S1 Supporting Information. Per-residue decomposition of the average electrostatic interaction energies $\langle V^{Ele} \rangle$ **(Figure A)**. Per-residue decomposition of the average Van der Waals interaction energies $\langle V^{VdW} \rangle$ **(Figure B)**. Structures and IC_{50} values from literature for the data set of compounds **(Table A)**. Reacting chemical groups in (quasi-)irreversible CYP inhibitors **(Table B)**. Overview of the average electrostatic $\langle V^{Ele} \rangle$ and van der Waals $\langle V^{VdW} \rangle$ interaction energies **(Table C)**.

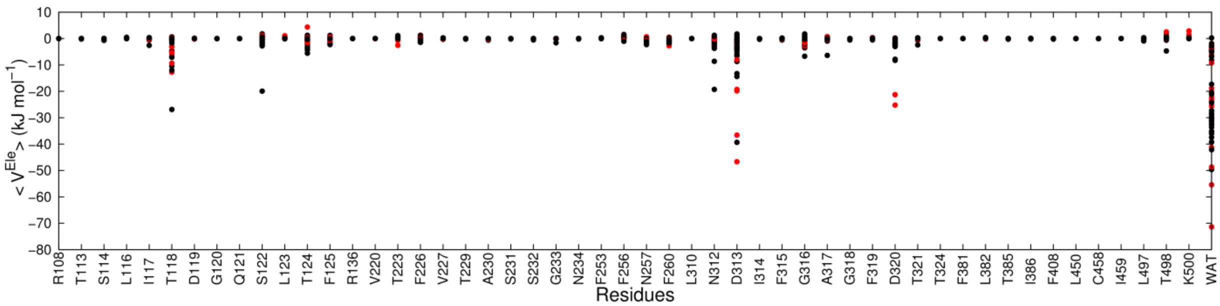


Figure A. Per-residue decomposition of the average electrostatic interaction energy <V^{Ele}>. Interaction energies are reported between CYP 1A2 active site residues and training (black) and test set (red) compounds during the multiple MD simulations of the CYP 1A2-ligand complex performed per compound.

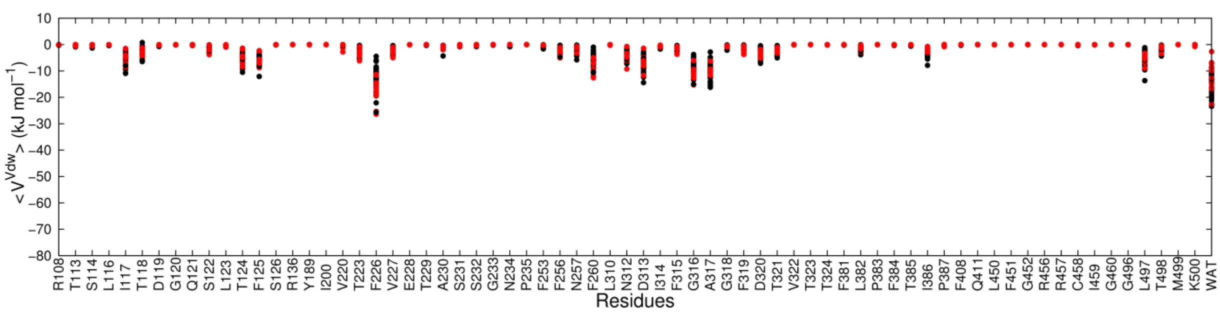
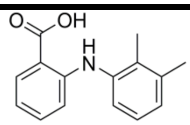
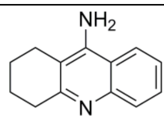
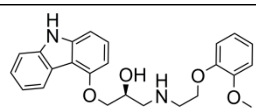
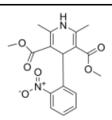
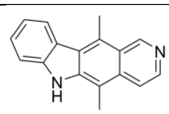
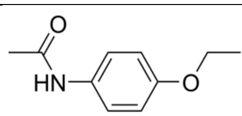
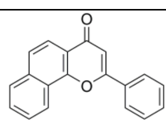
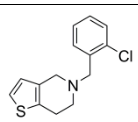
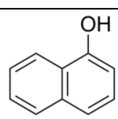
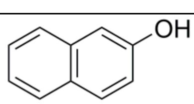
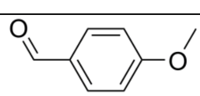
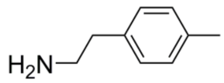
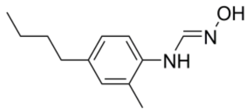
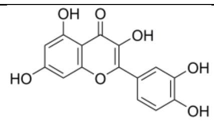
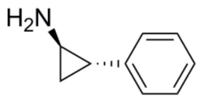
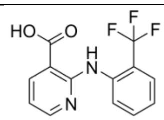
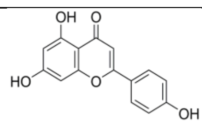
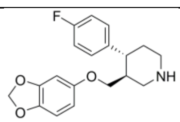
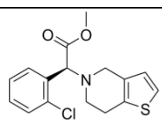
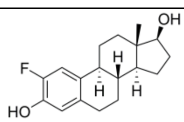
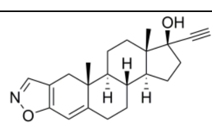
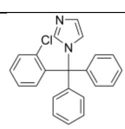
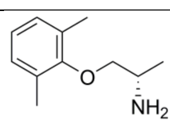
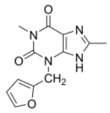
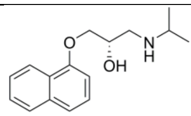
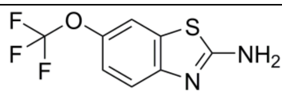
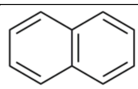
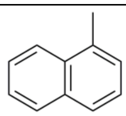
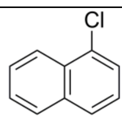
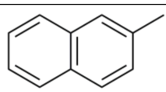
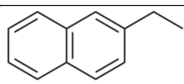
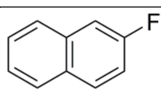
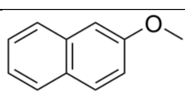
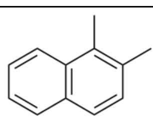
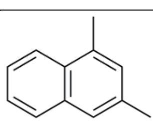
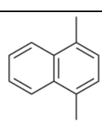


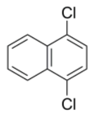
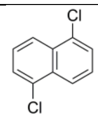
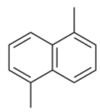
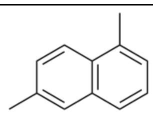
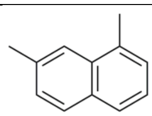
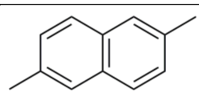
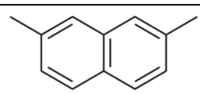
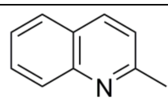
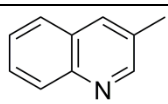
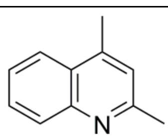
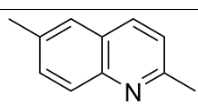
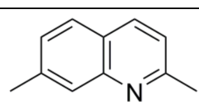
Figure B. Per-residue decomposition of the average van der Waals interaction energy <V^{VdW}>. Interaction energies are reported between CYP 1A2 active site residues and training (black) and test set (red) compounds during the multiple MD simulations of the CYP 1A2-ligand complex performed per compound.

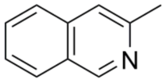
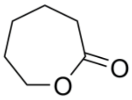
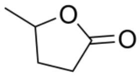
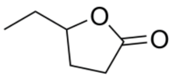
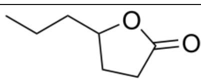
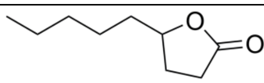
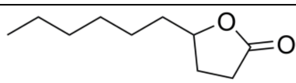
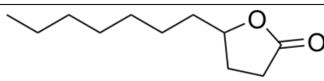
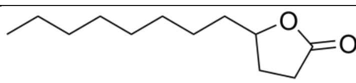
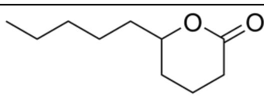
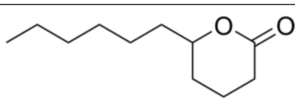
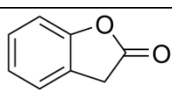
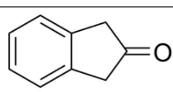
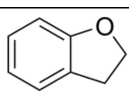
Table A. Structures and IC_{50} values from literature for the data set of compounds. Compounds are classified into LIE model training (Train) and test (Test) set. Inhibitors that are predicted to not be competitive are also reported (NC).

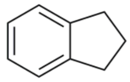
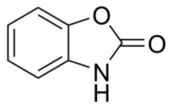
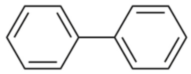
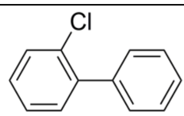
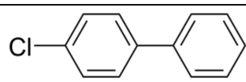
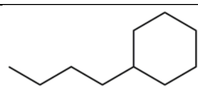
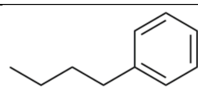
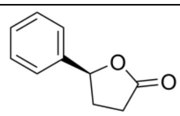
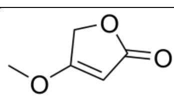
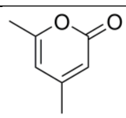
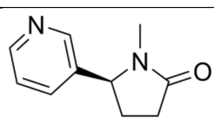
ID	Structure	Molecule	IC_{50} (µM)	Source	Classification
1		Mefenamic Acid	13.98	1	Train
2		Tacrine	5.20	1	Train
3		Carvedilol	5.10	1	NC
4		Nifedipine	5.74	1	Train
5		Ellipticine	0.11	2	NC
6		Phenacetin	28.00	2	Train
7		alpha-Naphthoflavone	0.08	2	Train
8		Ticlopidine	22.43	2	NC
9		1-naphthol	3.2	3	Test
10		2-naphthol	17	3	Test
11		p-methoxybenzaldehyde	270	3	Test

12		p-tolylethylamine	14	3	Test
13		HET-0016	1.09	1	Train
14		Quercetin	5.52	1	Test
15		Tranylcypromine	10.42	1	NC
16		Niflumic Acid	11.59	1	Train
17		Naringenin	12.35	1	Test
18		Paroxetine	23.46	1	NC
19		Clopidogrel	24.15	1	NC
20		2-Fluoroestradiol	26.75	1	Test
21		Danazol	45.32	1	NC
22		Clotrimazole	5.83	1	NC
23		Mexiletine	1.84	2	Train

24		Furafylline	1.50	2	NC
25		Propranolol	3.84	2	Train
26		Riluzole	15.8	2	NC
27		Naphthalene	700	3	Train
28		1-Methylnaphthalene	110	3	Train
29		1-Chloronaphthalene	50	3	Test
30		2-Methylnaphthalene	120	3	Train
31		2-Ethylnaphthalene	19	3	Test
32		2-Fluoronaphthalene	49	3	Train
33		2-Methoxynaphthalene	13	3	Test
34		1,2-Dimethylnaphthalene	5.5	3	Test
35		1,3-Dimethylnaphthalene	7.9	3	Train
36		1,4-Dimethylnaphthalene	3.6	3	Train

37		1,4-Dichloronaphthalene	2.3	3	Test
38		1,5-Dichloronaphthalene	14	3	Train
39		1,5-Dimethylnaphthalene	42	3	Test
40		1,6-Dimethylnaphthalene	25	3	Test
41		1,7-Dimethylnaphthalene	7.5	3	Test
42		2,6-Dimethylnaphthalene	52	3	Train
43		2,7-Dimethylnaphthalene	65	3	Test
44		Quinaldine	40	3	NC
45		3-Methylquinoline	13	3	NC
46		2-4-Dimethylquinoline	2.4	3	NC
47		2,6-Dimethylquinoline	3.3	3	NC
48		2,7-Dimethylquinoline	4.4	3	NC

49		3-Methylisoquinoline	21	3	NC
50		ε-Caprolactone	40,000	3	Train
51		γ-Valerolactone	15,000	3	Train
52		γ-Caprolactone	9,900	3	Train
53		γ-Heptalactone	4,500.	3	Train
54		γ-Nonanoiclactone	310	3	Train
55		γ-Decanolactone	230	3	Train
56		γ-Undecanoiclactone	72	3	Train
57		γ-Dodecanolactone	58	3	Test
58		δ-Decanolactone	230	3	Train
59		δ-Undecanolactone	72	3	Test
60		2-Coumarone	260	3	Train
61		2-Indanone	80	3	Train
62		2,3-Dihydrobenzofuran	1,200	3	Train

63		Indan	550	3	Test
64		2-Benzoxazolinone	370	3	Train
65		Biphenyl	160	3	Train
66		2-Chlorobiphenyl	230	3	Test
67		4-Chlorobiphenyl	49	3	Train
68		Butylcyclohexane	55	3	Train
69		Butylbenzene	3,700	3	Test
70		γ-Phenyl-γ-butyrolactone	2,300	3	Train
71		4-Methoxyfuran-2-(5H)-one	40,000	3	Test
72		4,6-Dimethyl-α-pyron	4,500	3	Train
73		Cotinine	5,400	3	Train

Source 1: Bayer HealthCare databases for CYP inhibition, made available within *eTOX* consortium. Source 2: Cohen, L.; Remley, M.; Raunig, D.; Vaz, A. In Vitro Drug Interactions of Cytochrome P450: An Evaluation of Fluorogenic to Conventional Substrates. Drug Metab. Dispos. 2003, 31, 1005–1015. Source 3: Korhonen, L. E.; Rahnasto, M.; Mähönen, N. J.; Wittekindt, C.; Poso, A.; Juvonen, R. O.; Raunio, H. Predictive Three-dimensional Quantitative Structure-activity Relationship of Cytochrome P450 1A2 Inhibitors. J. Med. Chem. 2005, 48, 3808–3815.

Table B. Reacting chemical groups in (quasi-)irreversible CYP inhibitors.

Chemical Group	Mechanism of inhibition*
Aromatic Nitrogens	Quasi-irreversible inhibition
Isothiocyanates	Mechanism-based inhibition
Thioureas	Mechanism-based inhibition
Thiophenes	Mechanism-based inhibition
Thiols	Mechanism-based inhibition
Thiocyanate	Mechanism-based inhibition
Clorinated groups	Mechanism-based inhibition
Alkenes/Alkynes	Mechanism-based inhibition
Tertiary amines in heterocyclic rings	Mechanism-based inhibition
Furanocumarines	Mechanism-based inhibition
Furanopyridins	Mechanism-based inhibition
Methylene dioxycompounds	Mechanism-based inhibition
Amines	Mechanism-based inhibition
Hydrazines	Mechanism-based inhibition
Dihydropyridines	Mechanism-based inhibition
Dyhydroquinolines	Mechanism-based inhibition
Aldehydes	Mechanism-based inhibition

*From: Correia, M. A., Ortiz de Montellano P. R. Inhibition of Cytochrome P450 Enzymes. In Cytochrome P450: Structure, Mechanism, and Biochemistry; 3e; Ortiz de Montellano, P. R., Ed; Kluwer Academic / Plenum Publishers, New York, 2005.

Table C. Overview of average electrostatic $\langle V^{Ele} \rangle$, and van der Waals $\langle V^{VdW} \rangle$ interaction energies. The energies and their standard deviations are obtained from MD for each ligand, simulated in solvent and in all the orientations obtained from docking and clustering. Relative weights W_i of the energy for each simulation contributing to the LIE model (maximum 6 poses, α=0.587, β=0.267) are also reported.

ID	Solvent		Protein-bound			
	$\langle V^{Ele} \rangle$	$\langle V^{VdW} \rangle$	Pose	$\langle V^{Ele} \rangle$	$\langle V^{VdW} \rangle$	W_i
1	-110.1 ± 21.4	-77.9 ± 11.2	1	-71.6 ± 11.5	-152.6 ± 10.0	0.32
			2	-53.6 ± 17.8	-139.0 ± 11.7	0.00
			3	-91.9 ± 18.3	-137.7 ± 11.2	0.09
			4	-50.1 ± 11.1	-146.6 ± 9.6	0.01
			5	-80.8 ± 10.8	-150.9 ± 9.7	0.58
2	-73.8 ± 18.1	-72.0 ± 10.2	1	-46.1 ± 14.8	-134.0 ± 9.8	0.15
			2	-48.5 ± 14.6	-130.8 ± 9.4	0.09
			3	-39.5 ± 14.0	-137.1 ± 9.2	0.16
			4	-48.2 ± 12.6	-133.1 ± 8.8	0.15
			5	-42.0 ± 11.7	-139.0 ± 9.1	0.32
			6	-36.0 ± 12.6	-137.6 ± 9.3	0.12
4	-129.4 ± 20.2	-101.1 ± 12.8	1	-83.5 ± 13.5	-169.5 ± 12.2	0.13
			2	-81.9 ± 18.9	-170.4 ± 11.5	0.13
			3	-73.3 ± 20.3	-165.0 ± 13.1	
			4	-61.6 ± 15.2	-183.5 ± 11.9	0.33
			5	-83.9 ± 19.1	-170.2 ± 12.2	0.16
			6	-69.1 ± 13.5	-167.9 ± 11.0	0.02
			7	-68.1 ± 15.6	-179.1 ± 12.6	0.24
6	-92.2 ± 16.7	-65.8 ± 10.0	1	-62.7 ± 11.2	-117.7 ± 9.4	0.12
			2	-70.9 ± 11.3	-116.4 ± 9.8	0.22
			3	-45.5 ± 11.5	-126.3 ± 9.2	0.15
			4	-54.0 ± 14.2	-118.9 ± 8.8	0.06
			5	-58.8 ± 12.9	-119.6 ± 9.9	0.13
			6	-56.2 ± 13.6	-124.7 ± 9.5	0.32
7	-63.3 ± 14.5	-96.8 ± 9.7	1	-21.7 ± 10.5	-183.2 ± 8.7	0.22
			2	-44.6 ± 11.8	-159.1 ± 9.7	0.01
			3	-43.7 ± 9.1	-167.6 ± 9.6	0.06
			4	-32.6 ± 10.7	-153.0 ± 9.9	0.00
			5	-39.6 ± 9.2	-179.9 ± 8.7	0.71
13	-101.7 ± 29.8	-72.7 ± 11.8	1	-30.8 ± 13.5	-150.5 ± 9.3	0.01

			2	-59.0 ± 19.2	-132.2 ± 12.1	0.00
			3	-83.4 ± 18.5	-133.4 ± 11.4	0.07
			4	-37.9 ± 16.9	-145.8 ± 10.8	0.01
			5	-31.2 ± 8.6	-149.3 ± 8.8	0.01
			6	-120.6 ± 19.8	-127.6 ± 12.7	0.90
16	-116.9 ± 31.3	-74.7 ± 13.5	1	-77.4 ± 18.4	-148.7 ± 11.9	0.17
			2	-65.3 ± 21.0	-149.9 ± 11.4	0.06
			3	-68.1 ± 23.6	-151.4 ± 11.8	0.12
			4	-77.9 ± 19.5	-149.5 ± 11.5	0.22
			5	-68.8 ± 15.0	-154.5 ± 10.3	0.27
			6	-79.1 ± 22.0	-147.8 ± 12.2	0.16
23	-63.8 ± 14.5	-65.5 ± 9.3	1	-41.7 ± 11.8	-116.1 ± 10.1	0.07
			2	-26.9 ± 17.0	-124.7 ± 8.3	0.10
			3	-24.7 ± 13.0	-127.4 ± 8.5	0.16
			4	-36.7 ± 10.7	-125.8 ± 8.0	0.38
			5	-41.4 ± 10.4	-122.4 ± 8.6	0.29
25	-94.2 ± 22.9	-92.2 ± 11.8	1	-39.3 ± 11.1	-166.5 ± 10.1	0.07
			2	-32.2 ± 11.0	-176.9 ± 8.7	0.39
			3	-47.3 ± 18.4	-167.7 ± 9.8	0.23
			4	-51.7 ± 12.9	-164.4 ± 10.0	0.17
			5	-52.0 ± 22.5	-163.2 ± 11.5	0.13
27	-22.7 ± 8.0	-53.2 ± 6.2	1	-11.3 ± 3.9	-90.4 ± 6.1	0.52
			2	-6.9 ± 4.4	-88.5 ± 6.3	0.21
			3	-3.6 ± 4.9	-90.2 ± 6.6	0.22
			4	-12.9 ± 7.0	-79.0 ± 7.1	0.04
28	-21.8 ± 7.5	-59.4 ± 6.1	1	-8.8 ± 4.2	-101.2 ± 6.4	0.17
			2	-6.3 ± 3.5	-101.2 ± 6.1	0.13
			3	-8.6 ± 4.0	-103.1 ± 6.2	0.26
			4	-8.6 ± 3.9	-105.5 ± 6.3	0.45
30	-22.4 ± 8.0	-59.9 ± 6.5	1	-7.7 ± 4.2	-100.6 ± 7.0	0.16
			2	-11.0 ± 5.1	-96.3 ± 6.9	0.08
			3	-6.8 ± 4.5	-103.2 ± 7.0	0.26
			4	-7.1 ± 3.5	-104.4 ± 6.0	0.35
			5	-6.5 ± 4.7	-101.1 ± 6.9	0.15
32	-19.4 ± 7.4	-55.0 ± 6.2	1	-10.1 ± 4.9	-95.2 ± 6.9	0.29
			2	-10.2 ± 4.3	-91.4 ± 6.9	0.12
			3	-11.5 ± 5.2	-95.4 ± 6.7	0.36
			4	-12.5 ± 4.9	-93.2 ± 6.9	0.23
35	-21.6 ± 7.8	-65.8 ± 6.7	1	-7.0 ± 3.9	-115.7 ± 6.0	0.34
			2	-4.4 ± 3.3	-111.6 ± 7.0	0.10
			3	-14.1 ± 5.6	-113.8 ± 6.1	0.48
			4	-8.9 ± 5.5	-108.5 ± 6.4	0.08
36	-21.4 ± 7.5	-65.4 ± 6.6	1	-7.3 ± 3.1	-115.6 ± 6.5	0.29
			2	-7.4 ± 4.9	-112.2 ± 6.8	0.13

			3	-7.0 ± 4.2	-113.2 ± 6.3	0.16
			4	-7.7 ± 3.8	-117.1 ± 6.5	0.43
38	-12.2 ± 5.5	-67.0 ± 6.3	1	-9.2 ± 4.6	-110.8 ± 6.5	0.13
			2	-3.9 ± 3.4	-117.3 ± 5.8	0.34
			3	-5.9 ± 3.7	-111.3 ± 6.6	0.10
			4	-10.3 ± 3.4	-115.4 ± 6.5	0.43
42	-21.8 ± 7.7	-66.1 ± 6.6	1	-9.8 ± 4.6	-113.6 ± 6.0	0.28
			2	-9.4 ± 3.3	-110.5 ± 7.0	0.13
			3	-5.0 ± 3.2	-104.3 ± 6.1	0.02
			4	-7.5 ± 3.7	-113.4 ± 6.6	0.21
			5	-5.0 ± 3.1	-117.0 ± 6.1	0.37
50	-58.1 ± 13.4	-45.2 ± 7.5	1	-42.6 ± 14.5	-80.3 ± 7.7	0.28
			2	-41.8 ± 13.1	-80.6 ± 7.5	0.27
			3	-41.3 ± 10.8	-81.0 ± 8.2	0.29
			4	-42.6 ± 13.0	-77.8 ± 9.0	0.16
51	-54.4 ± 13.0	-39.9 ± 7.4	1	-44.4 ± 13.2	-71.2 ± 7.8	0.22
			2	-47.7 ± 11.7	-72.3 ± 7.8	0.40
			3	-37.4 ± 15.4	-72.7 ± 8.1	0.15
			4	-34.8 ± 8.3	-72.9 ± 7.4	0.12
			5	-33.2 ± 13.2	-73.5 ± 7.1	0.11
52	-54.7 ± 13.6	-46.5 ± 7.4	1	-41.9 ± 13.5	-83.7 ± 8.5	0.50
			2	-35.5 ± 10.0	-84.2 ± 7.3	0.28
			3	-37.6 ± 12.1	-78.3 ± 7.9	0.09
			4	-32.4 ± 15.1	-82.2 ± 8.2	0.13
53	-54.3 ± 13.0	-52.8 ± 8.1	1	-36.8 ± 11.4	-94.2 ± 8.2	0.19
			2	-57.7 ± 14.2	-88.1 ± 8.1	0.41
			3	-32.2 ± 9.6	-95.9 ± 7.8	0.17
			4	-23.9 ± 11.4	-96.2 ± 8.4	0.07
			5	-42.5 ± 11.7	-90.9 ± 8.7	0.16
54	-54.0 ± 13.0	-65.9 ± 8.7	1	-41.7 ± 12.1	-115.9 ± 8.3	0.25
			2	-27.7 ± 14.6	-121.1 ± 8.0	0.19
			3	-42.6 ± 12.3	-112.1 ± 8.9	0.11
			4	-45.1 ± 11.5	-112.5 ± 11.5	0.16
			5	-36.3 ± 10.5	-108.9 ± 9.8	0.03
			6	-42.1 ± 12.2	-116.1 ± 8.7	0.27
			7	-36.5 ± 12.5	-105.3 ± 8.6	
55	-53.3 ± 12.9	-72.5 ± 8.5	1	-32.7 ± 12.5	-122.9 ± 9.1	0.09
			2	-38.2 ± 11.6	-123.4 ± 9.0	0.18
			3	-35.6 ± 10.3	-124.9 ± 8.8	0.20
			4	-44.1 ± 10.8	-123.4 ± 9.6	0.34
			5	-28.7 ± 13.4	-124.2 ± 9.7	0.08
			6	-27.1 ± 16.9	-126.4 ± 8.6	0.11
56	-52.6 ± 13.0	-79.8 ± 9.0	1	-35.3 ± 10.9	-131.4 ± 9.0	0.06
			2	-33.8 ± 7.8	-133.8 ± 8.7	0.08

			3	-35.7 ± 12.2	-136.4 ± 8.8	0.19
			4	-39.4 ± 11.7	-139.6 ± 9.4	0.60
			5	-33.1 ± 10.3	-133.6 ± 9.3	0.07
58	-57.5 ± 13.6	-70.5 ± 8.7	1	-48.4 ± 11.4	-119.7 ± 8.7	0.25
			2	-42.7 ± 14.1	-120.2 ± 9.4	0.15
			3	-42.5 ± 13.7	-105.7 ± 9.3	0.01
			4	-38.2 ± 10.7	-126.1 ± 8.9	0.38
			5	-35.5 ± 11.6	-124.1 ± 9.1	0.18
			6	-43.5 ± 12.5	-114.0 ± 10.7	0.04
60	-46.5 ± 12.8	-50.9 ± 7.7	1	-41.1 ± 10.7	-90.1 ± 7.6	0.27
			2	-11.3 ± 9.7	-95.5 ± 7.4	0.04
			3	-33.8 ± 9.4	-91.5 ± 7.2	0.17
			4	-35.4 ± 9.4	-94.1 ± 7.0	0.38
			5	-33.6 ± 10.9	-90.6 ± 7.8	0.14
61	-45.7 ± 12.1	-51.5 ± 7.4	1	-13.6 ± 14.8	-94.3 ± 7.0	0.10
			2	-25.7 ± 9.0	-92.2 ± 7.3	0.22
			3	-30.4 ± 9.7	-89.7 ± 7.3	0.20
			4	-33.2 ± 8.8	-89.7 ± 7.5	0.28
			5	-32.8 ± 9.9	-88.5 ± 7.4	0.20
62	-25.3 ± 8.9	-50.4 ± 6.4	1	-10.2 ± 7.3	-85.6 ± 6.3	0.15
			2	-12.9 ± 6.6	-87.4 ± 6.3	0.30
			3	-13.4 ± 6.8	-87.7 ± 6.9	0.34
			4	-13.0 ± 6.6	-86.1 ± 6.4	0.22
64	-64.0 ± 14.6	-48.0 ± 8.1	1	-61.7 ± 11.8	-86.2 ± 8.9	0.21
			2	-59.3 ± 12.5	-82.4 ± 8.3	0.07
			3	-48.8 ± 12.8	-88.4 ± 8.7	0.09
			4	-67.7 ± 17.8	-83.7 ± 9.0	0.22
			5	-70.1 ± 14.4	-85.5 ± 8.7	0.43
65	-27.4 ± 9.4	-62.5 ± 7.0	1	-10.7 ± 4.5	-108.7 ± 6.0	0.16
			2	-6.9 ± 4.8	-107.3 ± 6.4	0.08
			3	-11.8 ± 4.8	-109.5 ± 6.3	0.22
			4	-12.5 ± 4.6	-108.1 ± 6.2	0.17
			5	-7.9 ± 5.4	-112.7 ± 6.8	0.31
			6	-9.1 ± 5.5	-105.9 ± 6.3	0.07
67	-22.9 ± 8.5	-69.9 ± 7.0	1	-5.4 ± 4.9	-123.1 ± 7.7	0.16
			2	-7.4 ± 3.8	-122.4 ± 6.3	0.16
			3	-10.1 ± 3.9	-121.2 ± 6.7	0.17
			4	-6.1 ± 5.0	-123.8 ± 7.5	0.21
			5	-12.9 ± 5.5	-119.0 ± 7.0	0.14
			6	-10.7 ± 4.6	-120.2 ± 6.7	0.15
68	2.7 ± 1.1	-68.3 ± 6.2	1	0.0 ± 0.9	-118.3 ± 7.9	0.52
			2	0.9 ± 0.8	-103.9 ± 8.4	0.02
			3	0.2 ± 0.9	-114.7 ± 7.1	0.22
			4	0.7 ± 0.8	-105.8 ± 7.0	0.03

			5	0.5 ± 0.8	-112.1 ± 7.1	0.12
			6	0.4 ± 1.0	-111.3 ± 9.3	0.10
70	-68.0 ± 14.7	-60.2 ± 8.2	1	-35.0 ± 12.6	-105.8 ± 8.8	0.05
			2	-48.0 ± 16.3	-106.7 ± 8.4	0.23
			3	-47.3 ± 13.3	-108.5 ± 8.8	0.32
			4	-46.0 ± 12.7	-110.0 ± 7.8	0.40
72	-52.9 ± 12.7	-47.4 ± 7.7	1	-45.8 ± 13.0	-84.2 ± 8.6	0.27
			2	-50.3 ± 11.8	-83.3 ± 8.3	0.36
			3	-37.3 ± 12.7	-85.1 ± 7.7	0.14
			4	-39.3 ± 10.0	-86.4 ± 7.1	0.23
73	-95.2 ± 17.6	-59.2 ± 10.0	1	-63.6 ± 17.1	-108.1 ± 10.2	0.11
			2	-55.1 ± 13.2	-118.8 ± 10.1	0.55
			3	-58.1 ± 16.6	-113.0 ± 10.5	0.20
			4	-48.5 ± 17.6	-111.2 ± 9.0	0.05
			5	-37.2 ± 19.1	-115.4 ± 11.5	0.04
			6	-45.8 ± 22.7	-113.2 ± 10.6	0.06
Test set compounds						
9	-57.0 ± 14.6	-50.2 ± 8.7	1	-49.1 ± 13.4	-92.5 ± 9.5	0.39
			2	-40.1 ± 10.1	-94.3 ± 8.0	0.23
			3	-51.5 ± 11.2	-87.4 ± 8.9	0.15
			4	-48.7 ± 13.3	-90.3 ± 9.2	0.22
10	-65.0 ± 15.4	-48.9 ± 9.2	1	-45.3 ± 13.2	-92.2 ± 9.2	0.10
			2	-49.9 ± 13.8	-90.8 ± 9.0	0.12
			3	-54.2 ± 14.7	-89.2 ± 9.1	0.13
			4	-56.4 ± 10.1	-94.4 ± 8.4	0.56
			5	-57.9 ± 13.5	-86.3 ± 9.7	0.10
11	-54.7 ± 13.4	-51.2 ± 7.8	1	-22.5 ± 8.4	-94.3 ± 6.5	0.07
			2	-40.3 ± 10.7	-94.2 ± 7.4	0.44
			3	-27.0 ± 10.1	-92.1 ± 7.3	0.06
			4	-37.2 ± 13.0	-85.3 ± 8.8	0.04
			5	-47.8 ± 9.6	-90.4 ± 7.8	0.39
12	-59.5 ± 15.3	-50.9 ± 9.0	1	-34.7 ± 14.1	-98.6 ± 8.2	0.13
			2	-49.0 ± 15.9	-87.0 ± 9.6	0.04
			3	-34.3 ± 13.3	-97.3 ± 8.7	0.09
			4	-19.6 ± 15.0	-100.3 ± 8.0	0.04
			5	-42.6 ± 13.1	-94.1 ± 9.0	0.11
			6	-41.7 ± 10.9	-101.8 ± 8.9	0.59
14	-171.0 ± 34.2	-78.0 ± 16.3	1	-120.1 ± 24.4	-161.0 ± 14.5	0.04
			2	-125.2 ± 23.8	-167.5 ± 13.3	0.31
			3	-71.3 ± 24.3	-172.9 ± 10.9	0.00
			4	-106.6 ± 32.7	-163.9 ± 14.3	0.02
			5	-146.2 ± 29.4	-158.9 ± 15.6	0.39
			6	-154.7 ± 35.2	-152.9 ± 18.0	0.24
17	-132.0 ± 29.2	-77.4 ± 14.1	1	-112.0 ± 18.2	-152.5 ± 13.9	0.53

			2	-50.7 ± 18.3	-168.3 ± 9.6	0.03
			3	-83.3 ± 17.1	-155.1 ± 11.7	0.05
			4	-100.5 ± 17.8	-140.5 ± 12.7	0.01
			5	-95.2 ± 17.1	-158.6 ± 13.4	0.38
20	-92.7 ± 20.9	-91.0 ± 11.8	1	-64.3 ± 20.3	-162.8 ± 12.3	0.19
			2	-56.8 ± 27.7	-146.9 ± 14.5	0.00
			3	-89.0 ± 17.6	-151.6 ± 12.4	0.20
			4	-54.8 ± 24.5	-154.7 ± 17.1	0.01
			5	-52.3 ± 16.1	-170.2 ± 10.7	0.30
			6	-70.5 ± 15.8	-161.7 ± 11.5	0.29
29	-17.1 ± 6.7	-60.2 ± 6.2	1	-7.7 ± 3.6	-101.1 ± 5.8	0.19
			2	-7.7 ± 3.8	-105.0 ± 6.4	0.48
			3	-6.3 ± 3.8	-102.7 ± 6.1	0.23
			4	-8.1 ± 4.3	-98.2 ± 6.5	0.10
31	-21.8 ± 7.7	-65.8 ± 6.6	1	-6.9 ± 3.4	-111.5 ± 6.3	0.06
			2	-11.1 ± 3.9	-116.0 ± 7.1	0.27
			3	-9.2 ± 5.3	-112.4 ± 6.5	0.10
			4	-8.7 ± 3.8	-115.6 ± 6.8	0.19
			5	-4.5 ± 3.1	-116.2 ± 6.2	0.14
			6	-10.6 ± 3.8	-115.5 ± 6.7	0.23
33	-30.0 ± 9.7	-63.6 ± 6.9	1	-12.3 ± 4.0	-108.8 ± 6.1	0.12
			2	-12.5 ± 6.8	-109.6 ± 7.1	0.14
			3	-14.5 ± 7.1	-111.1 ± 7.1	0.26
			4	-19.0 ± 6.6	-107.8 ± 6.6	0.19
			5	-14.8 ± 7.1	-109.9 ± 7.2	0.20
			6	-13.2 ± 5.9	-107.5 ± 6.6	0.10
34	-21.7 ± 7.8	-65.1 ± 6.6	1	-5.9 ± 3.7	-111.4 ± 7.1	0.06
			2	-7.6 ± 4.0	-116.9 ± 6.5	0.27
			3	-8.1 ± 3.7	-117.9 ± 7.4	0.37
			4	-6.6 ± 4.4	-117.7 ± 6.9	0.30
37	-12.8 ± 6.0	-66.9 ± 6.2	1	-8.4 ± 3.6	-117.4 ± 6.9	0.46
			2	-7.4 ± 3.7	-115.5 ± 6.3	0.26
			3	-4.6 ± 3.8	-114.4 ± 6.1	0.15
			4	-9.7 ± 4.1	-111.4 ± 7.0	0.13
39	-21.3 ± 7.6	-65.5 ± 6.6	1	-10.3 ± 4.1	-110.6 ± 7.2	0.17
			2	-8.4 ± 4.1	-115.9 ± 6.8	0.48
			3	-5.2 ± 3.7	-114.6 ± 6.6	0.25
			4	-5.8 ± 3.5	-110.5 ± 6.9	0.10
40	-21.5 ± 7.6	-65.8 ± 6.6	1	-11.2 ± 5.7	-106.1 ± 7.0	0.03
			2	-6.2 ± 3.6	-119.9 ± 7.1	0.49
			3	-5.0 ± 4.7	-115.6 ± 6.9	0.16
			4	-7.3 ± 4.1	-116.7 ± 7.0	0.26
			5	-4.4 ± 2.9	-112.0 ± 6.5	0.06
41	-21.7 ± 7.4	-65.7 ± 6.5	1	-5.5 ± 4.3	-110.6 ± 6.3	0.08

			2	-8.3 ± 4.1	-113.5 ± 7.2	0.21
			3	-5.7 ± 4.3	-115.2 ± 6.7	0.24
			4	-6.4 ± 3.9	-117.6 ± 7.1	0.45
			5	-4.3 ± 3.4	-104.6 ± 6.7	0.02
43	-21.6 ± 7.6	-66.4 ± 6.5	1	-5.7 ± 3.6	-113.6 ± 6.4	0.10
			2	-7.7 ± 4.0	-117.3 ± 7.4	0.30
			3	-4.6 ± 3.4	-115.3 ± 6.1	0.13
			4	-4.3 ± 3.7	-110.1 ± 7.0	0.04
			5	-6.7 ± 3.5	-119.2 ± 6.4	0.42
57	-53.7 ± 12.9	-85.1 ± 9.0	1	-38.4 ± 9.4	-148.5 ± 9.8	0.57
			2	-29.1 ± 8.9	-144.9 ± 9.5	0.09
			3	-23.5 ± 13.5	-145.5 ± 8.4	0.06
			4	-15.8 ± 9.9	-148.9 ± 8.9	0.06
			5	-37.6 ± 10.9	-144.9 ± 9.8	0.22
			6	-32.9 ± 9.6	-132.1 ± 9.9	0.01
59	-56.1 ± 13.1	-77.5 ± 8.7	1	-45.8 ± 10.9	-137.7 ± 9.7	0.56
			2	-30.2 ± 10.2	-131.6 ± 9.3	0.02
			3	-33.2 ± 12.0	-128.3 ± 9.0	0.02
			4	-43.3 ± 12.7	-128.5 ± 9.0	0.05
			5	-42.0 ± 11.4	-136.1 ± 9.4	0.25
			6	-32.6 ± 11.9	-136.3 ± 8.5	0.10
63	-17.6 ± 7.4	-52.3 ± 6.0	1	-3.1 ± 5.1	-82.7 ± 8.1	0.06
			2	-2.5 ± 3.8	-90.0 ± 6.6	0.34
			3	-3.1 ± 2.5	-89.2 ± 6.0	0.29
			4	-2.7 ± 3.5	-89.5 ± 5.9	0.31
66	-20.7 ± 8.3	-68.2 ± 7.1	1	-3.3 ± 4.0	-116.8 ± 7.1	0.10
			2	-7.4 ± 4.2	-117.6 ± 7.2	0.19
			3	-12.9 ± 5.0	-116.7 ± 7.5	0.27
			4	-6.7 ± 5.6	-118.6 ± 6.8	0.22
			5	-10.8 ± 4.8	-116.0 ± 7.6	0.18
			6	-8.0 ± 4.8	-110.4 ± 6.5	0.04
69	-16.1 ± 7.6	-60.6 ± 6.5	1	-4.9 ± 6.0	-100.8 ± 6.8	0.14
			2	-2.3 ± 2.1	-102.9 ± 6.0	0.17
			3	-4.6 ± 3.7	-99.8 ± 6.5	0.11
			4	-3.9 ± 3.0	-104.0 ± 7.5	0.27
			5	-5.2 ± 3.7	-103.9 ± 6.6	0.31
71	-58.0 ± 13.5	-42.3 ± 7.7	1	-43.4 ± 11.6	-76.5 ± 7.7	0.30
			2	-31.1 ± 11.6	-79.8 ± 7.4	0.18
			3	-26.0 ± 12.6	-80.0 ± 8.1	0.11
			4	-39.4 ± 12.5	-76.8 ± 9.0	0.21
			5	-38.8 ± 12.5	-77.0 ± 7.6	0.21