

Supplementary Information 1

Name or Code	PAHIV	A _{HIV-IP}	Series	Smiles
CHEMBL258205	CCR2	1	Training	<chem>OCC(C1CCN(CC1)C(=O)\C=C\c2ccc(Cl)c(Cl)c2)N3CCC(CC3)c4c[nH]e5ccccc45</chem>
CHEMBL1090893	CCR2	1	Prediction	<chem>CCN(C(C)C)[C@@H]1CC[C@@H]([C@H](CS(=O)(=O)c2ccccc2)C1)N3CC[C@H](NC(=O)c4cccc(c4)C(F)(F)F)C3=O</chem>
CHEMBL497202	CCR2	1	Training	<chem>CSc1ccc(cc1)S(=O)(=O)C[C@@H]2C[C@@H](CC[C@@H]2NC(=O)CNC(=O)c3cccc(c3)C(F)(F)F)N(C)C</chem>
CHEMBL1092678	CCR2	1	Training	<chem>CC(C)N(C)[C@@H]1CC[C@@H]([C@H](CS(=O)(=O)c2ccc(C)cc2)C1)N3CC[C@H](NC(=O)c4cccc(c4)C(F)(F)F)C3=O</chem>
CHEMBL230281	CCR2	1	Training	<chem>CNC(=O)Nc1nc(cs1)[C@H](CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL256301	CCR2	1	Prediction	<chem>CS(=O)(=O)Nc1ccc2[nH]cc(C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5ccc(Cl)c(Cl)c5)c2c1</chem>
CHEMBL257191	CCR2	1	Training	<chem>OCC(C1CCN(CC1)C(=O)\C=C\c2cc(F)cc(F)c2)N3CCC(CC3)c4c[nH]e5ccccc45</chem>
CHEMBL389771	CCR2	1	Training	<chem>CNC(=O)Nc1nc(cs1)[C@H](CCN2CCC3(CC2)C=Cc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL1092941	CCR2	1	Training	<chem>CC(C)N(C)[C@@H]1CC[C@@H]([C@H](CS(=O)(=O)c2ccccc2)C1)N3CC[C@H](NC(=O)c4cc(F)cc(c4)C(F)(F)F)C3=O</chem>
CHEMBL1091604	CCR2	1	Prediction	<chem>CC(C)N(C)[C@@H]1CC[C@H](NC(=O)CNC(=O)c2ccccc2)C(F)(F)F[C@H](CS(=O)(=O)c3ccccc3)C1</chem>
CHEMBL495924	CCR2	1	Training	<chem>CSc1ccc(CNC2CCN(C)CC2NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F)cc1</chem>
CHEMBL1290636	CCR2	1	Training	<chem>CCO[C@H]1CN(C[C@@H]1NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@@H]3CC[C@@H](CC3)c4ccccc4</chem>
CHEMBL403889	CCR2	1	Training	<chem>Nc1ccc2[nH]cc(C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5cc(F)c(F)c(F)c5)c2c1</chem>
CHEMBL254772	CCR2	1	Prediction	<chem>CS(=O)(=O)Nc1ccc2[nH]cc(C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5cc(F)c(F)c(F)c5)c2c1</chem>
CHEMBL404904	CCR2	1	Training	<chem>OCC(C1CCN(CC1)C(=O)\C=C\c2cc(F)c(F)c(F)c2)N3CCC(CC3)c4c[nH]e5ccc(O)cc45</chem>
CHEMBL1091605	CCR2	1	Training	<chem>CC(C)N(C)[C@@H]1CC[C@@H]([C@H](CS(=O)(=O)c2ccccc2)C1)N3CC[C@H](NC(=O)c4cccc(c4)C(F)(F)F)C3=O</chem>
CHEMBL226066	CCR2	1	Training	<chem>C[C@H]1CN(CC[C@@H]12C=Cc3ccccc23)[C@@H]4CC[C@@H](C)(C4)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL397749	CCR2	1	Prediction	<chem>NC(=N)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(c(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL229316	CCR2	1	Training	<chem>C[C@H]1CN(CCC(C(=O)NCc2cc(cc(c2)C(F)(F)F)C(F)(F)F)c3sc(N)n3)CCC14C=Cc5ccccc45</chem>
CHEMBL502247	CCR2	1	Training	<chem>CSc1ccc(cc1)S(=O)(=O)C[C@@H]2C[C@@H](CC[C@@H]2NC(=O)CNC(=O)c3cccc(c3)C(F)(F)F)N(C)C(C)C</chem>
CHEMBL502793	CCR2	1	Training	<chem>CCN(CC)[C@@H]1CC[C@H](NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@H](CS(=O)(=O)c3ccc(SC)cc3)C1</chem>
CHEMBL397948	CCR2	1	Prediction	<chem>CC(=O)Nc1nc(cs1)[C@H](CCN2CCC3(CC2)C=Cc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL226065	CCR2	1	Training	<chem>C[C@H]1CN(CC[C@@H]12C=Cc3ccccc23)[C@@H]4CC[C@@H](C4)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL526752	CCR2	1	Training	<chem>CSc1ccc(cc1)S(=O)(=O)C[C@@H]2C[C@@H](CC[C@@H]2N</chem>

				<chem>C(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F)N(C)C(C)C</chem>
CHEMBL272369	CCR2	1	Training	<chem>CC(C)[C@@]1(CC[C@H](C1)N2CC[C@@]3(C=Cc4ccccc34)[C@@H](C)C2)C(=O)NCc5cc(F)cc(c5)C(F)(F)F</chem>
CHEMBL388487	CCR2	1	Prediction	<chem>CC(=O)Nc1nc(cs1)C(CCN2CCC3(CC2)C=Cc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL397996	CCR2	1	Training	<chem>CC(=O)Nc1nc(cs1)[C@H](CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL230790	CCR2	1	Training	<chem>CC(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccc(F)cc3)C(=O)NCc4c(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL496343	CCR2	1	Training	<chem>CSc1ccc(cc1)C(=O)NC2CCN(C)CC2NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F</chem>
CHEMBL402442	CCR2	1	Prediction	<chem>OCC(C1CCN(CC1)C(=O)\C=C\c2ccc(F)c(Br)c2)N3CCC(CC3)c4c[nH]c5ccccc45</chem>
CHEMBL255302	CCR2	1	Training	<chem>CC(=O)Nc1ccc2[nH]cc(C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5cc(F)c(F)c(F)c5)c2c1</chem>
CHEMBL502516	CCR2	1	Training	<chem>CSc1ccc(cc1)S(=O)(=O)C[C@@H]2C[C@@H](CC[C@@H]2N)C(=O)CNC(=O)c3cccc(c3)C(F)(F)F)NC(C)C</chem>
CHEMBL437552	CCR2	1	Training	<chem>CN(C)C(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL1289203	CCR2	1	Prediction	<chem>CCO[C@H]1CN(C[C@@H]1NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@@H]3CC[C@@](O)(CC3)c4ccc(C)cc4</chem>
CHEMBL1289083	CCR2	1	Training	<chem>CCO[C@H]1CN(C[C@@H]1NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@@H]3CC[C@@](O)(CC3)c4ccccc4</chem>
CHEMBL505722	CCR2	1	Training	<chem>CSc1ccc(cc1)C(=O)NC2CC(CCC2NC(=O)CNC(=O)c3cccc(c3)C(F)(F)F)NC(=O)OCc4ccccc4</chem>
CHEMBL481010	CCR2	1	Training	<chem>CSc1ccc(CNC2CC(CCC2NC(=O)CNC(=O)c3cccc(c3)C(F)(F)F)N(C)C)cc1</chem>
CHEMBL387583	CCR2	1	Prediction	<chem>COC(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL450231	CCR2	1	Training	<chem>CSc1ccc(cc1)S(=O)(=O)C[C@@H]2CCCC[C@@H]2NC(=O)NC(=O)c3cc(ccc3NC(=O)N4CCOCC4)C(F)(F)F</chem>
CHEMBL1681819	CCR2	1	Training	<chem>CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3C[C@@H]4C[C@H]3CN4C(=O)OC(C)(C)C</chem>
CHEMBL1290637	CCR2	1	Training	<chem>CCCO[C@H]1CN(C[C@@H]1NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@@H]3CC[C@@H](CC3)c4ccccc4</chem>
CHEMBL230166	CCR2	1	Prediction	<chem>CNC(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL388486	CCR2	1	Training	<chem>CC(=O)Nc1nc(cs1)C(CCN2CCC(CC2)n3cnc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL438304	CCR2	1	Training	<chem>C[C@H]1CN(CCC(C(=O)NCc2cc(cc(c2)C(F)(F)F)C(F)(F)F)c3cs(c(NC(=O)C)n3)CCC14C=Cc5ccccc45</chem>
CHEMBL1683074	CCR2	1	Training	<chem>CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4cc(ccn4)C(F)(F)F</chem>
CHEMBL521275	CCR2	1	Prediction	<chem>CN(C)C1CCC(NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)C(C1)NCc3ccc4[nH]ccc4c3</chem>
CHEMBL1684712	CCR2	1	Training	<chem>CC(C)[C@@]1(CC[C@H](C1)NC2CCOCC2F)C(=O)N3C[C@@H]4C[C@H]3CN4C(=O)OC5CCCC5</chem>
CHEMBL1683059	CCR2	1	Training	<chem>CC(C)[C@@]1(CC[C@H](C1)N[C@H]2CCOC[C@H]2C)C(=O)N3CCN(CC3)c4ccccc4)C(F)(F)F</chem>
CHEMBL256629	CCR2	1	Training	<chem>Cc1ccc(CN2CC[C@H](C2)NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F</chem>

				F)c(C)c1
CHEMBL1683190	CCR2	1	Prediction	CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@@](CC(F)(F)F)(C2)C(=O)N3CCN(CC3)c4cc(ccn4)C(F)(F)F
CHEMBL1684706	CCR2	1	Training	CC(C)[C@@]1(CC[C@H](C1)NC2CCOCC2F)C(=O)N3C[C@@H]4C[C@H]3CN4C(=O)OC(C)C(F)(F)F
CHEMBL497788	CCR2	1	Training	CCCN1CCC(NC2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F
CHEMBL230684	CCR2	1	Training	CCC(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F
CHEMBL397997	CCR2	1	Prediction	COC(=O)Nc1nc(cs1)[C@H](CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F
CHEMBL1684694	CCR2	1	Training	CC(C)[C@@]1(CC[C@H](C1)NC2CCOCC2)C(=O)N3C[C@@H]4C[C@H]3CN4C(=O)OC(C)C(F)(F)F
CHEMBL1092748	CCR2	1	Training	CC(C)N(C)[C@@H]1CC[C@H]([C@H](CS(=O)(=O)c2ccccc2)C1)N3CC[C@H](NC(=O)c4cc(cc(c4)C(F)(F)F)C(F)(F)F)C3=O
CHEMBL496630	CCR2	1	Training	CN[C@@H]1CC[C@H](NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@H](CS(=O)(=O)c3ccc(SC)cc3)C1
CHEMBL502513	CCR2	1	Prediction	CCCN1CCC(NC2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(ccc3N)C(=O)NC(C)C(F)(F)F
CHEMBL516224	CCR2	1	Training	CSc1ccc(cc1)C(=O)NC2CCC(CC2NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F)NC(C)C
CHEMBL447937	CCR2	1	Training	CSc1ccc(cc1)S(=O)(=O)C[C@@H]2CCCC[C@@H]2NC(=O)CN(C(=O)c3cc(ccc3NC(=O)N4CCCC4)C(F)(F)F
CHEMBL230794	CCR2	1	Training	FC(F)(F)c1cc(CNC(=O)C(CCN2CCC(CC2)c3ccccc3)c4csc(NC(=O)C5CC5)n4)cc(c1)C(F)(F)F
CHEMBL397747	CCR2	1	Prediction	FC(F)(F)c1cc(CNC(=O)C(CCN2CCC(CC2)c3ccccc3)c4csc(NC(=O)n4)cc(c1)C(F)(F)F
CHEMBL441856	CCR2	1	Training	C[C@H]1CN(CC[C@@H](C2CC2)C(=O)NCc3cc(cc(c3)C(F)(F)F)C(F)(F)F)CC[C@@]14C=Cc5ccccc45
CHEMBL255478	CCR2	1	Training	OCC(C1CCN(CC1)C(=O)\C=C\c2cc(F)c(F)c(F)c2)N3CCC(CC3)c4c[nH]c5ccccc45
CHEMBL257062	CCR2	1	Training	Nc1ccc(cc1C(=O)NCC(=O)N[C@@H]2CCN(Cc3ccc(Cl)c(N)c3)C2)C(F)(F)F
CHEMBL1684702	CCR2	1	Prediction	CC(C)[C@@]1(CC[C@H](C1)NC2CCOCC2F)C(=O)N3C[C@@H]4C[C@H]3CN4C(=O)OC(C)(C)C
CHEMBL526859	CCR2	1	Training	CCCCN1CCC(NC(=O)c2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F
CHEMBL1684713	CCR2	1	Training	CC(C)COC(=O)N1C[C@@H]2C[C@H]1CN2C(=O)[C@]3(CC[C@H](C3)NC4CCOCC4F)C(C)C
CHEMBL1782377	CCR2	1	Training	CO[C@@H]1COCC[C@@H]1N(C)[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4cc(ccn4)C(F)(F)F
CHEMBL1683063	CCR2	1	Prediction	CC[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4ccccc4)C(F)(F)F
CHEMBL402532	CCR2	1	Training	C[C@H]1CN(CC[C@@]12C=Cc3ccccc23)[C@@H]4CC[C@@]5(CCO[C@H]5OCc6cc(F)cc(c6)C(F)(F)F)C4
CHEMBL495368	CCR2	1	Training	CC(C)[C@@]1(CC[C@H](C1)NC2CCOCC2)C(=O)NCc3cc(cc(c3)C(F)(F)F)C(F)(F)F
CHEMBL481009	CCR2	1	Training	CSc1ccc(cc1)C(=O)NC2CC(N)CCC2NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F
CHEMBL1684683	CCR2	1	Prediction	CC(C)[C@@]1(CC[C@H](C1)NC2CCOCC2)C(=O)N3C[C@@H]

				<chem>]4C[C@H]3CN4C(=O)OC(C)(C)C</chem>
CHEMBL391459	CCR2	1	Training	<chem>OC(=O)C(C1CCN(CC1)C(=O)\C=C\c2cc(F)c(F)c(F)c2)N3CCC(CC3)c4c[nH]c5ccccc45</chem>
CHEMBL1289316	CCR2	1	Training	<chem>CCO[C@H]1CN(C[C@@H]1NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@@H]3CC[C@@H](O)(CC3)c4ccc5OCOc5c4</chem>
CHEMBL273083	CCR2	1	Training	<chem>CSc1ccc(cc1)C(=O)N[C@@H]2CCCC[C@@H]2NC(=O)CNC(=O)c3cc(ccc3NC(=O)NC(C)C)C(F)(F)F</chem>
CHEMBL389888	CCR2	1	Prediction	<chem>CC(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(c(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL270435	CCR2	1	Training	<chem>COc1ccc(CN2CC[C@H](C2)NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F)cc1N</chem>
CHEMBL492569	CCR2	1	Training	<chem>CC(C)[C@]1(CC[C@@H](C1)NC2CCOCC2C(F)(F)F)C(=O)NCc3cc(cc(c3)C(F)(F)F)C(F)(F)F</chem>
CHEMBL522688	CCR2	1	Training	<chem>CCC1COCCC1N[C@H]2CC[C@](C2)(C(C)C)C(=O)NCc3cc(cc(c3)C(F)(F)F)C(F)(F)F</chem>
CHEMBL1683067	CCR2	1	Prediction	<chem>CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4ccccc4)C(F)(F)F</chem>
CHEMBL388868	CCR2	1	Training	<chem>CNC(=O)Nc1nc(cs1)[C@@H](CCN2CCC3(CC2)C=Cc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL499467	CCR2	1	Training	<chem>CSc1ccc(cc1)S(=O)(=O)C[C@@H]2CCCC[C@@H]2NC(=O)CNC(=O)c3cc(ccc3NC(=O)N4CCC4)C(F)(F)F</chem>
CHEMBL255499	CCR2	1	Training	<chem>COc1ccc2[nH]cc(C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5cc(F)c(F)c(F)c5)c2c1</chem>
CHEMBL257173	CCR2	1	Prediction	<chem>OCC(C1CCN(CC1)C(=O)\C=C\c2ccc(F)c(F)c2)N3CCC(CC3)c4c[nH]c5ccccc45</chem>
CHEMBL271725	CCR2	1	Training	<chem>Cc1ccc(CN2CC[C@H](C2)NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F)cc1N</chem>
CHEMBL496959	CCR2	1	Training	<chem>CCCN1CCC(NCc2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(N)cc(c3)C(F)(F)F</chem>
CHEMBL496344	CCR2	1	Training	<chem>CCCN1CCC(NC(=O)c2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(N)cc(c3)C(F)(F)F</chem>
CHEMBL497577	CCR2	1	Prediction	<chem>CSc1ccc(CNC2CCNCC2NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F)cc1</chem>
CHEMBL388867	CCR2	1	Training	<chem>CC(=O)Nc1nc(cs1)[C@@H](CCN2CCC3(CC2)C=Cc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL452509	CCR2	1	Training	<chem>CCN(CC)C(=O)Nc1ccc(cc1C(=O)NCC(=O)N[C@H]2CCCC[C@H]2CS(=O)(=O)c3ccc(SC)cc3)C(F)(F)F</chem>
CHEMBL257628	CCR2	1	Training	<chem>COc1ccc2[nH]cc(C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5ccc(Cl)c(Cl)c5)c2c1</chem>
CHEMBL495151	CCR2	1	Prediction	<chem>CC(C)[C@@]1(CC[C@@H](C1)NC2C(C)COCC2C)C(=O)NCc3cc(cc(c3)C(F)(F)F)C(F)(F)F</chem>
CHEMBL396517	CCR2	1	Training	<chem>Nc1nc(cs1)C(CCN2CCC3(CC2)C=Cc4ccccc34)C(=O)NCc5cc(cc(c5)C(F)(F)F)C(F)(F)F</chem>
CHEMBL1782376	CCR2	1	Training	<chem>CC(C)[C@@]1(CC[C@H](C1)NC2C3CCCC2COC3)C(=O)N4CCN(CC4)c5cc(ccn5)C(F)(F)F</chem>
CHEMBL395721	CCR2	1	Training	<chem>CC(C)C(=O)Nc1nc(cs1)C(CCN2CCC(CC2)c3ccccc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F</chem>
CHEMBL1290412	CCR2	1	Prediction	<chem>O[C@H]1CN(C[C@@H]1NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)[C@@H]3CC[C@@H](CC3)c4ccccc4</chem>
CHEMBL226017	CCR2	1	Training	<chem>FC(F)(F)c1cc(CNC(=O)[C@H]2CC[C@H](C2)N3CCC4(CC3)C=</chem>

				Cc5ccccc45)cc(c1)C(F)(F)F
CHEMBL480621	CCR2	1	Training	CN(C)C1CCC(NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)C(C1)NCc3ccc(NC(=O)C)cc3
CHEMBL494540	CCR2	1	Training	CCCC1COCCC1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)NCc3cc(c(c3)C(F)(F)F)C(F)(F)F
CHEMBL526091	CCR2	1	Prediction	CCCCN1CCC(NC2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(ccc3N)C(F)(F)F
CHEMBL380258	CCR2	1	Training	CN(C)CCCN(C)[C@H](C(=O)NCc1cc(cc(c1)C(F)(F)F)C(F)(F)F)c2cccc2
CHEMBL502795	CCR2	1	Training	CSc1ccc(cc1)S(=O)(=O)C[C@@H]2CCCC[C@@H]2NC(=O)CNC(=O)c3ccc(ccc3NC(=O)N(C)C)C(F)(F)F
CHEMBL1782572	CCR2	1	Training	CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4cc(cnn4)C(F)(F)F
CHEMBL451340	CCR2	1	Prediction	CSc1ccc(cc1)S(=O)(=O)C[C@@H]2C[C@@H](CC[C@@H]2NC(=O)CNC(=O)c3cccc(c3)C(F)(F)F)NCc4cccc4
CHEMBL1684700	CCR2	1	Training	CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3C[C@@H]4C[C@H]3CN4C(=O)C5CCCC5
CHEMBL449672	CCR2	1	Training	CCCN1CCC(NC2ccc(SC)cc2)C(C1)NC(=O)CNC(=O)c3cc(ccc3NC(=O)N4CCCC4)C(F)(F)F
CHEMBL1782573	CCR2	1	Training	CO[C@@H]1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4ncc(s4)C(F)(F)F
CHEMBL215020	CCR2	1	Prediction	C[C@H]1CN(CC[C@H](CC2CC2)C(=O)NCc3cc(cc(c3)C(F)(F)F)C(F)(F)F)CC[C@@]14C=Cc5ccccc45
CHEMBL257385	CCR2	1	Training	OCC(C1CCN(CC1)C(=O)\C=C\c2cccc(Br)c2)N3CCC(CC3)c4c[nH]c5ccccc45
CHEMBL271828	CCR2	1	Training	NS(=O)(=O)c1ccc(cc1)C(=O)N[C@@H]2CCCC[C@@H]2NC(=O)CNC(=O)c3ccc(ccc3NC(=O)C4CCCC4)C(F)(F)F
CHEMBL438353	CCR2	1	Training	OCC(C1CCN(CC1)C(=O)Nc2ccc(Cl)c(Cl)c2)N3CCC(CC3)c4c[nH]c5ccccc45
CHEMBL230727	CCR2	1	Prediction	Nc1nc(cs1)C(CCN2CCC(CC2)c3ccc(F)cc3)C(=O)NCc4cc(cc(c4)C(F)(F)F)C(F)(F)F
CHEMBL1782578	CCR2	1	Training	CCC1COCC[C@@H]1N[C@@H]2CC[C@](C2)(C(C)C)C(=O)N3CCN(CC3)c4cc(ccn4)C(F)(F)F
CHEMBL481202	CCR2	1	Training	CN(C)C1CCC(NC(=O)CNC(=O)c2cccc(c2)C(F)(F)F)C(C1)NCc3ccc(C)cc3
CHEMBL209411	CCR2	1	Training	CN(C)CC\C=N[C@H](C(=O)NCc1cc(cc(c1)C(F)(F)F)C(F)(F)F)c2cccc2
CHEMBL403581	CCR2	1	Prediction	OCC(C1CCN(CC1)C(=O)Nc2ccc(Cl)c(Cl)c2)N3CCC(CC3)c4c[nH]c5ccc(cc45)C(=O)O
CHEMBL255500	CCR2	1	Training	COc1cccc2c(c[nH]c12)C3CCN(CC3)C(CO)C4CCN(CC4)C(=O)\C=C\c5cc(F)c(F)c(F)c5
CHEMBL403250	CCR2	1	Training	OCC(C1CCN(CC1)C(=O)\C=C\c2cccc(c2)C(F)(F)F)N3CCC(CC3)c4c[nH]c5ccccc45
CHEMBL257768	CCR2	1	Training	OC[C@@H](C1CCN(CC1)C(=O)\C=C\c2cc(F)c(F)c(F)c2)N3CC(C(CC3)c4c[nH]c5ccccc45
Acetofenac	CCR2	-1	Prediction	Clc2cccc(Cl)c2Nc1cccc1CC(=O)OCC(=O)O
Acetaminophen	CCR2	-1	Training	Oc1ccc(NC(C)=O)cc1
Acetazolamide	CCR2	-1	Training	O=S(N)(=O)c1nnc(NC(C)=O)s1
Acetophenazine	CCR2	-1	Training	CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4cccc4Sc3cc2

Amantadine	CCR2	-1	Prediction	<chem>NC13CC2CC(CC(C1)C2)C3</chem>
Ambenonium	CCR2	-1	Training	<chem>Clc2ccccc2C[N+](CC)(CC)CCNC(=O)C(=O)NCC[N+](Cc1ccccc1Cl)(CC)CC</chem>
Amineptine	CCR2	-1	Training	<chem>O=C(O)CCCCCNC2c3ccccc3CCc1ccccc12</chem>
Amiodarone	CCR2	-1	Training	<chem>CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC</chem>
Amitriptyline	CCR2	-1	Prediction	<chem>CN(C)CC\C=C\c3ccccc3CCc2ccccc12</chem>
Aprobarbital	CCR2	-1	Training	<chem>O=C1NC(=O)NC(=O)C1(CC=C)C(C)C</chem>
Artane	CCR2	-1	Training	<chem>OC(CC1CCCCC1)(c2ccccc2)C3CCCCC3</chem>
Aspirin	CCR2	-1	Training	<chem>O=C(C)Oc1ccccc1C(=O)O</chem>
Atenolol	CCR2	-1	Prediction	<chem>CC(C)NCC(O)COc1ccc(cc1)CC(N)=O</chem>
Atropine	CCR2	-1	Training	<chem>CN3C1CCC3C[C@@H](C1)OC(=O)C(CO)c2ccccc2</chem>
Baclofen	CCR2	-1	Training	<chem>Clc1ccc(cc1)C(CN)CC(=O)O</chem>
Beclomethasone	CCR2	-1	Training	<chem>OCC(=O)[C@@]4(O)[C@@H](C)CC3C2CCC1=CC(=O)C=C[C@@]1(C)[C@@]2(Cl)[C@@H](O)C[C@@]34C</chem>
Benzonatate	CCR2	-1	Prediction	<chem>O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NC(C)C)cc1</chem>
Biperiden	CCR2	-1	Training	<chem>OC(CC1CCCCC1)(c2ccccc2)C4CC3C=CC4C3</chem>
Bromocriptine	CCR2	-1	Training	<chem>BrC3nc2cccc1C4=C[C@H](CN(C)C4Cc3c12)C(=O)N[C@@]7(O[C@]6(O)N([C@@H](CC(C)C)C(=O)N5CCCC56)C7=O)C(C)C</chem>
Bucizine	CCR2	-1	Training	<chem>CC(C)(C)c1ccc(cc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Budesonide	CCR2	-1	Prediction	<chem>OCC(=O)[C@@]53OC(O[C@@H]5CC2C1CCC4=CC(=O)C=C[C@@]4(C)C1[C@@H](O)C[C@@]23C)CCC</chem>
Buprenorphine	CCR2	-1	Training	<chem>CC(C)(C)C(C)(O)[C@H]1C[C@]75CC[C@]1(OC)[C@@H]2Oc4c(O)ccc3C[C@H]7[N@](CC[C@]25c34)CC6CCC6</chem>
Caffeine	CCR2	-1	Training	<chem>O=C2c1n(C)ncn1N(C)C(=O)N2C</chem>
Cantil	CCR2	-1	Training	<chem>O=C(OC1CCC[N+](C)(C)C1)C(O)(c2ccccc2)c3ccccc3</chem>
Carbachol	CCR2	-1	Prediction	<chem>C[N+](C)(C)CCOC(=O)N</chem>
Carbamazepine	CCR2	-1	Training	<chem>NC(=O)N2c3ccccc3C=Cc1ccccc12</chem>
Carisoprodol	CCR2	-1	Training	<chem>O=C(NC(C)C)OCC(C)(COC(=O)N)CCC</chem>
Carvedilol	CCR2	-1	Training	<chem>COc4ccccc4OCCNCC(O)COc2ccccc3nc1ccccc1c23</chem>
Cefoperazone	CCR2	-1	Prediction	<chem>O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O</chem>
Chloral hydrate	CCR2	-1	Training	<chem>ClC(Cl)(Cl)C(O)O</chem>
Chlordiazepoxide	CCR2	-1	Training	<chem>Clc1ccc2N=C(C[N+](O-))=C(c2c1)c3ccccc3)NC</chem>
Chlorpropamide	CCR2	-1	Training	<chem>O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1</chem>
Chlorthalidone	CCR2	-1	Prediction	<chem>NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2ccccc23</chem>
Clidinium	CCR2	-1	Training	<chem>OC(c1ccccc1)(c2ccccc2)C(=O)OC4C[N+](C)CCC4CC3</chem>
Clobazam	CCR2	-1	Training	<chem>Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3ccccc3</chem>
Clofazimine	CCR2	-1	Training	<chem>Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5</chem>
Clomipramine	CCR2	-1	Prediction	<chem>CN(C)CCCN2c3ccccc3CCc1ccc(Cl)cc12</chem>
Clonidine	CCR2	-1	Training	<chem>Clc2ccccc(Cl)c2N=C1/NCCN1</chem>
Codeine	CCR2	-1	Training	<chem>COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23</chem>
Colchicine	CCR2	-1	Training	<chem>CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12</chem>

Cyclizine	CCR2	-1	Prediction	CN1CCN(CC1)C(c2cccc2)c3ccccc3
Cyclosporin	CCR2	-1	Training	CC(C\C=C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C
Dextropropoxyphene	CCR2	-1	Training	CN(C)CC(C)C(OC(=O)CC)(Cc1cccc1)c2cccc2
Diazepam	CCR2	-1	Training	C1c1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3
Diflucortolone	CCR2	-1	Prediction	OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C
Dimercaprol	CCR2	-1	Training	OCC(S)CS
Diphenhydramine	CCR2	-1	Training	CN(C)CCOC(c1cccc1)c2cccc2
Diphenidol	CCR2	-1	Training	OC(CCCN1CCCC1)(c2cccc2)c3ccccc3
Dobutamine	CCR2	-1	Prediction	Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O
Dofetilide	CCR2	-1	Training	CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O
Domperidone	CCR2	-1	Training	C1c4cc5NC(=O)N(C3CCN(CCCN1c2cccc2NC1=O)CC3)c5cc4
Dopamine	CCR2	-1	Training	Oc1ccc(CCN)cc1O
Doxazosin	CCR2	-1	Prediction	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4
Doxepin	CCR2	-1	Training	CN(C)CC\C=C1/c3cccc3OCc2cccc12
Dronabinol	CCR2	-1	Training	CCCCCc3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3
Droxicam	CCR2	-1	Training	O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O
Entacapone	CCR2	-1	Prediction	Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+])([O-])=O)c1O
Epinephrine	CCR2	-1	Training	Oc1ccc(cc1O)[C@@H](O)CNC
Eprosartan	CCR2	-1	Training	OC(=O)C(/Cc1cccs1)=C/c3enc(CCCC)n3Cc2ccc(cc2)C(=O)O
Ergotamine	CCR2	-1	Training	CN2C[C@@H](C=C1c3cccc4ncc(CC12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O
Ethosuximide	CCR2	-1	Prediction	CC1(CC)CC(=O)NC1=O
Fentanyl	CCR2	-1	Training	CCC(=O)N(C2CCN(CCc1cccc1)CC2)c3ccccc3
Fexofenadine	CCR2	-1	Training	O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4
Flecainide	CCR2	-1	Training	FC(F)(F)COc2cc(C(=O)NCC1CCCCN1)c(OCC(F)(F)F)cc2
Flunarizine	CCR2	-1	Prediction	Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4
Flunisolide	CCR2	-1	Training	OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C
Fluoxetine	CCR2	-1	Training	FC(F)(F)c2ccc(OC(CCNC)c1cccc1)cc2
Fluvoxamine	CCR2	-1	Training	FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN
Gabapentin	CCR2	-1	Prediction	NCC1(CC(=O)O)CCCC1
Gestodene	CCR2	-1	Training	O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2
Glutethimide	CCR2	-1	Training	CCC1(CCC(=O)NC1=O)c2cccc2
Glycopyrrolate	CCR2	-1	Training	C[N+]3(C)CCC(OC(=O)C(O)(c1cccc1)C2CCCC2)C3
Guanadrel	CCR2	-1	Prediction	N=C(N)NCC2COC1(CCCCC1)O2
Halofantrine	CCR2	-1	Training	CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F
Haloperidol	CCR2	-1	Training	Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3
Halothane	CCR2	-1	Training	BrC(Cl)C(F)(F)F

Hydromorphone	CCR2	-1	Prediction	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	CCR2	-1	Training	<chem>Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	CCR2	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C</chem>
Indomethacin	CCR2	-1	Training	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	CCR2	-1	Prediction	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	CCR2	-1	Training	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	CCR2	-1	Training	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	CCR2	-1	Training	<chem>CNC1(CCCCC1=O)c2ccccc2Cl</chem>
Labetalol	CCR2	-1	Prediction	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2</chem>
Lacidipine	CCR2	-1	Training	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	CCR2	-1	Training	<chem>Clc1cccc(c1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	CCR2	-1	Training	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCN(C(=O)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2ccccc23)NC(=O)C(Cc4ennc4)NC(=O)C5CCC(=O)N5</chem>
Levodopa	CCR2	-1	Prediction	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>
Lidocaine	CCR2	-1	Training	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	CCR2	-1	Training	<chem>Clc3cc4CCc1cccn1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	CCR2	-1	Training	<chem>CNCCCC24CCC(c1ccccc12)c3ccccc34</chem>
Meclizine	CCR2	-1	Prediction	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Medroxyprogesterone	CCR2	-1	Training	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	CCR2	-1	Training	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	CCR2	-1	Training	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	CCR2	-1	Prediction	<chem>C[C@H](NC)Cc1ccccc1</chem>
Methantheline	CCR2	-1	Training	<chem>CC[N+](C)(CC)CCOC(=O)C1c3ccccc3Oc2ccccc12</chem>
Methocarbamol	CCR2	-1	Training	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	CCR2	-1	Training	<chem>ClC(Cl)C(F)(F)OC</chem>
Methscopolamine	CCR2	-1	Prediction	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+]3(C)C</chem>
Methylphenidate	CCR2	-1	Training	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	CCR2	-1	Training	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3ccccc1c23)N(C)C4</chem>
Metoclopramide	CCR2	-1	Training	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	CCR2	-1	Prediction	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	CCR2	-1	Training	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	CCR2	-1	Training	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	CCR2	-1	Training	<chem>CC(C)(O)c5ccccc5CC[C@@H](SCC1(CC(=O)O)CC1)c2ccccc2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	CCR2	-1	Prediction	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	CCR2	-1	Training	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@@H]45</chem>
Nalmefene	CCR2	-1	Training	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C[N@@]3CC2CC2)c45</chem>
Neostigmine	CCR2	-1	Training	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>

Nifedipine	CCR2	-1	Prediction	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	CCR2	-1	Training	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	CCR2	-1	Training	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	CCR2	-1	Training	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	CCR2	-1	Prediction	<chem>CSC[C@@H]4CC1C(Cc2enc3cccc1c23)N(C4)CCC</chem>
Phenylbutazone	CCR2	-1	Training	<chem>O=C3C(CCCC)C(=O)N(c1cccc1)N3c2ccccc2</chem>
Phenytoin	CCR2	-1	Training	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	CCR2	-1	Training	<chem>Cn2cnc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	CCR2	-1	Prediction	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	CCR2	-1	Training	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	CCR2	-1	Training	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	CCR2	-1	Training	<chem>OC(CCN1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	CCR2	-1	Prediction	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	CCR2	-1	Training	<chem>OC(C(C)NC)c1cccc1</chem>
Pyrantel	CCR2	-1	Training	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>
Quinidine	CCR2	-1	Training	<chem>COc1cc2c(cc1)nc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	CCR2	-1	Prediction	<chem>[O-][N+](=O)C=C(/NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	CCR2	-1	Training	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oe4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	CCR2	-1	Training	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	CCR2	-1	Training	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	CCR2	-1	Prediction	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>
Selegiline	CCR2	-1	Training	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>
Sulfinpyrazone	CCR2	-1	Training	<chem>O=C4C(CCS(=O)c1cccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	CCR2	-1	Training	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>
Terpin	CCR2	-1	Prediction	<chem>C[C@@]1(O)CC[C@@H](CC1)C(C)(C)O</chem>
Tolcapone	CCR2	-1	Training	<chem>Oc1cc(cc([N+](O-)=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranlycypromine	CCR2	-1	Training	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	CCR2	-1	Training	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	CCR2	-1	Prediction	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@@]23C</chem>
Valproic acid	CCR2	-1	Training	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	CCR2	-1	Training	<chem>O=C(O)[C@@H]10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	CCR2	-1	Training	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	CCR2	-1	Prediction	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wytensin	CCR2	-1	Training	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	CCR2	-1	Training	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>

Zileuton	CCR2	-1	Training	<chem>NC(=O)N(O)C(C)c1cc2ccccc2s1</chem>
Zonisamide	CCR2	-1	Prediction	<chem>NS(=O)(=O)Cc2noc1ccccc12</chem>
CHEMBL429323	CCR3	1	Training	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nccn4C</chem>
CHEMBL399495	CCR3	1	Training	<chem>C[C@H](NC(=O)Nc1cccc(c1)c2nnnn2C)[C@@H](O)CN3CCC[C@@H](Cc4ccc(F)cc4)C3</chem>
CHEMBL403838	CCR3	1	Prediction	<chem>CC(C)[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL217987	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2)cc(c1)C(=O)C</chem>
CHEMBL257029	CCR3	1	Training	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(C)cc(c3)c4nnnn4C</chem>
CHEMBL402331	CCR3	1	Training	<chem>CNC(=O)O[C@H](C[C@@H](C)NC(=O)Nc1cccc(c1)c2nnnn2C)N3CCC[C@@H](Cc4ccc(F)cc4)C3</chem>
CHEMBL404585	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)N[C@H](C)C[C@@H](N(C)C)N2CCC[C@@H](Cc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL361369	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3cccc(Cl)c3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL269933	CCR3	1	Training	<chem>CCC[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL404586	CCR3	1	Training	<chem>C[C@H](C[C@@H](NC(=O)C)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL43423	CCR3	1	Prediction	<chem>Cn1nnnc1c2cccc(NC(=O)NCCCN3CCC[C@@H](Cc4ccc(F)cc4)C3)c2</chem>
CHEMBL362179	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@H]2CN(CCc3ccc(F)cc3)CCC2(C)C)cc(c1)c4nnnn4C</chem>
CHEMBL386073	CCR3	1	Training	<chem>CCCN1CC[C@@H](Cc2ccc(F)cc2)C[C@@H]1CCCN(C(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL404618	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(c(c3)C(C)(C)C(=O)O)c4nnnn4C</chem>
CHEMBL270806	CCR3	1	Prediction	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)c4nccs4)c5nccs5</chem>
CHEMBL256068	CCR3	1	Training	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL376737	CCR3	1	Training	<chem>CC(=O)CN1CC[C@@H](Cc2ccc(F)cc2)C[C@@H]1CCCN(C(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL218568	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CCO)cc(c1)C(=O)C</chem>
CHEMBL218262	CCR3	1	Prediction	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CC=C)cc(c1)C(=O)C</chem>
CHEMBL401545	CCR3	1	Training	<chem>CCc1cc(NC(=O)NCCCN2CCC[C@@H](Cc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL270583	CCR3	1	Training	<chem>CC[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL257293	CCR3	1	Training	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)c4nnnn4C)C(C)C</chem>
CHEMBL363840	CCR3	1	Prediction	<chem>Cn1nnnc1c2cccc(NC(=O)N[C@@H]3CCCC[C@H]3CN4CCC[C@@H](Cc5ccc(F)cc5)C4)c2</chem>
CHEMBL272068	CCR3	1	Training	<chem>Cn1nnnc1c2cc(NC(=O)NCCCN3CCC[C@@H](Cc4ccc(F)cc4)C3)cc(c2)C(C)(C)C(=O)O</chem>

CHEMBL429846	CCR3	1	Training	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)c4ccn4)c5ccn5</chem>
CHEMBL180746	CCR3	1	Training	<chem>CCc1cc(NC(=O)N[C@@H]2CCCN(CCCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL46404	CCR3	1	Prediction	<chem>CC(=O)c1cc(NC(=O)NCCCN2CCC[C@@H](Cc3ccc(F)cc3)C2)c(c1)C(=O)C</chem>
CHEMBL257737	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(C)cc(c3)c4nnnn4C</chem>
CHEMBL258322	CCR3	1	Training	<chem>C[C@H](C[C@@H](N)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL257073	CCR3	1	Training	<chem>CC(C)C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL384199	CCR3	1	Prediction	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CCCO)cc(c1)C(=O)C</chem>
CHEMBL182086	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@H]2CN(CCc3ccc(F)cc3)CC[C@@H]2C)cc(c1)c4nnnn4C</chem>
CHEMBL428775	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL219048	CCR3	1	Training	<chem>CC(=O)c1cccc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CN2)c1</chem>
CHEMBL272067	CCR3	1	Prediction	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)n4ccnn4)n5ccnn5</chem>
CHEMBL257074	CCR3	1	Training	<chem>CCC[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)C(C)(C)O)c4nnnn4C</chem>
CHEMBL444568	CCR3	1	Training	<chem>Cc1cc(NC(=O)NCCCN2CCC[C@@H](Cc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL270582	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(c(c3)c4nnnn4C)C(=O)C</chem>
CHEMBL178503	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)NC[C@H]2CN(CCc3ccc(F)cc3)CC[C@@H]2C(C)C)cc(c1)c4nnnn4C</chem>
CHEMBL178230	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL403839	CCR3	1	Training	<chem>Fc1ccc(C[C@@H]2CCCN(CCCNC(=O)Nc3cc(cc(c3)n4cccn4)n5cccn5)C2)cc1</chem>
CHEMBL218174	CCR3	1	Training	<chem>CN1CC[C@@H](Cc2ccc(F)cc2)C[C@@H]1CCCN(C(=O)Nc3ccc(c3)C(=O)C</chem>
CHEMBL403331	CCR3	1	Prediction	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(Br)cc(c3)c4nnnn4C</chem>
CHEMBL270147	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(c(c3)n4cccn4)n5cccn5</chem>
CHEMBL178506	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(F)cc3F)C2)cc(c1)c4nnnn4C</chem>
CHEMBL258156	CCR3	1	Training	<chem>C[C@H](C[C@@H](C)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL402983	CCR3	1	Prediction	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(Br)cc(c3)c4nnnn4C</chem>
CHEMBL437031	CCR3	1	Training	<chem>CCc1cc(NC(=O)N[C@H](C)C[C@@H](O)N2CCC[C@@H](Cc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL220765	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CC#C)cc(c1)C(=O)C</chem>

CHEMBL180042	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL221067	CCR3	1	Prediction	<chem>CCCN1CC[C@@H](Cc2ccc(F)cc2)C[C@@H]1CCCN(C(=O)Nc3cccc(c3)C(=O)C</chem>
CHEMBL427728	CCR3	1	Training	<chem>CCc1cc(NC(=O)N[C@H](C)CCN2CCC[C@@H](Cc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL441334	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(c(c3)n4ccnn4)n5ccnn5</chem>
CHEMBL250689	CCR3	1	Training	<chem>CC(=O)c1cccc(NC(=O)N[C@@H]2CCCC[C@H]2CN3CCC[C@@H](Cc4ccc(F)cc4)C3)c1</chem>
CHEMBL178671	CCR3	1	Prediction	<chem>CC[C@H]1CCN(CCc2ccc(F)cc2)C[C@@H]1CNC(=O)Nc3cc(C)cc(c3)c4nnnn4C</chem>
CHEMBL360039	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@H]2CCCN(CCCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL20921	CCR3	1	Training	<chem>Nc1ccc2nc(SCC(=O)NC3CCN(Cc4ccc(Cl)c(Cl)c4)CC3)sc2c1</chem>
CHEMBL220713	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CCF)cc(c1)C(=O)C</chem>
CHEMBL270146	CCR3	1	Prediction	<chem>CC[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)C(C)(C)O)c4nnnn4C</chem>
CHEMBL220819	CCR3	1	Training	<chem>CC(=O)c1cccc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CN2CC4CC4)c1</chem>
CHEMBL46905	CCR3	1	Training	<chem>CC(=O)c1cccc(NC(=O)NCCCN2CCC[C@@H](Cc3ccc(F)cc3)C2)c1</chem>
CHEMBL429604	CCR3	1	Training	<chem>CC(C)c1cc(NC(=O)NCCCN2CCC[C@@H](Cc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL404122	CCR3	1	Prediction	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(c(c3)c4nnnn4C)C(C)C</chem>
CHEMBL295415	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCCN2CCC[C@@H](Cc3ccc(F)cc3)C2)c(c1)c4nnnn4C</chem>
CHEMBL401879	CCR3	1	Training	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)n4cccn4)n5cccn5</chem>
CHEMBL258309	CCR3	1	Training	<chem>C[C@@H](C[C@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL255399	CCR3	1	Prediction	<chem>C[C@H](C[C@@H](O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)c4ocnn4)c5ocnn5</chem>
CHEMBL255398	CCR3	1	Training	<chem>C[C@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(c(c3)C(=O)C)C(=O)C</chem>
CHEMBL361130	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@H]2CN(CCc3ccc(F)cc3)CC[C@@H]2c4cccc4)cc(c1)c5nnnn5C</chem>
CHEMBL180728	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@H]2CN(CCc3ccc(F)cc3)CC[C@@H]2C(F)(F)F)cc(c1)c4nnnn4C</chem>
CHEMBL180351	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(F)c(F)c3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL366710	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL178287	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(Cl)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL385607	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CC(=O)N)cc(c1)C(=O)C</chem>
CHEMBL359609	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3cccc3)C2)cc(c1)c4nn</chem>

				nn4C
CHEMBL383879	CCR3	1	Training	<chem>CC(=O)N1CC[C@@H](Cc2ccc(F)cc2)C[C@@H]1CCCN(C(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL258323	CCR3	1	Training	<chem>C[C@@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)c4nnnn4C</chem>
CHEMBL221903	CCR3	1	Training	<chem>CC(=O)c1cccc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CN2CC=C)c1</chem>
CHEMBL428071	CCR3	1	Prediction	<chem>C[C@H](CC(=O)N1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cccc(c3)c4nnnn4C</chem>
CHEMBL220766	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2C(=N)N)cc(c1)C(=O)C</chem>
CHEMBL362490	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NC[C@@H]3CCCN(CCc4ccc(F)cc4)C3)c2</chem>
CHEMBL180229	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(Cl)cc3Cl)C2)cc(c1)c4nnnn4C</chem>
CHEMBL369331	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccccc3F)C2)cc(c1)c4nnnn4C</chem>
CHEMBL384649	CCR3	1	Training	<chem>CCC(=O)N1CC[C@@H](Cc2ccc(F)cc2)C[C@@H]1CCCN(C(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL404202	CCR3	1	Training	<chem>C[C@@H](CCN1CCC[C@@H](Cc2ccc(F)cc2)C1)NC(=O)Nc3cc(cc(c3)C(=O)C)C(=O)C</chem>
CHEMBL181575	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NCC3CCCN(CCc4ccc(F)cc4)C3)c2</chem>
CHEMBL218581	CCR3	1	Prediction	<chem>CC(=O)c1cccc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccccc3)CCN2)c1</chem>
CHEMBL220801	CCR3	1	Training	<chem>CC(=O)c1cccc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CN2CCO)c1</chem>
CHEMBL181528	CCR3	1	Training	<chem>CCc1cc(NC(=O)N[C@@H]2CCCN(CCCCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL360529	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(C)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL360062	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccccc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL386493	CCR3	1	Training	<chem>CC(=O)c1cc(NC(=O)NCCC[C@H]2C[C@H](Cc3ccc(F)cc3)CCN2CC(F)F)cc(c1)C(=O)C</chem>
CHEMBL180694	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NC[C@H]3CCCN(CCc4ccc(F)cc4)C3)c2</chem>
CHEMBL178278	CCR3	1	Training	<chem>CCc1cc(NC(=O)N[C@@H]2CCCN(CCc3ccc(F)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL362613	CCR3	1	Prediction	<chem>Cn1nnnc1c2cccc(NC(=O)NC[C@H]3CCCN(CCCc4ccc(F)cc4)C3)c2</chem>
CHEMBL21143	CCR3	1	Training	<chem>CCOc1ccc2nc(SCC(=O)NC3CCN(Cc4ccc(Cl)c(Cl)c4)CC3)sc2c1</chem>
CHEMBL218997	CCR3	1	Training	<chem>O=C(NCCC[C@H]1C[C@H](Cc2ccccc2)CCN1)Nc3ccccc3)C#N</chem>
CHEMBL426422	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NCC3CCCN(CCCCc4ccc(F)cc4)C3)c2</chem>
CHEMBL20532	CCR3	1	Prediction	<chem>Clc1ccc(CN2CCC(CC2)NC(=O)CSc3nc4ccccc4s3)cc1Cl</chem>
CHEMBL182087	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NCC3CCCN(CCCc4ccc(F)cc4)C3)c2</chem>
CHEMBL266181	CCR3	1	Training	<chem>CCOC(=O)c1ccc2nc(SCC(=O)NC3CCN(Cc4ccc(Cl)c(Cl)c4)CC3)sc2c1</chem>
CHEMBL180534	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NCC3CCN(Cc4ccc(F)cc4)CC3)c2</chem>
CHEMBL282285	CCR3	1	Prediction	<chem>Clc1ccc(CN2CCC(CC2)NC(=O)CSc3nc4ccccc4s3)cc1</chem>

CHEMBL181302	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(cc3)C(F)(F)F)C2)cc(c1)c4nnnn4C</chem>
CHEMBL180860	CCR3	1	Training	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(OC)cc3)C2)cc(c1)c4nnnn4C</chem>
CHEMBL220800	CCR3	1	Training	<chem>O=C(NCCCC[C@H]1C[C@H](Cc2ccccc2)CCN1)Nc3cccc(c3)C#N</chem>
CHEMBL221901	CCR3	1	Prediction	<chem>O=C(NCC[C@H]1C[C@H](Cc2ccccc2)CCN1)Nc3cccc(c3)C#N</chem>
CHEMBL181311	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NCC3CCN(CCCc4ccc(F)cc4)CC3)c2</chem>
CHEMBL20612	CCR3	1	Training	<chem>Clc1cccc(CN2CCC(CC2)NC(=O)CSc3nc4cccc4s3)c1</chem>
CHEMBL360653	CCR3	1	Training	<chem>Cn1nnnc1c2cccc(NC(=O)NCC3CCN(CCc4ccc(F)cc4)CC3)c2</chem>
CHEMBL180082	CCR3	1	Prediction	<chem>CCc1cc(NC(=O)NC[C@@H]2CCCN(CCc3ccc(cc3)N(C)C)C2)cc(c1)c4nnnn4C</chem>
CHEMBL220866	CCR3	1	Training	<chem>O=C(NCCC[C@@H]1C[C@H](Cc2ccccc2)CCN1)Nc3cccc(c3)C#N</chem>
Aceclofenac	CCR3	-1	Training	<chem>Clc2cccc(Cl)c2Nc1cccc1CC(=O)OCC(=O)O</chem>
Acetaminophen	CCR3	-1	Training	<chem>Oc1ccc(NC(C)=O)cc1</chem>
Acetazolamide	CCR3	-1	Prediction	<chem>O=S(N)(=O)c1nnc(NC(C)=O)s1</chem>
Acetophenazine	CCR3	-1	Training	<chem>CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4cccc4Sc3cc2</chem>
Amantadine	CCR3	-1	Training	<chem>NC13CC2CC(CC(C1)C2)C3</chem>
Ambenonium	CCR3	-1	Training	<chem>Clc2ccccc2C[N+](CC)(CC)CCNC(=O)C(=O)NCC[N+](Cc1ccccc1Cl)(CC)CC</chem>
Amineptine	CCR3	-1	Prediction	<chem>O=C(O)CCCCCNC2c3ccccc3CCc1ccccc12</chem>
Amiodarone	CCR3	-1	Training	<chem>CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC</chem>
Amitriptyline	CCR3	-1	Training	<chem>CN(C)CC\C=C\c3ccccc3CCc2ccccc12</chem>
Aprobarbital	CCR3	-1	Training	<chem>O=C1NC(=O)NC(=O)C1(CC=C)C(C)C</chem>
Artane	CCR3	-1	Prediction	<chem>OC(CCN1CCCCC1)(c2ccccc2)C3CCCCC3</chem>
Aspirin	CCR3	-1	Training	<chem>O=C(C)Oc1ccccc1C(=O)O</chem>
Atenolol	CCR3	-1	Training	<chem>CC(C)NCC(O)COc1ccc(cc1)CC(N)=O</chem>
Atropine	CCR3	-1	Training	<chem>CN3C1CCC3C[C@@H](C1)OC(=O)C(CO)c2ccccc2</chem>
Baclofen	CCR3	-1	Prediction	<chem>Clc1ccc(cc1)C(CN)CC(=O)O</chem>
Beclomethasone	CCR3	-1	Training	<chem>OCC(=O)[C@@]4(O)[C@@H](C)CC3C2CCC1=CC(=O)C=C[C@@]1(C)[C@@]2(Cl)[C@@H](O)C[C@@]34C</chem>
Benzonatate	CCR3	-1	Training	<chem>O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NC(C)C)cc1</chem>
Biperiden	CCR3	-1	Training	<chem>OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3</chem>
Bromocriptine	CCR3	-1	Prediction	<chem>BrC3nc2cccc1C4=C[C@H](CN(C)C4Cc3c12)C(=O)N[C@@]7(O[C@]6(O)N([C@@H](CC(C)C)C(=O)N5CCCC56)C7=O)C(C)C</chem>
Buclizine	CCR3	-1	Training	<chem>CC(C)(C)c1ccc(cc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Budesonide	CCR3	-1	Training	<chem>OCC(=O)[C@@]53OC(O[C@@H]5CC2C1CCC4=CC(=O)C=C[C@@]4(C)C1[C@@H](O)C[C@@]23C)CCC</chem>
Buprenorphine	CCR3	-1	Training	<chem>CC(C)(C)C(C)(O)[C@H]1C[C@]75CC[C@]1(OC)[C@@H]2Oc4c(O)ccc3C[C@H]7[N@](CC[C@]25c34)CC6CC6</chem>
Caffeine	CCR3	-1	Prediction	<chem>O=C2c1n(C)enc1N(C)C(=O)N2C</chem>
Cantil	CCR3	-1	Training	<chem>O=C(OC1CCC[N+](C)(C)C1)C(O)(c2ccccc2)c3ccccc3</chem>
Carbachol	CCR3	-1	Training	<chem>C[N+](C)(C)CCOC(=O)N</chem>
Carbamazepine	CCR3	-1	Training	<chem>NC(=O)N2c3ccccc3C=Cc1ccccc12</chem>

Carisoprodol	CCR3	-1	Prediction	<chem>O=C(NC(C)C)OCC(C)(COC(=O)N)CCC</chem>
Carvedilol	CCR3	-1	Training	<chem>COc4cccc4OCCNCC(O)COc2cccc3nc1cccc1c23</chem>
Cefoperazone	CCR3	-1	Training	<chem>O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O</chem>
Chloral hydrate	CCR3	-1	Training	<chem>ClC(Cl)(Cl)C(O)O</chem>
Chlordiazepoxide	CCR3	-1	Prediction	<chem>Clc1ccc2N=C(C[N+](O-)=C(c2c1)c3ccccc3)NC</chem>
Chlorpropamide	CCR3	-1	Training	<chem>O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1</chem>
Chlorthalidone	CCR3	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2ccccc23</chem>
Clidinium	CCR3	-1	Training	<chem>OC(c1cccc1)(c2ccccc2)C(=O)OC4C[N+](C)CCC4CC3</chem>
Clobazam	CCR3	-1	Prediction	<chem>Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3ccccc3</chem>
Clofazimine	CCR3	-1	Training	<chem>Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5</chem>
Clomipramine	CCR3	-1	Training	<chem>CN(C)CCCN2c3ccccc3CCc1ccc(Cl)cc12</chem>
Clonidine	CCR3	-1	Training	<chem>Clc2ccccc(Cl)c2N=C1NCCN1</chem>
Codeine	CCR3	-1	Prediction	<chem>COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23</chem>
Colchicine	CCR3	-1	Training	<chem>CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12</chem>
Cyclizine	CCR3	-1	Training	<chem>CN1CCN(CC1)C(c2ccccc2)c3ccccc3</chem>
Cyclosporin	CCR3	-1	Training	<chem>CC(C\C=C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C</chem>
Dextropropoxyphene	CCR3	-1	Prediction	<chem>CN(C)CC(C)C(OC(=O)CC)(Cc1cccc1)c2ccccc2</chem>
Diazepam	CCR3	-1	Training	<chem>Clc1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3</chem>
Diflucortolone	CCR3	-1	Training	<chem>OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C</chem>
Dimercaprol	CCR3	-1	Training	<chem>OCC(S)CS</chem>
Diphenhydramine	CCR3	-1	Prediction	<chem>CN(C)CCOC(c1cccc1)c2ccccc2</chem>
Diphenidol	CCR3	-1	Training	<chem>OC(CCCN1CCCC1)(c2ccccc2)c3ccccc3</chem>
Dobutamine	CCR3	-1	Training	<chem>Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O</chem>
Dofetilide	CCR3	-1	Training	<chem>CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O</chem>
Domperidone	CCR3	-1	Prediction	<chem>Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4</chem>
Dopamine	CCR3	-1	Training	<chem>Oc1ccc(CCN)cc1O</chem>
Doxazosin	CCR3	-1	Training	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4</chem>
Doxepin	CCR3	-1	Training	<chem>CN(C)CC\C=C1/c3ccccc3OCc2ccccc12</chem>
Dronabinol	CCR3	-1	Prediction	<chem>CCCCCc3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3</chem>
Droxicam	CCR3	-1	Training	<chem>O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O</chem>
Entacapone	CCR3	-1	Training	<chem>Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+](O-)=O)c1O</chem>
Epinephrine	CCR3	-1	Training	<chem>Oc1ccc(cc1O)[C@@H](O)CNC</chem>
Eprosartan	CCR3	-1	Prediction	<chem>OC(=O)C(/Cc1cccs1)=C/c3cnc(CCCC)n3Cc2ccc(cc2)C(=O)O</chem>
Ergotamine	CCR3	-1	Training	<chem>CN2C[C@@H](C=C1c3cccc4ncc(CC12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O</chem>
Ethosuximide	CCR3	-1	Training	<chem>CC1(CC)CC(=O)NC1=O</chem>

Fentanyl	CCR3	-1	Training	<chem>CCC(=O)N(C2CCN(CCc1cccc1)CC2)c3cccc3</chem>
Fexofenadine	CCR3	-1	Prediction	<chem>O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3cccc3)c4cccc4</chem>
Flecainide	CCR3	-1	Training	<chem>FC(F)(F)COc2cc(C(=O)NCC1CCCCN1)c(OCC(F)(F)F)cc2</chem>
Flunarizine	CCR3	-1	Training	<chem>Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4cccc4</chem>
Flunisolide	CCR3	-1	Training	<chem>OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C</chem>
Fluoxetine	CCR3	-1	Prediction	<chem>FC(F)(F)c2ccc(OC(CCNC)c1cccc1)cc2</chem>
Fluvoxamine	CCR3	-1	Training	<chem>FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN</chem>
Gabapentin	CCR3	-1	Training	<chem>NCC1(CC(=O)O)CCCC1</chem>
Gestodene	CCR3	-1	Training	<chem>O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2</chem>
Glutethimide	CCR3	-1	Prediction	<chem>CCC1(CCC(=O)NC1=O)c2cccc2</chem>
Glycopyrrolate	CCR3	-1	Training	<chem>C[N+]3(C)CCC(OC(=O)C(O)(c1cccc1)C2CCCC2)C3</chem>
Guanadrel	CCR3	-1	Training	<chem>N=C(N)NCC2COC1(CCCCC1)O2</chem>
Halofantrine	CCR3	-1	Training	<chem>CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F</chem>
Haloperidol	CCR3	-1	Prediction	<chem>Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3</chem>
Halothane	CCR3	-1	Training	<chem>BrC(Cl)C(F)(F)F</chem>
Hydromorphone	CCR3	-1	Training	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	CCR3	-1	Training	<chem>Clc1ccc(cc1)C(c2cccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	CCR3	-1	Prediction	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3cccc3CC2C</chem>
Indomethacin	CCR3	-1	Training	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	CCR3	-1	Training	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	CCR3	-1	Training	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	CCR3	-1	Prediction	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	CCR3	-1	Training	<chem>CNC1(CCCCC1=O)c2cccc2C1</chem>
Labetalol	CCR3	-1	Training	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2cccc2</chem>
Lacidipine	CCR3	-1	Training	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	CCR3	-1	Prediction	<chem>Clc1cccc(c1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	CCR3	-1	Training	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCN(=N)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2cccc23)NC(=O)C(Cc4cncn4)NC(=O)C5CCC(=O)N5</chem>
Levodopa	CCR3	-1	Training	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>
Lidocaine	CCR3	-1	Training	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	CCR3	-1	Prediction	<chem>Clc3cc4CCc1ccnc1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	CCR3	-1	Training	<chem>CNCCCC24CCC(c1cccc12)c3cccc34</chem>
Meclizine	CCR3	-1	Training	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4cccc4</chem>
Medroxyprogesterone	CCR3	-1	Training	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	CCR3	-1	Prediction	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	CCR3	-1	Training	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	CCR3	-1	Training	<chem>C[C@H](NC)Cc1cccc1</chem>
Methantheline	CCR3	-1	Training	<chem>CC[N+](C)(CC)CCOC(=O)C1c3cccc3Oc2cccc12</chem>

Methocarbamol	CCR3	-1	Prediction	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	CCR3	-1	Training	<chem>ClC(Cl)C(F)(F)OC</chem>
Methscopolamine	CCR3	-1	Training	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+]3(C)C</chem>
Methylphenidate	CCR3	-1	Training	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	CCR3	-1	Prediction	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3ccccc1c23)N(C)C4</chem>
Metoclopramide	CCR3	-1	Training	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	CCR3	-1	Training	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	CCR3	-1	Training	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	CCR3	-1	Prediction	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	CCR3	-1	Training	<chem>CC(C)(O)c5ccccc5CC[C@@H](SCC1(CC(=O)O)CC1)c2ccccc2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	CCR3	-1	Training	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	CCR3	-1	Training	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@@H]45</chem>
Nalmefene	CCR3	-1	Prediction	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C[C@N@]3CC2CC2)c45</chem>
Neostigmine	CCR3	-1	Training	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>
Nifedipine	CCR3	-1	Training	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	CCR3	-1	Training	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	CCR3	-1	Prediction	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	CCR3	-1	Training	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	CCR3	-1	Training	<chem>CSC[C@@H]4CC1C(Cc2cnc3cccc1c23)N(C4)CCC</chem>
Phenylbutazone	CCR3	-1	Training	<chem>O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2</chem>
Phenytoin	CCR3	-1	Prediction	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	CCR3	-1	Training	<chem>Cn2cnc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	CCR3	-1	Training	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	CCR3	-1	Training	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	CCR3	-1	Prediction	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	CCR3	-1	Training	<chem>OC(CC1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	CCR3	-1	Training	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	CCR3	-1	Training	<chem>OC(C(C)NC)c1ccccc1</chem>
Pyrantel	CCR3	-1	Prediction	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>
Quinidine	CCR3	-1	Training	<chem>COc1cc2c(cc1)nccc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	CCR3	-1	Training	<chem>[O-][N+](=O)C=C(NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	CCR3	-1	Training	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oc4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	CCR3	-1	Prediction	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	CCR3	-1	Training	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	CCR3	-1	Training	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>
Selegiline	CCR3	-1	Training	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>

Sulfinpyrazone	CCR3	-1	Prediction	<chem>O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	CCR3	-1	Training	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>
Terpin	CCR3	-1	Training	<chem>C[C@@]1(O)CC[C@H](CC1)C(C)(C)O</chem>
Tolcapone	CCR3	-1	Training	<chem>Oc1cc(cc([N+])([O-])=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranlycypromine	CCR3	-1	Prediction	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	CCR3	-1	Training	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	CCR3	-1	Training	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@@]23C</chem>
Valproic acid	CCR3	-1	Training	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	CCR3	-1	Prediction	<chem>O=C(O)[C@@H]%10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	CCR3	-1	Training	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	CCR3	-1	Training	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wytensin	CCR3	-1	Training	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	CCR3	-1	Prediction	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>
Zileuton	CCR3	-1	Training	<chem>NC(=O)N(O)C(C)c1cc2ccccc2s1</chem>
Zonisamide	CCR3	-1	Training	<chem>NS(=O)(=O)Cc2noc1ccccc12</chem>
CHEMBL515193	CCR5	1	Prediction	<chem>CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)NCc4ccc(Cl)c(Cl)c4</chem>
CHEMBL460845	CCR5	1	Training	<chem>CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)Cc4ccc(Cl)c(Cl)c4</chem>
CHEMBL21106	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CC1)N2C[C@H](CN3CCC(CCC(F)(F)c4cc(F)cc4)CC3)[C@H](C2)c5ccccc(F)c5</chem>
CHEMBL457043	CCR5	1	Training	<chem>CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)Cc4ccc(cc4)S(=O)(=O)C</chem>
CHEMBL20896	CCR5	1	Prediction	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCCc4ccccc4)CC3)[C@H](C2)c5ccccc5</chem>
CHEMBL320386	CCR5	1	Training	<chem>OC(=O)[C@@H](C1CCC1)N2C[C@H](CN3CCC(CCCc4ccccc4)CC3)[C@H](C2)c5ccccc5</chem>
CHEMBL316475	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CC1)N2C[C@H](CN3CCC(CCCc4ccccc4)CC3)[C@H](C2)c5ccccc5</chem>
CHEMBL20345	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCCc4ccc(F)cc4)CC3)[C@H](C2)c5ccccc(F)c5</chem>
CHEMBL473558	CCR5	1	Prediction	<chem>CC(C)c1nnc(C)n1C2CCN(CC2)C(C)C[C@H](NC(=O)C3CCCC3)c4ccccc4</chem>
CHEMBL461687	CCR5	1	Training	<chem>CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)NCc4ccccc4</chem>
CHEMBL319593	CCR5	1	Training	<chem>OC1(CCCc2ccc(cc2)c3nn[nH]3)CCN(C[C@H]4CN(CC5CCCC5)C[C@@H]4c6ccccc6)CC1</chem>
CHEMBL322422	CCR5	1	Training	<chem>Cn1nnnc1c2ccc(CCCC3(O)CCN(C[C@H]4CN(CC5CCCC5)C[C@@H]4c6ccccc6)CC3)cc2</chem>
CHEMBL99909	CCR5	1	Prediction	<chem>OC(=O)[C@@H](C1CCCC1)N2C[C@H](CN3CCC(CCCc4ccccc4)CC3)[C@H](C2)c5ccccc5</chem>
CHEMBL1201187	CCR5	1	Training	<chem>CC(C)c1nnc(C)n1[C@@H]2C[C@H]3CC[C@@H](C2)N3CC[C@H](NC(=O)C4CCC(F)(F)CC4)c5ccccc5</chem>

CHEMBL21147	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCCc4ccc(c4)C(F)(F)F)CC3)[C@H](C2)c5cccc(F)c5
CHEMBL20622	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCC(F)(F)c4ccc(F)cc4)CC3)[C@H](C2)c5cccc5
CHEMBL212731	CCR5	1	Prediction	CCN(C1CCN(CC[C@H](c2ccc(cc2)S(=O)(=O)C)c3cccc(F)c3)CC1)C(=O)Cc4ccc(cc4)S(=O)(=O)C
CHEMBL520091	CCR5	1	Training	OC(=O)[C@@H](CC1CC1)N2C[C@H](CN3CCC(CC3)c4cnc(Cc5ccccc5)s4)[C@H](C2)c6cccc6
CHEMBL511493	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4cnc(Cc5ccccc5)s4)[C@H](C2)c6cccc6
CHEMBL480503	CCR5	1	Training	OC(=O)[C@@H](C1CCCC1)N2C[C@H](CN3CCC(CC3)c4cnc(Cc5ccccc5)s4)[C@H](C2)c6cccc6
CHEMBL317710	CCR5	1	Prediction	OC1(CCCc2cccc2)CCN(C[C@H]3CN(CC4CCCC4)C[C@@H]3c5ccccc5)CC1
CHEMBL194497	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4cnc5ccc(F)cn45)[C@H](C2)c6cccc(F)c6
CHEMBL21117	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCC(F)(F)c4ccc(F)cc4)CC3)[C@H](C2)c5cccc(F)c5
CHEMBL455073	CCR5	1	Training	OC(=O)[C@@H](CC1CCCC1)N2C[C@H](CN3CCC(CCC(F)(F)c4ccc(F)cc4)CC3)[C@H](C2)c5cccc5
CHEMBL212689	CCR5	1	Prediction	CCN(C1CCN(CC[C@H](c2ccc(cc2)S(=O)(=O)C)c3cc(F)cc(F)c3)CC1)C(=O)Cc4ccc(cc4)S(=O)(=O)C
CHEMBL459384	CCR5	1	Training	CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)Cc4ccc(Cl)cc4
CHEMBL480693	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4oc(Cc5ccccc5)nc4)[C@H](C2)c6cccc6
CHEMBL193984	CCR5	1	Training	CCc1ccn2c(cnc2c1)C3CCN(C[C@H]4CN(C[C@@H]4c5cccc(F)c5)[C@H](CC6CCC6)C(=O)O)CC3
CHEMBL489513	CCR5	1	Prediction	CC(C)c1nnc(C)n1C2CCN(CC2)C(C)C[C@H](NC(=O)C3CC(F)(F)C3)c4ccccc4
CHEMBL103790	CCR5	1	Training	C[n+]1n[nH]c(n1)c2ccc(CCCC3(O)CCN(C[C@H]4CN(CC5CCC(C5)C[C@@H]4c6ccccc6)CC3)cc2
CHEMBL20453	CCR5	1	Training	OC(CCC1CCN(C[C@H]2CN(C[C@@H]2c3cccc(F)c3)[C@H](C4CC4)C(=O)O)CC1)c5ccc(F)cc5
CHEMBL464132	CCR5	1	Training	Cn1nnc(n1)c2ccc(CCCC3(O)CCN(C[C@H]4CN(CC5CCCC5)C[C@@H]4c6ccccc6)CC3)cc2
CHEMBL371584	CCR5	1	Prediction	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4cnc5cccn45)[C@H](C2)c6cccc6
CHEMBL456226	CCR5	1	Training	CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)Cc4ccc(cc4)C(F)(F)F
CHEMBL491319	CCR5	1	Training	CC(C)c1nnc(C)n1C2CCN(CC2)[C@H](C)C[C@H](NC(=O)C3CC(F)(F)C3)c4ccccc4
CHEMBL371177	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4cnc5c(Cl)cc(Cl)cn45)[C@H](C2)c6cccc(F)c6
CHEMBL471920	CCR5	1	Prediction	CC(C)C[C@@H](N1C[C@H](CN2CCC(CCC(F)(F)c3ccc(F)cc3)CC2)[C@H](C1)c4cccc(F)c4)C(=O)O
CHEMBL472464	CCR5	1	Training	Cc1cccc(C)c1C(=O)N2CCC(C)(CC2)N3CCC(CC3)N(Cc4ccccc4)C(=O)C5CC5
CHEMBL278085	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCCc4ccccc4)CC3)[C@H](C2)c5cccc(F)c5

CHEMBL513564	CCR5	1	Training	<chem>CC(C)[C@@H](N1C[C@H](CN2CCC(CC2)c3nc(Cc4ccccc4)s3)[C@H](C1)c5ccccc5)C(=O)O</chem>
CHEMBL473759	CCR5	1	Prediction	<chem>CC(C)c1nnc(C)n1C2CCN(CC2)C(C)C[C@H](NC(=O)C3CCCCC3)c4ccccc4</chem>
CHEMBL500631	CCR5	1	Training	<chem>CCc1nc(Cc2ccccc2)[nH]c1C3CCN(C[C@H]4CN(C[C@@H]4c5ccccc5)[C@H](CC6CCC6)C(=O)O)CC3</chem>
CHEMBL195753	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4nc5ccc(en45)[N+](=O)[O-])[C@H](C2)c6cccc(F)c6</chem>
CHEMBL472412	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4[nH]c(Cc5ccccc5)nc4Cl)[C@H](C2)c6ccccc6</chem>
CHEMBL520755	CCR5	1	Prediction	<chem>OC(=O)[C@@H](C1CCCC1)N2C[C@H](CN3CCC(CC3)c4nc(Cc5ccccc5)[nH]4)[C@H](C2)c6ccccc6</chem>
CHEMBL377914	CCR5	1	Training	<chem>Fc1ccc(CC(=O)NC2CCN(CC[C@H](NC(=O)C3CCC3)c4ccccc4)CC2)cc1</chem>
CHEMBL318406	CCR5	1	Training	<chem>CC(C)[C@@H](N1C[C@H](CN2CCC(CCCc3ccccc3)CC2)[C@H](C1)c4ccccc4)C(=O)O</chem>
CHEMBL211866	CCR5	1	Training	<chem>CCN(C1CCN(CC[C@H](c2ccccc2)c3ccc(cc3)S(=O)(=O)C)CC1)C(=O)Cc4ccc(cc4)S(=O)(=O)C</chem>
CHEMBL471251	CCR5	1	Prediction	<chem>CCc1nc(Cc2ccccc2)sc1C3CCN(C[C@H]4CN(C[C@@H]4c5ccccc5)[C@H](CC6CCC6)C(=O)O)CC3</chem>
CHEMBL193822	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4nc5ccc(en45)c6ccccc6)[C@H](C2)c7cccc(F)c7</chem>
CHEMBL328297	CCR5	1	Training	<chem>[O-][N+](=O)c1ccc(COC(=O)N(CC=C)C2CCN(C[C@H]3CN(C[C@@H]3c4ccccc4)C(=O)c5ccccc5Cl)CC2)cc1</chem>
CHEMBL471909	CCR5	1	Training	<chem>CC(C)C[C@@H](N1C[C@H](CN2CCC(CCSccc(F)cc3)CC2)[C@H](C1)c4cccc(F)c4)C(=O)O</chem>
CHEMBL172854	CCR5	1	Prediction	<chem>CCn1nc(Cc2ccccc2)cc1C3CCN(C[C@H]4CN(C[C@@H]4c5ccccc5)[C@@H](C(=O)O)C(C)(C)C)CC3</chem>
CHEMBL281607	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CCCc4ccc(F)cc4)CC3)[C@H](C2)c5cccc(F)c5</chem>
CHEMBL101961	CCR5	1	Training	<chem>OC(=O)[C@H](N1C[C@H](CN2CCC(O)(CCc3ccccc3)CC2)[C@H](C1)c4ccccc4)c5ccccc5</chem>
CHEMBL511634	CCR5	1	Training	<chem>OC(=O)[C@@H](C1CCCC1)N2C[C@H](CN3CCC(CC3)c4onc(Cc5ccccc5)c4)[C@H](C2)c6ccccc6</chem>
CHEMBL435886	CCR5	1	Prediction	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4nc5ccc(en45)C(F)(F)F)[C@H](C2)c6cccc(F)c6</chem>
CHEMBL193440	CCR5	1	Training	<chem>OC(=O)[C@@H](C1CCCC1)N2C[C@H](CN3CCC(CCCn4nc5ccccc45)CC3)[C@H](C2)c6ccccc6</chem>
CHEMBL193988	CCR5	1	Training	<chem>OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4nc5ccc(Cl)en45)[C@H](C2)c6cccc(F)c6</chem>
CHEMBL449758	CCR5	1	Training	<chem>CCc1nc(Cc2ccccc2)oc1C3CCN(C[C@H]4CN(C[C@@H]4c5ccccc5)[C@H](CC6CCC6)C(=O)O)CC3</chem>
CHEMBL435727	CCR5	1	Prediction	<chem>CCC(CC)[C@@H](N1C[C@H](CN2CCC(CC2)c3cc(Cc4ccccc4)nn3CC)[C@H](C1)c5cccc(F)c5)C(=O)O</chem>
CHEMBL470510	CCR5	1	Training	<chem>CC(C)C[C@@H](N1C[C@H](CN2CCC(CCS(=O)(=O)c3ccc(F)c3)CC2)[C@H](C1)c4cccc(F)c4)C(=O)O</chem>
CHEMBL461690	CCR5	1	Training	<chem>CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)Cc4ccc(F)cc4</chem>
CHEMBL379082	CCR5	1	Training	<chem>CCN(C1CCN(CC[C@H](c2ccc(cc2)S(=O)(=O)C)c3cccc(Cl)c3)C</chem>

				C1)C(=O)Cc4ccc(cc4)S(=O)(=O)C
CHEMBL420465	CCR5	1	Prediction	OC1(CCCc2ccc(Cc3nn[nH]n3)cc2)CCN(C[C@H]4CN(CC5CCC CC5)C[C@@H]4c6ccccc6)CC1
CHEMBL93139	CCR5	1	Training	CN(C[C@@](C)(CCN1CCC(CC1)N(CC=C)C(=O)OCc2ccc(cc2)[N+](=O)[O-])c3ccccc3)S(=O)(=O)c4ccccc4
CHEMBL196497	CCR5	1	Training	OC(=O)[C@@H](CC1CCC1)N2C[C@H](CN3CCC(CC3)c4nc5 cncn45)[C@H](C2)c6ccccc6
CHEMBL471623	CCR5	1	Training	Cc1cccc(C)c1C(=O)N2CCC(CC2)N3CC[C@H](C3)N(Cc4ccccc4)C(=O)C5CC5
CHEMBL481068	CCR5	1	Prediction	Cc1cccc(C)c1C(=O)N2[C@@H]3CC[C@H]2[C@@H](C3)N4C C[C@H](C4)N(Cc5ccccc5)C(=O)C6CC6
CHEMBL480890	CCR5	1	Training	CCc1nc(Cc2ccccc2)sc1C3CCN(C[C@H]4CN(C[C@@H]4c5cccc c5)[C@H](CC(C)C)C(=O)O)CC3
CHEMBL99788	CCR5	1	Training	COC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(O)(CCCc 4ccccc4)CC3)[C@H](C2)c5ccccc5
CHEMBL198758	CCR5	1	Training	CCN(C1CCN(CCC(c2ccccc2)c3ccc(cc3)C#N)CC1)C(=O)Cc4ccc (cc4)S(=O)(=O)C
CHEMBL382435	CCR5	1	Prediction	CCN(C1CCN(CC[C@H](c2ccc(cc2)S(=O)(=O)C)c3cc(F)cc(Cl)c3)CC1)C(=O)Cc4ccc(cc4)S(=O)(=O)C
CHEMBL207182	CCR5	1	Training	CC(=O)N1CCC(CC1)C(=O)N(CCCN2CCC(Cc3ccc(F)cc3)CC2)c 4ccc(Cl)c(Cl)c4
CHEMBL471542	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)c4cc (Cc5ccccc5)on4)[C@H](C2)c6ccccc6
CHEMBL175327	CCR5	1	Training	CCn1nc(Cc2ccccc2)cc1C3CCN(C[C@H]4CN(C[C@@H]4c5cccc (F)c5)[C@H](CC6CC6)C(=O)O)CC3
CHEMBL173095	CCR5	1	Prediction	CCn1nc(Cc2ccccc2)cc1C3CCN(C[C@H]4CN(C[C@@H]4c5cccc (F)c5)[C@H](CC6CCC6)C(=O)O)CC3
CHEMBL353331	CCR5	1	Training	CCn1nc(Cc2ccccc2)cc1C3CCN(C[C@H]4CN(C[C@@H]4c5cccc c5)[C@H](C6CCCCC6)C(=O)O)CC3
CHEMBL481080	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)c4csc (Cc5ccccc5)n4)[C@H](C2)c6ccccc6
CHEMBL1222769	CCR5	1	Training	O[C@@]1(CN(C[C@@H]1CN2CCC(CC2)N(CC=C)C(=O)NCc3 ccc(cc3)C(F)(F)F)C(=O)C4CCCC4)c5cccc(F)c5
CHEMBL455570	CCR5	1	Prediction	CC(C)c1nc(C)nn1C2CC3CCC(C2)N3CC[C@H](NC(=O)C4CCC (F)(F)CC4)c5ccccc5
CHEMBL174304	CCR5	1	Training	CCn1nc(Cc2ccccc2)cc1C3CCN(C[C@H]4CN(C[C@@H]4c5cccc (F)c5)[C@H](C(C)C)C(=O)O)CC3
CHEMBL481274	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)c4oc (Cc5ccccc5)n4)[C@H](C2)c6ccccc6
CHEMBL283788	CCR5	1	Training	COC(=O)C(CCC1CCN(C[C@H]2CN(C[C@@H]2c3cccc(F)c3)[C@H](CC4CC4)C(=O)O)CC1)c5ccc(F)cc5
CHEMBL457044	CCR5	1	Prediction	CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O) Cc4cccc(Cl)c4
CHEMBL20598	CCR5	1	Training	CC(O)(CCC1CCN(C[C@H]2CN(C[C@@H]2c3cccc(F)c3)[C@H (CC4CC4)C(=O)O)CC1)c5ccc(F)cc5
CHEMBL480504	CCR5	1	Training	OC(=O)[C@@H](CC1CC1)N2C[C@H](CN3CCC(CC3)c4oc(Cc5 ccccc5)nc4)[C@H](C2)c6ccccc6
CHEMBL352514	CCR5	1	Training	CCn1nc(Cc2ccccc2)cc1C3CCN(C[C@H]4CN(C[C@@H]4c5cccc c5)[C@H](C6CCC6)C(=O)O)CC3
CHEMBL380447	CCR5	1	Prediction	CCCCOCCOc1ccc(cc1)c2ccc3N(CCC)CCC\C(=C/c3c2)\C(=O)N

				c4ccc(cc4)[S+][O-]Ce5nncn5CCC
CHEMBL198150	CCR5	1	Training	CCN(C1CCN(CCC(c2ccccc2)c3ccc(cc3)S(=O)(=O)C)CC1)C(=O)Cc4ccc(cc4)S(=O)(=O)C
CHEMBL207630	CCR5	1	Training	CS(=O)(=O)N1CCC(CC1)C(=O)N(CCCN2CCC(Cc3ccc(cc3)C#N)CC2)c4ccc(Cl)c(Cl)c4
CHEMBL437494	CCR5	1	Training	CC(=O)N1CCC(CC1)C(=O)N(CCCN2CCC(CC2)Sc3ccc(F)cc3)c4ccc(Cl)c(Cl)c4
CHEMBL204743	CCR5	1	Prediction	CCCCOCCOc1ccc(cc1)c2ccc3N(Cc4cnn(C)c4)CCC\C(=C/c3c2)\C(=O)Nc5ccc(cc5)[S+][O-]Cc6nncn6CCC
CHEMBL428104	CCR5	1	Training	CCCN(C1CCN(C[C@H]2CN(C[C@@H]2c3ccccc(F)c3)[C@H](C4CCC4)C(=O)O)CC1)c5ncccn5
CHEMBL204821	CCR5	1	Training	CCCCOCCOc1ccc(cc1)c2ccc3N(CC(C)C)CCC(=Cc3c2)C(=O)Nc4ccc(cc4)[S+][O-]Ce5nncn5CCC
CHEMBL179141	CCR5	1	Training	CN(CC(C)(CCN1CCC2C(CCN2C(=O)OC(C)(C)C)C1)c3ccccc3)S(=O)(=O)c4ccccc4
CHEMBL179209	CCR5	1	Prediction	CN(CC(C)(CCN1CCC2C(CCN2C(=O)OCc3ccc(cc3)[N+](=O)[O-])C1)c4ccccc4)S(=O)(=O)c5ccccc5
CHEMBL85086	CCR5	1	Training	CCN(C1CCN(CC[C@H](CN(C)S(=O)(=O)c2ccccc2)c3ccccc3)C1)C(=O)OCc4ccccc4
CHEMBL214818	CCR5	1	Training	Cc1nc2ccccc2n1C3CC4CCC(C3)N4CC[C@H](NC(=O)C5CCCC5)c6ccccc6
CHEMBL320149	CCR5	1	Training	OC(=O)CCc1ccc(CCCC2(O)CCN(C[C@H]3CN(CC4CCCC4)C[C@@H]3c5ccccc5)CC2)cc1
CHEMBL469724	CCR5	1	Prediction	CC(C)c1nnc(C)n1C2CCN(CC2)C(C)C[C@H](NC(=O)C3CCC3)c4ccccc4
CHEMBL318210	CCR5	1	Training	CC(C)[C@@H](N1C[C@H](CN2CCC(O)(CCCc3ccccc3)CC2)[C@H](C1)c4ccccc4)C(=O)O
CHEMBL511494	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)c4ncc(Cc5ccccc5)s4)[C@H](C2)c6ccccc6
CHEMBL499483	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)c4cc([nH]4)C(F)(F)c5ccccc5)[C@H](C2)c6ccccc6
CHEMBL202814	CCR5	1	Prediction	CCCCOCCOc1ccc(cc1)c2ccc3N(CCC)CCC\C(=C/c3c2)\C(=O)Nc4ccc(cc4)[S+][O-]Ce5nncn5CCC
CHEMBL207487	CCR5	1	Training	CS(=O)(=O)N1CCC(CC1)C(=O)N(CCCN2CCC(Cc3ccc(cc3)S(=O)(=O)C)CC2)c4ccc(Cl)c(Cl)c4
CHEMBL172659	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)c4cc(Cc5ccccc5)n[nH]4)[C@H](C2)c6ccccc6
CHEMBL197641	CCR5	1	Training	CCN(C1CCN(CCC(c2ccccc2)c3ccc(cc3)C(F)(F)F)CC1)C(=O)Cc4ccc(cc4)S(=O)(=O)C
CHEMBL366626	CCR5	1	Prediction	CCn1cc(CCc2ccccc2)c(n1)C3CCN(C[C@H]4CN(C[C@@H]4c5ccccc5)[C@H](C6CCCCC6)C(=O)O)CC3
CHEMBL457960	CCR5	1	Training	CCN(C1CCN(CC1)C(C)C[C@H](NC(=O)C2CCC2)c3ccccc3)C(=O)Cc4ccc(Cl)cc4Cl
CHEMBL203536	CCR5	1	Training	CCCCOCCOc1ccc(cc1)c2ccc3N(CC(C)C)CCC\C(=C/c3c2)\C(=O)Nc4ccc(cc4)[S+][O-]Ce5nncn5CCC
CHEMBL364070	CCR5	1	Training	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CC3)n4cnc5ccccc5)[C@H](C2)c6ccccc6
CHEMBL193972	CCR5	1	Prediction	OC(=O)[C@@H](C1CCCCC1)N2C[C@H](CN3CCC(CCn4cnc5ccccc5)CC3)[C@H](C2)c6ccccc6
CHEMBL382252	CCR5	1	Training	CS(=O)(=O)N1CCC(CC1)C(=O)N(CCCN2CCC(Cc3ccccc3)C(=

Bromocriptine	CCR5	-1	Training	BrC3nc2cccc1C4=C[C@H](CN(C)C4Cc3c12)C(=O)N[C@@]7(O[C@]6(O)N([C@@H](CC(C)C)C(=O)N5CCCC56)C7=O)C(C)C
Buclicine	CCR5	-1	Training	CC(C)(C)c1ccc(cc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4cccc4
Budesonide	CCR5	-1	Training	OCC(=O)[C@@]53OC(O[C@@H]5CC2C1CCC4=CC(=O)C=C[C@]4(C)C1[C@@H](O)C[C@@]23C)CCC
Buprenorphine	CCR5	-1	Prediction	CC(C)(C)C(C)(O)[C@H]1C[C@]75CC[C@]1(OC)[C@@H]2Oc4c(O)ccc3C[C@H]7[N@](CC[C@]25c34)CC6CC6
Caffeine	CCR5	-1	Training	O=C2c1n(C)cnc1N(C)C(=O)N2C
Cantil	CCR5	-1	Training	O=C(OC1CCC[N+](C)(C)C1)C(O)(c2cccc2)c3cccc3
Carbachol	CCR5	-1	Training	C[N+](C)(C)CCOC(=O)N
Carbamazepine	CCR5	-1	Prediction	NC(=O)N2c3cccc3C=Cc1cccc12
Carisoprodol	CCR5	-1	Training	O=C(NC(C)C)OCC(C)(COC(=O)N)CCC
Carvedilol	CCR5	-1	Training	COc4cccc4OCCNCC(O)COc2cccc3nc1cccc1c23
Cefoperazone	CCR5	-1	Training	O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O
Chloral hydrate	CCR5	-1	Prediction	ClC(Cl)(Cl)C(O)O
Chlordiazepoxide	CCR5	-1	Training	Clc1ccc2N=C(C[N+](O-)=C(c2c1)c3cccc3)NC
Chlorpropamide	CCR5	-1	Training	O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1
Chlorthalidone	CCR5	-1	Training	NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2cccc23
Clidinium	CCR5	-1	Prediction	OC(c1cccc1)(c2cccc2)C(=O)OC4C[N+](3(C)CCC4CC3
Clobazam	CCR5	-1	Training	Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3cccc3
Clofazimine	CCR5	-1	Training	Clc1ccc(cc1)NC3=CC4=Nc2cccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5
Clomipramine	CCR5	-1	Training	CN(C)CCCN2c3cccc3CCc1ccc(Cl)cc12
Clonidine	CCR5	-1	Prediction	Clc2cccc(Cl)c2\N=C1/NCCN1
Codeine	CCR5	-1	Training	COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23
Colchicine	CCR5	-1	Training	CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12
Cyclizine	CCR5	-1	Training	CN1CCN(CC1)C(c2cccc2)c3cccc3
Cyclosporin	CCR5	-1	Prediction	CC(C\C=C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C
Dextropropoxyphene	CCR5	-1	Training	CN(C)CC(C)C(OC(=O)CC)(Cc1cccc1)c2cccc2
Diazepam	CCR5	-1	Training	Clc1ccc2c(c1)C(=NCC(=O)N2C)c3cccc3
Diflucortolone	CCR5	-1	Training	OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C
Dimercaprol	CCR5	-1	Prediction	OCC(S)CS
Diphenhydramine	CCR5	-1	Training	CN(C)CCOC(c1cccc1)c2cccc2
Diphenidol	CCR5	-1	Training	OC(CCCN1CCCC1)(c2cccc2)c3cccc3
Dobutamine	CCR5	-1	Training	Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O
Dofetilide	CCR5	-1	Prediction	CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O
Domperidone	CCR5	-1	Training	Clc4cc5NC(=O)N(C3CCN(CCCN1c2cccc2NC1=O)CC3)c5cc4
Dopamine	CCR5	-1	Training	Oc1ccc(CCN)cc1O
Doxazosin	CCR5	-1	Training	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5cccc5O4

Doxepin	CCR5	-1	Prediction	<chem>CN(C)CC\C=C1/c3ccccc3OCc2ccccc12</chem>
Dronabinol	CCR5	-1	Training	<chem>CCCCCc3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3</chem>
Droxicam	CCR5	-1	Training	<chem>O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O</chem>
Entacapone	CCR5	-1	Training	<chem>Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+])([O-])=O)c1O</chem>
Epinephrine	CCR5	-1	Prediction	<chem>Oc1ccc(cc1O)[C@@H](O)CNC</chem>
Eprosartan	CCR5	-1	Training	<chem>OC(=O)C(/Cc1cccs1)=C/c3cnc(CCCC)n3Cc2ccc(cc2)C(=O)O</chem>
Ergotamine	CCR5	-1	Training	<chem>CN2C[C@@H](C=C1c3ccccc4ncc(CC12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O</chem>
Ethosuximide	CCR5	-1	Training	<chem>CC1(CC)CC(=O)NC1=O</chem>
Fentanyl	CCR5	-1	Prediction	<chem>CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3</chem>
Fexofenadine	CCR5	-1	Training	<chem>O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4</chem>
Flecainide	CCR5	-1	Training	<chem>FC(F)(F)COc2cc(C(=O)NCC1CCCCN1)c(OCC(F)(F)F)cc2</chem>
Flunarizine	CCR5	-1	Training	<chem>Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4</chem>
Flunisolide	CCR5	-1	Prediction	<chem>OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C</chem>
Fluoxetine	CCR5	-1	Training	<chem>FC(F)(F)c2ccc(OC(CCNC)c1ccccc1)cc2</chem>
Fluvoxamine	CCR5	-1	Training	<chem>FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN</chem>
Gabapentin	CCR5	-1	Training	<chem>NCC1(CC(=O)O)CCCC1</chem>
Gestodene	CCR5	-1	Prediction	<chem>O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2</chem>
Glutethimide	CCR5	-1	Training	<chem>CCC1(CCC(=O)NC1=O)c2ccccc2</chem>
Glycopyrrolate	CCR5	-1	Training	<chem>C[N+](3(C)CCC(OC(=O)C(O)(c1ccccc1)C2CCCC2)C3</chem>
Guanadrel	CCR5	-1	Training	<chem>N=C(N)NCC2COC1(CCCCC1)O2</chem>
Halofantrine	CCR5	-1	Prediction	<chem>CCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F</chem>
Haloperidol	CCR5	-1	Training	<chem>Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3</chem>
Halothane	CCR5	-1	Training	<chem>BrC(Cl)C(F)(F)F</chem>
Hydromorphone	CCR5	-1	Training	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	CCR5	-1	Prediction	<chem>Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	CCR5	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C</chem>
Indomethacin	CCR5	-1	Training	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	CCR5	-1	Training	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	CCR5	-1	Prediction	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	CCR5	-1	Training	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	CCR5	-1	Training	<chem>CNC1(CCCCC1=O)c2ccccc2Cl</chem>
Labetalol	CCR5	-1	Training	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2</chem>
Lacidipine	CCR5	-1	Prediction	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	CCR5	-1	Training	<chem>Clc1cccc(c1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	CCR5	-1	Training	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCN(C(=N)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2ccccc23)NC(=O)C(Cc4cncn4)NC(=O)C5CCC(=O)N5</chem>
Levodopa	CCR5	-1	Training	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>

Lidocaine	CCR5	-1	Prediction	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	CCR5	-1	Training	<chem>Clc3cc4CCc1ccnc1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	CCR5	-1	Training	<chem>CNCCCC24CCC(c1cccc12)c3ccccc34</chem>
Meclizine	CCR5	-1	Training	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Medroxyprogesterone	CCR5	-1	Prediction	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	CCR5	-1	Training	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	CCR5	-1	Training	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	CCR5	-1	Training	<chem>C[C@H](NC)Cc1ccccc1</chem>
Methantheline	CCR5	-1	Prediction	<chem>CC[N+](C)(CC)CCOC(=O)C1c3ccccc3Oc2ccccc12</chem>
Methocarbamol	CCR5	-1	Training	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	CCR5	-1	Training	<chem>ClC(Cl)C(F)(F)OC</chem>
Methscopolamine	CCR5	-1	Training	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+]3(C)C</chem>
Methylphenidate	CCR5	-1	Prediction	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	CCR5	-1	Training	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3ccccc1c23)N(C)C4</chem>
Metoclopramide	CCR5	-1	Training	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	CCR5	-1	Training	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	CCR5	-1	Prediction	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	CCR5	-1	Training	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	CCR5	-1	Training	<chem>CC(C)(O)c5ccccc5CC[C@@H](SCC1(CC(=O)O)CC1)c2cccc(c2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	CCR5	-1	Training	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	CCR5	-1	Prediction	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@@H]45</chem>
Nalmefene	CCR5	-1	Training	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C)C[N@@]3CC2CC2)c45</chem>
Neostigmine	CCR5	-1	Training	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>
Nifedipine	CCR5	-1	Training	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	CCR5	-1	Prediction	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	CCR5	-1	Training	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	CCR5	-1	Training	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	CCR5	-1	Training	<chem>CSC[C@@H]4CC1C(Cc2enc3ccccc1c23)N(C4)CCC</chem>
Phenylbutazone	CCR5	-1	Prediction	<chem>O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2</chem>
Phenytoin	CCR5	-1	Training	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	CCR5	-1	Training	<chem>Cn2cncc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	CCR5	-1	Training	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	CCR5	-1	Prediction	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	CCR5	-1	Training	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	CCR5	-1	Training	<chem>OC(CCN1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	CCR5	-1	Training	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	CCR5	-1	Prediction	<chem>OC(C(C)NC)c1ccccc1</chem>
Pyrantel	CCR5	-1	Training	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>

Quinidine	CCR5	-1	Training	<chem>COc1cc2c(cc1)nccc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	CCR5	-1	Training	<chem>[O-][N+](=O)C=C(/NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	CCR5	-1	Prediction	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oc4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	CCR5	-1	Training	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	CCR5	-1	Training	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	CCR5	-1	Training	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>
Selegiline	CCR5	-1	Prediction	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>
Sulfinpyrazone	CCR5	-1	Training	<chem>O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	CCR5	-1	Training	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>
Terpin	CCR5	-1	Training	<chem>C[C@@]1(O)CC[C@@H](CC1)C(C)(C)O</chem>
Tolcapone	CCR5	-1	Prediction	<chem>Oc1cc(cc([N+])([O-])=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranylepromine	CCR5	-1	Training	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	CCR5	-1	Training	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	CCR5	-1	Training	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@@]23C</chem>
Valproic acid	CCR5	-1	Prediction	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	CCR5	-1	Training	<chem>O=C(O)[C@@H]10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	CCR5	-1	Training	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	CCR5	-1	Training	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wyntensin	CCR5	-1	Prediction	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	CCR5	-1	Training	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>
Zileuton	CCR5	-1	Training	<chem>NC(=O)N(O)C(C)c1cc2ccccc2s1</chem>
Zonisamide	CCR5	-1	Training	<chem>NS(=O)(=O)Cc2noc1ccccc12</chem>
CHEMBL1242210	CXCR4	1	Training	<chem>CN(Cc1nc2cccc(N3CCN(C)CC3)n2c1CO)[C@H]4CCc5ccnc45</chem>
CHEMBL218806	CXCR4	1	Training	<chem>CN1[C@H](CCCN(C(=N)N)C(=O)N[C@H](Cc2ccc(O)cc2)C(=O)NCC(=O)N[C@@H](Cc3ccc4ccccc4c3)C(=O)N[C@@H](CCCN(C(=N)N)C1=O</chem>
CHEMBL508054	CXCR4	1	Training	<chem>C(S/C(=N/C1CCCCC1)\NC2CCCCC2)C3=CSC4=NCCN34</chem>
CHEMBL1096504	CXCR4	1	Prediction	<chem>CN(C)CCCc1c(CN(C)[C@H]2CCc3ccnc23)ncc4ccccc14</chem>
CHEMBL219474	CXCR4	1	Training	<chem>NC(=N)NCCC[C@@H]1NC(=O)[C@H](CCCN(C(=N)N)NC(=O)[C@H](Cc2ccc3ccccc3c2)NC(=O)CNC(=O)[C@@H](Cc4ccc(O)cc4)NC1=O</chem>
CHEMBL1092637	CXCR4	1	Training	<chem>CC(C)N1CCC[C@H](Cn2c(CN(C)[C@H]3CCc4ccnc34)nc5ccccc25)C1</chem>
CHEMBL454896	CXCR4	1	Training	<chem>C(S/C(=N/C1CCCCC1)\NC2CCCCC2)C3=CSC4=NCCN34</chem>
CHEMBL219339	CXCR4	1	Prediction	<chem>NC(=N)NCCC[C@@H]1NC(=O)[C@H](Cc2ccc3ccccc3c2)NC(=O)CNC(=O)[C@@H](Cc4ccc(O)cc4)NC(=O)[C@@H](CCCN(C(=N)N)NC1=O</chem>

CHEMBL460298	CXCR4	1	Training	C(S\C(=N/C1CCCCC1)\NC2CCCCCCC2)C3=CSC4=NCCN34
CHEMBL518501	CXCR4	1	Training	CC1(C)CN2C(=CSC2=N1)CS\C(=N/C3CCCCC3)\NC4CCCCC4
CHEMBL1682996	CXCR4	1	Training	NCCCCN(Cc1ncccc1N)[C@H]2CCCc3ccnc23
CHEMBL373636	CXCR4	1	Prediction	C[C@H]1NC(=O)[C@@H](Cc2ccc(O)cc2)NC(=O)[C@@H](CCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc3cc4cccc4c3)NC1=O
CHEMBL375990	CXCR4	1	Training	C[C@H]1NC(=O)[C@@H](Cc2ccc(O)cc2)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc3cc4cccc4c3)NC1=O
CHEMBL518924	CXCR4	1	Training	NCCCCN(Cc1nc2ccccc2[nH]1)[C@H]3CCCc4ccnc34
CHEMBL1094864	CXCR4	1	Training	CN(C)CC(=O)NCc1c(CN(C)[C@H]2CCCc3ccnc23)nc4cccc14
CHEMBL1682997	CXCR4	1	Prediction	C[C@H](N(CCCCN)Cc1nc2ccccc2[nH]1)c3cccn3
CHEMBL1644080	CXCR4	1	Training	NCc1ncccc1CN(Cc2nc3ccccc3[nH]2)[C@H]4CCCc5ccnc45
CHEMBL376219	CXCR4	1	Training	CN1[C@@H](CCCNC(=N)N)C(=O)N[C@H](CCCNC(=N)N)C(=O)N[C@H](Cc2ccc(O)cc2)C(=O)NCC(=O)N[C@@H](Cc3ccc4cccc4c3)C1=O
CHEMBL1088913	CXCR4	1	Training	NCCCCN(Cc1nc2ccccc2[nH]1)C3CCCc4ccnc34
CHEMBL374421	CXCR4	1	Prediction	CN1[C@@H](CCCNC(=N)N)C(=O)N[C@H](Cc2ccc(O)cc2)C(=O)NCC(=O)N[C@@H](Cc3ccc4cccc4c3)C(=O)N[C@@H](CCNC(=N)N)C1=O
CHEMBL541728	CXCR4	1	Training	C(S\C(=N/C1CCCCC1)\NC2CCCCCCC2)C3=CSC4=NCCN34
CHEMBL436283	CXCR4	1	Training	NC(=N)NCCC[C@@H]1NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@@H](Cc2ccc(O)cc2)NC(=O)CNC(=O)[C@H](Cc3ccc4cccc4c3)NC1=O
CHEMBL1682998	CXCR4	1	Training	C[C@H](N(CCCCN)Cc1ncccc1C)c2cccn2
CHEMBL1644082	CXCR4	1	Prediction	NCc1cocc1N(Cc2nc3ccccc3[nH]2)[C@H]4CCCc5ccnc45
CHEMBL375991	CXCR4	1	Training	NC(=N)NCCC[C@@H]1NC(=O)[C@H](Cc2ccc3ccccc3c2)NC(=O)CCNC(=O)[C@@H](Cc4ccc(O)cc4)NC(=O)[C@H](CCCNC(=N)N)NC1=O
CHEMBL577268	CXCR4	1	Training	CN(Cc1nc2ccccc2n1CCCN)C3CCCc4ccnc34
CHEMBL452864	CXCR4	1	Training	C(S\C(=N/C1CCCCC1)\NC2CCCCC2)C3=CSC4=NCCN34
CHEMBL516630	CXCR4	1	Prediction	C(S\C(=N/C1CCCCC1)\NC2CCCCC2)C3=CSC4=NCCCN34
CHEMBL1682995	CXCR4	1	Training	Cc1nc(CN(CCCCN)[C@H]2CCCc3ccnc23)c(C)c1
CHEMBL374108	CXCR4	1	Training	C[C@@H]1NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc2ccc(O)cc2)NC(=O)CNC(=O)[C@@H](Cc4ccc(O)cc4)NC1=O
CHEMBL461358	CXCR4	1	Training	CCCCCN\C(=N/C1CCCCC1)\SCC2=CSC3=NCCN23
CHEMBL1091591	CXCR4	1	Prediction	CN(Cc1nc2ccccc2n1C3CCN(C)CC3)C4CCCc5ccnc45
CHEMBL461359	CXCR4	1	Training	C(S\C(=N/C1CCCCC1)\NC2C3CC4CC(CC2C4)C3)C5=CSC6=NCCN56
CHEMBL1644081	CXCR4	1	Training	NCc1cscc1N(Cc2nc3ccccc3[nH]2)[C@H]4CCCc5ccnc45
CHEMBL376811	CXCR4	1	Training	C[C@@H]1NC(=O)[C@@H](Cc2ccc(O)cc2)NC(=O)[C@@H](CCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc3ccc4cccc4c3)NC1=O
CHEMBL1682994	CXCR4	1	Prediction	Cc1cccc(CN(CCCCN)[C@H]2CCCc3ccnc23)n1
CHEMBL436536	CXCR4	1	Training	CN1[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@H](Cc2ccc(O)cc2)C(=O)NCC(=O)N[C@@H](Cc3ccc4cccc4c3)C1=O
CHEMBL506505	CXCR4	1	Training	NC(=N)NCCC[C@@H]1NC(=O)[C@H](Cc2ccc(O)cc2)NC(=

				O)CNC(=O)[C@@H](NC(=O)[C@H](CCCNC(=N)N)NC1=O)c3ccc4cccc4c3
CHEMBL1093137	CXCR4	1	Training	C(NCc1cccn1)c2ccc(CN(Cc3nc4cccc4[nH]3)[C@H]5CCCc6ccnc56)cc2
CHEMBL219096	CXCR4	1	Prediction	CN1[C@H](Cc2ccc(O)cc2)C(=O)NCC(=O)N[C@@H](Cc3ccc4cccc4c3)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCNC(=N)N)C1=O
CHEMBL373440	CXCR4	1	Training	C[C@H]1NC(=O)[C@@H](CCCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc2ccc3cccc3c2)NC(=O)CNC1=O
CHEMBL375993	CXCR4	1	Training	CN1[C@H](Cc2ccc(O)cc2)C(=O)NCC(=O)N[C@@H](Cc3ccc4cccc4c3)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@H](CCCN C(=N)N)C1=O
CHEMBL219075	CXCR4	1	Training	C[C@@H]1NC(=O)CN(C)C(=O)[C@@H](Cc2ccc(O)cc2)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC1=O
CHEMBL387120	CXCR4	1	Prediction	C[C@@H]1NC(=O)[C@@H](Cc2ccc(O)cc2)NC(=O)[C@H](CCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc3ccc4cccc4c3)NC1=O
CHEMBL460299	CXCR4	1	Training	C(S/C(=N/C1CCCC1)\NC2CCCC2)C3=CSC4=NCCN34
CHEMBL1093149	CXCR4	1	Training	NCCCCN(Cc1nc2cccc2[nH]1)[C@@H]3CCCc4ccnc34
CHEMBL384429	CXCR4	1	Training	C[C@H]1NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](Cc2ccc3cccc3c2)NC(=O)CNC(=O)[C@@H](Cc4ccc(O)cc4)NC1=O
CHEMBL375850	CXCR4	1	Prediction	CN1[C@@H](Cc2ccc3cccc3c2)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@H](Cc4ccc(O)cc4)C(=O)NCC1=O
CHEMBL1089434	CXCR4	1	Training	C(NCc1cccn1)c2ccc(CN(Cc3nc4cccc4[nH]3)C5CCCc6ccnc56)cc2
CHEMBL374862	CXCR4	1	Training	CN1CC(=O)N[C@@H](Cc2ccc3cccc3c2)C(=O)N[C@@H](CCNC(=N)N)C(=O)N[C@H](CCCNC(=N)N)C(=O)N[C@H](Cc4ccc(O)cc4)C1=O
CHEMBL219135	CXCR4	1	Training	NC(=N)NCCC[C@@H]1NC(=O)[C@H](Cc2ccc3cccc3c2)NC(=O)CCNC(=O)[C@@H](Cc4ccc(O)cc4)NC(=O)[C@@H](CCCNC(=N)N)NC1=O
CHEMBL462588	CXCR4	1	Prediction	CC(C)(C)C1CCC(CC1)N\C(=N\C2CCCC2)\SCC3=CSC4=NCCN34
CHEMBL426169	CXCR4	1	Training	CN1[C@@H](Cc2ccc3cccc3c2)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@H](CCCNC(=N)N)C(=O)N[C@H](Cc4ccc(O)cc4)C(=O)NCC1=O
CHEMBL373637	CXCR4	1	Training	NC(=N)NCCC[C@@H]1NC(=O)[C@H](Cc2ccc3cccc3c2)NC(=O)[C@@H]4CCCCN4C(=O)[C@@H](Cc5ccc(O)cc5)NC(=O)[C@@H](CCCNC(=N)N)NC1=O
CHEMBL450815	CXCR4	1	Training	CC(C)C[C@H](NC(=N)N)C(=O)Nc1ccc2c(c1)cc(C(=O)NCCc3c[nH]c4cccc34)n2CCCNC(=N)N
CHEMBL508684	CXCR4	1	Prediction	NC(=N)NCCCN1c(cc2cc(NC(=O)[C@H](Cc3cccc3)NC(=N)N)cc12)C(=O)NCCc4c[nH]c5cccc45
CHEMBL518041	CXCR4	1	Training	C(S/C(=N/C1CCCC1)\NC23CC4CC(CC(C4)C2)C3)C5=CSC6=NCCN56
CHEMBL450041	CXCR4	1	Training	CC(C)C[C@@H](NC(=N)N)C(=O)Nc1ccc2c(c1)cc(C(=O)NCCc3c[nH]c4cccc34)n2CCCNC(=N)N
CHEMBL480502	CXCR4	1	Training	NC(=N)NCCc1cc2cc(NC(=O)CCc3ccc(O)cc3)ccc2n1CCc4ccc5ccc5c4
CHEMBL472323	CXCR4	1	Prediction	NC(=N)NCCCN1c(cc2cc(NC(=O)CNC(=N)N)ccc12)C(=O)NCCc

Cefoperazone	CXCR4	-1	Training	<chem>O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O</chem>
Chloral hydrate	CXCR4	-1	Training	<chem>ClC(Cl)(Cl)C(O)O</chem>
Chlordiazepoxide	CXCR4	-1	Training	<chem>Clc1ccc2N=C(C[N+])([O-])=C(c2c1)c3ccccc3)NC</chem>
Chlorpropamide	CXCR4	-1	Prediction	<chem>O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1</chem>
Chlorthalidone	CXCR4	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2ccccc23</chem>
Clidinium	CXCR4	-1	Training	<chem>OC(c1cccc1)(c2ccccc2)C(=O)OC4C[N+](C)CCC4CC3</chem>
Clobazam	CXCR4	-1	Training	<chem>Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3ccccc3</chem>
Clofazimine	CXCR4	-1	Prediction	<chem>Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5</chem>
Clomipramine	CXCR4	-1	Training	<chem>CN(C)CCCN2c3ccccc3CCc1ccc(Cl)cc12</chem>
Clonidine	CXCR4	-1	Training	<chem>Clc2ccccc(Cl)c2N=C1/NCCN1</chem>
Codeine	CXCR4	-1	Training	<chem>COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23</chem>
Colchicine	CXCR4	-1	Prediction	<chem>CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12</chem>
Cyclizine	CXCR4	-1	Training	<chem>CN1CCN(CC1)C(c2ccccc2)c3ccccc3</chem>
Cyclosporin	CXCR4	-1	Training	<chem>CC(C\C=C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C</chem>
Dextropropoxyphene	CXCR4	-1	Training	<chem>CN(C)CC(C)C(OC(=O)CC)(Cc1cccc1)c2ccccc2</chem>
Diazepam	CXCR4	-1	Prediction	<chem>Clc1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3</chem>
Diflucortolone	CXCR4	-1	Training	<chem>OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C</chem>
Dimercaprol	CXCR4	-1	Training	<chem>OCC(S)CS</chem>
Diphenhydramine	CXCR4	-1	Training	<chem>CN(C)CCOC(c1cccc1)c2ccccc2</chem>
Diphenidol	CXCR4	-1	Prediction	<chem>OC(CCCN1CCCC1)(c2ccccc2)c3ccccc3</chem>
Dobutamine	CXCR4	-1	Training	<chem>Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O</chem>
Dofetilide	CXCR4	-1	Training	<chem>CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O</chem>
Domperidone	CXCR4	-1	Training	<chem>Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4</chem>
Dopamine	CXCR4	-1	Prediction	<chem>Oc1ccc(CCN)cc1O</chem>
Doxazosin	CXCR4	-1	Training	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4</chem>
Doxepin	CXCR4	-1	Training	<chem>CN(C)CC\C=C1/c3ccccc3OCc2ccccc12</chem>
Dronabinol	CXCR4	-1	Training	<chem>CCCCC3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3</chem>
Droxicam	CXCR4	-1	Prediction	<chem>O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O</chem>
Entacapone	CXCR4	-1	Training	<chem>Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+])([O-])=O)c1O</chem>
Epinephrine	CXCR4	-1	Training	<chem>Oc1ccc(cc1O)[C@@H](O)CNC</chem>
Eprosartan	CXCR4	-1	Training	<chem>OC(=O)C(/Cc1cccs1)=C/c3cnc(CCCC)n3Cc2ccc(cc2)C(=O)O</chem>
Ergotamine	CXCR4	-1	Prediction	<chem>CN2C[C@@H](C=C1c3ccccc4ncc(C12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O</chem>
Ethosuximide	CXCR4	-1	Training	<chem>CC1(CC)CC(=O)NC1=O</chem>
Fentanyl	CXCR4	-1	Training	<chem>CCC(=O)N(C2CCN(CCc1cccc1)CC2)c3ccccc3</chem>
Fexofenadine	CXCR4	-1	Training	<chem>O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4</chem>

Flecainide	CXCR4	-1	Prediction	<chem>FC(F)(F)COc2cc(C(=O)NCC1CCCN1)c(OCC(F)(F)F)cc2</chem>
Flunarizine	CXCR4	-1	Training	<chem>Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4</chem>
Flunisolide	CXCR4	-1	Training	<chem>OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C</chem>
Fluoxetine	CXCR4	-1	Training	<chem>FC(F)(F)c2ccc(OC(CCNC)c1ccccc1)cc2</chem>
Fluvoxamine	CXCR4	-1	Prediction	<chem>FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN</chem>
Gabapentin	CXCR4	-1	Training	<chem>NCC1(CC(=O)O)CCCCC1</chem>
Gestodene	CXCR4	-1	Training	<chem>O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2</chem>
Glutethimide	CXCR4	-1	Training	<chem>CCC1(CCC(=O)NC1=O)c2ccccc2</chem>
Glycopyrrolate	CXCR4	-1	Prediction	<chem>C[N+]3(C)CCC(OC(=O)C(O)(c1ccccc1)C2CCCC2)C3</chem>
Guanadrel	CXCR4	-1	Training	<chem>N=C(N)NCC2COC1(CCCCC1)O2</chem>
Halofantrine	CXCR4	-1	Training	<chem>CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F</chem>
Haloperidol	CXCR4	-1	Training	<chem>Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3</chem>
Halothane	CXCR4	-1	Prediction	<chem>BrC(Cl)C(F)(F)F</chem>
Hydromorphone	CXCR4	-1	Training	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	CXCR4	-1	Training	<chem>Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	CXCR4	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C</chem>
Indomethacin	CXCR4	-1	Prediction	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	CXCR4	-1	Training	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	CXCR4	-1	Training	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	CXCR4	-1	Training	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	CXCR4	-1	Prediction	<chem>CNC1(CCCCC1=O)c2ccccc2Cl</chem>
Labetalol	CXCR4	-1	Training	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2</chem>
Lacidipine	CXCR4	-1	Training	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	CXCR4	-1	Training	<chem>Clc1cccc(c1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	CXCR4	-1	Prediction	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCNC(=N)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2ccccc23)NC(=O)C(Cc4cncn4)NC(=O)C5CCCC(=O)N5</chem>
Levodopa	CXCR4	-1	Training	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>
Lidocaine	CXCR4	-1	Training	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	CXCR4	-1	Training	<chem>Clc3cc4CCc1cccn1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	CXCR4	-1	Prediction	<chem>CNCCCC24CCC(c1ccccc12)c3ccccc34</chem>
Meclizine	CXCR4	-1	Training	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Medroxyprogesterone	CXCR4	-1	Training	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	CXCR4	-1	Training	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	CXCR4	-1	Prediction	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	CXCR4	-1	Training	<chem>C[C@H](NC)Cc1ccccc1</chem>
Methantheline	CXCR4	-1	Training	<chem>CC[N+](C)(CC)CCOC(=O)C1c3ccccc3Oc2ccccc12</chem>
Methocarbamol	CXCR4	-1	Training	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	CXCR4	-1	Prediction	<chem>ClC(Cl)C(F)(F)OC</chem>

Methscopolamine	CXCR4	-1	Training	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+](C)C</chem>
Methylphenidate	CXCR4	-1	Training	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	CXCR4	-1	Training	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3cccc1c23)N(C)C4</chem>
Metoclopramide	CXCR4	-1	Prediction	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	CXCR4	-1	Training	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	CXCR4	-1	Training	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	CXCR4	-1	Training	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	CXCR4	-1	Prediction	<chem>CC(C)(O)c5ccccc5CC[C@H](SCC1(CC(=O)O)CC1)c2cccc(c2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	CXCR4	-1	Training	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	CXCR4	-1	Training	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@H]45</chem>
Nalmefene	CXCR4	-1	Training	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C[C@N@]3CC2CC2)c45</chem>
Neostigmine	CXCR4	-1	Prediction	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>
Nifedipine	CXCR4	-1	Training	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	CXCR4	-1	Training	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	CXCR4	-1	Training	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	CXCR4	-1	Prediction	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	CXCR4	-1	Training	<chem>CSC[C@H]4CC1C(Cc2cnc3cccc1c23)N(C4)CCC</chem>
Phenylbutazone	CXCR4	-1	Training	<chem>O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2</chem>
Phenytoin	CXCR4	-1	Training	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	CXCR4	-1	Prediction	<chem>Cn2cncc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	CXCR4	-1	Training	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	CXCR4	-1	Training	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	CXCR4	-1	Training	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	CXCR4	-1	Prediction	<chem>OC(CCN1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	CXCR4	-1	Training	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	CXCR4	-1	Training	<chem>OC(C(C)NC)c1ccccc1</chem>
Pyrantel	CXCR4	-1	Training	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>
Quinidine	CXCR4	-1	Prediction	<chem>COc1cc2c(cc1)nccc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	CXCR4	-1	Training	<chem>[O-][N+](=O)C=C(NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	CXCR4	-1	Training	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oc4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	CXCR4	-1	Training	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	CXCR4	-1	Prediction	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	CXCR4	-1	Training	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>
Selegiline	CXCR4	-1	Training	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>
Sulfinpyrazone	CXCR4	-1	Training	<chem>O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	CXCR4	-1	Prediction	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>

Terpin	CXCR4	-1	Training	<chem>C[C@@]1(O)CC[C@@H](CC1)C(C)(C)O</chem>
Tolcapone	CXCR4	-1	Training	<chem>Oc1cc(cc([N+])([O-])=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranylcypromine	CXCR4	-1	Training	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	CXCR4	-1	Prediction	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	CXCR4	-1	Training	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@]23C</chem>
Valproic acid	CXCR4	-1	Training	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	CXCR4	-1	Training	<chem>O=C(O)[C@@H]10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	CXCR4	-1	Prediction	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	CXCR4	-1	Training	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wyntensin	CXCR4	-1	Training	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	CXCR4	-1	Training	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>
Zileuton	CXCR4	-1	Prediction	<chem>NC(=O)N(O)C(C)c1cc2ccccc2s1</chem>
Zonisamide	CXCR4	-1	Training	<chem>NS(=O)(=O)Cc2noc1ccccc12</chem>
CHEMBL433165	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccnc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccc6ccccc56</chem>
CHEMBL76289	HIV-1 PR	1	Training	<chem>CC[C@@H](C)[C@@H](NC(=O)[C@H](C\C=C\C1CCCC1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C(=O)NC3nc4c4ccc4[nH]3</chem>
CHEMBL53254	HIV-1 PR	1	Training	<chem>O[C@@H](C[C@@H](Cc1ccccc1)C(=O)NC2[C@H](O)Cc3cccc23)[C@H](Cc4ccccc4)NC(=O)OC5CCOC5</chem>
CHEMBL52669	HIV-1 PR	1	Prediction	<chem>Cc1cccc(Cl)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45</chem>
CHEMBL421568	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc(Br)cs2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45</chem>
CHEMBL52702	HIV-1 PR	1	Training	<chem>Cc1cccc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45</chem>
CHEMBL319092	HIV-1 PR	1	Training	<chem>O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23)[C@H](Cc4ccccc4)NC(=O)O[C@@H]5CCOC5</chem>
CHEMBL96352	HIV-1 PR	1	Prediction	<chem>CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccnc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccc6ccccc56</chem>
CHEMBL430469	HIV-1 PR	1	Training	<chem>O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23)[C@H](Cc4ccccc4)NC(=O)O[C@H]5CCOC5</chem>
CHEMBL319408	HIV-1 PR	1	Training	<chem>O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23)[C@H](Cc4ccccc4)NC(=O)O[C@H]5CCOC5</chem>
CHEMBL319792	HIV-1 PR	1	Training	<chem>O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23)[C@H](Cc4ccccc4)NC(=O)O[C@@H]5CCOC5</chem>
CHEMBL295414	HIV-1 PR	1	Prediction	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)CC(Cc2ccc(OCC(=O)O)cc2)C(=O)NC3[C@H](O)Cc4ccccc34</chem>
CHEMBL300140	HIV-1 PR	1	Training	<chem>CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccc(s4)c5cccs5)C[C@H]3C(=O)</chem>

				NC(C)(C)C
CHEMBL298189	HIV-1 PR	1	Training	Cc1cccc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45
CHEMBL433270	HIV-1 PR	1	Training	CC1(C)SCN([C@@H]1C(=O)NCc2c(Cl)cccc2Cl)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL96697	HIV-1 PR	1	Prediction	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3secc3s2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56
CHEMBL100310	HIV-1 PR	1	Training	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCC(O)CO
CHEMBL300754	HIV-1 PR	1	Training	Cc1nsc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL96100	HIV-1 PR	1	Training	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3ccsc3s2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56
CHEMBL94824	HIV-1 PR	1	Prediction	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3nc4ccccc4[nH]3
CHEMBL52645	HIV-1 PR	1	Training	Cc1ccccc1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL314510	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](C(=O)NCc3nc4ccccc4[nH]3)c5ccccc5
CHEMBL297720	HIV-1 PR	1	Training	Cc1onc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL79236	HIV-1 PR	1	Prediction	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc6ccccc6c5
CHEMBL49768	HIV-1 PR	1	Training	COCCOCOCOCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1
CHEMBL295442	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCCN3CC[S+](O-])CC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45
CHEMBL416082	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCCN3CCS(=O)(=O)CC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45
CHEMBL312238	HIV-1 PR	1	Prediction	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)C(C)(C)c5oc6ccccc6c5
CHEMBL297294	HIV-1 PR	1	Training	COC(CCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1)OC
CHEMBL316454	HIV-1 PR	1	Training	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3secc3s2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56
CHEMBL295549	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCCO)cc2)C(=O)NC3[C@H](O)Cc4ccccc34
CHEMBL419923	HIV-1 PR	1	Prediction	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)[C@H](O)c4ccccc34
CHEMBL44489	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H]

				(Ce2ccc(CCCO)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL293992	HIV-1 PR	1	Training	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc5ccccc5s4)C[C@H]3C(=O)NC(C)(C)C
CHEMBL285759	HIV-1 PR	1	Training	CC(C)[C@]1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C
CHEMBL318777	HIV-1 PR	1	Prediction	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc(Br)cs2)CCN1C[C@@H](O)C[C@@H](Cc3ccncc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45
CHEMBL294392	HIV-1 PR	1	Training	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc5ccsc5s4)C[C@H]3C(=O)NC(C)(C)C
CHEMBL96645	HIV-1 PR	1	Training	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3ccsc3s2)CCN1C[C@@H](O)C[C@@H](Cc4ccncc4)C(=O)N[C@@H]5[C@H](O)Cc6cccc56
CHEMBL297066	HIV-1 PR	1	Training	COCCOCOCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)N)C(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1
CHEMBL301571	HIV-1 PR	1	Prediction	Cc1ccncc1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL318525	HIV-1 PR	1	Training	CC(C)(C)NC(=O)[C@@H]1CN(Cc2c(F)cccc2F)CCN1C[C@@H](O)C[C@@H](Cc3ccncc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45
CHEMBL311953	HIV-1 PR	1	Training	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)C(F)(F)F)c5oc6ccncc6c5
CHEMBL295470	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(O)cc1)[C@@H](O)C[C@@H](Cc2ccc(O)cc2)C(=O)NC3[C@H](O)Cc4ccccc34
CHEMBL431999	HIV-1 PR	1	Prediction	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCC(O)CO
CHEMBL299884	HIV-1 PR	1	Training	Cc1ccncc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL298316	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(O)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL291196	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(CCO)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL290987	HIV-1 PR	1	Prediction	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(O)cc2)C(=O)NC3[C@H](O)Cc4ccccc34
CHEMBL295530	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C\C=C\c2ccc(O)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL47610	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](CCc2enc3ccccc3n2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45
CHEMBL46114	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(CO)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL295471	HIV-1 PR	1	Prediction	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(cc2)S(=O)(=O)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL111143	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34
CHEMBL45451	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCc3ccccc3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45

CHEMBL292193	HIV-1 PR	1	Training	<chem>CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc(Br)cs4)C[C@H]3C(=O)NC(C)(C)C</chem>
CHEMBL322984	HIV-1 PR	1	Prediction	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](CCc2ccccc2)C(=O)N[C@@H]3[C@H](O)[C@H](O)c4ccccc34</chem>
CHEMBL77786	HIV-1 PR	1	Training	<chem>CC(C)C1(CCc2csc(CO)c2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C</chem>
CHEMBL48565	HIV-1 PR	1	Training	<chem>CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccccc4)C(C)C</chem>
CHEMBL297673	HIV-1 PR	1	Training	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCC(=O)N3CCOCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45</chem>
CHEMBL46274	HIV-1 PR	1	Prediction	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCC[N+](=O)[O-])CCOCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45</chem>
CHEMBL276447	HIV-1 PR	1	Training	<chem>CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3nc4ccccc4[nH]3</chem>
CHEMBL44578	HIV-1 PR	1	Training	<chem>CN1CCN(CCOc2ccc(C[C@H](C[C@H](O)[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C)C(=O)NC4[C@H](O)Cc5ccccc45)cc2)CC1</chem>
CHEMBL99267	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccccc5c4)NC(=O)C(F)(F)F</chem>
CHEMBL100040	HIV-1 PR	1	Prediction	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc(F)cc4)NC(=O)C(F)(F)F</chem>
CHEMBL98589	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccccc5c4)NS(=O)(=O)C</chem>
CHEMBL297189	HIV-1 PR	1	Training	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(O)c2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34</chem>
CHEMBL95228	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccccc5c4)NC(=O)C(F)(F)F</chem>
CHEMBL98954	HIV-1 PR	1	Prediction	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc(F)cc4)NS(=O)(=O)C</chem>
CHEMBL9544	HIV-1 PR	1	Training	<chem>CC(C)C(NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@@H](O)[C@H](Cc3ccccc3)NC(=O)C(NC(=O)OCc4ccccc4)C(C)C</chem>
CHEMBL9705	HIV-1 PR	1	Training	<chem>CC(C)C(NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@@H](O)[C@H](Cc3ccccc3)NC(=O)C(NC(=O)OCc4ccccc4)C(C)C</chem>
CHEMBL295357	HIV-1 PR	1	Training	<chem>CSc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1</chem>
CHEMBL265514	HIV-1 PR	1	Prediction	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C/C=C/c2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34</chem>
CHEMBL413515	HIV-1 PR	1	Training	<chem>CN(C)c1ccc(CNC(=O)[C@@H](NC(=O)c2ccccc2c3ccccc3)[C@@H]4N[C@@H](C(=O)NCCNC(=O)[C@@H]5N[C@H](SC5(C)C)[C@H](NC(=O)c6ccccc6c7ccccc7)C(=O)NCc8ccc(cc8)N(C)C)C(C)(C)S4)cc1</chem>
CHEMBL296115	HIV-1 PR	1	Training	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H]</chem>

				(Ce2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL47480	HIV-1 PR	1	Training	CC(C)C[C@H](NC(=O)[C@H](C\C=C\c1ccccc1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C(=O)N[C@@H](Cc3ccccc3)C(=O)N
CHEMBL77497	HIV-1 PR	1	Prediction	CC(C)C1(CCc2cnsc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C
CHEMBL52670	HIV-1 PR	1	Training	CC1(C)SCN([C@@H]1C(=O)NCc2c(F)cccc2F)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5cccc45
CHEMBL329750	HIV-1 PR	1	Training	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccc3
CHEMBL410311	HIV-1 PR	1	Training	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccc(Br)s4)C[C@H]3C(=O)NC(C)(C)C
CHEMBL108918	HIV-1 PR	1	Prediction	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](CSc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL164045	HIV-1 PR	1	Training	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](CSc2ccc3ccccc3c2)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4
CHEMBL351834	HIV-1 PR	1	Training	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](CSc3ccc4ccccc4c3)NC(=O)[C@H](CC(=O)N)NC(=O)c5ccc6ccccc6n5
CHEMBL296484	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(cc2)C(F)(F)F)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL297620	HIV-1 PR	1	Prediction	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(cc2)C(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL295904	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(cc2)[N+](=O)[O-])C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL298393	HIV-1 PR	1	Training	Cc1cccc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45
CHEMBL305814	HIV-1 PR	1	Training	CC(C)C1(CCc2cc[nH]n2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C
CHEMBL295924	HIV-1 PR	1	Prediction	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C\C=C\c2ccc(CCN3CCOCC3)cc2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45
CHEMBL265516	HIV-1 PR	1	Training	Cc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1
CHEMBL308780	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@H](Cc1ccccc1)C(O)C[C@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34
CHEMBL296493	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(N)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34
CHEMBL301269	HIV-1 PR	1	Prediction	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc5ccccc5s4)C[C@H]3C(=O)NC(C)(C)C
CHEMBL101560	HIV-1 PR	1	Training	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23)[C@H](Cc4ccccc4)NC(=O)OC5CCCC5
CHEMBL78261	HIV-1 PR	1	Training	CC(C)C1(CCc2cocc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C
CHEMBL277908	HIV-1 PR	1	Training	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34

CHEMBL77431	HIV-1 PR	1	Prediction	<chem>CC(C)C1(CCc2cccs2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C</chem>
CHEMBL297045	HIV-1 PR	1	Training	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccc(O)cc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34</chem>
CHEMBL291195	HIV-1 PR	1	Training	<chem>CC(C)C[C@H](NC(=O)[C@H](CCCc1ccccc1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)N</chem>
CHEMBL82245	HIV-1 PR	1	Training	<chem>CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NC5CCCC5)c6oc7cncnc7c6</chem>
CHEMBL429722	HIV-1 PR	1	Prediction	<chem>CC(C)C(NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)C(NC(=O)OCc4ccccc4)C(C)C</chem>
CHEMBL310417	HIV-1 PR	1	Training	<chem>CC(C)CNC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)C(C)(C)c5oc6cncnc6c5</chem>
CHEMBL49002	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)c4ccc5ccccc5c4)NS(=O)(=O)C</chem>
CHEMBL73880	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@H]1C[C@@H]2CCCC[C@@H]2CN1CC(O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4</chem>
CHEMBL115	HIV-1 PR	1	Prediction	<chem>CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccccc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45</chem>
CHEMBL265975	HIV-1 PR	1	Training	<chem>CC(C)C1(CCc2cscc2C)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C</chem>
CHEMBL289195	HIV-1 PR	1	Training	<chem>CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)N[C@@H](Cc3ccccc3)C(=O)N</chem>
CHEMBL99357	HIV-1 PR	1	Training	<chem>CC(=O)N[C@H](CS(=O)(=O)c1cccc2ccccc12)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCSC[C@H]5C[C@H]4C(=O)NC(C)(C)C</chem>
CHEMBL75363	HIV-1 PR	1	Prediction	<chem>CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C</chem>
CHEMBL49544	HIV-1 PR	1	Training	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(CCCN3CCOCC3)cc2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45</chem>
CHEMBL298788	HIV-1 PR	1	Training	<chem>CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccc(cc2)c3ccccc3)C(=O)N[C@@H](Cc4ccccc4)C(=O)N</chem>
CHEMBL95413	HIV-1 PR	1	Training	<chem>CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCO</chem>
CHEMBL296137	HIV-1 PR	1	Prediction	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(F)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34</chem>
CHEMBL202345	HIV-1 PR	1	Training	<chem>O[C@@H](C[C@]1(Cc2ccccc2)N=CC(=C1O)C3C4OC(=O)N[C@@H]4c5ccccc35)[C@H](Cc6ccccc6)NC(=O)O[C@H]7CCOC7</chem>
CHEMBL306963	HIV-1 PR	1	Training	<chem>CC(C)C1(CCc2nc(C)cs2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C</chem>
CHEMBL97253	HIV-1 PR	1	Training	<chem>CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCN</chem>
CHEMBL98129	HIV-1 PR	1	Prediction	<chem>CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCO</chem>

CHEMBL47712	HIV-1 PR	1	Training	<chem>CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCCN3CCSCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45</chem>
CHEMBL60697	HIV-1 PR	1	Training	<chem>CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4csc5ccc(Cl)cc45)C[C@H]3C(=O)NC(C)(C)C</chem>
CHEMBL319053	HIV-1 PR	1	Training	<chem>CC(C)(C)NC(=O)[C@@H]1CN(Cc2c(F)cccc2F)CCN1C[C@@H](O)C[C@@H](Cc3cncnc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45</chem>
CHEMBL100089	HIV-1 PR	1	Prediction	<chem>CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc5ccccc5c4)NS(=O)(=O)C</chem>
CHEMBL432550	HIV-1 PR	1	Training	<chem>CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC5CC5)c6oc7cncnc7c6</chem>
CHEMBL316694	HIV-1 PR	1	Training	<chem>CC(=O)N[C@H](CS(=O)(=O)c1ccc2ccccc2c1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCS[C@H]5C[C@H]4C(=O)NC(C)(C)C</chem>
Aceclofenac	HIV-1 PR	-1	Training	<chem>Clc2cccc(Cl)c2Nc1cccc1CC(=O)OCC(=O)O</chem>
Acetaminophen	HIV-1 PR	-1	Prediction	<chem>Oc1ccc(NC(C)=O)cc1</chem>
Acetazolamide	HIV-1 PR	-1	Training	<chem>O=S(N)(=O)c1nnc(NC(C)=O)s1</chem>
Acetophenazine	HIV-1 PR	-1	Training	<chem>CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2</chem>
Amantadine	HIV-1 PR	-1	Training	<chem>NC13CC2CC(CC(C1)C2)C3</chem>
Ambenonium	HIV-1 PR	-1	Prediction	<chem>Clc2ccccc2C[N+](CC)(CC)CCNC(=O)C(=O)NCC[N+](Cc1ccccc1Cl)(CC)CC</chem>
Amineptine	HIV-1 PR	-1	Training	<chem>O=C(O)CCCCCNC2c3ccccc3CCc1ccccc12</chem>
Amiodarone	HIV-1 PR	-1	Training	<chem>CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC</chem>
Amitriptyline	HIV-1 PR	-1	Training	<chem>CN(C)CC\C=C\c3ccccc3CCc2ccccc12</chem>
Aprobarbital	HIV-1 PR	-1	Prediction	<chem>O=C1NC(=O)NC(=O)C1(CC=C)C(C)C</chem>
Artane	HIV-1 PR	-1	Training	<chem>OC(CCN1CCCCC1)(c2ccccc2)C3CCCCC3</chem>
Aspirin	HIV-1 PR	-1	Training	<chem>O=C(C)Oc1ccccc1C(=O)O</chem>
Atenolol	HIV-1 PR	-1	Training	<chem>CC(C)NCC(O)COc1ccc(cc1)CC(N)=O</chem>
Atropine	HIV-1 PR	-1	Prediction	<chem>CN3C1CCC3C[C@@H](C1)OC(=O)C(CO)c2ccccc2</chem>
Baclofen	HIV-1 PR	-1	Training	<chem>Clc1ccc(cc1)C(CN)CC(=O)O</chem>
Beclomethasone	HIV-1 PR	-1	Training	<chem>OCC(=O)[C@@]4(O)[C@@H](C)CC3C2CCC1=CC(=O)C=C[C@@]1(C)[C@@]2(Cl)[C@@H](O)C[C@@]34C</chem>
Benzonatate	HIV-1 PR	-1	Training	<chem>O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NCCC)cc1</chem>
Biperiden	HIV-1 PR	-1	Prediction	<chem>OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3</chem>
Bromocriptine	HIV-1 PR	-1	Training	<chem>BrC3nc2cccc1C4=C[C@H](CN(C)C4Cc3c12)C(=O)N[C@@]7(O[C@]6(O)N([C@@H](CC(C)C)C(=O)N5CCCC56)C7=O)C(C)C</chem>
Bucizine	HIV-1 PR	-1	Training	<chem>CC(C)(C)c1ccc(cc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Budesonide	HIV-1 PR	-1	Training	<chem>OCC(=O)[C@@]53OC(O[C@@H]5CC2C1CCC4=CC(=O)C=C[C@@]4(C)C1[C@@H](O)C[C@@]23C)CCC</chem>
Buprenorphine	HIV-1 PR	-1	Prediction	<chem>CC(C)(C)C(C)(O)[C@H]1C[C@]75CC[C@]1(OC)[C@@H]2Oc4c(O)ccc3C[C@H]7[N@](CC[C@]25c34)CC6CC6</chem>
Caffeine	HIV-1 PR	-1	Training	<chem>O=C2c1n(C)cnc1N(C)C(=O)N2C</chem>
Cantil	HIV-1 PR	-1	Training	<chem>O=C(OC1CCC[N+](C)(C)C1)C(O)(c2ccccc2)c3ccccc3</chem>
Carbachol	HIV-1 PR	-1	Training	<chem>C[N+](C)(C)CCOC(=O)N</chem>

Carbamazepine	HIV-1 PR	-1	Prediction	<chem>NC(=O)N2c3ccccc3C=Cc1ccccc12</chem>
Carisoprodol	HIV-1 PR	-1	Training	<chem>O=C(NC(C)C)OCC(C)(COC(=O)N)CCC</chem>
Carvedilol	HIV-1 PR	-1	Training	<chem>COc4ccccc4OCCNCC(O)COc2cccc3nc1ccccc1c23</chem>
Cefoperazone	HIV-1 PR	-1	Training	<chem>O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O</chem>
Chloral hydrate	HIV-1 PR	-1	Prediction	<chem>ClC(Cl)(Cl)C(O)O</chem>
Chlordiazepoxide	HIV-1 PR	-1	Training	<chem>Clc1ccc2N=C(C[N+])([O-])=C(c2c1)c3ccccc3)NC</chem>
Chlorpropamide	HIV-1 PR	-1	Training	<chem>O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1</chem>
Chlorthalidone	HIV-1 PR	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2ccccc23</chem>
Clidinium	HIV-1 PR	-1	Prediction	<chem>OC(c1ccccc1)(c2ccccc2)C(=O)OC4C[N+](C)(CCC4CC3</chem>
Clobazam	HIV-1 PR	-1	Training	<chem>Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3ccccc3</chem>
Clofazimine	HIV-1 PR	-1	Training	<chem>Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5</chem>
Clomipramine	HIV-1 PR	-1	Training	<chem>CN(C)CCCN2c3ccccc3CCc1ccc(Cl)cc12</chem>
Clonidine	HIV-1 PR	-1	Prediction	<chem>Clc2ccccc(Cl)c2N=C1/NCCN1</chem>
Codeine	HIV-1 PR	-1	Training	<chem>COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23</chem>
Colchicine	HIV-1 PR	-1	Training	<chem>CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12</chem>
Cyclizine	HIV-1 PR	-1	Training	<chem>CN1CCN(CC1)C(c2ccccc2)c3ccccc3</chem>
Cyclosporin	HIV-1 PR	-1	Prediction	<chem>CC(C\C=C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C</chem>
Dextropropoxyphene	HIV-1 PR	-1	Training	<chem>CN(C)CC(C)C(OC(=O)CC)(Cc1ccccc1)c2ccccc2</chem>
Diazepam	HIV-1 PR	-1	Training	<chem>Clc1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3</chem>
Diflucortolone	HIV-1 PR	-1	Training	<chem>OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C</chem>
Dimercaprol	HIV-1 PR	-1	Prediction	<chem>OCC(S)CS</chem>
Diphenhydramine	HIV-1 PR	-1	Training	<chem>CN(C)CCOC(c1ccccc1)c2ccccc2</chem>
Diphenidol	HIV-1 PR	-1	Training	<chem>OC(CCCN1CCCCC1)(c2ccccc2)c3ccccc3</chem>
Dobutamine	HIV-1 PR	-1	Training	<chem>Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O</chem>
Dofetilide	HIV-1 PR	-1	Prediction	<chem>CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O</chem>
Domperidone	HIV-1 PR	-1	Training	<chem>Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4</chem>
Dopamine	HIV-1 PR	-1	Training	<chem>Oc1ccc(CCN)cc1O</chem>
Doxazosin	HIV-1 PR	-1	Training	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4</chem>
Doxepin	HIV-1 PR	-1	Prediction	<chem>CN(C)CC\C=C1/c3ccccc3OCc2ccccc12</chem>
Dronabinol	HIV-1 PR	-1	Training	<chem>CCCCCc3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3</chem>
Droxicam	HIV-1 PR	-1	Training	<chem>O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O</chem>
Entacapone	HIV-1 PR	-1	Training	<chem>Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+])([O-])=O)c1O</chem>
Epinephrine	HIV-1 PR	-1	Prediction	<chem>Oc1ccc(cc1O)[C@@H](O)CNC</chem>
Eprosartan	HIV-1 PR	-1	Training	<chem>OC(=O)C(/Cc1cccs1)=C/c3cnc(CCCC)n3Cc2ccc(cc2)C(=O)O</chem>
Ergotamine	HIV-1 PR	-1	Training	<chem>CN2C[C@@H](C=C1c3ccccc4ncc(CC12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O</chem>

Ethosuximide	HIV-1 PR	-1	Training	<chem>CC1(CC)CC(=O)NC1=O</chem>
Fentanyl	HIV-1 PR	-1	Prediction	<chem>CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3</chem>
Fexofenadine	HIV-1 PR	-1	Training	<chem>O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4</chem>
Flecainide	HIV-1 PR	-1	Training	<chem>FC(F)(F)COc2cc(C(=O)NCC1CCCCN1)c(OCC(F)(F)F)cc2</chem>
Flunarizine	HIV-1 PR	-1	Training	<chem>Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4</chem>
Flunisolide	HIV-1 PR	-1	Prediction	<chem>OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C</chem>
Fluoxetine	HIV-1 PR	-1	Training	<chem>FC(F)(F)c2ccc(OC(CCNC)c1ccccc1)cc2</chem>
Fluvoxamine	HIV-1 PR	-1	Training	<chem>FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN</chem>
Gabapentin	HIV-1 PR	-1	Training	<chem>NCC1(CC(=O)O)CCCCC1</chem>
Gestodene	HIV-1 PR	-1	Prediction	<chem>O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2</chem>
Glutethimide	HIV-1 PR	-1	Training	<chem>CCC1(CCC(=O)NC1=O)c2ccccc2</chem>
Glycopyrrolate	HIV-1 PR	-1	Training	<chem>C[N+]3(C)CCC(OC(=O)C(O)(c1ccccc1)C2CCCC2)C3</chem>
Guanadrel	HIV-1 PR	-1	Training	<chem>N=C(N)NCC2COC1(CCCCC1)O2</chem>
Halofantrine	HIV-1 PR	-1	Prediction	<chem>CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F</chem>
Haloperidol	HIV-1 PR	-1	Training	<chem>Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3</chem>
Halothane	HIV-1 PR	-1	Training	<chem>BrC(Cl)C(F)(F)F</chem>
Hydromorphone	HIV-1 PR	-1	Training	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	HIV-1 PR	-1	Prediction	<chem>Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	HIV-1 PR	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C</chem>
Indomethacin	HIV-1 PR	-1	Training	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	HIV-1 PR	-1	Training	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	HIV-1 PR	-1	Prediction	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	HIV-1 PR	-1	Training	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	HIV-1 PR	-1	Training	<chem>CNC1(CCCCC1=O)c2ccccc2Cl</chem>
Labetalol	HIV-1 PR	-1	Training	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2</chem>
Lacidipine	HIV-1 PR	-1	Prediction	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	HIV-1 PR	-1	Training	<chem>Clc1ccccc1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	HIV-1 PR	-1	Training	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCNC(=N)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2ccccc23)NC(=O)C(Cc4cncn4)NC(=O)C5CCCC(=O)N5</chem>
Levodopa	HIV-1 PR	-1	Training	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>
Lidocaine	HIV-1 PR	-1	Prediction	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	HIV-1 PR	-1	Training	<chem>Clc3cc4CCc1cccn1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	HIV-1 PR	-1	Training	<chem>CNCCCC24CCC(c1ccccc12)c3ccccc34</chem>
Meclizine	HIV-1 PR	-1	Training	<chem>Cc1ccccc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Medroxyprogesterone	HIV-1 PR	-1	Prediction	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	HIV-1 PR	-1	Training	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	HIV-1 PR	-1	Training	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	HIV-1 PR	-1	Training	<chem>C[C@H](NC)Cc1ccccc1</chem>

Methantheline	HIV-1 PR	-1	Prediction	<chem>CC[N+](C)(CC)CCOC(=O)C1c3ccccc3Oc2ccccc12</chem>
Methocarbamol	HIV-1 PR	-1	Training	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	HIV-1 PR	-1	Training	<chem>ClC(Cl)C(F)(F)OC</chem>
Methscopolamine	HIV-1 PR	-1	Training	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+](C)C</chem>
Methylphenidate	HIV-1 PR	-1	Prediction	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	HIV-1 PR	-1	Training	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3ccccc1c23)N(C)C4</chem>
Metoclopramide	HIV-1 PR	-1	Training	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	HIV-1 PR	-1	Training	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	HIV-1 PR	-1	Prediction	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	HIV-1 PR	-1	Training	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	HIV-1 PR	-1	Training	<chem>CC(C)(O)c5ccccc5CC[C@H](SCC1(CC(=O)O)CC1)c2cccc(c2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	HIV-1 PR	-1	Training	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	HIV-1 PR	-1	Prediction	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@@H]45</chem>
Nalmefene	HIV-1 PR	-1	Training	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C[C@N@]3CC2CC2)c45</chem>
Neostigmine	HIV-1 PR	-1	Training	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>
Nifedipine	HIV-1 PR	-1	Training	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	HIV-1 PR	-1	Prediction	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	HIV-1 PR	-1	Training	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	HIV-1 PR	-1	Training	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	HIV-1 PR	-1	Training	<chem>CSC[C@@H]4CC1C(Cc2cnc3ccccc1c23)N(C4)CCC</chem>
Phenylbutazone	HIV-1 PR	-1	Prediction	<chem>O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2</chem>
Phenytoin	HIV-1 PR	-1	Training	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	HIV-1 PR	-1	Training	<chem>Cn2cncc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	HIV-1 PR	-1	Training	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	HIV-1 PR	-1	Prediction	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	HIV-1 PR	-1	Training	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	HIV-1 PR	-1	Training	<chem>OC(CCN1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	HIV-1 PR	-1	Training	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	HIV-1 PR	-1	Prediction	<chem>OC(C(C)NC)c1ccccc1</chem>
Pyrantel	HIV-1 PR	-1	Training	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>
Quinidine	HIV-1 PR	-1	Training	<chem>COc1cc2c(cc1)nccc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	HIV-1 PR	-1	Training	<chem>[O-][N+](=O)C=C(/NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	HIV-1 PR	-1	Prediction	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oc4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	HIV-1 PR	-1	Training	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	HIV-1 PR	-1	Training	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	HIV-1 PR	-1	Training	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>

Selegiline	HIV-1 PR	-1	Prediction	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>
Sulfinpyrazone	HIV-1 PR	-1	Training	<chem>O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	HIV-1 PR	-1	Training	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>
Terpin	HIV-1 PR	-1	Training	<chem>C[C@@]1(O)CC[C@@H](CC1)C(C)(C)O</chem>
Tolcapone	HIV-1 PR	-1	Prediction	<chem>Oc1cc(cc([N+])([O-])=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranylcypromine	HIV-1 PR	-1	Training	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	HIV-1 PR	-1	Training	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	HIV-1 PR	-1	Training	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@]23C</chem>
Valproic acid	HIV-1 PR	-1	Prediction	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	HIV-1 PR	-1	Training	<chem>O=C(O)[C@@H]10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	HIV-1 PR	-1	Training	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	HIV-1 PR	-1	Training	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wytenzin	HIV-1 PR	-1	Prediction	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	HIV-1 PR	-1	Training	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>
Zileuton	HIV-1 PR	-1	Training	<chem>NC(=O)N(O)C(C)c1cc2ccccc2s1</chem>
Zonisamide	HIV-1 PR	-1	Training	<chem>NS(=O)(=O)Cc2noc1ccccc12</chem>
CHEMBL338099	HIV-1 RT	1	Training	<chem>Cc1nc(CCCCCC(=O)c2ccccc2)n3nc(ccc13)n4ccnc4</chem>
CHEMBL88677	HIV-1 RT	1	Training	<chem>Fc1cccc(F)c1CC\N=C(/S)\Nc2ccc(Br)cn2</chem>
CHEMBL132756	HIV-1 RT	1	Prediction	<chem>COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1C#N</chem>
CHEMBL253186	HIV-1 RT	1	Training	<chem>COc1ccc(OC)c(CCNC(=S)Nc2ccc(Cl)cn2)c1F</chem>
CHEMBL135380	HIV-1 RT	1	Training	<chem>Clc1ccc(NC(=S)NCCN2C(=O)c3ccccc3C2=O)nc1</chem>
CHEMBL57	HIV-1 RT	1	Training	<chem>Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12</chem>
CHEMBL37024	HIV-1 RT	1	Prediction	<chem>CCOc1ccc(F)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1F</chem>
CHEMBL37835	HIV-1 RT	1	Training	<chem>CCOc1ccc(Cl)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1F</chem>
CHEMBL541204	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(C2CC2NC(=O)Nc3ccc(Cl)cn3)c1F</chem>
CHEMBL436376	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1C#N</chem>
CHEMBL436177	HIV-1 RT	1	Prediction	<chem>CCOc1ccc(Cl)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1F</chem>
CHEMBL103706	HIV-1 RT	1	Training	<chem>Fc1cc(F)c(CC\N=C(/S)\Nc2ccc(Cl)cn2)c(F)c1</chem>
CHEMBL341201	HIV-1 RT	1	Training	<chem>Clc1ccc(NC(=S)NCCN2C(=O)c3c(Cl)ccc(Cl)c3C2=O)nc1</chem>
CHEMBL37762	HIV-1 RT	1	Training	<chem>Fc1cccc(F)c1[C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3</chem>
CHEMBL38341	HIV-1 RT	1	Prediction	<chem>COc1ccc(OC)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1F</chem>
CHEMBL408273	HIV-1 RT	1	Training	<chem>CC[C@@H]1NC(=O)C([C@H](O)[C@H](C)C\C=C\C)N(C)C(=O)[C@H](C(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](C)NC(=O)[C@H](C)NC(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](NC(=O)[C@H](CC(C)C)N(C)C(=O)C(SCCN(CC)CC)N(C)C1=O)C(C)C</chem>
CHEMBL134278	HIV-1 RT	1	Training	<chem>CCC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(Cl)cn3)c1O</chem>
CHEMBL133658	HIV-1 RT	1	Training	<chem>CCOc1ccc(Cl)c(C2CC2NC(=O)Nc3ccc(cn3)C#N)c1F</chem>
CHEMBL382553	HIV-1 RT	1	Prediction	<chem>Cc1c(Cl)cccc1n2nnnc2SCC(=O)Nc3ccccc3[N+](=O)[O-]</chem>
CHEMBL435600	HIV-1 RT	1	Training	<chem>COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(cn2)C#N)c1C#N</chem>

CHEMBL398766	HIV-1 RT	1	Training	<chem>Cc1ccc(NC(=S)NCCc2c(F)cccc2F)nc1</chem>
CHEMBL207512	HIV-1 RT	1	Training	<chem>Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3Cl)C(=O)N</chem>
CHEMBL334983	HIV-1 RT	1	Prediction	<chem>COc1ccc(F)c(F)c1CC\N=C(/S)\Nc2ccc(Br)cn2</chem>
CHEMBL207839	HIV-1 RT	1	Training	<chem>Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3cccc3[N+](=O)[O-]</chem>
CHEMBL133195	HIV-1 RT	1	Training	<chem>Brclccc(NC(=S)NCCn2nc3cccc3n2)nc1</chem>
CHEMBL206522	HIV-1 RT	1	Training	<chem>NS(=O)(=O)c1ccc(NC(=O)CSc2nnnn2c3cc(Cl)ccc3Cl)c(Cl)c1</chem>
CHEMBL381134	HIV-1 RT	1	Prediction	<chem>Cc1ccc(c(Br)c1)n2nnnc2SCC(=O)Nc3cccc3[N+](=O)[O-]</chem>
CHEMBL56135	HIV-1 RT	1	Training	<chem>Cc1cc(Br)cc(c1)S(=O)(=O)c2cccc(N)c2C#N</chem>
CHEMBL287317	HIV-1 RT	1	Training	<chem>COc1ccc(OC)c(CCNC(=O)Nc2ccc(Cl)cn2)c1F</chem>
CHEMBL133559	HIV-1 RT	1	Training	<chem>CC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(Br)cn3)c1O</chem>
CHEMBL134026	HIV-1 RT	1	Prediction	<chem>CCC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(Br)cn3)c1O</chem>
CHEMBL36424	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(CCNC(=O)Nc2ccc(Br)cn2)c1Cl</chem>
CHEMBL253169	HIV-1 RT	1	Training	<chem>COCc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F</chem>
CHEMBL205152	HIV-1 RT	1	Training	<chem>Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(Cl)cc3[N+](=O)[O-]</chem>
CHEMBL379722	HIV-1 RT	1	Prediction	<chem>Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3Cl)S(=O)(=O)N</chem>
CHEMBL252964	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F</chem>
CHEMBL207929	HIV-1 RT	1	Training	<chem>[O-][N+](=O)c1cccc1NC(=O)CSc2nnnn2c3cc(Cl)ccc3Cl</chem>
CHEMBL38318	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c([C@H]2C[C@H]2NC(=O)Nc3ccc(cn3)C#N)c1Cl</chem>
CHEMBL206962	HIV-1 RT	1	Prediction	<chem>[O-][N+](=O)c1cccc1NC(=O)CSc2nnnn2c3c(Cl)cccc3Cl</chem>
CHEMBL134630	HIV-1 RT	1	Training	<chem>Fe1ccoc1CC\N=C(/S)\Nc2ccc(Cl)cn2</chem>
CHEMBL340047	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(C2CC2NC(=O)Nc3ccc(cn3)C#N)c1Cl</chem>
CHEMBL399976	HIV-1 RT	1	Training	<chem>CCOc1cccc(F)c1CCNC(=S)Nc2ccc(C)cn2</chem>
CHEMBL377010	HIV-1 RT	1	Prediction	<chem>Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3cccc3Cl</chem>
CHEMBL135254	HIV-1 RT	1	Training	<chem>COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Cl)cn2)c1C#N</chem>
CHEMBL236161	HIV-1 RT	1	Training	<chem>CC(C1=C(C)C(=O)NC(=N1)SC2CCCC2)c3c(F)cccc3F</chem>
CHEMBL253822	HIV-1 RT	1	Training	<chem>COc1ccc(OC)c(CCNC(=S)Nc2ccc(Cl)cn2)c1</chem>
CHEMBL399503	HIV-1 RT	1	Prediction	<chem>CCOc1ccc(OC)c(CCNC(=S)Nc2ccc(Cl)cn2)c1F</chem>
CHEMBL207920	HIV-1 RT	1	Training	<chem>CN(C)CCNC(=O)c1ccc(NC(=O)CSc2nnnn2c3c(C)cc(C)cc3C)c(Cl)c1</chem>
CHEMBL306904	HIV-1 RT	1	Training	<chem>CC1CN2C(=S)Nc3ccc(Cl)c(CN1CC=C(C)C)c23</chem>
CHEMBL402265	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(F)c1CCNC(=S)Nc2ccc(Br)cn2</chem>
CHEMBL429488	HIV-1 RT	1	Prediction	<chem>CCOc1ccc(F)c(CCNC(=S)Nc2ccc(en2)C#N)c1Cl</chem>
CHEMBL135259	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(CC\N=C(/S)\N[n+]2ccc(Cl)cn2)c1Cl</chem>
CHEMBL400547	HIV-1 RT	1	Training	<chem>CCc1csc(NC(=S)NCCc2c(F)cccc2F)n1</chem>
CHEMBL207900	HIV-1 RT	1	Training	<chem>[O-][N+](=O)c1cccc1NC(=O)CSc2nnnn2c3cccc4cccc34</chem>
CHEMBL291983	HIV-1 RT	1	Prediction	<chem>Cc1cc(Cl)cc(c1)S(=O)(=O)c2cccc(N)c2C#N</chem>
CHEMBL131972	HIV-1 RT	1	Training	<chem>CCOc1ccc(Cl)c(C2CC2NC(=O)Nc3cc(Cl)cnn3)c1F</chem>
CHEMBL135105	HIV-1 RT	1	Training	<chem>CC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(cn3)C#N)c1O</chem>
CHEMBL254007	HIV-1 RT	1	Training	<chem>Fe1cccc(F)c1CCNC(=S)Nc2nc(cs2)C#N</chem>
CHEMBL398890	HIV-1 RT	1	Prediction	<chem>COc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F</chem>
CHEMBL253369	HIV-1 RT	1	Training	<chem>CCOc1cccc(F)c1CCNC(=S)Nc2ccc(Br)cn2</chem>
CHEMBL253170	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(CCNC(=S)Nc2ccc(Cl)cn2)c1Cl</chem>
CHEMBL252137	HIV-1 RT	1	Training	<chem>Fe1cccc(Cl)c1CCNC(=S)Nc2nccs2</chem>

CHEMBL129	HIV-1 RT	1	Prediction	<chem>CC1=CN([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)C(=O)NC1=O</chem>
CHEMBL132425	HIV-1 RT	1	Training	<chem>CCC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(en3)C#N)c1O</chem>
CHEMBL137111	HIV-1 RT	1	Training	<chem>COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)en2)c1OC</chem>
CHEMBL299001	HIV-1 RT	1	Training	<chem>Cc1cc(C)cc(c1)S(=O)(=O)c2cccc(N)c2C#N</chem>
CHEMBL443063	HIV-1 RT	1	Prediction	<chem>CN(C)c1ccc(F)c(CCNC(=S)Nc2ccc(Br)en2)c1F</chem>
CHEMBL37834	HIV-1 RT	1	Training	<chem>CCOc1ccc(OC)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Br)en3)c1F</chem>
CHEMBL381513	HIV-1 RT	1	Training	<chem>Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3cccc3Br</chem>
CHEMBL83412	HIV-1 RT	1	Training	<chem>CCc1cc(NCc2cc(C)c(C)cc2OC)c(O)nc1C</chem>
CHEMBL252963	HIV-1 RT	1	Prediction	<chem>CN(C)c1ccc(F)c(CCNC(=S)Nc2ccc(Cl)en2)c1F</chem>
CHEMBL35729	HIV-1 RT	1	Training	<chem>CCOc1ccc(OC)c(CCNC(=O)Nc2ccc(Cl)en2)c1F</chem>
CHEMBL253171	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c(CCNC(=S)Nc2ccc(I)en2)c1Cl</chem>
CHEMBL593	HIV-1 RT	1	Training	<chem>CC(C)Nc1cccn1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3</chem>
CHEMBL135808	HIV-1 RT	1	Prediction	<chem>CN(C)c1ccc(CC\N=C(/S)\Nc2ccc(Br)en2)c(F)c1C#N</chem>
CHEMBL37025	HIV-1 RT	1	Training	<chem>CCOc1ccc(F)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)en3)c1Cl</chem>
CHEMBL46745	HIV-1 RT	1	Training	<chem>Fc1ccc(OCC(=O)Nc2cccc2)c(c1)C(=O)c3cccc3</chem>
CHEMBL84621	HIV-1 RT	1	Training	<chem>CCc1cc(NCc2cc(C)c(C)nc2OC)c(O)nc1C</chem>
CHEMBL383088	HIV-1 RT	1	Prediction	<chem>NS(=O)(=O)c1ccc(NC(=O)CSc2nnnn2c3cccc(Cl)c3Cl)c(Cl)c1</chem>
CHEMBL319224	HIV-1 RT	1	Training	<chem>Fc1ccc(C#N)c(F)c1CC\N=C(/S)\Nc2ccc(Cl)en2</chem>
CHEMBL78882	HIV-1 RT	1	Training	<chem>Clc1ccc2NC(=O)NC(C#Cc3occc3)(C4CC4)c2c1</chem>
CHEMBL252136	HIV-1 RT	1	Training	<chem>Fc1cccc(F)c1CCNC(=S)Nc2nccs2</chem>
CHEMBL381888	HIV-1 RT	1	Prediction	<chem>CC1CN(C2C[C@H](CO)C(C2)N=[N+]=[N-])C(=O)NC1=O</chem>
CHEMBL55187	HIV-1 RT	1	Training	<chem>COc1cc(C)cc(c1)S(=O)(=O)c2cccc(N)c2C#N</chem>
CHEMBL142837	HIV-1 RT	1	Training	<chem>CCN1c2ncccc2C(=O)Nc3c(C)cc(Cl)nc13</chem>
CHEMBL144744	HIV-1 RT	1	Training	<chem>CCN1c2nc(cc(C)c2NC(=O)c3cccn13)N(C)CCO</chem>
CHEMBL438146	HIV-1 RT	1	Prediction	<chem>CCOc1cccc(F)c1CCNC(=S)Nc2nccs2</chem>
CHEMBL250438	HIV-1 RT	1	Training	<chem>COc1cccc(F)c1CCNC(=S)Nc2nccs2</chem>
CHEMBL103386	HIV-1 RT	1	Training	<chem>CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CSc4cccc4)cnc13</chem>
CHEMBL205764	HIV-1 RT	1	Training	<chem>[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3ccc(F)ccc3Cl</chem>
CHEMBL366017	HIV-1 RT	1	Prediction	<chem>CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCOc4ccc(cc4C)C(=O)O)cnc13</chem>
CHEMBL81227	HIV-1 RT	1	Training	<chem>Clc1ccc2NC(=O)NC(C#Cc3cccc3C#N)(C4CC4)c2c1</chem>
CHEMBL79526	HIV-1 RT	1	Training	<chem>Clc1ccc2NC(=O)NC(C#Cc3nccs3)(C4CC4)c2c1</chem>
CHEMBL171919	HIV-1 RT	1	Training	<chem>CCc1cc(SCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C</chem>
CHEMBL309896	HIV-1 RT	1	Training	<chem>Clc1ccc2NC(=O)N[C@](C#Cc3cccn3)(C4CC4)c2c1</chem>
CHEMBL207105	HIV-1 RT	1	Training	<chem>[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3cccc(Cl)c3Cl</chem>
CHEMBL398891	HIV-1 RT	1	Prediction	<chem>CCOc1ccc(F)c(CCNC(=S)Nc2ccc(Br)en2)c1Cl</chem>
CHEMBL131643	HIV-1 RT	1	Training	<chem>CCOc1ccc(Cl)c(C2CC2NC(=O)Nc3ccc(Cl)en3)c1F</chem>
CHEMBL368116	HIV-1 RT	1	Prediction	<chem>CCc1cc(CCc2oc3cccc(F)c3n2)c(S)nc1C</chem>
CHEMBL377820	HIV-1 RT	1	Training	<chem>CN(C)CCCOc1ccc(NC(=O)CSc2nnnn2c3c(C)cc(C)cc3C)c(Cl)c1</chem>
CHEMBL177271	HIV-1 RT	1	Training	<chem>CCc1cc(CCc2oc3c(F)ccc(F)c3n2)c(O)nc1C</chem>
CHEMBL99235	HIV-1 RT	1	Training	<chem>CCc1cc(CCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C</chem>
CHEMBL192231	HIV-1 RT	1	Prediction	<chem>CCN1c2ncccc2N(C)C(=O)c3ccc(CCOc4ccc5ccc(ccc5c4)C(=O)O)cn</chem>

				c13
CHEMBL288971	HIV-1 RT	1	Training	Clc1ccc(OCC(=O)N2CCc3ccccc3C2)c(c1)C(=O)c4ccccc4
CHEMBL191163	HIV-1 RT	1	Training	CCN1c2ncc(CCOc3ccc(cc3C)C(=O)O)cc2C(=O)N(C)c4ccc(OC)n c14
CHEMBL39999	HIV-1 RT	1	Training	Brclccc(NC(=S)NCCc2ccccc2)nc1
CHEMBL189942	HIV-1 RT	1	Prediction	CCN1c2nc(F)ccc2N(C)C(=O)c3cc(CCOc4ccc(cc4C)C(=O)O)cnc1 3
CHEMBL176362	HIV-1 RT	1	Training	CCc1cc(CCc2oc3ccccc(F)c3n2)c(O)nc1C
CHEMBL336237	HIV-1 RT	1	Training	CCc1c(C)nc(O)c(N)c1Sc2cc(C)cc(C)c2
CHEMBL175162	HIV-1 RT	1	Training	CCc1cc(CCc2oc3c(F)ccc(F)c3n2)c(S)nc1C
CHEMBL317356	HIV-1 RT	1	Prediction	Brclccc(NC(=S)NCCc2ccccc2)nc1
Aceclofenac	HIV-1 RT	-1	Training	Clc2cccc(Cl)c2Nc1ccccc1CC(=O)OCC(=O)O
Acetaminophen	HIV-1 RT	-1	Training	Oc1ccc(NC(C)=O)cc1
Acetazolamide	HIV-1 RT	-1	Training	O=S(N)(=O)c1nnc(NC(C)=O)s1
Acetophenazine	HIV-1 RT	-1	Prediction	CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2
Amantadine	HIV-1 RT	-1	Training	NC13CC2CC(CC(C1)C2)C3
Ambenonium	HIV-1 RT	-1	Training	Clc2ccccc2C[N+](CC)(CC)CCNC(=O)C(=O)NCC[N+](Cc1ccccc 1Cl)(CC)CC
Amineptine	HIV-1 RT	-1	Training	O=C(O)CCCCCNC2c3ccccc3CCc1ccccc12
Amiodarone	HIV-1 RT	-1	Prediction	CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC
Amitriptyline	HIV-1 RT	-1	Training	CN(C)CC\C=C\c3ccccc3CCc2ccccc12
Aprobarbital	HIV-1 RT	-1	Training	O=C1NC(=O)NC(=O)C1(CC=C)C(C)C
Artane	HIV-1 RT	-1	Training	OC(CCN1CCCCC1)(c2ccccc2)C3CCCCC3
Aspirin	HIV-1 RT	-1	Prediction	O=C(C)Oc1ccccc1C(=O)O
Atenolol	HIV-1 RT	-1	Training	CC(C)NCC(O)COc1ccc(cc1)CC(N)=O
Atropine	HIV-1 RT	-1	Training	CN3C1CCC3C[C@@H](C1)OC(=O)C(CO)c2ccccc2
Baclofen	HIV-1 RT	-1	Training	Clc1ccc(cc1)C(CN)CC(=O)O
Beclomethasone	HIV-1 RT	-1	Prediction	OCC(=O)[C@@]4(O)[C@@H](C)CC3C2CCC1=CC(=O)C=C[C@ @]1(C)[C@@]2(Cl)[C@@H](O)C[C@@]34C
Benzonatate	HIV-1 RT	-1	Training	O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NC CCC)cc1
Biperiden	HIV-1 RT	-1	Training	OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3
Bromocriptine	HIV-1 RT	-1	Training	Br3nc2ccccc1C4=C[C@H](CN(C)C4Cc3c12)C(=O)N[C@@] [C@]6(O)N([C@@H](CC(C)C)C(=O)N5CCCC56)C7=O)C(C)C
Bucizine	HIV-1 RT	-1	Prediction	CC(C)(C)c1ccc(cc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4
Budesonide	HIV-1 RT	-1	Training	OCC(=O)[C@@]53OC(O[C@@H]5CC2C1CCC4=CC(=O)C=C[C@ @]4(C)C1[C@@H](O)C[C@@]23C)CCC
Buprenorphine	HIV-1 RT	-1	Training	CC(C)(C)C(C)(O)[C@H]1C[C@]75CC[C@]1(OC)[C@@H]2Oc4 c(O)ccc3C[C@H]7[N@](CC[C@]25c34)CC6CC6
Caffeine	HIV-1 RT	-1	Training	O=C2c1n(C)cnc1N(C)C(=O)N2C
Cantil	HIV-1 RT	-1	Prediction	O=C(OC1CCC[N+](C)(C)C1)C(O)(c2ccccc2)c3ccccc3
Carbachol	HIV-1 RT	-1	Training	C[N+](C)(C)CCOC(=O)N
Carbamazepine	HIV-1 RT	-1	Training	NC(=O)N2c3ccccc3C=Cc1ccccc12
Carisoprodol	HIV-1 RT	-1	Training	O=C(NC(C)C)OCC(C)(COC(=O)N)CCC
Carvedilol	HIV-1 RT	-1	Prediction	COc4ccccc4OCCNCC(O)COc2ccccc3nc1ccccc1c23

Cefoperazone	HIV-1 RT	-1	Training	<chem>O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O</chem>
Chloral hydrate	HIV-1 RT	-1	Training	<chem>ClC(Cl)(Cl)C(O)O</chem>
Chlordiazepoxide	HIV-1 RT	-1	Training	<chem>Clc1ccc2N=C(C[N+]([O-])=C(c2c1)c3ccccc3)NC</chem>
Chlorpropamide	HIV-1 RT	-1	Prediction	<chem>O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1</chem>
Chlorthalidone	HIV-1 RT	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2ccccc23</chem>
Clidinium	HIV-1 RT	-1	Training	<chem>OC(c1cccc1)(c2ccccc2)C(=O)OC4C[N+](C)CCC4CC3</chem>
Clobazam	HIV-1 RT	-1	Training	<chem>Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3ccccc3</chem>
Clofazimine	HIV-1 RT	-1	Prediction	<chem>Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5</chem>
Clomipramine	HIV-1 RT	-1	Training	<chem>CN(C)CCCN2c3ccccc3CCc1ccc(Cl)cc12</chem>
Clonidine	HIV-1 RT	-1	Training	<chem>Clc2ccccc(Cl)c2N=C1/NCCN1</chem>
Codeine	HIV-1 RT	-1	Training	<chem>COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23</chem>
Colchicine	HIV-1 RT	-1	Prediction	<chem>CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12</chem>
Cyclizine	HIV-1 RT	-1	Training	<chem>CN1CCN(CC1)C(c2ccccc2)c3ccccc3</chem>
Cyclosporin	HIV-1 RT	-1	Training	<chem>CC(C\C=C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C</chem>
Dextropropoxyphene	HIV-1 RT	-1	Training	<chem>CN(C)CC(C)C(OC(=O)CC)(Cc1ccccc1)c2ccccc2</chem>
Diazepam	HIV-1 RT	-1	Prediction	<chem>Clc1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3</chem>
Diflucortolone	HIV-1 RT	-1	Training	<chem>OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C</chem>
Dimercaprol	HIV-1 RT	-1	Training	<chem>OCC(S)CS</chem>
Diphenhydramine	HIV-1 RT	-1	Training	<chem>CN(C)CCOC(c1ccccc1)c2ccccc2</chem>
Diphenidol	HIV-1 RT	-1	Prediction	<chem>OC(CCCN1CCCCC1)(c2ccccc2)c3ccccc3</chem>
Dobutamine	HIV-1 RT	-1	Training	<chem>Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O</chem>
Dofetilide	HIV-1 RT	-1	Training	<chem>CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O</chem>
Domperidone	HIV-1 RT	-1	Training	<chem>Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4</chem>
Dopamine	HIV-1 RT	-1	Prediction	<chem>Oc1ccc(CCN)cc1O</chem>
Doxazosin	HIV-1 RT	-1	Training	<chem>COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4</chem>
Doxepin	HIV-1 RT	-1	Training	<chem>CN(C)CC\C=C1/c3ccccc3OCc2ccccc12</chem>
Dronabinol	HIV-1 RT	-1	Training	<chem>CCCCCc3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3</chem>
Droxicam	HIV-1 RT	-1	Prediction	<chem>O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O</chem>
Entacapone	HIV-1 RT	-1	Training	<chem>Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+]([O-])=O)c1O</chem>
Epinephrine	HIV-1 RT	-1	Training	<chem>Oc1ccc(cc1O)[C@@H](O)CNC</chem>
Eprosartan	HIV-1 RT	-1	Training	<chem>OC(=O)C(/Cc1cccs1)=C/c3cnc(CCCC)n3Cc2ccc(cc2)C(=O)O</chem>
Ergotamine	HIV-1 RT	-1	Prediction	<chem>CN2C[C@@H](C=C1c3ccccc4ncc(CC12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O</chem>
Ethosuximide	HIV-1 RT	-1	Training	<chem>CC1(CC)CC(=O)NC1=O</chem>
Fentanyl	HIV-1 RT	-1	Training	<chem>CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3</chem>
Fexofenadine	HIV-1 RT	-1	Training	<chem>O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4</chem>

Flecainide	HIV-1 RT	-1	Prediction	<chem>FC(F)(F)COc2cc(C(=O)NCCC1CCCN1)c(OCC(F)(F)F)cc2</chem>
Flunarizine	HIV-1 RT	-1	Training	<chem>Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4</chem>
Flunisolide	HIV-1 RT	-1	Training	<chem>OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C</chem>
Fluoxetine	HIV-1 RT	-1	Training	<chem>FC(F)(F)c2ccc(OC(CCNC)c1ccccc1)cc2</chem>
Fluvoxamine	HIV-1 RT	-1	Prediction	<chem>FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN</chem>
Gabapentin	HIV-1 RT	-1	Training	<chem>NCC1(CC(=O)O)CCCCC1</chem>
Gestodene	HIV-1 RT	-1	Training	<chem>O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2</chem>
Glutethimide	HIV-1 RT	-1	Training	<chem>CCC1(CCC(=O)NC1=O)c2ccccc2</chem>
Glycopyrrolate	HIV-1 RT	-1	Prediction	<chem>C[N+](3)(C)CCC(OC(=O)C(O)(c1ccccc1)C2CCCC2)C3</chem>
Guanadrel	HIV-1 RT	-1	Training	<chem>N=C(N)NCC2COC1(CCCCC1)O2</chem>
Halofantrine	HIV-1 RT	-1	Training	<chem>CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F</chem>
Haloperidol	HIV-1 RT	-1	Training	<chem>Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3</chem>
Halothane	HIV-1 RT	-1	Prediction	<chem>BrC(Cl)C(F)(F)F</chem>
Hydromorphone	HIV-1 RT	-1	Training	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	HIV-1 RT	-1	Training	<chem>Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	HIV-1 RT	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C</chem>
Indomethacin	HIV-1 RT	-1	Prediction	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	HIV-1 RT	-1	Training	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	HIV-1 RT	-1	Training	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	HIV-1 RT	-1	Training	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	HIV-1 RT	-1	Prediction	<chem>CNC1(CCCCC1=O)c2ccccc2Cl</chem>
Labetalol	HIV-1 RT	-1	Training	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2</chem>
Lacidipine	HIV-1 RT	-1	Training	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	HIV-1 RT	-1	Training	<chem>Clc1cccc(c1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	HIV-1 RT	-1	Prediction	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCNC(=N)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2ccccc23)NC(=O)C(Cc4cncn4)NC(=O)C5CCCC(=O)N5</chem>
Levodopa	HIV-1 RT	-1	Training	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>
Lidocaine	HIV-1 RT	-1	Training	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	HIV-1 RT	-1	Training	<chem>Clc3cc4CCc1cccn1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	HIV-1 RT	-1	Prediction	<chem>CNCCCC24CCC(c1ccccc12)c3ccccc34</chem>
Meclizine	HIV-1 RT	-1	Training	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Medroxyprogesterone	HIV-1 RT	-1	Training	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	HIV-1 RT	-1	Training	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	HIV-1 RT	-1	Prediction	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	HIV-1 RT	-1	Training	<chem>C[C@H](NC)Cc1ccccc1</chem>
Methantheline	HIV-1 RT	-1	Training	<chem>CC[N+](C)(CC)CCOC(=O)C1c3ccccc3Oc2ccccc12</chem>
Methocarbamol	HIV-1 RT	-1	Training	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	HIV-1 RT	-1	Prediction	<chem>ClC(Cl)C(F)(F)OC</chem>

Methscopolamine	HIV-1 RT	-1	Training	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+](C)C</chem>
Methylphenidate	HIV-1 RT	-1	Training	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	HIV-1 RT	-1	Training	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3ccccc1c23)N(C)C4</chem>
Metoclopramide	HIV-1 RT	-1	Prediction	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	HIV-1 RT	-1	Training	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	HIV-1 RT	-1	Training	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	HIV-1 RT	-1	Training	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	HIV-1 RT	-1	Prediction	<chem>CC(C)(O)c5ccccc5CC[C@H](SCC1(CC(=O)O)CC1)c2cccc(c2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	HIV-1 RT	-1	Training	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	HIV-1 RT	-1	Training	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@@H]45</chem>
Nalmefene	HIV-1 RT	-1	Training	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C[C@N@]3CC2CC2)c45</chem>
Neostigmine	HIV-1 RT	-1	Prediction	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>
Nifedipine	HIV-1 RT	-1	Training	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	HIV-1 RT	-1	Training	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	HIV-1 RT	-1	Training	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	HIV-1 RT	-1	Prediction	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	HIV-1 RT	-1	Training	<chem>CSC[C@H]4CC1C(Cc2cnc3ccccc1c23)N(C4)CCC</chem>
Phenylbutazone	HIV-1 RT	-1	Training	<chem>O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2</chem>
Phenytoin	HIV-1 RT	-1	Training	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	HIV-1 RT	-1	Prediction	<chem>Cn2cncc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	HIV-1 RT	-1	Training	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	HIV-1 RT	-1	Training	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	HIV-1 RT	-1	Training	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	HIV-1 RT	-1	Prediction	<chem>OC(CCN1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	HIV-1 RT	-1	Training	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	HIV-1 RT	-1	Training	<chem>OC(C(C)NC)c1ccccc1</chem>
Pyrantel	HIV-1 RT	-1	Training	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>
Quinidine	HIV-1 RT	-1	Prediction	<chem>COc1cc2c(cc1)nccc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	HIV-1 RT	-1	Training	<chem>[O-][N+](=O)C=C(/NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	HIV-1 RT	-1	Training	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oc4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	HIV-1 RT	-1	Training	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	HIV-1 RT	-1	Prediction	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	HIV-1 RT	-1	Training	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>
Selegiline	HIV-1 RT	-1	Training	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>
Sulfinpyrazone	HIV-1 RT	-1	Training	<chem>O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	HIV-1 RT	-1	Prediction	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>

Terpin	HIV-1 RT	-1	Training	<chem>C[C@@]1(O)CC[C@@H](CC1)C(C)(C)O</chem>
Tolcapone	HIV-1 RT	-1	Training	<chem>Oc1cc(cc([N+])([O-])=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranylcypromine	HIV-1 RT	-1	Training	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	HIV-1 RT	-1	Prediction	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	HIV-1 RT	-1	Training	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@@]23C</chem>
Valproic acid	HIV-1 RT	-1	Training	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	HIV-1 RT	-1	Training	<chem>O=C(O)[C@@H]10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	HIV-1 RT	-1	Prediction	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	HIV-1 RT	-1	Training	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wytenzin	HIV-1 RT	-1	Training	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	HIV-1 RT	-1	Training	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>
Zileuton	HIV-1 RT	-1	Prediction	<chem>NC(=O)N(O)C(C)c1cc2ccccc2s1</chem>
Zonisamide	HIV-1 RT	-1	Training	<chem>NS(=O)(=O)Cc2noc1ccccc12</chem>
CHEMBL414850	HIV-IN	1	Training	<chem>Oc1c(nc(N2CCCCS2(=O)=O)c3ccnc13)C(=O)NCc4ccc(F)cc4</chem>
CHEMBL196391	HIV-IN	1	Prediction	<chem>COc1ccc2c(c1)c(en2Cc3ccc(F)cc3)\C=C\C(=O)C(=O)O)\O</chem>
CHEMBL212412	HIV-IN	1	Training	<chem>COc1c2c(C(=O)N(Cc3ccc(F)cc3)C24CC4)c(O)c5ncccc15</chem>
CHEMBL210234	HIV-IN	1	Training	<chem>CN(C(=O)C(=O)N1CCCCC1)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24</chem>
CHEMBL212213	HIV-IN	1	Training	<chem>COc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncc(F)cc14</chem>
CHEMBL204656	HIV-IN	1	Prediction	<chem>COc1cc2N(C=C(C(=O)O)C(=O)c2cc1Cc3cccc(Cl)c3F)[C@H](CO)C(C)C</chem>
CHEMBL206604	HIV-IN	1	Training	<chem>CC(C)[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12</chem>
CHEMBL203443	HIV-IN	1	Training	<chem>COc1cc2N(CCO)C=C(C(=O)O)C(=O)c2cc1Cc3cccc(Cl)c3F</chem>
CHEMBL371007	HIV-IN	1	Training	<chem>Oc1c(nc(C2CC(=O)NC(=O)N2)c3ccnc13)C(=O)NCc4ccc(F)cc4</chem>
CHEMBL379658	HIV-IN	1	Prediction	<chem>CCN1CCN(C(=O)C1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24</chem>
CHEMBL193759	HIV-IN	1	Training	<chem>OC(=O)C(=O)\C=C(/O)c1cccc(Cc2ccccc2)c1</chem>
CHEMBL32865	HIV-IN	1	Training	<chem>Oc1c(ncc2ccnc12)C(=O)c3cc(CN4CCCS4(=O)=O)cc(Cc5ccccc5)c3</chem>
CHEMBL425924	HIV-IN	1	Training	<chem>CN1C(CC(=O)NC1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24</chem>
CHEMBL382965	HIV-IN	1	Prediction	<chem>CN1C(=O)CC(NC1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24</chem>
CHEMBL378029	HIV-IN	1	Training	<chem>CNC(=O)C(=O)N(C)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13</chem>
CHEMBL377501	HIV-IN	1	Training	<chem>OC(=O)C(=O)\C=C(/O)C1=CN(Cc2ccc(F)cc2)c3ccc(cc3C1=O)\C=C\C(=O)C(=O)O)\O</chem>
CHEMBL210233	HIV-IN	1	Training	<chem>CN(C(=O)C(=O)N)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13</chem>
CHEMBL368084	HIV-IN	1	Prediction	<chem>O\C=C/C(=O)c1nc[nH]n1)\c2oc(Cc3ccc(F)cc3)cc2</chem>
CHEMBL379664	HIV-IN	1	Training	<chem>OCCN1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12</chem>
CHEMBL377759	HIV-IN	1	Training	<chem>CN(C(=O)C)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13</chem>

CHEMBL209872	HIV-IN	1	Training	<chem>CC(=O)N1CCN(CC1)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24</chem>
CHEMBL212982	HIV-IN	1	Prediction	<chem>CN(C)S(=O)(=O)Oc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncnc14</chem>
CHEMBL199145	HIV-IN	1	Training	<chem>Oc1c(ncc2ccnc12)C(=O)NCc3ccc(F)cc3</chem>
CHEMBL198160	HIV-IN	1	Training	<chem>CN1C(CC(=O)N(C)C1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4nccc24</chem>
CHEMBL212000	HIV-IN	1	Training	<chem>COc1c2C(O)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14</chem>
CHEMBL36070	HIV-IN	1	Prediction	<chem>Oc1c(ncc2ccnc12)C(=O)c3cccc(Cc4cccc4)c3</chem>
CHEMBL380588	HIV-IN	1	Training	<chem>NC(=O)C(=O)Nc1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13</chem>
CHEMBL209307	HIV-IN	1	Training	<chem>CN(C(=O)C(=O)N1CCCC1)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4nccc24</chem>
CHEMBL441683	HIV-IN	1	Training	<chem>CN1CCN(CC1)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24</chem>
CHEMBL426686	HIV-IN	1	Prediction	<chem>CN(C)C(=O)C(=O)N(C)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13</chem>
CHEMBL270717	HIV-IN	1	Training	<chem>OC(=O)C1=CNc2ccc(Cc3cccc(Cl)c3F)cc2C1=O</chem>
CHEMBL209440	HIV-IN	1	Training	<chem>COc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14</chem>
CHEMBL421353	HIV-IN	1	Training	<chem>OC(=O)C(=O)\C=C(/O)\c1cccn1Cc2ccc(F)cc2</chem>
CHEMBL142072	HIV-IN	1	Training	<chem>Oc1c(ccc2ccnc12)C(=O)c3cc(Cc4cccc4)ccn3</chem>
CHEMBL208776	HIV-IN	1	Training	<chem>CN(C)C(=O)CN(C)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13</chem>
CHEMBL320261	HIV-IN	1	Prediction	<chem>OC(=O)C(=O)\C=C(/O)\c1cc(OCc2cccc2)cc(OCc3cccc3)c1</chem>
CHEMBL384912	HIV-IN	1	Training	<chem>COC1N(Cc2ccc(F)cc2)C(=O)c3c(O)c4ncccc4c(OC)c13</chem>
CHEMBL409132	HIV-IN	1	Training	<chem>CC1C=C(NC(=O)C2=CC(=CC2)NC(=O)C3=CC(=CC3)N(C)C(=O)c4ccc(cc4)C(=O)N(C)C5=CC(C)C(=C5)C(=O)NC6=CC(C)C(=C6)C(=O)NC7=CC(C)C(=C7)C(=O)NCCCN(C)C)C=C1C(=O)NCCCN(C)C</chem>
CHEMBL365604	HIV-IN	1	Training	<chem>CCOC(=O)C(=O)\C=C(/O)\c1cn(Cc2ccc(F)cc2)c3ccc(Cl)cc13</chem>
CHEMBL29660	HIV-IN	1	Prediction	<chem>OC(=O)[C@@H](OC(=O)\C=C\c1ccc(O)c(O)c1)[C@H](OC(=O)\C=C\c2ccc(O)c(O)c2)C(=O)O</chem>
CHEMBL209958	HIV-IN	1	Training	<chem>Oc1c2C(=O)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14</chem>
CHEMBL377267	HIV-IN	1	Training	<chem>COc1c2C(C)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14</chem>
CHEMBL216058	HIV-IN	1	Training	<chem>CC1C=C(NC(=O)C2=CC(=CC2)NC(=O)C3=CC(=CC3)NC(=O)c4ccc(cc4)C(=O)NC5=CC(C)C(=C5)C(=O)NC6=CC(C)C(=C6)C(=O)NC7=CC(C)C(=C7)C(=O)NCCC(=N)N)C=C1C(=O)NCCC(=N)N</chem>
CHEMBL386055	HIV-IN	1	Prediction	<chem>COc1cnc2c(O)c3C(=O)N(Cc4ccc(F)cc4)Cc3c(OC)c2c1</chem>
CHEMBL403498	HIV-IN	1	Training	<chem>CC1C=C(NC(=O)C2=CC(=CC2)NC(=O)C3=CC(=CC3)NC(=O)c4ccc(nc4)C(=O)NC5=CC(C)C(=C5)C(=O)NC6=CC(C)C(=C6)C(=O)NC7=CC(C)C(=C7)C(=O)NCCC(=N)N)C=C1C(=O)NCCC(=N)N</chem>
CHEMBL143614	HIV-IN	1	Training	<chem>OC(=O)C(=O)CC(=O)c1csc(Cc2ccccc2)c1</chem>
CHEMBL194833	HIV-IN	1	Training	<chem>COc1ccc(Cc2ccccc2)cc1\C=C\C(=O)C(=O)O)\O</chem>
CHEMBL343646	HIV-IN	1	Prediction	<chem>CC(C)Oc1ccc(Cc2ccccc2)cc1C(=O)CC(=O)C(=O)O</chem>
CHEMBL147147	HIV-IN	1	Training	<chem>OC(=O)C(=O)CC(=O)c1cccc(Cc2ccc(F)cc2)c1</chem>
CHEMBL357909	HIV-IN	1	Training	<chem>OC(=O)C(=O)CC(=O)c1cccc(Cc2ccccc2Cl)c1</chem>
CHEMBL19464	HIV-IN	1	Training	<chem>OC(=O)C(=O)CC(=O)c1cccc(Cc2ccccc2)c1</chem>
CHEMBL145705	HIV-IN	1	Prediction	<chem>COc1ccc(Cc2ccccc2)cc1C(=O)CC(=O)C(=O)O</chem>
CHEMBL148241	HIV-IN	1	Training	<chem>CCOc1ccc(Cc2ccccc2)cc1C(=O)CC(=O)C(=O)O</chem>

CHEMBL145280	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1cccc(Cc2ccccc2F)c1
CHEMBL145335	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1cccc(Cc2ccccc(Cl)c2)c1
CHEMBL63592	HIV-IN	1	Prediction	OC(=O)C(OC(=O)\C=C\c1ccc(O)c(O)c1)C(OC(=O)\C=C\c2ccc(O)c(O)c2)C(=O)O
CHEMBL147317	HIV-IN	1	Training	COc1cc(Cc2ccccc2)cc(c1)C(=O)CC(=O)C(=O)O
CHEMBL371471	HIV-IN	1	Training	COc1cc(Cc2ccccc2)cc(c1)\C(=C\C(=O)C(=O)O)\O
CHEMBL197584	HIV-IN	1	Training	COc1ccc(cc1Cc2ccccc2)\C(=C\C(=O)C(=O)O)\O
CHEMBL213852	HIV-IN	1	Prediction	COc1c2C(=C)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14
CHEMBL20342	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1ccc(CN=[N+]=[N-])c(CN=[N+]=[N-])c1
CHEMBL146777	HIV-IN	1	Training	COc1ccc(cc1Cc2ccccc2)C(=O)CC(=O)C(=O)O
CHEMBL379132	HIV-IN	1	Training	CN(CCN(C)c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13)C(=O)C
CHEMBL50605	HIV-IN	1	Prediction	OC(=O)C(=O)CC(=O)c1cccn1Cc2ccc(F)cc2
CHEMBL198000	HIV-IN	1	Prediction	OC(=O)C(=O)\C=C(/O)c1cccc(Cc2ccccc(F)c2)c1
CHEMBL144727	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1cccc(Cc2ccccc(F)c2)c1
CHEMBL214371	HIV-IN	1	Training	CN(C)S(=O)(=O)Oc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14
CHEMBL1159993	HIV-IN	1	Training	OC(=O)C(=O)\C=C(/O)/c1ccc(CN=[N+]=[N-])c(CN=[N+]=[N-])c1
CHEMBL144613	HIV-IN	1	Prediction	CC(=O)Nc1cc(cc2cc(cc(O)c12)S(=O)(=O)O)S(=O)(=O)O
CHEMBL213467	HIV-IN	1	Training	COc1c2C(SCCCC(=O)O)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14
CHEMBL37869	HIV-IN	1	Training	OC(=O)c1ccc2ccc\C=C\c3cc(O)c(O)c(O)c3)nc2c1O
CHEMBL209641	HIV-IN	1	Training	COC(=O)CCSC1N(Cc2ccc(F)cc2)C(=O)c3c(O)c4ncccc4c(OC)c13
CHEMBL278545	HIV-IN	1	Prediction	OC(=O)C(=O)CC(=O)c1ccc2C(CCC(N=[N+]=[N-])c2c1)N=[N+]=[N-]
CHEMBL1159989	HIV-IN	1	Training	OC(=O)C(=O)\C=C(/O)/c1ccc2C(CCC(N=[N+]=[N-])c2c1)N=[N+]=[N-]
CHEMBL32711	HIV-IN	1	Training	OC1=C(C(C2=C(O)Oc3cc(O)ccc3C2=O)c4ccc(cc4)C(C5=C(O)Oc6cc(O)ccc6C5=O)C7=C(O)Oc8cc(O)ccc8C7=O)C(=O)c9ccc(O)c9O1
CHEMBL108253	HIV-IN	1	Training	OC(=O)C(=O)\C=C(/O)c1cccc(OCc2ccccc2)c1
CHEMBL18927	HIV-IN	1	Prediction	OC(=O)C(=O)CC(=O)c1cccc(OCc2ccccc2)c1
CHEMBL379974	HIV-IN	1	Training	CN(C)S(=O)(=O)Oc1c2c(C(=O)N(Cc3ccc(F)cc3)C24CC4)c(O)c5ncccc15
CHEMBL1159988	HIV-IN	1	Training	OC(=O)C(=O)\C=C(/O)/c1ccc2C(CC(N=[N+]=[N-])c2c1)N=[N+]=[N-]
CHEMBL20592	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1ccc2C(CC(N=[N+]=[N-])c2c1)N=[N+]=[N-]
CHEMBL35842	HIV-IN	1	Prediction	Oc1c(ccc2cccn12)C(=O)c3ccccc(Cc4ccccc4)c3
CHEMBL145946	HIV-IN	1	Prediction	OC(=O)C(=O)CC(=O)c1ccn(Cc2ccccc2)c1
CHEMBL144118	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1cccc(Cc2ccc(Cl)cc2)c1
CHEMBL358506	HIV-IN	1	Training	OC(=O)C(=O)CC(=O)c1ccc(Cc2ccccc2)s1
Aceclofenac	HIV-IN	-1	Training	Clc2ccccc(Cl)c2Nc1ccccc1CC(=O)OCC(=O)O
Acetaminophen	HIV-IN	-1	Prediction	Oc1ccc(NC(C)=O)cc1
Acetazolamide	HIV-IN	-1	Training	O=S(N)(=O)c1nnnc(NC(C)=O)s1
Acetophenazine	HIV-IN	-1	Training	CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2

Amantadine	HIV-IN	-1	Training	NC1CC2CC(CC(C1)C2)C3
Ambenonium	HIV-IN	-1	Prediction	Clc2ccccc2C[N+](CC)(CC)CCNC(=O)C(=O)NCC[N+](Cc1ccccc1Cl)(CC)CC
Amineptine	HIV-IN	-1	Training	O=C(O)CCCCCNC2c3ccccc3CCc1ccccc12
Amiodarone	HIV-IN	-1	Training	CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC
Amitriptyline	HIV-IN	-1	Training	CN(C)CC\C=C1\c3ccccc3CCc2ccccc12
Aprobarbital	HIV-IN	-1	Prediction	O=C1NC(=O)NC(=O)C1(CC=C)C(C)C
Artane	HIV-IN	-1	Training	OC(CCN1CCCCC1)(c2ccccc2)C3CCCCC3
Aspirin	HIV-IN	-1	Training	O=C(C)Oc1ccccc1C(=O)O
Atenolol	HIV-IN	-1	Training	CC(C)NCC(O)COc1ccc(cc1)CC(N)=O
Atropine	HIV-IN	-1	Prediction	CN3C1CCC3C[C@@H](C1)OC(=O)C(CO)c2ccccc2
Baclofen	HIV-IN	-1	Training	Clc1ccc(cc1)C(CN)CC(=O)O
Beclomethasone	HIV-IN	-1	Training	OCC(=O)[C@@]4(O)[C@@H](C)CC3C2CCC1=CC(=O)C=C[C@]1(C)[C@@]2(Cl)[C@@H](O)C[C@@]34C
Benzonatate	HIV-IN	-1	Training	O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NCCC)cc1
Biperiden	HIV-IN	-1	Prediction	OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3
Bromocriptine	HIV-IN	-1	Training	BrC3nc2ccccc1C4=C[C@H](CN(C)C4Cc3c12)C(=O)N[C@@]7(O[C@]6(O)N([C@@H](CC(C)C)C(=O)N5CCCC56)C7=O)C(C)C
Buclizine	HIV-IN	-1	Training	CC(C)(C)c1ccc(cc1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4
Budesonide	HIV-IN	-1	Training	OCC(=O)[C@@]53OC(O[C@@H]5CC2C1CCC4=CC(=O)C=C[C@]4(C)C1[C@@H](O)C[C@@]23C)CCC
Buprenorphine	HIV-IN	-1	Prediction	CC(C)(C)C(C)(O)[C@H]1C[C@]75CC[C@]1(OC)[C@@H]2Oc4c(O)ccc3C[C@H]7[N@](CC[C@]25c34)CC6CC6
Caffeine	HIV-IN	-1	Training	O=C2c1n(C)nc1N(C)C(=O)N2C
Cantil	HIV-IN	-1	Training	O=C(OC1CCC[N+](C)(C)C1)C(O)(c2ccccc2)c3ccccc3
Carbachol	HIV-IN	-1	Training	C[N+](C)(C)CCOC(=O)N
Carbamazepine	HIV-IN	-1	Prediction	NC(=O)N2c3ccccc3C=Cc1ccccc12
Carisoprodol	HIV-IN	-1	Training	O=C(NC(C)C)OCC(C)(COC(=O)N)CCC
Carvedilol	HIV-IN	-1	Training	COc4ccccc4OCCNCC(O)COc2ccccc3nc1ccccc1c23
Cefoperazone	HIV-IN	-1	Training	O=C1C(=O)N(CC)CCN1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C5SCC(CSc3nnnn3C)=C4C(=O)O
Chloral hydrate	HIV-IN	-1	Prediction	ClC(Cl)(Cl)C(O)O
Chlordiazepoxide	HIV-IN	-1	Training	Clc1ccc2N=C(C[N+](O-))=C(c2c1)c3ccccc3)NC
Chlorpropamide	HIV-IN	-1	Training	O=S(=O)(NC(=O)NCCC)c1ccc(Cl)cc1
Chlorthalidone	HIV-IN	-1	Training	NS(=O)(=O)c1cc(ccc1Cl)C3(O)NC(=O)c2ccccc23
Clidinium	HIV-IN	-1	Prediction	OC(c1ccccc1)(c2ccccc2)C(=O)OC4C[N+](3(C)CCC4CC3
Clobazam	HIV-IN	-1	Training	Clc1ccc2c(c1)N(C(=O)CC(=O)N2C)c3ccccc3
Clofazimine	HIV-IN	-1	Training	Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5
Clomipramine	HIV-IN	-1	Training	CN(C)CCCN2c3ccccc3CCc1ccc(Cl)cc12
Clonidine	HIV-IN	-1	Prediction	Clc2cccc(Cl)c2\N=C1/NCCN1
Codeine	HIV-IN	-1	Training	COc1ccc2C[C@H]5[N@@](C)CC[C@@]43C5C=C[C@H](O)[C@@H]4Oc1c23
Colchicine	HIV-IN	-1	Training	CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12

Cyclizine	HIV-IN	-1	Training	CN1CCN(CC1)C(c2ccccc2)c3ccccc3
Cyclosporin	HIV-IN	-1	Prediction	CC(C\C=C\C\C)C(O)C1C(=O)NC(CC)C(=O)N(C)CC(=O)N(C)C(C(C(C)C)C(=O)NC(C(=O)N(C)C(CC(C)C)C(=O)NC(C)C(=O)NC(C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C(=O)N1C)C(C)C
Dextropropoxyphene	HIV-IN	-1	Training	CN(C)CC(C)C(OC(=O)CC)(Cc1ccccc1)c2ccccc2
Diazepam	HIV-IN	-1	Training	Clc1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3
Diflucortolone	HIV-IN	-1	Training	OCC(=O)[C@H]4[C@H](C)CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)[C@@]2(F)[C@@H](O)C[C@@]34C
Dimercaprol	HIV-IN	-1	Prediction	OCC(S)CS
Diphenhydramine	HIV-IN	-1	Training	CN(C)CCOC(c1ccccc1)c2ccccc2
Diphenidol	HIV-IN	-1	Training	OC(CCCN1CCCCC1)(c2ccccc2)c3ccccc3
Dobutamine	HIV-IN	-1	Training	Oc2ccc(CCNC(C)CCc1ccc(O)cc1)cc2O
Dofetilide	HIV-IN	-1	Prediction	CS(=O)(=O)Nc1ccc(cc1)CCN(C)CCOc2ccc(cc2)NS(C)(=O)=O
Domperidone	HIV-IN	-1	Training	Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4
Dopamine	HIV-IN	-1	Training	Oc1ccc(CCN)cc1O
Doxazosin	HIV-IN	-1	Training	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5O4
Doxepin	HIV-IN	-1	Prediction	CN(C)CC\C=C1/c3ccccc3OCc2ccccc12
Dronabinol	HIV-IN	-1	Training	CCCCCc3cc2OC(C)(C)C1CCC(C)=CC1c2c(O)c3
Droxicam	HIV-IN	-1	Training	O=C(N2C3=NC=CC=C3)C(N1C)=C(OC2=O)C(C=CC=C4)=C4S1(=O)=O
Entacapone	HIV-IN	-1	Training	Oc1cc(\C=C(/C#N)C(=O)N(CC)CC)cc([N+])([O-])=O)c1O
Epinephrine	HIV-IN	-1	Prediction	Oc1ccc(cc1O)[C@@H](O)CNC
Eprosartan	HIV-IN	-1	Training	OC(=O)C(/Cc1cccs1)=C/c3enc(CCCC)n3Cc2ccc(cc2)C(=O)O
Ergotamine	HIV-IN	-1	Training	CN2C[C@@H](C=C1c3ccccc4ncc(C12)c34)C(=O)N[C@]8(C)O[C@]7(O)N([C@@H](Cc5ccccc5)C(=O)N6CCCC67)C8=O
Ethosuximide	HIV-IN	-1	Training	CC1(CC)CC(=O)NC1=O
Fentanyl	HIV-IN	-1	Prediction	CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3
Fexofenadine	HIV-IN	-1	Training	O=C(O)C(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4
Flecainide	HIV-IN	-1	Training	FC(F)(F)COc2cc(C(=O)NCC1CCCCN1)c(OCC(F)(F)F)cc2
Flunarizine	HIV-IN	-1	Training	Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4
Flunisolide	HIV-IN	-1	Prediction	OCC(=O)[C@@]54OC(C)(C)O[C@@H]5CC3C2C[C@H](F)C1=CC(=O)C=C[C@]1(C)C2[C@@H](O)C[C@@]34C
Fluoxetine	HIV-IN	-1	Training	FC(F)(F)c2ccc(OC(CCNC)c1ccccc1)cc2
Fluvoxamine	HIV-IN	-1	Training	FC(F)(F)c1ccc(cc1)C(\CCCCOC)=N\OCCN
Gabapentin	HIV-IN	-1	Training	NCC1(CC(=O)O)CCCCC1
Gestodene	HIV-IN	-1	Prediction	O=C2CCC3C4CC[C@@]1(CC)C(C=C[C@@]1(O)C#C)C4CCC3=C2
Glutethimide	HIV-IN	-1	Training	CCC1(CCC(=O)NC1=O)c2ccccc2
Glycopyrrolate	HIV-IN	-1	Training	C[N+]3(C)CCC(OC(=O)C(O)(c1ccccc1)C2CCCC2)C3
Guanadrel	HIV-IN	-1	Training	N=C(N)NCC2COC1(CCCCC1)O2
Halofantrine	HIV-IN	-1	Prediction	CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F
Haloperidol	HIV-IN	-1	Training	Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3
Halothane	HIV-IN	-1	Training	BrC(Cl)C(F)(F)F

Hydromorphone	HIV-IN	-1	Training	<chem>O=C1CCC3[C@H]2Cc5ccc(O)c4O[C@@H]1[C@]3(CC[N@@]2C)c45</chem>
Hydroxyzine	HIV-IN	-1	Prediction	<chem>Clc1ccc(cc1)C(c2ccccc2)N3CCN(CC3)CCOCCO</chem>
Indapamide	HIV-IN	-1	Training	<chem>NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C</chem>
Indomethacin	HIV-IN	-1	Training	<chem>Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC</chem>
Isoetharine	HIV-IN	-1	Training	<chem>Oc1ccc(cc1O)C(O)C(CC)NC(C)C</chem>
Isoproterenol	HIV-IN	-1	Prediction	<chem>Oc1ccc(cc1O)C(O)CNC(C)C</chem>
Isosorbide	HIV-IN	-1	Training	<chem>[O-][N+](=O)O[C@H]2COC1C2OCC1O[N+](O-)=O</chem>
Ketamine	HIV-IN	-1	Training	<chem>CNC1(CCCCC1=O)c2ccccc2Cl</chem>
Labetalol	HIV-IN	-1	Training	<chem>O=C(N)c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2</chem>
Lacidipine	HIV-IN	-1	Prediction	<chem>CC(N2)=C(C(OCC)=O)C(C(C(OCC)=O)=C2C)C(C=CC=C1)=C1/C=C/C(OC(C)(C)C)=O</chem>
Lamotrigine	HIV-IN	-1	Training	<chem>Clc1cccc(c1Cl)c2nnc(N)nc2N</chem>
Leuprorelin	HIV-IN	-1	Training	<chem>O=C(NCC)[C@@H]6CCCN6C(=O)C(N)CCCN(C(=N)NC(=O)C(CC(C)C)NC(=O)[C@@H](CC(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc3cnc2ccccc23)NC(=O)C(Cc4cncn4)NC(=O)C5CCC(=O)N5</chem>
Levodopa	HIV-IN	-1	Training	<chem>Oc1ccc(C[C@H](N)C(=O)O)cc1O</chem>
Lidocaine	HIV-IN	-1	Prediction	<chem>O=C(Nc1c(C)cccc1C)CN(CC)CC</chem>
Loratadine	HIV-IN	-1	Training	<chem>Clc3cc4CCc1cccn1C(=C2/CCN(CC2)C(=O)OCC)\c4cc3</chem>
Maprotiline	HIV-IN	-1	Training	<chem>CNCCCC24CCC(c1ccccc12)c3ccccc34</chem>
Meclizine	HIV-IN	-1	Training	<chem>Cc1cccc(c1)CN2CCN(CC2)C(c3ccc(Cl)cc3)c4ccccc4</chem>
Medroxyprogesterone	HIV-IN	-1	Prediction	<chem>CC(=O)[C@@]2(O)CCC1C3C[C@H](C)C4=CC(=O)CC[C@]4(C)C3CC[C@@]12C</chem>
Melfalan	HIV-IN	-1	Training	<chem>O=C(O)[C@@H](N)Cc1ccc(cc1)N(CCCl)CCCl</chem>
Meprobamate	HIV-IN	-1	Training	<chem>O=C(N)OCC(C)(COC(=O)N)CCC</chem>
Methamphetamine	HIV-IN	-1	Training	<chem>C[C@H](NC)Cc1ccccc1</chem>
Methantheline	HIV-IN	-1	Prediction	<chem>CC[N+](C)(CC)CCOC(=O)C1c3ccccc3Oc2ccccc12</chem>
Methocarbamol	HIV-IN	-1	Training	<chem>NC(=O)OCC(O)COc1ccccc1OC</chem>
Methoxyflurane	HIV-IN	-1	Training	<chem>ClC(Cl)C(F)(F)OC</chem>
Methscopolamine	HIV-IN	-1	Training	<chem>OC[C@H](c1ccccc1)C(=O)OC2CC3C4OC4C(C2)[N+]3(C)C</chem>
Methylphenidate	HIV-IN	-1	Prediction	<chem>O=C(OC)C(C1CCCCN1)c2ccccc2</chem>
Methysergide	HIV-IN	-1	Training	<chem>CC[C@@H](CO)NC(=O)[C@@H]4C=C1C(Cc2cn(C)c3ccccc1c23)N(C)C4</chem>
Metoclopramide	HIV-IN	-1	Training	<chem>Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC</chem>
Midodrine	HIV-IN	-1	Training	<chem>COc1ccc(cc1C(O)CNC(=O)CN)OC</chem>
Mirtazapine	HIV-IN	-1	Prediction	<chem>CN1CC2N(CC1)c4ncccc4Cc3ccccc23</chem>
Modafinil	HIV-IN	-1	Training	<chem>O=S(CC(N)=O)C(c1ccccc1)c2ccccc2</chem>
Montelukast	HIV-IN	-1	Training	<chem>CC(C)(O)c5ccccc5CC[C@@H](SCC1(CC(=O)O)CC1)c2ccccc2)/C=C/c3ccc4ccc(Cl)cc4n3</chem>
Moricizine	HIV-IN	-1	Training	<chem>O=C(OCC)Nc1cc2N(c3ccccc3Sc2cc1)C(=O)CCN4CCOCC4</chem>
Morphine	HIV-IN	-1	Prediction	<chem>Oc1ccc2C[C@H]4N(C)CC[C@@]35[C@@H](Oc1c23)[C@@H](O)C=C[C@@H]45</chem>
Nalmefene	HIV-IN	-1	Training	<chem>C=C1CC[C@@]6(O)[C@H]3Cc5ccc(O)c4O[C@@H]1[C@]6(C[N@@]3CC2CC2)c45</chem>
Neostigmine	HIV-IN	-1	Training	<chem>O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C</chem>

Nifedipine	HIV-IN	-1	Training	<chem>CC(N2)=C(C(OC)=O)C(C(C(OC)=O)=C2C)C1=CC=CC=C1[N+](O-)=O</chem>
Oxycodone	HIV-IN	-1	Prediction	<chem>O=C1CC[C@@]5(O)[C@H]2Cc4ccc(OC)c3O[C@@H]1[C@]5(CC[N@@]2C)c34</chem>
Paroxetine	HIV-IN	-1	Training	<chem>Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2</chem>
Pecazine	HIV-IN	-1	Training	<chem>CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23</chem>
Pergolide	HIV-IN	-1	Training	<chem>CSC[C@@H]4CC1C(Cc2cnc3cccc1c23)N(C4)CCC</chem>
Phenylbutazone	HIV-IN	-1	Prediction	<chem>O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2</chem>
Phenytoin	HIV-IN	-1	Training	<chem>O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3</chem>
Pilocarpine	HIV-IN	-1	Training	<chem>Cn2cnc2C[C@H]1COC(=O)[C@H]1CC</chem>
Pimozide	HIV-IN	-1	Training	<chem>Fc1ccc(cc1)C(CCCN2CCC(CC2)N3c4ccccc4NC3=O)c5ccc(F)cc5</chem>
Pramipexole	HIV-IN	-1	Prediction	<chem>CCCN[C@@H]1Cc2sc(N)nc2CC1</chem>
Probenecid	HIV-IN	-1	Training	<chem>O=S(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)O</chem>
Procyclidine	HIV-IN	-1	Training	<chem>OC(CCN1CCCC1)(c2ccccc2)C3CCCCC3</chem>
Propantheline	HIV-IN	-1	Training	<chem>CC(C)[N+](C)(CCOC(=O)C1c3ccccc3Oc2ccccc12)C(C)C</chem>
Pseudoephedrine	HIV-IN	-1	Prediction	<chem>OC(C(C)NC)c1ccccc1</chem>
Pyrantel	HIV-IN	-1	Training	<chem>CN2CCCN=C2/C=C/c1cccs1</chem>
Quinidine	HIV-IN	-1	Training	<chem>COc1cc2c(cc1)nc2[C@H](O)C4CC3CCN4CC3C=C</chem>
Ranitidine	HIV-IN	-1	Training	<chem>[O-][N+](=O)C=C(/NC)NCCSCc1ccc(CN(C)C)o1</chem>
Rifampin	HIV-IN	-1	Prediction	<chem>CN1CCN(CC1)/N=C/c3c2NC(=O)C(C)=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)C=CO[C@@]5(C)Oe4c(C)c(O)c(c2O)c(c3O)c4C5=O</chem>
Risperidone	HIV-IN	-1	Training	<chem>FC3=CC1=C(C=C3)C(C2CCN(CCC4=C(C)N=C5N(CCCC5)C4=O)CC2)=NO1</chem>
Ropinirole	HIV-IN	-1	Training	<chem>CCCN(CCC)CCc1cccc2NC(=O)Cc12</chem>
Salmeterol	HIV-IN	-1	Training	<chem>OCc1cc(ccc1O)C(O)CNCCCCCOCCCCc2ccccc2</chem>
Selegiline	HIV-IN	-1	Prediction	<chem>C#CCN(C)[C@H](C)Cc1ccccc1</chem>
Sulfinpyrazone	HIV-IN	-1	Training	<chem>O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3</chem>
Tegafur	HIV-IN	-1	Training	<chem>FC1=CN(C(=O)NC1=O)C2CCCO2</chem>
Terpin	HIV-IN	-1	Training	<chem>C[C@@]1(O)CC[C@@H](CC1)C(C)(C)O</chem>
Tolcapone	HIV-IN	-1	Prediction	<chem>Oc1cc(cc([N+](O-)=O)c1O)C(=O)c2ccc(C)cc2</chem>
Tranlycypromine	HIV-IN	-1	Training	<chem>N[C@@H]2C[C@H]2c1ccccc1</chem>
Trazodone	HIV-IN	-1	Training	<chem>Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O</chem>
Triamcinolone	HIV-IN	-1	Training	<chem>OCC(=O)[C@@]3(O)[C@H](O)C[C@H]2[C@@H]4CCCC1=CC(=O)C=C[C@]1(C)[C@@]4(F)C(O)C[C@@]23C</chem>
Valproic acid	HIV-IN	-1	Prediction	<chem>CCCC(CCC)C(=O)O</chem>
Vancomycin	HIV-IN	-1	Training	<chem>O=C(O)[C@@H]1%10NC(=O)[C@H]2NC(=O)[C@H](NC(=O)[C@@H]6NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](NC(=O)[C@@H](CC(C)C)NC)[C@H](O)c7ccc(Oc5cc6cc(Oc1ccc(cc1Cl)[C@H]2O)c5OC4OC(CO)C(O)C(O)C4OC3CC(C)(N)C(O)C(C)O3)c(Cl)c7)c8ccc(O)c(c8)c9c(O)cc(O)cc9%10</chem>
Venlafaxine	HIV-IN	-1	Training	<chem>OC1(CCCCC1)C(CN(C)C)c2ccc(OC)cc2</chem>
Verapamil	HIV-IN	-1	Training	<chem>COc1cc(ccc1OC)C(C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C</chem>
Wytensin	HIV-IN	-1	Prediction	<chem>Clc1cccc(Cl)c1/C=N/NC(=N)N</chem>
Zafirlukast	HIV-IN	-1	Training	<chem>Cc1ccccc1S(=O)(=O)NC(=O)c5ccc(Cc3cn(C)c2ccc(cc23)NC(=O)OC4CCCC4)c(OC)c5</chem>

Zileuton	HIV-IN	-1	Training	NC(=O)N(O)C(C)c1cc2ccccc2s1
Zonisamide	HIV-IN	-1	Training	NS(=O)(=O)Cc2noc1ccccc12

A_{HIV-IP}: is referred to the observed anti-HIV activity through the inhibition of a specific protein.

Name or Code: in the specific case of codes, these are represented by numbers belonging to ChEMBL Database.

PA_{HIV}: the code used for the different proteins associated to HIV.

Note #1: From Eq. 3 and Table 2 you can see that both, average (*avg*) and deviation (*dif*) descriptors enter in the discriminant function. In the case of the mt-QSAR-LDA model, “*dif*” descriptors are calculated as the difference between the original descriptor corresponding to each compound (calculated by MODESLAB v1.5) and the “*avg*” descriptors, as explained in the manuscript. All the “*avg*” descriptors are:

Target	avgμ(Gas) ₁	avgμ(Ab-R2) ₉	avgμ(Ab-sumB20) ₃
CCR2	-1.6744831	167885.7351	125.979124
CCR3	-1.6156685	65331.34729	89.15693307
CCR5	-1.87367	115615.2178	104.5659475
CXCR4	-2.2545632	85794.40879	97.29456735
HIV-1 PR	-2.507272	148198.2698	134.9628535
HIV-1 RT	-0.9233859	77250.56134	68.64206873
HIV-IN	-1.2659498	93054.98893	78.50327219

These values were use also for the calculation of fragment contributions

Note #2: From Table 3 you can see that both, average (*avg*) and deviation (*dif*) descriptors enter in the mt-QSAR-ANN model. Thus, “*dif*” descriptors are calculated as the difference between the original descriptor corresponding to each compound (calculated by DRAGON v5.3) and the “*avg*” descriptors, as explained in the manuscript. All the “*avg*” descriptors are:

Target	avgGATS1v	avgS3K	avgIVDM	avgMATS1v	avgGATS2e	avgEEig01r	avgGGI3	avgJGI1
CCR2	1.12175207	7.28015703	5.15690083	0.00940496	0.53038017	4.35392562	2.939	0.25307438
CCR3	1.09866964	7.41675893	5.04959821	-0.00504464	0.63215179	3.99840179	2.11047321	0.20960714
CCR5	1.12833858	7.11389764	5.22399213	0.00734646	0.73353543	4.1956378	2.68989764	0.18461417
CXCR4	1.05994118	8.06647059	5.11477941	0.03952941	0.83564706	4.08075	2.3715	0.16925
HIV-1 PR	1.08446721	9.84102459	5.41062295	0.03856557	0.70295902	4.25598361	3.62610656	0.23077869
HIV-1 RT	0.92906306	4.66269369	4.53279279	-0.00592793	0.70856757	4.14401802	2.02621622	0.20396396
HIV-IN	0.92583333	4.54425	4.6787381	0.04915476	0.64822619	4.17967857	2.27091667	0.20285714