

Supplementary Materials

Figure S1. Docking scores of actives and decoys.

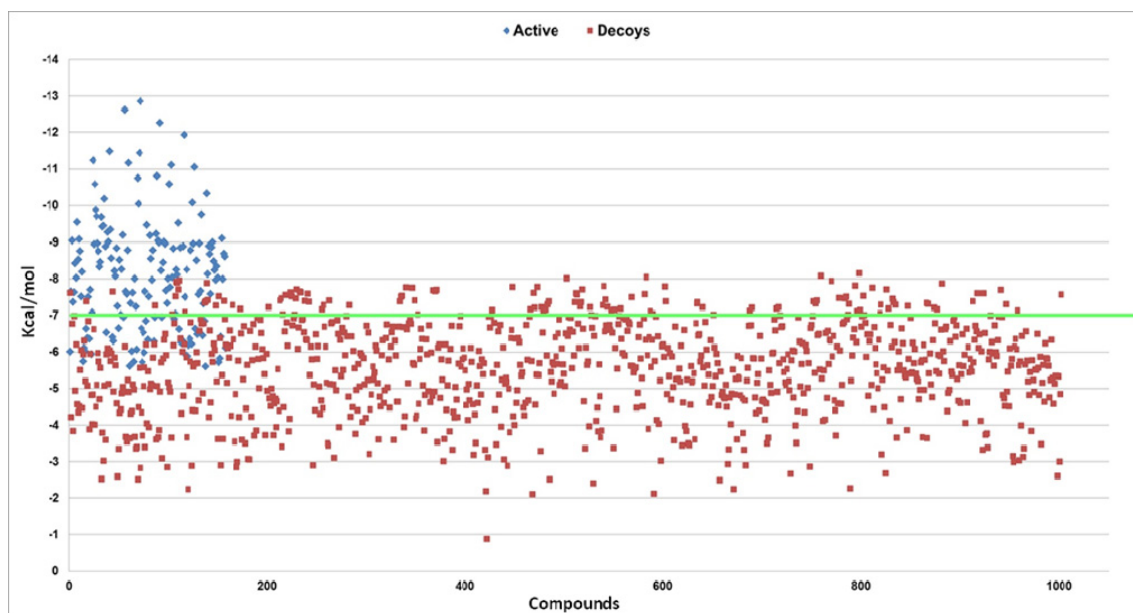


Table S1. Chemical and physical properties of the 12 best hits. MW, LogP, HBA, HBD and PSA indicate, respectively, molecular weight, lipophilicity, hydrogen bond acceptor groups, hydrogen bond donor groups and polar surface area.

Hit	MW	LogP	HBA	HBD	PSA
ZINC79190432	378.38	1.29	5	2	116.31
ZINC77031588	270.28	3.17	4	3	69.92
ZINC32124244	374.44	3.48	3	2	79.78
ZINC20760949	441.91	2.79	4	2	83.66
ZINC14610063	338.35	4.41	5	2	72.06
ZINC12902036	420.46	1.95	4	4	108.24
ZINC12664647	404.46	2.46	3	3	88.15
ZINC12377179	290.32	2.92	3	2	62.22
ZINC04252698	288.25	2.26	6	5	118.22
ZINC03985155	403.43	2.51	6	1	89.85
ZINC03843477	352.34	2.36	6	0	86.74
ZINC02131213	349.38	3.9	4	1	69.28

Table S2. SMILES chemical formula, reference code and IC₅₀ values of the active compounds.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cccc2c1c(c3n2[c@]45c)c6c(c(=O)nc6)c7c8c(cccc8)n(c37)[c@h](o5)c[c@h](nc)[c@@h]4oc</chem>	CHEMBL162 [1] IC ₅₀ = 8,32 µM
<chem>cn(c)ccnc1nc(cccc2)c2c3[nh]c(c4c13)c5c(cc4)ccc(c5)oc</chem>	CHEMBL10763 [2] IC ₅₀ = 9,8 µM
<chem>c1cccc[n+]1l(c)ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)cc(cc4)nc(=O)cc[n+]5(c)ccccc5</chem>	CHEMBL14832 [3] IC ₅₀ = 7,8 µM
<chem>c1cccc(c12)ccc(c2)c(\c)=c\c(=O)nc(c3c(=O)o)cccc3</chem>	CHEMBL27323 [4] IC ₅₀ = 5 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)ccc(c4)nc(=O)ccn5ccccc5</chem>	CHEMBL33618 [3] IC ₅₀ = 4,5 µM
<chem>cc[n+]1ccccc1/c=c2/n(cc)c(=O)/c(s2)=c(/n3c)sc(c34)cccc4</chem>	CHEMBL33859 [3] IC ₅₀ = 5 µM
<chem>ccn(cc)ccc(=O)nc(c1)ccc(c12)c(=O)c3c(c2=O)ccc(c3)nc(=O)ccn(cc)cc</chem>	CHEMBL34683 [3] IC ₅₀ = 3,5 µM
<chem>o=p(o)(o)o[p@](=O)(o)o[p@](=O)(o)oc[c@h]1cc[c@h](o1)n(en2)c(c23)nc(n)[nh]c3=O</chem>	CHEMBL54224 [5] IC ₅₀ = 8,6 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn5ccccc5</chem>	CHEMBL79900 [6] IC ₅₀ = 5,2 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn5ccccc5</chem>	CHEMBL81268 [7] IC ₅₀ = 2,8 µM
<chem>oc[c@h]1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn5cccc[c@@h]5co</chem>	CHEMBL81271 [7] IC ₅₀ = 5,4 µM
<chem>oc1ccn(cc1)ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn(cc5)ccc5o</chem>	CHEMBL81516 [8] IC ₅₀ = 8 µM
<chem>cc[c@h]1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn5cccc[c@@h]5cc</chem>	CHEMBL81747 [7] IC ₅₀ = 2,7 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1ccccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL82008 [8] IC ₅₀ = 3,1 µM
<chem>c[c@@h]1cccn(c1)ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn(c5)ccc[c@h]5c</chem>	CHEMBL83173 [8] IC ₅₀ = 1,35 µM
<chem>c1cccc(c12)n(cc2c)cccn(c(c34)cccc4)cc3cc(=O)nccccccccccco[p@](=O)(o)oc5c(c1)cccc5</chem>	CHEMBL83388 [9] IC ₅₀ = 3,6 µM
<chem>cc(c)(c)oc(=O)n1ccc[c@h]1c(=O)n[c@@h](cc2c[nh]c(c23)cccc3)c(=O)nccccccccccco[p@@](=O)(o)oc4c(c1)cccc4</chem>	CHEMBL86984 [9] IC ₅₀ = 9,5 µM
<chem>c1cccc1coc(=O)cc[c@@h](nc(=O)oc(c)(c)c)c(=O)n[c@@h](cc2c[nh]c(c23)cccc3)c(=O)nccccccccccco[p@](=O)(o)oc4c(c1)cccc4</chem>	CHEMBL87237 [9] IC ₅₀ = 6,4 µM
<chem>c1ccccn1ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)cc(cc4)nc(=O)ccn5cccc5</chem>	CHEMBL89250 [10] IC ₅₀ = 3,1 µM
<chem>cn(c)ccc(=O)nc(c1)ccc(c12)c(=O)c3c(c2=O)cc(cc3)nc(=O)ccn(c)c</chem>	CHEMBL89977 [9] IC ₅₀ = 4,7 µM
<chem>c1cccc[n+]1(c)ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)cc(cc4)nc(=O)cc[n+]5(c)cccc5</chem>	CHEMBL90901 [10] IC ₅₀ = 7,8 µM
<chem>ccn(cc)ccc(=O)nc(c1)ccc(c12)c(=O)c3c(c2=O)cc(cc3)nc(=O)ccn(cc)cc</chem>	CHEMBL91163 [3] IC ₅₀ = 4,3 µM
<chem>c1ccccn1ccc(=O)nc(cc2)cc(c2-3)c(=O)c4c3ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL91935 [10] IC ₅₀ = 9 µM
<chem>ccoc(c1)ccc(c12)nc3c(c2n)ccc(c3)n</chem>	CHEMBL94007 [11] IC ₅₀ = 8,2 µM
<chem>c1ccccn1ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL109382 [5] IC ₅₀ = 4,5 µM
<chem>c[n+](c)(c)ccc(=O)nc1ccc(nc(=O)cc[n+](c)(c)c)(c12)c(=O)c3c(c2=O)cccc3</chem>	CHEMBL111417 [8] IC ₅₀ = 7 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5c(sc)cccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL137809 [7] IC ₅₀ = 0,15 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nccn(c)c)cc(cc4)nc(=O)ccn5cccc5</chem>	CHEMBL137928 [7] IC ₅₀ = 0,57 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5cccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL137973 [7] IC ₅₀ = 0,21 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3ncccn(c)c)ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL138187 [7] IC ₅₀ = 0,08 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc(cc5)ccc5n(c)c)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL138357 [7] IC ₅₀ = 0,17 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5cccc5)cc(cc4)nc(=O)ccn6cccc6</chem>	CHEMBL138369 [7] IC ₅₀ = 1,29 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc(ccc5)cc5n(c)c)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL138487 [7] IC ₅₀ = 0,1 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5cc(sc)ccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL138761 [7] IC ₅₀ = 0,1 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5cc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL138811 [7] IC ₅₀ = 0,05 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5cccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL139287 [7] IC ₅₀ = 0,09 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc(ccc5)cc5n(c)c)cc(cc4)nc(=O)ccn6cccc6</chem>	CHEMBL139443 [7] IC ₅₀ = 0,6 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5cc(n)ccc5)cc(cc4)nc(=O)ccn6cccc6</chem>	CHEMBL139500 [7] IC ₅₀ = 1,09 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5c(n)cccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL139511 [7] IC ₅₀ = 0,02 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nccn(c)c)ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL140084 [7] IC ₅₀ = 0,27 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nccn(c)c)ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL140180 [7] IC ₅₀ = 0,01 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5ccccc5)ccc(c4)nc(=O)ccn6ccccc6</chem>	CHEMBL140354 [7] IC ₅₀ = 1,33 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3ncn5ccccc5)ccc(c4)nc(=O)ccn6ccccc6</chem>	CHEMBL141540 [7] IC ₅₀ = 0,05 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc(ccc5)cc5nc(=O)c)ccc(c4)nc(=O)ccn6ccccc6</chem>	CHEMBL141661 [7] IC ₅₀ = 0,1 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5ccc(cc5)oc)cc(cc4)nc(=O)ccn6ccccc6</chem>	CHEMBL141740 [7] IC ₅₀ = 0,46 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5ccc(n)cc5)cc(cc4)nc(=O)ccn6ccccc6</chem>	CHEMBL142036 [7] IC ₅₀ = 0,2 µM
<chem>c1ccc[n+]1(c)ccc(=O)nc2ccc(c(c23)c(=O)c4c(c3=O)cccc4)nc(=O)cc[n+]5(c)ccccc5</chem>	CHEMBL143452 [3] IC ₅₀ = 5 µM
<chem>c1ccc[n+]1(c)ccc(=O)nc2cccc(c23)c(=O)c4c(c3=O)c(ccc4)nc(=O)cc[n+]5(c)ccccc5</chem>	CHEMBL144219 [3] IC ₅₀ = 8,2 µM
<chem>cc[n+](c)(cc)ccc(=O)nc1ccc(nc(=O)cc[n+](c)(cc)cc)c(c12)c(=O)c3c(c2=O)cccc3</chem>	CHEMBL144303 [8] IC ₅₀ = 3,1 µM
<chem>c1cccc[n+]1(c)ccc(=O)nc2cccc(c23)c(=O)c4c(c3=O)cccc4nc(=O)cc[n+]5(c)ccccc5</chem>	CHEMBL144334 [8] IC ₅₀ = 8,6 µM
<chem>c1cccn1ccc(=O)nc2cccc(c23)c(=O)c4c(c3=O)c(ccc4)nc(=O)ccn5ccccc5</chem>	CHEMBL144386 [8] IC ₅₀ = 3,7 µM
<chem>ccn(cc)ccc(=O)nc1cccc(c12)c(=O)c3c(c2=O)cccc3nc(=O)ccn(cc)cc</chem>	CHEMBL144664 [8] IC ₅₀ = 2,7 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)cc(cc4)nc(=O)ccn5ccccc5</chem>	CHEMBL144757 [12] IC ₅₀ = 6,7 µM
<chem>c1cccn1ccc(=O)nc2cccc(c23)c(=O)c4c(c3=O)cccc4nc(=O)ccn5ccccc5</chem>	CHEMBL144848 [3] IC ₅₀ = 7,8 µM
<chem>cn(c)ccc(=O)nc1cccc(c12)c(=O)c3c(c2=O)c(ccc3)nc(=O)ccn(c)c</chem>	CHEMBL144984 [8] IC ₅₀ = 6,4 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>cc[n+](c)(cc)ccc(=O)nc1cccc(c12)c(=O)c3c(c2=O)c(ccc3)nc(=O)cc[n+](c)(cc)cc</chem>	CHEMBL145311 [8] IC ₅₀ = 7,5 µM
<chem>ccn(cc)ccc(=O)nc1cccc(c12)c(=O)c3c(c2=O)c(ccc3)nc(=O)ccn(cc)cc</chem>	CHEMBL145575 [8] IC ₅₀ = 4,2 µM
<chem>cc(c1)cc2n(cc)c(cccc3)c3c4[n+](cc)c(c5c1c24)cccc5</chem>	CHEMBL154643 [13] IC ₅₀ = 2 µM
<chem>c1c(cl)ccc(c12)n(cc2)ccn(c(c34)cccc4)cc3cc(=O)nccccccccccco[p@@](=O)(o)oc5ccccc5</chem>	CHEMBL155030 [14] IC ₅₀ = 6,7 µM
<chem>cc(c1)cc2n(c)c(ccc(cl)c3)c3c4[n+](c)c(c5c1c24)ccc(cl)c5</chem>	CHEMBL156480 [13] IC ₅₀ = 0,25 µM
<chem>cc(c1)cc2n(c)c(cccc3)c3c4[n+](c)c(c5c1c24)cccc5</chem>	CHEMBL156492 [13] IC ₅₀ = 0,76 µM
<chem>c1ccc2n(c)c(cccc3)c3c4[n+](c)c(c5c1c24)cccc5</chem>	CHEMBL157766 [13] IC ₅₀ = 0,38 µM
<chem>cc(c1)cc2n(c)c(ccc(f)c3)c3c4[n+](c)c(c5c1c24)ccc(f)c5</chem>	CHEMBL158083 [13] IC ₅₀ = 0,33 µM
<chem>cc(c1)cc2n(c)c(ccc(c)c3)c3c4[n+](c)c(c5c1c24)ccc(c)c5</chem>	CHEMBL158365 [13] IC ₅₀ = 0,25 µM
<chem>c1cccn1c(=O)cccc(=O)nc2ccc(cc2)nc3c(ccc(c4)nc(=O)ccn5cccc5)c4nc(c36)cc(cc6)nc(=O)ccn7cccc7</chem>	CHEMBL181970 [7] IC ₅₀ = 0,31 µM
<chem>ccn(cc)ccccccnc(=O)cccc(=O)nc1ccc(cc1)nc2c(ccc(c3)nc(=O)ccn4cccc4)c3nc(c25)cc(cc5)nc(=O)ccn6cccc6</chem>	CHEMBL182871 [7] IC ₅₀ = 0,08 µM
<chem>ccn(cc)ccnc(=O)cccc(=O)nc1ccc(cc1)nc2c(ccc(c3)nc(=O)ccn4cccc4)c3nc(c25)cc(cc5)nc(=O)ccn6cccc6</chem>	CHEMBL184587 [7] IC ₅₀ = 0,09 µM
<chem>cn(c)cccnc(c1c(n2)cccc1)c(c2c34)[nh]c3cccc4</chem>	CHEMBL219728 [15] IC ₅₀ = 0,63 µM
<chem>c1c(cl)c(o)c(o)c(c12)oc(cc2=O)-c3cc(o)c(o)cc3</chem>	CHEMBL222132 [16] IC ₅₀ = 0,82 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cc(o)c(o)c(c12)oc(c(f)c2=O)-c3cc(o)c(o)cc3</chem>	CHEMBL222354 [16] IC ₅₀ = 0,6 µM
<chem>coc(cc1)c(oc)c(c12)oc(cc2=O)-c3cc(n)c(n)cc3</chem>	CHEMBL222490 [16] IC ₅₀ = 7,4 µM
<chem>c1cc(o)c(o)c(c12)oc(cc2=O)-c3cc(n)c(n)cc3</chem>	CHEMBL222539 [16] IC ₅₀ = 3,6 µM
<chem>c1cc(o)c(o)c(c12)oc(cc2=O)-c3cc(o)c(o)cc3</chem>	CHEMBL222541 [16] IC ₅₀ = 0,2 µM
<chem>coc(cc1)c(oc)c(c12)oc(cc2=O)-c(c3)ccc(c34)[nh]cn4</chem>	CHEMBL222547 [16] IC ₅₀ = 2,2 µM
<chem>c1cc(o)c(o)c(o)c1c(=O)/C=C/C2cc(o)c(o)cc2</chem>	CHEMBL222557 [16] IC ₅₀ = 6 µM
<chem>n1c(o)[nh]c(c12)ccc(c2)-c(cc3=O)oc(c34)c(o)c(o)cc4</chem>	CHEMBL222757 [16] IC ₅₀ = 1,2 µM
<chem>c[n+](c)(c)ccn(c(=O)c1c2c34)c(=O)c2ccc4c5c6c7c(c(=O)n(cc[n+](c)(c)c)c(=O)c7cc5)ccc6c3cc1</chem>	CHEMBL224754 [17] IC ₅₀ = 0,03 µM
<chem>c1cccn1ccn(c2)cc3ccc4c5ccc6cn(ccn7cccc7)cc(cc8)c6c5c8c9ccc2c3c49</chem>	CHEMBL224755 [17] IC ₅₀ = 0,4 µM
<chem>cn(c)ccn(c(=O)c1c2c34)c(=O)c2ccc4c5c6c7c(c(=O)n(ccn(c)c)c(=O)c7cc5)ccc6c3cc1</chem>	CHEMBL225001 [17] IC ₅₀ = 0,16 µM
<chem>occnccn(c(=O)c1c2c34)c(=O)c2ccc4c5c6c7c(ccc6c3cc1)c(=O)n(c(=O)c7cc5)ccncco</chem>	CHEMBL225205 [17] IC ₅₀ = 0,06 µM
<chem>c1cc(o)c(o)cc1-c(c(c#n)c2=O)oc(c23)c(o)c(o)cc3</chem>	CHEMBL225211 [16] IC ₅₀ = 0,13 µM
<chem>coc(cc1)c(o)c(c12)oc(cc2=O)-c3cc(o)c(o)cc3</chem>	CHEMBL225228 [16] IC ₅₀ = 7,8 µM
<chem>c[n+](c)(c)ccn(c(=O)c1cc2)c(=O)c3ccc4c(=O)n(c(=O)c2c4c13)cc[n+](c)(c)c</chem>	CHEMBL225507 [17] IC ₅₀ = 2,5 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cc(o)c(o)cc1c(=o)/c=c/c2cc(o)c(o)cc2</chem>	CHEMBL225618 [16] IC ₅₀ = 1,7 µM
<chem>c1cccc(c12)[n+](c)cc(c2)nc(=o)c(n3)ccc4ccc(c5c34)ccc(n5)c(=o)nc(c6)c[n+](c)c(c67)cccc7</chem>	CHEMBL259739 [18] IC ₅₀ = 0,001 µM
<chem>o1cccc1-c2cc(c[n+](c)c2)-c3c(n4)ccc4c(-c(c[n+](c)c5)cc5-c6cccc6)c([nh]7)ccc7c(-c(c[n+](c)c8)cc8-c9cccc9)c([nh]1)ccc1c(c(n1)ccc13)-c(c[n+](c)c1)cc1-c1cccc1</chem>	CHEMBL265594 [19] IC ₅₀ = 8 µM
<chem>cn(c)ccnc1nc(cccc2)c2c3[nh]c(c4c13)c5c(cc4)cc(cc5)oc</chem>	CHEMBL274096 [2] IC ₅₀ = 1 µM
<chem>cn(c)ccnc1[nh]c(cccc2)c2c3nc(c4c13)c5c(cc4)ccc(c5)[n+](o-)=o</chem>	CHEMBL274335 [2] IC ₅₀ = 0,5 µM
<chem>c[n+](c)(c)cccn(c(=o)c1cc2)c(=o)c3ccc4c(=o)n(c(=o)c2c4c13)ccc[n+](c)(c)c</chem>	CHEMBL275860 [17] IC ₅₀ = 2,5 µM
<chem>cn(c)ccnc1nc(cccc2)c2c3[nh]c(c4c13)c5c(cc4)ccc(c5)oc</chem>	CHEMBL276202 [2] IC ₅₀ = 1,1 µM
<chem>c1cccc(c12)ccc(c2)c(\c)=c/c(=o)nc(c3c(=o)o)cccc3</chem>	CHEMBL282105 [4] IC ₅₀ = 5 µM
<chem>c1c(n)ccc2c1[n+](cc)c(c(c23)cc(n)cc3)-c4cccc4</chem>	CHEMBL284328 [11] IC ₅₀ = 3,3 µM
<chem>cn(c)cccn(c(=o)c1cc2)c(=o)c3ccc4c(=o)n(c(=o)c2c4c13)cccn(c)c</chem>	CHEMBL287201 [4] IC ₅₀ = 3,5 µM
<chem>ccn(cc)ccoc(cc1)cc(c12)o[c@@h]3[c@h]2c(=o)c4c(c3=O)cccc4</chem>	CHEMBL292475 [20] IC ₅₀ = 7 µM
<chem>cc1ccn(cc1)ccc(=O)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=O)ccn(cc5)ccc5c</chem>	CHEMBL309919 [8] IC ₅₀ = 1,35 µM
<chem>ccn(cc)ccc(=O)nc(cc1)cc(c12)nc3c(c2)ccc(c3)nc(=O)ccn(cc)cc</chem>	CHEMBL309982 [7] IC ₅₀ = 5,8 µM
<chem>cn(c)ccc(=O)nc(cc1)cc(c12)nc3c(c2)ccc(c3)nc(=O)ccn(c)c</chem>	CHEMBL311072 [7] IC ₅₀ = 8,2 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cccc1c[c@@h](nc(=o)oc(c)(c)c(=o)n[c@@h](cc2c[nh]c(c23)cccc3)c(=o)ccccccccccco[p@@](=o)(o)oc4c(cl)cccc4</chem>	CHEMBL314040 [9] IC ₅₀ = 6,8 µM
<chem>c1cccc1coc(=o)n[c@h](cc2c[nh]c(c23)cccc3)c(=o)ccccccccccco[p@](=o)(o)oc4c(cl)cccc4</chem>	CHEMBL314864 [9] IC ₅₀ = 3,6 µM
<chem>c1ccc[c@h](co)[n@@+]1(c)ccc(=o)nc2ccc(c(c23)c(=o)c4c(c3=O)cccc4)nc(=o)cc[n@@+]5(c)[c@@h](co)cccc5</chem>	CHEMBL322686 [5] IC ₅₀ = 9,4 µM
<chem>oc[c@@h]1cccc1ccc(=o)nc(cc2)cc(c2-3)c(=o)c4c3ccc(c4)nc(=o)ccn5cccc[c@h]5co</chem>	CHEMBL328065 [10] IC ₅₀ = 8 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3nccn(c)c)ccc(c4)nc(=o)ccn5cccc5</chem>	CHEMBL335132 [9] IC ₅₀ = 0,06 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3nccoc)ccc(c4)nc(=o)ccn5cccc5</chem>	CHEMBL335564 [7] IC ₅₀ = 0,14 µM
<chem>c1cccc(c12)[n+](c)cc(c2)-c3c(n4)ccc4c(-c(c5)c[n+](c)c(c56)cccc6)c([nh]7)ccc7c(-c8ccc[n+](c)c8)c([nh]9)ccc9c(c(n1)ccc13)-c(c1)c[n+](c)c(c12)cccc2</chem>	CHEMBL335814 [19] IC ₅₀ = 5 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3nc5ccc(n)cc5)ccc(c4)nc(=o)ccn6cccc6</chem>	CHEMBL335819 [7] IC ₅₀ = 0,07 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3nc5cc(n)ccc5)ccc(c4)nc(=o)ccn6cccc6</chem>	CHEMBL336417 [7] IC ₅₀ = 0,06 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3nc(cc5)ccc5n(c)c)ccc(c4)nc(=o)ccn6cccc6</chem>	CHEMBL336434 [17] IC ₅₀ = 0,04 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3nc(cc5)ccc5c(=o)c)ccc(c4)nc(=o)ccn6cccc6</chem>	CHEMBL336444 [7] IC ₅₀ = 0,04 µM
<chem>c1c[n+](c)ccc1-c2c(n3)ccc3c(-c4cc[n+](c)cc4)c([nh]5)ccc5c(-c6cc[n+](c)cc6)c([nh]7)ccc7c(c(n8)ccc28)-c9cc[n+](c)cc9</chem>	CHEMBL337559 [19] IC ₅₀ = 8 µM
<chem>c1cccn1ccc(=o)nc(c2)ccc(c23)nc4c(c3nc5ccc(n)cc5)ccc(c4)nc(=o)ccn6cccc6</chem>	CHEMBL337762 [7] IC ₅₀ = 0,08 µM
<chem>c1cccn1ccc(=o)nc(c2)ccc(c23)nc4c(c3nc(cc5)ccc5n(c)c)cc(cc4)nc(=o)ccn6cccc6</chem>	CHEMBL341985 [7] IC ₅₀ = 0,5 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5cc(n)ccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL342480 [7] IC ₅₀ = 0,21 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5cc(oc)ccc5)cc(cc4)nc(=O)ccn6cccc6</chem>	CHEMBL342921 [7] IC ₅₀ = 2,73 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5c(o)cccc5)cc(cc4)nc(=O)ccn6cccc6</chem>	CHEMBL343041 [7] IC ₅₀ = 1,03 µM
<chem>c1cccc[n+](c)ccc(=O)nc2cccc(c23)c(=O)c4c(c3=O)c(ccc4)nc(=O)cc[n+](c)cccc5</chem>	CHEMBL343238 [3] IC ₅₀ = 7,8 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)c(=O)c4c(c3=O)ccc(c4)nc(=O)ccn5cccc5</chem>	CHEMBL343445 [8] IC ₅₀ = 1,8 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5c(n)cccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL343609 [7] IC ₅₀ = 0,11 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5ccc(f)cc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL343795 [7] IC ₅₀ = 0,07 µM
<chem>c1ccc[n+](c)ccc(=O)nc2cccc(c23)c(=O)c4c(c3=O)cccc4nc(=O)cc[n+](c)cccc5</chem>	CHEMBL344072 [8] IC ₅₀ = 8,8 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)nc4c(c3nc5c(n)cccc5)cc(cc4)nc(=O)ccn6cccc6</chem>	CHEMBL345035 [8] IC ₅₀ = 0,17 µM
<chem>c1c(cl)ccc(c12)n(cc2)ccn(c(c34)cccc4)cc3cc(=O)nccccccccccc[p@@](=O)(o)oc5cccc5</chem>	CHEMBL345715 [14] IC ₅₀ = 8,7 µM
<chem>c1cccn1ccn(c(c23)cccc3)cc2cc(=O)nccccccccccc[p@@](=O)(o)c4c(cl)cccc4</chem>	CHEMBL349085 [14] IC ₅₀ = 4,2 µM
<chem>c1c(cl)ccc(c12)n(cc2)ccn(c(c34)cccc4)cc3cc(=O)nccccccccccc[p@@](=O)(o)oc5cc(cl)ccc5</chem>	CHEMBL351995 [14] IC ₅₀ = 2,5 µM
<chem>cn(c)ccc(=O)nc1cccc(c12)c(=O)c3c(c2=O)cccc3nc(=O)ccn(c)c</chem>	CHEMBL356077 [8] IC ₅₀ = 1,3 µM
<chem>c1cccn1ccn(c(=O)c2c3c45)c(=O)c3ccc5c6c7c8c(ccc7c4cc2)c(=O)n(c(=O)c8cc6)ccn9cccc9</chem>	CHEMBL359594 [17] IC ₅₀ = 0,2 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>cn(c)cccc(n1)[nh]c(c12)ccc(c2)-c(cc3=o)oc(c34)c(oc)c(cc4)oc</chem>	CHEMBL376279 [16] IC ₅₀ = 0,47 µM
<chem>n1c[nh]c(c12)ccc(c2)-c(cc3=o)oc(c34)c(o)c(o)cc4</chem>	CHEMBL390725 [16] IC ₅₀ = 4 µM
<chem>c1cccc(c12)[n+](c)cc(c2)nc(=o)c3cccc(n3)c(=o)nc(c4)c[n+](c)c(c45)cccc5</chem>	CHEMBL409247 [17] IC ₅₀ = 0,06 µM
<chem>c1cccc(c12)n(cc2c)cccn(c(c34)cccc4)cc3cc(=o)ccccccccccco[p@](=o)(o)oc5cc(cl)ccc5</chem>	CHEMBL413033 [14] IC ₅₀ = 3,4 µM
<chem>c1cc(o)c(o)c(c12)oc(cc2=o)-c3ccc(o)cc3</chem>	CHEMBL420982 [16] IC ₅₀ = 3 µM
<chem>clc1cccc(cl)c1esc(c2c#n)nc(cc2)/c=n/c(c3c)cccn3</chem>	CHEMBL421825 [21] IC ₅₀ = 1 µM
<chem>c[n+](c)(c)ccc(=o)nc1cccc(c12)c(=o)c3c(c2=o)c(ccc3)nc(=o)cc[n+](c)(c)c</chem>	CHEMBL422120 [3] IC ₅₀ = 4,4 µM
<chem>c1cc(o)c(o)c(c12)oc(c(cl)c2=o)-c3cc(o)c(o)cc3</chem>	CHEMBL426182 [16] IC ₅₀ = 0,8 µM
<chem>c[c@h]1ccccn1ccc(=o)nc(cc2)cc(c23)nc4c(c3)ccc(c4)nc(=o)ccn5cccc[c@h]5c</chem>	CHEMBL431404 [7] IC ₅₀ = 3,1 µM
<chem>c1cccc(c12)[nh]c(c2)c[c@h](nc(=o)oc(c)(c)c)c(=o)n[c@@h](cc3c[nh]c(c34)cccc4)c(=o)ccccccccccco[p@](=o)(o)oc5c(cl)cccc5</chem>	CHEMBL432562 [9] IC ₅₀ = 0,3 µM
<chem>cc1oc(n2)-c(c(o3)c)nc3[c@h](cs4)n=c4c(co5)nc5-c(co6)nc6-c(co7)nc7-c(co8)nc8-c(co9)nc9-c12</chem>	CHEMBL443683 [18] IC ₅₀ = 1,15 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(ccc(c4)nc(=o)ccn5cccc5)c3ncncncnc6c(ccc(c7)nc(=o)ccn8cccc8)c7nc(c69)cc(cc9)nc(=o)ccn1cccc1</chem>	CHEMBL443702 [22] IC ₅₀ = 7,5 µM
<chem>cn(c)ccc(=o)nc(c1)ccc(c12)c(=o)c3c(c2=o)ccc(c3)nc(=o)ccn(c)c</chem>	CHEMBL444347 [8] IC ₅₀ = 4,1 µM
<chem>c1cccn1ccc(=o)nc(cc2)cc(c23)nc4c(ccc(c4)nc(=o)ccn5cccc5)c3ccccccnc6c(ccc(c7)nc(=o)ccn8cccc8)c7nc(c69)cc(cc9)nc(=o)ccn1cccc1</chem>	CHEMBL448813 [22] IC ₅₀ = 4 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>cn(c)cccnc(c1c([n+]2c)cccc1)c(c2c34)oc3cccc4</chem>	CHEMBL482414 [25] IC ₅₀ = 0,37 µM
<chem>ccn(cc)cccnc(c1c([n+]2c)cccc1)c(c2c34)[nh]c3cccc4</chem>	CHEMBL484670 [25] IC ₅₀ = 0,16 µM
<chem>cn(c)cccnc(c1c([n+]2c)cccc1)c(c2c34)[nh]c3c(f)cc(f)c4</chem>	CHEMBL489811 [25] IC ₅₀ = 0,4 µM
<chem>ccn(cc)cccnc(c1c([n+]2c)cccc1)c(c2c34)[nh]c3c(f)cc(f)c4</chem>	CHEMBL490013 [25] IC ₅₀ = 0,27 µM
<chem>cn(c)cccnc(c1c([n+]2c)cccc1)c(c2c34)[nh]c3ccc(f)c4</chem>	CHEMBL491432 [25] IC ₅₀ = 0,31 µM
<chem>ccn(cc)cccnc(c1c([n+]2c)cccc1)c(c2c34)[nh]c3ccc(f)c4</chem>	CHEMBL491633 [25] IC ₅₀ = 0,2 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(ccc(c4)nc(=O)ccn5cccc5)c3ncocccocnc6c(ccc(c7)nc(=O)ccn8cccc8)c7nc(c69)cc(cc9)nc(=O)ccn1cccc1</chem>	CHEMBL506865 [22] IC ₅₀ = 9 µM
<chem>cn(c)cccnc(c1c([n+]2c)cccc1)c(c2c34)[nh]c3cccc4</chem>	CHEMBL507633 [25] IC ₅₀ = 0,22 µM
<chem>c1ccc[n+]1(c)ccc(=O)ncc(ccc2)c(c23)nc4c(c3)cccc4cnc(=O)cc[n+]5(c)cccc5</chem>	CHEMBL566078 [1] IC ₅₀ = 4 µM
<chem>c[n+](c)(c)cc(=O)ncc(ccc1)c(c12)nc3c(c2)cccc3cnc(=O)c[n+](c)(c)c</chem>	CHEMBL572616 [1] IC ₅₀ = 7,3 µM
<chem>cn(c)ccncc1cccc(c12)cc3c(n2)c(ccc3)cncn(c)c</chem>	CHEMBL574042 [1] IC ₅₀ = 5,6 µM
<chem>c[n+](c)(c)ccc(=O)ncc(ccc1)c(c12)nc3c(c2)cccc3cnc(=O)cc[n+](c)(c)c</chem>	CHEMBL575809 [1] IC ₅₀ = 3 µM
<chem>c1cccn1ccc(=O)ncc(ccc2)c(c23)nc4c(c3)cccc4cnc(=O)ccn5cccc5</chem>	CHEMBL5771₅₀[1] IC ₅₀ = 6 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)c(=O)[c@@h]4[c@@h](c3=O)c=cc(=c4)nc(=O)ccn5cccc5</chem>	CHEMBL609670 [6] IC ₅₀ = 4,5 µM

<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)c(=O)[c@h]4[c@h](c3=O)c=cc(=c4)nc(=O)ccn5cccc5</chem>	CHEMBL612102 [6] IC ₅₀ = 1,8 µM
<chem>c[c@h]1cccn1ccc(=O)nc(c2)ccc(c23)n=c4[c@@h](c3=O)c=c(c=c4)nc(=O)ccn5cccc[c@@h]5c</chem>	CHEMBL1076521 [7] IC ₅₀ = 1,5 µM
<chem>occ[c@h]1cccn1ccc(=O)nc(cc2)cc(c23)n=c4[c@h](c3=O)c=c(c=c4)nc(=O)ccn5cccc[c@h]5cco</chem>	CHEMBL1077669 [7] IC ₅₀ = 0,2 µM
<chem>ccn(cc)ccc(=O)nc(cc1)cc(c12)n=c3[c@h](c2=O)c=c(c=c3)nc(=O)ccn(cc)cc</chem>	CHEMBL1077950 [7] IC ₅₀ = 0,7 µM
<chem>c1cccc[n+](1([O-])c(=O)ccccc(=O)nc2ccc(cc2)nc3c(ccc(c4)nc(=O)ccn5cccc5)c4nc(c36)cc(cc6)nc(=O)ccn7cccc7</chem>	CHEMBL1078222 [7] IC ₅₀ = 0,27 µM
<chem>c1cccn1ccc(=O)nc(cc2)cc(c23)nc4c(c3nc5cccccc5)ccc(c4)nc(=O)ccn6cccc6</chem>	CHEMBL1078502 [7] IC ₅₀ = 0,21 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)n=c4[c@@h](c3=O)c=c(c=c4)nc(=O)ccn5cccc5</chem>	CHEMBL1078516 [7] IC ₅₀ = 5,8 µM
<chem>oc1ccn(cc1)ccc(=O)nc(c2)ccc(c23)n=c4[c@h](c3=O)c=c(c=c4)nc(=O)ccn(cc5)ccc5o</chem>	CHEMBL1078525 [7] IC ₅₀ = 2,3 µM
<chem>cn(c)ccc(=O)nc(c1)ccc(c12)n=c3[c@h](c2=O)c=c(c=c3)nc(=O)ccn(c)c</chem>	CHEMBL1078925 [7] IC ₅₀ = 0,6 µM
<chem>c1cncc[n+](1(c)ccc(=O)nc(c2)ccc(c23)n=c4[c@h](c3=O)c=c(c=c4)nc(=O)cc[n+](5(c)ccncc5</chem>	CHEMBL1079036 [7] IC ₅₀ = 1,9 µM
<chem>c1cccn1ccc(=O)nc(c2)ccc(c23)n=c4[c@@h](c3=O)c=c(c=c4)nc(=O)ccn5cccc5</chem>	CHEMBL1079201 [7] IC ₅₀ = 1,9 µM
<chem>cc1ccn(cc1)ccc(=O)nc(cc2)cc(c23)n=c4[c@@h](c3=O)c=cc(=c4)nc(=O)ccn(cc5)ccc5c</chem>	CHEMBL1080613 [7] IC ₅₀ = 1,7 µM
<chem>c1nc(cl)ccc1coc(cc2o)cc(c23)oc(cc3=O)-c4ccc(cc4)occ5ccc(cl)nc5</chem>	CHEMBL1169924 [23] IC ₅₀ = 0,8 µM
<chem>c1nc(cl)ccc1coc(cc2)cc(c23)occ(c3=O)-c4ccc(cc4)oc</chem>	CHEMBL1170488 [13] IC ₅₀ = 2,5 µM
<chem>c1nc(cl)ccc1coc(cc2)cc(c23)oc(cc3=O)-c4ccc(cc4)oc</chem>	CHEMBL1170702 [23] IC ₅₀ = 3,1 µM

Table S2. Cont.

SMILES chemical formula	Reference code and IC ₅₀
<chem>c1nc(Cl)ccc1coc(cc2)ccc2-c(cc3=O)oc(c34)cc(O)cc4O</chem>	CHEMBL1172458 [23] IC ₅₀ = 3,5 µM
<chem>c1cc(O)ccc1[C@@H](c2)n(c(=O)c)n=c2c(c3)c(=O)oc(c34)cccc4Br</chem>	CHEMBL1257134 [23] IC ₅₀ = 4 µM
<chem>c1cccc(Cl)c1[C@H](c2)n(c(=O)c)n=c2c(c3)c(=O)oc(c34)cccc4</chem>	CHEMBL1258868 [23] IC ₅₀ = 6,5 µM
<chem>c1nc(Cl)ccc1csc(O2)nnc2-c3cccc(c34)cccc4</chem>	CHEMBL1276872 [23] IC ₅₀ = 4,2 µM
<chem>c1nc(Cl)ccc1csc(O2)nnc2-c3c(O)cc(cc3)oc</chem>	CHEMBL1278128 [23] IC ₅₀ = 2,3 µM
<chem>CN(C)CCCN1CCN(CC1)C(C2)C3C4CCC(C(=O)N(C(=O)C5CC6)CCN7CCCC7)C5C4C6C8CCC9C(=O)N(C(=O)C2C9C38)CCN1CCCC1</chem>	CHEMBL1689442 [24] IC ₅₀ = 3 µM
<chem>c1cccc1c(=O)n(n=c2c)[C@H](c2)c3c(O)cccc3</chem>	CHEMBL1770486 [24] IC ₅₀ = 4 µM
<chem>c1ccc(c)cc1csc(O2)nnc2-c3ccc(c34)occo4</chem>	CHEMBL1917259 [24] IC ₅₀ = 3,26 µM
<chem>S1CC(C)[N+](CC)C1/C=C2/N(CC)C(=O)/C(S2)=C(/N3C)SC(C34)CCCC4</chem>	CHEMBL1956189 [25] IC ₅₀ = 2 µM
<chem>OC1CCN(CC1)CC(=O)N(N=C2C)[C@H](C2)C3C(O)CCCC3</chem>	CHEMBL2012469 [25] IC ₅₀ = 9,11 µM
<chem>Fc(F)(F)C1CCN(CC1)CC(=O)N(N=C2C)[C@H](C2)C3C(O)CCCC3</chem>	CHEMBL2012474 [25] IC ₅₀ = 8,81 µM
<chem>CC1CCN(CC1)CC(=O)N([C@H](C2)C3CCCC3)N=C2C(C4)C(=O)OC(C45)CCCC5</chem>	CHEMBL2012477 [25] IC ₅₀ = 2 µM

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