Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

1. Molecular datasets used
2. Complexity graphs
3. Scaffolds founded

1. Molecular datasets used
    a. LasR Dataset

Molecule	Activity	pIC_{50}	Reference
S(SCCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O)(=O)(=O)C	INACTIVE	5.82	1
S=C=NC[C@H](F)CCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	INACTIVE	3.81	1
Br[C@H](CCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O)CN=C=S	INACTIVE	4.02	1
Cl[C@H](CCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O)CN=C=S	INACTIVE	3.84	1
SCCCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	INACTIVE	3.94	1
O1CC[C@H](NC(=O)CC(=O)CCCCCCC[C@H]2OC2)C1=O	AGONIST	7.64	1
S(SCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O)(=O)(=O)C	INACTIVE	5	1
S(SCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O)(=O)(=O)C	INACTIVE	5.22	1
O1CC[C@H](NC(=O)CC(=O)CCCCCCCC)C1=O	AGONIST	8.82	2
O1CC[C@H](OC(=O)CC(=O)CCCCCCCCNC(=O)CC(=O)CCCCCCCC)C1=O	INACTIVE	3.6	2
S1CC[C@@H](NC(=O)CC(=O)CCCCCCCC)C1=O	AGONIST	8.82	2
O=C1NCC[C@H]1NC(=O)CC(=O)CCCCCCCC	AGONIST	7.52	2
O=C1CCC[C@H]1NC(=O)CC(=O)CCCCCCCC	AGONIST	7.82	2
O=C(CCCCCCCC)CC(=O)NC1CCCC1	AGONIST	6.8	2
O1C[C@H](NC(=O)CC(=O)CCCCCCCC)CC1	AGONIST	6.04	2
O[C@H]1CCC[C@H]1NC(=O)CC(=O)CCCCCCCC	INACTIVE	5.72	2
O1CCC[C@H]1CNC(=O)CC(=O)CCCCCCCC	AGONIST	6.59	2
O1CC[C@@H](n2nnc(c2)CCCCCCCC)C1=O	INACTIVE	3.51	3
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1Cl	AGONIST	6.43	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1C	AGONIST	6.12	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1cc(ccc1)C	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(cc1)C	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1OC	AGONIST	6.61	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1[N+](=O)[O-]	AGONIST	6.31	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(F)cc1Br	AGONIST	6.36	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1c(Cl)cccc1Cl	AGONIST	6.5	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OCc1c(Cl)cccc1Cl	AGONIST	6.79	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1cc(Cl)ccc1	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2cc([N+](=O)[O-])ccc2)c1OC(=O)c1ccccc1Cl	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2ccc([N+](=O)[O-])cc2)c1OC(=O)c1ccccc1Cl	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2cc(F)c(F)cc2[N+](=O)[O-])c1OC(=O)c1ccccc1Cl	AGONIST	6.48	4
Brc1cc(Br)cc(CC(=O)Nc2ncncc2)c1OC(=O)c1ccccc1Cl	AGONIST	6.22	4
Brc1cc(Br)cc(CC(=O)Nc2cc[nH+]cc2[N+](=O)[O-])c1OC(=O)c1ccccc1Cl	AGONIST	6.35	4
Brc1cc(Br)cc(CC(=O)N[C@H]2CCOC2=O)c1OC(=O)c1ccccc1Cl	AGONIST	9.05	4
Brc1cc(Br)cc(CC(=O)Nc2ncccc2)c1OC(=O)c1ccccc1Cl	INACTIVE	4.38	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(Cl)cc1	INACTIVE	4.3	4
Brc1cc(Br)cc(CNC(=O)c2ncccc2)c1OC(=O)c1ccccc1Cl	INACTIVE	4.1	4
Brc1cc(Br)cc(CC(=O)Nc2cccc(F)c2F)c1OC(=O)c1ccccc1Cl	AGONIST	7.34	4
Brc1cc(Br)cc(CNC(=O)c2cccc(F)c2F)c1OC(=O)c1ccccc1Cl	INACTIVE	4.19	4
Brc1cc(Br)cc(CNC(=O)c2ncncc2)c1OC(=O)c1ccccc1Cl	INACTIVE	5.79	4
Brc1cc(Br)cc(CNC(=O)c2cccnc2)c1OC(=O)c1ccccc1Cl	AGONIST	6.31	4

Brc1cc(Br)cc(CNC(=O)c2ncccc2)c1OC(=O)CCCN1C(=O)C=CC1=O	INACTIVE	4.11	4
Brc1cc(Br)cc(CC(=O)N[C@@H]2CCOC2=O)c1OC(=O)CCCN1C(=O)C=CC1=O	INACTIVE	4	4
Brc1cc(Br)cc(CC(=O)N[C@@H]2CCOC2=O)c1OC(=O)CCN1C(=O)C=CC1=O	INACTIVE	4.62	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1Br	AGONIST	6.57	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1cc(Br)ccc1	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(Br)cc1	INACTIVE	4.3	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1F	INACTIVE	5.89	4
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(F)cc1	INACTIVE	4.3	4
Ic1ccccc1C(Oc1c(cc(Br)cc1Br)CC(=O)Nc1ccccc1[N+](=O)[O-])=O	INACTIVE	5.8	4
O1CC[C@H](NC(=O)CCCCCC)C1=O	INACTIVE	4.29	5
O1CC[C@H](NC(=O)C[C@H]2CCC=C2)C1=O	INACTIVE	4.48	5
O=C1CCCC[C@H]1NC(=O)CC(=O)CCCCCCCCC	ANTAGONIST	5	5
O=C([O-])Cc1nn(nn1)CCCCCCCCCCCC	ANTAGONIST	7.52	5
S1CC[C@H](NC(=O)CCCCCCCCCCC)C1=O	ANTAGONIST	7.4	5
Brc1ccc(cc1)CCC(=O)N[C@H]1CCOC1=O	ANTAGONIST	6.47	5
BrCC(=O)NCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4	5
O1CC[C@H](NC(=O)CCCCCCC)C1=O	ANTAGONIST	5.76	5
O1CC[C@H](NC(=O)CCCCCCCCC)C1=O	ANTAGONIST	6.6	5
O1CC[C@H](NC(=O)CC(=O)CCCCC)C1=O	ANTAGONIST	6.96	5
Ic1ccc(cc1)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.76	5
O1CC[C@H](NC(=O)CC(=O)CCCCCCC)C1=O	AGONIST	7.82	5
O1CC[C@H](NC(=O)C[C@H](O)CCCCCCCCC)C1=O	AGONIST	7.27	5
O1CC[C@H](NC(=O)CC(=O)CCCCCCCCCCC)C1=O	AGONIST	8	5
O1CC[C@H](NC(=O)CC(=O)Cc2ccccc2)C1=O	AGONIST	6.27	5
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)CCN1C(=O)CCC1=O	AGONIST	8.44	5
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)CCCN1C(=O)CCC1=O	AGONIST	6.92	5
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1Cl	AGONIST	7.55	5
O1CC[C@H](NC(=O)CCCc2c3c([nH]c2)cccc3)C1=O	INACTIVE	4.83	6
Oc1ccccc1NC(=O)CC(=O)CCCCC	INACTIVE	4.43	6
O=C(CCCCCCCCC)CC(=O)Nc1ccccc1	ANTAGONIST	5.32	6
O1CC[C@H](NC(=O)Cc2cc([N+](=O)[O-])ccc2)C1=O	ANTAGONIST	6.29	6
S(Cc1nnn(c1)-c1ccc(cc1)C(=O)N[C@H]1CCOC1=O)c1ccccc1	ANTAGONIST	5.58	7
FC(F)(F)Oc1ccc(OCC(=O)N[C@H]2CCOC2=O)cc1	ANTAGONIST	5.33	8
O1CC[C@H](NC(=O)CCCCCCCCCCC)C1=O	AGONIST	7.48	8
S1CC[C@@H](NC(=O)CC(=O)CCCCCCCCC)C1=O	AGONIST	8.15	8
O1CC[C@H](NC(=O)CC(=O)CC\C=C\CCCCC)C1=O	AGONIST	8	8
ClCC(=O)NCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.96	9
O=C([O-])Cc1nn(nn1)CCCCCCCCCCCCC	INACTIVE	4.52	9
S1CC[C@H](NC(=O)CC(=O)CCC)C1=O	INACTIVE	4.89	10
Brc1ccc(cc1)CC(=O)N[C@H]1CCSC1=O	AGONIST	6.4	10
S1CC[C@H](NC(=O)Cc2ccc(cc2)-c2ccccc2)C1=O	INACTIVE	5.54	10
S1CC[C@H](NC(=O)CCc2[nH]c3c(c2)cccc3)C1=O	ANTAGONIST	5.74	10
S1CC[C@H](NC(=O)CCCCC)C1=O	INACTIVE	5.96	10
S1CC[C@H](NC(=O)CCCCCC)C1=O	AGONIST	6.1	10
S1CC[C@H](NC(=O)CCCCCCC)C1=O	AGONIST	6.85	10
S1CC[C@H](NC(=O)Cc2ccccc2)C1=O	INACTIVE	5.6	10

S1CC[C@H](NC(=O)Cc2cc([N+](=O)[O-])ccc2)C1=O	ANTAGONIST	5.39	10
S1CC[C@H](NC(=O)Cc2ccc(OC)cc2)C1=O	INACTIVE	5.14	10
Brc1ccc(cc1)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.32	11
ClCC(=O)NCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.51	11
BrCC(=O)NCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4.57	11
S=C=NCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4.41	11
S=C=NCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.41	11
S=C=NCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	AGONIST	5.59	12
O(C)c1cc(NC(=O)CC(=O)CCCCCCCCC)ccc1	INACTIVE	3.7	12
Brc1cc(OCCCC(=O)N[C@H]2CCSC2=O)ccc1	INACTIVE	5.38	12
O=C(NC1CCCC1)CCCCCCCCC	INACTIVE	4.3	12
O=C(CC(=O)NCCCCCCCCC)c1ccccc1	ANTAGONIST	5.28	12
Clc1cc(ccc1)C(=O)Nc1ccccc1NC(=O)c1cc(Cl)ccc1	INACTIVE	4.16	12
O1CC[C@H](NC(=O)CC(=O)CCC)C1=O	INACTIVE	4.4	12
Oc1ccccc1NC(=O)CC(=O)CCCCCCCCC	INACTIVE	4.77	12
O1CC[C@H](NC(=O)CCCc2ccccc2)C1=O	INACTIVE	3.76	12
FC(F)(F)c1ccc(cc1)CCC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.52	12
Clc1ccc(OCCCC(=O)N[C@H]2CCOC2=O)cc1	INACTIVE	4.68	12
Brc1cc(Br)cc(CNC(=O)c2ccccc2Cl)c1OC(=O)c1ccc(F)cc1	ANTAGONIST	6.62	13
Brc1cc(Br)cc(CNC(=O)c2ccccc2Cl)c1OC(=O)c1ccccc1C	ANTAGONIST	7.27	13
Clc1cc(Cl)ccc1C(Oc1c(cc(cc1C)C)CNC(=O)c1ccccc1Cl)=O	ANTAGONIST	6.04	13
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)CNC(=O)CCl	INACTIVE	4	14
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)N1C(=O)C=CC1=O	INACTIVE	4.06	14
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)CC	ANTAGONIST	5.44	14
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)CCN1C(=O)C=CC1=O	INACTIVE	4.11	14
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)CN1C(=O)C=CC1=O	INACTIVE	4.28	14
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)CCN1C(=O)C=CC1=O	ANTAGONIST	5.82	14
O1CC[C@H](NC(=O)CC(=O)CCCCCCCCCC)C1=O	INACTIVE	4.52	14
[Br+](c1cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c(OC(=O)CCCN=C=S)c(Br)c1)[CH2-]	INACTIVE	3.83	14
[Br+](c1cc(CNC(=O)c2ccccc2[N+](=O)[O-])c(OC(=O)CCCN=C=S)c(Br)c1)[CH2-]	INACTIVE	3.7	14
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OCCCN=C=S	INACTIVE	3.7	14
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OCCCCN=C=S	INACTIVE	3.84	14
Brc1cc(Br)cc(CC(=O)Nc2ccccc2[N+](=O)[O-])c1OC(=O)[N-]C(=O)CCl	INACTIVE	4.13	14
O1CC[C@H](NC(=O)CC(=O)CCCCCCCCC)C1=O	AGONIST	8.75	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(Br)cc1	AGONIST	8.79	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(OC)cc1	AGONIST	8.04	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)CCCCCCC	AGONIST	7.91	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)C	AGONIST	7.69	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OCOC	AGONIST	7.42	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC	AGONIST	7.22	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1O	AGONIST	6.05	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2Cl)c1OC(=O)c1ccccc1[N+](=O)[O-]	AGONIST	8.29	15
Brc1cc(Br)cc(CNC(=O)c2ccccc2Cl)c1OC(=O)c1ccccc1Cl	AGONIST	8.1	15
Fc1cc(ccc1)CNC(=O)c1ccccc1[N+](=O)[O-]	INACTIVE	4.68	16

FC(F)(F)c1ccc(cc1)CNC(=O)c1ccccc1[N+](=O)[O-]	INACTIVE	4.46	16
O=C(NC[C@@H](C)c1ccccc1)c1ccccc1[N+](=O)[O-]	INACTIVE	4.43	16
O=C(NCCc1ccccc1)c1ccccc1[N+](=O)[O-]	INACTIVE	4.68	16
O=C(NCCCCCC)c1ccccc1[N+](=O)[O-]	INACTIVE	4.4	16
O=C(NCCC=1CCCCC=1)c1ccccc1[N+](=O)[O-]	INACTIVE	4.28	16
O=C(NCc1cc([N+](=O)[O-])ccc1)c1ccccc1[N+](=O)[O-]	INACTIVE	4.6	16
O=C(NCCCCCCCCCCC)c1ccccc1[N+](=O)[O-]	AGONIST	6.45	16
Fc1cc(cc(F)c1)CNC(=O)c1ccccc1[N+](=O)[O-]	ANTAGONIST	5.18	16
Fc1cc(ccc1F)CNC(=O)c1ccccc1[N+](=O)[O-]	INACTIVE	4.8	16
Fc1cc(F)ccc1CNC(=O)c1ccccc1[N+](=O)[O-]	INACTIVE	4.35	16
Clc1cc(ccc1)CNC(=O)c1ccccc1[N+](=O)[O-]	ANTAGONIST	5.05	16
Brc1cc(ccc1)CNC(=O)c1ccccc1[N+](=O)[O-]	ANTAGONIST	5.02	16
Ic1cc(ccc1)CNC(=O)c1ccccc1[N+](=O)[O-]	ANTAGONIST	5.19	16
Brc1ccc(cc1)CCNC(=O)c1ccccc1[N+](=O)[O-]	ANTAGONIST	5.32	16
O=C(NCc1ccccc1[N+](=O)[O-])c1ccccc1[N+](=O)[O-]	ANTAGONIST	5.01	16
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1	AGONIST	8.94	16
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1[N+](=O)[O-]	AGONIST	9.17	16
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1OC	AGONIST	8.96	16
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccccc1C#N	AGONIST	8.25	16
Brc1cc(Br)cc(CNC(=O)c2ccccc2[N+](=O)[O-])c1OC(=O)c1ccc(Cl)cc1	AGONIST	8.68	16
BrC/1=CC(O\C\1=C/Br)=O	ANTAGONIST	5.7	17
S(Cc1ccccc1)CC(=O)N[C@@H]1CCOC1=O	INACTIVE	4	17
S(CCc1ccccc1)CC(=O)N[C@@H]1CCOC1=O	INACTIVE	4	17
S(CC(=O)N[C@@H]1CCOC1=O)c1cc2c(cc1)cccc2	INACTIVE	3.82	17
S(CCCCCCC)CC(=O)NC1CCCC1	INACTIVE	3.82	17
S(CCCCCCC)CC(=O)NC1CCCCC1	INACTIVE	4.12	17
S(CCCCCCC)CC(=O)N[C@@H]1CCC[C@H]1O	INACTIVE	4	17
S(CCCCCCC)CC(=O)N[C@@H]1CCCC1=O	INACTIVE	3.82	17
S(CCCCCCC)CC(=O)N[C@@H]1CCCCC1=O	INACTIVE	3.82	17
S(CCCCC)CC(=O)N[C@@H]1CCOC1=O	INACTIVE	3.52	17
S(=O)(CCCCC)CC(=O)N[C@H]1CCOC1=O	INACTIVE	3.52	17
S(=O)(CCCCCCC)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4.3	17
S(CCCCCCC)CC(=O)N[C@@H]1CCOC1=O	ANTAGONIST	5.22	17
S(CCCCCCCCC)CC(=O)N[C@@H]1CCOC1=O	INACTIVE	4.3	17
S(CC(=O)N[C@@H]1CCOC1=O)c1ccccc1	INACTIVE	3.52	17
S(CC(=O)N[C@@H]1CCOC1=O)c1ccc(cc1)C	INACTIVE	4.3	17
S(CC(=O)N[C@@H]1CCOC1=O)c1ccc(O)cc1	INACTIVE	4	17
S1CC[C@@H](NC(=O)Cn2c3c(nc2)N(C)C(=O)N(C)C3=O)C1=O	INACTIVE	3.7	18
O(CC(=O)NN1C(=Nc2c(cccc2)C1=O)C)c1ccccc1	INACTIVE	3.92	18
O=C(Nc1ncccc1C)c1n(nc(c1)C(=O)Nc1ncccc1C)C	INACTIVE	4.46	18
s1ccnc1NS(=O)(=O)c1ccc(NS(=O)(=O)c2ccccc2[N+](=O)[O-])cc1	INACTIVE	4.22	18
s1ccnc1NS(=O)(=O)c1ccc(N)cc1	ANTAGONIST	5.05	18
O1CC[C@H](NC(=O)Cn2nnc(c2)CCCC)C1=O	INACTIVE	4.75	19
O1CC[C@H](NC(=O)Cn2nnc(c2)CCCCC)C1=O	ANTAGONIST	5.49	19
O1CC[C@H](NC(=O)Cn2nnc(c2)C2CCCC2)C1=O	INACTIVE	4.79	19
O1CC[C@H](NC(=O)Cn2nnc(c2)C2CCCCC2)C1=O	INACTIVE	4.91	19

O1CC[C@H](NC(=O)Cn2nnc(c2)-c2ccccc2)C1=O	INACTIVE	4.8	19
Fc1cc(cc(F)c1)-c1nnn(c1)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4.86	19
O1CC[C@H](NC(=O)CCc2nnn(c2)-c2ccc(OC)cc2)C1=O	INACTIVE	4.78	19
O1CC[C@H](NC(=O)CCc2nnn(c2)-c2ccc(cc2)C)C1=O	INACTIVE	4.96	19
O1CC[C@H](NC(=O)CCc2nnn(c2)-c2cc(N)ccc2)C1=O	ANTAGONIST	5.39	19
O=C1NC=Nc2[nH]nnc12	ANTAGONIST	6.14	20
Fc1cc(ccc1)C[C@@H]([NH3+])C(=O)[O-]	ANTAGONIST	5.74	20
O=C1NC(Nc2[nH]nnc12)=N	ANTAGONIST	6.19	20
O=C([O-])[C@@H]([NH3+])[C@H](O)c1ccccc1	ANTAGONIST	5.44	20
O=C([O-])c1c2c([nH]c1)cccc2	ANTAGONIST	5.68	20

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b. PqsR dataset

Molecule	Activity	pIC_{50}	Reference
O=C(N)c1ccc(cc1)C(C)(C)C	AGONIST	6.05	1
o1c(nnc1N)-c1cc(ccc1)C	INACTIVE	4.91	1
FC(F)(F)c1cc(ccc1)-c1oc(nn1)C	INACTIVE	4.89	1
FC(F)(F)c1cc(ccc1)-c1ocnn1	INACTIVE	5.19	1
s1cccc1-c1[nH]nc(c1)C(F)(F)F	INACTIVE	5.07	1
o1c(nnc1N)-c1cc(ccc1)C(C)(C)C	INACTIVE	5.51	1
O=C(N)c1cc2c(cc1)cccc2	AGONIST	6.1	1
Brc1cc(ccc1)C(=O)N	INACTIVE	5.17	1
Brc1nc(N)ccc1	INACTIVE	5.17	1
Clc1ccc(cc1)-c1oc(nn1)N	INACTIVE	3.7	1
Clc1ccc(cc1)-c1sc(nn1)N	INACTIVE	5.43	1
o1c(nnc1N)-c1cc(ccc1)C#N	INACTIVE	4.75	1
FC(F)(F)c1cc(ccc1)-c1oc(nn1)N	AGONIST	5.89	1
Clc1cc(ccc1)-c1oc(nn1)N	INACTIVE	4.57	1
Fc1cc2N=C(N([O-])C(=O)c2cc1)CCCCCCCCC	INACTIVE	4.68	2
Clc1cc2N=C(N(OC)C(=O)c2cc1)CCCCCCCCC	INACTIVE	4.43	2
Fc1cc2N=C(N(OC)C(=O)c2cc1)CCCCCCCCC	AGONIST	5.66	2
Fc1cc2c(N=C(N(OC)C2=O)CCCCCCCCC)cc1F	INACTIVE	4.27	2
O=C1N(N)C(=Nc2c1cccc2)CCCCCCC	INACTIVE	4.27	2
O=C1N(N)C(=Nc2c1cccc2)CCCCCCCCC	INACTIVE	4.11	2
O=C1N(N)C(=Nc2c1cccc2)CCCCCCCCCCC	INACTIVE	3.68	2
Clc1cc2N=C(N(N)C(=O)c2cc1)CCCCCCCCC	ANTAGONIST	5.3	2
Fc1cc2N=C(N(N)C(=O)c2cc1)CCCCCCCCC	ANTAGONIST	5.41	2
Fc1cc2c(N=C(N(N)C2=O)CCCCCCCCC)cc1F	ANTAGONIST	5.92	2
O=C1N(CC[NH3+])C(=Nc2c1cccc2)CCCCCCCCC	INACTIVE	3.77	2
Clc1cc2c(N=C(N(CC[NH3+])C2=O)CCCCCCCCC)cc1	ANTAGONIST	5.03	2
Clc1cc2N=C(N(CC[NH3+])C(=O)c2cc1)CCCCCCCCC	INACTIVE	4.71	2
Clc1cc2N=C(N(CCC[NH3+])C(=O)c2cc1)CCCCCCCCC	INACTIVE	4.81	2
Clc1cc2N=C(N(CC[NH3+])C(=O)c2cc1)CCCc1ccccc1	INACTIVE	4.1	2
Clc1cc2N=C(N(N)C(=O)c2cc1)CCCc1ccccc1	INACTIVE	4.4	2
O=C1C=C(Nc2c1cccc2)CCCCCCCCC	AGONIST	6.4	2

OC=1C(=O)c2c(NC=1CCCCCCCCC)cccc2	AGONIST	5.96	2
Clc1cc2NC(CCCCCCC)=C(O)C(=O)c2cc1	AGONIST	7.85	2
O=C1c2c(NC(CCCCCCC)=C1N)cccc2	AGONIST	6.4	2
O=C1N([O-])C(=Nc2c1cccc2)CCCCCCC	INACTIVE	4.27	2
O=C1N([O-])C(=Nc2c1cccc2)CCCCCCCCC	INACTIVE	4.52	2
Clc1cc2N=C(N([O-])C(=O)c2cc1)CCCCCCCCC	INACTIVE	4.9	2
FC(F)(F)c1cc2c(NC(=CC2=O)CCCCCCC)cc1	ANTAGONIST	7.27	3
O=C1C=C(Nc2c1cc([N+](=O)[O-])cc2)CCCCOCC	ANTAGONIST	5.45	3
O=C1c2cc([N+](=O)[O-])ccc2NC(CCCCCCC)=C1CO	ANTAGONIST	7.14	3
O=C1c2cc([N+](=O)[O-])ccc2NC(CCCCCCC)=C1C(=O)N	ANTAGONIST	7.46	3
O=C1C=C(Nc2c1cc([N+](=O)[O-])cc2)CCCCCCC	ANTAGONIST	7.29	3
OC=1C(=O)c2c(NC=1CCCCCCC)cccc2	AGONIST	8.2	3
OC=1C(=O)c2cc([N+](=O)[O-])ccc2NC=1CCCCCCC	AGONIST	8.55	3
FC(F)(F)c1cc2c(N(C)C(=CC2=O)CCCCCCC)cc1	ANTAGONIST	6.57	3
FC(F)(F)c1cc2c(N(C)C(=CC2=O)CCCCCC)cc1	ANTAGONIST	6.64	3
FC(F)(F)c1cc2c(NC(=CC2=O)COCCCCC)cc1	ANTAGONIST	6.76	3
O=C1C=C(Nc2c1cc([N+](=O)[O-])cc2)COCCCCC	ANTAGONIST	6.6	3
FC(F)(F)c1cc2c(NC(=CC2=O)CCCCOCC)cc1	ANTAGONIST	5.77	3
O=C(N[O-])c1ccc(cc1)C(C)(C)C	INACTIVE	4.63	4
S(=O)(=O)(C)c1nc(-n2nnnc2)ccn1	INACTIVE	4.82	4
S(=O)(=O)(CCCCCC)c1nc(-n2nncc2)ccn1	INACTIVE	4.3	4
Brc1cc(ccc1)-c1oc(nn1)N	ANTAGONIST	5.12	5
FC(F)(F)Oc1cc(ccc1)-c1oc(nn1)N	INACTIVE	4.33	5

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c. RhlR dataset

Molecule	Activity	pIC_{50}	Reference
O1CC[C@H](NC(=O)CCC)C1=O	INACTIVE	5.09	1
O1CC[C@H](NC(=O)CC2CC2)C1=O	AGONIST	5.56	1
S1CC[C@H](NC(=O)CCC)C1=O	AGONIST	5.42	1
O=C1CCC[C@@H]1NC(=O)CCC	INACTIVE	4.84	1
O1CC[C@H](NC(=O)CCC=C)C1=O	INACTIVE	5.1	1
O=C1CCC[C@@H]1NC(=O)C1CCC1	INACTIVE	5.23	1

Ic1ccc(OCC(=O)NC[C@H]2OCCC2)cc1	INACTIVE	4	1
Ic1ccc(OCC(=O)N[C@H]2CCSC2=O)cc1	INACTIVE	4.5	1
S1CC[C@H](NC(=O)C2CCC2)C1=O	AGONIST	5.76	1
O=C1CCC[C@@H]1NC(=O)CC(C)C	INACTIVE	5.12	1
S1CC[C@H](NC(=O)CC(C)C)C1=O	AGONIST	6.33	1
O1CC[C@H](NC(=O)CC(C)C)C1=O	AGONIST	5.99	1
O=C(NC1CCCC1)C1CCC1	INACTIVE	4.57	1
O1CC[C@H](NC(=O)C2CCCC2)C1=O	AGONIST	5.91	1
O1CC[C@H](NC(=O)CCCC)C1=O	INACTIVE	4.97	1
O1CC[C@H](NC(=O)C(C)C)C1=O	AGONIST	5.31	1
O1CC[C@H](NC(=O)[C@@H](CC)C)C1=O	INACTIVE	5.11	1
O1CC[C@H](NC(=O)C\C=C\C)C1=O	INACTIVE	5.16	1
O1CC[C@H](NC(=O)C2CCC2)C1=O	AGONIST	5.85	1
O1CC[C@H](NC(=O)Cc2cc(ccc2)C)C1=O	AGONIST	5.7	2
O1CC[C@H](NC(=O)Cc2cc(OC)ccc2)C1=O	AGONIST	5.33	2
O1CC[C@H](NC(=O)Cc2cc(ccc2)C#N)C1=O	AGONIST	5.77	2
S(C)c1cc(ccc1)CC(=O)N[C@H]1CCOC1=O	INACTIVE	5.18	2
Clc1ccc(cc1)CCC(=O)N[C@H]1CCOC1=O	INACTIVE	5.18	2
Brc1cc(ccc1)CCC(=O)N[C@H]1CCOC1=O	INACTIVE	4.95	2
O1CC[C@H](NC(=O)CCc2ccc([N+](=O)[O-])cc2)C1=O	INACTIVE	4.57	2
O1CC[C@H](NC(=O)CC2CCCC2)C1=O	AGONIST	5.51	2
Ic1ccc(cc1)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.09	2
O1CC[C@H](NC(=O)Cc2ccc([N+](=O)[O-])cc2)C1=O	INACTIVE	4.75	2
O1CC[C@H](NC(=O)Cc2ccc(cc2)C)C1=O	INACTIVE	4.7	2
FC(F)(F)c1ccc(cc1)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4.61	2
Clc1cc(ccc1Cl)CC(=O)N[C@H]1CCOC1=O	ANTAGONIST	5.47	2
O1CC[C@H](NC(=O)Cc2ccccc2)C1=O	INACTIVE	4.83	2
O1CC[C@H](NC(=O)Cc2cc3c(cc2)cccc3)C1=O	INACTIVE	4.68	2
O1CC[C@H](NC(=O)COc2ccc(cc2)C)C1=O	ANTAGONIST	4.97	2
O1CC[C@H](NC(=O)COc2ccc(OC)cc2)C1=O	ANTAGONIST	4.92	2
Brc1ccc(OCC(=O)N[C@H]2CCOC2=O)cc1	ANTAGONIST	5.23	2
Ic1ccc(OCC(=O)N[C@H]2CCOC2=O)cc1	INACTIVE	4.76	2
S(C)c1ccc(cc1)CCC(=O)N[C@H]1CCOC1=O	INACTIVE	4.66	2
Fc1ccc(cc1)CC(=O)N[C@H]1CCOC1=O	INACTIVE	5.05	2
Clc1cc(ccc1)CC(=O)N[C@H]1CCOC1=O	INACTIVE	5.26	2
Ic1cc(ccc1)CC(=O)N[C@H]1CCOC1=O	INACTIVE	5.24	2
Brc1cc(OCCCC(=O)N[C@H]2CCSC2=O)ccc1	ANTAGONIST	5.4	3
[Br+](c1cc(OCCCC(=O)N[C@@H]2CCSC2=O)ccc1)[CH2-]	INACTIVE	4	3
Clc1cc(OCCCC(=O)N[C@@H]2CCSC2=O)ccc1	ANTAGONIST	5.05	3
S=C=NCCCCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O	INACTIVE	4.25	3
O=C(CC(=O)NCCCCCCCCC)c1ccccc1	INACTIVE	4.74	3

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2. Complexity graphs

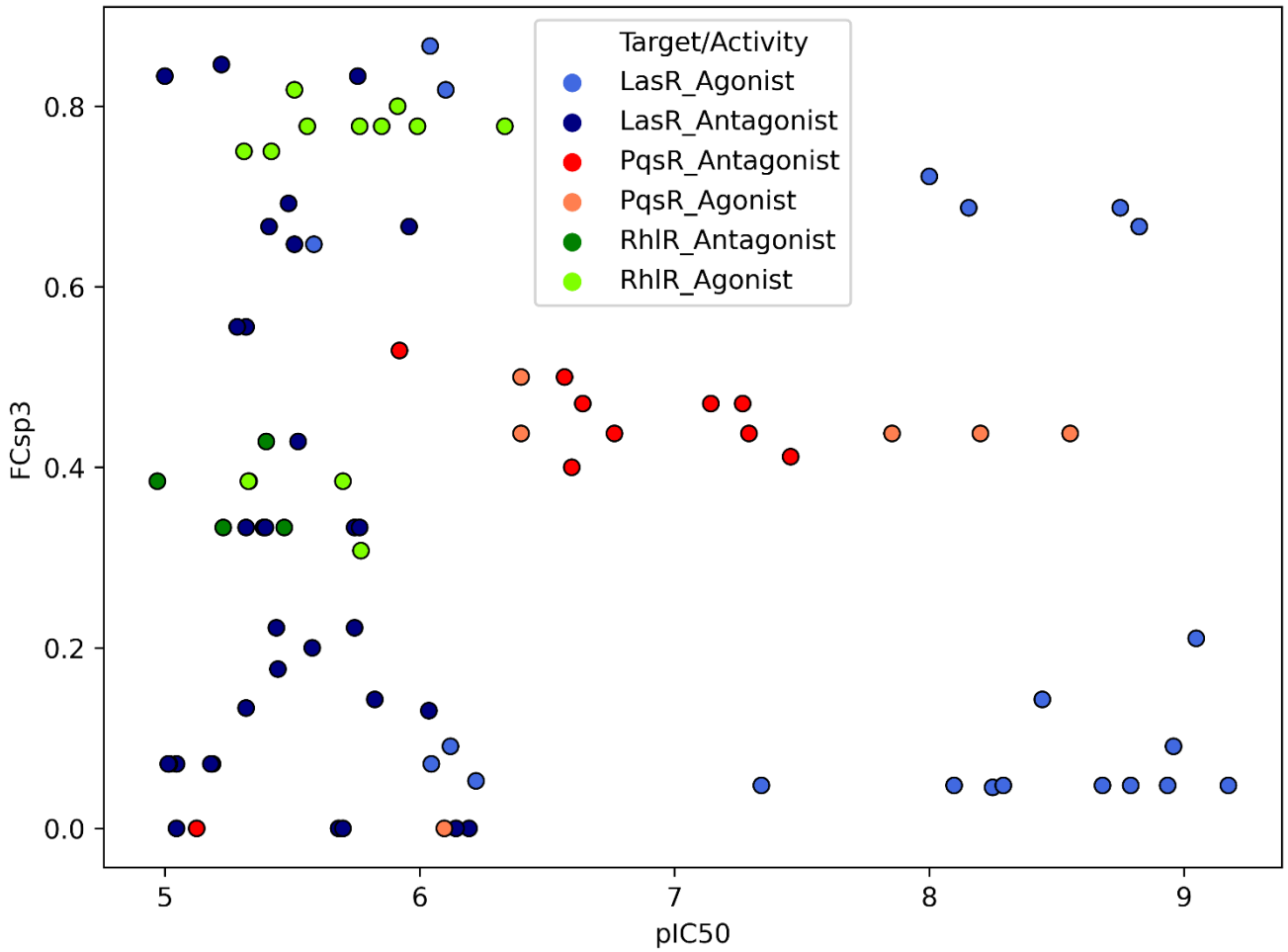

Fig. 1 Distribution of biological activity values against fraction of sp^3 carbons complexity. Molecules with activity against LasR, PqsR and RhlR appear in blue, red and green respectively; light colors represent agonist compounds and dark colors antagonist compounds.

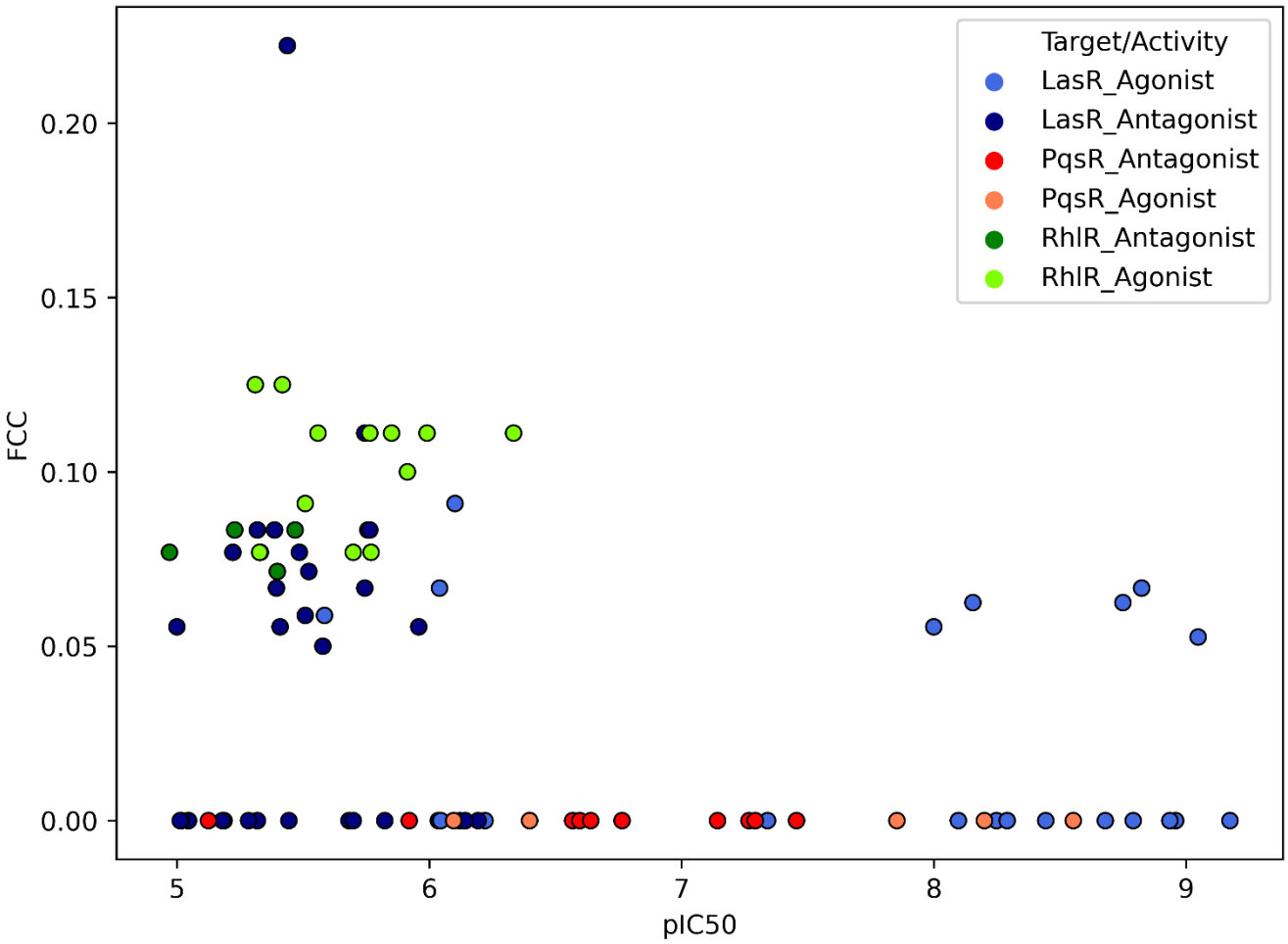

Fig. 2 Distribution of biological activity values against fraction of chiral centers complexity. Molecules with activity against LasR, PqsR and RhlR appear in blue, red and green respectively; light colours represent agonist compounds and dark colours antagonist compounds.

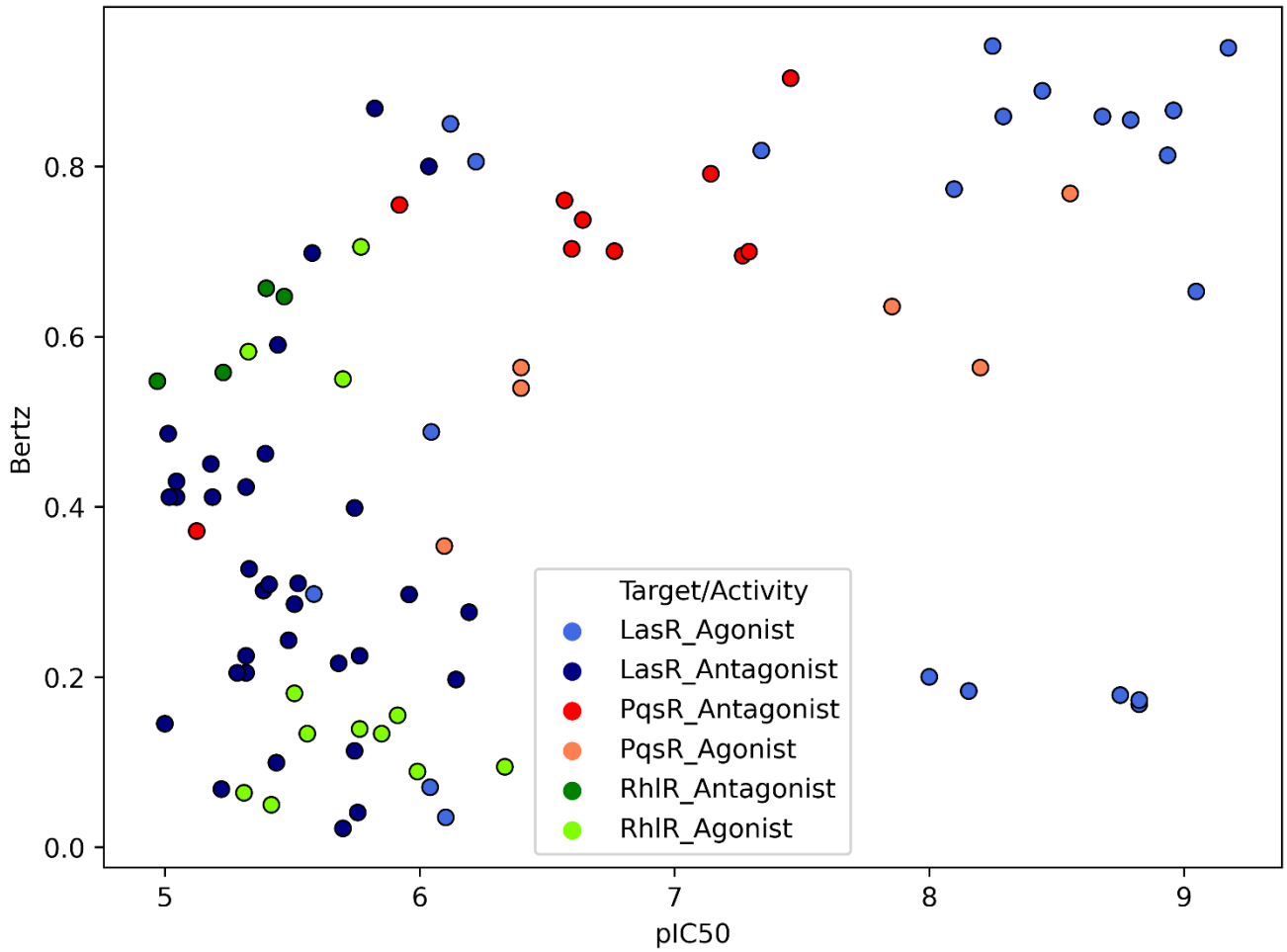

Fig. 3 Distribution of biological activity values against Bertz complexity. Molecules with activity against LasR, PqsR and RhlR appear in blue, red and green respectively; light colours represent agonist compounds and dark colours antagonist compounds.

3. Scaffolds founded
    (a) LasR Scaffolds

Scafold	Frecuency
c1ccoc1	22
O=C(Cc1ccccc1OC(=O)c1ccccc1)Nc1ccccc1	21
O=C(NCc1ccccc1)c1ccccc1	16
O=C(NCc1ccccc1OC(=O)c1ccccc1)c1ccccc1	14
O=C1CCCO1	11
c1ccccc1	9
O=C(Cc1ccccc1)Nc1ccccc1	5
C1CCCC1	5
O=C(Cc1ccccc1)NC1CCSC1=O	4
O=C1CCCS1	4
O=C(CSc1ccccc1)NC1CCOC1=O	3
O=C(CCc1cn(-c2ccccc2)nn1)NC1CCOC1=O	3
O=C(NCCc1ccccc1)c1ccccc1	3
c1ccsc1	3
O=C(Cc1ccccc1)NC1CCOC1=O	3
O=C(Cn1ccnn1)NC1CCOC1=O	2
c1nn[nH]n1	2
O=C(CCc1ccccc1)NC1CCOC1=O	2
O=C(Cn1cc(-c2ccccc2)nn1)NC1CCOC1=O	2
O=C1CCCCC1	2
C1CCOC1	2
O=C1CCCC1	2
O=C(CCCn1cccc1)Oc1ccccc1CNC(=O)c1ccccc1	1
O=C(Cc1ccccc1OC(=O)c1ccccc1)N=c1cc[nH]cc1	1
C=C1C=CC(=O)O1	1
O=C(Cc1ccccc1OC(=O)CCn1cccc1)Nc1ccccc1	1
O=C(Cc1ccccc1OC(=O)CCN1C(=O)C=CC1=O)NC1CCOC1=O	1
O=C(COc1ccccc1)Nn1cnc2ccccc2c1=O	1
O=S(=O)(N=c1[nH]ccs1)c1ccccc1	1
O=S(=O)(N=c1[nH]ccs1)c1ccc(NS(=O)(=O)c2ccccc2)cc1	1
O=C(Cc1ccccc1OC(=O)c1ccccc1)N=c1cc[nH]cn1	1
O=C(CSCCc1ccccc1)NC1CCOC1=O	1
O=C(N=c1cccc[nH]1)c1cc(C(=O)N=c2cccc[nH]2)[nH]n1	1
O=C(Oc1ccccc1CNC(=O)c1ccncn1)c1ccccc1	1
O=C(NCCC1=CCCCC1)c1ccccc1	1
O=C([CH-]c1ccccc1)Nc1ccccc1	1
O=C(Cc1ccccc1OC(=O)c1ccccc1)NC1CCOC1=O	1

c1ccc2[nH]ccc2c1	1
O=C1OCCC1n1ccnn1	1
O=C(Cn1cnc2[nH]c(=O)[nH]c(=O)c21)NC1CCSC1=O	1
O=C(Cc1ccccc1OC(=O)CCN1C(=O)C=CC1=O)Nc1ccccc1	1
O=C(Cn1cc(C2CCCC2)nn1)NC1CCOC1=O	1
O=C(CCCOc1ccccc1)NC1CCSC1=O	1
O=C(CSc1ccc2ccccc2c1)NC1CCOC1=O	1
O=C(CCCc1ccccc1)NC1CCOC1=O	1
O=C(CSCc1ccccc1)NC1CCOC1=O	1
O=c1[nH]cnc2[nH]nnc12	1
O=C(Cc1ccccc1OC(=O)c1ccccc1)N=c1cccc[nH]1	1
O=C(Cn1cc(C2CCCCC2)nn1)NC1CCOC1=O	1
O=C(CCCCCCCCCC1CO1)Nc1ccoc1	1
O=C(CCCOc1ccccc1)NC1CCOC1=O	1
O=C(Cc1ccc(-c2ccccc2)cc1)NC1CCSC1=O	1
O=C(Oc1ccccc1CNC(=O)c1ccccn1)c1ccccc1	1
O=C(CCN1C(=O)C=CC1=O)Oc1ccccc1CNC(=O)c1ccccc1	1
N=c1[nH]c(=O)c2[nH]nnc2[nH]1	1
O=C(NCc1ccccc1OC(=O)c1ccccc1)c1cccnc1	1
O=C(Cc1ccccc1OCc1ccccc1)Nc1ccccc1	1
C1CCCCC1	1
O=C(Cc1ccccc1OC(=O)N1C(=O)C=CC1=O)Nc1ccccc1	1
O=C(NC1CCOC1=O)c1ccc(-n2cc(CSc3ccccc3)nn2)cc1	1
O=C(Nc1ccccc1NC(=O)c1ccccc1)c1ccccc1	1
c1cc[nH]c1	1
O=C(CCCc1c[nH]c2ccccc12)NC1CCOC1=O	1
O=C(COc1ccccc1)NC1CCOC1=O	1
O=C(CN1C(=O)C=CC1=O)Oc1ccccc1CNC(=O)c1ccccc1	1
O=C(CCc1cc2ccccc2[nH]1)NC1CCSC1=O	1
O=C(CCCc1ccccc1)Nc1ccoc1	1
O=C(CCCN1C(=O)C=CC1=O)Oc1ccccc1CNC(=O)c1ccccn1	1
O=C(CC1C=CCC1)NC1CCOC1=O	1
O=C(Cc1ccccc1OC(=O)CCCN1C(=O)C=CC1=O)NC1CCOC1=O	1

(b) PqsR Scaffolds

Scaffold	Frecuency
O=c1[nH]cnc2ccccc12	17
O=c1cc[nH]c2ccccc12	16
N=c1[nH]nc(-c2ccccc2)o1	8
c1ccccc1	3
c1ccc(-c2nnco2)cc1	2

O=c1[nH]c(CCCc2ccccc2)nc2ccccc12	2
N=c1cccc[nH]1	1
N=c1[nH]nc(-c2ccccc2)s1	1
c1ccc2ccccc2c1	1
c1cc(-n2cnnn2)ncn1	1
c1csc(-c2ccn[nH]2)c1	1
c1cc(-n2ccnn2)ncn1	1

(c) RhlR Scaffolds

Scaffold	Frecuency
O=C(Cc1ccccc1)NC1CCOC1=O	13
O=C1CCCO1	6
O=C(CCc1ccccc1)NC1CCOC1=O	4
O=C(COc1ccccc1)NC1CCOC1=O	4
O=C1CCCS1	2
O=C1CCCC1	2
O=C(CCCOc1ccccc1)NC1CCSC1=O	2
c1ccoc1	2
O=C(COc1ccccc1)NCC1CCCO1	1
c1ccccc1	1
O=C(NC1CCCC1)C1CCC1	1
O=C(NC1CCSC1=O)C1CCC1	1
O=C([CH-]CCOc1ccccc1)NC1CCSC1=O	1
O=C(Cc1ccc2ccccc2c1)NC1CCOC1=O	1
O=C(NC1CCCC1=O)C1CCC1	1
O=C(CC1CC1)NC1CCOC1=O	1
O=C(NC1CCOC1=O)C1CCCC1	1
O=C(NC1CCOC1=O)C1CCC1	1
O=C(CC1CCCC1)NC1CCOC1=O	1
O=C(COc1ccccc1)NC1CCSC1=O	1