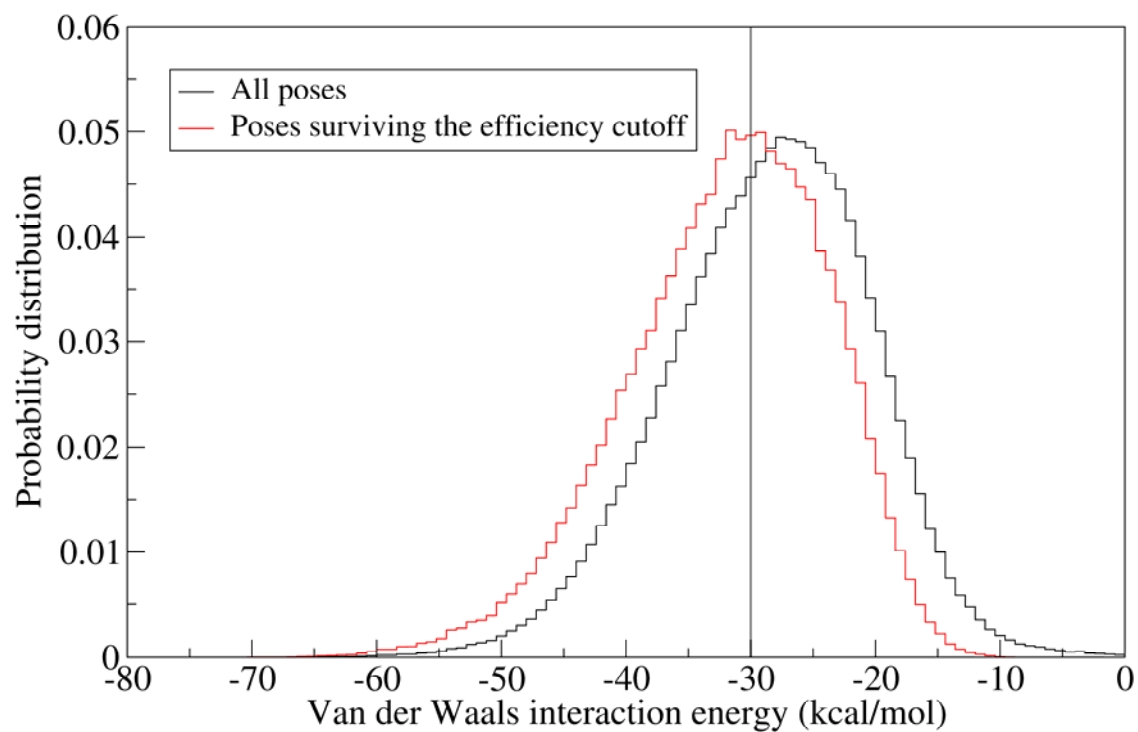


Supplemental Table S1. Identification codes and source of 29 putative inhibitors of human cathepsin B. The ZINC-codes are those of the database 2005 [Irwin, J. J., and Shoichet, B. K. (2005) J. Chem. Inf. Model. 45, 177-182]. [2-(2,4-dioxothiazolidin-3-yl) ethylcarbamoylmethyl 2-(furan-2-carbonylamino) acetate (DOFA) is shown in boldface.

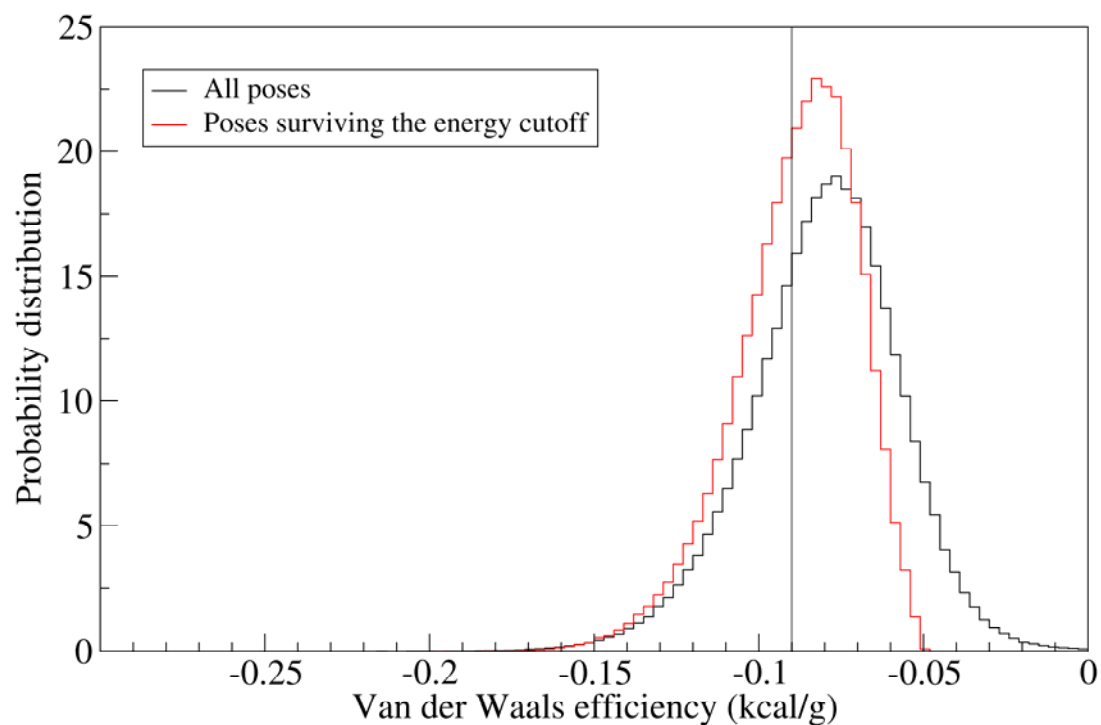
Source	ZINC 2005-codes
ChemDiv (San Diego, USA)	33816, 978038, 2487954, 2560859
Ambinter (Paris, France)	1271923, 1414169
ChemBridge (San Diego, USA)	958753, 2904166, 2973678, 2990182
Pharmerks (Moscow, Russia)	989395, 1755678, 1837733, 1871954
Life Chemicals (Burlington, Canada)	1797383
Enamine (Kiev, Ukraine)	2616818 , 2667966, 3247330, 3333255, 3340535, 3417832, 3439551, 3451184
IBScreen (Moscow, Russia)	1419203, 2128374, 2131752
National Cancer Institute, U.S.A.	1581881, 1628238, 1682930

Van der Waals interaction energies distribution



Supplemental Figure S1. **Van der Waals interaction energies distribution.** The histogram represents the distribution of van der Waals interaction energies before and after the efficiency cutoff. The vertical line marks the cutoff on van der Waals energy.

Van der Waals interaction energy efficiencies distribution



Supplemental Figure S2. **Van der Waals interaction energy efficiencies distribution.**

The histogram represents the distribution of van der Waals interaction energy efficiencies before and after the energy cutoff. The vertical line represents the cutoff of van der Waals efficiency.