

A Sobering Assessment of Classical Force Field

Methods for Low Energy Conformer

Predictions

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Table S1. A list of Simplified Molecular Input Line Entry Specification (SMILES) for the molecules in this study.

CODE	SMILES
astex_1g9v	C(=O)(O)C(C)(C)Oc1ccc(cc1)CC(=O)Nc1cc(cc(c1)C)C
astex_1gkc	CC(C)([C@@H](C(=O)NC)NC(=O)[C@@H](CN(C=O)O)CC(C)C)C
astex_1gm8	O=C1N2[C@@H](C(=O)[O-])C(C)(C)[S@](=O)[C@@H]2[C@H]1NC(=O)Cc1cccc1
astex_1hnn	c1cc(cc2c1CC[NH2+]C2)S(=O)(=O)N
astex_1hp0	OC[C@H]1O[C@H]([C@@H]([C@@H]1O)O)n1cnc2c(N)nc2c12
astex_1hq2	C1Nc2nc(N)[nH]c(=O)c2N=C1CO
astex_1hvyy	n1c(C)[nH]c(=O)c2cc(ccc12)CN(c1sc(cc1)C(=O)N[C@@H](CCC(=O)O)C(=O)O)C
astex_1hwii	c12c(cccc1)n(c(c2c1ccc(cc1)F)/C=C/[C@H](C[C@@H](O)CC(=O)O)O)C(C)C
astex_1ia1	c12c(c(nc([nH+]1)N)N)c(cce2)Sc1cccc1
astex_1ig3	Cc1nc(N)c(C[n+])csc(CC O)c2C)cn1
astex_1j3j	n1c([nH+]c(c(c1N)c1ccc(cc1)Cl)CC)N
astex_1jd0	c1(nnc(NC(=O)C)s1)S(=O)(=O)[NH-]
astex_1jje	[C@H](C(=O)O)(Cc1cccc1)[C@@H](C(=O)O)Cc1cc2OCOc2cc1
astex_1jla	c1(cccc1)Cc1n(c(=O)[nH]c(=O)c1C(C)C)COCc1cccc1
astex_1k3u	O=C(O)C[C@@H](C(=O)O)NC(=O)Cc1c[nH]c2c1cccc2
astex_1ke5	N1C(=O)/C=C\Nc2ccc(cc2)S(=O)(=O)NC/c2cccc12
astex_1kzk	c1(O)cccc(c1C)C(=O)N[C@@H](Cc1cccc1)[C@H](O)C(=O)N1CSC(C)(C)[C@H]1C(=O)NCc1c(ccc1)C
astex_1l2s	N(c1ccc(cc1)Cl)S(=O)(=O)c1c(sc1)C(=O)O
astex_1l7f	[C@H]1(NC(=[NH2+])N)[C@H]([C@H](C(CC)CC)NC(=O)C)[C@H](O)[C@@H](C(=O)O)C1
astex_1lpz	c1cc2c(c(c1)C)cc(n2Cc1cccc(c1)C(=[NH2+])N)C(=O)NCc1cc(cc(c1)Cl)C1
astex_1lrh	c12c(cccc1cccc2)CC(=O)O
astex_1m2z	C1=CC(=O)C=C2CC[C@@H]3[C@@]([C@@]12C)([C@H](C[C@]1([C@H]3C[C@H]([C@@]1(C(=O)CO)O)
astex_1meh	C1(=O)c2c(CO1)c(C)c(c2O)C/C=C/[CCC(=O)O)C)OC
astex_1mmv	[NH3+] [C@H](C(=O)O)CCCNC(=[NH2+])NCCCC
astex_1mzc	[C@@]1(c2cc(Oc3c(ccc(c3)[C@](c3n(cnc3)C)(C)[NH3+])C#N)ccc2)(C(=O)N(CCCC1)C)CC
astex_1n1m	C1CN(CC1)C(=O)[C@H](C(C)C)[NH3+]
astex_1n2j	O=C(O)[C@H](O)C(C)(C)CO
astex_1n2v	[nH]1c(CCCC)nc2c(=O)[nH][nH]c(=O)c12
astex_1n46	O=c1[nH]c(=O)cnn1c1cc(C)c(c1)C)Oc1ccc(c1)C(C)C)O
astex_1nav	O=C(O)Cc1cc(c(Oc2ccc(O)c2)C(C)C)c(c1)Cl)Cl
astex_1of1	OC[C@@H]1[C@@H](O)C[C@]2(n3c(=O)[nH]c(=O)c3)C)[C@H]1C2
astex_1of6	[NH3+] [C@H](C(=O)O)Cc1ccc(cc1)O
astex_1opk	OCc1cccc(Nc2nec3cc(c(=O)n(c3n2)C)c2c(Cl)cccc2Cl)c1
astex_1oq5	S(=O)(=O)(c1ccc(cc1)n1c(c2ccc(C)cc2)cc(C(F)F)F)n1)[NH-]
astex_lowe	[NH2+]=C(N)c1ccc2cc(ccc2c1)C(=O)Nc1cccc1
astex_1oyt	O=C1N(Cc2ccc(F)cc2)C(=O)[C@H]2[C@H]3N(CCC3)[C@@H](c3ccc(cc3)C(=[NH2+])N)[C@@H]12
astex_1p2y	n1cc(ccc1)[C@H]1[N@@H+]([C@H]1C)
astex_1p62	OC[C@H]1O[C@@H](n2ccc(nc2=O)N)C(F)F)[C@@H]1O
astex_1pmn	n1(c(nc(c1c1ccn(c1)Nc1CC1)c1cc(c(cc1)Cl)Cl)[C@H]1CC)N@@H+(CC1)C)CCC
astex_1q1g	CSC[C@H]1[NH2+][C@H]([C@H](O)[C@@H]1O)c1c[nH]c2c(=O)[nH]cnc12
astex_1q41	c12/C(=N\O)/C(=C\3/C(=O)Nc4c3cccc4)/Nc1cccc2
astex_1q4g	c1cc([C@@H](C(=O)O)C)cccc1c1cccc1
astex_1r1h	C[C@H]([NH3+])[P@](=O)(O)C[C@H](C(=O)N[C@@H](C)C(=O)O)Cc1ccc(cc1)c1cccc1
astex_1r55	N(C(=O)C[C@@H](C[C@@H](C(=O)NO)O)CC(C)C)[C@@H](C(C)C(C)C)C(=O)NC
astex_1r58	C(O)(C)SCC[C@@H](N)[C@H](O)C(=O)NNC(=O)c1cccc(c1)Cl
astex_1r90	c1cc(ccc1)c1ccc(cc1F)[C@H](C)C(=O)O
astex_1s3v	c1([nH+]c2c(c(n1)N)C[C@@H](CC2)CN(c1cc(c(c1)OC)OC)OC)C)N
astex_1sg0	c1(cc(cc(c1)C=C\c1ccc(cc1)O)O)O
astex_1sj0	[C@H]1([C@@H](Oc2ccc(O)cc2S1)c1ccc(cc1)OCC[NH+]1CCCCC1)c1ccc(O)cc1
astex_1sq5	OCC(C)(C)[C@@H](O)C(=O)NCCCC(=O)O
astex_1t40	c1c(c(ccc1F)C(=O)NCc1nc2c(s1)c(F)cc(F)c2F)OCC(=O)O
astex_1t46	c1cc(cnc1)c1ccn(c1)Nc1c(ccc(c1)NC(=O)c1ccc(cc1)CN1CC[N@@H+](C)CC1)C
astex_1t9b	COc1nc(C)nc(N/C(=N/S(=O)(=O)c2cccc2Cl)/O)n1
astex_1tow	O=C(O)CCCn1c2cccc2c2c1cccc2
astex_1tt1	[NH2+]\1C[C@@H]([C@@H]([C@H]1C(=O)O)CC(=O)O)C(=C)C
astex_1tz8	CC/C(=C\c1cccc(O)cc1)/CC)c1ccc(O)cc1
astex_1u1c	OCCOCn1c(=O)[nH]c(=O)c(c1)Cc1cccc1
astex_1u4d	O=C1NCC/C(=C\2/NC(=NC2=O)N)c2c1[nH]cc2
astex_1um1	c1n(cnc1C(=O)N)[C@@H](CO)CCn1ccc2c1cc(cc2)NC(=O)CCc1cccc1

CODE	SMILES
astex_1unl	OC[C@@@H](CC)Nc1nc2n(C(C)C)cnc2c(n1)NCc1cccc1
astex_1uou	Clc1c(CN2CCCC2=[NH2+])[nH]c(=O)[nH]c1=O
astex_1v0p	n1c(nc2n(C(C)C)cnc2c1Nc1ccc(c(Cl)c1)C(=O)O)N[C@H](C(C)C)CO
astex_1v48	n1(cnc2c(=O)[nH]c(N)nc12)CCCC(F)(F)P(=O)(O)O
astex_1v4s	s1ccnc1NC(=O)c1c(cc(c(c1)Sc1n(ccn1)C)F)N
astex_1vcj	c1c(c(cc(c1)C(=O)O)NC(CC)CC)N1[C@@@](CCC1=O)(CO)C[NH3+]
astex_1w1p	O=C1[C@@@H]2CCCN2C(=O)CN1
astex_1w2g	OC[C@H]1O[C@H](C[C@@H]1O)n1c(=O)[nH]c(=O)c(C)c1
astex_1xm6	O=C1O[C@](CN1)(C)c1ccc(OC)c(c1)OCCC
astex_1xoq	O=C(c1ccc(OC(F)F)c(OCC2CC2)c1)Nc1c(Cl)cnc1Cl
astex_1xoz	c1ccc2c3c([nH]c2c1)[C@H](N1C(=O)CN(C(=O)[C@H]1C3)C)c1ccc2OCOc2c1
astex_1y6b	O=S(=O)(NCC1CC1)c1ccc(c(c1)Nc1oc(cn1)c1cc(ccc1)c1c[nH+]ccc1)OC
astex_1ygc	Oc1cc(N[C@@H](C(=O)NS(=O)(=O)c2cccc(N)c2)c2c(F)c(OCC)cc(OCC)c2)ccc1C(=[NH2+])N
astex_1yqy	c1(cc(c(cc1)F)C)S(=O)(=O)N[C@@H](C(=O)NO)C1CCOCC1
astex_1yvf	C(=C(=NC(=O)c1cccc1)C(=O)O)c1ccc(cc1)Oc1c(cccc1)Br
astex_1ywr	c1c(ccc(c1)F)c1c(c2nc(N[C@H](c3cccc3)C)nc2)n(n(C2CC[NH2+]CC2)c1=O)C
astex_1z95	c1cc(F)ccc1S(=O)(=O)C[C@@](O)(C)C(=O)Nc1cc(c(c1)C#N)C(F)(F)F
astex_2bm2	c1(cc(c(c1)C[NH3+])C@H)CCN(C(=O)c2cc(CCc3cccc3)nc2)CC1
astex_2br1	COc1ccc(cc1)c1c2c(NCCO)ncnc2oc1c1ccc(OC)cc1
astex_2bsm	COc1ccc(cc1)c1c(C(=O)NCC)N[nH]c1c1cc(Cl)c(O)cc1O
omegacsd_ABHYTZ	C(=O)(c1cccc1)NNc1n[nH]c(=S)n1N
omegacsd_ABIMAZ	Brc1n(c(C(C)C)c(n1)NC(=O)C)C
omegacsd_ABSBPP	c1(c(ncc1NS(=O)(=O)c1cccc1)C(C)(C)N(C)C)c1cccc1
omegacsd_ABVPRO	Brc1ccc(cc1)C(=C/c1cccc1)/C1=CC(=O)N(C1)C(=O)C
omegacsd_ABXBPC	c12c(ccc(c1c(=O)cc(C(=O)[O-])o2)OCCC(C)C)CC=C
omegacsd_ABZNPS	S(=O)(=O)(c1ccc(N(=O)=O)c1)Cc1ccc(N(C)C)c1
omegacsd_ACENHT	s1cc(n(/c/1=C/N(=O)=O)CCNC(=O)C)c1cccc1
omegacsd_ACPIXZ	c1cc(c2c(c3cccc3)c(N(C(=O)C)C(=O)C)on2)ccc1
omegacsd_ACTHBZ	c1(cc(c(cc1)NC(=O)C)SC)c1ccc(cc1)NC(=O)C
omegacsd_ADPRTR	n1cnc2c(c1N)ncn2CCC(=O)NCCc1c[nH]c2c1cccc2
omegacsd_AMOCMS10	ClCS(=O)(=O)C(=C(c1cccc1)N1CCOCC1)/C
omegacsd_AMPDAM	n1c(Cl)c(ccc1)NCC1nc(Cl)c(N)cc1
omegacsd_ANOPPS	c12c(=O)n(c3cccc3)[nH]c1nc(Nc1cccc1)s2
omegacsd_ANTZOA	s1c(nc(c1N(c1cccc1)C)C)Nc1cccc1
omegacsd_ANTZOB	s1c(nc(c1N(c1cccc1)C)c1cccc1)Nc1cccc1
omegacsd_AOPCHY	c1cc(ccc1C(=C1CCCCC1)c1ccc(cc1)OC(=O)C)OC(=O)C
omegacsd_APRTAM	n1cnc2c(c1N)ncn2CCC(=O)NCCc1ccc(cc1)O
omegacsd_AURMIN	N(C)C)c1ccc(cc1)C(=[NH2+])c1ccc(N(C)C)cc1
omegacsd_AZLNPR	c1(CCC(=O)O)cc(c2cccccc12)CCC(=O)O
omegacsd_BAFJEX10	O1CC[NH+](CC1)CCNc1ccc(n[nH+]1)c1cccc1
omegacsd_BAFREF	n1c(nc(cc1)N)SSc1nccc(n1)N
omegacsd_BAFYOW	Fc1c(=O)[nH]c(=O)n(c1)c1nc(nc(c1)O)Cc1ccc(OC)cc1
omegacsd_BAJZOB10	Oc1cc(O)c(cc1CN1C(=O)CCCCC1)CN1C(=O)CCCCC1
omegacsd_BATROD	[nH]1c(c(cc1C(=O)NC/C=C/c1[nH]c(=[NH2+])][nH]c1)Br)Br
omegacsd_BATXID	c1(cnn(c2cccc2)c1)c1ccccn1)[C@@@H]1OC(=O)c2c1cccc2
omegacsd_BAXOZO	Brc1cc(ccc1)c1nc(cc(=O)o1)OC(=O)C
omegacsd_BBSPRT10	Brc1ccc(S(=O)(=O)N[C@@H]2C(=O)SC2)cc1
omegacsd_BEDLUR	c1(ccc(cc1)F)CNc1nc(c(cc1)NC(=O)OCC)N
omegacsd_BEHHOL10	n1c(c2c(NS(=O)(=O)c3ccc(cc3)C)cccc2)oc(=O)c2cc(ccc12)Br
omegacsd_BEK DIE	Brc1ccc(C(=O)NCC(=O)O)[C@H]2[C@@H](CCC2O)cc1
omegacsd_BELWOE	Cl/C(=C(/S(=O)(=O)C)C(C)C)c1cccc1
omegacsd_BENPRL	[C@@@H]1(CCN(CC1)CCCC(=O)c1ccc(cc1)F)n1c2c(cccc2)[nH]c1=O
omegacsd_BESCEH	S(=O)(=O)(Nc1c(cc(cc1)C)c1oc2c(n1)cccc2)c1ccc(cc1)C
omegacsd_BETFAH	c1(=S)c(c(nc(o1)c1cccc1)SC)C(=O)N
omegacsd_BEWLIY10	O=c1n(nc(c2n1nc(c2)C(=O)OC)c1cccc1)C
omegacsd_BEWLOE10	o1c(cc2c(nn(c12)c1cccc1)C)C(=O)OC
omegacsd_BEXVOP	n1c(nc(c(c1)Cc1cc(c(c(c1)OC)OC)OC)OC)N
omegacsd_BHMPET	c1(cc(c(cc1)OC)O)CCc1cc(c(cc1)OC)O
omegacsd_BIBHID	n1([nH]c(=O)n(c1=O)c1cccc1)C(CC(C)(C)C)C(C)C
omegacsd_BIBSEK	N1(CC[C@@](CC1)(O)c1ccc(cc1)Br)CCCC(=O)c1ccc(cc1)F
omegacsd_BSBTHP	Brc1cc(S(=O)(=O)N)sc1S(=O)(=O)c1cccc1
omegacsd_BTHYDX	c1(cccc1)C(=O)NOC(=O)c1ccc(cc1)C

CODE	SMILES
omegacsd_BUDCUY	C(=C(c1ccc(cc1)N(C)C)/CC)(/c1ccc(cc1)N(=O)=O)\C#N
omegacsd_BUFXOP	N(C)(C)c1ccc(NC(=O)NC(=O)CCc2cccc2)cc1
omegacsd_BUHNIB	c1(nc(nc(c1SC)Cl)NCc1cccc1)N1CCN(CC1)C
omegacsd_BUNFUL	n1nc(n(Nc2cccc2)c1c1cccc1)C
omegacsd_BUSNIM	Brc1c(c(cc(Br)c1)C[N@H+](C)C1CCCCC1)N
omegacsd_BUTDID	O=C(Nc1ccc(N(=O)=O)cc1)c1cccc1
omegacsd_BUVYIA	ClC(Cl)(Cl)COC(=O)c1nc(sc1C)C(=O)NC(=O)Cc1cccc1
omegacsd_BUYZIE	[nH]1cc(c2cccc12)CCNC(=O)NC1CCCC1
omegacsd_BZAPCX10	n1cnc2c(c1N)n(cn2)C(=O)OCc1cccc1
omegacsd_BZAPUC20	O=C(OCc1cccc1)n1c2ncn(N)c2nc1
omegacsd_CABCUD	C1CCCCN1NC(=O)NS(=O)(=O)c1ccc(cc1)C
omegacsd_CAFGIZ	Brc1cc(C(=O)COC(=O)/C=C\2/C[C@@H](CCC2)C)cc1
omegacsd_CAGXEN	c1(c(ccn1)C(=O)[O-])Nc1cc(ccc1)C(F)(F)F
omegacsd_CALLEG	s1c[n+](c(c1CCO)C)Cc1c(=O)[nH]c(nc1)C
omegacsd_CANPUC	Brc1n(cc(c2cccc2)c(=O)c1cc(ccc1)C(F)(F)F)C
omegacsd_CARNID	n1(c(nc1N(=O)=O)O)CCNC(=S)OC
omegacsd_CATXIE	O=C([O-])c1cccc1C(=O)NCCc1[nH+]c2c([nH]1)CCCC2
omegacsd_CAVNUI	c1(cccc1O)C(=O)N(c1cccc1)OC(=O)C
omegacsd_CBMHZP	C1CN(C(=C)C=C(C)N1C(=O)c1ccc(cc1)Cl)C(=O)c1ccc(cc1)Cl
omegacsd_CBSTHP	Clc1c(S(=O)(=O)c2sc(S(=O)(=O)N)cc2)cc(Cl)cc1
omegacsd_CBZHGX	Clc1c(ccc1)C(=O)NOC(=O)c1c(Cl)cccc1
omegacsd_CDBMPI10	O=C(N1 C[@H](CN C[@H](C1)C)C(=O)c1cccc1)C)c1cccc1
omegacsd_CEJTIU	CN(C)c1ccc(cc1)NC(=O)NC(=O)Cc1cccc1
omegacsd_CEKNOV	O(c1c(ccc1)C(=C/c1c(OC)ccc1)\C)/C/C
omegacsdCELDEC	S=C(c1ccc(OC)cc1)c1ccc(OC)cc1
omegacsdCELXOG	[nH]1c(c(c2CCCCc12)c1cccc1)C(=O)OCC
omegacsdCENNIS	o1sc2c(SCc3ccc(Br)cc3)cccc(=O)c2c1=O
omegacsdCETZOQ	[C@@]12(CCCCCC[C@H]1C(=C2C(=O)OC)N1CCCCC1)C(=O)OC
omegacsdCEVTUS	C1(=O)C(Cc2cc(cc12)NC(=O)C)C(C)(C)C(C)
omegacsdCEWFUF	c1cccc1c1noc(n1)N(C)Cc1nc(no1)c1cccc1
omegacsdCFBPBI	Clc1cc2[nH]c(=O)n(c2cc1)CCCN1CC[C@@H](CC1)C(=O)c1ccc(F)cc1
omegacsdCIBPEI	c1c(ccc2cccc12)NC(=O)c1c(ccc1)C(=O)O
omegacsdCIBPOS	c1(cccc1)c1oc(nn1)c1c(ccc1)C(=O)O
omegacsdCIDSIR	N(OC(=O)c1cccc1)C(=O)c1cccc1c1cccc1C
omegacsdCIHFAA	S(=O)(=O)(c1ccc(cc1)NC(=O)c1cccc1C(=O)O)NC(=O)C
omegacsdCIHJAE	n1(c(c(c1cccc1)c1c(ccc1)Cl)C(=O)OCC)C(=O)OCC
omegacsdCIJFEG	O=C(C(=O)c1cc(ccc1)C(=O)C(=O)c1cccc1)c1cccc1
omegacsdCIJVAS	[S@@](=O)(c1oc(N(C)c2cccc2)c1)c1cccc1c1ccc(cc1)C
omegacsdCIPXEE	Clc1ccc(cc1)C(=O)N(Cc1cccc1)C(C)C
omegacsdCIXFIY	Brc1e(ccc1)C(=O)N(Cc1cccc1)C(C)C
omegacsdCIXTOS	n1cnc2c(c1N)ncn2CCC(=O)NCCc1[nH+]c[nH]c1
omegacsdCLPHAC	Clc1ccc(cc1)[C@@H](c1ccc(Cl)cc1)C(=O)O
omegacsdCLPNXA	S1c2ccc(Cl)cc2/C=C\CCN2CCN(CC2)CCO/c2cccc12
omegacsdCLPSAM	Clc1c(ccc1)NS(=O)(=O)c1ccc(cc1)N
omegacsdCLPTBU	Clc1c(/C=C/C=C/c2cccc2)c(Cl)ccc1
omegacsdCMANPQ	C1(=O)C(=C(C(=O)c2cccc12)CN(C)c1ccc(cc1)C(=O)OCC)Cl
omegacsdCMAPTX	Clc1cc2c(cc1)Sc1c(ccc1)C/2=C/CCN(C)C
omegacsdCMPEPI	C(C[n+]1ccc(cc1)C#N)c1ccc(cc1)OC
omegacsdCMSMOC	C1CC C[@H](C(=C1)N1CCOCC1)S(=O)(=O)CC#N
omegacsdCMXPMB	c1c(cc(c1C)Oc1c(cc(cc1)C(=O)OC)N)C)C
omegacsdCMXPYO	c1cccc1c1c(c(=O)n(c(C)c1cccc1)NC(=O)OC)C
omegacsdCNBPCT	Brc1ccc(cc1)NC(=O)Nc1c(cnc(C)n1)CN(/C(=C\1/CCS1)/C)C=O
omegacsdCNINDO	N(c1ccc(/C=C/C(=C2/C(=O)c3cccc3C2=O)/O)cc1)(C)C
omegacsdCOCHOL	C1(=O)C(=C(C(=O)C(=C1c1[nH]c2ccc(cc12)CC=C(C)O)c1c[nH]c2c1cc(cc2)CC=C(C)C)O
omegacsdCODYUP10	n1(c(=O)sc(c1C)CCO)Cc1c(nc(nc1)C)N
omegacsdCOFHIO10	n1c(sc2ncn(Nc3cccc3)c12)SC
omegacsdCOKBOT	[S@@](=O)(CC C[@H]1C(=O)N(N(C1=O)c1cccc1)c1cccc1)c1cccc1
omegacsdCOKSUQ	c12(cccc1)OC=C(O2)[C@@H](O)CNCCc1ccc(c(OC)c1)OC
omegacsdCOKTAX	c12(cccc1)OC=C(O2)[C@@H](O)CN1CCN(CC1)c1cccc1OC
omegacsdCOTXUE	O=C(N(Cc1[nH]c2c(n1)cccc2)c1c(NC(=O)C)cccc1)C
omegacsdCOVXIU	c1(ccc(cc1)S(=O)(=O)Nc1nc(cc(n1)C)C)N
omegacsdCOYHUT10	c1(cc(c(cc1)OC)C(=O)NCc1cccc1)C(=O)NCc1cccc1

CODE	SMILES
omegacsd_COYPIP	C1C(=C(c1ccc(OC)cc1)c1ccc(cc1)OC)Cl
omegacsd_COYTOZ	O=C1O[C@H](CNC)CN1c1ccc(cc1)OCc1cccc(c1)Cl
omegacsd_COYVIV	s1c(nn1c1cccc1S(=O)(=O)NC)N
omegacsd_COZFOM	O=C(ON1C(=O)c2c(C1=O)cccc2)c1cccc1C(=O)ON1C(=O)c2c(C1=O)cccc2
omegacsd_CPIPLA	Clc1ccc(cc1)N1[C@H](c2cccc2)[C@H](C(C)C)C1=O
omegacsd_CPPHAM	Clc1ccc(cc1)NC(=O)c1c(ccc1)C(=O)O
omegacsd_CPQZOL	n1(c(=O)nc(c2cccc2)c2cc(ccc12)OC)CC1CC1
omegacsd_CPYPTZ	Clc1cnc(cc1)c1c(c2cccc2)nc(N(CC)CC)s1
omegacsd_CUHNEY10	Clc1cnc(N2C(=O)c3ncnc3[C@@H]2OC(=O)N2CCN(CC2)C)cc1
omegacsd_CUJSAB	Clc1c(OCCn2nc(SC)nc2N)c(Cl)ccc1
omegacsd_CUNTIO	n1(ncnc1)/C(=C/C(=O)C(C)(C)C/c1cccc2c1cccc2
omegacsd_CUSLUX	Clc1c(SC)n(S(=O)(=O)c2ccc(cc2)C)c2c1cc(cc2)C
omegacsd_CUWRIV	c1ccc(CS/(C(=C\c2esc3c(c2=O)cccc3)c2cccc2)(=O)=O)cc1
omegacsd_CYCLIZ10	c1ccc(cc1)[C@H](N1CC[N@H+](C)C1)c1cccc1
omegacsd_DABGUI	c1(ccc(cc1)S(=O)(=O)Nc1cc(nc(n1)C)OC)N
omegacsd_DADDUH	Clc1cc(Cl)cnc1Oc1ccc(cc1)Oc1c(Cl)cc(cn1)Cl
omegacsd_DAFTOT	n1c(C)nc(N)c(c1)CNC(=O)CCc1c[nH]c2cccc12
omegacsd_DAFVUB	O=c1n(c2c(n1Cc1cccc1)c(=O)n(c2=O)Cc1cccc1)Cc1cccc1
omegacsd_DAHNIJ	c1ccc(c2c1nc(cn2)NS(=O)(=O)c1ccc(cc1)N)Cl
omegacsd_DAKGEB	S=c1n(cc(n1c1cccc1)[C@@H]1OCC=C1)c1ccc(cc1)C
omegacsd_DANNEL	n1c(C(=O)c2ccc(cc2)Cl)c(cnc1cccc1)C)O
omegacsd_DAWRAU	c1(ccc(cc1)S(=O)(=O)NC(=O)c1cccc1)N
omegacsd_DAXKAO	C1CC(c2cc(ccc2S1)/C(=C\c1ccc(cc1)C(=O)OCC/C)C)C
omegacsd_DCLPET	Clc1ccc(cc1)[C@H](c1ccc(Cl)cc1)C(Cl)Cl
omegacsd_DCTXAN	Clc1ccc(NC(=S)C(=S)Nc2ccc(cc2)Cl)cc1
omegacsd_DEBBER	n1cccc2cccc(N[C@@H](Nc3cccc4ccenc34)c3ncnc3)c12
omegacsd_DEBBOB	c1(ccc(cc1)C)N(C(=O)C)Cc1c(cc(c1)C)N(C(=O)C)C
omegacsd_DEBFAR	O=c1n([nH]c(c1C(=O)c1cccc1)C)c1cccc1
omegacsd_DECZIU	Clc1ccc(NC2=C(C(=O)CO2)C(=O)OCC)cc1
omegacsd_DENBUT	o1ct(c2cccc2)nnc1Cc1ccc(OC)cc1
omegacsd_DENDAC	s1nc(N(C)C)nc1C(=O)c1cn(C(=O)C)c2cccc12
omegacsd_DERZAB	s1c(=S)n(nc1N(C(=O)NC)C)Cc1cc(F)ccc1
omegacsd_DIAVER	n1c(nc(c1)Cc1cc(c(cc1)OC)OC)N)N
omegacsd_DIGSIV	O=C1C[C@H](Cc2nn(c12)COCc1cccc1)C)C
omegacsd_DIPJAN10	c1(ccc(c1)O[C@H](C)CNC(=[NH2+])Cc1cccc(c1)C)OC
omegacsd_DISHOC	Clc1cc(OCC(=O)c2ccc(cc2)CCC)ccc1
omegacsd_DIWPUU	s1nc(c(n1)C(=O)N1CCCCC1)C(=O)N1C(CCCC1(C)C)C)C
omegacsd_DIWWUB	S=c1oc(nc(N(CC)CC)c1C)c1cccc1
omegacsd_DIZREJ	O=C(N(Cc1cccc1)C)c1c(C)cc[n+](C)c1C
omegacsd_DIZWAK	N(C(=O)c1ccc(cc1)Cl)CC[NH+]1CCOCC1
omegacsd_DOHREX	C\1(=C\c2ccc(cc2)[S@@H](=O)C)/C(=C(c2cc(ccc12)F)CC(=O)O)C
omegacsd_DOLJIX	S(=O)(=O)(Nc1ncnc(OC)c1OC)c1ccc(N)cc1
omegacsd_DOPXIP	Brc1cccc(NC(=O)N2CC[C@H]3N(c4c([C@H]3C2)cc(cc4)F)c2ccc(cc2)F)c1
omegacsd_DOTFEX	S(=O)(=O)(NCC(=O)O)c1cccc2c1cccc2N(C)C
omegacsd_DOXANN	C(=O)(c1ccc(cc1)OC)Cc1ccc(cc1)OC
omegacsd_DUDNUL	s1s/c(=N\c2cccc2)/n(c/1=N/c1cccc1)CC
omegacsd_DUDPAT	s1n(c(=S)n/c/1=N/c1cccc1)c1cccc1)CC
omegacsd_DUHSUU	s1nc(n(c/1=N/C(=O)C)c1cccc1)Nc1cccc1
omegacsd_DUMTAG	O1C(=O)c2c(/C/1=C(/c1cccc1)OC(=O)c1cccc1)cccc2
omegacsd_DUPKII	S1Cc2n(nc(c2c2cccc2)C(=O)OCC)c2cccc12
omegacsd_DUXYOK	S1(=O)(=O)N(C(=O)CCc2cc(OC)c(OC)cc12)c1ncc(cc1)C
omegacsd_DUZDAD	n1c(n(c1n)CC)c1ccc(cc1)OC)c1ccc(cc1)N(C)C
omegacsd_DUZRAR	Clc1c(NC)cc(OC)c(c1)C(=O)N[C@H]1C[N@H+](C)C1Cc1cccc1
omegacsd_EBTNIC	c1(cccc1)C(=O)Nc1c(C(=O)OCC)c(c(c(=S)[nH]1)C(=O)c1cccc1)N(C)C
omegacsd_ECBHMP	N1(C(=O)CC/C/1=C\c1[nH]c(c(c1C)C)C(=O)OCC)CC
omegacsd_EHMPYX10	N1C(=O)CC/C/1=C\c1[nH]c(c(c1C)C)C(=O)OCC
omegacsd_EITDZL	s1n(c(=N\c2cccc2)/n(c/1=N/CC)CC)c1cccc1
omegacsd_EMZPPO	c12c(=O)n(CC)c(=O)c1cn(CC)c(=O)c2c1n(ccn1)C
omegacsd_EPCMPO	O=C1N(C(C)C)CC(=C1CC(=O)Nc1cccc1)CC
omegacsd_EXOADN	n1cnc2(c1N)ncn2[C@H]1CO[C@H](OC1)OCC
omegacsd_FABSOQ10	s1c(ccc1[C@H](O)c1ccc(OC)cc1)[C@H](O)c1ccc(OC)cc1
omegacsd_FABWUA10	[nH]1/c(=C\C(=O)c2cccc2)/n(c(=O)c2cccc12)c1cccc1C

CODE	SMILES
omegacsd_FACCER10	c1(cc(ccc1)N1Cc2c(cc(c2OC1=O)C)C(=O)OC
omegacsd_FAGHIE	Brc1ccc(C(=O)N2/C(=C\c3cc(OC)c(OC)cc3)/c3c(CC2)cc(OC)c(OC)c3)cc1
omegacsd_FAHTUD	Clc1ccc(Nc2nn3c(=O)c(nnc3n2c2ccc(Cl)cc2)C)cc1
omegacsd_FAHXIV	N1(C(=O)N(C(=O)[C@H]1CC(=O)OC)Cc1cccc1)C(=O)C
omegacsd_FAJVAN	s1c[n+](c(C)c1CCO)Cc1c(nc([nH+]c1)C)N
omegacsd_FANPUF	N1C(=O)N([C@@H](C21CCCCC2)O)CN(Cc1cccc1)Cc1cccc1
omegacsd_FANRER	[nH+]1c(N2CCN(CC2)C(=O)[C@H]2Oc3cccc3O2)nc(N(C)C)c2cc(OC)c(OC)cc12
omegacsd_FAVYEG	S=c1oc2c(n1C(=O)OCc1cccc1)cccc2
omegacsd_FAWREA	s1nc(NNc2cccc2)c2c1ccc(c2)CC(=O)OC
omegacsd_FAXPUP	N1C(=O)/C(=C(CCC(=O)OC)c2cccc2)/C=C1c1cccc1
omegacsd_FBAZD	C1[C@]2(C(=O)NCN2c2cccc2)CCN(CCCC(=O)c2ccc(cc2)F)C1
omegacsd_FECPUY	s1c(=S)n(c(c1C)c1cccc1)[C@H](C)c1cccc1
omegacsd_FEFPOV	o1nc(nc1c1cccc1)CCNc1cccc1
omegacsd_FEKYEZ	S(=O)(=O)(C)Nc1ccc([C@H](O)Cn2c[nH+]cc2)cc1
omegacsd_FEMMAL	Brc1ccc(C(=O)Nc2c3c([C@@H](CN(C3)C)c3cccc3)ccc2)cc1
omegacsd_FEVZUB	[n+]1(cccc1)CCCc1c[nH]j2cccc12
omegacsd_FEWBAK	n1(nc(c(c1=O)O)C(=O)c1cccc1)c1cccc1e1cccc1
omegacsd_FEYJEY	n1c(c2c(NS(=O)(=O)c3ccc(ec3)C)cc(cc2)OC)oc(=O)c2cccc12
omegacsd_FEYKUP	S=c1c2cccc2ccn1/C(=CN1CCOCC1)c1ccc(Br)cc1
omegacsd_FHFPBY	C(CCC(=O)c1ccc(cc1)F)N1CC[C@](c2ccc(cc2)F)(CC1)O
omegacsd_FIBREN	n1c(nc(c2c1oc(n2)C)N[C@@H](CC(=O)O)c1cccc1)C
omegacsd_FIJJUD	S(=O)(=O)(c1ccc(cc1)N1C(=O)c2cccc2C1=O)/N=c/1\sc[nH]1
omegacsd_FIVPUV	O=C1O[C@H](CN1c1cccc1)COc1cccc1
omegacsd_FIWLUS	s1c(nc1N(=O)=O)NC(=O)c1sccc1
omegacsd_FIXNUV	c1(cc(cc1N)S(=O)(=O)Nc1ccnn1c1cccc1
omegacsd_FLPNTX10	c1c2c(ccc1C(F)(F)F)Sc1c(ccc1)/C/2=C/CCN1CCN(CC1)CCO
omegacsd_FOBZIF	O=c1[nH]c(c[nH]1)C(=O)c1ccc(cc1)n1ccn1)CC
omegacsd_FOGWAZ	c1(nc2c(c(n1)N)c(c2)CNc1cc(c(c1)OC)OC)OC)C)N
omegacsd_FOJZUZ	S(Cc1cccc1)C(=S)N1CCOCC1
omegacsd_FOLMEY	S1C(=O)CN2[C@H]1[C@@H](C2=O)NC(=O)Cc1cccc1
omegacsd_FOLYIO	[nH+]1c(nc([NH2+])c2cc(c(cc12)OC)OC)N1CCN(CC1)C(=O)c1occc1
omegacsd_FOMDUG	n1c(cc(cc1C)C)N(C(=O)c1cccc1)CC
omegacsd_FOPMIG	c1(c(C(=O)[O-])cccc1)Nc1c(Cl)c(C)ccc1Cl
omegacsd_FOWPOW	O=c1[nH]c2nnnn2nc1Nc1ccc(OC)cc1
omegacsd_FOYLIO	N1(C(=O)C(=C([C@@H]1c1cccc1)C)CC(=O)OCC)c1cccc1
omegacsd_FPAMCA	c1(c(ccc1)C(=O)O)Nc1cccc(C(F)(F)F)c1
omegacsd_FUCFIS	s1n(c(=O)cc1c1cccc1)/C=C/c1cccc1
omegacsd_FUDVUV	N(=O)(=O)c1ccc(N2[C@H](CCC2)CO)cc1
omegacsd_FUGSIJ	c1(c(OC)c(Br)ccc1OC)C(=O)NC[C@H]1CCCN1CC
omegacsd_FUHHAR	n1(enc(c1N)c1nn(cn1)C)Cc1cccc1
omegacsd_FUHLID	S=C(N(C(C)C)C(C)C)/N=c/1\sc(Sc2cccc2)n1C
omegacsd_FUJRUX	N1([C@@H]([C@H]([C@@H](O1N(O)c1cccc1)CC)CCC)c1cccc1
omegacsd_FUMBOE	O(C(=O)c1ccc(N(=O)=O)cc1)C(C)C)c1cccc1
omegacsd_FUNXUH	o1c(cc2cccc12)C(=O)c1ccc(cc1)OC
omegacsd_FUNYAO	o1cc(c2cccc12)C(=O)c1ccc(cc1)OC
omegacsd_FUPFIF	O=C(N(C)C[C@H](C)c1cccc1)c1c(cc[nH+]c1)C
omegacsd_FURACM	Clc1cc(Cn2c(=O)[nH]c(=O)c(F)c2)ccc1OC
omegacsd_FURKEI	[C@]1([C@](C1)C(=O)OC)Sc1cccc1)(C(=O)OC)Sc1cccc1
omegacsd_FURSEM01	Clc1cc(NCc2occc2)cc1S(=O)(=O)N)C(=O)O
omegacsd_FUSZOI	Brc1c(OCC(=O)c2ccc(cc2)CC)cccc1
omegacsd_GAKWIY	n1c(Nc2cc(ccc2)C(F)(F)F)c(ccc1)C(=O)OCCN1CCOCC1
omegacsd_GALMOV	n1(cc(c(=O)c2cc(c(cc12)N1CC[N@H+](CC1)C)F)C(=O)O)CC
omegacsd_GALSEM	S(=O)(=O)(NC(=O)CC)c1c(Nc2cc(ccc2)C(F)(F)F)ccn1
omegacsd_GANFIK	n1(c2cccc2c(c1)CCNC(=O)C(F)(F)F)C(=O)C(F)(F)F
omegacsd_GASPUL	n1(c(cc2cccc12)[C@](O)c1cccc1)C[C@](O)(C)c1cccc1)C
omegacsd_GASXED	c1cc(ccc1NC1=C(C(=O)OC1)C(=O)Nc1cccc1)C
omegacsd_GATPOG	Clc1cc(ecc1Cl)C(=O)CC1CCCC1
omegacsd_GAVMIZ	[C@H]1(CC(=O)N(C1=O)Nc1cccc1)c1ccc(cc1)OC(C)C
omegacsd_GEBJOM	O1c2cc(ccc2OC1)CCN1C(=O)CCC2=C1C(=O)CC2
omegacsd_GEHKIN	c1c(c(c1C)C(=O)Nc1cc(cc1)C(=O)OC)O)C
omegacsd_GEJJUA	Brc1ccc(O/C(=C/C(C)(C)C)/n2ncnc2)cc1
omegacsd_GEJLAI	O=N(=O)c1ccc(CCNc2cccc2)cc1

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omegacsd GEKWAU	c1(c(ccc1F)Cn1c2c(c([nH]cn2)NC)nc1
omegacsd GIFZAW	S1CN([C@H](C)[C@@H]1CCO)Cc1c(nc(nc1)C)N
omegacsd GIHKAJ	N1(CCCC1)C(=N)Nc1nc(no1)c1cccc1
omegacsd GIHTUM	Clc1ccc(cc1)[C@@]1(C[C@H](COc2ccc(Cl)cc2)ON1C)Cn1cncc1
omegacsd GIHWUP	n1(c(=O)n/c(=N/c2c(cc(cc2)C)C)/cc1c1cc(c(cc1)OC)OC)C)CC
omegacsd GIKJOZ	s1c(nc(c1C(=O)c1cccc1)C)N(C)c1cccc1
omegacsd GINKUJ	[nH]1c(=O)n(c(=O)nc1C(=O)OCC)c1ccc(cc1)Cl
omegacsd HADLAZ	[nH]1/c(=C\C(=O)c2ccncc2)/n(c(=O)c2cccc12)c1cccc1C
omegacsd HALDOL	Clc1ccc(cc1)[C@@]1(CCN(CCCC(=O)c2ccc(cc2)F)CC1)O
omegacsd HALJOT	[C@H]1(C2=C(C(=O)N1CCO)CCCC2)c1ccc(cc1)C
omegacsd HALOPE	Clc1cc2[nH]c(=O)n(c2cc1)[C@@H]1CCN(CC1)CCNC(=O)c1cc(F)cc1
omegacsd HALSES	n1(c(nc2cc(cnc12)Cl)CC(CC(=O)O)(C)C)Cc1ccc(cc1)Cl
omegacsd HASCOT	Oc1c(c2nnN(c3cccc3)C)c(n2)c2cccc2)cccc1
omegacsd HATKES	n1c(ccc(c1OC(=O)c1ccc(cc1)Cl)C#N)OC(=O)c1cccc1
omegacsd HAVJET	n1[nH]c(=O)ccc1c1ccc(cc1OC)NC(=O)C
omegacsd HAVLUL	N1(C(=O)N(C(=O)[C@]1(c1cccc1)c1cccc1)Cc1ccc(cc1Cl)Cl)CC(=O)O
omegacsd HAVRUR	S=c1n(c2c(c(=O)n1C(=O)c1cccc1)cccc2)CC
omegacsd HBFRAN	O1C[C@@H](c2cccc12)CC(=O)Nc1cccc1
omegacsd HECHEC	N(C)c1c(C(=O)c2c(OC)cccc2)cc(Br)cc1
omegacsd HEHVOF	n1c(n(N(C(=O)C)C(=O)[C@H](C)c2cccc2)c(=O)c2cccc12)C(C)C
omegacsd HEJTAR	S=C1N([C@H]2CCCC[C@H]2N1)C(=O)Nc1cccc1
omegacsd HEKROE	n1(c(nc2cccc12)Oc1c(ccc1)OC)C
omegacsd HEKZAY	n1(ccc2cc(ncc12)C(=O)OCC)S(=O)(=O)c1ccc(cc1)C
omegacsd HEMLOA	s1c(nn1C(NC(=S)c1cccc1)(C)C)c1cccc1
omegacsd HEMWUR	s1nc2n(/c1=N/C(=O)NCc1cccc1)ccs2
omegacsd HEMXIG	Clc1ccc2oc3ns/c(=N\c(=O)NCc4cccc4)/n3c2c1
omegacsd HEPGAK	Clc1c(Sc2cc(ccc2)C(F)(F)F)e(Cl)cc(n2ncc(=O)[nH]c2=O)c1
omegacsd HEPKUI	Br[C@H](C(=O)N1C(=O)N(C)[C@@H]([C@H]1c1cccc1)C)CN1C(=O)c2cccc2C1=O
omegacsd HEPYAC	Clc1cc(CC(=O)N2[C@H](c3ccoc3CC2)C[N@H]2C[C@@H](O)CC2)ccc1Cl
omegacsd HEVJAT	Clc1c(Ne2c(ccc2)CC(=O)[O-])e(Cl)ccc1
omegacsd HEVRIJ	O=C(c1cccc1)c1ccc(NCNC2ccc(C(=O)c3cccc3)cc2)cc1
omegacsd HEVXEL	O1COc2cc(c(OCC)cc12)[C@@H](C)c1ccc(OC)cc1
omegacsd HEXFEV	O(c1nc(nc(n1)N(C)C)N(C)C)Cc1occc1
omegacsd HEXYIS	S(=O)(=O)(N1C2cccc2C(=O)[C@@H]1c1cccc1)c1ccc(cc1)C
omegacsd JOTDAX	s1sc(Nc2cccc2)c(/c1=N/c1cccc1)C(=S)Nc1cccc1
omegacsd JOXFIL	O1/C(=C(/c2cccc2)c2ccc(OC)cc2)/CCC1=O
omegacsd JUBGES	O1Cc2cccc2C(=O)c2c1ccc(c2)CC(=O)OC
omegacsd JUBJOF	[n+]1(ccc(N(C)C)cc1)C(=O)Oc1cccc1
omegacsd JUDLUP	S(=O)(=O)(/N=c1/onc(o1)c1c(cc1C)C)C)c1ccc(cc1)C
omegacsd JUDWEK	s1c(=S)n(c(c1C(=O)OC)SC)c1cccc1
omegacsd JUHHEZ	C1C=C(Cl)[C@@H](OC)N(C1=O)[C@H]1C(=O)N([C@H]1c1cccc1)c1cccc1
omegacsd JUKZUK	o1c(=O)c(cc2C(=O)CC(C)C)Cc12NC(=O)c1cccc1
omegacsd JUVPAR	C1(=O)C(C)(C)[C@H]2N1C(=C(C)O2)C(=O)OCc1ccc(cc1)N(=O)=O
omegacsd KABJOM	Clc1cccc(c1)N1CCN(C1=O)CCN1CC(C1)C
omegacsd KACKII	N1(C=Cc2c(C(=O)C1)cccc2)C(=O)Nc1ccc(cc1)OC
omegacsd KAVLIC	Clc1ccc(cc1)Cc1nn(c(=O)c2c1cccc2)[C@@H]1CCN(C)CCC1
omegacsd KAVNOK	n1c(c(n2cccc(c12)C/C=C/c1cccc1)CC#N)C
omegacsd KAXXAI	Clc1cccc(Nc2c(C(=O)O)cccc2)c1C
omegacsd KEBVES	C1(CCC(c2ccc(cc12)NC(=O)c1ccc(cc1)C(=O)O)(C)C)C
omegacsd KECDUR	S=C1N(CC[C@@H]1[C@H](CC(=O)c1c(cc1C)C)C)C
omegacsd KEJBEG	Clc1cc(C(=O)c2cccc2)c(n2c(nn2CN(CC)CC)C)cc1
omegacsd KEJGEL	c1(c(cc(c1)OC)OC)Br)c1cnenc1c1ccc(c(c1O)OC)OC
omegacsd KEMHOZ	[C@H]1([N@H+]([C@H](Cc2cc(O)cc(OC)c12)C)Cc1cccc1)C
omegacsd KICRIX	c1cc(cc(c1C(=O)c1cccc1)C(=O)O)OC
omegacsd KIFZAA	O(C(=O)Nc1cccc(c1)C)c1cccc(NC(=O)OC)c1
omegacsd KIHWAZ	S(=O)(=O)(c1ccc(cc1)C)c1cc(c(cc1cccc1)C)C
omegacsd KIHWED	S(=O)(=O)(C1=C([C@H]2[C@H]1CCC=C2)c1cccc1)c1ccc(cc1)C
omegacsd KINJIA	N1C(=C([C@H](C(=C1C)C(=O)OCC)c1oc(cc1)c1ccc(cc1)C)C(=O)OCC)C
omegacsd KIXLOS	c1(c(O)cc(O)cc1OC)C(=O)CCc1ccc(OC)cc1
omegacsd KOFKUL	o1c(nc(c1cccc1)C(C)C)NC(=O)OCc1cccc1
omegacsd KOFLIA	o1c(ncc1cccc1)NC(=O)OCc1cccc1
omegacsd KOFLOG	o1c(ncc1C(C)C)NC(=O)OCc1cccc1

CODE	SMILES
omegacsd_KOFMIB	o1c(c(nc1c1cccc1)C)NC(=O)OCc1cccc1
omegacsd_KOJMEB	O1C(=O)C=C2CCCCC2=C1c1ccc(OC(=O)CCC)cc1
omegacsd_KOKBIV	O=C(/C=c1[nH]c2cccc2[nH]c1=C/C(=O)c1cccc1)c1cccc1
omegacsd_KOTGIJ	C(=O)(c1ccc(cc1)N(=O)=O)OC[C@H](c1cccc1)F
omegacsd_KUBHEU	S1[C@H](COc2cccc2)C[C@H](n2c(=O)nc(N)cc2)C1
omegacsd_KUFPIK	n1c(nc(nc1N)Nc1ccc(cc1)C(C)(C)C)Nc1ccc(cc1)C(C)(C)C
omegacsd_KUHNUW	Cc1cccn2c1nc(c(c2=O)CCN1CC[C@H](CC1)c1noc2cc(ccc12)F)C
omegacsd_LABLOP	n1(cnc(c1NCc1cccc1)N(=O)=O)C
omegacsd_LACCEX	[nH]1cc(c2cccc2)CC(=O)NC(C(=O)O)(C)C
omegacsd_LACPAG	[S@@]1(=O)(=NC(=O)[C@](O)(C1)CC(=O)OCc1cccc1)C
omegacsd_LADTOZ	S(=O)(=O)(n1cnc([C@H](c2c(c(ccc2)C)C)C)c1)c1ccc(cc1)C
omegacsd_LANXED	S(=O)(=O)(C[C@H]([C@@H](N1CCCC1)c1cccc1)C)c1cccc1
omegacsd_LAWJEY	o1c2cccc(c2nc1c1c(NC2CC2)nc1)C
omegacsd_LAXWEM	[C@@H]1(C(C)(C)C)N(CC(=O)O1)C(=O)Oc1cccc1
omegacsd_LEDWAS	O=C(O)CCCNC1ccc(N(=O)=O)cc1
omegacsd_LEKMET	O=C1N(Cc2c1cccc2)c1ccc(cc1)[C@H](C)C(=O)O
omegacsd_LELROJ	S(=O)(=O)(NC(=O)Nc1nc1(n1)C)c1c(eccc1)C(=O)OCC
omegacsd_LEMXIK	Clc1ccc(NC(=O)O[C@@H]2CCC[C@@H]3C[C@H]([C@H](OC(=O)Nc4ccc(Cl)cc4)[C@H]23)C)cc1
omegacsd_LERKAU	n1c(nn2C(=O)N(CCC2)C[C@H](C)c1cccc1)c1cccc1
omegacsd LETBAN	S1(=O)(=O)c2cccc2C(=O)N1CCC(=O)O
omegacsd LETBUH	n1c(OC)nc(OC)nc1ON1C(=O)CCC1=O
omegacsd LEVTOV	n1(Nc2cccc2)cc(c(c1cccc1)C(=O)OCC)C(=O)OCC
omegacsd LEZGOM	S(=O)(=O)(N(Cc1cccc1)[C@H](c1cccc1)C(=O)O)c1ccc(cc1)C
omegacsd LIKBUC	S(=O)(=O)(N(Cc1ccc(OC)c(OC)c1)[C@H](c1cccc1)CO)c1ccc(cc1)C
omegacsd LIKGIV	[S@@]1(=O)(c1ccc(cc1)C)c1ccc1[C@@H](O)c1cccc1
omegacsd LIKMEX	S=C(NCCc1ccc(Cl)cc1)N1Cc2cc(O)c(O)cc2CCCC1
omegacsd LINLAV	O=c1n(cnc2c1cccc2)[C@H](Nc1c(cc(c1)C)C)Cc1cccc1
omegacsd MAMNAQ	CN(CC1=C(C(=O)c2c(C1=O)cccc2)C)c1cccc1
omegacsd MATSTA10	s1n(c(n/c/1=N/S(=O)(=O)c1ccc(cc1)C)c1ccc(cc1)OC)C
omegacsd MBZTWT10	c1(=S)[nH]nc(CCN2CCOCC2)n1Cc1cccc1
omegacsd MICONZ	n1(cncc1)C[C@@H](c1c(cc(cc1)Cl)Cl)OCc1c(cc(cc1)Cl)Cl
omegacsd MINTSA	c1(ccc(cc1)C)S(=O)(=O)Nc1n(c2cccc12)C
omegacsd MLDPHE10	O=C1N(C)[C@H](C(=O)N([C@@H]1Cc1cccc1)C)Cc1cccc1
omegacsd MOPBZA	Brc1ccc(cc1)C(=O)NCCCCc1ccc(cc1)OC
omegacsd MRMPYR	c1cccc1[C@]1(C)C(=O)N(C(=O)C1)CN1CCOCC1
omegacsd MTBPNP	n1c(nc2c(c1NC(=O)c1cccc1)[nH]cn2)SC
omegacsd MVERIQ	COc1c(ecc(c1)Cc1c2cc(c(cc2)CC)OC)OC)OC
omegacsd NADYIA	O([C@@H]1C(=O)N([C@@H]1[C@H]1N(CCC1)C(=O)OC(C)(C)C)c1ccc(OC)cc1)C
omegacsd NADZIB	O=C1N([C@@H]([C@@H]1O)[C@H]1N(CCC1)C(=O)OC(C)(C)C)c1cccc1
omegacsd NBPENC	C1(=C(C)S[C@H]2CC(=O)N12)C(=O)OCc1ccc(cc1)N(=O)=O
omegacsd NFCSEY	Clc1ccc(S(=O)(=O)/C=C/c2oc(N(=O)=O)cc2)cc1
omegacsd PACVUK	Clc1c([C@@H](O)c2c(sc(c2)CC)n2c(nnc2)CN)cccc1
omegacsd PAPPHI	O=C1N(C(=O)c2cccc12)c1ccc(Nc2cccc2)cc1
omegacsd PBBSHD	C(Cc1ccc(cc1)C(=O)[C@@H]1C[C@]1C(=O)c1cccc1C2=O)C
omegacsd PBYXCH	O([C@@H]1CCCC(=C1)N1CCCC1)C(=O)c1cccc1
omegacsd PCPTZA	s1c(nc(c1CC(=O)O)c1ccc(cc1)Cl)c1cccc1
omegacsd PEBHAF	O=C(OC)[C@@H](N1C(=O)c2cccc2)C1=O)[C@H](O)c1cccc1
omegacsd PEKCEO	Brc1ccc(C(=O)O[C@H](c2nc([C@@H](OC(=O)c3ccc(Br)cc3)C)cc2)C)cc1
omegacsd PEPHEX	[O-][N+](CCC[C@H]1C(=O)N[C@@H](C)c1cccc1)Cc1cccc1
omegacsd PEXFED	O1[C@H](N([C@]2(C(C)C)C)C1=O)C(=O)c1cccc1)C(C)(C)C
omegacsd PEXJEH	O=C(c1c([nH]c(c1C(=O)OC)C)C)c1cccc1Cc1cccc1
omegacsd PIBSXM	C(c1cccc1)[S@@]1(=NN1C(=O)c2c(ccc2)C1=O)(=O)Cc1cccc1
omegacsd PIDSIE	O=C1N(OCc2cccc2)C(=O)C2(C1)CCCC2
omegacsd PIDWOO	o1c(nc(c1c1cccc1)c1cccc1)c1ocnc1c1cc(ccc1)OCC(=O)O
omegacsd PIKDIW	S(=O)(=O)(Nc1cc(OC)cc2cc(nc12)C)c1ccc(C)cc1
omegacsd PILCOC	c1(cccc1)COc(=O)N1CCCC1C(=O)NC(C)C
omegacsd PINSAG	S1C[C@@H]([C@@H](N(C)C)C=C1c1ccc(cc1)C(F)F)C(=O)Nc1cccc1
omegacsd PKOJSI	c1cccc1C(=O)COc1coc(cc1=O)CO
omegacsd PMAANO01	c1(cccc1)N1C(C)C[C@](C)(N(c2cccc2)O)O1
omegacsd PMANAQ	O=C1C(=C(C(=O)c2c1cccc2)C(=O)CN(C)c1ccc(OC)cc1)c1cccc1
omegacsd PMBSAN10	c1(ccc(cc1)OC)S(=O)(=O)N(C(C)C)c1ccc(cc1)OC
omegacsd PMCPRC10	[C@@]1([C@@]1(C)c1cccc1)c1cccc1(C(=O)O)C

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omegacsd_PMEPEN	CC1([C@@H](C(=O)O)N2[C@H]([C@H](C2=O)NC(=O)COc2cccc2)S1)C
omegacsd_PMPAIN	O(c1ccc(Nc2c3cccc3[nH]c2c2cccc2)cc1)C
omegacsd_PMPBTZ	c12cccc1c(c1cc(n(c3cccc3)n1)OC)ns2
omegacsd_PMTSVD	s1n(c2cccc2)c(=O)n(/c/1=N/S(=O)(=O)c1ccc(cc1)C)C
omegacsd_PNBPIP	c1(ccc(cc1)N(=O)=O)C(=O)N1CCCCC1
omegacsd_PNPAUR	OC(=O)CNC(=O)Cc1ccc(cc1)N(=O)=O
omegacsd_PONXUL	S1C(=O)NC(=O)[C@H]1Cc1ccc(OCCN(C)c2[nH+]cccc2)cc1
omegacsd_PTHPAL	C(=O)([C@H](Cc1cccc1)N1C(=O)c2cccc2C1=O)O
omegacsd_PXBVCP10	BrC(=C[C@@H]1C(C)(C)[C@@H]1C(=O)O[C@H](C#N)c1cc(ccc1)Oc1cccc1)Br
omegacsd_PXEZSD	C1[C@]2(C(=O)NCN2c2cccc2)CCN(CCOC2cccc2)C1
omegacsd_PXMPEN	N(C(=O)COc1cccc1)[C@@H]1[C@H]2N(/C(=C/C)\C)/C(=O)S2)C1=O
omegacsd_PYMSBZ	S(=O)(=O)(N)c1ccc(OC)c1C(=O)NC[C@H]1N(CCC1)CC
omegacsd_QQQHDG10	S(=O)(=O)(Nc1nn([nH]1)c1cccc1)c1cccc1
omegacsd_SADXIE	O=c1n(Cc2cccc2)c2nc(=O)n(c(=O)n2cc1)Cc1cccc1
omegacsd_SAGMUI	c1(c(c(ccc1)O)O)c1scc(n1)C(=O)NCCc1nc[nH]c1
omegacsd_SAGWOM	C(=O)(C[n+])lcsc(c1)NC(=O)Cc1cccc1)[O-]
omegacsd_SAVXOC	S1(=O)(=O)N(C(=C(c2cccc12)OC)C(=O)/N=c\1/n(ccc1)C)C
omegacsd_SAVYET	S(c1c(oc(c1)c1cccc1)C(=O)c1cccc1)C
omegacsd_SAVZEU	c1(c(ccc1)Nc1nc(c(cc1C(=O)OCC)C#N)N)C(=O)OCC
omegacsd_SAWZUL	c1(nc(cc2cccc12)NC(=[NH2+])Cc1cccc1)Cc1cccc1
omegacsd_SEFLIY	O1[C@@H](c2c(C1=O)cccc2)CC(=O)N1[C@H](CSC1=S)C(C)C
omegacsd_SEMDET	c1(nen(n1)CN1CCCCC1)C1(1CCCCC1)O
omegacsd_SEMXEN	s1c(=O)n(c2cccc12)CC(=O)OCc1cccc1
omegacsd_SEYMIS	o1nc(c(C(=O)Nc2cn(C)c2)C(=O)OCC)c1C)c1cccc1
omegacsd_SEYPUH	Clc1ccc(cc1)C[C@H](n1ncn1)C(=O)C(C)(C)C
omegacsd_SFDMOX	c1(ccc(cc1)N)S(=O)(=O)Nc1cc(nc(n1)OC)OC
omegacsd_SIFJIA	o1c(=O)cc(c2ccc(cc12)C)COc1ccc(cc1)C
omegacsd_SIHDDES	N1(C(=S)SC[C@@H]1[C@@H](C)C)C(=O)[C@H](C)[C@@H]1N(C(=O)CC1)C
omegacsd_SIHDIW	N1(C(=S)SC[C@@H]1C(C)C)C(=O)[C@H](C[C@H]1N(C(=O)CC1)C)SC1CCCCC1
omegacsd_SIHGIZ	Brc1ccc(NC(=S)O[C@@H](C)C[C@H]2[NH2+])C[C@H](CCC2)C)C)cc1
omegacsd_SIHVUA	Brc1ccc(cc1)C(=O)NC1(C(=O)O)CC1
omegacsd_SILTUC	c1(c(ccc1)OC)NC(=O)Nc1c(ccc1)OC
omegacsd_SINKUV	O=C(OC)[C@]1(N2C(=O)c3cccc3C2=O)C[C@H]1C(=O)OC
omegacsd_SISYIC	o1c2c(ccc2c(OC(C)C)c1C(=O)Nc1nn[nH]1)c1cccc1
omegacsd_SIZDOU	S(=O)(=O)([C@@H]1C=C[C@H](NC(=O)OCc2cccc2)[C@@H](C1)C(=O)c1cccc1)c1cccc1
omegacsd_SLFNMB04	c1(ccc(cc1)S(=O)(=O)Nc1cc(on1)C)N
omegacsd_SLFNMF02	Nc1ccc(cc1)S(=O)(=O)Nc1nn(cc1)OC
omegacsd_SOPNAM	S(=O)(=O)(Nc1c(n(n(c1=O)c1cccc1)C)C)c1ccc(N)cc1
omegacsd_SOPSIZ	N(c1c(ccc(c1)C)C)C(=O)[C@H](C)SC(=O)N
omegacsd_SORCOR	S(=O)(=O)(n1cc(cc1)C(=O)c1cccc1)c1ccc(cc1)C
omegacsd_SOWCOW	O=C(N1C(=CCC1)c1cccc1)CN1C(=O)c2cccc2C1=O
omegacsd_SPIRIL	C1[C@]2(C(=O)NCN2c2cccc2)CCN(CC/C=C(/c2ccc(cc2)F)C)C1
omegacsd_SUKEPET	[nH+]1c(CC)cc(c2CCCCc12)OCc1ccc(cc1)c1cccc1c1[nH]nnn1
omegacsd_SURREC	O=C(N(c1c(N(C)C)C(=O)c2cccc2)cccc1)C)c1cccc1
omegacsd_TAJSEC	S=c1n(cc(c1)Nc1cccc1)C(=O)c1cccc1C
omegacsd_TANNOL	[nH]1cc(c2cccc12)CCNC(=O)Cc1ccc(cc1)O
omegacsd_TAPBZO	S(=O)(=O)(Nc1c(c2oc(=O)c3c(n2)cccc3)cccc1)c1ccc(cc1)C
omegacsd_TAPSOS	Clc1ccc(S[C@@H]2C(=O)O[C@H](N2C(=O)Cc2cccc2)C(C)(C)C)cc1
omegacsd_TAPZEP	N1(C(=O)C[C@H](CC1=O)c1cc(ccc1)Br)CN1CCOCC1
omegacsd_TAZPUF	O=C(O)[C@H]([C@@H](c1cccc1)c1ccc(Cn2c3nc(cc(c3nc2CC)C)C)cc1)C
omegacsd_TAZXAT	S(c1[nH+]cccc1)c1nnn(Sc2[nH+]cccc2)c2c1cccc2
omegacsd_TECSUP	O=C(N[C@H](C)c1cccc1)[C@@]1(C=Cc2cccc12)C
omegacsd_TEDBUZ	O=C(NC(=O)Nc1c(=O)n(n(c1C)C)c1cccc1)c1cccc1
omegacsd_TEKBIU	Fc1c(N2CC[NH2+]CC2)cc2c(c(=O)c(en2C2CC2)C(=O)O)c1
omegacsd_TPHPRO	c1(ccc(cc1)C)S(=O)(=O)N1CCC[C@H]1C(=O)N1C[C@H](C[C@H]1C(=O)O)O
omegacsd_VADTAV	o1nc(c2cccc2)c2n[nH]c(C(=O)c3cccc3)c12
omegacsd_VAMBOA	Clc1ccc(cc1)C(=O)NCCc1ccc(OC(C)C)C(=O)O)cc1
omegacsd_VAMCUH	C1OC(=O)Cc2cc(c1cc1)OCc1cccc1)OC
omegacsd_VAYXOI	n1cc(c(c(c1C[S@](=O)c1[nH]c2e(n1)ccc(c2)OC)C)OC)C
omegacsd_VEMCIZ	s1c(c(c1c1ccc(N(C)C)cc1)c1ccc(OC)cc1)C(=O)c1ccc(OC)cc1
omegacsd_VENRUB	n1(nn2c1cccc2)COc1cc2c(cc1)cccc2
omegacsd_VEXROF	C1(=O)[C@H]([C@@H](C1)c1cccc1)N(C)S(=O)(=O)c1ccc(cc1)C

CODE	SMILES
omegacsd VEYRAS	COc1cccc1OC[C@H](c1ccc(cc1)O)O
omegacsd VIBNID	[C@@@H]1(N(C)C(=O)N(C)[C@@@]21C=CN(C(=O)C)C=C2)NC(=O)c1cc(C)cc(C)c1
omegacsd VIBWIM	O1C(=O)C[C@@H](c2c(O)cc(O)c(c12)C(=O)CCc1cccc1)c1cccc1
omegacsd VIMYUL	c1(c(O)c(Br)ccc1OC)C(=O)NC[C@H]1CCCC[N@H+]1Cc1ccc(F)cc1
omegacsd VIPHOR	O1[C@@H](C=C[C@]21NC(=O)N(C2=O)Cc1ccc(OC)cc1)COCc1cccc1
omegacsd VOPDIN	O=C1N([C@@]2([C@@H](C2)c2cccc2)C(=O)OC)C(=O)c2cccc2
omegacsd VORBAF	S(=O)(=O)(NC(=O)Nc1nc(nc(n1)C(C)C)OC)c1c(Cl)cccc1
omegacsd VORDAH	c1(ccccc1)[C@@H](O)C(=O)N1CC=C[C@@H](O1)N1C(=O)CC[C@H]1C(=O)OC
omegacsd VORJER	c1cc(ccc1C(=O)C1=C(C(=O)OC1)Nc1c(=O)n(c(=O)n(c1N)C)C)OC
omegacsd VOWXEK	c1cccc1c1cc(/C=C/Cc2cccc2)no1
omegacsd VOXHAR	Clc1cccc(N2CCN(C[C@H](O)CN3C(=O)CCC3)CC2)c1
omegacsd VOXMOK	n1c(cc(cc1C)C)NC(=O)c1n(c2cccc2c1)C
omegacsd VOXNOL	C(=O)(Cc1ccc(cc1)N(=O)=O)c1cccc1
omegacsd VUGDEG	O=C(Nc1cccc1)c1[nH]c(cc1c1cccc1)C
omegacsd VURTOR	[nH+]1c(C)cc(OCc2ccc(cc2)c2cccc2c2[nH]nnn2)c2cccc12
omegacsd VUSKID	S(c1cccc1)c1nc(n1C)[C@H](O)c1cccc1
omegacsd WAMZAL	n1(c(=O)nc(NC(=O)c2cccc2)cc1)[C@H]1CC[C@H](O1)CO
omegacsd WASTEP	Fc1ccc2c(c1)onc2[C@H]1CCN(CC1)Cc1c(=O)n2c(nc1C)CCCC2
omegacsd WAVTIW	n1c(cc(c2cccc12)C)c1c(ccc1)NC(=O)c1ccc(cc1)OC
omegacsd WEBCOV	[NH+]1[C[C@H](O)[C@@H]1Oc2c(CC1)cc(cc2)F)Cc1cccc1
omegacsd WELGAV	n1c(nc(c2CCC(=O)N(c12)Cc1ccc(cc1)c1c(ccc1)c1[nH]nnn1)C)C
omegacsd WESFOP	Br[C@]1(CC21CCCCC2)C(=O)N[C@H](c1cccc1)C
omegacsd WESZOJ	C[C@H](n1nc2c(n1)cccc2)[C@H](C)n1nc2c(n1)cccc2
omegacsd WEVTIA	n1(cc(c(c1c1oc(e1N)Cl)c1cc(cc1)OC)Cl)C
omegacsd WEXBEG	S(=O)(=O)(NC(=O)Nc1nc(OC)nc(n1)C)c1c(n(c2cccc12)C)C(=O)OC
omegacsd WIDDIW	C1CC[C@H](c2c(c3cccc3)[nH+]1c12)NCc1cccc1)O
omegacsd WIFREI	s1c(nnc1C(NC(=S)c1cccc1)C)C(=O)OCC
omegacsd WIKJOP	Clc1ccc(C(=O)Sc2c(SC)nn3c2cccc3)cc1
omegacsd YABKOB	O=c1[nH]c(c(n1C(=O)c1cccc1)C(=O)c1ccc(cc1)n1ccn1C)CC
omegacsd YAGWOS	n1(nn2cccc12)[C@H]1OCC[C@H]1[C@H](c1cccc1)N1CCOCC1
omegacsd YAHBOY	O1[C@H](C)Cc2c(n(c(=O)nc12)C)NCc1cccc1
omegacsd YAHFAO	Brc1cc(c(NS(=O)(=O)c2ccc(cc2)C)cc1)C(=O)c1cccc1
omegacsd YAYDEH	[NH+]1CCCC(CC1)(Oc1ccc(cc1)C(F)F)c1cccc1
omegacsd YAZBAC	C1=C([C@H](CCC1)NC(=O)O[C@H]1[C@H](CC[C@H](C1)C)C(C)C)c1ccc2OCoc2c1
omegacsd YAZHUC	[C@@H]1([C@](CC1)O)c1cccc1)NC(=O)c1ccc(cc1)Cl
omegacsd YEMNEJ	c1(c(c(cc1)OC(=O)c1cccc1)NC(=O)c1cccc1)C(=O)O
omegacsd YENLEI	n1c(OC)nc(nc1O)c1cccc1C(=O)OCC
omegacsd YESPIV	N1(C(=C)[C@](c2cccc12)(Cc1n(c2cccc2n1)c1cccc1)C)C
omegacsd YEYVED	S1/C(=C\c2oc(N(=O)=O)cc2)/SC(=C1SC)SC
omegacsd YICPIJ	O=C1N(C[C@H](O)[C@@H]1[C@H](Nc1cccc1)c1cccc1)c1ccc(N)cc1
omegacsd YIHJAA	Clc1c(Cl)cc(CC(=O)N([C@H](C[NH+]2CCCC2)c2cccc2)C)cc1
omegacsd YILDOM	s1nc(c(n1)NC(=O)C(=O)c1cccc1)c1cccc1
omegacsd YINDII	o1[nH]c(c(c1=O)C(=O)c1cccc1)c1cccc1
omegacsd YITLES	s1c(c2nc3cccc3[nH]2)c(nc1NC(=O)C)C
omegacsd YOPRAW	Brc1ccc(C(=O)O[C@H]2C(CN(C2=O)c2cccc2)(C)C)cc1
omegacsd YOPWOP	O(c1cc2c(c[nH]2cc1)CCNC(=O)C1CCC1)C
omegacsd YOSMOI	S(=O)(=O)(Nc1nc(O)c1c(N)cc1)
omegacsd YOWVOV	Oc1ccc(cc1OC)CC(=O)NCCCCc1cc(c(cc1)C)C
omegacsd YOWYAK	S(c1n(cnc1N(=O)=O)Cc1cccc1)CC(=O)OC
omegacsd YOXDEU	O1c2cc(O)c(cc2OC1)[C@H](O)[C@H]1N(CCC1)C(=O)OC(C)C(C)C
omegacsd YUKKUK	c1(ccc2c(eccc12)N(C)C)S(=O)(=O)Nc1nc(c1C)C
omegacsd YUKNAT	O(c1ccc(F)cc1C(=O)c1cccc1)CC(=O)Nc1cccc1
omegacsd YULXIM	[S@](=O)(O)[C@H]1N(C(=O)C1)C(=C(C)C)C(=O)NCc1cccc1
omegacsd YULZOU	Sc1c(N(C)CCN(C)c2cccc2S)cccc1
omegacsd YUYJEH	O(C)c1ccc2[nH]c(cc2c1)C(=O)Nc1cccc(OC)c1
omegapdb 1b6l	C1CC(=O)N[C@H](C(=O)N[C@@H](Cc2ccc(cc2)OC1)[C@H](O)CN1[C@H](CCCC1)C(=O)NC(C)(C)C)CC
omegapdb 1bxh	c1ccc(cc1)CS(=O)(=O)N[C@H]1C(=O)N2[C@H](CC1)SC[C@H]2C(=O)NCCCC(=N)N
omegapdb 1bto	[S@@]1(=O)C[C@H](CC1)CCCC
omegapdb 1c1u	c1(ccc2c(c1)nc(Cc1[nH]c3cccc3n1)[nH]2)C(=N)N
omegapdb 1d09	P(=O)(O)(O)CC(=O)N[C@H](C(=O)O)CC(=O)O
omegapdb 1d3g	Cc1c(nc2c(c1C(=O)O)cc(cc2)F)c1ccc(cc1)c1cccc1
omegapdb 1d3h	c1cc(ccc1NC(=O)[C@H](C#N)[C@H](O)C)C(F)(F)F

CODE	SMILES
omegapdb_1d4i	c1(ccccc1)CO[C@H]([C@@H](C[C@@H](OCc1cccc1)C(=O)N[C@H]1c2c(ccc2)C[C@H]1O)O)C(=O)N[C@]
omegapdb_1d4l	C1CC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc2ccc(cc2)OCCCC1)[C@H](O)CN(CCC)S(=O)(=O)c1ccc(cc1)
omegapdb_1d8d	CC(=CCC/C(=C/CC/C(=C/CONC(=O)CP(=O)(O)O)/C/C)C
omegapdb_1dfo	n1c(C)e(O)c(CNCC(=O)O)c1COP(=O)(O)O
omegapdb_1e2m	O=c1c(C)c([nH]c(=O)[nH]1)CCCC
omegapdb_1eby	c1(ccccc1)CO[C@H]([C@@H]([C@H]([C@@H](OCc1cccc1)C(=O)N[C@H]1c2c(ccc2)C[C@H]1O)O)O)C(=
omegapdb_1ec0	c1(ccccc1F)CO[C@H]([C@@H]([C@H]([C@@H](OCc1c(ccc1)F)C(=O)N[C@H]1c2c(ccc2)C[C@H]1O)O)O
omegapdb_1exa	c1(cc(ccc1NC(=O)[C@@H](c1cc2c(cc1)C(CCC2(C)C)(C)O)C(=O)O)F
omegapdb_1ezf	c12[C@@H](c3cccc4cccc34)O[C@H](CC(=O)N[C@@H](CC(=O)O)C(=O)O)C(=O)N(c1ccc(Cl)c2)CC(C)(C)C
omegapdb_1f06	C(=O)(O)[C@@H](N)CCCC(=C)C(=O)O
omegapdb_1f8b	C(=O)(C1=C[C@@H]([C@H]([C@H]([C@H](CO)O)O)1)NC(=O)C)O
omegapdb_1fm9	N([C@@H](Cc1ccc(cc1)OCCc1nc(oc1C)c1cccc1)C(=O)O)c1c(ccc1)C(=O)c1cccc1
omegapdb_1g2k	N1(S(=O)(=O)N([C@@H]([C@H]([C@H]1COc1cccc1)O)O)COc1cccc1)Cc1cc(cc1)C(
omegapdb_1g4s	Cc1ncc(c(n1)N)C[n+]1csc(c1C)CCOP(=O)(O)O
omegapdb_1g6c	n1csc(c1C)CCOP(=O)(O)O
omegapdb_1gi6	c1(c(cc2(c1)cc([nH]2)c1cccc(c1O)c1cccc1)Cl)C(=[NH2+])N
omegapdb_1gia	c1(ccc(cc1)NC(=O)c1cccc1O)C(=N)N
omegapdb_1gid	c1(c(Cl)cc(cc1)NC(=O)c1cc(C)cc(I)c1O)C(=N)N
omegapdb_1gs5	[C@@H](C(=O)O)(CCC(=O)O)NC(=O)C
omegapdb_1gse	N[C@H](C(=O)O)CCC(=O)N[C@H](C(=O)NCC(=O)O)CS
omegapdb_1gz8	c1(nc2c(c(n1)OCC(=O)C(C)C)[nH]cn2)N
omegapdb_1h1p	n1c(nc2c(c1OCC1CCCCC1)nc[nH]2)N
omegapdb_1h1s	c1(nc(OCC2CCCCC2)c2nc[nH]c2n1)Nc1ccc(cc1)S(=O)(=O)N
omegapdb_1h2k	C(=O)(C(=O)NCC(=O)O)O
omegapdb_1h6h	[C@H]1([C@@H]([C@H]([C@H]([C@H]1O)O)O)OP(=O)(O)O)O[P@@@](=O)(O)OC[C@H](C
omegapdb_1hwk	c1c(ccc1)c1c(c2cc(cc2)F)n(CC[C@H](C[C@H](O)CC(=O)O)O)c1C(=O)Nc1cccc1)C(C)C
omegapdb_1hyo	OC(=O)CC(=O)C[P@](=O)(O)C
omegapdb_1ik4	C(=O)(COP(=O)(O)O)NO
omegapdb_1is0	CNC(=O)[C@H]1[C@H](C(=O)[C@H]1c1ccc(cc1)OP(=O)(O)O
omegapdb_1iy7	c1(cccc1)C[C@@H](C(=O)O)NS(=O)(=O)N
omegapdb_1j3f	Oc1c(ccc1/C=N/c1cccc1/N=C/c1cccc(c1O)C)C
omegapdb_1jsl	N[C@H](CCCCO)C(=O)O
omegapdb_1k2t	N/C(=N/c1cccc1)/SCC
omegapdb_1k2u	N/C(=N/c1ccc(cc1)C(F)F)/SCC
omegapdb_1koj	[C@@H]([C@@H]([C@@H]([C@@H](COP(=O)(O)O)O)O)C(=O)NO
omegapdb_1kz8	OCc1sc(c1)cc(c1)Nc1ncnc2c1cc(OCC)c2OCC
omegapdb_1l7g	[C@H]1(NC(=N)N)[C@H]([C@H](C(CC)CC)NC(=O)C)[C@H](O)[C@@H](C(=O)O)C1
omegapdb_1lww	n1c2nc(N)[nH]c(=O)c2[nH]1cBr
omegapdb_1m2x	O=C(O)[C@H]1CCCC1C(=O)[C@H](C)CS
omegapdb_1m5b	OC(=O)[C@@H](N)Cc1c(onc1O)c1nn(nn1)C
omegapdb_1m5d	OC(=O)[C@@H](N)Cc1c(Br)c(O)no1
omegapdb_1m5f	OC(=O)c1noc(c1C[C@H](N)C(=O)O)C
omegapdb_1n2b	[O-]C(=O)[C@H](O)C(C)C(C)CO
omegapdb_1n3z	OC[C@H]1O[C@H]([C@@H]([C@@H]([C@@H]1O)O)n1cnc2c(N)ncnc12
omegapdb_1nms	CC(=O)[C@H](CC(=O)O)NC(=O)c1ccc(cc1)CNS(=O)(=O)c1cc(c(cc1)O)C(=O)O
omegapdb_1nnk	CC(c1c(c([O-])no1)C[C@@H](C(=O)[O-])[NH3+])C(C)C
omegapdb_1nqu	OC[C@@H](O)[C@@H](O)[C@@H](O)Cn1c(=O)c(=O)[nH]c2c1[nH]c(=O)[nH]c2=O
omegapdb_1nqv	[nH]1c(=O)[nH]c(=O)c1NC[C@H](O)C[C@H](O)[C@H](O)CO)N=O
omegapdb_1o2q	c1(c(Cl)cc2c(c1)cc([nH]2)c1cccc(OC2CCCC2)c1[O-])C(=[NH2+])N
omegapdb_1o2y	c1(ccc2c(c1)nc([nH]2)c1cc([C@H](C(=O)O)CC(=O)O)cc(c1O)Br)C(=N)N
omegapdb_1o37	c1(ccc2c(c1)nc([nH]2)c1cc(CC[NH3+])cc(c1[O-])c1cccc1)C(=[NH2+])N
omegapdb_1o3l	c1(ccc2c(c1)cc([nH]2)c1cc(CC(=O)[O-])cc(c1[O-])Br)C(=[NH2+])N
omegapdb_1o3m	c1(ccc2c(c1)nc([nH]2)c1cc(OC(F)F)cc1[O-])C(=[NH2+])N
omegapdb_1ofd	C(=O)(O)C(=O)CCC(=O)O
omegapdb_1oiu	c1(Nc2cc(ccc2)S(=O)(=O)N)nc(OCC2CCCCC2)c2nc[nH]c2n1
omegapdb_1oks	C1CC(CCC1)NCCS(=O)(=O)O
omegapdb_1p1o	C(=O)([C@H](Cn1c(=O)[nH]c(=O)o1)N)O
omegapdb_1pa9	S(=O)(=O)(Oc1cc([N+](=O)[O-])ccc1O)O
omegapdb_1pck	OC(=O)[C@H](OP(=O)(O)O)CC
omegapdb_1q72	CO[C@H]1[C@@H]2N(C)[C@@H](CC2)C[C@H]1OC(=O)c1cccc1
omegapdb_1q91	c1cc(ccc1)[C@H](OC[C@H]2O[C@H](n3c(=O)[nH]c(=O)c3)C)C[C@H]2O1)P(=O)(O)O
omegapdb_1qin	C(=O)(O)[C@@H](N)CCCC(=O)N[C@@H](CS[C@H](N(O)c1ccc(cc1)I)O)C(=O)NCC(=O)O

CODE	SMILES
omegapdb_1qnf	n1c(=O)[nH]c(=O)c2cc3ccc(O)cc3n(c12)C[C@@H](O)[C@H](O)[C@@H](O)CO
omegapdb_1qxw	C1CC1NCC([C@@H](N)CCCC)(O)O
omegapdb_1qy5	C(=O)(NCC)[C@H]1O[C@H]([C@@H]([C@@H]1O)O)n1cnc2c(N)ncnc12
omegapdb_1r34	[C@@H]1(S[C@H](NC(=N)Cc2cccc2)[C@@H](O)[C@H](O)[C@@H]1O)CO
omegapdb_1r4p	[n+]1(cccc1)CCCS(=O)(=O)[O-]
omegapdb_1r6w	O=C(O)[C@H]1[C@@H](C=CC=C1C(=O)CCC(=O)O)O
omegapdb_1rf6	P(=O)(O)(O)C[NH2+][CC](=O)O
omegapdb_1ros	N1(C(=O)c2c(ccc2)C1=O)CC[C@@H](CC(=O)c1ccc(cc1)c1ccc(cc1)OCC)C(=O)O
omegapdb_1s63	N1(CCNC(=O)C1)c1cc(ccc1)Cl)Cc1n(Cc2ccc(cc2)C#N)cnc1
omegapdb_1s8j	C1(CCCC(=C1/C=C/C(=C/C=C/C/C/C)C)(C)C
omegapdb_1sa4	Cn1cnc1[C@](c1ccc(Cl)cc1)(N)c1cc2c(cc1)n(C)c(=O)cc2c1cc(Cl)ccc1
omegapdb_1sn5	c1(cc(c(c(c1)O)c1cc(c(c1)O)I)I)C[C@@H](C(=O)O)N
omegapdb_1syh	C(n1c(=O)[nH]c(=O)c2c1CCC2)[C@@H](C(=O)O)N
omegapdb_1t32	O=C(N1CC[C@H](N(C(=O)c2c(C(=O)[C@H](P(=O)(O)O)c3cccc4c3cccc4)ec3cccc3e2)C)CC1)c1ccc2c(c1)ccc
omegapdb_1toj	C(=O)(O)CCc1cccc1
omegapdb_1uf5	NC(=O)N[C@H](CCSC)C(=O)O
omegapdb_1uf7	NC(=O)N[C@H](C(C)C)C(=O)O
omegapdb_1uf8	N([C@@H](C(=O)O)Cc1cccc1)C(=O)N
omegapdb_1ur8	C1[C@@H]([C@H]([C@@H]([C@@H](CO)O)O)O)NC(=O)C
omegapdb_1urw	c1c(ccc(c1)S(=O)(=O)NCCCN(C)C)Nc1nc(c2cnc3ccnn23)ccn1
omegapdb_1utt	c12c(cc2c2)[C@H]2CN(Cc3cccc3)C(=O)CO2)CS(=O)(=O)N1C
omegapdb_1uu9	NCCN1cc(c2c1cccc2)C1=C(C(=O)NC1=O)c1c2cccc2[nH]c1
omegapdb_1uwc	c1(ccc(cc1OC)/C=C/C(=O)O)O
omegapdb_1uy8	CCCCN1c2ncnc(c2nc1Cc1cccc(c1)OC)N
omegapdb_1v2k	n1cccc(c1)N1CC[C@H](CC1)C(=O)N1CCN(CC1)S(=O)(=O)c1cc2c(cc1)cc(cc2)Cl
omegapdb_1v2n	C(c1ccc(cc1)C(=N)N)[C@H]1CCCC[C@H](Cc2ccc(cc2)C(=N)N)C1=O
omegapdb_1v97	c1cnccc1c1nc([nH]1)c1cc(ncc1)C#N
omegapdb_1w1q	CC(=CCNc1c2nc[nH]c2ncn1)C
omegapdb_1w4l	C1=C[C@@H](C[C@H]2[C@]31CC[N+](=Cc1ccc(c31)O2)OC)CCCCCCCCN1C(=O)c2cccc2C1=O)O
omegapdb_1w5v	c1(cccc(c1)F)CO[C@H]([C@@H]([C@@H](OCc1cc(ccc1)F)C(=O)N)C@H]1c2c(ccc2)C[C@H]1O)O
omegapdb_1w7x	O=C(N[C@H](c1cccc1)C(=O)O)[C@H](Nc1ccc(cc1)C(=N)N)c1cc(OC)c(cc1)OCc1cccc1
omegapdb_1w9u	C(=O)(O)CCC[C@H](C(=O)N)
omegapdb_1wvj	OC(=O)[C@H](N)CC1=CCCCc2c1c(no2)O
omegapdb_1xap	C/C(=Cc1ccc(C(=O)O)cc1)/c1ccc2c(c1)C(C)(C)CCC2(C)C
omegapdb_1xge	O=C1N[C@H](CC(=O)N1)C(=O)O
omegapdb_1xn0	c1(cc(c(cc1)OC)OC1CCCC1)[C@@H]1CC(=O)NC1
omegapdb_1xom	OC(=O)[C@H]1CC[C@](CC1)(C#N)c1cc(OC)c(c1)OC1CCCC1
omegapdb_1xon	Clc1ncc(Cl)c1NC(=O)c1ccc(OC)c(c1)OC1CCCC1
omegapdb_1xp0	CCOc1ccc(cc1c1nc(=O)c2n([nH]1)c(nc2C)CCC)S(=O)(=O)N1CCN(CC1)CC
omegapdb_1xqc	Oc1ccc2c(c1)CCN([C@@H]2c1ccc(cc1)N1CCN2[C@H](C1)CCCC2)c1cccc1
omegapdb_1y6q	c1nc(c2c(c(CN3C)C[C@H](CSC)[C@H](C3)O)c[nH]2)n1N
omegapdb_1yc1	c1c2OCOc2ccc1c1c(C(=O)O)[nH]nc1c1cc(CC)c(O)cc1O
omegapdb_1yc4	Oc1cc(O)c(CC)c1c1n[nH]cc1c1c[nH]cn1
omegapdb_1yc5	n1cc(ccc1)C(=O)N
omegapdb_1yvx	N(C(C)C)(C(=O)c1ccc(cc1)C)c1c(sc(c1)c1cccc1)C(=O)O
omegapdb_1z1r	[C@H]1(Cc2ccc(cc2)OCCCC(=O)N[C@H](C(=O)N1)CC(=O)N)[C@H](O)CNS(=O)(=O)c1cccc1
omegapdb_1zvx	c1(ccc(cc1)OC)c1ccc(cc1)S(=O)(=O)N[C@H](C(C)C)P(=O)(O)O
omegapdb_1zz2	c1cccc(c1O)CN[C@H]1CCN(CC1)S(=O)(=O)Nc1cc(ccc1)Oc1ccc(cc1)F
omegapdb_2aj8	n1(c(=O)n(c2c(c1=O)n(c2n)N1CC[NH2+][C@H]1Cc1cccc1)C)C
omegapdb_2aw1	S(=O)(=O)(N)c1ccc(cc1)c1c(C)onc1c1cccc1
omegapdb_2ayr	c1(ccc(cc1)S(=O)(=O)C)c1ccc2cc(ccc2c1Oc1ccc(cc1)OCCN1CCCCC1)O
omegapdb_2b7d	c1(ccc2c(c1)[nH]c(n2)c1cc([C@H](C(=O)O)CC(=O)O)cc(c1O)c1c(ccc(CNC(=O)N)c1)O)C(=N)N
omegapdb_2bgd	O=C1NS(=O)(=O)N(C1)c1cc(ccc1OC)c1cccc1
omegapdb_2brc	c1c2OCCOc2ccc1c1c(C)n[nH]c1c1cc(CC)c(O)cc1O
omegapdb_2btr	O=C(/N=c\1/[nH]cc(s1)C(C)Cc1cccn1
omegapdb_2bts	O=S(=O)(N)c1ccc(Nc2sc(cn2)C(C)C)c1
omegapdb_2byh	O=C(C)c1ccc(cc1)NC(=O)c1en[nH]c1c1cc(Cl)c(O)cc1O
omegapdb_2byi	Clc1cc(O)c(c1)c1[nH]nc1C(=O)NCc1ccc(cc1)S(=O)(=O)N)O
omegapdb_2c4w	O=S(=O)(/N=c\1/[nH]nn[nH]1)c1cc2c(cc1)oc1cccc1c2=O
omegapdb_2cbs	C1(CCC(c2ccc(cc12)C(=C/C=C/C(=C/C(=O)O)C/C)C(C)C)C
omegapdb_2cji	Clc1ccc2cc(ccc2c1)S(=O)(=O)N[C@H]1CCN(C1=O)[C@@H](C(C)C(=O)N1CCOCC1
omegapdb_2evc	o1c(C(=O)O)ccc1c1c(cccc1)C(F)(F)F

CODE	SMILES
omegapdb_2ewb	c1c(cccc1)S[C@H]1C[C@@H](C(=O)O)N(C1)C(=O)[C@H](C)CS
omegapdb_2f14	S(=O)(=O)(N)c1ccc(cc1)CCNC(=S)Nc1ccc(c(c1)C(=O)O)c1c2ccc(cc2oc2cc(=O)ccc12)O
omegapdb_2f34	O=C(O)[C@@H](N)Cn1c(=O)n(c(=O)c(C)c1)Cc1ccsc1C(=O)O
omegapdb_2f4j	N1(CCNC(C)C1)c1cc(nc(n1)Sc1ccc(cc1)NC(=O)C1CC1)Nc1cc(n[nH]1)C)C
omegapdb_2f6v	OS(=O)(=O)Nc1cccc2c(c1)CN([C@H](C(=O)NC)C2)C(=O)OCc1cccc1
omegapdb_2f70	OS(=O)(=O)Nc1cccc(c1)CNC(=O)Cc1cc(NS(=O)(=O)O)ccc1
omegapdb_2f71	OS(=O)(=O)Nc1cccc2c(c1)CN([C@H](C2)C(=O)NC)C(=O)C
omegapdb_2f7p	[C@H]1(NCc2cccc2)[C@@H](O)[C@@H](O)[C@@H](O)[C@@H]1S
omegapdb_2flb	c1(ccc2c(c1)nc([nH]2)c1c(O)c([nH]n1)c1cccc1)C(=N)N
omegapdb_2fm0	FC(F)Oc1c(OC2CC2)cc(cc1)[C@@H](c1ncc(s1)C(O)(C(F)(F)F)C(F)(F)F)Cc1ccc[n+](c1)[O-]
omegapdb_2fq1	OC(=O)[C@@H](N)CCSC[C@@H](O)[C@@H](O)C(=O)NO
omegapdb_2fwz	CC(C)NCCCCn1c2ncnc(N)c2nc1Sc1cc2OCOc2cc1
omegapdb_2fyv	[C@H]1(O)[C@H](O)CN([C@H]1CO)C[C@H](O)[C@@H](O)[C@H](O)[C@H](O)C(=O)O
omegapdb_2g8n	OC[C@@H]1NCc2cc(ccc2C1)S(=O)(=O)Nc1ccc(cc1)Cl
omegapdb_2ggd	C1(=C[C@H]([C@H]([C@@H](C1)O)O)OP(=O)(O)O)C(=O)O
omegapdb_2gss	c1(OCC(=O)O)c(Cl)c(Cl)c(cc1)C(=O)C(=C)CC
omegapdb_2h03	N(c1ccc(CC(C(=O)OCC)(CCNC(=O)OC(C)(C)C)C(=O)OCC)cc1)S(=O)(=O)O
omegapdb_2h42	CCCc1nn(C)c2c(=O)[nH]c(nc12)c1cc(ccc1OCC)S(=O)(=O)N1CCN(C)CC1
omegapdb_2hb1	c1c(c(c(s1)C(=O)O)OCC(=O)O)Br
omegapdb_2hd6	NS(=O)(=O)c1ccc(cc1)NC(=O)c1cccc1S
omegapdb_2i0a	O=C(C)c1ccc(cc1)N1C(=O)O[C@@H](C1)C(=O)N[C@@H](Cc1cccc1)[C@H](O)CN(CC(C)C)S(=O)(=O)c1cc
omegapdb_2iko	c1(nc(c1c1ccc(cc1)NCc1cc(cc(c1)F)F)CC)N)N
omegapdb_2iuz	O=c1c2n(C)cnc2n(C)c(=O)n1CCn1c(=O)c2n(C)cnc2n(C)c1=O
omegapdb_2izl	C(=O)(O)CCCC[C@@H]1SC[C@@H]2NC(=N)N[C@H]12
omegapdb_2j34	Clc1cc2c(cc(S(=O)(=O)N[C@H]3CCN(C3=O)[C@@H](C)C(=O)N3CCOCC3)s2)cc1
omegapdb_2j47	O=C(C)N[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)[n+]2c1[nH]c(c2)C(=O)Nc1cccc1
omegapdb_2j4i	CS(=O)(=O)NCCN(C(C)C)C(=O)[C@H](C)N1C(=O)[C@H](CC1)NS(=O)(=O)c1cccc2cc(ccc2c1)Cl
omegapdb_3cbs	c1(cc(c(c(c1)C)/C=C/C=C/C=C/C(=O)O)/C/C)C)O

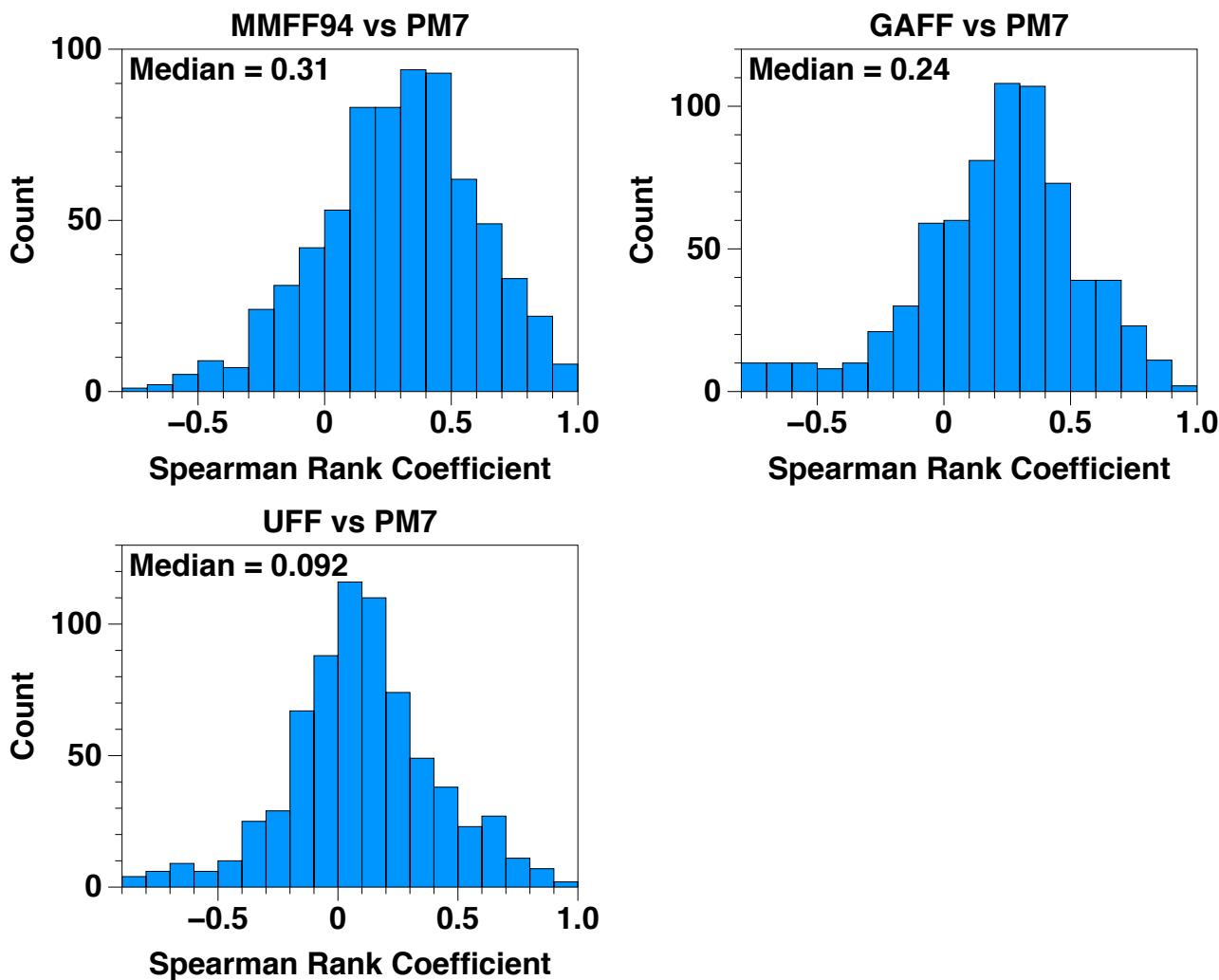


Figure S1. Spearman rank correlations for each of the data set combinations which are discussed in the text with regard to R^2 values. In determining the accuracy of a method, the researcher would expect either the absolute energy values to be accurate, which is explained through the R^2 values or the expectation would be that even if the energy values are not accurate than the order of the ranking of energies from largest to smallest should be accurate. These values show that the ranking of MM methods are poor, compared to PM7.

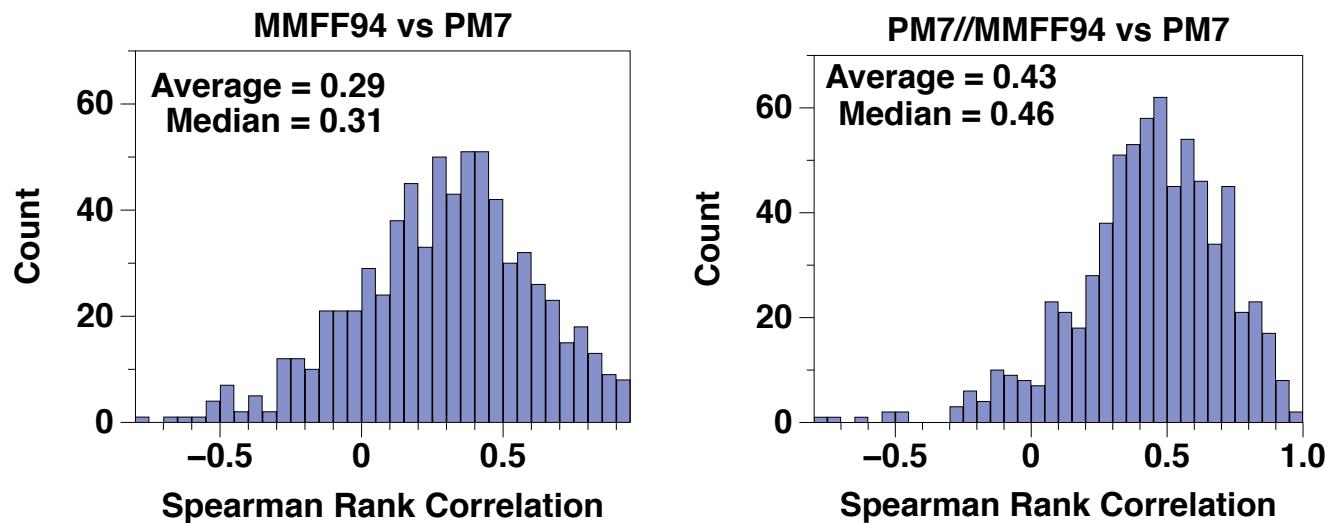


Figure S2. Spearman Rank correlations for MMFF94 and single point PM7 calculations at MMFF94 geometries compared with PM7 calculations.

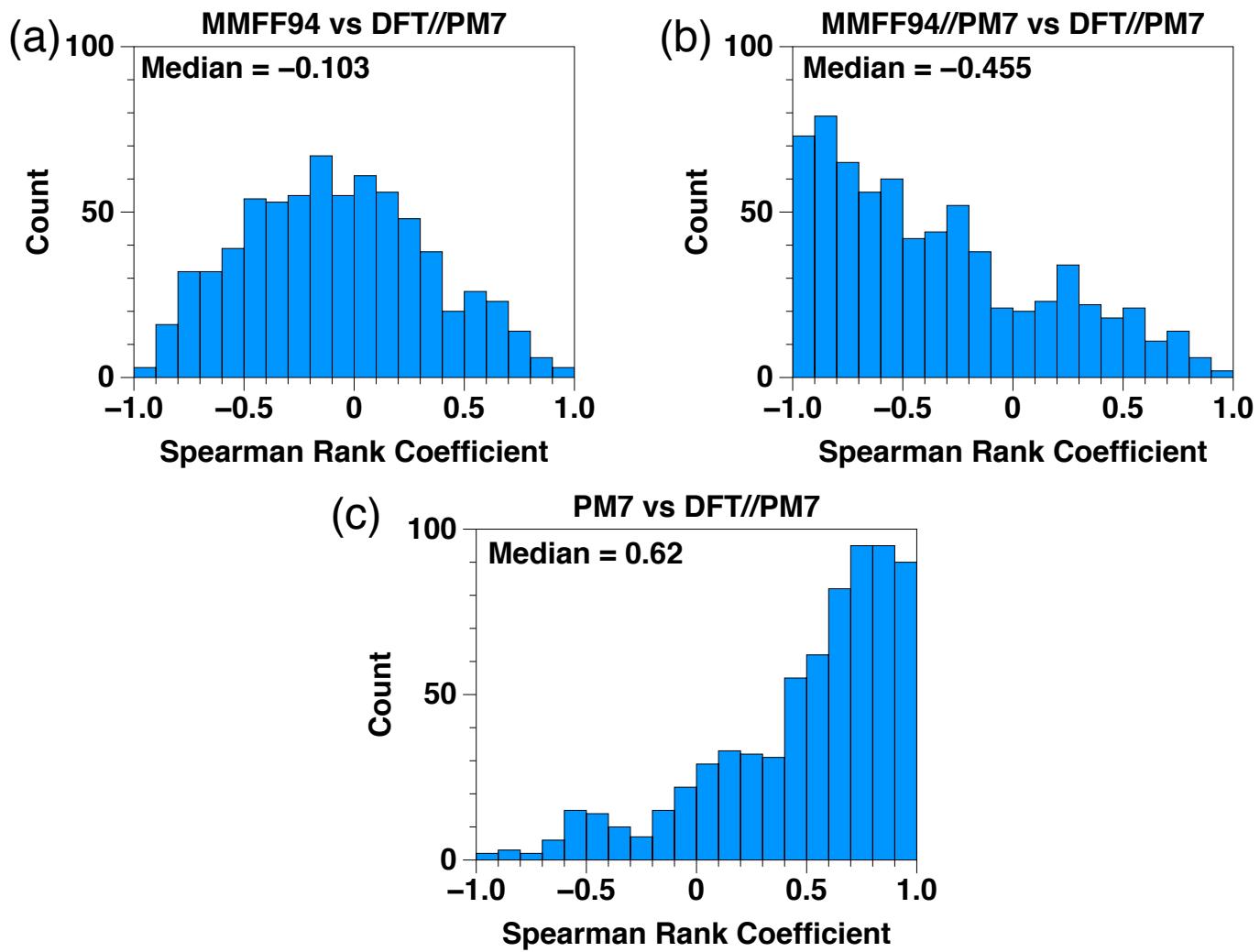


Figure S3. Spearman rank correlation data for MMFF94, MMFF94//PM7 and PM7 calculations vs. DFT//PM7 calculations. The results show poor correlation of the ordered ranking of the energies of the molecules between MMFF94 and MMFF94//PM7 with DFT//PM7 and good correlation between the PM7 and DFT//PM7 energies ordered rankings. This suggests that MMFF94 provides poor ordered rankings even when performed on a molecule already optimized with PM7 and that PM7 provides molecule energies in similar orders to the energies of DFT.

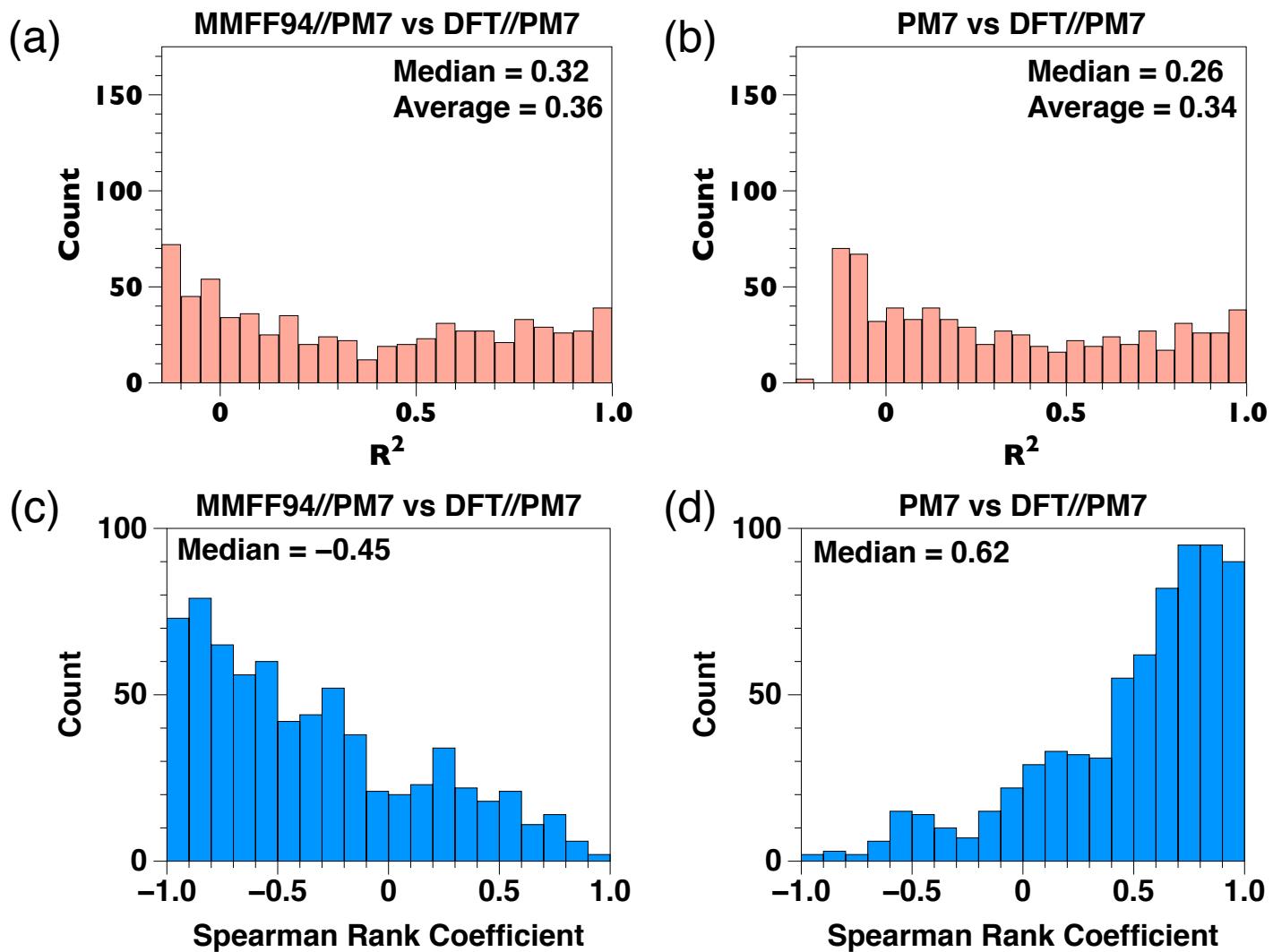


Figure S4. Comparison of R^2 values and Spearman Rank correlations of MMFF94//PM7 and PM7 vs. DFT//PM7 calculations. Although the R^2 values for these two analyses look similar, it is clear that the PM7 and DFT lists of conformers for each molecule are similar to one another while there is no correlation between the MMFF94//PM7 and DFT conformer ranked lists. These plots support the idea that molecular mechanics calculations are inaccurate for energy calculations.

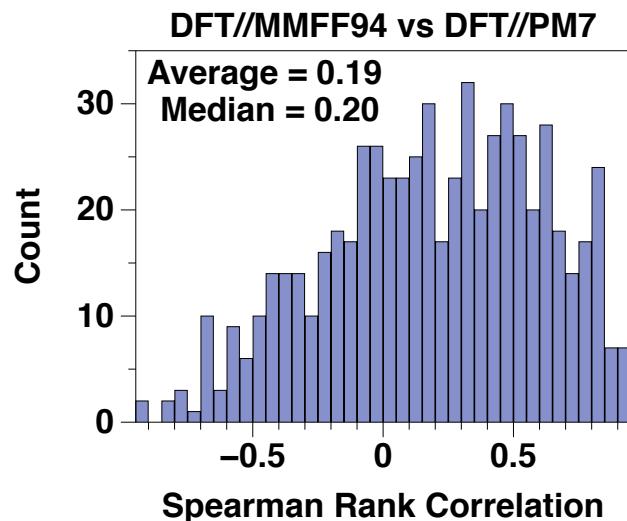


Figure S5. Spearman rank correlation data for DFT//MMFF94 geometries compared with DFT//PM7 geometries corroborates the trend shown with the R^2 data. Poor correlation between these methods lead to the conclusion that these calculations should not be relied upon for conformer screening.

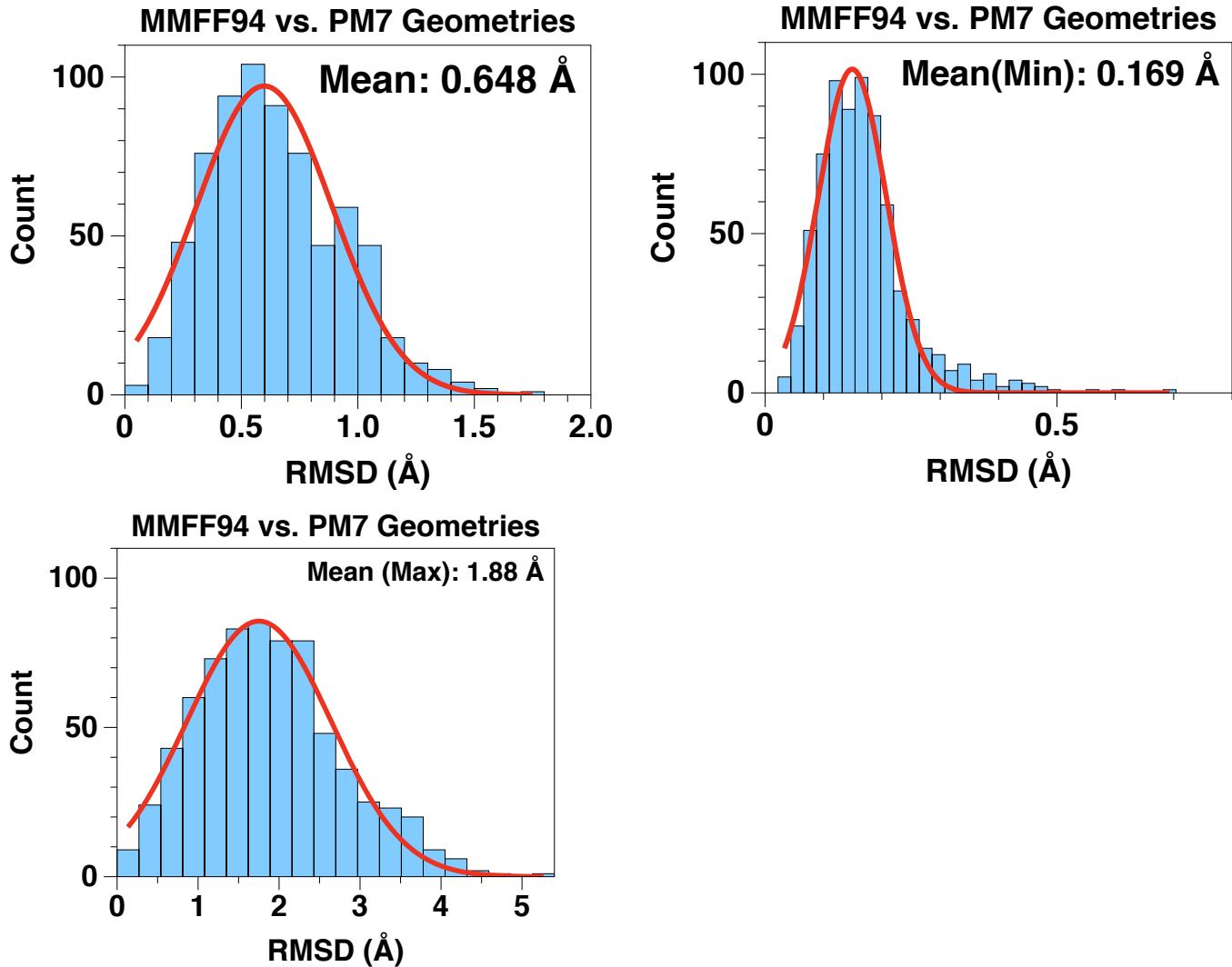


Figure S6: RMSD data shows that when beginning with the same starting pose, the optimized MMFF94 and PM7 geometries differ on average by $\sim 0.6\text{\AA}$ per heavy atom. The mean of the minimum RMSD values shows that beginning with the same starting pose, the optimized MMFF94 and PM7 geometries minima differ on average by $\sim 0.2\text{\AA}$ per heavy atom and the maxima of the average RMSD differ by $\sim 1.9\text{\AA}$ per heavy atom.

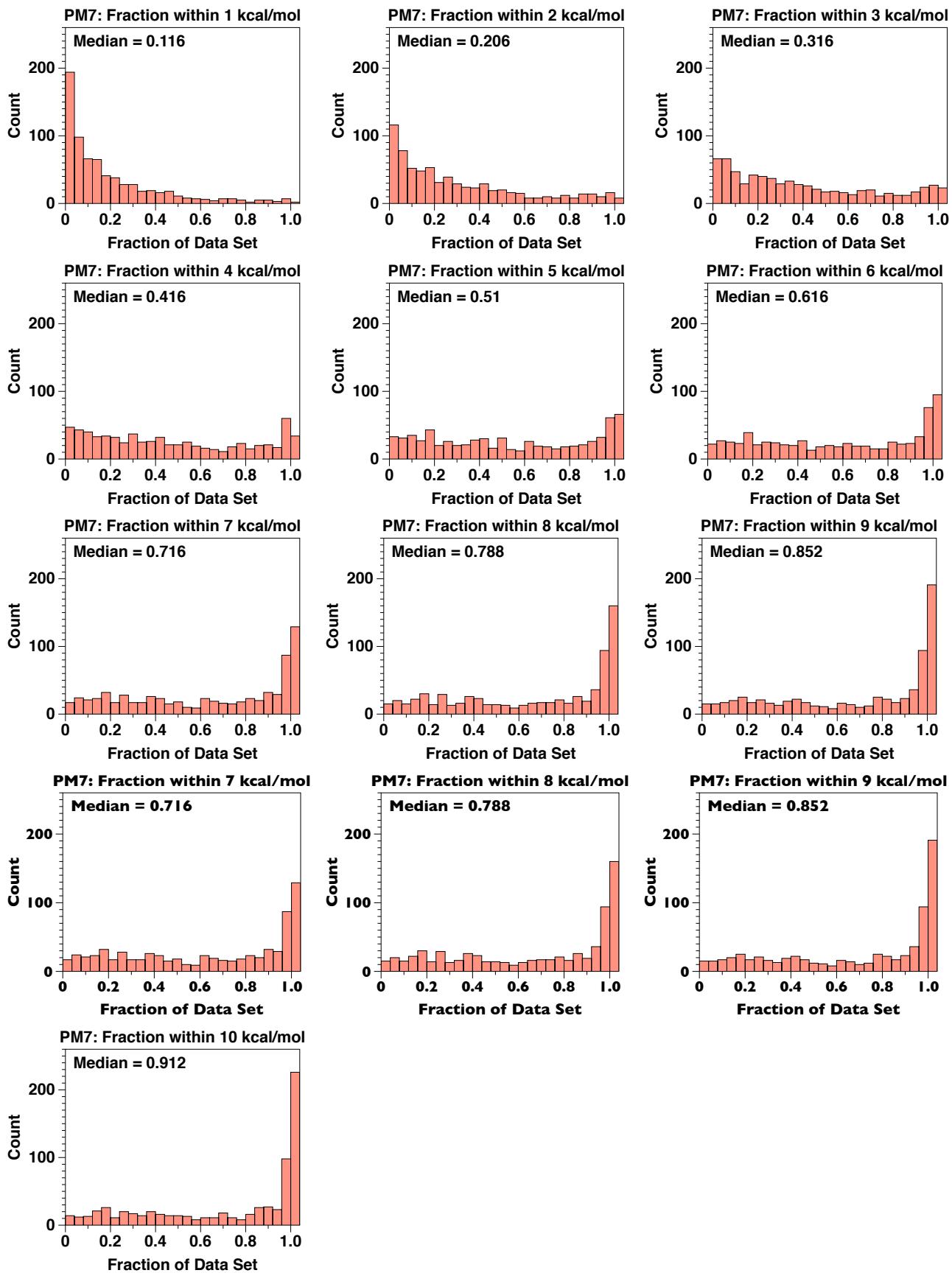


Figure S7: Histograms portraying the number of conformers for each molecule in the PM7 data sets that are within 1 – 10 kcal/mol of the lowest energy conformer for each molecule.

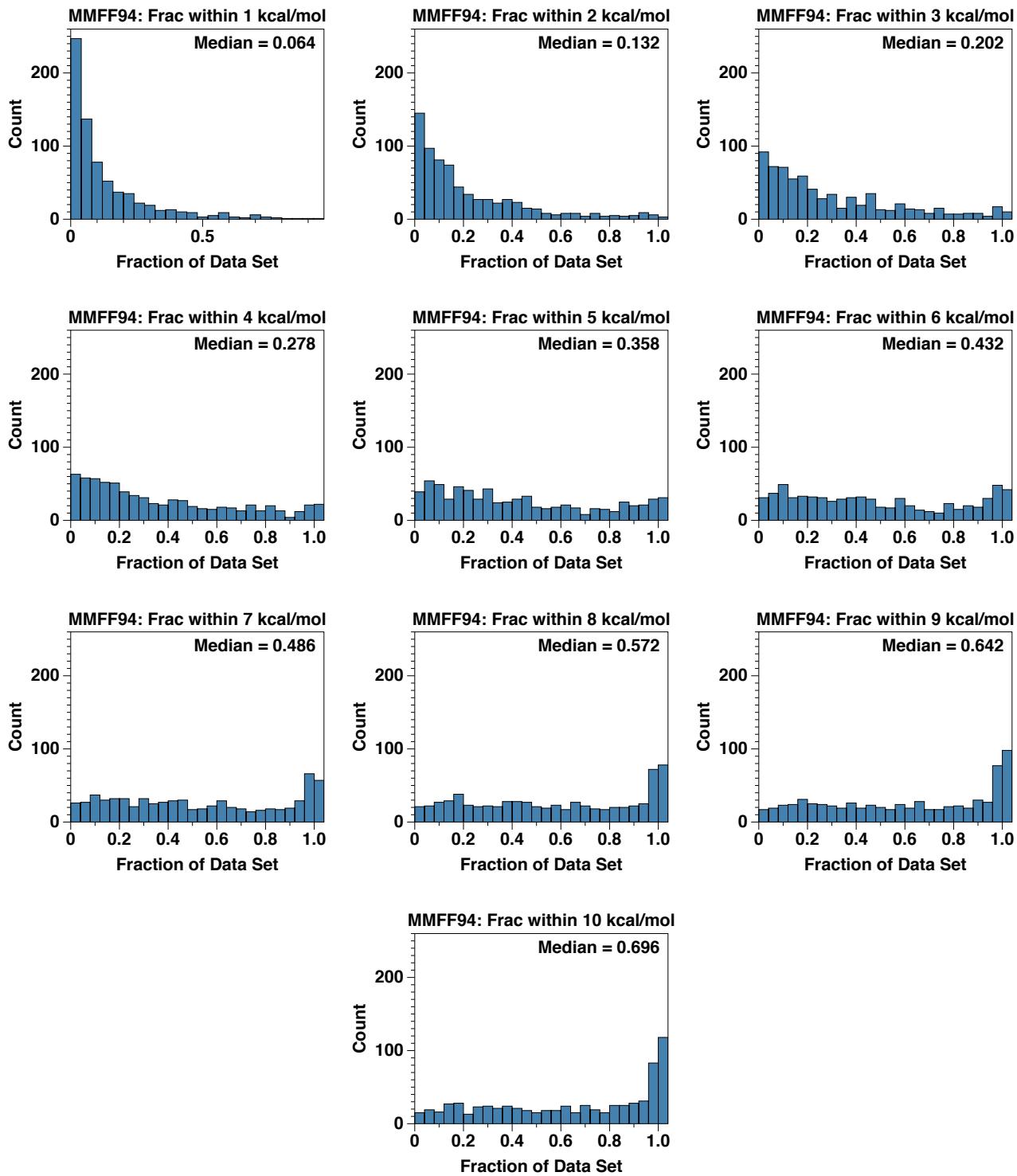


Figure S8: Histograms portraying the number of conformers for each molecule in the MMFF94 data sets that are within 1 – 10 kcal/mol of the lowest energy conformer for each molecule.

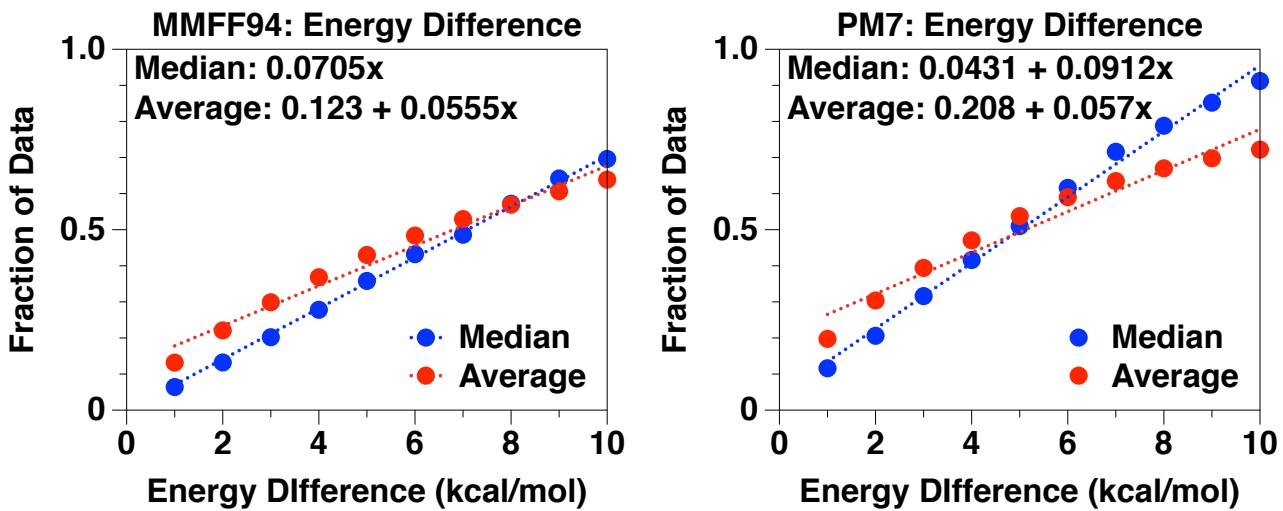


Figure S9. Plots of median and average values for the fraction of the data with energy differences ranging from 1-10 kcal/mol for MMFF94 and PM7 data indicate that while most of the conformers energies are not within 1 kcal/mol of one another, the energies of most of the conformers are indeed within 10 kcal/mol of the energy of the lowest conformer.

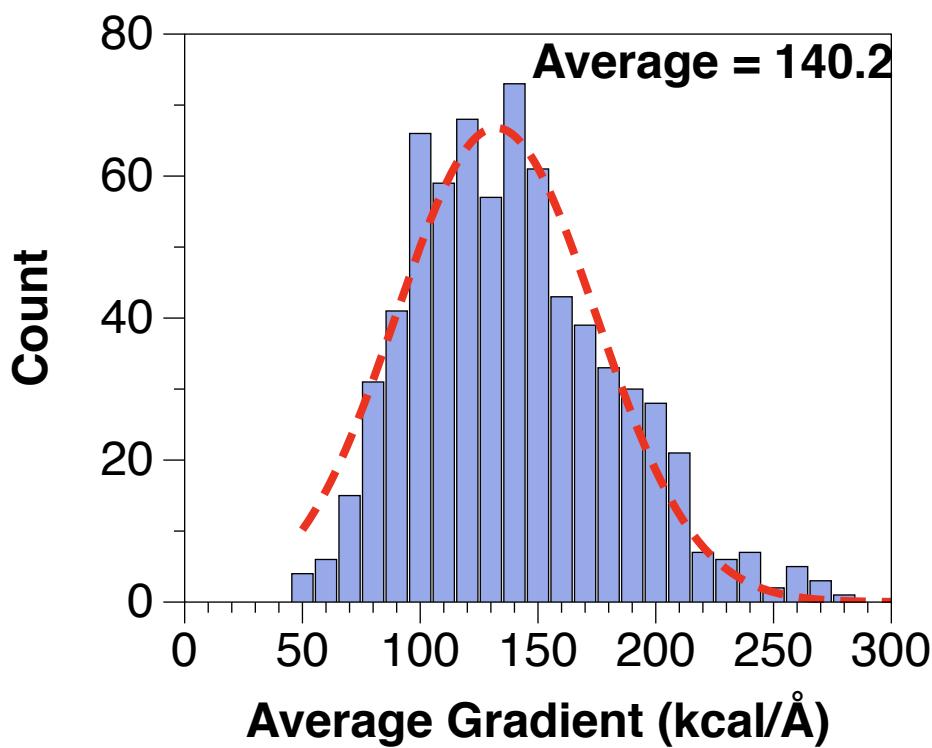


Figure S10: Histogram of the average gradient norm across all conformers for a molecule using PM7 on an MMFF94 optimized geometry. The gradients are expected to be close to 0. An analogy to this figure would indicate that if you are on flat ground (i.e., low energy) in MMFF94 world, then when teleported to PM7 world, on average you would be on a steep slope. Roughly the same gradients are found for the initial non-optimized conformers. PM7 world is not the same as MMFF94 world. The potential energy surfaces do not map, as expected.

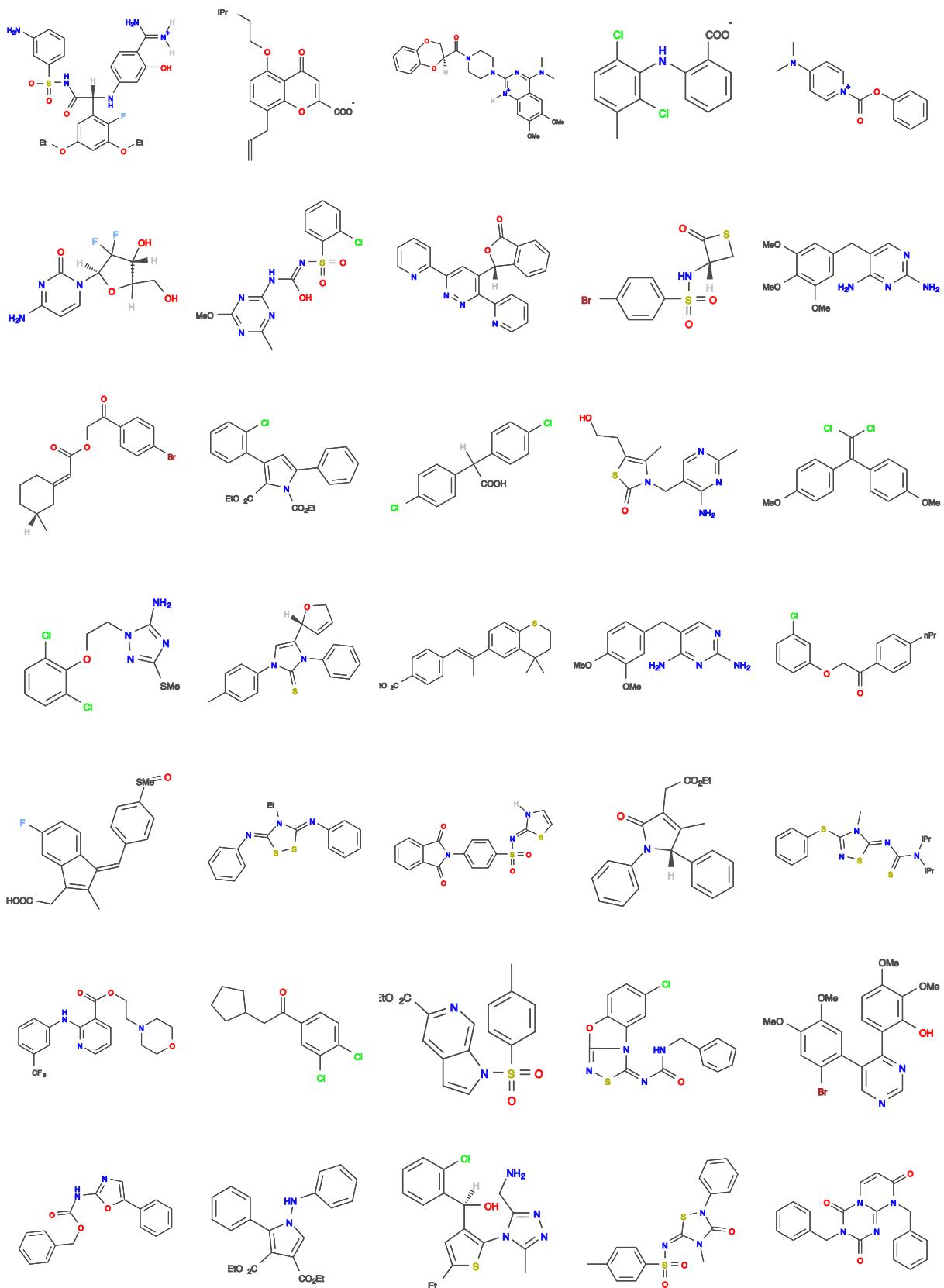


Figure S11. Molecules that resulted in R^2 values below 0.05 with MMFF94 vs DFT//PM7, MMFF94 vs PM7 and PM7 vs. DFT//PM7. (Part 1 of 2)

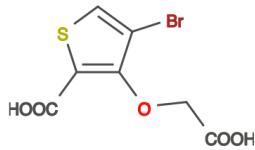
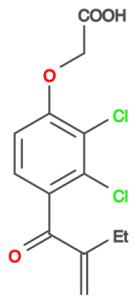
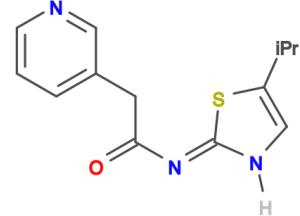
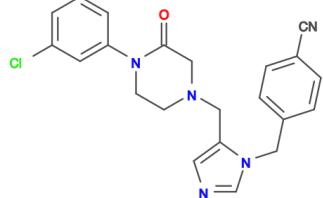
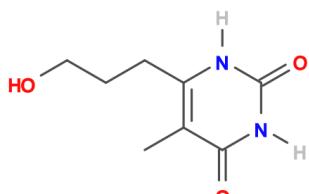
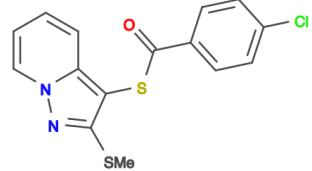
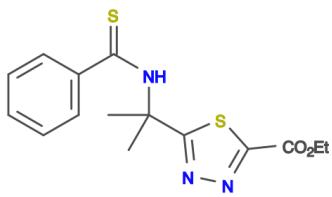
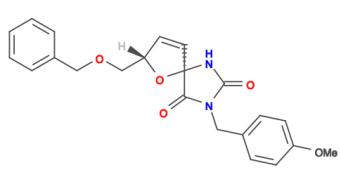
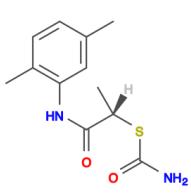


Figure S12. Molecules that resulted in R^2 values below 0.05 with MMFF94 vs DFT//PM7, MMFF94 vs PM7 and PM7 vs. DFT//PM7. (Part 2 of 2)

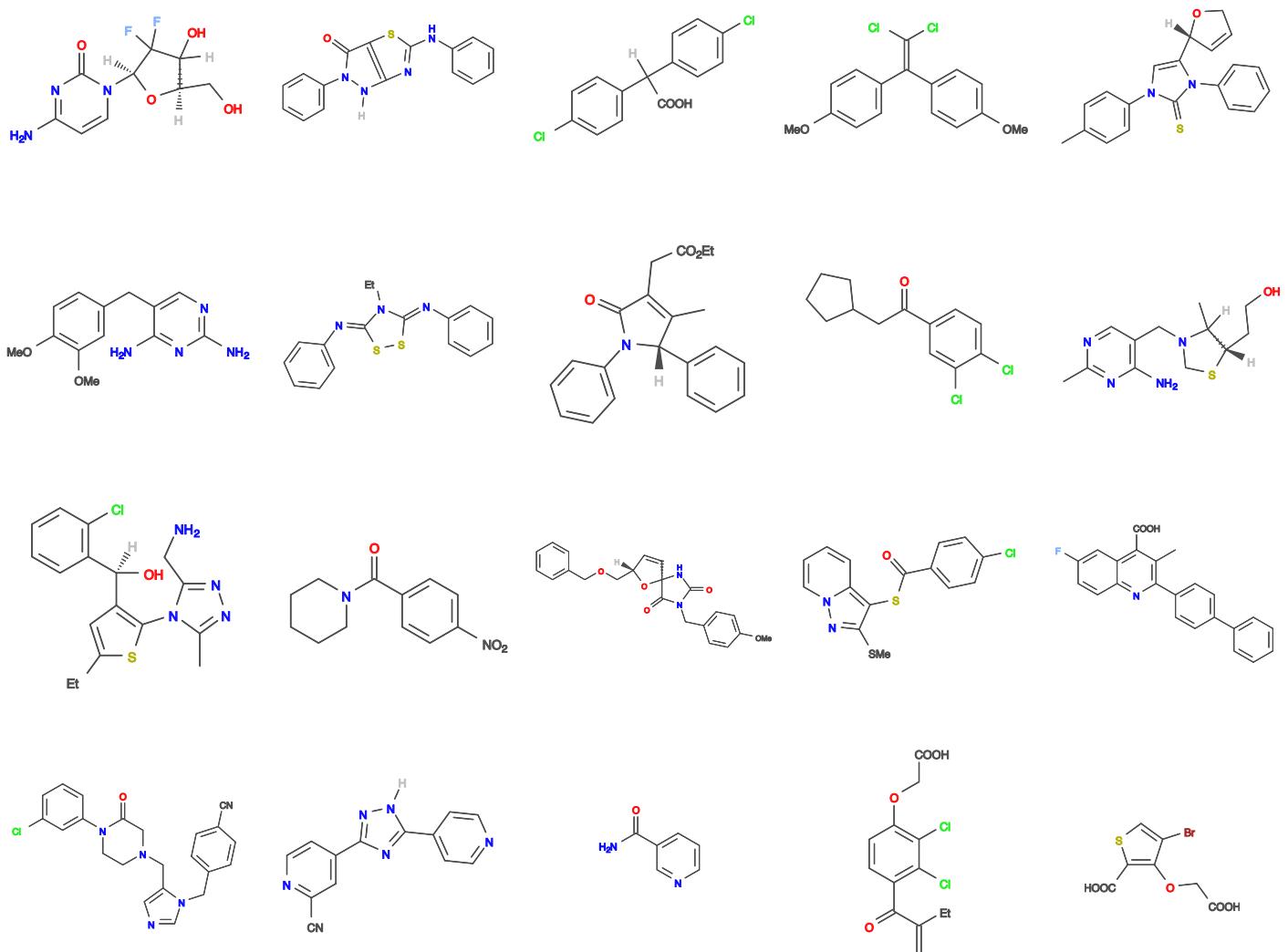


Figure S13: Molecules in both the MMFF94 vs PM7 and PM7 vs DFT//PM7 calculations with poor R^2 values.

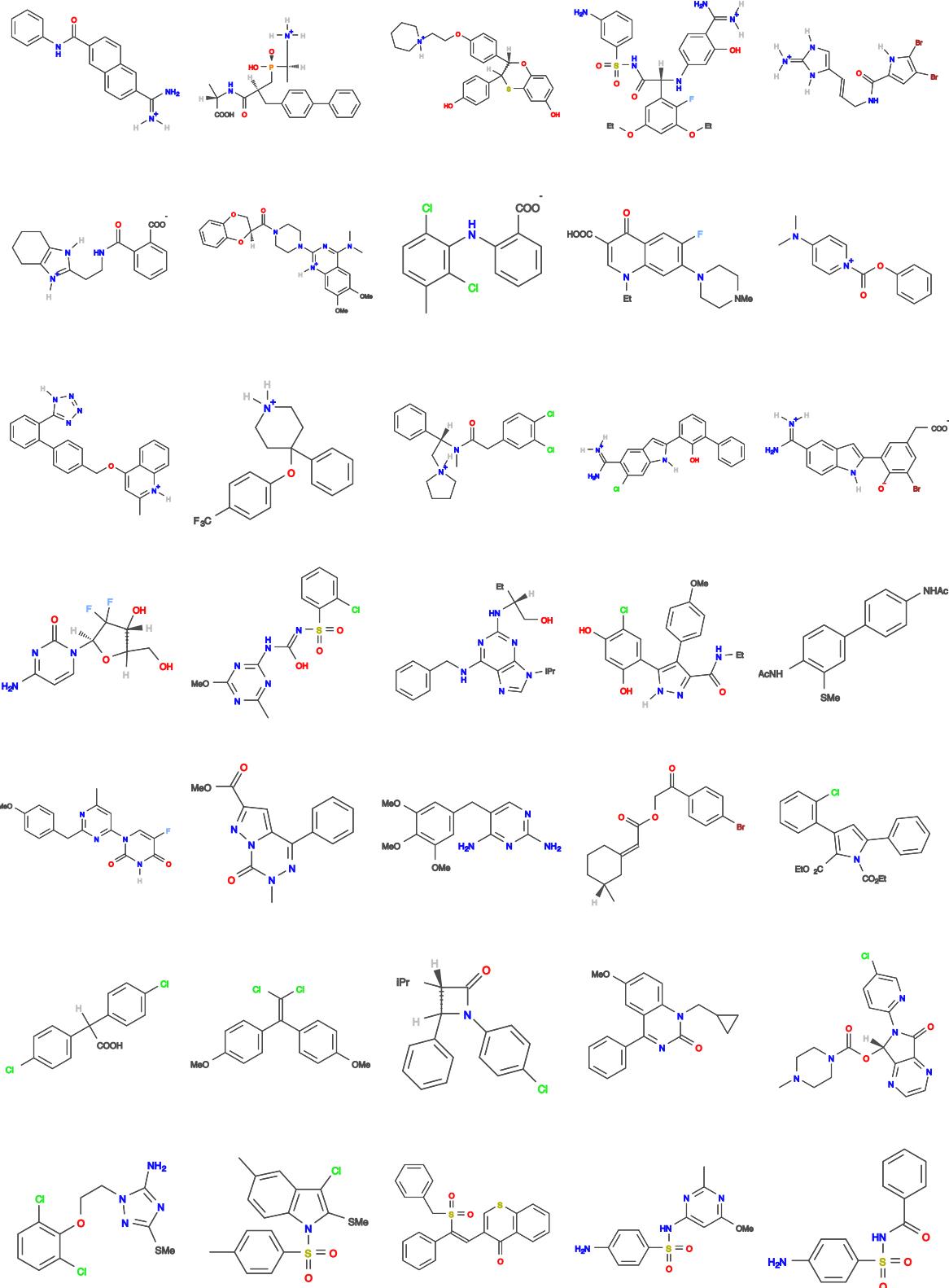


Figure S14: Molecules in both the MMFF94 vs DFT//PM7 and the PM7 vs DFT//PM7 calculations with poor R^2 values. (Part 1 of 3)

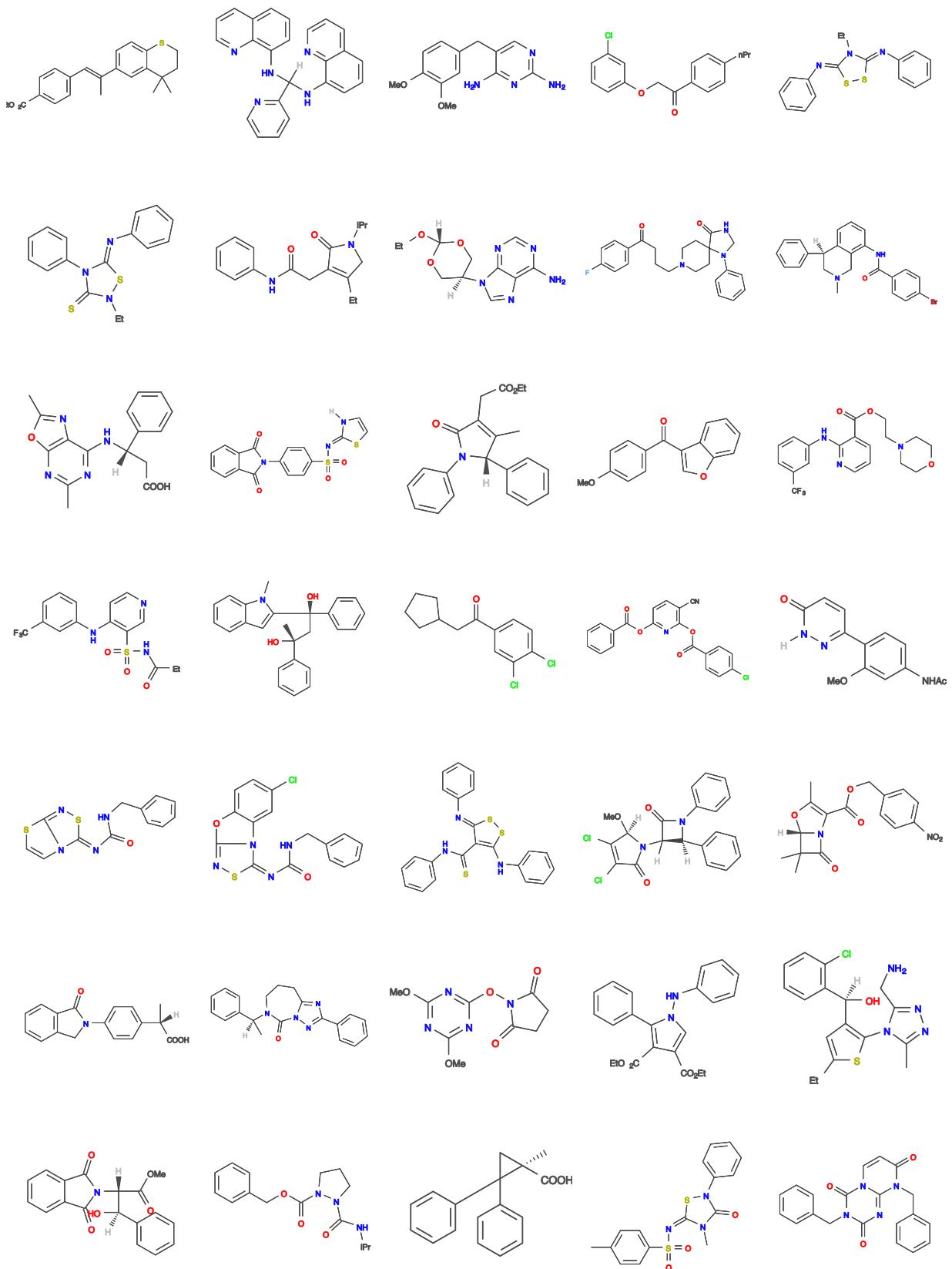


Figure S15: Molecules in both the MMFF94 vs DFT//PM7 and the PM7 vs DFT//PM7 calculations with poor R² values. (Part 2 of 3)

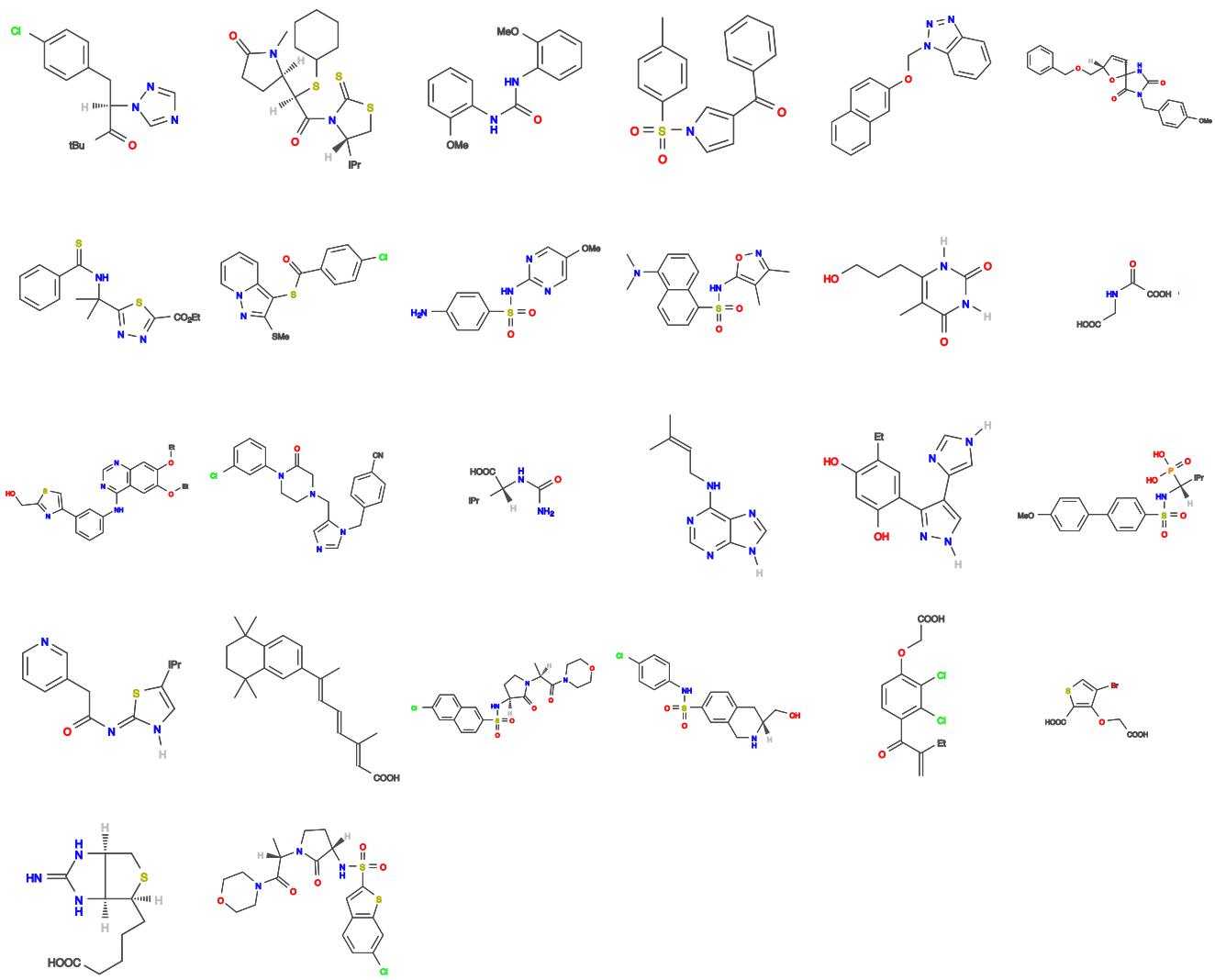


Figure S16: Molecules in both the MMFF94 vs DFT//PM7 and the PM7 vs DFT//PM7 calculations with poor R^2 . (Part 3 of 3)

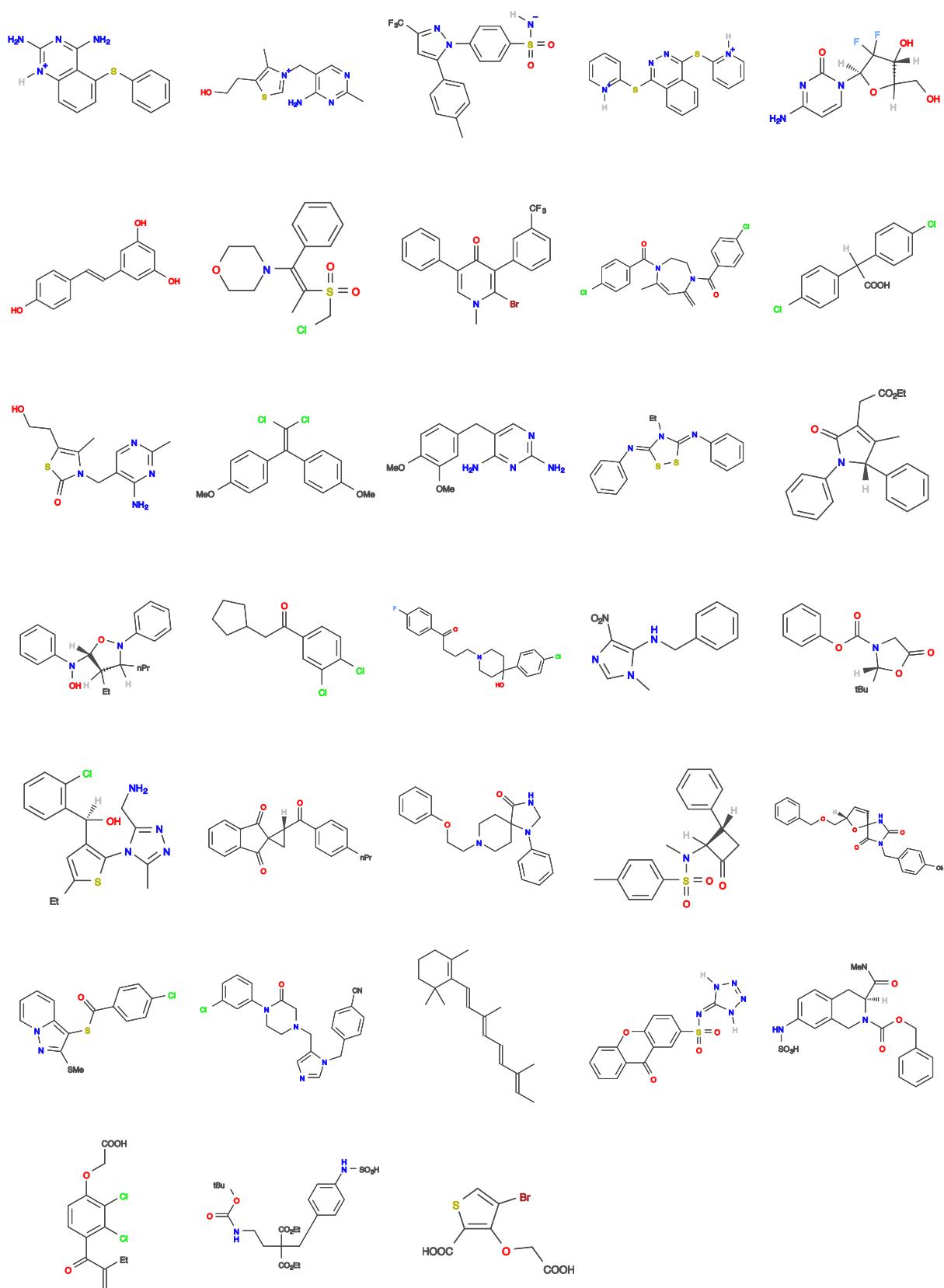


Figure S17: Molecules in both the MMFF94 vs DFT//PM7 and MMFF94 vs PM7 calculations with poor R^2 values.

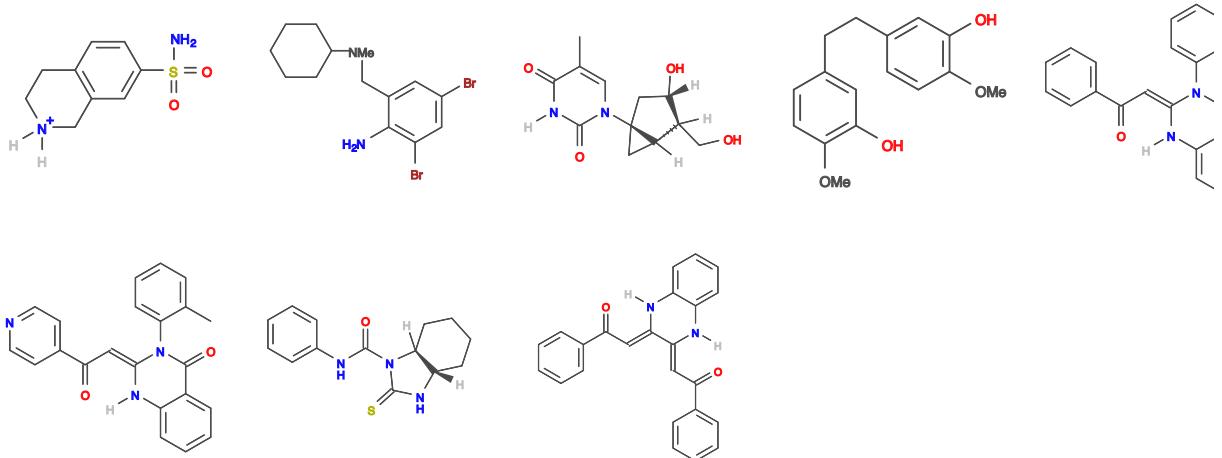


Figure S18: Molecules in both the MMFF94 vs PM7 and PM7 vs DFT//PM7 calculations with high R^2 values greater than 0.8.

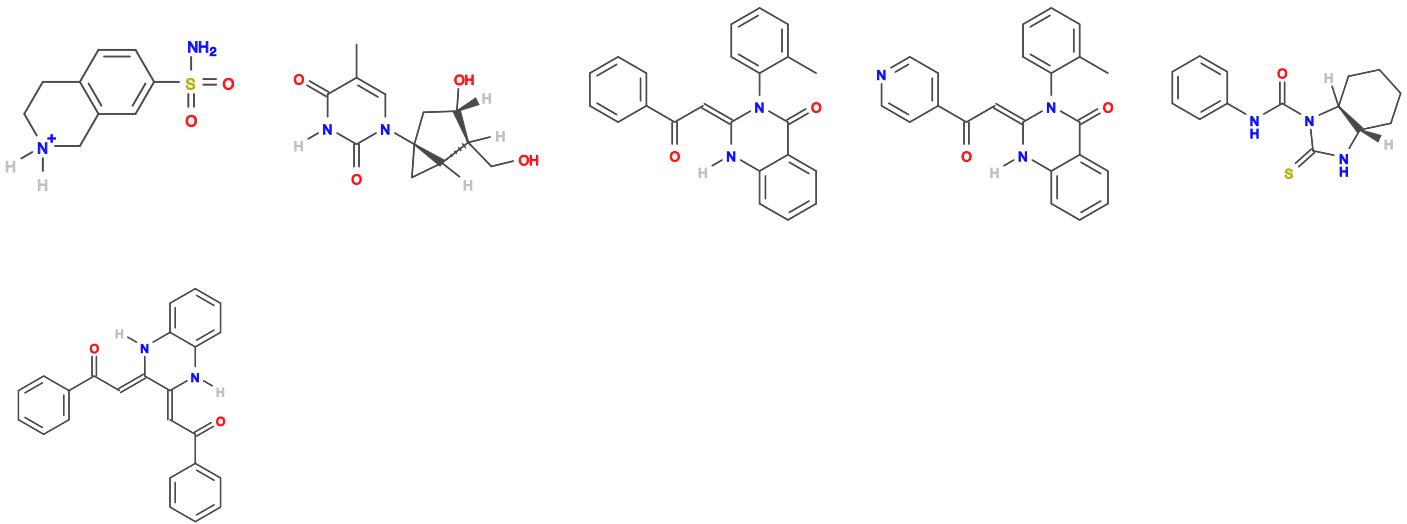


Figure S19: Molecules in both the MMFF94 vs DFT//PM7 and MMFF94 vs PM7 calculations with R^2 values greater than 0.8.

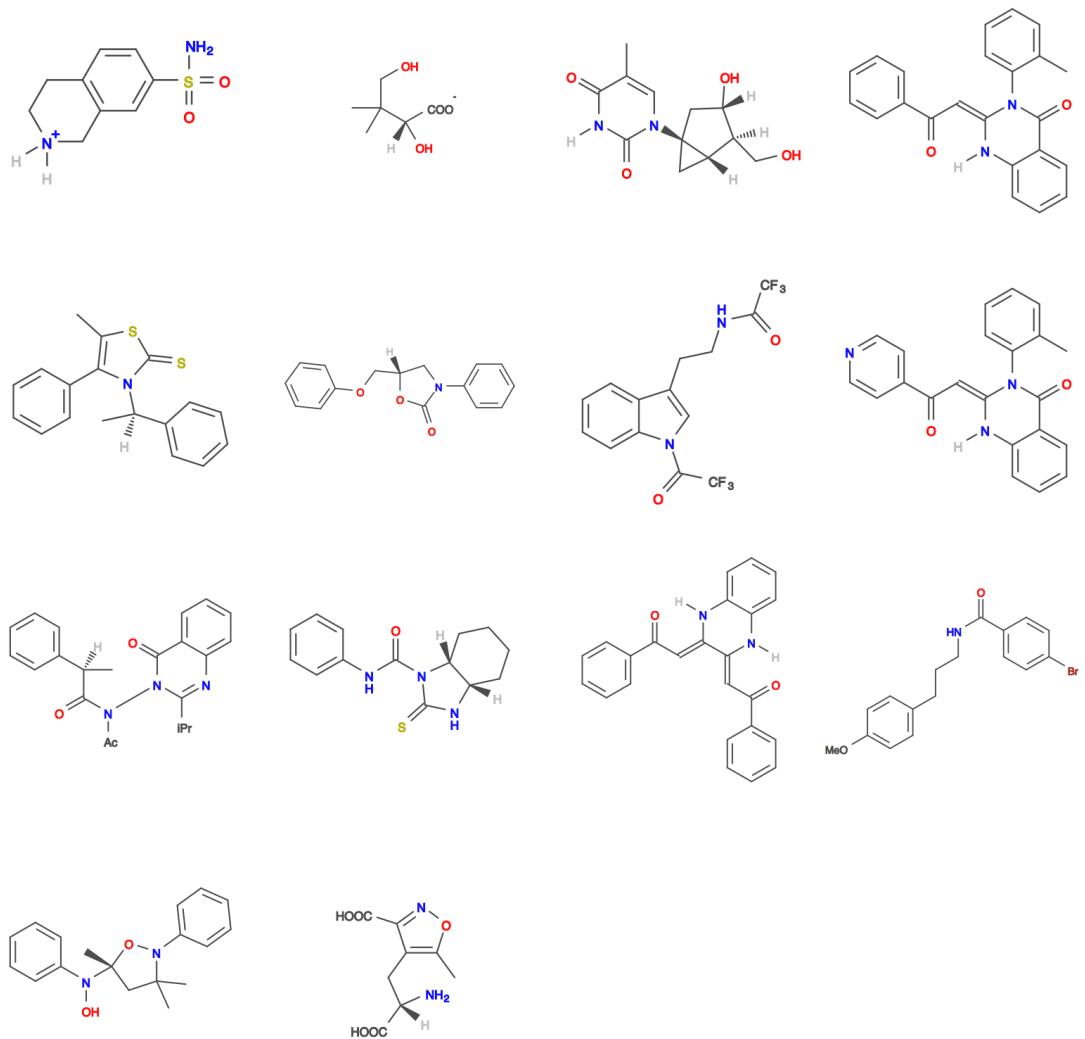


Figure S20: Molecules in both the MMFF94 vs DFT//PM7 and the PM7 vs DFT//PM7 calculations with R2 values greater than 0.8.