Article

Computational tools in the discovery of FABP4 ligands: a statistical and molecular modeling approach

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Table S1. Chemical structures of the FABP4 inhibitors used as benchmark for docking methodology validation, including both experimental and calculated p*K*i binding affinities.

Compound[a]	SMILES	Exp. p*K*i	Calcd. p*K*i
BMS309403	CCC1=C(C2=CC=CC=C2)C(C3=CC=CC=C3)=NN1C4=CC=CC=C4C5=CC=CC(OCC(O)=O)=C5	7.82	7.46
1a	[H]C(C(O)=O)(OC1=CC(C2=CC=CC=C2C3=NN(C(C4=CC=CC=C4)=C3)C5=CC=C(C=C5)[H])=CC=C1)[H]	7.49	8.00
1b	[H]C(C([O-])=O)OC1=CC(C2=CC=CC=C2C3=NN(C4=CC=C(Cl)C=C4)C(C5=CC=CC=C5)=C3)=CC=C1	7.89	7.82
1c	[H]C(C(O)=O)(OC1=CC(C2=CC=CC=C2C3=NN(C(C4=CC=CO4)=C3)C5=CC=C(C=C5)Cl)=CC=C1)[H]	8.15	8.22
1d	[H]C(C(O)=O)(OC1=CC(C2=CC=CC=C2C3=NN(C(C4=CC=CS4)=C3)C5=CC=C(C=C5)Cl)=CC=C1)[H]	8.30	7.68
1f	[H]C(CC)(C([O])=O)OC1=CC(C2=CC=CC=C2C3=NN(C4=CC=C(Cl)C=C4)C(C5=CC=CS5)=C3)=CC=C1	8.22	7.28
2a	O=C([O-])CCCCOC1=C(C2=NC(C3=CC=CC=C3)=C(C4=CC=CC=C4)O2)C=CC=C1	7.24	6.70
2b	O=C(COC1=CC=CC(C2=C(C=CC=C2)C3=NC(C4=CC=CC=C4)=C(O3)C5=CC=CC=C5)=C1)[O-]	8.22	8.17
3a	O=C(COC1=CC(C2=CC=CC=C2C3=NC(C4=CC=CC=C4)=C(C5=CC=CC=C5)N3)=CC=C1)[O-]	8.03	7.96
3b	O=C(CNC1=CC(C2=CC=CC=C2C3=NC(C4=CC=CC=C4)=C(C5=CC=CC=C5)N3)=CC=C1)[O-]	7.74	8.30
3d	CN1C(C2=CC=CC=C2C3=CC=CC(NCC([O-])=O)=C3)=NC(C4=CC=CC=C4)=C1C5=CC=CC=C5	8.57	6.62
3g	[O-]C(CNC1=CC(C2=CC=CC=C2C3=NC(C4=CC=CC=C4)=C(C5=CC=CC=C5)N3CC(C)C)=CC=C1)=O	6.89	6.21
3f	[O-]C(CNC1=CC(C2=CC=CC=C2C3=NC(C4=CC=CC=C4)=C(C5=CC=CC=C5)N3CC)=CC=C1)=O	8.47	6.39
18	O=C([O-])CCN1C(C2=CC=CC(OC(C)C)=C2)=C(C3=C(C)NN=C3C)C4=C1C=CC(C5CC5)=C4	7.52	7.57
19	O=C([O-])CCN1C(C2=CC=CC=C2)=C(C3=C(OC)C=NC=C3)C4=C1C=CC(C5CC5)=C4	7.00	6.83
20	O=C([O-])CCN1C(C2=CC=CC=C2)=C(C3=CC=CC=C3)C4=C1C=CC(C5CC5)=C4	6.92	6.69
33	ClC(C=C1)=CC2=C1N=C(C)C(C(O)=O)=C2C3=CC=CC=C3	6.98	6.26
34a	ClC1=CC2=C(N=C(C([O-])=O)C(C(C)C)=C2C3=CC=CC([H])=C3)C([H])=C1	7.92	6.34
34b	ClC1=CC2=C(N=C(C([O-])=O)C(N3CCCCC3)=C2C4=CC=CC([H])=C4)C([H])=C1	7.66	6.91
34c	ClC1=CC2=C(N=C(C([O-])=O)C(N3CCCCC3)=C2C4=CC=CC([H])=C4)C(Cl)=C1	7.80	6.37
34d	ClC1=CC2=C(N=C(C([O-])=O)C(N3CCCCC3)=C2C4=CC=CC([H])=C4)C(C)=C1	7.89	6.97
34e	ClC1=CC2=C(C=C1)N=C(C(C(C)C)=C2C3=CC=CC(C(C)C)=C3)C([O-])=O	7.80	5.41
34f	ClC1=CC2=C(N=C(C3=NN=NN3)C(N4CCCCC4)=C2C5=CC=CC([H])=C5)C=C1	7.96	8.15
34g	ClC1=CC2=C(N=C(C3=NNC(O3)=O)C(N4CCCCC4)=C2C5=CC=CC([H])=C5)C=C1	7.70	7.62
34h	ClC1=CC2=C(N=C(C3=NNC(O3)=S)C(N4CCCCC4)=C2C5=CC=CC([H])=C5)C=C1	8.15	6.95
39	O=C(/C(S1)=C\C2=CC(OCC)=C(O)C=C2)N(CCC([O-])=O)C1=S	5.60	5.69
41	O=S(NC1=CC(SCC([O-])=O)=C(O)C2=CC=CC=C21)(C3=CC=C(Cl)C=C3)=O	5.64	6.68

42	O=C([O-])C(C1C2C(Cl)C(SC3=CC=CC=C3[N+]([O-])=O)C1)[NH+]4CC5C(CCC5)C6=CC=CC2=C64	5.50	6.64
42a	[O-]C(C1C2C(C=CC2)C3=C(C)C=C(C)C4=C3[NH+]1CC5C4C=CC5)=O	6.21	7.19
42b	[O-]C(C1C2C(C=CC2)C3=CC(Br)=CC4=C3[NH+]1CC5C4C=CC5)=O	6.54	6.59
42c	[O-]C(C1C2C(C=CC2)C3=CC(C)=CC4=C3[NH+]1CC5C4C=CC5)=O	6.42	6.60
42d	[O-]C(C1C2C(C=CC2)C3=CC(Cl)=CC4=C3[NH+]1CC5C4C=CC5)=O	6.16	6.79
44	CC1=C(C)C=CC(/C=C2NC(/C(S/2)=C/C3=CC=CN3C4=CC=CC(C([O-])=O)=C4)=O)=C1	5.44	7.24
45	O=S(C1=CC(OCCC)=C(Cl)C=C1)(NC2=CC=C(C([O-])=O)C=C2)=O	5.37	5.67

[a] The numbers correspond to that reported in the reference [1].

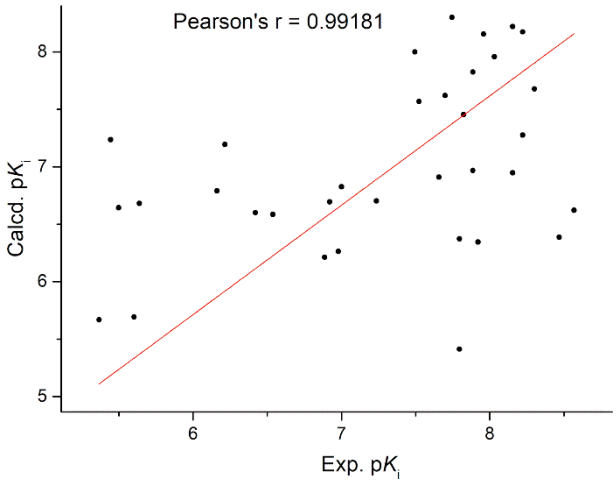

Figure S1. Linear regression plot of experimental *vs*. calculated pK_i values reported in Table S1.

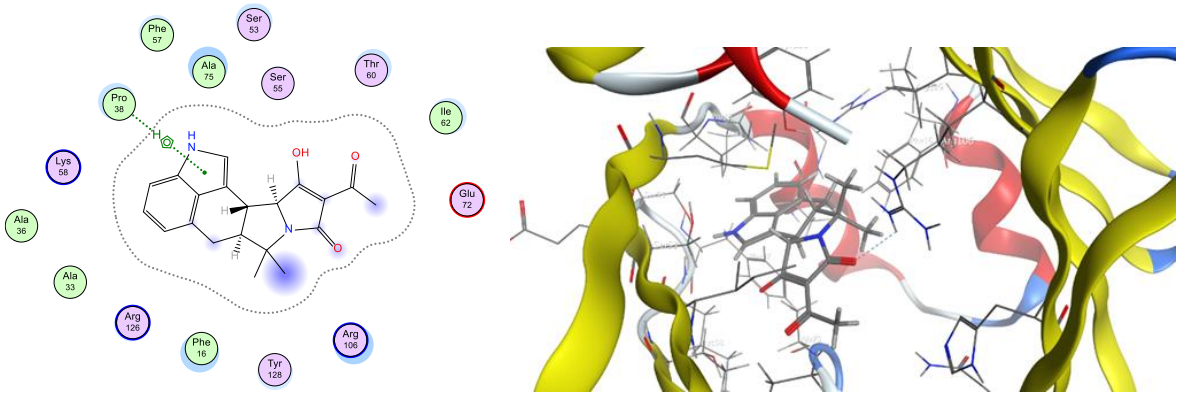

Figure S2. Docking binding pose of 5339.

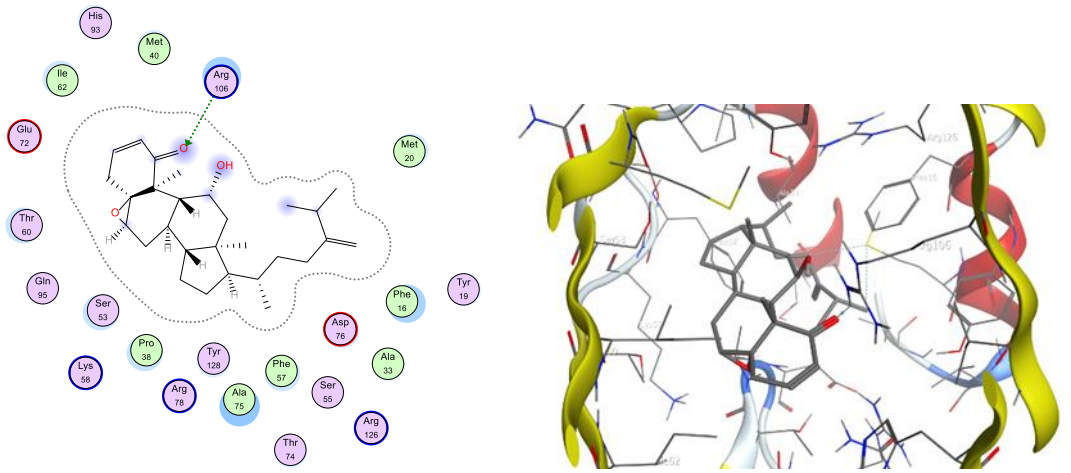

Figure S3. Docking binding pose of 14123.

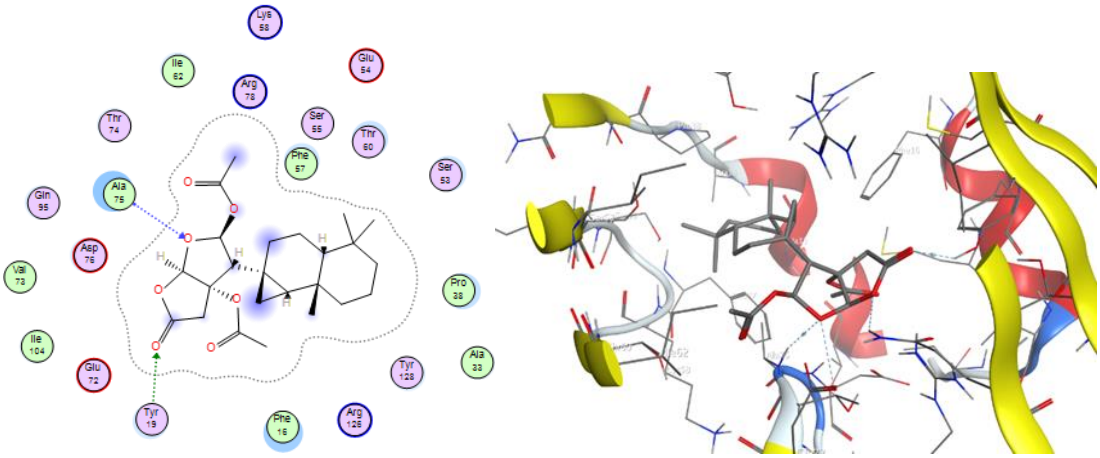

Figure S4. Docking binding pose of 13575.

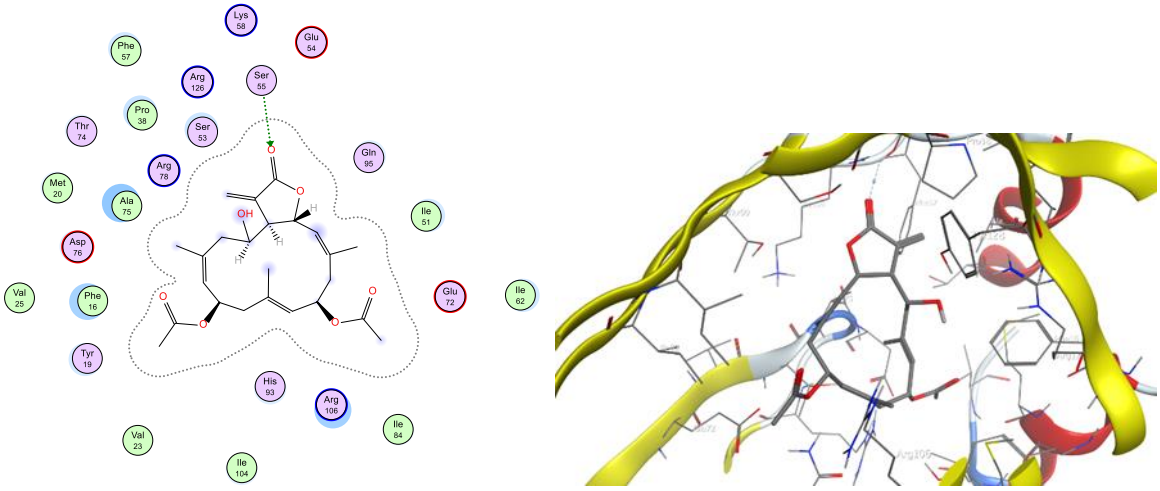

Figure S5. Docking binding pose of 7846.

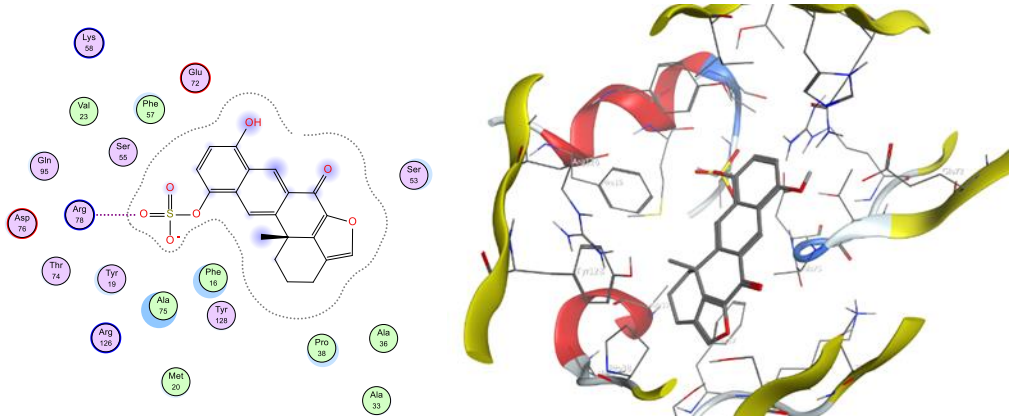

Figure S6. Docking binding pose of 3164.

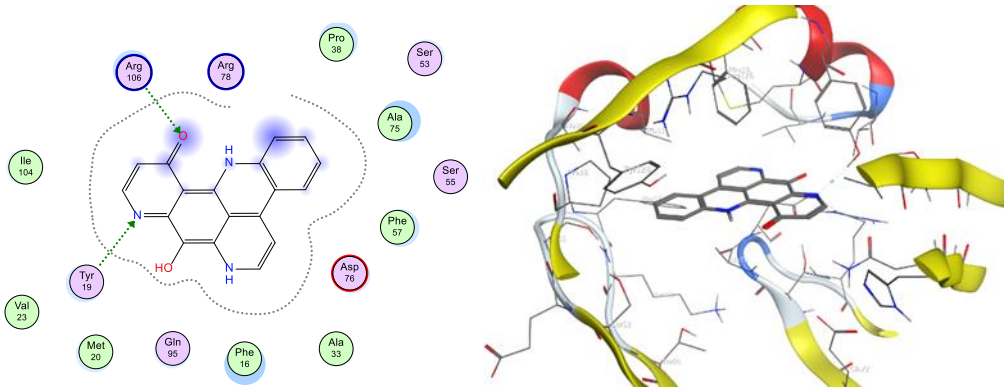

Figure S7. Docking binding pose of 2076.

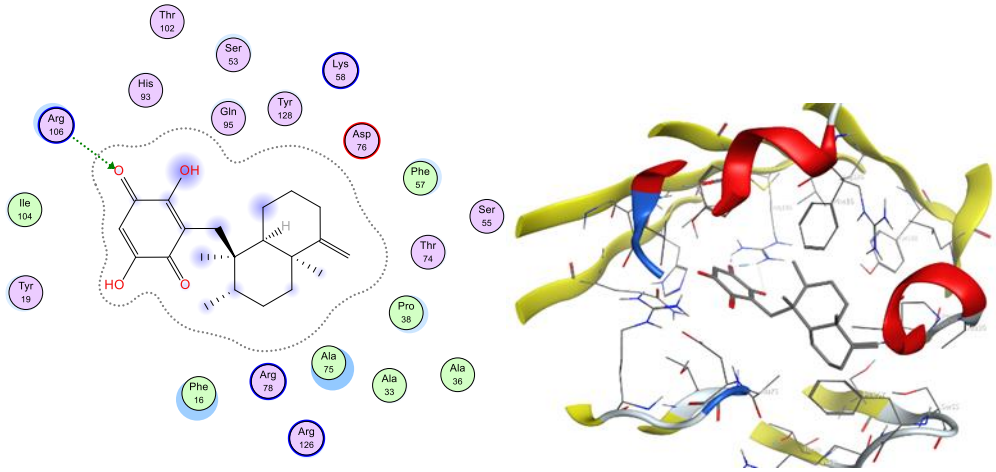

Figure S8. Docking binding pose of 1534.

Table S2. Chemical structures of the marine dataset that passed the first statistical filter including the ligand- (pIC_{50}) and structure-based (pK_i) calculated binding affinities.

MNP ID[a]	SMILES	pIC_{50}[b]	3D-QSAR description	pK_i[c]
13469	O1c2c(CC13C1(C(C45C(CC1)C(CCC4)(C)C(OC5)=O)CCC3(O)C)C)cc(O)cc2	5.4	Excellent	8.9
2549	O=C1C2C3(Nc4c1cccc4)C=1C(=NC2)CCNC=1c1nc2c(c4c1c3ncc4)cccc2	6.6	Good	8.7
2550	O=C1C2C3(Nc4c1cccc4)c1c(nccc1NC2)-c1nc2c(c4c1c3ncc4)cccc2	5.2	Excellent	8.6
8107	O(C)c1c2nccc3-c4c(N5c(c(C6C(C)C5(C)C(=O)NC6=O)c1)c23)cccc4			8.5

3305	O1C2n3c4c(c5c(c6c7c(n(c46)C1(C)C(OC)C(O)C2)cccc7)C(=O)NC5)c1c3cccc1	5.5	Good	8.5
1589	O(C)c1c2nccc3-c4c(N5c(c(C6C(C)C5(C)C(=O)NC6=O)c1)c23)cccc4			8.5
1404	n1c2c3c(c4c1cccc4)ccnc3c1nccc3c1c2nc1c3cccc1	5.3	Bad	8.5
1256	O(C)c1c2nccc3-c4c(N5c(c(C6C(C)C5(C)C(=O)NC6=O)c1)c23)cccc4			8.5
3556	O1C(C1(C)C)C1N2C3N(CCC34C3(CC2)c2c1cccc2N(C3Nc1c4cccc1)C)C(=O)C			8.3
711	O1C2CC(OC(=O)C)C3(C(Cc4c(occ4C)C=C(C=CC3)C)C12C)C	4.2	Poor	8.3
3085	O1C(COC(c2ccccc2)(c2ccccc2)c2ccccc2)C(O)CC1N1C=CC(=O)NC1=O	4.5	Bad	8.1
7770	O(C(=O)CC(O)C)C1CC2C(C3CC(=O)C(=CC13C)C(=O)C)(CCC1C3(CC3C)CCCC12C)C	5.4	Good	8.0
3983	O1C2CC(CC=C3CC(OC3=O)CC(C(OC)=O)C(=O)CC(=O)C12C)C(C)=C	5.1	Poor	8.0
13575	O1C2OC(=O)CC2(OC(=O)C)C(C23C(C2)C2(C(CC3)C(CCC2)(C)C)C)C1OC(=O)C	6.1	Bad	7.9
7313	O1C2C(CC3C(C)(C(OC(=O)C)C(=O)C=C3C)C(OC(=O)C(=CC)C)CCC(=C2)C)=C(C)C1=O	5.6	Bad	7.9
6794	O1C2CCC(C)C(CCC3=C(C)C(=O)CC4C(C)(C)C(=O)CCC34C)C2(CCC(=O)C1(C)C)C	5.2	Poor	7.9
1257	O(C)c1c2nccc3-c4c(N5c(c(C6C(C)(C5C)C(=O)NC6=O)c1)c23)cccc4	5.0	Excellent	7.9
7850	O1C2C(CCC(=CC(OC(=O)C)CC(=CC(O)CC(=C2)C)C)C)C(=C)C1=O	5.6	Poor	7.8
7354	O(C(=O)C=1c2[nH]c3c(c2C=C(c2[nH]c4c(c2C=1)cccc4)C(OC)=O)cccc3)C	5.1	Good	7.8
5339	OC=1C2N(C(=O)C=1C(=O)C)C(C1C2c2c3c(C1)cccc3[nH]c2)(C)C	6.4	OK	7.8
1065	BrC1=CC23C4=C(NC(SC2=CC1=O)C3)C(=O)c1[nH]cc2CCN=C4c12	5.5	Poor	7.8
13477	o1c2c3c(c1)C(=O)CCC3(c1c(cc3c(c1)C(=O)C=CC3=O)C2=O)C	4.9	Excellent	7.7
12059	O=C1N(C)C(=O)C=2N(C3Nc4c(cccc4)C3(C=2)c2c3c([nH]c2)cccc3)C1=O	5.0	Poor	7.7
11051	O1CC23C4CCC(O)(C)C(CC5=CC(=O)C=C(OC)C5=O)C4(CCC2C(CCC3)(C)C1=O)C	5.0	Excellent	7.7
9329	O1C23C(CCC(C)C2(CC2=C1C(=O)C=C(N)C2=O)C)C(CCC3)(C)C	5.1	OK	7.7
8422	O1C2CCC1(C)C(OC(=O)C)C(OC(=O)C)C=1C(OC(=O)C=1C)CC(=CCCC2C)C	5.8	Excellent	7.7
8421	O1C2CCC1(C)C(OC(=O)C)C(OC(=O)C)C=1C(OC(=O)C=1C)CC(=CCCC2C)C	4.8	Poor	7.7
6663	BrC1=CC23C4=C(NC(SC2=CC1=O)C3)C(=O)c1[nH]cc2c1c4ncc2	4.9	Excellent	7.7
5744	O1C(C2(C(CC1=O)=C1C(CC2)C2(C)C(CC(OC)=O)C(C)(C)C(=O)C(C1)C2=O)C)c1ccoc1			7.7
4152	OC12C=C(C3C4(C1N1C(C4)C=CCCCC1)CN(CC3)CCCCC=CCC2)CO	4.2	Good	7.7
3742	O1C2=CC(=O)C(O)=CC2=C(C2C3(C(CCC12C)C(CCC3)(C)C)C)C#N	4.4	OK	7.7
1869	O1C2n3c4c(c5c(CNC5=O)c5c6c(n(c45)C1(C)C(OC)C(O)C2)cccc6)c1c3cccc1	5.0	Good	7.7
488	ClC1CC2C3(SC(=O)NC3C1(C=C)C)c1c3c(cccc3[nH]c1)C2(C)C	5.9	OK	7.7
14086	S(OC=C1CCC2C(CCC3C(CCCC23C)(C)C)(C)C1CCc1ccoc1)(O)(=O)=O	4.7	Poor	7.6
13431	O1C2CCC(O)(C)C(CCC3(C=4C(OC(C)(C)C(O)CC=4)CCC3C)C)C2(CCC(=O)C1(C)C)C	4.4	Bad	7.6
11107	O1C2CCC(=CCCC(=CC3OC(=O)C(C3CC(=O)C12C)=C)C)C	5.4	Excellent	7.6
8920	O1C(C(C)C)C(=O)N2C3=C(CC2)c2nc4c(c5c2c(ncc5)C13O)cccc4	4.4	Excellent	7.6
7410	S1CC(=O)Nc2c3nccc4c3c3n(c5c4cccc5)c(N(C)C)cc3c12	4.9	Bad	7.6
6778	O=C1C(=CC(=O)C=C1C)CC1(C2CCC(=C(C)C)C(CCC(O)=O)C2(CCC1C)C)C	5.6	Poor	7.6
6066	S(OC=C1CCC2C(CCC3C(CCCC23C)(C)C)(C)C1CCc1ccoc1)(O)(=O)=O	5.2	Good	7.6
4859	O=C1NC(C=2N(C1Cc1c3c([nH]c1)cccc3)C(=O)c1c(N=2)cccc1)C	5.0	Excellent	7.6
4852	O=C1NC(C=2N(C1Cc1c3c([nH]c1)cccc3)C(=O)c1c(N=2)cccc1)C	5.0	OK	7.6
4667	O1C(=O)C(C2C3C(C4OC3C1(CCC(O)C(C4)=C)C)C(OC(=O)CCC)(CC2)C)C	3.6	OK	7.6
3750	O1C=C2C(CCC=C2C)(c2c(cc3c(c2)C(=O)C=CC3=O)C1=O)C	4.9	Good	7.6
3000	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)C(OC)CNC(=O)C=C(C)C	4.7	Good	7.6
2999	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)C(O)CNC(=O)C(=CC)C	4.0	Good	7.6
2998	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)C(O)CNC(=O)C=C(C)C	4.6	Poor	7.6
2912	OC12C=C(C3C4(C1N1C(C4)C=CCCCC1)CN(CC3)CCCCC=CCC2)C=O	3.1	OK	7.6
2571	O1C2N3CC1(CC3C1C23C(CCC1C(OC)=O)C1(C(CC3OC(=O)C)C(CCC1)(C)C)C)C			7.6

2216	OC1C2C(C3CCC(C(O)(C=C(CC(C)C)C)C)C3(C1)C)C(=O)CC1CCC=CC12C	5.9	Poor	7.6
1950	O1C(OC(=O)C)C2C(C(O)CC3C4(C(CCC23C)C(CCC4)(C)C)C)C1OC(=O)C	4.2	OK	7.6
346	O1C2C(C(=C)C1=O)C(OC(=O)C)CC(=CCCC(=CC(OC(=O)C)CC(=C2)C)C)C	5.3	Bad	7.6
169	O1C2C(CCCC(=O)C(CC(O)C1(C)C)=C2CC1(Oc2c(cc(O)cc2C)CC1)C)(C)C	5.1	Poor	7.6
160	O1C2C(CCCC(=O)C(CC(O)C1(C)C)=C2CC1(Oc2c(cc(O)cc2C)CC1)C)(C)C	4.8	Poor	7.6
13812	O=C1CC2C(CCC3C(C)(C)C(=O)CCC23C)(C)C1=C(C=CC=C(C(O)=O)C)C	6.0	Good	7.5
13678	O1C(=O)C(C2CC3OC3(CCC(OC(=O)C)C3(OC(CC3)C1(CC2)C)C)C)=C	6	Excellent	7.5
10265	O1C23C(OC(=O)C12C)C=C(CCC(OC(=O)C)C1(C(C(C)C(=O)C=C1)C3O)C)C	5.4	Excellent	7.5
9401	Oc1ccc(cc1)C=1NC(=C2N(C=1)C(=O)C(=N2)Cc1ccccc1)Cc1ccccc1	5.6	Bad	7.5
9043	O1C2C(C(=C)C1=O)C(O)CC(=C)C(OC(=O)C)CCC(=CC(OC(=O)C)CC(=C2)C)C	5.3	OK	7.5
7472	O1C2CC(C(=C)C1=O)C(O)CC(=CCCC(=CCCC2(O)C)C)C	4.9	Good	7.5
5275	O1C23CC(O)CC(=O)C2(C2C(C4CCC(C(CCC(C(C)C)C)C)C4(CC2OC(=O)C)C)CC13)C	4.0	OK	7.5
5273	O1C23CC(O)CC(=O)C2(C2C(C4CCC(C(CCC(C(C)C)=C)C)C4(CC2OC(=O)C)C)CC13)C	3.7	Poor	7.5
5104	O1C2C(=CC1=O)C(O)CC1C2(C)C(OC(=O)C)CC2C1(CCC1C(CCCC12C)(C)C)C	5.1	Good	7.5
4292	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCNC(=O)C=C(C)C)cccc4	5.1	Poor	7.5
3831	O1C2(C=CC1(O)C(=CC1C(CC2OC(=O)Cc2ccccc2)C(=CC(=O)C1C(C)C)C)C)C	4.7	Poor	7.5
3001	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)C(OC)CNC(=O)C(=CC)C	3.8	Poor	7.5
2070	O1C2n3c4c(c5c(CNC5=O)c5c6c(n(c45)C1(C)C(OC)C(N(C)C)C2)cccc6)c1c3cccc1	5.7	Poor	7.5
1280	O1C2CC(O)(CC(=O)C=C(C)C(=O)CC(CCC(=C2)C1=O)C(C)=C)C	5.7	OK	7.5
919	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)CCNC(=O)C(=CC)C	5.9	Good	7.5
916	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)CCNC(=O)C=C(C)C	5.7	Good	7.5
395	BrC1=CC2(C=C(Br)C1=O)C1=C(NCC2)C(=O)c2[nH]cc3CCN=C1c23	5.4	Good	7.5
348	O1C2C(CCC(=CCCC(=CC(OC(=O)C)CC(=C2)C)C)C)C(=C)C1=O	4.1	Poor	7.5
14443	O1C2C(CC=C(C3OOC(CC3)(C)C(OC(=O)C)CCC(=C2)C)C)C(=C)C1=O	5.4	OK	7.4
14126	O1C23C1CC1C(C2(C)C(=O)C=CC3)C(O)CC2(C1CCC2C(CCC(C(C)C)C)C)C	5.4	Poor	7.4
14123	O1C23C1CC1C(C2(C)C(=O)C=CC3)C(O)CC2(C1CCC2C(CCC(C(C)C)=C)C)C	6.3	OK	7.4
13420	O=C1CC2C3(CC(C2CCC3C)(C)C)C1CN1C=2N=CNC(=O)C=2NC1=O			7.4
13330	O=C1C=2C(=CC(=O)N(C=2)C)c2nc3c(c4c2c1ncc4)cccc3	5.1	Excellent	7.4
13184	O1C2c3oc(CC(CCC45OC4C(OC5=O)CC12C)C(C)=C)c(c3)C=O	5.1	Poor	7.4
11162	O1CC2C(CC3C(OC(=O)C=C3C)C2=C)C(=CC=CC(O)(C)C)C1=O	5.1	Poor	7.4
11161	O1CC2C(CC3C(OC(=O)C=C3C)C2=C)C(=CC=CC(O)(C)C)C1=O	5.2	Bad	7.4
10708	O1C2n3c4c(c5c(CNC5=O)c5c6c(n(c45)C1(C)C(OC)C(NC)C2)cccc6)c1c3cccc1	4.9	Poor	7.4
9456	O1C=C(C2C(CN3C(C2)C2(CC3)c3c(NC2=O)cccc3)C1C)C(OC)=O	4.4	Good	7.4
9396	O1C=C(C2C(CN3C(C2)C2(CC3)c3c(NC2=O)cccc3)C1C)C(OC)=O	3.9	Excellent	7.4
9214	O(C)C1c2c(C(=O)N(C)C1OC)c(O)c1nccc3-c4c(Nc2c13)cccc4	5.5	Excellent	7.4
8139	ClC=1CCC2OC(C(OC(=O)CC(OC(=O)C)C(=CCC=1)C)C2)C1OC(=O)CC(=C1)C	5.4	Poor	7.4
7851	O1C2C(CCC(=CCCC(=CC(OC(=O)C)CC(=C2)C)C)C)C(=C)C1=O	3.5	Bad	7.4
7182	Brc1c(cc2C3C(CCC3C(C)C)(C)C(O)(C(OC)=O)C(=O)c2c1O)C	4.7	Excellent	7.4
6935	O1CC(=C(c2c3c([nH]c2)cccc3)C1=O)c1c2c([nH]c1)cccc2	5.3	Excellent	7.4
6443	Oc1c2c(ncc1)-c1nc3c(c4c1c(ncc4)C2=O)cccc3	5.2	Excellent	7.4
5891	O=C1C2=CC(=O)CCC2(C2C(C3CCC(C(CC=CC(OO)(C)C)C)C)C3(CC2)C)C1)C	4.7	Bad	7.4
5731	O1C2CCC(C)C(O)(CCC3(C4C5(OC(C(O5)CC4)(C)C)CCC3C)C)C2(CCC(=O)C1(C)C)C	5.0	Bad	7.4
5443	OC12N(C(c3[nH]c4c(c3C1=O)cccc4)C=C(C)C)C(=O)C1N(CCC1)C2=O	5.7	Excellent	7.4
5215	ClC1=CC(O)C=CC(C2C3(N4C(CCC3)CC=C(C4)C(OCC1)=O)CCC2)C	4.1	Good	7.4
4837	ClC1=C(O)C(=O)c2c(cc3c(c2)C(=O)c2occ4c2C3(CCC4)C)C1=O	5.4	OK	7.4

4301	O1C2=C3C(C1)C(O)CCC3(c1c(cc3c(c1)C(=O)C=CC3=O)C2=O)C	5.6	Poor	7.4
2076	O=C1C=2C(=NC=C1)C(=O)c1nccc-3c1C=2Nc1c-3cccc1	6.1	Good	7.4
822	O=C1N2C(Cc3c([nH]c4c3cccc4)C2C=C(C)C)C(=O)N2C1CCC2	5.7	Poor	7.4
14256	O1C2OC(=O)C3C2C2(C(CC3)C3(C(CC2OC(=O)C)C(CCC3)(C)C)C)C1O	4.7	Poor	7.3
14229	o1c2c3c(c1)C(=O)CCC3(c1c(cc3c(c1)c(O)ccc3O)C2=O)C	4.8	Good	7.3
13896	OC12C(CCCC1(C)C)C(CCC(=CCn1c3c(nc1)N(C)C(=NC3=O)C)C)(C)C(CC2)C	6.0	Good	7.3
12945	Oc1cccc(C)c1C(OC(C)c1c2nc3c(nc2ccc1)c(ccc3)C(O)=O)=O	5.8	OK	7.3
12346	O1C2C(CC(O)C(CCC(=CCCC(=C2)C)C)C(=O)C)C(=C)C1=O	5.6	OK	7.3
12188	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC3(OC3CC(OC(=O)C)C12C)C)C	4.7	Poor	7.3
12164	O(C(=O)C)C1CC2(C(=C1C(C)C)C(OC(=O)C)CC1(C)C(O)(C2)C(CCC1O)=C)C	6.0	Good	7.3
11977	O1C2C3C(C1CC(=CCCC2(OC(=O)C)C)C)C(C)=C(OC(=O)C)CC3C(OC(=O)C)(C)C	5.6	Excellent	7.3
11745	O1C2C(CC(O)C(CCC(=CCCC(=C2)C)C)C(=O)C)C(=C)C1=O	5.4	Excellent	7.3
11044	S1C2=CC(=O)C=CC23C2=C(NC1C3)C(=O)c1[nH]cc3CCN=C2c13	4.9	Excellent	7.3
8909	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCNC(=O)C(CC)C)cccc4	4.0	Excellent	7.3
8908	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCNC(=O)C(C)C)cccc4	4.4	Poor	7.3
8120	O1c2c3c(cccc3O)c(O)c3c2-c2c(c(ccc2OC3=O)C)C1=O	5.1	Excellent	7.3
7846	O1C2C(C(=C)C1=O)C(O)CC(=CC(OC(=O)C)CC(=CC(OC(=O)C)CC(=C2)C)C)C	6.4	Poor	7.3
7758	O1C(C2=C(C3(C(CC2)C2(C(CC3OC(=O)CC(O)C)C3(C(CC2)C2(CC2C)CCC3)C)C)C)C1=O)C	4.9	Poor	7.3
7757	O1C(C2=C(C3(C(CC2)C2(C(CC3OC(=O)CC(O)C)C3(C(CC2)C2(CC2C)CCC3)C)C)C)C1=O)C	5.2	Good	7.3
6857	O1C(C2C3(CC=C4C(=CC(C5CC(O)CCC45C)(C)C)C3(CC2)C)C1=O)(CCCC(O)(C)C)C	4.8	Poor	7.3
6792	O1C23C(OC(O)(CC2)C1(C)C)CCC(C)C3(CCC=1C2(C(OC(C)(C)C(=O)CC2)CCC=1C)C)C	5.0	Poor	7.3
5889	OC1C2=CC(=O)CCC2(C2C(C3CCC(C(CC=CC(OO)(C)C)C)C3(CC2)C)C1)C	5.0	Bad	7.3
5818	o1c2c(cc1)C(=O)CC1C3(C(CCC12C)C(CCC3)(C)C)COC(=O)C	5.4	Good	7.3
5220	O1CC2(C3C(CCC2C1=O)C1(C(CC3O)C(CCC1)(C)C)C)C	4.7	Excellent	7.3
5123	O1C2(OC(=CC3(CCCC23C)C)CC(=CCC2=CC(=O)C=C(C)C2=O)C)C=CC1(C)C	4.3	Bad	7.3
4822	O1C2CCC1(C)C(O)CC1C(OC(=O)C1=C)C(O)C(CCCC2=C)C	4.8	Excellent	7.3
4306	O1C2C3C(C1CC(O)(C)C(OC(=O)CC(C)C)CCC2(OC(=O)C)C)C(CCC3C(C)C)=C	4.4	OK	7.3
4298	S(C)C=1C(=O)c2nccc3c2c(nc2c3cccc2)C=1CCNC(=O)C(=CC)C	4.4	Good	7.3
3691	O1C2CCC(O)(C)C(CCC3=C(C)C(=O)C(O)=C4C(C)(C)C(=O)CCC34C)C2(CCC(=O)C1(C)C)C	4.4	Bad	7.3
3498	OC1CC2=CC(=O)C3C4CCC(C(C=CC(=O)C)C)C4(CCC3C2(CC1)C)C	5.7	Poor	7.3
3455	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(OC(=O)C)CC=C(C(OC)=O)C	5.8	Poor	7.3
3164	S(Oc1c2c(cc3c(c2)C2(CCCc4c2c(oc4)C3=O)C)c(O)cc1)(O)(=O)=O	6.3	OK	7.3
2853	s1c2c3cc(n4c3c3c(c5c4cccc5)ccnc3c2nc1)N(C)C	5.3	Excellent	7.3
2708	O1CC(C2CC(C)C(OC(=O)C)C3C2C2OC3CC(=CCCC12C)C)C	5.1	Good	7.3
2680	O1CC(C2CC(C)C(OC(=O)C)C3C2C2OC3CC(=CCCC12C)C)C	5.0	Good	7.3
2570	O1C2N3CC1(CC3C1C23C(CCC1C(OC)=O)C1(C(CC3OC(=O)CCC)C(CCC1)(C)C)C)C			7.3
2478	O1C2c3oc(CC(CC(OC(=O)C)C4=CC(OC4=O)CC12C)C(C)=C)c(c3)C=O	5.7	Poor	7.3
2458	O1C2C(CC(O)C(CCC(=CCCC(=C2)C)C)C(=O)C)C(=C)C1=O	5.3	Poor	7.3
1667	ClC1CC2C(O)(C([NH+]=[CH-])C1(C=C)C)C(=O)c1c(cccc1NC=O)C2(C)C	4.7	Excellent	7.3
1666	O=C1C2C(CCC(C=C)(C)C2[NH+]=[CH-])C(c2c1c(NC=O)ccc2)(C)C	3.7	OK	7.3
1534	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(O)=CC1=O	6.1	Excellent	7.3
1127	O1C2OC(OC(=O)C)C(C2C2(CCC3=C(CCCC3(C)C)C2C)C)C(OC(=O)C)C1=O	5.4	Bad	7.3
1009	O1C(=O)C(CCC1C(C)C1CCC2C3C(CCC12COC(=O)C)C1(C(=CC(=O)C=C1)CC3)C)C	4.6	Bad	7.3

14257	O1C2OC(=O)C3C2C2(C(CC3)C3(C(CC2O)C(CCC3)(C)C)C)C1O	4.3	Excellent	7.2
14185	O1C2c3oc(CC(CCC45OC4C(OC5=O)CC12C)C(C)=C)c(c3)C(OC)=O	4.2	Good	7.2
14124	O1C23C1CC1C(C2(C)C(=O)C=CC3)C(O)CC2(C1CCC2C(C=CC(C(C)C)C)C)C	4.5	Poor	7.2
13810	O=C1CC2C(CCC3C(C)(C)C(=O)CCC23C)(C)C1=C(C=O)C	5.2	Good	7.2
13809	O=C1CC2C(CCC3C(C)(C)C(=O)CCC23C)(C)C1=C(C=O)C	3.7	Excellent	7.2
13410	S=C=NC(CC1C2C3C(CCC(C)C3([NH+]=[CH-])CCC2=C)C(C1)C)(C)C	3.8	Good	7.2
13405	O1C2C3C(C1CC(O)(C)C(OC(=O)CCC)CCC2(OC(=O)C)C)C(=C)C(O)CC3C(C)C	4.1	Poor	7.2
12773	O(C(=O)C)C1CC(C(=CCC=C(C)C)C)C(C2C(C)C(O)CC2=O)C1C=O	6.1	Excellent	7.2
12766	O1C2CC(=O)CC(CC=C3C(O)C(OC3=O)CC1(CC2=O)C)C(C)=C	4.7	Good	7.2
12391	O1C2C(CC3OC3(CCC=C(CCC=C(C)C2O)C)COC(=O)C)C(=C)C1=O	6.3	Excellent	7.2
12388	O1C2C(CC3OC3(CCC=C(CCC=C(C)C2O)C)COC(=O)C)C(=C)C1=O	4.5	Good	7.2
12079	O1C2CCC(=CCCC(=CC3OC(=O)C(C3CC(OC(=O)C)C12C)=C)C)C	4.1	Good	7.2
11973	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=CCC(OC(=O)C)C12C)C)C	5.5	OK	7.2
11944	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=CCC(OC(=O)C)C12C)C)C	4.7	Excellent	7.2
11844	ClC=1C=2C(OC3(C(C=2)C2(C(CC3)C(CCC2)(C)C)C)C)=CC(=O)C=1O	4.6	Bad	7.2
11480	O1C2C(CCC(O)(C)C(O)CCC(=CCCC(=C2)C)C)=C(C)C1=O	5.1	Excellent	7.2
11471	O=CNC(CC1C2C3C(CCC(C)C3([NH+]=[CH-])CCC2=C)C(C1)C)(C)C	4.7	Excellent	7.2
10174	O1C2c3oc(CC(CCC4=CC(OC4=O)CC12C)C(C)=C)c(c3)C(OC)=O	5.7	Poor	7.2
9979	O=C1C2N(C(=O)C1=C(O)C)C(C1C2C2c3c(C1)cccc3N(C)C2=O)(C)C	5.0	Excellent	7.2
9778	O1C2C3(C(C4C5(C(CCC(C)C5(O)C2=O)C(C4)C)C3=O)C1(C)C)C			7.2
9400	Oc1ccc(cc1)-c1nc(Cc2ccccc2)c(nc1)NC(=O)Cc1ccccc1	5.1	Bad	7.2
9349	O1C2=CC(=O)C3(O)CC(OC3C2=CC2C3(C(CCC12C)C(CCC3)(C)C)C)OC	6.2	Poor	7.2
9211	O(C)c1c2c3c(nc1)C(=O)C1=C(C=CN(C)C1=O)c3nc1c2cccc1	5.8	Excellent	7.2
8934	O1C2CCC(=C)C(CCC3C4(C(OC(C)(C)C(=O)CC4)CCC3(O)C)C)C2(CCC(O)C1(C)C)C	3.5	Poor	7.2
8832	OC12C3=C(C(=O)C(O)=C1C)C(CCC3C(CC2C=C(C)C)C)C	6.0	Excellent	7.2
8673	O1C2CC3(C(CCC(=C)C(OO)CCC12C)C(=C(C)C)C(=O)C3)C	5.3	Excellent	7.2
8530	O1CC2=C(CCC3C2(CCC2C(C)=C(O)C(=O)CC23C)CO)C1=O	5.2	Good	7.2
8369	OC1C2CC(O)CCC2(C=2C(C3CCC(C(CC(=O)C=C(C)C)C)C3(CC=2)C)C1)C	4.6	Poor	7.2
7848	O1C2C(C(=C)C1=O)C(OC(=O)C)CC(=CCCC(=CC(O)CC(=C2)C)C)C	4.7	Poor	7.2
7503	OC1CC2=CCC3C4CCC(=NO)C4(CCC3C2(CC1)C)C	4.8	Good	7.2
7414	O1c2c(C(CCC3(C)C(CCC=C3C)C)(C)C1C)c(O)cc1c2C(=O)C(C)=C(O)C1=O	4.6	OK	7.2
7386	O1C23C(C4CCC(C(CCCC(C)C)C)C4(CC12C)=CC(OC(=O)C)C1(O)CC(O)CCC13C	6.2	OK	7.2
7289	O1C2CC(=O)CC(CC=C3C(O)C(OC3=O)CC1(CC2=O)C)C(C)=C	5.4	Excellent	7.2
7263	OC1=C(C)C(=O)C23C4(CC(=CC2CC(C3CCC4C)C)C)C1=O	4.4	Good	7.2
7083	S=C=NC(CC1C2C3C(CCC2=C)C([NH+]=[CH-])(CCC3C(C1)C)C)(C)C	5.1	OK	7.2
6936	O=C(c1c2c([nH]c1)cccc2)c1nccc2c1[nH]c1c2cccc1	6.0	Excellent	7.2
6889	O1C23C1(C1CCC(C(C=CC(C(C)C)C)C)C1(CC2)C)C(O)C1OC12CC(O)CCC23C	5.4	Poor	7.2
6829	Oc1c2c3C(=C(C)C(=O)C(=O)c3c(c1)C)C(CC2C)C=C(C)C	5.7	Excellent	7.2
6784	O=C1NC(C=2N(c3c1cccc3)C(=O)c1c(N=2)cccc1)C	5.0	Excellent	7.2
6249	O1C23C=4C(CCC2(C)C(CC13)C(C=CC(C(C)C)C)C)C1(C(CC(=O)CC1)C(=O)C=4)C	4.5	Bad	7.2
5670	O1CC2C(=CC(OC(=O)C)C3C2(C=O)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	6.0	Good	7.2
5477	OC1(CC(O)C=C(CC(=O)C(CCC(C=C1)C(C)C)(COC(=O)C)C)C)C	6.1	OK	7.2
5274	O1C23CC(O)CC(=O)C2(C2C(C4CCC(C(C=CC(C(C)C)C)C)C)C4(CC2OC(=O)C)C)CC13)C	5.6	Poor	7.2
5131	S=C=NC(CC1C2C3C(CCC2=C)C([NH+]=[CH-])(CCC3C(C1)C)C)(C)C	4.9	Poor	7.2
4827	O1C2(CCC(CC(O)C3(OC(CC3)C(O)(CCC2=O)C)C)C(=C)C1=O)C	4.9	Poor	7.2
3933	O1C2CC(=O)CC(CC=C3C(O)C(OC3=O)CC1(CC2=O)C)C(C)=C	5.9	Excellent	7.2

3912	O1C2CC(=O)CC(CC=C3C(O)C(OC3=O)CC1(CC2=O)C)C(C)=C	5.1	Excellent	7.2
3784	O1C2C3C(C1C=C(C)C(=O)CCC2(OC(=O)C)C)C(OC(=O)C)(CCC3C(C)C)C	6.0	OK	7.2
3639	O1C2C(CC3OC3(CCC=C(CCCC(C)C2=O)C)C)C(=C)C1=O	4.3	Excellent	7.2
3403	O1C2=C(C3C(CCC(=C3)C)C1(CCC=C(C)C)C)C(=O)c1c(C2=O)c(O)cc(O)c1	4.1	Poor	7.2
3287	O1C2C(C(=C)C1=O)C(OC(=O)C)CC(=CC(OC(=O)C)CC(=CCCC1(OC12)C)C)C	5.6	Excellent	7.2
3281	Oc1ccc(cc1)-c1nc(Cc2ccccc2)c(nc1)NC(=O)Cc1ccccc1	5.2	Poor	7.2
3062	O1C2=C3C(C1)C(O)CCC3(c1c(cc3c(c1)C(=O)CCC3O)C2=O)C	5.3	Bad	7.2
2910	OC1CC2=CCC3C4CCC(=NO)C4(CCC3C2(CC1)C)C	5.0	Good	7.2
2722	O1CC(C2(C3C(CC2OC(=O)C)C(CCCC3=C)(C)C)C)C(CC1=O)COC(=O)C	5.3	Poor	7.2
2106	O(C(=O)C)C1=C(CC2(C3CCC=C(C)C3(CCC2C)C)C)C(=O)C=CC1=O	4.9	Excellent	7.2
2075	Oc1c-2c(ncc1)C(=O)c1nccc3c1c-2nc1c3cccc1	5.2	Good	7.2
1785	O1C2C3OC(CC(=O)C=C(C)C(=O)CC(CCC3(O)C1=O)C(C)=C)(C2)C	4.7	Excellent	7.2
1658	O1C2OC(=O)CC2C(C2(C3C4(C(CC2)C(CCC4)(C)C)C3)C)C1OC(=O)C	4.5	Excellent	7.2
1643	OC1CC2=CCC3C4CCC(=NO)C4(CCC3C2(CC1)C)C	4.8	Poor	7.2
1535	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(NCCc2ccccc2)=CC1=O	5.3	Good	7.2
1430	O1C2C3C(C1CC(=C)C(=O)CCC2(OC(=O)CCC)C)C(CCC3C(C)C)=C	5.1	Excellent	7.2
1123	O1CC(C(COC(=O)C)C(O)C1=O)C1(C2C(CC1)C(CCCC2=C)(C)C)C	5.6	Good	7.2
1010	O1C(=O)C(CCC1C(C)C1CCC2C3C(CCC12C)C1(C(CC(=O)CC1)CC3)C)C	5.6	Good	7.2
999	O1C2CCC(O)(C=CCC(=CC3OC(=O)C(C3CC(=O)C12C)=C)C)C	5.9	Excellent	7.2
938	o1c2c3c(CCCC3(c3c(cc4c(c3)C(O)CCC4O)C2=O)C)c1	5.3	Poor	7.2
626	O1C2OC(=O)C3C2C2(C(CC3)C3(C(C(CCC3)(C)C)C(OC(=O)C)C2)C)C1OC(=O)C	5.9	OK	7.2
495	ClC1CC2C(c3c4c(cccc4[nH]c3)C2(C)C)C([NH+]=[CH-])C1(C)C1OC1	5.3	Excellent	7.2
486	ClC1CC2C(c3c4c(cccc4[nH]c3)C2(C)C)C([NH+]=[CH-])C1(C)C1OC1	4.2	Poor	7.2
460	Oc1cc2[nH]c3c(CC4N(C3C=C(C)C)C(=O)C3N(CCC3)C4=O)c2cc1	5.9	Poor	7.2
245	O1C2C(CC=C(CCC=C(CCC=C(C2)C)C)COC(=O)C)C(=C)C1=O	5.4	OK	7.2
162	O1C2C(CCCC(=O)C(C=CC1(C)C)=C2CC1(Oc2c(cc(O)cc2C)CC1)C)(C)C	5.2	Excellent	7.2
13492	O1C2CCC(O)(C)C(CCC3C(=C)C(=O)CC4C(CCC4(O)C)C3(C)C)C2(CCC(=O)C1(C)C)C	5.2	Poor	7.1
13045	O1CC12C1OC3C=C(CCC3(COC(=O)C=C(CCO)C)C2(C)C(O)C1)C	4.5	OK	7.1
12947	O(C(=O)C)C1C2C(C3CCC(C(CCC(O)=O)C)C3(C1)C)CCC1=CC(=O)CCC12C	3.7	Poor	7.1
12875	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(OC(=O)C)C(OC(=O)C)C=C(C)C	6.2	Bad	7.1
12603	O(C(=O)C)C1CC=2C(CC3(O)C1(C)C(OC(=O)C)CCC3=C)(CCC=2C(C)C)C	4.6	OK	7.1
12227	S1CC(NC1=O)C1(OC2CCC(C=CC=CCCC(=CC(OC(C1)C2)=O)C)C)O	4.8	Poor	7.1
12033	N#CC1(CC2CC(C3C4C(CCC(C24)C1C)C(CC3)(C#N)C)C)C	5.7	Good	7.1
11736	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(OC(=O)C)C(OC(=O)C)C=C(C)C	5.4	Good	7.1
11413	O1C2=C(CC13C1(C(CCC3C)C(CCC1)(C)C)C)C(=O)C(OC)=CC2=O	4.9	Poor	7.1
11393	O(C(=O)C(=O)c1c-2n(C=Cc3c-2[nH]c2c3cccc2)c2c1cccc2)CC	4.2	Poor	7.1
10774	O1C2(C3C(CCC3C)C(=CC2C=C(CCCc2ccoc2)C)C)C(=O)C(C)=C1O	5.0	OK	7.1
10665	O1C2(CCC(CC3OC3(CCC=C(CCC2=O)C)C)C(=C)C1=O)C	5.4	Excellent	7.1
10654	O1C(CC(=CCCC(C=CC=C(CCCC2=CC(=O)N(C2)CC(O)=O)C)C)C(O)=C(C)C1=O	5.5	Bad	7.1
10087	OC1CC2=CCC3C4CCC(C(CC=CC(O)(C)C)C)C4(CCC3C2(CC1)C)C	4.3	Bad	7.1
10086	OC1CC2=CCC3C4CCC(C(CC=CC(O)(C)C)C)C4(CCC3C2(CC1)C)C	5.1	OK	7.1
9821	O1C2CCC1(C)C(O)C1OC(=O)C(=C1C(=O)CC(=CCCC2C)C)C	3.9	Excellent	7.1
9155	O1C2CC(O)(C3C2C(C2C(=CC(=O)CC(C2)C(C)=C)C3=O)C1=O)C	4.5	Good	7.1
9106	OC1C2C(C3CCC(C(CCC(C(C)C)C)C)C3(C1)C)CC(O)C1=CC=CC(=O)C12C	5.4	Bad	7.1
8235	OC1CC2=CC(=O)C3C4CCC(C(CC#CC(O)(C)C)C)C4(CCC3C2(CC1)C)C	4.5	Poor	7.1
8040	ClC1C(C2CC(OC(=O)C)C(=C)C(CC(O)C3CC(=O)NC3=O)C2(CC1Cl)C)(C)C	4.8	Bad	7.1

8022	O1C(O)C(=CC1=O)C(O)CC1C2(C(CCC1=C)C1(C(CC2)C(CCC1)(C)C)C)C	4.9	OK	7.1
7944	Oc1c2N=C3N(c4c(cccc4)C(=O)NC3C)C(=O)c2ccc1	5.1	Excellent	7.1
7935	OC=1C(=O)c2c3c(C=1C)c(cc(c3c(O)cc2C)C)C=C(C)C	4.8	Excellent	7.1
7486	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=O)C)C)C1(C(OC)=O)C)C	5.9	OK	7.1
7417	O1C2=C(C=3C(CCC(OC)(C=3)C)C1(CCC=C(C)C)C)C(=O)c1c(C2=O)c(O)cc(O)c1	5.3	Poor	7.1
7415	Brc1c(O)c2c(cc1O)C(=O)C1=C(OC(C3C1C=C(CC3)C)(CCC=C(C)C)C)C2=O	4.5	Poor	7.1
7273	O1C2(O)C3(C(C4C5(C(CCC(C)C5(O)C2=O)C(C4)C)C3=O)C1(C)C)C	5.2	OK	7.1
6633	Oc1cc2c(N3C(=Nc4c(cccc4)C3=O)C(NC2=O)C)cc1	5.3	Excellent	7.1
6599	O(C(C)c1c2nc3c(nc2ccc1)c(ccc3)C(O)=O)C(=O)c1ccccc1	6.0	Bad	7.1
6583	O(C)c1cc2C3=NC(CC(=O)C)C(c4c([nH]c5c4cccc5)C3=Nc2cc1)CC(=O)C	5.0	Poor	7.1
6548	O1C(OC)C2=C(CCC3C4(C(CCC23C)C(CCC4)(C(O)=O)C)C)C1=O	5.4	Excellent	7.1
6134	O1C(O)C(=CC1=O)C(OC(=O)C)CC1(C=2C(CCC1C)C(CCC=2)(CCCC(C)=C)C)C	4.9	Poor	7.1
6124	Oc1ccc(O)cc1C1C2=C(CCC(C)C1=C)C(CCC2)(C)C	5.6	OK	7.1
5888	OC1C2=CC(=O)CCC2(C2C(C3CCC(C(CCC(OO)C(C)=C)C)C3(CC2)C)C1)C	5.4	Bad	7.1
5673	Oc1ccc(O)cc1C1C2=C(CCC(C)C1=C)C(CCC2)(C)C	4.6	Excellent	7.1
5539	Brc1cc2[nH]cc(c2cc1)C1=C(c2n(cnc2)C)C(=O)NC1=O	5.1	Excellent	7.1
5358	O1C2(CCC(CC(O)C(=CCC=C(CCC2O)C)C)C(=C)C1=O)C	5.4	Excellent	7.1
5269	O=C1N2C(CCC2)C(=O)NC1Cc1c2c([nH]c1CC=C(C)C)cccc2	5.5	Excellent	7.1
5218	O1CC2=C(CC(OC(=O)C)C3C2(C)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	5.4	OK	7.1
4838	ClC1=C(O)C(=O)c2c(cc3c(c2)C2(CCCc4c2c(oc4)C3=O)C)C1=O	5.1	Excellent	7.1
4793	O1c2c(cc(O)c(O)c2)C(=O)C2C3(C(CCC12C)C(CCC3)(C)C)C	5.6	Good	7.1
4276	O(C)c1ccc(cc1)C(=O)Cn1cc(c(-c2ccc(O)cc2)c1C(OC)=O)-c1ccc(O)cc1	5.0	Poor	7.1
3692	O1C2CCC(C)C(CCC3=C(C)C(=O)C(O)=C4C(C)(C)C(=O)CCC34C)C2(CCC(=O)C1(C)C)C	5.4	Poor	7.1
3684	O1CC(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C(CC1=O)COC(=O)C	6.4	Good	7.1
3485	O1c2cc(ccc2OC1)Cc1n(C)c(nc1Cc1cc2OCOc2cc1)N	4.1	Good	7.1
3402	Brc1c2c(C(=O)C=3OC(C4C(C=3C2=O)C=C(CC4)C)(CCC=C(C)C)C)c(O)cc1O	5	Good	7.1
3337	O1C2OC(=O)C=C2C(O)CC=C(CCC=2C3(C(CCC=2C)C(CCC3)(C)C)C)C1O	4.7	Good	7.1
3165	O1C2=C3C(C1)C(O)CCC3(c1c(cc3c(c1)C(O)CCC3=O)C2=O)C	5.0	OK	7.1
2707	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=CCCC12C)C)C	4.5	OK	7.1
2679	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=CCCC12C)C)C	4.7	Excellent	7.1
2520	O1C2C3C(CCC3(CCC(CC(=O)CC(C2)C)=C)C)=C(C)C1=O	5.2	Good	7.1
2417	O1C23C1C(O)C=1C4CCC(C(C=CCC(C)C)C)C4(CCC=1C2(CCC(O)C3)C)C	4.8	Poor	7.1
2345	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCNC(=O)CC(C)C)cccc4	4.9	Good	7.1
2015	O1C2OC(OC(=O)C)C(C(OC(=O)C)C1=O)C2C(=C)C1CCC2C1(CCCC2(C)C)C			7.1
1659	O1CC(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C(CC1=O)COC(=O)C	6.1	Good	7.1
1624	Oc1ccc(cc1CC1(C2CCCC(=C)C2(CCC1C)C)C)C(OC)=O	4.8	Good	7.1
1484	O1C(O)C(=CC1=O)C(OC(=O)C)CC1C2(C(CCC1C=O)C1(C(CC2)C(CCC1)(C)C)C)C	5.0	Poor	7.1
1279	O1C2CC(CC(=O)C=C(C)C(=O)CC(CCC(=C2)C1=O)C(C)=C)=C	5.0	Good	7.1
1008	O1C(=O)C(CCC1C(C)C1CCC2C3C(CCC12C)C1(C(=CC(=O)C=C1)CC3)C)C	4.7	Excellent	7.1
1006	O1C(=O)C(C)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C(=CC(=O)C=C1)CC3)C)C	3.9	Bad	7.1
869	BrC1=CC23C4=C(NC(SC2CC1=O)C3)C(=O)c1[nH]cc2CCN=C4c12	5.2	Excellent	7.1
633	ClC1CC2C(C([NH+]=[CH-])C1(C=C)C)C(=O)c1c(cccc1NC=O)C2(C)C	4.9	Excellent	7.1
459	O1C2OC(=O)CC2C(C(=CC2(CC(CCC2)(C)C)C)C=C)C1OC(=O)C	6.0	Good	7.1
447	O1CC2C(CCC3C2(COC(=O)C)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	6.2	OK	7.1
14455	O(C)c1c2c(cc(C)c1C(=O)C)cc1c(C(=O)C(C)(C)C(=O)C1(C)C)c2O	4.6	Poor	7.0
14447	O1C2C=C(CCC(C(C)=C)C(OC(=O)C)c3oc(cc3C)C2C(C)=C)C1=O	5.7	OK	7.0

14259	O1C2OC(=O)C3C2C2(C(CC3)C3(C(CC2OC(=O)CCC)C(CCC3)(C)C)C)C1O	4.4	Excellent	7.0
14114	O=C1N(Cc2ccccc2)C(=O)N(c2nccnc12)Cc1ccccc1	5.8	OK	7.0
13425	O1C23CC(=O)CC(CC2C2C4C(C1(CC4OC2=O)C)C3=O)C(C)=C	4.5	Good	7.0
13331	O1C2C1(C=CC(=O)C(=CC1C(CCC(CC2=O)C)C1(C)C)C)C	5.9	Excellent	7.0
12940	O=C1C2N(C(=O)C1=C(O)C)C(C1C2c2c3c(C1)cccc3[nH]c2)(C)C	4.7	Excellent	7.0
12806	O1C2(CCC=C(CCC(=CC=C(CCC2O)C)C(C)C)C1=O)C	5.3	Good	7.0
12431	O1C(O)C2C(=CCC3C4(C(CCC23C)C2(C(CC4)C(CCC2)(C)C)COC(=O)C)C)C1=O	5.8	Good	7.0
12229	O1C2=CC(O)(CCC(OC(=O)CC(C)C)C3(C(CC2=C(C)C1=O)C(=CCC3OC(=O)C)C)C)C	4.4	Excellent	7.0
12103	O1CC2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1=O	4.9	Bad	7.0
12064	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(NC=O)(CC1)C	4.3	Poor	7.0
12001	O1C(C)(C)C1C(OC(=O)C)CC(C)C1CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)CC3)C	4.3	Bad	7.0
11857	O1C2=CC(=O)C(O)=CC2=CC2C3(C(CCC12C)C(CCC3)(C)C)C	5.4	Poor	7.0
11601	O1C2(CCC=C(CCC(=CC=C(CCC2O)C)C(C)C)C1=O)C	4.9	Excellent	7.0
11475	O1c2c(cc(O)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C(O)=O)C)C)C	5.2	Bad	7.0
11379	Brc1cc2n3c(-c4[nH]c5c(c4C=C3)cccc5)c(c2cc1)C(=O)C(OCC)=O	4.9	OK	7.0
11261	O1CC(=C2CC(O)C(=CCCC(=CCCC(=CC12)C)C(OC)=O)C)C	4.3	Good	7.0
11090	O1C2C(CC3OC3(CCC=C(CCC=C(C)C2=O)C)C)C(=C)C1=O	5.3	Poor	7.0
10923	O(C(=O)C=1c2n(c3c(c2C=C(c2n(c4c(c2C=1)cccc4)C)C(OC)=O)cccc3)C)C	4.9	OK	7.0
10900	O1CC=2C(C3(C(CC=2)C2(C(CC3OC(=O)C)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1O	6.0	Poor	7.0
10838	O1C2C(CC3OC3(CCC=C(CCC=C(C2)C)C)COC(=O)C)C(=C)C1=O	5.6	Poor	7.0
9690	O1C2C(CC(O)C(=CCCC(=CCCC(=C2)C)C(OC)=O)C)=C(C)C1=O	4.4	Poor	7.0
9276	S(C)c1c2c3c(nc4c2cccc4)C(=CC(=O)c3nc1)CCNC(=O)C	5.3	Excellent	7.0
9026	O1C(=CC(CCC=C(CCCC2=CC(OC2=O)(OC)Cc2ccoc2)C)C)C(O)=C(C)C1=O	3.3	Bad	7.0
9025	O1C(=CC(CCCC(=CCCC2=CC(OC2=O)(OC)Cc2ccoc2)C)C)C(O)=C(C)C1=O	3.8	Bad	7.0
8447	O1C2C(CC3OC3(CCC=C(CCCC(C)C2OC(=O)C)C)C)C(=C)C1=O	4.5	Excellent	7.0
8082	ClC1C(C2C(C3CC(OC3(CC2=O)C)C2CC(=O)NC2=O)(CC1Cl)C)(C)C	4.7	Excellent	7.0
7491	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=O)C)C)C1(C(O)=O)C)C	6.0	Bad	7.0
6998	O1C(O)C2=C(C3(C(CC2)C2(C(CC3)C(CCC2)(CO)C)C)C)C1=O	5.0	Good	7.0
6996	O1C(O)C2=C(C3(C(CC2)C2(C(CC3)C(CCC2)(C(O)=O)C)C)C)C1=O	5.2	Excellent	7.0
6995	O1C(O)C2=C(CCC3C4(C(CCC23C)C(CCC4)(C(O)=O)C)C)C1=O	4.2	OK	7.0
6937	O=C1C23C(CCC2(C)C(CC1)C(C=CC(C(C)C)C)C)C1(C(=CC(=O)CC1)C(=O)C3)C	2.9	Bad	7.0
6738	O1C2Oc3cc(OC)c4c(Oc5c(C4=O)c(O)ccc5OC)c3C2C=C1	4.7	Excellent	7.0
6625	O1C23C1C(O)C=1C(CCC4(C=1CCC4C(C=CC(C(C)C)C)C)C)C2(CCC(O)C3)C	5.5	Excellent	7.0
6310	S1CC(=O)Nc2c1c(c1Nc3c(-c4c1c2ncc4)cccc3)CCN(C)C	4.9	Bad	7.0
6008	O1CC23C(C(CCC2C2(C(C(OC(=O)CCC)C3O)C(CCC2)(C)C)C)C(OC)=O)C1=O	5.0	Poor	7.0
5994	O1C2CCC1(C)C(OC(=O)C)CC1C(OC(=O)C1=C)C(O)C(CCCC2=C)C	4.3	Poor	7.0
5165	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=O)C)C)C)C1(C(O)=O)C)C	6.2	Poor	7.0
5156	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=O)C)C)C)C1(C(O)=O)C)C	5.9	Poor	7.0
5122	O1C2(OC(=CC3(CCCC23C)C)CC2(Oc3c(cc(O)cc3C)CC2)C)C=CC1(C)C	4.4	Bad	7.0
5071	O1C2C3C(C1CC(=C)C(N(C(=O)C)C)CCC2(OC(=O)C)C)C(OC(=O)C)(CCC3C(C)C)C	5.0	Bad	7.0
4982	O1C2CCC(C)C(CCC3=C(C)C(=O)CC4C(C)(C)C(O)CCC34C)C2(CCC(=O)C1(C)C)C	5.0	Bad	7.0
4835	o1c2c3c(CCCC3(c3c(cc4c(c3)C(=O)C=C(OC)C4=O)C2=O)C)c1	4.6	OK	7.0
4244	O(CC1C2(C(CC=C1C=O)C1(C(CC2)C(CCC1)(C)C)C)COC(=O)C)C(=O)C	5.6	Poor	7.0
4062	[nH]1c2c(CCN=C2c2c3c([nH]c2)cccc3)c2c1cccc2	5.2	Poor	7.0
3769	O1C2=CC(=O)C(=O)C=C2C=C2C3(C(CCC12C)C(CCC3)(C)C)C	4.1	Bad	7.0
3596	O1C2CCC3(OC3CCC(=CC=C(C(C)=C)C(O)CC12C)C)C	4.7	Excellent	7.0

3496	OC1CC2=CC(=O)C3C4CCC(C(C=CC(=O)C(C)C)C)C4(CCC3C2(CC1)C)C	6	Poor	7.0
3394	O1C23C(CCC(C)C2(CC2=C1C(=O)C=C(OC)C2=O)C)C(CCC3)(C)C	4.4	Excellent	7.0
3317	O1C(CC=C(CCC=2C3(C(CCC=2C)C(CCC3)(C)C)C)C1O)C1=CC(OC1O)=O	4.1	Excellent	7.0
2913	OC12C=C(C3C4(C1NCCCCC=CCC4)CN(CC3)CCCCC=CCC2)C=O	3.0	Poor	7.0
2465	O1C2C3C(C1CC(=CCCC2(OC(=O)C)C)C)C(=CC(OC(=O)C)C3C(C)C)C	4.4	OK	7.0
2294	O(C(=O)C(=O)c1c-2n(C=Cc3c-2[nH]c2c3cccc2)c2c1cccc2)C	4.0	Poor	7.0
2105	O(C(=O)C)c1c(CC2(C3CCC=C(C)C3(CCC2C)C)C)c(O)ccc1O	5.3	Poor	7.0
1748	OC1C2C(C3CCC(C(CCCC(C)C)C)C3(C1)C)CC(=O)C1CC(=O)CCC12C	5.2	Good	7.0
1721	OC1CC2C(C=3C(C4CCC(C(C=CCC(C)C)C)C4(CC=3)C)=CC2O)(CC1)C	5.2	Poor	7.0
1657	O1C2C(CCC3C(CCCC23C)(C)C)(C)C(COC(=O)C)C(CC(OC)=O)C1=O	5.8	Good	7.0
1655	O1C(C=CC2C(CC=CCCCC1=O)C(=O)CC2OC(=O)C)CC=CCC	4.5	Excellent	7.0
1596	S1CC(N(CO)C1=O)C1(OC2CCC(C=CCCC(=CC(OC(C1)C2)=O)C)C)O	4.6	Excellent	7.0
1566	O1C(CCCC=CC=CC(=O)CC(O)CC=CC=CC(O)CC=CC=CC1=O)C	4.7	Poor	7.0
1155	BrC1=CC23C4=C(NC(SC2CC1=O)C3)C(=O)c1[nH]cc2c1c4ncc2	5.1	Excellent	7.0
1138	O1C2OC(=O)CC(C2C2(CCC3=C(C2C)C(O)CCC3(C)C)C)C1OC(=O)C	4.3	Good	7.0
1126	O1C2OC(=O)CC(C2C2(CCC3=C(C2C)C(O)CCC3(C)C)C)C1OC(=O)C	6.0	Good	7.0
997	O1C2CCC(O)(C=CCC(=CC3OC(=O)C(C3CC(OC(=O)C)C12C)=C)C)C	5.2	Excellent	7.0
949	ClC1C2OC(=O)C(C)C2(O)C(O)C2C(C=CC(=O)C2C)(C)C(OC(=O)C)CCC1=C	6.3	Excellent	7.0
666	S=C=NC1(C2C(C(CC1)C1(OC(CC1)C([NH+]=[CH-])(C)C)C)C([NH+]=[CH-])C(O)(CC2)C)C	5.1	OK	7.0
630	O1C2OC(=O)C3C2C2(C(CC3)C3(C(C(CCC3)(C)C)C(OC(=O)C)C2)C)C1O	5.2	Excellent	7.0
619	O=C1Nc2c(cccc2)C12C1C2([NH+]=[CH-])C(CCC1C(C)=C)(C=C)C	3.5	Excellent	7.0
552	O1C2CC(=Cc3oc(CC(CCC4(OC24)C1=O)C(C)=C)c(c3)C)C	4.6	OK	7.0
489	ClC1CC2C(O)(c3c4c(cccc4[nH]c3)C2(C)C)C([NH+]=[CH-])C1(C=C)C	3.4	Excellent	7.0
448	O1CC2C3C(CCC2C1=O)C1(C(CC3COC(=O)C)C(CCC1)(C)C)C	6.4	Excellent	7
324	Fc1c(N2CCN(CC2)C)c(F)c2N(C=C(C(O)=O)C(=O)c2c1N)c1ccccc1	5.8	Poor	7
14478	O1C2C(CCC(=CCCC(C)C(=O)CCC(=C2)C)C)=C(C)C1=O	4.9	Excellent	6.9
14477	O1C2C(CCC(=CCCC(O)(C)C(O)CCC(=C2)C)C)=C(C)C1=O	4.2	Excellent	6.9
14364	S1CC(NC1=O)C(=O)CC1OC(=O)C=C(CCC=CC(CCC(OC)C1)C)C	4.9	Bad	6.9
13943	O1C2C(CC3C(C)(C(OC(=O)C)CCC(=C2)C)C(OC(=O)C)CC=C3C)=C(C)C1=O			6.9
13941	O1C2OC(=O)CC2C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1OC(=O)C	4.9	Bad	6.9
13767	O1C2(CCC(CC3OC3(CCC=C(CCC2O)C)C)C(=C)C1=O)C	4.5	Excellent	6.9
13728	O(C(=O)C)CC(c1c2c([nH]c1)cccc2)c1c2c([nH]c1)cccc2	4.4	Good	6.9
13606	o1c2c(c3c1c(C=O)c(O)c(O)c3)C1(C(CCC2C)C(CCC1)(C)C)C	5.5	Good	6.9
13364	O1C2C=C(CC(=O)C=C(CCC=C(CC(OC(=O)C)C2C(C)C)C)C)C1=O	5.3	Poor	6.9
13133	O1C2OC(=O)CC2C(C(=C)C2CCC3C2(CCCC3(C)C)C)C1OC(=O)C	4.5	Good	6.9
13010	O=C1C=C(NC)C(=O)C=C1CC1(C2CCC=C(C)C2(CCC1C)C)C	5.8	Excellent	6.9
12996	O1C2CCC(=CCC(CCC(=CC(OC(=O)C)CC12C)C)C(OC(=O)C)(C)C)C	4.5	Bad	6.9
12851	O=C1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	4.3	Bad	6.9
12808	O1C2(CCC=C(CCC(=CC=C(CCC2OC(=O)C)C)C(C)C)C1=O)C	3.3	OK	6.9
12749	O1C2(CCC=C(CCC(=CC=C(CCC2=O)C(OC)=O)C(C)C)C1=O)C	4.5	Excellent	6.9
12503	O(C(=O)C)C1C2C3C(CCC2(C)C(C1)C=C)C1(C(=CC(=O)C=C1)CC3)C	4.6	Good	6.9
12081	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)C1O)C1=CC(OC1OC(=O)C)=O	6.7	Bad	6.9
11951	O1C2CCC(C3C(CCC12C)C(=COC3OC(=O)C)C(OC(=O)C)CC=C(C)C)=C	4.7	OK	6.9
11945	O1CC(C2CC(C)C(O)C3C2C2OC3CC(=CCC(O)C12C)C)C	5.2	Excellent	6.9
11470	[NH+](C12C3C(C(CC(C3CCC1C)C)CC([NH+]=[CH-])(C)C)C(CC2)=C)=[CH-]	4.3	Excellent	6.9
11035	O1CC2C(CCC(=CC(O)CC2=C)C)C(C=CCC(O)(C)C)C1=O	4.4	Excellent	6.9

10992	O(C(=O)C)C1CC(O)C2(C(C1)CCC1C3CCC(C=C)C3(CCC12)C)C	3.9	Good	6.9
10982	O1C2CC(CCC3(OC3CCC(=CCCC2(O)C)C)C)C(C)C1=O	5	Good	6.9
10678	O(C(=O)C)C1(CC(O)C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC=C1)C)C)C	4.3	Good	6.9
10292	n1cccc(c1-c1cccnc1)-c1cc(ncc1)-c1cccnc1	6.1	Poor	6.9
9943	O1C2(CCC(CC3OC3(CCC=C(CCC2O)C)C)C(=C)C1=O)C	4.8	Excellent	6.9
9929	O(C(=O)C)CC(NC(=O)C(NC(=O)c1ccccc1)Cc1ccccc1)Cc1ccccc1	4.1	Poor	6.9
9822	O1C2CCC1(C)C(O)C1OC(=O)C(C1C(=O)CC(=CCCC2C)C)C	4.7	Good	6.9
9820	O1C2CCC1(C)C(O)CC=1C(OC(=O)C=1C)CC(=CCCC2C)C	5.8	Good	6.9
9819	O1C2CCC1(C)C(O)CC=1C(OC(=O)C=1C)CC(=CCCC2C)C	4.6	Excellent	6.9
9508	OC1CCC2C3C(CCC12C)C1(C(CC(O)CC1)=CC3)C	5.2	Excellent	6.9
9192	O1C2CC3C4C(C)(C(=O)CC3(CC(=O)C12C)C)C(=O)C=C4C(C)C	6.5	Excellent	6.9
9154	O1C2CC(O)(C3C2C(C2=C(CC(=O)CC(C2)C(C)=C)C3=O)C1=O)C	6.1	OK	6.9
9126	O1C(CCC1C(O)(C)C)(C(O)CCC(=C)C1OC2(C(OC(CC2)C2(OC(=O)CC2)C)CC1)C)C	5	Bad	6.9
9109	O1C2C(CCC(=CC(OC(=O)C)CC(=CC(OC(=O)C)CC(=C2)C)C)C)C(=C)C1=O	5.1	Good	6.9
9031	O1C(CC(=CCCC(C=CC(OC)C(O)(CCCc2ccoc2)C)C)C)C(O)=C(C)C1=O	3.7	Bad	6.9
8919	O=C1c2nccc3c2c(nc2c3cccc2)-c2c1[nH]cc2	4.2	Excellent	6.9
8606	OC12CC(O)CCC1(C1C(C3CCC(C(CCC(C(COC(=O)C)C)=C)C)C3(CC1)C)CC2=O)C	4.7	Bad	6.9
8589	O1C2C(CCC(=CCCC(C)C(=O)CCC(=C2)C)C)=C(C)C1=O	4.5	Excellent	6.9
8021	O1C(CC2C3(C(CCC2=C)C2(C(CC3)C(CCC2)(C)C)C)C)C(=CC1=O)CO	6.2	Excellent	6.9
8020	O1C(O)C(=CC1=O)C=CC1C2(C(CCC1=C)C1(C(CC2)C(CCC1)(C)C)C)C	3.8	Bad	6.9
7379	Oc1c(cc(cc1O)C(OC)=O)CC1(C2CCC=C(C)C2(CCC1C)C)C	4.1	OK	6.9
7378	Oc1c(cc(cc1O)C(OC)=O)CC1(C2CCC=C(C)C2(CCC1C)C)C	4.3	Good	6.9
7377	Oc1ccc(cc1CC1(C2CCC=C(C)C2(CCC1C)C)C)C(OC)=O	4.9	OK	6.9
7376	Oc1ccc(cc1CC1(C2CCC=C(C)C2(CCC1C)C)C)C(OC)=O	3.7	Excellent	6.9
7315	O1C2C(CC3C(C)(C(OC(=O)C)C(=O)C=C3C)C(OC(=O)CC)CCC(=C2)C)=C(C)C1=O	6.1	Excellent	6.9
7314	O1C2C(CC3C(C)(C(OC(=O)C)C(=O)C=C3C)C(OC(=O)C(C)C)CCC(=C2)C)=C(C)C1=O	6	OK	6.9
7184	Brc1c(cc2C3C(CCC3C(C)C)(C)C(OC(=O)C)C(=O)C(=O)c2c1O)C	6.5	Good	6.9
7052	O1C2C=C(CCC=C(CCC=C(CCC2C(O)(C)C)C)C)C1=O	6.4	OK	6.9
6691	O1C2C(CC3OC2C(CCCC(=CCCC3(O)C)C)C)C(=C)C1=O	6	Excellent	6.9
6431	O1C2C(CCC(=CCCC(O)(C)C(O)CCC(=C2)C)C)=C(C)C1=O	6	Good	6.9
6387	n1cnc2N(CN(c2c1N)CC=C(CCC1C2(CCCC(C)C2(CCC1=C)C)C)C)C	4.4	Bad	6.9
6266	O1C2C=C(CCC(C(C)=C)C(O)C(=O)C(=CC(=O)C3CC23C)C)C1=O	5.4	Poor	6.9
6265	O1C2C=C(CCC(C(C)=C)C(O)C(=O)C(=CC(=O)C3CC23C)C)C1=O	5.9	Excellent	6.9
6014	O1CC2C3(C(CCC2(O)C1=O)C1(C(CC3OC(=O)C)C(CCC1)(C)C)C)COC(=O)C	5.5	Poor	6.9
5843	O1C2(C3(OC1(CC3)C(CCCC(C)C)C)C1C(CC2OC(=O)C)C2(C(=CC(=O)C=C2)CC1)C)C	4.6	Good	6.9
5669	O1CC2C(CC(OC(=O)C)C3C2(C=O)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	5.4	Poor	6.9
5625	O(C(=O)C1C2(CCC3(C(CCC=C3C)C2(CCC1C)C)C)C)CC(O)COC(=O)C	3.9	Bad	6.9
5622	O(C(=O)C=C(CCC1C2(C(CCC1=C)C(CCC2)(C)C)C)C)CC(O)COC(=O)C	3.5	Bad	6.9
5302	O=C1CCC2(C3C(C4CCC(C(CC(O)C(OC)=O)C)C4(CC3)C)CCC2=C1)C	4.5	Bad	6.9
5219	O1CC2C(=CC(OC(=O)C)C3C2(C)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	5.4	Good	6.9
5204	O1C(O)C(=CC1=O)C(O)CC=C(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C	4.6	Good	6.9
5126	O=C=NC1(C2C3C(CC1)C(CC1CC(C)C(C(C13)CC2)(C#N)C)C)C	4.6	Poor	6.9
4814	O1C2CCC(=CCC3(C(CCC12C)C(C=C3)=C(COC(=O)C)COC(=O)C)C)C	5.2	Bad	6.9
4792	Clc1c2C=C3C4(C(CCC3(Oc2cc(O)c1O)C)C(CCC4)(C)C)C	3.8	OK	6.9
4757	O1C=C(C2C(C(CC=CC(OC(=O)C)(CC2)C)=C)C1OC(=O)C)C(=O)CC=C(C)C	4.1	OK	6.9
4746	O1C2C1(C(=O)C(=CCCC=CC(=CC(=CC)C(OC)=O)C)C)C(=O)NC2(O)C	5.4	Poor	6.9

4660	O1C2C34N5C6(OC(CC(C6)C)C5)CCC3(C)C(C3C(C5C(CC3=O)C(=O)C=C(C5)C)(C4)C)(C)C12O			6.9
4615	O1C2C1(CCC=C(CCC1(C3=C(CCC1C)C2(OC3)O)C)C)C	5.6	Excellent	6.9
4310	O1C2C3C(C1CC(O)(C)C(O)CCC2(OC(=O)CCC)C)C(CCC3C(C)C)=C	5.7	OK	6.9
4217	O1C2C(CCC3(OC3CCC(O)(C=CCC(=C2)C)C)C)C(=C)C1=O	4.9	Excellent	6.9
4189	O(C(COC(=O)c1ccccc1)c1cc(ccc1)CC)C(=O)c1ccccc1	4.5	Poor	6.9
3862	O1C(C(C)C2OC(CC)=C(C)C(=O)C2C)C(C)C(=O)C(C)=C1CC	6.6	Good	6.9
3834	O1C2(C=CC1(O)C(=CC1C(CC2OC(=O)C=C(C)C)C(=CC(=O)C1C(C)C)C)C)C	5.1	Good	6.9
3782	O1C2C3C(C1CC(O)(C)C(OC)CCC2(OC(=O)C)C)C(O)(CCC3C(C)C)C	4.1	Excellent	6.9
3657	O1C(C2C(C=CCC=CCC=CCCCC1=O)C(O)C(O)C2)CC	4.7	Bad	6.9
3549	O1c2c(cc(OC)cc2C)CCC1(CC=1CC2(CCCC2(C)C(=O)C=1CC(O)(C)C)C)C	5	Bad	6.9
3547	O1c2c(cc(OC)cc2C)CCC1(CC=1CC2(CCCC2(C)C(=O)C=1CC(O)(C)C)C)C	4.8	Bad	6.9
3539	O1C2CC(CCC(=CCCC(=CCCC2(O)C)C)C)C(=C)C1=O	4.1	Excellent	6.9
3499	OC1CC2=CC(=O)C3C4CCC(C(CCC(C(O)(C)C)=C)C)C4(CCC3C2(CC1)C)C	6.3	Bad	6.9
3497	OC1CC2=CC(=O)C3C4CCC(C(CCC(=O)C(C)C)C)C4(CCC3C2(CC1)C)C	5.5	Excellent	6.9
3399	O1CC(C2CC(C)C(=O)C3C2C2OC3CC(=CCC(OC(=O)CCCCCCC)C12C)C)C	5.1	Poor	6.9
3322	O1CC(CC1=O)C(O)CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)CO	3.9	Good	6.9
3299	O1CC(=CC1=O)CCC=C(CCC1C2C3(C)C1(CCC3(C)C(CC2=O)C)C)C	6.3	Poor	6.9
3249	o1ccc(C(C)C)c1CC(C(O)=O)C1CCC2C3C(CCC12C)C1(C=C(O)C(=O)CC1CC3)C	4.9	Bad	6.9
2857	O1C2C3C(C1CC(C)C(=O)CCC2(OC(=O)CCC)C)C(=C)C(O)CC3C(C)C	5.1	Good	6.9
2718	O1C2C(CCC(=CCCC(O)(C)C(O)CCC(=C2)C)C)=C(C)C1=O	4.9	Excellent	6.9
2564	OC12CC(O)CCC1(C1C(C3CCC(C(C=CCC(C)C)C)C3(CC1)C)=CC2=O)C	3.8	Good	6.9
2532	O1C2C3C(CCC3(CC=C(CC(=O)CC(C2)C)C)C)=C(C)C1=O	4.7	Excellent	6.9
2479	O1C2c3oc(CC(CCC4=CC(OC4=O)CC12C)C(C)=C)c(c3)C=O	5.4	Excellent	6.9
2346	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCNC(=O)CC)cccc4	4.9	Good	6.9
2240	O1OC(CCC1(CCC1C(C2C(CC1=C)CC(CC2)=C)(C)C)C)C(C(O)=O)C	5.9	Bad	6.9
2082	O=C1c2c(NC=C1)c1nc3c(c4C=Nc(c14)c2NC)cccc3	4.7	OK	6.9
1595	S1CC(N(CO)C1=O)C1(OC2CCC(C=CC=CCCC(=CC(OC(C1)C2)=O)C)C)O	4.4	Poor	6.9
1418	O1CC2(C3C(=O)C(C4C(CC(=CC4=O)C)C3(C=C3N4C5(OC(CC(C5)C)C4)CCC23C)C)C)CC1=O			6.9
1416	O1CC2(C3C(=O)C(C4C(CC(=CC4=O)C)C3(C=C3N4C5(OC(CC(C5)C)C4)CCC23C)C)C)CC1=O			6.9
1400	O1CC(C2CCC3(C(CCc4c3coc4)C2(CC1=O)C)C)C(OC)=O	4.4	Good	6.9
1264	O1C(OC(=O)C)C2C(CC=C(C3(CC(CCC3)(C)C)C)C2=CC)C1=O	5.6	Good	6.9
1151	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(OC(=O)C)C=C=C	5.4	Poor	6.9
1079	O(C(=O)C1C2(CC=C3C(CCCC3(C)C)C2(CCC1C)C)C)CC(O)COC(=O)C	5.8	OK	6.9
1078	O(C(COC(=O)C1C2(CC=C3C(CCCC3(C)C)C2(CCC1C)C)C)CO)C(=O)C	4.9	Bad	6.9
1014	O1C(=O)C(C)=C(CC1C(C)C1CCC2C3C(CCC12COC(=O)C)C1(C(=CC(=O)C=C1)CC3)C)C	5.3	Bad	6.9
996	O1C2C(CCC3(OC3CCC(O)(C=CCC(=C2)C)C)C)C(=C)C1=O	5.5	Good	6.9
920	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)CCNC(=O)CC(O)(C)C	3	Good	6.9
909	O1C2C3C(CCC3(CC=C(CC(=O)CC(C2)C)C)C)=C(C)C1=O	4.7	Poor	6.9
719	O1C(C2OC1(C1C3(CCCC3(C)C1(O)C2)C)CC(=CCc1cc(OC)cc(C)c1O)C)(C)C	6.1	Good	6.9
651	Brc1cc2nc3c4c(nccc4c2cc1)-c1ncccc1C3=O	5.9	Poor	6.9
587	O1C(CC=C(CCC=C(CCC2(CCCC2C)C(C)=C)C)C1O)C1=CC(OC1O)=O	6.6	Bad	6.9
445	O(C(=O)C)C1CC(CCC(C)C(OC(=O)C)CCC(CC(=O)CC1C)C)C(C)=C	4.2	OK	6.9
338	Oc1c(cc(cc1O)C(OC)=O)CC1(C2CCCC(=C)C2(CCC1C)C)C	4.8	Poor	6.9
336	O=C1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	3.8	Bad	6.9
58	O1C2OC(=O)C3C2C2(C(CC3)C3(C(C(O)C2OC(=O)CCC)C(CCC3)(C)C)C)C1O	4.7	Excellent	6.9
14297	O1C=C2C(C3(C(C(OC(=O)C)C2OC(=O)C)C(CCC3)(C)C)C)C1OC(=O)C	6	Good	6.8

13771	O1C2(OC)C3=C(CCC(CCC(CC(O)C=C(C2)C)=C)C3(C)C)C1=O	4.9	Excellent	6.8
13434	O1CC2C3(C(CCC3C(=CC=CC(O)(C)C)C=O)(C)C(O)CC2)C1=O	6.6	Excellent	6.8
13363	O1C2CCC(=CC=C(CCC(=CCCC12C)C(OC)=O)C(C)C)C(OC)=O	4.2	Good	6.8
13069	O(C(=O)C)C1CC(C2CC=C(C(C1C(CCC=C(C)C)C)C2OC(=O)C)C=O)=C	4.7	Poor	6.8
13009	O1C23C4C(CCC4C)C(=CC2CC(OC3=C(C)C1=O)(CCCc1ccoc1)C)C	5.6	Excellent	6.8
12997	O1C2CCC(=CCC(CCC(=CC(OC(=O)C)CC12C)C)C(O)(C)C)C	5.2	Excellent	6.8
12992	O1OC(CCC1(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C)C(C(O)=O)C	5.6	Bad	6.8
12767	O1C2CC(=O)CC(CCC3=CC(OC3=O)CC1(CC2=O)C)C(C)=C	5.4	Excellent	6.8
12685	O1C2C(CCC(=CCCC(=CCCC(=C2)C)C(O)=O)C)C(=C)C1=O	4.4	Excellent	6.8
12465	O1C2CCC(O)(C)C(CCC3C(C4C(CC=C3C)C(O)(CC4)C)(C)C)C2(CCC(=O)C1(C)C)C	5.6	Poor	6.8
12352	O1C2C(=CC1=O)C(OC(=O)C)CC1C2(C)C(O)CC2C1(CCC1C(CCCC12C)(C)C)C	4.2	OK	6.8
12325	OC1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	4.1	OK	6.8
12230	o1cc(c2CC3C(C)(C(OC(=O)C)C(=O)CC(=Cc12)C)C(OC(=O)C)CC=C3C)C	5.5	OK	6.8
12214	O1c2c(C3C1c1c(OC3)cc3occc3c1)ccc(OC)c2OC	3.8	Excellent	6.8
12163	O(C(=O)C)C1CC2C(CC1C(=O)C)(C)C(=O)CC1C2(CCC2C(CCCC12C)(CC)C)C	5.1	Bad	6.8
12105	OC1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	3.8	Poor	6.8
11943	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=CCC(O)C12C)C)C	5.6	OK	6.8
11941	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=C)C(O)CC(OC(=O)C)C12C)C	4.7	Good	6.8
11925	O=C1C=C2CCC3C4CCC(C=C)C4(CCC3C2(C=C1)C)COC(=O)C	4.4	Excellent	6.8
11830	O1OC(CCC1(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C)C(C(O)=O)C	4.6	Bad	6.8
11566	O1CC2C(CCC(=CC(O)CC2=C)C)C(=CC=CC(O)(C)C)C1=O	6.1	Excellent	6.8
11563	O1CC2C(CCC3(OC3C(O)CC2=C)C)C(=CC=CC(O)(C)C)C1=O	4.6	Poor	6.8
11506	o1cc(cc1)C(OC(=O)C)CC1C(CC2C1(CCC1C(CCCC12C)(C=O)C)C)(C=O)C	4	OK	6.8
11491	O1CC2C(CCC(=CC(O)CC2=C)C)C(=CC=CC(O)(C)C)C1=O	6.3	Excellent	6.8
11464	O(C(=O)C)C1C2C(C3CCC(C=C)C3(C1)C)CCC1=CC(=O)CCC12C	4.6	Poor	6.8
11412	O1C2=C(CC3C4(C(CCC13C)C(CCC4)(C)C)C)C(=O)C(OC)=CC2=O	4.6	OK	6.8
11411	O(C)C1=CC(=O)C(O)=C(C=C2C3(C(CCC2C)C(CCC3)(C)C)C)C1=O	4.2	Poor	6.8
11378	Brc1cc2n3c(-c4[nH]c5c(c4C=C3)cccc5)c(c2cc1)C(=O)C(OC)=O	4	Poor	6.8
11192	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	5.4	OK	6.8
11163	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	5.3	Bad	6.8
10983	O1C2CC(CCC3(OC3CCC(=CCCC2(O)C)C)C)C(=C)C1=O	5.4	Good	6.8
10862	O1C=C(C2C(C(CC(O)C=C(CC2)C)=C)C1O)C(OC(=O)C)C(OC(=O)C)C=C(C)C	5.1	OK	6.8
10807	OC1CC2=CCC3C4CCC(C(CCC(OC)=O)C)C4(CCC3C2(CC1)C)C	3.8	Bad	6.8
10544	O1C(=O)C(=CC1=CC(CC=CC(=CCCc1cc(oc1)Cc1ccoc1)C)C)C	5	Poor	6.8
10407	O(C(=O)c1ccccc1)c1c2nc3c(nc2ccc1)cccc3	4.8	Excellent	6.8
10285	O1C2C(CCC(=CCCC(=CCCC(=C2)C)C(O)=O)C)C(=C)C1=O	4.2	Excellent	6.8
10075	Oc1ccc(cc1CC1C2(C(CCC1=C)C(CCC2)(C)C)C)C(O)=O	5.1	Excellent	6.8
9823	O1C2CCC1(C)C(O)C1OC(=O)C(O)(C1C(=O)CC(=CCCC2C)C)C	6.4	Excellent	6.8
9156	O1C2CC(=O)CC(CC(OC)C3=CC(OC3=O)CC1(CC2=O)C)C(C)=C	6.1	Excellent	6.8
8792	O1CC(=CC1=O)C(O)CC=C(CCC1(C2CCCC(=C)C2(CC(O)C1C)C)C)C	4.8	Bad	6.8
8605	OC12CC(O)CCC1(C1C(C3CCC(C(CCC(C(COC(=O)C)C)=C)C)C3(CC1)C)CC2=O)C	5.2	Bad	6.8
8555	OC1(CCC2C3C(CCC12C)C1(C(CC(O)CC1)=CC3)C)C(=O)C	3.6	Excellent	6.8
8546	O1C23CCCC(=C)C2(CCC(C)C3(CC2=C1C(=O)C=C(OC)C2=O)C)C	5.8	Excellent	6.8
8545	O1C23CCCC(=C)C2(CCC(C)C3(CC2=C1C(=O)C=C(OC)C2=O)C)C	5.5	OK	6.8
8395	ClC1CC(C2C(C3CC(OC3(CC2=O)C)C2CC(=O)NC2=O)(C1)C)(C)C	4.3	OK	6.8
8393	ClC1CC2(C(C(C1)(C)C)C(=O)CC(=C)C2CC(O)C1CC(=O)NC1=O)C	4.9	OK	6.8
8330	O(O)C1CCC(=C)C(=O)CC2(CC(=O)C(=C2CCC1=C)C(C)C)C	4.7	Excellent	6.8

7946	ClC1CC2C(C3(C)C1(O)CC=CC3=O)C(O)CC1(C2CCC1C(C=CC(C(C)C)C)C)C	4	Poor	6.8
7931	O1C(=O)C(=C2CC3C(C4OC3(CC4)C)(CCC=C(CC12O)C)C)C	5.2	Good	6.8
7783	O1C2C1(CC=C(CCC=C(CCC=C(CO)C)C)C)C(=O)C=C(CO)C2OC(=O)C	5.2	Bad	6.8
7778	O1C2C1(CC=C(CCC=C(CCC=C(C)C)C)C)C(=O)C=C(COC(=O)C)C2=O	3.5	Poor	6.8
7521	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(C#N)(C)C2O)C(CC1O)(C#N)C	6.3	Excellent	6.8
7297	O1C23C1C=CC(=O)C2(C1C(C2CCC(C(CCC(C(C)C)C)C)C)C2(CC1O)C)CC3O)C	5.1	Excellent	6.8
7133	O1C23C4C(CCC4C)C(=CC2CC(OC3=C(C)C1=O)(CCCc1ccoc1)C)C	5.3	Excellent	6.8
6679	O1C2C(CC3OC2C(CCCC(=CCCC3(OC(=O)C)C)C)C)C(=C)C1=O	6.2	Excellent	6.8
6572	O1C2C(=CC1=O)CCC1C2(CCC2C3(C(CCC12C)C(CCC3)(C)C)C)C=O	4.5	Excellent	6.8
6214	O1C2CC(=O)CC(CCC3=CC(OC3=O)CC1(CC2=O)C)C(C)=C	5.3	Excellent	6.8
6125	O1C2=C(C3=C(C1)C(CCC1(O)C3=CC(=O)C=C1)C)CCCC2(C)C	6	Good	6.8
6070	OC1CC2=CCC3C4CCC(C(CCC(OC)=O)C)C4(CCC3C2(CC1)C)C	4.7	Poor	6.8
6058	O1C23C1C(O)C1C4CCC(C(CCC=C(C)C)C)C4(CCC1C2(CCC(O)C3)C)C	4.5	Poor	6.8
6056	OC1C2CC(O)CCC2(C)C(=O)C(=C1)C1CCC(C(C=CCC(C)C)C)C1(CCOC(=O)C)C	5	OK	6.8
6049	O1C2C(=CC1=O)C(OC(=O)C)CC1C2(C)C(O)CC2C1(CCC1C(CCCC12C)(C)C)C	4.5	Bad	6.8
6013	O1C(O)C2C(CCC3C2(C)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	5.3	OK	6.8
5996	Brc1cc2NC(=C3c4c(NC3=O)cccc4)C(=O)c2cc1	5.8	OK	6.8
5959	O1CC2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(CO)C)C)C)C)C1=O	3.8	Excellent	6.8
5901	O=C1c2c(NCC1)c1nc3c(c4C=Nc(c14)c2N)cccc3	4.2	Poor	6.8
5782	S(OCC(CC=CC(C)C1CCC2C=3C(CCC12C)C1(C(CC(O)CC1)C(=O)C=3)C)C)(O)(=O)=O	5.6	Bad	6.8
5781	S(OCC(CCCC(C)C1CCC2C=3C(CCC12C)C1(C(CC(O)CC1)C(=O)C=3)C)C)(O)(=O)=O	5.1	Poor	6.8
5756	OC1C2C3CCC(C(CCCC(CO)C)C)C3(CCC2C2(C(C1)=CC(=O)CC2)C)C	5.5	Bad	6.8
5676	O1C2=C(C3=C(C1)C(CCC1(O)C3=CC(=O)C=C1)C)CCCC2(C)C	5.8	Excellent	6.8
5638	OC1(CCC2C3C(CCC12C)C1(C(CC(O)CC1)=CC3)C)C(=O)C	5.1	Excellent	6.8
5217	O1CC2(O)C(=CC(OC(=O)C)C3C2(CCC2C(CCCC23C)(C)C)C)C1=O	5.6	Excellent	6.8
5047	O1C2(C(CC1=O)C1(C(C3(C(CC1)C(CCC3)(C)C)C)C(OC(=O)C)C2)COC(=O)C)C	5	Poor	6.8
4981	O1C2CCC3(OC3)C(CCC3=C(C)C(=O)C(O)=C4C(C)(C)C(=O)CCC34C)C2(CCC(=O)C1(C)C)C	5	Good	6.8
4940	O(C)c1cc2[nH]c(CC=C(C)C)c(c2cc1)CC1NC(=O)C2N(CCC2)C1=O	4.3	Good	6.8
4936	O1C2C(C=CCC1=O)=C(C1C(C3CCC(C(C=CC(C(C)C)C)C)C)C3(CC1O)C)C2)C	4.8	Good	6.8
4929	O1CC(C2C3C(C4OC3C1(C)C(O)(CC(=O)C(C4)=C)C(=O)CCCCCCC)C(O)(CC2)C)C	5.1	OK	6.8
4919	O1C(=O)C(=C2CC3C(C)(C(OC(=O)C)CCC(=CC12O)C)C(OC(=O)C)CC=C3C)C			6.8
4836	o1c2c3c(CCCC3(c3c(cc4c(c3)C(=O)C(OC)=CC4=O)C2=O)C)c1	5.7	Good	6.8
4811	O1C2CCC(=CCC3(C(CCC12C)C(=C(C)C)C(=O)C3)C)COC(=O)C	5.5	Poor	6.8
4718	O1CC(=CC1=O)C(O)CC1CC2C(CCCC2(C2CCC(CC12C)=C)C)(C)C	5.5	Excellent	6.8
4663	O1C(=O)C(C2C3C(C(O)(CC2)C)C(OC3C1(C=CC=O)C)CC(=O)C)C	5.5	Excellent	6.8
4448	O1C=2C(=CC13C1(C(CCC3C)C(CCC1)(C)C)C)C=C(O)C(=O)C=2C=O	4.7	Good	6.8
4441	O1C=2C(=CC13C1(C(CCC3C)C(CCC1)(C)C)C)C=C(O)C(=O)C=2C=O	4.5	Excellent	6.8
4307	O1C2C3C(C1C(CC(=O)CCC2(OC(=O)C)C)C)C(CCC3C(C)C)=C	5.6	Excellent	6.8
4297	S(C)C=1C(=O)c2nccc3c2c(nc2c3cccc2)C=1CCNC(=O)CC(C)C	4.4	Poor	6.8
4230	o1cc2c(CCC3C2(CCC2C(C)(C)C(=O)C(O)CC23C)CO)c1	4.6	OK	6.8
4229	o1cc2c(CCC3C2(CCC2C(C)(C)C(=O)C(O)CC23C)CO)c1	4.4	Good	6.8
4131	Oc1cc(CC(OC)=O)c(O)cc1CC1C2(C(CCC1=C)=C(C)C(CC2)C)C	4.7	Poor	6.8
3783	O1C2C3C(C1CC(=C)C(=O)CCC2(OC(=O)C)C)C(OC(=O)C)(CCC3C(C)C)C	5.7	Bad	6.8
3736	OC1CC2(C(C3C1(C)C(O)C=C3C(C)C)CCC(=CC2)C)C	5.1	Good	6.8
3682	O1C2OC(=O)CC2C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1O	4	Excellent	6.8

3649	OC1CC2=CCC3C4CCC(C(CCC(OC)=O)C)C4(CCC3C2(CC1)C)C	4.2	Poor	6.8
3445	O1C2CCC1(C)C(OC(=O)C)CCC(=CC=C(CCC2(O)C)C(C)C)C	3.9	Poor	6.8
3401	O1CC(C2CC(C)C(OC(=O)C)C3C2C2OC3CC(CCC(=O)C12C)=C)C	4.8	Good	6.8
3400	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(CCC(=O)C12C)=C)C	4.8	Good	6.8
3347	O1C(CC=C(CCC=2C3(C(CCC=2C)C(CCC3)(C)C)C)CO)C(=CC1=O)CO	4.4	Bad	6.8
3338	O1C(CC=C(CCC=2C3(C(CCC=2C)C(CCC3)(C)C)C)CO)C(=CC1=O)CO	4.1	Poor	6.8
3292	OC1CC2=CC(O)C3C4CCC(C(C=CCC(C)C)C)C4(CCC3C2(CC1)C)C	3.8	Poor	6.8
3291	OC1CC2=CC(O)C3C4CCC(C(C=CCC(C)C)C)C4(CCC3C2(CC1)C)C	5.4	Poor	6.8
3132	O1C(C)(C)C(O)CC(=O)C1(CCCC(=CC(=O)CC(=CCc1cc(O)cc(C)c1OC)C)C)C	4.1	Poor	6.8
3122	O1C(C)(C)C(O)CC(=O)C1(CCCC(=CC(=O)CC(=CCc1cc(O)cc(C)c1OC)C)C)C	6.2	Poor	6.8
2989	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)C1=O)C1CC(OC1)=O	5.3	Poor	6.8
2985	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)C1O)C1CC(OC1)=O	4.3	OK	6.8
2965	OC1(CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)CC3)CC)C(=O)COC(=O)C	4.4	Bad	6.8
2938	O1C(=O)C(CCC2C3(C(CCC12C)C(CCC3)(C)C)C)=CCC(OC(=O)C)C1=CC(OC1)=O	4.5	Bad	6.8
2591	O1C2OC(=O)CC2C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1O	4	Bad	6.8
2589	Oc1c(cc(cc1O)C(OC)=O)CC1C2(C(CC=C1C)C(CCC2)(C)C)C	4.5	Good	6.8
2519	O1C2C3C(CCC3(CCC(=CC(=O)CC(C2)C)C)C)=C(C)C1=O	4.8	Good	6.8
2381	O1C2OC(=O)CC2C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1O	4	Good	6.8
2347	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCNC(=O)C)cccc4	6.3	Excellent	6.8
2236	O1CC1C1(CC2C(=CC1)C1(C(CC2O)C2(C(C2)C(OC(=O)C)C1)CO)C)C	5.2	Good	6.8
2122	O1C2C3=C4COC3(O)C(O)C1(CCC=C(CCC4(C)C(C2)C)C)C	4.9	Excellent	6.8
2104	OC1=CC(=O)C=C(CC2(C3CCC=C(C)C3(CCC2C)C)C)C1=O	4.9	Good	6.8
1938	O1C2CC(OC(=O)C)C3(C(Cc4c(occ4C)C=C(C)C(O)CC3)C12C)C			6.8
1786	O1C2CC(=CC(=O)C=C(C)C(=O)CC(CCC3(OC23)C1=O)C(C)=C)C	5.1	Good	6.8
1482	O1C2OC(=O)CC(C2C2(C3C4(C(CC2)C(CCC4)(C)C)C3)C)C1OC(=O)C	5.7	Bad	6.8
1421	O1OC(CCC1(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C)C(C(O)=O)C	4.2	Good	6.8
1281	O1C2C3C(C1CC(=CCCC2(OC(=O)CCC)C)C)C(=C)C(O)CC3C(C)C	4.7	OK	6.8
1125	O1C2OC(=O)CC(C2C2(CCC3=C(CCCC3(C)C)C2C)C)C1OC(=O)C	6	Excellent	6.8
1020	ClC1=CC(O)(C2Cc3c(occ3C)CC(=CCCC2(C)C1=O)C)C	5.3	Excellent	6.8
1019	o1cc(c2CC3C(CCC=C(Cc12)C)(C)C(=O)C=CC3(O)C)C	4.9	Excellent	6.8
665	S=C=NC(C)(C)C1OC(CC1)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	4.2	Good	6.8
627	O1C2OC(=O)C3C2C2(C(CC3)C3(C(C(CCC3)(C)C)C(OC(=O)CCC)C2)C)C1OC(=O)C	5.8	Good	6.8
588	O1C(O)C(=CC1=O)C(O)CC=C(CCC=C(CCC1(CCCC1C)C(C)=C)C)C=O	4.9	Poor	6.8
551	O1C23OC4C(OC(=O)C4(O)CCC(CC1(O)C(=C2)C)C(C)=C)CC(=C3)C	5.3	Excellent	6.8
462	O1Cc2c(c(C(C(OC)=O)C)c(cc2)C2(CC(CCC2)(C)C)C)C1=O	4.8	Good	6.8
367	O1C2OC(=O)CC2C(C2(CCC3C(=CCCC3(C)C)C2C)C)C1OC(=O)C	5.4	Good	6.8
335	OC1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	4	Bad	6.8
194	O1OC(CCC1(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C)C(C(O)=O)C	5.6	Excellent	6.8
59	O1C2OC(=O)C3C2C2(C(CC3)C3(C(C(OC(=O)CCC)C2O)C(CCC3)(C)C)C)C1O	3.7	Poor	6.8
7	O1C2CC(=O)CC(CCC3=CC(OC3=O)CC1(CC2=O)C)C(C)=C	5.8	Excellent	6.8
14491	O1C2CC(=O)CC(CC=C(CC(=O)CC1(CC2=O)C)C(OC)=O)C(C)=C	4.9	Poor	6.7
14444	O1C(C2(C=C(C=C(C)C2C(=CC(C(=O)CC)C)C)C)C)=C(C)C(=O)C(C)=C1OC	5.3	Good	6.7
14434	O1C(C2(C=C(C=C(C)C2C(=CC(C(=O)CC)C)C)C)C)=C(C)C(=O)C(C)=C1OC	5.4	Excellent	6.7
14404	O1C(O)C(=CC1=O)C=CC=C(CCC=C(CCC=1C(CCCC=1C)(C)C)C)C=O	5.9	Poor	6.7
14011	O1C2C(CC3OC3(CCC=C(CCCC(C)C2O)C)C)C(=C)C1=O	5.1	Excellent	6.7
13770	O1C2CCC(CCC(CC(O)C=C(CC1=O)C)=C)C(C)(C)C2=O	5.2	Excellent	6.7

13722	O1C2=C(C=CC1(CCC1(CCC=C(C)C1C)C)C)C(=O)C(OC)=CC2=O	4.9	Good	6.7
13403	O1C2C3C(C(OC(=O)C)(CCC3C(C)C)C)C(=O)CC(O)(C1CCC2(O)C)C	4.7	Good	6.7
13011	O=C1C(=CC(=O)C=C1NC)CC1(C2CCC=C(C)C2(CCC1C)C)C	4.1	Poor	6.7
12858	O1C2C1(C)C(=O)CC(CCC1=CC(OC1=O)CC(=CC2=O)C)C(C)=C	5.3	OK	6.7
12323	O1C2OC(O)C3C2C(CC3)C(CCC=C(CCC=C(C)C)C)C1O	5.2	Good	6.7
12170	O1C2C(CC(OC(=O)C)C(=CCCC(=CCCC(=C2)C)C(OC)=O)C)=C(C)C1=O	6.4	Good	6.7
12058	S(C)C12N(C3Nc4c(cccc4)C3(C1)c1c3c([nH]c1)cccc3)C(=O)C(SC)N(C)C2=O	5	Excellent	6.7
11846	ClC1CCC2(C(C1(C)C)C(=O)C=C(C)C2CC(O)C1CC(=O)NC1=O)C	4.7	Excellent	6.7
11791	O1C2CCC1(C)C(O)C(OC(=O)C)c1c(occ1C)CC(=CCCC2C)C	4.4	Excellent	6.7
11653	O(C(=O)C)C1C2C(C3C(C1)(C)C(CC3OC(=O)C)C=C)CCC1=CC(=O)CCC12C	4.3	Good	6.7
11468	O(C(=O)C)C1CC2C(C=C(C)C(=O)C=CC1(O)C)C2(CCC=C(C)C)C			6.7
11460	O(C(=O)C)C1CC2C(C=C(C)C(=O)C=CC1(O)C)C2(CCC=C(C)C)C			6.7
11414	O1C2=C(C=C3C4(C(CCC13C)C(CCC4)(C)C)C)C(=O)C(OC)=CC2=O	4.6	OK	6.7
11288	O1C(C)(C)C1CC(OC(=O)C)C=1C2C(C(CC(O)C=C(CC2)C)=C)C(OC=1)O	5.5	OK	6.7
11193	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	5.2	Poor	6.7
11164	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	5.9	Poor	6.7
11091	O=C1C2C(C3CCC(C(=O)CO)C3(C1)C)CCC1=CC(=O)C=CC12C	4.7	OK	6.7
11032	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	4.7	Poor	6.7
11029	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	6.2	Good	6.7
10922	O1CC2=C(C3C(C3)C(CC(OC(=O)C)C2C(CCC=C(C)C)C)C)C1=O	5.3	Excellent	6.7
10797	Oc1ccc(O)cc1CC1C2(C(CC=C1C)C(CCC2)(C)C)C	4.7	Excellent	6.7
10653	O1C(CC(=CCCC(C=CC=C(CCCC2=CCN(CC(O)=O)C2=O)C)C)C(O)=C(C)C1=O	5.5	Bad	6.7
10542	O1C(=O)C(=CC1=CC(CC=CC(=CCCc1cc(oc1)Cc1ccoc1)C)C)CO	4.5	Poor	6.7
9834	OC(=O)c1ccccc1N1Cc2[nH]c3c(c2C=C1)cccc3	4.3	Excellent	6.7
9716	O1C23C1(C1CCC(C(CCCC(C)C)C)C1(CC2)C)CC(O)C1CC(O)CCC13C	5.1	Poor	6.7
9656	O1C2C(c3c1cc(OC)cc3)COc1c2cc2c(occ2)c1	4.5	Poor	6.7
9520	O1C2C(CC3OC3(CCC=C(CCCC(C)C2O)C)C)C(=C)C1=O	5.5	Good	6.7
9486	Oc1cc(C)c(CCC(=CCC2=CC(=O)C=CC2=O)C)c(C)c1C=O	5.3	Poor	6.7
9454	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	4.8	Good	6.7
9277	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)C(OC)CNC(=O)C	6.8	Excellent	6.7
9195	O(O)C1(CCC2C3C(C)(C(=O)CC2(C=C1)C)C(=O)C=C3C(C)C)C	6.5	Poor	6.7
9148	O1C(C)(C)C1CC=C(COC(=O)C)C1CCC2(OC2CCC(=C)C1C(OC)=O)C	5.5	Bad	6.7
9143	O=C1c2c(NC1=C1c3c(NC1=O)cccc3)cccc2	6.1	Poor	6.7
9048	O1C2(O)C3=C(CCC(CCC(CC(O)C=C(C2)C)=C)C3(C)C)C1=O	4.9	Excellent	6.7
8790	O1CC(=CC1=O)C(O)CC=C(CCC1(C2CCCC(=C)C2(CC(OC(=O)C)C1C)C)C)C	5.2	Bad	6.7
8620	Oc1ccc(O)cc1CC1C2(C(CC=C1C)C(CCC2)(C)C)C	5.2	Excellent	6.7
8603	O1C23C1C(O)C1C4CCC(C(CCC(C(C)C)=C)C)C4(CCC1C2(CCC(O)C3)C)C	4.4	Bad	6.7
8423	O1C2CCC1(C)C(O)C(O)C=1C(OC(=O)C=1C)CC(=CCCC2C)C	4.8	Bad	6.7
8409	O1C(=CC(CCCC(=CCCc2cc(oc2)Cc2ccoc2)C)C)C(O)=C(C)C1=O	5.6	Bad	6.7
8394	ClC1CC2(C(C(C1)(C)C)C(=O)C=C(C)C2CC(O)C1CC(=O)NC1=O)C	4.8	Bad	6.7
8263	OC1(CCC(O)CC1=CC(=O)C1C2CCC(C(CCCC(C)C)C)C2(CCC1)C)C	5.6	Good	6.7
8083	ClC1C(C2C(CC1Cl)(C)C(CC(O)C1CC(=O)NC1=O)C(=CC2=O)C)(C)C	5.5	Excellent	6.7
7782	O1C2C1(CC=C(CCC=C(CCC=C(CO)C)C)C)C(=O)C=C(COC(=O)C)C2O	4.4	Bad	6.7
7779	O1C2C1(CC=C(CCC=C(CCC=C(C)C)C)C)C(=O)C=C(CO)C2OC(=O)C	5	Poor	6.7
7544	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(N)=CC1=O	5.2	Good	6.7
7525	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=O)C)C)C1(CO)C)C	5.1	OK	6.7
7524	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=O)C)C)C1(CO)C)C	5.3	OK	6.7

7523	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=O)C)C)C)C1(CO)C)C	5.1	Good	6.7
7500	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC(O)=O)C)C)C1(C(O)=O)C)C	7.2	Poor	6.7
7499	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C(O)=O)C)C)C1(C(O)=O)C)C	6.1	Good	6.7
7316	O1C2C(CC3C(C)(C(OC(=O)C)C(=O)C=C3C)C(OC(=O)c3ccccc3)CCC(=C2)C)=C(C)C1=O	6	Poor	6.7
7237	O1C23C(CCC(C2)C)C2(C(C1(O)C(CC2=O)C(C)C)C(=C3)C(OC)=O)C			6.7
7191	O1C23C(CC=C(C2)C)C2(C(C(=O)C(CC12O)C(C)C)C(=C3)C(OC)=O)C	5	Poor	6.7
6681	O1CC=2C3(C(CCC=2)C(CCc2ccoc2)(C)C(CC3O)C)C1O	3.9	OK	6.7
6610	O1C23C(CCC(C2)=C)C2(C(C(=O)C(CC12O)C(C)C)C(=C3)C(OC)=O)C	5.2	Good	6.7
6526	O=C1NC(=O)C2=C1c1c3c([nH]c1-n1c2cnc1)cccc3	6.1	Excellent	6.7
6471	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(=CC1)C	5.1	Good	6.7
6323	OC1CC2=CC(=O)C3C4CCC(C(CCC(C(C)C)=C)C)C4(CCC3C2(CC1)CO)C	4.7	OK	6.7
6307	O1OC(CCC1(CCC1=C(C)C(=O)CC2C1(CCCC2(C)C)C)C)C(C(OC)=O)C	5.1	Bad	6.7
6018	O1C2C1(C(OC)=O)C(=O)C1(C(C3(C(CC1)C(CCC3)(C)C)C)C2OC(=O)C)C	5.1	Good	6.7
6017	O(C(=O)C)C1C2C(CCC3C(CCCC23C)(C)C)(C)C(=O)C(=C1)C(OC)=O	4.8	OK	6.7
6011	O(C(=O)C)C1CC2C(CCCC2(C2CCC(C(OC)=O)C(C=O)C12C)C)(C)C	4.8	Poor	6.7
5995	Brc1cc2NC(=O)C(c2cc1)=C1Nc2c(cccc2)C1=O	4.3	OK	6.7
5958	O1CC2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(CO)C)C)C)C)C1=O	4.3	Excellent	6.7
5940	O1C2CC(CCC(=CCCC(O)(C=CCC12C)C)C)C(C(OC)=O)=C	5.1	OK	6.7
5858	O1CC2C(CCC(=CCCC2=C)C)C(=CCC(OC(=O)C)C(C)=C)C1=O	5.1	Good	6.7
5838	O1C2(CC(O)C1(C)C)C1(CCCC1(C)C2C(=O)C(Cc1cc(OC)cc(C)c1O)C(C)=C)C	5.8	Poor	6.7
5777	O1C(CC)C(O)CC=CCC=CCC=CCCCCC1=O	4.8	Excellent	6.7
5623	ClC1(CCC2C(CCC3C(CCCC23C)(C)C)(C)C1C(OCC(O)COC(=O)C)=O)C	5.5	Poor	6.7
5569	Brc1cc2[nH]cc(c2cc1)C1=NCCc2c1[nH]c1c2cccc1	4.4	Excellent	6.7
5503	s1c2c(nc1)-c1nccc3c1c(nc1c3cccc1)C2(O)CCNC(=O)CC	4.8	Bad	6.7
5301	O=C1CCC2(C3C(C4CCC(C(CC(O)C(OC)=O)C)C4(CC3)C)C=CC2=C1)C	5.4	Poor	6.7
5216	O1CC2(O)C(=CC(OC(=O)C)C3C2(C)C(OC(=O)C)CC2C(CCCC23C)(C)C)C1=O	4.8	Good	6.7
5166	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=O)C)C)C1(C(O)=O)C)C	5.8	Excellent	6.7
5157	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=O)C)C)C1(C(O)=O)C)C	5	Excellent	6.7
5127	O=C=NC1(C2C3C4C(CC2)C([NH+]=[CH-])(CCC4C(CC3CC1C)C)C)C	4.4	Poor	6.7
4930	O1CC(C2C3C(C4OC3C1(C)C(=O)CC(O)C(C4)=C)C(OC(=O)CCCCCCC)(CC2)C)C	5.1	Poor	6.7
4926	O1C2C(CC3C(C)(C(OC(=O)CC)CCC(=C2)C)C(OC(=O)C)CC=C3C)=C(C)C1=O			6.7
4923	O1C2(C3OC(C4C3C(CC(O)C4(O)C)C(C)C1=O)CC(=CCC2OC(=O)CCCCCCC)C)C	4.1	OK	6.7
4820	ClC1C(=CC2C3(C(CCC2(O)C)C(CCC3)(C)C)C)C(O)=CC1=O	5.5	OK	6.7
4717	ClC1C(C2CC(=O)C3=C(C2(CC1O)C)C(OC3)=O)(CCC(C(C)=C)C)C	4.4	Poor	6.7
4693	O1C2C(CC3OC3(CCC(O)C(CCCC(C)C2OC(=O)C)=C)C)C(=C)C1=O	4.5	Bad	6.7
4682	O1C2C(CC3OC3(CCC(O)C(CCCC(C)C2OC(=O)C)=C)C)C(=C)C1=O	4.4	Bad	6.7
4593	O1C2CCC(C)C(O)(CCC3C4(C5(OC(C(O5)CC4)(C)C)CCC3C)C)C2(CCC(=O)C1(C)C)C			6.7
4575	O1C2C3C(C1C(OC(=O)CCC)(CCC(O)C(=C)C2O)C)C(CCC3=C)C(C)C	4.2	Excellent	6.7
4491	O1c2c(CCC1(CC=1CC3(CCCC3(C)C(=O)C=1CC(O)(C)C)C)C)c(O)c(cc2OC)C	4.3	Bad	6.7
4228	o1cc2c(CCC3C2(CCC2C(C)(C)C(O)C(=O)CC23C)CO)c1	5.6	Good	6.7
4227	o1cc2c(CCC3C2(CCC2C(C)(C)C(O)C(=O)CC23C)CO)c1	5.3	Good	6.7
4225	O1c2c(CC(O)C1(CCC=C(CCC=C(C)C)C)C)c(O)cc1c2CN(CC(=O)C)C1=O	4.2	Bad	6.7
4190	O(C(COC(=O)c1ccccc1)c1ccc(cc1)CC)C(=O)c1ccccc1	5.3	OK	6.7
3946	O1C(CC=C(CCC=C(CCC2=C(C)C(=O)CCC2(C)C)C)C1O)C1=CC(OC1O)=O	3.9	Bad	6.7
3796	O(C)C1=CC(=O)C(O)=C(CC2C3(C(CCC2=C)C(CCC3)(C)C)C)C1=O	4.4	Excellent	6.7
3654	O1C(C2C(C=CCC=CCCCCC1=O)C(O)C(O)C2)CC	5.2	Good	6.7

3326	O1C(=O)C(CC1C=C(C)C)=CCCC(=CCCC(=CCC(OC(=O)C)C1=CC(OC1)=O)C)C	4.8	Bad	6.7
3306	O1CC1(C(C)C)CCC(C)C1CCC2C3C(CCC12C)C1(C(CC(O)CC1)=CC3O)C	3.6	Poor	6.7
3239	Oc1ccc(cc1CC1C2(C(CC=C1C)C(CCC2)(C)C)C)C(OC)=O	5	Poor	6.7
3189	OC1=C(CC=C(CCC2(CCCC(C)C2=C)C)C)C(=O)C(NCCC(C)C)=CC1=O	4.2	Bad	6.7
3187	O(CCCC)C1=CC(=O)C(O)=C(CC=C(CCC2(CCCC(C)C2=C)C)C)C1=O	4.7	Bad	6.7
3104	O1C2C3C(CC1=O)C(OC(=O)C)CCC3(C)C(C2)C(CCC=C(C)C)C	4.8	OK	6.7
2990	O1C2C1(CCC=C(CCC1(C)C(C)C(O)C=C(C1(O)C)C2=O)C)C	4.5	Excellent	6.7
2858	O1C2CCC(=CCCC(=CC3OC(=O)C(C3CC(=O)C12C)CN(C)C)C)C	4.1	Excellent	6.7
2807	O1C2C(c3oc(CC(C(C)=C)C(O)C=C(C2O)C1=O)c(c3)C(OC)=O)C(C)=C	6.1	Good	6.7
2522	O1C(C2C(C3(C(CC2O)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1=O)C	4.8	Bad	6.7
2382	O1C2OC(=O)CC(C2C(=C)C2CCC3C2(CCCC3(C)C)C)C1OC(=O)C	5.6	OK	6.7
2281	OC1(C=2N(C=CC3C=2Nc2c3cccc2)c2c1cccc2)CC(=O)C	3.3	Good	6.7
2245	O1C(C=CC2C(CC=CCCCC1=O)C(O)CC2OC(=O)C)CCCCC	4.9	Good	6.7
2218	O=C1c2c(N3C1=Nc1c(cccc1)C3=O)cccc2	4.4	Good	6.7
2118	O1C2C1(CCC=C(CCC1(C)C(C)C(O)C=C(C1(O)C)C2=O)C)C	5.1	Excellent	6.7
2107	O(C)C1=CC(=O)C(CC2(C3CCC=C(C)C3(CCC2C)C)C)=C(O)C1=O	6.1	Good	6.7
2068	O1C2CC(=CC3(O)C(C(=O)C(=C3)C)C(CCC3(OC23)C1=O)C(C)=C)C	6.3	Excellent	6.7
1912	O(C)C1=CC(=O)C(O)=C(CC23C4(C(CCC2C)C(CCC4)(C)C)C3)C1=O	5.2	OK	6.7
1769	O1C2(CC(O)C1(C)C)C1(CCCC1(C)C2C(=O)C(Cc1cc(OC)cc(C)c1O)C(C)=C)C	3	Poor	6.7
1759	O1C2(CC(O)C1(C)C)C1(CCCC1(C)C2C(=O)C(Cc1cc(OC)cc(C)c1O)C(C)=C)C	3.7	Bad	6.7
1429	O1C2C3C(C1CC(=C)C(O)CCC2(OC(=O)CCC)C)C(CCC3C(C)C)=C	4.9	Good	6.7
1377	O1C2CCC1(C)C(O)C(O)C=1C(OC(=O)C=1C)CC(=CCCC2C)C	4.7	Excellent	6.7
1349	O1C(=CC(CCCC(=CCCC(=CCC(O)c2ccoc2)C)C)C)C(O)=C(C)C1=O	5.6	Bad	6.7
1122	O1CC(C(COC(=O)C)C(OC(=O)C)C1=O)C1(C2C(CC1)C(CCCC2=C)(C)C)C	5.7	Good	6.7
1096	O1C2C3C(C1CC(=C)C(OO)CC(OC(=O)C)C2(O)C)C(=CCC3C(C)C)C	5.1	Good	6.7
1011	O1C(=O)C(CCC1C(C)C1CCC2C3C(CCC12COC(=O)C)C1(C(=CC(=O)CC1)CC3)C)C	5	Bad	6.7
1007	O1C(=O)C(C)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)CC3)C)C	5.5	Poor	6.7
908	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(N)=CC1=O	5.3	Poor	6.7
668	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(CC1)=C	5.6	Excellent	6.7
658	O1C(Cc2c(C1=O)c(O)cc1c2c(O)c2c(c1)C(C)(C)C(=O)C(CCC(=O)C)(C)C2=O)C	4.8	OK	6.7
487	S=C=NC1C2C(CC(O)C1(C=C)C)C(c1c3c2c[nH]c3ccc1)(C)C	4.2	Good	6.7
449	O1C2OC(=O)C3C2C2(C(CC3)C3(C(CC2)C(CCC3)(C)C)C)C1O	4.8	Poor	6.7
435	O1OC(CCC1(CCC=1C(C2C(CC=1C)C=C(CC2)C)(C)C)C)C(C(O)=O)C	4.6	Good	6.7
368	O1C2OC(=O)CC(C2C2(CCC3C(=CCCC3(C)C)C2C)C)C1OC(=O)C	3.9	Bad	6.7
164	O1C(OC(=O)C)c2c(ccc(C3(CC(CCC3)(C)C)C)c2C(=O)C)C1=O	4.6	Good	6.7
163	O1C(OC(=O)C)c2c(ccc(C3(CC(CCC3)(C)C)C)c2C(=O)C)C1=O	5.8	Good	6.7
14490	O1C2CC(=O)CC(CCC34OC3C(OC4=O)CC1(CC2=O)C)C(C)=C	5.5	Excellent	6.6
14470	O(C(=O)C)C1CC2C(C3CC(O)C(CC13C)C(=O)C)(CCC1C(CCCC12C)(CC)C)C	5.1	Good	6.6
14451	O(C)c1cc2c(c(CCC)c1C(OC)=O)C(=O)C1=C(C(C)(C)C(=O)C(C)=C1O)C2=O	5.2	Good	6.6
14131	O1C(=CC(CC=CC(=CCCc2cocc2Cc2ccoc2)C)C)C(O)=C(C)C1=O	5.8	Excellent	6.6
13762	O1C(C)(C)C1CC=C1C2C(C(CC(O)C=C(CC2)C)=C)C(OC1)O	4.4	Good	6.6
13761	O1C(C)(C)C1CC=C1C2C(C(CC(O)C=C(CC2)C)=C)C(OC1)=O	5.3	Poor	6.6
13725	O1C(=O)C(CC1C=C(C)C)=CCC(OC(=O)C)C(=CCCC(=CCCC1=CC(OC1)=O)C)C	4.9	Good	6.6
13546	OC12CC(=O)CCC1(C1CCC3(C(CCC3C(C=CC(C(C)C)C)C)C)C1(O)C=C2)C)C	5.2	Good	6.6
13471	O1CC2C(CCC(=CC(=O)CC2=C)C)C(=CC=CC(O)(C)C)C1=O	6.3	Excellent	6.6
13433	OC1=C(CC2C3(C(CC=C2C)C(CCC3)(C)C)C)C(=O)C=CC1=O	5.5	Excellent	6.6
13377	O=C1C=C2CCC3C4CCC(C(C=CC(C(OC)=O)C)C)C4(CCC3C2(C=C1)C)C	4.2	Bad	6.6

13373	O=C1C=C2CCC3C4CCC(C(C(OC(=O)C)CC=C(C(OC)=O)C)C)C4(CCC3C2(C=C1)C)C	5.3	Bad	6.6
13344	P(Oc1ccccc1)(Oc1ccccc1)(=O)NC1CCCCCCC1	6	Good	6.6
13202	O1C(C=2C(C3(C(CC=2)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1O)C	4.4	OK	6.6
13183	O1C2CCC(C3C(CC(O)C12C)C(=CC(C=C(C)C)C3O)C=O)=C	4.8	Good	6.6
13111	OC1C2(C3CCC(=C)C(C(OC)=O)C3(CCC2C(CC1=O)(C)C)C)C	4.4	Excellent	6.6
12965	O1C2C=C(C3OC3C(Cc3oc(cc3C(OC)=O)C2C(C)=C)C(C)=C)C1=O	5.4	Excellent	6.6
12854	O=C1CC2C(CCC3C(C)(C)C(=O)CCC23C)(C)C1=C(C=CC=C(C(=O)C=CC(=O)C)C)C	4.3	Bad	6.6
12853	O=C1CC2C(CCC3C(C)(C)C(=O)CCC23C)(C)C1=C(C=CC=C(C(=O)C=CC(=O)C)C)C	4.8	Bad	6.6
12762	OC1CC2=CCC3C4CCC(C(C=CCC(C)C)C)C4(CCC3C2(CC1)CO)C	4.4	OK	6.6
12345	O1C2C(CC(OC(=O)C)C(CCC(=CCCC(=C2)C)C)C(=O)C)C(=C)C1=O	4.8	Good	6.6
12146	O=C1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)CO	5.1	Bad	6.6
12080	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)C1O)C1=CC(OC1O)=O	3.6	Bad	6.6
11950	O1C(C)=C(C2C(C(CCC=CCC2)=C)C1OC(=O)C)C(O)CC=C(C)C	5.7	Poor	6.6
11847	ClC1CCC2(C(C1(C)C)C(=O)CC(=C)C2CC(O)C1CC(=O)NC1=O)C	4.6	Good	6.6
11602	O1C2(CCC=C(CCC(=CC=C(CCC2=O)C)C(C)C)C1=O)C	4.5	Excellent	6.6
11590	o1cc2c(CCC3C4(C(CCC23C)C(COC(=O)C)(C)C(OC(=O)C)C(=O)C4)C)c1	4	OK	6.6
11584	o1cc2c(CCC3C4(C(CCC23C)C(COC(=O)C)(C)C(OC(=O)C)C(=O)C4)C)c1	3.8	Bad	6.6
11168	O1C(O)C2C(CCC(C3(CC(CCC3)(C)C)C)=C2C(C(OC)=O)C)C1=O	5.7	OK	6.6
11167	O1C(OC)C2C(CCC(C3(CC(CCC3)(C)C)C)=C2C(C(O)=O)C)C1=O	6.4	Poor	6.6
11108	O1C2C(CC(OC(=O)C)C(CCC(=CCCC(=C2)C)C)C(=O)C)C(=C)C1=O	5.7	Good	6.6
10934	O(C(=O)C)C1CC2CCC3C4CCC(C(C=CC(OC)=O)C)C4(CCC3C2(CC1)C)C	4.5	Bad	6.6
10680	OC1(CC(O)C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC=C1)C)C)C	4.7	Poor	6.6
10679	O(C(=O)C)C1(CC(OC(=O)C)C2C(CCC2C(O)(C)C)(C=CC(CC=C1)C)C)C	5.2	Good	6.6
10676	OC1(CC(O)C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC=C1)C)C)C	4.7	Good	6.6
10664	O1C2(CCC(CC3OC3(CC(O)C=C(CCC2O)C)C)C(=C)C1=O)C	5.3	Excellent	6.6
10592	O1C(C=CC2C(CC=CCCCC1=O)C(=O)CC2OC(=O)C)CCCCC	5.6	Excellent	6.6
10460	O(C(=O)C)c1ccc(OC(=O)C)cc1CC1(C2CCC=C(C)C2(CCC1C)C)C	5.9	OK	6.6
9766	Brc1cc(N2Cc3[nH]c4c(c3C=C2)cccc4)c(cc1)C(O)=O	4.7	Poor	6.6
9324	O1C(=CC(CCCC(=CC=CC2(CCCc3c2occ3)C)C)C)C(O)=C(C)C1=O	5.3	Good	6.6
9323	O1C(=CC(CCCC(=CC=CC2(CCCc3c2occ3)C)C)C)C(O)=C(C)C1=O	4.6	Poor	6.6
9204	O=C1CC2(CC(=O)C(=CCC2C2C1(C)C(=O)C=C2C(C)C)C)C	5.8	Excellent	6.6
9190	O1C2CC3C4C(CCC3(CC(O)C12C)C)(C)C(O)C=C4C(C)C	4.4	Excellent	6.6
9137	O(C(=O)C)C1CC2C(C3CC(O)C(C(=O)C)C(O)C13C)(CCC1C(CCCC12C)(C)C)C	5.9	OK	6.6
8980	O1C2C(CC3OC2C(CCCC(OO)(C=CCC3(O)C)C)C)C(=C)C1=O	6.1	OK	6.6
8943	O=C1NC(=CC(C)C2CCC3C=4C(CCC23C)C2(C(CC(N)CC2)CC=4)C)C(=C1)C(C)C	4.3	Bad	6.6
8925	O=C1C2CC(=O)CCC2(C2C(C3CCC(C(O)(C=CCC(C)C)C)C3(CC2)C)C1)C	5.1	OK	6.6
8858	O1C2C3C(C4C(C(C2C(=O)C)C(=O)C3)C(=O)CC(C4)C(C)=C)C1=O	4.3	Poor	6.6
8828	O1C2=C(CC3(C4CCCC(=C)C4(CCC13C)C)C)C(=O)C(OC)=CC2=O	5	Good	6.6
8827	O1C2=C(CC3(C4CCCC(=C)C4(CCC13C)C)C)C(=O)C(OC)=CC2=O	4.7	OK	6.6
8549	O=C1CC2C(CCC3C(C)(C)C(=O)CCC23C)(C)C1=C(C=CC=C(C(=O)C=CC(=O)C)C)C	6.1	Bad	6.6
8300	O1C(=CC(CCCC(=CCCc2cc(oc2)Cc2ccoc2)C)C)C(O)=C(C)C1=O	4	Bad	6.6
8197	O1C2C1(CC1C3(C(CCC1=C)C(CCC3)(C)C)C)C(=O)C=C(CO)C2=O	5	OK	6.6
8128	OC1C2CC(O)CCC2(C=2C(C3CCC(C(CC(=O)CC(C)C)C)C3(CC=2)C)C1)C	4.3	Poor	6.6
8081	ClC1C(C2C(CC1Cl)(C)C(CC(O)C1CC(=O)NC1=O)C(CC2=O)=C)(C)C	5.7	Excellent	6.6
7936	OC1=C(C)C(=O)C2=C(C1=O)C(CCC2C(CC=CC(O)(C)C)C)C	4.9	Bad	6.6
7569	O1C(c2c(c3CC(C)(C)C(O)c3cc2C)C1=O)CO[N+](=O)[O-]	5.1	Poor	6.6

7488	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC(OC)=O)C)C)C1(C(OC)=O)C)C	4.8	Poor	6.6
7421	O(C(=O)C)C1C(C)=C(CCC(=CCO)C)C2(C(C1OC(=O)C)C(CC(OC(=O)C)C2)(C)C)C	5.3	OK	6.6
7370	O1C23C4C(CCC(C2)(C)C(O)CC13)C(=CC(C=C(C)C)C4O)C=O	6.2	OK	6.6
7296	O1C23C1C=CC(=O)C2(C1C(C2CCC(C(C=CC(C(C)C)C)C)C2(CC1O)C)CC3O)C	4.5	Poor	6.6
7272	O1C(=O)C2(C(C3C4(C(CCC(C)C4=O)C(C3)C)C2=O)C1(C)C)C	4.7	Excellent	6.6
7271	O(C(=O)C)C=1C(=O)C2(O)C3(C(CCC2C)C(CC3C=C(C)C)C)C(=O)C=1C	4.6	Good	6.6
7270	OC12C3(C(CCC1C)C(CC3C=C(C)C)C)C(=O)C(C)=C(O)C2=O	4.7	Good	6.6
7249	O(C(=O)C)C1C=C2C(CCC3(C2CCC3C(C=CC(C(C)C)C)C)C)C2(CCC(O)CC12O)C	5.8	Bad	6.6
7179	OC1(C(OC)=O)C2(C(c3c(C1=O)c(O)cc(c3)C)C(CC2)C(C)C)C	4.4	Excellent	6.6
7053	O1C2C=C(CCC=C(CCC=C(CCC2C(OC(=O)C)(C)C)C)C)C1=O	5.7	Excellent	6.6
6955	O(C(=O)C)C1CC(C(=CCC=C(C)C)C)C(C2C(C)C(OC(=O)C)CC2=O)C1C=O	5.6	Good	6.6
6890	O1C23C1C(O)C=1C4CCC(C(C=CC(C(C)C)C)C)C4(CCC=1C2(CCC(O)C3)C)C	5	Poor	6.6
6831	OC1(CC(=O)C(CCC(C=CC(O)(CC=C1)C)C(C)C)(COC(=O)C)C)C	5	Bad	6.6
6747	O1c2c(c(cc(OC)c2)C)C(=O)c2c1cc(O)cc2O	5	Poor	6.6
6736	O1C(O)C(OC)=C(C(=O)CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	4.4	Excellent	6.6
6617	OC1C(=O)C(=CC=C(CCC=C(CO)C(=O)CCC1C)C)C(C)C	4.9	Excellent	6.6
6602	O1C23C(CCC(=C2)C)C2(C(C(=O)C(CC12O)C(C)C)C(=C3)C(OC)=O)C	4.4	Excellent	6.6
6547	O1C(OC)C2=C(C3(C(CC2)C2(C(CC3)C(CCC2)(C(O)=O)C)C)C)C1=O	5.1	OK	6.6
6546	O1C(OC)C2=C(C3(C(CC2)C2(C(CC3)C(CCC2)(C(O)=O)C)C)C)C1=O	5	Excellent	6.6
6545	O1C2C1(CC1C3(C(CCC1=C)C(CCC3)(C)C)C)C(=O)C=C(CO)C2OC(=O)CC(O)=O	6.1	Bad	6.6
6544	O1C2C1(CC1C3(C(CCC1=C)C(CCC3)(C)C)C)C(=O)C=C(COC(=O)CC(O)=O)C2O	5.1	Bad	6.6
6472	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(CC1)=C	3.5	Excellent	6.6
6412	O1C(=O)C2(C(C3C4(C(CCC(C)C4=O)C(C3)C)C2=O)C1(C)C)C	4.7	Excellent	6.6
6409	OC1=C(C)C(=O)C23C(C1=O)C(CCC2C(CC3C=C(C)C)C)C	4.4	Excellent	6.6
6267	O1C2C=C(CCC(C(C)=C)C(=O)C(O)C(=CC(=O)C3CC23C)C)C1=O	4.9	Excellent	6.6
6255	O1C(O)C(=CC1=O)C=CC1C2(C(CCC1C(O)=O)C1(C(CC2)C(CCC1)(C)C)C)C	6.2	Good	6.6
6055	O1C2CC(=Cc3oc(C(O)C(CCC(=C2)C1=O)C(C)=C)c(c3)C)C	5.5	Excellent	6.6
6054	O1C23C(CCC(C2)C)C2(C(C(=O)C(CC12O)C(C)C)C(=C3)C(OC)=O)C	5.1	OK	6.6
6012	O1CC23C(CCC(C2COC(=O)C)C1=O)C1(C(CC3)C(CCC1)(C)C)C	5	Good	6.6
5993	O1C2C(CC3OC2C(CCCC(OO)(C=CCC3(O)C)C)C)C(=C)C1=O	5.3	Poor	6.6
5950	O1OC(CCC1(CCC1C2(C(CCC1(O)C)C(CCC2)(C)C)C)C)C(C(OC)=O)C	4.2	Good	6.6
5890	O=C1C2=CC(=O)CCC2(C2C(C3CCC(C(CCC(OO)C(C)=C)C)C3(CC2)C)C1)C	4.6	Bad	6.6
5819	O1CC=C(CC(OC(=O)C)C2C3(C(CCC2=C)C(CCC3)(C)C)C)C1=O	4.5	Excellent	6.6
5706	O(C(=O)C)C1CC2=CC(O)C3C(C2(CC1)C)C(O)CC1(C3CCC1C=C)C	4.1	Poor	6.6
5637	O1C2CCC1(C)C(O)CC1(C(CC=C2C)C(=C(C)C)C(=O)C1)C	5.4	Excellent	6.6
5401	Oc1ccc(cc1)-c1c2c([nH]c1)C(=O)c1n(cc3CCN=C2c13)C	4.1	Poor	6.6
5290	O1C2C=C(CCC(OC(=O)CCC)C3(C(C(C)C(=O)C=C3)C(=O)C12C(C(OC)=O)C)C)C	6.3	Excellent	6.6
5270	O1C2C(CCC(=CCCC(=CCCC(O)(C2)C)C)C)C(=C)C1=O	6.2	Excellent	6.6
5175	O1C(CCC(C)C)C(C2C3(C(CC2=O)C2C(CC3)C3(C(=CC(=O)CC3)CC2)C)C1O)C	4.3	OK	6.6
5064	Oc1ccc(cc1)CCNC1=CC=2N(CCC=3C=2C(=NC=3)C1=O)C	3.5	OK	6.6
5031	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(NC=O)(CC1)C	5.4	Excellent	6.6
5023	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(NC=O)(CC1)C	4.8	Good	6.6
5007	O1C2C=C(C(O)CC(Cc3oc(cc3C(OC)=O)C2C(C)=C)C(C)=C)C1=O	4.5	Poor	6.6
4960	O1C(C)(C)C1CCC(C)C1CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)C(O)C3)C	5	Bad	6.6
4937	O1C2C(C=CCC1=O)=C(C1C(C3CCC(C(CCC(C)(C)C)C)C)C3(CC1O)C)C2)C	4.6	Bad	6.6
4922	O1C2CC(=C3C2C(C2=C(CC(=O)CC(C2)C(C)=C)C3=O)C1=O)C	5.8	Good	6.6
4920	O1C(=O)C(=C2CC3C(C)(C(OC(=O)CC)CCC(=CC12O)C)C(OC(=O)C)CC=C3C)C			6.6

4829	O1C2CCC1(C)C(O)CC1C(OC(=O)C1=C)C(OC(=O)C)C(CCCC2=C)C	5.5	Good	6.6
4823	O1C2CCC1(C)C(O)CC1C(OC(=O)C1=C)C(OC(=O)C)C(CCCC2=C)C	6.8	Good	6.6
4720	o1c2c(nc1)cc(O)c(O)c2CC1(C2CCC=C(C)C2(CCC1C)C)C	4.5	Good	6.6
4714	ClC1C(C2CC=C3C(C2(CC1O)C)C(OC3)=O)(CCC(C(C)=C)C)C	5.2	Good	6.6
4671	O1C2(C3OC(C4C3C(CCC4(O)C)C(C)C1=O)CC(=C)C(O)CC2OC(=O)CCCCCCC)C	5	Poor	6.6
4669	O1C2(C3OC(C4C3C(CCC4(O)C)C(C)C1=O)CC(=C)C(O)CC2OC(=O)CCCCCCC)C	5.5	OK	6.6
4613	O1C2C1(CCC1OC1(CCC1(C)C(O)(C(=CCC1C)C2=O)C)C)C	4.5	Excellent	6.6
4559	O1C23C1C(O)C=1C4CCC(C(C=CC(C(C)C)C)C)C4(CCC=1C2(CCC(O)C3)C)C	5.1	Poor	6.6
4359	O1C2C(CCC(=CCCC(=CCC=C(C2)C)C(OC)=O)C)C(COC)C1=O	5.1	Poor	6.6
4226	o1cc2c(CCC3C4(C(CCC23C)C(C)(C)C(O)C(=O)C4)C)c1	4.7	OK	6.6
4195	O1CC(C2CC(C)C(OC(=O)C)C3C2C(OC3CC(=O)C)C1(C=CC=O)C)C	6.1	Poor	6.6
3720	O=C1CC2C(CCC3C(CCCC23C)(C)C)(C)C(CCC(C(O)=O)C)C1C	6.2	Bad	6.6
3600	O(C(=O)C)C1C2C(CC=C2C)C(=C)C(O)CC1C(C(OC(=O)C)C(OC(=O)C)C=C(C)C)C	4.6	Poor	6.6
3346	O1C(O)C(=CC1=O)C=CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)CO	4.2	Bad	6.6
3319	O1C(O)C(=CC1=O)C=CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)CO	4.9	Good	6.6
3258	S(O)(=O)(=O)CCNC1=CC(=O)C=C(CC2(C3CCC=C(C)C3(CCC2C)C)C)C1=O	6.3	OK	6.6
2976	O1C2C3C(C1CC(=C)C(OC(=O)C)CCC2(O)C)C(=CCC3C(C)C)C	4.9	Poor	6.6
2809	O(C)C1=CC(=O)C(O)=C(CC2(C3C(=CCC2C)C(CCC3)(C)C)C)C1=O	4.4	Excellent	6.6
2808	O1C2C=C(C(OC)C(O)C(Cc3oc(cc3C(OC)=O)C2C(C)=C)C(C)=C)C1=O	5.8	Good	6.6
2806	O1C2C=C(C(O)C(O)C(Cc3oc(cc3C(OC)=O)C2C(C)=C)C(C)=C)C1=O	5.3	Good	6.6
2805	O1C2C=C(CC(=O)C(Cc3oc(cc3C(OC)=O)C2C(C)=C)C(C)=C)C1=O	3.9	Poor	6.6
2798	s1c2c3c(C(=O)c4c(-c3c1C(OC)=O)cccc4O)c(O)cc2	4.6	Excellent	6.6
2530	O1C2C3C(C1CC(=C)C(OC(=O)C)CCC2(OC(=O)CCC)C)C(CCC3C(C)C)=C	4.8	Poor	6.6
2518	O1C2C3C(CCC3(CCC(CC(=O)CC(C2)C)C)C)=C(C)C1=O	4.5	Bad	6.6
2385	O1C2CC=C(C3C(C(COC3=O)CCC=C(C)C)C(O)CC12C)C=O	6.2	OK	6.6
2239	O1C2(c3c(CC(C)C2(CC1C1(OOC(CC1)C(C(O)=O)C)C)C)cc(cc3)C)C	4.9	Bad	6.6
2224	O1C2C=C(CCC(Cc3oc(cc3C(OC)=O)C2C(C)=C)C(C)=C)C1=O	4.6	Good	6.6
2120	O1CC(C2CCC3(C(CCc4c3coc4)C2(CC1=O)C)CO)(C(O)=O)C	5.3	Good	6.6
1881	ClC(C)(C)C1OC(CC1)(C)C1C2C(CCC([NH+]=[CH-])(C)C2O)C([NH+]=[CH-])(CC1)C	3.7	Good	6.6
1878	O1C2C(c3oc(CC(C(C)=C)C(O)C=C(C2N(C)C)C1=O)c(c3)C(OC)=O)C(C)=C	4.8	Excellent	6.6
1789	s1c2c(nc1)C=1CCN3C=1C1=C(C=C[NH+](C)[C-]12)c1c3cccc1	4	Good	6.6
1787	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCN(C)C)cccc4	4	OK	6.6
1717	O(C)C1=CC(=O)C(O)=C(CC=C(CCC2(CCC=C(C)C2C)C)C)C1=O	4.7	Good	6.6
1712	O=C1c2c(NCC1)c1nc3c(c4C=Nc(c14)c2N(C)C)cccc3	5.9	OK	6.6
1682	S(C)C=1C(=O)c2nccc3c2c(nc2c3cccc2)C=1CCNC(=O)C	5.8	Excellent	6.6
1656	O1C(C=CC2C(CC=CCCCC1=O)C(=O)CC2O)CC=CCC	6.2	Good	6.6
1536	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(NCCC(C)C)=CC1=O	5.5	Good	6.6
1523	O1C2CC(=O)C(C3C(C1)C(OC(=O)C)CC3C(=CCC=C(C)C)C)C2C			6.6
1464	Oc1ccc(cc1)C1CC(CCC1C(C)C)(C)c1ccc(O)cc1	5.6	OK	6.6
1401	O=C1CC(CCC(C)C(=O)CCC(CC(=O)CC1C)C)C(C)=C	4.6	Poor	6.6
1389	O=C1CC(CCC(C)C(=O)CCC(CC(=O)CC1C)C)C(C)=C	4.8	Excellent	6.6
1329	O(C)c1cc2[nH]c3c(CC4N(C3C=C(C)C)C(=O)C3N(CCC3)C4=O)c2cc1	5.1	OK	6.6
1320	O(C)c1cc2[nH]c3c(CC4N(C3C=C(C)C)C(=O)C3N(CCC3)C4=O)c2cc1	3.4	Good	6.6
1211	O1C2(CC3OC(C4C3C(CCC4C(C)C)=C)C1(CCC2OC(=O)C)C)C			6.6
1143	O1C2C=C(CCC(CC(=O)C(=CC(=O)C3CC23C)C)C(C)=C)C1=O	5.2	Excellent	6.6
1037	s1c2c(nc1)c1N(C=Cc3c1c(nc1c3cccc1)c2CCN(C)C)C	4.3	Excellent	6.6

952	O1C(CC=C(CCC=C(CCC2(CCCC2C)C(C)=C)C)C1O)C1=CC(OC1)=O	3.6	Bad	6.6
895	O1C2C(CC3C(C)(C(OC(=O)C)CC4OC34C)C(OC(=O)CCC)CCC(=C2)C)=C(C)C1=O	4.2	Poor	6.6
631	ClC1CC2C(=CC1(C=C)C)C(=O)c1c(cccc1NC=O)C2(C)C	3.5	Excellent	6.6
451	O1CC23C(C(CCC2C2(C(C(O)C3O)C(CCC2)(C)C)C)C(OC)=O)C1=O	4.9	Poor	6.6
345	O1C2C(C(=C)C1=O)C(O)CC(=CCCC(=CC(OC(=O)C)CC(=C2)C)C)C	5.6	Excellent	6.6
297	o1c(ccc1CO)-c1nc(cc2c1[nH]c1c2cccc1)C(OC)=O	3.7	Bad	6.6
210	OC1(C2CC(=O)C(C=CCC(O)(C=CC2(CC1)C)C)C)C(C)C	4.7	Excellent	6.6
198	OC1(C2CC(=O)C(C=CCC(O)(C=CC2(CC1)C)C)C)C(C)C	4.2	Excellent	6.6
18	O1C(C(C(=O)C(C)C=2OC(CC)=C(C)C(=O)C=2C)C)=C(C)C(=O)C(C)=C1CCCCC	4.2	Poor	6.6
16	O1C(C(C(=O)C(C)C=2OC(CC)=C(C)C(=O)C=2C)C)=C(C)C(=O)C(C)=C1CCCCC	5.9	Poor	6.6
14439	O1C(C2(C=C(C)C(=O)C(C)=C2C(=CC(C(=O)CC)C)C)C)=C(C)C(=O)C(C)=C1OC	5.8	Excellent	6.5
14435	O1C(C2(C=C(C)C(=O)C(C)=C2C(=CC(C(=O)CC)C)C)C)=C(C)C(=O)C(C)=C1OC	5.4	Good	6.5
14433	O1C(C2(C3C2(C)C(=O)C(C)C3C(C(=O)CC)=C)C)=C(C)C(=O)C(C)=C1OC	5.5	Good	6.5
14237	O(C)C1=CC(=O)C(O)=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	4.7	Good	6.5
14232	O1C(CCC1C(OC(=O)C)(C)C)(C)C1CCC(C2C(C1O)C(=CC2)C)=C	4.1	Excellent	6.5
14215	O1C(OC(=O)C)C2C(CC=C(C3(CC(CCC3)(C)C)C)C2=CC)C1OC(=O)C	4.2	OK	6.5
14125	O1C23C1CC1C(C2(C)C(=O)C=CC3)C(O)CC2(C1CCC2C(C)C1CC1C(C(C)C)C)C	4	Poor	6.5
14029	O(C(=O)C)C1CC2(C(CC=C(CCC=C1C=O)C)C(CC2)C(C)=C)C	6.5	Excellent	6.5
13996	OC1CCC(O)(C2C3C(CCC12C)C(CC=C3C)C(C)C)C	5	Excellent	6.5
13717	O1CC1(C(C)C)CC(O)C(C)C1CCC2C3C(CCC12C)C1(C(CC(O)CC1)=CC3)C	5.1	Bad	6.5
13677	O1C2C(CCC(=CCCC(OC)(C)C(O)CCC(=C2)C)C)=C(C)C1=O	5.1	Bad	6.5
13561	O1C2CCC(=C)C(C(OC)=O)C(CCC12C)C(=CCC(O)C(O)(C)C)COC(=O)C	5.4	Good	6.5
13547	OC12CC(=O)CCC1(C1CCC3(C(CCC3C(C=CC(C(C)C)CC)C)C1(O)C=C2)C)C	4.1	Poor	6.5
13516	O1C2CC(OC(=O)C)C3(C(CC(=C(C(OC)=O)C)C(=O)C=C(CCC3)C)C12C)C	4.4	Excellent	6.5
13464	O1CC2C(CCC3(OC3CCC2=C)C)C(=CC=CC(O)(C)C)C1=O	6	Excellent	6.5
13359	O1CC2C(=CCC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(COC(=O)C)C)C)C1=O	5.3	Poor	6.5
13358	O1CC2C(=CCC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(COC(=O)C)C)C)C1=O	5.3	Poor	6.5
13351	O1C(C2C(C(CCC=C(CC2)C)=C)C1=O)(C=CC=C(C)C)CO	5.6	Excellent	6.5
13297	O1C2C1(CC1C3(C(CCC1=C)C(C)(C)C(=O)CC3)C)C(=O)C=C(CO)C2O	4.8	OK	6.5
13187	O1C2C(CC3OC3(CCC=C(CCC=C(C)C2O)C)C)C(=C)C1=O	5	Excellent	6.5
13186	O1C2C(CC3OC3(CCC=C(CCC=C(C)C2O)C)CO)C(=C)C1=O	4.9	Poor	6.5
12998	O1C2CCC(=CCC(CCC(=CC(O)CC12C)C)C(O)(C)C)C	3.7	Good	6.5
12969	O1C2C(c3oc(CC(C(C)=C)C(O)C=C(C2OC)C1=O)c(c3)C(OC)=O)C(C)=C	5.4	OK	6.5
12860	O1C2CC(=CC(=O)C=C(C)C(=O)CC(CCC(=C2)C1=O)C(C)=C)C	5.7	Excellent	6.5
12857	O1C2CC(=CC(=O)C=C(C)C(=O)CC(CCC(=C2)C1=O)C(C)=C)C	6.1	Excellent	6.5
12834	O1C(=CC(CCCC(=CCCC(O)(CCCc2ccoc2)C)C)C)C(O)=C(C)C1=O	5.5	Poor	6.5
12786	O1C(C2C(C3(C(CC2O)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)COC(=O)C)C)C)C1=O)C	4.9	Excellent	6.5
12712	O=C1CC2CCC3C4CCC(C(OC(=O)C)C)C4(CCC3C2(C=C1)C)C	3.9	Bad	6.5
12628	O1C(O)C(=CC1=O)C(O)CC=C(CCC=C(CCC=1C(CCCC=1C)(C)C)C)C=O	4.7	OK	6.5
12467	O1CC2=C3C(O)CC(C)C2(CCC1(C)C(O)CCC1(OC1C3=O)C)C	5.1	Excellent	6.5
12320	O1C2(CCC=C(CCC(=CC=C(CCC2OC(=O)C)C(OC)=O)C(C)C)C1=O)C	5.7	Excellent	6.5
12239	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(NCC(C)C)=CC1=O	4.5	Bad	6.5
12228	S1CC(NC1=O)C1(OC2CCC(C=CCCC(=CC(OC(C1)C2)=O)C)C)O	4.2	Bad	6.5
11953	O1C2C1(CCC1C(C(CC2O)=C)C(OCC1=CC=CC(O)(C)C)=O)C	5	Poor	6.5
11875	OC1C=C2C3(C(C1C)C(O)=CC(=C3)C)C(CC2C)C=C(C)C	4.2	Excellent	6.5

11790	O1C2CCC1(C)C(O)C(O)c1c(occ1C)CC(=CCCC2C)C	5.4	OK	6.5
11619	O(C)C1=CC(=O)C(O)=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	4.6	Excellent	6.5
11435	O(C)c1cc(c2c(c1)C(=O)c1c(C2=O)c(O)ccc1)C	5.1	Poor	6.5
11410	O(C)C1=CC(=O)C(O)=C(CC2(C3CCC=C(C)C3(CCC2C)C)C)C1=O	4.7	Good	6.5
11384	Brc1cc(N2C=Cc3c([nH]c4c3cccc4)C2=O)c(cc1)C(O)=O	4.2	OK	6.5
11221	O1C2CCC(C3C(CCC12C)C(C3)(C(=O)C=CC(O)(C)C)C)=C	5.7	Excellent	6.5
11173	O1C(C2=C(C(CCC2C2(CC(CCC2)(C)C)C)C(OC)=O)C1=O)C	5.4	Good	6.5
10974	O=C(C(=O)c1c2c([nH]c1)cccc2)c1c2c([nH]c1)cccc2	5.7	Poor	6.5
10899	O1C(O)C2C(=CCC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	4.5	Poor	6.5
10601	Oc1ccc(cc1)C=1N=C(C=2N(C=1)C(=O)C(N=2)=Cc1ccc(O)cc1)Cc1ccccc1	4.8	Bad	6.5
10412	O1C2CC(=CC(=O)C(OCC)CC(=O)CC(CC=C(C2O)C1=O)C(C)=C)C	5.9	Excellent	6.5
10411	OC1CC2=CCC3C4CCC(C(=NO)C)C4(CCC3C2(CC1)C)C	4.6	OK	6.5
9226	O1C(OC)(C=2OC3(CCC4(C(CCCC4=C)C3(CC=2C1=O)C)C)C)CC(OC)=O	6.2	Good	6.5
9225	O1C(OC)(C=2OC3(CCC4(C(CCCC4=C)C3(CC=2C1=O)C)C)C)CC(OC)=O	6	OK	6.5
9224	O1C(OC)(C=2OC34CCCC(=C)C3(CCC(C)C4(CC=2C1=O)C)C)CC(OC)=O	5.9	Good	6.5
9223	O1C(OC)(C=2OC34CCCC(=C)C3(CCC(C)C4(CC=2C1=O)C)C)CC(OC)=O	5.8	Good	6.5
9193	O1C2CC3C4C(CCC3(CC(O)C12C)C)(C)C(=O)C=C4C(C)C	5.2	Excellent	6.5
9191	O1C2CC3C4C(C)(C(=O)CC3(CC(O)C12C)C)C(=O)C=C4C(C)C	6.1	Good	6.5
9150	O=C1CCC2C(CCC3(C2CCC3C=C)C)C1(CCC(OC)=O)COC(=O)C	5.8	OK	6.5
9147	O1C(OC)C(C2C(C(CCC=C(CC2)C)=C)C1OC)=CC=CC(O)(C)C	5.7	Poor	6.5
9016	O1C(CC=C(CCC=C(CCC2C(CCC=C2C)(C)C)C)C1OC)C1=CC(OC1O)=O	4.1	Bad	6.5
8922	OC12CC(O)CCC1(C1C(C3CCC(C(CCC(C(C)C)C)C)C3(CC1)C)=CC2=O)C	5.6	Bad	6.5
8864	O1CC2C(CCC(=C)C(O)CCC2=C)C(=CC=CC(O)(C)C)C1=O	5.1	Excellent	6.5
8791	O1CC(=CC1=O)C(O)CC=C(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C	5.1	Excellent	6.5
8750	O1C(O)C2C(=CCC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	4.8	Poor	6.5
8591	O1CC2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(C)(C)C(OC(=O)C)CC3)C)C)C)C1=O	4.7	Poor	6.5
8548	OC12CC(O)CCC1(C1C(C3CCC(C(CCCC(C)C)C)C3(CC1)C)=CC2=O)C	4.7	Bad	6.5
8465	OC1C2CC(O)CCC2(C=2C(C3CCC(C(=O)C)C3(CC=2)C)C1)C	4.6	Excellent	6.5
8410	O1C(=CC(CCC=C(CCCc2cc(oc2)Cc2ccoc2)C)C)C(O)=C(C)C1=O	5.4	Poor	6.5
8302	O1C(=CC(CCC=C(CCCc2cc(oc2)Cc2ccoc2)C)C)C(O)=C(C)C1=O	5.2	Poor	6.5
8165	O1C(CC=C(CCC2(C3CCCC(=C)C3(CCC2C)C)COC(=O)C)C)C(=CC1=O)CO	5.2	Bad	6.5
7849	O1C2C(CCC(=CC(O)CC(=CC(OC(=O)C)CC(=C2)C)C)C)C(=C)C1=O	5.2	Poor	6.5
7576	O=C(C(C)(c1c2c([nH]c1)cccc2)c1c2c([nH]c1)cccc2)C	4.4	Excellent	6.5
7561	O1C(c2c(c3CC(Cc3cc2C)(C)C)C1=O)CO[N+](=O)[O-]	5.3	OK	6.5
7545	Oc1cc(c2c(CC3C4(C(CCC23C)C(CCC4)(C)C)C)c1O)C(OC)=O	5.1	OK	6.5
7522	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=O)C)C)C)C1(CO)C)C	5.8	Poor	6.5
7508	OC12CC(O)CCC1(C1C(C3CCC(C(CCC=C(COC(=O)C)C)C)C3(CC1)C)CC2=O)C	3.8	Bad	6.5
7465	O1C2C3OC(=O)C(C3CC(O)C1(CCC=C(CCCC2C)C)C)=C	5.5	Poor	6.5
7227	O=C1CC2C3C(CCC2(C)C1C(O)(CCCC(C)C)C)C1(C(CC(=O)C=C1)CC3)C	4.5	Good	6.5
7195	O1C23C(OC(=O)C12C)C=C(CCC(O)C1(C(C(C)C(=O)C=C1)C3O)C)C	5.3	Excellent	6.5
6582	O(C)c1cc2C3=NC=Cc4c([nH]c5c4cccc5)C3=Nc2cc1	4.3	Poor	6.5
6564	O(C(=O)C1C2(C(CCC1=C)C1(C(CC2)C(CCC1)(C)C)C)C)CC(O)COC(=O)C	4.4	Bad	6.5
6550	O1CC2=C(C3(C(CC2)C2(C(CC3)C(CCC2)(C(O)=O)C)C)C)C1=O	5.6	Excellent	6.5
6473	S=C=NC1C2C(CCC1(O)C)C(CCC2C1(OC(CC1)C([NH+]=[CH-])(C)C)C)=C	4.3	OK	6.5
6469	O(C(=O)C)C1C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC(=O)CC(=C1)C)C)C	5	OK	6.5
6356	O(C(=O)C)C1CC2(C(CC=C(C=O)C2COC(=O)C)C(C1)(C)C)C	5.1	Poor	6.5
6264	O1C2C=C(CCC(C(C)=C)C(OC(=O)C)C(=O)C(=CC(=O)C3CC23C)C)C1=O	5.8	Good	6.5

6048	O1C23CC(O)CCC2(C)C(=O)C(=CC13)C1CCC(C(CCC(C(C)C)=C)C)C1(CC=O)C	4.6	Bad	6.5
6016	O(C(=O)C)C1CC2C(CCCC2(C2CCC(C(OC)=O)C(O)C12C)C)(C)C	4.7	Excellent	6.5
6015	O(C(=O)C)C1CC2C(CCCC2(C2CCC(C(OC)=O)C(O)C12C)C)(C)C	5.3	Good	6.5
6000	O1C(C)C(O)C=CC(OC(CC=CC(OC(CC1=O)C)=O)C)=O	4	Excellent	6.5
5985	O1C(C)C(O)C=CC(OC(CC=CC(OC(CC1=O)C)=O)C)=O	4.8	Excellent	6.5
5688	O=C(NC1(C2CC(C3CC2(CC1C3)C)C(C)C)C)NCCc1ccccc1	4.8	Bad	6.5
5624	ClC1(CCC2C(CCC3C(CCCC23C)(C)C)(C)C1C(OCC(OC(=O)C)CO)=O)C	4.5	OK	6.5
5558	O(C(=O)C)C1CC2C(C3CC=C(C=O)C(CO)C13C)(CCC1C(CCCC12C)(C)C)C	4.6	Excellent	6.5
5521	O(C)c1cc(cc(CC2(C3CCCC(=C)C3(CCC2C)C)C)c1O)C(OC)=O	5.5	Excellent	6.5
5478	O(C)C1(CCC=C(CC(=O)C(CCC(C=C1)C(C)C)(CO)C)C)C	4.6	Poor	6.5
5447	O1C(=O)C(C2CC(O)C(=CCC(O)C3(OC(CC3)C1(CC2)C)C)C)=C	5.3	Excellent	6.5
5335	O1CC2C(CCC(=CCCC2=C)C)C(=CC=CC(O)(C)C)C1=O	6.2	OK	6.5
5291	O1C2C(=C(C)C1=O)C(O)C1C(C)(C(OC(=O)CCC)CCC(=C2)C)C(OC(=O)C)CC=C1C	3.8	Poor	6.5
5164	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=CC=O)C)C)C)C1(C(O)=O)C)C	5.7	Bad	6.5
5155	OC1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=CC=O)C)C)C)C1(C(O)=O)C)C	5.1	Bad	6.5
5065	Oc1ccc(cc1)CCNC1=CC2=NCCc3c2c(n(c3)C)C1=O	4.1	Excellent	6.5
5055	O1C(CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	3.7	Bad	6.5
4984	O1C2CCC(C)C1(CCC1C34OC(O)(CC3)C(OC4CCC1C)(C)C)C2(CCC(=O)C(C)C)C	5.3	Poor	6.5
4957	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(O)CC(O)C(C)=C	4.6	Bad	6.5
4932	Brc1cc2NC(=O)C(c2cc1)=C1Nc2c(ccc(Br)c2)C1=O	6.1	Bad	6.5
4812	O1C2C1(CCC1C(=C(C)C)C(=O)CC1(CC=C(CC2OC(=O)C)C)C)C	4.5	Poor	6.5
4750	O(C(=O)C)C1CC2C3C(CCC2(C)C1C=C)C1(C(CC(=O)C=C1)CC3)C	4.1	OK	6.5
4659	O1c2c(cc(O)cc2)C=CC1(CCC1C(CC(=O)C=C1C)(C)C)C	4.9	Excellent	6.5
4653	O1c2c(cc(O)cc2)C=CC1(CCC1C(CC(=O)C=C1C)(C)C)C	5.3	Bad	6.5
4598	O1C=2C3C=C(CCC(OC(=O)C)C1(CCC(=O)C=2CCC3(O)C(C)=C)C)C	5.6	Excellent	6.5
4382	O1C2(CC(OOC2CC1=O)(CC(CCCCCCc1ccccc1)C)C)C	5.3	Good	6.5
4293	O=C1C=C(c2nc3c(c4c2c1ncc4)cccc3)CCNC(=O)C	5.3	Excellent	6.5
3730	o1c2c3c(c1)C(=O)CCC3(c1c(cc3c(c1)C(=O)C=C(OC)C3=O)C2=O)C	5.8	OK	6.5
3655	O1C(C2C(C=CCCCCCCCC1=O)C(O)C(O)C2)CC	5.2	Excellent	6.5
3447	OC1(CCC(=CC=C(CCC(=O)C(CCC1O)C)C)C(C)C)C	5.2	Good	6.5
3321	O1CC(=CC1=O)C(O)CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)CO	5.3	Good	6.5
3186	O1C2=C(C=CC1(CCC1(CCCC(C)C1=C)C)C)C(=O)C(OC)=CC2=O	5.6	Excellent	6.5
2991	O1C2C1(CCC=C(CCC1(C)C(C)C(O)C=C(C1=C)C2=O)C)C	5.5	Good	6.5
2981	O=C1N(CC2=C1C1(C(CC2)C2(C(CC1)C(CCC2)(C(O)=O)C)C)C)CCc1ccccc1	5.4	Excellent	6.5
2860	O1C2C(CC(OC(=O)C)C(CCC(=CCCC(=C2)C)C)C(=O)C)C(CN(C)C)C1=O	6.2	Excellent	6.5
2814	O(C(=O)CC(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)C)CC(O)COC(=O)C	4.5	Bad	6.5
2551	O1C(=O)C(=C2CC3(C(CC12OC)C(OC(=O)C(=CC)C)CCC3C)C)C	5.6	Excellent	6.5
2344	s1c2c(nc1)-c1nccc3c1c(nc1c3cccc1)C2=O	6.1	OK	6.5
2326	O1C(C=CC2C(CC=CCCCC1=O)C(=O)C=C2)CC=CCC	4.9	Poor	6.5
2283	O=C1N(C=Cc2c1[nH]c1c2cccc1)c1ccccc1C(OC)=O	4.6	Good	6.5
2251	O1C(C=CC2C(CC=CCCCC1=O)C(O)CC2OC(=O)C)CC=CCC	5.7	Good	6.5
2206	O1C2CCC(O)(C=CCC(=CC3OCC(=C3CCC12C)C)C)C	4.9	OK	6.5
2094	O1C2CC3(C(CCC4(OC4CCC12C)C)C(=CC3)C(O)(C)C)C	5.9	Excellent	6.5
1851	O1C23CC(O)CCC2(C2C(C4CCC(C(CCC(C)(C)C)=C)C)C4(CC2)C)CC13)CO	5	OK	6.5
1788	s1c2c(nc1)c(c1Nc3c(-c4c1c2ncc4)cccc3)CCNC	4.2	OK	6.5
1745	S(OC1CC2=CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C)(O)(=O)=O	4.2	Excellent	6.5
1632	O(C)C1=CC(O)(C(OC)=O)C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	5.5	Good	6.5

1631	O(C)C1=CC(O)(C(OC)=O)C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	5.2	Good	6.5
1630	O(C)C1=CC(O)(C(OC)=O)C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	5	Good	6.5
1623	O(C)C1=CC(O)(C(OC)=O)C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	4.8	Excellent	6.5
1593	S1CC(NC1=O)C1(OC2CCC(C=CC3OC3CCC(=CC(OC(C1)C2)=O)C)C)O	4.1	Poor	6.5
1547	S(C)c1c(c2Nc3c(-c4c2c(ncc4)c1OC)cccc3)CCNC(=O)CC	6.1	Good	6.5
1537	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(NCC(C)C)=CC1=O	4.5	OK	6.5
1533	O(CC)C1=CC(=O)C(O)=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C1=O	4.7	Good	6.5
1480	O1CC(C(COC(=O)C)C2(C3C(CC2)C(CCCC3=C)(C)C)C)C(OC(=O)C)C1=O	5.4	OK	6.5
1455	O1c2c(cc(O)cc2C)CC2C3(C(CCC12C)C1(C(CC3)C(C)(C)C(=O)CC1)C)C	3.9	Bad	6.5
1454	S(OC(CC1C2(C(CC=C1C)C(CCC2)(C)C)C)C(CCCc1ccoc1)C)(O)(=O)=O	5.4	Poor	6.5
1364	O1C2C3C(C1CC(O)(C)C(O)CCC2(OC(=O)C)C)C(CCC3C(C)C)=C	5.2	Good	6.5
1284	O1C2CC(=CC(=O)C=C(C)C(=O)CC(CCC(=C2)C1=O)C(C)=C)C	6.3	Excellent	6.5
1283	O1C2C=C(CCC(CC(=O)C(=CC(=O)C2=C(C)C)C)C(C)=C)C1=O	5	Excellent	6.5
1278	O1C2C=C(CCC(CC(=O)C(=CC(=O)C2=C(C)C)C)C(C)=C)C1=O	4.6	Good	6.5
1258	O(C)c1cc(c2Nc3c(-c4c2c1ncc4)cccc3)C(OC)=O	4.6	Excellent	6.5
1162	O1C2CC(=CCCC(=C(C2C(CCC=C(C)C)C)C1=O)COC(=O)C)C			6.5
981	O(C)C1=CC(=O)C(O)=C(CC=C(CCC2(CCCC(C)C2=C)C)C)C1=O	5.3	Good	6.5
963	OC12C(CCCC1(C)C)C(CCC(=CCn1c3c(nc1)N(C=NC3=NC)C)C)(C)C(CC2)C	4	Poor	6.5
953	O1CC(=CC1=O)C(O)CC=C(CCC=C(CCC1(CCCC1C)C(C)=C)C)C=O	4.6	Poor	6.5
792	O1C(C(=C)C2C3C4C(CCC4C)C3(C)C(O)C2)C1C=C(COC(=O)C)C	4.2	Poor	6.5
629	O1C2OC(=O)C3C2C2(C(CC3)C3(C(C(CCC3)(C)C)C(OC(=O)CCC)C2)C)C1O	5.4	OK	6.5
570	O=C(Cc1ccccc1)c1nccc2c1[nH]c1c2cccc1	5.1	OK	6.5
569	Brc1cc2c3c([nH]c2cc1)c(ncc3)C(=O)Cc1ccccc1	6.2	Good	6.5
568	Brc1cc2[nH]c3c(c2cc1)ccnc3C(=O)Cc1ccccc1	5.7	Excellent	6.5
564	O1CC(=C2C1C=C(CCC(O)C(O)(CCC=C(CC2)C)C)C)C	4.6	Good	6.5
545	O1C(CC(CCCC(=CC=CC2(CCCc3c2occ3)C)C)=C)C(O)=C(C)C1=O	3.3	Good	6.5
465	O1C2CC(=CC(=O)C=C(C)C(=O)CC(CCC(=C2)C1=O)C(C)=C)C	5.6	Poor	6.5
433	S1CC(NC1=O)C1(OC2CCC(C=CCCC(=CC(OC(C1)C2)=O)C)C)OC	6.8	OK	6.5
243	O1C(C2C(C(=CC(C(=O)CC)C)C)C(=CC(C)=C2C)C)=C(C)C(=O)C(C)=C1OC	5.8	OK	6.5
240	O1C(CC(CCCC(=CC=CC2(CCCc3c2occ3)C)C)=C)C(O)=C(C)C1=O	4.7	Bad	6.5
14489	O1C(CC(=CC=CC(=CCCc2cc(oc2)Cc2ccoc2)C)C)C(O)=C(C)C1=O	4.2	Bad	6.4
14488	O1C(CC(=CCCC(=CCCc2cc(oc2)Cc2ccoc2)C)C)C(O)=C(C)C1=O	5.2	Bad	6.4
14448	O1C2C=C(CCC(C(C)=C)C(O)C(=O)C(C)=C(O)C(=O)C2C(C)=C)C1=O	4	Excellent	6.4
14432	O1C(C2(C3C2(C=C(C)C3C(C(=O)CC)=C)C)C)=C(C)C(=O)C(C)=C1OC	6.3	OK	6.4
14033	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	4.7	Poor	6.4
14032	O1C23N4C5(OC(CC(C5)C)C4)CCC2(C)C(C2C(=O)C(C4C(CC(=CC4=O)C)C2(C3)C)C)(CC1=O)C			6.4
13933	O(C(=O)C)C1CC2(C(CC=C(CCC=C1CO)C)C(CC2)C(C)=C)C	4.6	Excellent	6.4
13669	O1OC(CC1(CC(C=CCC(C=Cc1ccccc1)C)C)C)(CC(O)=O)C	5.1	Bad	6.4
13467	O1CC23C(CCC4(C5Cc6cc(O)ccc6OC5(CCC24)C)C)C(CCC3)(C)C1O	4.6	Bad	6.4
13463	O1CC2C(CCC(=CCCC2=C)C)C(=CC=CC(O)(C)C)C1=O	5	Excellent	6.4
13200	O(C(=O)C)C1CC2=CCC3C4CCC(=O)C4(CCC3C2(CC1)C)C	4.7	Poor	6.4
13094	O1C(O)C2C(CCC3C4(C(CCC23C)C(CCC4)(C)C)C)C1O	5.4	Excellent	6.4
12850	O1CC=2C(C3(C(CC=2)C2(C(CC3=O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1OC(=O)C	5	OK	6.4
12711	O=C1CC2CCC3C4CCC(C(COC(=O)C)C)C4(CCC3C2(C=C1)C)C	5.2	Good	6.4
12631	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)CO)C(=CC1=O)CO	4.1	Poor	6.4
12617	S(=O)(=O)(n1cc(c2c1cccc2)C=O)c1ccccc1	5.7	OK	6.4

12199	O=C(C)C1CCC2C3C(CCC12C)C1(C(CC(=NO)CC1)CC3)C	3.7	Bad	6.4
12198	O=C(C)C1CCC2C3C(CCC12C)C1(C(CC(=NO)CC1)CC3)C	3.9	Bad	6.4
12134	FC1=CN(Cc2ccccc2)C(=O)N(Cc2ccccc2)C1=O	6.4	Excellent	6.4
12102	OC1CC(CCC(C)C(=O)CCC(CC(=O)CC1C)C)C(C)=C	5.8	Excellent	6.4
11942	O1CC(C2CC(C)C(OC(=O)CCC)C3C2C2OC3CC(=C)C(=O)CC(OC(=O)C)C12C)C	3.7	Poor	6.4
11874	OC1CC2C3(C(C1C)C(O)=CC(=C3)C)C(CC2C)C=C(C)C	5	Excellent	6.4
11806	O1C(=O)C(c2c(c(ccc2C2(CC(CCC2)(C)C)C)C=O)C1OC)C	5.7	Good	6.4
11795	O=C1N2C(CCC2)C(=O)NC1Cc1c2c([nH]c1)cccc2	4.4	Excellent	6.4
11792	O1C2CCC1(C)C(O)C(O)c1c(occ1C)CC(=CCCC2C)C	4.3	Excellent	6.4
11456	O1C(C2(C3C2(C)C(=O)C(C)C3C(=CC(C(=O)CC)C)C)C)=C(C)C(=O)C(C)=C1OC	5.6	Poor	6.4
11383	Brc1cc(N2C=Cc3c([nH]c4c3cccc4)C2=O)c(cc1)C(OC)=O	5	OK	6.4
11332	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)C1OC)C1=CC(OC1O)=O	3.7	Poor	6.4
11331	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)C1OC)C1=CC(OC1O)=O	3.6	Bad	6.4
11326	Clc1cc(N=C2C=C(Oc3c2cc(Cl)cc3)c2ccc(OC)cc2)ccc1OC	6.5	Good	6.4
11276	n1c2c(n(C)c1N)C1=NC(=NC1=CC=C2C)N(C)C	5.9	Excellent	6.4
11174	O1CC2C(C(C(C(OC)=O)C)=C(CC2)C2(CC(CCC2)(C)C)C)C1=O	5.6	Excellent	6.4
11141	O1C(C(C)C2(O)CCC3C4C(CCC23C)C2(C(CC(O)CC2)=CC4)C)C1CC(C)C	4	Poor	6.4
10800	OC1CC2CCC3C4CCC(C(CCC(OC)=O)C)C4(CCC3C2(CC1)C)C	4.8	Poor	6.4
10756	O1C2CC3(CC(O)C4(C(C3CCC12C)C(=CC4=O)C(C)C)C)C	6.2	Excellent	6.4
10675	O(C(=O)C)C1C2C(CCC2C(O)(C)C)(C=CC(CCC=C(C1)C)C)C	4.5	Excellent	6.4
10652	O1C(CC(=CCCC(C=CC=C(CCCC2=CC(OC2=O)OC)C)C)C)C(O)=C(C)C1=O	4.8	Bad	6.4
10558	O1C23C1C(O)C1C4CCC(C(CCCC(C)C)C)C4(CCC1C2(CCC(O)C3)C)C	5.7	OK	6.4
10529	OC1CC2=CCC3C4CCC(C(=NO)C)C4(CCC3C2(CC1)C)C	4.6	OK	6.4
10414	O1C2CC(=CC(=O)C(OCC)CC(=O)CC(CC=C(C2O)C1=O)C(C)=C)C	5.5	Excellent	6.4
10413	O1C2CC(=CC(=O)C(OCC)CC(=O)CC(CC=C(C2O)C1=O)C(C)=C)C	5.4	Excellent	6.4
10410	OC1CC2=CCC3C4CCC(C(=NO)C)C4(CCC3C2(CC1)C)C	4.3	Good	6.4
10366	O(C(=O)C)C1C2C(CCC2C(O)(C)C)(C=CC(CCC=C(C1)C)C)C	4.2	Excellent	6.4
9677	Oc1cc(c2c(CC3C4(C(CCC23C)C(CCC4)(C)C)C)c1O)COC	5.5	Excellent	6.4
9608	Oc1c2c(ccc1)C(=O)c1c(c(cc(O)c1)C)C2=O	4.2	Excellent	6.4
9555	O=C1N(CCc2c1[nH]c1c2cccc1)C(=O)c1ccccc1NC	4.5	Poor	6.4
9197	O(O)C1(CCC2C3C(C)(C(O)CC2(C=C1)C)C(=O)C=C3C(C)C)C	5	Poor	6.4
9159	ClC1CC2(C(CCC(=C)C2CC(O)C2CC(=O)NC2=O)C(C1)(COC(=O)C)C)C	5.1	Bad	6.4
9120	O(C)c1cc(CC2(C3CCC(=O)C(CCC(O)=O)C3(CCC2C)C)C)c(O)c(c1)C	4.8	Excellent	6.4
9024	O1C(CC(=CCCC(C=CC=C(CCCC2=CC(OC2=O)OC)C)C)C)C(O)=C(C)C1=O	4.5	Bad	6.4
8977	O1C2CCC(=C)C(O)CCC(O)(C=CC(CCC12C)C(C)C)C	5.3	Excellent	6.4
8976	O1C2CCC(=C)C(O)CCC(O)(C=CC(CCC12C)C(C)C)C	5.8	Good	6.4
8845	OC1=C(C)C(=O)C2=C(C1=O)C(CCC2C(CCC=C(C)C)C)C	4.7	Excellent	6.4
8735	O=C1N2C(CCC2)C(=O)NC1Cc1c2c([nH]c1)cccc2	4.8	Poor	6.4
8619	Oc1ccc(O)cc1CC1C2(C(CCC1=C)C(CCC2)(C)C)C	5.3	Excellent	6.4
8542	O1C2(O)C(=CC1=O)CC1C(CCC(=C1)C)C2(C)C	4.5	Poor	6.4
8493	O=C1N2C(CCC2)C(=O)NC1Cc1c2c([nH]c1)cccc2	4.3	OK	6.4
8436	Oc1ccc(cc1)-c1nc(Cc2ccccc2)c(nc1)N	4.8	Poor	6.4
8188	O1c2c(C=CC1(CCC1(CCCC(C)C1=C)C)C)c(O)c(O)cc2OC	4.5	Excellent	6.4
8185	O(C(=O)C)C1CC2=CCC3C4CCC(C(CC(O)=O)C)C4(CCC3C2(CC1)C)C	5.3	Bad	6.4
8177	O(C)C1=CC(O)(C(OC)=O)C(CC2(CCC3(C(CCC=C3C)C2C)C)C)C1=O	4.7	Good	6.4
8176	O(C)C1=CC(O)(C(OC)=O)C(CC2(CCC3(C(CCC=C3C)C2C)C)C)C1=O	4.2	Good	6.4
8043	OC1CC2=CC(=O)C3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	4.9	Excellent	6.4

7998	O(C(=O)C)C1CC2=CCC3C4CCC(=O)C4(CCC3C2(CC1)C)C	4.6	Poor	6.4
7933	O1C(=O)C(=C2CC3C(C4OC3(CC4)C)(CCC=C(CC12OC)C)C)C	5.5	Excellent	6.4
7932	O1C(=O)C(=C2CC3C(C4OC3(CC4)C)(CCC=C(CC12OC)C)C)C	5.7	Good	6.4
7723	O1CC2=C(C3(C(CC2OC(=O)C)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1=O	4.2	Bad	6.4
7540	Brc1cc(ccc1O)C1=C(Cl)C(OC1=Cc1cc(Br)c(O)cc1)=O	5.3	Excellent	6.4
7490	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=O)C)C)C)C1(C(O)=O)C)C	5.8	Bad	6.4
7481	O1C(O)C(OC)=C(C(=O)CC2(CCC3(C(CCC=C3C)C2C)C)C)C1=O	4.6	Good	6.4
7400	O(C(=O)C)C12C3(C(CC1)C(CCCC)C3C=CC(OC(=O)C)CCC(OC)=O)C(=O)C=C2	6.2	OK	6.4
7180	Brc1c(C)c(Br)c2C3C(CCC3C(C)C)(C)C(=O)C(=O)c2c1O	6	Excellent	6.4
7058	O=C1CC2CCC3C4CCC(C(C(O)C(O)C=C(C)C)C)C4(CCC3C2(C=C1)C)C	5.3	OK	6.4
7000	O1CC=2C(C3(C(CC=2)C2(C(CC3=O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1O	4.1	Bad	6.4
6997	O1C(O)C2=C(CCC3C4(C(CCC23C)C(CCC4)(CO)C)C)C1=O	4.6	Poor	6.4
6856	O1C(C2C3(CC=C4C(=CCC5C(C)(C)C(O)CCC45C)C3(CC2)C)C1=O)(CCCC(OC)(C)C)C	5.3	Poor	6.4
6769	O1CCCCC1n1c2ncnc(NCc3ccccc3)c2nc1	5.3	Good	6.4
6631	O1C(C2=C(C3(C(CC2)C2(C(CC3=O)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	4.1	Poor	6.4
6565	O(C(COC(=O)C1C2(C(CCC1=C)C1(C(CC2)C(CCC1)(C)C)C)C)CO)C(=O)C	4.6	Bad	6.4
6551	O1CC2=C(CCC3C4(C(CCC23C)C(CCC4)(C(O)=O)C)C)C1=O	4.4	Good	6.4
6454	O(C(=O)C(=CC(CCCC)C)C)C1C2=CC(=O)C(CC2(C)C(CC1)C(O)=O)C(C=O)=C	5	Good	6.4
6453	O(C(=O)C(=CC(CCCC)C)C)C1C2=CC(=O)C(CC2(C)C(CC1)C(O)=O)C(C=O)=C	4.4	Bad	6.4
6452	O(C(=O)C(=CC(CCCC)C)C)C1C2=CC(=O)C(CC2(C)C(CC1)C(O)=O)C(C=O)=C	3.9	Bad	6.4
6451	O(C(=O)C(=CC(CCCC)C)C)C1C2=CC(=O)C(CC2(C)C(CC1)C(O)=O)C(C=O)=C	4.8	OK	6.4
6227	O1CC=2C(C3(C(C4C(CC3O)C3(C(CC4)C(CCC3)(C)C)C)CC=2)C)C1O	4.9	Bad	6.4
6132	O1OC(CCC1(CCC=C(CCC1(O)C(CCCC1=C)(C)C)C)C)C(C(O)=O)C	5.5	Bad	6.4
6128	OC12C=C3CC(O)CC3C(C=C(C=CC1CCCCCCC)C)C2=O	6	Excellent	6.4
6113	O1C2CC(=CC(=O)CC(OCC)C(=O)CC(C(C)=C)C(=O)CC(=C2)C1=O)C	5.2	Good	6.4
6102	O(C)c1ccc(cc1)CC=1N(C)C(=N)N(C=1)Cc1ccc(O)cc1	3.8	OK	6.4
6090	s1c2c(nc1)c1nccc3-c4c(Nc(c13)c2CCN)cccc4	3.9	OK	6.4
6033	o1c(-c2c3c([nH]c2)cccc3)c(nc1C(N(C)C)CC(CC)C)C(O)=O	4.3	Good	6.4
6001	O1C(C)C(O)C=CC(OC(CC(OC(CC=CC1=O)C)=O)C)=O	5.5	Excellent	6.4
5957	O1CC2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(C)(C)C(O)CC3)C)C)C)C1=O	3.9	Poor	6.4
5896	OC1(CC(c2c(C1)ccc(C)c2C=CC=CC(O)=O)C)C	5.3	Excellent	6.4
5828	OC(=O)CCc1ncc2c(c1)C1(C(CC2)C2(C(CC1)C(CCC2)(C)C)C)C	6.2	Good	6.4
5705	O(C(=O)C)C1C2C3CCC(C=C)C3(CCC2C2(C(CC(O)CC2)=C1)C)C	4.4	OK	6.4
5704	O(C(=O)C)C1CC2=CC(O)C3C4CCC(C=C)C4(CCC3C2(CC1)C)C	5	OK	6.4
5568	O(C(=O)C)C1CC2C(C3C=CC(=CC13C)C=O)(CCC1C(CCCC12C)(C)C)C	5.4	Excellent	6.4
5492	O1C(O)C(CCC1C(C)C)C1(O)CCC2C3C(CCC12C)C1(C(CC(=O)CC1)CC3)C	3.8	Bad	6.4
5490	O1C(O)C(CCC1C(C)C)C1(O)CCC2C3C(CCC12C)C1(C(CC(=O)C=C1)CC3)C	4.3	Poor	6.4
5459	O(C(=O)C)C1CC2=CCC3C4CCC(=O)C4(CCC3C2(CC1)C)C	4.6	Good	6.4
5412	OC12C=C3CC(O)CC3C(C=C(C=CC1CCCCCCC)C)C2=O	4.1	Good	6.4
5359	O=C1C(=C2NC(CC2C)CC(CC=CC#CC#CCCCCC)C)C(=O)N(C)C1C	4.3	Bad	6.4
5267	O(C)c1cc(O)cc(C=C2C3(C(CCC2C)C(CCC3)(C)C)C)c1O	3.8	Bad	6.4
5115	OC(=O)[C-]1[NH+]2C(CCCC2)=CC=C1c1ccccc1	5.1	Excellent	6.4
5100	O1C2C3OCC(=C3CCC(=CCCC(O)(C1CCC2(O)C)C)C)C	4.9	Excellent	6.4
4918	O1C2C(CC3C(C)(C(OC(=O)CCC)CCC(=C2)C)C(OC(=O)C)CC=C3C)=C(C)C1=O	5	Poor	6.4
4882	O1C2(C3C(CCC2C2(CC(CCC2)(C)C)C)C(OC3O)O)C1C	4.6	Excellent	6.4
4858	O1CC2C(CCC(O)(C=CCC2=C)C)C(=CC=CC(O)(C)C)C1=O	6.2	OK	6.4

4843	O1CC2C(CCC(O)(C=CCC2=C)C)C(=CC=CC(O)(C)C)C1OC	5.7	Good	6.4
4842	O(C)c1ccc(O)c(O)c1C=C1C2(C(CCC1C)C(CCC2)(C)C)C	4.4	Good	6.4
4756	O1C=C(C2C(C(CC=CC(OC(=O)C)(CC2)C)=C)C1OC(=O)C)C(=O)C=CC(O)(C)C	5.1	Poor	6.4
4724	O1CC2C(CCC(O)(C=CCC2=C)C)C(=CC=CC(O)(C)C)C1=O	5.6	OK	6.4
4710	OC1CC2=CC(=O)C3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	5.3	Poor	6.4
4709	OC1CC2=CC(=O)C3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	6.2	Good	6.4
4640	O=C(C1=NCCc2c1[nH]c1c2cccc1)c1n(cnc1)C	4.9	OK	6.4
4551	O(C)c1ccc(O)c(O)c1C=C1C2(C(CCC1C)C(CCC2)(C)C)C	4.3	OK	6.4
4528	O(C(=O)C)c1c2c(cc3c1c(OC(=O)C)ccc3)cccc2OC(=O)C	5.1	Excellent	6.4
4473	O=C(CNC(=O)C(N(C)C)Cc1ccccc1)c1c2c([nH]c1)cccc2	4.7	Excellent	6.4
4245	O=C1C2C(CCC3C(CCCC23C)(C)C)(C)C(COC(=O)C)C(=C1)COC(=O)C	4.6	Good	6.4
3895	Brc1cc2c3c4c(ncc3)C(=O)C(N)=Cc4nc2cc1	5.4	Excellent	6.4
3795	ClC1(CCC=C(CCC=C(CC2OC(=O)C(C2CC1O)=C)C)C)C	5.2	Excellent	6.4
3679	O1CC(CC(OC)=O)C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1=O	5.1	Excellent	6.4
3616	O1OC(CCC1(CCC1(C)C(CCC2C1(O)CCCC2(C)C)C)C)C(C(O)=O)C	4.6	Bad	6.4
3568	O(c1cc(ccc1OC)C1C=C(CC1)C(OC)=O)C1CCCC1	5	Good	6.4
3444	O1C2CCC1(C)C(O)CCC(=CC=C(CCC2(O)C)C(C)C)C	4.5	Excellent	6.4
3362	O1C2(CCC=C(CCC(=CC3C2(O)CCC3=C)C(C)C)C1=O)C	4.4	Excellent	6.4
3344	O1CC(=CC1=O)C=CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)CO	4.7	Good	6.4
3320	O1CC(=CC1=O)C=CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)CO	5	Poor	6.4
3318	O1C(O)C(=CC1=O)C=CC=C(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)C(OC)OC	4.8	Poor	6.4
3285	O1C=2C(=CC1=O)C(OC(=O)C)CC1C(CCC3C4(C(CCC13C)C(CCC4)(C)C)C)C=2	4.6	Bad	6.4
2936	O1C2(O)CCC3C4CCC(C(CCCC(C)C)C)C4(CCC3C2(CC1=O)C)C	5.3	Poor	6.4
2859	O1C2CCC(=CCCC(=CC3OC(=O)C(C3CC(OC(=O)C)C12C)CN(C)C)C)C	5.3	OK	6.4
2791	O(C(=O)C)C1CCC(=CC2C(C(O)(CCC2C(C)C)C)C(OC(=O)C)CC1=C)C	4.6	Good	6.4
2581	O=C1CC(=CC(=O)C=C(CCC=C(C)C(=O)CC1C(C)C)C)C(OC)=O	6.5	Excellent	6.4
2119	O1CC2(C(CCC3(C2CCc2c3coc2)CO)C(CO)(C)C1=O)C	6	Poor	6.4
1914	OC1=C(CC2(C3CCCC(=C)C3(CCC2C)C)C)C(=O)C(NCCCCC)=CC1=O	4.8	OK	6.4
1805	O1C2(CC(=O)C=CC2=O)CC2C3(C(C45C(CC3)C(CCC4)(C)C(OC5)=O)CCC12C)C	4.3	Bad	6.4
1798	O1C2(CC(=O)C=CC2=O)CC2C3(C(C45C(CC3)C(CCC4)(C)C(OC5)=O)CCC12C)C	4	Bad	6.4
1598	O1C(C(C)C)C(C)C(=O)C(C)=C1C(C)C=1OC(CC)=C(C)C(=O)C=1C	5.2	Excellent	6.4
1513	O(C)c1ccc(cc1O)CC=1N(C)C(=N)N(C)C=1Cc1ccc(OC)cc1	5	Excellent	6.4
1388	OC1CC(CCC(C)C(O)CCC(CC(=O)CC1C)C)C(C)=C	5.1	Excellent	6.4
1120	O1CC(C(OC(=O)C)C(OC)=O)C(=C1)C1(C2C(CC1)C(CCCC2=C)(C)C)C	4.9	Good	6.4
964	OC12C(CCCC1(C)C)C(CCC(=CCn1c3c(nc1)N(CN(C)C3=N)C)C)(C)C(CC2)C	3.7	Bad	6.4
652	Oc1c2c(cc(C)c1C(=O)C)cc1c(C(=O)C(C)(C)C(=O)C1(C)C)c2O	3.4	Bad	6.4
628	O1C(OC(=O)C)C2C3(C(CCC2C(OC)=O)C2(C(CC3)C(CCC2)(C)C)C)C1OC(=O)C	5	Poor	6.4
347	O1C2C(CCC(=CCC(OC(=O)C)C(=CCCC(=C2)C)C)C)C(=C)C1=O	5	OK	6.4
344	O1C2C(C(=C)C1=O)C(O)CC(=CCCC(=CC(O)CC(=C2)C)C)C	4.4	Good	6.4
14352	S=C(NC1(C2C(C3C(CC1)C3(C)C)C(CC2)C)C)NCCc1ccccc1	4.2	OK	6.3
14351	S=C(NC1(C2C3C(CCC2(CCC1)C)C3(C)C)C)NCCc1ccccc1	5.5	Poor	6.3
14300	O(C(COC(=O)C1C2(C(CC=C1C)C1(C(CC2)C(CCC1)(C)C)C)C)CO)C(=O)C	5.3	Good	6.3
14299	O(C(=O)C1C2(C(CC=C1C)C1(C(CC2)C(CCC1)(C)C)C)C)CC(O)COC(=O)C	3.9	Good	6.3
14156	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(O)CC=C(CO)C	4.7	Excellent	6.3
14127	O1C2CC3OC(CC4=CCC(C(C)C)C4(CC(=O)C3(O)C)C)C12C	4.1	Excellent	6.3
14061	O(C(=O)C)C1CC(C(C(OC(=O)C)CC=C(C)C)C)C(O)C2C(CC=C2C)C1=C	5.5	OK	6.3
14035	O1C(CCC1C(C)=C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	4.2	OK	6.3

14034	ClC(C)(C)C1OC(CC1)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	5.1	Excellent	6.3
13892	OC1CC2=CCC3C4CCC(C(O)C)C4(CCC3C2(CC1)C)C	4.8	OK	6.3
13891	OC1CC2=CCC3C4CCC(C(O)C)C4(CCC3C2(CC1)C)C	4.5	OK	6.3
13858	O1C2(O)C(=CC1=O)C(C1C(C2)C=C(CC1)C)(C)C	5.1	Excellent	6.3
13793	O1C(=CC(NCCO)=C(C=O)C1=O)C1C2C(CCCC2)C=CC1C	7.6	Bad	6.3
13723	O1c2c(C=CC1(CCC1(CCC=C(C)C1C)C)C)c(O)c(OC)c(OC)c2OC	4.3	Excellent	6.3
13558	O1C2CCC3(C1)C(C(OC)=O)C(CCC23C)C(=CCC(O)C(O)(C)C)COC(=O)C	4.3	Good	6.3
13488	O1C2CCC(O)(C)C(CCC3C(C4C(CC5OC35C)C(O)(CC4)C)(C)C)C2(CCC(=O)C1(C)C)C	5	Excellent	6.3
13468	O1CC23C(CCC4(C5Cc6cc(O)ccc6OC5(CCC24)C)C)C(CCC3)(C)C1O	4.3	Bad	6.3
13406	O1C2C3C(C(CCC3C(CO)C)=C)C(=O)CC(O)(C1CCC2(OC(=O)CCC)C)C	6	Excellent	6.3
13204	O1C2CC3C4(C(CCC3(C3CC=C(C(C23C)C1=O)C(O)C)C)C(CCC4)(C)C)CO	5	Bad	6.3
13113	O(C(=O)C)CC(CCC=C(CCC1C(CCCC1C)(C)C)C)=CC=O	5.4	Poor	6.3
13022	OC1CC(=CCC=C(C=O)C(COC(=O)C)C1C(CCC=C(C)C)C)C	5.3	Poor	6.3
12879	ClCC(O)(C)C1C2OC(CC1)(C)C(OC(=O)C)CCC(=CCCC(=C2)C)C	5.2	Excellent	6.3
12774	O(C(=O)C)C1CC(C(=CCC=C(C)C)C)C(C2C(C)C(OC(=O)C)CC2=O)C1CO	5.3	Good	6.3
12351	OC1=C(C)C(=O)c2c(C1=O)c(ncc2)COC(=O)C(=CC)C	5.2	Excellent	6.3
12301	OC1CC(C2C3C(CCC3C)C12C)C(CC=CC(O)(C)C)=C	5.5	OK	6.3
12151	O(C(=O)CC(O)C)C1CC2C(C3CC=C(C(=O)C)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	6.1	OK	6.3
12039	o1cc2c(CCC3C4(C(CCC23C)C(CCC4)(C(O)=O)C)C)c1	5.1	Excellent	6.3
12012	O1C2C=C(C(C)C)C(=O)C(O)C(CCC(=O)C(CCCC12C)CO)C	5.8	OK	6.3
11890	O(C)C1=C(C)C(=O)c2c(C1=O)c(ncc2)COC(=O)C(=CC)C	5.2	Excellent	6.3
11679	O(C(=O)C)C1C2C(CCCC2(C2CCC(O)(CC2(C1)C)C1CC(=O)C(=CC1)C)C)(C)C	4.4	Good	6.3
11588	o1cc2c(CCC3C4(C(CCC23C)C(CO)(C)C(O)C(=O)C4)C)c1	4.9	Excellent	6.3
11586	o1cc2c(CCC3C4(C(CCC23C)C(CO)(C)C(O)C(=O)C4)C)c1	5.2	Good	6.3
11298	BrC1CCC(=C)C(C=CC(O)(C)C2CC(Br)C(O)(CC2)C)C1(C)C	4.8	Poor	6.3
11175	O1CC2C(C(C(C(O)=O)C)=C(CC2)C2(CC(CCC2)(C)C)C)C1OC	5.4	Poor	6.3
11170	O(C(=O)C)C1C=C(C)C(=O)CC1C1(O)CC2(C(CC1)C1(C(C(CCC1)(C)C)C(OC(=O)C)C2)C)C	3.6	Poor	6.3
11166	O1CC2C(C(C(C(O)=O)C)=C(CC2)C2(CC(CCC2)(C)C)C)C1OC	5.6	Good	6.3
11165	O=C1C(C(C(O)=O)C)=C(CCC1COC=O)C1(CC(CCC1)(C)C)C	4.9	Excellent	6.3
11140	O1C(C(C)C2(O)CCC3C4C(CCC23C)C2(C(CC(O)CC2)=CC4)C)C1C(C(C)C)C	4.4	Bad	6.3
10959	O1OC(CCC1(CC=CC(O)(CCC=1C(CCCC=1C)(C)C)C)C)C(C(O)=O)C	4.5	Bad	6.3
10908	O1c2c(cc(O)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C)C)C=O)C	5.7	OK	6.3
10823	OC(=O)C1(C2CCC(=C)C(CCC(=CC(O)=O)C)C2(CCC1)C)C	6	Excellent	6.3
10683	OC1C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC(O)C=C(C1)C)C)C	4.4	Poor	6.3
10491	OC1C2CC(O)CCC2(C=2C(C3CCC(C(CC(=O)C)C)C3(CC=2)C)C1)C	3.9	Poor	6.3
10392	O(C(=O)C)C1C2C(CC=C2C)C(CCC1C(CCC(=O)C(C)C)C)=C	4.6	Good	6.3
10368	O(C(=O)C)C1C=C2C(CC3(O)C1(CCCC3=C)C)(CCC2(O)C(C)C)C	4.9	OK	6.3
10357	[NH+](C1(C2C3C4C(CC2)C([NH+]=[CH-])(CCC4C(CC3CC1C)C)C)C)=[CH-]	5.5	Excellent	6.3
10213	OC1CC2=CCC3C4CCC(C(O)C)C4(CCC3C2(CC1)C)C	4	OK	6.3
9837	Oc1ccc(O)cc1CC1(C2CCC=C(C)C2(CCC1C)C)C	5	OK	6.3
9777	O1C2=CC(C)(C(O)C(CCC3=CC(OC3=O)C2C(C)=C)C(C)=C)C1=O	5	Excellent	6.3
9626	o1cc(cc1CC(=CCCC(=CC(OCc1ccoc1)=O)C)C)C	5.5	OK	6.3
9550	OC1CC2=CCC3C4CCC(C(CCC(O)=O)C)C4(CCC3C2(CC1)C)C	4.2	Bad	6.3
9266	O(C(=O)C)C1CC2C(C3CCC(C(CC(O)C(C(C)C)C)C)C13C)CC=C1CC(O)CCC12C	4.5	Bad	6.3

9222	O1C2=C(CC3(CCC4(C(CCCC4=C)C13C)C)C)C(=O)C(OC)=CC2=O	5.1	Good	6.3
9199	OC1C=C(C2C3CCC(O)(C=CC3(CC(=O)C12C)C)C)C(C)C	5.9	Good	6.3
9196	OC1(CCC2C3C(C)(C(=O)CC2(C=C1)C)C(=O)C=C3C(C)C)C	5.7	Excellent	6.3
9194	O1C2CC3C4C(CCC3(CC(=O)C12C)C)(C)C(=O)C=C4C(C)C	4.3	Excellent	6.3
9189	OC1C=C(C2C3CCC(=C)C(O)CC3(CCC12C)C)C(C)C	5.1	Excellent	6.3
9053	OC1CC2=CCC3C4CCC(C(CCC(O)=O)C)C4(CCC3C2(CC1)C)C	4.2	Bad	6.3
9017	O1C(O)C(=CC1=O)C(O)CC=C(CCC=C(CCC1C(CCC=C1C)(C)C)C)C=O	4.9	Bad	6.3
8966	O1C23C1C(O)C=1C4CCC(C(CCC(C(C)C)CC)C)C4(CCC=1C2(CCC(O)C3)C)C	5	Poor	6.3
8829	OC1CCC2(C(CC(=O)C3=C2CCC(C3)(C=C)C)C1(CO)C)C	5.5	Good	6.3
8523	O1C2(O)C(=CC1=O)C(C1CC(O)C(=CC1C2)C)(C)C	5.1	Excellent	6.3
8411	O=C1C=C(C)C(=O)C=C1CC=C(CCC=C(CC(=O)CC(C)C)C)C	3.6	Bad	6.3
8327	O1C2CCC(=C)C(=O)CC3(C(=CCC12C)C(C(C)C)C(=O)C3)C	5	Excellent	6.3
8189	O1c2c(C=CC1(CCC1(CCCC(C)C1=C)C)C)c(O)c(OC)cc2O	5.3	OK	6.3
8164	O1C(CC=C(CCC2(C3CCCC(=C)C3(CCC2C)C)C)C)C(=CC1=O)CO	4.6	Poor	6.3
8010	O1CC12C1(C3(OC3C2O)C(O)C2C1C(OC(=O)CCCCCCC)C(C2)(C)C)C			6.3
7947	ClC1CC2C(C3(C)C1(O)CC=CC3=O)C(O)CC1(C2CCC1C(CCC(C(C)C)C)C)C	5.5	Bad	6.3
7833	O1C2(O)C(=CC1=O)C(C1C(C2)C=C(CC1)C)(C)C	5.5	Good	6.3
7798	O1C(O)C(=CC1=O)CCC1(C2C3(CC3(CCC2)C)CCC1C)C	5.2	Excellent	6.3
7777	O1C2C1(CC=C(CCC=C(CCC=C(C)C)C)C)C(=O)C=C(COC(=O)C)C2O	3.4	Poor	6.3
7743	OC12C(O)(C)C(=O)C34C(C1=O)C(CCC3C(CC4C2C(C)=C)C)C	5	Excellent	6.3
7721	O1CC2=C(C3(C(CC2O)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1=O	5.6	Good	6.3
7183	Brc1c(cc2C3C(CCC3C(C)C)(C)C(=O)C(=O)c2c1O)C	5.7	Excellent	6.3
7161	O1C(CC(=CCCC(C=CC=C(CCCC2=CC(=O)N(C2)CCO)C)C)C)C(O)=C(C)C1=O	5	Bad	6.3
7160	O1C(CC(=CCCC(C=CC=C(CCCC2=CCN(CCO)C2=O)C)C)C)C(O)=C(C)C1=O	5.3	Bad	6.3
7075	O1C2C3=C(C(CCC3C(CC(C=C(C)C)C2(O)C)C)C)C1=O	5.7	Excellent	6.3
7059	O(C(COC(=O)C)CO)C(=O)CC(CCC1(C=2C(CCC1C)C(CCC=2)(C)C)C)C	4.4	Excellent	6.3
6894	O1C2(OC)C(C3C(C(OC(=O)C)CC3C(=CCC=C(C)C)C)C1OC)C(C=C2)C	5	Excellent	6.3
6892	O1C2(OC)C(C3C(C(OC(=O)C)CC3C(=CCC=C(C)C)C)C1OC)C(C)C(OC)C2	4.5	Poor	6.3
6810	O1C(C2C3(CC=C4C(CCC5C(C)(C)C(O)CCC45C)C3(CC2=O)C)C1=O)(CCC=C(C)C)C	4.6	Poor	6.3
6803	OC(=O)c1c2nc3c(nc2ccc1)c(ccc3)C(O)=O	5.2	Excellent	6.3
6693	O1C2C(CC3C(C)(C(OC(=O)C=C(C)C)CCC(=C2)C)C(OC(=O)C)CC=C3C)=C(C)C1=O	5	Good	6.3
6640	OC1CCC2(C(CC=C3C2CCC(C3)(C=C)C)C1(CO)C)C	5.9	Poor	6.3
6566	OC1(CCC2C(CCC3C(CCCC23C)(C)C)(C)C1C(OCC(O)COC(=O)C)=O)C	5	Bad	6.3
6462	Oc1cc(c2Nc3c(-c4c2c1ncc4)cccc3)C=O	5.7	Excellent	6.3
6438	BrC1CC(CCC1(O)C)C(=CC(O)C1C(=C)C(CCC1=C)C)C	5.7	OK	6.3
6042	O1C2(C(=C(C(=O)CCCCCC(O)C)C1=O)C(=C1C(=COC(=C1)C)C2O)C=O)C	6.4	Bad	6.3
6041	O1C2(C(=C(C(=O)CCCCCCC)C1=O)C(=C1C(=COC(=C1)C)C2O)C=O)C	4.7	Excellent	6.3
6019	O1C2C1(C(OC)=O)C(=O)C1(C(C3(C(CC1)C(CCC3)(C)C)C)C2=O)C	5	Good	6.3
5878	O(C(=O)C)c1c2c(ccc1)C(=O)c1c(C2=O)c(OC(=O)C)ccc1	4.8	Excellent	6.3
5778	O1C(CC=CCC=CCCCCCCCC1=O)C(O)CC	4	Excellent	6.3
5776	O1C(CC)C(O)CC=CCC=CCCCCCCCC1=O	4.5	Good	6.3
5754	S(OC1=C(C)C(OC1CC(=CCCC(C=CC=C(CCCc1ccoc1)C)C)C)=O)(O)(=O)=O	4.7	Bad	6.3
5522	O(C)c1cc(cc(CC2(C3CCCC(=C)C3(CCC2C)C)CO)c1O)C(OC)=O	4.5	Poor	6.3
5438	o1cc(cc1C=C(CCCc1cc(oc1)C=C(C(=O)NCCN)C)C)CCCc1ccoc1	4	Bad	6.3
5340	O1C(O)(CC)C(C)C(OC(=O)C(C(O)C(C(=O)CC)C)C)C(C)C1C(C)C	4	Good	6.3
5201	S(C)C=1N(CN(C)C=1C(=O)c1nccc2c1[nH]c1c2cc(O)cc1)C	4.7	Good	6.3

5194	O1C2C=C(C1CC(=CCCC(=CCCC2(O)C)C)C)C(O)(C)C	5	Good	6.3
5125	S=C=NC1(C2C3C(CC1)C(CC1CC(C)C(C(C13)CC2)(C#N)C)C)C	4	Excellent	6.3
4916	O1C2C(CC3C(C)(C(OC(=O)CC)CCC(=C2)C)C(OC(=O)C)CC=C3C)=C(C)C1=O			6.3
4851	O1CC2C(CCC(O)(C=CCC2=C)C)C(=CC=CC(C)C)C1=O	5.7	Excellent	6.3
4758	O1C=C(C2C(C(CCC=C(CC2)C)=C)C1OC(=O)C)C(O)CC=C(C)C	5.1	OK	6.3
4715	ClC1C(C2CC=C3C(C2(CC1O)C)C(OC3)O)(CCC(C(C)=C)C)C	5	Excellent	6.3
4699	O1C2C(CC3OC3(CCC(O)C(CCCC(C)C2O)=C)C)C(=C)C1=O	5.4	Poor	6.3
4674	OC1CCC(C2CC=C(C(=O)C)C(C=O)C12C)(C(CC=C(CC)C)C)C	5.6	Poor	6.3
4665	O1C2OC2C(CCC=C(CCC=C(CC(O)C=C(C)C)C)C)C1=O	4.9	Bad	6.3
4614	O1C2C1(CCC=C(CCC1(C)C(O)(C(=CCC1C)C2=O)C)C)C	5.1	Poor	6.3
4518	OC1(CCC=C(CC(=O)C(CCC(C=C1)C(C)C)(COC(=O)C)C)C)C	4.5	Poor	6.3
4482	O1C2CCC(C3C(CCC12C)C(=CC(C=C(C)C)C3O)C=O)=C	5.1	Excellent	6.3
4431	O(C(=O)C)C1C2C(C=CC=C2C)(C)C(=O)CC2C1(CCC2(O)C(C)C)C	4.7	Excellent	6.3
4420	O(C(=O)C)C1C2C(C=CC=C2C)(C)C(=O)CC2C1(CCC2(O)C(C)C)C	4.7	Good	6.3
3936	O1C2CC(=CCCC(C(C2C(CCC=C(C)C)C)C1=O)=COC(=O)C)C	5.6	OK	6.3
3929	O1C2C3C(C1CC(O)(C)C(OC)CCC2(O)C)C(CCC3C(C)C)=C	5.2	Excellent	6.3
3907	O1C2(CCC1(C=CC(O)(CCC=C(CCC2O)C)C)C(C)=C)C	5.7	Excellent	6.3
3696	O(C(COC(=O)C1C2(C(CC=C1C)C1(C(CC2)C(CCC1)(C)C)C)C)CO)C(=O)C	4.2	Bad	6.3
3683	O1CC(CC(OC)=O)C(C(=C)C2CCC3C2(CCCC3(C)C)C)C1=O	5.6	Excellent	6.3
3617	O1OC(CCC1(CCC1(O)C2(C(CCC1C)C(CCC2)(C)C)C)C)C(C(O)=O)C	4.9	OK	6.3
3601	OC1C2C(CC=C2C)C(=C)C(O)CC1C(C(OC(=O)C)C(OC(=O)C)C=C(C)C)C	4.7	OK	6.3
3446	O1C2CCC(O)(C1CCC(=CC=C(CCC2(O)C)C(C)C)C)C	4.3	Excellent	6.3
3339	O1C(=O)C(CC1C=C(C)C)=CCCC(=CCCC(=CCC(O)C1=CC(OC1)=O)C)C	5.1	Bad	6.3
3335	O(C)C1=CC(=O)C(O)=C(CC=C(CCC2C(CCC=C2C)(C)C)C)C1=O	5.6	OK	6.3
3242	O1C23CC(OC(=O)C)CCC2(C)C(=O)C(=CC13)C1CCC(C(C=CC(C)C)C)C1(CCOC(=O)C)C	4.4	Poor	6.3
3038	O1c2c(cc(O)cc2C)C=CC1(C=CC=C(C=O)C)C	5.6	Excellent	6.3
2813	O(C(COC(=O)C)CO)C(=O)CC(CCC=1C2(C(CCC=1C)C(CCC2)(C)C)C)C	3.4	Poor	6.3
2578	O(C(=O)C)C1C2C(CCC3C1(CCC3(O)C(C)C)C)(C=CC=C2C)C	4.2	OK	6.3
2399	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2NC=O)C(N=C=S)(CC1)C	4.3	Good	6.3
2378	O1CC2=C(C3C(C3)C(CC(O)C2C(CCC=C(C)C)COC(=O)C)C)C1=O	5.1	Poor	6.3
2370	O1OC(CCC1(CCC1C2(CCCC(C)(C)C2(O)CCC1C)C)C)C(C(OC)=O)C	5	Poor	6.3
2350	O1C2C(c3c(cc(OC)c(c3)C)C(C)C2O)=C(C)C1=O	6	Excellent	6.3
2123	o1cc2c(CCC3C4(C(CCC23C)C(C)=C(O)C(=O)C4)C)c1	5.1	Excellent	6.3
2095	OC1CC2(C(CCC(=C)C(O)CC=C1C)C(CC2)=C(C)C)C	5.3	Excellent	6.3
2017	O1CC(C(C(=C)C2CCC3C2(CCCC3(C)C)C)COC(=O)C)C(O)C1=O	6.3	Good	6.3
2016	O1CC(CC(OC)=O)C(C(=C)C2CCC3C2(CCCC3(C)C)C)C1=O	5.7	Excellent	6.3
1978	O1C23CC(CCC(=O)C(C)C)(C)C1(O)CCC2(COC(=O)C)C(O)CCC3=C	4.2	Excellent	6.3
1854	O(C)C1C=C2C(CCC3(C2CCC3C(C=CC(C(C)C)C)C)C)C2(CCC(O)CC12O)C	5.2	OK	6.3
1668	O=C1c2c(cccc2NC=O)C(C2C1=CC(CC2)(C=C)C)(C)C	3.7	Excellent	6.3
1649	O1C(O)(CC=C(C(O)CC=C(C)C)C)C2(C(CCC2)=C(C)C1=O)C	4.7	Good	6.3
1600	O1C(C2C3(CC=C4C(CCC5C(C)(C)C(O)CCC45C)C3(CC2=O)C)C1=O)(CC(=O)CC(C)C)C	5.6	Good	6.3
1599	O1C(CC)C(C)C(=O)C(C)=C1C(C)C=1OC(CC)=C(C)C(=O)C=1C	4.8	Excellent	6.3
1548	S(C)c1c(c2Nc3c(-c4c2c(ncc4)c1OC)cccc3)CCNC(=O)C	4.2	Excellent	6.3
1486	O(C(=O)C)C1C2(CCCC(=C)C2(O)CC2(C(C1OC(=O)C)=C(CC2)C(C)C)C)C	4.6	OK	6.3
1423	OC(=O)c1c2nc3c(nc2ccc1)c(ccc3)C(=O)C	5.4	Excellent	6.3
1288	O1C(O)C2=C(C3C(C3)C(CC(OC(=O)C)C2C(CCC=C(C)C)C)C)C1O	5.1	Poor	6.3

1286	OC1=C(C)C(=O)C2=C(C1=O)C(CCC2C(CC(O)C=C(C)C)C)C	5.5	Good	6.3
1124	O1CC(C(CO)C(O)C1=O)C1(C2C(CC1)C(CCCC2=C)(C)C)C	5.5	Excellent	6.3
945	O(C)C1=CC(=O)C(O)=C(CC2(C3CCCC(C)(C)C3(O)CCC2C)C)C1=O	5.3	Excellent	6.3
655	O(C)c1cc2c(c(CCC)c1C(OC)=O)c(O)c1c(c2)C(C)(C)C(=O)C(CCC(=O)C)(C)C1=O	4.1	Bad	6.3
86	OC1CC2=CCC3C4CCC(C(O)C)C4(CCC3C2(CC1)C)C	4.2	Good	6.3
14462	O1C2C=C(CCC(C(C)=C)C(O)c3oc(cc3C)C2C(C)=C)C1=O	3.9	Excellent	6.2
14441	OC1C2C3C(CCC2(CC(=O)C(=C1)COC(=O)C)C)(CCC3C(C)=C)C	6.3	Excellent	6.2
14436	O1C(C2(C=C(C3OC3(C)C2C(=CC(C(=O)CC)C)C)C)C)=C(C)C(=O)C(C)=C1OC	5.2	Excellent	6.2
14431	O1C(C2(C=C(C3OC3C2C(C(O)C(C(=O)CC)C)=C)C)C)=C(C)C(=O)C(C)=C1OC			6.2
14347	O(C(=O)C)C1CC2C(C3CC=C(CC13C)C=O)(CCC1C(CCCC12C)(C)C)C	5.7	Bad	6.2
14071	O1CC2(CC2C=C(CCC=C(C)C)C)C2C(C(=CC2)C=O)C1=O	4	OK	6.2
13911	O1OC(CCC1(CCC=1C(CCCC=1C)(C)C)C)C(C(OC)=O)C	4.8	Excellent	6.2
13560	O1C(OC)C(C2C(C(CC(O)C=C(CC2)C)=C)C1OC)=CC=CC(C)C	5.2	Excellent	6.2
13446	O(C(=O)C=CC(O)(C)C)C1C=C(CCC(O)C(CCC1C(=O)C)=C)C	4.2	Poor	6.2
13237	O1c2c(cc(O)cc2C)CCC1(CCC=C(CCC=C(C=O)C)C)C	4.2	Bad	6.2
13221	O1C(O)C2=C(C3C(C3)C(CC(OC(=O)C)C2C(CCC=C(C)C)C)C)C1=O	3.9	Poor	6.2
13220	O1C(O)C2=C(C3C(C3)C(CC(O)C2C(CCC=C(C)C)C)C)C1=O	4.9	OK	6.2
13208	O1C=C2C(C3(C(CC2OC(=O)C)C(CCC3)(C)C)C)C1OC(=O)C	5.3	Good	6.2
13205	O1C2CC3C4(C(CCC3(C3CC=C(C(C23C)C1=O)C(O)C)C)C(CCC4)(C)C)COC(=O)C	4.6	Poor	6.2
13195	O1C2CCC3(C1)C(C=O)C(CCC23C)C(=CC=CC(O)(C)C)C=O	5.7	Poor	6.2
13188	O1C2C(CC=C(CCC=C(CCC=C(C2)C)C)CO)C(=C)C1=O	4.6	Excellent	6.2
13122	O1CC23C(CCC2C2C(CC3)C3(C(=CC(=O)C=C3)CC2)C)C(C)C1(O)CCC(C)C	4.3	OK	6.2
13070	OC1CC2C3C(CCC2(C)C1C(O)(CCCC(C)C)C)C1(C(=CC(=O)CC1)CC3)C	4.8	OK	6.2
13034	BrC1CCC(C)(C1(C)C)C1=CC2(O)C(CC1=O)(C)C(Br)CCC2(O)C	4.4	Excellent	6.2
12878	O1C2C=C(CCC=C(CCC(O)C1(CCC2C1(OC1)C)C)C)C	4.9	Excellent	6.2
12877	O1C2C=C(CCC=C(CCC(OC(=O)C)C1(CCC2C1(OC1)C)C)C)C	4.8	Excellent	6.2
12839	O1C(O)C(=CC1=O)C=CC=C(CCC1(C2CCCC(=C)C2(CCC1C)C)C)C	3.8	Bad	6.2
12772	O(C(=O)C)C1CC(=O)C(C2C(C=O)C(O)CC2C(=CCC=C(C)C)C)C1C	5	Good	6.2
12627	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)CO)C(=CC1=O)CO	5.5	Bad	6.2
12447	O(C)c1c(OC)c2c(cc1OC)C(=O)c1c(C2=O)c(O)cc(c1)C	5.5	Good	6.2
12065	O1C(CCC1C(NC=O)(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(CC1)(C#N)C	4.1	Poor	6.2
12035	[NH+](C1(C2C3C(C(CC(C3CC1)C)CC([NH+]=[CH-])(C)C)C(CC2)=C)C)=[CH-]	4.8	OK	6.2
12011	OC1C(=O)C(=CC=C(CCCC(CO)C(=O)CCC1C)C)C(C)C	4.7	Excellent	6.2
11866	O(C(=O)c1c2nc3c(nc2ccc1)c(ccc3)C(O)C)C	4.7	Excellent	6.2
11865	O(C(C)c1c2nc3c(nc2ccc1)c(ccc3)C(OC)=O)C	5.6	Good	6.2
11808	O1C(OC)c2c(ccc(C3(CC(CCC3)(C)C)C)c2C(C(O)=O)C)C1OC	5.7	Good	6.2
11807	O1C(OC)c2c(ccc(C3(CC(CCC3)(C)C)C)c2C(C(O)=O)C)C1OC	5.9	OK	6.2
11781	OC1C2CC(O)CCC2(C=2C(C3CCC(=C(CC(=O)CC(C)C)C)C3(CC=2)C)C1)C	3.8	Bad	6.2
11774	OC1C2CC(O)CCC2(C=2C(C3CCC(=C(CC(=O)CC(C)C)C)C3(CC=2)C)C1)C	4.3	Bad	6.2
11704	O(C(=O)C)C1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	5.2	Poor	6.2
11703	O(C(=O)C)C1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	4.1	Poor	6.2
11593	n1c2c(n(C)c1N)C1=NC(=NC1=CC=C2C)NC	5.9	Excellent	6.2
11514	O(C(=O)C(NC(=O)c1ccccc1)CCCNC(=O)c1ccccc1)C	4.9	Good	6.2
11492	O1CC(C2C(C(CC(O)C=C(CC2)C)=C)C1=O)=CC=CC(O)(C)C	5.3	Excellent	6.2
11048	O1C2=CC(=O)C=3NC(CC(OC)C=3C2=Nc2c1cccc2)C	4.6	Excellent	6.2
11036	O(C(=O)C)C1CC(=C)C(COC(=O)C)C(CCC(=C1)C)C(=CC=CC(O)(C)C)COC(=O)C	5.4	Poor	6.2
10848	o1c2c(cc1)C(O)CC1C2(C)C(OC(=O)C)CC2C1(CCC1C(CCCC12C)(C)C)C	4.9	Poor	6.2

10799	O(C(=O)C)C1CC2=CCC3C4CCC(C(CCC(OC)=O)C)C4(CCC3C2(CC1)C)C	3.7	Bad	6.2
10757	OC1CC2C3C(CCC2(CC1(C=O)C)C)(C)C(=O)C=C3C(C)C	5.3	Excellent	6.2
10650	O1C(O)C(=CC1=O)CCCC(=CC=CC(CCC=C(CC(O)C(OC)=O)C)C)C	5.1	Bad	6.2
10462	O(C(=O)C)C1CC2C(CCC3(C2CCC3C(CCCC(C)C)C)C)C2(CCC(O)CC12O)C	5.4	OK	6.2
10181	O(C(CO)CO)C(=O)CC(CCC1(C=2C(CCC1C)C(CCC=2)(C)C)C)C	4.3	Good	6.2
10072	[nH]1c2C3=NC(=NC3=C(C=Cc2nc1N(C)C)C)NC	5	Excellent	6.2
9630	O(C(=O)C)C1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	5.5	Bad	6.2
9291	O1OC(CCC1(CCC1(C=2C(CCC1C)C(CCC=2)(C)C)C)C)C(C(O)=O)C	5.4	Bad	6.2
9200	OC1C=C(C2C3CCC(O)(C=CC3(CCC12C)C)C)C(C)C	5.2	Excellent	6.2
9187	O1C2CC3(CC(O)C4(C(C3CCC12C)C(=CC4O)C(C)C)C)C	5.2	Excellent	6.2
9181	Oc1c2c(cc(c1)C)C(=O)c1c(C2=O)c(O)ccc1	5.5	Poor	6.2
9166	O1c2c(cc(OC)c(O)c2)C(OC)C2C3(C(CCC12C)C(CCC3)(C)C)C	5.6	Bad	6.2
9045	O(C(=O)C)C1CC2C3C(CCC2(C)C1C(O)(CCCC(C)C)C)C1(C(=CC(=O)CC1)CC3)C	4	Poor	6.2
8580	OC1CC2C3C(CCC2(C)C1C(O)(CCCC(C)C)C)C1(C(=CC(=O)CC1)CC3)C	4.7	OK	6.2
8541	O1C2=CC3(C(CC2=C(C)C1=O)C(=CC=C3)COC(=O)C)C	5.7	Excellent	6.2
8536	O1C2CC3(C(CC2=C(C)C1=O)C(=CC=C3)COC(=O)C)C	5.5	Excellent	6.2
8526	O(C)c1c2c(cc(C)c1O)cc1c(c2)C(=O)C(=O)C=C1	5.9	Excellent	6.2
8463	O1OC(CCC1(CCC1(O)C(CCCC1=C)(C)C)C)C(C(OC)=O)C	5.1	Excellent	6.2
8293	o1cc(cc1)CCCC(=CC(=O)CC(=CCCc1ccoc1)C)C	4.8	Good	6.2
8267	OC1CC2CCC3C4CCC(C(CCC(O)=O)C)C4(CCC3C2(CC1)C)C	4.5	Bad	6.2
8011	O1CC12C1(C3(OC3C2=O)C(O)C2C1C(OC(=O)C(O)CCCCCC)C(C2)(C)C)C			6.2
7939	O1C2C(CCC(=C)C(=O)CCC(=C2)C)C(=C)C1=O	5.5	Excellent	6.2
7847	O1C2C(C(=C)C1=O)C(OC(=O)C)CC(=CC(OC(=O)C)CC(=CC(O)CC(=C2)C)C)C	5.2	Poor	6.2
7590	O=C1N2C(=CCC2)C(=O)NC1Cc1c2c([nH]c1)cccc2	4.6	Excellent	6.2
7543	BrC1=C(C(OC1=O)=Cc1cc(Br)c(O)cc1)c1cc(Cl)c(O)cc1	5.8	Excellent	6.2
7458	O=C1CC23C(CCC1(C2)C)C1(C(CC3)C(CCC1)(C(O)=O)C)C	5.5	Good	6.2
7371	O1C2CCC(=C)C(C(OC)=O)C(CCC12C)C(=CC=CC(O)(C)C)COC(=O)C	5.7	Poor	6.2
7295	O(C(=O)C)C1CC2C(C3(C)C1(O)CC=CC3=O)C(O)CC1(C2CCC1C(CCC(C(C)C)C)C)C	6.3	Good	6.2
7082	[NH+](C1(C2C3C(C(CC(C3CC1)C)CC([NH+]=[CH-])(C)C)C(CC2)=C)C)=[CH-]	4.4	Good	6.2
6893	O1C2(OC)C(C3C(C(OC(=O)C)CC3C(=CCC=C(C)C)C)C1OC)C(C)C(OC)C2	5.5	Good	6.2
6600	O1C2(O)C3CC(CCC2=CC1=O)(C)C(=C)C(C3)C	4.5	Excellent	6.2
6570	O1C(=CC(N)=C(C=O)C1=O)C1C2C(CC(O)CC2)C=CC1C	5.4	Excellent	6.2
6569	O1C(=CC(N)=C(C=O)C1=O)C1C2C(CC(O)CC2)C=CC1C	6.4	Excellent	6.2
6450	o1c2c(cc1)C(=O)CC1C2(C)C(O)CC2C1(CCC1C(CCCC12C)(C)C)C	4.3	Poor	6.2
6366	O1C=C(COC(=O)C)C(C2(CCC3C(CCCC3(C)C)(C)C2C=O)C)C1OC(=O)C	5.1	OK	6.2
6311	S(CCN(C)C)C=1C=C(O)C2=NCCc3c2c(nc2c3cc(O)cc2)C=1	3.8	Excellent	6.2
6135	O1C(O)C(=CC1=O)C(O)CC1(C=2C(CCC1C)C(CCC=2)(CCCC(C)=C)C)C	4.3	OK	6.2
6129	O1OC(CCC1(CCC1C(CCCC1=C)(C)C)C)C(C(O)=O)C	4.8	OK	6.2
6060	O(C)c1cc(O)c2c(c1)C(=O)c1c(C2=O)c(O)cc(c1)COC(=O)C	6.6	Good	6.2
5760	o1c2c(CCCC2(CC(=O)CC(=CCCc2ccoc2)C)C)cc1	4.6	Excellent	6.2
5557	O(C(=O)C)C1CC2C(C3CC=C(C=O)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	4.8	Good	6.2
5437	o1cc(cc1CC(CCCc1cc(oc1)C=C(C(O)=O)C)C)CCCc1ccoc1	5.1	Bad	6.2
5417	O(C)C1C(O)(c2c(NC1=O)cccc2)c1ccc(OC)cc1	4.6	OK	6.2
5311	Oc1ccc(cc1)CC1N(C(=O)C=C(OC)CCNC(=O)CCCCC(C)(C)C)C(=O)C=C1	7.1	Poor	6.2
5097	O=C1N2C(CC3(c4c(NC23)cccc4)C(C=C)(C)C)C(=O)NC1=Cc1n(cnc1)CC	4.3	Poor	6.2
5096	O(C(=O)c1[nH]ccc1)CC1=CCCC2C(CCC(O)(C=C)C)(C)C(CCC12C)C	4	Bad	6.2

4931	O1CC(C2CC(O)(C(=O)CCCCCCC)C(O)(C3C2C2OC3CC(CCCC12C)=C)C)C	5	Poor	6.2
4841	O(C)c1ccc(O)c(O)c1CC=1C2(C(CCC=1C)C(CCC2)(C)C)C	4.9	OK	6.2
4828	O(C(=O)CC(CCC1(C=2C(CCC1C)C(CCC=2)(C)C)C)C)CC(O)CO	4.9	Bad	6.2
4815	O1C2(CCC=C(CCC(CC=C(CCC2O)C)C(C)=C)C1=O)C	5	OK	6.2
4798	O1C23CC(O)CCC2(C)C(=O)C(=CC13)C1CCC(C(C=CCC(C)C)C)C1(CCO)C	4.8	Poor	6.2
4677	O(C(=O)C)C1CCC(C2CC=C(C(=O)C)C(C=O)C12C)(C(CC=C(CC)C)C)C	4.5	Bad	6.2
4550	O(C)c1ccc(O)c(O)c1CC=1C2(C(CCC=1C)C(CCC2)(C)C)C	5.8	Good	6.2
4517	OC1(CCC=C(CC(=O)C(CCC(C=C1)C(C)C)(CO)C)C)C	6.1	Excellent	6.2
4375	o1c(ccc1COC)-c1nc(cc2c1[nH]c1c2cccc1)C(O)=O	6.8	Good	6.2
4317	O(C(=O)C)C1CC=C(C)C(=O)CC2C(CCC2(O)C(C)C)(CC=C1C)C	4	Excellent	6.2
4158	O1c2c(cc(O)cc2)C=CC1(CCc1c(C)c(CO)c(OC)cc1C)C	4.9	Poor	6.2
4087	Clc1c([nH]cc1Cl)-c1oc(-c2ccc(O)cc2)c(Cl)n1	4.9	Poor	6.2
3964	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	5.2	Good	6.2
3947	O1C(CC=C(CCC=C(CCC(=O)C(CCCC(=O)C)(C)C)C)C1O)C1=CC(OC1O)=O	4.2	Bad	6.2
3906	O1C2(CCC1(C=CC(O)(CCC=C(CCC2O)C)C)C(C)C)C	5.8	Excellent	6.2
3843	O1c2c(c(cc(OC)c2)C)C(=O)c2c1cc(OC)cc2O	5	Poor	6.2
3747	O1CC=2C(C3(C(CC=2)C2(C(CC3OC(=O)C)C3(C(C(CCC3)(C)C)C(=O)C2)C)C)C)C1O	4.3	OK	6.2
3719	OC(=O)C(CC1C(CCC2C1(CCC1C(CCCC12C)(C)C)C)(C=O)C)C	5.5	Good	6.2
3697	O(C(=O)C1C2(C(CC=C1C)C1(C(CC2)C(CCC1)(C)C)C)C)CC(O)COC(=O)C	4.7	Bad	6.2
3652	OC1CCC2C3C(CCC12C)C1(C(=CC(=NO)CC1)CC3)C	4.2	Poor	6.2
3651	OC1CCC2C3C(CCC12C)C1(C(=CC(=NO)CC1)CC3)C	5	OK	6.2
3619	O=C1NCCCC1NC(=O)C=C(CCC1(C)C(CCC=C1C)C)C	5.4	Bad	6.2
3597	O1C2C3C(C1CC(=C)C(O)CCC2(O)C)C(CCC3C(C)C)=C	4.8	Excellent	6.2
3259	S(O)(=O)(=O)CCNC1=CC(=O)C(=CC1=O)CC1(C2CCC=C(C)C2(CCC1C)C)C	6.2	OK	6.2
3206	O1C2C1(CCC=C(CCC1(C)C(C(=CCC1C)C2=O)C=O)C)C	5.1	Excellent	6.2
3098	O1C2CC3C4(C(CCC3(C3CC(O)C(C(C23C)C1=O)C(=O)C)C)C(CCC4)(C)C)CO	3.6	Excellent	6.2
3060	O(C(C(=CC(OC(=O)C)OC(=O)C)C=O)CC=C(C#CC=C(C)C)C)C(=O)C	4.7	Good	6.2
2995	O1C(CC=C(CCC=C(CCC=2C(CCCC=2C)(C)C)C)CO)C(CC1=O)CO	4.6	Bad	6.2
2994	O1CC(=CC1=O)C(O)CC=C(CCC=C(CCC=1C(CCCC=1C)(C)C)C)CO	4.8	Poor	6.2
2815	O=C1CC2C(CCCC2(C)C)(C)C(CCC(CC(OCC(O)CO)=O)C)=C1C	4.5	Good	6.2
2631	Brc1cc(cc(Br)c1O)C1=CC(OC1=Cc1ccc(O)cc1)=O	5.7	Good	6.2
2515	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	5.6	Good	6.2
2426	OC12CC(O)CCC1(C1C(C3CCC(C(CCC(C(C)C)C)C)C3(CC1)C)CC2=O)C	4.4	Poor	6.2
2379	O1C(CCC1C(O)(C)C)(C)C1CCC(C2C(C1O)C(=CC2)C)=C	4.3	OK	6.2
2376	O1CC(C2C(C(=CCC=C(CC2O)C)C=O)C1=O)CCC=C(C)C	6.2	Excellent	6.2
2241	O1C2(C34OOC(CC3)(C=C4CC(C)C2(CC1C1(OOC(CC1)C(C(O)=O)C)C)C)C)C	5.1	Good	6.2
2091	O1C23C(CCC(C2)C)C2(C(C1(O)C(CC2)C(C)C)C(=C3)C(OC)=O)C	4.7	Good	6.2
1936	o1cc(c2CC3C(CCCC(=Cc12)C)(C)C(=O)C=CC3(O)C)C	5.2	OK	6.2
1665	Brc1cc2c3CCN4OCSCC(NC(=O)C)C4c3[nH]c2cc1	5.6	Good	6.2
1549	S(OC1CCC2(C(=CCC3C4CCC(C(=O)C)C4(CCC23)C)C1O)C)(O)(=O)=O	4.9	Poor	6.2
1263	O1C(OC(=O)C)C2C(CCC(C(C)=C3CCCC3(C)C)C2(C)C)C1OC(=O)C	5.1	OK	6.2
1003	O=C1NC(Cc2c3c([nH]c2)c(ccc3N(C)C1C(C)C)C(CCC=C(C)C)(C=C)C)COC	4.5	Bad	6.2
982	O1c2c(C=CC1(CCC1(CCCC(C)C1=C)C)C)c(O)c(OC)cc2OC	4.1	Excellent	6.2
928	O1C2C3C(CC2C1=O)=C(CCC3COC(=O)CC(C)C)C1(CC(CCC1)(C)C)C	6.2	Good	6.2
752	o1cc2c(CCC3C4(C(CCC23C)C(CO)(C)C(=O)C(O)C4)C)c1	4.7	OK	6.2
667	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C(N=C=S)(CC1)C	4.8	Excellent	6.2

566	O1C2CC(c3cc(O)c(cc3C2=C(C)C1=O)C)C	5.9	Excellent	6.2
267	O1C2(O)C(C)C3(OC1(CC)C(C(O3)C2C)C)C(C(O)C(=CC(=CCC)C)C)C	4.8	Good	6.2
253	O1C23CC(CCC(=O)C(C)C)(C)C1(O)CCC2(C)C(OC(=O)C)CCC3=C	5.6	Poor	6.2
218	O1C2CC=C(C1CC1=CCC(C(C)C)C1(CC(=O)C2(O)C)C)C	4	OK	6.2
17	O1C(C(C(=O)C(C)C=2OC(CC)=C(C)C(=O)C=2C)C)=C(C)C(=O)C(C)=C1CC(C)C	4.6	Bad	6.2
14322	o1c2c(CCC3C4(C(CCC23C)C(CCC4)(C)C)C(O)=O)cc1	5.2	Excellent	6.1
14289	BrC1CCC(O)(C2C3C4(CC(O)C3CC4C(C)C)CCC12C)C	5.5	Good	6.1
14160	BrC1CCC2(C(CC(O)C3C2=CCC(C3)(C(Br)CO)C)C1(C)C)C	5	OK	6.1
14098	O(C(C)c1c2nc3c(nc2ccc1)c(ccc3)C(O)=O)C(=O)CO	5.6	Excellent	6.1
14097	OC(C)c1c2nc3c(nc2ccc1)c(ccc3)C(O)=O	4.8	Excellent	6.1
14081	N1C=2C(N=C1N)=C(C=CC1=NC(=NC1=2)N(C)C)C	4.7	Bad	6.1
14010	OC1C2CCC3C4CCC(C=C)C4(CCC3C2(CCC1O)C)C	4.1	Excellent	6.1
13951	O1OC(CCC1(CCC=1C(CCCC=1C)(C)C)C)C(C(O)=O)C	5.1	Good	6.1
13848	O(C(=O)C)C1Cc2c(C1(O)C)c(ccc2C=O)C=C(C)C	6.6	Excellent	6.1
13733	OC1C2(C3CCC(=C)C(C(OC)=O)C3(CCC2C(CC1O)(C)C)C)C	5.4	OK	6.1
13634	OC1CC2CCC3C4CCC(C=C)C4(CCC3C2(CC1)CO)C	4.5	Bad	6.1
13617	O(C(=O)C)C1C(=CC2(C(=CC(=O)CC2C)CCC1=O)C)C	4.5	Good	6.1
13567	O=C1NC(N(C)C1CC(CC)C)C(=O)c1c2c([nH]c1)cccc2	5.5	Poor	6.1
13311	O1c2c(cc(O)cc2C)C=CC1(CCC=C(C=O)C)C	5.6	Excellent	6.1
13291	O1C2C1(CC1C3(C(CCC1=C)C(CCC3)(C)C)C)C(=O)C=C(CO)C2O	4.8	Excellent	6.1
13206	o1cc(cc1)CCC=C(CC=CC(O)(CC=Cc1ccoc1)C)C	5.1	Excellent	6.1
13194	O(C(=O)C)c1ccc(O)c(CC2C3(C(CC=C2C)C(CCC3)(C)C)C)c1O	4.1	Poor	6.1
13117	O1C2(O)C(C3CCC(C(C=CC(C(C)C)CC)C)C3(CC2)C)=CC1=O	4.3	Bad	6.1
13116	O1C2(O)C(C3CCC(C(C=CC(C(C)C)C)C)C3(CC2)C)=CC1=O	4.6	Excellent	6.1
13002	O1C2=CC(O)(C)C3(O)C(CC2=C(C)C1=O)C(CC3)=C	5.3	Excellent	6.1
13001	O1C2=CC(O)(C)C3(O)C(CC2=C(C)C1=O)C(CC3)=C	6.2	Excellent	6.1
12975	O(C(=O)C)C1C2C(CCC(C1CC=C2C=O)=C)C(CCC=C(C)C)C			6.1
12935	BrC(CO)C1(CC2C(=CC1)C1(C(CC2O)C2(C(C2)C(OC(=O)C)C1)C)C)C	5.1	OK	6.1
12785	O(C(=O)C)C1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)CO	5.7	Poor	6.1
12779	OC12C(C3C1(C)C(O)CC3C(=CCC=C(C)C)C)C(CC2)C	5.2	Excellent	6.1
12736	Brc1cc(OC)c2[nH]ccc2c1-c1c2cc(Br)ccc2[nH]c1Br	5.2	Excellent	6.1
12616	Oc1cc(O)ccc1C=CC(OCC1C2(C(CCC1=C)C(CCC2)(C)C)C)=O	4.6	Bad	6.1
12437	O1C=CC(=C)C1OC(=O)C=C(CCC=C(Cc1occ(c1)C)C)C	3.9	Poor	6.1
12314	OC1CC(C2C3C(CCC3C)C12C)C(CCC(O)C(C)=C)=C	4.8	Good	6.1
12284	O(C(=O)C)C1CC2=CCC3C4CCC(C(O)C)C4(CCC3C2(CC1)C)C	4.4	Poor	6.1
12002	O(C(=O)C)C1CC2C(C3CCC(C(CCC(=O)C(C)C)C)C13C)CCC1=CC(=O)CCC12C	4.8	Bad	6.1
11958	O1C2CCC(C3C(CCC12C)C(C3)(CCC(OC(=O)C)C(O)(C)C)C)=C	4.8	Excellent	6.1
11505	o1cc(cc1)C(O)CC1C(CC2C1(CCC1C(CCCC12C)(C=O)C)C)(C=O)C	5.7	Poor	6.1
11477	O1CC23C(CCC4(C5Cc6cc(OC)ccc6OC5(CCC24)C)C)C(CCC3)(C)C1=O	4	Bad	6.1
11450	O(C)c1cc(cc(OC)c1O)Cc1n(C)c(nc1Cc1ccc(OC)cc1)N	5.1	Excellent	6.1
11215	o1cc(cc1)CCCC(CC1CC2(C(CCC1=C)C(CCC2)(CO)C)C)CO	5.8	Poor	6.1
11077	O1C2C3C(C1CC(=CCCC2(O)C)C)C(O)(CCC3C(C)C)C	4.4	Excellent	6.1
11052	O1C2=C(CC1C(O)(C)C)C(=O)c1c(cccc1)C2=O	4.7	Poor	6.1
11001	O1C(C2(C=C(C3OC3(C)C2C(=CCC)C)C)C)=C(C)C(=O)C(C)=C1OC	5.2	Excellent	6.1
10907	O1c2c(cc(O)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C)C)CO)C	5	Bad	6.1
10783	OC1CC2CC(C3C(C4CCC(C(O)(C(OC(=O)C)C=CC)C)C4(CC3)C)=CC2=O)=CC1	3.9	Poor	6.1
10649	O1C(=O)C(=CC1CC(=CCCc1ccoc1)C)CC=Cc1ccoc1	6.2	Excellent	6.1

10136	O=C(c1nccc2c1[nH]c1c2cccc1)c1[nH]cnc1	4.6	Excellent	6.1
9833	O(C(=O)c1ccccc1[NH+]1C=Cc2c([nH]c3c2cccc3)[CH-]1)C	4.4	Good	6.1
9560	O1c2c(cc(O)cc2C)CC2C3(C(CCC12C)C1(C(CC3)C(C)(C)C(O)CC1)C)C	4.8	Bad	6.1
9509	O(C)c1cc(O)c2c(c1)C(=O)c1c(C2=O)c(O)cc(c1)C	6.4	Poor	6.1
9478	O(C)c1cc(C)c(CCC(=CCC2=CC(=O)C=CC2=O)C)c(C)c1C	4.5	Poor	6.1
9357	O1C(CC(O)CC=CC(OC(CC=CC1=O)C)=O)C	5.2	Excellent	6.1
9151	O=C1CCC2C(CCC3(C2CCC3C=C)C)C1(CCC(OC)=O)C	5.1	OK	6.1
9146	O1CC(C2C(C(CCC=C(CC2)C)=C)C1O)=CC=CC(O)(C)C	5.3	Excellent	6.1
9124	O(C)c1c2c(cc(C)c1O)C(=O)c1c(C2=O)c(O)ccc1	4.6	Excellent	6.1
8992	O1C23CC(O)CCC2(C)C(=O)C(CC13)C1CCC(C(CCC(C)C)C)C)C1(CCO)C	4.6	Good	6.1
8640	O(C)C1CC2=CCC3C4CCC(O)(C(=O)C)C4(CCC3C2(CC1)C)C	3.9	Poor	6.1
8584	O(C(=O)C)C1CC2=CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	4.2	Bad	6.1
8539	O1C(=O)C(=C2CC3C(CC12O)(C=CC=C3C)C)C	4.9	Good	6.1
8538	O1C(=O)C(=C2CC3C(CC12O)(C=CC=C3COC(=O)C)C)C	5.7	Excellent	6.1
8500	OC12CC3(C(CC1)C1(C(CC3)C(CCC1)(CO)C)C)CC2=C	3.5	Excellent	6.1
8356	O(C(=O)C)C1CC2=CCC3C4CCC(C(CCC(OC)=O)C)C4(CCC3C2(CC1)C)C	3.7	Bad	6.1
8292	o1cc(cc1)CCCC(=CC(=O)CC(=CCCc1ccoc1)C)C	5.5	Good	6.1
8097	O(C(=O)C)C1CC2=CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	4.1	Excellent	6.1
8095	O(C(=O)C)C1CC2=CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	4.2	Bad	6.1
8094	O(C)c1c2c(cc(OC)c1O)C(=O)c1c(C2=O)c(O)cc(c1)C	5.2	OK	6.1
8063	O=C(NN=C(CCc1ccccc1)c1ccccc1)N	5.5	Bad	6.1
7913	O1C(=O)C(=C2CC3(C(CC12OC)C(OC(=O)C)CCC3C)C)C	4.9	Good	6.1
7900	BrC1C2C(CCC2(O)C)C(C)(C)C1C(=C)C1CC(Br)C(O)(CC1)C	4.7	Good	6.1
7776	O1C2C1(CC=C(CCC=C(CCC=C(C)C)C)C)C(=O)C=C(CO)C2O	4	Excellent	6.1
7562	O([N+](=O)[O-])C(CO)c1c(c2CC(Cc2cc1C)(C)C)C	5.1	OK	6.1
7559	O=C1c2c(CC1(C)C)c(C)c(CCO[N+](=O)[O-])c(c2)C	4.8	Good	6.1
7541	Brc1cc(cc(Br)c1O)C=C1OC(=O)C(Cl)=C1c1ccc(O)cc1	5.3	OK	6.1
7420	O(C(=O)C)C1C(C)=C(CCC(=CCO)C)C2(C(C1OC(=O)C)C(CCC2)(C)C)C	4.9	OK	6.1
7076	O1C2(O)C3=C(C(CCC3C(CC(C=C(C)C)C2(O)C)C)C)C1=O	6.1	Excellent	6.1
6983	O(C(=O)C)C1CC(C2C3C(CCC3C)C12C)C(CC(O)C=C(C)C)=C	4.6	OK	6.1
6965	Brc1cc2n(cc(S(=O)(=O)c3c4c([nH]c3)cc(Br)cc4)c2cc1)C(O)=O	5	Poor	6.1
6842	OC(CO)C1(CC=2C(CC1)C1(C(CC=2)C(CCC1)(C)C)C)C	4.2	Bad	6.1
6618	O1C2C=C(C(C)C)C(=O)C(O)C(CCC(=O)C(=CCCC12C)CO)C	5.2	Excellent	6.1
6567	OC1(CCC2C(CCC3C(CCCC23C)(C)C)(C)C1C(OCC(OC(=O)C)CO)=O)C	4.7	Poor	6.1
6476	OC1(CCC2C(C1[NH+]=[CH-])C(CCC2([NH+]=[CH-])C)C(CCC=C(C)C)C)C	4.9	Excellent	6.1
6375	Brc1cc2[nH]cc(c2cc1)-c1nc(ncc1)N	4.2	OK	6.1
6247	O1C(CC2C3(C(CCC12COC(=O)C)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	4.5	Bad	6.1
6246	O1C(CC2C3(C(CCC12COC(=O)C)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	4.2	Bad	6.1
6192	O(C(=O)C)c1cc(ccc1O)CCC=CC=CC=CCCOC(=O)C	3.7	Bad	6.1
6169	O1C(CC=C(CC=CC(=CC(O)C)C)C)=C(C)C(=O)C(C)=C1OC	5	Good	6.1
6047	O1C23CC(O)CCC2(C)C(=O)C(=CC13)C1CCC(C(C=CC(C(C)C)C)C)C1(CC=O)C	3.8	Bad	6.1
6044	O1C2(C(C=C3C(=COC(=C3)C)C2O)=C(C(=O)CCCCCCC)C1=O)C	7.1	Excellent	6.1
5827	O=C1CC2C(C=C1CC(O)=O)CCC1C3(C(CCC12C)C(CCC3)(C)C)C	4.6	Bad	6.1
5797	OC1(C2C3C(CCC(O)(C2CC1)C)C3(CCC=C(C)C)C)C	5.8	Good	6.1
5748	O1CC(=CC1=O)CCC=C(CCC(O)C(CCC1(C)C(CC(=O)C=C1C)C)=C)C	5.5	OK	6.1
5691	O(C)c1c(O)c(ccc1OC)Cc1n(C)c(nc1Cc1ccc(OC)cc1)N	4.5	OK	6.1
5567	O(C(=O)C)C1CC2C(C3CC(O)C(=CC13C)C=O)(CCC1C(CCCC12C)(C)C)C	4.4	Excellent	6.1

5501	O1C23CC(OC(=O)C)CCC2(C)C(=O)C(=CC13)C1CCC(C(C=CC(C(C)C)C)C)C1(CC=O)C	5.1	Bad	6.1
5491	O1C(O)C(CCC1C(C)C)C1(O)CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)CC3)C	4.9	Poor	6.1
5489	O1C(O)C(CCC1C(C)C)C1(O)CCC2C3C(CCC12C)C1(C(=CC(=O)C=C1)CC3)C	4.2	Bad	6.1
5403	O(C(=O)C)C1CC(C)(C)C(=C=CC(=CC=CC(=O)C)C)C(O)(C1)C	5.3	Poor	6.1
5387	O1C(CC(CCC(CC(C)C(=O)N(C=CCC1=O)C)C)C)C(C)(C)C	4.6	Excellent	6.1
5350	O1C(O)C(=CC1=O)C(O)CC1(C2C(=CCC1C)C(CCC2)(CCCC(C)=C)C)C	3.9	Bad	6.1
5198	O(C(=O)C)C1CC2=CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	4.1	Bad	6.1
5103	O(C(=O)C)c1c2c(cccc2)c(OC(=O)C)cc1CC=C(C)C	3.9	Excellent	6.1
5009	O1C2C(C=C(C)C1C=CCCCCCCC)C1CC(O)CC1=CC2=O	4.3	Poor	6.1
4831	O1CC2C(CCC(O)(C=CCC2=C)C)C(=CC=CC(OC)(C)C)C1OC	5.3	Poor	6.1
4825	O1C2C(CC3OC(CCC3(OC)C)C(O)(CCCC(C)C2OC(=O)C)C)C(=C)C1=O	6.8	Good	6.1
4787	O(C(=O)C)C1CC(=O)C=C2CCC3C(C12C)C(O)CC1(C3CCC1C(=O)COC(=O)C)C	5.7	Poor	6.1
4775	O(C(=O)CO)C1CC2C(NC1C)CCCC2C=CC=CCCC(=O)C	3.6	OK	6.1
4719	O1C(CCC1=O)C=CC=C1C(OC(=O)C)(C=CC1=O)C=CCCCCCC	6.6	Good	6.1
4703	O1C2(O)C(C3CCC(C(C=CC(C(C)C)C)C)C3(CC2)C)=CC1=O	4	Bad	6.1
4683	O1C2C(CC3OC3(CCC(OC(=O)C)C(CCCC(C)C2OC(=O)C)=C)C)C(=C)C1=O	5.4	Poor	6.1
4539	O1C2C3C(C1CC(O)(C)C(O)CCC2(OC(=O)CCC)C)C(=C)C(OC(=O)C)CC3C(C)C	4.6	Good	6.1
4367	O(C)c1c2c(cc(OC)c1)C(=O)c1c(C2=O)c(O)cc(O)c1C(=O)CCC	6	OK	6.1
4360	o1c2c(CCC3C(CC(OC(=O)C)CC23C)(CO)C)cc1	4.8	Good	6.1
4206	ClC1CC(OC(=O)C)C(OC(CC1OC(=O)C)C(OC(=O)C)CC)CC=CC#C	4.9	OK	6.1
4199	S=C=NC(C)(C)C1OC(CC1)(C)C1C2C(CCC(=C2)C)C(CC1)(C#N)C	4.9	Poor	6.1
4159	Oc1ccc(O)cc1CC=C(CCC1C(CC(=O)C=C1C)(C)C)C	5	Bad	6.1
4154	O(C)C1=CC(C)(C)C(CCC(=CCc2cc(O)ccc2O)C)=C(C)C1=O	4.2	OK	6.1
3987	O1C(CC2C3(C(CCC12COC(=O)C)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	5.8	OK	6.1
3986	O1C(CC2C3(C(CCC12COC(=O)C)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	4.6	Good	6.1
3978	O1C2C1(CCC=C(CCC1(C)C(C(CCC1C)C2=O)C=O)C)C	5.5	Good	6.1
3935	O1C2C3C(C1CC(O)(C)C(OCC)CCC2(O)C)C(CCC3C(C)C)=C	4.6	Excellent	6.1
3739	O1C2CC(=CCC(OC)C3=C(C1NC3=O)C2C(CCC=C(C)C)C)C	5.7	Poor	6.1
3408	OC1C2C(C=CC2(O)C)C(CCC1C(CC(OC(=O)C)C=C(C)C)C)=C	5.4	OK	6.1
3265	O1C23CC(O)CCC2(C)C(=O)C(=CC13)C1CCC(C(CCCC(C)C)C)C1(CCO)C	5.2	Bad	6.1
2765	o1cc(cc1)C(O)CC1C(CC2C1(CCC1C(CCCC12C)(C)C)C)(C=O)C	5.3	OK	6.1
2698	O=C1C=C2CCC3C4CCC(C(O)(C=CCC(C)C)C)C4(CCC3C2(C=C1)C)CO	4.4	Good	6.1
2632	O1C(=Cc2ccc(O)cc2)C(=CC1=O)c1ccc(O)cc1	5.5	Excellent	6.1
2630	Brc1cc(cc(Br)c1O)C=C1OC(=O)C=C1c1ccc(O)cc1	5	OK	6.1
2435	O1C(CNCC1c1c2c([nH]c1)cccc2)c1cc(OC)c(OC)c(OC)c1	3.6	Poor	6.1
2418	O1C23C1C(O)C=1C4CCC(C(CCC(C(C)C)=C)C)C4(CCC=1C2(CCC(O)C3)C)C	4.8	Bad	6.1
2371	O1OC(CCC1(CCC1(C2CCCC(C)(C)C2(O)CCC1C)C)C)C(C(O)=O)C	6.3	Excellent	6.1
2359	O1C(CCC(C)C(O)CC1=O)C(C(=O)C(=CCC(O)C(C)C)C)C	4.9	Poor	6.1
2336	O1C2C(c3c(cc(OC)c(c3)CO)C(C)C2O)=C(C)C1=O	6.6	Excellent	6.1
2309	o1cc(c2-c(c1)c(cc2)C=O)CC(OC(=O)C)C=C(CCC=C(C)C)C	5.9	Poor	6.1
2116	O=C1c2c(cccc2)C(=O)C1=C(NN(C(=O)C)C(OCC)=O)C	4.8	Excellent	6.1
1524	O(C(=O)C)C1CC(C(=CCC=C(C)C)C)C(C2C(C=CC2=O)C)C1COC(=O)C	5.6	Bad	6.1
1212	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC([NH+]=[CH-])(C)C2O)C([NH+]=[CH-])(CC1)C	4.2	Good	6.1
1173	O1C2CC(=CCCC(C(C2C(CCC=C(C)C)C)C1=O)C=O)C			6.1
1101	O(C(=O)C)C1CC(C(CC=CC(O)(C)C)C)C(O)C2C(CC=C2C)C1=C	5.8	Poor	6.1
872	OC1C2C(CC=C2C)C(=C)C(O)CC1C(C(OC(=O)C)CC=C(C)C)C	5.8	Good	6.1

759	O1C2OC(=O)C3(CC4(C(C3)C(=CC=C4)COC(=O)C)C)C12C	5.3	Good	6.1
537	O=C1CC2C3(C(CCC2(C2CC=C(CC12C)C(=O)C)C)C(CCC3)(C)C)C(O)=O	6.1	Bad	6.1
521	O(C(=O)C)C1C(=CC2(C(=CC(OC(=O)C)CC2C)CCC1=O)C)C	4.7	Good	6.1
14301	O(C(=O)C1C2(C(CC=C1C)C(CCC2)(C)C)C)CC(O)COC(=O)C	4.1	OK	6
14183	Brc1cc(OC)c2[nH]cc(Br)c2c1-c1c2cc(Br)ccc2[nH]c1	4.5	Excellent	6
14073	O(CC=1CCC(C(CCC=C(CCC=C(C)C)C)C=O)C=1C=O)C(=O)C	3.7	Bad	6
14040	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	5.6	Good	6
13950	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	4.4	Good	6
13831	OC1C(C2CCC3(C(CC=C(C)C3C(OCCC)=O)C2(CC1O)C)C)(C)C	4.8	Excellent	6
13795	O1C(=CC(OC)=C(C=O)C1=O)C1C2C(CCCC2)C=CC1C	4.7	Excellent	6
13760	O1C2CCC(C3C(CCC12C)C(C3)(CCC(O)C(O)(C)C)C)=C	4.1	Poor	6
13709	O(CC=1CCC(C(CCC=C(CCC=C(C)C)C)C=O)C=1C=O)C(=O)C	4.1	Bad	6
13684	OC1C2C(CC=C2C)C(CCC1C(CCC(O)C(C)=C)C)=C	4.7	Good	6
13564	O1C(=O)C(C)=C(O)C(C)=C1C(=CC(CC(CC(CCC)C)C)C)C	4.9	Good	6
13523	O(C(=O)C)C1CC(C2C3C(CCC3C)C12C)C(=CC=CC(O)(COC(=O)C)C)COC(=O)C	4.9	Poor	6
13404	O1C2C3C(C(OC(=O)CCC)(CCC3C(C)C)C)C1(O)CC(=C)C(OC(=O)C)CCC2(O)C	5.6	Good	6
13400	O1c2c(cc(O)cc2C)CC2C3(C(CCC12C)C1(C(CC3)C(C)(C)C(O)CC1)C)C	4.4	Poor	6
13395	O1C2CC(O)C3C(CCC3C(O)(C)C)(C=CC(CCC12)C)C	5.2	Excellent	6
13256	OC1CC2=CCC(C3CCC(C(CCCC(C)C)C)C3(CCO)C)C(=O)C2(CC1)C	4	Bad	6
13209	O1C(OC(=O)C)C2C(=CCC3C(CCCC23C)(C)C)C1OC	5.3	OK	6
13203	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)CO)C)C)C1=O)C	4.4	OK	6
12993	O1CC2=C(C3C(C3)C(CC(O)C2C(CCC=C(C)C)C)C)C1=O	4.7	Good	6
12917	O(C)c1c(cc2c(c1OC)C(=O)c1c(cccc1O)C2=O)C	4.1	Excellent	6
12735	Brc1cc(OC)c2[nH]cc(Br)c2c1-c1c2cc(Br)ccc2[nH]c1	4.9	Excellent	6
12615	Oc1cc(ccc1O)C=CC(OCC1C2(C(CCC1=C)C(CCC2)(C)C)C)=O	4.9	Bad	6
12538	O1C(C2(C3C2(C=C(C)C3C(=CC(C(=O)CC)C)C)C)C)=C(C)C(=O)C(C)=C1OC	5.7	OK	6
12302	OC1CC(C2C3C(CCC3C)C12C)C(CC(O)C=C(C)C)=C	4.9	Excellent	6
12201	O(C(=O)C)C1CC(=CCC=C(C=O)C(C=O)C1C(CCC=C(C)C)C)C	5	Excellent	6
12152	O(C(=O)C)C1CC2C(C3CC=C(C(=O)C)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	5	Bad	6
12150	O1c2c(cc(O)cc2C)CC2C3(C(CCC12C)C1(C(CC3)C(C)(C)C(O)CC1)C)C	4.1	Poor	6
12128	O(C)c1c(O)c(CC=C(CCC=C(C)C)C)c(C)c(O)c1OC	4.8	OK	6
12095	O1C(CCC=C(CCC=C(CC(=O)C=C(C)C)C)C)(C)C1CO	3.1	Good	6
11685	O1C2C=3C(CCC2C(=C)C1=O)(C)C(O)CCC=3C	5.3	Excellent	6
11615	O(C(C(O)(C)C)CC=C(COC(=O)C)C1CC(C(C)=C)C(CC1)(C=C)C)C(=O)C	5.9	Good	6
11512	S(CC=1CCC2C(C=1)Cc1c(occ1)C2(C)C)C(=O)C	4.5	Poor	6
11442	O(C(C(C=COC(=O)C)=COC(=O)C)CC=C(C#CC=C(C)C)C)C(=O)C	4.2	Bad	6
11380	Brc1cc([NH+]2C=Cc3c([nH]c4c3cccc4)[CH-]2)c(cc1)C(OC)=O	4.4	OK	6
11222	O1C2CCC(C3C(CCC12C)C(C3)(C(=O)CCC(OC(=O)C)C)C)=C	4.8	Good	6
11049	O=C1N(C)C(=NC)N(C)C1=Cc1c2c([nH]c1)cccc2	4.3	OK	6
10837	O1C2CCC(=CC(O)C(CCC(=CCCC12C)C)C(C)=C)CO	4.4	Poor	6
10682	O(C(=O)C)C1C2C(CCC2C(O)(C)C)(C=CC(CC(OC(=O)C)C=C(C1)C)C)C	4	Good	6
10677	O(C(=O)C)C1C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC=CC(O)(C1)C)C)C	4.2	Excellent	6
10436	O1c2c(c(cc(c2)C)CO)C(=O)c2c1cccc2O	4.7	Excellent	6
10365	OC1C2C(CCC2C(O)(C)C)(C=CC(CCC=C(C1)C)C)C	4	Excellent	6
10330	O=C1N2NC(c3ccccc3)=C(C2=NC=C1C(OCC)=O)C	5.8	Good	6
9985	O(C)c1c(O)c(CC=C(CCC=C(C)C)C)c(C)c(O)c1OC	5	Excellent	6
9937	OC1CC2(CC(O)C3(C(C2C2CC12C=O)C(CC3)C(C)C)C)C	4.8	Excellent	6

9496	O1C2OC(=O)CC12CCCC(CC(O)CC(=CCCc1ccoc1)C)C	4.4	Poor	6
9403	O(C(=O)CN(CC(=O)NC1C2(C=C(CC2)C)C(CCC1C(C)C)C)C)C	5	OK	6
9283	O1C23C1C(O)C=1C(CCC4(C=1CCC4C(CCCC(C)C)C)C)C2(CCC(O)C3)C	5.5	OK	6
9063	O(C(C(C(O)CC=CC=CC(=O)N)C)C(CC)C)C(=O)C=Cc1ccccc1	4.6	Good	6
8724	o1cc(cc1Cc1ccoc1)CCC=C(CCCC(CC(O)=O)C)C	4.7	Poor	6
8705	O1CC2C(=CCC3C2(C)C(O)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	4.4	OK	6
8654	O=C1CC2C(CC(CCC2C)C(OC(=O)C)(C)C)=C1C	6	OK	6
8417	O1c2cc(C)c(O)cc2C=CC1(CCC=C(CC(=O)CC(C)C)C)C	4.2	Excellent	6
8412	O=C1C=C(C)C(=O)C=C1CC=C(CCCC(=CC(=O)CC(C)C)C)C	4.9	Poor	6
8299	O1c2c(c(cc(O)c2)C)C(=O)c2c1cc(OC)cc2O	5.8	Poor	6
8227	O1C(=O)C2C(=CCC3C(CCCC23C)(C)C)C1=O	5.4	Excellent	6
8226	O1C(=O)C2C(=CC(O)C3C(CCCC23C)(C)C)C1=O	4.8	Excellent	6
8224	O1C(=O)C2C(=CCC3C(C)(C)C(O)CCC23C)C1=O	4.6	Excellent	6
8132	O1c2c(cc(O)cc2C)CC2C3(C(CCC12C)C1(C(CC3)C(C)(C)C(O)CC1)C)C	4.5	Poor	6
8104	O1CC2C(CCC(=CCCC2=C)C)C(CC=CC(O)(C)C)C1=O	3.6	Excellent	6
8093	O(C)c1c2c(cc(OC)c1)C(=O)c1c(C2=O)c(O)cc(c1)CO	5.2	Excellent	6
8065	O1C(=O)C(CC1C=C(CCCc1ccoc1)C)CCCc1ccoc1	4.6	Bad	6
7974	O(CC1=CCCC2C(CCC(O)(C=C)C)(C)C(CCC12C)C)C(=O)C	4.1	Bad	6
7965	O1C2CCC(O)(C)C(CC=C3C(C4C(CCC3C)C(O)(CC4)C)(C)C)C2(CCC(=O)C1(C)C)C	4.9	Poor	6
7869	OC1CC2C3C(CCC2(C)C1C(CCCC(C)C)C)C1(C(CC(=O)CC1)C(=O)C3)C	4.4	Poor	6
7566	O=C1c2c(CC1(C)C)c(CO)c(CCO[N+](=O)[O-])c(c2)C	4.4	Excellent	6
7542	Brc1cc(ccc1O)C=C1OC(=O)C(Cl)=C1c1ccc(O)cc1	5.6	Excellent	6
7372	O1CC(C2C(C(CCC(O)C(=CC2)C)=C)C1=O)=CC=CC(C)C	5.9	Good	6
7293	OC(=O)C1(C2CCC3(C(CCC(=C3)C=O)C2(CCC1)C)C)C	5.5	Excellent	6
7269	O1C2OC(=O)CC12CCC=C(CCC=C(CC(O)C=C(C)C)C)C	5.5	OK	6
7226	OC1CC2C3C(CCC2(C)C1C(O)(CCCC(C)C)C)C1(C(CC(=O)CC1)CC3)C	3.4	Bad	6
7091	O1CC(C2C(C(CCC=C(CC2)C)=C)C1=O)=CCC=C(CO)CO	5.4	Excellent	6
6814	O(C(=O)c1c2nc3c(nc2ccc1)c(ccc3)C(OC)=O)C	4.5	Good	6
6746	Oc1ccc(cc1)CC(NC(=O)C=CC(=CC(CCCCCC)C)C)C(OC)=O	5	Poor	6
6682	OC1CC2=CCC3C4CC(=O)C(C(O)(CCC(C(C)C)=C)C)C4(CCC3C2(CC1)C)C	4.4	Poor	6
6632	O1C(C2=C(C3(C(CC2)C2(C(CC3=O)C3(C(CC2)C(CCC3)(C)C)C)C)C)C1=O)C	3.7	Bad	6
6571	O1C(=CC(N)=C(C=O)C1=O)C1C2C(CCCC2)C=CC1C	4.7	Excellent	6
6559	O(C)c1c(cc(O)cc1C)CC=C(CC(=O)C=C(CCCC(=O)C)C)C	5.6	OK	6
6558	O(C)c1c(cc(O)cc1C)CC=C(CC(=O)C=C(CCCC(=O)C)C)C	5.5	Poor	6
6524	O1CC12C1OC3C=C(CCC3(COC(=O)C)C2(C)C(OC(=O)C)C1)C	5.8	Excellent	6
6475	S=C=NC1(C2C(C(CC1)C1(OC(CC1)C(C)=C)C)C([NH+]=[CH-])C(O)(CC2)C)C	4.4	OK	6
6437	BrC1CC(CCC1(O)C)C(=CC(O)C1C(C)=C(CCC1=C)C)C	5.5	Excellent	6
6386	O1C2(C3C(CC(C)C2(CC1C1(OOC(CC1)C(C(O)=O)C)C)C)C=C(CC3)C)C	4.6	Bad	6
6385	O1C2(C3C(CC(C)C2(CC1C1(OOC(CC1)C(C(O)=O)C)C)C)C=C(CC3)C)C	3.6	Bad	6
6291	OC1CC2(C(CC=C1C)C(CC2)C(O)(CCC=C(C)C)C)C	5.1	OK	6
6260	O(C(=O)C)C1C23C(CCC2(C=C(C(OC)=O)C3C)C)C(C1)C	4.6	Poor	6
6225	O1CC=2C(C3(C(C4C(CC3O)C3(C(CC4)C(C)(C)C(=O)CC3)C)CC=2)C)C1O	4.9	Good	6
6212	O1C(C2CCC3(C(CCc4c3coc4)C2(CC1=O)C)C)(CO)C	5.1	Good	6
6211	O1C(C2CCC3(C(CCc4c3coc4)C2(CC1=O)C)C)(CO)C	5	Excellent	6
5962	OC1C2C(C(C=CC=CC(O)=O)C(C(=CC)C)C(=C2)C)C(CC1)C	4.5	Poor	6
5820	O1C2(OC)C(=CC1=O)C(C1CC(=O)C(=CC1C2)C)(C)C	5	Excellent	6
5807	O1C(CC2C(CCC3C4(C(CCC23C)C(CCC4)(C)C)C)C1OC(=O)C)C1=CC(OC1O)=O	4.1	Bad	6

5779	O1C(CC=CCC=CCC=CCCCCC1=O)C(O)CC	5.1	Good	6
5667	O(C(=O)C)C1CC2C=3C(C(C=C(C)C)C(=O)C2C)C(CCC=3C1C)=C	4.4	Good	6
5629	o1cnc(C(O)=O)c1-c1c2c([nH]c1C(N(C)C)CC(CC)C)cccc2	5.2	Good	6
5526	O1C23CC(O)CCC2(C)C(=O)C(=CC13)C1CCC(C(CCCC(C)C)C)C1(CC=O)C	4.1	Poor	6
5502	O1C23CC(OC(=O)C)CCC2(C)C(=O)C(=CC13)C1CCC(C(C=CCC(C)C)C)C1(CC=O)C	6.3	Poor	6
5500	O1C23CC(OC(=O)C)CCC2(C)C(=O)C(=CC13)C1CCC(C(CCCC(C)C)C)C1(CC=O)C	5.5	Bad	6
5441	o1cc(cc1C=C(CCCc1cc(oc1)C(=O)NCCNC(=O)C)C)CCCc1ccoc1	4.7	Bad	6
5354	N1C=2C3C(CC(C)C=2C=CCC)CCC3N=C1N	4.2	Excellent	6
5298	O1C(CC=CCCC1=O)C1CC1C(O)C=CC(O)CC=CCC=CCC	4.1	Good	6
5285	O1C(CCCCCC1=O)C1CC1C=CC(O)C(O)CC=CCCCCC	4.5	Poor	6
5284	O1C(CC=CCCC1=O)C1CC1C(O)C=CC(O)CC=CCC=CCC	3.7	Bad	6
5180	O1C(C)(C)C1CC=C(C)C1C2C3C(=CCCC2CC1)COC3O	4.8	Excellent	6
5019	O1C2C(C=C(C)C1C=CCCCCCCC)C1CC(O)CC1=CC2=O	5.1	OK	6
5016	O1C2C(C=C(C)C1C=CCCCCCCC)C1CC(O)CC1=CC2O	3.4	Good	6
4875	O(C(COC(=O)C)COC(=O)C)C(=O)C=C(CCC=1C(CCCC=1C)(C)C)C	4.8	Bad	6
4868	O(C(C(C(O)CC=CC=CC(=O)N)C)C(CC)C)C(=O)C=Cc1ccccc1	4.7	Good	6
4857	O1CC2C(CCC(O)(C=CCC2=C)C)C1(C=CC=C(C)C)CO	4.5	Good	6
4799	O1C23CC(O)CCC2(C)C(=O)C(=CC13)C1CCC(C(C=CC(C(C)C)C)C)C1(CCO)C	4.9	Poor	6
4778	Brc1cc2n(c3c(c2cc1)ccnc3)Cc1nc[nH]c1SC	5.3	Excellent	6
4725	O1CC2C(CCC(O)(C=CCC2=C)C)C1(C=CC=C(C)C)CO	5.7	Good	6
4716	ClC1C(C2CC=C(C=O)C(C=O)C2(CC1O)C)(CCC(C(C)=C)C)C	5.8	Excellent	6
4711	O1C(CCC1=O)C=CC=C1C(OC(=O)C)(C=CC1=O)C=CCCCCCC	5	Good	6
4694	O1C2C(CC3OC3(CCC(OC(=O)C)C(CCCC(C)C2OC(=O)C)=C)C)C(=C)C1=O	4.5	Bad	6
4684	OC1C2C(C(C=CC=CC(O)=O)C(C(=CC)C)C(=C2)C)C(CC1)C	4.5	Bad	6
4510	O1C2C(C(C)C1(O)CCC(C)C)C1(C(C3C(CC1)C1(C(=CC(=O)C=C1)CC3)C)C2)C	5.3	OK	6
4423	O1C(CCCC1=O)C1CC1C=CC(O)C(O)CC=CCC=CCC	3.4	OK	6
4380	O1OC(CC1(CC(CCCCCCc1ccccc1)C)C)(CC(O)=O)C	5.7	Excellent	6
4362	O(C(=O)C)C1CC2(O)C(CC1)(C)C(=O)C(=CC2O)C1CCC(C(CCCC(C)C)C)C1(CC=O)C	4.7	Bad	6
4316	O(C(=O)C)C1CC=C(C)C(=O)CC2C(CCC2(O)C(C)C)(CC=C1C)C	5.4	Poor	6
4130	BrC1CCC2(C(CCC(=C)C2Cc2cc(O)c(cc2O)C=O)C1(C)C)C	5.2	Bad	6
4100	OC1(C2CCC(=CCCC(C=CC2(CC1)C)C)C)C(O)(C)C	4.6	Excellent	6
3780	O1C2C3C(C1CC(O)(C)C(OC)CCC2(OC(=O)C)C)C(OC(=O)C)(CCC3C(C)C)C	5.2	Poor	6
3752	S1(=O)(=O)C2=C(NCC1)C(=O)c1c(cc3c(c1)C1(C(=COC3=O)C(=CCC1)C)C)C2=O	5.9	OK	6
3748	OC1CC2C(C3CCC(C(CCC(OC)=O)C)C13C)C(O)CC1CC(=O)CCC12C	3.3	Bad	6
3670	O1C(CC=CC#C)C(OC(=O)C)CC(O)C(O)CC1C(OC(=O)C)CC	5.1	Excellent	6
3598	O(C(C(C=COC(=O)C)=COC(=O)C)CC(O)C(C#CC=C(C)C)=C)C(=O)C	3.9	Bad	6
3506	OC1CC2C(C3CCC(C(CCC(OC)=O)C)C13C)C(O)CC1CC(=O)CCC12C	3.7	Excellent	6
3476	O1C2(C3C(CC(C)C2(CC1C1(OOC(CC1)C(C(O)=O)C)C)C)C=C(CC3)C)C	5.3	OK	6
3302	O=C1CCC2(C3C(C4CCC(C(CCC(O)=O)C)C4(CC3)C)CCC2=C1)C	5.2	Bad	6
3257	O1c2c(cc(O)cc2C)CC2C3(C(CCC12C)C1(C(CC3)C(C)(C)C(O)CC1)C)C	4.9	Bad	6
3012	o1c2c(CCCC2(C=CC=C(CCCC(CC(O)=O)=C)C)C)cc1	4.8	Excellent	6
3003	O(C(=O)CO)C1CC2C(NC1C)CCCC2C=CC=CCCCC	3.8	OK	6
2667	O1C(CCCCCC(CCCCc2ccc(O)cc2)C)(C)C(O)=C(C)C1=O	5.9	Bad	6
2514	O1C(C2C(C3(C(CC2O)C2(C(CC3=O)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	4.4	Poor	6
2377	OC1CC(=CCC=C(C=O)C(C=O)C1C(CCC=C(C)C)COC(=O)C)C	6.3	Good	6
2358	O1C(C(=O)C(C)C2OC(=O)CC(O)C(CC2)C)(C)C1CC(O)C(C)C	5.3	Excellent	6

2134	O1C2CC=C3C(C(CCC12C)C(CCC=C(C)C)C)C(OC3)O	4.5	Excellent	6
1947	O1C(=O)C(=C2CC3(C(CC12O)C(OC(=O)C)CCC3C)C)C	4.5	Excellent	6
1810	O1C2C=3C(CCC2C(=C)C1=O)(C)C(O)CCC=3C	4.6	Excellent	6
1799	O1Cc2c(C=C1C(CC(CC)C)C)cc1c(C(=O)C(=O)C(OC)=C1)c2O	5.1	Good	6
1796	O1c2c(cc(O)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C=O)C)C)C	4.5	Poor	6
1594	S1CC(NC1=O)C1(OC(CCC1)CCC(C=CCCC(=CC(OC)=O)C)C)O	4.7	OK	6
1481	O1CC(C(OC(=O)C)C(OC)=O)C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1OC(=O)C	4.6	OK	6
1247	O(C)C1C=C2C(CCC3(C2CCC3C(CCCC(C)C)C)C)C2(CCC(O)CC12O)C	5	Poor	6
1134	O(C(=O)C)C1c2c(C(=O)C1(C)C)c(C)c(OC)cc2C(C)C	5.6	Excellent	6
1084	O1C(=O)C(=CC1CC(=CCCc1ccoc1)C)CC=Cc1ccoc1	5	Good	6
884	O1C2CCC(CCC3(C4(OC4CC12CO)C(CC3)C(O)(C)C)C)=C	5.9	Excellent	6
858	[nH]1c(ccc1C=C1N=C(C)C(=C1)CCCCC)-c1[nH]ccc1	6.1	Good	6
771	O1c2c(c(OC)c(OC)c3c2c(OC)cc(O)c3)C(=O)C=C1CCC	5.6	Excellent	6
680	ClC1CCC(OC1(C)C)(C)C1C2C(CCC(O)(C)C2[NH+]=[CH-])C([NH+]=[CH-])(CC1)C	5.2	Good	6
654	O(C)c1cc2c(c(CCC)c1C(OC)=O)c(O)c1c(c2)C(C)(C)C(O)=C(C)C1=O	4.7	Good	6
582	O1c2c(OC1)cc1c(C(=O)c3c(ccc(O)c3OC)C1=O)c2OC	4.7	Excellent	6
538	S(OC1CC2CCC3C4CCC(C(CCCC(C)C)C)C4(CCC3C2(CC1)C)C)(O)(=O)=O	3.8	Bad	6
499	O1C(=CC(OC)=C(C=O)C1=O)C1C2C(CCCC2)C=CC1C	5.8	Excellent	6
216	OC1(C2C=C(CCC(=CCCC(O)(C(C1)C2)C)C)C(C)C)C	4.9	Good	6
14481	O1C(OC)C2=C(C3C(C3)C(CC(OC(=O)C)C2C(CCC=C(C)C)C)C)C1OC	4.9	OK	5.9
14476	O1C(C2C(C3(C(CC2O)C2(C(CC3OC(=O)C)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	4.2	Good	5.9
14450	O(C)c1cc2c(c(CCC)c1C(OC)=O)c(O)c1c(c2)C(C)(C)C(=O)C(O)(C)C1=O	4.4	Poor	5.9
14332	O=C1C23C(CCC2(C=C(C(O)=O)C3C)C)C(C1)C	5.3	Good	5.9
13902	O1C(=O)C(C)=C(O)C(C)=C1C(=CC(CC(CC(CC)C)C)C)C	3.5	Excellent	5.9
13794	O1C(=CC(OC)=C(CO)C1=O)C1C2C(CCCC2)C=CC1C	5.4	OK	5.9
13774	Brc1cc2c3c([nH]c2cc1)c(ncc3)C1=NCCC1	4.8	Excellent	5.9
13758	OC1CCC(C2C(CCC1=C)C(C2)(CC(O)C=C(C)C)C)=C	4.8	Excellent	5.9
13662	O1C(O)(C(C(=O)C(CC(=CCC)C)C)C)C(C)C(O)C(C)C1C(C(=O)CC)C	4.4	Good	5.9
13646	O1C(O)(C(C(=O)C(CC(=CCC)C)C)C)C(C)C(O)C(C)C1C(C(=O)CC)C	3.6	Good	5.9
13640	O1C(C)C(OC(=O)C)C(O)C(O)C1OC1CC2CCC3C4CCC(C=C)C4(CCC3C2(CC1)C)C	4.4	Bad	5.9
13559	O(C(=O)C)CC(=CCC(O)C(O)(C)C)C1CCC(=CCCC(=C)C1C(OC)=O)C	5.3	OK	5.9
13470	O1CC(C2C(C(CCC(O)C(CC2)=C)=C)C1=O)=CC=CC(O)(C)C	6.7	OK	5.9
13352	O1C2CCC(=CC(CCC12C)C(=CC=CC(O)(C)C)C=O)C=O	4.8	Excellent	5.9
13080	O1C2CCC(O)(C3C(C3)C(CCC12C)(CC=CC(OO)(C)C)C)C	5.8	Good	5.9
13079	O1C2CCC(O)(C3C(C3)C(CCC12C)(CC=CC(O)(C)C)C)C	5.2	Good	5.9
13066	O=C1C23C(CCC2(C=C(C(O)=O)C3C)C)C(C1)C	5.2	Good	5.9
13000	O1C2=CC(O)(C3C(CC2=C(C)C1=O)C(CC3)=C)C	4.8	Excellent	5.9
12999	O1C2=CC(O)(C3C(CC2=C(C)C1=O)C(CC3)=C)C	6.1	Excellent	5.9
12971	O(C=C1C2(C(CC=C1C=O)C(CCC2)(C)C)C)C(=O)C	4	Excellent	5.9
12769	O(C(=O)C)C1C2(C=O)C(CCC1(CC=C2C=O)C)C(CCC=C(C)C)C	5	OK	5.9
12641	O(C(=O)C)c1ccc(O)cc1CC=C(CCC=C(C)C)C	4.7	OK	5.9
12439	o1cc(cc1)COC(=O)C=C(CCC=C(CC(=O)CC(C)C)C)C	4.1	Bad	5.9
12424	O1C(C2C3(CCC4C(=CCC5C(C)(C)C(O)CCC45C)C3(CC2)C)C1=O)(CC(O)CC(C)=C)C	4.4	Bad	5.9
12397	O1C23CC(CCC(=O)C(C)C)(C)C1(O)CCC2(CCC(O)C3=C)C	4.9	Good	5.9
12373	O(C)c1c2c(cc(c1)C(=O)CC)C(=O)c1c(C2=O)c(OC)cc(OC)c1	5.3	Poor	5.9
12250	O1C(C2OC2C(=C)C2C3C4C(CCC4C)C3(C)C(O)C2)C1(C)C	5.1	Excellent	5.9

12166	OC12CC3(C(CCC1(CCC(O)C2=C)C)=C(CC3)C(C)C)C	4.5	Good	5.9
12165	OC12CC3(C(CCC1(C)C(O)CCC2=C)=C(CC3)C(C)C)C	5.3	Excellent	5.9
11956	OC(C(O)CCC1(C2C(C1)C(CCC=C(CC2)C)=C)C)(C)C	5	Excellent	5.9
11882	O(C(=O)C)C1CC2C(C)(C(C=O)C1C(=O)C)C(O)CC1C2(CCC2C(CCCC12C)(CC)C)C	4.3	Poor	5.9
11742	O1c2c(C(=O)C=C1c1cc(O)c(OC)cc1)c(OC)cc(O)c2	4.9	Good	5.9
11651	O=C1NCCC=C1CC(=O)c1c2c([nH]c1)cccc2	4.6	Excellent	5.9
11473	O1c2c(cc(OC)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C(O)=O)C)C)C	5.7	Excellent	5.9
11394	Oc1ccccc1[NH+]1C=Cc2c([nH]c3c2cccc3)[CH-]1	4.1	Poor	5.9
11382	Brc1cc([NH+]2C=Cc3c([nH]c4c3cccc4)[CH-]2)c(O)cc1	4.5	Good	5.9
10960	O1OC(CCC1(CCC(O)C(CCC=1C(CCCC=1C)(C)C)=C)C)C(C(O)=O)C	3.8	Poor	5.9
10745	O(C(=O)C)C1CCC(O)(C=CC(CCC1=C)C(C)C)C	4.6	Excellent	5.9
10612	O1C23CC(CCC(=O)C(C)C)(C)C1(O)CCC2(C)C(=O)CCC3=C	5.2	Excellent	5.9
10415	O(C)C=1C(=O)C(CC=C(CCC=C(C)C)C)=C(C)C(=O)C=1OC	3.9	Good	5.9
10003	O1C(=O)C(=CC1O)CCC1C(CC=CC1=C)(C)C	5	Excellent	5.9
9935	OC1CC2(C(C3C(CC2)(CCC3C(C)C)C)C2CC12CO)C	4.6	Excellent	5.9
9934	OC1CC2(CC(O)C3(C(C2C2C1(CCC2C(C)C)C)C3)C)C	4.5	Excellent	5.9
9839	BrC12OC1C1OC1(C)C1(CC(Br)C(Cl)(CC1O)C)C2(C)C			5.9
9798	BrC12OC3C(CC(Br)C(Cl)(C3)C)(C1(C)C)C(=C)C(O)C2O	4.2	Excellent	5.9
9547	BrC1=CC2(Oc3c(C2)cc(cc3Br)CO)C=C(Br)C1=O	4.3	Excellent	5.9
9498	O1c2c(c(O)c(OC)c(O)c2)C(=O)C=C1c1ccc(OC)cc1	6	Good	5.9
9494	O1C2OC2C(CCCC(CC(O)CC(=CCCc2ccoc2)C)C)C1=O	5.2	Excellent	5.9
9493	O1C(O)C(=CC1=O)CCC=C(CC(O)CC(CCCc1ccoc1)C)C	5.1	Excellent	5.9
9490	O1C(=O)C(=CC1O)CCCC(CC(O)CC(=CCCc1ccoc1)C)C	5.8	Poor	5.9
9391	O1C(O)C2C(=CCC3C2(C)C(O)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	4.3	Bad	5.9
9321	ClC=C1CCNc2c1cc(OC1OCC(OC)C(O)C1OC)cc2C	4.4	Excellent	5.9
9310	O=C1C(=C(O)CCCCCCCCC(CC)C)C(=O)N(C)C1C	5.3	Bad	5.9
9241	O(C)c1c2nc3c(nc2c(cc1)CO)cccc3C(O)=O	5.2	Poor	5.9
8995	Brc1cc2[nH]c3c(c2cc1)ccnc3C1ON(CC1)C	4.2	Excellent	5.9
8863	OC1(C=CC(=O)c2c1n(O)c1c2cccc1C(OC)=O)C=O	5	Excellent	5.9
8725	o1cc(cc1Cc1ccoc1)CCCC(=CCCC(CC(O)=O)C)C	4.9	OK	5.9
8515	O1CC23C(CCC1(C)C2C(O)Cc1ccoc1)C(CCC3)(C)C	4.9	OK	5.9
8450	Brc1c2c(n(C)c1Br)C(=O)N1C3(N=C(NC23)N)CCC1	2.9	OK	5.9
8294	BrC12OC3C(CC(Br)C(Cl)(C3)C)(C1(C)C)C1(OC1C2O)C	5.6	Excellent	5.9
8230	O1C(OCC)C2=C(C(O)CC3C(CCCC23C)(C)C)C1=O	5.1	Excellent	5.9
8229	O1C(OCC)C2=C(C(O)CC3C(CCCC23C)(C)C)C1=O	5.1	Excellent	5.9
8146	O1c2c(C(=O)C=C1CCC)c(O)cc1c2c(OC)cc(O)c1	5.7	Excellent	5.9
8103	O1CC2C(CCC(=CCCC2=C)C)C(CCC=C(CO)C)C1=O	4.9	Poor	5.9
8064	O1C(=O)C(CC1C=C(CCCc1ccoc1)C)=CCCc1ccoc1	4.4	Poor	5.9
7902	O(C(=O)c1c2nc3c(nc2ccc1)cccc3)C	5.1	OK	5.9
7787	O1CC2C(CCC(=CC(O)CC2=C)C)C1(C=CC=C(C)C)CO	4.5	Poor	5.9
7568	ClCC1OC(=O)c2c1c(cc1c2CC(C)(C)C1O)C	5	Excellent	5.9
7564	O([N+](=O)[O-])C1c2c(CC1(C)C)c(C)c(CCO)c(c2)C	4	Excellent	5.9
7487	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C(OC)=O)C)C)C1(C(OC)=O)C)C	5.3	Poor	5.9
7485	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=O)C)C)C)C1(C(OC)=O)C)C	4.1	OK	5.9
7454	O(C(=O)C)CC=C(CCC=C(CCC1C(CCCC1C)(C)C)C)C=O	6.1	Poor	5.9
7397	OC(=O)c1c2c(n(c1)Cc1ccccc1)cccc2	7	Excellent	5.9

7170	OC1(CCC2C(CCCC2(C)C)(C)C1CCC(=CCO)C)C	4.7	Excellent	5.9
7147	OC(=O)CCc1nc2c(nc1)cc1c(c2)cccc1	3.5	Good	5.9
7090	O1CC(C2C(C(CCC=C(CC2)C)=C)C1=O)=CC=CC(CO)=C	5.6	Excellent	5.9
7019	O(C)c1c2c(cc(OC)c1)C(=O)c1c(C2=O)c(OC)cc(OC)c1	5.3	Poor	5.9
6895	O1C2(OC)C(C3C(C(OC(=O)C)CC3C(=CCC=C(C)C)C)C1OC)C(CC2)C	4.8	Bad	5.9
6851	O(C(=O)c1ccccc1)CC(=O)c1c2c([nH]c1)cccc2	5	Bad	5.9
6766	O1C(=O)C(CCC=CC=CN(C)C(=O)C(CCC(CC1C(C)(C)C)C)C)C	4.9	Good	5.9
6504	O1C(=CC(OC)=C(CO)C1=O)C1C2C(CCCC2)C=CC1C	4.9	OK	5.9
6489	OC1(CCC2C(=C1)C(CCC2(C#N)C)C(C)C)C	5.7	Excellent	5.9
6468	O(C(=O)C)C1C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC(=O)C=C(C1)C)C)C	4.6	Good	5.9
6467	O(C(=O)C)C1C2C(CCC2C(OC(=O)C)(C)C)(C=CC(CC(=O)C=C(C1)C)C)C	4.5	Poor	5.9
6442	OC1CC2(C(CC1C(=O)C)C(CC2)C(O)(CCC=C(C)C)C)C	5.3	Good	5.9
6327	N(CCCN1CCCCCCCCC=CCCCC1)CCCN	2.3	Bad	5.9
6292	OC(CC=CC(O)(C)C)(C)C1C2CCC(=CCC2(CC1)C)C	5.1	Good	5.9
6252	O1C(CC2C(CCC3C4(C(CCC23C)C(CCC4)(C)C)C)C1OC(=O)C)C1=CC(OC1O)=O	5.1	Bad	5.9
6250	OC1CC2C(CCC3C2(CCC2C(CCCC23C)(C)C)C)(CC)C(C=O)C1C(=O)C	5	Poor	5.9
6145	O=C1NC(=NC1(CC(=O)C)c1c2c([nH]c1)cccc2)N(C)C	5.5	OK	5.9
6043	O1C2(C(C=C3C(=COC(=C3)C)C2O)=C(C(=O)CCCCCC(O)C)C1=O)C	5.8	Poor	5.9
5892	O(C(=O)C)C1C(C=2C(C1(C)C)C(OC(=O)C)CC(C)C=2C=O)(C=O)C	5.1	Excellent	5.9
5824	O1CC(OC)C(O)C(OC)C1Oc1cc(c2nccc(c2c1)C)C	4.3	Good	5.9
5753	Brc1cc2NC(=C3Nc4c(ccc(Br)c4)C3=O)C(=O)c2cc1	4.8	Poor	5.9
5746	O1C2=CC(=O)C(NC(=O)C)=CC2=Nc2c1cccc2	4.2	Good	5.9
5566	O(C(=O)C)C1CC2C(C3CC(O)C(=CC13C)C=O)(CCC1C(CCCC12C)(C)C)C	4.6	Good	5.9
5440	o1cc(cc1C=C(CCCc1cc(oc1)C(=O)NCCN)C)CCCc1ccoc1	4.3	Bad	5.9
5419	OC(CCCCC(O)=O)C=CC=1CC2C(CC=CC2)C=1CCCCC	4.4	OK	5.9
5362	n1c2c3C(CC(C)C2CC=CCCC)CCc3nc1N	4.4	Excellent	5.9
5351	n1c2c3C(CC(C)C2CC=CCCC)CCc3nc1N	5	Excellent	5.9
5296	O1C(CCCCCC1=O)C1CC1C(O)C=CC(O)CC=CCC=CCC	4.9	Poor	5.9
5283	O1C(CC=CCCC1=O)C1CC1C(O)C=CC(O)CC=CCCCCC	5.2	Poor	5.9
5282	O1C(CCCCCC1=O)C1CC1C(O)C=CC(O)CC=CCC=CCC	5.6	Poor	5.9
4874	O(C(COC(=O)C)CO)C(=O)C=C(CCC=1C(CCCC=1C)(C)C)C	4.5	Poor	5.9
4780	S(C)c1[nH]cnc1Cn1c2c(c3c1cncc3)cccc2	4.7	Excellent	5.9
4537	O1C2CC3C4(CCC(C(CCC=C(C)C)C)C4(C)C(O)CC3(C)C(CCCO)C12C(=O)C)C	4.8	Bad	5.9
4463	O(C)c1cc(O)cc(C(=O)c2cc(cc(OC)c2O)C)c1C=O	6.2	Poor	5.9
4296	O=C1N=C(NC)N(C)C1=Cc1c2c([nH]c1)cccc2	4.8	Poor	5.9
4271	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(=C2)C)C([NH+]=[CH-])(CC1)C	4	Good	5.9
4270	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(=C2)C)C([NH+]=[CH-])(CC1)C	5	Good	5.9
3625	o1cc(cc1)CCC=C(CC(=O)CC(CC=Cc1ccoc1)C)C	4.2	Poor	5.9
3620	O=C1NCCCCC1NC(=O)C=C(CCC1(C)C(CCC=C1C)C)C	4.9	Bad	5.9
3523	O1C2OC=C(C3C2C(CC3)C1OC(=O)C)C(=O)CC=C(C)C	5	Excellent	5.9
3284	O1C2C(=CC1=O)C(OC(=O)C)CC1C(CCC3C4(C(CCC13C)C(CCC4)(C)C)C)C2O	4.8	Bad	5.9
3058	O(C(C(=CC=O)COC(=O)C)CC=C(C#CC=C(C)C)C)C(=O)C	4.6	OK	5.9
2953	OC1(CCC(C(=CCC=C(C)C)C)C1C1C(C=CC1=O)C)COC(=O)C	5	OK	5.9
2699	O=C1C=C2CCC3C4CCC(C(O)(C=CC(C(C)C)C)C)C4(CCC3C2(C=C1)C)CO	4.8	Poor	5.9
2685	O1C2C1(CC=C(C)C)C(=O)c1c(cccc1)C2=O	4.1	Excellent	5.9
2416	O1C23C1C(O)C=1C4CCC(C(CCCC(C)C)C)C4(CCC=1C2(CCC(O)C3)C)C	5.4	OK	5.9
2332	O(C)c1cc(CC=C(CC(=O)CCCC(=O)C=C(C)C)C)c(O)c(c1)C	5.9	Excellent	5.9

2285	O1CC(C2C(C3(O)CC(CC2)(C)C(O)CC3)C1=O)=CC=CC(C)C	3.6	OK	5.9
2146	O1C(=CC(OC)=CC1=O)C(NC(=O)C)Cc1ccccc1	5.1	OK	5.9
1880	O1C(CCC1C([NH+]=[CH-])(C)C)(C)C1C2C(CCC(=C2)C)C([NH+]=[CH-])(CC1)C	5	Good	5.9
1705	O(C)C=1C(=O)C(=CC(=O)C=1OC)CC=C(CCC=C(C)C)C	4.1	Good	5.9
1432	O1C2C3C(C1CC(=CCCC2(OC(=O)CCC)C)C)C(=C)C(OC(=O)C)C(OC(=O)C)C3C(C)C	4.9	Good	5.9
1163	O1C2CC(=CCCC(=O)C(C2C(CCC=C(C)C)C)C1=O)C	4.3	Poor	5.9
1012	O1C(=O)C(CCC1C(C)C1CCC2C3C(C4(C(CC(=O)CC4)CC3)C)C(OC(=O)C)CC12C)C	3.6	Bad	5.9
780	O(C)C1=NC(=Cc2ccccc2)C(=O)NC1=Cc1ccccc1	5.8	Bad	5.9
774	O1c2c(C(=O)C=C1CCC)c(O)cc1c2c(O)cc(OC)c1	6	OK	5.9
770	O1c2c(c(O)c(OC)c3c2c(OC)cc(O)c3)C(=O)C=C1CCC	5.8	Excellent	5.9
461	O1C(OC(=O)C)C2C(CCC(C3(CC(CCC3)(C)C)C)C2=CC)C1OC(=O)C	4.9	OK	5.9
252	O1C23CC(CCC(=O)C(C)C)(C)C1(O)CCC2(C)C(O)CCC3=C	4.8	Excellent	5.9
251	O1C23CC(CCC(=O)C(C)C)(C)C1(O)C(O)CC2(CCCC3=C)C	5.8	Poor	5.9
244	O=C1N=C(N=C1c1c2c([nH]c1)cccc2)N(C)C	4.8	Excellent	5.9
221	O1C2C(=CC1OO)C(C1C(C=C(CC1)C)C2OC)(C)C	5.4	Excellent	5.9
177	Brc1cc(O)c2[nH]c3c(c2c1)ccnc3C1=NCCC1	3.9	Excellent	5.9
14471	O1CC2C(CCC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(CC)C)C)C1(O)C	3.8	OK	5.8
14440	OC1C2C3C(CCC2(CC(=O)C(=C1)CO)C)(CCC3C(C)=C)C	5	Excellent	5.8
14370	OC(=O)C1C2(C(CC=C1C=O)C(CCC2)(C)C)C	6.1	Excellent	5.8
13821	O(C(=O)C1C2(C(CC=C1C)C(CCC2)(C)C)C)CC(O)CO	4.8	Good	5.8
13775	Brc1cc2c3c([nH]c2cc1O)c(ncc3)C1=NCCC1	4.3	Excellent	5.8
13734	O(C(=O)C1C2(C(CCC1=C)C(C(O)=O)(C)C(CC2)C(C=O)(C)C)C)C	5.5	Excellent	5.8
13639	O1C(C)C(O)C(OC(=O)C)C(O)C1OC1CC2CCC3C4CCC(C=C)C4(CCC3C2(CC1)C)C	4.2	Bad	5.8
13635	O(C(=O)C)C1CC2CCC3C4CCC(C=C)C4(CCC3C2(CC1)C=O)C	4.2	OK	5.8
13447	O(C(=O)C=CC(O)(C)C)C1C=C(CCC(=O)C(CCC1C(=O)C)=C)C	5.6	Good	5.8
13445	O(C(=O)C=CC(O)(C)C)C1C2C(CCC1C(=O)C)(C)C(O)CCC2=C	5.3	Good	5.8
13139	Brc1cc2[nH]cc(c2cc1)C=C1N(C)C(=N)N(C)C1=O	4.2	Excellent	5.8
13125	O(C(=O)c1ccccc1C(OCCCC)=O)Cc1ccccc1	3.8	Good	5.8
13115	O1C2(O)C(C3CCC(C(C=CCC(C)C)C)C3(CC2)C)=CC1=O	4.4	Good	5.8
13083	OC1(C2C(C2)C(CCC(=CCC1)C)(CC=CC(O)(C)C)C)C	4.4	Excellent	5.8
13082	O1C2CCC(O)(C3C(C3)C(CCC12C)(CCC(OO)C(C)=C)C)C	4.6	OK	5.8
12784	O=C1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)C(O)=O	5.2	Bad	5.8
12525	OCC=C(CCC(=O)C(CCC=C(CC(=O)C=C(C)C)C)=C)C	5.2	Poor	5.8
12368	O1C2CC3(C(CC(=O)CC3(C)C)C1=O)C=CC2(O)C	5.6	Excellent	5.8
12147	O=C1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)COC(=O)C	4.7	OK	5.8
12018	O1C2C(C3(C(=CC(=O)CC3C)CC2)C)C(C)C1=O	5.5	Excellent	5.8
12014	O1C2C(C3(C(=CC(O)CC3C)CC2)C)C(C)C1=O	4.9	Excellent	5.8
12003	O1C(C)(C)C1CCC(C)C1CCC2C3C(CC(OC(=O)C)C12C)C1(C(=CC(=O)CC1)CC3)C	5.1	OK	5.8
11885	O1CC2C(C1(O)C)C(OC(=O)C)CC1C2(C)C(=O)CC2C1(CCC1C(CCCC12C)(CC)C)C	4	Bad	5.8
11776	OC1C2CC(O)CCC2(C=2C(C3CCC(=C(CC(=O)C=C(C)C)C)C3(CC=2)C)C1)C	5	Bad	5.8
11775	OC1C2CC(O)CCC2(C=2C(C3CCC(=C(CC(=O)C=C(C)C)C)C3(CC=2)C)C1)C	5.5	Poor	5.8
11630	OC1C2CC(O)CCC2(C=2C(C1)C1=C(CC=2)C(CC1)(C(CC(=O)CC(C)C)C)C)C	3.5	Excellent	5.8
11179	O(C(=O)C)C=CC(=CCC1C(CCCC1=C)(C)C)C=O	6	Poor	5.8
11137	BrC1CCC(O)(CC1(C)C)CC1C2C(CC1)(C)C(Br)CCC2(O)C	4.7	Good	5.8
10928	S(OC1CC2=CCC3C4CCC(=O)C4(CCC3C2(CC1)C)C)(O)(=O)=O	5.5	OK	5.8
10829	O(C)c1c2c(ccc1)C(=O)c1c(C2=O)c(OC)ccc1	3.8	OK	5.8

10812	OC1C2C(C=CC2(O)C)C(CCC1C(CCC=C(C)C)C)=C	4.6	Poor	5.8
10780	O=C(Cc1ccccc1)C(=O)Nc1ccccc1	5.9	Excellent	5.8
10730	O1CC(C2C3(C(=CC(=O)CC3C)CCC12O)C)C	5.2	Excellent	5.8
10674	OC1C2C(CC=C2C)C(CCC1C(O)(CCC=C(C)C)C)=C	4	OK	5.8
10661	OC1C2C(CC=C2C)C(O)(CCC1C(CCC=C(C)C)C)C	4.7	Good	5.8
10396	O1C2CC3C(C(O)C(CCC3=C)C(CC(O)C=C(C)C)C)C12C	4.9	Excellent	5.8
10394	O(C(=O)C)C1C2C(CC=C2C)C(CCC1C(CCC(O)C(O)(C)C)C)=C	4	Excellent	5.8
10393	O(C(=O)C)C1C2C(CC=C2C)C(CCC1C(CCC(O)C(C)=C)C)=C	4.2	Poor	5.8
9846	O(C)c1c2c(ccc1)C(=O)c1c(C2=O)c(O)ccc1	5	Excellent	5.8
9812	N1C=2C(N=C1N(C)C)=C(C1=NC(=NC1=CC=2)N(C)C)C	6.1	Good	5.8
9810	n1c2c(n(C)c1NC)C(=C1N=C(N=C1C=C2)N(C)C)C	4.8	Good	5.8
9722	Brc1cc(cc(Br)c1OCC1OC(=O)NC1)C1OC(=O)NC1	5.3	Excellent	5.8
9666	N1C=2C(N=C1N)=C(C1=NC(=NC1=CC=2)N(C)C)C	3.6	Excellent	5.8
9530	O(C)C1=CC(=NC1=Cc1[nH]c(cc1)CCCCCCCCCCC)c1[nH]ccc1	3.6	Poor	5.8
9495	O1C2OC2C(CCC=C(CC(O)CC(CCCc2ccoc2)C)C)C1=O	4.8	OK	5.8
9492	O1C(O)C(=CC1=O)CCCC(CC(O)CC(=CCCc1ccoc1)C)C	5.4	OK	5.8
9491	O1C(=O)C(=CC1O)CCC=C(CC(O)CC(CCCc1ccoc1)C)C	4.7	Poor	5.8
9358	O1C(CC=CC(OC(CCC(O)C=CC1=O)C)=O)C	4.3	Excellent	5.8
8341	O1C=C2C(=CC(=O)C(C(O)=O)=C2O)C(C)=C1C(CC)C	5	Excellent	5.8
8284	O1C2CCC(O)(C3C(C=CCCC12C)C(O)(CC3)C)C	4.5	Excellent	5.8
8266	O1C(=O)C(=C2CC3(C(CC12O)C(=O)CCC3C)C)C	5.4	Excellent	5.8
8225	O1C(=O)C2C(=CCC3C(CCCC23C)(CO)C)C1=O	4.3	Excellent	5.8
8170	O(C(=O)C)C1C=C(CO)C(=O)C(O)C1C(=CC=CC(C=CCC(C)C)C)C	4	Good	5.8
8105	O1OC(CCC1(CCC=C(CCC(=O)C(CCCC(=O)C)(C)C)C)C)C(C(O)=O)C	5.1	Poor	5.8
7914	O=C1NC(=O)N(c2nccnc12)c1ccccc1	5.1	Excellent	5.8
7839	O(C)C1=CC(=O)C=C(CC=C(CCC=C(C)C)C)C1=O	5	Excellent	5.8
7808	O1C2C(CCC(=C)C(OO)CCC(=C2)C)C(=C)C1=O	5	OK	5.8
7294	O(C(=O)C)C1CC2C(C3(C)C1(O)CC=CC3=O)C(O)CC1(C2CCC1C(C=CC(C(C)C)C)C)C	6.6	Poor	5.8
7225	O=C1CC2C3C(CCC2(C)C1C(O)(CCCC(C)C)C)C1(C(CC(=O)CC1)CC3)C	3.8	Bad	5.8
6811	O1C(C2C3(CC=C4C(CCC5C(C)(C)C(O)CCC45C)C3(CC2=O)C)C1=O)(CCCC(O)(C)C)C	3.8	Bad	5.8
6789	O1C2CCC3(C(CCC3=O)C2(CCC(O)C1(C)C)C)C	4.4	OK	5.8
6606	OC1C=C(C)C2(C(C1)C(CCC(O)(C=C)C)(C)C(CC2)C)C	4.5	Poor	5.8
6605	OC1C=C(C)C2(C(C1)C(CCC(O)(C=C)C)(C)C(CC2)C)C	5.3	Excellent	5.8
6200	OC(=O)c1ccccc1N(C(=O)CCc1ccccc1)C	5.6	Excellent	5.8
6130	O1OC(CCC1(CCC1C(CCCC1=C)(C)C)C)C(C(OC)=O)C	4.7	Good	5.8
6127	O1C23C(C=C(C)C1C=CCCCCCCC)C1CC(O)CC1(OC2=O)CC3O	5.2	Poor	5.8
5895	OC1(C2C(CC(CC2C)C)C=CC1C)C=CC=CC(O)=O	5.3	Excellent	5.8
5736	OC1(c2nc(nc3CCC(CC1C)c23)N)CCCC	4.8	Good	5.8
5525	O1C(O)C2=C(C=CC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	5.5	Bad	5.8
5524	BrC=1CC23N(C=1Br)C(=O)C=1N(C2NC(=O)N3)CCC=1	6.5	Excellent	5.8
5516	O1C(=O)C(=C2CC=3C(CCC=3C)C(CC12O)C)C	5	Excellent	5.8
5436	o1cc(cc1CC(CCCc1cc(oc1)CC(C(O)=O)C)C)CCCc1ccoc1	5.6	Good	5.8
5413	O1C23C(C=C(C)C1C=CCCCCCCC)C1CC(O)CC1(OC2=O)CC3O	3.3	Bad	5.8
5336	O1CC(C2C(C(CCC=C(CC2)C)=C)C1=O)=CC=CC(O)(C)C	5.9	OK	5.8
5297	O1C(CC=CCCC1=O)C1CC1C(O)C=CC(O)CC=CCCCCC	5.1	OK	5.8
5295	O1C(CCCCCC1=O)C1CC1C(O)C=CC(O)CC=CCCCCC	5.1	Good	5.8

5281	O1C(CCCCCC1=O)C1CC1C(O)C=CC(O)CC=CCCCCC	5.3	OK	5.8
5211	O1OC(OC)(CC(C)C1CC(O)=O)CCCC=CC(=CCC)C	4.8	Excellent	5.8
5210	O1OC(OC)(CC(C)C1CC(O)=O)CCCC=CC(=CC)C	6	Good	5.8
4885	O1C(O)C(=CC1=O)CCC=C(CCC=C(C)C)C	4.1	Bad	5.8
4873	O1C(O)(C)C(C)C(O)CC1CC=CC=CC(CC(=CCCC=C)C)C	3.7	Bad	5.8
4580	[nH]1cnc(CCN)c1CC=C(CCC1C(CCCC1=C)(C)C)C	4.6	Excellent	5.8
4462	O(C)c1c(cc(cc1OC)C)C(=O)c1cc(O)cc(OC)c1C=O	5.6	Good	5.8
4347	OC1C=C(C)C2(C(C1)C(CCC(O)(C=C)C)(C)C(CC2)C)C	5.6	Excellent	5.8
4346	O(C)c1c2c(cc(CCC)c1C(OC)=O)C(=O)c1c(C2=O)c(OC)cc(OC)c1	5	OK	5.8
4241	O1C(C1(C)C)C1OC2OC(O)C3C(C2=C1)CCC(O)(C1OC1CC3=C)C	4.8	Good	5.8
4089	Clc1c([nH]cc1Cl)-c1oc(cn1)-c1ccc(O)cc1	4.2	Bad	5.8
3892	[NH+]12CCc3c([nH]c4c3cccc4)[C-]1C=C1NC=NC1=C2	4.7	Excellent	5.8
3860	O1C(C(C(OC(=O)C(CC)C)C(C(=O)CC)C)C)C(C)C(=O)C(C)=C1CC	5.6	Excellent	5.8
3575	OC1=C(C)C(=O)c2c(C1=O)c(ncc2)COC(=O)C	4.4	Good	5.8
3550	O(C(=O)C)C1C(=CC2(C(CCC1=O)=CCCC2C)C)C	5.4	Good	5.8
3535	BrC1C(C)C2(C3(C(CC3OC(=O)C)(C)C(Br)C2)C(C)C1O)C	4.7	Excellent	5.8
3452	O(C(=O)CCCCC=CCC(=CC=CC=CC(=O)CC)C=O)C	5.7	Good	5.8
3396	O1CC2C(C1(O)C)C(OC(=O)C)CC1C2(C)C(=O)CC2C1(CCC1C(CCCC12C)(CC)C)C	5.8	Poor	5.8
3207	O(C(=O)C)C1C2C(CCCC2(C)C)(C)C(CCC(=CCO)C)=C(C)C1O	3.6	OK	5.8
3185	O1c2c(C=CC1(CCC1(CCCC(C)C1=C)C)C)c(O)c(OC)c(OC)c2OC	4.8	Bad	5.8
3059	O(C(C(C=COC(=O)C)=COC(=O)C)CC=C(C#CC=C(C=O)C)C)C(=O)C	5.9	Bad	5.8
2882	O1C(=O)C(=C2CC=3C(CC12O)(CCCC=3C)C)C	4.9	Excellent	5.8
2797	S(=O)(=O)(C)c1c2c([nH]c3c2cccc3)c(nc1)CC	4.9	Excellent	5.8
2633	O1C(=Cc2ccc(OC)cc2)C(=CC1=O)c1ccc(O)cc1	4.8	Excellent	5.8
2628	O1C(O)C(O)C(CCC=C(CCC=C(CC(=O)C=C(C)C)C)C)C1=O	4.9	Bad	5.8
2577	OC1C2C(CCC3C1(CCC3(O)C(C)C)C)(C=CC=C2C)C	4.5	Excellent	5.8
2425	OC12CC(O)CCC1(C1C(C3CCC(C(CCC(C(OC(=O)C)(C)C)C)C)C)C3(CC1)C)CC2=O)C	3.7	Bad	5.8
2389	O=C1C23C(C(C)C(=CC2C=CCC(C=C(CC(=O)C=C1)C)C)C)C(NC3=O)Cc1c2c([nH]c1)cccc2	3.8	Bad	5.8
2237	O1C2(c3c(CC(C)C2(CC1C1(OOC(CC1)C(C(OC)=O)C)C)C)cc(cc3)C)C	5	Bad	5.8
2183	O1OC(C=C(CC)C1CC(O)=O)(CC(CC(CC)C=CCC)C)CC	4.9	Good	5.8
1962	Brc1cc2[nH]cc(c2cc1)C1N(C)C(=NC1)C(=O)c1c2c([nH]c1)cc(Br)cc2	4.5	Bad	5.8
1872	O(C)C1=CC(=NC1=CNCCc1ccccc1)c1[nH]ccc1	4.4	Excellent	5.8
1858	o1cc(cc1)CCCC(=CC(=O)C=C(CCCc1ccoc1)C)C	4	Poor	5.8
1857	o1cc(cc1)CCCC(=CC(=O)C=C(CCCc1ccoc1)C)C	3.9	Good	5.8
1856	o1cc(cc1)CCCC(=CC(=O)C=C(CCCc1ccoc1)C)C	5.5	Poor	5.8
1731	OC1CC(=CCCC(C2C(C=C1C(C)C)C(O)(CC2)C)=C)C	4.8	Excellent	5.8
1699	O1C(CC=CCCCC1=O)C1CC1C(O)C=CC(O)CC=CCC	4.6	Good	5.8
1587	S(CC=1CCC2C(CC3(OC(=O)C=C3C2(C)C)O)C=1)C(=O)C	4.5	Good	5.8
1434	O1CC12CCCC1C(CCC(CC(O)=O)C)(C)C(CCC12C)C	5.6	Excellent	5.8
1422	O(C(C)c1c2nc3c(nc2ccc1)c(ccc3)C(O)=O)C	4.6	Good	5.8
1420	Brc1cc(cc(Br)c1OCC1OC(=O)NC1)C1OC(=O)NC1	4.8	Excellent	5.8
1347	BrC(C(OC(=O)C)CC1OC(OC=C=C)CC1OC(=O)C)CC=CCC	5.2	Excellent	5.8
1066	O1C(=O)C(=C2CC3(C(CC12O)C(=O)CCC3C)C)C	5.3	Excellent	5.8
995	O1C(C=C(CCC=C(CCCC(=O)C)C)C)C(CCO)C(=C)C1=O	4.2	Good	5.8
661	S(OC1CC2=CCC3C4CCC(=O)C4(CCC3C2(CC1)C)C)(O)(=O)=O	6	Excellent	5.8
192	o1cc(cc1)CCCC(CC(=O)C=C(CCCc1ccoc1)C)C	4.1	OK	5.8

191	o1cc(cc1)CCCC(CC(=O)C=C(CCCc1ccoc1)C)C	5	Poor	5.8
30	ClC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	5.3	OK	5.8
14472	O(C(=O)C)C1C23C(C(C(=O)C)C(O)CC2C2(C(C1)C1(C(CC2)C(CCC1)(CC)C)C)C)C(O)C3	5.9	OK	5.7
13903	O1C(O)(C)C(=O)C(C)=C1C(=CC(CC(CC(CC)C)C)C)C	5.1	Good	5.7
13609	O(C=O)C1CCC2=CC(O)CC(C)C2(C)C1C(=O)C	5	Excellent	5.7
13607	O1C2(OCC)C(=CC1=O)C(C1CC(O)C(=CC1C2)C)(C)C	4.9	Excellent	5.7
13527	OC(C(CCC=C(CCC=C(CC(=O)C=C(C)C)C)C)=C)CO	3.8	OK	5.7
13525	OC(CC(=O)CC(=CCCC(=CCCC(=CCO)C)C)C)(C)C	4.7	Excellent	5.7
13442	O1C2C3C(CCC2C(C)C1=O)(C)C(O)CCC3=C	5.4	Good	5.7
13386	OC(=O)CC1C(CCC2CC(CCC12C)(C=C)C)(C(=O)C)C	4.9	Excellent	5.7
13350	O1CC(C2C(C34CCC(OC3)C4(CC2)C)C1=O)=CC=CC(O)(C)C	5.1	Excellent	5.7
13340	OC1(CCC(C)(C1=C)c1cc(O)c(cc1)C)C	4.6	Excellent	5.7
13327	O1CC(=C)C2(CC3CC(O)CC(C)C3(C)C2O)C1OC	4.4	Excellent	5.7
13253	O1OC(CC(CC)C1CC(O)=O)(CCCC(CC)C=CC(=O)C)CC	5.7	Good	5.7
13081	O1C2CCC(O)(C3C(C3)C(CCC12C)(CCC(O)C(C)=C)C)C	4.4	Excellent	5.7
12846	O1C2C3C(CCC2C(C)C1=O)(C)C(O)CCC3=C	4.7	Good	5.7
12843	O1C(CCC(=O)C=CC=CC)(C)C(OC(=O)C)=C(C)C1=O	4.9	Good	5.7
12562	O1C(C2C3(CCC4C(=CCC5C(C)(C)C(O)CCC45C)C3(CC2=O)C)C1=O)(CCCC(C)=C)C	4.5	Bad	5.7
12438	O1C=CC(=C)C1OC(=O)C=C(CCC=C(CC(=O)CC(C)C)C)C	4.1	Bad	5.7
12425	O1C(C2C3(CCC4C(=CCC5C(C)(C)C(O)CCC45C)C3(CC2)C)C1=O)(CC(O)CC(C)C)C	3.5	Poor	5.7
12310	O(C=O)C1CCC2=CC(O)CC(C)C2(C)C1C(=O)C	5.2	Excellent	5.7
12187	O(C(=O)C=C(CCC=C(CCC=C(C)C)C)C)CC(O)CO	5.9	OK	5.7
12140	O(C)c1ccc(cc1O)CCNC(=O)C=C(CCCCCCCCC)C	5.1	Bad	5.7
12116	s1nc(nc1C(=O)c1c2c([nH]c1)cccc2)N(C)C	4.9	OK	5.7
12051	O=C1C=CC(CCC(=O)CCCCC)C1CC=CCCCC(O)=O	5.1	Good	5.7
11773	O(C(=O)C)c1c2c(cc(OC(=O)C)c1)cccc2OC(=O)C	3.2	Excellent	5.7
11643	n1c2c(n(C)c1N)C(=C1N=C(N=C1C=C2)NC)C	4.4	Excellent	5.7
11612	O(C(=O)C)CC(=CCC(O)C(O)(C)C)C1CC(C(C)=C)C(CC1)(C=C)C	4.6	OK	5.7
11564	O1C2=C(CC13C1(C(CCC3C)C3(C(CC1)C(C)(C)C(O)CC3)C)C)C(=O)C(=O)C=C2C	5.5	Good	5.7
11474	O1CC23C(CCC4(C5Cc6cc(O)ccc6OC5(CCC24)C)C)C(CCC3)(C)C1=O	5	Bad	5.7
11131	O1C(O)C2=C(C(O)CC3C(CCCC23C)(C)C)C1=O	5.2	Excellent	5.7
10729	O1C(=O)C(C2C3(C(CCC12O)=CCCC3C)C)C	4.7	Good	5.7
10704	IC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	5.9	Good	5.7
10662	OC1C2C(C(CCC1C(CCC=C(C)C)C)=C)C(O)C=C2C	4.2	OK	5.7
10611	O1C23C(O)C(CCC(=O)C(C)C)(C)C1(O)CCC2(CCCC3=C)C	4.5	Good	5.7
10546	Brc1cc(O)c(cc1O)C(=O)C=C(CCC=C(C)C)C	6.3	Poor	5.7
10545	Brc1cc(O)c(cc1O)C(=O)C=C(CCC=C(C)C)C	5.4	Excellent	5.7
10391	o1cc(cc1)CCCC(C(=O)CC=C(CCCc1ccoc1)C)C	4.3	Excellent	5.7
10390	o1cc(cc1)CCCC(C(O)CC=C(CCCc1ccoc1)C)C	5.1	OK	5.7
10307	O(C)c1c2NC(=O)CN3C=Cc4nccc(c1)c4c23	5.1	Excellent	5.7
9939	O(C)C1=CC(=NC1=Cc1[nH]c(cc1)CCCCCCCCCCC)c1[nH]ccc1	5.1	OK	5.7
9721	O(C(C(CCC(=CC=O)C)CC=C(CCC(O)C(C)=C)C)(C)C)C(=O)C	5.4	Excellent	5.7
9718	O1CC2(CC(C3C2(O)C(C(CC3OC(=O)C)C)C1O)(C)C)C	4.3	Good	5.7
9636	O1C(C2C3(CC=C4C(CCC5C(C)(C)C(O)CCC45C)C3(CC2=O)C)C1=O)(CCCC(OC)(C)C)C	3.5	Bad	5.7
9604	S(OC1CC2=CC(=O)C3C4CCC(C(CCCC(C)C)C)C4(CCC3C2(CC1)C)C)(O)(=O)=O	5.8	Bad	5.7

9529	O(C(=O)C1N(Cc2ccccc2)C(CC1)C(OCC)=O)CC	4.3	Excellent	5.7
9489	O1C2OC(=O)CC12CCC=C(CC(O)CC(CCCc1ccoc1)C)C	5.3	Excellent	5.7
9392	O1C(O)C2=C(C(OC)CC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	5.7	Poor	5.7
9173	O(C(=O)C)C1C(C2C(CC1=O)(C1C(CC2OC(=O)C)=CC(CC1)(C=C)C)C)(C)C	5.2	Good	5.7
9136	O(C(=O)C)C1CC2C(C3CC(O)C(CC13C)C(=O)C)(CCC1C(CCCC12C)(C)C)C	5	Poor	5.7
9027	o1cc(cc1)CCCC(=CC=CC(CCC=C(CC(O)C(O)=O)C)C)C	4.7	Bad	5.7
8917	O1C(C(O)C(C(=O)C(C(O)CC(=O)CC)=C)COC(=O)C)(C)C1C(C=CC)C	5.4	Good	5.7
8631	O=CNCCCNCCCN1CCCCCCCCC=CCCCC1	4	Bad	5.7
8590	O1C2(O)C(CC3(C(CCCC3C)C2=O)C)=C(C)C1=O	5.8	Excellent	5.7
8381	O(C)c1cc(OC)ccc1C=CC(=O)c1ccc(OC)cc1O	6.1	Good	5.7
8232	O1C(O)C2=C(C(O)CC3C(CCCC23C)(C)C)C1=O	5.3	Excellent	5.7
8231	O1C(O)C2=C(C(O)CC3C(CCCC23C)(C)C)C1=O	5.4	Excellent	5.7
8220	O1C(O)C2C(=CCC3C(CCCC23C)(C)C)C1=O	4.9	Good	5.7
8181	O1C23CC(O)CCC2(C)C(=O)C(CC13)C1CCC(C(C)C2CC2(C(C(C)C)C)C)C1(CCO)C	4.4	Poor	5.7
7863	O1c2c(C(=O)C=C1CCC)c(OC)c1c(cc(O)cc1OC)c2	5.6	Good	5.7
7731	O1C(=O)C(=CC1CC(=O)C)CCC(C(O)c1oc(cc1C)C=O)C(C)=C	5.4	Poor	5.7
7261	OCC=C(CCC=C(CCC(=O)C(CC(=O)C=C(C)C)=C)C)C	6.1	Poor	5.7
6787	O1C2(CCC1C1(CCC3OC(C)(C)C(O)CCC13C)C)C1(C(OC(C)(C)C(=O)CC1)CCC2C)C	4.4	Bad	5.7
6749	O(C(=O)C)c1ccc(OC(=O)C)cc1C#CC(C)=C	4.2	Poor	5.7
6649	Oc1cccc(-c2cc(ncc2)C)c1NC(=O)CCCCCCCCC	4.7	OK	5.7
6515	BrC1=C2C(C=3S(=O)(=O)C=CNC=3C1=O)=CN(CC2)C	4.9	Excellent	5.7
6317	Brc1cc2c3c([nH]c2cc1Br)c(ncc3)C1=NCCC1	4.2	Bad	5.7
6190	O(C(=O)C)c1ccc(cc1)CCC=CC=CC=CCCOC(=O)C	5.4	Bad	5.7
5822	O1C(=O)C(=CC1OC)CCC1(C)C(CC(=O)C=C1C)C	5.3	Excellent	5.7
5821	O1C(=O)C(=CC1O)CCC1(C)C(CC(=O)C=C1C)C	5	Excellent	5.7
5613	O1C(O)(C)C(=O)C(C)=C1C(=CC(CC(CC(CCC)C)C)C)C	4.9	Good	5.7
5159	O1c2c(c(cc(O)c2)C)C(=O)c2c1cc(O)cc2OC	5.3	Excellent	5.7
4319	O(CC(OC)=O)c1c2nc3c(nc2ccc1)cccc3	5.6	Good	5.7
4282	O1C2CC(C=C)(C)C(CC2=C(C)C1=O)C(C(OC)=O)=C	5.5	Excellent	5.7
4135	S(CC1N2C3(C(CCCC3)C(=O)CC2CCCCCC)CC1)C#N	4.8	Excellent	5.7
4134	O=C1CC(N2C3(C1CCCC3)CCC2COC(=O)C)CCCCCC	4.4	Good	5.7
4088	Clc1c([nH]c(Cl)c1Cl)-c1oc(cn1)-c1ccc(O)cc1	4.2	Bad	5.7
3979	O1C2OC=C(C3C2C(CC3)C1OC(=O)C)CCC=C(C)C	4.5	Good	5.7
3861	O1C(C(C(OC(=O)CC)C(C(=O)CC)C)C)C(C)C(=O)C(C)=C1CC	5.4	Excellent	5.7
3522	O1C2OC=C(C3C2C(CC3)C1OC(=O)C)C(=O)CCC(C)C	5.9	Good	5.7
3520	OC1C2CC(O)CCC2(C)C(=O)C(=C1)C1CCC(C(C=CC(C)C)C)C1(CCOC(=O)C)C	5.1	Poor	5.7
3332	O1C(=O)C(CC1C=C(C)C)=CCCC(=CCCC(=O)C)C	6	Good	5.7
3093	Brc1cc2[nH]c3c(c2cc1)ccnc3C(=O)CC(C)C	4.7	Bad	5.7
2734	O1c2c(C=C(OC)C1=O)cc1C=C(OCc1c2O)C(=CC(CC)C)C	4.2	Poor	5.7
2728	OC1C2CC(O)CCC2(C)C(=O)C(=C1)C1CCC(C(CCCC(C)C)C)C)C1(CC=O)C	4.5	Good	5.7
2412	OC12CC3(C(CCC1(CCCC2=C)CO)=C(CC3)C(C)C)C	4.6	Good	5.7
2409	O(C(=O)C)C1C(=CC2(C(=CC(O)CC2C)CCC1=O)C)C	4.5	Excellent	5.7
2117	O=C1c2c(cccc2)C(=O)C1=CNN(C(OCC)=O)C	4.2	Excellent	5.7
2102	OC(C=CC(=O)C(O)(C)C)(C)C1CC(C(C)=C)C(CC1)(C=C)C	4.3	OK	5.7
1951	S(CC=1CCC2C(C=1)Cc1occc1C2(C)C)C(=O)C	4.4	Excellent	5.7
1934	O1C(O)(C)C(=O)C(C)=C1C(=CC(CC(CCC)C)C)C)C	4.1	Excellent	5.7

1438	O1CC12CCCC1C(CCC(CC(O)=O)C)(C)C(CCC12C)C	6.3	OK	5.7
1346	BrC(C(OC(=O)C)CC1OC(OC(Br)C#C)CC1O)CC=CCC	5.3	Good	5.7
1160	O(C(=O)C)C1CC2C(C)(C(C(=O)C1C(=O)C)C(=O)CC1C2(CCC2C(CCCC12C)(C)C)C	5.6	Poor	5.7
1159	o1cc(cc1)CCCC(=CC(O)CC(=CCCc1ccoc1)C)C	5.2	Excellent	5.7
1132	O(C)c1cc(c2c(C(=O)C(C)(C)C2=O)c1C)C(C)C	4.7	Excellent	5.7
1121	O1C(C(OC)=O)C(CO)C(C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1O	3.9	Good	5.7
939	S1(=O)(=O)C2=C(NCC1)C(=O)c1c(cc3c(c1)C(=O)c1occ4c1C3(CCC4)C)C2=O	5.6	Poor	5.7
769	O1c2c(C(=O)C=C1CCC)c(O)c1c(cc(O)cc1OC)c2OC	5.3	Good	5.7
709	S1CC(N)C2N(OC1)CCc1c2[nH]c2c1cccc2	4	OK	5.7
664	O(C)C1=CC(=O)C=C(CC=C(CCC=C(C)C)C)C1=O	4.1	Excellent	5.7
535	O(C(=O)C)C1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)C=O	5.4	OK	5.7
298	Oc1ccc(O)cc1CC=C(CCC=C(C)C)C	4.3	OK	5.7
25	ClC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	6.6	Good	5.7
14340	OC(CC=CCC)C=CC=CCC=CCC=CCCCC(O)=O	5	Excellent	5.6
14325	O=C1C23C(CCC2(C=C(C(OC)=O)C3C)C)C(C1)C	4.2	Excellent	5.6
14316	O(C)C1=C(C)C(=O)c2c(C1=O)c(ncc2)COC(=O)C	4.8	Poor	5.6
14059	OC1C2C(CC=C2C)C(CCC1C(CC(O)C=C(C)C)C)=C	4.2	Poor	5.6
13932	OC1CC2(C(CC=C(CCC=C1CO)C)C(CC2)C(C)=C)C	5.1	Good	5.6
13778	Brc1cc2c3CCN4OCSCC(N)C4c3[nH]c2cc1	3.9	Excellent	5.6
13739	O1C(=O)C(=CC1=CC1(OOC(CC1)C(=CCO)C)C)C	3.4	Excellent	5.6
13738	O1C(=O)C(=CC1=CC1(OOC(CC1)C(=CCO)C)C)C	4.9	Excellent	5.6
13737	O1C(=O)C(=CC1=CC1(OOC(CC1)C(=CCO)C)C)C	3.9	OK	5.6
13736	O1C(=O)C(=CC1=CC1(OOC(CC1)C(=CCO)C)C)C	3.6	Excellent	5.6
13690	O(Cc1ccc(cc1[N+](=O)[O-])C(OC)=O)c1ccccc1	5.9	Good	5.6
13626	O1C(=O)C(C)=C(O)C(C)=C1C(=CC(=CC(CC(CCC)C)C)C)C	5.2	Excellent	5.6
13625	O1C(=O)C(C)=C(O)C(C)=C1C(=CC(=CC(CC(CCC)C)C)C)C	4.6	OK	5.6
13287	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(C(OC(=O)C)C)C)C)C)C)C1=O)C	4.3	Poor	5.6
13138	O1CC2(C3=C(C(C)(C)C2O)C(O)CC(C3=C1)C)C	4.4	Excellent	5.6
12970	O1C2(CC(=O)C(=CC=CC(=O)C)C)C(CC(O)CC12C)(C)C	5.7	Poor	5.6
12755	Oc1c(cc(O)cc1C)CC=C(CCC=C(C)C)C	4.8	Good	5.6
12722	O1C(O)C2=C(CCC3C(CCCC23C)(C)C)C1=O	4.8	Poor	5.6
12614	OC(CO)(C)C1=CC2(C(CC1)=CCCC2C)C	3.9	Excellent	5.6
12526	OC(CCC=C(CC(=O)C=C(C)C)C)(C=CCC(=CCO)C)C	5.1	OK	5.6
12374	O1C2(OC)C3CC(CCC2=CC1=O)(C)C(O)(C)C(C3)=C	5.3	OK	5.6
12315	O1C2C(C3(C(=CC(O)CC3C)CC2)C)C(C)C1O	4.7	Excellent	5.6
12155	O1c2c(CC13C1(C(CCC3C)C3(C(CC1)C(C)(C)C(O)CC3)C)C)cc(O)cc2C	4.2	Bad	5.6
12144	O1c2c(CC13C1(C(CCC3C)C3(C(CC1)C(C)(C)C(O)CC3)C)C)cc(O)cc2C	3.9	Bad	5.6
11848	O1C2C13C(CCC1(C3CCC1C(CCCC(C)C)C)C)C1(CCC(OC(=O)C)CC1(O)C2O)C	3.3	Poor	5.6
11571	O(C(=O)C)C=C(C(O)CC=C(C=CC=C(C)C)C)C=CO	5.3	Poor	5.6
11381	Brc1cc([NH+]2C=Cc3c([nH]c4cc(Br)ccc34)[CH-]2)c(cc1)C(OC)=O	3.6	OK	5.6
11039	O1C2C3C(CCC2C(C)C1=O)(C)C(=O)CCC3=C	4.9	Excellent	5.6
10968	OC(C=CC=C(CO)C1CC2C(CC1)(CCCC2=C)C)(C)C	3.9	Excellent	5.6
10905	O1C2C(CCC(=C)C(O)CCC(=C2)C)C(=C)C1=O	4.6	Excellent	5.6
10603	ClC1C2OC(C(C1)C2C=CCC=CCCCCC(O)=O)CC	5.4	Bad	5.6
10548	BrC1CCC(=C)C(Cc2cc(O)c(Br)cc2O)C1(C)C	5.2	Excellent	5.6
10472	OC1C2C(CC=C2C)C(=C)C(O)CC1C(CCC=C(C)C)C	4.5	Excellent	5.6

10376	O(C(=O)C)c1c2nc3c(nc2ccc1)cccc3	5.4	Good	5.6
10324	OC1CC(=O)C(CCC(=O)CCCCC)C1CC=CCCCC(O)=O	6.8	Excellent	5.6
9875	BrC1CCC(CC1(C)C)=CC1C2C(CC1O)(C)C(Br)CCC2(O)C	5	Good	5.6
9719	O1C=C(c2ccc(OC)cc2OC)C(=O)c2c1cc(OC)cc2O	3.4	Poor	5.6
9298	O=C1C(=C(O)CCCC(CCCCCCC)C)C(=O)N(C)C1C	4.5	Excellent	5.6
9278	O(C)c1ccc(cc1)CC=1N(C)C(=N)N(C)C=1Cc1ccc(OC)cc1	4.5	Poor	5.6
9145	O1CC(C2C(C(CC(OO)CC(CC2)=C)=C)C1=O)=CC=CC(O)(C)C	5.8	Poor	5.6
8745	Brc1cc2OC(CC(=O)c2cc1O)(CCCC(O)(C)C)C	5.6	Poor	5.6
8741	O(Cc1ccccc1)c1cc2c([nH]cc2CCO)cc1	5	OK	5.6
8616	O1OC(CC(CC)C1CC(OC)=O)(CC)C=CCC(C)C	5	Good	5.6
8290	O1C(O)(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	3.7	Good	5.6
8283	OC1(CCC=C(CCC=C(CCC(O)C=C1)C)C)C	4.1	Excellent	5.6
8210	BrC1C(C)(C)C2(CCC(O)(C=C2)C(Br)Br)C(CC1O)=C	4.7	Excellent	5.6
8101	O(C(C=CC(OC(=O)C)C(C=CC=C(C=C)C)C)(C)C)C(=O)C	5.4	Good	5.6
7866	OC1CC(=O)C(CC=CCCCC(OC)=O)C1C=CC(O)CCCCC	6.2	Excellent	5.6
7837	OC(CCC)C=Cc1cc(ccc1C=CCC(=O)N)C	4.8	Good	5.6
7369	O1CC(C2C(C3(OC)CC(CC2)(C)C(O)CC3)C1=O)=CC=CC(C)C	5.9	Good	5.6
7210	OC1C(C2C(=CC1=O)C=CC2)C=C(C=CC(O)CCCCCCC)C	4.7	Bad	5.6
7081	O(C)c1cc(OC)ccc1C(=O)C=Cc1ccc(OC)cc1OC	4.4	Poor	5.6
6869	O1C(O)C2=C(CCC3C(CCCC23C)(C)C)C1=O	4.8	Excellent	5.6
6760	O1c2c(C(=O)C1=Cc1cc(OC)c(OC)cc1)c(OC)cc(OC)c2	4.6	OK	5.6
6657	O(C)c1cc(ccc1C(C=CC=C(C)C)C)C(O)=O	5.4	Excellent	5.6
6603	O(O)C1C=C(C)C2(C(C1)C(CCC(O)(C=C)C)(C)C(CC2)C)C	4.9	Excellent	5.6
6490	O1c2c(Oc3c1ccc(O)c3C=O)ccc(O)c2C=O	5.6	Excellent	5.6
6374	Brc1cc2c([nH]cc2-c2nc(ncc2)N)cc1	4.3	Poor	5.6
6243	O1C(=O)C(=CC1OC)CCC=C(C(O)CC=C(C)C)C	4.5	Excellent	5.6
6191	Oc1ccc(cc1)CCC=CC=CC=CCCOC(=O)C	4.3	Bad	5.6
6173	Oc1c2c(c3[nH]c(cc3c1C)COC)C(=O)CC2	4.4	Excellent	5.6
6122	O(C(C(O)(C)C)CC=C(C)C1CC(C(C)=C)C(CC1)(C=C)C)C(=O)C	4.3	Poor	5.6
5759	o1cc(cc1)CCC=C(CC(=O)CC(=CCCc1ccoc1)C)C	5.7	OK	5.6
5482	O1C(CCC1=O)C=CCC1C(C=CC1=O)C=CCCCCCC	6.9	Excellent	5.6
5361	n1c2c3C(CC(C)C2CCCC)CCc3nc1N	4.9	OK	5.6
5188	O1C2(C)C(O)C(COC(=O)C)C1(OC2C(C=CC)C)C(C(O)CC(=O)CC)=C	3.9	Bad	5.6
5053	O1C(O)C(=CC1=O)C1OCC2(O)C(C1)C1(C(CC2)C2(C(CC1)C(CCC2)(C)C)C)C	4.6	Bad	5.6
5052	O1C(O)C(=CC1=O)C1OCC2(O)C(C1)C1(C(CC2)C2(C(CC1)C(CCC2)(C)C)C)C	5.8	Poor	5.6
5051	O1C(O)C(=CC1=O)C1OCC2(O)C(C1)C1(C(CC2)C2(C(CC1)C(CCC2)(C)C)C)C	4.2	Bad	5.6
5050	O1C(O)C(=CC1=O)C1OCC2(O)C(C1)C1(C(CC2)C2(C(CC1)C(CCC2)(C)C)C)C	4.6	Bad	5.6
4889	O1C(=O)C(=CC1O)CCC=C(CCC=C(C)C)C	4.7	Poor	5.6
4832	O(C(=O)C)C1C2C(CCCC2(C2CCC(=CC2(C1)C)C1CC(=O)C(=CC1O)C)C)(C)C	4.5	Bad	5.6
4592	O1C2CCC(C)C(O)(CCC3C4(C(OC(C)(C)C(=O)CC4)CCC3=C)C)C2(CCC(=O)C1(C)C)C	4.1	Bad	5.6
4090	Clc1cc[nH]c1-c1oc(cn1)-c1ccc(O)cc1	5	Excellent	5.6
4016	S1CC(N=C1C1CC1C)C=CCCC=CC=C(CCC(OC)CC=C)C	4.3	Bad	5.6
3994	O1CC=2C(C3(C(CC=2)C2(C(CC3OC(=O)C)C3(C(CC2)C(C)(C)C(=O)CC3)C)C)C)C1O	4.8	OK	5.6
3980	O(C(=O)C)C=C(CCC=C(CCC=C(C)C)C=O)C=COC(=O)C	6	Bad	5.6
3922	ClC=C(CNC(=O)CCC=CCC(OC)CCCCC)C=1C(=O)C(CCC=1C)C	4.7	Bad	5.6

3921	O1CC=2C(C3(C(CC=2)C2(C(CC3OC(=O)C)C3(C(CC2)C(C)(C)C(=O)CC3)C)C)C)C1O	4	Poor	5.6
3587	O(C(=O)C)C1CC2CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	4.3	Poor	5.6
3581	OC1C2C(CC=C2C)C(CCC1C(CCC(O)C(OC)(C)C)C)=C	4.6	Good	5.6
3415	Oc1ccc(cc1)C=CNC1=CC2=NCCc3c2c(n(c3)C)C1=O	3.3	Bad	5.6
3395	O1CC2C(=CCC3C2(C)C(=O)CC2C3(CCC3C(CCCC23C)(CC)C)C)C1(O)C	4.9	Bad	5.6
3199	O1C23C1C(OC(=O)C)CC(C)C2(C)C(C(=O)C)C(=O)CC3	4.6	Good	5.6
3092	Brc1cc2[nH]c3c(c2cc1)ccnc3C(N)CC(C)C	3.7	Poor	5.6
2862	O1C(=O)C(=CCC1C(O)(C)C)C1CC(C(C)=C)C(CC1)(C=C)C	6.4	OK	5.6
2548	O(Cc1ccccc1)c1ccc(cc1[N+](=O)[O-])C(OC)=O	5.4	Good	5.6
2380	O1C2OCC(OC(=O)C)C(C2C2(C3C(CC2)C(CCCC3=C)(C)C)C)C1OC(=O)CC(C)C	5.6	Bad	5.6
2112	O1C(CCCC1=O)C1CC1C(O)C=CC(O)CC=CCCCCC	4.9	OK	5.6
2110	O1C(CCCC1=O)C1CC1C(O)C=CC(O)CC=CCCCCC	3.9	Bad	5.6
2092	O(C(C(CC=O)=COC(=O)C)CC=C(C#CC=C(C)C)C)C(=O)C	5.4	Poor	5.6
1946	O1C(=O)C(=C2CC3(C(CC12O)=CCCC3C)C)C	5.4	Excellent	5.6
1935	O1C2=CC(C=C)(C)C(CC2=C(C)C1=O)C(C(OC)=O)=C	6.1	Excellent	5.6
1797	O1c2c(cc(O)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(CO)C)C)C	4.1	Bad	5.6
1761	O(C)C1=C(C)C(=O)c2c(C1=O)c(ncc2)COC(=O)CC	5	Excellent	5.6
1741	o1cc(cc1)CCCC(O)(CC(O)C=C(CC=Cc1ccoc1)C)C	3.9	Bad	5.6
1698	O1C(CC=CCCCC1=O)C1CC1C(O)C=CC(O)CCCCC	4.5	Poor	5.6
1686	OC1CCC23C(CCC4C2(CCC2(C)C4(CCC2C(CC(=O)C=C(C)C)C)C)C3)C1(C(O)=O)C	6.3	Poor	5.6
1554	O1C2C(OC3CC4OC(CC(O)C4OC3(CC2)C)CC(C=O)=C)CCC(O)(C)C1CCC=CC=C	4.2	Poor	5.6
1519	OC1C2C(CC=C1C)C(O)(CCC2C(CCC=C(C)C)C)C	4.5	Excellent	5.6
1259	ClC(Cl)(Cl)C(CC1N(C(=O)CC(C(Cl)(Cl)Cl)C)C(=O)C(C)(C)C1O)C	6.1	Excellent	5.6
1053	Brc1cc2[nH]c3C4N(OCS(=O)CC4N)CCc3c2cc1	3.7	Poor	5.6
861	ClC1C2C(CCC1(O)C)C([NH+]=[CH-])(CCC2C1(OC(CC1)C([NH+]=[CH-])(C)C)C)C	4.2	Poor	5.6
518	OC1(C2C(C=C(CC1)C(CC(=O)CC(C)C)C)C(O)(CC2)C)C	5.5	Excellent	5.6
517	OC1(C2C(C=C(CC1)C(CC(=O)CC(C)C)C)C(O)(CC2)C)C	3.9	Good	5.6
224	O1C(=O)C(=CC1O)CC1C=C(CCC1C(C)=C)C	6	Excellent	5.6
74	O1C(C2C3(CC=C4C(CCC5C(C)(C)C(O)CCC45C)C3(CC2)C)C1=O)(CC(=O)CC(C)C)C	5.2	Good	5.6
29	ClC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	4.7	OK	5.6
13867	O(C(=O)C)C=1C(=O)C(=CC(=O)C=1C)C(CCC=C(C)C)C	4.3	Poor	5.5
13791	OC(CC=CCC)C=CC=CCC=CCC=CCCCC(O)=O	5.3	Bad	5.5
13777	Brc1cc2[nH]c3C4N(OCSCC4N)CCc3c2cc1	4.2	Excellent	5.5
13759	OC1CCC(C2C(CC=C1C)C(C2)(CC(O)C=C(C)C)C)=C	5.4	Excellent	5.5
13701	N1C=2C3C(CC(C)C=2CCCC)CCC3N=C1N	3.8	Poor	5.5
13605	O=CC1(CC1C=C(CCC=C(C)C)C)C1CC=C(C=O)C1C=O	4.5	Good	5.5
13453	N1C=2C3C(CC(C)C=2CCCC)CCC3N=C1N	3.6	Excellent	5.5
13422	OC1CC(CCC(=C)C(O)CCC1=C)C(C)=C	4.6	Excellent	5.5
13389	OC(CC=CCC)C=CC=CCC=CCC=CCCCC(O)=O	4.3	Bad	5.5
13259	O1C(=O)C(=CC1O)CCC1C(CCCC1=C)(C)C	5	Excellent	5.5
13214	o1cc(cc1)CCC=C(CC(O)C=C(CC=Cc1ccoc1)C)C	4.7	Poor	5.5
13207	O1C(C=2C(C3(C(CC=2)C2(C(CC3OC(=O)C)C3(C(CC2)C(CCC3)(C)C)CO)C)C)C1O)C	4.6	OK	5.5
13047	O=C1N(CCCCN=C(N)N)C(CC1)=CC=CCC=CCC	5.1	OK	5.5
13046	O=C1N(CCCCCN=C(N)N)C(CC1)=CC=CCC=CCC	5	Poor	5.5
12938	BrC(COC(=O)C)C1(CC2C(=CC1)C1(C(CC2O)C2(O)C(CC2)C(OC(=O)C)C1)C)C	5	Good	5.5

12842	O1C(CCC(=O)C=CC=CC)(C)C(OC)=C(C)C1=O	6.5	Poor	5.5
12771	OC1CC(C(=CCC=C(C)C)C)C(C2C(C=CC2=O)C)C1C=O	4.8	Excellent	5.5
12768	OC1C2(C=O)C(CCC1(CC=C2C=O)C)C(CCC=C(C)C)C	4	Bad	5.5
12726	OC(C(O)CCC(=CCCC(=CCCC(=O)C)C)C)(C)C	3.7	Good	5.5
12477	N1C2C3C(CC(C)=C2CCCC)CCC3N=C1N	3.4	Excellent	5.5
12476	N1C=2C3C(CC(C)C=2CCCC)CCC3N=C1N	4.2	Poor	5.5
12185	BrC1CC2OC2CC(OC1CC)C(O)C(Cl)C=CC#C	4.8	Poor	5.5
12013	O1C2C(C3(C(=CC(O)CC3C)CC2)C)C(C)C1O	4	Good	5.5
11949	BrC12OC3C(CC(Br)C(O)(C3)C)(C1(C)C)C(O)(C=C2)C	4.4	Excellent	5.5
11476	O1CC23C(CCC4(C5Cc6cc(OC(=O)C)ccc6OC5(CCC24)C)C)C(CCC3)(C)C1=O	4.5	Bad	5.5
11339	O1C2C(CCC(=C)C(=O)CCC(=C2)C)C(C)C1=O	5.4	Excellent	5.5
10744	OC1CCC(O)(C=CC(CCC1=C)C(C)C)C	5.4	Excellent	5.5
10591	OC1=CC(=O)C(C=CC(O)CCCCC)C1CC=CCCCC=O	4.8	Poor	5.5
10147	ON=CCc1c2c([nH]c1)cc(cc2)CC=C(C)C	4	OK	5.5
9884	O=C1CCC(C=CC(O)CCCCC)=C1CC=CCCCC(OC)=O	5.1	Good	5.5
9811	N1C=2C(N=C1NC)=C(C1=NC(=NC1=CC=2)N(C)C)C	4.6	Poor	5.5
9720	O(C(C(CCC(=CC=O)C)CC=C(CCC(O)C(C)=C)C)(C)C)C(=O)C	4.6	Bad	5.5
9476	O(CC)C1=C(C)C(=O)C2=C(c3n(C=C2)c(nc3)C)C1=O	4.8	Excellent	5.5
9432	S(OC1CC2C(C=3C(C4CCC(C(=O)C)C4(CC=3)C)CC2O)(CC1)C)(O)(=O)=O	5.5	Poor	5.5
9304	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCCC(CC)C	5.2	Bad	5.5
9039	Brc1cc(cc(Br)c1OCC[C-]([N+](C)(C)C)C(O)=O)CCNC(=O)C	4.4	Bad	5.5
8965	O1C23C1C(O)C=1C(CCC4(C=1CCC4C(CCC(C(C)C)CC)C)C)C2(CCC(O)C3)C	4.1	Poor	5.5
8678	O1CC2=C(C3C(CO)C2(CCC3C(C)C)C)C1=O	5.2	Excellent	5.5
8630	N(CCCN1CCCCCC=CCC=CCCCC1)CCCN	3.7	Poor	5.5
8519	IC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	4.2	Good	5.5
8296	o1cc(cc1)CCCC(CC(=O)CC(=CCCc1ccoc1)C)C	4.3	Excellent	5.5
8228	O1C(OCC)C2=C(C3(C(CC2O)C(CCC3)(C)C)C)C1=O	5	Excellent	5.5
8221	O1CC=2C(C3(C(CC=2)C(CC(O)C3)(C)C)C)C1=O	5.9	Excellent	5.5
8217	o1cc(cc1)CCCC(CC(O)CC(=CCCc1ccoc1)C)C	4.5	Poor	5.5
7899	BrC1CC(CCC1(O)C)C(=CC=CC(O)(CCC=C(C)C)C)C	4.2	Excellent	5.5
7858	Oc1cc([n+]([O-])c2c1cccc2)CCCCCCCCC	4.3	Excellent	5.5
7772	O1C(C2=C(C3(C(CC2)C2(C(CC3OC(=O)CC(O)C)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	4.8	Poor	5.5
7771	O1C(C2=C(C3(C(CC2)C2(C(CC3OC(=O)CC(O)C)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	4.2	Good	5.5
7600	S(OC1CC2C(C=3C(C4CCC(C(=O)C)C4(CC=3)C)CC2O)(CC1)C)(O)(=O)=O	4.5	Bad	5.5
7563	O([N+](=O)[O-])Cc1c2CC(Cc2cc(C)c1CCO)(C)C	4.7	Good	5.5
7399	o1cc(cc1)CCCC(O)(CC(O)C=C(CC=Cc1ccoc1)C)C	5.7	Poor	5.5
7305	O1C(C=2C(C3(C(CC=2)C2(C(CC3O)C3(C(CC2)C(CCC3)(C)C)COC(=O)C)C)C)C1O)C	5.1	Bad	5.5
6656	Oc1c(O)c(ccc1C(C=CC=C(C)C)C)C=O	5	Excellent	5.5
6394	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)CO	4.9	OK	5.5
6179	O1OC(C=C(CC)C1CC(O)=O)(CC(CCCC)C)CC	5.6	Poor	5.5
6004	OC(CC=CCC)C=CC=CCC=CCCCCC(O)=O	5.4	Bad	5.5
5936	O1C(O)C2(O)C(C3(C(CC2)C(CCC3)(C)C)C)C1OC	4.6	Excellent	5.5
5794	O=C1C(=CC=C2CC(=O)CCC12C)C1CCC(C(CCCC(C)C)C)C1(CC=O)C	3.8	Bad	5.5
5481	O1C(CCC1=O)C=CCC1C(C=CC1=O)C=CCCCCCC	4.2	Poor	5.5
5408	OC(C(CCCC(CCC1C(CCCC1C)(C)C)C)=C)CO	5.8	Excellent	5.5

5061	BrC1CCC(CC1(C)C)C1(Cl)C2OC2C(O)(CC1)CO	5.1	Poor	5.5
4648	S1CC(N=C1C1CC1C)C=CCCC=CC=CCCC(OC)CC=C	4.7	Bad	5.5
4210	O1C2CC(OC(C=CC2O)CC)C1C(O)C=CC#C	3.7	Excellent	5.5
4132	O=C1CC(N2C3(C1CCCC3)CCC2CO)CCCCCC	4.2	Bad	5.5
4065	O1OC(CCC1(OC)CCCC=CC(=CCC)C)C(C(O)=O)C	4.5	Poor	5.5
4064	O1OC(CCC1(OC)CCCC=CC(=CCC)C)C(C(O)=O)C	5	Excellent	5.5
4060	O1OC(CCC1(OC)CCCC=CC(=CCC)C)C(C(O)=O)C	6.6	Excellent	5.5
3992	O1OC(C=CC1(OC)CCCC1OOC(C=C1)CCC)CC(OC)=O	3.3	Good	5.5
3898	O1OC(CC(CC)C1CC(O)=O)(CCCC(CC)C=CCC)CC	4.5	Bad	5.5
3450	O(C(=O)CCCCC=CCC(=CC=CC=CC(O)CC)C=O)C	5.9	OK	5.5
2733	O1Cc2c(C=C1C(=CC(CC)C)C)cc1c(C(=O)C(=O)C(OC)=C1)c2O	4.4	Poor	5.5
2604	o1c(ccc1CC(O)=O)CC=CCC=CCC=CCC=CCC	5.1	Excellent	5.5
2598	Brc1c2c3c4n(c2ccc1O)CN(C)C(c4ncc3)CSC	3.5	Good	5.5
2398	S=C=NC1(C2C(=CC(O)(CC2)C)C(CC1)C(C)C)C	4.5	Excellent	5.5
1980	O1C23CC(CCC(=O)C(C)C)(C)C1(O)CCC2(CCCC3=C)C	4.3	Excellent	5.5
1921	OC1CC(C=CCC(=C)C(O)CCC1=C)(C)C	4.4	Excellent	5.5
1826	S(OC1CC2=CCC3C4CCC(C(CCCC(C)C)C)C4(CCC3C2(CC1)C)C)(O)(=O)=O	5.4	Bad	5.5
1650	OC(C(=CCC(=O)C1(CCCC1C(=O)C)C)C)CC=C(C)C	3.9	Poor	5.5
1133	O(C)c1cc(c2c(C(=O)C(C)(C)C2O)c1C)C(C)C	5.3	Excellent	5.5
1062	OC(CC=CCC=CCCCC(O)=O)C=CC=CC(=O)C=CCC	4.9	Bad	5.5
889	O1C2(CC(=O)C(=CC=CC(O)C)C)C(CC(O)CC12C)(C)C	4.3	Good	5.5
637	OC1CCC(O)(C=CC(CCC1=C)C(C)C)C	4.7	Good	5.5
536	OC1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)C(O)=O	5.3	Bad	5.5
436	O1C(CC2C(C3C(CC12C)C=C(CC3)C)(C)C)C1(OOC(CC1)C(C(O)=O)C)C	5.7	Good	5.5
308	OC(CC=CCC)C=CC=CCC=CCC=CCCCC(O)=O	5.2	OK	5.5
31	ClC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	5.6	Good	5.5
14070	O(C(=O)C)C=C(C(O)CC=C(CCC=C(C)C)C)C=CO	3.5	Excellent	5.4
14069	OCC=1CCC(C(CCC=C(CCC=C(C)C)C)C=O)C=1C=O	4.3	Bad	5.4
13957	O1C(O)(CC)C(C)C(=O)C(C)C1C(=CC(CCC)C)C	3.8	Excellent	5.4
13946	ClC(Cl)(Cl)C(CC(OC)=CC(=O)N1C(C(C)C)C(OC)=CC1=O)C	4.3	Excellent	5.4
13849	O(C)C1(c2c(CC1O)c(ccc2C=C(C)C)C=O)C	4.6	Excellent	5.4
13843	OC1CC(=CCC=C(C=O)C(C=O)C1C(CCC=C(C)C)C)C	4.9	Bad	5.4
13720	O(C)C1=CC(=NC1=CNCCC=CCCCCCCCC)c1[nH]ccc1	5.4	Poor	5.4
13612	OC1CCC2=CC(O)CC(C)C2(C)C1C(=O)C	4.5	Poor	5.4
13611	OC1CCC2=CC(O)CC(C)C2(C)C1C(=O)C	4.6	Poor	5.4
13610	OC1CCC2=CC(O)CC(C)C2(C)C1C(=O)C	4.8	Excellent	5.4
13500	Oc1ccc(O)cc1C1C=C(CCC1C(OC)(C)C)C	4.5	Excellent	5.4
13019	O(C(CC(=CCCC(=CC(O)CC(O)(C=C)C)C)C)C=C(C)C)C(=O)C	5.2	Poor	5.4
12821	OC1(C=CC(=O)C1=CC=CCC)CCCCCCCC(O)=O	7.1	Excellent	5.4
12655	S(OC1CC2=CCC3C4CCC(C(C=CCC(C)C)C)C4(CCC3C2(CC1)C)C)(O)(=O)=O	6.5	Excellent	5.4
12568	O1C(OC(=O)C)C2C(=CCC3C4(C(CCC23C)C2(C(CC4)C(CCC2)(C)C)C)C)C1=O	5.3	Excellent	5.4
12139	O(C)c1cc(ccc1O)CCNC(=O)C=C(CCCCCCCCCC)C	4.4	Bad	5.4
12137	Oc1ccc(cc1)CCNC(=O)C=C(CCCCCCCCCC)C	6.1	Poor	5.4
11947	O1OC(CC(CC)C1CC(OC)=O)(CC(CC)C=CCC)C	4.8	Good	5.4
11614	OC(C(O)CC=C(C)C1CC(C(C)=C)C(CC1)(C=C)C)(C)C	3.7	Poor	5.4
11507	O1C(O)C2=C(C(O)CC3C2(C)C(OC(=O)C)CC2C3(CCC3C(CCCC23C)(C)C)C)C1=O	5.3	Bad	5.4
11486	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	3.6	Excellent	5.4

11316	O1OC(CC(CC)C1CC(OC)=O)(CC)C=CCCC	4.5	Poor	5.4
11305	O=C1N(CCCCN=C(N)N)C(CC1)=CC=CCC=CCC	4.7	Bad	5.4
11304	O=C1N(CCCCCN=C(N)N)C(CC1)=CC=CCC=CCC	4.5	Bad	5.4
10731	ClC(Cl)(Cl)C(CC(OC)=CC(=O)N1C(C(C)C)C(OC)=CC1=O)C	4	Poor	5.4
10703	IC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	5	Good	5.4
10389	OC1C2C3C(C(=C)C2(CCC3C(C)C)C)C1O	5.3	Excellent	5.4
10055	O(C(C)(C)C)C(=O)n1cc(c2c1cccc2)C=O	6.5	Excellent	5.4
9958	OCC1=CCCC2C(CCC(O)(C=C)C)(C)C(CCC12C)C	4.5	Excellent	5.4
9857	OC1C2C3C(C(=C)C2(CCC3C(C)C)C)C1O	4.3	Poor	5.4
9748	O=C(NCCc1ccccc1)NCCc1ccccc1	5.3	Excellent	5.4
9488	S1SC2(N(C)C(=O)C1(N(C)C2=O)Cc1ccccc1)CO	3.6	Poor	5.4
9435	OC(=O)C12C3(C(CC1(C1C(C3)C(CC1)C)C=O)C=C2C(C)C)CO	4.9	Poor	5.4
9303	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCCCC(C)C	4.3	Poor	5.4
9301	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCCCC(CC)C	4.4	Bad	5.4
9300	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCCCCC(C)C	4.2	Bad	5.4
8964	O(C(=O)CCC(O)=O)C1CC2=CCC3C4CCC(C(=O)C)C4(CCC3C2(CC1)C)C	5.5	Bad	5.4
8746	Brc1cc2OC(C=Cc2cc1O)(CCCC(O)(C)C)C	3.9	Excellent	5.4
8660	S1SC2(N(C)C(=O)C1(N(C)C2=O)Cc1ccccc1)CO	4	OK	5.4
8615	O1OC(CC(CC)C1CC(OC)=O)(CC)C=CC(=O)CC	4.3	Good	5.4
8592	O1CC2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CCC3)(COC(=O)C)C)C)C)C)C1=O	4.5	Bad	5.4
8572	OC1CC(=O)C(CC=CCCCC(OC)=O)C1C=CC(O)CCCCC	4.9	OK	5.4
8223	O1C(=O)C2(O)C(C3(C(CC2)C(CCC3)(C)C)C)C1O	5.1	Excellent	5.4
8222	O1CC=2C(C3(C(C(CCC3)(C)C)C(O)C=2)C)C1O	4.9	Excellent	5.4
8116	Oc1cc([n+]([O-])c2c1cccc2)CCCCCCC	4.9	Excellent	5.4
7975	OCC1=CCCC2C(CCC(O)(C=C)C)(C)C(CCC12C)C	5.1	Excellent	5.4
7886	ClC(Cl)C(C=C1N(C)C(=O)C(N(C)C1=O)CC(CCl)C)C	4.9	Poor	5.4
7884	ClC(Cl)(Cl)C(CC1NC(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	4.5	Excellent	5.4
7648	O=C1C=C(Nc2c1cccc2)CCCCCCCCCO	4.5	Excellent	5.4
7592	O1C(CCCCC(CC(=CC(=CC(O)=O)C)C)C(CO)C1=O	5.8	Excellent	5.4
7222	Brc1cc(Br)cc(C(=O)Nc2ccccc2)c1O	5.5	OK	5.4
6953	OC(C(=C)C1CCC(NC=O)(CC1)C)C=CC(C)C	5.4	Excellent	5.4
6952	O=C(C(=C)C1CCC(NC=O)(CC1)C)C=CC(C)C	4.7	Poor	5.4
6807	O1c2c(CC(NC(=O)C=CC(=CC(CCCCCC)C)C)C1O)cccc2	6	Good	5.4
6767	O1C(CC(CCCCC(C)C(=O)N(C=CCC1=O)C)C)C(C)(C)C	4.2	Poor	5.4
6647	O1C23CC(OC(=O)C)CCC2(C)C(=O)C(=CC13)C1CCC(C(CCCC(C)C)C)C1(CCO)C	3.9	Bad	5.4
6389	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	4.8	OK	5.4
6382	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C)=C(Cl)Cl)C	4.4	OK	5.4
6335	O1OC(C=C(CC)C1CC(OCC)=O)(CC(CCCC)C)CC	3.6	Good	5.4
6259	OC1C23C(CCC2(C=C(C(OC)=O)C3C)C)C(C1)C	4.6	Good	5.4
6182	O1OC(C=C(CC)C1CC(OC)=O)(CC(CCCC)C)CC	4.5	Excellent	5.4
6171	O=C1CCc2c1c1[nH]c(cc1c(c2)C)COC	4.8	Excellent	5.4
5661	ClC(Cl)C(CC(N(C(=O)CC(C(Cl)Cl)C)C)C(=O)NCc1sccn1)C	4.1	Good	5.4
5409	OC(CCCC(CCC1C(CCCC1C)(C)C)C)(CCO)C	5.1	OK	5.4
5062	BrC1CCC(CC1(C)C)C12OC1C(O)C(Cl)(CC2)CO	4.9	Good	5.4
5060	BrC1CCC(CC1(C)C)C12OCC(O)(CC1)C(Cl)C2O			5.4
4821	O1C(O)C(=CC1=O)CCCC(CCCC(CCCC(C)C)C)C	4	Bad	5.4
4647	S1CC(N=C1C1CC1C)C=CCCC=CC=C(CCC(OC)CC=C)C	3.8	Bad	5.4

4509	O1C2C(C(C)C1(O)CCC(C)C)C1(C(C3C(CC1)C1(C(CC(=O)C=C1)CC3)C)C2)C	3.9	Poor	5.4
4432	O1C(CCCC1=O)C1CC1C=CC(O)C(O)CC=CCCCCC	5.7	Good	5.4
4422	O1C(CCCC1=O)C1CC1C=CC(O)C(O)CC=CCCCCC	5.9	Good	5.4
4248	O1C(=O)C(=CC1O)CCC1(C)C(CC=CC1=C)C	5.1	Good	5.4
4205	Brc1[nH]c(cc1)C1=NC(=CNCC(CC)C)C(OC)=C1	4.3	Good	5.4
4204	Brc1[nH]c(cc1)C1=NC(=CNCC(C)C)C(OC)=C1	4.5	Good	5.4
4183	S1CC(N=C1C1CC1C)C=CCCC=CC=C(CCC(OC)CC=C)C	4.5	Bad	5.4
4136	S(CC1N2C3(C(CCCC3)C(=O)CC2CCCC)CC1)C#N	4.5	Excellent	5.4
3991	O1OC(C=CC1(OC)CCCC1OOC(C=C1)CCC)CC(O)=O	3.7	Excellent	5.4
3671	ClC(Cl)(Cl)C(CC1NC(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	4.7	Excellent	5.4
3566	O(Cc1ccccc1)C(=O)NCCCC(NC(=O)C)C(OC)=O	4.7	Poor	5.4
3486	O1c2cc(ccc2OC1)C=C1N=C(N)N(C)C1=O	4.4	Excellent	5.4
3250	o1ccc(C(C)C)c1CC(C(O)=O)C1CCC2C3C(CCC12C)C1(CC(=O)C(O)=CC1CC3)C	5.9	OK	5.4
2606	o1c(ccc1CC(O)=O)CC=CCC=CCC=CCC=CCC	5.1	Poor	5.4
2474	Brc1cc2[nH]cc(c2cc1)C=CC(OC)=O	4.1	OK	5.4
2393	ClC(Cl)C(CC1N(C(=O)CC(C(Cl)Cl)C)C(=O)C(C)(C)C1O)C	4.7	Excellent	5.4
2391	O=C1CCC(C=CC(O)CCCCC)=C1CC=CCCCC(O)=O	6.1	Poor	5.4
2013	O1c2c(CC1C=CC=CC)cc(OC(=O)C)cc2OC(=O)C	4.2	OK	5.4
1742	o1cc(cc1)CCC=C(CC(O)C=C(CC=Cc1ccoc1)C)C	4.2	OK	5.4
1661	O1C2=C(C=CC(=O)C2(CC)C)C(=O)C(C)=C1C	5.9	Excellent	5.4
1491	O(C(=O)C=CC=CC(CC)C)C1C=CC2=CC(=O)C(O)CC2(C)C1C	5	OK	5.4
1277	OC1C23C(CCC2(C=C(C(O)=O)C3C)C)C(C1)C	5.5	Excellent	5.4
697	OCC(CO)=C1CC=2C(CC1)(CCCC=2C)C	5.4	Excellent	5.4
673	O1C=C(c2ccc(OC)cc2OC)C(=O)c2c1cc(OC)cc2OC	3	OK	5.4
663	O(C)C1=CC(=O)C=C(CC=C(CCCC(O)(C)C)C)C1=O	4.6	Excellent	5.4
662	O(C)C1=CC(=O)C=C(CC=C(CCCC(O)(C)C)C)C1=O	4.5	OK	5.4
14338	O(C(=O)C)c1c(C(CCC=C(C)C)C)c(O)cc(C)c1O	3.8	Excellent	5.3
14128	BrC1C(C23CC(CC2)C(CC3(O)CC1O)=C)(C)C	4.6	Excellent	5.3
13970	OC(CCCC(O)=O)C=CC=CCC=CCC=CCC=CCC	4.9	Bad	5.3
13658	o1cc(cc1)CCCC(O)(CCC=C(CCCC(O)=O)C)C	4.2	Excellent	5.3
13613	OC1CC(C)C2(C(=C1)CCC(=O)C2C(=O)C)C	3.8	Excellent	5.3
13598	O(C(=O)CC(O)C(CC(=CC(=O)CC(CC)C=CCC)C)CC)C	5.7	OK	5.3
13597	O1OC(CC(CC)C1CC(OC)=O)(CC(CC)C=CCC)C	4.7	Good	5.3
13557	O1CC(C2C(C=3CC(CC2)(C)C(O)CC=3)C1=O)=CC=CC(O)(C)C	5.8	Poor	5.3
13532	Brc1cc(C(CCCC(O)(C)C)C)c(O)cc1C	5.5	Excellent	5.3
13531	Clc1cc(C(CCCC(O)(C)C)C)c(O)cc1C	4.5	Excellent	5.3
13444	O(C(=O)C=CC(O)(C)C)C1C(C(C)=C)C(CCC1C(=O)C)(C=C)C	5.3	Excellent	5.3
13443	O1C2C(CCC(=C)C(O)CCC(=C2)C)C(C)C1=O	5.6	Excellent	5.3
13268	o1cc(cc1CC(CCC=C(C=C)C)C)C(O)=O	4.9	Excellent	5.3
13212	O1C(CCC=C(C)C)(C)C1C=CC(=CC(=O)c1[nH]ccc1)C	5.5	Bad	5.3
12587	Oc1c(C)c(O)c(cc1C(=O)C=CC=CC)C	4.3	Excellent	5.3
12586	O1C(CCC(=O)C=CC=CC)(C)C(O)=C(C)C1=O	6.4	Excellent	5.3
12532	OC1CCC2(O)CC1(CCC1C2CC1(C)C)C	4.5	Excellent	5.3
12375	O1C2(OC)C3CC(CCC2=CC1=O)(C)C(=C)C(O)(C3)C	5.1	Excellent	5.3
12309	O(C(=O)C)C1CCC2=CC(O)CC(C)C2(C)C1C(C=O)C	4.8	Good	5.3
12207	O1C(C(=CC2(OOC(CC(OC)=O)C(C2)CC)CC)CC)C1CC	4.6	Poor	5.3
12206	O1C(C(=CC2(OOC(CC(OC)=O)C(C2)CC)CC)CC)C1CC	4.6	Poor	5.3

12138	Oc1ccc(cc1)CCNC(=O)C=C(CCCCCCCCC)C	5.6	Poor	5.3
12100	O1C(OC)(CCCCCCCCC(OC)=O)C(C)=C(C)C1=O	4.6	Bad	5.3
11933	O1OC(CC(CC)C1CC(OC)=O)(CC(CCCC)CC)C	4.4	Good	5.3
11716	O1C2C3C(CCC(C)(C(C2)C)C3=C)(CC=O)C1=O	3.8	Excellent	5.3
11543	O(C(=O)C(C(O)C(C=C(CC)C=C(C=Cc1ccccc1)C)C)C)C	3.4	OK	5.3
11457	OC1CCC2(C(=CCC(O)CC2)C1C(C)C)C	3.7	Excellent	5.3
11369	Oc1cc(C)c(O)cc1C(CCC=C(C)C)C	4.7	Excellent	5.3
11340	O1C2C(CCC(=C)C(O)CCC(=C2)C)C(C)C1=O	5.5	Excellent	5.3
10981	O(C(=O)C)c1c2c(ccc1)cccc2OC(=O)C	5	Excellent	5.3
10547	Brc1cc(O)c(cc1O)CC=C(CCC=C(C)C)C	5.5	Excellent	5.3
9916	O(C)C1=CC(=O)C(O)=C(CCCCCCCCCCC)C1=O	5.2	Good	5.3
9829	O1OC(CC(CC)C1CC(O)=O)(CC)C=CCC(CC)C=CCC	5	Bad	5.3
9527	Oc1c(C=O)c(CCCCCCC)c(O)cc1CC=C(C)C	5.7	Excellent	5.3
9306	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCC(C)C	4.8	Poor	5.3
8747	Brc1cc2OC(C=Cc2cc1O)(CCC(O)C(C)=C)C	5.3	Excellent	5.3
8684	O1CC12C1C3C(C2(CCC3C(C)C)C)C(O)C1O	4.4	Excellent	5.3
8618	O1OC(CC(CC)C1CC(O)=O)(CC)C=CCCC	4.7	Excellent	5.3
8617	O1OC(CC(CC)C1CC(OC)=O)(CC)C=CCCC	4.8	Excellent	5.3
8575	O(C)c1cc(cc(OC)c1O)C=CC(OC(C)C)=O	4.8	Excellent	5.3
8488	Brc1c2c3c([nH]c2ccc1O)c(ncc3)C(N(C)C)CSC	3.6	Excellent	5.3
8376	O=C1C=CC(C=CC(O)CC=CCC)C1CC=CCCCC(O)=O	6.1	Good	5.3
8334	OC=1C(=O)C(=CC(=O)C=1C(CCC=C(C)C)C)C	4.7	Excellent	5.3
8295	o1cc(cc1)CCCC(CC(=O)CC(CCCc1ccoc1)C)C	5	Poor	5.3
8051	O(C)c1ccc(cc1)C=Cc1cc(O)cc(O)c1	4	OK	5.3
8014	O(C)C=1C(=O)C(=CC(=O)C=1C(CCC=C(C)C)C)C	5.4	OK	5.3
7801	O1OC(CC(CC)C1CC(O)=O)(CC)C=CCC(CC)C=CCC	4.1	Bad	5.3
7567	ClCCc1c(c2CC(C)(C)C(O)c2cc1C)CO	4.1	Excellent	5.3
7304	OC1CC2C3(C(CCC2(C2CC=C(C(=O)C)C(C=O)C12C)C)C(CCC3)(C)C)COC(=O)C	4.9	Good	5.3
7007	S1CC(N=C1CC(C(CC(CCN(C(=O)C(CC)C)C)C)C)C=C	4.5	Bad	5.3
6393	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)Cl)C)C	4.5	Good	5.3
6392	ClC(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)Cl)C)C	4.6	Excellent	5.3
6329	O1OC(CC(CC)C1CC(OCC)=O)(CC)C=CCC	5.5	Excellent	5.3
6318	O1C(O)(c2c(C1=O)c(O)ccc2)CCCCCC	5	Excellent	5.3
6270	ClC(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)Cl)C)C	5	Excellent	5.3
6254	O1C(CC2C(CCC3C4(C(CCC23C)C(CCC4)(COC(=O)C)C)C)C1O)C1=CC(OC1O)=O	4.1	Bad	5.3
6244	O1C(CC2C3(C(CCC12CO)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	3.7	Bad	5.3
5732	O1C2CCC(=C)C(CCC3(O)C4(C(OC(C)(C)C(=O)CC4)CCC3C)C)C2(CCC(O)C1(C)C)C	4.7	Bad	5.3
5551	OC=1C=C(C)C(=O)C(=O)C=1C(CCC=C(C)C)C	5.2	Excellent	5.3
5528	O1c2c(cc(O)cc2)C=CC1(CC(=O)CC(C)C)C	4.7	Excellent	5.3
5414	OC1C2C3C(CCCC2(C)C)(C)C1(CC3O)C	4	Excellent	5.3
5027	Oc1ccc(cc1[N+](=O)[O-])CCNC(=O)CC(C)C	4.6	Excellent	5.3
5026	Oc1ccc(cc1[N+](=O)[O-])CCNC(=O)C(C)C	5.4	Excellent	5.3
3224	O1C2C(C(CC2O)C1CC=CCC)C=CCC=CCCCC(O)=O	5.3	Bad	5.3
3223	O1C2C(C(CC2O)C1CC=CCC)C=CCCCCC(O)=O	4.9	Excellent	5.3
3200	O(C)c1c2c(c(O)c(c1)C=O)C(CCC2C)C(C)C	5.1	Excellent	5.3
2600	O1C(C2=C(C3(C(CC2)C2(C(CC3OC(=O)C)C3(C(CC2)C(CCC3)(CC)C)C)C)C)C1=O)C	5.2	Good	5.3

2488	BrC1CC(O)C(=C)C(CCC(O)(C=C)C)C1(C)C	3.9	Good	5.3
2353	O=C1C=CC(C=CC(O)CCCCC)C1CC=CCCCC(O)=O	4.6	OK	5.3
1922	O1c2c(CC1(C=CC=CC)C)cc(O)cc2O	4.4	Poor	5.3
1746	OC12CC(=O)C(C)C1(C1CC(CC1(O)C2)(C)C)C	5.3	Excellent	5.3
1490	o1cc(cc1CC(CCC=C(C=C)C)C)C(O)=O	5.6	Excellent	5.3
555	OC(C(=O)c1c2c([nH]c1)cccc2)CC(=O)C	5.5	Excellent	5.3
55	O(C)C=1C(=O)C(=CC(=O)C=1C(CCC=C(C)C)C)C	5.6	Excellent	5.3
14409	O=C1C=CC(CC=CCCCCC)C1CC=CCCCC(OC)=O	5.9	Good	5.2
14348	Oc1cc(O)cc(C(OC)=O)c1C(=O)CCCCCCC	2.9	Good	5.2
14302	O(C(=O)C=C(CCC1C(CCCC1=C)(C)C)C)CC(O)CO	4.8	Bad	5.2
14177	o1cc(cc1)CC1=CC(O)(CCC1C(C)C)CO	4.7	Excellent	5.2
13671	O1OC(CC(CC)C1CC(O)=O)(CC(CC)C=CCC)C	4.8	Excellent	5.2
13650	OC1(C2C(C=C(CC1)C(C)C)C(O)(CC2)C)C	4.4	Excellent	5.2
13601	OC1(CCC(C)(C1C)c1ccc(cc1O)C)C	4.6	Excellent	5.2
13342	OC1(CCC(C)(C1=C)c1ccc(cc1O)C)C	4.4	Excellent	5.2
13308	O(C)C1=CC(=NC1=CNCC(C)C)c1[nH]ccc1	4.4	Excellent	5.2
12807	ClC(Cl)(Cl)C(CC(N(C(=O)CC(C(Cl)Cl)C)C)C(=O)NCc1sccn1)C	4.4	Excellent	5.2
12750	BrC(CCOc1ccc(Cl)cc1Cl)(C(O)=O)C(O)=O	5.8	Bad	5.2
12674	O(C(CCCC=CC#CCCC=CCC=CCC)C(O)=O)C	4.4	OK	5.2
12653	O1C2(C=CC(=CC=O)C)C(CC(O)CC12C)(C)C	4.2	Excellent	5.2
12582	Brc1cc(cc(Br)c1OCCCN(C)C)C(O)CNC(=O)CC	4.5	Poor	5.2
12204	OC(=O)CC1C2CCC(C)C1(CC2(C)C)C(=O)C			5.2
12175	O1C(Cc2c(C1=O)c(O)ccc2)CCCCCCCCCCC	5.2	Poor	5.2
12092	O1C(O)C(C2C3(C(CCC12O)=CCCC3C)C)C	3.5	Good	5.2
12042	OC(CC=CCC=CCC)C=CC=CCC=CCCCC(O)=O	4.6	Poor	5.2
12005	OC1(C2C(C=C(CC1)C(C)C)C(O)(CC2)C)C	4.3	Excellent	5.2
11626	S(C)C1(N(C)C(=O)C(SC)(N(C)C1=O)CO)Cc1ccccc1	5	Excellent	5.2
11458	O1C(C)(C2CC(O)CCC23OC3)C1CC=C(C)C	5.5	Excellent	5.2
11427	OC1(CCCCCCC)C(=O)c2c(NC1=O)cccc2	5	Excellent	5.2
11301	o1c(ccc1C)CC(CCC(=O)c1ccoc1)C	4.2	Excellent	5.2
10868	o1cc(cc1C=C(CCC=C(C=C)C)C)C(O)=O	4.6	Excellent	5.2
10639	O(C(=O)C1N(CC(C1)C#N)Cc1ccccc1)CC	3.7	OK	5.2
10263	OC1(C2C(C=C(CC1)C(C)C)C(O)(CC2)C)C	4.4	Excellent	5.2
10103	O(C(=O)C(Cc1c2c([nH]c1)cccc2)C)CC	5.2	Excellent	5.2
10094	o1c(CCCCCCCCC(O)=O)c(C)c(C)c1CCC	4.9	Bad	5.2
9725	BrC1CCC(O)(C)C2(CC(Br)C(Cl)(CC2O)C)C1(C)C	4.5	Excellent	5.2
9504	S(C)C1(N(C)C(=O)C(SC)(N(C)C1=O)CO)Cc1ccccc1	5.3	Good	5.2
9499	S(C)C1(N(C)C(=O)C(SC)(N(C)C1=O)CO)Cc1ccccc1	3.9	Poor	5.2
9379	S(C)C1(N(C)C(=O)C(SC)(N(C)C1=O)CO)Cc1ccccc1	4.9	OK	5.2
9299	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCCCCC	4.2	OK	5.2
9111	O(C)c1cc(cc(OC)c1O)C=CC(OCCCC)=O	5	Good	5.2
8960	Oc1ccc(O)cc1C=CC(OC)(CCC=C(C)C)C	4.6	Good	5.2
8574	OC1(CC=C(C)C2(CCC(O)(C=C2)C)C1=C)C	4.4	Excellent	5.2
8466	OC1C2CC(O)CCC2(C=2C(C3CCC(C(=CC(=O)CC(C)C)C)C3(CC=2)C)C1)C	5.1	Bad	5.2
8130	O(C(=O)C)C12C3CC(CC(C1(CC2)CO)C(=C3)C)(C)C			5.2
7855	O1c2c(cc(OC(=O)C)cc2)CC2C3(C(CCC12C)C1(C(CC3)C(CCC1)(C(O)=O)C)C)C	5.4	Bad	5.2
7832	OC1C(C(=O)C)C(O)C=C(C)C1=CC=CC(=CC=CC(C)C)C	4.2	OK	5.2

7587	O=C1C=CC(CC=CCCCCC)C1CC=CCCCC(OC)=O	7	OK	5.2
7570	OCc1c2CC(Cc2cc(C)c1CCO)(C)C	5	Excellent	5.2
7388	O=C1C(=C(O)CCC(CCCCCCCCC)C)C(=O)N(C)C1C	5.3	Good	5.2
7308	O(C)C1=CC(=O)c2c(C1=O)c(OC)c(OC)cc2OC	5.4	Excellent	5.2
6391	ClC(Cl)(Cl)C(C=C1N(C)C(=O)C(N(C)C1=O)CC(C(Cl)Cl)C)C	4.9	Poor	5.2
6390	ClC(Cl)(Cl)C(C=C1N(C)C(=O)C(N(C)C1=O)CC(C(Cl)Cl)C)C	4.8	Excellent	5.2
6326	N(CCCN1CCCCCCCCCCCCC1)CCCN	3.3	Bad	5.2
6245	O1C(CC2C3(C(CCC12CO)C1(C(CC3)C(CCC1)(C)C)C)C)C1=CC(OC1O)=O	4.7	Bad	5.2
5247	O=C(NCCc1c2c([nH]c1)cccc2)CC(C)C	3.5	Excellent	5.2
5094	O=[N+]([O-])CCCCCCCCCCCC#CCCc1cccnc1	4.1	Bad	5.2
4751	O(C(=O)C)C1CC2C3C(CCC2(C)C1C=C)C1(C(CC(OC(=O)C)C=C1)CC3)C	4.4	Bad	5.2
4508	ClC(Cl)(Cl)C(C=C1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	5.1	Excellent	5.2
4066	O1OC(CCC1(OC)CCCC=CC=CCC)C(C(O)=O)C	5.4	Good	5.2
4061	O1OC(CCC1(OC)CCCC=CC=CCC)C(C(O)=O)C	5.8	OK	5.2
3629	ClC(Cl)(Cl)C(C=C1N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	4.2	Poor	5.2
3628	ClC(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)CC(C(Cl)Cl)C)C	4.4	OK	5.2
3614	ClC1C2CCC3C4CCC(C(CC(=O)C(C(C)C)=C)C(O)=O)C4(CCC3C2(CCC1O)C)C	5.6	Poor	5.2
3613	ClC1=C2CCC3C4CCC(C(CC(=O)C(C(C)C)=C)C(O)=O)C4(CCC3C2(CCC1=O)C)C	4.5	Good	5.2
3418	O1c2cc(ccc2OC1)Cc1nc(n(c1)C)N	4.2	Good	5.2
2804	O1C(=O)C(CC1CO)C(O)CCCCC(C)C	4.9	Excellent	5.2
2559	O1C(CCC=C(CCC=C(C)C)C)(C)C1CCC(=CCO)CO	5.4	Good	5.2
2341	S(C)c1n(c2c3c1CCN=C3C=C(N)C2=O)C	3.8	Excellent	5.2
2340	ClC=1C2=NCCc3c2c(n(C)c3SC)C(=O)C=1N	5	Excellent	5.2
2250	O(C)c1c2c(C(=O)C=C(O)C2=O)c(OC)cc1OC	5.3	Excellent	5.2
2238	O1C2(C34OOC(CC3)(C=C4CC(C)C2(CC1C1(OOC(CC1)C(C(OC)=O)C)C)C)C)C	4.7	Good	5.2
1896	O1C2CCC(=CC3C(CCC12C)C3(C)C)COO	5.8	Excellent	5.2
1749	OC(=O)CC(NC(=O)C=CC=CC=CC)c1ccccc1	5.4	Good	5.2
1213	O=C1C=CC(CC=CCCCCC)C1CC=CCCCC(O)=O	6.2	Excellent	5.2
988	s1cc(nc1C(C(O)CC=CC(CCNC(OC)=O)=C)(C)C)CC=CCC=C	3.6	Poor	5.2
607	Oc1cc(ccc1C(CCCC(O)(C)C)C)C	4.5	Excellent	5.2
561	O1C(C)(C2C(OC)C(O)CCC23OC3)C1CC=C(C)C	3.6	Excellent	5.2
391	IC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	6.3	Good	5.2
208	o1cc(cc1)CCCC(CC(=O)CC(CCCc1ccoc1)C)C	4.8	Poor	5.2
13600	O1OC(CC(CC)C1CC(OC)=O)(CC(CC)C=CCC)CC	4.8	OK	5.1
13586	OC1CCC(C2=CC(CCC12C)C(O)(C)C)C	4.6	OK	5.1
13581	OC(=O)CCCCC(=O)C=CC=CCC=CCCC	4.1	Good	5.1
13580	OC(CC=CCCCCC(O)=O)C=CC=CCC=C	4.4	Poor	5.1
13528	OC(C(CCC=C(CC(=O)CC(C)C)C)=C)CCC(=CCO)C	5.8	Excellent	5.1
13476	BrC1CCC(O)(C)C(CCC(O)(C=C)C)C1(CCC=C(C)C)C	4.4	Excellent	5.1
13360	O1C(OC(=O)C)C2C(=CCC3C4(C(CCC23C)C2(C(CC4)C(CCC2)(COC(=O)C)C)C)C)C1=O	3.7	Bad	5.1
13230	O(C)c1c2NC=Cc3nccc(cc1OC)c23	4.7	Excellent	5.1
13166	Clc1c(O)c2c(CC(OC2=O)C)cc1OC	4.3	OK	5.1
12933	BrC1C(C23CC(Cl)C(CC2(O)CC1O)(CC3)C)(C)C	4.7	Excellent	5.1
12696	OC(CC=CCC=CCC)C=CC=CCC=CCCCC(O)=O	3.4	Bad	5.1
12398	O1OC(CC(CC)C1CC(OC)=O)(CC(CC)C=CCC)CC	3.9	OK	5.1
12225	O1CC(=C2C1CC1CCCC(C)C1(C)C2O)CO	4.4	Excellent	5.1

12212	OC(CC=CCC=CCCCCC)C#CCCCC(O)=O	4.9	OK	5.1
12098	O1C(OC)(CCCCCCCCCCC(OC)=O)C(C)=C(C)C1=O	5.8	OK	5.1
11780	OC1C2CC(O)CCC2(C=2C(C3CCC(C(=CC(=O)CC(C)C)C)C3(CC=2)C)C1)C	3.6	Poor	5.1
11625	S(C)C1(N(C)C(=O)C(SC)(N(C)C1=O)CO)Cc1ccccc1	5.9	Good	5.1
11280	O1C(CCC1(C)C)C1(OC(=O)C23CC=C4C(=CCC5C(C)(C)C(O)CCC45C)C2(CCC13O)C)C	4.4	OK	5.1
11263	O1CCC2(CC(=O)C(CCC(=O)C)C2(C)C)C1=O	5.6	Excellent	5.1
11202	O1C(CCC2OC2(C)C)(C)C1CCC(=CC(OC)=O)C	4.8	OK	5.1
11171	O(C(=O)C)C1C2C(CCCC2(C2CC=C(CC2(C1)C)C1CC(=O)C(=CC1O)C)C)(C)C	5.1	Bad	5.1
11118	OC1CC(CC2C(CCC2(O)CC1=C)C)(C)C	4.2	Excellent	5.1
11082	O1OC(CC(CC)C1CC(OC)=O)(CC(CC)C=CCC)C	5.6	Excellent	5.1
9790	OC1=C(CCCCCCCCCCC)C(=O)C(O)=CC1=O	5.3	Good	5.1
9309	O=C1C(=C(O)CCCCCCCCCC(C)C)C(=O)N(C)C1C	4.8	Excellent	5.1
9308	O=C1C(=C(O)CCCCCCCCCCC)C(=O)N(C)C1C	4.4	Bad	5.1
9307	O=C1C(=C(O)CCCCCCCCCCCC)C(=O)N(C)C1C	4.4	OK	5.1
8742	Brc1cc(OC)c(cc1O)CC=C(CCCC(O)(C)C)C	4.8	Poor	5.1
8680	O1CC2C(C3C(=C)C2(CCC3C(O)(C)C)C)C1=O	5.3	Excellent	5.1
8521	OC1C2CC=C3C4CCC(C(CC5=[N+]([O-])CCC5=C(C)C)C)C4(CCC3C2(CCC1N(C)C)C)C	3.7	Poor	5.1
8049	Brc1cc2c(n(cc2OC(=O)C)C(=O)C)cc1	4.5	Excellent	5.1
7489	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=CC=O)C)C)C)C1(C(O)=O)C)C	5.8	Bad	5.1
7197	Brc1cc(cc(Br)c1OCCCNC(=O)C#N)CCNC	2.9	Poor	5.1
6954	O(C(C=CC(O)C(C)C)(C)C1CCC(NC=O)(CC1)C)C	5.7	Excellent	5.1
6398	ClC(Cl)(Cl)C(CC1(O)N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	6.2	Excellent	5.1
6397	ClC(Cl)(Cl)C(CC1(O)N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	3.7	Good	5.1
6396	ClC(Cl)(Cl)C(CC1(O)N(C)C(=O)C(N(C)C1=O)=CC(C(Cl)(Cl)Cl)C)C	3.7	Excellent	5.1
6330	O1OC(CC(CC)C1CC(OC)=O)(CC)C=CCC	4.4	Excellent	5.1
6167	O1C2(CCC1C1(CCC3OC(C)(C)C(=O)CCC13C)C)C1(C(OC(C)(C)C(=O)CC1)CCC2C)C	5.6	OK	5.1
5708	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)CC(C(Cl)Cl)C)C	5.8	Excellent	5.1
5435	O(CCCCCCCC)c1cc(O)c(cc1)C(=O)c1ccccc1	5.6	Bad	5.1
5143	Brc1cc(cc(Br)c1OCCCNC(=O)C#N)CCN	4.5	Poor	5.1
4740	BrC=1C(O)C2(ON=C(C2)C(=O)N)C=C(Br)C=1OC	5.1	OK	5.1
4255	Clc1c(O)c2c(CC(OC2=O)C)cc1OC	5.5	Excellent	5.1
4221	O1C=C(OCc2ccccc2)C(=O)C=C1CO	4.7	Excellent	5.1
4203	Brc1[nH]c(cc1)C1=NC(=CNCCC)C(OC)=C1	4.3	Good	5.1
3836	O1C2OC3OC2(CC1=O)C(OC(=O)C)CC1C3CCC2C3(C(CCC12C)C(CCC3)(C)C)C			5.1
3832	O1C2OC3OC2(CC1=O)C(OC(=O)C)CC1C3CCC2C3(C(CCC12C)C(CCC3)(C)C)C			5.1
3804	ClC(Cl)(Cl)C(CC(N(C(=O)CC(C(Cl)(Cl)Cl)C)C)c1sccn1)C	5.4	OK	5.1
3555	O1C23C1C(O)CC(C)C2(C)C(C(=O)C)C(=O)CC3	4.4	Excellent	5.1
3554	O1C23C1C(O)CC(C)C2(C)C(C(=O)C)C(=O)CC3	5.1	OK	5.1
3364	ClC(Cl)(Cl)C(CC(N(C(=O)C=CCC(C(Cl)(Cl)Cl)C)C)C(OC)=O)C	6.1	Good	5.1
3342	ClC1CCC(C)C(CC(=O)C)(C)C12OC(=O)CC2	5.5	Excellent	5.1
3198	O1C23C1C(O)CC(C)C2(C)C(C(=O)C)C(=O)CC3	3.6	Excellent	5.1
2803	O1C(=O)C(CC1CO)C(O)CCCCC(C)C	5.7	OK	5.1
2706	OC(=O)CC(CCCC(CCC(=O)C(C)C)C)C	5.1	Excellent	5.1
2554	OC(CC=CCC=CCC)C=CC=CCCCCC(O)=O	5.7	Bad	5.1

2553	O(C(=O)C)CC=CC=CCC=CCCCC(OC)=O	3.9	Good	5.1
2489	BrC1CC(O)C(C)=C(CCC(O)(C=C)C)C1(C)C	4.9	Excellent	5.1
2243	BrC1CCC(=C)C2(O)CC(CCC12C)C(=CC=CC(O)(C)C)C	4.7	Bad	5.1
1415	O1C(CCC2OC2(C)C)(C)C1CCC(=CC(OC)=O)C	4.8	OK	5.1
1226	OC(CC=CCCCC(O)=O)C=CC=CCC=CCC=CCC	5	OK	5.1
1140	OC(CC=CCC=CCC)C=CC=CCC=CCCCC(O)=O	4.6	Bad	5.1
639	OC(CC=CCC=CCC)C=CC=CCC=CCCCC(O)=O	5.2	Poor	5.1
638	OC(CC=CCC=CCCCC(O)=O)C=CC=CCC=CCC	3.9	Bad	5.1
214	O1CC1(C(CCC)C=C=CC)C(O)C=CCC=CCCCC(O)=O	5.1	Good	5.1
13615	O1C23C1C(O)CC(C)C2(C)C(C(=O)C)C(O)CC3	5	Excellent	5
13614	O1C23C1C(O)CC(C)C2(C)C(C(=O)C)C(O)CC3	3.6	Excellent	5
13582	OC(CCCCC(O)=O)C=CC=CCC=CCCC	5.7	Bad	5
13579	OC(CCCCC(O)=O)C=CC=CCC=CCC=C	5.2	OK	5
13578	OC(=O)CCCCC(=O)C=CC=CCC=CCC=C	4.8	Bad	5
13577	OC(CC=CCCCCC(O)=O)C=CC=CCCC	4.5	Excellent	5
13309	Brc1cc[nH]c1C1=NC(=CNCC(C)C)C(OC)=C1	3	Excellent	5
13260	OC=C(CCC1C(CCCC1=C)(C)C)C=CO	4.9	Excellent	5
13007	OC(CCCC(O)=O)C=CC=CCC=CCC=CCC=CCC	5.2	Poor	5
12861	OC1(CCC=C(CCC(C=C1)C(O)(C)C)C)C	5.3	Excellent	5
12585	Oc1c(C)c(O)c(cc1C(=O)CCC=CC)C	4.1	Good	5
12558	OC=C(CCC1C(CCC=C1C)(C)C)C=CO	4.2	Excellent	5
12326	OC(CC(O)c1ccccc1)c1ccccc1	4.4	Excellent	5
12283	O1C(=O)C(CCC1(CCCCCCCCC)CO)C	4.2	Excellent	5
12205	OC(=O)C12CC(C(CCC1C)C2CC(O)=O)(C)C			5
12195	O1C(=O)C(CCC1(CCCCCCCCC)CO)C	3.9	Excellent	5
12168	OC1CC2C(C3CC=C(C(=O)C)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	5.3	Excellent	5
11952	O1CC(C2C(C(CC(OC(=O)C)C=C(CC2)C)=C)C1=O)=CC=CC(O)(C)C	4.7	Good	5
11408	OC=C(CCC=C(CCC=C(C)C)C)C=CO	4.2	OK	5
10970	O(C)C1=C(OC)C(=O)c2c(C1=O)c(OC)cc(OC)c2	4.8	Excellent	5
9758	OC(CC(O)c1ccccc1)c1ccccc1	3.5	Good	5
9652	OC(CC(O)c1ccccc1)c1ccccc1	4.3	OK	5
9634	OC(CC(O)c1ccccc1)c1ccccc1	4.6	Poor	5
9305	O=C1C(=C(O)CCCCCCCCCCCCCC)C(=O)N(C)C1C	4.5	Poor	5
9302	O=C1CN(C)C(=O)C1=C(O)CCCCCCCCCCCCCC	4.3	Poor	5
8753	Oc1c(C=O)c(C=CC=CC=CC)c(O)cc1CC=C(C)C	5.9	Good	5
8147	OCC1C2(C(CC=C1CO)C(CCC2)(C)C)C	4.4	Excellent	5
7867	O=C1C=CC(C=CC(O)CCCCC)C1CC=CCCCC(OC)=O	5.7	OK	5
7611	ON=CCCCCCCCCCCCCc1cccnc1	4.6	Bad	5
6896	O1C(=Cc2c(c(O)c(OC)c(OC)c2)C1=O)C	5.1	Excellent	5
6790	O1C2CCC(=O)CC2(CCC1C(O)(C)C)C	4.8	Excellent	5
6695	OCC1C2(C(CC=C1CO)C(CCC2)(C)C)C	3.6	Excellent	5
5865	ClC1C(O)C2(OC(OC)C(NC(=O)C=CC(=CC(CCCCCC)C)C)C2)C=C(Cl)C1=O	4.1	Bad	5
5662	BrC1CC(O)C(OC1CC)CC(=O)CCC=CC#C	4.2	Good	5
5254	O(CC#CC#CCCCCCCCC=C)CC(O)=O	4.9	Bad	5
5086	O=[N+]([O-])CCCCCCCCCCCCc1cccnc1	4.4	Excellent	5
4782	BrC=1C(O)C2(ON=C(C2)C(O)=O)C=C(Br)C=1OC	4.7	Excellent	5
4498	O1C(C)(C1C=CC(OC)(CO)C)C1CC(C(C)=C)C(CC1)(C=C)C	3.9	Bad	5

4285	ClC(CCCC(CCCC(C)C)C)(C(OC)=O)C(O)=O	5.9	Excellent	5
4202	Brc1[nH]c(cc1)C1=NC(=CNCC)C(OC)=C1	4.3	Excellent	5
4119	O(C(=O)C=CC=1[N+](C)(C)[C-]=NC=1CC=C(C)C)C	4.3	Excellent	5
3807	ClC(Cl)C(CC(N(C(=O)CC(C(Cl)Cl)C)C)c1sccn1)C	5	Excellent	5
3803	ClC(Cl)(Cl)C(CC(NC(=O)CC(C(Cl)(Cl)Cl)C)c1sccn1)C	5.1	Excellent	5
3634	ClC(Cl)(Cl)C(CC1N(C)C(=O)C(N(C)C1=O)CC(C(Cl)(Cl)Cl)C)C	4.5	OK	5
3615	ClC1=C2CCC3C4CCC(C(CC(=O)C(C(C)C)CC)C(O)=O)C4(CCC3C2(CCC1=O)C)C	5.6	Bad	5
3518	Oc1ccc(cc1)C(CCC(O)C(C)=C)(C=C)C	5.5	Excellent	5
3385	O1C(CCC2OC2(C)C)(C)C1CCC(=CC(OC)=O)C	5.5	OK	5
3090	O(C(=O)C=CC=1[N+](C)(C)[C-]=NC=1CC=C(C)C)C	4.8	Excellent	5
2929	O1C2(CCC1=O)C(CC(=O)C)(C)C(CCC2O)C	5.2	Excellent	5
2339	OC(CCCCCCCCC(O)=O)C=CC=CCC=CCC	4.8	Bad	5
2330	O(C(=O)c1c2c(n(c1)C(OCC)=O)cccc2)CC	6.1	Excellent	5
1897	O1C2CCC(=C)C(OO)C3C(CCC12C)C3(C)C	4.4	Excellent	5
1207	O=C(NN)CCCCCCCCCCCc1ccccc1	4.6	Bad	5
904	S(C)C1(N(C)C(=O)C(SC)N(C)C1=O)Cc1ccc(OCC(OC)=CC)cc1	4.8	Good	5
573	OC(CC(O)c1ccccc1)c1ccccc1	4.5	Excellent	5
437	O1C(C(O)C=CCCCCCCCC(O)=O)C1CC=CCC	5.4	Bad	5
392	BrC1=CC(O)(CC=CCCCCC)C(=CC=CCCCC(OC)=O)C1=O	4.5	Poor	5
187	O=C1N(CCCCCC)C(=O)N(c2ncn(c12)C)C	5.4	Good	5
15	O1C(C(CC)C)C(C)C(=O)C(C)=C1C(C(O)CC)C	4.9	Excellent	5
14239	Ic1c(OC(=O)C)cc(OC(=O)C)cc1OC(=O)C	3.7	Good	4.9
14150	O(C)C1=CC(=O)C=C(CCCCCCCCCCC)C1=O	4.2	Bad	4.9
13958	O(C(C(C(=O)CC)C)C(=CC(CCC)C)C)C(=O)CC	4.3	Excellent	4.9
13622	BrC=1C(O)C2(ON=C(C2)C(OC)=O)C=C(Br)C=1OC	4.2	Poor	4.9
13616	O1C23C1CCC(C)C2(C)C(C(=O)C)C(O)CC3	5.1	Excellent	4.9
13142	O1C(CCCC1=O)C=CC=CC=CC(O)CC=CCCCCC	4.7	Poor	4.9
12710	OC(CC=CCCCCCCCC(O)=O)C=CC=CCC	4.1	Poor	4.9
12430	O1C(OC(=O)C)C2C(=CCC3C4(C(CCC23C)C2(C(CC4)C(CCC2)(C)C)COC(=O)C)C)C1=O	4.6	Bad	4.9
11863	O(C(CC=CCCC(O)=O)C=C(CCCCCCC)C)C	5	Bad	4.9
11611	O1C(=O)C(CCC1(CCCCCCCCC)CO)C	5.1	Excellent	4.9
11313	O1C(OCC)(CC(OCC)=O)C(CC1(CC)C=CCCC)CC	3.2	Good	4.9
11059	o1c(CCCCC)c(C)c(C)c1CCC(O)=O	4.5	Excellent	4.9
10798	O(C(=O)C)C1CC2=CCC3C4CCC(C(C=CC(OC)=O)C)C4(CCC3C2(CC1)C)C	3.8	Poor	4.9
10177	S(O)(=O)(=O)n1cccc1CCCCCC	3.8	Excellent	4.9
10175	S(O)(=O)(=O)n1cccc1CCCCCCCC	3.7	Excellent	4.9
10095	o1c(CCCCCCCCC(O)=O)c(cc1CCCCC)C	4.7	Bad	4.9
9281	O(C)c1ccc(cc1)C=C1N=C(N)N(C)C1=O	4.4	Excellent	4.9
8938	O1C2CC3C4(C(CCC3(C3CC=C(C(C23C)C1=O)C(=O)C)C)C(CCC4)(C)C)CO	5.3	Bad	4.9
8683	O1CC2C3C(C=O)C1(CO)C2(CCC3C(C)C)C			4.9
7916	O1C2=C(CC3C4(C(OC(CC4)C(O)(C)C)CCC13C)C)C(=O)C=C(C(C(=O)C(CC)C)C)C2=O	4.8	Poor	4.9
7612	ON=CCCCCCCCCCCCc1cccnc1	3.7	Bad	4.9
6724	Oc1cc(ccc1C(CC(O)CC(C)C)C)C=O	4.6	Excellent	4.9
6655	Oc1cc(ccc1C(CC(OC(=O)C)CC(C)C)C)C=O	4.7	Poor	4.9
6535	O(CC(O)CO)C=CC#CCCCCCCC(C)C	4.4	Bad	4.9
6457	Brc1cc(cc(Br)c1OCCCN(C)C)CCNC(=O)C	4	Good	4.9

5458	Brc1c2c(NC(=O)C2(O)CC(=O)C)cc(Br)c1	5.6	Poor	4.9
5263	BrC=1C(O)C2(ON=C(C2)C(OC)=O)C=C(Br)C=1OC	4.5	Poor	4.9
4606	Brc1c2c(NC(=O)C2(O)CC(=O)C)cc(Br)c1	4	Excellent	4.9
4277	ClCC(=O)C1(C2C(CC(C)(C)C2O)C=C1CO)C	5.1	Excellent	4.9
4169	O1C2=C(CC3C4(C(OC(CC4)C(O)(C)C)CCC13C)C)C(=O)C=C(C(C(=O)C(CC)C)C)C2=O	4.1	Poor	4.9
3805	ClC(Cl)(Cl)C(CC(NC(=O)CC(C(Cl)Cl)C)c1sccn1)C	5.2	OK	4.9
3532	O1C2CC(OC2CC=CC#C)C1CC(O)C(O)C=C	3	OK	4.9
1591	O1C(C=CC=CC=CCCCCCC)C(O)CC=CCCC1=O	4.6	OK	4.9
1496	O(C(=O)C=CC=CC(CC)CO)C1C=CC2=CC(=O)C(O)CC2(C)C1C	5.1	Poor	4.9
269	S(OC1CC2CCC3C4CCC(C(CCC(C(C)C)=C)C)C4(CCC3C2(CC1)C)C)(O)(=O)=O	4.4	Bad	4.9
14151	O(C(=O)C)C1C(C=CC2(C(C(CC2)C(O)(C)C)C(OC(=O)C)CC(=CC1OC(=O)C)C)C)C	5.9	Poor	4.8
13307	Brc1[nH]c(cc1)C1=NC(=CN)C(OC)=C1	3.9	Excellent	4.8
13298	S(=O)(=O)(CCC(OC)(OC)C)c1ccccc1	3.9	Excellent	4.8
12096	O=Cc1[nH]c(cc1)CCCCCC=CCCCCCC#N	4.6	OK	4.8
12032	O1C(=O)C(CCC1(CCCCCCCCC)CO)C	4.7	Poor	4.8
11980	O1C(CCCCC)C(O)CC1C(O)CCCCCCCCC=C	3.7	Poor	4.8
11259	OC1(CC2(C(=CCC3C4CCC(C(C(=CC(C(C)C)CC)C)C4(CCC23)C)C1=O)C)C(OC)=O	5.5	Bad	4.8
11257	OC1(CC2(C(=CCC3C4CCC(C(C(=CC(C(C)C)CC)C)C4(CCC23)C)C1=O)C)C(OC)=O	4.4	Poor	4.8
11169	O(C(=O)C)C1C2C(CCCC2(C2CC=C(CC2(C1)C)c1cc(O)c(cc1)C)C)(C)C	4.1	Bad	4.8
10176	S(O)(=O)(=O)n1cccc1CCCCCCC	5.2	Excellent	4.8
8475	OC(C(O)CC=CC#C)CC=CCC=CCC	5.4	Excellent	4.8
8244	O(C)C1=C[C-]([NH+](C=C1)CC(O)=O)CCCCCCCCC=C	5.6	Bad	4.8
7548	OC1(CCC(C(O)(CCC=C(C)C)C)C1C)C	4	Excellent	4.8
7030	O1C(CCCC1=O)(CCCCCCCCCCC)CO	3.6	OK	4.8
6536	O(C(=O)CCCCCCC=CC(O)C#C)C	3.7	Good	4.8
6531	O(CC(O)CO)C=CC#CC=CCCCCC(C)C	5	Bad	4.8
6530	O(CC(O)CO)C=CC#CC=CCCCCCC	5	Bad	4.8
6395	ClC(Cl)(Cl)C(CC1(O)N(C)C(=O)C(N(C)C1=O)CC(C(Cl)(Cl)Cl)C)C	3.5	Excellent	4.8
6328	O1OC(CC(CC)C1CC(OCC)=O)(CCCC)CC	5.3	Good	4.8
5594	ClC(Cl)C(CCC(=O)C(CCOC(=O)C)C)=CCl	4.6	Bad	4.8
5593	ClC(Cl)C(CCC(=O)C(CCOC(=O)C)C)=CCl	5.1	OK	4.8
5253	O(CC#CC#CCCCCCCC)CC(O)=O	5.5	Bad	4.8
4748	OC(CC=CCCCCCCCC(O)=O)C=CC=CCC	5.6	Bad	4.8
4713	OC(CCCCCCCC(O)=O)C=CC=CCC=CCC	4.4	Poor	4.8
3806	ClC(Cl)(Cl)C(CC(N(C(=O)CC(C(Cl)Cl)C)C)c1sccn1)C	5.1	Excellent	4.8
3724	O(C(=O)C)c1cc2c([nH]cc2)cc1OC(=O)C	3.8	Excellent	4.8
1825	OC(=O)CCCCCCCC(=O)C=CC=CCC=CCC	4.5	Poor	4.8
1592	O1C(C=CC=CC=CCCCCCC)C(O)CC=CCCC1=O	4.3	Poor	4.8
1583	O1C(C=CC=CC=CCCCCC)C(O)CC=CCCCC1=O	4.5	OK	4.8
1338	O(C(=O)C)c1c(OC(=O)C)cc(cc1OC(=O)C)COC	4	Good	4.8
717	O(CC(O)CO)C=CC#CC=CCCCCCCC(C)C	5.2	Bad	4.8
454	O1C(C(O)C=CCCCCCCCC(O)=O)C1CC=CCC	5.1	Poor	4.8
14100	OC(=O)CCCCCCCC=CCC(=O)C=CC=CCC	4.1	Bad	4.7
12581	Brc1cc(cc(Br)c1OCCCN(C)C)C(O)CN	4.3	Poor	4.7
12049	Brc1cc(cc(Br)c1OC(=O)C)COC(=O)C	3.6	Good	4.7
9418	OC(CCCCCCCC(O)=O)C=CC=CCC=CCC	5	Bad	4.7

9135	O(C(=O)C)C1CC2C(C3CC(O)C(C(=O)C)C(C=O)C13C)(CCC1C(CCCC12C)(C)C)C	5.5	Good	4.7
8497	O1C(CCCC1=O)(CCCCCCCCCCC)CO	3.6	Excellent	4.7
8355	O(CC#CC#CCCCCCC=C)CC(O)=O	5.5	Excellent	4.7
8351	O(CC#CC#CCCCCCC=C)CC(O)=O	3.9	Poor	4.7
6692	O1C2C(CC3C(C)(C(OC(=O)c4ccccc4)CCC(=C2)C)C(OC(=O)C)CC=C3C)=C(C)C1=O			4.7
6532	O(CC(O)CO)C=CC#CC=CCCCCCC(CC)C	4.7	Bad	4.7
6406	OC(CCCCCCCC(O)=O)C=CC=CCC=CCC	4.5	Bad	4.7
6232	O1C(C(O)CC=C(C)C)(C)C1CCc1ccoc1	4.8	Excellent	4.7
5554	O1C(C=CC=CC=CC(=O)C)=C(C)C(OC)=CC1=O	5.2	Bad	4.7
5099	OC1C2C3CCC1(C)C3(CCCC2(CO)C)C			4.7
4968	Brc1cc(cc(Br)c1OC)C[C-]([N+](C)(C)C)C(=O)NCCc1nc[nH]c1	5.6	Bad	4.7
4607	Brc1c2c(NC(=O)C2(O)CCCl)cc(Br)c1	5.2	Excellent	4.7
4476	Brc1c(CCNCC(O)C)c(Br)cc(Br)c1OC	3.6	OK	4.7
2727	O1C(C=CC=CC=CCCCCC)C(O)CC=CCCCC1=O	4.4	Poor	4.7
2462	Brc1cc(cc(Br)c1OCCCN(C)C)C=CC(O)=O	4.1	Bad	4.7
2007	BrC1=CC(O)(C=C(Br)C1(OCCCC)OC)CC(=O)N	5.6	Good	4.7
1967	S1CCc2c(c(SSC)c(OC)c(OC)c2N(C)C)C1=O	5.5	Excellent	4.7
1311	OC(CC=CCCCCCCCC(O)=O)C=CC=CCC	5	Bad	4.7
723	O(CC(O)CO)C=CC#CC=CCCCCCCC(C)C	4.7	Bad	4.7
720	O(CC(O)CO)C=CC#CC=CCCCCCC(C)C	4.8	Bad	4.7
714	O(CC(O)CO)C=CC#CC=CCCCCCCC	4.9	Bad	4.7
691	s1ccnc1C(=O)c1cc(OC)c(O)cc1	5.8	Poor	4.7
14422	Brc1cc2[nH]cc(c2cc1)CSCCN	3.9	Excellent	4.6
13865	OC(CCCCCCCC(O)=O)C=CC=CCC=CCC	4.3	Bad	4.6
11880	O(C(=O)C)C1CC2C(C)(C(C(=O)C1C(=O)C)C(O)CC1C2(CCC2C(CCCC12C)(C)C)C	4.3	OK	4.6
9674	OC1(C)C(CCC(O)(C=C)C)C(=CCC1C)C	4.2	Excellent	4.6
9673	OC1(C)C(CCC(O)(C=C)C)C(=CCC1C)C	4.1	Excellent	4.6
9637	OCC1=CC2C(CCO)C1(CCCC2(C)C)C	4.6	Poor	4.6
8106	O(C(CCCC=CCCCCCC(C)C)C(O)=O)C	4.6	Excellent	4.6
7162	O1C(CCCC(C)C)(C)C2(O)C3(CC=C4C(=CCC5C(C)(C)C(O)CCC45C)C3(CC2)C)C1=O	3.7	Good	4.6
7073	OC(CCCCCCCCCCCCC)C(O)=O	4.4	Bad	4.6
7013	BrC1=CC(O)(C=C(Br)C1=O)CC(OCC)=O	5.4	Good	4.6
6756	Brc1c(OC(=O)C)c(Br)cc(OC(=O)C)c1Br	4.5	Excellent	4.6
6332	O(C(=O)CC(O)C(CC(O)(CCCC)CC)=CC)CC	3.8	Good	4.6
5979	BrC1CC(OCC1(O)C)C(O)(C=CCl)C	4.2	Poor	4.6
5978	BrC1CC(OCC1(O)C)C(O)(C=CCl)C	5.7	OK	4.6
5977	BrC1CC(OCC1(O)C)C(O)(C=CBr)C	4.7	Excellent	4.6
4504	ClC(Cl)(Cl)C(CC=CC=CC(=O)NC(C(C)C)c1sccn1)C	5	Bad	4.6
4484	OC(CC=CCCCCCCCC(O)=O)C=CC=CCC	4.9	OK	4.6
4236	O1C(C=CC=CC=CCC=CCC)C(O)CC=CCCCC1=O	4.2	Poor	4.6
3313	BrC(C(=O)CCC(OC(=O)C)CC)=C(Br)Br	5.1	Excellent	4.6
3286	O1C(CC2C(CCC3C4(C(CCC23C)C(CCC4)(C)C)C)C1OC(=O)C)C1=CC(OC1)=O	3.7	Bad	4.6
2952	O1C(C(CC)C)=C(C)C(=O)C=C1CC(O)C	6.4	Excellent	4.6
2904	Brc1cc(cc(Br)c1O)CC(=O)C(O)=O	4.6	Excellent	4.6
2726	O1C(C=CC=CC=CCC=CCC)C(O)CC=CCCCC1=O	5.1	Poor	4.6
2373	O(C(=O)C=CC=CC(CC(O)=O)C)C1C=CC2=CC(=O)C(O)CC2(C)C1C	5.2	Bad	4.6

2338	OC(CC=CCCCCCCCC(O)=O)C=CC=CCC	4.4	Good	4.6
2008	BrC1=CC(O)(C=C(Br)C1(OCCCCC)OC)CC(=O)N	4.9	Excellent	4.6
1601	O1C(C2C3(CCC4=C(CCC5C(C)(C)C(O)CCC45C)C3(CC2=O)C)C1=O)(CC(=O)CC(C)C)C	4.4	Poor	4.6
1495	O(C(=O)C=CC=CC(O)(CC)C)C1C=CC2=CC(=O)C(O)CC2(C)C1C	5.8	Bad	4.6
1354	Brc1c2c([nH]c(S(=O)C)c2SC)cc(Br)c1	3.7	Excellent	4.6
716	O(CC(O)CO)C=CC#CC=CCCCCCCCCC	4.8	Bad	4.6
14475	O(C(=O)C)C1CC2C3(C(CCC2(C2=CC(=O)C(C(=O)C)=C(C(O)=O)C12C)C)C(CCC3)(CC)C)C	6.6	Poor	4.5
13576	OC(CCCCCCC)C=CCCCCCC(O)=O	4.7	Bad	4.5
12571	O1C(C)(C)C(CC12OC1C3C45C(C6C(C(OC4OC23C)C5)C2(C(CC(OC(=O)C)CC2)CC6)C)C1)C	3.7	Bad	4.5
11520	O(C(CCCCCCC)CC=CCCC(O)=O)C	5.6	Good	4.5
11434	[Si](O[Si](O[Si](O[Si](OC(=O)C)(C)C)(C)C)(C)C)(C(=O)C)(C)C	5.4	Excellent	4.5
11358	BrC=1C(=O)C(Br)=C(Br)OC=1C(=O)CC	5.4	Excellent	4.5
11319	O(C(=O)CC(O)C(CC(O)(CC)C=CCCC)CC)CC	4.3	Good	4.5
11315	O(C(=O)CC(O)C(CC(O)(CC)C=CCCC)CC)CC	4.4	Excellent	4.5
9574	Brc1c(O)c(O)cc(COCCC)c1Br	5.5	Excellent	4.5
7074	OC(CCCCCCCCCCCC)C(O)=O	4	Bad	4.5
7015	Brc1cc(cc(Br)c1O)CC(OCC)=O	5	Good	4.5
6745	Clc1cc([N+]([O-])=NC(=O)N)cc(Cl)c1OC	5	Bad	4.5
6331	O(C(=O)CC(O)C(CC(O)(CCCC)CC)CC)CC	5	Good	4.5
1355	Brc1c2c([nH]c(SC)c2S(=O)C)cc(Br)c1	4.3	Good	4.5
722	O(CC(O)CO)C=CC#CC=CCCCCCCCC	4.7	Bad	4.5
715	O(CC(O)CO)C=CC#CC=CCCCCCCCC	5.1	Bad	4.5
231	[As](=O)(CC1OC(OCC2OC(OC2)(C)C)C2OC(OC12)(C)C)(C)C	5.2	Excellent	4.5
230	[As](CC1OC(OCC2OC(OC2)(C)C)C2OC(OC12)(C)C)(C)C	4.5	Excellent	4.5
11521	OC(CCCCCCC)CC=CCCC(O)=O	4.4	Excellent	4.4
11105	BrC1CC(O)C(=CC1(C)C)C(O)CCl	3.7	Excellent	4.4
9727	Brc1c(O)c(O)cc(COCC)c1Br	4.5	Excellent	4.4
9511	BrC=1C(O)C(O)(C=C(Br)C=1OC)CC#N	5.3	Excellent	4.4
8732	Brc1cc2c([nH]cc2CCN)cc1Br	4.2	Excellent	4.4
8677	OCC1C2C=C(CO)C1(CCC2C(C)C)C	4.9	Excellent	4.4
8474	OC(C(O)CC=CC#C)CC=CCC=CCC	5.1	Excellent	4.4
8461	Brc1c(O)c(cc(Br)c1OC)CC(O)=O	5.7	Excellent	4.4
8069	S(C(=O)C)CCC(=O)CCCCCCCC	4.6	Good	4.4
8067	S(C(=O)C)CCC(=O)C=CCCCCCC	5.7	Poor	4.4
7791	BrC=1C(O)C(O)(C=C(Br)C=1OC)CC#N	4.9	Excellent	4.4
7527	BrC=1C(O)C(O)(C=C(Br)C=1OC)CC#N	4.3	Excellent	4.4
7513	Brc1c(O)c(cc(Br)c1OC)CC(=O)N	5	Excellent	4.4
7012	BrC1=CC(O)(C=C(Br)C1(OC)OC)CC(=O)N	4.6	OK	4.4
6534	O(CC(O)CO)C=CC#CCCCCCC(CC)C	4	Bad	4.4
6533	O(CC(O)CO)C=CC#CCCCCCCCC	4.2	Bad	4.4
5787	O(C(OC)CCCCCCCCCC(OC)=O)C	4.8	OK	4.4
4457	O(C(=O)CCCCCCCCCCCC=O)C	4.3	Excellent	4.4
2394	ClC(Cl)C(CC1NC(=O)C(C)(C)C1O)C	5.6	Excellent	4.4
1969	S1CCc2c(c(SSC)c(OC)c(OC)c2N(C)C)C1(OC)C(=O)C	3.8	OK	4.4
927	O(C(=O)C=CC=CC(CCO)C)C1C=CC2=CC(=O)C(O)CC2(C)C1C	4.9	Bad	4.4

812	S=C=NC=CCCCCCCCCCC=O	4.7	Poor	4.4
721	O(CC(O)CO)C=CC#CC=CCCCCCCCC	5.7	Bad	4.4
434	Brc1cc(cc(Br)c1O)COC(=O)C	4.6	Excellent	4.4
11748	O(C(=O)CCCCC(=O)CCCCC)CC	3.4	Excellent	4.3
11109	OC(CCCCCCCCCCCCC)C(O)=O	4.2	Good	4.3
8767	BrC1=CC(O)(C=C(Br)C1(OCC)OC)CC(=O)N	5.7	Excellent	4.3
7361	OC(CCCCCCCCCCCCC)C(O)=O	4.4	Poor	4.3
4833	O(C(=O)C)C1C2C(CCCC2(C2CCC(O)(CC2(C1)C)C1CC(=O)C(=CC1O)C)C)(C)C	4.8	Bad	4.3
1970	S1CCc2c(C1OC)c(SOC)cc(O)c2N(C)C	5.6	Excellent	4.3
13201	O(C(=O)CCCCCCCCCC=O)CC	5.5	Poor	4.2
11405	ClC=CCCCC(O)CC(O)CCCCC	5.1	Poor	4.2
10932	OC(=O)CCCCCCCCCCCC=O	5	Poor	4.2
9949	OC1CCC2(C(CCC3(C2CC=C2C4CC(CCC4(CCC23C)C)(C(O)=O)C)C)C1(C)C)C	5.4	Bad	4.2
9149	BrC(C(O)CC(Cl)C(O)(C=CBr)C)(CCl)C	5.6	Excellent	4.2
7211	Brc1c(COC)c(Br)c(Br)c(O)c1O	4.4	Excellent	4.2
5864	ClC1=CC2(OC(O)C(NC(=O)C=CC(=CC(CCCCCC)C)C)C2)C=C(Cl)C1=O	4.8	Bad	4.2
5511	S(C(SC)=NC=Cc1ccc(O)cc1)C	4.9	Poor	4.2
5510	S(C(SC)=NC=Cc1ccc(O)cc1)C	4.1	Excellent	4.2
3768	Brc1cc(cc(Br)c1OCCCN)CCN	4.3	Poor	4.2
1971	S1CCc2c(c(SSC)c(OC)c(OC)c2N(C)C)C1OC	3.9	Excellent	4.2
12050	Brc1cc(cc(Br)c1OC(=O)C)C=O	4.3	Excellent	4.1
11881	O1CC2C(C1(O)C)C(OC(=O)C)CC1C2(C)C(=O)CC2C1(CCC1C(CCCC12C)(C)C)C	6.1	Good	4.1
10901	Brc1cc(Br)cc(C(OCC)=O)c1O	4.9	Excellent	4.1
9228	O1C2(CCC1C1(CCC3OC(C)(C)C(=O)CCC13C)C)C1(C(OC(C)(C)C(O)CC1)CCC2C)C	4.8	Poor	4.1
8777	BrCC(Cl)(C(O)CC=C(C(O)CBr)C)C	4.8	Excellent	4.1
7484	O(C(=O)C)C1CCC2(C(CCC3(C2CC(=O)C3=C(C=CC=C(C=CC=O)C)C)C)C1(C(OC)=O)C)C	5.2	Bad	4.1
1567	O1C(CCCC=CCCC(=O)CC(O)CC=CC=CC(O)CC=CC=CC1=O)C	5.2	OK	4.1
1492	O(C(=O)C=CC=CC(CC)C)C1C=CC2=CC(=O)C(O)(CC2(C)C1C)C(CO)=C	4.6	Bad	4.1
14469	O(C(=O)C)C1CC2C(C3CC(O)C(C(=O)C)C(C=O)C13C)(CCC1C(CCCC12C)(CC)C)C	5.7	Good	4
8776	BrC(C(O)CC=C(C(O)CBr)C)(CCl)C	4.4	Excellent	4
4299	S(C)c1c(OC)c(O)cc(CCN)c1SC	3.8	Excellent	4
876	O1C(CCC1(C)C)C1(OC(=O)C23CC(=O)C4C(=CCC5C(C)(C)C(O)CCC45C)C2(CCC13O)C)C	4.7	Poor	4
649	BrC(Br)C(O)CC(OC(=O)C)CCC	5	Excellent	4
11887	Brc1c(CO)c(Br)c(Br)c(O)c1OC	4.5	Excellent	3.9
11152	O1C(CCC1(C)C)C1(OC(=O)C23C1CCC2(C=1C(=CC3)C2(C(CC=1)C(C)(C)C(O)CC2)C)C)C	4.1	Bad	3.9
4011	O(C(=O)C=CC=CC(CC)C)C1C=CC2=CC(=O)C(O)(CC2(C)C1C)C(C=O)=C	4	Poor	3.9
2114	O1C(C)(C)C1CCC1(C=C(CCC1O)C=CC=CC1=CC(CCC2OC2(C)C)(C)C(O)CC1)C	4.4	Bad	3.9
2111	O1C(C)(C)C1CCC1(C=C(CCC1O)C=CC=CC1=CC(CCC2OC2(C)C)(C)C(O)CC1)C	4.7	Bad	3.9
8288	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CC)(C)C(OC(=O)C)CC3)C)C)C)C1=O)C	4.6	Bad	3.8
13638	O1C(C)C(O)C(OC(=O)C)C(O)C1OC1CC2=CCC3C4CCC(C=C)C4(CCC3C2(CC1)C)C	4.9	Bad	3.6
8287	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CC)(C)C(OC(=O)CC)CC3)C)C)C)C1=O)C	4.9	Bad	3.6
2374	O(C(=O)C=CC=CC(CC)C)C1C=CC2=CC(=O)C(CC2(C)C1C)C(C)=C	4	Poor	3.6
3854	Oc1ccc(cc1)C=CNC1=C[C-]2[NH+](CCc3c2c(n(c3)C)C1=O)C	3.7	Poor	3.5

2375	O(C(=O)C=CC=CC(CC)C)C1C=CC2=CC(=O)C(CC2(C)C1C)=C(C)C	5.3	Bad	3.5
7970	O1C(O)(C=CC2C3(C(OC(C)(C)C(=O)CC3)CCC2(O)C)C)C(CCC2C(CCCC12C)(C)C)C	4	Poor	3.2
9390	OC1CCC2(C(CCC3(C2CC=C2C4CC(CCC4(CCC23C)C(O)=O)(C)C)C)C1(C)C)C	4.6	Bad	3
4378	OC1C2CC=C3C4CCC(C(CC5=NCCC5=C(C)C)C)C4(CCC3C2(CCC1NC(=O)C)C)C	5.3	Bad	3
5929	O1C(C)C(OC(=O)C)C(O)C(O)C1OC1CC2=CCC3C4CCC(C=C)C4(CCC3C2(CC1)C)C	4.6	Bad	2.9
1845	O1CC2C(C1(OC)C)C(OC(=O)C)CC1C2(C)C(=O)CC2C1(CCC1C(CCCC12C)(CC)C)C	4.7	Bad	2.9
12287	OC1CCC2(C(CCC3(C2CC=C2C4C(C)C(CCC4(CCC23C)C(O)=O)C)C)C1(C)C)C	4.9	Poor	2.5
12063	OC1CCC2(C(CCC3(C2CC=C2C4C(C)C(CCC4(CCC23C)C(O)=O)C)C)C1(C)C)C	4.3	Bad	2.5
9003	OC1CCC2(C3C(CCC2C1(C)C)(C)C1(C(C2CC(CCC2(CC1)C)(C(O)=O)C)=CC3=O)C)C	5.1	Bad	2.3
7821	O(C(=O)C=CC(=CC(CC)C)C)C1C=CC2=CC(=O)C(O)(CC2(C)C1C)C(COC(=O)C)=C	4.2	Bad	2.1
8286	O1C(C2=C(C3(C(CC2)C2(C(CC3O)C3(C(CC2)C(CC)(C)C(OC(=O)CCC)CC3)C)C)C)C1=O)C	4	Bad	1.9
7720	O1C(C)(C2C(OC)C(OC(=O)C=CC=CC=CC(OC)=O)CCC23OC3)C1CC=C(C)C	4.2	Bad	1.8
6687	O1C2(CC(=O)C(=CC=CC(=CC=CC=C(C=CC=O)C)C)C)C(CC(O)CC12C)(C)C	6.1	Bad	1.8
10633	O(C(=O)C)c1ccc(cc1)C=CC=CC=CC(=O)C	4	Bad	1.7
10381	O1C(C)(C2C(OC)C(OC(=O)C=CC=CC=CC(OC)=O)CCC23OC3)C1CC=C(C)C	4.8	Bad	1.5
4262	Brc1cc[nH]c1C=CC=CC=CC=1OC(=O)C(C)=C(O)C=1	5.2	Bad	1.5
6768	O1C(C)(C2C(OC)C(OC(=O)C=CC=CC=CC(O)=O)CCC23OC3)C1CC=C(C)C	5.8	Bad	1.3
13322	O1C(C)(C)C(CC12OC1C(C2(O)C)C2(CC(=O)C3C(C2C1)CCC1CC(O)CCC13C)C)C	4.8	Poor	1.1
4263	Brc1c([nH]cc1Br)C=CC=CC=CC=1OC(=O)C(C)=C(O)C=1	4.6	Bad	0.4
2760	[As](=O)(CC1OC(OC)C2OC(OC12)(C)C)(C)C	5.3	Poor	0.3

[a] Were the QSAR values are missing the alignment calculation failed. [b] From QSAR calculations. [c] From Docking calculations.

References

1. Floresta, G.; Pistarà, V.; Amata, E.; Dichiara, M.; Marrazzo, A.; Prezzavento, O.; Rescifina, A., Adipocyte fatty acid binding protein 4 (FABP4) inhibitors. A comprehensive systematic review. *Eur J Med Chem* **2017**, 138, 854-873.