Table S1. Data sets used in the study

Training set	
Canonical_Smiles	LOAEL [mg/kg_bw/day]
ClC1=C(Cl)C2(Cl)C3C4CC(C=C4)C3C1(Cl)C2(Cl)Cl	0.01
ClC1(Cl)C2(Cl)C3C4(Cl)C(Cl)(Cl)C5(Cl)C3(Cl)C1(Cl)C5(Cl)C24Cl	0.01
Nc1c(c(nn1c2c(Cl)cc(cc2Cl)C(F)(F)F)C#N)S(=O)C(F)(F)F	0.06
CNC(=O)ON=CC(C)(C)SC	0.1
CC(Oc1ccc(Oc2ncc(cc2Cl)C(F)(F)F)cc1)C(=O)O	0.1
ClC1C2OC2C3C1C4(Cl)C(=C(Cl)C3(Cl)C4(Cl)Cl)Cl	0.1125
CCOP(=S)(OCC)SCCSCC	0.12
CCOP(=S)(OCC)SCSCC	0.16
ClC1=C(Cl)C2(Cl)C3C4CC(C5OC45)C3C1(Cl)C2(Cl)Cl	0.1875
CC1CCCC(O)CCCCCc2cc(O)cc(O)c2C(=O)O1	0.2
S=C1NCCN1	0.24
COP(=S)(OC)Oc1ccc(cc1)[N+](=O)[O-]	0.25
CCOP(=O)(SC(C)CC)SC(C)CC	0.25
ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	0.27
Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	0.29
COC(=O)C=C(C)OP(=O)(OC)OC	0.35
CNC(=O)C=C(C)OP(=O)(OC)OC	0.45
CCOc1cc(OP(=S)(OC)OC)nc(CC)n1	0.45
COP(=S)(OC)Oc1ccc(c(C)c1)[N+](=O)[O-]	0.46
CCOP(=S)(NC(C)C)Oc1ccccc1C(=O)OC(C)C	0.5
CNC(=O)CCSCCSP(=O)(OC)OC	0.54
COP(=O)(N)SC	0.565
C1C[n+]2ccccc2c3cccc[n+]13	0.575
ClC1C2(Cl)C3C4C5OC5C6C4C1(Cl)C(Cl)(C36)C2(Cl)Cl	0.7
ClC1(Cl)C2(Cl)C3(Cl)C4(Cl)C(Cl)(Cl)C5(Cl)C(Cl)(C1(Cl)C35Cl)C24Cl	0.7
CCOP(=S)(OCC)SCSC(C)(C)C	0.703
CCOP(=S)(OCC)SCSc1ccc(Cl)cc1	1
Clc1cccc(n1)C(Cl)(Cl)Cl	1
COC(=O)C(C)Oc1ccc(Oc2ncc(cc2Cl)C(F)(F)F)cc1	1
Clc1ccccc1Nc2nc(Cl)nc(Cl)n2	1.15
CCCCSP(=O)(SCCCC)SCCCC	1.25
CCNc1nc(Cl)nc(NC(C)(C)C#N)n1	1.25
CCOP(=S)(OCC)Oc1ccc2C(=C(Cl)C(=O)Oc2c1)C	1.25
ClC=C	1.3
CCOP(=S)(OCC)Oc1ncn(n1)c2ccccc2	1.3
COC1=NN(CSP(=S)(OC)OC)C(=O)S1	1.4125
[O-][N+](=O)N1CN(CN(C1)[N+](=O)[O-])[N+](=O)[O-]	1.5
CNC(=O)Oc1cc(C)c(N(C)C)c(C)c1	1.5

CCOP(=O)(OCC)OC(=CCl)c1ccc(Cl)cc1Cl	1.5
COP(=O)(OC)OC=C(Cl)Cl	1.6
CCOP(=O)(NC(C)C)Oc1ccc(SC)c(C)c1	1.6
COP(=S)(OC)Oc1ccc(SC)c(C)c1	1.64
CC(CN1CC(C)OC(C)C1)Cc2ccc(cc2)C(C)(C)C	1.7
COP(=S)(OC)SCN1N=Nc2ccccc2C1=O	1.73
ClC1CC2C(C1Cl)C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	1.755
CCOP(=S)(CC)Sc1ccccc1	1.94
CCOP(=S)(OCC)Oc1ccc(cc1)[N+](=O)[O-]	1.96
COP(=O)(OC)OC(Br)C(Cl)(Cl)Br	2
CCOP(=S)(OCC)SCSP(=S)(OCC)OCC	2
Cc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	2
CCOP(=S)(OCC)SCN1C(=O)Oc2cc(Cl)ccc12	2
COC(=O)Nc1nc2ccc(cc2[nH]1)S(=O)c3ccccc3	2
OC(c1ccc(Cl)cc1)(c2cncnc2)c3ccccc3Cl	2.3
CC(C)C(Nc1ccc(cc1Cl)C(F)(F)F)C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	2.5
CCOP(=S)(OCC)SC(CCl)N1C(=O)c2ccccc2C1=O	2.5
Clc1ccc(OS(=O)(=O)c2ccc(Cl)cc2)cc1	2.5
Clc1cccc(Cl)c1C#N	2.5
CC1(C)C(C=C(Br)Br)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	2.5
OC(c1ccc(F)cc1)(c2cncnc2)c3ccccc3Cl	2.5
CNC(=O)CSP(=S)(OC)OC	2.625
CCCSP(=O)(OCC)SCCC	2.7
ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)C2(Cl)Cl	2.9
CC1(C)C(C(Br)C(Br)(Br)Br)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	3
COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl	3
CCSC(=O)N(CC)C1CCCCC1	3
CCCCOC(=O)C(C)Oc1ccc(Oc2ccc(cn2)C(F)(F)F)cc1	3
Cc1nn(C)c(Oc2ccccc2)c1C=NOCc3ccc(cc3)C(=O)OC(C)(C)C	3.08
ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	3.14
C[n+]1ccc(cc1)c2cc[n+](C)cc2	3.15
CP(=O)(O)CCC(N)C(=O)O	3.5
COC(=O)N(C(=O)N1COC2(Cc3cc(Cl)ccc3C2=N1)C(=O)OC)c4ccc(OC(F)(F)F)cc4	3.6
CSC(=O)c1c(CC(C)C)c(C(=O)SC)c(nc1C(F)F)C(F)(F)F	3.63
CCOP(=S)(OCC)Oc1cc(C)nc(n1)C(C)C	3.65
CCOC(=O)C(C)Oc1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1	3.7
Nc1ncn[nH]1	3.75
Clc1cccc(c1)c2ccccc2	4
CNP(=O)(OC)Oc1ccc(cc1Cl)C(C)(C)C	4
Clc1c(Cl)c(C#N)c(Cl)c(C#N)c1Cl	4
Cc1cc(Cl)ccc1OCC(=O)O	4
CCOC(=O)c1cn2nc(OP(=S)(OCC)OCC)cc2nc1C	4

CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1	4.375
Cc1c(F)c(F)c(COC(=O)C2C(C=C(Cl)C(F)(F)F)C2(C)C)c(F)c1F	4.6
CCCCC(O)(Cn1cncn1)c2ccc(Cl)cc2Cl	4.7
Cc1c(COC(=O)C2C(C=C(Cl)C(F)(F)F)C2(C)C)cccc1c3ccccc3	4.85
CC(N)Cc1ccccc1	5
CC(C)Oc1cc(N2N=C(OC2=O)C(C)(C)C)c(Cl)cc1Cl	5
CNC(=O)ON=C(SC)C(=O)N(C)C	5
CCN(CC)C(=O)SCc1ccc(Cl)cc1	5
OC(=O)COc1ccc(Cl)cc1Cl	5
FC(F)(F)c1cccc(c1)N2CC(CCl)C(Cl)C2=O	5
CNC(=O)Oc1cccc2CC(C)(C)Oc12	5
Oc1c(Cl)cc(Cl)c(Cl)c1Cc2c(O)c(Cl)cc(Cl)c2Cl	5
CC1(C)CNC(=NN=C(C=Cc2ccc(cc2)C(F)(F)F)C=Cc3ccc(cc3)C(F)(F)F)NC1	5
CCCN(CC1CC1)c2c(cc(cc2[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	5
ClCC=CCl	5.1
Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl	5.125
CCNc1nc(Cl)nc(NCC)n1	5.15
Nc1ccc(Cl)cc1	5.5
CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl	5.5
Cc1cccc(C)c1O	6
CNC(=O)ON=C(CSC)C(C)(C)C	6
CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c3ccc(OC(F)F)cc3	6
[O-]Br(=O)=O	6.1
CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1	6.125
Cc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])C(=O)N	6.25
CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)n2ccnc2	6.3
Clc1ccc(c(Cl)c1)C2(Cn3cncn3)CC(Br)CO2	6.48
CCN(CC)C(=O)C(=C(C)OP(=O)(OC)OC)Cl	6.9
CC(C)NCC(O)COc1cccc2[nH]c3ccccc3c12	7
Cc1ccc2nc3SC(=O)Sc3nc2c1	7.5
Fc1cccc(F)c1C(=O)NC(=O)Nc2ccc(Cl)cc2	7.6
CCCCC(Cn1cncn1)(C#N)c2ccc(Cl)cc2	7.9
Cc1ccc(cc1N)[N+](=O)[O-]	8
O=C1C2=C(SC(=C(S2)C#N)C#N)C(=O)c3ccccc13	8
CCN(CC)c1nc(C)cc(OP(=S)(OC)OC)n1	8.15
CCSC(=O)N1CCCCCC1	8.405
CC(Oc1cc(Cl)c(Cl)cc1Cl)C(=O)O	8.7
CC(C)N1C(=NC(C)(C)C)SCN(C1=O)c2ccccc2	8.7
CC(C)OC(=O)C(O)(c1ccc(Cl)cc1)c2ccc(Cl)cc2	9
CC(Oc1ccc(Cl)cc1Cl)C(=O)O	9
CCOC(=O)C(C)Oc1ccc(Oc2oc3cc(Cl)ccc3n2)cc1	9
CON(C(=O)OC)c1ccccc1COc2ccn(n2)c3ccc(Cl)cc3	9

CNC(=O)Oc1cc(C)c(SC)c(C)c1	9.3
CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c2ccc(F)c(Oc3ccccc3)c2	9.5
CN(C=Nc1ccc(C)cc1C)C=Nc2ccc(C)cc2C	9.9
CC1=C(C)S(=O)(=O)CCS1(=O)=O	10
Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	10
OC(=O)COc1cc(Cl)c(Cl)cc1Cl	10
CSC(=NOC(=O)N(C)SN(C)C(=O)ON=C(C)SC)C	10
Clc1ccc(c(Cl)c1)C2(Cn3cncn3)OCCO2	10
CNC(=O)Oc1cc(C)c(C)c(C)c1	10
CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1	10
Cc1cc(C(C#N)c2ccc(Cl)cc2)c(Cl)cc1NC(=O)c3cc(I)cc(I)c3O	10
Clc1ccccc1c2nnc(nn2)c3ccccc3Cl	10.125
CN(C)C(=S)SSC(=S)N(C)C	11
OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(Cl)(Cl)Cl	11.25
CCCSP(=S)(OCC)Oc1ccc(SC)cc1	11.5
CCNc1cc2[o+]c3cc(NCC)c(C)cc3c(c4ccccc4C(=O)OCC)c2cc1C	12
CCOC(=O)C(Cl)Cc1cc(N2N=C(C)N(C(F)F)C2=O)c(F)cc1Cl	12
CCOc1ccc2NC(C)(C)C=C(C)c2c1	12
CC(C)C(O)(c1ccc(OC(F)(F)F)cc1)c2cncnc2	12.1
CN(C)C(=O)Oc1nc(nc(C)c1C)N(C)C	12.4
CNC(=O)Oc1cccc(c1)N=CN(C)C	12.5
CC(C)N(C(C)C)C(=O)SCC(=C(Cl)Cl)Cl	12.5
CCOC(=O)CN1C(=O)Sc2cccc(Cl)c12	12.5
CON(C)C(=O)Nc1ccc(Br)cc1	12.5
COC(=O)c1ccccc1S(=O)(=O)NC(=O)N(C)c2nc(C)nc(OC)n2	12.5
CCN(CC(=C)C)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	12.5
CCOP(=S)(OCC)Oc1nc(Cl)n(n1)C(C)C	12.5
CC1(C)C(C=C(Cl)C(F)(F)F)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	12.5
[O-][N+](=O)c1cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-]	13.31
ClC(Cl)C(Cl)(Cl)SN1C(=O)C2CC=CCC2C1=O	13.5
CCOCn1c(c2ccc(Cl)cc2)c(C#N)c(Br)c1C(F)(F)F	13.6
Cc1ccc(O)cc1C	14
ClC(=C)Cl	14
CCc1cccc(CC)c1N(COC)C(=O)CCl	14.5
COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O	14.5
Nc1nc(N)nc(NC2CC2)n1	15
COC(=O)Nc1nc2ccc(Sc3ccccc3)cc2[nH]1	15
CSC1=NN=C(C(=O)N1N)C(C)(C)C	15
CCNc1nc(NC(C)(C)C)nc(SC)n1	15
CC12CC1(C)C(=O)N(C2=O)c3cc(Cl)cc(Cl)c3	15
CC(C)OP(=S)(OC(C)C)SCCNS(=O)(=O)c1ccccc1	15
CN(C)C(=O)Nc1cccc(c1)C(F)(F)F	15
CCOc1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	15

CNC(=O)ON=C(C)SC	15
Cc1ncc([N+](=O)[O-])n1C	15
CC(C)(C)C(O)(CCc1ccc(Cl)cc1)Cn2cncn2	15.9
CCCC(=NOCC)C1C(=O)CC(CC(C)SCC)CC1=O	16.56
CC(CN1c2ccccc2Sc3ccccc13)N(C)C	16.6
CC1(OC(=O)N(Nc2ccccc2)C1=O)c3ccc(Oc4ccccc4)cc3	16.8
CCCN(CCC)C(=O)SCC	17
[O-][N+](=O)NC1=NCCN1Cc2ccc(Cl)nc2	17
CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccc(C)cc1	18
CCOC(=O)C(O)(c1ccc(Cl)cc1)c2ccc(Cl)cc2	18.4
COP(=O)(NC(=O)C)SC	18.75
NC(=NCCCCCCCCNCCCCCCCCCN=C(N)N)N	19
Clc1ccc(cc1)C(C#N)c2c(Cl)ccc(N3N=CC(=O)NC3=O)c2Cl	19
CC(Cl)(Cl)C(=O)O	19.085
CC(C)C1(C)N=C(NC1=O)c2nc3ccccc3cc2C(=O)O	20
CS(=O)(=O)c1cc(ccc1C(=O)c2cnoc2C3CC3)C(F)(F)F	20
COP(=O)(OC)C(O)C(Cl)(Cl)Cl	20
CCCSc1ccc2nc(NC(=O)OC)[nH]c2c1	20
CC1(C)CON(Cc2ccccc2Cl)C1=O	21.5
Nc1nc(NC2CC2)nc(N)c1C#N	22
CC1(C)C(C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2)C1(C)C	22.225
CC(C)N(C(=O)CCl)c1ccccc1	23
CCC1CCCC(OC2CCC(C(C)O2)N(C)C)C(C)C(=O)C3CC4C(CCC5CC(CC45)OC6CC(C)C(OC)C(OC)C6OC)C3CC(=O)O1	24
c1ccc2[nH]c(nc2c1)c3cscn3	24
COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2Cl)n1	25
Nc1ccc(O)c(N)c1	25
COC(=O)c1sccc1S(=O)(=O)NC(=O)Nc2nc(C)nc(OC)n2	25
CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc2cccc(Oc3ccccc3)c2	25
COC(=O)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1	25
CCOC(=O)COC(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	25
CC(C)(C)C(O)C(Oc1ccc(cc1)c2ccccc2)n3cncn3	25
CCCCC1=C(C)NC(=NC1=O)NCC	25
Clc1ccc(CN(C2CCCC2)C(=O)Nc3ccccc3)cc1	25
CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c3ccc(Cl)cc3	25
CC(C)c1cc(ccc1O)C(C)(C)c2ccc(O)c(c2)C(C)C	25
CCCCN(CCCC)SN(C)C(=O)Oc1cccc2CC(C)(C)Oc12	25
CCNc1nc(Cl)nc(NC(C)C)n1	25
Fc1cccc(F)c1C(=O)NC(=O)Nc2cc(Cl)c(F)c(Cl)c2F	25.5
CC(C)OC(=O)C(O)(c1ccc(Br)cc1)c2ccc(Br)cc2	26
CCOc1ccc(cc1)C(C)(C)COCc2cccc(Oc3ccccc3)c2	26
CCN1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC4	26
CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n2cncn2	26.585

Clc1ccc(C(Cn2ccnc2)OCC=C)c(Cl)c1	27.5
CC(=O)Nc1cc(NS(=O)(=O)C(F)(F)F)c(C)cc1C	27.6
N(c1ccccc1)c2ccccc2	28
CCCC(=C1C(=O)CC(CC1=O)C2CCCSC2)NOCC	28
ClC(Br)Br	28.5
CN1C=C(C(=O)C(=C1)c2cccc(c2)C(F)(F)F)c3ccccc3	28.75
CC(=O)OCCCCCCCCCCCCCNC(=N)N	29
CCCN(CCC)c1c(cc(c(N)c1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	29.4
CC1=C(SCCO1)C(=O)Nc2ccccc2	30
OC(=O)CCl	30
CN(C)C(=O)C(c1ccccc1)c2ccccc2	30
O=C(Nc1ccccc1)Nc2cnns2	30
Clc1cc(Cl)cc(c1)C2(CC(Cl)(Cl)Cl)CO2	30
CN1CSC(=S)N(C)C1	30
CCNC(=O)NC(=O)C(=NOC)C#N	30.3
Cc1cccc2sc3nncn3c12	31
COC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OC	32
Cc1cc(C)nc(NS(=O)(=O)c2ccc(N)cc2)n1	33
Cc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]	34
CNC1=C(Cl)C(=O)N(N=C1)c2cccc(c2)C(F)(F)F	35
Clc1ccc(CCC(Cn2cncn2)(C#N)c3ccccc3)cc1	35
Cc1cc(nc(Nc2ccccc2)n1)C3CC3	35.6
OC(=O)COc1nc(Cl)c(Cl)cc1Cl	36
FC(OC(F)(F)F)C(F)(F)Oc1ccc(NC(=O)NC(=O)c2c(F)cccc2F)cc1Cl	36
CC(C)N1C(=O)c2ccccc2NS1(=O)=O	37.5
CC(=CC1C(C(=O)OC2CC(=O)C(=C2C)CC=C)C1(C)C)C	37.77
CNC(=O)Oc1cccc2ccccc12	37.8
CC(C)(C)C(O)C(=Cc1ccc(Cl)cc1)n2cncn2	39.41
CNC(=O)N(C)c1nnc(s1)C(C)(C)C	40
COCC(=O)Nc1cc(Sc2ccccc2)ccc1NC(=NC(=O)OC)NC(=O)OC	40
CC(C)N(C(C)C)c1c(cc(cc1[N+](=O)[O-])S(=O)(=O)N)[N+](=O)[O-]	40.93
COC(=O)c1c(CC(C)C)c(C2=NCCS2)c(nc1C(F)F)C(F)(F)F	44.2
CON=C(Cc1cccnc1)c2ccc(Cl)cc2Cl	45
CCC(C)(O)C#C	46
COC(C)(C)CCCC(C)CC=CC(=CC(=O)OC(C)C)C	46
CC(C)NC(=O)N1CC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2	46
COC(=O)C(C)N(C(=O)Cc1ccccc1)c2c(C)cccc2C	46
COc1ccc(cc1OC)C(=CC(=O)N2CCOCC2)c3ccc(Cl)cc3	46.3
Nc1ccc2cc3ccc(N)cc3nc2c1	47
CCc1ccc(cc1)C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C	48
CCC(=O)Nc1ccc(Cl)c(Cl)c1	48
CCOCN(C(=O)CCl)c1c(C)cccc1CC	50
CNC(=O)Oc1ccccc1OC(C)C	50

CN(C)C1=NC(=O)N(C2CCCCC2)C(=O)N1C	50
COP(=S)(OC)Oc1cc(Cl)c(Cl)cc1Cl	50
CC(C)Nc1nc(Cl)nc(NC(C)C)n1	50
COC(=O)c1ccc(C)cc1C2=NC(C)(C(C)C)C(=O)N2	50
IC(=C(I)I)I	50
CN1CC(O)N(C1=O)c2nnc(s2)C(C)(C)C	50
CC(C)(C)C(O)C(=Cc1ccc(Cl)cc1Cl)n2cncn2	50
COCC(=O)N(N1CCOC1=O)c2c(C)cccc2C	50
CCC(C)Nc1c(cc(cc1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-]	50
CS(=O)(=O)NC(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	50
CCN(Cc1c(F)cccc1Cl)c2c(cc(cc2[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	50
CCOC(=O)CN(C(=O)CCl)c1c(CC)cccc1CC	50
CCOC(=O)C(C)OC(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	50
CC(C)(c1ccc(O)cc1)c2ccc(O)cc2	50
CCOC(=O)C(C)OC(=O)c1cc(Oc2cc(ccc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	50
CN1CC2CC1CN2c3cc4N(C=C(C(=O)O)C(=O)c4cc3F)C5CC5	50
CCC(C)(CC)c1cc(NC(=O)c2c(OC)cccc2OC)on1	50.7
ClCCl	51.29
CCCCCCCCc1cc(c(OC(=O)C=CC)c(c1)[N+](=O)[O-])[N+](=O)[O-]	57
CNC(=O)Oc1cc(C)cc(C)c1C	59.2
NC1CCCCC1	59.25
CC(C)(C)c1ccc(OC2CCCCC2OS(=O)OCC#C)cc1	59.5
O=Cc1occc1	60
Nc1c(Cl)c(Cl)nc(C(=O)O)c1Cl	60
ClC(Cl)Cl	60
CON=C(C(=O)OC)c1ccccc1CON=C(C)c2cccc(c2)C(F)(F)F	60
CCCC1COC(Cn2cncn2)(O1)c3ccc(Cl)cc3Cl	60.5
COC=C(C(=O)OC)c1ccccc1Oc2cc(Oc3ccccc3C#N)ncn2	62.25
COCC(=O)N(C(C)C(=O)OC)c1c(C)cccc1C	62.5
CCC(C)N1C(=O)NC(=C(Br)C1=O)C	62.5
CCc1cccc(CC)c1N(CNC(=O)C)C(=O)CCl	62.5
CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	62.5
Cc1cc(C)c(N)cc1C	63
CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n2cncn2	65
CC1=NN(C(=O)N1C(F)F)c2cc(NS(=O)(=O)C)c(Cl)cc2Cl	67
CCCCCCCCSC(=O)Oc1cc(Cl)nnc1c2ccccc2	67.5
ClC#N	70
CC1CC=CC=CC=CC(CC2(C)OC(O)(CC(O)CC3(C)OC3C=CC(=O)O1)CC(O)C2C(=O)O)OC4(C)OC(C)C(O)C(N)C4O	72
Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccn3	72.5
CC1(OC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2)C=C	72.9

NC(=N)NC(=N)NCCc1ccccc1	73
COP(=O)(OC)OC(=CCl)c1cc(Cl)c(Cl)cc1Cl	75
COC(=O)Nc1nc2ccccc2[nH]1	75
NCCNc1cccc2ccccc12	79
COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2CCC(F)(F)F)n1	79.9
Cc1cc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2C(=O)OC3COC3)n1	83
Nc1ccc(N)c(c1)[N+](=O)[O-]	87
CCSC(C)CC1CC(=O)C(=C(CC)NOCC=CCl)C(=O)C1	93
CC(=CC1C(C(=O)OC2CC(=O)C(=C2C)CC#C)C1(C)C)C	95
COP(=O)OC	100
CC(Oc1cccc(Cl)c1)C(=O)O	100
ClC(Cl)(Cl)SN1C(=O)C2CC=CCC2C1=O	100
CCN(CC)C(=O)C(C)Oc1cccc2ccccc12	100
CCSC(=O)N(CC(C)C)CC(C)C	100
ClC(Cl)(Cl)C(NC=O)N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl	100
OC(=O)c1cc(Oc2ccc(cc2Cl)C(F)(F)F)ccc1[N+](=O)[O-]	102.5
ClC(Cl)C(Cl)Cl	108
FC1(F)Oc2cccc(c2O1)c3c[nH]cc3C#N	110
OC(=O)C1C2CCC(O2)C1C(=O)O	115
COc1c(Cl)ccc(Cl)c1C(=O)O	115
Clc1ccccc1	120
BrC#N	122
CC1CC(OC(=O)C)OC(C)O1	125
C[n+]1c(cc(c2ccccc2)n1C)c3ccccc3	125
COc1ccc(cc1)C(c2ccc(OC)cc2)C(Cl)(Cl)Cl	125
CN(C)C(=O)Nc1ccc(Cl)cc1	125
CC(=CC1C(C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C)C	125
COc1cc(Cl)c(OC)cc1Cl	125
COC(=O)c1ccc(cc1)C(=O)OC	125
O=C1CCCCCN1	125
CCOC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc2nc(Cl)cc(OC)n2	125
CCCCOCC(C)OCC(C)O	128
ClC(Cl)Br	130
[O-][N+](=O)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	132.5
OC(O)C(Cl)(Cl)Cl	135
COC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc2nc(OC(F)F)cc(OC(F)F)n2	140
CC(COc1ccc(Oc2ccccc2)cc1)Oc3ccccn3	140
Oc1cccc2cccnc12	143
COC(=O)C(Cc1ccccc1)NC(=O)C(N)CC(=O)O	147
FC(F)(Cl)Cl	150
C[N+]1(C)CCCCC1	150
COC(=O)C1(O)c2ccccc2c3ccc(Cl)cc13	150
CCc1cccc(C)c1N(C(C)COC)C(=O)CCl	150

CC(C)C12CCC(C)(O1)C(C2)OCc3ccccc3C	150
CC(=CC1C(C(=O)OCc2cccc(Oc3ccccc3)c2)C1(C)C)C	150
Cc1ncc([N+](=O)[O-])n1CCO	150
CN(C)C1C2CC3C(=C(O)c4c(O)cccc4C3(C)O)C(=O)C2(O)C(=O)C(=C(N)O)C1=O	150
CC1C(SC(=O)N1C(=O)NC2CCCCC2)c3ccc(Cl)cc3	160
[O-][N+](=O)c1cccc2ccccc12	165
CCOC(=O)C1OC1(C)c2ccccc2	175
CCCCOCCOCCOCc1cc2OCOc2cc1CCC	175
CC1=CC(=O)CC(C)(C)C1	179
COC(=O)NS(=O)(=O)c1ccc(N)cc1	180
Oc1ccc2cc(ccc2c1N=Nc3ccccc3)S(=O)(=O)O	180
Cc1cc(N)ccc1NOS(=O)(=O)O	184
Nc1c(Cl)cc(cc1Cl)[N+](=O)[O-]	195
ClC(Cl)(Cl)SN1C(=O)c2ccccc2C1=O	196
CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	200
CCCN(CCCl)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	202.4
OP(=O)(O)CCCl	202.67
CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC	205
CCCCNC(=O)n1c(NC(=O)OC)nc2ccccc12	215
CC(C)(C)c1ccc(O)c(Cl)c1	216
COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2OCCCl)n1	220.8
CC(C)(C)c1cc(O)ccc1O	225
OCCNc1ccc(cc1OCCO)[N+](=O)[O-]	229
Clc1ccc(cc1)S(=O)(=O)c2cc(Cl)c(Cl)cc2Cl	230
C=Cc1ccccc1	235.33
CCOC(=O)C=C	248
CC(=C)C(=O)O	248
c1ccc(cc1)c2ccccc2	250
CC(=CC1C(C(=O)OCN2C(=O)C3=C(CCCC3)C2=O)C1(C)C)C	250
CCCOC(=O)c1ccc(nc1)C(=O)OCCC	250
NCC(O)c1ccc(O)cc1	250
COC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc2nc(C)nc(OC)n2	250
COC(=O)c1c(Cl)c(Cl)c(C(=O)OC)c(Cl)c1Cl	255
C[N+](C)(C)CCCl	262.5
COc1ccc(N)c(OC)c1	276
CC1(CCCCC1)C(=O)Nc2ccc(O)c(Cl)c2Cl	292
Clc1ccc(Cl)cc1	300
COC(=O)c1ccccc1CS(=O)(=O)NC(=O)Nc2nc(OC)cc(OC)n2	309
Oc1ccccc1	344
COc1ccc(C=CC)cc1	344
FC(Cl)(Cl)Cl	349
CCc1ccccc1	349.5

COC(=O)c1ccccc1O	360
CON=C(C(=O)OC)c1ccccc1COc2ccccc2C	372.5
CC(C)Oc1cccc(NC(=O)c2ccccc2C(F)(F)F)c1	387.5
CC(C)c1ccccc1	396.5
CCOP(=O)O	400
CC1CCc2cc(F)cc3C(=O)C(=CN1c23)C(=O)O	400
COc1cccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)c1C	411
ClCC#CCOC(=O)Nc1cccc(Cl)c1	450
CCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2	470
COc1ccc(N)cc1	474
COC(=O)C(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C)C)C	500
CC(CCC(=O)O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C	500
Nc1c(Cl)c(F)nc(OCC(=O)O)c1Cl	500
C(Oc1ccccc1c2ccccc2)C3CO3	500
CC(C)C1(C)N=C(NC1=O)c2ncccc2C(=O)O	500
O=C1NNC(=O)C=C1	500
CC(C)N(C(C)C)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	520
CC(C)C1CCC(C)CC1O	593
CCCCOC(=O)c1ccccc1C(=O)OCCCC	600
OC(=O)CNCP(=O)(O)O	650
CCCOC(=O)NCCCN(C)C	680
Nc1ccc(O)cc1	686
CCN(Cc1cccc(c1)S(=O)(=O)O)c2ccc(cc2)C(=C3C=CC(=[N+](CC)Cc4cccc(c4)S(=O)(=O)O)C=C3)c5ccc(cc5)N(C)C	720
OCc1cc(N=Nc2ccc(c3ccccc23)S(=O)(=O)O)c(O)c(N=Nc4ccc(c5ccccc45)S(=O)(=O)O)c1O	736
S=C1Nc2ccccc2S1	750
CC(C)OC(=O)Nc1cccc(Cl)c1	750
OC(=O)c1c(Cl)ccc2cc(Cl)cnc12	757
NC(=O)c1cnccn1	789
OCCO	803.335
CCCOC(=O)c1cc(O)c(O)c(O)c1	864
O=C1CCCCC1	910
NC(=S)NNC(=S)N	947
Oc1ccccc1c2ccccc2	1000
OC(=O)C=CC(=O)O	1081
CCOc1ccc(NC(=O)C)cc1N	1185
Nc1cc(ccc1C(=O)O)[N+](=O)[O-]	1185
O=C1OC(=O)c2ccccc12	1185
OCC(O)C1OC(=O)C(=C1O)O	1330.335
COC(=O)c1ccc(O)cc1	1500
CCCOC(=O)c1ccc(O)cc1	1500

CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC	1500
CC(=O)Nc1ccc(cc1)C(=O)CCl	1580
CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2c(C)c(OC(=O)C)c(C)c(C)c2O1	2000
COC(=O)c1ccccc1C(=O)OC	2000
OC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccc(O)c(O)c3	2034
COc1ccc(cc1N=Nc2c(O)c(cc3ccccc23)C(=O)Nc4cccc(c4)[N+](=O)[O-])[N+](=O)[O-]	2100
CCOC(=O)COC(=O)c1ccccc1C(=O)OCC	2500
Nc1ccccc1C(=O)O	2751
O=C1NS(=O)(=O)c2ccccc12	3602
OS(=O)(=O)NC1CCCCC1	3602
COc1cc(c(C)cc1N=Nc2c(O)ccc3cc(ccc23)S(=O)(=O)O)S(=O)(=O)O	3739
CCOC(=O)c1ccccc1C(=O)OCC	4435
CN(C)C1C2C(O)C3C(=C(O)c4c(O)ccc(Cl)c4C3(C)O)C(=O)C2(O)C(=O)C(=C(N)O)C1=O	5200
OCC(O)CO	6883
CCCCCCCCCCCC(=O)OCC(O)C1OCC(O)C1O	6883
CCCCCCCCCCCCCCCCCCC(=O)OCC(O)C1OCC(O)C1O	7203
External validation set	
Canonical_Smiles	LOAEL [mg/kg_bw/day]
CNC(=O)\C=C(/C)\OP(=O)(OC)OC	0.005
CCS(=O)CCSP(=O)(OC)OC	0.028
Nc1c(c(nn1c2c(Cl)cc(cc2Cl)C(F)(F)F)C#N)C(F)(F)F	0.032
COP(=O)(OC)O\C(=C\C(=O)N(C)C)\C	0.045
CCOP(=S)(OCC)OC(Cl)C(Cl)(Cl)Cl	0.311
C[C@@H](Oc1ccc(Oc2ncc(Cl)cc2F)cc1)C(=O)OCC#C	0.32
COC(=O)\C=C(/C)\OP(=O)(OC)OC	0.35
CCNP(=S)(OC)O\C(=C/C(=O)OC(C)C)\C	0.3645
N#CSCSC#N	0.4
CCCCC[C@H](C)OC(=O)COc1ccc(Cl)c2cccnc12	0.42
CNC(=O)O\N=C\C(C)(C)SC	0.47
CS(=O)(=O)c1ccc(C(=O)C2C(=O)CCCC2=O)c(c1)[N+](=O)[O-]	0.48
CNC(=O)Oc1cccc2OC(C)(C)Oc12	0.7745
[O-][N+](=O)C(Cl)(Cl)Cl	1
CCCSP(=O)(OCC)Oc1ccc(Br)cc1Cl	1
CC(C)N(C(=O)COc1nnc(s1)C(F)(F)F)c2ccc(F)cc2	1.2
CCOP(=S)(OC(C)C)Oc1cnc(nc1)C(C)(C)C	1.71
COc1cc2OC[C@H]3Oc4c5C[C@@H](Oc5ccc4C(=O)[C@H]3c2cc1OC)C(=C)C	1.88
COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1	2
COC(=O)N(C(=O)N1CO[C@]2(Cc3cc(Cl)ccc3C2=N1)C(=O)OC)c4ccc	2.13

(OC(F)(F)F)cc4	
CCOP(=O)(SC(C)CC)N1CCSC1=O	2.375
CC1(C)[C@@H](C=C(Br)Br)[C@H]1C(=O)O[C@H](C#N)c2cccc(Oc3ccccc3)c2	2.5
Clc1ccc(CN2CCS/C/2=N\C#N)cn1	2.5
Cc1nn(C)c(Oc2ccccc2)c1\C=N\OCc3ccc(cc3)C(=O)OC(C)(C)C	3
CC1(C)[C@@H](C(Br)C(Br)(Br)Br)[C@H]1C(=O)O[C@H](C#N)c2cccc(Oc3ccccc3)c2	3
CN(\C=N\c1ccc(C)cc1C)\C=N\c2ccc(C)cc2C	3.13
CCCCOC(=O)[C@@H](C)Oc1ccc(Oc2ccc(cc2F)C#N)cc1	3.44
CCCOC\C(=N/c1ccc(Cl)cc1C(F)(F)F)\n2ccnc2	3.5
Cl[C@@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H](Cl)[C@H]1Cl	3.655
[O-][N+](=O)c1cc(c(Cl)c(c1Nc2ncc(cc2Cl)C(F)(F)F)[N+](=O)[O-])C(F)(F)F	3.7
CC1=NNC(=O)N(C1)\N=C\c2cccnc2	3.76
Cc1c(ccc(c1C2=NOCC2)S(=O)(=O)C)C(=O)c3cnn(C)c3O	3.895
CNC(=O)O\N=C(/SC)\C(=O)N(C)C	4.17
Cc1c(F)c(F)c(COC(=O)[C@@H]2[C@H](\C=C(/Cl)\C(F)(F)F)C2(C)C)c(F)c1F	4.6
CC1(C)CNC(=NC1)NN=C(\C=C\c2ccc(cc2)C(F)(F)F)\C=C\c3ccc(cc3)C(F)(F)F	4.9
CC(C)(C)N1N=CC(=C(Cl)C1=O)SCc2ccc(cc2)C(C)(C)C	5
CCCCN(CC)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	5.4
Cc1c(COC(=O)C2C(\C=C(/Cl)\C(F)(F)F)C2(C)C)cccc1c3ccccc3	6.1
CCc1nn(C)c(C(=O)NCc2ccc(cc2)C(C)(C)C)c1Cl	6.52
CN1SC(=CC1=O)Cl	6.6
CN1CCN(Cc2occ(c2)c3ccc4nc(O)oc4c3)[C@H](C1)c5ccc(F)cc5	7
CSC1=N[C@](C)(C(=O)N1Nc2ccccc2)c3ccccc3	7.07
NC#N	7.5
CCNc1nc(O)nc(NC(C)C)n1	7.75
COP(=O)(OC)SCN1C(=O)Oc2cc(Cl)cnc12	8.1
CC(C)N1\C(=N\C(C)(C)C)\SCN(C1=O)c2ccccc2	8.7
CC(CN1C[C@@H](C)O[C@@H](C)C1)Cc2ccc(cc2)C(C)(C)C	8.8
CCCCCCCCCCCCC1=C(OC(=O)C)C(=O)c2ccccc2C1=O	9.02
COc1ccc(cc1NNC(=O)OC(C)C)c2ccccc2	9.7
CCOC(=O)Nc1cccc(OC(=O)Nc2ccccc2)c1	10.595
C[C@H](Oc1ccc(Cl)cc1Cl)C(=O)O	11.01
CBr	11.1
CN1C(=O)N(C(=O)C=C1C(F)(F)F)c2ccc(Cl)c(c2)C(=O)OC(C)(C)C(=O)OCC=C	11.4
CCOC(=O)CSc1nc(nn1C(=O)N(C)C)C(C)(C)C	11.5
CCCCOCN(C(=O)CCl)c1c(CC)cccc1CC	11.85
CNC(=O)Oc1cccc(c1)\N=C\N(C)C	12

CS\C(=N\OC(=O)N(C)SN(C)C(=O)O\N=C(/C)\SC)\C	12
Clc1cc(Cl)c(cc1OCC#C)N2N=C3CCCCN3C2=O	12.1
ClC\C=C\Cl	12.5
CC1(C)C(\C=C(/Cl)\C(F)(F)F)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2	12.5
CCOC(=O)CC(SP(=O)(OC)OC)C(=O)OCC	13
CCC(C)(C)C(=O)OC1=C(C(=O)OC12CCCCC2)c3ccc(Cl)cc3Cl	14.7
Oc1cc(Cl)ccc1Oc2ccc(Cl)cc2Cl	15
CC(C1CC1)C(O)(Cn2cncn2)c3ccc(Cl)cc3	15.59
FC(F)(F)c1cccc(OCCCOc2c(Cl)cc(OCC=C(Cl)Cl)cc2Cl)n1	17.1
CN(Cc1ccc(Cl)nc1)\C(=N\C#N)\C	17.5
Fc1cc2OCC(=O)N(CC#C)c2cc1N3C(=O)C4=C(CCCC4)C3=O	18
CNC(=O)O\N=C(/C)\SC	20
NC(=O)CN1C(=O)C=C(CCN2CCN(CC2)c3nccc4sccc34)c5ccc(F)cc15	20
CCCCNC(=O)OCC#CI	20.1
CCNc1nc(NC(C)C)nc(SC)n1	20.9
CON(C)C(=O)Nc1ccc(Oc2ccc3c(OC(C)(CC3(C)C)OC)c2)cc1	23.1
COc1nc(NC(C)C)nc(NC(C)C)n1	23.3
CC[C@H]1CCC[C@H](O[C@H]2CC[C@@H]([C@@H](C)O2)N(C)C)[C@@H](C)C(=O)C3=C[C@H]4[C@@H]5C[C@@H](C[C@H]5C(=C[C@H]4[C@@H]3CC(=O)O1)C)O[C@@H]6O[C@@H](C)[C@H](OC)[C@@H](OC)[C@H]6OC	24.1
CC1COC(Cn2cncn2)(O1)c3ccc(Oc4ccc(Cl)cc4)cc3Cl	24.12
CC(C)c1ccc(cc1S(=O)(=O)C)C(=O)N=C(N)N	25
OC(=O)C1(CC1)C(=O)Nc2ccc(Cl)cc2Cl	25.5
FC(F)C(F)(F)OCC(Cn1cncn1)c2ccc(Cl)cc2Cl	27.7
CO\N=C(/C(=O)OC)\c1ccccc1CO\N=C(/C)\c2cccc(c2)C(F)(F)F	29.7
OC(=O)CCCOc1ccc(Cl)cc1Cl	30
Oc1ccc(Cl)cc1Cc2ccccc2	30
CCNC(=O)NC(=O)\C(=N\OC)\C#N	30.3
COC(=O)c1cccc(C)c1S(=O)(=O)NC(=O)Nc2nc(OCC(F)(F)F)nc(n2)N(C)C	30.6
CCCN(CC)CC1COC2(CCC(CC2)C(C)(C)C)O1	32.81
COCC(C)N(C(=O)CCl)c1c(C)csc1C	36
CC(C)(C)C(O)\C(=C/c1ccc(Cl)cc1Cl)\n2cncn2	39.4
CC(C)(C)[C@H](O)\C(=C/c1ccc(Cl)cc1)\n2cncn2	39.41
OCC(Br)(CO)[N+](=O)[O-]	40
NC1=C(Cl)C(=O)N(N=C1)c2ccccc2	40.095
CC1OC(C)OC(C)OC(C)O1	44
O=CCCCC=O	45.63
CCCC(=C1C(=O)CC(CC(C)SCC)CC1=O)NOCC	48
CC(C)(NC(=O)c1cc(Cl)cc(Cl)c1)C#C	48.8
CCOC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OCC	50
CCC(CC)Nc1c(cc(C)c(C)c1[N+](=O)[O-])[N+](=O)[O-]	51

CCCN(CCC)c1c(cc(cc1[N+](=O)[O-])S(=O)(=O)N)[N+](=O)[O-]	51.445
COc1ccc(cc1OC)\C(=C\C(=O)N2CCOCC2)\c3ccc(Cl)cc3	55.55
CSc1nc(NC(C)C)nc(NC(C)C)n1	60.88
CC(C)(C)C(O)C(Cc1ccc(Cl)cc1)n2cncn2	62.5
CN1COCN(Cc2cnc(Cl)s2)/C/1=N/[N+](=O)[O-]	63
CCCCCCCCCC[N+](C)(C)CCCCCCCCCC	64
NC(=O)C(Br)(Br)C#N	71.29
Clc1ccc(cc1)c2ccccc2NC(=O)c3ccenc3Cl	73
Brc1ccc(OC(=O)N2CCN3CCC2CC3)cc1	75
Fc1ccc(Oc2ccnc3cc(Cl)cc(Cl)c23)cc1	80
CO\C=C(\C(=O)OC)/c1ccccc1Oc2cc(Oc3ccccc3C#N)ncn2	82.4
CC(=C[C@@H]1[C@@H](C(=O)O[C@H]2CC(=O)C(=C2C)CC=C)C1(C)C)C	82.6
CCOC(=O)COc1cc(c(F)cc1Cl)c2nn(C)c(OC(F)F)c2Cl	86.7
CCCCCCCCCCCCC[N+](C)(C)[O-]	87.4
CCCCCCCCCCCCCC[N+](C)(C)Cc1ccccc1	88
Clc1cc(NC(=O)Nc2ccccc2)ccn1	93
CC\C(=N/OC\C=C\Cl)\C1=C(O)CC(CC1=O)C2CCOCC2	94.5
C\N=C(\NCc1cnc(Cl)s1)/N[N+](=O)[O-]	97.8
CCSC(C)CC1CC(=O)C(=C(CC)NOC\C=C\Cl)C(=O)C1	100
CCOc1nc(F)cc2nc(nn12)S(=O)(=O)Nc3c(Cl)cccc3Cl	102.2
CC(C)(C)C(=O)[C@@H](Oc1ccc(Cl)cc1)n2cncn2	114
CCONC(=C1C(=O)CC(CC1=O)c2c(C)cc(C)cc2C)CC	117.9
CCCCCCC(C)c1cc(cc(c1OC(=O)\C=C/C)[N+](=O)[O-])[N+](=O)[O-]	120.8
CCS(=O)(=O)c1cccnc1S(=O)(=O)NC(=O)Nc2nc(OC)cc(OC)n2	121
COC(=O)CSc1cc(\N=C\2/SC(=O)N3CCCCN23)c(F)cc1Cl	130
COC(=O)c1c(Cl)nn(C)c1S(=O)(=O)NC(=O)Nc2nc(OC)cc(OC)n2	138.6
CC(C)[C@]12CC[C@](C)(O1)[C@@H](C2)OCc3ccccc3C	150
OC(=O)c1nc(Cl)ccc1Cl	150
CCCCC(CC)CN1C(=O)C2C3CC(C=C3)C2C1=O	150
C[C@H]1[C@@H](SC(=O)N1C(=O)NC2CCCCC2)c3ccc(Cl)cc3	163
CCCN(CCC)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]	169
CC1(C)[C@@H](C=C(Cl)Cl)[C@H]1C(=O)OCc2cccc(Oc3ccccc3)c2	170.75
CCOc1cc(ccc1C2COC(=N2)c3c(F)cccc3F)C(C)(C)C	201.5
Cc1cc(C)nc(Nc2ccccc2)n1	221
CCS(=O)(=O)c1nc2ccccn2c1S(=O)(=O)NC(=O)Nc3nc(OC)cc(OC)n3	244.2
COS(=O)(=O)[O-].C[n+]1c(cc(c2ccccc2)n1C)c3ccccc3	250
COc1cnc(OC)n2nc(NS(=O)(=O)c3c(OCC(F)F)cccc3C(F)(F)F)nc12	254
CO\N=C(\C1=NOCCO1)/c2ccccc2Oc3ncnc(Oc4ccccc4Cl)c3F	271.9
CC1(C)CC\C(=C\c2ccc(Cl)cc2)\C1(O)Cn3cncn3	286.6
CCC[N+](C)(C)CC[N+](C)(C)CCOC	300
CSC(=O)c1cccc2nnsc12	312
CCCCCOC(=O)COc1cc(N2C(=O)C3=C(CCCC3)C2=O)c(F)cc1Cl	360.4

CCN(CC)C(=O)c1cccc(C)c1	400
Oc1ccc(Cl)cc1C(=O)Nc2ccc(cc2Cl)[N+](=O)[O-]	410
CCOC1Oc2ccc(OS(=O)(=O)C)cc2C1(C)C	469
CC1(C)N(Cl)C(=O)N(Cl)C1=O	634.5
C\N=C(\NCC1CCOC1)/N[N+](=O)[O-]	991
CC1(C)NC(=O)NC1=O	1000
Cc1ccn2nc(nc2n1)S(=O)(=O)Nc3c(F)cccc3F	1000
NNC(=O)C=CC(=O)O	1956

Table S2. The SVM parameters C and γ for all models.

Threshold	Fingerprint type	C	γ
5	Estate	1.4142	0.25
	Extend	5.6569	0.0078
	FP	11.3137	0.0078
	MACCS	2	0.0221
	Pubchem	2.8284	0.0039
	SubFP	8	0.0625
10	Estate	0.7071	0.25
	Extend	1.4142	0.0055
	FP	16	0.0078
	MACCS	1	0.0625
	Pubchem	2.8284	0.0078
	SubFP	1	0.125
50	Estate	1	0.5
	Extend	0.7071	0.011
	FP	1	0.0078
	MACCS	1	0.0312
	Pubchem	2	0.0055
	SubFP	1.4142	0.125
100	Estate	1	0.7071
	Extend	1.4142	0.011
	FP	1.4142	0.011
	MACCS	2.83	0.0884
	Pubchem	4	0.0039
	SubFP	2	0.0884
10&50	Estate	0.70711	0.3536
	Extend	1	0.0884
	FP	2	0.011
	MACCS	2	0.0884
	Pubchem	2.8284	0.0055
	SubFP	2.8284	0.011

Table S3. Performance of models on 5-fold cross validation

Threshold=5 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.775	0.3936	0.8813	0.6917	0.2964
Estate_SVM	0.8307	0.3617	0.9614	0.7578	0.4281
Estate_Random Forest	0.8329	0.3298	0.9733	0.7666	0.4313
Estate_Naive Bayes	0.8051	0.3936	0.9199	0.7478	0.3641
Estate_Classification Tree	0.7819	0.4255	0.8813	0.7035	0.3259
Extend_kNN	0.8051	0.3936	0.9199	0.7131	0.3641
Extend_SVM	0.8098	0.2447	0.9674	0.7545	0.3248
Extend_Random Forest	0.8051	0.2128	0.9703	0.7427	0.2971
Extend_Naive Bayes	0.7331	0.5532	0.7834	0.6833	0.3063
Extend_Classification Tree	0.7354	0.4043	0.8279	0.6359	0.2304
FP_kNN	0.8098	0.383	0.9288	0.7083	0.3719
FP_SVM	0.819	0.2553	0.9763	0.751	0.3648
FP_Random Forest	0.8004	0.2234	0.9614	0.7353	0.2831
FP_Naive Bayes	0.7099	0.4787	0.7745	0.6275	0.2327
FP_Classification Tree	0.7262	0.4787	0.7953	0.672	0.2565
MACCS_kNN	0.7749	0.4468	0.8665	0.7577	0.3223
MACCS_SVM	0.8353	0.3617	0.9674	0.7611	0.4444
MACCS_Random Forest	0.8214	0.3298	0.9585	0.7847	0.3893
MACCS_Naive Bayes	0.7726	0.5106	0.8457	0.7469	0.3486
MACCS_Classification Tree	0.7632	0.4362	0.8546	0.6897	0.2954
Pubchem_kNN	0.7888	0.4043	0.8961	0.6753	0.3307
Pubchem_SVM	0.8283	0.3723	0.9555	0.7325	0.4227
Pubchem_Random Forest	0.8376	0.4149	0.9555	0.7746	0.462
Pubchem_Naive Bayes	0.733	0.4894	0.8012	0.6953	0.2728
Pubchem_Classification Tree	0.7796	0.4894	0.8605	0.7094	0.3513
SubFP_kNN	0.7772	0.4255	0.8754	0.732	0.3166
SubFP_SVM	0.8143	0.3298	0.9496	0.7437	0.3667
SubFP_Random Forest	0.8422	0.3936	0.9674	0.771	0.4738
SubFP_Naive Bayes	0.7704	0.4362	0.8635	0.7207	0.3083
SubFP_Classification Tree	0.8098	0.4787	0.9021	0.711	0.4085
Threshold=10 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.7053	0.4436	0.8221	0.7002	0.2799
Estate_SVM	0.7588	0.3158	0.9564	0.6965	0.3768
Estate_Random Forest	0.7449	0.2707	0.9564	0.7451	0.3304
Estate_Naive Bayes	0.731	0.3835	0.8859	0.7081	0.3127
Estate_Classification Tree	0.6892	0.4436	0.7987	0.6377	0.2503
Extend_kNN	0.7356	0.4662	0.8557	0.7119	0.3463
Extend_SVM	0.7588	0.3383	0.9463	0.7255	0.3772

Extend_Random Forest	0.7262	0.2632	0.9329	0.7025	0.2714
Extend_Naive Bayes	0.6568	0.6015	0.6812	0.6905	0.2659
Extend_Classification Tree	0.6683	0.5188	0.7349	0.6149	0.2468
FP_kNN	0.7426	0.4511	0.8725	0.7058	0.3566
FP_SVM	0.7495	0.3308	0.9362	0.7257	0.3492
FP_Random Forest	0.7355	0.2556	0.9497	0.7064	0.2987
FP_Naive Bayes	0.6474	0.6015	0.6678	0.6971	0.2524
FP_Classification Tree	0.6661	0.4361	0.7685	0.5905	0.2072
MACCS_kNN	0.696	0.4662	0.7987	0.7384	0.2715
MACCS_SVM	0.7518	0.3835	0.9161	0.7647	0.3631
MACCS_Random Forest	0.754	0.3684	0.9262	0.7671	0.3668
MACCS_Naive Bayes	0.7007	0.5414	0.7718	0.7145	0.3089
MACCS_Classification Tree	0.7285	0.5564	0.8054	0.6588	0.3625
Pubchem_kNN	0.71	0.4436	0.8289	0.6857	0.2887
Pubchem_SVM	0.7587	0.3609	0.9362	0.7126	0.3788
Pubchem_Random Forest	0.7424	0.3684	0.9094	0.767	0.3367
Pubchem_Naive Bayes	0.6684	0.4887	0.7483	0.6861	0.2338
Pubchem_Classification Tree	0.6915	0.5263	0.7651	0.6433	0.2874
SubFP_kNN	0.7054	0.4586	0.8154	0.7158	0.2855
SubFP_SVM	0.7541	0.3233	0.9463	0.751	0.3623
SubFP_Random Forest	0.7495	0.2782	0.9597	0.75	0.3462
SubFP_Naive Bayes	0.6824	0.4962	0.7651	0.681	0.2598
SubFP_Classification Tree	0.7217	0.4887	0.8255	0.6785	0.3264
Threshold=50 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.6844	0.7481	0.5818	0.7204	0.3307
Estate_SVM	0.7076	0.8797	0.4303	0.7211	0.3533
Estate_Random Forest	0.659	0.7331	0.5394	0.7184	0.2741
Estate_Naive Bayes	0.6774	0.7368	0.5818	0.7351	0.3183
Estate_Classification Tree	0.6472	0.7218	0.5273	0.6655	0.2503
Extend_kNN	0.6218	0.6278	0.6121	0.6852	0.2339
Extend_SVM	0.6843	0.8759	0.3758	0.7105	0.2951
Extend_Random Forest	0.6634	0.7406	0.5394	0.6907	0.2824
Extend_Naive Bayes	0.6657	0.6955	0.6182	0.6833	0.3085
Extend_Classification Tree	0.6404	0.7218	0.5091	0.6363	0.2329
FP_kNN	0.638	0.6165	0.6727	0.6825	0.2812
FP_SVM	0.6819	0.8571	0.4	0.7192	0.2921
FP_Random Forest	0.6473	0.7218	0.5273	0.6654	0.2503
FP_Naive Bayes	0.6565	0.6729	0.6303	0.675	0.2967
FP_Classification Tree	0.6471	0.7444	0.4909	0.6145	0.2405
MACCS_kNN	0.6705	0.7669	0.5152	0.701	0.2892
MACCS_SVM	0.7307	0.8835	0.4848	0.7536	0.4094

MACCS_Random Forest	0.6984	0.7519	0.6121	0.7419	0.3632
MACCS_Naive Bayes	0.6751	0.688	0.6545	0.7259	0.3352
MACCS_Classification Tree	0.6404	0.703	0.5394	0.632	0.2416
Pubchem_kNN	0.6799	0.7632	0.5455	0.702	0.3135
Pubchem_SVM	0.7168	0.8684	0.4727	0.7494	0.377
Pubchem_Random Forest	0.7007	0.782	0.5697	0.7317	0.3577
Pubchem_Naive Bayes	0.6613	0.6767	0.6364	0.7001	0.3063
Pubchem_Classification Tree	0.652	0.7105	0.5576	0.6511	0.2669
SubFP_kNN	0.6728	0.7632	0.5273	0.6916	0.2964
SubFP_SVM	0.7169	0.8759	0.4606	0.7364	0.3763
SubFP_Random Forest	0.6915	0.8233	0.4788	0.7182	0.3228
SubFP_Naive Bayes	0.6868	0.7406	0.6	0.714	0.3395
SubFP_Classification Tree	0.6473	0.6955	0.5697	0.6592	0.2625
Threshold=100 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.7171	0.7803	0.5635	0.7581	0.3352
Estate_SVM	0.7797	0.941	0.3889	0.7739	0.4141
Estate_Random Forest	0.7656	0.9049	0.4286	0.7891	0.3847
Estate_Naive Bayes	0.7354	0.8164	0.5397	0.776	0.3578
Estate_Classification Tree	0.7194	0.8131	0.4921	0.7069	0.3105
Extend_kNN	0.7194	0.7639	0.6111	0.7536	0.3587
Extend_SVM	0.7842	0.9475	0.3889	0.7928	0.4276
Extend_Random Forest	0.7493	0.8787	0.4365	0.7684	0.3499
Extend_Naive Bayes	0.6892	0.7213	0.6111	0.7158	0.3122
Extend_Classification Tree	0.652	0.7082	0.5159	0.6127	0.2127
FP_kNN	0.6985	0.7246	0.6349	0.749	0.3368
FP_SVM	0.7842	0.9443	0.3968	0.7903	0.4282
FP_Random Forest	0.7285	0.8557	0.4206	0.7489	0.301
FP_Naive Bayes	0.6822	0.7016	0.6349	0.7218	0.3129
FP_Classification Tree	0.7126	0.7934	0.5159	0.6578	0.3079
MACCS_kNN	0.7749	0.859	0.5714	0.8092	0.4426
MACCS_SVM	0.8005	0.9443	0.4524	0.8263	0.4784
MACCS_Random Forest	0.7843	0.8852	0.5397	0.7989	0.4532
MACCS_Naive Bayes	0.7171	0.7377	0.6667	0.759	0.3788
MACCS_Classification Tree	0.7264	0.7934	0.5635	0.7026	0.3507
Pubchem_kNN	0.7216	0.8098	0.5079	0.7271	0.3208
Pubchem_SVM	0.7865	0.941	0.4127	0.796	0.4362
Pubchem_Random Forest	0.7634	0.8754	0.4921	0.7697	0.396
Pubchem_Naive Bayes	0.7077	0.7443	0.619	0.724	0.3439
Pubchem_Classification Tree	0.7216	0.8197	0.4841	0.6774	0.3116
SubFP_kNN	0.7449	0.8361	0.5238	0.7476	0.3691
SubFP_SVM	0.768	0.9344	0.3651	0.7929	0.3783

SubFP_Random Forest	0.7493	0.9279	0.3175	0.7763	0.318
SubFP_Naive Bayes	0.747	0.8066	0.6032	0.7739	0.4018
SubFP_Classification Tree	0.7217	0.823	0.4762	0.6755	0.3085

Table S4. Performance of models on external validation.

Threshold=5 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.8621	0.5833	0.9541	0.8481	0.6053
Estate_SVM	0.8000	0.2500	0.9817	0.8096	0.3780
Estate_Random Forest	0.7931	0.1944	0.9908	0.7877	0.3506
Estate_Naive Bayes	0.8000	0.2778	0.9725	0.6988	0.3784
Estate_Classification Tree	0.7517	0.3611	0.8807	0.6304	0.2724
Extend_kNN	0.8276	0.5000	0.9358	0.8265	0.4984
Extend_SVM	0.8345	0.4444	0.9633	0.8588	0.5108
Extend_Random Forest	0.8345	0.3611	0.9908	0.8140	0.5148
Extend_Naive Bayes	0.7793	0.5000	0.8716	0.7167	0.3871
Extend_Classification Tree	0.7793	0.5000	0.8716	0.7132	0.3871
FP_kNN	0.8276	0.5000	0.9358	0.7866	0.4984
FP_SVM	0.8345	0.4444	0.9633	0.8372	0.5108
FP_Random Forest	0.7862	0.2222	0.9725	0.8108	0.3177
FP_Naive Bayes	0.7241	0.4444	0.8165	0.6593	0.2610
FP_Classification Tree	0.7724	0.4722	0.8716	0.7180	0.3623
MACCS_kNN	0.8483	0.6667	0.9083	0.7852	0.5862
MACCS_SVM	0.8138	0.3056	0.9817	0.8160	0.4343
MACCS_Random Forest	0.8000	0.2778	0.9725	0.7987	0.3784
MACCS_Naive Bayes	0.7862	0.4444	0.8991	0.7852	0.3812
MACCS_Classification Tree	0.7931	0.5833	0.8624	0.7715	0.4457
Pubchem_kNN	0.8345	0.5833	0.9174	0.8099	0.5341
Pubchem_SVM	0.8000	0.2500	0.9817	0.8119	0.3780
Pubchem_Random Forest	0.8207	0.3333	0.9817	0.8005	0.4607
Pubchem_Naive Bayes	0.7379	0.3889	0.8532	0.7201	0.2582
Pubchem_Classification Tree	0.8138	0.4167	0.9450	0.7150	0.4439
SubFP_kNN	0.7793	0.5556	0.8532	0.8001	0.4088
SubFP_SVM	0.8207	0.3611	0.9725	0.8135	0.4600
SubFP_Random Forest	0.8000	0.2500	0.9817	0.7252	0.3780
SubFP_Naive Bayes	0.7517	0.3333	0.8899	0.6095	0.2595
SubFP_Classification Tree	0.8207	0.3889	0.9633	0.7231	0.4614
Threshold=10 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.7655	0.5510	0.8750	0.7894	0.4544
Estate_SVM	0.7241	0.2041	0.9896	0.7752	0.3460
Estate_Random Forest	0.7241	0.2041	0.9896	0.7230	0.3460
Estate_Naive Bayes	0.7172	0.3265	0.9167	0.6649	0.3095
Estate_Classification Tree	0.6966	0.4898	0.8021	0.6602	0.3023
Extend_kNN	0.7448	0.5510	0.8438	0.7927	0.4117
Extend_SVM	0.7724	0.4286	0.9479	0.7950	0.4642

Extend_Random Forest	0.7724	0.4082	0.9583	0.7755	0.4665
Extend_Naive Bayes	0.6552	0.4694	0.7500	0.6644	0.2217
Extend_Classification Tree	0.7034	0.5918	0.7604	0.6956	0.3474
FP_kNN	0.7517	0.5306	0.8646	0.7787	0.4216
FP_SVM	0.7724	0.4286	0.9479	0.8031	0.4642
FP_Random Forest	0.7448	0.3265	0.9583	0.7511	0.3908
FP_Naive Bayes	0.6414	0.4490	0.7396	0.6576	0.1906
FP_Classification Tree	0.7448	0.5714	0.8333	0.7248	0.4164
MACCS_kNN	0.7655	0.6122	0.8438	0.7891	0.4662
MACCS_SVM	0.7517	0.4082	0.9271	0.7759	0.4074
MACCS_Random Forest	0.6897	0.3061	0.8854	0.7636	0.2362
MACCS_Naive Bayes	0.6828	0.4490	0.8021	0.7292	0.2637
MACCS_Classification Tree	0.7034	0.5306	0.7917	0.6622	0.3275
Pubchem_kNN	0.7655	0.5918	0.8542	0.7908	0.4619
Pubchem_SVM	0.7241	0.3469	0.9167	0.7580	0.3301
Pubchem_Random Forest	0.7586	0.2857	1.0000	0.7765	0.4576
Pubchem_Naive Bayes	0.6207	0.4694	0.6979	0.6682	0.1650
Pubchem_Classification Tree	0.6897	0.5306	0.7708	0.6700	0.3030
SubFP_kNN	0.7103	0.5918	0.7708	0.8055	0.3592
SubFP_SVM	0.7241	0.2653	0.9583	0.7722	0.3288
SubFP_Random Forest	0.7241	0.2245	0.9792	0.6848	0.3372
SubFP_Naive Bayes	0.6138	0.4286	0.7083	0.6437	0.1369
SubFP_Classification Tree	0.6897	0.5102	0.7812	0.6400	0.2962
Threshold=50 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.6345	0.7419	0.4423	0.6318	0.1888
Estate_SVM	0.6759	0.8925	0.2885	0.6705	0.2297
Estate_Random Forest	0.6069	0.8172	0.2308	0.6380	0.0575
Estate_Naive Bayes	0.6276	0.7849	0.3462	0.6203	0.1430
Estate_Classification Tree	0.6483	0.7634	0.4423	0.5985	0.2133
Extend_kNN	0.6552	0.7204	0.5385	0.6721	0.2568
Extend_SVM	0.6138	0.8817	0.1346	0.6262	0.0238
Extend_Random Forest	0.6414	0.8280	0.3077	0.6546	0.1569
Extend_Naive Bayes	0.5793	0.7634	0.2500	0.4642	0.0151
Extend_Classification Tree	0.6207	0.7097	0.4615	0.5804	0.1720
FP_kNN	0.6552	0.7097	0.5577	0.6683	0.2634
FP_SVM	0.6276	0.8817	0.1731	0.6337	0.0762
FP_Random Forest	0.6552	0.8065	0.3846	0.6827	0.2084
FP_Naive Bayes	0.5517	0.7419	0.2115	0.4844	-0.0521
FP_Classification Tree	0.6276	0.7097	0.4808	0.5734	0.1904
MACCS_kNN	0.6414	0.7742	0.4038	0.6536	0.1882
MACCS_SVM	0.6621	0.8710	0.2885	0.6420	0.1964

MACCS_Random Forest	0.6621	0.8387	0.3462	0.6308	0.2115
MACCS_Naive Bayes	0.5379	0.6774	0.2885	0.5167	-0.0354
MACCS_Classification Tree	0.6621	0.7957	0.4231	0.6048	0.2330
Pubchem_kNN	0.6483	0.8065	0.3654	0.6798	0.1890
Pubchem_SVM	0.6276	0.8602	0.2115	0.5860	0.0926
Pubchem_Random Forest	0.6414	0.8280	0.3077	0.6094	0.1569
Pubchem_Naive Bayes	0.4966	0.6129	0.2885	0.4711	-0.0991
Pubchem_Classification Tree	0.6552	0.7849	0.4231	0.5699	0.2199
SubFP_kNN	0.6552	0.7634	0.4615	0.6469	0.2318
SubFP_SVM	0.6483	0.8387	0.3077	0.6610	0.1713
SubFP_Random Forest	0.6828	0.8495	0.3846	0.6857	0.2650
SubFP_Naive Bayes	0.6138	0.7634	0.3462	0.5719	0.1176
SubFP_Classification Tree	0.7103	0.8495	0.4615	0.6889	0.3392
Threshold=100 mgkgday					
Model	Q	SE	SP	AUC	MCC
Estate_kNN	0.6621	0.8495	0.3269	0.6474	0.2063
Estate_SVM	0.6897	0.9677	0.1923	0.6524	0.2687
Estate_Random Forest	0.6414	0.9570	0.0769	0.6666	0.0712
Estate_Naive Bayes	0.6138	0.8495	0.1923	0.6455	0.0539
Estate_Classification Tree	0.6828	0.9140	0.2692	0.5999	0.2449
Extend_kNN	0.6621	0.8172	0.3846	0.6608	0.2220
Extend_SVM	0.6345	0.9462	0.0769	0.5905	0.0460
Extend_Random Forest	0.5931	0.8817	0.0769	0.5679	-0.0651
Extend_Naive Bayes	0.5655	0.7742	0.1923	0.4272	-0.0392
Extend_Classification Tree	0.6345	0.8387	0.2692	0.5842	0.1294
FP_kNN	0.6345	0.8065	0.3269	0.6441	0.1495
FP_SVM	0.6276	0.9247	0.0962	0.6283	0.0364
FP_Random Forest	0.6552	0.9892	0.0577	0.6010	0.1374
FP_Naive Bayes	0.5655	0.7742	0.1923	0.4434	-0.0392
FP_Classification Tree	0.5724	0.7849	0.1923	0.4704	-0.0269
MACCS_kNN	0.6552	0.8710	0.2692	0.6112	0.1753
MACCS_SVM	0.6483	0.9032	0.1923	0.6183	0.1358
MACCS_Random Forest	0.6276	0.9140	0.1154	0.6714	0.0477
MACCS_Naive Bayes	0.5448	0.7204	0.2308	0.4944	-0.0532
MACCS_Classification Tree	0.5793	0.7849	0.2115	0.4773	-0.0041
Pubchem_kNN	0.6414	0.8710	0.2308	0.6641	0.1313
Pubchem_SVM	0.6483	0.9462	0.1154	0.5773	0.1116
Pubchem_Random Forest	0.6207	0.9032	0.1154	0.5701	0.0293
Pubchem_Naive Bayes	0.5241	0.6989	0.2115	0.4815	-0.0968
Pubchem_Classification Tree	0.6138	0.8387	0.2115	0.5693	0.0628
SubFP_kNN	0.6690	0.8602	0.3269	0.6295	0.2216
SubFP_SVM	0.6828	0.9570	0.1923	0.6308	0.2424

SubFP_Random Forest	0.6345	0.9032	0.1538	0.5949	0.0851
SubFP_Naive Bayes	0.6552	0.8602	0.2885	0.6532	0.1806
SubFP_Classification Tree	0.6759	0.8925	0.2885	0.7093	0.2297