1, 98, 0.19259, 0.22295, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0219, c1cnccc1CNC(=O)CC#N, FMOPL000694a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.19, 0.029, 51.4, 1.5, 99.9, 91.8, 100, 0.17391, 0.20376, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0220, Cc1ccc(cc1)Nc2c3cn[nH]c3ncn2, FMOPL000679a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.81, 0.022, 70, 1.2, 97.4, 99.3, 100, 0.22226, 0.2477, 0.22733, 0.25547, P 3 2 1, 6 - Deposited, 5QGK

NUDT7A-x0221, Cc1c(cco1)C(=O)Nc2ccncc2, FMOPL000393a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.28, 0.037, 38.1, 1.4, 96, 96.1, 77.9, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0222, c1ccc(cc1)C(=O)Nc2ccc(cc2)C(=O)N, FMOPL000381a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.32, 0.027, 67, 1.9, 99.4, 95.2, 93, 0.18608, 0.22799, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0223, c1cc(cnc1)C(=O)OCc2ccc(cc2)Cl, FMOPL000726a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.31, 0.025, 61.4, 1.2, 99.5, 94.6, 95, 0.18718, 0.22603, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0224, CCC(=O)OCc1cc2cc(ccc2[nH]c1=O)C, FMOPL000681a, None, success, P 3 2 1, 126 126 41 90 90 120, 3.47, 0.339, 8.8, 3.7, 100, 98.8, 100, 0.16411, 0.22719, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0225, c1cc(ccc1NC(=S)N)OC(F)(F)F, FMOPL000276a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.3, 0.04, 61, 0.6, 96.7, 98.6, 93.3, 0.27535, 0.34037, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0226, CC1(CC(CC(N1O)(C)C)NC(=O)N(C)C)C, FMOPL000350a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.95, 0.023, 84, 2.6, 99.9, 97.4, 99, 0.18418, 0.21456, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0227, CC(C)(C)CC(=O)Nc1ccc(cc1F)F, FMOPL000718a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.46, 0.029, 59.1, 2, 98.8, 94.5, 95.6, 0.17051, 0.20738, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0228, c1ccc(cc1)C[NH2+][C@H]2CS(=O)(=O)C=C2, FMOPL000666a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.79, 0.023, 88.3, 2.2, 99.8, 97.4, 98.2, 0.18134, 0.21028, 0.18134, 0.21028, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0229, COc1ccc(cc1)C(=O)C2CC[NH2+]CC2, FMOPL000277a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.77, 0.018, 108.6, 2.5, 99.9, 97.5, 99.1, 0.18968, 0.21512, 0.18968, 0.21512, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0230, c1ccc(cc1)SCC[NH+]2CCOCC2, FMOPL000323a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.94, 0.038, 35.6, 0.7, 99.2, 97.8, 95.2, 0.19743, 0.22442, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0231, Cc1cccc1OCC(=O)Nc2ncccn2, FMOPL000757a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.59, 0.046, 40.2, 1.9, 99.3, 93, 91.9, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0232, Cc1cccc(c1)Nc2c3cnn(c3ncn2)C, PKTTA024495b, None, success, P 3 2 1, 126 126 41 90 90 120, 1.82, 0.017, 96.8, 2.3, 99.9, 97.2, 98.5, 0.18254, 0.20572, 0.18254, 0.20572, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0233, c1ccc(cc1)C(c2ccccc2)[NH+]3CC(C3)O, FMOPL000279a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.79, 0.072, 39.1, 1.6, 99.3, 91.8, 92.4, 0.23799, 0.29951, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0234, Cc1ccc(c([nH+]1)CCc2ccc(cc2)OC)[O-], FMOPL000378a, None, success, P 3 2 1, 126 126 42 90 90 120, 2, 0.026, 59.8, 1.6, 99.1, 97.7, 100, 0.20187, 0.23644, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0235, Cc1ccc(c(c1)O)NC(=O)c2ccccc2C, FMOPL000755a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.29, 0.02, 93.9, 2.3, 99.8, 95.7, 98.4, 0.17566, 0.20875, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0236, COC(=O)N1CCN(CC1)c2ccc(cc2)F, FMOPL000423a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.97, 0.02, 89, 1.9, 99.8, 96.9, 99.2, 0.18658, 0.21402, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0237, c1ccc(cc1)C(=O)N[C@H]2CS(=O)(=O)C=C2, FMOPL000671a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.33, 0.023, 72.8, 1.8, 99.7, 95.4, 96.9, 0.1782, 0.21116, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0238, Cc1cc(nc(n1)Nc2ccc(cc2)N)C, FMOPL000278a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.84, 0.026, 65.6, 2, 99.8, 91.8, 98.7, 0.15419, 0.2002, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0239, c1cc(ccc1C[NH+]2CCOCC2)C(F)(F)F, FMOPL000345a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.8, 0.018, 104.4, 2.1, 99.7, 97.8, 97.6, 0.19468, 0.22756, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0240, c1ccc(cc1)N2[C@H]3CC[C@H](O2)C=C3, FMOPL000700a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.33, 0.023, 81.1, 2.1, 99.8, 95.5, 97.7, 0.17343, 0.20661, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0241, CCOC(=O)C[NH+]1CCS(=O)(=O)CC1, FMOPL000614a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.82, 0.026, 50, 1.3, 97.5, 98.3, 100, 0.20944, 0.23325, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0242, c1cnc(nc1)N2CCC(CC2)CO, FMOPL000274a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.03, 0.025, 68.4, 3.3, 99.6, 99.8, 100, 0.20269, 0.23131, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0243, COc1ccc(cc1O)C[NH+]2CCCCC2, FMOPL000356a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.94, 0.021, 95.8, 1.7, 99.8, 96.7, 98.4, 0.19179, 0.22035, 0.19179, 0.22035, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0244, CCc1cccc1NC(=O)c2c(nns2)C, FMOPL000736a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.3, 0.031, 50.2, 0.9, 99.5, 98.8, 99.5, 0.19052, 0.23225, 0.19052, 0.23225, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0245, CCOC(=O)C1CCN(CC1)c2ccc(cc2)N, FMOPL000615a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.02, 0.036, 39.8, 0.7, 97.1, 95.2, 97.9, 0.21987, 0.24854, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0247, CC[C@H](C#CC[NH+]1CCCC1)OC(=O)C, FMOPL000337a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.11, 0.02, 72.6, 1.6, 94.9, 99.1, 100, 0.19147, 0.2284, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0248, Cc1ccc(cc1)N2CCN(CC2)C(=O)N, FMOPL000723a, None, success, P 3 2 1, 126 126 41 90 90 120, 3.03, 0.038, 41.4, 1.9, 99.7, 78.5, 100, 0.15314, 0.20224, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0249, CCOC(=O)c1cc2c([nH]1)ccs2, FMOPL000613a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.53, 0.022, 77.6, 2.1, 99.6, 94.4, 95.2, 0.16096, 0.20392, 0.16096, 0.20392, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0251, CN(CCO)S(=O)(=O)c1ccc(cc1)N, FMOPL000328a, None, success, P 3 2 1, 125 125 41 90
90 120, 2.19, 0.04, 41, 1.3, 100, 99.4, 100, 0.18378, 0.21721, 0.18378, 0.21721, P 3 2 1, 2 - PANDDA
model, None

NUDT7A-x0252, c1cc(ccc1N2CCN(CC2)C(=O)N)F, FMOPL000716a, None, success, P 3 2 1, 124 124 41 90
90 120, 2.66, 0.023, 67.2, 2.1, 99.7, 93.2, 96.9, 0.15875, 0.21001, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0253, c1cc(sc1)C[NH2+]Cc2ccc(cc2)O, FMOPL000619a, None, success, P 3 2 1, 125 125 41
90 90 120, 2.01, 0.023, 69.2, 1.9, 99.8, 96.4, 98.6, 0.18457, 0.22179, 0.18457, 0.22179, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0254, COc1cc(cc(c1OC)OC)C(=O)[O-], FMOPL000275a, None, success, P 3 2 1, 125 125 41 90
90 120, 2.27, 0.019, 81.1, 3.6, 99.6, 95.8, 95.4, 0.19466, 0.24422, 0.20154, 0.24945, P 3 2 1, 6 -
Deposited, 5QGL

NUDT7A-x0255, CC(=O)N1CCC(CC1)[NH2+]CCc2ccccc2, FMOPL000369a, None, success, P 3 2 1, 125 125
41 90 90 120, 2.53, 0.052, 34.8, 1.3, 100, 99.2, 100, 0.17075, 0.21559, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0256, C[C@@H]1CCCCN1C(=O)c2cncn2, FMOPL000391a, None, success, P 3 2 1, 126 126 41 90
90 120, 1.95, 0.046, 45.9, 1.2, 99.5, 97.1, 100, 0.19115, 0.22461, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0273, CC1=NN=C2N1N=C(NC(C)CN(C)C)C3=CC=CC=C32, BD065150b, None, success, P 3 2 1, 126
126 41 90 90 120, 3.07, 0.203, 4.1, 0.4, 99.9, 98.4, 100, , , None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0274, O=C1[C@]2(C)[C@](C2)(C(OCC)=O)[C@]3([H])CCC[C@@]31[H], FM010729a, None, success, P 3
2 1, 126 126 41 90 90
120, 3.12, 0.03, 44.3, 1.1, 90.6, 85.6, 91.5, 0.30445, 0.40384, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0276, [H][C@@]12[C@@](C2)(C(OCC)=O)[C@]3([H])CCC[C@]3([H])[C@@H]1NCC4=CC=CC=C4, FM010693
a, None, success, P 3 2 1, 125 125 41 90 90
120, 2.14, 0.027, 62, 1.2, 98.2, 95.5, 100, 0.20286, 0.24414, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0278, C=C(C(OCC)=O)CC(C1=CC=C(N(C)C)C=C1)NC2=CC=C(OC)C=C2, FM010696a, None, success, P 3 2
1, 126 126 41 90 90
120, 2.16, 0.025, 63.2, 1.9, 99.3, 95.6, 92.1, 0.18506, 0.21793, 0.18506, 0.21793, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0279, C=C(C(OCC)=O)CC(C1=CC=CC=C1F)NC2=CC=C(OC)C=C2, FM010697a, None, success, P 3 2
1, 126 126 41 90 90 120, 2.2, 0.078, 16.6, 0.7, 100, 99.7, 100, 0.32985, 0.36639, None, None, None, 1
- Analysis Pending, None

NUDT7A-x0280, O=C(N(C1=CC=C(OC)C=C1)C(C2=CC=CC=C2)C3)C3=C, FM010699a, None, success, P 3 2
1, 128 128 41 90 90 120, 3.31, 0.047, 32.6, 1.6, 98, 89.6, 99.7, 0.24032, 0.31447, None, None, None, 1
- Analysis Pending, None

NUDT7A-x0281, O=C1CC[C@@](C)(CCC2=CC=C(OC)C=C2)C1, FM010700a, None, success, P 3 2 1, 126 126
41 90 90 120, 2.02, 0.023, 73.5, 1.5, 97.7, 97.1, 100, 0.19852, 0.23167, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0282, C[C@]1(OC)OC2=CC(N)=CC=C2O[C@]1(C)OC, FM010701a, None, success, P 3 2 1, 126 126
41 90 90 120, 1.97, 0.015, 97.4, 2.3, 99.8, 96.8, 97.6, 0.18391, 0.21139, 0.18391, 0.21139, P 3 2
1, 2 - PANDDA model, None

NUDT7A-x0283,OC(CCNC1=CC=NC(C2=NNC=C2)=N1)=O,KD001536b, None, success, P 3 2 1,125 125 41
 90 90 120,2.06,0.044,43.6,1.4,99.5,96,100,0.22163,0.25193,0.22163,0.25193,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0284,S=C1C(O)=CC=CN1C,FM000368b, None, success, P 3 2 1,126 126 41 90 90
 120,2.42,0.049,39.1,3.2,100,99.9,100,0.17952,0.22115, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-
 x0285,O=C1CN=C(C2=CC=CC=C2C3=C(F)C=CC=C3)C4=CC(C1)=CC=C4N1,BD067750b, None, success, P 3 2
 1,126 126 41 90 90
 120,2.02,0.025,69.7,2.6,99.9,99.8,100,0.19945,0.22642,0.19945,0.22642,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0286,COc1ccc(-c2ccccc2N2CCCC2=O)cc1,FM010686a, None, success, P 3 2 1,126 126 41 90
 90 120,1.95,0.021,97.6,2.3,99.9,96.7,99.2,0.19314,0.22726,0.19198,0.22061,P 3 2 1,6 -
 Deposited,5QGM

NUDT7A-x0287,CC(C=CC=C1)=C1C2=C(SC3=CC=CC=C3)N=CN=C2NCCO,PK010474b, None, success, P 3 2
 1,126 126 41 90 90
 120,1.83,0.017,103.2,2.7,99.9,97.5,99.5,0.18863,0.21622,0.18863,0.21622,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-
 x0289,N#C[C@@]1(C2=CC=CC=C2)[C@@H](C3=CN=CC=C3)NC4=CC=CC=C41,FM010704a, None, success, P 3
 2 1,126 126 41 90 90
 120,2.02,0.031,52.1,0.4,95,98.6,99.3,0.24909,0.27971, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0290,COC1=CC=C(C(C#N)N(C)C)C=C1,FM010705a, None, success, P 3 2 1,126 126 41 90 90
 120,2.01,0.059,44.8,1.6,96.8,96.8,99.9,0.19483,0.22949, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0291,N#CC1CCOCCN1CC2=CC=CC=C2,FM010706a, None, success, P 3 2 1,126 126 41 90 90
 120,1.77,0.025,76.7,1.1,99.7,95.6,100,0.19211,0.21747,0.19211,0.21747,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0292,N#C[C@@H](N1CCC[C@H]1C(OC)=O)C2=CC=CC=C2,FM010707a, None, success, P 3 2
 1,127 127 41 90 90 120,2.7,0.031,54.6,1.5,98.6,93.3,88.4,0.2663,0.31808, None, None, None, 1
 - Analysis Pending, None

NUDT7A-
 x0293,O=C([C@@H]1CCCN1[C@H](C#N)[C@@H](NC(OC(C)(C)C)=O)C(C)C)OC,FM010708a, None, success,
 P 3 2 1,126 126 41 90 90
 120,2.07,0.05,40.3,1.7,97.2,99.7,100,0.20271,0.23943,0.20271,0.23943,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0295,CN(C(C1=NN=N1)C2=CC=CC=C2)C,FM010710a, None, success, P 3 2 1,126 126 41 90
 90 120,1.97,0.022,79.3,1.9,99.7,97,96.6,0.19249,0.2204, None, None, None, 2 - PANDDA
 model, None

NUDT7A-
 x0296,O=S([C@H]1C[C@H](C2=CC=CC=C2)NC3=CC=C(OC)C=C31)(C4=CC=CC=C4)=O,FM010711a, None, suc
 cess, P 3 2 1,126 126 41 90 90
 120,1.97,0.026,65.6,1.5,98.1,99.4,100,0.20568,0.23769, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0297,O=P(OCC)(OCC)C(CC(NC1=CC=C(OC)C=C1)C2=CC=CC=C2)=C,FM010712a, None, success, P
 3 2 1,126 126 41 90 90
 120,1.95,0.023,92.2,3.4,99.8,96.9,98.2,0.18398,0.21562, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0298,CC(NC1=CC(B(O)O)=CC(C(O)=O)=C1)=O,FM010713a, None, success, P 3 2 1,127 127 41
 90 90 120,2.32,0.038,41.6,1,99.3,94.5,91.1,0.17398,0.20396, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0299,O=C(CC1=CC=CS1)NC2=CC(B(O)O)=CC(C(O)=O)=C2,FM010687a, None, success, P 3 2
 1,126 126 41 90 90 120,1.95,0.03,71.1,3.3,99.9,97.4,99,0.19151,0.2173,0.19234,0.21118,P
 3 2 1,6 - Deposited,5QGN

NUDT7A-x0300,COC(=O)C12CC(=C)c3ccccc3CN1CC2,FM009905b, None, success, P 3 2 1,124 124 41 90
 90 120,2.63,0.059,29,1.1,99.4,94.8,99.1,0.19566,0.2391, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0303,O[C@@H]1C[C@H](c2ccccc2)[C@H]3C[C@@H]4CNC[C@]41N3,NU000598b, None, success, P
 3 2 1,126 126 41 90 90
 120,1.82,0.022,93.8,2.3,99.9,97.6,99.3,0.19367,0.21948,0.2016,0.22347,P 3 2 1,6 -
 Deposited,5QGO

NUDT7A-x0304,O[C@H]1C[C@H](c2ccccc2)[C@H]3C[C@@H]4CNC[C@]41N3,NU000598c, None, success, P
 3 2 1,126 126 41 90 90
 120,2.09,0.02,86.6,2.3,99.8,96.4,97.6,0.18179,0.2136,0.18831,0.22383,P 3 2 1,6 -
 Deposited,5QGP

NUDT7A-x0305,C1c2[nH]c[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2,FM010716a, None, success, P 3 2
 1,126 126 41 90 90
 120,2.28,0.02,85.2,1.5,99.4,94.7,93.2,0.18401,0.21529,0.18401,0.21529,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0306,CC(C)C1(CC(=O)c2ccccc2CN1)C(=O)NC1CC1,FM010717a, None, success, P 3 2 1,126
 126 41 90 90 120,2,0.04,39.6,1.4,99.4,97,93.2,0.18592,0.21242, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-
 x0307,O[C@H]1[C@@H](C(C)=C2)C[C@H](CC1)N2S(C3=CC=C(C)C=C3)(=O)=O,FM010694a, None, success
 , P 3 2 1,126 126 41 90 90
 120,1.98,0.02,74.9,0.9,96,99.6,99.8,0.21592,0.25507, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0308,O=C1[C@@H]2C[C@H](C(C)=C1)NC[C@H]2C,FM010698a, None, success, P 3 2 1,126 126
 41 90 90 120,1.98,0.023,82.8,2.7,99.8,97.3,97.9,0.18961,0.21773,0.18961,0.21773,P 3 2
 1,2 - PANDDA model, None

NUDT7A-x0309,O=C1C[C@]2(CCC#C[Si](C)(C)C)CCC[C@]2([H])O1,FM010702a, None, success, P 3 2
 1,126 126 41 90 90
 120,2.27,0.018,98.6,4.4,99.8,95.9,97.5,0.18016,0.21212,0.18016,0.21212,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0310,OC1CCCC12CC/C(C2C(OC)=O)=C\[Si](C)(C)C,FM010718a, None, success, P 3 2 1,126
 126 41 90 90 120,1.97,0.019,88.9,2.2,99.5,96.9,93.8,0.1837,0.21154, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0311,FC1=CC=C(S(N2CCN(CC2)C)(=O)=N)C=C1,FM010719a, None, success, P 3 2 1,126 126
 41 90 90 120,2.39,0.046,56.3,1.7,99.6,92.5,100,0.19668,0.23951, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0312,FC1=CC=C(S(=NCCC#N)(N)=O)C=C1,FM010720a, None, success, P 3 2 1,126 126 41 90
 90 120,1.84,0.028,69.9,1.4,98.9,96.9,100,0.19601,0.22261,0.19601,0.22261,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0313,O=S(C1CC1)(N2CCN(CC2)C(OCC3=CC=CC=C3)=O)=N,FM010721a, None, success, P 3 2
 1,126 126 41 90 90
 120,1.81,0.03,62.8,1.9,99.7,96.7,96.5,0.18504,0.21006,0.18504,0.21006,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0314,O=C1[C@@]2([H])[C@@](C(C=C(SC)C=C3)=C3O2)(C)CCC1,FM010722a,None,success,P 3 2 1,126 126 41 90 90
 120,1.76,0.041,49.7,1.4,99.1,98.5,100,0.22764,0.25965,None,None,None,1 - Analysis Pending,None

NUDT7A-x0315,O=C1[C@@]2([H])[C@@](C(C=CC(N(C)C)=C3)=C3O2)(C)CCC1,FM010723a,None,success,P 3 2 1,126 126 41 90 90
 120,2.28,0.018,86,0.3,99.5,95.6,94.7,0.17692,0.21513,0.17692,0.21513,P 3 2 1,2 - PANDDA model,None

NUDT7A-x0316,O=C1[C@@]2([H])[C@@](C(C=CC=C3C1)=C3O2)(C)CCC1,FM010724a,None,success,P 3 2 1,126 126 41 90 90
 120,1.84,0.02,84.9,1.9,99.7,97.5,96.6,0.19155,0.22014,None,None,None,1 - Analysis Pending,None

NUDT7A-x0317,BrC(C(O)O1)=C(OC2=CC=CC=C2)C1=O,FM010725a,None,success,P 3 2 1,126 126 41 90 90
 120,2.29,0.031,82.1,3.2,99.7,94.6,97.4,0.18021,0.21534,0.18021,0.21534,P 3 2 1,2 - PANDDA model,None

NUDT7A-x0318,CC(CC1)=C(OC2=CN=CC=C2)C1=O,FM010688a,None,success,P 3 2 1,126 126 41 90 90
 120,1.95,0.022,75.7,3,99.7,97.4,96.6,0.1888,0.21662,0.20312,0.22688,P 3 2 1,6 - Deposited,5QGQ

NUDT7A-x0319,OC1=NN=C(O)C2=CC=NC=C21,FM010726a,None,success,P 3 2 1,126 126 41 90 90
 120,1.93,0.025,56,2.5,96.6,97.8,77.9,0.22907,0.26251,None,None,None,1 - Analysis Pending,None

NUDT7A-x0320,CC1=NN=C2N1N=C(N(CC3)CC3N(C)C)C4=CC=CC=C42,BD066070b,None,success,P 3 2 1,126 126 41 90 90
 120,2.02,0.024,87.4,2.3,99.7,96.8,97.6,0.17986,0.21043,None,None,None,1 - Analysis Pending,None

NUDT7A-x0321,OC1=NN=C(O)C2=CC(F)=C(F)C=C21,FM010727a,None,success,P 3 2 1,126 126 41 90 90
 120,1.93,0.026,72.3,2.1,99.5,96.9,94.4,0.1856,0.21313,0.18560,0.21313,P 3 2 1,2 - PANDDA model,None

NUDT7A-x0322,CC1=NN=C2N1N=C(C1)C3=CC=CC=C32,FM010728a,None,success,P 3 2 1,127 127 41 90 90
 120,2.47,0.051,26.5,1.4,95.1,92.5,95.5,0.2067,0.26114,None,None,None,1 - Analysis Pending,None

NUDT7A-x0323,CC1=NN=C2N1N=C(NC(C)CN(C)C)C3=CC=CC=C32,BD065150b,None,success,P 3 2 1,126 126 41 90 90
 120,3,0.412,20.8,0,99.7,99.2,100,,None,None,None,1 - Analysis Pending,None

NUDT7A-x0324,O=C1[C@]2(C)[C@](C2)(C(OCC)=O)[C@]3([H])CCC[C@@]31[H],FM010729a,None,success,P 3 2 1,126 126 41 90 90
 120,2.33,0.026,69.9,2,99.8,95.5,98,0.17021,0.20404,None,None,None,1 - Analysis Pending,None

NUDT7A-x0325,O=C1[C@]2([H])[C@]([C@H]2C3=CC=CC(F)=C3)(C(OCC)=O)[C@]4([H])CCC[C@@]41[H],FM010730a,None,success,P 3 2 1,126 126 41 90 90
 120,2.32,0.03,61.5,1.4,99.5,95,94.6,,None,None,None,1 - Analysis Pending,None

NUDT7A-x0326,[H][C@@]12[C@@](C2)(C(OCC)=O)[C@]3([H])CCC[C@]3([H])[C@@H]1NCC4=CC=CC=C4,FM010693a,None,success,P 3 2 1,126 126 41 90 90
 120,2.29,0.02,84.2,-0.3,99.8,95.8,97.6,0.17636,0.21453,None,None,None,1 - Analysis Pending,None

NUDT7A-x0327,C=C(C(OCC)=O)CC(C1=CC=CN=C1)NC2=CC=C(OC)C=C2,FM010695a,None,success,P 3 2 1,126 126 41 90 90
 120,1.94,0.022,80.8,2.1,99.5,96.8,94.2,0.184,0.21428,None,None,None,1 - Analysis Pending,None

NUDT7A-
 x0328, C=C (C (OCC) =O) CC (C1=CC=C (N (C) C) C=C1) NC2=CC=C (OC) C=C2, FM010696a, None, success, P 3 2
 1,126 126 41 90 90
 120,1.95,0.023,86.4,2.6,99.8,97,98.4,0.18918,0.21668,0.18918,0.21668,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0329, C=C (C (OCC) =O) CC (C1=CC=CC=C1F) NC2=CC=C (OC) C=C2, FM010697a, None, success, P 3 2
 1,126 126 41 90 90
 120,1.97,0.029,70.8,0.9,96.9,99.8,97.5,0.26284,0.29862, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0330, O=C (N (C1=CC=C (OC) C=C1) C (C2=CC=CC=C2) C3) C3=C, FM010699a, None, success, P 3 2
 1,125 125 41 90 90 120,2.66,0.034,48.5,1.7,99.4,93.3,93,0.19888,0.25783, None, None, None, 1
 - Analysis Pending, None

NUDT7A-x0331, O=C1CC [C@@] (C) (CCC2=CC=C (OC) C=C2) C1, FM010700a, None, success, P 3 2 1,126 126
 41 90 90 120,2.08,0.026,72.3,3.3,93.5,95.5,88.6,,, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0332, C [C@] 1 (OC) OC2=CC (N) =CC=C2O [C@] 1 (C) OC, FM010701a, None, success, P 3 2 1,126 126
 41 90 90 120,1.78,0.018,91.7,1.5,99.9,98,100,0.18855,0.21597,0.18855,0.21597,P 3 2 1,2
 - PANDDA model, None

NUDT7A-x0333, OC (CCNC1=CC=NC (C2=NNC=C2) =N1) =O, KD001536b, None, success, P 3 2 1,126 126 41
 90 90 120,1.96,0.021,74.1,1.7,96.9,97.8,96.2,0.22132,0.2439,0.22429,0.262,P 3 2 1,3 - In
 Refinement, None

NUDT7A-x0334, S=C1C (O) =CC=CN1C, FM000368b, None, success, P 3 2 1,126 126 41 90 90
 120,2.01,0.036,48.8,1.6,99.4,96.5,94.1,0.18338,0.2152, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-
 x0335, O=C1CN=C (C2=CC=CC=C2C3=C (F) C=CC=C3) C4=CC (C1) =CC=C4N1, BD067750b, None, success, P 3 2
 1,126 126 41 90 90
 120,1.83,0.026,78.9,2.9,99.8,97.5,98.2,0.18799,0.21715,0.18799,0.21715,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0336, COc1ccc (-c2ccccc2N2CCCC2=O) cc1, FM010686a, None, success, P 3 2 1,125 125 41 90
 90 120,1.66,0.043,55.3,2.8,99.9,98.1,99.6,0.18918,0.21038,0.18918,0.21038,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0337, CC (C=CC=C1) =C1C2=C (SC3=CC=CC=C3) N=CN=C2NCCO, PK010474b, None, success, P 3 2
 1,126 126 41 90 90 120,1.64,0.054,39.1,1.1,99.5,99.9,100,,, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0338, O=C1C2=C (C=CC=C2) CC (C3=CC=CC=C3N4C) 1C4=O, FM010703a, None, success, P 3 2
 1,127 127 41 90 90
 120,2.33,0.015,94.8,0.7,99.8,92.9,100,0.18149,0.22022, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-
 x0339, N#C [C@@] 1 (C2=CC=CC=C2) [C@@H] (C3=CN=CC=C3) NC4=CC=CC=C41, FM010704a, None, success, P 3
 2 1,127 127 41 90 90 120,3.29,0.039,45,2.1,99,86,96.9,,, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0340, COC1=CC=C (C (C#N) N (C) C) C=C1, FM010705a, None, success, P 3 2 1,126 126 41 90 90
 120,1.98,0.02,91.5,2.4,99.8,96.9,97.9,0.17901,0.20844, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0341, N#CC1CCOCCN1CC2=CC=CC=C2, FM010706a, None, success, P 3 2 1,126 126 41 90 90
 120,1.89,0.024,76.3,1,99.6,94.6,98.9,0.18802,0.2179,0.18802,0.21790,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0342,N#C[C@@H](N1CCC[C@H]1C(OC)=O)C2=CC=CC=C2,FM010707a, None, success, P 3 2
 1,126 126 41 90 90 120,1.95,0.03,68.3,2.4,99.7,97,96.4,0.1836,0.21372, None, None, None,1
 - Analysis Pending, None

NUDT7A-
 x0343,O=C([C@@H]1CCCN1[C@H](C#N)[C@@H](NC(OC(C)(C)C)=O)C(C)C)OC,FM010708a, None, success,
 P 3 2 1,126 126 41 90 90
 120,1.92,0.034,51.6,1.6,97.5,99.6,81.9,0.20477,0.22488,0.20477,0.22488,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0345,CN(C(C1=NN=N1)C2=CC=CC=C2)C,FM010710a, None, success, P 3 2 1,126 126 41 90
 90 120,2.15,0.021,63.6,1.3,99.4,96.8,100,0.19284,0.23143,0.19284,0.23143,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-
 x0346,O=S([C@H]1C[C@H](C2=CC=CC=C2)NC3=CC=C(OC)C=C31)(C4=CC=CC=C4)=O,FM010711a, None, suc
 cess, P 3 2 1,127 127 41 90 90
 120,2.8,0.035,47,1.3,99.5,92.6,96.8,0.22955,0.28603, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0347,O=P(OCC)(OCC)C(CC(NC1=CC=C(OC)C=C1)C2=CC=CC=C2)=C,FM010712a, None, success, P
 3 2 1,126 126 41 90 90
 120,1.81,0.031,50.4,1.3,99.5,97.2,93.9,0.18836,0.2204, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0348,CC(NC1=CC(B(O)O)=CC(C(O)=O)=C1)=O,FM010713a, None, success, P 3 2 1,126 126 41
 90 90 120,2.33,0.026,56.3,0.3,95.8,99,100,0.27537,0.30592, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0349,O=C(CC1=CC=CS1)NC2=CC(B(O)O)=CC(C(O)=O)=C2,FM010687a, None, success, P 3 2
 1,126 126 41 90 90
 120,1.67,0.028,78.9,1.1,99.8,97.6,99.9,0.19657,0.21828, None, None, None,2 - PANDDA
 model, None

NUDT7A-x0350,COC(=O)C12CC(=C)c3ccccc3CN1CC2,FM009905b, None, success, P 3 2 1,125 125 41 90
 90 120,1.95,0.027,80.1,2.6,99.9,97.1,98.7,0.18753,0.23167,0.18753,0.23167,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0351,C[C@]12OC(=O)N[C@H]1C[C@@]13CNC[C@@H]1C[C@@H]2O3,FM010715a, None, success, P
 3 2 1,126 126 41 90 90
 120,1.98,0.024,79.9,2.4,99.9,97.3,98.4,0.18297,0.21408,0.18297,0.21408,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0352,O[C@H]1C[C@H]([C@@H]2C[C@H]3CNC[C@@]31N2)c1ccccc1,NU000598b, None, success, P
 3 2 1,126 126 41 90 90
 120,1.94,0.02,93.2,1.9,99.1,97.1,88,0.19467,0.22357,0.19467,0.22357,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-
 x0353,O[C@H]1[C@@H](C(C)=C2)C[C@H](CC1)N2S(C3=CC=C(C)C=C3)(=O)=O,FM010694a, None, success
 , P 3 2 1,126 126 41 90 90
 120,1.94,0.02,86,1.4,99.8,96.9,97.7,0.1886,0.21775, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0354,O=C1[C@@H]2C[C@H](C(C)=C1)NC[C@H]2C,FM010698a, None, success, P 3 2 1,126 126
 41 90 90 120,1.88,0.022,60.1,0.6,98.2,97.8,93.1,0.21469,0.25042, None, None, None,1 -
 Analysis Pending, None

NUDT7A-x0356,OC1CCCC12CC/C(C2C(OC)=O)=C\[Si](C)(C)C,FM010718a, None, success, P 3 2 1,125
 125 41 90 90 120,1.71,0.021,80.7,1.1,99.8,99.4,100,0.19063,0.21879, None, None, None,1 -
 Analysis Pending, None

NUDT7A-x0357,FC1=CC=C(S(N2CCN(CC2)C)(=O)=N)C=C1,FM010719a, None, success, P 3 2 1,126 126
 41 90 90 120,1.96,0.02,77.8,1.4,98.9,97.7,99.6,0.20816,0.23855,0.20816,0.23855,P 3 2 1,2
 - PANDDA model, None

NUDT7A-x0358,FC1=CC=C(S(=NCCC#N)(N)=O)C=C1,FM010720a, None, success, P 3 2 1,126 126 41 90
 90 120,1.81,0.031,42.9,1.2,98.3,96.2,100,0.20347,0.22482, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0359,O=S(C1CC1)(N2CCN(CC2)C(OCC3=CC=CC=C3)=O)=N,FM010721a, None, success, P 3 2
 1,126 126 41 90 90 120,2.04,0.059,17.8,2.1,100,99.8,100,0.3066,0.34567, None, None, None, 1
 - Analysis Pending, None

NUDT7A-x0360,O=C1[C@@]2([H])[C@@](C(C=C(SC)C=C3)=C3O2)(C)CCC1,FM010722a, None, success, P
 3 2 1,126 126 41 90 90
 120,1.84,0.022,71.6,1.3,99.9,98,100,0.19263,0.22453,0.19263,0.22453,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-
 x0361,O=C1[C@@]2([H])[C@@](C(C=CC(N(C)C)=C3)=C3O2)(C)CCC1,FM010723a, None, success, P 3 2
 1,126 126 41 90 90 120,2,0.028,54.5,1.6,99.6,97.2,95,0.18292,0.21472, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0362,O=C1[C@@]2([H])[C@@](C(C=CC=C3C1)=C3O2)(C)CCC1,FM010724a, None, success, P 3
 2 1,126 126 41 90 90
 120,1.81,0.031,43.7,1.4,99.8,96.5,99.8,0.19174,0.21519, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0363,BrC(C(O)O1)=C(OC2=CC=CC=C2)C1=O,FM010725a, None, success, P 3 2 1,126 126 41
 90 90 120,2.07,0.09,50.5,2.1,100,99.7,100,, , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0364,CC(CC1)=C(OC2=CN=CC=C2)C1=O,FM010688a, None, success, P 3 2 1,126 126 41 90 90
 120,2.57,0.327,4.7,2.1,100,99.5,100,0.31381,0.36336, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0365,OC1=NN=C(O)C2=CC=NC=C21,FM010726a, None, success, P 3 2 1,126 126 41 90 90
 120,1.81,0.021,68,1.5,99.8,97.9,97.1,0.18839,0.21597, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0366,CC1=NN=C2N1N=C(N(CC3)CC3N(C)C)C4=CC=CC=C42,BD066070b, None, success, P 3 2
 1,126 126 41 90 90
 120,2.51,0.039,52.2,0.9,97.9,95.2,99.2,0.2426,0.29489, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0367,OC1=NN=C(O)C2=CC(F)=C(F)C=C21,FM010727a, None, success, P 3 2 1,127 127 41 90
 90 120,2.79,0.037,44.5,0.8,94.9,91.8,82.2,, , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0368,CC1=NN=C2N1N=C(C1)C3=CC=CC=C32,FM010728a, None, success, P 3 2 1,126 126 41 90
 90 120,1.84,0.023,69.6,2,99.6,97.1,95.3,0.1836,0.21086, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0369,C1c2[n]cc[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2,FM010714a, None, success, P 3 2
 1,126 126 41 90 90
 120,3.19,0.055,22.3,1.4,87.3,96.9,99.1,0.28455,0.42321, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-
 x0370,O[C@@H]1C[C@H]([C@@H]2C[C@H]3CNC[C@@]31N2)c1cccc1,NU000598c, None, success, P 3 2
 1,126 126 41 90 90 120,2.22,0.045,15,5.6,99.2,99.4,95.2,0.74899,0.66987, None, None, None, 1
 - Analysis Pending, None

NUDT7A-x0371,C1c2[nH]c[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2,FM010716a, None, success, P 3 2
 1,126 126 41 90 90
 120,3.19,0.055,22.3,1.4,87.3,96.9,99.1,0.28455,0.42321, None, None, None, 1 - Analysis
 Pending, None

120,1.79,0.026,61.6,1.9,99.7,97.7,96.4,0.18496,0.20913,0.18496,0.20913,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x0372,CC(C)C1(CC(=O)c2ccccc2CN1)C(=O)NC1CC1,FM010717a,None,success,P 3 2 1,126
126 42 90 90 120,2.28,0.022,33.6,4.9,91.2,94,64.4,0.35244,0.40035,None,None,None,1 -
Analysis Pending,None

NUDT7A-x0373,c1cnc(cn1)c2ncc(c(n2)N)C#N,FM0PL000086a,None,success,P 3 2 1,125 125 41 90
90 120,2.71,0.026,54.5,1.3,99.5,92.1,95,0.18792,0.24858,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0374,c1ccnc(c1)c2ccc(s2)C(=S)N,FM0PL000022a,None,success,P 3 2 1,126 126 41 90
90 120,1.96,0.017,84,1.6,97.6,97.6,99.9,0.21088,0.24249,0.21419,0.24384,P 3 2 1,6 -
Deposited,5QGR

NUDT7A-
x0375,CC(C)(C)NC(=O)c1ccc2c(c1)nns2,FM0PL000178a,None,None,None,None,None,None,Non
e,None,None,None,,None,None,None,1 - Analysis Pending,None

NUDT7A-x0376,c1cc(ccc1c2ccc(o2)CO)N,FM0PL000551a,None,success,P 3 2 1,126 126 41 90 90
120,2.28,0.03,52.6,0.8,99.6,95.9,95.1,0.17787,0.21795,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0377,CC(C)NC(=O)N[C@@H]1CCCCNC1=O,FM0PL000087a,None,success,P 3 2 1,125 125 41
90 90 120,2.42,0.036,42.3,1,99.1,95,88.4,0.17985,0.2217,0.17985,0.22170,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x0378,c1cc(ccc1c2cc(c(s2)C#N)N)F,XST00000578b,None,success,P 3 2 1,125 125 41 90
90 120,2.37,0.034,52.9,0.2,98.2,94.7,86.3,0.2551,0.299,0.25510,0.29900,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x0379,c1cc(cnc1)C[NH2+][C@H]2CS(=O)(=O)C[C@@H]2O,FM0PL000179a,None,success,P 3 2
1,126 126 41 90 90
120,2.37,0.078,24.7,2.3,99.9,99.8,99.7,0.30794,0.35984,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0380,Cc1ccc(cc1)c2cc(on2)C#N,FM0PL000556a,None,success,P 3 2 1,126 126 41 90 90
120,2.01,0.026,59.6,1.7,99.6,96.4,95.2,0.18149,0.21657,0.18149,0.21657,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x0381,COC(=O)c1cccc(c1)NS(=O)(=O)C,FM0PL000089a,None,success,P 3 2 1,126 126 41
90 90 120,2.76,0.059,16.3,0.8,94.9,95.1,97.9,0.30496,0.32979,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0382,c1ccc(cc1)Coc2cccc(c2)N,FM0PL000023a,None,success,P 3 2 1,126 126 41 90 90
120,2,0.018,85.1,1.2,96.1,95.6,100,0.21477,0.24085,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0383,C[NH+]1CCC(CC1)[NH+]2CCC[C@H](C2)C(=O)[O-],FM0PL000180a,None,success,P 3 2
1,126 126 41 90 90 120,1.77,0.02,73.5,1.5,99.8,98.2,100,0.19276,0.2175,None,None,None,1
- Analysis Pending,None

NUDT7A-x0384,C[C@@H](C[NH2+])Cc1c(ccc1Cl)ClO,FM0PL000555a,None,success,P 3 2 1,126 126
41 90 90 120,1.99,0.036,61.3,1.2,98.8,97.9,99.5,0.23257,0.27258,0.24831,0.29199,P 3 2
1,3 - In Refinement,None

NUDT7A-x0385,c1csc(c1NC(=O)C(F)(F)F)C(=O)N,FM0PL000092a,None,success,P 3 2 1,125 125 41
90 90 120,2.92,0.029,67,1.6,99.2,90.8,94.6,0.21921,0.29119,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0386,c1ccc(cc1)C[NH+]2CCO[C@H](C2)CO,FM0PL000024a,None,success,P 3 2 1,126 126
41 90 90 120,2.15,0.015,98.3,1.2,97.9,97.2,100,0.19408,0.22864,None,None,None,1 -
Analysis Pending,None

NUDT7A-x0387, C[NH+]1CCN(CC1)C(=O)c2ccc(c(c2)F)F, FMOPL000181a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.97, 0.019, 88.6, 2, 99.7, 97.1, 96.3, 0.17809, 0.20839, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0389, c1cc(scl)c2ccc(s2)c3ccn[nH]3, FMOPL000091a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.77, 0.021, 62.4, 1.3, 98.8, 98, 100, 0.1997, 0.23156, 0.20029, 0.22739, P 3 2 1, 3 - In Refinement, None

NUDT7A-x0390, CC(C)(C)OC(=O)N1CCC(CC1)[NH2+]C2CC2, FMOPL000025a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.88, 0.024, 82.6, 1.2, 99.9, 96.7, 99.9, 0.18381, 0.21362, 0.18381, 0.21362, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0391, c1ccc(cc1)COCc2c[nH]c(=O)[nH]c2=O, FMOPL000182a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.31, 0.027, 49.6, 0.6, 99.6, 95.4, 100, 0.18661, 0.23506, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0392, Cc1ccc2c(c1)c3c([nH]2)[C@H](CCC3)[NH3+], FMOPL000564a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.82, 0.035, 41.4, 1.1, 88.2, 89.4, 77.1, 0.26189, 0.32446, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0393, COC(=O)NNc1cc(ccn1)C(F)(F)F, FMOPL000096a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.34, 0.026, 72.1, 1.3, 99.3, 92.8, 100, 0.1963, 0.2351, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0394, c1ccc(c(c1)CNC2ccc(cc2)F)CO, FMOPL000183a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.3, 0.023, 66.8, 1, 99.5, 95.8, 99.6, 0.19104, 0.23753, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0395, c1ccc(cc1)C[NH+]2CC(=O)NC(=O)C2, FMOPL000558a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.97, 0.023, 62.8, 1, 98.8, 99.4, 99.5, 0.20261, 0.23505, 0.20261, 0.23505, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0396, COc1cccc(c1)c2nc(c(o2)N)C#N, FMOPL000097a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.32, 0.025, 55.7, 1.1, 99.6, 96.4, 100, 0.18864, 0.23717, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0397, c1cc(ccc1NNC(=S)N)F, FMOPL000055a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.45, 0.044, 35.5, 1.2, 99.2, 92.4, 99.9, 0.19253, 0.23483, 0.19253, 0.23483, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0398, c1cc(ccc1CC(=O)NC2CCCCC2)F, FMOPL000184a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.86, 0.036, 37.6, 1.5, 97.9, 93.3, 100, 0.22748, 0.29131, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0399, CCOc1cccc(c1)c2nnc(s2)N, FMOPL000560a, None, success, P 3 2 1, 126 126 41 90 90 120, 2, 0.021, 67.1, 1.3, 98.4, 97.9, 100, 0.20952, 0.23727, 0.21479, 0.24721, P 3 2 1, 3 - In Refinement, None

NUDT7A-x0401, c1cc(ccc1NC(=O)CC#N)Cl, FMOPL000056a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.23, 0.045, 32.8, 0.7, 98.4, 96.6, 90.4, 0.23021, 0.27454, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0402, CC(C)CC(=O)NCc1ccc2c(c1)OCO2, FMOPL000185a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.61, 0.034, 49.5, 0.4, 99.1, 92.2, 92.8, 0.20767, 0.26606, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0403, c1ccc(cc1)C#CC[NH+]2CCCCC2, FMOPL000559a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.85, 0.021, 73.9, 1.7, 99.7, 97.8, 95.9, 0.18492, 0.21659, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0404, Cc1c(c(c([nH]1)C)C(=O)OC)c2cc[nH]n2, FMOPL000098a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.36, 0.029, 42.3, 1.4, 96.8, 95.7, 100, 0.25541, 0.30154, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0405, c1ccc(cc1)c2cc(on2)C[NH3+], FMOPL000057a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.81, 0.019, 81, 1.4, 96.9, 97.2, 100, 0.21661, 0.24413, 0.21661, 0.24413, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0406, CC(=O)Nc1ccc(cc1)Nc2ccccc2, FMOPL000186a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.78, 0.016, 109.9, 1.5, 97.2, 99.3, 100, 0.20974, 0.23515, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0407, c1cc(cc(c1)Cl)NC(=O)C[NH+]2CCCC2, FMOPL000567a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.1, 0.029, 51.1, 1.3, 99, 97.2, 99.1, 0.19675, 0.23422, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0408, CC(=O)c1ccc(o1)c2ccc(cc2F)F, FMOPL000095a, None, success, P 3 2 1, 124 124 41 90 90 120, 2.66, 0.031, 54.7, 1.1, 98.9, 92.4, 92.8, 0.30181, 0.37036, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0409, c1cc(ccc1n2cc(nn2)CO)Cl, FMOPL000058a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.35, 0.049, 22.6, 1.1, 100, 99.3, 100, 0.27005, 0.32976, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0410, CC(=O)Nc1cc(ccc1O)c2ccccc2, FMOPL000187a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.24, 0.033, 46.3, 1.6, 98.3, 96.9, 90.5, 0.22273, 0.27365, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0411, CC(=O)Nc1ccc(cc1)c2csc(n2)N, FMOPL000568a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.69, 0.022, 79.1, 1.2, 99.9, 96.2, 100, 0.19142, 0.21506, 0.1925, 0.22113, P 3 2 1, 3 - In Refinement, None

NUDT7A-x0412, c1cc(sc1)c2nc(no2)N3CCCCC3, FMOPL000093a, None, success, P 3 2 1, 126 126 42 90 90 120, 2.24, 0.031, 42.9, 2.9, 94.5, 97.1, 51.9, 0.25305, 0.30579, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0413, CC(=O)Nc1ccc(cc1)OCC(=O)[O-], FMOPL000059a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.55, 0.037, 43.3, 1, 98.4, 94.3, 95, 0.20474, 0.25823, 0.20474, 0.25823, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0414, Cc1nc(c(s1)NC(=O)OC)c2ccccc2, FMOPL000188a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.78, 0.083, 28.1, 1.5, 99.3, 96.9, 100, 0.19777, 0.2214, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0415, Cc1cc(nn1c2ccccc2)NC(=O)OC, FMOPL000105a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.94, 0.109, 49.3, 1.9, 98.3, 97.4, 82, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0416, c1cc(oc1)CNC(=O)Nc2ccc(cc2)F, FMOPL000189a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.62, 0.02, 76.2, 1.3, 99, 98.4, 100, 0.20282, 0.22557, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0417, None, None, None, success, P 3 2 1, 126 126 41 90 90 120, 1.82, 0.024, 85.1, 2.5, 99.8, 97.9, 98.2, 0.18248, 0.21079, 0.18248, 0.21079, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0418, None, None, None, success, P 3 2 1, 125 125 41 90 90 120, 1.78, 0.024, 59.2, 1.3, 99.2, 98.1, 100, 0.20194, 0.23268, 0.20194, 0.23268, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0419, None, None, None, success, P 3 2 1, 126 126 41 90 90 120, 1.95, 0.024, 83.7, 2.4, 99.9, 97, 99.1, 0.18556, 0.2142, 0.18556, 0.21420, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0420, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.24, 0.034, 46.7, 1.3, 98.9, 94.4, 85.7, 0.19632, 0.23144, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0422, None, None, None, success, P 3 2 1, 127 127 41 90 90
 120, 1.85, 0.026, 77.3, 2, 99.7, 97.2, 95.8, 0.18488, 0.21306, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0423, None, None, None, success, P 3 2 1, 127 127 42 90 90
 120, 2.8, 0.037, 38.4, 0.9, 94.6, 97.8, 96.3, 0.2678, 0.34222, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0424, C[C@@H](CNC(=O)Nc1cccc1)O, FMOPL000464a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.81, 0.063, 36.3, 2.3, 99.9, 97.9, 98.3, 0.18123, 0.20778, 0.18123, 0.20778, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0425, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.97, 0.023, 68.4, 2, 99.6, 96.9, 95.4, 0.18148, 0.21423, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0426, None, None, None, success, P 3 2 1, 124 124 41 90 90
 120, 3.12, 0.055, 29, 0.9, 90.8, 85.2, 76.9, 0.26722, 0.33717, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0427, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.46, 0.137, 26.5, 1.5, 99.7, 98.9, 100, 0.2516, 0.30497, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0428, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.15, 0.022, 59.1, 1.5, 99.5, 97.2, 100, 0.18681, 0.22532, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0429, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.32, 0.027, 61.8, 1.1, 99.4, 95.5, 93.4, 0.22327, 0.28365, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0430, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.92, 0.028, 52.3, 2.1, 97.9, 97.9, 85.5, 0.21574, 0.24837, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0431, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.42, 0.037, 48.7, 1, 99.2, 95.9, 100, 0.22208, 0.26477, 0.22208, 0.26477, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0432, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.84, 0.019, 94, 1.6, 97.5, 96, 100, 0.20265, 0.22557, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0434, CC(C)C(=O)Nc1nnn(n1)C, FMOPL000547a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.13, 0.115, 44.5, 1.4, 100, 99.6, 100, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0435, c1ccc(cc1)NS(=O)(=O)c2ccc(cc2)N, FMOPL000432a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.95, 0.017, 86.2, 1.2, 95.5, 98.2, 90.5, 0.21544, 0.25557, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0436, CC[C@H](CO)NC(=O)Nc1ccc(cc1)Cl, FMOPL000476a, None, success, P 3 2 1, 125 125 41
 90 90 120, 1.55, 0.047, 46.2, 1.1, 99.9, 98.9, 99.9, 0.19793, 0.21942, 0.16575, 0.19511, P 3 2 1, 6
 - Deposited, 5QGS

NUDT7A-x0437, COc1cccc(c1)C[NH+]2CCC(CC2)C(=O)N, FMOPL000305a, None, success, P 3 2 1, 125 125
 41 90 90 120, 1.85, 0.028, 75.4, 2.6, 99.8, 97.7, 97.5, 0.18498, 0.21372, 0.18498, 0.21372, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0438, c1ccc(cc1)Coc2ccccc2C(=O)NN, FMOPL000587a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.98, 0.028, 60.7, 1.3, 98.8, 97.5, 99.7, 0.21607, 0.24873, 0.22011, 0.24757, P 3 2 1, 3 - In Refinement, None

NUDT7A-x0439, c1c(c(=O)[nH]c(=O)[nH]1)NC2CCCC2, FMOPL000388a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.68, 0.026, 62.1, 1.9, 99.7, 98.1, 96.1, 0.18274, 0.20647, 0.18274, 0.20647, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0440, C[C@H](C[NH2+])C1CCCC1O, FMOPL000461a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.4, 0.021, 73.2, 1.9, 99.3, 93.7, 94.8, 0.18825, 0.24319, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0441, c1c(nns1)C(=O)N2CCOCC2, FMOPL000281a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.14, 0.029, 63.5, 0.5, 94, 96.6, 99.4, 0.27266, 0.31552, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0442, C[C@@H](C(=O)OC)NC(=O)N1CCOCC1, FMOPL000563a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.77, 0.016, 116.6, 2.4, 99.9, 97.5, 98.7, 0.18265, 0.21138, 0.18265, 0.21138, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0445, c1cc(c(cc1C(F)(F)F)N)N2CCCC2, FMOPL000263a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.14, 0.029, 50.1, 1.4, 99.7, 97.1, 100, 0.18862, 0.22577, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0446, COc1cc(cc(c1)OC)C(=O)Nn2cnnc2, FMOPL000451a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.65, 0.029, 48.6, 2.2, 95.7, 93.2, 93, 0.26369, 0.29632, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0447, c1ccnc(c1)NC(=O)c2cnccn2, FMOPL000469a, None, success, P 3 2 1, 127 127 41 90 90 120, 3.19, 0.058, 31.6, 1.6, 99.2, 89, 95.2, 0.28632, 0.34633, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0448, COC(=O)c1cccc2c1-c3ccccc3C2=O, FMOPL000264a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.01, 0.024, 68.7, 1.7, 99.6, 97.2, 95.8, 0.18452, 0.21703, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0450, Cc1c(sc(n1)NC(=O)OC)C(=O)N(C)C, FMOPL000409a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.34, 0.021, 71.3, 1.1, 99.1, 96.9, 100, 0.21103, 0.25957, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0451, COc1ccc2c(c1)sc(n2)NC(=O)C3CC3, FMOPL000487a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.94, 0.054, 9.1, 1.9, 100, 98.7, 100, 0.27613, 0.32556, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0452, CCOC(=O)Nc1cccc(c1)Cl, FMOPL000260a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.76, 0.021, 73.6, 1.9, 99.6, 97.7, 95.7, 0.18382, 0.20913, 0.18531, 0.20932, P 3 2 1, 3 - In Refinement, None

NUDT7A-x0453, c1cc(cnc1)Nc2nnc(s2)C(F)(F)F, FMOPL000643a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.96, 0.028, 57.6, 1.5, 99.5, 97.3, 93.3, 0.19084, 0.22052, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0454, CC(C)C(=O)N1CCC(CC1)Cc2ccccc2, FMOPL000438a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.38, 0.09, 7.4, 1.1, 100, 99.6, 100, 0.40388, 0.4596, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0455, CC(C)NC(=O)c1ccc2ccccc2n1, FMOPL000474a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.8, 0.023, 83.9, 2.9, 99.9, 97.6, 99.3, 0.17933, 0.2059, 0.17933, 0.20590, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0456, Cc1ccc(o1)C[NH+] (C)C, FMOPL000259a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.02, 0.032, 53, 1.5, 96.9, 99.6, 100, 0.20139, 0.23812, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0457, CN(C)C(=O)Nc1cnc1C(F)(F)F, FMOPL000641a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.68, 0.033, 60.5, 2.4, 99.8, 98.2, 97.7, 0.18347, 0.20824, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0458, C[NH+]1CCN(CC1)C(=O)Nc2ccccc2, FMOPL000408a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.66, 0.026, 71.3, 1.3, 99.9, 96.7, 100, 0.19035, 0.21268, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0459, CCC(=O)Nc1ccc2c(c1)[nH]c(=O)[nH]2, FMOPL000468a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.84, 0.023, 64.3, 1.2, 99.3, 97.3, 91.5, 0.18995, 0.22063, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0460, C1CC[NH+](C1)C[C@H](CO)O, FMOPL000258a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.55, 0.027, 80.5, 2.6, 99.8, 98.3, 97.8, 0.1837, 0.2041, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0461, COC(=O)c1c(ccs1)NC(=O)C2CC2, FMOPL000637a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.67, 0.456, 8.5, 2.9, 100, 99.4, 100, 0.30772, 0.35423, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0462, COCC1nnc(s1)NC(=O)c2ccccc2, FMOPL000424a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.77, 0.023, 78.2, 2, 99.6, 97.6, 95.2, 0.18445, 0.21146, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0463, CC(C)C(=O)NCc1[nH]c2ccccc2n1, FMOPL000473a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2, 0.031, 54.2, 1.6, 99.3, 97.2, 91.3, 0.18858, 0.22189, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0464, c1cc(cc(c1)C1)C[NH+]2CCOCC2, FMOPL000312a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.69, 0.024, 72, 2, 99.6, 98.1, 94.8, 0.18457, 0.21027, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0465, CC(=O)Nc1ccc(cc1)C[NH+]2CCOCC2, FMOPL000349a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.7, 0.035, 66, 2.5, 99.9, 98.2, 98.8, 0.18232, 0.20467, 0.18232, 0.20467, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0466, Cc1cccc(c1)C[NH+]2CCOCC2, FMOPL000319a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.97, 0.029, 73.6, 2.4, 99.7, 97, 96.4, 0.18268, 0.21732, 0.18268, 0.21732, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0467, CC(C)(C)C1CCC(CC1)[NH2+]Cc2ccncc2, FMOPL000368a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.83, 0.026, 63.4, 1.2, 98.8, 96.8, 100, 0.20242, 0.22651, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0468, Cc1cc(cc(c1NC)C)[N+](C)(C)C, FMOPL000318a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.82, 0.039, 43.5, 1.1, 95.9, 98.4, 100, 0.2477, 0.27499, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0469, c1cc(ccc1OCC(=O)N2CCCC2)F, FMOPL000332a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.77, 0.038, 57.9, 2.7, 99.9, 98, 98.3, 0.17973, 0.20867, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0470, COCC(=O)Nc1nc(cs1)c2ccccc2, FMOPL000355a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.67, 0.032, 59.2, 1.2, 99.7, 96.4, 99.9, 0.18973, 0.21141, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0471, c1ccc(cc1)CCC(=O)Nc2ccc(cc2)O, FMOPL000363a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.93, 0.03, 71.4, 1.8, 99.8, 97.3, 97.4, 0.20577, 0.24352, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0472, c1ccc2c(c1)OC[C@H](O2)C(=O)N3CCOCC3, FMOPL000366a, None, success, P 3 2 1, 125
 125 41 90 90 120, 2.13, 0.028, 72.9, 2.2, 99.6, 96.6, 94.4, 0.18727, 0.23534, 0.18727, 0.23534, P 3
 2 1, 2 - PANDDA model, None

NUDT7A-x0473, c1ccc(cc1)CNC2ccc(cc2)C(=O)[O-], FMOPL000343a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.62, 0.026, 80.5, 2.5, 99.8, 98.5, 97.8, 0.18009, 0.20232, 0.18009, 0.20232, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0474, c1ccc(cc1)SCC(=O)NC2CCCCC2, FMOPL000344a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.8, 0.033, 57.6, 2.5, 99.9, 97.9, 98.6, 0.17805, 0.2039, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0475, COCC(=O)Nc1cccc1C(=O)N, FMOPL000329a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.53, 0.031, 71.9, 3.1, 99.9, 98.2, 98.3, 0.17983, 0.20236, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0476, c1ccc(cc1)COc2ccc(cc2)C(=O)N, FMOPL000099a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.94, 0.026, 66.2, 1.1, 99.9, 99.6, 99.9, 0.19557, 0.23806, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0477, CCOC1ccc(cc1)NC(=O)NC(C)(C)C, FMOPL000041a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.75, 0.024, 93.1, 2.4, 99.8, 97.8, 97.2, 0.19112, 0.22596, 0.19112, 0.22596, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0478, CC[NH+]1CCN(CC1)C(=O)NC2CCCCC2, FMOPL000190a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.8, 0.033, 67.9, 2.5, 99.9, 97.6, 98.3, 0.18786, 0.22292, 0.18786, 0.22292, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0479, COc1ccc2cc(ccc2c1)c3cc[nH]n3, FMOPL000102a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.23, 0.029, 50.5, 1.3, 99.2, 96.8, 93.3, 0.19284, 0.23716, 0.19284, 0.23716, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0480, CC1(CC(=CC(=O)C1)Nc2cccc(c2)O)C, FMOPL000040a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.03, 0.029, 50.5, 1.1, 100, 99.5, 99.9, 0.19173, 0.22455, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0481, c1cnc1c2nc(on2)C3CCCC3, FMOPL000191a, None, success, P 3 2 1, 125 125 42 90 90 120, 2.23, 0.033, 40.8, 1.2, 99.1, 96.4, 90.5, 0.19274, 0.23114, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0482, CCCn1c(nnn1)NC(=O)c2cccs2, FMOPL000569a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.07, 0.035, 40, 0.5, 98.9, 96.5, 85.4, 0.17747, 0.20808, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0484, C[C@H]1CC[C@H](C1)[NH2+]Cc2ccc3c(c2)OCO3, FMOPL000043a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.34, 0.049, 47.1, 1.3, 99, 95.2, 95.3, 0.25245, 0.30386, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0485, c1ccn(c1)c2ccc(cc2)N3CCOCC3, FMOPL000192a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.02, 0.019, 80.3, 1.3, 99.4, 97.1, 95.6, 0.19791, 0.23092, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0486, COc1cccc1N2CC[NH+](CC2)CC#N, FMOPL000103a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.29, 0.026, 58.7, -2, 99.5, 95.7, 94.1, 0.18586, 0.23003, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0487, c1cc(oc1)C(=O)N2CC[NH+](CC2)CC(=O)N, FMOPL000038a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.45, 0.029, 52.2, 1.3, 99.4, 93.3, 92.7, 0.17606, 0.2168, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0488, CC1CCN(CC1)c2ccc(cc2N)C(=O)[O-], FMOPL000193a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.48, 0.052, 27, 1.1, 98.8, 93.5, 99.5, 0.21242, 0.25059, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0489, Cc1ccc(cc1)S(=O)(=O)N(C)CCC#N, FMOPL000571a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.99, 0.022, 64.6, 1.4, 97.5, 99.2, 100, 0.20442, 0.23657, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0490, Cc1cc(nol)c2nc(on2)c3cccc3, FMOPL000106a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.73, 0.023, 65.2, 1.3, 99.4, 97.1, 98.8, 0.19266, 0.21438, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0491, Cc1ccc(cc1)C(=O)n2cnc3c2cccc3, FMOPL000194a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.89, 0.021, 86.6, 1.5, 99.8, 97.8, 99.6, 0.19978, 0.22861, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0492, Cc1cc(nol)C(=O)NNc2cccc2F, FMOPL000104a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.13, 0.025, 62.4, 1.8, 99.3, 96.7, 93.2, 0.17819, 0.21899, 0.17819, 0.21899, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0493, c1ccc2c(c1)ccc(c2O)C[NH+]3CCOCC3, FMOPL000195a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.17, 0.027, 47.5, 1.2, 99.6, 96.9, 100, 0.19266, 0.23052, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0494, c1cc(ccc1C(=O)[O-])Oc2ccc(cc2)N, FMOPL000584a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.32, 0.035, 46.4, 0.8, 98.7, 95.5, 88.6, 0.21673, 0.25816, 0.21673, 0.25816, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0495, c1cc2c(cc1NC(=O)NCC3CC3)CCO2, FMOPL000100a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.46, 0.029, 62.6, 1.4, 99.5, 95.8, 99.9, 0.1957, 0.24767, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0496, CC(C)(C)NC(=O)Nc1cccc1C(=O)N, FMOPL000039a, None, success, P 3 2 1, 126 126 41
 90 90 120, 3.47, 0.059, 22.5, 2.3, 92.7, 85.8, 74.2, 0.2661, 0.34042, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0497, c1cc2c(cc1[NH2+]Cc3ccncc3)OCO2, FMOPL000196a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.97, 0.019, 80, 2, 99.7, 96.6, 97, 0.18182, 0.21447, 0.18814, 0.2162, P 3 2 1, 3 - In
 Refinement, None

NUDT7A-x0498, CC1CC[NH+](CC1)Cc2c[nH]c3c2cccc3, FMOPL000576a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.2, 0.026, 64.7, 1.8, 100, 99.2, 100, 0.2117, 0.24173, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0499, COc1ccc(cn1)NC(=O)Nc2cccs2, FMOPL000101a, None, success, P 3 2 1, 125 125 41 90
 90 120, 3.31, 0.078, 14.9, 1.3, 91.2, 91, 93.4, 0.34913, 0.3731, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0500, c1cc(ccc1N2C(=O)CCC2=O)OCC(=O)[O-], FMOPL000045a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.95, 0.024, 59.7, 1.2, 99.9, 94.2, 99.7, 0.18763, 0.21463, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0501, Cc1cccc1OCC(=O)Nc2ccnc2, FMOPL000197a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.86, 0.032, 43.8, 1.2, 99.6, 98.4, 99.8, 0.20395, 0.23509, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0502, c1ccc2c(c1)ncn2Cc3ccc(cc3)F, FMOPL000574a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.08, 0.061, 45.3, 1.6, 98.8, 97.5, 96.2, 0.22129, 0.25131, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0503, Cc1nccc(n1)c2cccc(c2)NC(=O)NC, FMOPL000110a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.9, 0.092, 21.4, 2, 99.9, 92.8, 100, 0.18172, 0.23751, 0.18771, 0.25895, P 3 2 1, 3 - In
 Refinement, None

NUDT7A-x0504, c1ccc(cc1)CCNC(=O)NC2CCCC2, FMOPL000046a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.27, 0.03, 56.5, 0.5, 99.7, 95.3, 96.6, 0.17891, 0.21454, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0505, Cc1cccc(c1C)NC(=O)C[NH+]2CCOCC2, FMOPL000198a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.27, 0.035, 49.8, 1.3, 99.5, 95.8, 93.7, 0.16931, 0.20721, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0506,CCOC(=O)c1cc(no1)c2ccc(cc2)C,FMOPL000579a, None, success, P 3 2 1,127 127 41
90 90 120,2.33,0.041,35.7,0.5,99.4,95.1,93,0.18319,0.23127, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0507,c1cc(ccc1CNC(=O)N2CCOCC2)C#N,FMOPL000108a, None, success, P 3 2 1,126 126 41
90 90 120,1.91,0.027,68.7,0.8,97.8,97.6,86.4,0.21517,0.24156,0.21517,0.24156,P 3 2 1,2
- PANDDA model, None

NUDT7A-x0510,c1c(cnc1C(=O)[O-])C#CCC2CCCC2,FMOPL000109a, None, success, P 3 2 1,125 125
41 90 90 120,2.23,0.041,53.8,1.3,98.9,93.9,94.4,0.2317,0.26977, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0511,c1ccc(cc1)NC(=O)N2CCC(CC2)C(=O)N,FMOPL000200a, None, success, P 3 2 1,124 124
41 90 90 120,2.58,0.034,46.8,1,99.4,93,99.4,0.18942,0.24169, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0512,CC(C)COc1ccc(cc1)c2csc(n2)N,FMOPL000575a, None, success, P 3 2 1,126 126 41 90
90 120,2.06,0.024,55.5,1.5,97.1,96.8,91.4,0.22621,0.25907,0.22621,0.25907,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0515,c1cc(cnc1)CNC2ccc(cc2N)C(=O)[O-],FMOPL000201a, None, success, P 3 2 1,126 126
41 90 90 120,2.01,0.028,53.2,1.6,99.7,97.3,100,0.20248,0.23734,0.20248,0.23734,P 3 2 1,2
- PANDDA model, None

NUDT7A-x0516,CCC(=O)Nc1c2cccc2oc1C(=O)N,FMOPL000577a, None, success, P 3 2 1,124 124 41 90
90 120,2.63,0.026,44.4,1.7,98.4,96.1,98.6,0.20585,0.26874, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0517,c1cc(cc(c1)c2ccc(cc2)O)C#N,FMOPL000261a, None, success, P 3 2 1,125 125 41 90
90 120,2.4,0.025,69.8,1.6,99.5,95,98.5,0.20435,0.25285,0.20435,0.25285,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0519,Cc1cc(nc(c1)NC(=O)Nc2cccc2)C,FMOPL000454a, None, success, P 3 2 1,125 125 41
90 90 120,2.44,0.037,37.2,1.1,99.1,94.8,89.4,0.16849,0.2135, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0520,CCcn1c(nnn1)NC(=O)c2ccc2,FMOPL000475a, None, success, P 3 2 1,125 125 41 90
90 120,2.08,0.026,63.3,2.2,97.9,94.6,92.1,0.20895,0.23297, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0521,c1cc(cc(c1)c2cccc(c2)O)C#N,FMOPL000262a, None, success, P 3 2 1,129 129 41 90
90 120,2.77,0.105,42.4,1.6,100,99,100,, None, None, None,1 - Analysis Pending, None

NUDT7A-x0522,CCOC(=O)c1c(nc(s1)c2cncn2)C,FMOPL000647a, None, success, P 3 2 1,127 127 41
90 90 120,2.37,0.021,67.9,1.1,98.1,92.7,99.1,0.20942,0.25232, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0523,CC(C)Oc1ccc(cc1)[C@@H]2CC(=O)NC2,FMOPL000402a, None, success, P 3 2 1,126 126
41 90 90 120,2.17,0.028,72.8,1.5,99.8,98.4,99.9,0.20368,0.24779, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0524,CC(=O)Nc1ccc(cc1)OC(=O)N2CCCC2,FMOPL000494a, None, success, P 3 2 1,126 126 41
90 90 120,2.46,0.034,54.2,1.5,99.6,94.7,95.7,0.17067,0.21711,0.17067,0.21711,P 3 2 1,2
- PANDDA model, None

NUDT7A-x0525,C[NH+](C)Cc1c[nH]c2c1cc(cc2)OC,FMOPL000690a, None, success, P 3 2 1,125 125 41
90 90 120,2.43,0.071,49.3,1.8,99.2,94.6,90.8,0.2328,0.2797,0.23280,0.27970,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0526,C1COCC[NH+]1Cc2c(snn2)C1,FMOPL000627a, None, success, P 3 2 1,126 126 41 90 90
120,3.45,0.03,51.2,6.8,98.7,86.3,88.6,0.20176,0.25188, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0527,CCc1nnc(s1)NC(=O)c2cnccn2,FMOPL000404a, None, success, P 3 2 1,126 126 41 90
 90 120,1.97,0.026,67.5,1.4,99.7,97,97.9,0.19504,0.22501, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0528,c1ccc(cc1)CC[NH+]2CCC(CC2)C(=O)N,FMOPL000481a, None, success, P 3 2 1,126 126
 41 90 90 120,1.94,0.024,70.7,3,99.8,99.8,99.3,0.20303,0.23045, None, None, None,1 -
 Analysis Pending, None

NUDT7A-x0529,CC(=O)c1ccc(cc1)OCC(=O)[O-],FMOPL000688a, None, success, P 3 2 1,126 126 41 90
 90 120,1.93,0.028,47,1.1,100,98.9,99.8,0.19533,0.22147,0.19533,0.22147,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0531,CC(=O)Nc1nc2ccc(cc2s1)C(=O)NC,FMOPL000419a, None, success, P 3 2 1,126 126 41
 90 90 120,3.16,0.076,17.9,2.2,98.6,93.4,96.7,0.20151,0.26918, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0532,Cc1c(sc2c1c(ncn2)N(C)C)C,FMOPL000466a, None, success, P 3 2 1,126 126 41 90 90
 120,2.22,0.02,67.7,4.5,95.2,95.7,73.8,0.25368,0.28971, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0533,COc1ccc2c(c1)non2,FMOPL000686a, None, success, P 3 2 1,125 125 41 90 90
 120,2.34,0.028,66.4,1.4,99.7,95.4,97.4,0.17397,0.21289, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0534,c1ccc(cc1)[C@@H](C[NH+]2CCC(CC2)C(=O)N)O,FMOPL000653a, None, success, P 3 2
 1,126 126 41 90 90
 120,2.46,0.025,60.9,1.7,99.5,94.8,93.6,0.16853,0.21635, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0535,c1cc(oc1)C(=O)NCCc2ccc(cc2)F,FMOPL000411a, None, success, P 3 2 1,126 126 41
 90 90 120,2.29,0.018,74.8,0.8,99.6,95.7,99.5,0.18668,0.22424, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0536,CC(C)c1ccc(cc1)C(=O)NC[C@@H]2CCCO2,FMOPL000493a, None, success, P 3 2 1,126
 126 41 90 90 120,2.45,0.028,57.1,1.7,99.7,94.2,97.3,0.1744,0.22303,0.17440,0.22303,P 3
 2 1,2 - PANDDA model, None

NUDT7A-x0537,c1ccc(cc1)COC(=O)NO,SDOOA000888b, None, success, P 3 2 1,126 126 41 90 90
 120,2.27,0.025,63,1.4,99.7,95.3,96.1,0.18184,0.22397,0.18184,0.22397,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0538,COC(=O)c1ccc(s1)c2cccn2,FMOPL000638a, None, success, P 3 2 1,125 125 41 90 90
 120,2.32,0.025,70,1.5,99.5,94.9,94.2,0.17875,0.21566,0.17875,0.21566,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0539,CCn1cc(cn1)CNC(=O)c2cccnc2,FMOPL000422a, None, success, P 3 2 1,126 126 41 90
 90 120,2.01,0.027,56.1,1.3,99.5,97.2,93.6,0.18576,0.21112, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0540,CC(=O)c1ccc(cc1)N2CCC(CC2)C(=O)N,FMOPL000495a, None, success, P 3 2 1,126 126
 41 90 90 120,2.57,0.029,71.5,1.4,99.4,92.6,96.1,0.24783,0.31027, None, None, None,1 -
 Analysis Pending, None

NUDT7A-x0541,CCN(CCO)c1ccc(c(c1)C)N,FMOPL000689a, None, success, P 3 2 1,126 126 41 90 90
 120,2.32,0.032,48.2,1.2,99.5,95.5,94,0.1761,0.21426, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0543,c1cc(oc1)C(=O)NC(=S)N2CCOCC2,FMOPL000401a, None, success, P 3 2 1,126 126 41
 90 90 120,1.83,0.028,57,1.2,99.5,97.8,94.3,0.18885,0.2217,0.18885,0.22170,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0545, c1ccc(cc1)COC(=O)N2CCC[C@H]2CO, FMOPL000691a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.08, 0.033, 49.5, 1.5, 98.8, 97.1, 93.9, 0.19822, 0.2272, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0546, Cc1ccc(cc1)C(=O)O[C@H]2C[NH+]3CCC2CC3, FMOPL000661a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.32, 0.025, 69, 1.8, 99.6, 95.5, 97.6, 0.19481, 0.23997, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0548, CC(=O)Nc1nc(ns1)SC, FMOPL000460a, None, success, P 3 2 1, 122 122 39 90 90 120, 1.6, 1.17, 1, 0.1, 36, 96.4, 6, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0550, C[C@H]1CN(C[C@H](O1)C)c2ccc(cc2C(=O)[O-])N, FMOPL000658a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.98, 0.079, 20.7, 1.4, 98.1, 98, 99.9, 0.2143, 0.28475, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0552, c1ccc(cc1)CCCC(=O)N2CCOCC2, FMOPL000501a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.28, 0.205, 16.5, 1.3, 99.7, 96.4, 98.6, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0553, COc1ccc(cc1N)N, FMOPL000685a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.6, 0.045, 34.4, 0.8, 98.6, 94, 98.5, 0.22746, 0.2765, 0.22746, 0.27650, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0554, Cc1c(c(n(n1)C)C)NC(=O)CC#N, FMOPL000633a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.96, 0.023, 68.6, 1.8, 95.7, 97.3, 97.8, 0.28589, 0.32666, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0556, COCC(=O)Nc1cccc1, FMOPL000504a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.84, 0.044, 37.6, 1, 99.5, 97.7, 94.1, 0.18857, 0.21791, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0557, c1ccc(cc1)NO, FMOPL000684a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.97, 0.019, 89.4, 2, 99.8, 97.3, 97.9, 0.1855, 0.21474, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0558, c1cc(oc1)C[NH+]2CCS(=O)(=O)CC2, FMOPL000629a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.28, 0.055, 33.7, 1.3, 99.3, 95.8, 91.8, 0.1863, 0.22671, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0559, COc1ccc(cc1)NCc2ccccc2O, FMOPL000426a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.02, 0.02, 74.4, 2.1, 99.7, 96.6, 96.8, 0.18564, 0.21883, 0.18564, 0.21883, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0560, c1ccc(c(c1)NC(=S)N)OC(F)(F)F, FMOPL000512a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.98, 0.023, 78.1, 1.9, 99.7, 96.6, 97.6, 0.19232, 0.22435, 0.19232, 0.22435, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0561, Cc1ccc(cc1)CNC(=O)Cc2cccs2, FMOPL000743a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.73, 0.089, 52.4, 2, 100, 99.3, 100, 0.28886, 0.35374, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0562, CC(=O)Nc1cccc1C(=O)NN, FMOPL000631a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.81, 0.021, 71.3, 1.7, 99.7, 97.4, 96.4, 0.19072, 0.21661, 0.19072, 0.21661, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0563, CCOc1ccc(cc1)NC(=O)c2cnccn2, FMOPL000446a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.51, 0.054, 40, 1.1, 98.8, 94.5, 86.1, 0.18901, 0.22552, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0564, CC(=O)NCCc1ccc(cc1)S(=O)(=O)N, FMOPL000513a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.01, 0.018, 93.2, 1.5, 99.6, 96.1, 96, 0.18702, 0.22013, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0565, Cc1ccc(c(c1)O)NC2=CC(=O)CC(C2)(C)C, FMOPL000379a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.32, 0.023, 60.4, 1.1, 99.4, 95.3, 93.1, 0.18025, 0.2248, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0567, c1ccc(c(c1)C(=O)NCCc2ccncc2)F, FMOPL000361a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.02, 0.024, 70.5, 1.9, 99.7, 96.5, 97, 0.18089, 0.21274, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0568, CC(=O)N1CCNC(=O)[C@@H]1CC(=O)OC, FMOPL000325a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.84, 0.022, 60.4, 1.4, 99.5, 97.7, 94.1, 0.1912, 0.21601, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0569, CCCC(=O)Nc1nnn(n1)CC, FMOPL000311a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.84, 0.028, 65.4, 1.3, 99.7, 97.6, 96.4, 0.18901, 0.2164, 0.18901, 0.21640, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0570, CCNC(=O)c1ccc(cc1)NS(=O)(=O)C, FMOPL000335a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.85, 0.021, 90.6, 1.5, 99.9, 96.6, 99.2, 0.19043, 0.21747, 0.19043, 0.21747, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0571, c1cc(cc(c1)NC(=O)CCC2CCCC2)C#N, FMOPL000364a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.1, 0.023, 64.5, 1.4, 99.5, 96.7, 93.5, 0.18637, 0.21986, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0572, CN(C)C(=O)Oc1ccc(cc1)c2nnco2, FMOPL000354a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.14, 0.034, 44.2, 1.5, 99.5, 96.3, 94.3, 0.17802, 0.21129, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0573, CC1CCN(CC1)C(=O)c2cc3ccccc3o2, FMOPL000372a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.57, 0.066, 34.6, 1, 98.2, 95, 100, 0.25276, 0.30692, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0574, CC(C)(CO)NC(=O)c1cccc(c1)Cl, FMOPL000324a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.04, 0.028, 57, 1.5, 99.8, 94.7, 99.9, 0.20321, 0.23552, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0575, Cc1c(nc[nH]1)C[NH+]2CCCCC2, FMOPL000317a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.09, 0.025, 71.1, 1.4, 99.2, 96.5, 92, 0.19562, 0.22963, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0576, CC[NH+]1CCC(CC1)Nc2ccccc2F, FMOPL000339a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.96, 0.025, 63.9, 1.2, 99.5, 97.4, 93.7, 0.19224, 0.22292, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0577, c1ccc(cc1)C#Cc2ccc(cc2)c3ccn[nH]3, FMOPL000111a, None, success, P 3 2 1, 126 126 42 90 90 120, 2.28, 0.022, 79.6, 1, 99.7, 95.2, 97.5, 0.17797, 0.21696, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0578, CCOC1ccc(cc1)C(=O)Nc2ccccc2, FMOPL000050a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.54, 0.039, 45.1, 1.3, 98.8, 95.5, 98.9, 0.21005, 0.26522, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0579, Cc1ccc(cc1)OCC(=O)N2CC[NH+](CC2)C, FMOPL000202a, None, success, P 3 2 1, 126 126 41 90 90 120, 1.88, 0.074, 52.6, 0.5, 99, 97.6, 97.7, 0.24304, 0.27256, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0580, Cc1cccc1c2nc(c(o2)N(C)C)C#N, FMOPL000583a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.01, 0.031, 48.1, 1.1, 99.6, 97, 95.1, 0.1856, 0.21023, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0581, CC(=O)N1CCC(CC1)C#N, XST00000907b, None, success, P 3 2 1, 126 126 41 90 90 120, 2.5, 0.064, 12, 2.6, 100, 99.2, 100, 0.28266, 0.33276, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0582,CC(=O)Nc1cccc1OCc2cccc2,FMOPL000047a, None, success, P 3 2 1,127 127 41 90
90 120,2.08,0.024,61,1.4,98.6,97.5,90.8,0.20129,0.23809, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0583,CCc1ccc(cc1)OCC(=O)N2CCCC2,FMOPL000203a, None, success, P 3 2 1,125 125 41 90
90 120,2.31,0.051,30.4,1.2,99.5,95.5,94.3,0.19619,0.22539, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0584,Cc1ccc(s1)CNc2cccc(c2)C(=O)[O-],FMOPL000582a, None, success, P 3 2 1,126 126
41 90 90 120,1.97,0.026,75,1.9,99.7,96.9,97,0.1839,0.21817,0.18390,0.21817,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0585,C[NH2+]Cc1ccc(cc1)C(F)(F)F,FMOPL000112a, None, success, P 3 2 1,126 126 41 90
90 120,1.84,0.032,53.6,1.5,99.4,97,92.1,0.1884,0.21589, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0586,COc1ccc2c(c1)cc([nH]2)C[NH3+],FMOPL000053a, None, success, P 3 2 1,126 126 41
90 90 120,2.11,0.044,54.6,1.6,99.8,92.9,100,0.19584,0.21979,0.19584,0.21979,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0587,CCOc1cccc(c1)C(=O)Nc2nnn(n2)C,FMOPL000204a, None, success, P 3 2 1,127 127 41
90 90 120,2.33,0.026,55.2,1.4,99.5,94.6,93.6,0.16971,0.20127, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0588,CCNC(=O)N1CCNC(=O)[C@H]1CC(=O)OC,FMOPL000578a, None, success, P 3 2 1,126 126
41 90 90 120,1.99,0.022,58.4,1.1,94.8,99.4,100,0.22395,0.26457, None, None, None,1 -
Analysis Pending, None

NUDT7A-x0589,c1ccc(cc1)CONC(=O)N,XST00001145b, None, success, P 3 2 1,126 126 41 90 90
120,1.83,0.028,58,1.6,99.8,97.7,97.2,0.18759,0.21488,0.18759,0.21488,P 3 2 1,2 - PANDDA
model, None

NUDT7A-x0590,COc1ccc(cc1)C#CC(=O)[O-],FMOPL000052a, None, success, P 3 2 1,126 126 41 90 90
120,2.02,0.021,84.2,1.3,99.7,96.8,96.1,0.1927,0.22379,0.19270,0.22379,P 3 2 1,2 - PANDDA
model, None

NUDT7A-x0591,CCOc1ccc(cc1)[C@@H](C)[NH3+],FMOPL000205a, None, success, P 3 2 1,126 126 41
90 90 120,2.19,0.057,31.7,1.6,99.8,97.1,99.8,0.21683,0.25686,0.21683,0.25686,P 3 2 1,2
- PANDDA model, None

NUDT7A-x0592,COc1cccc(c1)Nc2c3c([nH]cn3)ncn2,FMOPL000596a, None, success, P 3 2 1,127 127
41 90 90 120,2.97,0.037,43.9,1.4,95,91,100,0.25506,0.31146, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0593,c1ccc(cc1)Nc2nnnc2,FMOPL000113a, None, success, P 3 2 1,126 126 41 90 90
120,2.2,0.073,33.1,1,99.4,96.3,99.4,0.29715,0.35024, None, None, None,1 - Analysis
Pending, None

NUDT7A-x0594,c1cc2c(ccc(c2nc1)O)C[NH+]3CCOCC3,FMOPL000054a, None, success, P 3 2 1,126 126
41 90 90 120,2.27,0.02,77.4,1.1,99.6,94.7,95,, None, None, None,1 - Analysis Pending, None

NUDT7A-x0595,c1cc2c(cc1C[NH2+])C[C@H]3CCCO3)OCO2,FMOPL000206a, None, success, P 3 2 1,126
126 41 90 90 120,1.75,0.023,79,2.2,99.8,97.9,97.3,0.18372,0.21006,0.18372,0.21006,P 3 2
1,2 - PANDDA model, None

NUDT7A-x0596,c1ccc(cc1)NC(=O)NCCN2CCCC2=O,FMOPL000589a, None, success, P 3 2 1,126 126 41
90 90 120,1.7,0.027,57.6,1.3,99.8,98.5,100,0.19424,0.21982,0.19424,0.21982,P 3 2 1,2 -
PANDDA model, None

NUDT7A-x0597,c1ccc(c(c1)N)Nc2ccccn2,FMOPL000114a, None, success, P 3 2 1,127 127 41 90 90
120,2.09,0.02,84.7,2.3,99.7,96.7,96.6,0.18424,0.22374,0.18424,0.22374,P 3 2 1,2 - PANDDA
model, None

NUDT7A-x0598, COC(=O)C#Cc1ccc(cc1)Cl, FMOPL000060a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.87, 0.022, 64.6, 1.1, 99.6, 94.9, 99.5, 0.19346, 0.21955, 0.19346, 0.21955, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0599, CCn1c(ccn1)C[NH2+]C, FMOPL000221a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.89, 0.026, 57.1, 0.7, 99.1, 99.6, 96.1, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0602, CCNC(=O)N1CCN(CC1)C(=O)C, FMOPL000061a, None, success, P 3 2 1, 127 127 41 90 90
 120, 2.47, 0.023, 62.6, 1.2, 98.1, 94.8, 100, 0.24003, 0.28672, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0603, CS(=O)(=O)NC1CCCC1, FMOPL000222a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.96, 0.019, 77.3, 1.4, 97.6, 99.8, 98.5, 0.21388, 0.24405, 0.21388, 0.24405, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0604, CN(C)c1ccc(cc1)c2cc(on2)C(=O)OC, FMOPL000595a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.7, 0.021, 77.9, 1.1, 99.4, 92.4, 94.5, 0.2008, 0.25502, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0605, c1cc(cc(c1)F)Nc2[nH]c(=O)ccn2, FMOPL000115a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.3, 0.043, 36.3, 1.3, 99.9, 95.4, 99.9, 0.18435, 0.22055, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0606, COC(=O)C#Cc1ccc2ccccc2c1, FMOPL000062a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.44, 0.081, 49.2, 1.1, 100, 99.1, 100, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0607, CC(=O)c1ccc(cc1)OC(F)F, FMOPL000223a, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.46, 0.097, 6.9, 1.2, 100, 99.6, 100, 0.37269, 0.41697, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0608, c1ccc2c(c1)[nH]c(n2)CNC(=O)c3ccco3, FMOPL000588a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.85, 0.023, 80.5, 1.6, 99.8, 97.8, 97.3, 0.18264, 0.21215, 0.18264, 0.21215, P 3
 2 1, 2 - PANDDA model, None

NUDT7A-x0611, CCSc1nnc(s1)NC(=O)OC, FMOPL000224a, None, success, P 3 2 1, 125 125 41 90 90
 120, 2.4, 0.053, 26.5, 1.4, 99.7, 96.7, 99.3, 0.19694, 0.24349, 0.19694, 0.24349, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0612, CC(C)(C(=O)NNc1ccc2ccccc2c1)O, FMOPL000590a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.42, 0.037, 37.9, 1, 98.7, 94.7, 82.5, 0.17329, 0.2062, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0613, Cc1c(nc(=O)[nH]n1)Nc2cccc(c2)O, FMOPL000117a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.37, 0.072, 21.6, 0.8, 99.9, 97.5, 99.7, 0.20305, 0.25106, 0.20305, 0.25106, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0614, c1cc(ccc1CO)c2ccc(cc2)CO, FMOPL000064a, None, success, P 3 2 1, 126 126 41 90 90
 120, 3.49, 0.083, 12, 2, 99.8, 97, 100, 0.26631, 0.38121, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0615, COc1ccccc1OCC(=O)NN, FMOPL000225a, None, success, P 3 2 1, 126 126 41 90 90
 120, 3.19, 0.037, 34.7, 1, 94.6, 88.3, 93.3, 0.22029, 0.30843, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0616, CC(=O)c1ccc(cc1)NC(=O)C[NH+]2CCCC2, FMOPL000591a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.32, 0.036, 24.1, 1.8, 100, 99.6, 100, 0.20003, 0.24222, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0617, CS(=O)(=O)Nc1ccc(cc1)c2ccccc2, FMOPL000121a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.35, 0.026, 53.4, 1.4, 99.5, 95.4, 94.3, 0.17687, 0.21527, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0618,CS(=O)(=O)Nc1ccc(cc1)C(=O)N, FMOPL000226a, None, success, P 3 2 1, 126 126 41 90
90 120, 2, 0.024, 62.4, 0.8, 99.8, 95.8, 99.9, 0.20693, 0.24173, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0619,CC1(C[C@@H](CCO1)C(=O)Nc2ccccc2)C, FMOPL000592a, None, success, P 3 2 1, 127
127 41 90 90 120, 2.88, 0.029, 54.2, 2.1, 99.5, 91.8, 95.5, 0.17629, 0.24918, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0620,CCCc1nnc(s1)NC(=O)c2ccccc2, FMOPL000119a, None, success, P 3 2 1, 125 125 41 90
90 120, 2, 0.025, 58.1, 1.4, 99.6, 97.2, 95.2, 0.18338, 0.20872, 0.18338, 0.20872, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0621,CCc1nnc(s1)NC(=O)C(F)(F)F, FMOPL000227a, None, success, P 3 2 1, 126 126 41 90
90 120, 2.45, 0.031, 57.6, 2, 99.8, 94.4, 98.8, 0.17511, 0.21365, 0.17511, 0.21365, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0622,Cc1cc(n2c(n1)ncn2)Nc3ccc(cc3)O, FMOPL000597a, None, success, P 3 2 1, 126 126 41
90 90 120, 1.85, 0.024, 69.1, 1.2, 99.5, 96.5, 99.9, 0.19792, 0.22689, 0.19792, 0.22689, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0623,CCC[C@H](C)C(=O)Nc1c(cccc1C)C, FMOPL000720a, None, success, P 3 2 1, 126 126 42
90 90 120, 2.52, 0.095, 20.9, 0.9, 99.3, 94.2, 91.1, 0.21582, 0.27203, 0.21582, 0.27203, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0624,CCOC(=O)NCc1cccc1, FMOPL000628a, None, success, P 3 2 1, 127 127 41 90 90
120, 1.97, 0.027, 66.8, 1.8, 99.7, 97.1, 97, 0.18112, 0.21532, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0625,COc1ccc(cc1)CNC(=O)c2cncn2, FMOPL000452a, None, success, P 3 2 1, 126 126 41 90
90 120, 3.01, 0.078, 23.1, 2.5, 98.2, 90.6, 99.2, 0.17978, 0.23695, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0626,c1csc1c[NH+]2CCC(CC2)O, FMOPL000505a, None, success, P 3 2 1, 126 126 41 90 90
120, 1.66, 0.024, 77.1, 2.3, 99.7, 97.9, 97.1, 0.18661, 0.21133, 0.18661, 0.21133, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x0627,CC(C)CC(=O)Nc1ccc(cc1)NC(=O)C, FMOPL000731a, None, success, P 3 2 1, 126 126 41
90 90 120, 1.97, 0.026, 79.3, 2.3, 99.5, 97.3, 93.9, 0.19287, 0.22908, 0.19287, 0.22908, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0629,c1cnc(cn1)C(=O)NCCC=CCCC2, FMOPL000415a, None, success, P 3 2 1, 126 126 41 90
90 120, 1.9, 0.016, 102, 1.9, 98.5, 97.9, 91.9, 0.20219, 0.23149, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0630,Cc1ccc(cc1)CNC(=O)COC, FMOPL000511a, None, success, P 3 2 1, 128 128 41 90 90
120, 2.09, 0.021, 81.8, 1.6, 99.6, 96.2, 95.5, , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0631,CCOc1ccc(cc1)C(=O)Nc2cc(on2)C, FMOPL000749a, None, success, P 3 2 1, 126 126 41
90 90 120, 2.59, 0.033, 38.2, 0.8, 98.3, 94.3, 83.3, 0.18193, 0.22553, 0.18193, 0.22553, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0633,c1ccc(cc1)CCC(=O)NN2CCOCC2, FMOPL000413a, None, success, P 3 2 1, 126 126 41 90
90 120, 2.33, 0.037, 39.8, 1.1, 99.3, 98.8, 99.9, 0.20867, 0.25744, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0635,c1cc(c(c(c1)F)C(=O)N2CCCCC2)F, FMOPL000729a, None, success, P 3 2 1, 126 126 41
90 90 120, 1.77, 0.025, 66.4, 1.9, 99.7, 97.8, 95.9, 0.18112, 0.20756, 0.18112, 0.20756, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x0637,CC(C)C(=O)Nc1ccc(cc1)N2CCCCC2, FMOPL000439a, None, success, P 3 2 1, 126 126 41
90 90 120, 2.32, 0.026, 60.3, 0.8, 99.7, 95.1, 97, 0.18581, 0.22476, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0639,Cc1ccc(cc1)CNC(=O)c2ccc(cc2)C,FMOPL000754a,None,success,P 3 2 1,126 126 41
 90 90 120,2.31,0.034,52,1.2,98.9,94.3,87.9,0.20552,0.24825,None,None,None,1 - Analysis
 Pending,None

NUDT7A-x0640,c1cc(cc(c1)NC(=O)c2ccno2)C(=O)[O-],FMOPL000648a,None,success,P 3 2 1,126
 126 41 90 90 120,1.82,0.024,60.8,1.3,96.1,96.6,100,0.2309,0.24793,0.23090,0.24793,P 3 2
 1,2 - PANDDA model,None

NUDT7A-x0641,C1CCC(CC1)CCC(=O)N2CCOCC2,FMOPL000400a,None,success,P 3 2 1,125 125 41 90
 90 120,1.6,0.036,70.5,2.8,99.9,98,99.3,0.18336,0.20276,None,None,None,1 - Analysis
 Pending,None

NUDT7A-x0642,C[NH+]1CCC(CC1)OC(=O)c2cccc(c2)F,FMOPL000739a,None,success,P 3 2 1,126 126
 41 90 90 120,1.6,0.044,48.5,1.1,99.9,98.7,100,0.19369,0.21644,0.19369,0.21644,P 3 2 1,2
 - PANDDA model,None

NUDT7A-x0643,c1cc(ccc1NNC(=O)C2CCC2)F,FMOPL000636a,None,success,P 3 2 1,126 126 41 90 90
 120,2.08,0.038,24.8,1.5,100,99.7,100,0.29425,0.32549,None,None,None,1 - Analysis
 Pending,None

NUDT7A-x0644,c1ccc(cc1)NC(=O)NCc2ccc(cc2)F,FMOPL000434a,None,success,P 3 2 1,126 126 41
 90 90 120,1.87,0.034,62.4,2,99.8,97.4,97.7,0.19295,0.22489,0.19295,0.22489,P 3 2 1,2 -
 PANDDA model,None

NUDT7A-x0645,CCC(=O)Nc1ccc(cc1O)C,FMOPL000506a,None,success,P 3 2 1,126 126 41 90 90
 120,1.77,0.031,60,1.2,100,96.9,100,0.19447,0.21888,0.19447,0.21888,P 3 2 1,2 - PANDDA
 model,None

NUDT7A-x0646,c1ccc2c(c1)nc(s2)N3CCOCC3,FMOPL000705a,None,success,P 3 2 1,126 126 41 90
 90 120,1.99,0.179,30.1,2,99.9,97.2,99.7,,None,None,None,1 - Analysis Pending,None

NUDT7A-x0647,c1ccc(c(c1)NNC(=O)c2ccno2)F,FMOPL000644a,None,success,P 3 2 1,125 125 41 90
 90 120,1.68,0.07,37.6,2.6,99.9,98.1,99.3,0.18109,0.20381,0.18109,0.20381,P 3 2 1,2 -
 PANDDA model,None

NUDT7A-x0648,COC(=O)Nc1cccc(c1)NC(=O)OC,FMOPL000406a,None,success,P 3 2 1,125 125 41 90
 90 120,1.66,0.041,62.7,2.8,99.6,98.1,98.3,0.186,0.20424,0.18600,0.20424,P 3 2 1,2 -
 PANDDA model,None

NUDT7A-x0649,CNC(=O)CCC1CCCCC1,FMOPL000503a,None,success,P 3 2 1,126 126 41 90 90
 120,1.7,0.023,102.9,2.5,99.9,97.9,98.8,0.18761,0.2144,0.18761,0.21440,P 3 2 1,2 - PANDDA
 model,None

NUDT7A-x0650,Cc1cccc(c1)NC(=O)Nc2nc(cs2)C,FMOPL000744a,None,success,P 3 2 1,125 125 41
 90 90 120,1.76,0.029,73.5,2.5,99.6,98.1,94.7,0.1834,0.2069,0.18340,0.20690,P 3 2 1,2 -
 PANDDA model,None

NUDT7A-x0651,c1ccc(cc1)C(=O)NNc2ccccc2F,FMOPL000649a,None,success,P 3 2 1,126 126 41 90
 90 120,1.7,0.021,96,2.5,99.8,97.8,97.8,0.18899,0.21276,0.18899,0.21276,P 3 2 1,2 -
 PANDDA model,None

NUDT7A-x0652,COc1ccc(cc1)CNC(=O)[C@@H]2CCCO2,FMOPL000425a,None,success,P 3 2 1,128 128
 41 90 90 120,1.93,0.035,79.5,1.5,98.2,96.7,85.4,0.25689,0.3029,None,None,None,1 -
 Analysis Pending,None

NUDT7A-x0653,COC(=O)COc1ccc(cc1)C#N,FMOPL000510a,None,success,P 3 2 1,126 126 41 90 90
 120,2.18,0.022,80.1,2,99.6,95.9,94.8,,None,None,None,1 - Analysis Pending,None

NUDT7A-x0655,CC(=O)Nc1ccc(cn1)NC(=O)c2ccco2,FMOPL000656a,None,success,P 3 2 1,125 125 41
 90 90 120,2.35,0.034,49.4,1.1,99.1,95,89.1,0.17801,0.22056,None,None,None,1 - Analysis
 Pending,None

NUDT7A-x0656, COC(=O)c1ccc(cc1)NC(=O)C2CCCC2, FMOPL000450a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.54, 0.024, 80.2, 1.4, 99.7, 94, 97.7, 0.18057, 0.23342, 0.18057, 0.23342, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0658, Cc1cc(no1)NC(=O)c2ccc(cc2)N(C)C, FMOPL000753a, None, success, P 3 2 1, 126 126
 41 90 90 120, 3.18, 0.028, 46.4, 1.1, 93, 86.2, 97.9, 0.28905, 0.38199, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0659, Cc1cc(no1)C(=O)Nc2ccc3c(c2)cc[nH]3, FMOPL000659a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.28, 0.03, 49.8, 1.3, 99.5, 95.8, 93.6, 0.17242, 0.20899, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x066, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.91, 0.028, 80.2, 2.3, 99.9, 97.5, 98.5, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0660, c1ccc(cc1)CCNc2c[nH]c(=O)[nH]c2=O, FMOPL000412a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.28, 0.03, 60.3, 2.2, 99.5, 94.8, 94.7, , , None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0661, CC(C)(C)[NH+]1CC(C1)O, FMOPL000515a, None, success, P 3 2 1, 127 127 41 90 90
 120, 1.97, 0.026, 64.2, 1.8, 98.5, 97.1, 95.2, 0.18303, 0.21205, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0662, COc1cc(ccc1O)C[NH2+]C2CCCC2, FMOPL000737a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.91, 0.039, 27.8, 1.9, 93.7, 86.7, 100, 0.37757, 0.41411, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0663, Cc1ccc(cc1)C[NH+]2CCS(=O)(=O)CC2, FMOPL000642a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.35, 0.027, 55.6, 0.9, 98.4, 96.9, 98.5, 0.22115, 0.25733, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0664, CCCC(=O)NCc1[nH]c2ccccc2n1, FMOPL000518a, None, success, P 31 2 1, 126 126 41 90
 90 120, 2.05, 0.113, 63.5, 2.6, 99.9, 98.9, 99.8, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0665, CC(=O)NCC1(CCOCC1)c2ccccc2, FMOPL000733a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.97, 0.024, 55, 1.3, 99.6, 98.2, 99.6, 0.18858, 0.22064, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0666, c1cc(c(cc1Cl)N)Nc2cc[nH+]cc2, FMOPL000639a, None, success, P 3 2 1, 125 125 41
 90 90 120, 3.06, 0.081, 17, 1.5, 98.2, 92.8, 99.9, 0.3036, 0.35228, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0667, Cc1ccc(c(c1)NC(=O)Nn2cnnc2)OC, FMOPL000455a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.09, 0.018, 94.8, 1.9, 99.7, 96.7, 97, 0.18083, 0.21246, 0.18083, 0.21246, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0668, c1cc2c(ccc(c2nc1)O)C[NH+]3CCCC3, FMOPL000519a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.27, 0.027, 52.1, 0.8, 95.7, 98.8, 70.6, 0.25686, 0.31304, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0669, c1cc(cnc1)NC(=O)CC2CCCC2, FMOPL000331a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.2, 0.038, 55.9, 1.2, 99.9, 94.6, 99.9, 0.18086, 0.21595, 0.18086, 0.21595, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x067, None, None, None, success, P 6 2 2, 125 125 41 90 90
 120, 1.68, 0.104, 28.9, 1.5, 100, 99.9, 100, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0670, c1nnnc1NC(=O)CC2CCCC2, FMOPL000321a, None, success, P 3 2 1, 126 126 42 90 90
 120, 2.39, 0.017, 84.3, 1.2, 97.5, 98.6, 93.7, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0671, c1ccnc(c1)C(=O)NCCc2ccc(cc2)O, FMOPL000362a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.01, 0.022, 87, 1.8, 99.8, 96.8, 98.3, 0.1847, 0.21656, 0.18470, 0.21656, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0673, c1ccc(c(c1)c2ccc(cc2)N)C(=O)[O-], FMOPL000342a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.6, 0.03, 50.7, 1, 99.5, 93.9, 94.3, 0.17907, 0.22522, 0.17907, 0.22522, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x0674, c1ccc(c(c1)C[NH+]2CCOCC2)O, FMOPL000382a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.4, 0.06, 32, 1, 97.8, 95.8, 95.7, 0.247, 0.28505, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0675, c1ccc(c(c1)CNc2[nH]c3ccccc3n2)O, FMOPL000383a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.8, 0.087, 41.4, 1.7, 99.8, 92.6, 99.4, 0.20372, 0.27493, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0676, C[NH+]1CCS(=O)(=O)CC1, FMOPL000267a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.28, 0.02, 77.8, 1.6, 99.6, 95.5, 94.9, 0.17757, 0.21242, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0677, c1ccc(cc1)COc2ccc(cc2)C(=O)[O-], FMOPL000270a, None, success, P 3 2 1, 125 125 41 90 90 120, 2.18, 0.027, 49, 0.6, 94.7, 99, 99.2, 0.2417, 0.2877, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0678, CC(=O)Oc1ccc2c(c1)nsn2, FMOPL000268a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.3, 0.022, 56.2, 0.9, 99.8, 97.1, 100, 0.17919, 0.22783, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0680, C1COCC[NH+]1CCO, FMOPL000265a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.27, 0.027, 61, 1.1, 99, 95.7, 87.4, 0.17054, 0.2036, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0682, CS(=O)(=O)NCCc1ccc(cc1)F, FMOPL000228a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.09, 0.025, 68.7, 1.7, 98.2, 97.4, 92.7, 0.21162, 0.24936, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0683, c1ccc(cc1)CONC(=O)Nc2ccccc2, FMOPL000122a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.28, 0.021, 78.2, 0.1, 99.6, 95.2, 95.3, 0.17383, 0.21332, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0684, COc1cc(nc(n1)N)c2ccccc2, FMOPL000229a, None, success, P 3 2 1, 127 127 41 90 90 120, 2.73, 0.051, 30.2, -0.2, 92.5, 94, 92, 0.39309, 0.41329, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0685, C[NH+]1CCN(CC1)c2ccc(cc2)C#N, FMOPL000230a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.31, 0.023, 57.1, 0.7, 99.1, 97.1, 100, 0.20684, 0.25294, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0686, COc1ccc2c(c1)nc(s2)N, FMOPL000602a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.39, 0.041, 45.2, 1, 96.8, 96.1, 100, 0.282, 0.31426, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0687, Cc1c(nc(=O)[nH]n1)Nc2ccc(cc2)C(C)C, FMOPL000125a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.47, 0.088, 23.3, 1.6, 99, 92.5, 100, 0.19062, 0.23012, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0688, CCc1ccc(cc1)c2c(sc(n2)N)C, FMOPL000231a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.34, 0.043, 50, 1.6, 99.5, 95.4, 94.8, 0.18262, 0.21734, None, None, None, 1 - Analysis Pending, None

NUDT7A-x0689, COc1ccc(cc1OC)C[NH3+], FMOPL000601a, None, success, P 3 2 1, 126 126 41 90 90 120, 2.19, 0.027, 59.3, 1.1, 99.7, 97.1, 100, 0.1921, 0.2333, 0.19210, 0.23330, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x069, None, None, None, success, P 3 2 1, 125 125 41 90 90 120, 1.95, 0.017, 113.2, 2.7, 99.9, 97.3, 99.1, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0690, COc1ccc(cc1)NC(=O)Nc2ccncc2, FMOPL000127a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.97, 0.025, 64.3, 1.7, 99.5, 97.3, 94.2, 0.18475, 0.21516, 0.18475, 0.21516, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0691, Cn1cc(c(n1)C(=O)NC2CCCC2)Cl, FMOPL000232a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.38, 0.029, 44.1, 1, 98, 99, 99.9, 0.24646, 0.29214, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0692, CCOc1ccc(cc1)CC(=O)[O-], FMOPL000603a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.71, 0.055, 36.1, 0.6, 99.3, 93.2, 94.4, 0.21477, 0.26036, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0693, c1cc(oc1)C(=O)N2CCN(CC2)C(=O)C3CC3, FMOPL000123a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.91, 0.028, 57.9, 0.3, 98.6, 96.1, 86.9, 0.20271, 0.23049, 0.20271, 0.23049, P 3
 2 1, 2 - PANDDA model, None

NUDT7A-x0694, CC(=O)c1cccc(c1)NC(=O)C(F)(F)F, FMOPL000233a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.05, 0.023, 73.2, 1.3, 99.4, 94.6, 98.1, 0.18467, 0.20871, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0695, c1cc(ccc1c2nnc(s2)N)O, FMOPL000605a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.72, 0.025, 88.8, 2.4, 99.9, 98.1, 98.4, 0.18877, 0.20819, 0.18877, 0.20819, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0696, CC(C)(C)C(=O)NCCc1[nH]c2cccc2n1, FMOPL000124a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.1, 0.021, 78.9, 2.4, 99.7, 96.3, 97.3, 0.17948, 0.21111, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0697, c1ccc(cc1)NC(=O)Nc2cccnc2, FMOPL000234a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.34, 0.023, 70.9, 1.1, 98.7, 93.4, 99.8, 0.21686, 0.25971, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0698, COc1ccc(cc1)NC(=O)C[NH3+], FMOPL000604a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.23, 0.055, 32.2, 1.6, 96, 96.2, 83.4, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0699, Cc1nc2ccc(cc2o1)O, FMOPL000128a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.26, 0.024, 65.8, 1.7, 99, 95.3, 88.1, 0.19073, 0.2271, 0.19073, 0.22710, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0700, CCS(=O)(=O)NCc1ccc2c(c1)OCO2, FMOPL000235a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.18, 0.029, 63.9, 2.1, 99.6, 96.2, 95.6, 0.17811, 0.20933, 0.17811, 0.20933, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0702, Cc1ccc(cc1C)c2c(sc(n2)N)C, FMOPL000129a, None, success, P 3 2 1, 127 127 41 90
 90 120, 2.16, 0.02, 70.9, 0.5, 95.4, 99.1, 100, 0.22695, 0.26544, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0703, CCOc1cccc1N2CC[NH2+]CC2, FMOPL000609a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.97, 0.024, 74.3, 2.1, 99.6, 97, 95.2, 0.18049, 0.20879, 0.19033, 0.21387, P 3 2 1, 6 -
 Deposited, 5QGT

NUDT7A-x0704, COc1ccc(cc1)N2C[C@@H](CC2=O)C(=O)N, FMOPL000131a, None, success, P 3 2 1, 124
 124 40 90 90 120, 3.12, 0.064, 26.8, 1.3, 90.5, 89, 99.2, 0.36647, 0.44442, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0706, CC1(C[C@H](CCO1)[NH2+]Cc2ccco2)C, FMOPL000607a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.93, 0.021, 85.2, 1.8, 98.4, 98.9, 88, 0.19994, 0.2306, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0707, c1cc(ccc1C(=O)[O-])Nc2cn[nH]c(=O)n2, FMOPL000130a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.09, 0.019, 81.2, 1.4, 99.5, 95.6, 95, 0.1874, 0.22047, 0.18740, 0.22047, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0708, c1ccc(cc1)Nc2ccc(cc2N)C#N, FMOPL000238a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.97, 0.025, 80.7, 2.5, 99.8, 97.3, 98.1, 0.18848, 0.21852, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0709, CC1CCN(CC1)c2ccc(cc2Cl)N, FMOPL000608a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.17, 0.026, 56, 1.3, 99.3, 96, 95.1, 0.20974, 0.2463, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x071, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.91, 0.021, 82.7, 2.5, 99.7, 97, 97.3, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0710, c1ccc2c(c1)CC[NH+](C2)Cc3ccc(cc3)O, FMOPL000132a, None, success, P 3 2 1, 126
 126 41 90 90 120, 1.86, 0.021, 83.4, 1.6, 97.8, 96.2, 100, 0.20842, 0.23729, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0711, CC(=O)N1CCN(CC1)c2ccc(cc2)Cl, FMOPL000239a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.33, 0.02, 85, 1.8, 99.7, 95.5, 96.1, 0.17982, 0.21746, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0712, CC(C)C(=O)N1CCN(CC1)c2ccc(cc2)N, FMOPL000610a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.85, 0.04, 29.3, 1.5, 93, 93.4, 94.6, 0.2997, 0.33627, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0713, CC(=O)c1ccc(cc1)OC(=O)c2cccs2, FMOPL000735a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.32, 0.031, 46.7, 1.3, 99.5, 94.1, 94.4, 0.17302, 0.20668, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0714, c1ccc2c(c1)c(cs2)NC(=O)NC3CC3, FMOPL000640a, None, success, P 3 2 1, 126 126 41
 90 90 120, 3.22, 0.042, 30.7, 1.4, 92.6, 93.8, 98.2, 0.25184, 0.3446, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0715, CC1(CC(=CC(=O)C1)Nc2c[nH]c(=O)[nH]c2=O)C, FMOPL000444a, None, success, P 3 2
 1, 126 126 41 90 90
 120, 1.93, 0.029, 50.6, 1.1, 99.8, 97.4, 98.1, 0.1918, 0.21937, 0.19180, 0.21937, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0716, COc1ccc(cc1)C[NH2+]C2CCCC2, FMOPL000707a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.06, 0.016, 104.2, 1.9, 96.8, 94.2, 99.2, 0.19802, 0.22998, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0717, CC(=O)Nc1ccc(cc1)NC(=O)[C@H]2CC2(C)C, FMOPL000655a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.54, 0.027, 66.7, 1.9, 99.6, 93.9, 96.3, 0.17814, 0.22499, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0719, C1CN(CCC1C(=O)N)C(=O)CC#N, FMOPL000517a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.7, 0.04, 33.2, 2.9, 99.6, 99.8, 99.2, 0.21321, 0.26246, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0720, c1cc(cc(c1)F)C[NH2+]Cc2ccco2, FMOPL000703a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.29, 0.019, 77.9, -1.4, 98.4, 95.8, 95, 0.30983, 0.36955, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0722, CC[C@H](C)NC(=O)c1cc(on1)c2ccccc2, FMOPL000448a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.7, 0.023, 53.6, 0.4, 97.2, 93.2, 93, 0.21061, 0.2666, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0723, C[NH2+]CCC1CCCCC1, FMOPL000516a, None, success, P 3 2 1, 127 127 41 90 90
 120, 2.33, 0.036, 50.5, 1.2, 99.1, 95.7, 89.4, 0.18133, 0.21792, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0724, COc1cccc(c1)C(=O)Nc2ccccc2F, FMOPL000752a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.34, 0.046, 42.5, 1, 98.2, 99.3, 99.7, 0.28981, 0.34343, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0725, Cn1c(cc(=O)[nH]1)Nc2ccccc2, FMOPL000632a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.79, 0.068, 25.7, 4.4, 99.7, 92.6, 98.2, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0726, CC1CCN(CC1)C(=O)CCCC2ccccc2, FMOPL000445a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.19, 0.037, 46.6, 1.6, 99.6, 95.5, 96.3, 0.18888, 0.22326, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0727, CC1CCC(CC1)[NH2+]C2CCC(CC2)O, FMOPL000520a, None, success, P 3 2 1, 124 124 41
 90 90 120, 2.55, 0.044, 30.7, 1.1, 99.3, 94, 100, 0.18051, 0.23922, 0.18051, 0.23922, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0728, CCC(=O)Nc1nnc(s1)C2CCCC2, FMOPL000719a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.27, 0.033, 44.2, 2.2, 98.4, 96.4, 80.5, 0.21345, 0.25578, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0730, Cc1cc(nol)NC(=O)c2ccc3c(c2)non3, FMOPL000660a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.023, 51.2, 1.2, 97.2, 95.6, 97.8, 0.23699, 0.28483, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0731, Cn1cc(cn1)CNC(=O)c2ccc2, FMOPL000397a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.6, 0.035, 63.1, 2.4, 99.8, 98.1, 98, 0.18472, 0.20401, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0732, c1ccc(cc1)C(=O)Nc2ccc3c(c2)cccn3, FMOPL000534a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.7, 0.024, 92, 2.4, 99.8, 98, 97.8, 0.18657, 0.20909, 0.18657, 0.20909, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0733, Cc1ccc(c(c1)OC(=O)c2ccncc2)C, FMOPL000742a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.82, 0.02, 87.3, 2, 99.6, 97.2, 94.8, 0.18465, 0.2132, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0734, c1cc2c(cc1C(=O)N3CCOCC3)nns2, FMOPL000645a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.98, 0.034, 54.7, 2.4, 99.9, 97.3, 98.7, 0.18061, 0.21079, 0.18061, 0.21079, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0735, Cn1ccc(n1)C(=O)NC[C@H]2CCCC2, FMOPL000398a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.97, 0.027, 64.8, 1.5, 99.6, 97, 95.8, 0.18773, 0.21784, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0736, c1ccc2c(c1)[nH]c(n2)C[NH+]3CCOCC3, FMOPL000717a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.8, 0.019, 99.9, 2.6, 99.9, 97.5, 98.5, 0.18272, 0.21124, 0.18272, 0.21124, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0737, CC(=O)N1CCC(CC1)c2c[nH]c3c2cccc3, XSTXX051512c, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.6, 0.029, 84.4, 2.8, 99.9, 98.2, 98.8, 0.18358, 0.20633, 0.18358, 0.20633, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0738, CCn1cc(cn1)C(=O)NCc2ccc(cc2)F, FMOPL000449a, None, success, P 3 2 1, 125 125 41
 90 90 120, 1.77, 0.044, 52.1, 2.4, 99.9, 97.8, 98.5, 0.17828, 0.20367, 0.17828, 0.20367, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0739, Cc1c(c(nol)c2ccc(cc2)F)C(=O)NC, FMOPL000529a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.94, 0.026, 57, 1.7, 99.6, 96.8, 95, 0.18333, 0.21641, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x074, None, None, None, success, P 3 2 1, 124 124 41 90 90
 120, 1.85, 0.021, 99.1, 2.7, 99.9, 97.6, 99.1, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0740, CC(C)(C)C1CCN(CC1)C(=O)c2ccccc2, FMOPL000747a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.71, 0.026, 66, 2.1, 99.8, 98.2, 97.2, 0.18856, 0.21525, 0.19975, 0.22055, P 3 2 1, 6
 - Deposited, 5QGU

NUDT7A-x0741, c1cc(ccc1C[NH+]2CCOCC2)CO, FMOPL000663a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.67, 0.069, 29.7, 1.3, 100, 99.9, 100, 0.20984, 0.24038, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0742, Cn1c(ccn1)C(=O)NCc2cccs2, FMOPL000396a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.04, 0.12, 41.1, 1.5, 99.3, 97.1, 95.6, 0.23744, 0.26419, 0.23744, 0.26419, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0743, CC(CO)(CO)NC(=O)Nc1cccc1, FMOPL000524a, None, success, P 3 2 1, 127 127 41 90
 90 120, 1.95, 0.024, 76.7, 1.8, 99.8, 97.1, 97.7, 0.19126, 0.22095, 0.19126, 0.22095, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0744, CC(=O)Nc1cccc(c1)NC(=O)N, FMOPL000701a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.45, 0.245, 32.9, 2.3, 100, 99.2, 100, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0745, COc1ccc(cc1)Nc2c3c([nH]cn3)ncn2, PKTTA033042b, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.95, 0.019, 73.2, 1.4, 97.9, 97.9, 96.1, 0.20365, 0.24308, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0746, CC(C)(C)c1ccc(cc1)C(=O)Nc2ccon2, FMOPL000437a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.05, 0.024, 75.9, 2.3, 99.8, 96.8, 98.1, 0.17998, 0.2168, 0.17998, 0.21680, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0747, c1cc(oc1)c2nnc(s2)NC(=O)C3CC3, FMOPL000522a, None, success, P 3 2 1, 127 127 41
 90 90 120, 2.09, 0.029, 172.9, 3.2, 99.9, 99.7, 100, 0.47102, 0.46422, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0748, Cn1c(c(cn1)Cl)C(=O)N2CCCC2, FMOPL000711a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.95, 0.028, 63.5, 1, 99.4, 96.9, 92.4, 0.18424, 0.21433, 0.18424, 0.21433, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0749, COC(=O)Nc1ccc(cc1)Cc2ccncc2, FMOPL000683a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.1, 0.023, 77.5, 2.4, 99.8, 96.8, 98.2, 0.18292, 0.21646, 0.18292, 0.21646, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x075, None, None, None, success, P 3 2 1, 127 127 41 90 90
 120, 2.32, 0.025, 69.5, 1.8, 99.2, 95.6, 90.2, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0750, CC[C@H](c1cccc1)C(=O)Nc2cncn2, FMOPL000447a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.81, 0.026, 61.6, 1.4, 98.9, 97.9, 100, 0.20426, 0.23637, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0751, CC(=O)Nc1ccc(cc1)N2CC[NH+](CC2)C, FMOPL000526a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.82, 0.029, 68.4, 2.6, 99.9, 97.9, 99.5, 0.18403, 0.21068, 0.18403, 0.21068, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0752, c1ccc(cc1)OCC(=O)NC2CCCC2, FMOPL000728a, None, success, P 3 2 1, 125 125 41 90
 90 120, 1.66, 0.023, 100.6, 2.9, 99.9, 98, 98.9, 0.18146, 0.20357, 0.18146, 0.20357, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0753, C1CCC2(CC1)OC[C@@H](O2)C[NH+]3CCCC3, FMOPL000669a, None, success, P 3 2 1, 125
 125 41 90 90 120, 1.82, 0.018, 99.1, 2.4, 99.9, 97.6, 98.5, 0.1801, 0.20781, 0.18010, 0.20781, P 3
 2 1, 2 - PANDDA model, None

NUDT7A-x0754, Cc1c(c(on1)C)C(=O)NCCC2=CCCC2, FMOPL000453a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.02, 0.02, 87.7, 2.6, 99.9, 97, 98.6, 0.17721, 0.2083, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0755, COc1ccc(cc1)NCc2ccc(cc2)F, FMOPL000528a, None, success, P 3 2 1, 125 125 41 90
 90 120, 1.72, 0.038, 56.7, 2.7, 99.8, 98.2, 98.2, 0.18349, 0.21064, 0.18349, 0.21064, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0756, CC(C)Oc1cc(c(cc1Cl)Cl)N, FMOPL000269a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.8, 0.031, 71.1, 2.8, 99.9, 97.9, 98.5, 0.17732, 0.20383, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0757, c1ccc(c(c1)N)N2CCOCC2, XST00000046b, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.72, 0.038, 58.1, 2.3, 99.6, 98.1, 94.7, 0.18322, 0.20307, 0.18322, 0.20307, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0758, c1ccc(cc1)COC(=O)N2CCC(CC2)O, FMOPL000543a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.53, 0.037, 50.5, 2.1, 99.6, 94.4, 95.8, 0.16909, 0.21778, 0.16909, 0.21778, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0759, COC(=O)C1CC1, FMOPL000535a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.7, 0.044, 54.7, 2.5, 99.9, 98.3, 99.5, 0.17783, 0.20118, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x076, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.93, 0.015, 127.4, 2.6, 99.9, 97.5, 98.9, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0760, CCOC(=O)c1ccoc1, FMOPL000537a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.6, 0.028, 72, 2.3, 99.6, 98.4, 95, 0.18579, 0.20829, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0761, C[NH+]1CCC[C@@H]1CO, FMOPL000536a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.64, 0.06, 43.1, 1.6, 100, 96.9, 100, 0.22151, 0.24442, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0762, c1ccc(cc1)COCC(=O)[O-], FMOPL000539a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.91, 0.042, 50, 2, 99.9, 97.2, 98.4, 0.18019, 0.20616, 0.18019, 0.20616, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0763, CCN(CCO)c1ccc(cc1)N, FMOPL000541a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.64, 0.024, 92, 2.7, 99.9, 98, 99.2, 0.17952, 0.20456, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0764, Cc1cc(nc(n1)Nc2ccccc2)C, FMOPL000542a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.68, 0.055, 42.3, 1.2, 100, 98.3, 100, 0.21297, 0.23793, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0765, CNC(=O)c1cc(ccn1)Cl, FMOPL000538a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.7, 0.028, 82.1, 2.6, 99.8, 98.1, 98, 0.17766, 0.1995, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0766, c1ccnc(c1)c2c[nH]nc2, FMOPL000133a, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.64, 0.044, 37.5, 1.1, 100, 99.9, 100, 0.19493, 0.21898, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0767, CC(C)C(=O)N1CCN(CC1)c2ccccc2N, FMOPL000611a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.95, 0.035, 58, 2.8, 99.8, 97.4, 97.5, 0.18311, 0.21189, 0.18311, 0.21189, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0768, CC(=O)N1CCC(CC1)[NH2+]CCOC, FMOPL000134a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.28, 0.025, 67.7, -0.1, 99.4, 95.8, 92.9, 0.18571, 0.21933, 0.18571, 0.21933, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x077, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.89, 0.045, 36.6, 1.3, 100, 99.9, 100, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0770, COc1ccc2c(cc(=O)oc2c1)CC(=O)[O-], FMOPL000612a, None, success, P 3 2 1, 125 125
 41 90 90 120, 3.44, 0.038, 38.8, 4.5, 95.8, 82.7, 92.2, , , None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0771, CNc1cccc1C(F)(F)F, FMOPL000136a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.13, 0.017, 89.4, 2.1, 99.5, 95.7, 93.7, 0.1816, 0.21527, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0772, CC(=O)Nc1cccc(c1)NC(=O)COC, FMOPL000242a, None, success, P 3 2 1, 125 125 41 90
 90 120, 2.17, 0.027, 51, 1.2, 99.7, 96.2, 100, 0.18778, 0.22382, 0.18778, 0.22382, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0774, CC1([C@H]2CC=C([C@@H]1C2)C[NH+]3CCC[C@@H]3CO)C, FMOPL000351a, None, success, P
 3 2 1, 126 126 41 90 90
 120, 2.71, 0.031, 53.9, 1, 99.6, 92.2, 96.4, 0.17781, 0.22869, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0775, C[C@H]1CC[C@H](C1)[NH+]2CCN(CC2)c3cccc3, FMOPL000376a, None, success, P 3 2
 1, 126 126 41 90 90
 120, 2.67, 0.03, 42.1, 0.9, 99.2, 93.9, 98.5, 0.19274, 0.24138, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0776, c1cc(ccc1C[NH+]2CC[C@H](C2)O)C1, FMOPL000314a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.32, 0.025, 72.5, 1.8, 99.6, 94.9, 95.6, 0.17191, 0.20962, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0777, Cc1ccsc1C[NH+]2CCC[C@@H]2CO, FMOPL000320a, None, success, P 3 2 1, 127 127 41 90
 90 120, 2.6, 0.057, 20.4, 1.1, 98, 94.7, 97.9, 0.22442, 0.27592, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0778, C[C@@H]1CCCC[NH+]1Cc2ccc(cc2)C(=O)OC, FMOPL000375a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.52, 0.042, 39.8, 1, 99.1, 94.5, 89, 0.17318, 0.22111, 0.17318, 0.22111, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0779, Cc1cc(c(cc1OC)C)C[NH+]2CC[C@H](C2)O, FMOPL000359a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.7, 0.095, 26.4, 3, 100, 99.5, 99.9, 0.16744, 0.21598, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x078, None, None, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.02, 0.025, 66.6, 1.9, 99.7, 97.1, 95.9, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0780, c1ccc2c(c1)CC[NH+](C2)Cc3cccc3O, FMOPL000367a, None, success, P 3 2 1, 126 126
 41 90 90 120, 3.11, 0.036, 35.3, 1.4, 97.5, 89.6, 99.9, 0.24835, 0.341, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0781, CCC1CCC(CC1)[NH+]2CCOCC2, FMOPL000315a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.33, 0.03, 49.2, 1.3, 99.5, 94.9, 93.3, 0.16983, 0.20571, 0.16983, 0.20571, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0782, CCC1CCC(CC1)[NH2+]C[C@H]2CCCO2, FMOPL000326a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.08, 0.031, 57.4, 1.8, 99.5, 96.2, 94.1, 0.18186, 0.2084, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0783, CC(=O)N1CC[NH+](CC1)CCC2cccc2, FMOPL000370a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.27, 0.021, 66.9, 1.1, 99.6, 95.3, 96.1, 0.16932, 0.19926, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0784, Cc1c(nc[nH]1)C[NH+]2CCc3cccc3C2, FMOPL000358a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.26, 0.029, 48.8, 0.9, 99, 95.9, 88.1, 0.19015, 0.23307, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0785, Cc1c(n2cccc2n1)C(=O)NCC(C)C, FMOPL000347a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.31, n/a, 37, 1, 100, 99.3, 100, 0.50087, 0.41977, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0786, COC(=O)C1CC[NH+] (CC1) CC(=O)N, FMOPL000077a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.01, 0.023, 69.4, 1.2, 99.6, 96.6, 95.4, 0.18266, 0.21596, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0787, C1CCN(CC1)C(=O)N2CCCC2, FMOPL000010a, None, success, P 3 2 1, 127 127 41 90 90
 120, 2.61, 0.088, 22, 1.4, 99.8, 94.7, 99.8, 0.19368, 0.23261, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0788, c1cc(ccc1C[NH2+]C[C@H]2CCCO2)F, FMOPL000166a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.68, 0.032, 41.4, 0.9, 97.3, 92.8, 88.9, 0.21836, 0.29747, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0789, CCOC(=O)C1CCN(CC1)c2cncn2, FMOPL000218a, None, success, P 3 2 1, 127 127 41 90
 90 120, 2.29, 0.086, 11.1, 0.9, 99.9, 99.4, 99.4, 0.29334, 0.47907, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x079, None, None, None, success, P 3 2 1, 125 125 41 90 90
 120, 1.72, 0.03, 74.6, 2.4, 99.9, 98.2, 98.7, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0790, c1ccnc(c1)NS(=O)(=O)c2ccc(cc2)N, FMOPL000078a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.52, 0.074, 40.6, 1.3, 98.4, 94, 87.5, 0.24649, 0.29611, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0791, c1ccc(c(c1)C(=O)[O-])OC(F)(F)F, FMOPL000013a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.28, 0.02, 83.9, 0.9, 99.7, 94.2, 96.4, 0.16954, 0.20609, 0.16954, 0.20609, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0792, C1CCCC(CC1)NC(=O)[C@H]2CCCO2, FMOPL000167a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.84, 0.136, 6.9, 0.4, 99.9, 98.8, 100, 0.34295, 0.42957, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0793, c1ccc2c(c1)ncn2Cc3ccc(cc3)C#N, FMOPL000219a, None, success, P 3 2 1, 125 125 41
 90 90 120, 1.99, 0.032, 44.4, 1.1, 99.4, 97.2, 92.7, 0.18451, 0.21413, 0.18451, 0.21413, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0794, COc1ccc2c(c1)sc(n2)C, FMOPL000079a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.45, 0.022, 71.1, 1.8, 99.5, 94.1, 94.8, 0.17787, 0.22614, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0795, COc1cc(cc(c1OC)OC)C[NH3+], FMOPL000011a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2, 0.03, 49.2, 0.8, 99.2, 97.2, 91.2, 0.18585, 0.21847, 0.18585, 0.21847, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0797, Cn1c(cc(n1)c2cccs2)N, XST00000599c, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.52, 0.021, 83.8, 1.8, 99.6, 94.4, 96.8, 0.18178, 0.2197, 0.18178, 0.21970, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0798, c1ccc(cc1)COc2ccccc2N, FMOPL000014a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.27, 0.037, 43.1, 0.4, 99, 95.9, 87.6, 0.19386, 0.23232, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0799, COc1ccc(cc1)[C@@H](c2ccccc2)[NH3+], FMOPL000169a, None, success, P 3 2 1, 125
 125 41 90 90 120, 3.27, 0.048, 23.7, 1.2, 94, 88, 96.9, 0.25778, 0.3684, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0800, COc1nnc(s1)N, FMOPL000544a, None, success, P 3 2 1, 125 125 41 90 90
 120, 3.31, 0.046, 33.3, 0.7, 81.9, 83.1, 76.4, 0.27418, 0.35714, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0802, c1ccc(cc1)c2ccc(cc2)CC(=O)[O-], FMOPL000015a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.72, 0.045, 43.5, 1.2, 99.5, 91.9, 95.2, 0.18444, 0.22396, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0803,CCOC(=O)Nc1nc2ccc(cc2s1)C, FMOPL000170a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.12, 0.023, 66.3, 1.3, 99.2, 94.4, 99.8, 0.18721, 0.21716, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0804, c1cnc([nH]1)c2[nH]ccn2, FMOPL000545a, None, success, P 3 2 1, 125 125 41 90 90
 120, 3.02, 0.036, 35.9, 1.3, 97.5, 94.8, 98.7, 0.21871, 0.31435, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0805, c1cc(sc1)c2ccc(cc2)C[NH3+], FMOPL000080a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.13, 0.035, 40.9, 1.6, 99.4, 96, 100, 0.19657, 0.23243, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0806, c1ccc(cc1)C[NH2+]C2ccc(cc2)F, FMOPL000016a, None, success, P 3 2 1, 127 127 41
 90 90 120, 2.76, 0.025, 66.3, 1.7, 99.5, 92.8, 95.4, 0.1982, 0.25163, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0808, C[C@H]([C@H](c1ccccc1)O)[NH2+]C, FMOPL000548a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.15, 0.044, 38.9, 1.4, 99.8, 95.1, 99.9, 0.18408, 0.20941, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0811, c1cc(cc(c1)F)NC(=O)c2cncn2, FMOPL000172a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.9, 0.077, 27.8, 1.7, 98.2, 93.3, 99.9, 0.25989, 0.30606, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0812, c1ccc2c(c1)[nH]c(n2)NC#N, FMOPL000546a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.85, 0.03, 77.4, 2.5, 99.9, 97.3, 99.1, 0.19123, 0.22054, 0.19123, 0.22054, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0813, c1cn[nH]c1c2cc(cc(c2O)F)F, FMOPL000085a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.89, 0.017, 101.4, 1.1, 99.2, 97.4, 96.2, 0.20193, 0.23004, 0.20193, 0.23004, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0814, CC(=O)N1CCC(CC1)[NH2+]C2CC2, FMOPL000018a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.28, 0.023, 76.8, 0.3, 99.6, 95.3, 96.5, 0.19498, 0.23488, 0.19498, 0.23488, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0815, CC(C)[NH+]1CCN(CC1)C(=O)c2cccs2, FMOPL000173a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.09, 0.023, 70.3, 1.8, 99.6, 96.8, 94.9, 0.17793, 0.2079, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0816, C[NH+](C)CC#Cc1ccccc1, FMOPL000549a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.94, 0.019, 77.4, 1.8, 97.1, 97.1, 81.1, 0.21598, 0.24332, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0817, CCc1nc(nol)c2ccc(cc2)Cl, FMOPL000083a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.85, 0.02, 100.8, 1.3, 99.9, 96.2, 99.9, 0.18917, 0.21414, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0818, CN(c1ccc(cn1)C(F)(F)F)N, FMSOA000815b, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.97, 0.024, 72.5, 1.6, 99.6, 97.3, 95.7, 0.18697, 0.21973, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0819, Cc1ccc(cc1C)C(=O)Nc2nc[nH]n2, FMOPL000174a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.89, 0.095, 16, 1.7, 95.8, 98.2, 100, 0.29846, 0.37238, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0820, Cc1ccc(o1)c2ccccc2N, FMOPL000550a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.8, 0.037, 66.4, 2.8, 99.9, 97.8, 99.6, 0.19215, 0.21999, 0.19215, 0.21999, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0822, Cc1ccc(o1)c2cccc(c2)N, FMOPL000020a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.27, 0.032, 51.9, 0.9, 99.9, 93.5, 100, 0.17705, 0.21183, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0823, c1cc(ccc1NC(=O)N2CCOCC2)O, FMOPL000175a, None, success, P 3 2 1, 124 124 41 90
 90 120, 3.34, 0.084, 16.4, -0.2, 99.8, 98.9, 100, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0825, COc1ccc(cc1)C(=O)NCC(=O)N, FMOPL000090a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.79, 0.055, 26.1, 1.5, 95.7, 95, 98.7, 0.21568, 0.27356, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0826, CS(=O)(=O)Nc1ccc(cc1)C[NH3+], FMOPL000019a, None, success, P 3 2 1, 127 127 41
 90 90 120, 2.41, 0.043, 47.3, 2.1, 99.1, 93.7, 89.6, 0.17244, 0.20657, 0.17244, 0.20657, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0827, c1ccc(cc1)C2CC[NH+](CC2)CC(=O)[O-], FMOPL000176a, None, success, P 3 2 1, 127
 127 41 90 90 120, 2.8, 0.038, 36.6, 1.1, 99.8, 93.6, 100, 0.17935, 0.2281, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0828, c1cc(ccc1c2cncnc2N)Cl, FMOPL000557a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.57, 0.026, 51.3, 0.7, 99, 95.3, 92.5, 0.20482, 0.26481, 0.20482, 0.26481, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0829, COC(=O)c1c(cc(s1)c2cccs2)N, FMOPL000088a, None, success, P 3 2 1, 127 127 41 90
 90 120, 2.74, 0.029, 53.8, 2.1, 100, 99.7, 100, 0.16885, 0.22764, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0830, c1cc(cc(c1)OC(C(F)F)(F)F)N, FMOPL000021a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.27, 0.024, 68.2, 0.9, 99.6, 95.3, 95.6, 0.17829, 0.21109, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0831, C[C@H]1CCCC[NH+]1Cc2ccccc2C#N, FMOPL000177a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.44, 0.043, 34.2, 1.4, 99.9, 96, 100, 0.18581, 0.22914, 0.18581, 0.22914, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0833, CNC(=O)c1cccc1NC(=O)c2ccco2, FMOPL000751a, None, success, P 3 2 1, 127 127 41
 90 90 120, 2.19, 0.036, 35.2, 0.4, 99.3, 97.4, 100, 0.19708, 0.23884, 0.19708, 0.23884, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0834, CC(=O)Nc1ccc(cc1)C(=O)Nn2cnnc2, FMOPL000443a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.32, 0.023, 66.8, 1.3, 99.6, 94.9, 95.8, 0.18487, 0.23089, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0835, c1ccc(cc1)CNC2c[nH]c(=O)[nH]c2=O, FMOPL000470a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.22, 0.055, 31.4, 1.5, 99.8, 96.4, 98.4, 0.18482, 0.21547, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0836, c1cc(cnc1)CNC2ccc(cc2C(=O)[O-])N, FMOPL000298a, None, success, P 3 2 1, 126 126
 41 90 90 120, 2.01, 0.028, 57.6, 1.2, 99.6, 97, 96.1, 0.18982, 0.22299, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0837, Cc1c(cccc1Cl)NC(=O)[C@@H]2CCCO2, FMOPL000722a, None, success, P 3 2 1, 125 125
 41 90 90 120, 2.14, 0.034, 44.5, 1, 98.8, 95.8, 84.9, 0.18084, 0.21059, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0839, c1ccc(cc1)CC(=O)N2CCc3c2cccc3, FMOPL000491a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.68, 0.032, 42.5, 1.2, 98.6, 97.4, 99.1, 0.21417, 0.2658, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0841, CC[C@@H](C)NC(=O)c1cc(on1)c2ccccc2, FMOPL000750a, None, success, P 3 2 1, 126
 126 41 90 90 120, 2.12, 0.021, 64.5, 1, 99.6, 96.9, 99.9, 0.20537, 0.24618, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0843, c1cc(ccc1C[NH2+])C2CCCC2)O, FMOPL000467a, None, success, P 3 2 1, 126 126 41 90
 90 120, 1.82, 0.028, 74.4, 1.8, 99.7, 96.8, 96.2, 0.19101, 0.21285, 0.19101, 0.21285, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0845, c1cc(ccc1NC(=O)CC#N)OC(F)(F)F, FMOPL000725a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.28, 0.025, 62.6, 2.3, 99.6, 95.3, 95.7, 0.1823, 0.21248, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0846, Cc1c(c(n[nH]1)C)CCOc2ccc(cc2)F, FMOPL000488a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.02, 0.018, 101.3, 2.4, 99.8, 96.3, 97.7, 0.18253, 0.21495, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0847, Cc1ccc(c(c1)C)OCC(=O)N2CCOCC2, FMOPL000306a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.98, 0.02, 77.2, 1.5, 99.7, 96.6, 97.9, 0.19456, 0.22815, 0.19456, 0.22815, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0848, c1cc(ccc1C(=O)N)NC(=O)c2cncn2, FMOPL000758a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.05, 0.016, 93.8, 1.4, 98.4, 97.9, 95.8, 0.19583, 0.22626, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0850, Cc1ccc(o1)C[NH+](C)Cc2ccccc2, FMOPL000479a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.87, 0.025, 68.1, 1.2, 99.8, 97.3, 97.3, 0.18842, 0.2178, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0851, CCOC(=O)c1c(nc(s1)N(C)C(=O)C)C, FMOPL000288a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.17, 0.02, 68.4, 1.3, 99.9, 96.2, 100, 0.26087, 0.26102, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0852, c1ccc(cc1)Nc2nnc3n2nc(cc3)Cl, FMOPL000745a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.6, 0.029, 50.6, 0.5, 98.4, 95.8, 99.7, 0.20885, 0.26335, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0853, c1cc2c(cc1C(=O)N3CCCCC3)OCO2, FMOPL000435a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.07, 0.03, 47.3, 1.4, 99.3, 96.3, 91.7, 0.18751, 0.21627, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0854, COc1ccc(cc1)C(=O)Nc2ccccc2F, FMOPL000496a, None, success, P 3 2 1, 124 124 41 90
 90 120, 2.91, 0.036, 36, 1.2, 97.5, 94, 97.8, 0.20736, 0.2792, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0855, Cn1nc(nn1)NC(=O)c2ccc(cc2)Cl, FMOPL000290a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.61, 0.044, 33.1, 0.5, 99.6, 95.4, 99.8, 0.20071, 0.261, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0856, CC(=O)Nc1ccc(cc1)C#N, FMSOA000445b, None, success, P 3 2 1, 125 125 41 90 90
 120, 3.24, 0.062, 22.4, 1.7, 91.4, 91.2, 99.8, 0.24185, 0.32249, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0857, Cn1c(c(cn1)NC(=O)c2ccccc2)C(=O)N, FMOPL000456a, None, success, P 3 2 1, 127 127
 41 90 90 120, 2.42, 0.025, 67.1, 1.4, 99.8, 96, 100, 0.18356, 0.23087, 0.18356, 0.23087, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x0859, Cn1nc(nn1)NC(=O)c2cc3ccccc3o2, FMOPL000309a, None, success, P 3 2 1, 126 126 41
 90 90 120, 3.48, 0.099, 13.8, 2.2, 99.2, 87.6, 95.4, 0.18947, 0.23462, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0860, c1cc(cnc1)C[NH2+][C][C@@H]2CCC=CC2, FMOPL000760a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.72, 0.022, 103.7, 2.4, 99.9, 97.8, 99.2, 0.18448, 0.21146, 0.18448, 0.21146, P 3 2
 1, 2 - PANDDA model, None

NUDT7A-x0862, C[C@H](c1ccccc1)NC(=O)COC, FMOPL000465a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.16, 0.035, 48.2, 1.4, 99.7, 97.2, 100, 0.18974, 0.23033, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0863, CCc1ccc(cc1)C(=O)Nc2nnn(n2)CC, FMOPL000303a, None, success, P 3 2 1, 127 127 41
 90 90 120, 2.44, 0.035, 43.8, 1.2, 97.4, 95.4, 90, 0.19974, 0.23858, 0.19974, 0.23858, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x0864, CNC(=O)OCc1nccn1C, FMOPL000759a, None, success, P 3 2 1, 125 125 41 90 90
 120, 3.44, 0.087, 11.2, 3.5, 100, 96.7, 100, 0.25559, 0.34386, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0865, COc1ccc(cc1)CNC(=O)CC#N, FMOPL000389a, None, success, P 3 2 1, 127 127 41 90 90
 120, 2.37, 0.039, 38.5, 1.4, 99.9, 95.1, 100, 0.17364, 0.21068, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0866, COCC(=O)Nc1ccc(cc1)O, FMOPL000462a, None, success, P 3 2 1, 126 126 41 90 90
 120, 2.28, 0.021, 77.8, 1.2, 99.6, 95.1, 94.9, 0.1799, 0.21822, 0.17990, 0.21822, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0867, CCOc1ccc(cc1)C(=O)Nc2nnn(n2)C, FMOPL000302a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.26, 0.044, 30.8, 1.4, 99.5, 96.7, 94.9, 0.18525, 0.22273, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0869, Cc1cc(no1)NC(=O)CSc2ccccc2, FMOPL000428a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.5, 0.098, 24.3, 1, 98.6, 95.6, 99.5, , , None, None, None, 1 - Analysis Pending, None

NUDT7A-x0870, Cc1ccc(cc1)OCC(=O)Nc2cc(on2)C, FMOPL000498a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.77, 0.037, 39.3, 1.2, 97.4, 92.9, 99.9, 0.24242, 0.30558, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0871, c1cc(oc1)C(=O)Nc2ccc3c(c2)[nH]c(=O)[nH]3, FMOPL000310a, None, success, P 3 2
 1, 126 126 41 90 90 120, 3.05, 0.088, 14.8, 1.2, 100, 98.3, 100, 0.26915, 0.32266, None, None, None, 1
 - Analysis Pending, None

NUDT7A-x0872, CCCc1cc(=O)oc2c1ccc(c2)OC(=O)C, FMOPL000594a, None, success, P 3 2 1, 125 125 41
 90 90 120, 2.78, 0.032, 54.7, 1.3, 99.3, 91.7, 92.4, 0.17922, 0.22866, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0873, Cc1c(ccol)C(=O)N2CCc3c2ccccc3, FMOPL000427a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.17, 0.03, 54, 1.3, 99.4, 96, 92.1, 0.1808, 0.21592, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0874, Cc1cccc(c1)C(=O)Nc2ccc(cc2O)C, FMOPL000499a, None, success, P 3 2 1, 126 126 41
 90 90 120, 2.28, 0.029, 54.8, 0.7, 99.4, 94.5, 93, 0.17617, 0.21169, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0875, Cc1ccc(cc1)C[NH2+]Cc2ccncc2, FMOPL000289a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.43, 0.046, 33.5, 1.2, 98.8, 95.9, 99.7, 0.20451, 0.26003, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0876, COC(=O)c1ccc(o1)C[NH+]2CCCC2, FMOPL000562a, None, success, P 3 2 1, 124 124 41
 90 90 120, 2.22, 0.038, 33.5, 1.1, 99.2, 95.6, 90.9, 0.19714, 0.24347, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0877, C1CCC(CC1)NC(=O)CC#N, FMOPL000385a, None, success, P 3 2 1, 126 126 41 90 90
 120, 1.94, 0.02, 70.5, 1.8, 99.7, 97.1, 96.9, 0.17871, 0.20998, 0.17871, 0.20998, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x0878, c1cc(oc1)CNC(=O)NCc2ccco2, FMOPL000471a, None, success, P 3 2 1, 126 126 41 90
 90 120, 2.32, 0.021, 80.8, 1.9, 99.7, 93.9, 97.4, 0.21195, 0.26264, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0879, c1cc(ccc1c[NH+]2CCC(CC2)C(=O)N)F, FMOPL000346a, None, success, P 3 2 1, 126 126
 41 90 90 120, 1.79, 0.026, 64.6, 2, 99.7, 97.7, 95.9, 0.17989, 0.20676, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0880, c1c(nc[nH]1)CC[NH2+]C2CCCCC2, FMOPL000322a, None, success, P 3 2 1, 126 126 41
 90 90 120, 1.82, 0.031, 68.7, 2.1, 99.7, 97.9, 96.6, 0.1849, 0.214, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0882,CC(C)c1ccc(cc1)C[NH+]2CCC(CC2)O,FMOP000348a, None, success, P 3 2 1,126 126
 41 90 90 120,1.81,0.028,59.5,1.5,99.5,97.9,93.6,0.18463,0.21365,0.18463,0.21365,P 3 2
 1,2 - PANDDA model, None

NUDT7A-x0883,CCOc1ccc(cc1)C[NH+]2CCSCC2,FMOP000336a, None, success, P 3 2 1,126 126 41 90
 90 120,1.75,0.028,64.5,2,99.7,97.9,95.8,0.18632,0.21099, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0884,C[NH+](C)CC(=O)c1ccc(cc1)c2ccccc2,FMOP000377a, None, success, P 3 2 1,126 126
 41 90 90 120,1.8,0.041,53.1,2.3,99.7,97.7,96.1,0.18609,0.21393, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0885,Cc1ccc(cc1)C(=O)N[C@@H]2C[C@H]3CC[C@@H]2C3,FMOP000360a, None, success, P 3 2
 1,126 126 41 90 90
 120,2.08,0.029,44.2,1.5,99.6,96.9,99.7,0.18448,0.21781, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0886,Cc1c(non1)NC(=O)N2CCCC2,FMOP000330a, None, success, P 3 2 1,126 126 42 90 90
 120,2.05,0.02,81,1.7,99.6,95.3,95.5,0.18274,0.20913, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0887,CN(C)c1ccc(cc1)C(=O)Nc2ccncc2,FMOP000374a, None, success, P 3 2 1,126 126 41
 90 90 120,1.78,0.029,77.6,2,99.8,97.8,97.6,0.19342,0.22293, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0888,CCN1c2ccccc2nc1NC(=O)CC,FMOP000352a, None, success, P 3 2 1,126 126 41 90 90
 120,2.07,0.036,44,1.3,99.7,97,98.8,0.18802,0.22155, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0889,COc1ccc(cc1OC)C[NH+]2CCOCC2,FMOP000357a, None, success, P 3 2 1,126 126 41 90
 90 120,1.82,0.022,79.7,2.6,99.8,97.9,97.4,0.18474,0.21057,0.18474,0.21057,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0890,C1c2[n]cc[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2,FM010714b, None, success, P 3 2
 1,124 124 41 90 90 120,3.01,0.03,52.2,3.3,99.2,91.2,96.1,0.21839,0.2784, None, None, None, 1
 - Analysis Pending, None

NUDT7A-
 x0891,CN1[C@H]2C[C@H]3CN(C[C@@]13[C@H](O)c1c2o[n]c1C)C=O,NU000903a, None, success, P 3 2
 1,124 124 41 90 90 120,2.17,0.021,82.1,1.6,99.7,96.3,97,0.18072,0.22014, None, None, None, 1
 - Analysis Pending, None

NUDT7A-x0892,C[C@]12OC(=O)N[C@H]1C[C@@]13CNC[C@@H]1C[C@@H]2O3,FM010715b, None, success, P
 3 2 1,125 125 41 90 90
 120,2.47,0.036,42.6,1.4,99.1,98.7,99.9,0.20902,0.25858,0.20902,0.25858,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x0893,C1NC[C@]23C[C@H]4NCCN[C@H]4[C@H](C[C@H]21)O3,NU000871a, None, success, P 3 2
 1,124 124 41 90 90 120,2.2,0.039,55.4,2.6,95.2,99.2,74.5,0.31903,0.37965, None, None, None, 1 -
 Analysis Pending, None

NUDT7A-x0894,CCN1C[C@@H]2C[C@@H]3O[C@]2(Cc2[nH]c[n]c23)C1,NU000872a, None, success, P 3 2
 1,124 124 41 90 90 120,2.46,0.035,37.4,1.4,99.7,99.9,100,0.188,0.2354, None, None, None, 1
 - Analysis Pending, None

NUDT7A-x0895,C1NC[C@]23C[C@@H]4NCCN[C@@H]4[C@H](C[C@H]21)O3,NU000871b, None, success, P 3
 2 1,124 124 40 90 90
 120,2.52,0.031,48.5,1.3,98.7,99.2,100,0.22739,0.27193, None, None, None, 1 - Analysis
 Pending, None

NUDT7A-x0896,C1c2[nH]c[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2,FM010716b, None, success, P 3 2
 1,124 124 41 90 90 120,2.16,0.023,76.6,1.9,99.7,96.4,97,0.1858,0.21791, None, None, None,1
 - Analysis Pending, None

NUDT7A-x0897,O=C1C[C@@H]2[C@@H]3C[C@H]4CNC[C@]14N3Cc1cccc12,NU000904a, None, success, P 3
 2 1,124 124 41 90 90
 120,1.96,0.03,65.3,2,99.7,97.6,95.9,0.19077,0.22269, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0898,C/C(N)=C1/C(=O)[C@@H]2C[C@H]3CNC[C@]3(N2)C/1=O,NU000905a, None, success, P 3
 2 1,124 124 41 90 90
 120,2.22,0.025,54.1,1.4,99.9,99.4,98.8,0.19206,0.23417, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0899,CN1[C@H]2C[C@H]3CN(C[C@@]13C(=O)c1c[nH]cc12)CC,NU000906a, None, success, P 3
 2 1,125 125 41 90 90 120,2.5,0.032,50.8,1,98.9,99.4,100,0.22648,0.28413, None, None, None,1
 - Analysis Pending, None

NUDT7A-
 x0900,CN1[C@H]2C[C@H]3CN(C[C@@]13C(=O)c1c[nH]cc12)C(N)=O,NU000907a, None, success, P 3 2
 1,124 124 41 90 90 120,2,0.021,87.4,2,99.9,97,98.6,0.18131,0.20888, None, None, None,1 -
 Analysis Pending, None

NUDT7A-x0901,CN1[C@H]2C[C@H]3CNC[C@@]13C(=O)c1c[nH]cc12,NU000873a, None, success, P 3 2
 1,124 124 40 90 90
 120,2.33,0.031,64.8,1.9,99.6,95.4,95.1,0.18638,0.2276, None, None, None,1 - Analysis
 Pending, None

NUDT7A-x0902,Cc1[n]oc2[C@@H]3C[C@H]4CNC[C@@]4([C@H](O)c12)N3C,NU000908a, None, success, P
 3 2 1,124 124 124 41 90 90
 120,2.25,0.02,90,0.7,99.8,95.8,98.5,0.17431,0.20861,0.17431,0.20861,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x0903,CN1[C@H]2C[C@H]3CN(C[C@@]13C(=O)c1c[nH]cc12)C=O,NU000909a, None, success, P 3
 2 1,124 124 41 90 90 120,2.97,0.029,48,1.3,98,99.2,98.8,0.2228,0.30713, None, None, None,1
 - Analysis Pending, None

NUDT7A-
 x0904,CN1[C@H]2C[C@H]3CN(C[C@@]13C(=O)c1c[nH]cc12)C(C)=O,NU000910a, None, success, P 3 2
 1,124 124 40 90 90 120,2.25,0.032,53.9,0.8,99.9,99.6,99,0.18892,0.2306, None, None, None,1
 - Analysis Pending, None

NUDT7A-x0905,O[C@H]1C[C@H]([C@@H]2C[C@H]3CNC[C@@]31N2)c1cccc1,NU000598f, None, success, P
 3 2 1,124 124 40 90 90
 120,2.41,0.031,41.4,1.4,99.8,99.9,100,0.1941,0.23863, None, None, None,1 - Analysis
 Pending, None

NUDT7A-
 x0906,O[C@@H]1C[C@H]([C@@H]2C[C@H]3CNC[C@@]31N2)c1cccc1,NU000598g, None, success, P 3 2
 1,124 124 41 90 90
 120,3.29,0.024,64.8,1.4,99.4,86.7,99.3,0.21088,0.26521, None, None, None,1 - Analysis
 Pending, None

NUDT7A-
 x0907,CN(C)C(=O)CN1[C@H]2C[C@H]3CNC[C@@]13[C@H](O)C=C2.CN(C)C(=O)CN1[C@H]2C[C@H]3CNC[C@
 @]13[C@@H](O)C=C2,NU000911a, None, success, P 3 2 1,124 124 41 90 90
 120,1.8,0.024,73.2,1.5,98.4,98.4,98.5,0.19037,0.22115, None, None, None,1 - Analysis
 Pending, None

NUDT7A-
 x0908,CS(=O)(=O)N1C[C@@H]2C[C@H]3C=C[C@@H](O)[C@]2(C1)N3CCO.CS(=O)(=O)N1C[C@@H]2C[C@H]3
 C=C[C@H](O)[C@]2(C1)N3CCO,NU000912a, None, success, P 3 2 1,124 124 40 90 90

120,2.07,0.028,57.9,1.8,99.6,96.7,94.9,0.18195,0.21569, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0909, C1c2[n]c3cccc3[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2, NU000874a, None, success, P 3
2 1,124 124 40 90 120,2.35,0.029,59.2,1.7,99.2,95.2,90.7,,, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0910, OC[C@@H]1C[C@H]2CN(Cc3[n]cc[s]3)C[C@@]2(CCO)O1, NU000875a, None, success, P 3
2 1,124 124 41 90 120,2.27,0.038,41.7,1,99.7,99.9,99.9,0.18839,0.23267, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0911, OCC[C@@]12CN(C[C@@H]1C[C@@H](CO)O2)C(=O)C1CCC1, NU000876a, None, success, P 3
2 1,124 124 41 90 120,2,0.021,84.1,2,99.7,97,97,0.18502,0.21566, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x0912, C(C)(C)CN1C[C@@H]2C[C@@H](CO)O[C@@]2(C1)CCO, NU000877a, None, success, P 3 2
1,124 124 41 90 120,1.93,0.023,74.7,1.7,98.1,96.4,99.6,0.20713,0.23347, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0913, C(C)(C)CN1C[C@@H]2C[C@H]3C[C@@H](O)[C@@H](O)[C@]2(C1)O3, NU000878a, None, success, P
3 2 1,124 124 41 90 120,2.26,0.019,87.9,1.8,99.6,95.8,95.2,0.17554,0.21177, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0914, O[C@@H]1C[C@@H]2C[C@H]3CN(C[C@]3(O2)[C@@H]1O)C(=O)C1CCC1, NU000879a, None, success, P
3 2 1,124 124 41 90 120,2.03,0.019,79,2.4,96.6,98.6,82.5,0.21933,0.25365, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0915, O[C@@H]1C[C@@H]2C[C@H]3CN(Cc4[n]cc[s]4)C[C@]3(O2)[C@@H]1O, NU000880a, None, success,
P 3 2 1,124 124 41 90 120,2.17,0.017,97.7,2.2,99.9,96.3,99.3,0.17889,0.21555, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0916, O[C@@H]1C[C@@H]2C[C@H]3CN(C[C@]3(O2)[C@@H]1O)c1cccc[n]1, NU000881a, None, success, P
3 2 1,124 124 41 90 120,2.78,0.032,46.1,2.7,95.5,99.9,100,0.18217,0.23833, None, None, None, 1 - Analysis
Pending, None

NUDT7A-
x0917, CC1(C)O[C@@H]2[C@H](CO)O[C@]3(CNC[C@H]3O)C[C@@H]2O1, NU000882a, None, success, P 3 2
1,125 125 41 90 120,2.27,0.02,84.2,1.3,99.6,95.8,96.3,0.18771,0.22155, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0918, C1[C@@H]2C[C@H]3CNC[C@]3(O2)c2[n]c3cccc3[n]c21, NU000883a, None, success, P 3
2 1,124 124 41 90 120,1.96,0.022,84,2.5,99.7,97.2,96.6,0.19645,0.22232, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x0919, O[C@@H]1C[C@@H]2C[C@H]3CNC[C@]3(O2)[C@@H]1O, NU000884a, None, success, P 3 2
1,124 124 41 90 120,1.73,0.031,63.4,1.2,100,99.8,100,0.19025,0.21816, None, None, None, 1
- Analysis Pending, None

NUDT7A-x0920, C1c2[nH]c[n]c2[C@@H]2C[C@H]3CNC[C@@]31O2, FM010716c, None, success, P 3 2
1,124 124 41 90 120,1.96,0.022,84,2.5,99.7,97.2,96.6,0.19645,0.22232, None, None, None, 1 - Analysis
Pending, None

120,1.92,0.034,63.5,1.6,95.7,98.2,84.7,0.25145,0.27924,0.25145,0.27924,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x0921,C1N(CC[C@@H]2C[C@H]3CNC[C@@]31O2)C1CC1,NU000885a,None,success,P 3 2 1,124
124 41 90 90 120,2.91,0.036,38.2,1.4,99.9,98.7,100,0.17057,0.23936,None,None,None,1 -
Analysis Pending,None

NUDT7A-x0922,O=S(=O)(C(F)(F)F)N1C[C@]23CNCC[C@H](C[C@H]2C1)O3,NU000886a,None,success,P
3 2 1,125 125 41 90 90
120,2.81,0.025,61.9,1.5,99.7,92.1,97.2,0.18098,0.23799,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0923,CC1(C)O[C@H]2CC3CN(C)CC=3C[C@H](O)[C@H]2O1,NU000913a,None,success,P 3 2
1,124 124 41 90 90
120,1.96,0.021,78.7,1.6,99.2,99.4,100,0.19979,0.22833,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0924,C[C@@]12OC(=O)N[C@@H]1C[C@@H]1C[C@H]3CNC[C@]23O1,NU000887a,None,success,P
3 2 1,124 124 40 90 90
120,2.52,0.041,39,2.2,95,99.5,93.7,0.17156,0.22681,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0926,C[C@@]1(O)[C@@H](C[C@@H]2C[C@H]3CNC[C@]13O2)NC(C)=O,NU000888a,None,success,P 3 2
1,124 124 41 90 90
120,1.87,0.027,80.2,1.3,99.6,97.6,95.5,0.18699,0.22001,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0927,C[C@@]1(O)[C@@H](C[C@@H]2C[C@H]3CNC[C@]13O2)N(C)C,NU000889a,None,success,P
3 2 1,125 125 41 90 90
120,2.73,0.033,49.6,0.5,92.9,99.4,95.2,0.31447,0.37531,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0928,C[C@@]1(O)[C@H](O)C[C@@H]2C[C@H]3CN(C[C@]13O2)C(C)=O,NU000890a,None,success,P 3 2
1,124 124 41 90 90 120,2.46,0.019,70.1,1.5,99.8,99.9,100,0.17866,0.2186,None,None,None,1
- Analysis Pending,None

NUDT7A-x0929,C[C@@]1(O)[C@H](O)C[C@@H]2C[C@H]3CN(C[C@]13O2)C=O,NU000891a,None,success,P
3 2 1,124 124 41 90 90
120,2.21,0.018,69,1.7,98.9,99.1,87.6,0.19606,0.2437,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0930,O=C1C=CC2C3CC1N2CCC3,NU000892a,None,success,P 3 2 1,126 126 41 90 90
120,2.33,0.019,94.2,1.1,100,99.3,100,0.18754,0.22985,0.18754,0.22985,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x0931,CCOC(=O)[C@@H](F)[C@H](O)c1ccc(Br)c[n]1,NU000917a,None,success,P 3 2 1,124
124 41 90 90 120,1.75,0.044,49,1.3,99.9,97.8,100,0.19451,0.22264,None,None,None,2 -
PANDDA model,None

NUDT7A-
x0932,COC(=O)N1C[C@@H]2C[C@@H]3O[C@@]2(C1)Cc1[nH]c[n]c13,NU000893a,None,success,P 3 2
1,124 124 41 90 90
120,1.87,0.022,70.6,2.4,91.8,98.3,65.5,0.24874,0.27565,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0933,COC(=O)N1C[C@@H]2C[C@@H]3O[C@@]2(C1)Cc1[n]cc[n]c13,NU000894a,None,success,P 3 2
1,124 124 40 90 90
120,2.12,0.034,72.4,0.6,96.5,99.5,100,0.27344,0.30144,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0934,CC(=O)N1C[C@@H]2C[C@@H]3O[C@]2(Cc2[nH]c[n]c23)C1,NU000895a,None,success,P 3 2 1,125 125 41 90 90
120,2.08,0.025,71.1,1.6,99.7,96.8,96.3,0.18173,0.21265,None,None,None,1 - Analysis
Pending,None

NUDT7A-x0935,O=CN1C[C@@H]2C[C@@H]3O[C@]2(Cc2[nH]c[n]c23)C1,NU000896a,None,success,P 3 2 1,124 124 41 90 90 120,2.39,0.059,31,1.5,99.3,99.3,100,0.20731,0.2587,None,None,None,1
- Analysis Pending,None

NUDT7A-
x0936,CCNC(=O)N1C[C@@H]2C[C@@H]3O[C@]2(Cc2[nH]c[n]c23)C1,NU000897a,None,success,P 3 2 1,124 124 40 90 90 120,1.99,0.028,55.7,1,99.5,97.1,94.3,0.1859,0.21468,None,None,None,1
- Analysis Pending,None

NUDT7A-
x0937,C[C@]12OC(=O)N[C@H]1C[C@@]13CN(C[C@@H]1C[C@@H]2O3)C(C)=O,NU000898a,None,success,P 3 2 1,124 124 41 90 90 120,1.78,0.02,79,1.4,98.3,99.7,100,0.20539,0.23485,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0938,C[C@]12OC(=O)N(C)[C@H]1C[C@@]13CN(C)[C@@H]1C[C@@H]2O3,NU000899a,None,success,P 3 2 1,124 124 41 90 90 120,2,0.023,76,1.1,99.7,97.1,96.4,0.18949,0.22393,None,None,None,1
- Analysis Pending,None

NUDT7A-
x0939,C[C@]12OC(=O)N[C@H]1C[C@@]13CN(C[C@@H]1C[C@@H]2O3)C=O,NU000900a,None,success,P 3 2 1,124 124 41 90 90 120,1.78,0.024,71.4,1.2,99.3,99.3,100,0.1948,0.22155,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0940,Cc1cccc1[C@@H]1C[C@H](O)[C@@]23CNC[C@@H]2C[C@@H]1N3,NU000914a,None,success,P 3 2 1,124 124 41 90 90 120,2.35,0.024,63.6,0.7,97.4,99.6,100,0.26839,0.32906,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0941,O[C@H]1C[C@H]([C@@H]2C[C@H]3CNC[C@@]31N2)c1ccc(F)cc1,NU000915a,None,success,P 3 2 1,125 125 41 90 90 120,2.92,0.035,41,1.6,98.8,98.1,100,0.21131,0.29101,None,None,None,1
- Analysis Pending,None

NUDT7A-x0942,CN1[C@H]2C[C@H]3CN(C[C@@]13[C@H](O)c1c2o[n]c1C)CC,NU000916a,None,success,P 3 2 1,124 124 41 90 90 120,1.86,0.029,70.9,2.6,99.8,97.6,97.3,0.18841,0.21871,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0943,C[C@]12OC(=O)N(C)[C@H]1C[C@@]13CNC[C@@H]1C[C@@H]2O3,NU000901a,None,success,P 3 2 1,125 125 41 90 90 120,2.32,0.052,36.5,0.9,99.3,99.3,99.7,0.19886,0.24632,None,None,None,1 - Analysis
Pending,None

NUDT7A-
x0944,C[C@]12OC(=O)N[C@H]1C[C@@]13CN(C)[C@@H]1C[C@@H]2O3,NU000902a,None,success,P 3 2 1,124 124 41 90 90 120,2.27,0.028,57.4,0.3,95.7,99.9,97,0.29503,0.33757,None,None,None,1
- Analysis Pending,None

NUDT7A-x1200,None,None,None,success,P 3 2 1,124 124 40 90 90
120,1.81,0.029,74.6,2.4,99.9,98,98.8,0.17988,0.20287,None,None,None,1 - Analysis
Pending,None

NUDT7A-x1201, COc1cccc (CC (Nc2cncnc2)=O) c1, NUOOA000151a, None, success, P 3 2 1, 123 123 40 90
90 120, 1.76, 0.046, 54.1, 2.6, 99.9, 98.2, 99, 0.17867, 0.20023, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x1202, COc1cccc (CC (Nc2cccnc2)=O) c1, NUOOA000152a, None, success, P 3 2 1, 123 123 40 90
90 120, 1.88, 0.034, 69.1, 2.9, 99.9, 97.8, 99.1, 0.17633, 0.20416, None, None, None, 2 - PANDDA
model, None

NUDT7A-x1203, COc1cccc (CC (Nc2cccc (c2) [Cl])=O) c1, UNUYB062989b, None, success, P 3 2 1, 124 124
41 90 90 120, 1.59, 0.039, 68.6, 2.7, 99.9, 98.7, 98.7, 0.1817, 0.19976, 0.19559, 0.21034, P 3 2 1, 6
- Deposited, 5QGV

NUDT7A-x1204, COc1ccc (CC (Nc2cncnc2)=O) cc1, NUOOA000153a, None, success, P 3 2 1, 124 124 40 90
90 120, 1.57, 0.041, 68.3, 2.9, 99.9, 98.7, 98.8, 0.18068, 0.19729, None, None, None, 2 - PANDDA
model, None

NUDT7A-x1205, COc1ccc (CC (Nc2cccnc2)=O) cc1, NUOOA000154a, None, success, P 3 2 1, 123 123 40 90
90 120, 1.94, 0.025, 85, 2.7, 99.9, 97.6, 99.4, 0.17453, 0.20187, 0.18789, 0.20773, P 3 2 1, 6 -
Deposited, 5QGW

NUDT7A-x1206, COc1ccc (CC (Nc2cccc (c2) [Cl])=O) cc1, NUOOA000155a, None, success, P 3 2 1, 124 124
40 90 90 120, 1.61, 0.029, 85.6, 2.6, 99.9, 98.7, 99.1, 0.18185, 0.19873, 0.19779, 0.20793, P 3 2
1, 6 - Deposited, 5QGX

NUDT7A-x1207, C (C (Nc1cncnc1)=O) c1cccc1, NUOOA000156a, None, success, P 3 2 1, 123 123 40 90
90 120, 1.69, 0.031, 79.8, 2.7, 99.9, 98.5, 98.5, 0.17884, 0.19587, None, None, None, 2 - PANDDA
model, None

NUDT7A-x1208, C (C (Nc1cccnc1)=O) c1cccc1, NUOOA000157a, None, success, P 3 2 1, 123 123 40 90
90 120, 1.9, 0.028, 85.4, 2.7, 99.9, 97.8, 99.5, 0.17588, 0.20455, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x1209, None, None, None, success, P 3 2 1, 124 124 40 90 90
120, 1.56, 0.033, 83.1, 3, 99.8, 98.8, 97.8, 0.18269, 0.20027, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x1210, C (C (Nc1cccc (c1) [Cl])=O) c1cccc1, NUOOA000158a, None, success, P 3 2 1, 124 124
40 90 90 120, 1.72, 0.051, 53.5, 2.8, 99.9, 98.3, 99, 0.17935, 0.20061, 0.19472, 0.21044, P 3 2 1, 6
- Deposited, 5QGY

NUDT7A-x1211, C (C (Nc1cncnc1)=O) c1ccc (cc1) F, NUOOA000159a, None, success, P 3 2 1, 124 124 40
90 90 120, 1.56, 0.036, 79, 2.9, 99.9, 98.7, 98.8, 0.18036, 0.19565, None, None, None, 2 - PANDDA
model, None

NUDT7A-x1212, C (C (Nc1cccnc1)=O) c1ccc (cc1) F, NUOOA000160a, None, success, P 3 2 1, 123 123 40
90 90 120, 1.76, 0.021, 107.3, 2.6, 99.9, 98.2, 98.8, 0.1773, 0.19907, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x1213, C (C (Nc1cccc (c1) [Cl])=O) c1ccc (cc1) F, NUOOA000161a, None, success, P 3 2 1, 123
123 40 90 90 120, 1.65, 0.027, 95.2, 2.7, 99.9, 98.6, 99.4, 0.18024, 0.19892, 0.1956, 0.21054, P 3
2 1, 6 - Deposited, 5QGZ

NUDT7A-x1214, Cc1ccc (C) c (CC (Nc2cncnc2)=O) c1, NUOOA000162a, None, success, P 3 2 1, 123 123 40
90 90 120, 1.63, 0.049, 53.1, 2.7, 99.9, 98.5, 98.5, 0.17931, 0.19495, None, None, None, 1 - Analysis
Pending, None

NUDT7A-x1215, Cc1ccc (C) c (CC (Nc2cccnc2)=O) c1, NUOOA000163a, None, success, P 3 2 1, 124 124 40
90 90 120, 1.5, 0.027, 54.7, 1.2, 100, 99.8, 100, 0.20522, 0.2235, None, None, None, 2 - PANDDA
model, None

NUDT7A-x1216, Cc1ccc (C) c (CC (Nc2cccc (c2) [Cl])=O) c1, NUOOA000164a, None, success, P 3 2 1, 123
123 40 90 90 120, 1.63, 0.041, 65.9, 2.8, 99.9, 98.6, 98.6, 0.18381, 0.20096, None, None, None, 1 -
Analysis Pending, None

NUDT7A-x1217, Cc1ccc(C)c(CC(Nc2cc(C)on2)=O)c1, NUOOA000165a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.79, 0.023, 100.6, 2.8, 99.9, 98.1, 99.5, 0.17563, 0.19647, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1218, None, None, None, success, P 3 2 1, 124 124 40 90 90 120, 1.58, 0.037, 67.8, 2.6, 99.8, 98.7, 97.2, 0.18086, 0.19789, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1219, C(C(Nc1cncnc1)=O)c1ccc(cc1)[Cl], NUOOA000166a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.88, 0.026, 87.1, 2.9, 99.9, 97.8, 99.2, 0.17541, 0.20077, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1220, C(C(Nc1cccnc1)=O)c1ccc(cc1)[Cl], NUOOA000167a, None, success, P 3 2 1, 124 124 40 90 90 120, 1.69, 0.032, 76.3, 2.7, 99.9, 98.4, 98.8, 0.18071, 0.20005, None, None, None, 2 - PANDDA model, None

NUDT7A-x1221, C(C(Nc1cccc(c1)[Cl])=O)c1ccc(cc1)[Cl], NUOOA000168a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.9, 0.02, 102, 2.6, 99.8, 97.8, 98, 0.17693, 0.20523, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1222, COc1cccc(c1)C(Nc1cccnc1)=O, NUOOA000169a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.82, 0.028, 89.3, 2.9, 100, 98, 99.7, 0.177, 0.20303, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1223, COc1cccc(c1)C(Nc1cccc(c1)[Cl])=O, NUOOA000170a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.59, 0.035, 76.7, 2.9, 99.9, 98.7, 99.2, 0.1818, 0.19868, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1224, c1cc(cc(c1)C(F)(F)F)C(Nc1cncnc1)=O, NUOOA000171a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.79, 0.041, 65.5, 2.9, 99.9, 98.1, 99.2, 0.17751, 0.20043, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1225, c1cc(cc(c1)C(F)(F)F)C(Nc1cccnc1)=O, NUOOA000172a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.69, 0.03, 90.3, 2.7, 99.8, 98.4, 98.1, 0.17901, 0.1962, None, None, None, 2 - PANDDA model, None

NUDT7A-x1226, c1cc(cc(c1)C(F)(F)F)C(Nc1cccc(c1)[Cl])=O, NUOOA000173a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.74, 0.043, 57.9, 3, 99.8, 98.3, 96.9, 0.17912, 0.19934, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1227, None, None, None, success, P 3 2 1, 123 123 40 90 90 120, 1.56, 0.029, 79.9, 2.7, 99.8, 98.7, 97.5, 0.18127, 0.19767, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1228, c1ccc(c(c1)C(Nc1cccnc1)=O)F, NUOOA000174a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.72, 0.054, 48, 2.7, 99.9, 98.3, 99.5, 0.18089, 0.20092, 0.18624, 0.20588, P 3 2 1, 3 - In Refinement, None

NUDT7A-x1229, c1ccc(c(c1)C(Nc1cccc(c1)[Cl])=O)F, NUOOA000175a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.67, 0.031, 83.9, 2.7, 99.9, 98.5, 99.2, 0.18072, 0.20048, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1230, c1ccc(cc1)C(Nc1cccnc1)=O, NUOOA000176a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.72, 0.033, 74.2, 2.6, 99.9, 98.3, 99.1, 0.17991, 0.19981, 0.18572, 0.20456, P 3 2 1, 3 - In Refinement, None

NUDT7A-x1231, c1ccc(cc1)C(Nc1cccc(c1)[Cl])=O, NUOOA000177a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.76, 0.022, 99.6, 2.9, 99.9, 98.2, 98.4, 0.17925, 0.2027, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1232, CN(C)c1ccc(cc1)C(Nc1cccnc1)=O, NUOOA000178a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.84, 0.026, 80.7, 2.8, 99.8, 97.9, 98.1, 0.17602, 0.20137, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1233, c1cc(cnc1)NC(c1ccc(cc1[C1])[C1])=O, BDCOA000036a, None, success, P 3 2 1, 124 124 40 90 90 120, 1.82, 0.027, 93.2, 3, 99.9, 98, 99.6, 0.17651, 0.19989, None, None, None, 2 - PANDDA model, None

NUDT7A-x1234, C(C(Nc1cncnc1)=O)c1cccc(c1)O, NUOOA000179a, None, success, P 3 2 1, 124 124 40 90 90 120, 1.56, 0.046, 59.2, 2.6, 99.8, 98.8, 97.2, 0.18131, 0.19611, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1235, C(C(Nc1cccnc1)=O)c1cccc(c1)O, NUOOA000180a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.57, 0.04, 70.9, 2.9, 99.8, 98.7, 97.9, 0.18072, 0.19465, 0.19636, 0.20593, P 3 2 1, 6 - Deposited, 5QH0

NUDT7A-x1236, None, None, None, success, P 3 2 1, 123 123 40 90 90 120, 1.67, 0.04, 69.8, 3, 99.9, 98.5, 99.5, 0.18069, 0.1988, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1237, C(C(Nc1cccc(c1)[C1])=O)c1cccc(c1)O, NUOOA000181a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.65, 0.025, 103, 2.9, 99.9, 98.5, 98.7, 0.18287, 0.20321, 0.19349, 0.20307, P 3 2 1, 6 - Deposited, 5QH1

NUDT7A-x1238, Cc1cc(NC(Cc2cccc(c2)O)=O)no1, NUOOA000182a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.67, 0.053, 52.6, 3, 99.9, 98.5, 99, 0.17752, 0.19237, 0.18496, 0.20106, P 3 2 1, 3 - In Refinement, None

NUDT7A-x1239, Cc1cccc1CC(Nc1cncnc1)=O, NUOOA000183a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.76, 0.024, 100.9, 2.8, 99.9, 98.2, 99.4, 0.17631, 0.19748, None, None, None, 2 - PANDDA model, None

NUDT7A-x1240, Cc1cccc1CC(Nc1cccnc1)=O, NUOOA000184a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.69, 0.036, 77.4, 2.8, 100, 98.4, 99.6, 0.18136, 0.19979, None, None, None, 2 - PANDDA model, None

NUDT7A-x1241, Cc1cccc1CC(Nc1ccccn1)=O, NUOOA000185a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.69, 0.045, 62.3, 3, 99.9, 98.4, 98.7, 0.18271, 0.20126, 0.18991, 0.20525, P 3 2 1, 3 - In Refinement, None

NUDT7A-x1242, Cc1cccc1CC(Nc1cccc(c1)[C1])=O, NUOOA000186a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.67, 0.036, 73.7, 2.8, 100, 98.4, 99.8, 0.1806, 0.19897, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1243, Cc1cccc(CC(Nc2cncnc2)=O)c1, NUOOA000187a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.65, 0.027, 95.5, 2.8, 99.9, 98.5, 99.1, 0.18172, 0.19961, None, None, None, 2 - PANDDA model, None

NUDT7A-x1244, Cc1cccc(CC(Nc2cccnc2)=O)c1, NUOOA000188a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.74, 0.026, 99.3, 3, 99.9, 98.3, 99.3, 0.17928, 0.20027, 0.19787, 0.20942, P 3 2 1, 6 - Deposited, 5QH2

NUDT7A-x1245, None, None, None, success, P 3 2 1, 123 123 40 90 90 120, 1.79, 0.031, 83.4, 2.8, 99.9, 98.2, 99.1, 0.17896, 0.20261, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1246, Cc1cccc(CC(Nc2cccc(c2)[C1])=O)c1, NUOOA000189a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.69, 0.03, 79.3, 2.9, 99.9, 98.4, 98.5, 0.182, 0.20197, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1247, C(C(Nc1cccc(c1)[C1])=O)c1cccc(c1)[C1], NUOOA000190a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.72, 0.045, 64, 3.2, 100, 98.3, 99.6, 0.18092, 0.19866, None, None, None, 2 - PANDDA model, None

NUDT7A-x1248, C(C(Nc1cccnc1)=O)c1ccc(cc1F)F, NUOOA000191a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.65, 0.036, 72.8, 2.5, 99.8, 98.6, 97.5, 0.18, 0.19621, 0.19634, 0.20512, P 3 2 1, 6 - Deposited, 5QH3

NUDT7A-x1249, C(C(Nc1cccc(c1)[Cl])=O)c1ccc(cc1F)F, NUOOA000192a, None, success, P 3 2 1, 123 123 40 90 90 120, 1.55, 0.073, 32.5, 1.1, 100, 99.8, 100, 0.19429, 0.21674, None, None, None, 1 - Analysis Pending, None

NUDT7A-x1250, COc1cccc(CC(Nc2ccon2)=O)c1, NUOOA000220a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.67, 0.024, 86.6, 2.7, 99.8, 98.3, 98, 0.18501, 0.20572, 0.20189, 0.2184, P 3 2 1, 6 - Deposited, 5QH4

NUDT7A-x1251, COc1cccc(CC(Nc2cccn2)=O)c1, NUOOA000221a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.6, 0.037, 65.3, 2.4, 99.9, 98.5, 98.6, 0.18674, 0.21139, None, None, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x1252, Cc1cc(NC(Cc2cccc(c2)OC)=O)no1, NUOOA000222a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.62, 0.026, 86.5, 2.5, 99.9, 98.4, 98.8, 0.18761, 0.20927, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1253, COc1ccc(CC(Nc2ccon2)=O)cc1, NUOOA000283a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.53, 0.044, 63.2, 3, 99.9, 98.7, 98.9, 0.18929, 0.20845, None, None, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x1254, COc1ccc(CC(Nc2cccn2)=O)cc1, NUOOA000223a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.58, 0.023, 89.8, 2.6, 99.9, 98.6, 98.3, 0.1955, 0.21476, None, None, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x1255, Cc1cc(NC(Cc2ccc(cc2)OC)=O)no1, NUOOA000284a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.76, 0.029, 71.7, 3, 99.9, 98, 98.8, 0.18091, 0.20454, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1256, C(C(Nc1ccon1)=O)c1cccc1, NUOOA000224a, None, success, P 3 2 1, 125 125 41 90 90 120, 1.85, 0.026, 80.2, 2.5, 99.8, 97.7, 98.2, 0.18009, 0.20336, 0.19158, 0.21101, P 3 2 1, 6 - Deposited, 5QH5

NUDT7A-x1257, C(C(Nc1cccn1)=O)c1cccc1, NUOOA000225a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.71, 0.028, 87.7, 3, 99.9, 98.2, 98.9, 0.1824, 0.2076, None, None, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x1258, Cc1cc(NC(Cc2ccccc2)=O)no1, NUOOA000226a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.72, 0.019, 103.5, 2.6, 99.8, 98.2, 97.1, 0.18122, 0.20417, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1259, C(C(Nc1ccon1)=O)c1ccc(cc1)F, NUOOA000227a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.81, 0.034, 60.9, 1.3, 99.9, 99.1, 99.8, 0.18497, 0.21269, None, None, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x1260, C(C(Nc1cccn1)=O)c1ccc(cc1)F, NUOOA000228a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.81, 0.036, 65.8, 3.1, 99.9, 97.9, 98.5, 0.17865, 0.20636, None, None, P 3 2 1, 2 - PANDDA model, None

NUDT7A-x1261, Cc1cc(NC(Cc2ccc(cc2)F)=O)no1, NUOOA000229a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.72, 0.021, 100.4, 2.5, 99.9, 98.1, 98.8, 0.18264, 0.20377, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1262, Cc1ccc(C)c(CC(Nc2ccon2)=O)c1, NUOOA000230a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.74, 0.029, 78.8, 2.7, 99.9, 98.1, 98.7, 0.18137, 0.20397, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1263, Cc1ccc(C)c(CC(Nc2cccn2)=O)c1, NUOOA000231a, None, success, P 3 2 1, 124 124 41 90 90 120, 1.71, 0.025, 91.9, 2.8, 99.9, 98.1, 98.8, 0.18136, 0.20254, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1264, Cc1ccc(C)c(CC(Nc2nccn2)=O)c1, NUOOA000285a, None, success, P 3 2 1, 124 124 40 90 90 120, 1.55, 0.032, 68.7, 1.4, 100, 99.8, 100, 0.18937, 0.20898, None, None, P 3 2 1, 1 - Analysis Pending, None

NUDT7A-x1265,C(C(Nc1ccon1)=O)c1ccc(cc1)[Cl],NUOOA000232a,None,success,P 3 2 1,124 124 41
90 90 120,2.76,0.033,53.7,1.8,99.7,97.9,99.5,0.16345,0.22338,0.15851,0.20863,P 3 2 1,1
- Analysis Pending,None

NUDT7A-x1266,C(C(Nc1ccccn1)=O)c1ccc(cc1)[Cl],NUOOA000233a,None,success,P 3 2 1,124 124
40 90 90 120,1.88,0.037,54.8,1.7,99.9,99.2,100,0.18288,0.21642,None,None,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x1267,Cc1cc(NC(Cc2ccc(cc2)[Cl])=O)no1,NUOOA000234a,None,success,P 3 2 1,124 124
40 90 90 120,1.72,0.027,81.3,2.6,99.8,98.3,98.1,0.18445,0.21015,None,None,P 3 2 1,2 -
PANDDA model,None

NUDT7A-x1268,COc1cccc(c1)C(Nc1ccon1)=O,NUOOA000235a,None,success,P 3 2 1,124 124 40 90
90 120,1.72,0.032,68.2,3,99.9,98.1,98.6,0.18157,0.2073,None,None,P 3 2 1,1 - Analysis
Pending,None

NUDT7A-x1269,COc1cccc(c1)C(Nc1cncn1)=O,NUOOA000236a,None,success,P 3 2 1,124 124 40 90
90 120,1.72,0.038,61.3,2.5,99.7,98.4,96,0.18251,0.21224,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1270,COc1cccc(c1)C(Nc1ccccn1)=O,NUOOA000237a,None,success,P 3 2 1,124 124 41 90
90 120,1.8,0.028,73.9,2.4,99.9,98.1,99.2,0.18385,0.21476,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1271,Cc1cc(NC(c2cccc(c2)OC)=O)no1,NUOOA000238a,None,success,P 3 2 1,124 124 41
90 90 120,1.74,0.022,89.1,2.6,99.9,98.1,99.2,0.18287,0.20884,None,None,P 3 2 1,1 -
Analysis Pending,None

NUDT7A-x1272,c1ccnc(c1)NC(c1cccc(c1)C(F)(F)F)=O,NUOOA000239a,None,success,P 3 2 1,124
124 41 90 90 120,1.8,0.02,93.8,2.3,99.9,97.9,99,0.18001,0.20365,None,None,P 3 2 1,1 -
Analysis Pending,None

NUDT7A-x1273,Cc1cc(NC(c2cccc(c2)C(F)(F)F)=O)no1,NUOOA000240a,None,success,P 3 2 1,124
124 40 90 90 120,1.74,0.035,62.4,2.6,99.8,98,98.1,0.18305,0.2067,0.18016,0.19773,P 3 2
1,1 - Analysis Pending,None

NUDT7A-x1274,c1ccc(c(c1)C(Nc1ccon1)=O)F,NUOOA000241a,None,success,P 3 2 1,124 124 40 90
90 120,1.74,0.024,77.7,1.1,99.8,99.2,98.9,0.19219,0.22217,0.19085,0.2207,P 3 2 1,3 - In
Refinement,None

NUDT7A-x1275,c1ccc(c(c1)C(Nc1ccccn1)=O)F,NUOOA000242a,None,success,P 3 2 1,124 124 41 90
90 120,1.85,0.022,86.6,2.4,99.8,97.6,97.7,0.18142,0.21299,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1276,c1ccc(c(c1)C(Nc1ccccn1)=O)F,NUOOA000243a,None,success,P 3 2 1,124 124 40 90
90 120,1.72,0.025,75,2.1,99.8,98.1,98.1,0.18555,0.21171,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1277,Cc1cc(NC(c2cccc2F)=O)no1,NUOOA000244a,None,success,P 3 2 1,124 124 40 90
90 120,1.74,0.035,65.3,3.1,99.9,98.3,98.4,0.18204,0.20621,None,None,P 3 2 1,1 - Analysis
Pending,None

NUDT7A-x1278,c1ccc(cc1)C(Nc1ccon1)=O,NUOOA000245a,None,success,P 3 2 1,123 123 40 90 90
120,1.78,0.03,61.2,1.9,99.7,97.9,96.7,0.18498,0.21283,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1279,c1ccc(cc1)C(Nc1cncn1)=O,NUOOA000246a,None,success,P 3 2 1,124 124 41 90 90
120,1.78,0.042,52.9,2.8,99.9,97.9,98.6,0.18143,0.21027,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1280,c1ccc(cc1)C(Nc1ccccn1)=O,NUOOA000247a,None,success,P 3 2 1,124 124 41 90 90
120,1.85,0.025,80.6,2.4,99.7,97.6,96.8,0.18371,0.21588,None,None,P 3 2 1,2 - PANDDA
model,None

NUDT7A-x1281, c1ccc(cc1)C(Nc1ncccn1)=O, NUOOA000248a, None, success, P 3 2 1, 124 124 41 90 90
120, 1.73, 0.039, 54.7, 3.2, 99.9, 98.2, 98.7, 0.18134, 0.20331, None, None, P 3 2 1, 2 - PANDDA
model, None

NUDT7A-x1282, Cc1cc(NC(c2ccccc2)=O)no1, NUOOA000249a, None, success, P 3 2 1, 124 124 40 90 90
120, 1.77, 0.033, 52, 2.8, 100, 99.9, 100, 0.18487, 0.21283, None, None, P 3 2 1, 1 - Analysis
Pending, None

NUDT7A-x1283, CN(C)c1ccc(cc1)C(Nc1ccon1)=O, NUOOA000250a, None, success, P 3 2 1, 124 124 40
90 90 120, 1.72, 0.064, 33.8, 1.2, 100, 99.7, 99.9, 0.18605, 0.21036, None, None, P 3 2 1, 1 -
Analysis Pending, None

NUDT7A-x1284, CN(C)c1ccc(cc1)C(Nc1cncnc1)=O, NUOOA000251a, None, success, P 3 2 1, 124 124 41
90 90 120, 1.65, 0.035, 69.9, 2.5, 99.8, 98.3, 97, 0.18504, 0.20824, None, None, P 3 2 1, 2 - PANDDA
model, None

NUDT7A-x1285, CN(C)c1ccc(cc1)C(Nc1ccccn1)=O, NUOOA000252a, None, success, P 3 2 1, 124 124 41
90 90 120, 1.74, 0.026, 81, 2.5, 99.9, 98.3, 98.6, 0.182, 0.20848, 0.18179, 0.20832, P 3 2 1, 3 - In
Refinement, None

NUDT7A-x1286, CN(C)c1ccc(cc1)C(Nc1cccc(c1)[Cl])=O, NUOOA000253a, None, success, P 3 2 1, 124
124 41 90 90 120, 1.72, 0.035, 65.1, 2.7, 99.8, 98.1, 98, 0.18249, 0.20612, None, None, P 3 2 1, 1 -
Analysis Pending, None

NUDT7A-x1287, Cc1cc(NC(c2ccc(cc2)N(C)C)=O)no1, FMOPL000753b, None, success, P 3 2 1, 124 124
40 90 90 120, 1.76, 0.037, 59.2, 2.5, 99.9, 98.2, 99.3, 0.18588, 0.21136, None, None, P 3 2 1, 1 -
Analysis Pending, None

NUDT7A-x1288, c1cc(C(Nc2ccon2)=O)c(cc1[Cl])[Cl], NUOOA000254a, None, success, P 3 2 1, 124 124
41 90 90 120, 1.83, 0.028, 78.3, 2.6, 99.8, 97.9, 97.9, 0.18424, 0.2153, None, None, P 3 2 1, 2 -
PANDDA model, None

NUDT7A-x1289, c1ccnc(c1)NC(c1ccc(cc1[Cl])[Cl])=O, NUOOA000255a, None, success, P 3 2 1, 124
124 41 90 90 120, 1.83, 0.035, 63.3, 2.8, 99.8, 97.7, 98, 0.17881, 0.20685, None, None, P 3 2 1, 1 -
Analysis Pending, None

NUDT7A-x1290, c1cnc(NC(c2ccc(cc2[Cl])[Cl])=O)nc1, NUOOA000256a, None, success, P 3 2 1, 124
124 41 90 90 120, 1.72, 0.066, 36.9, 2.4, 99.9, 98.2, 98.6, 0.18303, 0.21003, None, None, P 3 2 1, 2
- PANDDA model, None

NUDT7A-x1291, c1cc(cc(c1)[Cl])NC(c1ccc(cc1[Cl])[Cl])=O, NUOOA000257a, None, success, P 3 2
1, 124 124 40 90 90 120, 1.63, 0.059, 38.2, 1.3, 100, 99.8, 99.9, 0.1885, 0.21131, None, None, P 3 2
1, 2 - PANDDA model, None

NUDT7A-x1292, Cc1cc(NC(c2ccc(cc2[Cl])[Cl])=O)no1, NUOOA000258a, None, success, P 3 2 1, 124
124 40 90 90 120, 1.65, 0.032, 79.6, 2.7, 99.9, 98.5, 99.2, 0.18536, 0.20904, None, None, P 3 2 1, 1
- Analysis Pending, None

NUDT7A-x1293, C(C(Nc1ccccn1)=O)c1cccc(c1)O, NUOOA000259a, None, success, P 3 2 1, 124 124 40
90 90 120, 1.57, 0.042, 55.4, 1.3, 100, 99.8, 99.9, 0.22013, 0.24833, 0.18649, 0.21523, P 3 2 1, 6 -
Deposited, 5QH6

NUDT7A-x1294, Cc1cccc1CC(Nc1ccon1)=O, NUOOA000260a, None, success, P 3 2 1, 124 124 41 90 90
120, 1.7, 0.04, 57, 2.5, 99.9, 98.4, 99.4, 0.18252, 0.20398, 0.18135, 0.20409, P 3 2 1, 3 - In
Refinement, None

NUDT7A-x1295, Cc1cccc1CC(Nc1ncccn1)=O, NUOOA000261a, None, success, P 3 2 1, 124 124 41 90 90
120, 1.74, 0.047, 49.5, 2.7, 99.9, 98.1, 99.6, 0.18325, 0.20933, None, None, P 3 2 1, 2 - PANDDA
model, None

NUDT7A-x1296, Cc1cccc1CC(Nc1cc(C)on1)=O, NUOOA000193a, None, success, P 3 2 1, 124 124 41 90
90 120, 1.78, 0.036, 56.5, 2.9, 99.9, 97.9, 99.1, 0.17916, 0.20469, 0.17743, 0.20418, P 3 2 1, 3 - In
Refinement, None

NUDT7A-x1297, Cc1cccc(CC(Nc2ccon2)=O)c1, NUOOA000194a, None, success, P 3 2 1, 124 124 41 90
 90 120, 1.74, 0.067, 37.6, 2.8, 99.9, 98.2, 99.4, 0.18308, 0.20691, 0.20019, 0.21881, P 3 2 1, 6 -
 Deposited, 5QH7

NUDT7A-x1298, Cc1cccc(CC(Nc2cccn2)=O)c1, NUOOA000195a, None, success, P 3 2 1, 124 124 41 90
 90 120, 1.76, 0.034, 66.4, 2.8, 99.8, 98, 98.1, 0.18329, 0.21036, None, None, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x1299, Cc1cccc(CC(Nc2ncccn2)=O)c1, NUOOA000196a, None, success, P 3 2 1, 124 124 41 90
 90 120, 1.78, 0.035, 70.7, 2.6, 99.9, 98.1, 98.6, 0.18373, 0.2137, None, None, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x1300, Cc1cccc(CC(Nc2cc(C)on2)=O)c1, NUOOA000197a, None, success, P 3 2 1, 124 124 40
 90 90 120, 1.85, 0.022, 87.2, 2.4, 99.8, 97.9, 98.2, 0.179, 0.20689, None, None, P 3 2 1, 1 -
 Analysis Pending, None

NUDT7A-x1301, C(C(Nc1cncnc1)=O)c1cccc(c1)[Cl], NUOOA000198a, None, success, P 3 2 1, 124 124
 40 90 90 120, 1.7, 0.041, 52.4, 1, 99.7, 99.4, 99.5, 0.19075, 0.21896, None, None, P 3 2 1, 2 - PANDDA
 model, None

NUDT7A-x1302, C(C(Nc1cccnc1)=O)c1cccc(c1)[Cl], NUOOA000199a, None, success, P 3 2 1, 124 124
 41 90 90 120, 1.76, 0.034, 65.2, 2.7, 99.9, 98, 98.4, 0.18351, 0.21149, 0.18698, 0.21214, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x1303, C(C(Nc1ccccn1)=O)c1cccc(c1)[Cl], NUOOA000200a, None, success, P 3 2 1, 124 124
 41 90 90 120, 1.99, 0.026, 78.6, 2.5, 99.8, 97, 98.4, 0.18334, 0.21217, 0.17562, 0.20252, P 3 2 1, 2
 - PANDDA model, None

NUDT7A-x1304, C(C(Nc1ncccn1)=O)c1cccc(c1)[Cl], NUOOA000201a, None, success, P 3 2 1, 124 124
 41 90 90 120, 1.7, 0.026, 88.4, 2.5, 99.7, 98.2, 96.4, 0.18608, 0.21238, None, None, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x1305, Cc1cc(NC(Cc2cccc(c2)[Cl])=O)no1, NUOOA000202a, None, success, P 3 2 1, 124 124
 41 90 90 120, 1.74, 0.022, 89.2, 2.7, 99.9, 98.1, 98.8, 0.18049, 0.20328, None, None, P 3 2 1, 1 -
 Analysis Pending, None

NUDT7A-x1306, C(C(Nc1ccon1)=O)c1ccc(cc1F)F, NUOOA000203a, None, success, P 3 2 1, 124 124 41
 90 90 120, 1.7, 0.037, 50.7, 1.4, 100, 98.4, 100, 0.19229, 0.21652, None, None, P 3 2 1, 1 - Analysis
 Pending, None

NUDT7A-x1307, C(C(Nc1cncnc1)=O)c1ccc(cc1F)F, NUOOA000204a, None, success, P 3 2 1, 124 124 41
 90 90 120, 1.76, 0.05, 46.6, 2.6, 99.9, 98, 99.1, 0.1797, 0.20451, 0.18487, 0.20992, P 3 2 1, 2 -
 PANDDA model, None

NUDT7A-x1308, C(C(Nc1ccccn1)=O)c1ccc(cc1F)F, NUOOA000205a, None, success, P 3 2 1, 124 124 40
 90 90 120, 1.88, 0.034, 70.8, 2.6, 99.8, 97.6, 98, 0.1766, 0.207, None, None, P 3 2 1, 1 - Analysis
 Pending, None

NUDT7A-x1309, C(C(Nc1ncccn1)=O)c1ccc(cc1F)F, NUOOA000206a, None, success, P 3 2 1, 124 124 40
 90 90 120, 1.7, 0.048, 50.1, 2.5, 99.8, 98.4, 97.5, 0.18445, 0.20878, None, None, P 3 2 1, 1 -
 Analysis Pending, None

NUDT7A-x1310, Cc1cc(NC(Cc2ccc(cc2F)F)=O)no1, NUOOA000207a, None, success, P 3 2 1, 124 124 40
 90 90 120, 1.65, 0.033, 69.2, 2.4, 99.8, 98.3, 98, 0.18425, 0.20632, None, None, P 3 2 1, 1 -
 Analysis Pending, None

NUDT7A-x1311, C(c1ccc(cc1)C(Nc1ccon1)=O)#N, NUOOA000208a, None, success, P 3 2 1, 124 124 40
 90 90 120, 1.67, 0.046, 49.5, 2.9, 99.9, 98.4, 99.6, 0.18621, 0.20843, None, None, P 3 2 1, 1 -
 Analysis Pending, None

NUDT7A-x1312, C(c1ccc(cc1)C(Nc1cncnc1)=O)#N, NUOOA000209a, None, success, P 3 2 1, 124 124 40
 90 90 120, 1.78, 0.05, 46.8, 2.7, 99.9, 98.1, 99.3, 0.18035, 0.20446, None, None, P 3 2 1, 1 -
 Analysis Pending, None

NUDT7A-x1313,C(c1ccc(cc1)C(Nc1cccnc1)=O)#N,NUOOA000210a, None, success, P 3 2 1,124 124 41
 90 90 120,1.72,0.02,108.9,2.6,99.9,98.1,98.7,0.184,0.20668, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1314,C(c1ccc(cc1)C(Nc1cccnc1)=O)#N,NUOOA000211a, None, success, P 3 2 1,124 124 40
 90 90 120,1.7,0.028,78.6,2.4,99.9,98.1,98.8,0.18437,0.2068, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1315,C(c1ccc(cc1)C(Nc1cccnc1)=O)#N,NUOOA000262a, None, success, P 3 2 1,124 124 40
 90 90 120,1.65,0.061,35.5,1,99.9,99.7,99.8,0.19046,0.21317, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1316,C(c1ccc(cc1)C(Nc1cccc(c1)[Cl])=O)#N,NUOOA000212a, None, success, P 3 2 1,124
 124 41 90 90 120,1.74,0.035,66.1,2.7,99.7,98,96.5,0.18157,0.205, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1317,Cc1cc(NC(c2ccc(C#N)cc2)=O)no1,NUOOA000213a, None, success, P 3 2 1,123 123 40
 90 90 120,1.67,0.027,86.5,2.6,99.8,98.4,97.7,0.18669,0.21267, None, None, P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x1318,Cc1ccc(cc1C(Nc1cncnc1)=O)F,NUOOA000214a, None, success, P 3 2 1,124 124 40 90
 90 120,1.83,0.028,70.9,2.9,99.9,98,99.2,0.18012,0.20627, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1319,Cc1ccc(cc1C(Nc1cccnc1)=O)F,NUOOA000215a, None, success, P 3 2 1,124 124 40 90
 90 120,2.51,0.043,38.6,1.2,99.9,99.9,100,0.18752,0.22679, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1320,Cc1ccc(cc1C(Nc1cccc(c1)[Cl])=O)F,NUOOA000216a, None, success, P 3 2 1,123 123
 40 90 90 120,1.72,0.059,43.2,2.8,99.9,98.3,99.4,0.18676,0.21223, None, None, P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x1321,c1cc(ccc1C(Nc1ccon1)=O)c1ccncc1,NUOOA000287a, None, success, P 3 2 1,124 124
 41 90 90 120,1.69,0.032,66.7,1.4,99.8,99.1,99.9,0.18923,0.21508, None, None, P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x1322,c1cc(ccc1C(Nc1cncnc1)=O)c1ccncc1,NUOOA000217a, None, success, P 3 2 1,123 123
 40 90 90 120,1.61,0.061,40.7,1.2,100,99.8,100,0.1962,0.22337, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1323,c1cc(cnc1)NC(c1ccc(cc1)c1ccncc1)=O,NUOOA000218a, None, success, P 3 2 1,123
 123 40 90 90 120,1.9,0.038,60.5,2.6,99.9,97.8,98.7,0.18192,0.21172, None, None, P 3 2 1,2
 - PANDDA model, None

NUDT7A-x1324, None, None, None, success, P 3 2 1,124 124 41 90 90
 120,1.85,0.029,60.7,2.7,100,99.9,100,0.18092,0.20813, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1325,COc1cccc(CC(Nc2cncnc2)=O)c1,NUOOA000151a, None, success, P 3 2 1,125 125 41 90
 90 120,1.89,0.028,66.8,1.6,99.9,99,99.8,0.18566,0.21388, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1326,COc1cccc(CC(Nc2cccnc2)=O)c1,NUOOA000152a, None, success, P 3 2 1,124 124 41 90
 90 120,1.75,0.031,62.2,1.3,100,98.7,100,0.18187,0.20754, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1327,COc1cccc(CC(Nc2cccc(c2)[Cl])=O)c1,UNUYB062989b, None, success, P 3 2 1,124 124
 41 90 90 120,1.98,0.021,95.7,2.2,99.8,97.2,98.1,0.17639,0.20826, None, None, P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x1328,COc1ccc(CC(Nc2cncnc2)=O)cc1,NUOOA000153a, None, success, P 3 2 1,124 124 41 90
 90 120,1.96,0.019,108.7,2.7,99.8,97.3,97.6,0.17672,0.20888, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1329,COc1ccc(CC(Nc2cccnc2)=O)cc1,NUOOA000154a, None, success, P 3 2 1,124 124 41 90
90 120,1.73,0.02,92.2,1.4,99.9,98.6,99.9,0.1831,0.21114, None, None, P 3 2 1,2 - PANDDA
model, None

NUDT7A-x1330,COc1ccc(CC(Nc2ccccc2)[Cl])=O)cc1,NUOOA000155a, None, success, P 3 2 1,124 124
41 90 90 120,1.91,0.032,55.9,2.5,100,99.8,100,0.17958,0.20628, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1331,C(C(Nc1cncnc1)=O)c1ccccc1,NUOOA000156a, None, success, P 3 2 1,124 124 41 90
90 120,1.93,0.023,83,2.7,99.9,97.3,99.1,0.17378,0.2059, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1332,C(C(Nc1cccnc1)=O)c1ccccc1,NUOOA000157a, None, success, P 3 2 1,124 124 41 90
90 120,1.9,0.042,50.2,2.6,99.8,97.5,97.6,0.17766,0.20849, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1333, None, None, None, success, P 3 2 1,124 124 41 90 90
120,1.76,0.029,79.5,2.5,99.9,98,99.1,0.18022,0.20479, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1334,C(C(Nc1cccc(c1)[Cl])=O)c1ccccc1,NUOOA000158a, None, success, P 3 2 1,124 124
41 90 90 120,1.88,0.024,67.7,1.5,99.9,99,100,0.17853,0.21206, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1335,C(C(Nc1cncnc1)=O)c1ccc(cc1)F,NUOOA000159a, None, success, P 3 2 1,124 124 41
90 90 120,2.02,0.053,46.8,3.1,99.9,96.9,98.6,0.17437,0.20804, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1336,C(C(Nc1cccnc1)=O)c1ccc(cc1)F,NUOOA000160a, None, success, P 3 2 1,124 124 41
90 90 120,1.8,0.029,74.2,2.9,99.9,97.9,98.8,0.17787,0.20369, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1337,C(C(Nc1cccc(c1)[Cl])=O)c1ccc(cc1)F,NUOOA000161a, None, success, P 3 2 1,124
124 41 90 90 120,1.76,0.038,59.3,2.8,99.9,98,98.4,0.17898,0.20366, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1338,Cc1ccc(C)c(CC(Nc2cncnc2)=O)c1,NUOOA000162a, None, success, P 3 2 1,124 124 41
90 90 120,1.85,0.02,102.7,2.7,99.9,97.6,98.8,0.17824,0.20753, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1339,Cc1ccc(C)c(CC(Nc2cccnc2)=O)c1,NUOOA000163a, None, success, P 3 2 1,124 124 41
90 90 120,2.28,0.028,67.1,2.5,99.9,95.6,99.2,0.17246,0.20866, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1340,Cc1ccc(C)c(CC(Nc2ccccc2)[Cl])=O)c1,NUOOA000164a, None, success, P 3 2 1,124
124 41 90 90 120,1.76,0.025,85.3,2.9,99.8,98,97.5,0.17814,0.20159, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1341,Cc1ccc(C)c(CC(Nc2cc(C)on2)=O)c1,NUOOA000165a, None, success, P 3 2 1,125 125
41 90 90 120,1.98,0.042,53.4,2.1,99.8,97.2,98.1,0.18187,0.21142, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1342, None, None, None, success, P 3 2 1,124 124 41 90 90
120,1.83,0.026,80.7,2.4,99.8,97.7,97.6,0.17919,0.20229, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1343,,,,,Failed - unknown,,,,,,,,,,,,, #NAME?,

NUDT7A-x1344,,,,,Failed - unknown,,,,,,,,,,,,, #NAME?,

NUDT7A-x1345,C(C(Nc1cccc(c1)[Cl])=O)c1ccc(cc1)[Cl],NUOOA000168a, None, success, P 3 2
1,124 124 41 90 90 120,1.68,0.05,43.3,1.1,99.9,98.2,100,0.18483,0.21071, None, None, P 3 2
1,2 - PANDDA model, None

NUDT7A-x1346,COc1cccc(c1)C(Nc1cccnc1)=O,NUOOA000169a, None, success, P 3 2 1,124 124 41 90
 90 120,1.99,0.074,36.7,2.4,95,99.9,80.3,0.18307,0.2193, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1347,COc1cccc(c1)C(Nc1cccc(c1)[Cl])=O,NUOOA000170a, None, success, P 3 2 1,124 124
 41 90 90 120,2.08,0.017,104.5,2.6,99.8,96.7,98.1,0.17354,0.20905, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1348,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1349,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1350,c1cc(cc(c1)C(F)(F)F)C(Nc1cccc(c1)[Cl])=O,NUOOA000173a, None, success, P 3 2
 1,124 124 41 90 90 120,1.75,0.026,60.4,1.2,99.9,99.4,100,0.18247,0.20812, None, None, P 3
 2 1,1 - Analysis Pending, None

NUDT7A-x1351, None, None, None, success, P 3 2 1,124 124 41 90 90
 120,1.78,0.016,124.3,2.6,99.8,97.9,98.1,0.17901,0.20646, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1352,c1ccc(c(c1)C(Nc1cccnc1)=O)F,NUOOA000174a, None, success, P 3 2 1,124 124 41 90
 90 120,1.72,0.031,65,1.2,100,99.7,100,0.18631,0.21002, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1353,c1ccc(c(c1)C(Nc1cccc(c1)[Cl])=O)F,NUOOA000175a, None, success, P 3 2 1,124 124
 41 90 90 120,1.76,0.028,78.8,2.6,99.9,98,98.7,0.17955,0.20144, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1354,c1ccc(cc1)C(Nc1cccnc1)=O,NUOOA000176a, None, success, P 3 2 1,124 124 41 90 90
 120,1.79,0.026,71.6,2.9,100,99.9,100,0.18162,0.20717, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1355,c1ccc(cc1)C(Nc1cccc(c1)[Cl])=O,NUOOA000177a, None, success, P 3 2 1,124 124 41
 90 90 120,1.74,0.028,64.9,1.6,99.9,99.1,99.5,0.18441,0.20955, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1356,CN(C)c1ccc(cc1)C(Nc1cccnc1)=O,NUOOA000178a, None, success, P 3 2 1,124 124 41
 90 90 120,1.77,0.024,72.9,1.4,100,99.5,100,0.1828,0.20617, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1357,c1cc(cnc1)NC(c1ccc(cc1[Cl])[Cl])=O,BDCOA000036a, None, success, P 3 2 1,126
 126 41 90 90 120,2.37,0.027,66.7,2.3,99.9,95.2,99.2,0.18649,0.2221, None, None, P 3 2 1,2
 - PANDDA model, None

NUDT7A-x1358,C(C(Nc1cncnc1)=O)c1cccc(c1)O,NUOOA000179a, None, success, P 3 2 1,124 124 41
 90 90 120,1.95,0.097,29.6,2.7,100,99.8,100,0.18715,0.22532, None, None, P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1359,C(C(Nc1cccnc1)=O)c1cccc(c1)O,NUOOA000180a, None, success, P 3 2 1,124 124 41
 90 90 120,1.73,0.053,47,1.4,99.9,99.2,99.8,0.18268,0.2087, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1360, None, None, None, success, P 3 2 1,124 124 41 90 90
 120,1.78,0.034,64.6,2.7,99.7,97.9,96.9,0.17858,0.20397, None, None, P 3 2 1,1 - Analysis
 Pending, None

NUDT7A-x1361,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1362,Cc1cc(NC(Cc2cccc(c2)O)=O)no1,NUOOA000182a, None, success, P 3 2 1,124 124 41
 90 90 120,1.85,0.037,51.3,1.5,100,99.2,99.9,0.18212,0.21078, None, None, P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1363,Cc1cccc1CC(Nc1cncnc1)=O,NUOOA000183a, None, success, P 3 2 1,124 124 41 90 90
120,1.88,0.031,56.7,2.6,100,99.8,100,0.18098,0.2068, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1364,Cc1cccc1CC(Nc1cccnc1)=O,NUOOA000184a, None, success, P 3 2 1,124 124 41 90 90
120,1.93,0.023,81.8,2.4,99.8,97.4,97.8,0.18067,0.21025, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1365,Cc1cccc1CC(Nc1ccccn1)=O,NUOOA000185a, None, success, P 3 2 1,124 124 41 90 90
120,1.72,0.037,58.6,1.1,100,99.3,99.9,0.1852,0.20964, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1366,Cc1cccc1CC(Nc1cccc(c1)[Cl])=O,NUOOA000186a, None, success, P 3 2 1,124 124 41
90 90 120,1.84,0.021,75.2,1.5,99.9,98.9,99.9,0.17672,0.20698, None, None, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1367,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1368,Cc1cccc(CC(Nc2cccnc2)=O)c1,NUOOA000188a, None, success, P 3 2 1,124 124 41 90
90 120,2.02,0.032,62.2,2.5,99.9,96.9,98.7,0.17776,0.20721, None, None, P 3 2 1,2 - PANDDA
model, None

NUDT7A-x1369, None, None, None, success, P 3 2 1,124 124 41 90 90
120,1.83,0.027,79.9,2.5,99.9,97.7,98.5,0.17656,0.20063, None, None, P 3 2 1,1 - Analysis
Pending, None

NUDT7A-x1370,Cc1cccc(CC(Nc2cccc(c2)[Cl])=O)c1,NUOOA000189a, None, success, P 3 2 1,124 124
41 90 90 120,1.85,0.036,60.8,2.6,99.8,97.7,98.3,0.1772,0.20491,0.17572,0.20344, P 3 2 1,1
- Analysis Pending, None

NUDT7A-x1371,C(C(Nc1cccc(c1)[Cl])=O)c1cccc(c1)[Cl],NUOOA000190a, None, success, P 3 2
1,124 124 41 90 90
120,1.8,0.032,77.2,2.5,99.9,97.9,99.4,0.17969,0.20539,0.17951,0.20549, P 3 2 1,1 -
Analysis Pending, None

NUDT7A-x1372,C1CCN(C1c1cc2c(cc1)OCCO2)C(=O)C,NU000793a, None, success, P 3 2 1,124 124 41
90 90 120,1.9,0.023,91.2,2.6,99.9,97.5,98.5,0.18174,0.21045,0.18635,0.21141, P 3 2 1,2 -
PANDDA model, None

NUDT7A-x1373,C1CCN(C1c1cc2c(cc1)OCCO2)C(=O)C,NU000796a, None, success, P 3 2 1,124 124 41
90 90 120,1.76,0.031,70.4,2.5,99.9,98,99.1,0.18835,0.21744,0.19502,0.21548, P 3 2 1,2 -
PANDDA model, None

NUDT7A-x1374,C1CCCN(C1c1ccc(cc1)OC)C(=O)C,NU000792a, None, success, P 3 2 1,124 124 41 90
90 120,1.75,0.088,36.9,2.8,100,99.8,100,0.20238,0.22975,0.20494,0.22591, P 3 2 1,6 -
Deposited, 5QH8

NUDT7A-x1375,C1CCN(C1c1cc(ccc1)OC)C(=O)C,NU000795a, None, success, P 3 2 1,124 124 41 90 90
120,1.72,0.017,108.5,2.6,99.8,98.1,98,0.18631,0.20752,0.18465,0.20578, P 3 2 1,6 -
Deposited, 5QH9

NUDT7A-x1376,C1CCN(C1c1ccc(cc1)OC)C(=O)C,NU000791a, None, success, P 3 2 1,124 124 41 90 90
120,1.68,0.022,84.3,2.2,99.9,98.1,98.4,0.18805,0.21031,0.19617,0.21311, P 3 2 1,2 -
PANDDA model, None

NUDT7A-x1377,C1CCC(C1)(NC(=O)C)c1cc2c(cc1)OCCO2,NU000794a, None, success, P 3 2 1,123 123
41 90 90 120,1.57,0.099,30,0.5,99.3,99.3,97.5,0.2206,0.25453,0.19586,0.233, P 3 2 1,5 -
Deposition ready, 5QHA

NUDT7A-x1378, None, None, None, success, P 3 2 1,124 124 41 90 90
120,1.65,0.046,56.6,3.1,99.9,98.4,99.5,0.1861,0.20918,0.1861,0.20918, P 3 2 1,2 - PANDDA
model, None

NUDT7A-x1379,C1CC(N(C1)c1cccc1c1ccc(cc1)O)=O,NU000609a, None, success, P 3 2 1,125 125 41
 90 90 120,1.73,0.032,82.2,1.4,99.4,99.6,99.9,0.1896,0.21267,0.1896,0.21267,P 3 2 1,2 -
 PANDDA model, None

NUDT7A-x1380,Cc1ccc(cc1)c1cccc1N1CCCC1=O,NU000610a, None, success, P 3 2 1,124 124 41 90
 90 120,1.57,0.04,66.7,1.2,99.8,99.8,99.7,0.19447,0.21461,0.20066,0.213,P 3 2 1,6 -
 Deposited,5QHB

NUDT7A-x1381,C1CC(N(C1)c1cccc1c1ccc(cc1)[N+]([O-])=O)=O,NU000611a, None, success, P 3 2
 1,125 125 41 90
 120,1.92,0.032,82.7,3.4,100,97.5,99.9,0.17826,0.20372,0.17802,0.20285,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-x1382,C1CC(N(C1)c1cccc1c1ccc(c1)C(F)(F)F)=O,NU000612a, None, success, P 3 2 1,124
 124 41 90 90 120,2.21,0.022,93.9,6,99.9,96.1,99.3,0.18203,0.22104,0.19073,0.2282,P 3 2
 1,6 - Deposited,5QHC

NUDT7A-x1383,C1C(=C(C=CC=1)N1C(CCC1)=O)C(=CC=C(C1)C(F)(F)F)C=1,NU000613a, None, success, P
 3 2 1,124 124 41 90 90
 120,1.63,0.035,78,1.2,99.7,99.2,99.9,0.19166,0.21548,0.19093,0.2143,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-
 x1384,C1C(=C(C=CC=1)N(C(CCC1)=O)C1)C(=CC=C(C1)NC(=O)NC(=CC(=C2)[C1])C=C2)C=1,NU000614a,N
 one, success, P 3 2 1,124 124 41 90 90
 120,1.61,0.027,99.7,1.2,99.7,99.6,99.9,0.18772,0.20951,0.18732,0.20992,P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-
 x1385,C1C(=C(C=CC=1)N(C(CCC1)=O)C1)C(=CC=C(C1)NC(=O)C[C1])C=1,NU000615a, None, success, P 3
 2 1,125 125 41 90 90
 120,1.8,0.028,89.9,1.3,99.6,99.5,100,0.18954,0.22203,0.1895,0.22193,P 3 2 1,2 - PANDDA
 model, None

NUDT7A-
 x1386,C1C(=C(C=CC=1)N(C(CCC1)=O)C1)C(=CC=C(C1)OC(=O)NC(=CC(=C2)[C1])C=C2)C=1,NU000616a,N
 one, success, P 3 2 1,124 124 41 90 90
 120,1.92,0.083,31.8,1.7,99.5,97.3,94.5,0.19017,0.2192,0.19019,0.21975,P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-
 x1387,C1C(=C(C=CC=1)N(C(CCC1)=O)C1)C(=CC=C(C1)NC(=O)C(=CC(=C2)[C1])C=C2)C=1,NU000617a,No
 ne, success, P 3 2 1,125 125 41 90 90
 120,1.67,0.039,57.2,1.2,99.3,99.6,100,0.19521,0.22093,0.19467,0.22038,P 3 2 1,1 -
 Analysis Pending, None

NUDT7A-x1388,C1C(=C(C=CC=1)N(C(CCC1)=O)C1)C(=CC=C(C1)N)C=1,NU000618a, None, success, P 3 2
 1,125 125 41 90 90 120,1.76,0.034,80.7,3,100,98,99.7,0.19046,0.21537,0.19046,0.21537,P
 3 2 1,2 - PANDDA model, None

NUDT7A-x1389,,,, success, P 3 2 1,126 126 41 90 90
 120,3.22,0.038,41,1.7,100,99.8,100,0.14855,0.21465,0.14855,0.21465,P 3 2 1,2 - PANDDA
 model,

NUDT7A-x1390,,,, success, P 3 2 1,126 126 41 90 90
 120,3.2,0.045,34.2,1.9,99.9,97.5,100,0.14499,0.21298,0.14499,0.21298,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1391,,,, success, P 3 2 1,125 125 41 90 90
 120,2.77,0.047,36.5,1.3,100,98.9,100,0.16175,0.2101,0.16175,0.2101,P 3 2 1,1 - Analysis
 Pending,

NUDT7A-x1392,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.87,0.046,45.2,1.8,99.5,91.7,93.9,0.15991,0.22696,0.15991,0.22696,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1393,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.46,0.041,50.4,2.3,99.6,94.7,96,0.16627,0.20567,0.16627,0.20567,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1394,,,,,success,P 3 2 1,124 124 41 90 90
 120,3.15,0.051,30.8,1.7,99.8,99.8,100,0.18424,0.26805,0.18424,0.26805,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1395,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.79,0.044,42.5,1.8,99.6,92.4,95.8,0.15387,0.20672,0.15387,0.20672,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1396,,,,,success,P 3 2 1,124 124 40 90 90
 120,3.18,0.05,31.8,1.7,99.8,98,100,0.17374,0.25117,0.17374,0.25117,P 3 2 1,1 - Analysis
 Pending,

NUDT7A-x1400,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1401,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.18,0.029,51.7,1.2,99.5,98.7,99.6,0.18498,0.22053,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1402,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.35,0.023,78.6,1.2,99.9,99.6,100,0.17789,0.22043,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1403,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.3,0.028,61.4,1.4,99.9,95.6,99.8,0.18111,0.22136,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1404,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.18,0.033,56,1.5,99.9,98.3,100,0.19005,0.22374,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1405,,,,,success,P 3 2 1,125 125 41 90 90
 120,2,0.038,55.2,1.6,99.9,99,99.9,0.186,0.21711,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1406,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.08,0.344,12.6,1,99.1,96.8,100,0.3706,0.40089,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1407,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.91,0.05,39.8,2.5,99.7,95.6,98.8,0.16737,0.22518,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1408,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.32,0.032,61.6,2,99.6,95.4,96,0.17947,0.22254,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1409,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1410,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.91,0.05,30.1,1.4,94.8,98.7,93.8,0.19406,0.25017,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1411,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.63,0.027,69.5,1.8,99.8,98.9,100,0.15719,0.20719,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1412,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.33,0.028,59.8,1.5,99.9,98.5,100,0.17801,0.21572,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1413,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1414,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1415,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.29,0.106,41.2,7.1,100,99.7,100,0.13629,0.18806,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1416,,,,,success,P 3 2 1,124 124 40 90 90
 120,2.5,0.032,47.4,1.4,100,99.5,100,0.17659,0.21713,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1417,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1418,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1419,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.01,0.051,31.3,2.7,100,99.7,100,0.15604,0.20703,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1420,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.21,0.036,52.3,2,99.8,97.3,100,0.14031,0.19379,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1421,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1422,,,,,Failed - low resolution,P 3 2 1,125 125 41 90 90
 120,8.29,0.163,32.2,26,98.9,79.4,98.9,0.15865,0.21257,0.15865,0.21257,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1423,,,,,Failed - unknown,P 3 2 1,126 126 41 90 90
 120,2.72,0.052,41.6,2.4,99.8,93,97.8,0.1583,0.21417,0.1583,0.21417,P 3 2 1,#NAME?,

NUDT7A-x1424,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.19,0.021,92.3,1.8,99.9,99.1,99.8,0.17151,0.22795,0.17151,0.22795,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1425,C(C(Nc1ccon1)=O)c1cccc2c1cn[nH]2,NUOOA000290a,,success,P 3 2 1,124 124 40
 90 90 120,1.53,0.057,36,1.2,100,99.9,100,0.19367,0.21443,0.19367,0.21443,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1426,C(C(Nc1ccccn1)=O)c1cccc2c1cn[nH]2,NUOOA000291a,,success,P 3 2 1,125 125 41
 90 90 120,1.93,0.034,64.5,2,99.9,97.5,98.5,0.17719,0.20505,0.17719,0.20505,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1427,C(C(Nc1cccnc1)=O)c1cccc2c1cn[nH]2,NUOOA000292a,,success,P 3 2 1,125 125 41
 90 90 120,1.72,0.023,84.9,2.4,99.9,98.1,98.5,0.18554,0.2082,0.18554,0.2082,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1428,C(C(Nc1ccon1)=O)c1ccc2c(c1)cn[nH]2,NUOOA000293a,,success,P 3 2 1,125 125 41
 90 90 120,1.73,0.043,45.1,1.3,99.9,99.1,100,0.18273,0.20645,0.18273,0.20645,P 3 2 1,2 -
 PANDDA model,

NUDT7A-x1429,C(C(Nc1ccccn1)=O)c1cccc2c1cn[nH]2,NUOOA000294a,,success,P 3 2 1,125 125 41
 90 90 120,1.93,0.036,56.2,2.9,99.9,97.4,99.1,0.17678,0.20291,0.17678,0.20291,P 3 2 1,1
 - Analysis Pending,

NUDT7A-x1430,C(C(Nc1cccnc1)=O)c1cccc2c1cn[nH]2,NUOOA000295a,,success,P 3 2 1,124 124 41
 90 90 120,1.75,0.049,42.7,1.3,98.9,99.7,100,0.22174,0.25333,0.22174,0.25333,P 3 2 1,2 -
 PANDDA model,

NUDT7A-
 x1431,C(C(Nc1cnccc1OCC(N1CCNC(C1)=O)=O)=O)c1cccc2c1cn[nH]2,NUOOA000296a,,success,P 3 2
 1,125 125 41 90 90
 120,1.93,0.026,76.1,3.3,99.2,97.3,95.6,0.18114,0.20562,0.18114,0.20562,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1432,COc1ccc(cc1)OC(Nc1cccc(c1)[Cl])=O,NUOOA000297a,,success,P 3 2 1,125 125 41
 90 90 120,1.82,0.03,71.5,2.8,99.8,97.8,97.8,0.17999,0.20529,0.17999,0.20529,P 3 2 1,2 -
 PANDDA model,

NUDT7A-x1433,C1C(=C(C=CC=1)N(C(CC1)=O)C1)C(=CC=C(C1)OCC)C=1,BD067591b,,success,P 3 2
 1,125 125 41 90 90
 120,2.67,0.027,68.1,1.8,99.9,99.3,100,0.16027,0.21641,0.16027,0.21641,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1434, C1C(=C(C=CC=1)N(C(CC1)=O)C1)C1=CC=C(C=C1)F, NU000619a,, success, P 3 2 1, 124 124 41 90 90 120, 1.93, 0.025, 80.9, 2.4, 99.9, 97.7, 99.4, 0.17984, 0.20472, 0.18565, 0.21721, P 3 2 1, 3 - In Refinement, 5QHD

NUDT7A-x1435, C1C(=C(C=CC=1)N(C(CC1)=O)C1)C(=CC=C(C1)N(C(C2)=O)C(C=2)=O)C=1, NU000620a,, success, P 3 2 1, 126 126 41 90 90 120, 2.38, 0.016, 123.1, 2.2, 99.8, 95.2, 98.3, 0.17485, 0.21439, 0.17485, 0.21439, P 3 2 1, 2 - PANDDA model,

NUDT7A-x1436, C1C(=C(C=CC=1)N(C(CC1)=O)C1)C1=CC=C(C=C1)F, NU000621a,, success, P 3 2 1, 125 125 41 90 90 120, 1.74, 0.071, 31.8, 1.4, 99.9, 99.4, 100, 0.18799, 0.21131, 0.19919, 0.21888, P 3 2 1, 6 - Deposited, 5QHE

NUDT7A-x1437, COc1ccc(CC(Nc2cc(ccn2)OCC(N2CCNC(C2)=O)=O)=O)cc1, NU00A000298a,, success, P 3 2 1, 125 125 41 90 90 120, 1.7, 0.036, 58.4, 2.3, 99.7, 98.2, 95.7, 0.18816, 0.21226, 0.18816, 0.21226, P 3 2 1, 2 - PANDDA model,

NUDT7A-x1438, CC(C(Nc1cc(ccn1)OCC(N1CCNC(C1)=O)=O)=O)c1cccc1, NU00A000299a,, success, P 3 2 1, 125 125 41 90 90 120, 1.65, 0.031, 77, 2.3, 99.9, 98.4, 98.6, 0.18543, 0.20204, 0.18543, 0.20204, P 3 2 1, 2 - PANDDA model,

NUDT7A-x1439, COc1ccc(CC(=Nc2cc(cnc2)O)OCC(N2CCNC(C2)=O)=O)cc1, NU00A000300a,, success, P 3 2 1, 124 124 40 90 90 120, 1.63, 0.059, 33.5, 1.5, 100, 99.9, 100, 0.19514, 0.22274, 0.19514, 0.22274, P 3 2 1, 1 - Analysis Pending,

NUDT7A-x1440, COc1ccc(CC(Nc2cc(cnc2)OCC(N2CCNC(C2)=O)=O)=O)cc1, NU00A000301a,, success, P 3 2 1, 124 124 41 90 90 120, 1.67, 0.066, 36.2, 2.7, 99.9, 98.3, 98.7, 0.18316, 0.20062, 0.1953, 0.21254, P 3 2 1, 6 - Deposited, 5QHF

NUDT7A-x1441, CC(C(=Nc1cc(cnc1)O)OCC(N1CCNC(C1)=O)=O)c1cccc1, NU00A000302a,, success, P 3 2 1, 124 124 41 90 90 120, 1.69, 0.061, 39, 2.5, 99.8, 98.2, 97.7, 0.18288, 0.20008, , , P 3 2 1, 1 - Analysis Pending,

NUDT7A-x1442, CC(C(Nc1cc(cnc1)OCC(N1CCNC(C1)=O)=O)=O)c1cccc1, NU00A000303a,, success, P 3 2 1, 124 124 41 90 90 120, 1.88, 0.024, 80.9, 2.5, 99.9, 97.6, 98.8, 0.17938, 0.20432, , , P 3 2 1, 1 - Analysis Pending,

NUDT7A-x1443, C1CN(Cc2cc(ccc12)OC(Nc1cccc(c1)[C1])=O)C(C[C1])=O, NU00A000304a,, success, P 3 2 1, 125 125 41 90 90 120, 1.77, 0.051, 46.4, 2.4, 99.9, 98, 99.1, 0.18708, 0.20809, 0.18708, 0.20809, P 3 2 1, 1 - Analysis Pending,

NUDT7A-x1444, C1Cc2ccc(cc2N(C1)C(C[C1])=O)OC(Nc1cccc(c1)[C1])=O, NU00A000305a,, success, P 3 2 1, 124 124 40 90 90 120, 1.5, 0.073, 32.9, 1.3, 100, 99.9, 99.9, 0.19403, 0.21677, 0.19589, 0.21307, P 3 2 1, 3 - In Refinement,

NUDT7A-x1445, CCC(N(C1)C(C(CC1)=CC=C1OC(NC(C=CC=C2[C1])=C2)=O)=C1)=O, NU00A000306a,, success, P 3 2 1, 124 124 41 90 90 120, 1.72, 0.043, 57.5, 3.1, 99.9, 98.2, 98.8, 0.18273, 0.20085, 0.18273, 0.20085, P 3 2 1, 2 - PANDDA model,

NUDT7A-x1446, C(C(Nc1cccn1)=O)c1ccc(cc1)[C1], NU00A000232a,, success, P 3 2 1, 124 124 41 90 90 120, 1.74, 0.048, 42, 2.7, 99.9, 98.1, 99, 0.18127, 0.19912, , , P 3 2 1, 2 - PANDDA model,

NUDT7A-x1447,C1C(=C(C=CC=1)N(C(CC1)=O)C1)C1=CC=CC(=C1)C(F)(F)F,NU000622a,, success,P 3 2
 1,126 126 41 90 90 120,2.36,0.025,68.1,2.9,100,99.7,100,0.17367,0.20872,,,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1448,,,, success,P 3 2 1,125 125 41 90 90
 120,2.83,0.027,60.3,1.5,99.7,98.1,99.8,0.15577,0.20051,0.15577,0.20051,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1449,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1450,,,, Failed - low resolution,P 3 2 1,124 124 41 90 90
 120,3.69,0.037,38.9,2.9,100,98.4,100,,,,,

NUDT7A-x1451,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1452,,,, success,P 3 2 1,126 126 41 90 90
 120,2.72,0.022,77.4,1.9,99.9,93,99.6,0.16541,0.2062,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1453,,,, success,P 3 2 1,125 125 41 90 90
 120,2.39,0.032,62.6,2,99.9,98.3,99.9,0.17864,0.21289,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1454,,,, success,P 3 2 1,125 125 41 90 90
 120,3.08,0.039,37.2,3.2,100,99.8,100,0.14688,0.19303,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1455,,,, success,P 3 2 1,125 125 41 90 90
 120,2.41,0.03,60.9,1.3,99.9,99.3,99.9,0.18039,0.21948,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1456,,,, success,P 3 2 1,125 125 41 90 90
 120,2.84,0.025,68.1,1.5,99.9,98.3,100,0.15205,0.19088,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1457,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1458,,,, success,P 3 2 1,125 125 41 90 90
 120,2.41,0.035,60.3,1.4,99.8,96,99.8,0.18262,0.22249,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1459,,,, success,P 3 2 1,126 126 41 90 90
 120,2.78,0.051,54.3,1.6,99.4,98.3,99.7,0.18204,0.23675,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1460,,,, success,P 3 2 1,125 125 41 90 90
 120,2.52,0.038,48.6,1.5,99.9,99.2,99.8,0.16821,0.21004,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1461,,,, success,P 3 2 1,125 125 41 90 90
 120,2.08,0.03,69.6,2,99.9,98,99.7,0.18456,0.21869,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1462,,,, Failed - low resolution,P 3 2 1,124 124 41 90 90
 120,4.97,0.188,10.4,2.8,99.9,96.2,100,,,,,

NUDT7A-x1463,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1464,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1465,,,, success,P 3 2 1,125 125 41 90 90
 120,2.2,0.019,86.4,1.5,99.5,96.2,97.6,0.19028,0.22237,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1466,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1467,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1468,,,, success,P 3 2 1,125 125 41 90 90
 120,2.18,0.057,49.6,0.6,97.6,98.8,96.3,0.18494,0.22236,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1469,,,, Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1470,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.29,0.026,84.3,2.6,99.9,95.6,99,0.18678,0.22362,,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1471,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.53,0.023,89.7,2,99.8,94.4,98.7,0.17042,0.21371,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1472,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.83,0.043,59.3,1.4,99.9,99.2,99.8,0.19289,0.21987,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1473,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1474,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1475,,,,,Failed - low resolution,P 3 2 1,125 125 41 90 90
 120,4.32,0.088,14.1,1.2,97.2,93.3,91.5,,,,,

NUDT7A-x1476,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1477,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.11,0.048,46.4,1.4,100,98.8,100,0.18447,0.22153,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1478,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1479,,,,,Failed - low resolution,P 3 2 1,125 125 41 90 90
 120,4.42,0.47,13.9,7.5,98.9,97.3,100,,,,,

NUDT7A-x1480,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.43,0.046,44.8,2.4,99.9,94.9,99.5,0.17386,0.20153,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1481,,,,,Failed - low resolution,P 3 2 1,126 126 41 90 90
 120,4.05,0.171,11.7,2.9,100,97.1,100,,,,,

NUDT7A-x1482,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.54,0.032,61.8,1.4,99.9,95.4,100,0.16349,0.20918,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1483,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.38,0.062,30.5,1.9,99.7,95,100,0.16504,0.23681,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1484,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.68,0.038,47.3,1.6,99.8,94.1,100,0.17285,0.22253,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1485,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.12,0.062,33.3,2.2,99.7,98.1,100,0.14411,0.19681,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1486,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.71,0.019,87.1,1.5,99.8,98.4,100,0.15919,0.20891,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1487,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.95,0.025,70,2.4,99.8,91,98.8,0.16109,0.21892,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1488,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,

NUDT7A-x1489,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.15,0.035,55,1.7,99.9,98.8,100,0.18742,0.22103,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1490,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.44,0.038,43.8,1.1,99.9,99.6,100,0.17506,0.22733,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1491,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.29,0.03,50.2,0.6,99.7,99.4,100,0.19077,0.23698,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1492,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.44,0.051,36.1,1.4,99.5,99.9,100,0.19272,0.22888,,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1493,,,,,success,P 3 2 1,124 124 40 90 90
 120,3.29,0.036,47.9,1.3,94.2,99.7,99.5,0.22466,0.29431,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1494,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1495,,,,,Failed - low resolution,P 3 2 1,122 122 40 90 90
 120,6.03,0.048,25.7,2.2,99.3,90.8,99.3,,,,,
 NUDT7A-x1496,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.2,0.025,68.5,1.8,99.6,95.9,94.9,0.17523,0.20273,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1497,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.96,0.052,44.1,1.4,99.5,99.4,99.7,0.18492,0.21533,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1498,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.79,0.017,113.7,2.8,99.8,97.9,98,0.18134,0.20669,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1499,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.75,0.024,76.3,1.6,99.9,97.7,99.9,0.18335,0.20745,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1500,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.96,0.026,77.3,2.6,99.8,97.3,97.2,0.17809,0.20441,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1501,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.78,0.034,64.5,2.7,99.8,98,98.1,0.18779,0.20939,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1502,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.85,0.033,58.1,1.3,100,99.5,100,0.18644,0.21505,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1503,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.04,0.032,64.4,2.8,99.9,97,98.9,0.18025,0.21574,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1504,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.8,0.025,77.8,2.4,99.8,97.9,97.8,0.18035,0.20268,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1505,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.33,0.055,39.6,1,99.4,95.4,93.4,0.18085,0.21941,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1506,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1507,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.38,0.024,63.4,1.1,98.1,99.3,99.8,0.2257,0.26855,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1508,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.69,0.029,72.6,1.3,99.9,98.3,100,0.18902,0.21007,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1509,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1510,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.29,0.038,42.2,1.1,99.9,99.3,99.8,0.17825,0.21877,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1511,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1512,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.32,0.032,44,1.5,99.3,99.6,100,0.19324,0.22635,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1513,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.03,0.034,43.8,0.9,99.3,99.7,97.4,0.19083,0.21939,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1514,,,,,success,P 3 2 1,125 125 41 90 90 120,2.24,0.071,30.2,-
 0.1,94.9,98.5,36.8,0.19724,0.23007,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1515,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.21,0.022,87.6,3.2,99.9,96.2,98.8,0.18227,0.2192,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1516,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.8,0.07,32.4,1.2,99.2,99.3,100,0.22691,0.28243,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1517,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1518,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1519,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.19,0.022,72,1.5,99.7,96.2,96.6,0.18518,0.2136,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1520,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.93,0.032,57.2,0.9,99.2,99.9,95.4,0.19414,0.21636,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1521,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.33,0.034,48.6,1.1,99.1,99,100,0.20463,0.24536,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1522,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.61,0.022,52.8,0.4,98,97.7,96.6,0.2145,0.26903,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1523,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.14,0.018,92.7,1.9,99.9,99.5,100,0.18333,0.21121,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1524,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.32,0.022,91.8,1.7,99.6,95.4,95.6,0.17716,0.2122,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1525,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.21,0.02,98.7,2.4,99.8,96.2,97.9,0.17826,0.20773,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1526,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.79,0.091,9.5,1.7,100,99.3,100,0.30253,0.34787,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1527,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.01,0.015,96,2,99.6,97.1,96,0.18139,0.21012,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1528,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.28,0.029,61.2,1.1,99.7,95.7,97,0.19028,0.22174,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1529,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.08,0.045,41.6,1.8,99.9,98.6,99.6,0.18262,0.21446,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1530,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.21,0.028,74.1,2,99.8,96.2,97.6,0.17899,0.20898,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1531,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.56,0.023,67.9,1.1,99.6,98.7,99.6,0.18132,0.23327,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1532,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.03,0.024,54.2,1.4,99.9,99.6,99.8,0.18375,0.21083,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1533,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.32,0.018,82.7,2,99.7,95.3,97.1,0.17155,0.20806,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1534,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.48,0.028,56.9,1.3,96.3,99.5,100,0.23086,0.26657,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1535,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.5,0.042,42.6,1.4,99.5,99.9,100,0.18875,0.23314,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1536,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.43,0.028,69.5,2.6,99.6,95,97.3,0.18173,0.22769,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1537,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.03,0.026,67.1,1.6,99.7,97,96,0.18326,0.21193,,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1538,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.31,0.038,42.4,0.8,99.2,86.7,96.3,0.20913,0.26351,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1539,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.02,0.019,80.5,1.5,99.8,99.4,99.3,0.18529,0.21304,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1540,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.08,0.034,50.5,1.2,99.6,99.7,99.3,0.19872,0.23048,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1541,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.29,0.047,41.1,2.6,100,99.8,100,0.18253,0.2187,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1542,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.09,0.031,56.9,2,99.7,98.3,99.6,0.19378,0.22858,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1543,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.49,0.033,47.9,2.4,99.6,100,100,0.17574,0.21737,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1544,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.21,0.03,64.9,2.7,99.6,96.1,95.4,0.18317,0.21396,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1545,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.64,0.021,63,1,98,99,92.6,0.20114,0.24467,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1546,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.17,0.055,34.6,0.9,99.2,98,100,0.20754,0.23955,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1547,,,,,Failed - low resolution,P 3 2 1,124 124 41 90 90
 120,3.82,0.044,35.5,1.9,99.4,98.3,95.2,,,,,,
 NUDT7A-x1548,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.07,0.028,50.8,1,98.8,99.5,93.6,0.18827,0.2196,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1549,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.58,0.034,62,2.1,99.2,94,92.4,0.17678,0.22697,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1550,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.05,0.035,42,1.3,99.4,99.7,99.9,0.18523,0.21504,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1551,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.4,0.032,56.6,2.7,98.1,99.6,100,0.17467,0.21471,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1552,,,,,success,P 3 2 1,125 125 41 90 90
 120,2,0.023,59.9,1.3,99.8,99.7,100,0.18815,0.21805,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1553,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.34,0.029,75.9,2.8,99.3,95.2,97,0.17316,0.20885,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1554,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.32,0.024,71.8,2.1,99.7,95.5,98,0.17877,0.21264,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1555,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.29,0.047,37.4,2.4,99.9,99.8,100,0.18129,0.21637,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1556,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.03,0.025,67.5,1.2,99.6,97,94.6,0.18599,0.21737,,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1557,,,,,success,P 3 2 1,125 125 41 90 90 120,2.2,0.024,61.7,-
 0.2,99.4,96.2,95.1,0.1962,0.23187,,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1558,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.2,0.028,60.4,1.3,99.6,96.2,95.6,0.18228,0.21196,,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1559,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.96,0.02,85.8,2.5,99.8,97.4,97.2,0.18057,0.20551,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1560,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.78,0.032,58.8,2.3,99.9,98,98.3,0.18431,0.20425,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1561,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.2,0.021,74.2,1.5,99.6,96.2,95.4,0.18157,0.21949,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1562,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.07,0.041,45.6,2.7,97.3,99.8,100,0.18343,0.21369,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1563,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.14,0.096,26.6,1.8,97.5,98.6,100,0.18975,0.22053,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1564,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.95,0.033,59.3,1.6,98.9,98.4,98.9,0.18759,0.21473,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1565,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.32,0.02,74.2,1.7,99.5,95.5,94.3,0.17622,0.20752,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1566,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.36,0.031,45.9,1.6,99.9,98.9,99.8,0.17431,0.21186,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1567,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.76,0.031,73,2.7,99.8,98,98.3,0.18584,0.20705,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1568,,,,,success,P 3 2 1,125 125 41 90 90
 120,2,0.053,37.4,2,99.6,97.1,94.6,0.17838,0.21186,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1569,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.96,0.019,97.7,2.8,99.8,97.3,97.6,0.17998,0.20969,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1570,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.83,0.033,66.1,1.3,99.8,99.6,99.9,0.19219,0.21658,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1571,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.03,0.027,64.5,1.6,99.3,97.1,91.7,0.17771,0.20891,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1572,,,,,Failed - unknown,,,,,,,,,,,,,#NAME?,
 NUDT7A-x1573,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.37,0.027,67,1.8,99.5,95.2,94.5,0.17119,0.2095,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1574,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.29,0.023,79.8,2,99.8,95.8,98.1,0.1767,0.20679,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1575,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.36,0.037,36,1.6,99.8,99.4,100,0.17844,0.221,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1576,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.58,0.089,21.1,2.1,97.7,99.8,84.1,0.17495,0.21973,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1577,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.51,0.027,48.4,1.3,99.6,99.5,100,0.17876,0.21743,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1578,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.94,0.026,70,1.3,99.8,99.8,99.6,0.18755,0.21661,,,,P 3 2 1,1 - Analysis Pending,
 NUDT7A-x1579,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.47,0.027,66.3,1.8,99.6,94.6,95.2,0.17104,0.21149,,,,P 3 2 1,2 - PANDDA model,
 NUDT7A-x1580,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.47,0.02,86,2.4,99.7,94.6,96.4,0.17858,0.22138,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1581,,,,,success,P 3 2 1,126 126 41 90 90
 120,2.04,0.018,88,1.7,99.6,97.1,96.5,0.18016,0.20548,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1582,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.2,0.025,65.1,2.2,99.6,96.1,94.8,0.18065,0.20992,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1583,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.93,0.026,81.9,2.2,99.9,97.5,99.3,0.1847,0.21511,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1584,,,,,success,P 3 2 1,125 125 41 90 90
 120,1.81,0.039,41.5,1.2,99.9,98.6,100,0.18712,0.21344,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1585,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.94,0.05,35.4,1.4,98.2,99.4,99.3,0.1932,0.21853,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1586,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.49,0.04,44.1,2.4,99.5,99.8,100,0.17445,0.21831,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1587,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.41,0.018,63,1,99.5,99.9,100,0.18323,0.22825,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1588,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.52,0.027,59.1,2.4,99.5,99.8,100,0.17712,0.22355,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1589,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.28,0.035,49.9,1.1,99.8,98.4,99.8,0.18022,0.21868,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1590,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.29,0.018,95.4,2.2,99.7,95.7,97.3,0.17446,0.21151,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1591,,,,,success,P 3 2 1,125 125 41 90 90
 120,2,0.035,51.8,1.5,99.6,97.9,99.1,0.1812,0.21198,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1592,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.16,0.042,50.4,1.1,98.3,98.7,100,0.18091,0.21749,,,,P 3 2 1,2 - PANDDA model,

NUDT7A-x1593,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.72,0.018,84,1.5,99.6,93,96.6,0.16198,0.21101,,,,P 3 2 1,1 - Analysis Pending,

NUDT7A-x1701,C(C(Nc1cccnn1)=O)c1cccc2c1cn[nH]2,NU000438a,,success,P 3 2 1,124 124 40 90
 90 120,1.51,0.032,66,2,100,99.9,100,0.19999,0.22394,0.19999,0.22394,P 3 2 1,1 - Analysis
 Pending,

NUDT7A-x1702,C(C(Nc1cccnn1)=O)c1ccc2c(c1)cn[nH]2,NU000439a,,success,P 3 2 1,124 124 41
 90 90 120,1.62,0.021,83.2,1.2,99.8,99.6,99.9,0.19417,0.21805,0.19417,0.21805,P 3 2 1,2
 - PANDDA model,

NUDT7A-x1703,C(C(Nc1cccnn1)=O)c1cccc(c1)O,NU000436a,,success,P 3 2 1,124 124 41 90 90
 120,1.6,0.024,70.1,1.4,100,99.7,100,0.18313,0.20292,0.18313,0.20292,P 3 2 1,2 - PANDDA
 model,

NUDT7A-x1704,COc1cccc(CC(Nc2cccnn2)=O)c1,NU000440a,,success,P 3 2 1,125 125 41 90 90
 120,1.71,0.03,67.6,1.1,99.9,98.8,100,0.18698,0.20798,0.18698,0.20798,P 3 2 1,2 - PANDDA
 model,

NUDT7A-x1705,C(C(Nc1cccnn1)=O)c1cccc(c1)F,NU000437a,,success,P 3 2 1,124 124 40 90 90
 120,1.62,0.027,64.6,2,100,99.9,100,0.20517,0.23431,0.20517,0.23431,P 3 2 1,1 - Analysis
 Pending,

NUDT7A-x1706,COc1cccc(CC(Nc2cccnn2)=O)cc1OC,NU000441a,,success,P 3 2 1,124 124 40 90 90
 120,1.46,0.049,48.1,1.9,100,99.9,100,0.20173,0.22171,0.20173,0.22171,P 3 2 1,2 - PANDDA
 model,

NUDT7A-x1707,C(C(Nc1cccc(c1)[Cl])=O)c1cccc(c1)O,NU000087a,,success,P 3 2 1,124 124 40 90
90 120,1.67,0.031,64.7,1.3,100,99.2,100,0.18651,0.20397,0.18651,0.20397,P 3 2 1,2 -
PANDDA model,

NUDT7A-x1708,C(C(Nc1cccc(c1)[Cl])=O)c1cccc(c1)O,NU000087a,,success,P 3 2 1,124 124 41 90
90 120,1.78,0.046,45.7,1.5,100,99.8,100,0.19119,0.21583,0.19119,0.21583,P 3 2 1,2 -
PANDDA model,

NUDT7A-x1709,C(C(Nc1cccc(c1)[Cl])=O)c1cccc(c1)O,NU000087a,,success,P 3 2 1,123 123 40 90
90 120,1.79,0.043,53.9,1.2,100,99.6,100,0.18506,0.20939,0.18506,0.20939,P 3 2 1,2 -
PANDDA model,

NUDT7A-x1710,C1CN(Cc2cc(ccc12)OC(Nc1cccc(c1)[Cl])=O)C(C[Cl])=O,NU000008a,,success,P 3 2
1,123 123 40 90 90 120,1.6,0.028,62.4,1.9,100,99.9,100,0.19306,0.2219,0.19306,0.2219,P
3 2 1,2 - PANDDA model,

NUDT7A-x1711,C1Cc2ccc(cc2N(C1)C(C[Cl])=O)OC(Nc1cccc(c1)[Cl])=O,NU000007a,,success,P 3 2
1,124 124 41 90 90
120,1.87,0.026,69,1.1,97.2,99.4,90.7,0.24938,0.32303,0.24938,0.32303,P 3 2 1,1 -
Analysis Pending,

NUDT7A-x1712,C=CC(N1CCCc2ccc(cc12)OC(Nc1cccc(c1)[Cl])=O)=O,NU000226a,,success,P 3 2
1,124 124 41 90 90
120,1.88,0.017,94.9,2.5,94.7,97.9,78.4,0.20686,0.23464,0.20686,0.23464,P 3 2 1,2 -
PANDDA model,

NUDT7A-x1713,C(C(Nc1cccn1)=O)c1ccc(cc1)[Cl],NU000093a,,success,P 3 2 1,124 124 40 90 90
120,1.57,0.02,88.4,1.3,99.9,99.6,99.7,0.17984,0.20402,0.17984,0.20402,P 3 2 1,2 - PANDDA
model,

NUDT7A-x1714,C=CC(N1CCCc2ccc(cc12)OC(Nc1cccc(c1)[Cl])=O)=O,NU000226a,,Failed -
unknown,None,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1715,C=CC(N1CCCc1c1cccc(CC(Nc2cccc(c2)[Cl])=O)c1)=O,NU000442a,,success,P 3 2
1,125 125 41 90 90
120,1.92,0.041,52.6,1.5,99.7,98.4,99.1,0.19479,0.22917,0.20328,0.23278,P 3 2 1,6 -
Deposited,5QHG

NUDT7A-x1716,C1CC(c2cccc(CC(Nc3cccc(c3)[Cl])=O)c2)N(C1)C(C[Cl])=O,NU000443a,,Failed -
unknown,None,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1717,,,,Failed - low resolution,P 3 2 1,127 127 41 90 90
120,3.76,0.027,65.1,1.1,99.9,99.3,99.6,,,,,

NUDT7A-x1718,O=C1CC(c2cccc2)C2CC3CNCC13N2,NU000596a,,success,P 3 2 1,124 124 40 90 90
120,1.64,0.024,62.2,2,100,99.9,100,0.19459,0.21565,0.19459,0.21565,P 3 2 1,2 - PANDDA
model,

NUDT7A-x1719,COCC(=O)N1C2CC3CNCC31C(O)CC2c1cccc1,NU000597a,,success,P 3 2 1,124 124 40
90 90 120,1.58,0.026,58.3,1.9,99.8,99.9,98.6,0.19277,0.21452,0.19277,0.21452,P 3 2 1,2
- PANDDA model,

NUDT7A-x1720,OC1CC(c2cccc2)C2CC3CNCC13N2,NU000598a,,success,P 3 2 1,124 124 40 90 90
120,1.68,0.028,57.9,1.3,100,99.3,100,0.18053,0.20434,0.18053,0.20434,P 3 2 1,2 - PANDDA
model,

NUDT7A-x1721,CC(=O)N1C2CC3CNCC31C(O)CC2c1cccc1,NU000599a,,success,P 3 2 1,124 124 41 90
90 120,1.61,0.048,44.6,1.2,99.7,99,97.7,0.1844,0.20302,0.1844,0.20302,P 3 2 1,1 -
Analysis Pending,

NUDT7A-x1722,COCCC(=O)N1C2CC3CNCC31C(O)CC2c1cccc1,NU000600a,,success,P 3 2 1,123 123 40
90 90 120,1.66,0.024,66.7,1.2,99.9,99.2,99.9,0.1805,0.20028,0.1805,0.20028,P 3 2 1,2 -
PANDDA model,

NUDT7A-x1723,O=C1CC(c2cccc(O)c2)C2CC3CNCC13N2,NU000601a,,success,P 3 2 1,124 124 41 90
 90 120,1.6,0.024,82.1,1.4,99.9,99.3,99.7,0.18342,0.20446,0.18342,0.20446,P 3 2 1,2 -
 PANDDA model,

NUDT7A-x1724,CC(=O)Nc1cccc(C2CC(O)C34CNCC3CC2N4)c1,NU000602a,,success,P 3 2 1,124 124 40
 90 90 120,1.67,0.025,62.7,1.3,99.9,99.3,99.8,0.1792,0.20086,0.1792,0.20086,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1725,Oc1cccc(C2CC(O)C34CNCC3CC2N4)c1,NU000603a,,success,P 3 2 1,124 124 40 90 90
 120,1.51,0.044,40.1,1.7,99.9,100,99.1,0.19395,0.21592,0.19395,0.21592,P 3 2 1,2 - PANDDA
 model,

NUDT7A-x1726,CN1C2CCC(=O)C13CNCC3C2,NU000604a,,success,P 3 2 1,124 124 40 90 90
 120,1.6,0.028,61.6,1.3,99.9,99.4,100,0.18006,0.19962,0.18006,0.19962,P 3 2 1,2 - PANDDA
 model,

NUDT7A-x1727,CN1C2CCC(O)C13CNCC3C2,NU000605a,,success,P 3 2 1,124 124 41 90 90
 120,1.63,0.023,70.8,1.4,99.9,99.3,99.9,0.18089,0.20395,0.18089,0.20395,P 3 2 1,2 -
 PANDDA model,

NUDT7A-x1728,CN(C)CC(=O)N1C2CC3CNCC31C(O)CC2c1cccc1,NU000606a,,success,P 3 2 1,124 124
 40 90 90 120,1.57,0.024,73.6,1.4,99.7,99.3,97.8,0.17929,0.19682,0.17929,0.19682,P 3 2
 1,1 - Analysis Pending,

NUDT7A-x1729,C=CC(=O)N1CC2CC3NC2(C1)C(O)CC3c1cccc1,NU000607a,,success,P 3 2 1,123 123
 40 90 90 120,1.56,0.024,62.3,1.9,100,99.9,100,0.18907,0.20837,0.18907,0.20837,P 3 2 1,1
 - Analysis Pending,

NUDT7A-x1730,C=CC(=O)N1CC2CC3NC2(C1)C(O)CC3c1cccc1,NU000607b,,success,P 3 2 1,124 124
 40 90 90 120,1.64,0.026,59.1,1.9,100,100,100,0.20765,0.23161,0.20765,0.23161,P 3 2 1,1
 - Analysis Pending,

NUDT7A-x1731,CC(=O)Nc1cccc(C2CC(=O)C34CNCC3CC2N4)c1,NU000608a,,success,P 3 2 1,123 123
 40 90 90 120,1.65,0.029,55.5,2,100,99.9,100,0.19076,0.212,0.19076,0.212,P 3 2 1,2 -
 PANDDA model,

NUDT7A-x1732,COCC(=O)N1C2CC3CNCC31C(O)CC2c1cccc1,NU000597b,,success,P 3 2 1,124 124 41
 90 90 120,1.71,0.019,79.6,1.2,100,99.7,100,0.17857,0.20083,0.17857,0.20083,P 3 2 1,2 -
 PANDDA model,

NUDT7A-x1733,CN(C)CC(=O)N1C2CC3CNCC31C(O)CC2c1cccc1,NU000606b,,success,P 3 2 1,124 124
 41 90 90 120,1.85,0.028,57.8,1.2,99.5,98.9,99.9,0.1897,0.22395,0.1897,0.22395,P 3 2 1,2
 - PANDDA model,

NUDT7A-x1734,CC(=O)N1CCC[C@H]1c1cccc(CC(=O)Nc2cccc(C1)c2)c1,NU000443a,,success,P 3 2
 1,123 123 40 90 90
 120,1.68,0.063,27.1,1.2,100,99.5,100,0.18192,0.20382,0.18192,0.20382,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1735,CC(=O)N1CCC[C@H]1c1cccc(CC(=O)Nc2cccc(C1)c2)c1,NU000443a,,success,P 3 2
 1,124 124 40 90 90 120,1.46,0.068,30.1,2.2,100,100,100,0.19484,0.21109,0.19484,0.21109,P
 3 2 1,1 - Analysis Pending,

NUDT7A-x1736,CC(=O)N1CCC[C@H]1c1cccc(CC(=O)Nc2cccc(C1)c2)c1,NU000443a,,success,P 3 2
 1,124 124 40 90 90 120,1.55,0.068,30.7,2.2,100,100,100,0.19747,0.2175,0.19747,0.2175,P
 3 2 1,1 - Analysis Pending,

NUDT7A-x1737,CC(=O)N1CCC[C@H]1c1cccc(CC(=O)Nc2cccc(C1)c2)c1,NU000443a,,success,P 3 2
 1,124 124 41 90 90
 120,1.52,0.049,49.5,1.2,100,99.2,100,0.19247,0.20586,0.19115,0.20523,P 3 2 1,6 -
 Deposited,5QHH

NUDT7A-x1738,CC(=O)N1CCC[C@@H]1c1cccc(CC(=O)Nc2cccc(Cl)c2)c1,NU000443a,,success,P 3 2
 1,123 123 40 90 120,1.63,0.052,39.7,2.1,100,100,100,0.19855,0.21904,0.2067,0.2256,P
 3 2 1,3 - In Refinement,

NUDT7A-x1868,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.69,0.048,36.1,1.4,98.0,99.0,100.0,0.21886,0.28436,0.21886,0.28436,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1869,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.46,0.031,43.6,1.4,99.9,98.8,100.0,0.15977,0.19982,0.15977,0.19982,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1870,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.98,0.035,43.4,1.6,99.9,99.2,99.9,0.16735,0.18611,0.16735,0.18611,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1871,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.81,0.035,49.3,1.4,99.9,98.9,99.7,0.17374,0.19984,0.17374,0.19984,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1872,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.18,0.056,33.3,1.2,100.0,100.0,100.0,0.17824,0.21023,0.17824,0.21023,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1873,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.75,0.036,54.3,1.4,99.9,98.2,99.5,0.17679,0.19882,0.17679,0.19882,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1874,,,,,success,P 3 2 1,124 124 40 90 90
 120,2.28,0.045,39.8,1.1,93.3,99.9,100.0,0.17293,0.2234,0.17293,0.2234,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1875,,,,,success,P 3 2 1,123 123 41 90 90
 120,1.81,0.032,55.4,1.3,99.6,99.7,100.0,0.18778,0.21339,0.18778,0.21339,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1876,,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1877,,,,,success,P 3 2 1,122 122 40 90 90
 120,2.40,0.027,46.0,1.4,99.9,98.7,100.0,0.16735,0.20513,0.16735,0.20513,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1878,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.84,0.037,48.2,1.6,100.0,99.5,100.0,0.17447,0.19756,0.17447,0.19756,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1879,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.99,0.035,42.9,1.6,99.9,99.0,99.9,0.16983,0.19528,0.16983,0.19528,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1880,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.06,0.030,50.2,1.8,99.7,98.6,100.0,0.17956,0.20709,0.17956,0.20709,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1881,,,,,success,P 3 2 1,124 124 40 90 90
 120,1.93,0.037,47.0,1.4,99.9,98.7,99.6,0.17655,0.2087,0.17655,0.2087,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1882,,,,,success,P 3 2 1,122 122 40 90 90
 120,1.90,0.035,44.3,1.6,99.9,97.3,99.8,0.1719,0.19652,0.1719,0.19652,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1883,,,,,success,P 3 2 1,122 122 40 90 90
 120,2.46,0.051,29.9,1.2,100.0,100.0,100.0,0.17445,0.22178,0.17445,0.22178,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1884,,,,,success,P 3 2 1,122 122 40 90 90
 120,3.21,0.075,21.6,1.7,99.8,97.2,99.8,0.15307,0.22019,0.15307,0.22019,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1885,,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,
 NUDT7A-x1886,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.12,0.045,38.9,1.5,99.9,97.0,99.9,0.17359,0.21133,0.17359,0.21133,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1887,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.00,0.036,49.5,1.5,99.9,98.0,99.8,0.17859,0.20837,0.17859,0.20837,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1888,,,,,success,P 3 2 1,124 124 40 90 90
 120,2.28,0.032,48.0,1.0,99.9,99.1,99.9,0.17554,0.22152,0.17554,0.22152,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1889,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.16,0.034,55.1,1.8,99.9,98.7,100.0,0.17891,0.21976,0.17891,0.21976,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1890,,,,,success,P 3 2 1,124 124 40 90 90
 120,3.35,0.083,23.6,1.4,100.0,99.9,100.0,0.17123,0.2592,0.17123,0.2592,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1891,,,,,Failed - low resolution,P 3 2 1,122 122 40 90 90
 120,3.51,0.066,26.6,1.4,100.0,99.5,100.0,,,,,
 NUDT7A-x1892,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.39,0.051,36.4,1.4,99.9,99.3,99.7,0.17541,0.21979,0.17541,0.21979,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1893,,,,,success,P 3 2 1,122 122 40 90 90
 120,2.80,0.050,31.3,1.5,99.9,98.8,100.0,0.15923,0.21451,0.15923,0.21451,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1894,,,,,success,P 3 2 1,122 122 40 90 90
 120,3.44,0.038,36.5,2.5,98.2,96.4,92.9,0.15417,0.23277,0.15417,0.23277,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1895,,,,,success,P 3 2 1,122 122 40 90 90
 120,2.11,0.058,33.7,1.3,99.7,98.3,99.5,0.17701,0.21433,0.17701,0.21433,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1896,,,,,success,P 3 2 1,121 121 40 90 90
 120,2.09,0.040,38.9,1.8,99.9,98.8,99.8,0.17069,0.20332,0.17069,0.20332,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1897,,,,,success,P 3 2 1,125 125 41 90 90
 120,3.13,0.033,48.8,1.9,99.9,94.6,100.0,0.1496,0.21743,0.14960,0.21743,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1898,,,,,success,P 3 2 1,124 124 40 90 90
 120,2.05,0.025,67.4,1.2,100.0,99.9,100.0,0.17456,0.21412,0.17456,0.21412,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1899,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.08,0.033,44.3,1.8,100.0,99.0,100.0,0.17272,0.20484,0.17272,0.20484,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1900,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.73,0.027,74.1,2.2,100.0,99.8,100.0,0.18839,0.21355,0.18839,0.21355,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1901,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.86,0.035,49.0,2.2,100.0,99.8,100.0,0.18403,0.21091,0.18403,0.21091,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1902,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.40,0.022,56.4,1.1,99.0,98.7,99.7,0.21356,0.27304,0.21356,0.27304,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1903,,,,,success,P 3 2 1,122 122 40 90 90
 120,3.15,0.050,32.1,1.9,99.5,97.5,99.6,0.18701,0.26293,0.18701,0.26293,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1904,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.32,0.049,35.5,1.3,99.6,99.3,100.0,0.17570,0.22598,0.17570,0.22598,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1905,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.76,0.060,27.7,1.4,99.9,99.3,100.0,0.16122,0.21651,0.16122,0.21651,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1906,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.31,0.036,38.5,1.5,99.9,98.3,100.0,0.16517,0.20716,0.16624,0.21070,P 3 2 1,3 - In
 Refinement,

NUDT7A-x1907,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.03,0.042,42.0,1.7,99.9,99.2,99.9,0.17499,0.20081,0.17499,0.20081,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1908,,,,,success,P 3 2 1,123 123 40 90 90
 120,2.48,0.096,20.8,1.3,100.0,98.0,100.0,0.16716,0.21453,0.16716,0.21453,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1909,,,,,Failed - unknown,None,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1919,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.59,0.049,45.2,0.9,98.1,99.9,100.0,0.19070,0.21526,0.19070,0.21526,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1920,,,,,success,P 3 2 1,125 125 41 90 90
 120,2.03,0.046,34.2,1.5,100.0,99.3,100.0,,,,,,

NUDT7A-x1921,,,,,success,P 3 2 1,124 124 40 90 90
 120,1.64,0.047,50.7,1.1,100.0,99.9,100.0,,,,,,

NUDT7A-x1922,,,,,success,P 3 2 1,122 122 40 90 90
 120,3.00,0.037,33.9,1.4,98.1,97.7,97.0,0.24764,0.34382,0.24764,0.34382,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1923,,,,,Failed - unknown,None,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1924,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.68,0.063,28.7,0.3,100.0,99.9,100.0,0.21126,0.23801,0.21126,0.23801,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1925,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.68,0.050,48.0,1.0,100.0,99.9,100.0,0.19788,0.22022,0.19788,0.22022,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1926,,,,,success,P 3 2 1,122 122 40 90 90
 120,2.25,0.038,38.7,7.0,100.0,99.4,100.0,0.17011,0.20339,0.17011,0.20339,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1927,,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1928,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.65,0.051,41.1,1.1,100.0,99.9,100.0,0.19339,0.21677,0.19339,0.21677,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1929,,,,,success,P 3 2 1,124 124 40 90 90
 120,1.65,0.047,47.6,1.0,100.0,99.7,100.0,0.18828,0.20965,0.18828,0.20965,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1930,,,,,success,P 3 2 1,124 124 40 90 90
 120,1.64,0.050,43.9,1.0,100.0,99.9,100.0,0.19264,0.21645,0.19415,0.21702,P 3 2 1,3 - In
 Refinement,

NUDT7A-x1931,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.52,0.064,35.5,1.1,100.0,100.0,100.0,0.19251,0.21148,0.19251,0.21148,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1932,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.47,0.060,39.7,1.2,100.0,99.9,100.0,0.19531,0.21527,0.19531,0.21527,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1933,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.48,0.065,37.5,1.2,100.0,99.9,100.0,0.19368,0.21283,0.19368,0.21283,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1934,,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1935,,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1936,,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x1937,,,,,success,P 3 2 1,124 124 41 90 90
 120,2.93,0.027,50.4,7.1,99.9,96.7,100.0,0.14995,0.21423,0.14995,0.21423,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1938,,,,,Failed - low resolution,P 3 2 1,123 123 40 90 90
 120,3.97,0.091,17.3,2.7,99.9,97.7,100.0,,,,,

NUDT7A-x1939,,,,,success,P 3 2 1,123 123 40 90 90
 120,3.11,0.039,37.5,1.4,98.0,95.1,99.8,0.21751,0.30576,0.21751,0.30576,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1961,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.76,0.021,72.7,1.0,99.9,98.2,99.5,0.18915,0.21811,0.18915,0.21811,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1962,,,,,success,P 3 2 1,124 124 41 90 90
 120,1.71,0.029,63.3,1.1,99.8,94.9,100.0,0.19059,0.21748,0.19059,0.21748,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1963,,,,,success,P 3 2 1,123 123 40 90 90
 120,1.78,0.037,43.4,1.1,100.0,98.9,100.0,0.19228,0.22684,0.19228,0.22684,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1964,,,,Failed - low resolution,P 3 2 1,123 123 40 90 90
 120,3.74,0.049,29.8,16.6,99.8,96.8,100.0,,,,,

NUDT7A-x1965,,,,Failed - low resolution,C 1 2 1,215 125 41 90 90
 90,4.13,0.357,5.3,2.0,99.8,94.9,100.0,,,,,

NUDT7A-x1966,,,,success,P 3 2 1,124 124 41 90 90
 120,1.87,0.026,62.7,1.3,100.0,99.8,100.0,0.19144,0.21854,0.19144,0.21854,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1967,,,,success,P 3 2 1,124 124 41 90 90
 120,1.99,0.022,61.8,1.2,99.7,98.9,100.0,0.19173,0.22096,0.19173,0.22096,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x1968,,,,success,P 3 2 1,124 124 41 90 90
 120,2.46,0.035,49.3,4.6,99.8,98.6,99.9,0.17144,0.21349,0.17144,0.21349,P 3 2 1,1 -
 Analysis Pending,

NUDT7A-x6264,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x6265,,,,success,P 3 2 1,125 125 41 90 90
 120,2.11,0.061,31.2,1.3,99.9,97.1,100.0,,,,,

NUDT7A-x8001,C1.C(NCC=1C=CN=CC1)C2=CC=CS2,counterion,,success,P 3 2 1,124 124 40 90 90
 120,2.04,0.046,131.4,5.8,100.0,99.7,100.0,,,,,

NUDT7A-x8002,,,,Failed - unknown,None,None,None,None,None,None,None,None,,,,,

NUDT7A-x8003,,,,success,P 3 2 1,124 124 40 90 90
 120,2.06,0.069,82.3,2.0,100.0,99.9,99.8,,,,,

NUDT7A-x8004,,,,success,P 3 2 1,124 124 40 90 90
 120,2.13,0.044,112.6,2.1,100.0,96.9,100.0,,,,,

NUDT7A-x8005,,,,Failed - unknown,P 3 2 1,124 124 40 90 90
 120,2.18,0.066,80.5,2.0,100.0,99.4,100.0,,,,,

SGC Dataset – PARP14A (csv format)

CrystalName,CompoundSMILES,CompoundCode,MountingResult,DataCollectionOutcome,DataProcessingSpaceGroup,DataProcessingUnitCell,DataProcessingResolutionHigh,DataProcessingRmergeLow,DataProcessingIsigLow,DataProcessingIsigHigh,DataProcessingCompletenessOverall,DataProcessingCompletenessLow,DataProcessingCompletenessHigh,DimpleRcryst,DimpleRfree,RefinementRcryst,RefinementRfree,RefinementSpaceGroup,RefinementOutcome,Deposition_PDB_ID

,Cc1cccc(c1)Cc2cnc(s2)NC(=O)C, FMOPL000486a,,,,,,,,,,,,,
,Cc1c(nc[nH]1)C[NH+]2CCc3cccc3C2, FMOPL000358a,Fail_Melted,,,,,,,,,,,,,
,CC(C)Oc1ccc(cc1)c2csc(n2)N, FMOPL000171a,,,,,,,,,,,,,
,CC(C)c1nnc(s1)NCC(C)(C)C, FMOPL000082a,,,,,,,,,,,,,
,c1cc(ccc1NC(=O)N2CCOCC2)O, FMOPL000175a,,,,,,,,,,,,,
,c1ccc(cc1)CNc2c[nH]c(=O)[nH]c2=O, FMOPL000470a,,,,,,,,,,,,,
,CCc1cc(=O)oc2c1ccc(c2)OC(=O)C, FMOPL000594a,,,,,,,,,,,,,
,Cc1c(cco1)C(=O)N2CCc3c2cccc3, FMOPL000427a,,,,,,,,,,,,,
,CN(C)c1ccc(cc1)C(=O)Nc2ccncc2, FMOPL000374a,,,,,,,,,,,,,
,CC(C)(C)NC(=O)c1ccc2c(c1)nns2, FMOPL000178a,,,,,,,,,,,,,
,c1cc(ccc1c2cc(c(s2)C#N)N)F, XST00000578b,,,,,,,,,,,,,
,Cc1ccc(cc1)c2cc(on2)C#N, FMOPL000556a,,,,,,,,,,,,,
,CNC(=O)c1nc(no1)c2cccs2, FMOPL000553a,,,,,,,,,,,,,
,c1ccc(cc1)OCC(=O)Nc2cccc(c2)F, FMOPL000433a,,,,,,,,,,,,,
,c1cc(ccc1C(=O)Nc2ccc(cc2)O)Cl, FMOPL000489a,,,,,,,,,,,,,
,COC(=O)c1c(ccs1)NC(=O)C2CC2, FMOPL000637a,,,,,,,,,,,,,
,c1cc(oc1)C(=O)N2CC[NH+](CC2)CC(=O)N, FMOPL000038a,,,,,,,,,,,,,
,Cc1ccc(cc1)S(=O)(=O)N(C)CCC#N, FMOPL000571a,,,,,,,,,,,,,
,Cc1nnc(s1)Nc2cccc(c2)F, FMOPL000635a,,,,,,,,,,,,,
,c1cc(ccc1NC(=O)Nc2ccc(cc2)F)F, FMOPL000662a,,,,,,,,,,,,,
,CC(=O)Nc1nc(ns1)SC, FMOPL000460a,,,,,,,,,,,,,
,CC(C)c1ccc(cc1)C(=O)Nc2nncs2, FMOPL000418a,,,,,,,,,,,,,
,Cc1ccc(c(c1)O)NC2=CC(=O)CC(C2)(C)C, FMOPL000379a,,,,,,,,,,,,,
,CCOc1ccc(cc1)C(=O)Nc2cccc2, FMOPL000050a,,,,,,,,,,,,,
,COC(=O)C#Cc1ccc2cccc2c1, FMOPL000062a,,,,,,,,,,,,,
,CCSc1nnc(s1)NC(=O)OC, FMOPL000224a,,,,,,,,,,,,,
,CC(C)(C(=O)NNc1ccc2cccc2c1)O, FMOPL000590a,,,,,,,,,,,,,
,CCOc1ccc(cc1)C(=O)Nc2cc(on2)C, FMOPL000749a,,,,,,,,,,,,,

,c1cc(c(cc1Cl)N)Nc2cc[nH+]cc2,FMOPL000639a,,,,,,,,,,,,,
,CC[C@H](C)NC(=O)c1ccc(cc1)NC(=O)C,FMOPL000120a,,,,,,,,,,,,,
,C[NH+]1CCN(CC1)c2ccc(cc2)C#N,FMOPL000230a,,,,,,,,,,,,,
,COc1ccc(cc1)N2C[C@@H](CC2=O)C(=O)N,FMOPL000131a,,,,,,,,,,,,,
,CC(C)CNC(=O)c1cc(ccc1OC)Cl,FMOPL000237a,,,,,,,,,,,,,
,c1cc(ccc1NC(=O)Nc2cncn2)Cl,FMOPL000431a,,,,,,,,,,,,,
,COc1ccc(cc1)Nc2c3c([nH]cn3)ncn2,PKTTA033042b,,,,,,,,,,,,,
,C[NH+]1CCC[C@@H]1CO,FMOPL000536a,Fail_Unpickable,,,,,,,,,,,,,
,CC(C)C(=O)N1CCN(CC1)c2cccc2N,FMOPL000611a,,,,,,,,,,,,,
,CNc1cccc1C(F)(F)F,FMOPL000136a,Fail_Unpickable,,,,,,,,,,,,,
,CCc1ccc(cc1)NC(=O)c2cncn2,FMOPL000244a,,,,,,,,,,,,,
,c1cc(sc1)C[NH2+]Cc2ccncc2,FMOPL000139a,Fail_Melted,,,,,,,,,,,,,
,C[C@H](C(=O)[O-])Oc1ccc(cc1)c2cccc2,FMOPL000250a,Fail_Melted,,,,,,,,,,,,,
,c1ccc(cc1)OCC(=O)N2CCNC(=O)C2,FMOPL000730a,Fail_Unpickable,,,,,,,,,,,,,
,C[C@@H](c1ccc(cc1)N2CCOCC2)[NH3+],FMOPL000390a,,,,,,,,,,,,,
,COC(=O)c1cccc1NC(=O)N2CCCC2,FMOPL000253a,,,,,,,,,,,,,
,CNC(=O)Nc1nc2ccc(cc2s1)OC,FMO3D000631b,,,,,,,,,,,,,
,c1ccc(cc1)CC2CCN(CC2)C(=O)CC#N,FMOPL000256a,,,,,,,,,,,,,
,c1ccc(cc1)c2nc(on2)c3cccc3O,FMOPL000051a,,,,,,,,,,,,,
,COC(=O)c1ccc(cc1)NC(=O)C(F)(F)F,FMOPL000149a,,,,,,,,,,,,,
,c1ccc(cc1)CC[NH+]2CCC(CC2)O,FMOPL000030a,,,,,,,,,,,,,
,c1ccc(cc1)c2ccc(cc2)NC(=O)N,FMOPL000257a,,,,,,,,,,,,,
,Cc1c(=O)n(c(nn1)Nc2cccc2OC)N,FMOPL000049a,,,,,,,,,,,,,
,Cc1c(nc2c(n1)c(nc(n2)N)OC(C)C)C,FMOPL000147a,,,,,,,,,,,,,
,CS(=O)(=O)N(CC(=O)N)C1CCCC1,FMOPL000032a,,,,,,,,,,,,,
,CCC(=O)NC(=S)N1CCCc2c1cccc2,FMOPL000148a,,,,,,,,,,,,,
,CC(=O)Nc1cc(cc(c1)C(=O)N)C(=O)N,FMOPL000034a,,,,,,,,,,,,,
,c1ccc(cc1)N(CCC#N)CC,FMOPL000540a,,,,,,,,,,,,,
,c1ccc(c(c1)C(=O)N)Nc2ccc(cc2)Cl,FMOPL000150a,,,,,,,,,,,,,
,CC(C)(CO)NC(=O)Nc1ccc(cc1)Cl,FMOPL000033a,,,,,,,,,,,,,
,c1cc(ccc1CCC(=O)[O-])c2ccc(cc2)O,FMOPL000151a,,,,,,,,,,,,,
,Cc1ccc(cc1)CC(=O)Nc2nccs2,FMOPL000037a,,,,,,,,,,,,,

,Cc1cc(nc(n1)Nc2ccc(cc2)N)C, FMOPL000278a,,,,,,,,,,,,,
,clcc(ccc1C[NH+]2CCOCC2)C(F)(F)F, FMOPL000345a,,,,,,,,,,,,,
,clccc(cc1)N2[C@H]3CC[C@H](O2)C=C3, FMOPL000700a,,,,,,,,,,,,,
,CCOC(=O)C[NH+]1CCS(=O)(=O)CC1, FMOPL000614a,,,,,,,,,,,,,
,clcnc(nc1)N2CCC(CC2)CO, FMOPL000274a,,,,,,,,,,,,,
,COc1ccc(cc1O)C[NH+]2CCCCC2, FMOPL000356a,,,,,,,,,,,,,
,CCc1cccc1NC(=O)c2c(nns2)C, FMOPL000736a,,,,,,,,,,,,,
,CCOC(=O)C1CCN(CC1)c2ccc(cc2)N, FMOPL000615a,,,,,,,,,,,,,
,clccc(c(c1)CO)N2CCOCC2, XST00000280c,,,,,,,,,,,,,
,CC[C@H](C#CC[NH+]1CCCC1)OC(=O)C, FMOPL000337a,,,,,,,,,,,,,
,Cc1ccc(cc1)N2CCN(CC2)C(=O)N, FMOPL000723a,,,,,,,,,,,,,
,CCOC(=O)c1cc2c([nH]1)ccs2, FMOPL000613a,,,,,,,,,,,,,
,CCOC(=O)c1ccc(cc1F)F, FMOPL000273a,,,,,,,,,,,,,
,CN(CCO)S(=O)(=O)c1ccc(cc1)N, FMOPL000328a,,,,,,,,,,,,,
,clcc(ccc1N2CCN(CC2)C(=O)N)F, FMOPL000716a,,,,,,,,,,,,,
,clcc(sc1)C[NH2+]Cc2ccc(cc2)O, FMOPL000619a,,,,,,,,,,,,,
,COc1cc(cc(c1OC)OC)C(=O)[O-], FMOPL000275a,,,,,,,,,,,,,
,CC(=O)N1CCC(CC1)[NH2+]CCc2cccc2, FMOPL000369a,,,,,,,,,,,,,
,C[C@H]1CCCCN1C(=O)c2cncn2, FMOPL000391a,,,,,,,,,,,,,

PARP14A-x0102,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
90,1.14,0.042,39.7,1.1,97.6,99.8,80.4,0.19515,0.22595,None,None,P 21 21 21,1 - Analysis
Pending,None

PARP14A-x0103,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
90,1.05,0.04,44.1,1.3,81.3,99,15.2,0.20411,0.22515,None,None,P 21 21 21,1 - Analysis
Pending,None

PARP14A-x0104,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
90,1.05,0.035,49.5,1.5,82.6,99.2,14.6,0.19497,0.22014,None,None,P 21 21 21,1 - Analysis
Pending,None

PARP14A-x0105,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
90,1.2,0.026,43.1,1.1,99.1,99.5,94.6,0.18803,0.21804,None,None,P 21 21 21,1 - Analysis
Pending,None

PARP14A-x0106,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
90,1.09,0.039,37,1,92.2,99.8,49.2,0.18636,0.21328,None,None,P 21 21 21,1 - Analysis
Pending,None

PARP14A-x0107,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
90,1.05,0.052,34.7,1.8,85.4,99.7,17,0.17942,0.19797,None,None,P 21 21 21,1 - Analysis
Pending,None

PARP14A-x0108,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.061,31.7,2.3,84.6,99.9,15.4,0.18224,0.20192, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0109,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.044,42.5,2.5,76.7,99.3,13.7,0.18331,0.20385, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0110,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.043,54.2,2.9,84.9,99.5,16.5,0.18483,0.20332, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0111,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.034,49.3,1.8,84.8,99.5,16.7,0.17947,0.19903, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0112,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.055,38.3,2.3,84.1,99.5,14.5,0.17877,0.19816, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0113,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.053,36.4,1.9,84.6,99.7,15.1,0.17966,0.19729, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0114,,,Mounted_Clear,success,P 21 21 21,33 41 110 90 90
 90,1.05,0.046,42.5,3,83.1,99.4,17.3,0.16962,0.1903, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0115,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.057,40.2,2.9,82.5,99.4,15.4,0.17922,0.19642, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0116,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.16,0.042,44.7,2,96,98.5,70.4,0.20347,0.22974, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0117,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.032,46.9,0.9,84.4,99.8,15.4,0.17464,0.19658, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0118,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.044,36.3,1.2,82.5,99.5,14.9,0.18335,0.20266, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0119,,,Mounted_Clear,success,P 21 21 21,33 41 110 90 90
 90,1.05,0.045,38.6,2,84,99.6,16.2,0.17233,0.195, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0120,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.027,62.3,1.1,84.4,99.6,15.4,0.17316,0.19722, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0121,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.037,54.4,3.2,82.3,99.4,14.9,0.18179,0.19958, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0122,,,Mounted_Clear,success,P 21 21 21,33 41 110 90 90
 90,1.05,0.045,38.3,1.6,84.5,99.5,14.8,0.16671,0.18413, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0123,,,Mounted_Clear,success,P 21 21 21,33 41 110 90 90
 90,1.05,0.034,52.8,1.4,83,99.5,14.7,0.18471,0.21065, None, None, P 21 21 21,1 - Analysis
 Pending, None

PARP14A-x0124,,,Mounted_Clear,success,P 21 21 21,33 41 110 90 90
 90,1.05,0.025,63.9,1.5,79.9,99.5,11.1,0.18052,0.20939,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0125,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.05,35.7,1.2,83.8,99.7,14.6,0.18969,0.21291,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0126,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.074,27.7,1.6,84.3,99.8,15.3,0.19718,0.21838,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0127,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.19,0.025,56.4,1.2,99.1,99.9,94.9,0.1961,0.224,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0128,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.027,63.7,1.3,83.2,99.7,15.6,0.19487,0.21948,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0129,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.06,35.7,2.1,85.7,99.8,15.2,0.1929,0.21526,0.1929,0.21526,P 21 21 21,3 - In
 Refinement,None

PARP14A-x0130,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.19,0.046,45.9,1.8,98.7,99.7,91.5,0.24125,0.26634,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0131,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.098,20.2,1.8,84.2,99.8,15.2,0.20084,0.22332,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0132,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.064,29.7,1.6,84.4,99.8,16.1,0.19368,0.21511,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0133,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.041,43.9,1.8,85.2,99.4,15.6,0.19302,0.21793,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0134,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.07,27.8,1.8,85,99.8,16.8,0.19557,0.21558,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0135,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.063,35.4,2.2,84.6,99.8,15.1,0.1987,0.22285,None,None,P 21 21 21,2 - PANDDA
 model,None

PARP14A-x0136,,,Mounted_Clear,success,P 21 21 21,34 41 110 90 90
 90,1.05,0.07,27.9,2,82.6,99.7,14.7,0.19935,0.22259,None,None,P 21 21 21,1 - Analysis
 Pending,None

PARP14A-x0137,COc1cc(ccc1N)N2CCOCC2,FMOPL000065a,Mounted_Clear,success,P 21 21 21,34 41
 111 90 90 90,1.05,0.04,43.1,2.4,71.5,98.6,9.3,0.17842,0.2013,0.13672,0.16584,P 21 21
 21,6 - Deposited,5QHT

PARP14A-x0138,CC[NH+]1CCCCC1,FMOPL000001a,Mounted_Clear,success,P 21 21 21,34 41 110 90
 90 90,1.05,0.043,38.3,1.5,80.5,99.5,12.3,0.17078,0.19102,None,None,P 21 21 21,1 -
 Analysis Pending,None

PARP14A-x0139,CC(=O)Nc1nnc(s1)COC,FMOPL000154a,Mounted_Clear,success,P 21 21 21,33 41
 110 90 90 90,1.2,0.026,43.1,1.1,99.3,99.9,96.8,0.19001,0.22478,None,None,P 21 21 21,1 -
 Analysis Pending,None

PARP14A-x0140, CCNC(=O)Nc1cc(on1)C, FMOPL000207a, Mounted_Clear, success, P 21 21 21, 33 41 108 90 90 90, 1.05, 0.029, 47.6, 0.9, 83.8, 99.9, 14.8, 0.17729, 0.19431, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0141, CC(C)(C)OC(=O)N1CC[NH+](CC1)CCO, FMOPL000067a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.05, 0.037, 50.1, 1, 83.8, 99.4, 15.4, 0.17602, 0.20097, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0142, CN(C)c1cc[nH+]cc1, XST00000847b, Mounted_Clear, success, P 21 21 21, 34 41 111 90 90 90, 1.05, 0.093, 22.8, 2.7, 77.8, 99.8, 8.4, 0.19304, 0.21206, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0143, Cc1c([nH]c2c1cc(cc2)F)C, FMOPL000155a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.05, 0.028, 53.4, 1.4, 83.9, 99.7, 14.4, 0.167, 0.18913, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0144, c1cc(ccc1NC(=O)C2CCC2)n3cnnn3, FMOPL000208a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.31, 0.024, 43.1, 1.1, 99.5, 99.7, 99.3, 0.18983, 0.23631, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0145, c1ccc(c(c1)C[NH3+])N2CCC(CC2)CO, FMOPL000066a, Mounted_Clear, success, P 21 21 21, 34 41 111 90 90 90, 1.1, 0.044, 33.1, 1, 89.3, 99.5, 41.4, 0.19055, 0.21508, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0146, COc1ccc(cc1)Cl, FMOPL000002a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.04, 49.3, 1.9, 83.9, 99.8, 13.9, 0.18023, 0.20198, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0147, C[NH+] (C) Cc1ccc(o1)C(=O) [O-], FMOPL000156a, Mounted_Clear, Failed - unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis Pending, None

PARP14A-x0148, c1ccc(cc1)Coc2ccc(cc2)C(=O)NN, FMOPL000209a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.049, 40, 2.1, 80.9, 99.4, 12.9, 0.18137, 0.20321, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0149, c1cc(ccc1c2ccn[nH]2)n3ccnc3, FMOPL000068a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.057, 33.5, 1.7, 81.8, 99.6, 13.2, 0.18793, 0.20991, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0150, C[NH2+]Cc1cccc(c1)Cl, FMOPL000004a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.041, 47.4, 1.6, 84.8, 99.7, 13.8, 0.19387, 0.21366, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0151, CS(=O)(=O)NCCc1cccc1, FMOPL000157a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.05, 41.3, 2.2, 80.9, 99.4, 13.8, 0.18441, 0.20604, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0152, COC(=O)c1ccc(cc1)c2ccc(cc2)N, FMOPL000070a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.056, 36, 1.7, 78.2, 99.2, 13.3, 0.19029, 0.21309, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0153, Cc1cc(ccc1F)OC, FMOPL000005a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.085, 26.8, 2.7, 84.4, 99.8, 14.7, 0.18684, 0.20765, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0154, CC(=O)Nc1cccc2c1non2, FMOPL000158a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.04, 43.9, 2, 77.6, 98.9, 14.4, 0.17841, 0.19892, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0155, CCC(=O)Nc1nc(cs1)C, FMOPL000211a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.05, 0.038, 52, 1.5, 85.4, 99.3, 15, 0.17252, 0.19585, 0.18834, 0.21447, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0156, c1ccc2c(c1)ncn2c3ccc(cc3)CO, FMOPL000069a, Mounted_Clear, success, P 21 21
21,33 41 110 90 90 90,1.05,0.042,44.5,2,82.5,99.4,14.1,0.16556,0.1856, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0157, C1COCC[NH+]1CCC#N, FMOPL000003a, Mounted_Clear, success, P 21 21 21,34 41 110
90 90 90,1.16,0.032,41.9,1,96.6,99.5,77.5,0.1847,0.21242, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0158, Cc1ccsc1C[NH2+]C(C)(C)CO, FMOPL000159a, Mounted_Clear, success, P 21 21 21,34
41 110 90 90 90,1.05,0.046,41.1,1.7,83.8,99.5,16.3,0.18358,0.2046, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0159, CNC(=O)c1ccc(cc1)S(=O)(=O)N, FMOPL000212a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.036,43.3,1.3,82.7,99.4,15.7,0.18418,0.21036, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0160, c1ccc2c(c1)nc(o2)c3cc(ccc3F)N, FMOPL000071a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.057,42.4,3.2,81.7,99.6,13.6,0.18729,0.20526, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0161, CC(=O)Nc1ccccc1O, FMSOA000341b, Mounted_Clear, success, P 21 21 21,34 41 110
90 90 90,1.05,0.026,58.2,1.2,82.8,99.6,14.3,0.18165,0.2025,0.14273,0.16562, P 21 21 21,6
- Deposited, 5QHU

PARP14A-x0162, c1cc(cnc1)C[NH2+]C2CCCC2, FMOPL000160a, Mounted_Clear, success, P 21 21 21,34
41 111 90 90 90,1.05,0.076,23.3,0.9,85,99.9,15.2,0.19474,0.21782, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0163, c1cnc(nc1)NC2CCCCC2, FMOPL000213a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.14,0.033,41.1,1,97.6,99.9,80.7,0.18452,0.20944, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0164, COC(=O)c1ccccc1Oc2ccc(cc2)N, FMOPL000072a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.088,22.1,1.6,82.4,99.7,13.9,0.19433,0.21799, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0165, COc1ccc(cc1)NC(=S)N, FMOPL000007a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.05,0.049,45.5,3.2,79,99.5,8.9,0.18384,0.20379, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0166, c1cocc1C[NH2+]C[C@H]2CCCCO2, FMOPL000161a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.038,48,1.4,83.8,99.5,16.4,0.18974,0.21277, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0167, c1cc(c(cc1n2cc(nn2)CO)Cl)Cl, FMOPL000214a, Mounted_Clear, success, P 21 21
21,33 41 110 90 90 90,1.05,0.042,45,2,81,99.7,14.6,0.16646,0.18667, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0168, c1cnc(nc1)Oc2ccc(cc2)c3cc[nH]n3, FMOPL000074a, Mounted_Clear, success, P 21
21 21,33 41 109 90 90 90,1.14,0.028,50.6,1.2,93.3,99.6,63.2,0.19266,0.22719, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0169, Cc1nc(nol)c2ccccc2, FMOPL000008a, Mounted_Clear, success, P 21 21 21,34 41 110
90 90 90,1.05,0.047,40,2.1,84.8,99.6,14.4,0.17483,0.19259, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0170, c1cc(scl)CNC2ccc(cc2)O, FMOPL000162a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.1,0.022,60.4,1,91.6,98.9,50.6,0.17487,0.19886, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0171, CN(C)C(=O)Nc1ccc(cc1)S(=O)(=O)N, FMOPL000215a, Mounted_Clear, success, P 21
21 21,33 41 110 90 90 90,1.06,0.036,46.5,0.9,86.4,99.5,24.6,0.1802,0.20268, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0172, COc1ccc(cc1)[C@H]2C=C(NC(=O)N2)C(=O)[O-], FMOPL000073a, Mounted_Clear, Failed - low resolution, P 21 21 21,34 41 110 90 90
 90,3.93,0.468,4.9,1.1,97.8,72.5,99.2,,,None, None, None, 1 - Analysis Pending, None

PARP14A-x0173, CCOC(=O)C[NH+]1CCCCC1, FMOPL000006a, Mounted_Clear, success, P 21 21 21,34 41
 110 90 90 90,1.05,0.051,39.8,2.3,85.6,99.6,17.5,0.18319,0.20111, None, None, P 21 21 21,1
 - Analysis Pending, None

PARP14A-x0174, CC[C@H](C)c1ccc(cc1)NS(=O)(=O)C, FMOPL000163a, Mounted_Clear, success, P 21
 21 21,34 41 110 90 90 90,1.08,0.031,45.4,0.9,91.2,99.8,42.4,0.20345,0.22633, None, None, P
 21 21 21,1 - Analysis Pending, None

PARP14A-x0175, c1cc(sc1)c2[nH]ccn2, FMOCR000171b, Mounted_Clear, success, P 21 21 21,34 41
 110 90 90 90,1.05,0.04,46.5,1.6,83.5,99.6,14.1,0.18965,0.21227, None, None, P 21 21 21,1 -
 Analysis Pending, None

PARP14A-x0176, C[NH+]1CCN(CC1)S(=O)(=O)N(C)C, FMOPL000075a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.05,0.042,50.4,2,83.8,99.6,15.7,0.19907,0.22044, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0177, c1ccc(c(c1)C[NH3+])OC(F)(F)F, FMOPL000009a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.05,0.028,53.4,1.2,84.8,99.2,16,0.17057,0.19125, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0178, COC(=O)Nc1ccc(cc1)Br, FMOPL000216a, Mounted_Clear, success, P 21 21 21,34 41
 110 90 90 90,1.13,0.042,35.9,1,94.1,99.8,60.8,0.18976,0.21514, None, None, P 21 21 21,1 -
 Analysis Pending, None

PARP14A-x0179, COc1cccc(c1)[C@H](CC(=O)[O-])[NH3+], FMOPL000012a, Mounted_Clear, success, P
 21 21 21,34 41 110 90 90 90,1.05,0.052,36.3,2,83.4,99.6,15.2,0.18225,0.20407, None, None, P
 21 21 21,1 - Analysis Pending, None

PARP14A-x0180, Cc1ccc(cc1)c2ccc([nH]2)C(=O)[O-], FMOPL000165a, Mounted_Clear, success, P 21
 21 21,33 41 110 90 90 90,1.05,0.036,54,0.9,83.2,99.8,15.4,0.18165,0.2087, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0181, c1ccc2c(c1)ccc(n2)C(=O)NO, FMOPL000217a, Mounted_Clear, Failed -
 unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis
 Pending, None

PARP14A-x0182, Cc1ccc(cc1)c2nc(on2)C[NH2+]C(C)C, FMOPL000293a, Mounted_Clear, success, P 21
 21 21,33 41 109 90 90 90,1.1,0.026,45.8,1,89.4,99.5,41,0.17892,0.20318, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0183, C[NH+]1CCN(CC1)C(=O)Nc2ccc(cc2)F, FMOPL000740a, Mounted_Clear, success, P 21
 21 21,33 41 110 90 90 90,1.05,0.038,50.5,1.5,83.9,99.8,15.1,0.16529,0.18429, None, None, P
 21 21 21,1 - Analysis Pending, None

PARP14A-x0184, CC(=O)Nc1nnc(s1)SCC(=O)[O-], FMOPL000618a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.18,0.04,51.8,1.3,98.3,99.7,84.1,0.20086,0.22411,0.21389,0.23698, P 21 21 21,1 -
 Analysis Pending, None

PARP14A-x0185, COC(=O)c1ccncc1, FMOPL000272a, Mounted_Clear, Failed -
 unknown, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 1 - Analysis
 Pending, None

PARP14A-x0186, c1cc(cc1C(=O)N2CCSCC2)Cl, FMOPL000284a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.13,0.027,50,1,97.1,99.6,75.1,0.17439,0.19488, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0187,CN(C)C(=O)OCCn1ccnc1,FMOPL000698a,Mounted_Clear,success,P 21 21 21,34 41
110 90 90 90,1.05,0.05,37.1,1.9,82.7,99.6,15.5,0.1692,0.19,None,None,P 21 21 21,1 -
Analysis Pending,None

PARP14A-x0188,c1cc(ccc1CN2CCC(=O)N2)C1,FMOPL000617a,Mounted_Clear,success,P 21 21 21,33
41 110 90 90 90,1.05,0.032,55.2,2,84.2,99.8,14.4,0.16804,0.18979,0.15805,0.17412,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0189,CCOC(=O)c1c[nH]nc1,FMOPL000271a,Mounted_Clear,success,P 21 21 21,34 41 110
90 90 90,1.05,0.036,47.4,1.2,82.4,99.6,13.8,0.17799,0.19949,0.16197,0.1808,P 21 21 21,1
- Analysis Pending,None

PARP14A-x0190,c1ccc(c(c1)N)Nc2[nH]c3ccccc3n2,FMOPL000295a,Mounted_Clear,success,P 21 21
21,33 41 110 90 90 90,1.05,0.034,47.1,1,85.5,99.5,16.3,0.17431,0.19714,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0191,c1cc(ccc1CC(=O)Nc2ccc(cc2)F)F,FMOPL000746a,Mounted_Clear,success,P 21 21
21,33 41 110 90 90 90,1.05,0.036,44.4,1.4,84.5,99.7,14.7,0.16854,0.19061,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0192,CCNC(=O)Oc1ccc(cc1)c2csnn2,FMOPL000621a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.09,0.03,51.5,2.6,87.2,99,43.6,0.17389,0.19739,None,None,P 21 21
21,2 - PANDDA model,None

PARP14A-x0193,CCOC(=O)c1c(nc(s1)C)C(F)(F)F,FMSOA000791b,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.18,0.037,41.6,2.7,97.8,99.7,87.8,0.18158,0.20774,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-
x0194,CC(C)COc1ccc(cc1)[C@@H]2C(=O)NC(=O)N2,FMOPL000301a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.072,28.2,6,83.1,99.3,13.8,0.1838,0.20521,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0195,CC(C)CNC(=O)c1ccc2ccccc2c1,FMOPL000732a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.1,0.031,55.1,1.3,92,98.9,48.6,0.19122,0.21456,None,None,P 21 21 21,1
- Analysis Pending,None

PARP14A-x0196,c1ccc(cc1)c2ccccc2NNC(=S)N,FMOPL000624a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.1,0.033,53.9,2.6,91.9,99,58.1,0.20324,0.22552,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0197,C[NH+]1CCN(CC1)c2nc3ccccc3s2,FMOPL000478a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.15,0.025,63.9,1.8,92.8,98.5,60,0.18961,0.22023,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0198,CC(=O)NCCc1c[nH]c2c1cc(cc2)F,FMOPL000287a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.1,0.045,39.4,2.6,95,99.6,70.7,0.18806,0.2102,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0199,c1c(cnc1Br)C(=O)ON,FMOPL000692a,Mounted_Clear,success,P 21 21 21,34 41
110 90 90 90,1.13,0.029,58.6,2.6,97.2,99.4,84,0.19777,0.22162,None,None,P 21 21 21,1 -
Analysis Pending,None

PARP14A-x0200,CC(C)(C)c1ccc(cc1)NNC(=S)N,FMOPL000620a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.14,0.031,55.7,2.6,98,99.6,88.8,0.19204,0.21805,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0201,C[NH+](C)CCN1C(=O)c2ccccc2C1=O,FMOPL000477a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.13,0.028,60.2,1.5,96.3,99.4,68.9,0.19099,0.2168,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0202, c1cncclCCNC(=O)NC2CCCC2, FMOPL000299a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.051, 41.6, 2.4, 85.1, 99.2, 14.7, 0.19557, 0.21073, 0.14205, 0.16306, P 21 21 21, 6 - Deposited, 5QHV

PARP14A-x0203, c1cc(oc1)C(=O)OCc2ccc(cc2)Cl, FMOPL000714a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.14, 0.03, 52.6, 1.7, 95.3, 99.3, 64.3, 0.20514, 0.22789, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0204, COC(=O)[C@@H]1C[C@H](CN1C(=O)c2ccco2)O, FMOPL000622a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.059, 37.4, 3.2, 85.3, 99.2, 15.2, 0.20182, 0.22057, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0205, CC(C)(C)NC(=O)Cn1ccc(n1)C(F)(F)F, FMOPL000482a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.051, 42.8, 2.8, 81.8, 98.9, 14.5, 0.19588, 0.21692, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0206, Cc1cc(=O)oc2c1ccc(c2C[NH+](C)C)O, FMOPL000294a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90, 1.17, 0.025, 51.9, 1.1, 98.4, 99.7, 88.9, 0.19881, 0.2258, 0.19972, 0.22519, P 21 21 21, 3 - In Refinement, None

PARP14A-x0207, Cc1cc(nol)NC(=O)CCC2CCCC2, FMOPL000741a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.028, 55.5, 1.4, 95, 99.2, 63.1, 0.19077, 0.21832, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0208, COC(=O)[C@@H]1C[C@@H](CN1C(=O)c2ccco2)O, FMOPL000622a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.03, 50.6, 2.6, 89.2, 99.3, 53.9, 0.1931, 0.21717, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0209, C[C@]1(C(=O)NC(=O)N1)CCc2ccc(cc2)OC, FMOPL000497a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90, 1.11, 0.032, 54.1, 2.5, 94.2, 99.5, 67.3, 0.18761, 0.21189, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0210, c1cc(oc1)CNC(=O)NC2CCCC2, FMOPL000286a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.059, 36.4, 2.1, 81.4, 99.4, 13.9, 0.20311, 0.22469, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0211, COc1ccc(cc1)CC(=O)Nc2nncs2, FMOPL000738a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.35, 0.027, 47.6, 1.1, 99.5, 99, 99, 0.19455, 0.23368, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0212, CC(=O)NCc1cc(nol)c2ccc(cc2)OC, FMOPL000625a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.14, 0.034, 43.1, 2.7, 96.1, 99.5, 76.5, 0.17046, 0.19165, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0213, CC(C)C(=O)Nc1nnc(s1)COC, FMOPL000282a, Mounted_Clear, success, P 21 21 21, 33 41 110 90 90 90, 1.46, 0.027, 44.2, 1.1, 99.4, 99.6, 98.9, 0.21675, 0.28125, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0214, c1c(nns1)C(=O)NO, SDOOA000892b, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.03, 56.8, 2.5, 93.6, 99.6, 64.9, 0.19373, 0.2202, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0215, CC(C)CC(=O)Nc1ccc(cc1)C(=O)NN, FMOPL000483a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.48, 0.032, 47.6, 2, 99.8, 99, 97.9, 0.1856, 0.22637, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0216, c1ccc2c(c1)c(c[nH]2)C[NH+]3CCCCC3, FMOPL000291a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.2, 0.029, 53.5, 1.6, 97, 99, 84.2, 0.19789, 0.22455, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0217, c1cc(ccc1NC(=O)C[NH+]2CCCC2)F, FMOPL000715a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.09,0.028,58.2,1.3,90.3,99.1,43.2,0.19058,0.21674, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0218, C#Cc1ccc(cc1)OCc2ccccc2, FMOOA000390b, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.1,0.024,60.6,1.2,93.3,99.1,54.3,0.18836,0.21379, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0219, CC(C)[NH2+]Cc1ccc(cc1)N(C)C, FMOPL000463a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.11,0.03,52.8,1.3,95.4,99.3,64.1,0.1929,0.21646, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0220, Cc1cccc(c1)C(=O)N2CCC(CC2)C(=O)N, FMOPL000307a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.13,0.027,61.8,2.7,94.4,99,70.5,0.17924,0.20531, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0221, CCC(=O)Nc1ccc(cc1)N2CCC(CC2)C, FMOPL000748a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.18,0.031,50.3,1.5,97.5,99.3,81.9,0.18827,0.21728, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0222, c1ccn(c1)CCNC(=O)C(F)(F)Cl, FMOPL000616a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.18,0.03,52.1,1.6,98.5,98.5,92.7,0.18089,0.20619, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0223, c1cc(oc1)C(=O)N[C@@H]2CCCCNC2=O, FMOPL000472a, Mounted_Clear, success, P 2 2
2,34 41 111 90 90 90,1.14,0.025,61.4,1.6,95,99,61.9,0.2016,0.22923, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-
x0224, CNC(=O)[C@@H]1CC(=O)N(C1)c2ccc(cc2)OC, FMOPL000304a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.12,0.035,45.9,2.4,93.3,99.6,64.6,0.19682,0.22411, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0225, C[C@@H](C[NH2+]Cc1ccc2c(c1)OCO2)O, FMOPL000709a, Mounted_Clear, success, P 2 2
2 2,34 41 110 90 90 90,1.11,0.031,50.8,1.2,95.3,99.4,63,0.18672,0.2136, None, None, P 21 21
21,2 - PANDDA model, None

PARP14A-x0226, CC(=O)NCCc1cccc2c1cc(cc2)OC, BDOOA011525c, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.16,0.03,52.3,1.3,97.9,99.2,85.9,0.18877,0.21288, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0227, c1ccc(cc1)C[NH+]2CCC(CC2)n3cccc3, FMOPL000492a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.2,0.03,48.9,1.8,99.6,99.2,95.7,0.18146,0.21031, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-
x0228, CC1([C@@H]2CC=C([C@@H]1C2)C[NH+]3CCC[C@@H]3CO)C, FMOPL000351a, Mounted_Clear, success
, P 2 2 2,34 41 110 90 90
90,1.05,0.043,48.1,2.8,81.4,98.7,13.7,0.18776,0.20872, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-
x0229, C[C@@H]1CC[C@@H](C1)[NH+]2CCN(CC2)c3cccc3, FMOPL000376a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.057,36.9,3,76.4,98.7,13,0.17993,0.20108, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0230, c1cc(ccc1C[NH+]2CC[C@@H](C2)O)Cl, FMOPL000314a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.049,39.3,2,83.5,99.4,15.2,0.18987,0.21149, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0231, Cc1ccsc1C[NH+]2CCC[C@@H]2CO, FMOPL000320a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.14,0.036,46.1,2.5,97.4,99.9,83.2,0.19012,0.2169, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0232,C[C@H]1CCCC[NH+]1Cc2ccc(cc2)C(=O)OC,FMOPL000375a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.1,0.024,65.3,1.2,93.5,99.2,53.4,0.18206,0.2075, None, None, P 21 21,1 - Analysis Pending, None

PARP14A-x0233,Cc1cc(c(cc1OC)C)C[NH+]2CC[C@H](C2)O,FMOPL000359a,Mounted_Clear,success,P 21 21,34 41 110 90 90,1.14,0.029,51.7,2.6,96.8,99.8,79.9,0.17692,0.20348, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0234,c1ccc2c(c1)CC[NH+](C2)Cc3ccccc3O,FMOPL000367a,Mounted_Clear,success,P 2 2 2,33 41 110 90 90,1.38,0.018,76.5,2,99.7,99.1,96.9,0.1699,0.20862, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0235,CCC1CCC(CC1)[NH+]2CCOCC2,FMOPL000315a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.05,40.4,2.3,85.7,99.5,15.1,0.18416,0.20559, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0236,CCC1CCC(CC1)[NH2+]C[C@H]2CCCO2,FMOPL000326a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.13,0.034,49.1,2.8,94.5,99.6,67.4,0.18263,0.20757, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0237,CC(=O)N1CC[NH+](CC1)CCCc2ccccc2,FMOPL000370a,Mounted_Clear,Failed - centring failed,,,,,,,,,,,,,#NAME?,

PARP14A-x0238,Cc1c(n2ccccc2n1)C(=O)NCC(C)C,FMOPL000347a,Mounted_Clear,success,P 2 2 2,34 41 111 90 90 90,1.12,0.023,67.5,2.1,90.9,99.2,44.1,0.18144,0.20933,0.13829,0.1696,P 21 21 21,6 - Deposited,5QHW

PARP14A-x0239,COC(=O)C1CC[NH+](CC1)CC(=O)N,FMOPL000077a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.13,0.023,63.6,1.6,92.2,98.9,52.8,0.1786,0.20437, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0240,C1CCN(CC1)C(=O)N2CCCCC2,FMOPL000010a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.09,0.025,57.8,1.3,83.2,98.7,31.5,0.1762,0.19853, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0241,c1cc(ccc1C[NH2+]C[C@H]2CCCO2)F,FMOPL000166a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.08,0.031,56.5,2.5,84.8,99.7,32.2,0.17789,0.20065, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0242,CCOC(=O)C1CCN(CC1)c2cncn2,FMOPL000218a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.17,0.029,49.8,2.5,99.1,99.9,94.2,0.18861,0.21422, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0243,c1ccnc(c1)NS(=O)(=O)c2ccc(cc2)N,FMOPL000078a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.13,0.033,48.6,2.5,95.5,99.8,73.2,0.19601,0.2221, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0244,c1ccc(c(c1)C(=O)[O-])OC(F)(F)F,FMOPL000013a,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,#NAME?,

PARP14A-x0245,C1CCCC(CC1)NC(=O)[C@H]2CCCO2,FMOPL000167a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.12,0.022,59.7,0.9,95.9,99.9,69.2,0.20102,0.22963, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0246,c1ccc2c(c1)ncn2Cc3ccc(cc3)C#N,FMOPL000219a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.036,58.6,3.2,70.8,98.2,6.9,0.19694,0.22333, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0247,CCOc1ccc2c(c1)sc(n2)C,FMOPL000079a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.1,0.027,63,1.5,86.4,99,38.8,0.19168,0.21828, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0248, COc1cc(cc(c1OC)OC)C[NH3+], FMOPL000011a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.068, 31, 6.8, 74.6, 98.8, 9.5, 0.20211, 0.22591, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0249, C1CCC(CC1)NC(=O)NC[C@H]2CCCO2, FMOPL000168a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.06, 0.033, 56.1, 1.6, 83.2, 98.6, 19.7, 0.20512, 0.22518, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0250, Cn1c(cc(n1)c2cccs2)N, XST00000599c, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.22, 0.023, 55.5, 1.9, 99.4, 98.5, 96.3, 0.19553, 0.22984, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0251, c1ccc(cc1)COc2ccccc2N, FMOPL000014a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.18, 0.029, 55.4, 2.4, 99.6, 99.9, 97.6, 0.19069, 0.21822, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0252, COc1ccc(cc1)[C@@H](c2ccccc2)[NH3+], FMOPL000169a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.27, 0.018, 67.3, 2, 99.5, 98.9, 94.9, 0.1855, 0.22356, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0253, COCc1nnc(s1)N, FMOPL000544a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.031, 58.9, 2.3, 79.4, 99.1, 11.5, 0.18637, 0.21136, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0254, CCc1cccc1NNC(=S)N, FMOPL000081a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.036, 49.1, 2.6, 88.1, 98.8, 43.2, 0.19933, 0.22359, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0255, c1ccc(cc1)c2ccc(cc2)CC(=O)[O-], FMOPL000015a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.047, 42.3, 2.4, 84.3, 99.4, 14.7, 0.19345, 0.21418, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0256, CCOC(=O)Nc1nc2ccc(cc2s1)C, FMOPL000170a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.09, 0.031, 54.2, 1.3, 92.9, 99.3, 48.9, 0.19977, 0.22402, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0257, c1cnc([nH]1)c2[nH]ccn2, FMOPL000545a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.033, 49, 2.7, 93, 98.7, 62.3, 0.20603, 0.22861, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0258, c1cc(sc1)c2ccc(cc2)C[NH3+], FMOPL000080a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.04, 45.1, 2.6, 90.7, 99.2, 50.7, 0.19916, 0.22072, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0259, c1ccc(cc1)C[NH2+]Cc2ccc(cc2)F, FMOPL000016a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.043, 49.8, 1.5, 76.1, 98.6, 12.6, 0.19954, 0.22438, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0260, C[C@H]([C@H](c1ccccc1)O)[NH2+]C, FMOPL000548a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.026, 61.2, 1.3, 95.5, 99.1, 66.2, 0.19124, 0.21956, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0261, CNC(=O)NCc1c(ccc1C1)F, FMOPL000084a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.16, 0.03, 50.7, 1.7, 97.2, 99.1, 73.7, 0.20319, 0.23049, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0262, C[NH2+]Cc1ccncc1, FMOPL000017a, Mounted_Clear, Failed - unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0263, c1cc(cc(c1)F)NC(=O)c2cncn2, FMOPL000172a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.15, 0.026, 59.2, 1.4, 98.2, 99.4, 82.2, 0.20417, 0.22953, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0264, c1ccc2c(c1)[nH]c(n2)NC#N, FMOPL000546a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.047, 40.8, 2, 84, 99.4, 14.8, 0.19309, 0.21606, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0265, c1cn[nH]c1c2cc(cc(c2O)F)F, FMOPL000085a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.14, 0.029, 48.9, 2.4, 97.1, 99.6, 85.2, 0.19293, 0.21877, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0266, Cc1cc(C)nc(Nc2ccc(cc2)N)n1, FMOPL000278a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.11, 0.026, 57.6, 1.2, 95.6, 99.2, 63.8, 0.179, 0.2037, 0.14173, 0.17052, P 21 21 21, 6 - Deposited, 5QHX

PARP14A-x0267, CC(C)[NH+]1CCN(CC1)C(=O)c2cccs2, FMOPL000173a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.09, 0.031, 58.6, 1.2, 91.8, 99.4, 45.7, 0.20266, 0.22855, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0268, C[NH+](C)CC#Cc1cccc1, FMOPL000549a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.13, 0.024, 60.1, 2.5, 97.5, 99.6, 85.7, 0.19057, 0.21465, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0269, CCc1nc(no1)c2ccc(cc2)Cl, FMOPL000083a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.047, 46.9, 1.8, 84.4, 99.4, 14.9, 0.19748, 0.21988, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0270, CN(c1ccc(cn1)C(F)(F)F)N, FMSOA000815b, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.044, 47.6, 2, 83.8, 99.3, 13.8, 0.19486, 0.21615, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0271, Cc1ccc(cc1C)C(=O)Nc2nc[nH]n2, FMOPL000174a, Mounted_Clear, Failed - unknown, #NAME?,

PARP14A-x0272, Cc1ccc(o1)c2ccccc2N, FMOPL000550a, Mounted_Clear, Failed - unknown, #NAME?,

PARP14A-x0273, Cc1ccc(o1)c2cccc(c2)N, FMOPL000020a, Mounted_Clear, Failed - no diffraction, P 2 2 2, 34 41 110 90 90 90, 9.56, 0, 0, 0, 93.1, 0, 72.2, , , , , , , ,

PARP14A-x0274, c1c(c(=O)[nH]c(=O)[nH]1)N2CCOCC2, FMOPL000552a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.16, 0.027, 50.6, 1.1, 95.8, 99.9, 76.5, 0.20945, 0.23298, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0275, COc1ccc(cc1)C(=O)NCC(=O)N, FMOPL000090a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.26, 0.024, 54.5, 1.7, 99, 99.2, 93.9, 0.21052, 0.24306, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0276, CS(=O)(=O)Nc1ccc(cc1)C[NH3+], FMOPL000019a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.06, 34, 3, 83.1, 99.3, 14.7, 0.19907, 0.22096, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0277, c1ccc(cc1)C2CC[NH+](CC2)CC(=O)[O-], FMOPL000176a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.1, 0.032, 50.2, 1.3, 89.6, 99.3, 41, 0.20074, 0.22377, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0278, c1cc(ccc1c2cncnc2N)Cl, FMOPL000557a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.068, 31.2, 2.5, 75.8, 99.1, 12.9, 0.20926, 0.23327, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0279, COC(=O)c1c(cc(s1)c2cccs2)N, FMOPL000088a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.051, 39.5, 2.8, 75.6, 99, 13, 0.19153, 0.21551, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0280, c1cc(cc(c1)OC(C(F)F)(F)F)N, FMOPL000021a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.029,53.5,2.5,87.3,99.1,41.2,0.1966,0.21962, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0281, C[C@H]1CCCC[NH+]1Cc2ccccc2C#N, FMOPL000177a, Mounted_Clear, Failed -
unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0282, COc1ccc(c(c1)O)c2cc[nH]n2, FMOPL000554a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.033,53.5,2.5,87.9,99.3,45.9,0.20552,0.22945, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0283, CNC(=O)c1cccc1NC(=O)c2ccco2, FMOPL000751a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.052,37,2.5,88.6,99.4,44.7,0.2093,0.23198, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0284, CC(=O)Nc1ccc(cc1)C(=O)Nn2cncn2, FMOPL000443a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.26,0.024,60.9,2,95,97.8,85.6,0.1905,0.21989, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0285, c1cc(cnc1)CNC2ccc(cc2C(=O)[O-])N, FMOPL000298a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.1,0.039,47.9,2.6,90.6,99.5,52.8,0.19197,0.21674, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0286, Cc1c(cccc1Cl)NC(=O)[C@@H]2CCCO2, FMOPL000722a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.12,0.023,68.1,2.7,91,98.8,56,0.20216,0.2273, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0287, C[C@H]1CCCCN1C(=O)N2CCOCC2, FMOPL000392a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.05,0.058,37.7,3,84.4,99.2,14.3,0.20104,0.21891, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0288, c1ccc(cc1)CC(=O)N2CCc3c2ccccc3, FMOPL000491a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.13,0.035,47.4,2.7,96.7,99,80.1,0.20034,0.22355, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0289, C1CCN(CC1)c2c(non2)N, FMOPL000280a, Mounted_Clear, success, P 21 21 21,34 41
111 90 90 90,1.13,0.029,57.3,2.5,97.1,99.4,82.7,0.18941,0.21784,0.19499,0.2183, P 21 21
21,3 - In Refinement, None

PARP14A-x0290, CC[C@@H](C)NC(=O)c1cc(on1)c2ccccc2, FMOPL000750a, Mounted_Clear, success, P 2
2 2,34 41 110 90 90 90,1.1,0.031,56.3,1.1,92.6,99.2,50.5,0.20324,0.22834, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0291, CC(C)c1ccc(cc1)NC(=O)N2CCOCC2, FMOPL000442a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.13,0.03,55.3,2.6,96.9,99.4,80.8,0.20206,0.22736, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0292, c1cc(ccc1C[NH2+])C2CCCC2)O, FMOPL000467a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.13,0.031,51.7,1.4,97.2,99.3,73.9,0.19346,0.21809, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0293, CC[C@H](C)c1ccc(c(c1)O)NC(=O)C, FMOPL000285a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.1,0.039,46,2.5,92.5,99.4,59.3,0.18851,0.2124, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0294, c1cc(ccc1NC(=O)CC#N)OC(F)(F)F, FMOPL000725a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.08,0.029,58.2,2.7,85.4,98,34.8,0.18573,0.2087, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0295, Cc1c(c(n[nH]1)C)CCOc2ccc(cc2)F, FMOPL000488a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.07,0.032,49,1.4,79.7,98.4,24.1,0.18996,0.21528, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0296, Cc1ccc(c(c1)C)OCC(=O)N2CCOCC2, FMOPL000306a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.09,0.025,68.9,1.2,91.8,99.2,45.3,0.19198,0.21857, None, None, P 21 21
 21 21,1 - Analysis Pending, None

PARP14A-x0297, c1cc(ccc1C(=O)N)NC(=O)c2cncn2, FMOPL000758a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.05,0.038,52.9,2.1,71.7,98,8.8,0.1911,0.21872, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0298, CCn1ccc(n1)C[NH2+]C, FMOPL000384a, Mounted_Clear, success, P 21 21 21,34 41
 110 90 90 90,1.1,0.026,60.6,2.6,89.6,99.1,47.5,0.20012,0.22767, None, None, P 21 21 21,1 -
 Analysis Pending, None

PARP14A-x0299, Cc1ccc(oc1)C[NH+] (C)Cc2ccccc2, FMOPL000479a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.11,0.046,37.5,2.6,95.4,99.5,72.9,0.19099,0.21513, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0300, CCOC(=O)c1c(nc(s1)N(C)C(=O)C)C, FMOPL000288a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.05,0.046,42.9,1.7,78.3,99.1,12.5,0.20189,0.22687, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0301, c1ccc(cc1)Nc2nnc3n2nc(cc3)Cl, FMOPL000745a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.15,0.023,63.7,2.7,98,99.8,86.7,0.17996,0.20437, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0302, c1cc2c(cc1C(=O)N3CCCCC3)OCO2, FMOPL000435a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.09,0.042,45.3,2.5,91.7,99.6,57.3,0.19327,0.21788, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0303, COc1ccc(cc1)C(=O)Nc2ccccc2F, FMOPL000496a, Mounted_Clear, Failed -
 unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0304, Cn1nc(nn1)NC(=O)c2ccc(cc2)Cl, FMOPL000290a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.17,0.024,60.1,1.5,99.1,99.3,91.4,0.18702,0.2139, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0305, CC(=O)Nc1ccc(cc1)C#N, FMSOA000445b, Mounted_Clear, Failed -
 unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0306, Cn1c(c(cn1)NC(=O)c2ccccc2)C(=O)N, FMOPL000456a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.08,0.033,51.4,1.3,88,99.2,36.5,0.19563,0.21966, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-x0307, ClCCC(CC1)C(=O)N2CCC(CC2)C(=O)N, FMOPL000480a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.19,0.02,72.4,2,98.8,99,91.1,0.1839,0.21061, None, None, P 21 21 21,1
 - Analysis Pending, None

PARP14A-x0308, Cn1nc(nn1)NC(=O)c2cc3ccccc3o2, FMOPL000309a, Mounted_Clear, success, P 2 2
 2,34 41 110 90 90 90,1.15,0.022,73.2,1.6,96.4,98.9,75.7,0.20439,0.23266, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0309, c1cc(cnc1)C[NH2+]C[C@@H]2CCC=CC2, FMOPL000760a, Mounted_Clear, success, P 2 2
 2,34 41 111 90 90 90,1.05,0.041,48.5,2,83.6,99.4,14.4,0.19452,0.21583, None, None, P 21 21
 21,1 - Analysis Pending, None

PARP14A-
 x0310, CC(C)COc1ccc(cc1)[C@@H]2C(=O)NC(=O)N2, FMOPL000441a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.14,0.046,31.6,0.9,96.5,99.8,76.7,0.21389,0.24416, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0311, C[C@H](c1ccccc1)NC(=O)COC, FMOPL000465a, Mounted_Clear, success, P 21 21
 21,34 41 110 90 90 90,1.13,0.026,60.4,2.6,97.5,99.6,85.7,0.19388,0.21847, None, None, P 21
 21 21,1 - Analysis Pending, None

PARP14A-x0312, CCc1ccc(cc1)C(=O)Nc2nnn(n2)CC, FMOPL000303a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90, 1.1, 0.029, 60.1, 1.4, 90.3, 98.9, 42.5, 0.21069, 0.23622, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0313, CNC(=O)OCc1nccn1C, FMOPL000759a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.09, 0.03, 59.9, 1.4, 90.6, 98.9, 44.5, 0.20289, 0.22961, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0314, COc1ccc(cc1)CNC(=O)CC#N, FMOPL000389a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.17, 0.023, 58.8, 1.8, 97.1, 98.9, 80.7, 0.19646, 0.22166, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0315, COCC(=O)Nc1ccc(cc1)O, FMOPL000462a, Mounted_Clear, success, P 2 2 2,34 41 111 90 90 90, 1.17, 0.032, 50.9, 1.4, 99, 99.5, 88.2, 0.19885, 0.22708, 0.15175, 0.18634, P 21 21 21,6 - Deposited, 5QHY

PARP14A-x0316, CCOC1ccc(cc1)C(=O)Nc2nnn(n2)C, FMOPL000302a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90, 1.09, 0.037, 48.7, 2.7, 85.9, 98.8, 43.5, 0.20949, 0.23448, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0317, c1ccc(c(c1)C(=O)N)Nc2cccc(c2)Cl, FMOPL000761a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.14, 0.023, 64, 1.5, 94, 99.2, 58.2, 0.20119, 0.2269, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0318, Cc1cc(nol)NC(=O)CSc2cccc2, FMOPL000428a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.05, 0.059, 37.4, 4.1, 84.3, 99.4, 14.6, 0.19358, 0.21424, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0319, Cc1ccc(cc1)OCC(=O)Nc2cc(on2)C, FMOPL000498a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.22, 0.029, 53.5, 2, 99.8, 99.3, 98.7, 0.20187, 0.23146, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0320, c1cc(oc1)C(=O)Nc2ccc3c(c2)[nH]c(=O)[nH]3, FMOPL000310a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90, 1.12, 0.03, 53.5, 2.5, 96.2, 99.4, 77.4, 0.20779, 0.23213, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0321, Cc1cccc(c1)C(=O)Nc2ccc(cc2O)C, FMOPL000499a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.05, 0.045, 47.1, 1.9, 75.6, 99.2, 12.1, 0.20995, 0.2359, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0322, Cc1ccc(cc1)C[NH2+]Cc2ccncc2, FMOPL000289a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.09, 0.024, 70.1, 1.1, 90.9, 99.2, 43.2, 0.19845, 0.22098, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0323, COC(=O)c1ccc(o1)C[NH+]2CCCC2, FMOPL000562a, Mounted_Clear, success, P 2 2 2,34 41 111 90 90 90, 1.14, 0.038, 45.8, 1.7, 95, 99.1, 61.3, 0.19397, 0.22255, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0324, ClCCC(CC1)NC(=O)CC#N, FMOPL000385a, Mounted_Clear, success, P 2 2 2,34 41 111 90 90 90, 1.15, 0.027, 60.7, 1.4, 97.1, 99.2, 75.4, 0.19264, 0.21674, 0.14129, 0.17403, P 21 21 21,6 - Deposited, 5QHZ

PARP14A-x0325, c1cc(oc1)CNC(=O)Nc2cccc2, FMOPL000471a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90, 1.14, 0.042, 37.7, 2.3, 94.5, 99.7, 63.4, 0.20603, 0.22934, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0326, c1cc(ccc1C[NH+]2CCC(CC2)C(=O)N)F, FMOPL000346a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90, 1.11, 0.02, 75.2, 1.3, 93, 99, 56.8, 0.19833, 0.22273, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0327, c1c(nc[nH]1)CC[NH2+]C2CCCCC2, FMOPL000322a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.25,0.022,53.7,2,99.6,99.3,94.7,0.19081,0.21953, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0328, c1cc(cc(c1)O)C[NH+]2CCSCC2, FMOPL000313a, Mounted_Clear, Failed -
unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0329, CC(C)c1ccc(cc1)C[NH+]2CCC(CC2)O, FMOPL000348a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.68,0.076,25,8.2,100,99.9,100,0.23008,0.28536, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0330, COc1ccc(cc1)C[NH+]2CCSCC2, FMOPL000336a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.09,0.037,49.9,1.3,89.7,99.4,41.7,0.21896,0.24808, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0331, C[NH+](C)CC(=O)c1ccc(cc1)c2ccccc2, FMOPL000377a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.13,0.031,50.5,2.7,95.6,99.1,85.3,0.1884,0.21041, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-
x0332, Cc1ccc(cc1)C(=O)N[C@@H]2C[C@H]3CC[C@@H]2C3, FMOPL000360a, Mounted_Clear, success, P 2
2 2,34 41 110 90 90 90,1.05,0.076,28,3.6,81.3,98.8,14.2,0.20989,0.2322, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0333, Cc1c(non1)NC(=O)N2CCCC2, FMOPL000330a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.05,0.058,38.1,3.9,83.6,99.4,13.6,0.19719,0.21607,0.22661,0.23522, P 21 21
21,3 - In Refinement, None

PARP14A-x0334, CCCn1c2ccccc2nc1NC(=O)CC, FMOPL000352a, Mounted_Clear, success, P 21 21 21,34
41 111 90 90 90,1.05,0.048,49.3,2.9,85.2,99.6,15.3,0.19685,0.21926,0.13653,0.15657, P 21
21 21,6 - Deposited, 5QIO

PARP14A-x0335, COc1ccc(cc1OC)C[NH+]2CCOCC2, FMOPL000357a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.05,0.035,54.4,2.1,85.3,99.2,15.1,0.20101,0.224, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0336, c1cnc(cn1)c2ncc(c(n2)N)C#N, FMOPL000086a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.14,0.034,49.8,2.6,94,99,72.6,0.20974,0.23791, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0337, c1ccnc(c1)c2ccc(s2)C(=S)N, FMOPL000022a, Mounted_Clear, Failed -
unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0338, c1cc(ccc1c2ccc(o2)CO)N, FMOPL000551a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.13,0.018,79.2,1.5,92.7,99.3,50.5,0.20475,0.22977, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0339, CC(C)NC(=O)N[C@@H]1CCCCNC1=O, FMOPL000087a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.08,0.03,68.7,1.8,84.2,98.8,22.9,0.20643,0.22822, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-
x0340, c1cc(cnc1)C[NH2+][C@H]2CS(=O)(=O)C[C@@H]2O, FMOPL000179a, Mounted_Clear, success, P 2
2 2,34 41 110 90 90 90,1.05,0.036,55.5,2.6,85.2,98.9,14.7,0.20204,0.22568, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0341, COC(=O)c1cccc(c1)NS(=O)(=O)C, FMOPL000089a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.1,0.034,49.3,1.1,93,99.5,51.3,0.20403,0.22754, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0342, c1ccc(cc1)Coc2cccc(c2)N, FMOPL000023a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.17,0.038,40.9,1.6,97.9,99,80.1,0.20009,0.22459, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0343,C[NH+]1CCC(CC1)[NH+]2CCC[C@H](C2)C(=O)[O-],FMOPL000180a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.09,0.027,60.3,2.7,90.9,99.2,55.7,0.1972,0.21895, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0344,C[C@H](C[NH2+]Cc1c(ccc1C1)C1)O,FMOPL000555a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.1,0.031,52.7,2.5,94,98.7,66.4,0.21181,0.23628, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0345,c1csc(c1NC(=O)C(F)(F)F)C(=O)N,FMOPL000092a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.1,0.024,69.2,2.6,93.6,98.9,62.3,0.21113,0.23653, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0346,c1ccc(cc1)C[NH+]2CCO[C@H](C2)CO,FMOPL000024a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.16,0.039,42.8,2.6,98.2,99.7,89.2,0.21016,0.23319, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0347,C[NH+]1CCN(CC1)C(=O)c2ccc(c(c2)F)F,FMOPL000181a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.12,0.031,48.1,1,95.4,99.8,65.5,0.20474,0.23166, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0348,c1cc(sc1)c2ccc(s2)c3ccn[nH]3,FMOPL000091a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 1.09,0.039,45.6,1.2,92.4,99.6,49.6,0.20586,0.22871, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0349,CC(C)(C)OC(=O)N1CCC(CC1)[NH2+]C2CC2,FMOPL000025a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 1.05,0.082,29.3,5,84.5,99.1,15.3,0.21751,0.23792, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0350,c1ccc(cc1)COCc2c[nH]c(=O)[nH]c2=O,FMOPL000182a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.11,0.033,49.8,2.5,93.9,98.6,65.6,0.20285,0.22704, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0351,Cc1ccc2c(c1)c3c([nH]2)[C@H](CCC3)[NH3+],FMOPL000564a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 1.11,0.028,62.2,1.7,91.1,98.8,46,0.20517,0.22896, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0352,COC(=O)NNc1cc(ccn1)C(F)(F)F,FMOPL000096a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.12,0.029,53.5,2.5,96.6,98.7,81,0.19237,0.21434, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0353,c1ccc(c(c1)CNC2ccc(cc2)F)CO,FMOPL000183a,Mounted_Clear,Failed - unknown,,,,,,,,,,,,,#NAME?,

PARP14A-x0354,c1ccc(cc1)C[NH+]2CC(=O)NC(=O)C2,FMOPL000558a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 1.14,0.035,51.3,1.2,97.2,99.4,75.1,0.22841,0.25392, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0355,COc1cccc(c1)c2nc(c(o2)N)C#N,FMOPL000097a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 1.05,0.084,26.3,6.3,83.1,99.3,14.7,0.19297,0.21336, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0356,c1cc(ccc1NNC(=S)N)F,FMOPL000055a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 1.08,0.03,57,1.1,90.9,99.4,41,0.20977,0.23303, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0357,c1cc(ccc1CC(=O)NC2CCCC2)F,FMOPL000184a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 1.14,0.034,47.8,2.6,96.9,99,82.4,0.19831,0.22023, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0358,CCOc1cccc(c1)c2nnc(s2)N,FMOPL000560a,Mounted_Clear,success,P 21 21 21,34
41 110 90 90 90,1.12,0.045,37.1,2.7,93.9,99.6,67.2,0.19743,0.22389,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0359,c1cc(cc(c1)Cl)N2CC[NH+](CC2)CC#N,FMOPL000094a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.09,0.034,50.6,2.5,91.3,98,55.4,0.20419,0.22544,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0360,c1cc(ccc1NC(=O)CC#N)Cl,FMOPL000056a,Mounted_Clear,success,P 21 21 21,34 41
110 90 90 90,1.11,0.021,72,2.6,93.6,99.1,65.6,0.19211,0.21454,None,None,P 21 21 21,1 -
Analysis Pending,None

PARP14A-x0361,CC(C)CC(=O)NCc1ccc2c(c1)OCO2,FMOPL000185a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.12,0.03,52.3,2.5,96.7,99.3,79.2,0.2063,0.22932,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0362,c1ccc(cc1)C#CC[NH+]2CCCCC2,FMOPL000559a,Mounted_Clear,Failed - loop
broken,,,,,,,,,,,,,#NAME?,

PARP14A-x0363,Cc1c(c(c([nH]1)C)C(=O)OC)c2cc[nH]n2,FMOPL000098a,Mounted_Clear,success,P
21 21 21,34 41 110 90 90 90,1.18,0.028,50,2.7,96.9,99.6,87.3,0.20382,0.22695,None,None,P
21 21 21,1 - Analysis Pending,None

PARP14A-x0364,c1ccc(cc1)c2cc(on2)C[NH3+],FMOPL000057a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.1,0.027,61.8,2.5,93.8,98.5,64.1,0.20263,0.22873,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0365,CC(=O)Nc1ccc(cc1)Nc2ccccc2,FMOPL000186a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.08,0.036,45.5,2.6,89.3,99.2,48.1,0.18976,0.20901,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0366,c1cc(cc(c1)Cl)NC(=O)C[NH+]2CCCC2,FMOPL000567a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.05,0.04,53,2.5,83.3,99.1,15.9,0.19564,0.22085,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0367,CC(=O)c1ccc(o1)c2ccc(cc2F)F,FMOPL000095a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.14,0.022,66.6,2.5,96.5,99.6,79.8,0.19562,0.21885,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0368,c1cc(ccc1n2cc(nn2)CO)Cl,FMOPL000058a,Mounted_Clear,success,P 21 21 21,34
41 110 90 90 90,1.05,0.047,50.2,2.6,85.8,99.3,16.4,0.19963,0.22421,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0369,CC(=O)Nc1cc(ccc1O)c2ccccc2,FMOPL000187a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.1,0.034,51.5,2.5,93.9,99.2,66,0.19966,0.2232,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0370,CC(=O)Nc1ccc(cc1)c2csc(n2)N,FMOPL000568a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.08,0.033,56.3,2.7,88.6,98.7,46,0.19574,0.21918,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0371,c1cc(sc1)c2nc(no2)N3CCCCC3,FMOPL000093a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.15,0.024,59.4,2.7,98,99,86.8,0.20581,0.23026,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0372,CC(=O)Nc1ccc(cc1)OCC(=O)[O-],FMOPL000059a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.21,0.017,85.9,2.1,98.4,98.6,90.7,0.20241,0.23239,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0373,Cc1nc(c(s1)NC(=O)OC)c2ccccc2,FMOPL000188a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.09,0.032,54.6,1.4,90.8,99.1,43.9,0.20663,0.22872,None,None,P 21
21 21,1 - Analysis Pending,None

PARP14A-x0374, Cc1cc(nnc2ccccc2)NC(=O)OC, FMOPL000105a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.049,46.4,2.9,80.6,99.3,14.2,0.19907,0.22246, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0375, c1cc(oc1)CNC(=O)Nc2ccc(cc2)F, FMOPL000189a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.08,0.03,57.8,2.6,90.7,98.5,50.7,0.19828,0.22019, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-
x0376, Cc1ccc2c(c1)c3c([nH]2)[C@@H](CCC3)C#N, FMOPL000572a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.12,0.035,48.3,2.7,95.1,99.3,73,0.19818,0.22113, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-
x0377, c1cc2c(cc1C[NH2+])C[C@@H]3CCC=CC3)OCO2, FMOPL000300a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.17,0.021,57.7,1.2,98.6,99.8,93.1,0.20095,0.23177, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0378, c1ccc2c(c1)[nH]c(n2)NCc3ccco3, FMOPL000565a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.15,0.023,67.9,1.4,97.4,99.4,82.4,0.20229,0.23631, None, None, P 21
21 21,2 - PANDDA model, None

PARP14A-x0379, CC(=O)N[C@@H](Cc1ccc(cc1)O)C(=O)NN, FMOPL000484a, Mounted_Clear, success, P
21 21 21,34 41 110 90 90,1.08,0.027,62.7,2.8,89.8,97.9,48.1,0.20888,0.23085, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0380, c1ccnc(c1)C[NH2+]Cc2ccc3c(c2)OCO3, FMOPL000297a, Mounted_Clear, success, P 21 21
21 21,34 41 111 90 90 90,1.1,0.025,66,2.7,90.7,98.7,53.6,0.1979,0.22231, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0381, c1ccc(cc1)CCNc2[nH]c3ccccc3n2, FMOPL000586a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.062,35.7,2.5,83.9,99.3,15,0.20103,0.22439, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0382, C[C@@H](CNC(=O)Nc1cccc1)O, FMOPL000464a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.094,27.2,3.5,81.5,99.5,15.4,0.19892,0.22027, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0383, CC(C)(C)NC(=O)N1CCC(CC1)C(=O)OC, FMOPL000292a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.11,0.024,66.1,1.5,91.6,99.1,47.5,0.19553,0.2206, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0384, c1ccc(cc1)CCNC(=O)c2ccc(=O)oc2, FMOPL000585a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.13,0.03,57.3,2.6,92.5,99.3,57.6,0.19773,0.22491, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0385, Cc1cc(nol)C(=O)NCC(=O)OC, FMOPL000387a, Mounted_Clear, success, P 21 21 21,34
41 110 90 90 90,1.08,0.038,48.2,2.8,86.2,98.4,37.6,0.19855,0.22318, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0386, c1cc(cc(c1)O)NC(=O)Nc2ccc(cc2)F, FMOPL000500a, Mounted_Clear, success, P 21 21
21 21,34 41 110 90 90 90,1.09,0.032,53.1,2.5,88.7,99.1,48.7,0.19565,0.2203, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0387, CCc1nnc(s1)NC(=O)C[NH+] (C)C, FMOPL000283a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.08,0.03,58.8,2.5,90.8,97.2,53.9,0.20094,0.22178, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0388, CC1(C[C@@H](CCO1)C(=O)NCc2ccccc2)C, FMOPL000592a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.031,71.6,2.1,80.5,98.6,14.1,0.19213,0.21311, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0389,Cn1ccc(n1)C(=O)Nc2cccc(c2)C(=O)[O-],FMOPL000457a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90,1.1,0.034,48.2,2.5,91.3,99.4,57.2,0.19171,0.21199, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0390,c1ccc(cc1)OCC(=O)Nc2cccc2O,FMOPL000490a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.059,39.9,3.2,84.2,99.4,15.2,0.20541,0.22446, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0391,c1cc(ccc1C[NH2+])Cc2ccc(cc2)F)C#N,FMOPL000296a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.064,35.7,2.1,80.3,99.1,12.9,0.20188,0.22127, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0392,CC(C)C(=O)Nc1nnn(n1)C,FMOPL000547a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.09,0.044,37.4,2.5,90.8,99.7,54.8,0.20017,0.22179, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0393,c1ccc(cc1)NS(=O)(=O)c2ccc(cc2)N,FMOPL000432a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.14,0.029,51.5,1.3,95.3,98.5,64.1,0.19546,0.22057, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0394,CC[C@H](CO)NC(=O)Nc1ccc(cc1)Cl,FMOPL000476a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.046,47.2,3,82.6,99.2,14.8,0.19752,0.22083, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0395,COc1cccc(c1)C[NH+]2CCC(CC2)C(=O)N,FMOPL000305a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.39,0.029,46.3,2.2,99.9,99.1,98.8,0.18672,0.22026, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0396,c1ccc(cc1)COc2cccc2C(=O)NN,FMOPL000587a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.057,38.8,2.5,84.6,99.2,14.6,0.19801,0.22181, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0397,c1c(c(=O)[nH]c(=O)[nH]1)NC2CCCC2,FMOPL000388a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.033,68.2,2.3,83.7,99.2,14.7,0.18984,0.20959, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0398,C[C@H](C[NH2+])C1CCCC1O,FMOPL000461a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.09,0.023,68,2.6,91.2,99.1,57.3,0.20042,0.22523, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0399,c1c(nns1)C(=O)N2CCOCC2,FMOPL000281a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.15,0.028,53.1,1.6,95,99,68.7,0.19454,0.21922, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0400,C[C@@H](C(=O)OC)NC(=O)N1CCOCC1,FMOPL000563a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.057,41,2.2,84.2,99.3,14.1,0.19895,0.22095, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0401,c1ccc(cc1)[C@@H]2C[C@H]2C(=O)Nc3nccs3,FMOPL000417a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.16,0.034,49.3,2.6,98.4,99.5,89.8,0.20156,0.2261, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0402,c1cc(c(cc1C(F)(F)F)N)N2CCCC2,FMOPL000263a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.052,44.2,4,79.4,99,12.1,0.19419,0.21727, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0403,COc1cc(cc(c1)OC)C(=O)Nn2cnnc2,FMOPL000451a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.07,0.026,71,1.2,89.6,99.1,33,0.18842,0.21256, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0404, c1ccnc(c1)NC(=O)c2cnccn2, FMOPL000469a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.13, 0.034, 52.8, 2.6, 97.1, 99.3, 81.9, 0.19208, 0.21744, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0405, COC(=O)c1cccc2c1-c3ccccc3C2=O, FMOPL000264a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.1, 0.089, 19.1, 2.5, 94.6, 99.1, 68, 0.20094, 0.22579, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0406, c1cc(cc(c1)F)NCc2ccc3c(c2)OCO3, FMOPL000650a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.076, 28, 3.8, 81.6, 99.1, 13.5, 0.19533, 0.21482, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0407, Cc1c(sc(n1)NC(=O)OC)C(=O)N(C)C, FMOPL000409a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.031, 50.6, 2.7, 84.1, 98.2, 31.3, 0.20161, 0.22133, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0408, COc1ccc2c(c1)sc(n2)NC(=O)C3CC3, FMOPL000487a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.12, 0.029, 56.6, 2.6, 94.9, 98.3, 70.7, 0.20706, 0.2311, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0409, CCOC(=O)Nc1cccc(c1)Cl, FMOPL000260a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.09, 0.023, 67, 1.7, 78.5, 97.9, 20.5, 0.19155, 0.21757, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0410, c1cc(cnc1)Nc2nnc(s2)C(F)(F)F, FMOPL000643a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.035, 50, 2.7, 89.7, 98.6, 46.7, 0.20844, 0.23154, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0411, CC(C)C(=O)N1CCC(CC1)Cc2ccccc2, FMOPL000438a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.027, 61.7, 2.6, 87.7, 98.9, 42.4, 0.19751, 0.22265, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0412, CC(C)NC(=O)c1ccc2ccccc2n1, FMOPL000474a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.046, 44.4, 2.3, 84.5, 99.2, 14.3, 0.19716, 0.22157, 0.14917, 0.17231, P 21 21 21, 6 - Deposited, 5QI1

PARP14A-x0413, Cc1ccc(ol)C[NH+](C)C, FMOPL000259a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.037, 52.1, 2.5, 83.9, 98.7, 14, 0.19774, 0.21795, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0414, CN(C)C(=O)Nc1cnccc1C(F)(F)F, FMOPL000641a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.12, 0.028, 64.3, 1.1, 94.9, 99.5, 62.1, 0.18712, 0.21177, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0415, C[NH+]1CCN(CC1)C(=O)Nc2ccccc2, FMOPL000408a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.036, 55.8, 2.5, 81.8, 99.4, 15.6, 0.19831, 0.22064, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0416, CCC(=O)Nc1ccc2c(c1)[nH]c(=O)[nH]2, FMOPL000468a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.048, 44, 2.4, 74.2, 98.4, 11.3, 0.20251, 0.22545, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0417, ClCC[NH+](Cl)C[C@H](CO)O, FMOPL000258a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.048, 41, 2.6, 79.2, 99.1, 13, 0.18328, 0.20479, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0418, COCc1nnc(s1)NC(=O)c2ccccc2, FMOPL000424a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.033, 62.3, 1.7, 76.6, 98.5, 13.4, 0.19791, 0.22006, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0419, CC(C)C(=O)NCc1[nH]c2ccccc2n1, FMOPL000473a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.046, 39.5, 2.7, 89.5, 98.6, 47, 0.20149, 0.22247, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0420, c1cc(cc(c1)C1)C[NH+]2CCOCC2, FMOPL000312a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.07, 0.037, 55.7, 1.5, 82.8, 98.8, 27.2, 0.20018, 0.22117, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0421, CC(=O)Nc1ccc(cc1)C[NH+]2CCOCC2, FMOPL000349a, Mounted_Clear, Failed - unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0422, Cc1cccc(c1)C[NH+]2CCOCC2, FMOPL000319a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.06, 35.7, 3.1, 79.4, 98.7, 12, 0.20328, 0.22465, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0423, CC(C)(C)C1CCC(CC1)[NH2+]Cc2ccncc2, FMOPL000368a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 2.48, 0.239, 16.8, 1.5, 100, 99.1, 100, 0.29534, 0.36733, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0424, Cc1cc(cc(c1NC)C)[N+](C)(C)C, FMOPL000318a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.19, 0.022, 59.7, 1.9, 99.5, 99.3, 93.7, 0.18847, 0.21368, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0425, c1cc(ccc1OCC(=O)N2CCCC2)F, FMOPL000332a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90, 1.14, 0.039, 48.5, 2.4, 92.1, 99.6, 63.7, 0.18871, 0.21342, 0.18923, 0.21384, P 21 21 21, 3 - In Refinement, None

PARP14A-x0426, COCC(=O)Nc1nc(cs1)c2ccccc2, FMOPL000355a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.035, 51.1, 1.9, 77.7, 98.7, 13.5, 0.19016, 0.21484, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0427, c1ccc(cc1)CCC(=O)Nc2ccc(cc2)O, FMOPL000363a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.14, 0.028, 54.9, 2.4, 96, 99.8, 80.5, 0.19487, 0.22128, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0428, c1ccc2c(c1)OC[C@@H](O2)C(=O)N3CCOCC3, FMOPL000366a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.17, 0.026, 58.4, 1.5, 99, 99.4, 88.7, 0.19375, 0.22271, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0429, c1ccc(cc1)Cnc2ccc(cc2)C(=O)[O-], FMOPL000343a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.025, 64.5, 2.6, 89.7, 99.5, 51.9, 0.18707, 0.21317, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0430, c1ccc(cc1)SCC(=O)NC2CCCC2, FMOPL000344a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.05, 42.9, 4.2, 78.9, 98.7, 8.5, 0.19214, 0.21337, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0431, COCC(=O)Nc1cccc1C(=O)N, FMOPL000329a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.032, 57.4, 2.7, 89.2, 98.4, 50.3, 0.19023, 0.21666, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0432, c1ccc(cc1)Coc2ccc(cc2)C(=O)N, FMOPL000099a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.27, 0.021, 65.1, 2.5, 99.9, 99.3, 98.8, 0.19703, 0.22596, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0433, CCOC1ccc(cc1)NC(=O)NC(C)(C)C, FMOPL000041a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.057, 39.6, 2.2, 84.9, 99.3, 14.9, 0.20619, 0.22604, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0434, CC[NH+]1CCN(CC1)C(=O)NC2CCCC2, FMOPL000190a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.051, 41.8, 2.6, 81.8, 99.1, 13.3, 0.19528, 0.21663, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0435, COc1ccc2cc(ccc2c1)c3cc[nH]n3, FMOPL000102a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.19, 0.017, 72.2, 1.2, 94.1, 98.8, 75.7, 0.19957, 0.22977, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0436,CC1(CC(=CC(=O)C1)Nc2cccc(c2)O)C,FMOPL000040a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.12,0.029,54.4,2.6,95.7,99.5,74.1,0.19802,0.22387, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0437,c1cnccc1c2nc(on2)C3CCCCC3,FMOPL000191a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.056,41.3,3.6,71,99,7.3,0.2036,0.22777, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0438,CCcn1c(nnn1)NC(=O)c2cccs2,FMOPL000569a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.12,0.032,49.6,2.6,95.6,98.6,77.8,0.19062,0.2146, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0439,Cn1c(c(c(n1)C(F)(F)F)c2cccc2)N,XST00000908c,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.1,0.032,47.5,2.5,92,99.2,57,0.19216,0.21233, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0440,C[C@H]1CC[C@H](C1)[NH2+]Cc2ccc3c(c2)OCO3,FMOPL000043a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.12,0.028,58,2.6,95.6,99.1,74.6,0.18671,0.21003, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0441,c1ccn(c1)c2ccc(cc2)N3CCOCC3,FMOPL000192a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.049,45.2,2.4,84.5,99.2,16.7,0.21399,0.2346, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0442,COc1cccc1N2CC[NH+](CC2)CC#N,FMOPL000103a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.025,76.1,2,81.8,98.9,13.8,0.19837,0.22014, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0443,CC1CCN(CC1)c2ccc(cc2N)C(=O)[O-],FMOPL000193a,Mounted_BadDispense,success,P 2 2 2,34 41 110 90 90 90,1.05,0.057,41.6,3.1,85.2,99,14.5,0.19453,0.21534, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0444,Cc1cc(nol)c2nc(on2)c3cccc3,FMOPL000106a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.14,0.024,58.9,1.2,96.9,99.4,72.7,0.20286,0.22946, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0445,Cc1ccc(cc1)C(=O)n2cnc3c2cccc3,FMOPL000194a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.07,0.031,55,2.6,89.1,98.6,42.3,0.19042,0.20804, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0446,Cc1cc(nol)C(=O)NNc2cccc2F,FMOPL000104a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.027,70.1,1.7,78,98.5,12.9,0.18777,0.2111, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0447,c1ccc2c(c1)ccc(c2O)C[NH+]3CCOCC3,FMOPL000195a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.34,0.018,74.1,2.5,99.7,99.2,97.2,0.18958,0.2254, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0448,c1cc(ccc1C(=O)[O-])Oc2ccc(cc2)N,FMOPL000584a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.05,0.06,37.4,4,73.3,98.6,10.8,0.19618,0.21935, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0449,c1cc2c(cc1NC(=O)NCC3CC3)CCO2,FMOPL000100a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90 90,1.13,0.025,63.4,1.5,96.2,99.5,69.1,0.20386,0.22979, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0450,CC(C)(C)NC(=O)Nc1cccc1C(=O)N,FMOPL000039a,Mounted_Clear,success,P 21 21 21,34 41 110 90 90 90,1.11,0.025,67.5,2.7,93.9,97.7,67.4,0.19911,0.22097, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0451, c1cc2c(cc1C[NH2+]Cc3ccncc3)OCO2, FMOPL000196a, Mounted_Clear, success, P 2 2
2,34 41 111 90 90 90,1.08,0.028,65.1,1.4,91.3,99.1,40.8,0.19846,0.22319, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0452, CC1CC[NH+] (CC1)Cc2c[nH]c3c2cccc3, FMOPL000576a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.21,0.021,66.5,1.7,97.4,98.9,86.8,0.19946,0.23173, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0453, COc1ccc(cn1)NC(=O)Nc2cccs2, FMOPL000101a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.05,0.054,40.5,3.5,78.5,98.9,7.8,0.19242,0.21327, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0454, c1cc(ccc1N2C(=O)CCC2(=O)OCC(=O)[O-], FMOPL000045a, Mounted_Clear, Failed -
unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0455, Cc1cccc1OCC(=O)Nc2cccnc2, FMOPL000197a, Mounted_Clear, success, P 2 2 2,34 41
111 90 90 90,1.05,0.047,44.5,2.6,76,98.8,9.7,0.18404,0.20708,0.185,0.20705, P 21 21 21,3
- In Refinement, None

PARP14A-x0456, c1ccc2c(c1)ncn2Cc3ccc(cc3)F, FMOPL000574a, Mounted_Clear, success, P 21 21
21,33 41 110 90 90 90,1.14,0.032,50.7,2.5,97.9,99.4,86.4,0.17028,0.19645, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0457, Cc1nccc(n1)c2cccc(c2)NC(=O)NC, FMOPL000110a, Mounted_Clear, success, P 21 21
21,34 41 111 90 90 90,1.08,0.035,51.2,2.5,89.3,98.8,48.6,0.19883,0.22257,0.14477,0.17042, P 21 21 21,6 -
Deposited, 5QI2

PARP14A-x0458, c1ccc(cc1)CCNC(=O)NC2CCCC2, FMOPL000046a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.1,0.05,34.8,2.6,94,98.6,67.1,0.20944,0.23077, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0459, Cc1cccc(c1C)NC(=O)C[NH+]2CCOCC2, FMOPL000198a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.05,0.04,51.9,2.6,85.5,99.5,18.1,0.19656,0.21761, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0460, CCOC(=O)c1cc(nol)c2ccc(cc2)C, FMOPL000579a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.044,49.4,2.3,75.3,99.1,10,0.20422,0.22762, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0461, c1cc(ccc1CNC(=O)N2CCOCC2)C#N, FMOPL000108a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.06,0.035,52.6,1.4,87.3,99.1,23.5,0.20339,0.22928, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-
x0462, CC[C@@H](C)[NH+]1CCN(CC1)C(=O)c2ccncc2, FMOPL000199a, Mounted_Precipitate, success, P
2 2 2,34 41 110 90 90 90,1.2,0.03,53.7,1.7,95.2,99,82.6,0.20777,0.23181, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0463, CCOC(=O)c1cc(nol)c2ccc(cc2)F, FMOPL000580a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.12,0.028,57.4,2.7,95.7,98.1,75.4,0.19878,0.21909, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0464, c1c(cnc1C(=O)[O-])C#CCC2CCCC2, FMOPL000109a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.21,0.028,60.2,2.3,99.5,99,95.1,0.20054,0.23385, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0465, c1ccc(cc1)NC(=O)N2CCC(CC2)C(=O)N, FMOPL000200a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.1,0.022,74.7,2.6,92.5,98.8,60.9,0.20841,0.2317, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0466,CC(C)COc1ccc(cc1)c2csc(n2)N,FMOPL000575a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.12,0.036,51.9,2.7,94.6,99,67.9,0.20652,0.23045,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0467,c1ccc(cc1)[C@@H](CNC(=O)c2ccccc2)O,FMOPL000107a,Mounted_Clear,success,P
21 21 21,34 41 110 90 90
90,1.05,0.041,51.9,2.3,85.6,99.1,16.8,0.19463,0.21611,None,None,P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0468,CC1(CC(=CC(=O)C1)Nc2ccccc2C#N)C,FMOPL000049a,Mounted_Precipitate,Failed -
unknown,,,,,,,,,,,,,#NAME?,

PARP14A-x0469,c1cc(cnc1)CNC2ccc(cc2N)C(=O)[O-],FMOPL000201a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.08,0.03,52,2.5,91,99.2,51.4,0.1955,0.21789,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0470,CCC(=O)Nc1c2ccccc2oc1C(=O)N,FMOPL000577a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.13,0.026,63,1.4,95.2,99.1,68.6,0.20085,0.22887,None,None,P 21 21 21,1
- Analysis Pending, None

PARP14A-x0471,c1cc(cc(c1)c2ccc(cc2)O)C#N,FMOPL000261a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.1,0.025,65.3,2.5,93.2,99.3,62.1,0.19332,0.21884,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0472,Cc1cc(nc(c1)NC(=O)Nc2ccccc2)C,FMOPL000454a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.054,42.5,4,77.1,99.1,9.4,0.19458,0.21727,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0473,CCCN1c(nnn1)NC(=O)c2ccco2,FMOPL000475a,Mounted_Clear,success,P 2 2 2,34 41
110 90 90 90,1.05,0.079,29.6,5.5,80.2,98.9,14.8,0.18772,0.20636,0.1408,0.15758,P 21 21
21,6 - Deposited,5QI3

PARP14A-x0474,c1cc(cc(c1)c2cccc(c2)O)C#N,FMOPL000262a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.09,0.022,63.3,1.1,91.2,99.2,43.2,0.19733,0.22097,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0475,CCOC(=O)c1c(nc(s1)c2cncn2)C,FMOPL000647a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.05,0.049,52,2.7,85,99.6,15.9,0.20094,0.2217,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0476,CC(C)Oc1ccc(cc1)[C@@H]2CC(=O)NC2,FMOPL000402a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.051,44.5,2.9,79.8,99.2,14.5,0.19524,0.21601,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0477,CC(=O)Nc1ccc(cc1)OC(=O)N2CCCC2,FMOPL000494a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.11,0.022,73.5,1.5,90.1,99,40.8,0.20252,0.22777,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0478,C[NH+](C)Cc1c[nH]c2c1cc(cc2)OC,FMOPL000690a,Mounted_Clear,success,P 2 2
2,34 41 111 90 90
90,1.05,0.079,28.2,4.7,84.8,99.2,14.7,0.20705,0.22556,0.21299,0.23428,P 21 21 21,3 - In
Refinement, None

PARP14A-x0479,C1COCC[NH+]1Cc2c(snn2)C1,FMOPL000627a,Mounted_Clear,success,P 2 2 2,34 41
110 90 90 90,1.05,0.047,42.3,2.8,78.5,99.4,10.7,0.19714,0.21957,None,None,P 21 21 21,1
- Analysis Pending, None

PARP14A-x0480,CCc1nnc(s1)NC(=O)c2cncn2,FMOPL000404a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.13,0.028,56.8,2.3,94.3,99.3,70.7,0.19169,0.22008,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0481, c1ccc(cc1)CC[NH+]2CCC(CC2)C(=O)N, FMOPL000481a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.16,0.031,49.9,2.6,98,99.6,87.2,0.19738,0.22636, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0482, CC(=O)c1ccc(cc1)OCC(=O)[O-], FMOPL000688a, Mounted_Clear, Failed - unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0483, CC(=O)Nc1nc2ccc(cc2s1)C(=O)NC, FMOPL000419a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.048,46.6,3.4,79.4,98.7,9.4,0.20105,0.22198, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0484, Cc1c(sc2c1c(ncn2)N(C)C)C, FMOPL000466a, Mounted_Clear, success, P 21 21 21,34 41 111 90 90 90,1.2,0.025,56.9,2.3,99.3,99.7,97.5,0.18826,0.21996,0.14741,0.18488, P 21 21 21,6 - Deposited,5QI4

PARP14A-x0485, COc1ccc2c(c1)non2, FMOPL000686a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.041,52.5,2.3,85.5,98.9,15.2,0.19589,0.21865, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0486, c1ccc(cc1)[C@@H](C[NH+]2CCC(CC2)C(=O)N)O, FMOPL000653a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.19,0.028,50.9,1.7,98.8,99.2,86.5,0.19346,0.22499, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0487, c1cc(oc1)C(=O)NCCc2ccc(cc2)F, FMOPL000411a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.09,0.031,55.2,2.5,93,98.6,60.7,0.19745,0.223, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0488, CC(C)c1ccc(cc1)C(=O)NC[C@@H]2CCCO2, FMOPL000493a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.18,0.03,46,1.6,97.9,99.5,78.9,0.19578,0.22516, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0489, c1ccc(cc1)COC(=O)NO, SDOOA000888b, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.09,0.038,44.1,2.7,87.8,98.5,42.6,0.196,0.22302, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0490, COC(=O)c1ccc(s1)c2cccn2, FMOPL000638a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.24,0.03,42.3,1.2,99.6,99.6,98.7,0.18722,0.22375, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0491, CCn1cc(cn1)CNC(=O)c2cccn2, FMOPL000422a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.055,40.2,2.6,71.9,98.7,8.9,0.18647,0.20836, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0492, CC(=O)c1ccc(cc1)N2CCC(CC2)C(=O)N, FMOPL000495a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.21,0.022,50,1.1,98.8,99.1,94.6,0.20111,0.2287, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0493, CCN(CCO)c1ccc(c(c1)C)N, FMOPL000689a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.11,0.033,50,1.3,94.6,99.2,63.4,0.20256,0.22275, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0494, c1ccc(cc1)[C@@H](C[NH2+])[C@@H]2CCCCNC2=O)O, FMOPL000651a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.051,46.1,2.3,76.7,98.6,13,0.21035,0.23318, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0495, c1cc(oc1)C(=O)NC(=S)N2CCOCC2, FMOPL000401a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.05,0.092,29.2,3.9,84.4,99.7,15.5,0.19864,0.21926, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0496, CC(=O)Nc1ccc(cc1)Oc2ncccn2, FMOPL000485a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.078, 31.5, 6.2, 84.5, 99, 14.2, 0.19823, 0.21855, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0497, c1ccc(cc1)COC(=O)N2CCC[C@H]2CO, FMOPL000691a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.05, 36.5, 1.9, 84.6, 99.3, 14.9, 0.19194, 0.21667, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0498, Cc1ccc(cc1)C(=O)O[C@@H]2C[NH+]3CCC2CC3, FMOPL000661a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.032, 53.5, 2.5, 91.4, 99, 53.7, 0.19423, 0.21931, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0499, Cc1ccc(cc1)CNC(=O)c2c(ccs2)C, FMOPL000429a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.049, 37.7, 2.7, 89.2, 99, 48.3, 0.20258, 0.22065, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0500, COc1cc2cccnc2c(c1)N, FMOPL000687a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.14, 0.071, 22.6, 1.4, 97.2, 99.5, 75.5, 0.2039, 0.22852, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0501, C[C@H]1CN(C[C@H](O1)C)c2ccc(cc2C(=O)[O-])N, FMOPL000658a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.15, 0.031, 48.3, 2.7, 97.7, 99.7, 85.3, 0.19963, 0.22288, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0502, C[C@@H]1C[C@H]1C(=O)NCCc2ccc(cc2)Cl, FMOPL000407a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.067, 35, 6.4, 84.2, 99, 14.6, 0.21089, 0.23034, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0503, c1ccc(cc1)CCCC(=O)N2CCOCC2, FMOPL000501a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.19, 0.024, 56.7, 1.6, 98.5, 98.3, 87.1, 0.19921, 0.22719, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0504, COc1ccc(cc1N)N, FMOPL000685a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.055, 42.3, 2.2, 84.5, 99.8, 14.3, 0.21202, 0.23455, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0505, Cc1c(c(n(n1)C)C)NC(=O)CC#N, FMOPL000633a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.033, 57.3, 2.2, 74.1, 98.8, 11.3, 0.18778, 0.21102, 0.14067, 0.16519, P 21 21 21, 6 - Deposited, 5QI5

PARP14A-x0506, COCC(=O)Nc1cccc1, FMOPL000504a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.044, 45.2, 2.3, 83.4, 99.1, 14.1, 0.20261, 0.22422, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0507, c1ccc(cc1)NO, FMOPL000684a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.032, 68.2, 1.8, 78.8, 99.1, 10.3, 0.19136, 0.21655, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0508, c1cc(oc1)C[NH+]2CCS(=O)(=O)CC2, FMOPL000629a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.058, 36.7, 2.4, 85.4, 99.1, 15.1, 0.19692, 0.22098, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0509, COc1ccc(cc1)NCc2ccccc2O, FMOPL000426a, Mounted_Crystalline, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.056, 38.5, 2.7, 83.5, 99.2, 14.9, 0.19224, 0.21337, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0510, c1ccc(c(c1)NC(=S)N)OC(F)(F)F, FMOPL000512a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.1, 0.087, 21.3, 2.6, 88, 99.6, 49.7, 0.20134, 0.22599, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0511, Cc1ccc(cc1)CNC(=O)Cc2cccs2, FMOPL000743a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.055, 38.3, 2.2, 83.1, 99.4, 14.3, 0.208, 0.2304, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0512, CC(=O)Nc1cccc1C(=O)NN, FMOPL000631a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.1, 0.037, 45.3, 2.6, 88.9, 99, 47.4, 0.19267, 0.21266, 0.19254, 0.21254, P 21 21 21, 3 - In Refinement, None

PARP14A-x0513, CCOc1ccc(cc1)NC(=O)c2cnccn2, FMOPL000446a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.1, 0.034, 52.6, 2.5, 91.9, 99, 57.6, 0.20762, 0.23169, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0514, CC(=O)NCCc1ccc(cc1)S(=O)(=O)N, FMOPL000513a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.047, 47.7, 2.9, 83.8, 99, 15.1, 0.19542, 0.21281, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0515, CC(C)(C)NC(=O)N1CCC(CC1)C(=O)N, FMOPL000334a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.052, 38.8, 2, 83.7, 99.4, 14.8, 0.20573, 0.22649, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0516, c1ccc(c(c1)C(=O)NCCc2ccncc2)F, FMOPL000361a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.031, 54.2, 2.5, 88.9, 98.7, 47.6, 0.19499, 0.21789, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0517, CC(=O)N1CCNC(=O)[C@@H]1CC(=O)OC, FMOPL000325a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.034, 51.3, 1.2, 84.7, 99.2, 14.6, 0.19372, 0.21611, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0518, CCCC(=O)Nc1nnn(n1)CC, FMOPL000311a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.054, 37.7, 3.4, 84.7, 99.2, 14.4, 0.19375, 0.21475, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0519, CCNC(=O)c1ccc(cc1)NS(=O)(=O)C, FMOPL000335a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.028, 65.4, 2.1, 79.7, 98.2, 11.6, 0.19554, 0.21716, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0520, c1cc(cc(c1)NC(=O)CCC2CCCC2)C#N, FMOPL000364a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.049, 45.3, 2.1, 83.8, 99, 14.1, 0.19879, 0.22196, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0521, CN(C)C(=O)Oc1ccc(cc1)c2nnco2, FMOPL000354a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.053, 37.4, 1.9, 84.8, 99.4, 14.1, 0.20392, 0.22499, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0522, CC1CCN(CC1)C(=O)c2cc3ccccc3o2, FMOPL000372a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.075, 30.9, 6.1, 83.7, 99, 15.3, 0.19469, 0.21509, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0523, CC(C)(CO)NC(=O)c1cccc(c1)Cl, FMOPL000324a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.031, 55.9, 2.8, 88.8, 98.8, 46, 0.1984, 0.22279, 0.1505, 0.17192, P 21 21 21, 3 - In Refinement, None

PARP14A-x0524, Cc1c(nc[nH]1)C[NH+]2CCCCC2, FMOPL000317a, Mounted_Precipitate, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.024, 62.4, 1.5, 96.9, 99.2, 72, 0.19395, 0.21619, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0525, CC[NH+]1CCC(CC1)Nc2ccccc2F, FMOPL000339a, Mounted_Precipitate, success, P 21 21 21, 34 41 110 90 90 90, 1.39, 0.087, 19.3, 1.6, 98.4, 99.9, 99.9, 0.22508, 0.26527, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0526, c1ccc(cc1)C#Cc2ccc(cc2)c3ccn[nH]3, FMOPL000111a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.07, 0.022, 80.2, 1.4, 88.3, 98.7, 32.5, 0.20794, 0.23246, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0527, Cc1ccc(cc1)OCC(=O)N2CC[NH+](CC2)C, FMOPL000202a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.052, 41, 3.4, 77.8, 98.8, 9.4, 0.19145, 0.21304, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0528, Cc1cccc1c2nc(c(o2)N(C)C)C#N, FMOPL000583a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.057, 39.4, 2.9, 83.4, 99.3, 15.5, 0.20804, 0.22593, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0529, CC(=O)N1CCC(CC1)C#N, XST00000907b, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.054, 41.1, 2.7, 81.8, 99.1, 14, 0.19851, 0.21719, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0530, CC(=O)Nc1cccc1OCc2cccc2, FMOPL000047a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.026, 59.9, 1.2, 96.3, 99.3, 70.1, 0.20125, 0.2286, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0531, CCc1ccc(cc1)OCC(=O)N2CCCC2, FMOPL000203a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.058, 41.4, 2.5, 82.8, 98.8, 14.1, 0.19623, 0.21603, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0532, Cc1ccc(s1)Cnc2cccc(c2)C(=O)[O-], FMOPL000582a, Mounted_Precipitate, success, P 21 21 21, 34 41 110 90 90 90, 1.12, 0.056, 28.9, 2.4, 90.4, 99.2, 50.5, 0.20361, 0.22786, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0533, C[NH2+]Cc1ccc(cc1)C(F)(F)F, FMOPL000112a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.12, 0.025, 58.2, 2.5, 93.2, 99.5, 65.9, 0.1955, 0.21871, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0534, COc1ccc2c(c1)cc([nH]2)C[NH3+], FMOPL000053a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.059, 38.1, 2.5, 84.4, 99, 15.6, 0.19734, 0.21577, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0535, CCOc1cccc(c1)C(=O)Nc2nnn(n2)C, FMOPL000204a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.08, 0.039, 52.3, 1.5, 86.4, 99.3, 34.9, 0.20107, 0.22146, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0536, CCNC(=O)N1CCNC(=O)[C@H]1CC(=O)OC, FMOPL000578a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.14, 0.026, 53.7, 1, 97.4, 99.4, 79, 0.20988, 0.23942, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0537, c1ccc(cc1)CONC(=O)N, XST00001145b, Mounted_Clear, Failed - loop broken, P 21 21 21, 34 41 110 90 90 90, 1.22, 0.497, 32, 1.2, 81.3, 71.8, 61.4, , , None, None, None, 1 - Analysis Pending, None

PARP14A-x0538, COc1ccc(cc1)C#CC(=O)[O-], FMOPL000052a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.037, 47, 2.6, 95.2, 99, 70.6, 0.20706, 0.229, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0539, CCOc1ccc(cc1)[C@@H](C)[NH3+], FMOPL000205a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.035, 51, 2.4, 90.8, 99.7, 52.4, 0.19013, 0.21434, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0540, COc1cccc(c1)Nc2c3c([nH]cn3)ncn2, FMOPL000596a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.14, 0.03, 49.1, 1.1, 96.3, 99.2, 71.1, 0.19487, 0.22025, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0541, c1ccc(cc1)Nc2nncc2, FMOPL000113a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.051, 38.6, 2.1, 82.9, 99.9, 15.3, 0.18935, 0.20541, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0542, c1cc2c(ccc(c2nc1)O)C[NH+]3CCOCC3, FMOPL000054a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.048,43,1.9,82.8,99.3,14.4,0.20044,0.21957, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0543, c1cc2c(cc1C[NH2+]C[C@H]3CCCO3)OCO2, FMOPL000206a, Mounted_Clear, success, P
21 21 21,34 41 110 90 90
90,1.14,0.026,59.1,2.5,97.4,98.8,83.5,0.21851,0.24977, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0544, c1ccc(cc1)NC(=O)NCCN2CCCC2=O, FMOPL000589a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.051,44.3,2.6,84.7,99.3,14.4,0.19813,0.22063, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0545, c1ccc(c(c1)N)Nc2cccn2, FMOPL000114a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.09,0.027,66.7,1.3,88.9,99,37,0.20495,0.22359, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0546, COC(=O)C#Cc1ccc(cc1)Cl, FMOPL000060a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.11,0.037,50.8,1.4,88.3,99.2,45.8,0.21157,0.23803, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0547, CCn1c(ccn1)C[NH2+]C, FMOPL000221a, Mounted_Clear, success, P 2 2 2,34 41 110
90 90 90,1.05,0.059,34.3,2,84.3,99.4,13.9,0.20982,0.22983, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0548, Cc1ccc(cc1N)c2cnc3ccccc3n2, FMOPL000598a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.11,0.037,46.1,2.7,93.4,98.8,64,0.20433,0.22735, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0549, C1C[C@@H](OC1)CNC(=O)N2CCOCC2, FMOPL000116a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.024,68,2.5,85,99.1,32.7,0.20292,0.22459, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0550, CCNC(=O)N1CCN(CC1)C(=O)C, FMOPL000061a, Mounted_Clear, success, P 21 21 21,34
41 110 90 90 90,1.05,0.053,41.5,2.1,83,99.2,15.1,0.21673,0.23996, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0551, CS(=O)(=O)NC1CCCC1, FMOPL000222a, Mounted_Clear, success, P 21 21 21,34 41 110
90 90 90,1.08,0.022,72.9,2.4,90.4,99.1,49.6,0.19899,0.22381, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0552, CN(C)c1ccc(cc1)c2cc(on2)C(=O)OC, FMOPL000595a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.06,0.019,86.4,1.1,83.1,99.1,21.9,0.20428,0.22904, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0553, c1cc(cc(c1)F)Nc2[nH]c(=O)ccn2, FMOPL000115a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.034,51.7,2.5,91.6,98.8,54.5,0.21593,0.24188, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0554, CC(=O)c1ccc(cc1)OC(F)F, FMOPL000223a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.08,0.029,61,2.4,90.1,98.4,50.1,0.20898,0.22836, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0555, c1ccc2c(c1)[nH]c(n2)CNC(=O)c3ccco3, FMOPL000588a, Mounted_Clear, success, P
21 21 21,34 41 110 90 90
90,1.08,0.029,56.3,2.7,90.1,98.3,49.8,0.18911,0.21204, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0556, c1cc(cc1c2ccc(o2)C(=O)NN)Cl, FMOPL000118a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.15,0.025,59.8,2.5,98.7,98.8,91.8,0.20302,0.22983, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0557, c1ccc(cc1)c2cnc(c(n2)C(=O)N)N, FMOPL000063a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.11,0.029,57.9,2.7,92.2,98.8,58.9,0.20137,0.22313, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0558, Cc1c(nc(=O)[nH]n1)Nc2cccc(c2)O, FMOPL000117a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.1,0.029,57.1,2.5,94.9,99,71.4,0.20995,0.233, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0559, c1cc(ccc1CO)c2ccc(cc2)CO, FMOPL000064a, Mounted_Clear, success, P 21 21 21,34
41 110 90 90 90,1.11,0.039,42.3,2.6,93.9,99.4,66.7,0.20627,0.22887, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0560, COc1cccc1OCC(=O)NN, FMOPL000225a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.09,0.025,68.7,2.7,90.1,99.3,51.2,0.19071,0.21539, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0561, CC(=O)c1ccc(cc1)NC(=O)C[NH+]2CCCC2, FMOPL000591a, Mounted_Clear, success, P 2
2 2,34 41 110 90 90 90,1.05,0.036,60,1.9,79.6,99.2,10.9,0.20482,0.22497, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0562, CS(=O)(=O)Nc1ccc(cc1)c2cccc2, FMOPL000121a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.036,50.5,2.6,91.5,98.7,55.6,0.21141,0.23456, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0563, CS(=O)(=O)Nc1ccc(cc1)C(=O)N, FMOPL000226a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.1,0.035,49.4,2.6,91.1,99.4,55.6,0.19898,0.22224, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0564, CC1(C[C@H](CCO1)C(=O)NCc2cccc2)C, FMOPL000592a, Mounted_Clear, success, P
21 21 21,34 41 110 90 90 90,1.15,0.034,46.7,2.5,97.6,99.7,84.6,0.20223,0.22907, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0565, CCCc1nnc(s1)NC(=O)c2ccccn2, FMOPL000119a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.08,0.042,44.7,2.8,90,98.1,51.6,0.207,0.22722, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0566, CCc1nnc(s1)NC(=O)C(F)(F)F, FMOPL000227a, Mounted_Clear, Failed -
unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0567, Cc1cc(n2c(n1)ncn2)Nc3ccc(cc3)O, FMOPL000597a, Mounted_Clear, success, P 21 21
21,34 41 111 90 90 90,1.1,0.023,69,2.6,88.8,99,47.7,0.18301,0.20419,0.14006,0.16196, P 21
21 21,6 - Deposited,5QI6

PARP14A-x0568, CCC[C@H](C)C(=O)Nc1c(cccc1C)C, FMOPL000720a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.05,0.047,50.1,2.4,82.8,99.4,16.2,0.21528,0.24088, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0569, CCOC(=O)NCc1cccc1, FMOPL000628a, Mounted_Clear, success, P 21 21 21,34 41 110
90 90 90,1.07,0.036,50.2,2.8,86.4,98.4,41.1,0.19822,0.22035, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0570, COc1ccc(cc1)CNC(=O)c2cncn2, FMOPL000452a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.06,0.022,87.2,1.6,78.4,98.3,14.9,0.19997,0.22394, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0571, c1cscc1C[NH+]2CCC(CC2)O, FMOPL000505a, Mounted_Clear, success, P 21 21 21,34
41 111 90 90 90,1.07,0.025,61.5,2.8,83.2,97.1,32.1,0.19625,0.21943, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0572, CC(C)CC(=O)Nc1ccc(cc1)NC(=O)C, FMOPL000731a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.043,47,1.8,80.1,99.3,11.5,0.20828,0.22852, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0573, CC(C)c1ccc(cc1)NNC(=O)c2ccno2, FMOPL000654a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.05, 0.045, 52, 3.2, 84.8, 99.3, 16.7, 0.19965, 0.22191, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0574, c1cnc(cn1)C(=O)NCCC2=CCCCC2, FMOPL000415a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.14, 0.026, 63.9, 2.9, 97, 98.8, 82, 0.20535, 0.22365, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0575, Cc1ccc(cc1)CNC(=O)COC, FMOPL000511a, Mounted_Clear, success, P 2 2 2, 34 41 110
90 90 90, 1.05, 0.067, 32.5, 3.4, 81.8, 99.1, 14.8, 0.20404, 0.22643, None, None, P 21 21 21, 1 -
Analysis Pending, None

PARP14A-x0576, CC(C)c1ccc(cc1)NNC(=O)C2CCC2, FMOPL000646a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.09, 0.036, 48.6, 2.6, 92, 98.2, 56.9, 0.21349, 0.24011, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0577, c1ccc(cc1)CCC(=O)NN2CCOCC2, FMOPL000413a, Mounted_Clear, success, P 2 2 2, 34
41 110 90 90 90, 1.13, 0.024, 59, 1.2, 96.1, 99.2, 71.6, 0.20519, 0.23076, None, None, P 21 21 21, 1
- Analysis Pending, None

PARP14A-x0578, COCC(=O)NCc1cccc1, FMOPL000507a, Mounted_Clear, success, P 2 2 2, 34 41 110 90
90 90, 1.22, 0.025, 48.1, 1.9, 99.8, 99.3, 99, 0.18611, 0.21678, None, None, P 21 21 21, 1 - Analysis
Pending, None

PARP14A-x0579, c1cc(c(c(c1)F)C(=O)N2CCCCC2)F, FMOPL000729a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.08, 0.038, 45.3, 2.4, 91.2, 99.5, 52.8, 0.19506, 0.2174, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0580, CCc1cccc1NNC(=O)c2cccc2, FMOPL000657a, Mounted_Clear, success, P 2 2 2, 34 41
110 90 90 90, 1.17, 0.035, 47.5, 1.4, 97.3, 99.3, 78.4, 0.218, 0.24215, None, None, P 21 21 21, 1 -
Analysis Pending, None

PARP14A-x0581, CC(C)C(=O)Nc1ccc(cc1)N2CCCCC2, FMOPL000439a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.11, 0.028, 60.1, 2.7, 91.6, 98.5, 55.4, 0.20702, 0.23029, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0582, CCOC(=O)N1CCOCC1, FMOPL000502a, Mounted_Clear, success, P 2 2 2, 34 41 110 90
90 90, 1.12, 0.018, 75.1, 1.4, 95.3, 99.1, 63.4, 0.19777, 0.22335, None, None, P 21 21 21, 1 -
Analysis Pending, None

PARP14A-x0583, Cc1ccc(cc1)CNC(=O)c2ccc(cc2)C, FMOPL000754a, Mounted_Clear, success, P 2 2
2, 34 41 110 90 90 90, 1.07, 0.027, 70.5, 1.3, 85.9, 98.9, 29.5, 0.20426, 0.22748, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0584, c1cc(cc(c1)NC(=O)c2ccno2)C(=O)[O-], FMOPL000648a, Mounted_Clear, success, P 2
2 2, 34 41 110 90 90 90, 1.07, 0.029, 62.8, 1.7, 88.4, 99.1, 33.1, 0.19567, 0.21664, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0585, C1CCC(CC1)CCC(=O)N2CCOCC2, FMOPL000400a, Mounted_Clear, success, P 2 2 2, 34 41
110 90 90 90, 1.13, 0.02, 72.4, 1.5, 96.1, 99.3, 68, 0.19298, 0.21806, None, None, P 21 21 21, 1 -
Analysis Pending, None

PARP14A-x0586, CC(=O)Nc1ccc2c(c1)[nH]c(=O)[nH]2, FMOPL000508a, Mounted_Clear, success, P 21
21 21, 34 41 110 90 90 90, 1.06, 0.032, 50.3, 2.4, 79.3, 98.5, 25.1, 0.20448, 0.2273, None, None, P
21 21 21, 1 - Analysis Pending, None

PARP14A-x0587, C[NH+]1CCC(CC1)OC(=O)c2cccc(c2)F, FMOPL000739a, Mounted_Clear, success, P 2 2
2, 34 41 110 90 90 90, 1.05, 0.051, 42.5, 2, 84.8, 99.5, 14.8, 0.19918, 0.21802, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0588, c1cc(ccc1)NNC(=O)C2CCC2)F, FMOPL000636a, Mounted_Clear, success, P 2 2 2, 34 41
110 90 90 90, 1.1, 0.022, 67.1, 1.1, 92.9, 99.2, 54.3, 0.196, 0.22148, None, None, P 21 21 21, 1 -
Analysis Pending, None

PARP14A-x0589, c1ccc(cc1)NC(=O)NCc2ccc(cc2)F, FMOPL000434a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.03, 52.6, 1.3, 96.2, 98.9, 73.7, 0.18287, 0.21021, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0590, CCC(=O)Nc1ccc(cc1)C, FMOPL000506a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.059, 37.1, 4.7, 81, 99.1, 12.7, 0.18342, 0.20238, 0.13882, 0.16273, P 21 21 21, 6 - Deposited, 5QI7

PARP14A-x0591, c1ccc2c(c1)nc(s2)N3CCOCC3, FMOPL000705a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.23, 0.027, 52.6, 2.1, 98.8, 98.9, 90.5, 0.18971, 0.21938, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0592, c1ccc(c(c1)NNC(=O)c2ccno2)F, FMOPL000644a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.16, 0.032, 36.7, 1.2, 96.1, 99.7, 67.9, 0.19549, 0.22439, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0593, COC(=O)Nc1cccc(c1)NC(=O)OC, FMOPL000406a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.07, 0.032, 59.5, 1.2, 85.9, 99.5, 29.1, 0.19317, 0.21597, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0594, CNC(=O)CCC1CCCCC1, FMOPL000503a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.037, 60.2, 2, 79.9, 98.5, 13.2, 0.20756, 0.22887, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0595, Cc1cccc(c1)NC(=O)Nc2nc(cs2)C, FMOPL000744a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.13, 0.024, 63.5, 2.7, 95.8, 99.6, 75.6, 0.19199, 0.21748, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0596, c1ccc(cc1)C(=O)NNc2cccc2F, FMOPL000649a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.029, 50.8, 1.1, 96.8, 99.1, 74.5, 0.20235, 0.2281, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0597, COc1ccc(cc1)CNC(=O)[C@@H]2CCCO2, FMOPL000425a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.06, 0.03, 61.5, 1.5, 86.1, 99.2, 22.9, 0.19023, 0.21332, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0598, COC(=O)COc1ccc(cc1)C#N, FMOPL000510a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.13, 0.032, 52.8, 2.6, 96.1, 99.3, 76.6, 0.19018, 0.21628, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0599, c1cc(sc1)C(=O)Nc2ccc(cc2)C#N, FMOPL000713a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.029, 61.1, 2.6, 92.4, 98.6, 57.9, 0.19797, 0.22435, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0600, CC(=O)Nc1ccc(cn1)NC(=O)c2ccc2, FMOPL000656a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.06, 0.025, 71.1, 1.3, 83.7, 98.2, 21.4, 0.20826, 0.2336, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0601, COC(=O)c1ccc(cc1)NC(=O)C2CCCC2, FMOPL000450a, Mounted_Clear, success, P 21 21 2, 34 41 110 90 90 90, 1.05, 0.036, 56.8, 2.6, 72.2, 98.4, 9.1, 0.19395, 0.21763, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0602, COC(=O)CNC(=O)C1CCCC1, FMOPL000509a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.068, 29.8, 3.8, 76.9, 99, 8.9, 0.2114, 0.23366, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0603, Cc1cc(nol)NC(=O)c2ccc(cc2)N(C)C, FMOPL000753a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.065, 33.5, 6.2, 81.5, 99, 13, 0.20171, 0.22122, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0604, Cc1cc(nol)C(=O)Nc2ccc3c(c2)cc[nH]3, FMOPL000659a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.059, 37, 2.8, 81.4, 99.4, 14.9, 0.19973, 0.21905, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0605, c1ccc(cc1)CCNc2c[nH]c(=O)[nH]c2=O, FMOPL000412a, Mounted_Clear, success, P 2 2, 34 41 110 90 90 90, 1.05, 0.046, 46.2, 2.5, 84.5, 99.5, 13.6, 0.19253, 0.21538, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0606, CC(C)(C)[NH+]1CC(C1)O, FMOPL000515a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.032, 51.5, 2.5, 91, 99.2, 51.3, 0.19899, 0.22065, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0607, COc1cc(ccc1O)C[NH2+]C2CCCCC2, FMOPL000737a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.035, 50.4, 2.6, 88.8, 98.1, 47.3, 0.20192, 0.22384, 0.21224, 0.2249, P 21 21 21, 3 - In Refinement, None

PARP14A-x0608, Cc1ccc(cc1)C[NH+]2CCS(=O)(=O)CC2, FMOPL000642a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.06, 0.026, 71.8, 1.4, 75, 98.2, 14.7, 0.19007, 0.2178, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0609, CCCC(=O)NCC1[nH]c2ccccc2n1, FMOPL000518a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.044, 41.9, 2.6, 91.6, 99.3, 55.2, 0.20186, 0.22175, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0610, CC(=O)NCC1(CCOCC1)c2ccccc2, FMOPL000733a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.05, 47.3, 2.5, 75.6, 98.7, 12.3, 0.19457, 0.21628, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0611, Cc1ccc(c(c1)NC(=O)Nn2cnnc2)OC, FMOPL000455a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.059, 39.4, 6.8, 81.4, 98.9, 14.6, 0.20912, 0.22712, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0612, c1cc2c(ccc(c2nc1)O)C[NH+]3CCCC3, FMOPL000519a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.086, 28.9, 6.4, 77.7, 98.8, 8.6, 0.19479, 0.21537, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0613, c1cc(cnc1)NC(=O)CC2CCCCC2, FMOPL000331a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.035, 59, 2, 84, 99, 14.8, 0.20743, 0.22546, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0614, c1nncn1NC(=O)CC2CCCCC2, FMOPL000321a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.049, 44.3, 2.7, 83.2, 99.4, 14.8, 0.20024, 0.22338, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0615, c1ccnc(c1)C(=O)NCCc2ccc(cc2)O, FMOPL000362a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.058, 36.1, 2.1, 85.6, 99.4, 14.8, 0.20673, 0.2277, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0616, CC[C@H](C)NC(=O)Nc1cccc(c1)Cl, FMOPL000327a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.04, 48.6, 2.1, 81.5, 98.8, 13.4, 0.22938, 0.25905, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0617, c1ccc(c(c1)c2ccc(cc2)N)C(=O)[O-], FMOPL000342a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.068, 33.5, 2.9, 82, 99.2, 13.6, 0.20095, 0.21994, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0618, c1ccc(c(c1)C[NH+]2CCOCC2)O, FMOPL000382a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.047, 45.5, 1.9, 82.3, 99.4, 13.6, 0.19756, 0.22075, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0619, c1ccc(c(c1)CNc2[nH]c3ccccc3n2)O, FMOPL000383a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.21, 0.026, 57, 1.5, 99.7, 98.9, 96.9, 0.20214, 0.22997, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0620, C[NH+]1CCS(=O)(=O)CC1, FMOPL000267a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.085, 26.9, 4.7, 84.2, 99.3, 14.3, 0.19539, 0.21738, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0621, c1ccc(cc1)Coc2ccc(cc2)C(=O)[O-], FMOPL000270a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.05, 42.9, 2, 80.9, 99.1, 13.8, 0.19686, 0.21752, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0622, CC(=O)Oc1ccc2c(c1)nsn2, FMOPL000268a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.1, 0.021, 78.6, 1.3, 89.2, 99.2, 38.5, 0.19977, 0.22051, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0623, CNc1ccc(cc1)O, FMOPL000266a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.1, 0.031, 53.4, 1.3, 93.7, 99.4, 55.4, 0.19588, 0.21752, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0624, C1COCC[NH+]1CCO, FMOPL000265a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.19, 0.057, 47.2, 1.6, 94.9, 99.5, 81.1, 0.24335, 0.28699, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0625, CS(=O)(=O)NCCc1ccc(cc1)F, FMOPL000228a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.039, 59, 2.1, 79.9, 98.8, 13.4, 0.18893, 0.20498, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0626, c1ccc(cc1)CONC(=O)Nc2ccccc2, FMOPL000122a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.22, 0.035, 41.8, 1.6, 98.9, 99.4, 89.9, 0.20131, 0.22802, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0627, COc1cc(nc(n1)N)c2ccccc2, FMOPL000229a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.023, 63, 1.3, 94.1, 99.1, 62.7, 0.20855, 0.23763, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0628, COc1ccc2c(c1)nc(s2)N, FMOPL000602a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.038, 50.2, 2.5, 92.4, 99.2, 58.5, 0.19446, 0.21813, 0.16377, 0.18642, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0629, Cc1c(nc(=O)[nH]n1)Nc2ccc(cc2)C(C)C, FMOPL000125a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.12, 0.04, 40.1, 1, 94.9, 99.5, 65.8, 0.21021, 0.23613, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0630, CCc1ccc(cc1)c2c(sc(n2)N)C, FMOPL000231a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.069, 30.1, 2.5, 83, 99.4, 14, 0.21258, 0.23235, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0631, COc1ccc(cc1OC)C[NH3+], FMOPL000601a, Mounted_Clear, success, P 2 2 2, 34 41 111 90 90 90, 1.05, 0.066, 33.8, 3.1, 83.7, 99.3, 14.5, 0.19953, 0.2199, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0632, COc1ccc(cc1)NC(=O)Nc2ccncc2, FMOPL000127a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.047, 42.2, 3.5, 71.2, 98.6, 7.6, 0.1885, 0.21079, 0.15978, 0.18042, P 21 21 21, 2 - PANDDA model, None

PARP14A-x0633, Cn1cc(c(n1)C(=O)NC2CCCC2)Cl, FMOPL000232a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.066, 33.1, 6, 72.9, 98.4, 8.3, 0.20698, 0.22876, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0634, COc1ccc(cc1)CC(=O)[O-], FMOPL000603a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.085, 24.6, 4.4, 75.7, 98.6, 12.5, 0.20686, 0.22716, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0635, c1cc(oc1)C(=O)N2CCN(CC2)C(=O)C3CC3, FMOPL000123a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90

90,1.08,0.032,54.7,2.6,87.3,98.6,41.7,0.19399,0.21843, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0636, CC(=O)C1CCCC(C1)NC(=O)C(F)(F)F, FMOPL000233a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.1,0.097,19.8,2.5,91.1,99.6,56.8,0.20597,0.22661, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0637, C1CC(CCC1C2NCC(S2)N)O, FMOPL000605a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.09,0.03,57.9,2.6,92.2,98.7,57.4,0.19564,0.21932,0.14326,0.16699, P 21 21 21,6 - Deposited,5QI8

PARP14A-x0638, CC(C)(C)C(=O)NCCC1[NH]C2CCCCC2N1, FMOPL000124a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.09,0.027,60.4,1.3,92,99,46.7,0.1953,0.21934, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0639, C1CCC(C1)NC(=O)NC2CCCN2, FMOPL000234a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.08,0.03,57.4,2.6,90.7,99.1,52.4,0.20475,0.22535, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0640, COC1CCC(C1)NC(=O)C[NH3+], FMOPL000604a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.17,0.026,49.3,1.2,97.8,98.9,80.9,0.20855,0.23592, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0641, Cc1nc2ccc(cc2o1)O, FMOPL000128a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.2,0.024,51.1,1.3,98.2,99.7,96.5,0.20945,0.23964, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0642, CCS(=O)(=O)NCC1CCC2C(C1)OCO2, FMOPL000235a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.09,0.055,34.9,2.6,91.3,99.3,54.4,0.19957,0.22283, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0643, C1CC(CCC1C2CCNC(N2)N)C1, FMOPL000606a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.056,37,2.4,81.2,98.9,14.5,0.20645,0.22444, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0644, Cc1ccc(cc1C)C2C(SC(N2)N)C, FMOPL000129a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.054,40,2.3,85.3,99.3,15,0.19477,0.2161, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0645, CCOC1CCCC1N2CC[NH2+]CC2, FMOPL000609a, Mounted_Clear, success, P 21 21 21,34 41 110 90 90 90,1.14,0.031,45.8,1.1,96.9,99.8,74.7,0.20247,0.22728, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0646, CC1(C[C@H](CCO1)[NH2+]Cc2ccco2)C, FMOPL000607a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.18,0.021,70.6,1.6,97.9,99.4,78.2,0.20202,0.22719, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0647, C1CC(CCC1C(=O)[O-])NC2CN[NH]C(=O)N2, FMOPL000130a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.034,60.8,2.4,82.9,99.2,13.5,0.19196,0.21395, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0648, C1CCC(C1)NC2CCC(CC2N)C#N, FMOPL000238a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.15,0.033,42.8,1.3,95.1,99.3,70.2,0.19554,0.2222, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0649, CC1CCN(CC1)C2CCC(CC2C1)N, FMOPL000608a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.15,0.031,53.5,2,88.5,98.9,45.2,0.19697,0.22458, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0650, C1CCC2C(C1)CC[NH+] (C2)Cc3ccc(cc3)O, FMOPL000132a, Mounted_Clear, success, P 2 2 2,34 41 110 90 90 90,1.05,0.037,59.2,2.2,85.3,98.9,13.9,0.20413,0.2246, None, None, P 21 21 21,1 - Analysis Pending, None

PARP14A-x0651,CC(=O)N1CCN(CC1)c2ccc(cc2)Cl,FMOPL000239a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.18,0.033,48.5,2.7,99.3,99.7,95.6,0.19437,0.22175, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0652,CC(C)C(=O)N1CCN(CC1)c2ccc(cc2)N,FMOPL000610a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.16,0.028,52.2,1.5,98.3,99.3,82.5,0.19605,0.22466, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0653,CC(=O)c1ccc(cc1)OC(=O)c2cccs2,FMOPL000735a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.1,0.021,76,2.7,86.9,99.2,47.3,0.19321,0.21878, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0654,c1ccc2c(c1)c(cs2)NC(=O)NC3CC3,FMOPL000640a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.09,22.8,4.1,82.1,99.1,14.2,0.20638,0.22566, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-
x0655,CC1(CC(=CC(=O)Cl)Nc2c[nH]c(=O)[nH]c2=O)C,FMOPL000444a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.13,0.025,65,2.6,97.8,99.5,87,0.18169,0.20783, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0656,CNc1cccc1,FMOPL000514a,Mounted_Clear,success,P 2 2 2,34 41 110 90 90
90,1.05,0.062,36.2,3.3,84.9,99.4,14.5,0.19646,0.21727, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0657,COc1ccc(cc1)C[NH2+]C2CCCC2,FMOPL000707a,Mounted_Precipitate,success,P 2 2
2,34 41 110 90 90 90,1.05,0.039,48,1.6,80.5,99.1,14.9,0.19374,0.21594, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0658,CC(=O)Nc1ccc(cc1)NC(=O)[C@H]2CC2(C)C,FMOPL000655a,Mounted_Clear,success,P
2 2 2,34 41 110 90 90 90,1.05,0.045,49.3,1.8,82,98.7,13.2,0.20435,0.22436, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0659,c1cc(ccc1C(=O)N)NC(=O)[C@@H]2CCCO2,FMOPL000416a,Mounted_Clear,success,P 2
2 2,34 41 110 90 90 90,1.05,0.045,49.5,2.3,82.6,99.2,14.3,0.21635,0.24041, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0660,C1CN(CCC1C(=O)N)C(=O)CC#N,FMOPL000517a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.08,0.026,66,2.7,87.5,98.5,46.3,0.2105,0.23572, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0661,c1cc(cc(c1)F)C[NH2+]Cc2ccco2,FMOPL000703a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.05,0.045,46.2,2.6,81.9,99.4,15,0.20329,0.2228, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0662,CC(C)[C@](C)(C#N)Nc1cccc1,FMOPL000630a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.05,0.037,51.9,1.7,83.4,98.6,15.3,0.20138,0.22623, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0663,CC[C@H](C)NC(=O)c1cc(on1)c2ccccc2,FMOPL000448a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.08,0.043,46.2,2.6,90.9,98.7,50.3,0.21257,0.23698, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0664,C[NH2+]CCC1CCCC1,FMOPL000516a,Mounted_Clear,success,P 2 2 2,34 41 110 90
90 90,1.13,0.022,71.5,1.4,96.2,99.3,69.5,0.19533,0.22048, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0665,COc1cccc(c1)C(=O)Nc2ccccc2F,FMOPL000752a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.06,0.031,57.6,1.5,86.2,99.1,22.7,0.20037,0.22223, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0666,Cn1c(cc(=O)[nH]1)Nc2ccccc2,FMOPL000632a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.05,0.048,43.8,2.5,84.5,99.4,14.5,0.19925,0.222, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0667,CC1CCN(CC1)C(=O)CCc2ccccc2,FMOPL000445a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.14,0.034,43.8,2.6,97.2,99.4,82,0.19886,0.22433, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0668,CC1CCC(CC1)[NH2+]C2CCC(CC2)O,FMOPL000520a,Mounted_Clear,success,P 21 21
21,34 41 111 90 90 90,1.13,0.037,43.8,2.6,96.7,99.8,79.6,0.21244,0.2422, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0669,CCC(=O)Nc1nnc(s1)C2CCCC2,FMOPL000719a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.12,0.045,45.6,2.8,93.3,98.8,62.9,0.20819,0.2313, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0670,c1cc2c(cc1NC(=O)N3CCOCC3)non2,FMOPL000652a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.15,0.038,37.5,1.1,97.8,99.6,82.1,0.20587,0.2367, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0671,CC(=O)Nc1nnc(s1)Coc2ccccc2,FMOPL000734a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.12,0.032,52.5,2.6,95,99,72.7,0.2107,0.23691, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0672,Cc1cc(nol)NC(=O)c2ccc3c(c2)non3,FMOPL000660a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.045,48.6,2.1,73.8,98.7,8,0.19798,0.21938, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0673,Cn1cc(cn1)CNC(=O)c2ccco2,FMOPL000397a,Mounted_Clear,success,P 2 2 2,34 41
110 90 90 90,1.08,0.025,66.7,1.5,89.7,99,37.8,0.19287,0.21394, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0674,c1ccc(cc1)C(=O)Nc2ccc3c(c2)ccn3,FMOPL000534a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.056,40,2.8,83.6,99.4,14.1,0.19917,0.22159, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0675,Cc1ccc(c(c1)OC(=O)c2ccncc2)C,FMOPL000742a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.11,0.033,51.2,2.6,93.3,99.3,63.8,0.19859,0.21958, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0676,c1cc2c(cc1C(=O)N3CCOCC3)nns2,FMOPL000645a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.032,57.5,1.8,85.6,99.1,15,0.20096,0.22443, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0677,Cn1ccc(n1)C(=O)NC[C@@H]2CCCO2,FMOPL000398a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.037,51,2.3,78.9,98.8,9,0.19598,0.21827, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0678,Cc1cc(cc(c1)NC(=O)NCc2ccco2)C,FMOPL000533a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.09,0.039,47.3,2.4,92.1,99,57.1,0.20108,0.22738, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0679,c1ccc2c(c1)[nH]c(n2)C[NH+]3CCOCC3,FMOPL000717a,Mounted_Clear,success,P 2 2
2 2,34 41 110 90 90 90,1.15,0.026,55.6,1.8,93.3,98.4,62,0.19399,0.22106, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0680,CC(=O)N1CCC(CC1)c2c[nH]c3c2ccccc3,XSTXX051512c,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.03,57.3,2,82.5,98.9,15,0.19698,0.21845, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0681,CCn1cc(cn1)C(=O)NCc2ccc(cc2)F,FMOPL000449a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.05,0.043,49.3,2.2,79.3,98.9,9.4,0.19817,0.22288, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0682, Cc1c(c(nol)c2ccc(cc2)F)C(=O)NC, FMOPL000529a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.15,0.04,39.4,2.5,97.1,99.5,85.8,0.211,0.23815, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0683, CC(C)(C)C1CCN(CC1)C(=O)c2ccccc2, FMOPL000747a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90 90,1.12,0.036,47.9,2.5,90.3,99.7,49.7,0.19485,0.22076, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0684, c1cc(ccc1C[NH+]2CCOCC2)CO, FMOPL000663a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.13,0.036,46,2.8,94.8,99.1,69.5,0.20187,0.22953, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0685, Cn1c(ccn1)C(=O)NCc2cccs2, FMOPL000396a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.05,0.038,58.4,2.3,78.1,99.1,12.8,0.19033,0.21148, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0686, CC(CO)(CO)NC(=O)Nc1ccccc1, FMOPL000524a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.15,0.034,46.2,2.6,98.4,99.7,90,0.19189,0.2207, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0687, CC(=O)Nc1cccc(c1)NC(=O)N, FMOPL000701a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.08,0.024,71.2,1.2,89.6,99.3,37.9,0.19272,0.21341, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0688, CC(C)(C)c1ccc(cc1)C(=O)Nc2ccon2, FMOPL000437a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.08,0.025,68.1,1.2,86.9,99.4,35.9,0.20686,0.23148, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0689, c1cc(oc1)c2nnc(s2)NC(=O)C3CC3, FMOPL000522a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.1,0.031,55.3,2.5,91.9,99.1,58.3,0.21011,0.23273, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0690, Cn1c(c(cn1)C1)C(=O)N2CCCCC2, FMOPL000711a, Mounted_Clear, success, P 2 2 2,34
41 111 90 90 90,1.05,0.058,36.4,2.6,81.7,99.1,13.4,0.19507,0.21374,0.1398,0.16164, P 21
21 21,6 - Deposited,5QI9

PARP14A-x0691, COC(=O)Nc1ccc(cc1)Cc2ccncc2, FMOPL000683a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.09,0.034,54.3,2.5,92.5,98.9,58.9,0.21514,0.24158, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0692, CC[C@H](c1ccccc1)C(=O)Nc2cncn2, FMOPL000447a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.06,0.02,78,1.3,87.7,98.8,24.7,0.20447,0.22558, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0693, CC(=O)Nc1ccc(cc1)N2CC[NH+](CC2)C, FMOPL000526a, Mounted_Clear, success, P 21
21 21,34 41 110 90 90
90,1.15,0.026,54.3,1.5,97.9,99.8,83.5,0.19386,0.2155,0.20486,0.21852, P 21 21 21,3 - In
Refinement, None

PARP14A-x0694, c1ccc(cc1)OCC(=O)NC2CCCCC2, FMOPL000728a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.05,0.081,28.9,4.4,83.4,99.1,13.9,0.20171,0.2248, None, None, P 21 21 21,1
- Analysis Pending, None

PARP14A-x0695, C1CCC2(CC1)OC[C@@H](O2)C[NH+]3CCCC3, FMOPL000669a, Mounted_Clear, success, P
21 21 21,34 41 110 90 90 90,1.09,0.031,53,2.6,90.5,98.2,53.1,0.20827,0.23134, None, None, P
21 21 21,1 - Analysis Pending, None

PARP14A-x0696, Cc1c(c(on1)C)C(=O)NCCC2=CCCC2, FMOPL000453a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.17,0.038,46.6,1.6,98.6,99.2,85.6,0.20441,0.23476, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0697, COc1ccc(cc1)Nc2ccc(cc2)F, FMOPL000528a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.18, 0.019, 73.1, 1.7, 97.3, 99.3, 83.2, 0.20349, 0.22447, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0698, CC(C)Oc1cc(c(cc1Cl)Cl)N, FMOPL000269a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.2, 0.025, 56.2, 1.2, 99.4, 99.5, 96, 0.18977, 0.2256, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0699, c1ccc(c(c1)N)N2CCOCC2, XST00000046b, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.1, 0.026, 63.3, 2.6, 93.1, 98.8, 61.4, 0.20162, 0.22364, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0700, c1ccc(cc1)COC(=O)N2CCC(CC2)O, FMOPL000543a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.16, 0.035, 43.6, 1.1, 98.1, 99.1, 84.3, 0.19947, 0.22923, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0701, COC(=O)ClCC1, FMOPL000535a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.08, 0.04, 48.8, 1.8, 85.5, 97.7, 26.2, 0.19794, 0.22004, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0702, CCOC(=O)c1ccoc1, FMOPL000537a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.08, 0.045, 39.6, 2.5, 90.6, 99.2, 48.7, 0.19839, 0.22162, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0703, c1ccc(cc1)COC(=O)[O-], FMOPL000539a, Mounted_Precipitate, success, P 2 2 2, 34 41 110 90 90 90, 1.26, 0.026, 55.7, 1.9, 99.6, 98.9, 98.6, 0.19373, 0.22051, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0704, CCN(CCO)c1ccc(cc1)N, FMOPL000541a, Mounted_Precipitate, Failed - unknown,,,,,,,,,,,,, #NAME?,

PARP14A-x0705, Cc1cc(nc(n1)Nc2ccccc2)C, FMOPL000542a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.12, 0.034, 48.1, 2.9, 86.4, 98.7, 45.7, 0.1946, 0.21626, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0706, CNC(=O)c1cc(ccn1)Cl, FMOPL000538a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.15, 0.023, 68.9, 2.6, 96.3, 99.1, 82.6, 0.19458, 0.21849, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0707, c1ccnc(c1)c2c[nH]nc2, FMOPL000133a, Mounted_Clear, success, P 21 21 21, 34 41 111 90 90 90, 1.14, 0.03, 50.4, 2.5, 98, 99.6, 88.2, 0.21545, 0.24448, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0708, Cc1cnc(s1)NC(=O)CCC2CCCC2, FMOPL000240a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.11, 0.03, 55.7, 2.7, 93.3, 98.4, 64.2, 0.21272, 0.23911, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0709, CC(=O)N1CCC(CC1)[NH2+]CCOC, FMOPL000134a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.23, 0.036, 36.5, 1.2, 99.6, 99.6, 98.4, 0.19261, 0.22824, None, None, P 21 21 21, 2 - PANDDA model, None

PARP14A-x0710, CS(=O)(=O)N1CCC(CC1)C(=O)NC2CC2, FMOPL000241a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.17, 0.023, 61.6, 2, 93.3, 98.3, 62.8, 0.19145, 0.21773, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0711, COc1ccc2c(cc(=O)oc2c1)CC(=O)[O-], FMOPL000612a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.046, 52.4, 2.3, 85.2, 99.4, 15.2, 0.20889, 0.22788, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0712, CC(=O)Nc1cccc(c1)NC(=O)COC, FMOPL000242a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.14, 0.025, 67.3, 1.2, 97.5, 99.5, 76.5, 0.21194, 0.24097, 0.1604, 0.19815, P 21 21 21, 6 - Deposited, 5QIA

PARP14A-x0713,CC[NH+](CC)c1cccc(c1)O,FMOPL000135a,Mounted_Clear,success,P 2 2 2,34 41
110 90 90 90,1.13,0.025,61.8,1.3,97.1,99.2,76.4,0.19893,0.22803,None,None,P 21 21 21,1
- Analysis Pending, None

PARP14A-x0714,COC(=O)Nc1nnc(s1)CC2CCCC2,FMOPL000243a,Mounted_BadDispense,success,P 21
21 21,34 41 110 90 90 90,1.14,0.025,59.5,2.6,95.3,99.6,77.5,0.18425,0.20744,None,None,P
21 21 21,1 - Analysis Pending, None

PARP14A-x0715,COc1cc(ccc1N)Nc2ccccc2,FMOPL000626a,Mounted_Clear,success,P 21 21 21,34 41
110 90 90 90,1.1,0.028,59.6,2.5,93.6,99.1,65.7,0.2108,0.23782,None,None,P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0716,CCc1c(c(on1)C)C(=O)Nc2cc(on2)C,FMOPL000245a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.09,0.029,58.7,1,91.9,99.3,45.7,0.21399,0.2387,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0717,C[C@@H](Cc1ccc(cc1)O)[NH+](C)C,FMOPL000138a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.05,0.041,58.1,2.1,84.5,99.5,14.6,0.20113,0.22334,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0718,Cc1ccc(s1)C(=O)Nc2ccccc2OC,FMOPL000247a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.12,0.03,56,2.6,95.8,99.3,74.5,0.18528,0.21074,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0719,CC(=O)c1cccc(c1)NC(=O)N2CCOCC2,FMOPL000248a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.12,0.038,42.8,1.2,93.5,99.4,60.9,0.18798,0.21265,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0720,c1cc(c2c(c1)c3c([nH]2)CCCC3)C#N,FMOPL000140a,Mounted_Clear,success,P 2 2
2,34 41 110 90 90 90,1.25,0.028,52.9,2.1,99,98.7,88.9,0.19891,0.23269,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-
x0721,c1cc(ccc1N2CCN(CC2)C(=O)C3CC3)F,FMOPL000249a,Mounted_BadDispense,success,P 21 21
21,34 41 110 90 90 90,1.1,0.025,62.6,2.5,92.9,98.6,60.8,0.19215,0.21557,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0722,Cc1cccc1CNc2nnnn2C,FMOPL000143a,Mounted_Crystalline,success,P 2 2 2,34 41
110 90 90 90,1.05,0.059,35.9,3.3,83.4,99.4,14.3,0.19819,0.22099,None,None,P 21 21 21,1
- Analysis Pending, None

PARP14A-x0723,CCC(=O)Nc1ccc(cc1)S(=O)(=O)N,FMOPL000141a,Mounted_Crystalline,success,P 2
2 2,34 41 110 90 90 90,1.21,0.022,65.6,1.9,99.6,99,96.9,0.19032,0.2201,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0724,c1ccc2c(c1)[nH]c(n2)NC(=O)C3CCCC3,FMOPL000251a,Mounted_Clear,success,P 2
2 2,34 41 110 90 90 90,1.08,0.035,48.2,1.2,89.4,99,37.5,0.1992,0.22514,None,None,P 21 21
21,1 - Analysis Pending, None

PARP14A-x0725,c1c(c(=O)[nH]c(=O)[nH]1)N2CCCC2,FMOPL000665a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.05,0.045,52.7,2.8,85.2,99.3,15,0.19051,0.21085,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0726,Cc1cc(nol)C(=O)NCc2cccs2,FMOPL000394a,Mounted_Clear,success,P 2 2 2,34 41
110 90 90 90,1.11,0.021,67.9,1.4,93,99.4,56.2,0.18929,0.21488,None,None,P 21 21 21,1 -
Analysis Pending, None

PARP14A-
x0727,Cc1ccc(cc1)CC(=O)NC[C@@H]2CCCO2,FMOPL000530a,Mounted_BadDispense,success,P 21 21
21,33 41 110 90 90 90,1.24,0.031,45.5,1.1,99.8,99.8,99.5,0.17565,0.21144,None,None,P 21
21 21,1 - Analysis Pending, None

PARP14A-x0728, C1CCC (C1) C (=O) N2CCNC (=O) C2, FMOPL000699a, Mounted_Clear, success, P 2 2 2, 34
41 110 90 90 90, 1.09, 0.021, 67.2, 1.4, 86.9, 98.5, 31.6, 0.19563, 0.21944, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0729, C [NH+] 1CCC [C@H] (C1) OC (=O) c2cccc2, FMOPL000668a, Mounted_Clear, success, P 21
21 21, 34 41 110 90 90 90, 1.09, 0.027, 57.2, 2.6, 90.8, 98.5, 57, 0.19246, 0.21622, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0730, COC (=O) NCc1cc2cc (ccc2 [nH] 1) C1, FMOPL000405a, Mounted_Clear, success, P 2 2
2, 34 41 110 90 90 90, 1.07, 0.025, 74.6, 1.6, 82.4, 99.2, 18.6, 0.19292, 0.2165, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0731, CCn1c2cccc2nc1NC (=O) C, FMOPL000521a, Mounted_Clear, success, P 2 2 2, 34 41
111 90 90 90, 1.21, 0.044, 31.2, 1.7, 99.1, 99.3, 89, 0.18871, 0.22142, 0.20482, 0.23377, P 21 21
21, 3 - In Refinement, None

PARP14A-x0732, Cc1ccc (s1) C [NH2+] C [C@H] (C) O, FMOPL000693a, Mounted_Clear, success, P 2 2
2, 34 41 110 90 90 90, 1.09, 0.024, 66.9, 1.3, 92.3, 99.3, 46.1, 0.19271, 0.21658, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0733, COCC (=O) NCc1 [nH] c2cccc2n1, FMOPL000672a, Mounted_Clear, success, P 2 2 2, 34
41 110 90 90 90, 1.05, 0.027, 69.6, 1.3, 83.7, 99.3, 14.3, 0.18909, 0.21103, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0734, CCOC (=O) Nc1c (ccs1) C (=O) N, FMOPL000386a, Mounted_BadDispense, success, P 2 2
2, 34 41 110 90 90 90, 1.2, 0.045, 39.8, 2, 98.6, 99.1, 90, 0.18774, 0.21976, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0735, COc1ccc (cc1) CNC (=O) c2csnn2, FMOPL000527a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.23, 0.031, 46, 1.1, 99.4, 99.6, 99.1, 0.19131, 0.22906, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0736, c1ccc (cc1) CNC (=O) c2cccc (c2) F, FMOPL000727a, Mounted_BadDispense, success, P
21 21 21, 34 41 110 90 90
90, 1.17, 0.025, 57.1, 1.1, 97.5, 99.5, 84.5, 0.18611, 0.21536, None, None, P 21 21 21, 1 - Analysis
Pending, None

PARP14A-x0737, Cc1cccc2c1nc (s2) NC (=O) OC, FMOPL000395a, Mounted_Clear, success, P 21 21 21, 34
41 110 90 90 90, 1.23, 0.035, 39.3, 1.2, 95.5, 98.6, 85.4, 0.18982, 0.23159, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0738, c1cc (sc1) CCNC (=O) C2CCCC2, FMOPL000523a, Mounted_Clear, success, P 21 21
21, 34 41 110 90 90 90, 1.15, 0.033, 45.8, 1.1, 98, 99.7, 82.6, 0.20121, 0.23219, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0739, CCC (CC) C (=O) Nc1nccs1, FMOPL000695a, Mounted_Clear, success, P 21 21 21, 34 41
110 90 90 90, 1.11, 0.029, 54.5, 0.9, 94.8, 99.3, 64.4, 0.20402, 0.22781, None, None, P 21 21 21, 1
- Analysis Pending, None

PARP14A-
x0740, CC1 (C [C@H] (CCO1) [NH2+] Cc2ccc (cc2) O) C, FMOPL000676a, Mounted_BadDispense, success, P 2
2 2, 34 41 110 90 90 90, 1.05, 0.031, 61.3, 1.9, 84.6, 99.1, 16.1, 0.191, 0.21057, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-
x0741, CC [C@H] (c1cccc1) C (=O) Nc2ccon2, FMOPL000420a, Mounted_BadDispense, success, P 21 21
21, 34 41 110 90 90 90, 1.09, 0.043, 42, 2.5, 88.1, 99.6, 43.6, 0.19826, 0.22045, None, None, P 21 21
21, 1 - Analysis Pending, None

PARP14A-x0742, C [NH+] 1CCN (CC1) C (=O) c2ccc3cc [nH] c3c2, FMOPL000532a, Mounted_Clear, success, P
2 2 2, 34 41 110 90 90 90, 1.13, 0.025, 64.1, 1.5, 94.5, 99, 61.1, 0.19677, 0.22202, None, None, P 21
21 21, 1 - Analysis Pending, None

PARP14A-x0743, Cc1cc(c(c(c1)C)NC(=O)COC)C, FMOPL000710a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.07,0.035,51.8,2.6,89.7,98.5,45.2,0.19596,0.22036, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0744, c1cc(oc1)C(=O)N2CCN(CC2)C(=O)N, FMOPL000670a, Mounted_BadDispense, success, P
21 21 21,34 41 110 90 90
90,1.1,0.027,58.3,2.6,93.8,99.1,67.7,0.19247,0.21332, None, None, P 21 21 21,1 - Analysis
Pending, None

PARP14A-x0745, CCc1ccc(s1)C(=O)NCc2cnn(c2)C, FMOPL000421a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.039,51.5,2.2,76.2,98.6,13.5,0.18504,0.20714, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0746, CC(C)NC(=O)c1ccc(cc1)NC(=O)NC, FMOPL000525a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.08,0.031,58,2.6,89.1,97.7,50.2,0.20946,0.23146, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0747, CCCC(=O)Nc1cccnc1Cl, FMOPL000696a, Mounted_Clear, success, P 2 2 2,34 41 110
90 90 90,1.24,0.026,55.7,2.2,97.9,99.1,89.5,0.18915,0.21844, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0748, C1CCC2(CC1)OC[C@@H](O2)C[NH+]3CCCCC3, FMOPL000674a, Mounted_Clear, success, P
2 2 2,34 41 110 90 90 90,1.15,0.027,56,1.3,98.1,99.4,81.7,0.18936,0.2152, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0749, CCC(=O)Nc1nnc(s1)c2ccncc2, FMOPL000403a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.15,0.032,51.1,2.5,96.3,99.7,77.1,0.19226,0.21659, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-
x0750, C1C[C@H](CC=C1)C[NH+]2CCC(CC2)C(=O)N, FMOPL000333a, Mounted_Precipitate, success, P 2
2 2,34 41 110 90 90 90,1.09,0.025,61.3,1.2,89.7,98.8,43.2,0.19652,0.2194, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0751, CCC(CC)C(=O)Nc1cccc1O, FMOPL000706a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.05,0.039,55.6,2.4,83,99.4,15.2,0.18175,0.204, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0752, CC(=O)Nc1ccc2c(c1)nsn2, FMOPL000664a, Mounted_Clear, success, P 21 21 21,34 41
110 90 90 90,1.14,0.044,34.5,2.6,97,99.4,81.7,0.18467,0.20601, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0753, c1cc(cc(c1)Cl)C(=O)Nc2ccon2, FMOPL000399a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.17,0.035,39.4,1.1,98.6,99.8,88.6,0.19734,0.22749, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0754, COc1ccc(cc1)C[NH+]2CCC(CC2)O, FMOPL000353a, Mounted_Clear, success, P 2 2
2,34 41 110 90 90 90,1.05,0.042,47.8,2.3,84.4,99.3,15,0.19337,0.2157, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0755, COc1cccc1OC(=O)C2CCCC2, FMOPL000721a, Mounted_Clear, success, P 2 2 2,34 41
110 90 90 90,1.13,0.024,62.6,1.4,96,99.2,71.8,0.19085,0.21542, None, None, P 21 21 21,1 -
Analysis Pending, None

PARP14A-x0756, Cc1cccc(c1)OCC(=O)Nn2cnc2, FMOPL000680a, Mounted_Clear, success, P 21 21
21,34 41 110 90 90 90,1.12,0.032,48.4,2.5,88.9,98.9,52.5,0.20234,0.22732, None, None, P 21
21 21,1 - Analysis Pending, None

PARP14A-x0757, Cc1cc(nc(n1)Nc2cccc(c2)O)C, FMOPL000341a, Mounted_Clear, success, P 2 2 2,34
41 110 90 90 90,1.15,0.019,76.2,1.6,97.1,99.2,75.4,0.18998,0.21585, None, None, P 21 21
21,1 - Analysis Pending, None

PARP14A-x0758, CSc1nnc (s1)NC(=O)c2ccco2, FMOPL000708a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.028, 56.2, 2.6, 84.6, 98.9, 41.1, 0.19709, 0.22212, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0759, CN(C)c1nc(nc(n1)SC)N(C)C#N, FMOPL000667a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.09, 0.029, 55.6, 2.5, 92, 99, 55.3, 0.18953, 0.21007, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0760, COC(=O)c1ccc(cc1)S(=O)(=O)N, FMOPL000316a, Mounted_BadDispense, success, P 2 2 2, 34 41 110 90 90 90, 1.05, 0.046, 42.8, 3.1, 75.1, 99.1, 11.7, 0.18846, 0.20908, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0761, CCCC(=O)Nc1nnc(s1)SC, FMOPL000697a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.13, 0.031, 48.8, 1, 96, 99.6, 69.6, 0.20043, 0.23299, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0762, C[NH+]1CCC[C@H](C1)OC(=O)c2cccc(c2)F, FMOPL000678a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.13, 0.03, 54.6, 1.3, 96.7, 99.3, 72, 0.1965, 0.21942, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0763, c1cc2c(cc1CNC(=O)[C@H]3CCCO3)OCO2, FMOPL000436a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90, 1.1, 0.025, 64.5, 2.6, 91.4, 99.2, 56.1, 0.18136, 0.20436, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0764, CCOC(=O)Nc1ccc2c(c1)c(=O)n(cn2)C, FMOPL000373a, Mounted_Clear, success, P 21 21 21, 32 41 110 90 90 90, 1.47, 0.052, 27.8, 1.2, 99.6, 99.8, 99.4, 0.20418, 0.26184, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0765, Cc1ccc(cc1O)NC(=O)c2ccco2, FMOPL000724a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.06, 0.036, 50.8, 1.9, 73, 98.8, 11.6, 0.19581, 0.22179, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0766, CN(C)c1ccc(cc1)CNn2cncn2, BDILV000151b, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.14, 0.024, 64.1, 2.8, 95.4, 99.5, 72.5, 0.1847, 0.20936, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0767, C1CCC(CC1)CCC(=O)NN2CCOCC2, FMOPL000414a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.15, 0.028, 53.6, 2.3, 91.1, 99.3, 61.8, 0.19571, 0.2262, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0768, Cc1c(nc(=O)[nH]n1)Nc2ccc(cc2)N(C)C, FMOPL000371a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90, 1.09, 0.031, 56.9, 2.6, 88.2, 98.5, 43.3, 0.20044, 0.22174, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0769, CN(c1ccc(cc1)C(=O)N)S(=O)(=O)C, FMOPL000142a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.035, 53.8, 1.7, 80.9, 98.9, 14.7, 0.20099, 0.2218, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0770, CC(C)Sc1nnc(s1)NC(=O)C, FMOPL000027a, Mounted_Clear, success, P 2 2 2, 34 41 110 90 90 90, 1.09, 0.027, 68.5, 1.3, 89.3, 99, 45.1, 0.20147, 0.22795, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0771, CC(C)c1ccc(cc1)C(=O)Nc2ccccc2, FMOPL000252a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.14, 0.023, 69.1, 2.7, 96, 99.7, 75.2, 0.1863, 0.20929, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0772, C[NH+](C)Cc1ccc(cc1)C#N, FMOPL000137a, Mounted_Clear, success, P 21 21 21, 34 41 110 90 90 90, 1.05, 0.035, 52.7, 2.7, 81.7, 99, 15.2, 0.18459, 0.20306, None, None, P 21 21 21, 1 - Analysis Pending, None

PARP14A-x0773,CC(C)[NH+]1CCN(CC1)c2ccc(cc2)O,FMOPL000145a,Mounted_BadDispense,success,P
2 2 2,33 41 110 90 90 90,1.62,0.059,30.1,0.8,96.9,97.5,71.8,0.22984,0.3009,None,None,P
21 21 21,1 - Analysis Pending,None

PARP14A-x0774,c1cc(cc(c1)F)C[NH+]2CCOCC2,FMOPL000028a,Mounted_Precipitate,Failed -
unknown,,,,,,,,,,,,,#NAME?,

PARP14A-
x0775,CC(C)C(=O)Nc1nnc(s1)[C@@H]2CCCO2,FMOPL000144a,Mounted_BadDispense,success,P 21 21
21,34 41 110 90 90 90,1.08,0.028,52.7,2.4,88.9,99.8,47.3,0.17319,0.1952,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0776,c1cc2c(cc1c3cc[nH]n3)OCO2,FMOPL000029a,Mounted_Clear,Failed -
unknown,,,,,,,,,,,,,#NAME?,

PARP14A-x0777,CN(CCc1ccccn1)C(=O)c2cccc2,FMOPL000254a,Mounted_Clear,success,P 21 21
21,34 41 110 90 90 90,1.13,0.028,57.4,2.6,97.3,99,84.7,0.19291,0.21573,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0778,CCOc1cccc1C[NH+]2CCC(CC2)O,FMOPL000042a,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.05,0.035,57.9,2.3,78.8,98.8,8.9,0.1874,0.21338,None,None,P 21 21 21,1
- Analysis Pending,None

PARP14A-x0779,CCN(CC)S(=O)(=O)c1ccc(cc1)C,FMOMB000142b,Mounted_Clear,success,P 2 2 2,34
41 110 90 90 90,1.05,0.069,31.5,8.4,79.8,98.7,14.8,0.18399,0.20531,None,None,P 21 21
21,1 - Analysis Pending,None

PARP14A-x0780,Cc1c(ccol)C(=O)Nc2cc(on2)C(C)(C)C,FMOPL000255a,Mounted_Clear,success,P 21
21 21,34 41 110 90 90 90,1.1,0.028,60.5,2.5,93.1,99.5,63.1,0.18248,0.20973,None,None,P
21 21 21,1 - Analysis Pending,None

PARP14A-x0781,COc1ccc(cc1)[C@@H](C(=O)[O-])[NH3+],FMOPL000076a,Mounted_Clear,success,P
21 21 21,33 41 110 90 90
90,1.1,0.026,62.1,2.7,92.4,99.4,60.1,0.16606,0.18686,None,None,P 21 21 21,1 - Analysis
Pending,None