SUPPORT INFORMATION

Table 1 with the compounds used in this study. The smiles represent the structural key of the compound. The class is defined for a threshold of 40 micromolar. The IC50 (micromolar) is included when information is available and the reference number is linking to the reference in the manuscript.

Name	smiles	class	IC50	Ref
9-HYDROXYRISPERIDONE	Fc1ccc2c(o[nH0]c2C2CC[N+](CC2)CCC2C(=O)[N+]=3CCCC(O)C=3N=C2C)c1	1	0.15	ref 16
ACEBUTOLOL	O=C(Nc1ccc(OCC(O)C[N+]C(C)C)c(c1)C(=O)C)CCC	0		ref 16
ACETAMINOPHEN	O=C(Nc1ccc(O)cc1)C	0		ref 16
ACETAZOLAMIDE	s1c([S+2]([O-])([O-])N)[nH0][nH0]c1NC(=O)C	0		ref 16
ACETYLSALICYLIC_ACID	O=C(Oc1ccccc1C(=O)[O-])C	0		ref 16
ACITRETIN	O=C([O-])/C=C(\C)/C=C\C=C(/C)\C=C/c1c(C)cc(OC)c(C)c1C	0		ref 16
ACRIVASTINE	O=C([O-])/C=C\c1[nH0]c(ccc1)/C(=C\C[N+]1CCCC1)/c1ccc(C)cc1	0		ref 16
ACYCLOVIR	O=C1N=C(N)Nc2[nH0](c[nH0]c21)COCCO	0		ref 16
ALBUTEROL	OCc1cc(ccc1O)C(O)C[N+]C(C)(C)C	0		ref 16
ALFUZOSIN	O=C(NCCCN(C)c1[nH0]c(C)c2cc(OC)c(OC)cc2[nH0]1)C1OCCC1	0	83.3	ref 16
ALOSETRON	O=C1N(CCc2[nH0](C)c3ccccc3c21)Cc1[nH]c[nH0]c1C	1	3.23	ref 21
ALPRAZOLAM	Clc1ccc2[nH0]3c([nH0][nH0]c3C)CN=C(c2c1)c1ccccc1	0		ref 16
ALTRETAMINE	[nH0]1c([nH0]c([nH0]c1N(C)C)N(C)C)N(C)C	0		ref 16
AMANTADINE	[N+]C12C[C@H](C[C@@H](C[C@H](C3)C2)C1)3	0		ref 16
AMBASILIDE	O=C(N1C[C@H](C[N+](C[C@H](C1)C1)Cc2ccccc2)1)c1ccc(N)cc1	1	3.63	ref 16
AMILORIDE	Clc1[nH0]c(c(N)[nH0]c1N)C(=O)NC(=[N+])N	0		ref 16
AMINOBENZOIC_ACID	O=C([O-])c1ccc(N)cc1	0		ref 16
AMINOSALICYLIC_ACID	O=C([O-])c1ccc(N)cc1[O-]	0		ref 16
AMIODARONE	Ic1cc(cc(I)c1OCC[N+](CC)CC)C(=O)c1c2ccccc2oc1CCCC	1	1	ref 16
AMITRIPTYLINE	[N+](C)(C)CCC=C1c2ccccc2CCc2ccccc21	1	10	ref 21
AMLODIPINE	Clc1ccccc1C1C(=C(NC(COCC[N+])=C1C(=O)OCC)C)C(=O)OC	1	2	ref 16
AMPHETAMINE	[N+]C(C)Cc1ccccc1	0		ref 16
AMPRENAVIR	[S+2]([O-])([O-])(NC(C(C)C)C[C@@H](O)[C@@H](NC(=O)O[C@H](COCC1)1)Cc1ccccc1)c1ccc(N)cc1	0		ref 16
ANAGRELIDE	Clc1ccc2[N+]=C3NC(=O)CN3Cc2c1Cl	0		ref 16
ANASTROZOLE	N#CC(C)(C)c1cc(cc(c1)C(C)(C)C#N)C[nH0]1[nH0]c[nH0]c1	0		ref 16
ASTEMIZOLE	Fc1ccc(cc1)C[nH0]1c2ccccc2[nH0]c1NC1CC[N+](CC1)CCc1ccc(OC)cc1	1	0.0115	ref 26
ATENOLOL	O=C(N)Cc1ccc(OCC(O)C[N+]C(C)C)cc1	0		ref 16
ATORVASTATIN	Fc1ccc(cc1)c1[nH0](CC[C@@H](O)C[C@@H](O)CC(=O)[O-])c(c(c1c1ccccc1)C(=O)Nc1ccccc1)C(C)C	0		ref 16
ATOVAQUONE	Clc1ccc(cc1)[C@H](CC[C@H](CC1)C2=CC(=O)c3ccccc3C2=O)1	0		ref 16

ATROPINE	O=C(O[C@H](C[C@@H]([N+](C)[C@@H](C1)CC2)2)1)C(CO)c1ccccc1	1	0.558	ref 26
AWD_23-111	O=[N+]([O-])c1ccc(cc1)C(=O)N(CCC[N+](CC)CC)CC(=O)N(C1CCCCC1)C1CCCCC1	1	0.32	ref 16
AZATADINE	[nH0]1cccc2CCc3ccccc3C(c12)=C1CC[N+](C)CC1	0		ref 16
AZIMILIDE	Clc1ccc(cc1)c1oc(cc1)C=NN1CC(=O)N(CCCC[N+]2CC[N+](C)CC2)C1=O	1	1.4	ref 16
BENDROFLUMETHIAZIDE	[S+2]1([O-])([O-])NC(Nc2cc(c([S+2]([O-])([O-])N)cc12)C(F)(F)F)Cc1ccccc1	0		ref 16
BENZONATATE	O=Cc1ccc(NCCCC)cc1	0		ref 16
BENZTROPINE	O([C@H](C[C@@H]([N+](C)[C@@H](C1)CC2)2)1)C(c1ccccc1)c1ccccc1	0		ref 16
BEPRIDIL	O(CC(C)C)C[C@H]([N+]1CCCC1)CN(Cc1ccccc1)c1ccccc1	1	0.55	ref 16
BETAXOLOL	OC(COc1ccc(cc1)CCOCC1CC1)C[N+]C(C)C	0		ref 16
BEXAROTENE	O=C([O-])c1ccc(cc1)C(=C)c1cc2c(cc1C)C(C)(C)CCC2(C)C	0		ref 16
BICALUTAMIDE	[S+2]([O-])([O-])(c1ccc(F)cc1)c1c(C)c(cc(NC(=O)C(O)C)c1C#N)C(F)(F)F	0		ref 16
BIPERIDEN	OC(CC[N+]1CCCCC1)(c1ccccc1)C1CC2C=CC1C2	0		ref 16
BISOPROLOL	OC(COc1ccc(cc1)COCCOC(C)C)C[N+]C(C)C	0		ref 16
BRL-37872	O=[N+]([O-])c1ccc(cc1)C(=O)N(CCC[N+](C)CCc1ccc(OC)c(OC)c1)c1ccc(OC)c(OC)c1	1	0.0198	ref 20
BROMPHENIRAMINE	Brc1ccc(cc1)C(CC[N+](C)C)c1[nH0]cccc1	0		ref 16
BUPIVACAINE	O=C(Nc1c(C)cccc1C)C1[N+](CCCC1)CCCC	1		ref 16
BUPROPION	Clc1cccc(c1)C(=O)C([N+]C(C)(C)C)C	0		ref 16
BUSULFAN	[S+2]([O-])([O-])(OCCCCO[S+2]([O-])([O-])C)C	0		ref 16
BUTALBITAL	O=C1NC(=O)C(CC=C)(CC(C)C)C(=O)N1	0		ref 16
CABERGOLINE	O=C(NCC)N(CCC[N+](C)C)C(=O)[C@@H](C[N+](CC=C)[C@H](Cc1c[nH]c2cccc(c21)[C@@H](C1)2)2)1	0		ref 16
CAFFEINE	O=C1N(C)c2[nH0]c[nH0](C)c2C(=O)N1C	1	4.9	ref 19
CALCITRIOL	O[C@H](C\C(=C/C=C/1\CCC[C@@](C)([C@@H](CC[C@H]([C@H](C)CCCC(O)(C)C)2)\1)2)\C(=C)[C@@H](O)C1)1	0		ref 16
CARBAMAZEPINE	O=C(N)N1c2ccccc2C=Cc2ccccc12	0		ref 16
CARBETAPENTANE	O=C(OCCOCC[N+](CC)CC)C1(CCCC1)c1ccccc1	0		ref 16
CARISOPRODOL	O=C(OCC(C)(COC(=O)NC(C)C)CCC)N	0		ref 16
CARTEOLOL	O=C1Nc2cccc(OCC(O)C[N+]C(C)(C)C)c2CC1	0		ref 16
CARVEDILOL	OC(COC1=CC=CC2=Nc3ccccc3C21)C[N+]CCOc1ccccc1OC	1	10.42	ref 21
CELECOXIB	[S+2]([O-])([O-])(N)c1ccc([nH0]2[nH0]c(cc2c2ccc(C)cc2)C(F)(F)F)cc1	0		ref 16
CERIVASTATIN	Fc1ccc(cc1)c1c(/C=C/[C@@H](O)C[C@@H](O)CC(=O)[O-])c([nH0]c(c1COC)C(C)C)C(C)C	0		ref 16
CETIRIZINE	Clc1ccc(cc1)C([N+]1CC[N+](CC1)CCOCC(=O)[O-])c1ccccc1	1	30	ref 26
CEVIMELINE	S1C[C@](O[C@H]1(C))(C[N+]1CCC2CC1)2	0		ref 16
CHLORAMBUCIL	ClCCN(CCCl)c1ccc(cc1)CCCC(=O)[O-]	0		ref 16
CHLORDIAZEPOXIDE	Clc1ccc2[N+]=C(NC)C[N+]([O-])=C(c2c1)c1ccccc1	0		ref 16
CHLOROQUINE	Clc1ccc2c([nH0]ccc2NC(C)CCC[N+](CC)CC)c1	1	2.5	ref 20
CHLOROTHIAZIDE	Clc1cc2[N+]=C[N-][S+2]([O-])([O-])c2cc1[S+2]([O-])([O-])N	0		ref 16
CHLORPHENIRAMINE	Clc1ccc(cc1)C(CC[N+](C)C)c1[nH0]cccc1	1	21	ref 21

CHLORPROMAZINE	Clc1ccc2Sc3ccccc3N(CCC[N+](C)C)c2c1	1	1.47	ref 20
CHLORPROPAMIDE	Clc1ccc([S+2]([O-])([O-])[N-]C(=O)NCCC)cc1	0		ref 16
CHLORTHALIDONE	Clc1ccc(cc1[S+2]([O-])([O-])N)C1(O)NC(=O)c2ccccc21	0		ref 16
CHLORZOXAZONE	Clc1ccc2OC(=O)Nc2c1	0		ref 16
CHROMANOL	[S+2]([O-])([O-])(C[N+]C1c2cc(ccc2OC(C)(C)C1O)C[N+])CC	1	6.6	ref 19
CILOSTAZOL	O=C1Nc2ccc(OCCCCc3[nH0][nH0][nH0][nH0]3C3CCCCC3)cc2CC1	0		ref 16
CIMETIDINE	S(CCNC(=[N+]C#N)NC)Cc1[nH]c[nH0]c1C	0		ref 16
CIPROFLOXACIN	FC1=CC2C(=[N+](C=C(C2=O)C(=O)[O-])C2CC2)C=C1N1CC[N+]CC1	0	966	ref 20
CISAPRIDE	Clc1cc(c(OC)cc1N)C(=O)N[C@H](CC[N@H+](C[C@@H](OC)1)CCCOc2ccc(F)cc2)1	1	0.02	ref 16
CITALOPRAM	Fc1ccc(cc1)C1(OCc2cc(C#N)ccc21)CCC[N+](C)C	1	3.98	ref 16
CLARITHROMYCIN	O=C1O[C@@H](CC)[C@](O)(C)[C@H](O)[C@H](C)C(=O)[C@H](C)C[C@@](OC)(C)[C@H](O[C@H](O[C@H](C)C[C@H]([N@@H+](C)C)[C@@H](O)2)2)[C@@H](C)[C@@H](O[C@H](O[C@@H](C)[C@H](O)[C@@](OC)(C)C2)2)[C@@H](C)1	0	59	ref 26
CLAVULANIC_ACID	O=C1N2[C@H](O/C(=C/CO)/[C@@H]2(C(=O)[O-]))C1	0		ref 16
CLEMASTINE	Clc1ccc(cc1)C(OCCC1[N+](C)CCC1)(C)c1ccccc1	1	0.012	ref 16
CLOFIBRATE	Clc1ccc(OC(C)(C)C(=O)OCC)cc1	0		ref 16
CLOMIPHENE	Cl/C(/c1ccccc1)=C(\c1ccccc1)/c1ccc(OCC[N+](CC)CC)cc1	1	0.18	ref 27
CLONAZEPAM	Clc1ccccc1C1=NCC(=O)Nc2ccc([N+](=O)[O-])cc21	0		ref 16
CLONIDINE	Clc1cccc(Cl)c1[N+]=C1NCCN1	0		ref 16
CLOPIDOGREL	Clc1ccccc1C([N+]1CCc2sccc2C1)C(=O)OC	0		ref 16
CLORAZEPATE	Clc1ccc2NC(=O)C(N=C(c2c1)c1ccccc1)C(=O)[O-]	0		ref 16
CLOZAPINE	Clc1ccc2Nc3ccccc3C(=Nc2c1)N1CC[N+](C)CC1	1	0.256	ref 20
COCAETHYLENE	O=C(O[C@@H](CC1[N+](C)C(CC1)[C@@H](C(=O)OCC)1)1)c1ccccc1	1	1.2	ref 16
COCAINE	O=C(O[C@H](C[C@@H]([N@H+](C)[C@H](CC1)[C@H](C(=O)OC)2)1)2)c1ccccc1	1	7.2	ref 20
CODEINE	O[C@@H](C=C[C@@H]([C@H]([N+](C)CC[C@]{c1c(ccc(OC)c1O[C@@H]12)C3)22)3)2)1	0	301	ref 16
CROMOLYN	O=C1C=C(Oc2cccc(OCC(O)COc3cccc4OC(=CC(=O)c43)C(=O)[O-])c12)C(=O)[O-]	0		ref 16
CYCLOBENZAPRINE	[N+](C)(C)CCC=C1c2ccccc2C=Cc2ccccc21	0		ref 16
CYCLOPHOSPHAMIDE	ClCCN([P+]1([O-])OCCCN1)CCCl	0		ref 16
CYPROHEPTADINE	[N+]1(C)CCC(CC1)=C1c2ccccc2C=Cc2ccccc21	1		ref 16
D600 (methoxyverapamil)	O(C)c1ccc(cc1OC)CC[N+](C)CCCC(C#N)(c1cc(OC)c(OC)c(OC)c1)C(C)C	1	2.7	ref 19
D617(R=CH3)	O(C)c1ccc(cc1OC)C(C#N)(CCC[N+]C)C(C)C	0	>30	ref 28
D620(R=H)	O(C)c1ccc(cc1OC)C(C#N)(CCC[N+])C(C)C	0	>30	ref 28
DANAZOL	O[C@@](C#C)(CC[C@@H]([C@H](CCC1=Cc2o[nH0]cc2C[C@@](C)1([C@@H](CC[C@@](C)12)3))3)1)2	0		ref 16
DANTROLENE	O=[N+]([O-])c1ccc(cc1)c1oc(cc1)C=NN1CC(=O)NC1=O	0		ref 16
DELAVIRDINE	[S+2]([O-])([O-])(NC1C=CC2=NC(=CC2=C1)C(=O)N1CCN(CC1)c1[nH0]cccc1NC(C)C)C	0		ref 16
DESIPRAMINE	[N+](C)CCCN1c2ccccc2CCc2ccccc12	1	1.39	ref 16
DESLORATIDINE	Clc1ccc2c(c1)CCc1ccc[nH0]c1C2=C1CC[N+]CC1	1	4.46	ref 16

DEXFENFLURAMINE	FC(F)(F)c1cccc(c1)C[C@@H]([N+]CC)C	1		ref 16
DIAZEPAM	Clc1ccc2N(C)C(=O)CN=C(c2c1)c1ccccc1	0		ref 16
DICHLORPHENAMIDE	Clc1cc([S+2]([O-])([O-])N)cc([S+2]([O-])([O-])N)c1Cl	0		ref 16
DICLOFENAC	Clc1cccc(Cl)c1Nc1ccccc1CC(=O)[O-]	0		ref 16
DIDANOSINE	O=C1N=CNc2[nH0](c[nH0]c21)C1OC(CC1)CO	0		ref 16
DIFENOXIN	O=C([O-])C1(CC[N+](CC1)CCC(C#N)(c1ccccc1)c1ccccc1)c1ccccc1	0		ref 16
DIFLUNISAL	Fc1ccc(c(F)c1)c1ccc([O-])c(c1)C(=O)[O-]	0		ref 16
DILTIAZEM	S1c2ccccc2N(CC[N+](C)C)C(=O)[C@H](OC(=O)C)[C@@H]1(c1ccc(OC)cc1)	1	17.30	ref 20
DIPHENHYDRAMINE	O(CC[N+](C)C)C(c1ccccc1)c1ccccc1	1	27	ref 16
DIPYRIDAMOLE	OCCN(CCO)c1[nH0]c(N2CCCCC2)c2[nH0]c([nH0]c(N3CCCCC3)c2[nH0]1)N(CCO)CCO	0		ref 16
DISOPYRAMIDE	O=C(N)C(CC[N+](C(C)C)C(C)C)(c1[nH0]cccc1)c1ccccc1	0	92	ref 20
DISULFIRAM	S=C(SSC(=S)N(CC)CC)N(CC)CC	0		ref 16
DOFETILIDE	[S+2]([O-])([O-])(Nc1ccc(OCC[N@H+](C)CCc2ccc(N[S+2]([O-])([O-])C)cc2)cc1)C	1	0.0103	ref 20
DOLASETRON	O=C1C[N+]2[C@@H](CC(OC(=O)C=3CN=C4C=CC=CC4=3)C[C@@H]2(CC1C1))1	1	5.95	ref 16
DOMPERIDONE	ClC=1C=CC2=[N+](C(=O)N=C2C=1)C1CC[N+](CC1)CCC[N+]1=C2C=CC=CC2=NC1=O	1	0.1621	ref 16
DONEPEZIL	O=C1c2cc(OC)c(OC)cc2CC1CC1CC[N+](CC1)Cc1ccccc1	0		ref 16
DOXAZOSIN	O=C(N1CCN(CC1)c1[nH0]c(N)c2cc(OC)c(OC)cc2[nH0]1)C1Oc2ccccc2OC1	1	0.585	ref 26
DOXEPINE	O1Cc2ccccc2\C(=C\CC[N+](C)C)\c2ccccc12	1		ref 16
DOXYLAMINE	O(CC[N+](C)C)C(C)(c1[nH0]cccc1)c1ccccc1	0		ref 16
DRONABINOL	Oc1cc(cc2OC(C)(C)C3CCC(C)=CC3c12)CCCCC	0		ref 16
DROPERIDOL	Fc1ccc(cc1)C(=O)CCC[N@H+](CC=C([N+]1=C2C=CC=CC2=NC1=O)CC1)1	1	0.032	ref 20
DYPHYLLINE	O=C1N(C)c2[nH0]c[nH0](CC(O)CO)c2C(=O)N1C	0		ref 16
E-4031	[S+2]([O-])([O-])(Nc1ccc(cc1)C(=O)C1CC[N+](CC1)CCc1[nH0]c(C)ccc1)C	1	0.012	ref 20
EFAVIRENZ	Clc1ccc2NC(=O)O[C@@](C#CC3CC3)(c2c1)[C@](F)(F)F	0		ref 16
EGIS7229	ClC=1C=NNC(=O)C=1NCCC[N+](C)CCc1ccc(OC)c(OC)c1	1	6.6	ref 19
EMD60263	S1C(=O)NN=C(c2ccc3N(CCCc3c2)C(=NCC)c2ccc(OC)c(OC)c2)C1C	1	6.6	ref 19
ENTACAPONE	O=[N+]([O-])c1cc(cc(O)c1[O-])/C=C(\C#N)/C(=O)N(CC)CC	0		ref 16
EPHEDRINE	O[C@H](c1ccccc1)[C@@H]([N+]C)C	0		ref 16
EPINASTINE	NC1=[N+]CC2N1c1ccccc1Cc1ccccc12	0	165.95	ref 19
EPROSARTAN	s1cccc1C\C(=C\c1[nH0](Cc2ccc(cc2)C(=O)[O-])c([nH0]c1)CCCC)\C(=O)[O-]	0		ref 16
ERGOTAMINE	O=C1[nH0]2cccc2C2(O)OC(NC(=O)c3c[nH0+](C)c4cc5C=Nc6cccc(c65)c4c3)(C)C(=O)N2C1Cc1ccccc1	0		ref 16
ERYTHROMYCYLAMINE	O=C1OC(CC)[C@](O)(C)[C@H](O)[C@@H](C)[C@@H]([N+])[C@H](C)C[C@@](O)(C)[C@H](O[C@H](O[C@H](C)C[C@H]([N@@H+](C)C)[C@@H](O)2)2)[C@@H](C)[C@H](O[C@H](O[C@@H](C)[C@H](O)[C@@](OC)(C)C2)2)[C@@H](C)1	0	273.9	ref 20
OMEPRAZOLE	[S+]([O-])(Cc1[nH0]cc(C)c(OC)c1C)c1[nH0]c2ccc(OC)cc2[nH]1	0		ref 16
ESTAZOLAM	Clc1ccc2[nH0]3c[nH0][nH0]c3CN=C(c2c1)c1ccccc1	0		ref 16
ESTRADIOL	Oc1ccc2c(c1)CC[C@@H]([C@H](CC[C@H](O)[C@@](C)(CC[C@H]21)2)2)1	0		ref 16

ESTRAMUSTINE	ClCCN(CCCl)C(=O)Oc1ccc2c(c1)CC[C@@H]([C@H](CC[C@H](O)[C@@](C)(CC[C@H]21)2)2)1	0		ref 16
ESTROPIPATE	[S+2]([O-])([O-])([O-])Oc1ccc2c(c1)CC[C@@H]([C@H](CCC(=O)[C@@](C)(CC[C@H]21)2)2)1	0		ref 16
ETHACRYNIC_ACID	Clc1c(OCC(=O)[O-])ccc(c1Cl)C(=O)C(=C)CC	0		ref 16
ETHAMBUTOL	OC[C@@H]([N+]CC[N+][C@H](CO)CC)CC	0		ref 16
ETHINYL_ESTRADIOL	Oc1ccc2c(c1)CC[C@@H]([C@H](CC[C@@](O)(C#C)[C@@](C)(CC[C@H]21)2)2)1	0		ref 16
ETHIONAMIDE	S=C(N)c1cc[nH0]c(c1)CC	0		ref 16
ETHOSUXIMIDE	O=C1NC(=O)C(C)(C1)CC	0		ref 16
ETODOLAC	O=C([O-])CC1(OCCc2c3cccc(CC)c3[nH]c21)CC	0		ref 16
ETOPOSIDE	O=C1OCC2[C@H]1([C@H](c1cc(OC)c(O)c(OC)c1)c1cc3OCOc3cc1[C@@H](O[C@H](O[C@H](CO[C@H](O[C@H]1([C@H](O)[C@@H](O)3))C)1)3)2)	0		ref 16
FAMOTIDINE	s1cc([nH0]c1[N+]=C(N)N)CSCCC(N)=[N+][S+2]([O-])([O-])N	0		ref 16
FELBAMATE	O=C(OCC(COC(=O)N)c1ccccc1)N	0		ref 16
FELODIPINE	Clc1cccc(c1Cl)C1C(=C(NC(C)=C1C(=O)OCC)C)C(=O)OC	0		ref 16
FENOPROFEN	O=C([O-])C(C)c1cccc(Oc2ccccc2)c1	0		ref 16
FENTANYL	O=C(N(c1ccccc1)C1CC[N+](CC1)CCc1ccccc1)CC	1	1.82	ref 29
FEXOFENADINE	O=C([O-])C(C)(C)c1ccc(cc1)C(O)CCC[N+]1CCC(CC1)C(O)(c1ccccc1)c1ccccc1	0		ref 26
FINASTERIDE	O=C1NC2CCC3C4CCC(C(=O)NC(C)(C)C)C4(C)CCC3C2(C)C=C1	0		ref 16
FK506	O=C1N2CCCC[C@H]2(C(=O)O[C@H](/C(/C)=C/[C@H](CC[C@@H](O)[C@H](OC)C2)2)[C@H](C)[C@@H](O)CC(=O)[C@@H](C=C(C)C[C@H](C)C[C@H](OC)[C@@H](O[C@@](O)(C1=O)[C@H](C)C[C@H](OC)1)1)CC=C)	0		ref 16
FLECAINIDE	FC(F)(F)COc1ccc(OCC(F)(F)F)c(c1)C(=O)NCC1[N+]CCCC1	1	3.91	ref 20
FLUOXETINE	FC(F)(F)c1ccc(OC(CC[N+]C)c2ccccc2)cc1	1	0.46	ref 20
FLUSPIRILENE	Fc1ccc(cc1)C(CCC[N+]1CCC2(N(CNC2=O)c2ccccc2)CC1)c1ccc(F)cc1	1	0.003	ref 16
FLUTAMIDE	FC(F)(F)c1cc(NC(=O)C(C)C)ccc1[N+](=O)[O-]	0		ref 16
FLUVASTATIN	Fc1ccc(cc1)c1c2ccccc2[nH0](c1/C=C\[C@@H](O)C[C@@H](O)CC(=O)[O-])C(C)C	0		ref 16
FLUVOXAMINE	FC(F)(F)c1ccc(cc1)C(=NOCC[N+])CCCCOC	1	3.8	ref 30
FUROSEMIDE	Clc1cc(NCc2occc2)c(cc1[S+2]([O-])([O-])N)C(=O)[O-]	0		ref 16
GANCICLOVIR	[O-]c1[nH0]c(N)[nH0]c2[nH0](c[nH0]c21)COC(CO)CO	0		ref 16
GATIFLOXACIN	Fc1cc2c([N+](=CC(C2=O)C(=O)[O-])C2CC2)c(OC)c1N1CC[N+][C@H](C)C1	0	128	ref 21
GEMFIBROZIL	O=C([O-])C(C)(C)CCCOc1cc(C)ccc1C	0		ref 16
GLIMEPIRIDE	[S+2]([O-])([O-])([N-]C(=O)NC1CCC(C)CC1)c1ccc(cc1)CCNC(=O)N1CC(C)=C(CC)C1=O	0	74.13	ref 19
GLIPIZIDE	[S+2]([O-])([O-])([N-]C(=O)NC1CCCCC1)c1ccc(cc1)CCNC(=O)c1[nH0]cc([nH0]c1)C	0		ref 16
GLIBENCLAMIDE	Clc1ccc(OC)c(c1)C(=O)NCCc1ccc([S+2]([O-])([O-])[N-]C(=O)NC2CCCCC2)cc1	0	74.13	ref 20
GRANISETRON	O=C(NC1C[C@@H]([N+](C)[C@H](CCC2)C1)2)c1[nH0][nH0](C)c2ccccc21	1	3.71	ref 20
GREPAFLOXACIN	Fc1c(N2CC[N+][C@H](C)C2)cc2[N+](=CC(C(=O)c2c1C)C(=O)[O-])C1CC1	0	66.07	ref 19
GUAIFENESIN	OCC(O)COc1ccccc1OC	0		ref 16
GUANFACINE	Clc1cccc(Cl)c1CC(=O)NC(=[N+])N	0		ref 16

H345_32	O=C(OC(C)(C)C)N1CCC2OC(C1)C[N+](C2)CC(O)COc1ccc(C#N)cc1	1	0.0891	ref 19
HALOFANTRINE	Clc1cc(Cl)c2cc(c3ccc(cc3c2c1)C(F)(F)F)[C@H](O)CC[N+](CCCC)CCCC	1	0.0308	ref 20
HALOPERIDOL	Clc1ccc(cc1)C1(O)CC[N+](CC1)CCCC(=O)c1ccc(F)cc1	1	0.019	ref 20
HYDROCHLOROTHIAZIDE	Clc1cc2NCN[S+2]([O-])([O-])c2cc1[S+2]([O-])([O-])N	0		ref 16
HYDROCODONE	O=C1CC[C@@H]([C@H]([N+](C)CC[C@](c2c(ccc(OC)c2O[C@@H]11)C2)11)2)1	0		ref 16
HYDROFLUMETHIAZIDE	[S+2]1([O-])([O-])NCNc2cc(c([S+2]([O-])([O-])N)cc12)C(F)(F)F	0		ref 16
HYDROMORPHONE	O=C1CC[C@@H]([C@H]([N+](C)CC[C@](c2c(ccc(O)c2O[C@@H]11)C2)11)2)1	0		ref 16
HYDROXYCHLOROQUINE	Clc1ccc2c([nH0]ccc2NC(C)CCC[N+](CC)CCO)c1	0		ref 16
HYDROXYUREA	O=C(N)N[O-]	0		ref 16
HYDROXYZINE	Clc1ccc(cc1)C([N+]1CC[N+](CC1)CCOCCO)c1ccccc1	0		ref 16
HYOSCYAMINE	O=C(O[C@H](C[C@@H]([N+](C)[C@@H](C1)CC2)2)1)[C@H](CO)c1ccccc1	1		ref 39
IBUPROFEN	O=C([O-])C(C)c1ccc(cc1)CC(C)C	0		ref 16
IBUTILIDE	[S+2]([O-])([O-])(Nc1ccc(cc1)C(O)CCC[N+](CC)CCCCCCC)C	1	0.028	ref 16
IMIPRAMINE	N1(CCC[N+](C)C)c2ccccc2CCc2ccccc12	1	3.4	ref 16
INDAPAMIDE	Clc1ccc(cc1[S+2]([O-])([O-])N)C(=O)NN1c2ccccc2CC1C	0		ref 16
INDINAVIR	O=C(NC(C)(C)C)[C@@H]([N+](CC[N+](C1)Cc2c[nH0]ccc2)C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](c2ccccc2C[C@@H](O)2)2)1	0		ref 16
INDOMETHACIN	Clc1ccc(cc1)C(=O)[nH0]1c2ccc(OC)cc2c(CC(=O)[O-])c1C	0		ref 16
IODOQUINOL	Ic1cc(I)c2ccc[nH0]c2c1O	0		ref 16
IQB-9302	O=C(Nc1c(C)cccc1C)C1[N+](CCCC1)CC1CC1	1	20	ref 16
IRBESARTAN	O=C1N(Cc2ccc(cc2)c2ccccc2c2[nH0][nH0][nH0-][nH0]2)C(=NC21CCCC2)CCCC	0		ref 16
ISOMETHEPTENE	[N+](C)C(C)CCC=C(C)C	0		ref 16
ISONIAZID	O=C(NN)c1cc[nH0]cc1	0		ref 16
ISOPRENALINE	Oc1ccc(cc1O)C(O)C[N+]C(C)C	1		ref 16
ISOSORBIDE	O=[N+]([O-])O[C@H](CO[C@H]([C@@H](O)CO[C@H]12)2)1	0		ref 16
ISOTRETINOIN	O=C([O-])/C=C(\C)/C=C/C=C(\C)/C=C\C1=C(C)CCCC1(C)C	0		ref 16
ISRADIPINE	O=C(OC)C1=C(NC(C)=C(C(=O)OC(C)C)C1c1cccc2[nH0]o[nH0]c21)C	1		ref 16
KETANSERIN	Fc1ccc(cc1)C(=O)C1CC[N+](CC1)CCN1C(=O)Nc2ccccc2C1=O	1	0.107	ref 20
KETOCONAZOLE	Clc1ccc(c(Cl)c1)[C@@](OCC(O1)COc2ccc(N3CCN(CC3)C(=O)C)cc2)1(C[nH0]1c[nH0]cc1)	1	1.9	ref 20
KETOPROFEN	O=C(c1ccccc1)c1cccc(c1)C(C)C(=O)[O-]	0		ref 16
KETOROLAC	O=C(c1[nH0]2CCC(c2cc1)C(=O)[O-])c1ccccc1	0		ref 16
LAAM	O=C(OC(CC)C(CC([N+](C)C)C)C)(c1ccccc1)c1ccccc1)C	1	2.18	ref 29
LABETALOL	O=C(N)c1cc(ccc1[O-])C(O)C[N+]C(C)CCc1ccccc1	0		ref 16
LAMIVUDINE	S1C[C@H](O[C@@H]1(CO))N1C=CC(N)=NC1=O	0		ref 16
LAMOTRIGINE	Clc1cccc(c1Cl)c1[nH0][nH0]c(N)[nH0]c1N	0		ref 16
LANSOPRAZOLE	[S+]([O-])(Cc1[nH0]ccc(OCC(F)(F)F)c1C)c1[nH0]c2ccccc2[nH]1	0		ref 16

LETROZOLE	N#Cc1ccc(cc1)C([nH0]1[nH0]c[nH0]c1)c1ccc(C#N)cc1	0		ref 16
LEVAMISOLE	S1CCN2CC(N=C12)c1ccccc1	0		ref 16
LEVETIRACETAM	O=C1N(CCC1)C(CC)C(=O)N	0		ref 16
LEVOFLOXACIN	Fc1cc2C(=O)C(=CN3c2c(OC[C@H]3(C))c1N1CC[N+](C)CC1)C(=O)[O-]	0	912	ref 19
LEVORPHANOL	Oc1ccc2C[C@@H]([N+](C)CC[C@@](CCCC[C@@H]34)(c2c1)4)3	0		ref 16
LEVOTHYROXINE	Ic1cc(Oc2c(I)cc(cc2I)C[C@H]([N+])C(=O)[O-])cc(I)c1O	0		ref 16
LIDOCAINE	O=C(Nc1c(C)cccc1C)C[N+](CC)CC	0		ref 16
LIDOFLAZINE	Fc1ccc(cc1)C(CCC[N+]1CC[N+](CC1)CC(=O)Nc1c(C)cccc1C)c1ccc(F)cc1	1	0.0158	ref 20
LISINOPRIL	O=C([O-])[C@@H](N(CCC1)C(=O)[C@@H]([N+][C@H](CCc2ccccc2)C(=O)[O-])CCCC[N+])1	0		ref 16
LOMEFLOXACIN	Fc1cc2C(=O)C(=CN(CC)c2c(F)c1N1CC[N+]C(C)C1)C(=O)[O-]	0		ref 16
LOMUSTINE	ClCCN(N=O)C(=O)NC1CCCCC1	0		ref 16
LOPERAMIDE	Clc1ccc(cc1)C1(O)CC[N+](CC1)CCC(c1ccccc1)(c1ccccc1)C(=O)N(C)C	0		ref 16
LORATADINE	Clc1ccc2c(c1)CCc1ccc[nH0]c1C2=C1CCN(CC1)C(=O)OCC	1	2.3	ref 20
LORAZEPAM	Clc1ccc2NC(=O)C(O)N=C(c2c1)c1ccccc1Cl	0		ref 16
LOSARTAN	Clc1[nH0]c([nH0](Cc2ccc(cc2)c2ccccc2c2[nH0][nH0][nH0-][nH0]2)c1CO)CCCC	1	7.76	ref 19
LOXAPINE	Clc1ccc2Oc3ccccc3N=C(N3CC[N+](C)CC3)c2c1	0		ref 16
MCI-154	O=C1NN=C(CC1)c1ccc(Nc2cc[nH0]cc2)cc1	1	1.04	ref 19
MDL_74156	O=C(OC1CC2[N+]3CC(O)C(C2)CC3C1)c1c[nH]c2ccccc21	1	12.02	ref 19
MECAMYLAMINE	[N+](C)C1(C)C2CCC(C2)C1(C)C	0		ref 16
MECLIZINE	Clc1ccc(cc1)C([N+]1CC[N+](CC1)Cc1cccc(C)c1)c1ccccc1	1	patent 20060035863	
MEFENAMIC	O=C([O-])c1ccccc1Nc1cccc(C)c1C	0		ref 16
MEFLOQUINE	FC(F)(F)c1[nH0]c2c(cccc2C(F)(F)F)c(c1)[C@H](O)[C@H]([N+]CCCC1)1	1	2.56	ref 21
MEGESTROL	O=C1C=C2C(C)=CC3C4CCC(OC(=O)C)(C(=O)C)C4(C)CCC3C2(C)CC1	0		ref 16
MELOXICAM	s1c([nH0]cc1C)NC(=O)C=1N([S+2]([O-])([O-])c2ccccc2C=1O)C	0		ref 16
MELPHALAN	ClCCN(CCCl)c1ccc(cc1)C[C@H]([N+])C(=O)[O-]	0		ref 16
MEPHOBARBITAL	O=C1NC(=O)C(CC)(C(=O)N1C)c1ccccc1	0		ref 16
MEPROBAMATE	O=C(OCC(C)(COC(=O)N)CCC)N	0		ref 16
MERCAPTOPURINE	S=C1NC=[N+]c2[nH0]c[nH]c21	0		ref 16
MESALAMINE	O=C([O-])c1cc(N)ccc1[O-]	0		ref 16
MESORIDAZINE	S1c2ccccc2N(CCC2[N+](C)CCCC2)c2cc([S+]([O-])C)ccc12	1	0.55	ref 20
METAPROTERENOL	Oc1cc(O)cc(c1)C(O)C[N+]C(C)C	0		ref 16
METAXALONE	O=C1OC(CN1)COc1cc(C)cc(C)c1	0		ref 16
METFORMIN	[N+]=C(N)NC(=[N+])N(C)C	0		ref 16
METHADONE	O=C(CC)C(CC([N+](C)C)C)(c1ccccc1)c1ccccc1	1	9.77	ref 29
METHAMPHETAMINE	[N+](C)C(C)Cc1ccccc1	0		ref 16
METHAZOLAMIDE	S1C([S+2]([O-])([O-])N)=NN(C)C1=NC(=O)C	0		ref 16

METHOCARBAMOL	O=C(OCC(O)COc1ccccc1OC)N	0		ref 16
METHOXSALEN	O=C1Oc2c(C=C1)cc1ccoc1c2OC	0		ref 16
METHSUXIMIDE	O=C1N(C)C(=O)C(C)(C1)c1ccccc1	0		ref 16
METHYCLOTHIAZIDE	ClCC1Nc2cc(Cl)c([S+2]([O-])([O-])N)cc2[S+2]([O-])([O-])N1C	0		ref 16
METHYLPHENIDATE	O=C(OC)C(c1ccccc1)C1[N+]CCCC1	0		ref 16
METOCLOPRAMIDE	Clc1cc(c(OC)cc1N)C(=O)NCC[N+](CC)CC	1	5.40	ref 31
METOLAZONE	Clc1cc2NC(N(C(=O)c2cc1[S+2]([O-])([O-])N)c1ccccc1C)C	0		ref 16
METOPROLOL	OC(COc1ccc(cc1)CCOC)C[N+]C(C)C	0		ref 16
METYROSINE	O=C([O-])[C@]([N+])(C)Cc1ccc(O)cc1	0		ref 16
MEXILETINE	O(CC([N+])C)c1c(C)cccc1C	0		ref 16
MIBEFRADIL	Fc1ccc2c(c1)CC[C@@](OC(=O)COC)(CC[N@@H+](C)CCCc1[nH0]c3ccccc3[nH]1)[C@@H]2([C@H](C)C)	1	1.44	ref 20
MIDAZOLAM	Clc1ccc2[nH0]3c(c[nH0]c3C)CN=C(c2c1)c1ccccc1F	0		ref 16
MIDODRINE	O=C(NCC(O)c1cc(OC)ccc1OC)C[N+]	0		ref 16
MIGLITOL	OCC[N+]1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1(CO)	0		ref 16
MIRTAZAPINE	[nH0]1cccc2Cc3ccccc3C3N(CC[N+](C)C3)c12	1		ref 16
MISOPROSTOL	O=C1C[C@@H](O)[C@H](/C=C/CC(O)(C)CCCC)[C@@H](CCCCCCC(=O)OC)1	0		ref 16
MITOTANE	Clc1ccc(cc1)C(c1ccccc1Cl)C(Cl)Cl	0		ref 16
MITOXANTRONE	O=C1c2c([O-])ccc([O-])c2C(=O)c2c(NCC[N+]CCO)ccc(NCC[N+]CCO)c12	1		ref 16
MIZOLASTINE	Fc1ccc(cc1)C[nH0]1c2ccccc2[nH0]c1N1CCC(CC1)CNC1=[N+]C=CC(=O)N1	1	0.44	ref 20
MK-499	[S+2]([O-])([O-])(Nc1ccc2OC3(CC[N+](CC3)C3CCc4cc(C#N)ccc4C3)CC(O)c2c1)C	1	0.021	ref 20
MODAFINIL	[S+]([O-])(CC(=O)N)C(c1ccccc1)c1ccccc1	0		ref 16
MOLINDONE	O=C1C2=C(N=C(C)C2CC)CCC1C[N+]1CCOCC1	0		ref 16
MONTELUKAST	Clc1ccc2ccc([nH0]c2c1)/C=C\c1cccc(c1)C(SCC1(CC1)CC(=O)[O-])CCc1ccccc1C(O)(C)C	0		ref 16
MORPHINE	Oc1ccc2C[C@@H]([N+](C)CC[C@](c2c1O[C@@H]([C@@H](O)C=C[C@@H]12)3)32)1	0	1000	ref 16
MOSAPRIDE	Clc1cc(c(OCC)cc1N)C(=O)NCC1OCC[N+](C1)Cc1ccc(F)cc1	1	7.76	ref 19
MOXIFLOXACIN	Fc1cc2c([N+](=CC(C2=O)C(=O)[O-])C2CC2)c(OC)c1N1C[C@H]([N+]CCC[C@H](C1)1)1	0	128.82	ref 20
Methylecgonidine	O=C(OC)C1=CCC2[N+](C)C1CC2	0	169.82	ref 19
N-DEMETHYL-ERYTHROMYCIN	O=C1O[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)C(=O)[C@H](C)C[C@](O)(C)[C@H](O[C@H](O[C@H](C)C[C@H]([N+]C)[C@@H](O)2)2)[C@@H](C)[C@H](O[C@H](O[C@@H](C)[C@H](O)[C@@](OC)(C)C2)2)[C@@H](C)1	0	147	ref 20
NABUMETONE	O=C(C)CCc1ccc2cc(OC)ccc2c1	0		ref 16
NADOLOL	O[C@H](Cc1cccc(OCC(O)C[N+]C(C)(C)C)c1C[C@H](O)1)1	0		ref 16
NALTREXONE	O=C1CC[C@@](O)([C@H]([N+](CC[C@](c2c(ccc(O)c2O[C@@H]11)C2)11)CC3CC3)2)1	0		ref 16
NAPA(R=COCH3)	O=C(Nc1ccc(cc1)C(=O)NCC[N+](CC)CC)C	0		ref 26
NAPROXEN	O=C([O-])[C@@H](C)c1ccc2cc(OC)ccc2c1	0		ref 16
NARATRIPTAN	[S+2]([O-])([O-])(NC)CCc1ccc2N=CC(c2c1)C1CC[N+](C)CC1	0		ref 16
NATEGLINIDE	O=C(N[C@H](Cc1ccccc1)C(=O)[O-])[C@H](CC[C@H](CC1)[C@H](C)C)1	0		ref 16

NEFAZODONE	Clc1cccc(N2CC[N+](CC2)CCCN2N=C(N(CCOc3ccccc3)C2=O)CC)c1	0		ref 16
NELFINAVIR	S(C[C@H](NC(=O)c1cccc(O)c1C)[C@H](O)C[N+]1C[C@@H](CCCC[C@@H](C[C@H]1(C(=O)NC(C)(C)C))1)1)c1ccccc1	1	11.5	ref 26
NEVIRAPINE	O=C1Nc2c([nH0]ccc2C)N(c2[nH0]cccc21)C1CC1	0		ref 16
NIACIN	O=C([O-])c1c[nH0]ccc1	0		ref 16
NICOTINE	[nH0]1cccc(c1)C1[N+](C)CCC1	0	245	ref 20
NIFEDIPINE	O=[N+]([O-])c1ccccc1C1C(=C(NC(C)=C1C(=O)OC)C)C(=O)OC	0	616.59	ref 19
NILUTAMIDE	FC(F)(F)c1cc(N2C(=O)NC(C)(C)C2=O)ccc1[N+](=O)[O-]	0		ref 16
NIMODIPINE	O=[N+]([O-])c1cccc(c1)C1C(=C(NC(C)=C1C(=O)OC(C)C)C)C(=O)OCCOC	0		ref 16
NISOLDIPINE	O=[N+]([O-])c1ccccc1C1C(=C(NC(C)=C1C(=O)OCC(C)C)C)C(=O)OC	0		ref 16
NITRENDIPINE	O=[N+]([O-])c1cccc(c1)C1C(=C(NC(C)=C1C(=O)OCC)C)C(=O)OC	0	114.81	ref 19
NIZATIDINE	s1cc([nH0]c1C[N+](C)C)CSCCN/C(/NC)=C\[N+](=O)[O-]	0		ref 16
NORASTEMIZOLE	Fc1ccc(cc1)C[nH0]1c2ccccc2[nH0]c1NC1CC[N+]CC1	1	0.028	ref 20
NORCLOZAPINE	Clc1ccc2Nc3ccccc3C(=Nc2c1)N1CC[N+]CC1	1	4.49	ref 21
NORTRIPTYLINE	[N+](C)CCC=C1c2ccccc2CCc2ccccc21	1		ref 16
OFLOXACIN	Fc1cc2C(=O)C(=CN3c2c(OCC3C)c1N1CC[N+](C)CC1)C(=O)[O-]	0	1412	ref 20
OLANZAPINE	s1c2Nc3ccccc3N=C(N3CC[N+](C)CC3)c2cc1C	1	0.181	ref 20
ONDANSETRON	O=C1c2c([nH0](C)c3ccccc32)CCC1C[nH0]1cc[nH0]c1C	1	0.81	ref 20
OPC18790	O=C1Nc2ccc(OCC(O)C[N+]Cc3ccc(OC)c(OC)c3)cc2C=C1	1	0.955	ref 19
ORLISTAT	O=CN[C@@H](CC(C)C)C(=O)O[C@@H](CCCCCCCCCCC)C[C@H](OC(=O)[C@@H](CCCCCC)1)1	0		ref 16
ORPHENADRINE	O(CC[N+](C)C)C(c1ccccc1)c1ccccc1C	0		ref 16
OXAPROZIN	O=C([O-])CCc1oc(c2ccccc2)c([nH0]1)c1ccccc1	0		ref 16
OXCARBAZEPINE	O=C1Cc2ccccc2N(c2ccccc21)C(=O)N	0		ref 16
OXYBUTYNIN	O=C(OCC#CC[N+](CC)CC)C(O)(c1ccccc1)C1CCCCC1	1	25.11	ref 19
OXYCODONE	O=C1CC[C@@](O)([C@H]([N+](C)CC[C@](c2c(ccc(OC)c2O[C@@H]11)C2)11)2)1	0		ref 16
PAMABROM	Brc1[nH0]c2N(C)C(=O)N(C)C(=O)c2[nH]1	0		ref 16
PANTOPRAZOLE	[S+]([O-])(Cc1[nH0]ccc(OC)c1OC)c1[nH0]c2cc(OC(F)F)ccc2[nH]1	0		ref 16
PAROXETINE	Fc1ccc(cc1)C1CC[N+]CC1COc1ccc2OCOc2c1	0		ref 16
PEMOLINE	O=C1N=C(OC1c1ccccc1)N	0		ref 16
PENTAZOCINE	Oc1ccc2C[C@@H]([N+](CC[C@@](C)(c2c1)C1C)CC=C(C)C)1	0		ref 16
PENTOBARBITAL	O=C1NC(=O)C(CC)(C(=O)N1)C(C)CCC	0	131.82	ref 19
PENTOXIFYLLINE	O=C1N(C)c2[nH0]c[nH0](C)c2C(=O)N1CCCCC(=O)C	0		ref 16
PERGOLIDE	S(C)C[C@@H](C[N+](CCC)[C@H](CC1C=Nc2cccc(c21)[C@@H](C1)2)2)1	1	0.12	ref 32
PERHEXILENE	[N+]1CCCC[C@H]1(CC(C1CCCCC1)C1CCCCC1)	1	7.8	ref 20
PERPHENAZINE	Clc1ccc2Sc3ccccc3N(CCC[N+]3CC[N+](CC3)CCO)c2c1	0		ref 16
PHENAZONE	O=C1N(N(C)C(C)=C1)c1ccccc1	0		ref 16
PHENAZOPYRIDINE	Nc1[nH0]c(N)c(N=Nc2ccccc2)cc1	0		ref 16

PHENDIMETRAZINE	O1CC[N+](C)[C@@H](C)[C@@H]1(c1ccccc1)	0		ref 16
PHENELZINE	NNCCc1ccccc1	0		ref 16
PHENOBARBITAL	O=C1NC(=O)C(CC)(C(=O)N1)c1ccccc1	0	3000	ref 20
PHENOXYBENZAMINE	ClCC[N+](Cc1ccccc1)C(C)COc1ccccc1	0		ref 16
PHENTERMINE	[N+]C(C)(C)Cc1ccccc1	0		ref 16
PHENYLEPHRINE	Oc1cccc(c1)[C@@H](O)C[N+]C	0		ref 16
PHENYLPROPANOLAMINE	OC(c1ccccc1)C([N+])C	0		ref 16
PHENYLTOLOXAMINE	O(CC[N+](C)C)c1ccccc1Cc1ccccc1	0		ref 16
PHENYL_SALICYLATE	O=C(Oc1ccccc1)c1ccccc1[O-]	0		ref 16
PHENYTOIN	O=C1NC(=O)C(N1)(c1ccccc1)c1ccccc1	0	240	ref 20
PILOCARPINE	O=C1OC[C@H](Cc2[nH0](C)c[nH0]c2)[C@H](CC)1	0		ref 16
PIMOZIDE	Fc1ccc(cc1)C(CCC[N+]1CCC([N+]2=C3C=CC=CC3=NC2=O)CC1)c1ccc(F)cc1	1	0.018	ref 26
PIOGLITAZONE	S1C(=O)NC(=O)C1Cc1ccc(OCCc2[nH0]cc(cc2)CC)cc1	0		ref 16
PIROXICAM	[S+2]1([O-])([O-])N(C)C(=C(O)c2ccccc12)C(=O)Nc1[nH0]cccc1	0		ref 16
POLYTHIAZIDE	Clc1cc2NC(N([S+2]([O-])([O-])c2cc1[S+2]([O-])([O-])N)C)CSCC(F)(F)F	0		ref 16
PRAMIPEXOLE	s1c2C[C@@H]([N+]CCC)CCc2[nH0]c1N	0		ref 16
PRAZOSIN	O=C(N1CCN(CC1)c1[nH0]c(N)c2cc(OC)c(OC)cc2[nH0]1)c1occc1	1	1.57	ref 20
PRENYLAMINE	[N+](CCC(c1ccccc1)c1ccccc1)C(C)Cc1ccccc1	1	<1	ref 29
PRIMIDONE	O=C1NCNC(=O)C1(CC)c1ccccc1	0		ref 16
PROCAINAMIDE	O=C(NCC[N+](CC)CC)c1ccc(N)cc1	1		ref 16
PROCARBAZINE	O=C(NC(C)C)c1ccc(cc1)CNNC	0		ref 16
PROCHLORPERAZINE	Clc1ccc2Sc3ccccc3N(CCC[N+]3CC[N+](C)CC3)c2c1	1	22.6	KIM
PROGUANIL	Clc1ccc(NC(=[N+])NC(=[N+])NC(C)C)cc1	0		ref 16
PROMETHAZINE	S1c2ccccc2N(CC([N+](C)C)C)c2ccccc12	1		ref 16
PROPAFENONE	O=C(CCc1ccccc1)c1ccccc1OCC(O)C[N+]CCC	1	0.44	ref 33
PROPIONYL PROCAINAMIDE-N	O=C(NC(=O)c1ccc(N)cc1CC[N+](CC)CC)CC	1		ref 16
PROPOXYPHENE	O=C(O[C@](Cc1ccccc1)(c1ccccc1)[C@H](C)C[N+](C)C)CC	0		ref 16
PROPRANOLOL	OC(COc1cccc2ccccc12)C[N+]C(C)C	1	10	ref 38
PROTRIPTYLINE	[N+](C)CCCC1c2ccccc2C=Cc2ccccc21	0		ref 16
PRUCALOPRIDE	Clc1cc(c2OCCc2c1N)C(=O)NC1CC[N+](CC1)CCCOC	1	4.1	ref 34
PSEUDOEPHEDRINE	Oc1cccc(c1)[C@H](O)[C@@H]([N+]C)C	0		ref 16
PYRIDOXINE	OCc1c[nH0]c(C)c(O)c1CO	0		ref 16
PYRILAMINE	O(C)c1ccc(cc1)CN(CC[N+](C)C)c1[nH0]cccc1	1	2.45	ref 19
PYRIMETHAMINE	Clc1ccc(cc1)c1c(N)[nH0]c(N)[nH0]c1CC	0		ref 16
QUETIAPINE	S1c2ccccc2N=C(N2CC[N+](CC2)CCOCCO)c2ccccc12	1	5.75	ref 38

QUINIDINE	O[C@@H](c1cc[nH0]c2ccc(OC)cc21)[C@H]([N+]1CC[C@@H](C2)[C@@H](C=C)C1)2	1	1.07	ref 20
RABEPRAZOLE	[S+]([O-])(Cc1[nH0]ccc(OCCCOC)c1C)c1[nH0]c2ccccc2[nH]1	0		ref 16
RALOXIFENE	s1c2cc(O)ccc2c(c1c1ccc(O)cc1)C(=O)c1ccc(OCC[N+]2CCCCC2)cc1	0		ref 16
RANITIDINE	S(CCN/C(/NC)=C/[N+](=O)[O-])Cc1oc(cc1)C[N+](C)C	0		ref 16
RENZAPRIDE	Clc1cc(c(OC)cc1N)C(=O)N[C@@H](CC[N+]1CCC[C@@H](C1)1)1	1		ref 16
REPAGLINIDE	O=C(NC(CC(C)C)c1ccccc1N1CCCCC1)Cc1ccc(c(OCC)c1)C(=O)[O-]	0		ref 16
RIBAVIRIN	O=C(N)c1[nH0][nH0](c[nH0]1)[C@@H](O[C@@H](CO)[C@H](O)[C@H](O)1)1	0		ref 16
RILUZOLE	s1c2cc(OC(F)(F)F)ccc2[nH0]c1N	0		ref 16
RIMANTADINE	[N+]C(C)C12CC3CC(CC(C3)C2)C1	0		ref 16
RISPERIDONE	Fc1ccc2c(o[nH0]c2C2CC[N+](CC2)CCC2C(=O)[N+]=3CCCCC=3N=C2C)c1	1	0.163	ref 20
RITONAVIR	s1c[nH0]cc1COC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](NC(=O)[C@@H](NC(=O)N(C)Cc1[nH0]c(sc1)C(C)C)C(C)C)Cc1ccccc1	1	8.2	ref 26
RIVASTIGMINE	O=C(Oc1cccc(c1)[C@@H]([N+](C)C)C)N(C)CC	0		ref 16
RIZATRIPTAN	[nH0]1[nH0](c[nH0]c1)Cc1ccc2N=CC(CC[N+](C)C)c2c1	0		ref 16
ROFECOXIB	[S+2]([O-])([O-])(C)c1ccc(cc1)C=1COC(=O)C=1c1ccccc1	0		ref 16
ROPINIROLE	O=C1Nc2cccc(CC[N+](CCC)CCC)c2C1	0		ref 16
ROSIGLITAZONE	S1C(=O)NC(=O)C1Cc1ccc(OCCN(C)c2[nH0]cccc2)cc1	0		ref 16
ROXITHROMYCIN	O=C1O[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)C(=NOCOCCOC)[C@H](C)C[C@](O)(C)[C@H](O[C@H](O[C@H](C)C[C@H]([N@@H+](C)C)[C@@H](O)2)2)[C@@H](C)[C@H](O[C@H](O[C@@H](C)[C@H](O)[C@@](OC)(C)C2)2)[C@@H](C)1	1	36.5	ref 20
SAQUINAVIR	O=C(N)C[C@H](NC(=O)c1[nH0]c2ccccc2cc1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[N+]1C[C@@H](CCCC[C@@H](C[C@H]1(C(=O)NC(C)(C)C))1)1	1	15.3	ref 26
SELEGILINE	[N+](C)(CC#C)[C@H](C)Cc1ccccc1	0		ref 16
SERTINDOLE	Clc1ccc2[nH0](cc(c2c1)C1CC[N+](CC1)CCN1CCNC1=O)c1ccc(F)cc1	1	0.0126	ref 20
SERTRALINE	Clc1ccc(cc1Cl)[C@H](CC[C@H]([N+]C)c1ccccc11)1	0		ref 16
SIBUTRAMINE	Clc1ccc(cc1)C1(CCC1)C([N+](C)C)CC(C)C	0		ref 16
SILDENAFIL	[S+2]([O-])([O-])(N1CC[N+](C)CC1)c1ccc(OCC)c(c1)C=1N=C2C(=[N+](N=C2CCC)C)C(=O)N=1	0	100	ref 20
SIMVASTATIN	O=C1O[C@@H](C[C@@H](O)C1)CC[C@@H]([C@@H](C)C=CC1=C[C@H](C)C[C@H](OC(=O)C(C)(C)CC)[C@@H]11)1	0		ref 16
SOTALOL	[S+2]([O-])([O-])(Nc1ccc(cc1)C(O)C[N+]C(C)C)C	0	74.13	ref 19
SPARFLOXACIN	Fc1c(N)c2c([N+](=CC(C2=O)C(=O)[O-])C2CC2)c(F)c1N1C[C@@H]([N+][C@H](C)C1)C	1	18	ref 20
SPIRONOLACTONE	S(C(=O)C)[C@H](CC1=CC(=O)CC[C@@](C)1([C@@H](CC[C@@](C)([C@@H](CC[C@@](OC(=O)CC1)11)[C@H]23)1)3))2	0		ref 16
STAVUDINE	O=C1NC(=O)C(C)=CN1C1OC(C=C1)CO	0		ref 16
SUFENTANIL	s1cccc1CC[N+]1CCC(N(c2ccccc2)C(=O)CC)(CC1)COC	1		ref 16
SULINDAC	[S+]([O-])(C)c1ccc(cc1)/C=C/1\c2ccc(F)cc2C(CC(=O)[O-])=C\1C	0		ref 16
SUMATRIPTAN	[S+2]([O-])([O-])(NC)Cc1ccc2N=CC(CC[N+](C)C)c2c1	0		ref 16
TACRINE	Nc1c2ccccc2[nH0]c2CCCCc21	0		ref 16
TAMOXIFEN	O(CC[N+](C)C)c1ccc(cc1)/C(/c1ccccc1)=C(\CC)/c1ccccc1	1	1.58	ref 19

TAMSULOSIN	[S+2]([O-])([O-])(N)c1cc(ccc1OC)CC([N+]CCOc1ccccc1OCC)C	0	104.8	ref 26
TELMISARTAN	O=C([O-])c1ccccc1c1ccc(cc1)C[nH0]1c2cc(ccc2[nH0]c1CCC)c1[nH0]c2c([nH0]1C)cccc2C	0		ref 16
TEMOZOLOMIDE	O=C1[N+]2=CN=C(C2=NN=[N+]1C)C(=O)N	0		ref 16
TERBUTALINE	Oc1cc(O)cc(c1)C(O)C[N+]C(C)(C)C	0		ref 16
TERFENADINE	O[C@@H](CCC[N+]1CCC(CC1)C(O)(c1ccccc1)c1ccccc1)c1ccc(cc1)C(C)(C)C	1	0.0084	ref 20
TERODILINE	[N+](C(C)CC(c1ccccc1)c1ccccc1)C(C)(C)C	1	1.51	ref 19
TESTOLACTONE	O=C1C=CC2(C)C(=C1)CCC1C3CCC(=O)OC3(C)CCC12	0		ref 16
THALIDOMIDE	O=C1NC(=O)C(N2C(=O)c3ccccc3C2=O)CC1	0		ref 16
THEOPHYLLINE	O=C1N(C)c2[nH]c[nH0]c2C(=O)N1C	0		ref 16
THIOGUANINE	S=C1N=C(N)Nc2[nH0]c[nH]c21	0		ref 16
THIOPENTAL	S=C1NC(=O)C(CC)(C(=O)N1)C(C)CCC	1		ref 16
THIORIDAZINE	S1c2ccccc2N(CC[C@H]([N@@H+](C)CCCC2)2)c2cc(SC)ccc12	1	0.096	ref 20
THIOTHIXENE	S1c2ccccc2\C(=C\CC[N+]2CC[N+](C)CC2)\c2cc([S+2]([O-])([O-])N(C)C)ccc12	0		ref 16
TIAGABINE	s1ccc(C)c1C(=CCC[N+]1CCC[C@H](C1)C(=O)[O-])c1sccc1C	0		ref 16
TICLOPIDINE	Clc1ccccc1C[N+]1CCc2sccc2C1	0		ref 16
TILUDRONIC_ACID	Clc1ccc(SC([P+]([O-])([O-])[O-])[P+]([O-])([O-])[O-])cc1	0		ref 16
TIMOLOL	s1[nH0]c(OC[C@@H](O)C[N+]C(C)(C)C)c([nH0]1)N1CCOCC1	0		ref 16
TIZANIDINE	Clc1ccc2[nH0]s[nH0]c2c1NC1=[N+]CCN1	0		ref 16
TOCAINIDE	O=C(Nc1c(C)cccc1C)C([N+])C	0		ref 16
TOLCAPONE	O=[N+]([O-])c1cc(cc(O)c1[O-])C(=O)c1ccc(C)cc1	0		ref 16
TOLMETIN	O=C([O-])Cc1[nH0](C)c(cc1)C(=O)c1ccc(C)cc1	0		ref 16
TOLTERODINE	Oc1ccc(C)cc1[C@H](CC[N+](C(C)C)C(C)C)c1ccccc1	1	0.017	ref 35
TOPIRAMATE	[S+2]([O-])([O-])(OC[C@](OC[C@@H](OC(O[C@H]1([C@H](OC(O2)(C)C)3))(C)C)1)23)N	0		ref 16
TOREMIFENE	ClCC\C(\c1ccccc1)=C(/c1ccccc1)\c1ccc(OCC[N+](C)C)cc1	0		ref 16
TORSEMIDE	[S+2]([O-])([O-])([N-]C(=O)NC(C)C)c1c[nH0]ccc1Nc1cccc(C)c1	0		ref 16
TRAMADOL	O[C@@](CCCC[C@H](C[N+](C)C)1)(c2cccc(OC)c2)1	0		ref 16
TRANYLCYPROMINE	[N+][C@H](C[C@@H](c1ccccc1)1)1	0		ref 16
TRIAMTERENE	Nc1[nH0]c(N)c2[nH0]c(c(N)[nH0]c2[nH0]1)c1ccccc1	1		ref 16
TRIAZOLAM	Clc1ccc2[nH0]3c([nH0][nH0]c3C)CN=C(c2c1)c1ccccc1Cl	0		ref 16
TRIFLUOPERAZINE	S1c2ccccc2N(CCC[N+]2CC[N+](C)CC2)c2cc(ccc12)C(F)(F)F	1	0.234	ref 32
TRIHEXYPHENIDYL	OC(CC[N+]1CCCCC1)(c1ccccc1)C1CCCCC1	0		ref 16
TRIMETHOBENZAMIDE	O=C(NCc1ccc(OCC[N+](C)C)cc1)c1cc(OC)c(OC)c(OC)c1	0		ref 16
TRIMIPRAMINE	N1(CC(C)C[N+](C)C)c2ccccc2CCc2ccccc12	1		ref 16
TRIPROLIDINE	[nH0]1ccccc1/C(=C/C[N+]1CCCC1)/c1ccc(C)cc1	0		ref 16
URSODEOXYCHOLIC ACID	O=C([O-])CC[C@H](C)[C@@H](CC[C@@H]([C@H]([C@@H](O)C[C@H](C[C@H](O)CC[C@@](C)1([C@@H](CC[C@@](C)23)4))1)4)2)3	0		ref 16

VALPROIC_ACID	O=C([O-])C(CCC)CCC	0		ref 16
VALSARTAN	O=C(N(Cc1ccc(cc1)c1ccccc1c1[nH0][nH0][nH0-][nH0]1)[C@H](C(=O)[O-])C(C)C)CCCC	0		ref 16
VENLAFAXINE	OC1(CCCCC1)C(C[N+](C)C)c1ccc(OC)cc1	1		ref 16
VERAPAMIL	O(C)c1ccc(cc1OC)CC[N@H+](C)CCC[C@@](C#N)(c1ccc(OC)c(OC)c1)C(C)C	1	0.136	ref 20
VESNARINONE	O=C1Nc2ccc(N3CCN(CC3)C(=O)c3ccc(OC)c(OC)c3)cc2CC1	1	1.1	ref 20
VINPOCETINE	O=C(OCC)C=1[nH0]2c3ccccc3c3CC[N+]4CCC[C@](C=1)(CC)[C@H]4(c23)	1	0.032	ref 32
WARFARIN	O=C1Oc2ccccc2C(O)=C1C(CC(=O)C)c1ccccc1	0		ref 16
WAY123398	[S+2]([O-])([O-])(Nc1ccc([S+2]([O-])([O-])N(C)CCN(C)c2[nH0]c3ccccc3[nH0]2C)cc1)C	1	0.2041	ref 19
YOHIMBINE	O=C(OC)[C@@H]([C@@H](O)CC[C@@H](C[N+]1CCc2c3ccccc3[nH]c2[C@@H]1(C[C@@H]12))1)2	0		ref 16
ZAFIRLUKAST	[S+2]([O-])([O-])([N-]C(=O)c1ccc(Cc2c[nH0](C)c3ccc(NC(=O)OC4CCCC4)cc32)c(OC)c1)c1ccccc1C	0		ref 16
ZALCITABINE	O=C1N=C(N)C=CN1[C@H](O[C@@H](CC1)CO)1	0		ref 16
ZALEPLON	O=C(N(CC)c1cccc(c1)c1[nH0+]2[nH0]cc(C#N)c2[nH]cc1)C	0		ref 16
ZIDOVUDINE	O=C1NC(=O)C(C)=CN1C1OC(CO)C(N=[N+]=[N-])C1	0		ref 16
ZIPRASIDONE	Clc1cc2NC(=O)Cc2cc1CC[N+]1CCN(CC1)c1[nH0]sc2ccccc21	1	0.12	ref 20
ZOLPIDEM	O=C(N(C)C)CC=1[N+]2=CC(C)=CCC2=NC=1c1ccc(C)cc1	0		ref 16
almokalant	[S+]([O-])(CCC)CCC[N+](CC)CC(O)COc1ccc(C#N)cc1	1	0.44	ref 19
amsacrine	[S+2]([O-])([O-])(Nc1ccc(Nc2c3ccccc3[nH0]c3ccccc32)c(OC)c1)C	1	0.21	ref 20
aprinidine	N(CCC[N+](CC)CC)(c1ccccc1)C1Cc2ccccc2C1	1	0.23	ref 33
artemisin	O=C1C=CC2(C)CC(O)C3C(OC(=O)C3C)C2=C1C	0	110	ref 19
bekm-1	Clc1ccc(cc1)C([nH0]1c[nH0+](cc1)CC(OCc1ccc(Cl)cc1Cl)c1ccc(Cl)cc1Cl)c1ccc(Cl)cc1	1	0.03	ref 38
benzoylecgonine	O=C(OC1CC2[N+](C)C(CC2)C1C(=O)[O-])c1ccccc1	0	3981	ref 19
berberine	O1COc2cc3c4[nH0+](cc5c(ccc(OC)c5OC)c4)CCc3cc12	0	66.069	ref 19
buprenorphine	Oc1ccc2CC3[N+](CCC45c2c1OC4C1(OC)CCC35CC1C(O)(C)C(C)(C)C)CC1CC1	1	7.58	ref 29
cibenzoline	[N+]=1CCNC=1C1CC1(c1ccccc1)c1ccccc1	1	23	ref 33
clofilium	Clc1ccc(cc1)CCCC[N+](CC)(CC)CCCCCCCC	1	0.012	ref 19
clotrimazole	Clc1ccccc1C([nH0]1c[nH0]cc1)(c1ccccc1)c1ccccc1	1	3.02	ref 19
cyamemazin	S1c2ccccc2N(CC(C)C[N+](C)C)c2cc(C#N)ccc12	1	0.87	ref 6
desmethylastemizole	Fc1ccc(cc1)C[nH0]1c2ccccc2[nH0]c1NC1CC[N+](CC1)CCc1ccc(O)cc1	1	0.03	ref 19
ebastine	O=C(CCC[N+]1CCC(OC(c2ccccc2)c2ccccc2)CC1)c1ccc(cc1)C(C)(C)C	1	0.331	ref 20
ecgonine_methyl_ester	O=C(OC)C1C2[N+](C)C(CC1O)CC2	0	6025	ref 19
eddp	S([P+](Sc1ccccc1)([O-])OCC)c1ccccc1	0	50	ref 17
erythromycin	O=C1OC(CC)C(O)(C)C(O)C(C)C(=O)C(C)CC(O)(C)C(OC2OC(C)CC([N+](C)C)C2O)C(C)C(OC2OC(C)C(O)C(OC)(C)C2)C1C	0	72.2	ref 20
gbr-12909	Fc1ccc(cc1)C(OCC[N+]1CC[N+](CC1)CCCc1ccccc1)c1ccc(F)cc1	1	0.001	ref 32
glyceryl-nonivamide	O=C(NCc1ccc(CC(O)CO)c(OC)c1)CCCCCCCC	1	0.1	ref 19
isobutylmethylxanthine	O=C1N(CC(C)C)c2[nH0]c[nH]c2C(=O)N1C	1	10	ref 19
lopinavir	O=C1NCCCN1C(C(=O)NC(Cc1ccccc1)CC(O)C(NC(=O)COc1c(C)cccc1C)Cc1ccccc1)C(C)C	1	8.6	ref 26

lovastatin	O=C1OC(CC(O)C1)CCC1C(C)C=CC2=CC(C)CC(OC(=O)C(C)CC)C21	1	12.5	ref 32
maprotiline	[N+](C)CCCC12CCC(c3ccccc31)c1ccccc12	1	3.1	ref 32
norpropoxyphene	O=C(OC(Cc1ccccc1)(c1ccccc1)C(C)C[N+]C)CC	1	3.63	ref 19
norverapamil	O(C)c1ccc(cc1OC)CC[N+]CCCC(C#N)(c1ccc(OC)c(OC)c1)C(C)C	1	3.16	ref 19
papaverine	O(C)c1ccc(cc1OC)Cc1[nH0]ccc2cc(OC)c(OC)cc21	1	7.3	ref 32
protopine	O=C1Cc2ccc3OCOc3c2C[N+](C)CCc2cc3OCOc3cc21	0	165	ref 19
ranolazine	O=C(Nc1c(C)cccc1C)C[N+]1CC[N+](CC1)CC(O)COc1ccccc1OC	1	14.6	ref 32
sematilide	[S+2]([O-])([O-])(Nc1ccc(cc1)C(=O)NCC[N+](CC)CC)C	0	50	ref 33
tedisamil	[N+]1(CC2C[N+](CC(C1)C12CCCC1)CC1CC1)CC1CC1	1	2.5	ref 33
trimebutine	O=C(OCC([N+](C)C)(CC)c1ccccc1)c1cc(OC)c(OC)c(OC)c1	0	89.12	ref 19
trimethoprin	O(C)c1cc(cc(OC)c1OC)Cc1c[nH0]c(N)[nH0]c1N	0	239	ref 26
vitamine_K	O=C1C(C)=C(C/C=C(\C)/CCCC(C)CCCC(C)CCCC(C)C)C(=O)c2ccccc12	1	5.75	ref 19
ABACAVIR	OCC1C=CC([nH0]2c[nH0]c3c2[nH0]c(N)[nH0]c3NC2CC2)C1	0		ref 16
2-hydroxymethylOLANZAPINE	s1c2Nc3ccccc3N=C(N3CC[N+](C)CC3)c2cc1CO	1	11.6	ref 36
N_demethylHALOFANTRINE	Clc1cc(Cl)c2cc(c3ccc(cc3c2c1)[C@](F)(F)F)[C@H](O)CC[N+]	1	0.71	ref 20
CLOZAPINE_N_OXYDE	Clc1ccc2Nc3ccccc3[C@H](N(O)c2c1)[N+]1CC[N+](C)CC1	0	133.3	ref 36
desmethyl_OLANZAPINE	s1c2Nc3ccccc3N=C(N3CC[N+]CC3)c2cc1C	1	14.2	ref 36
sertindole1	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=O)1)c1ccccc1	0	88	ref 24
sertindole2	Clc1ccc2[nH0](cc(c2c1)C1=CC[N+](CC1)CCN1CCNC1=O)c1ccc(F)cc1	1	10	ref 24
sertindole3	Fc1ccc([nH0]2cc(c3ccccc23)[C@H](CC[N+](CC2)CCN3CCNC3=O)2)cc1	1	7	ref 24
sertindole4	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=O)1)c1ccc(cc1)CCO	0	579	ref 24
sertindole5	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=O)1)c1ccc(cc1)C(=O)[O-]	0	75000	ref 24
sertindole6	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=O)1)[C@H](CCCCC1)1	0	137	ref 24
sertindole7	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=O)1)c1ccc(cc1)CCOC	0	131	ref 24
sertindole8	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=O)1)c1ccc(cc1)COC	1	36	ref 24
sertindole10	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+](CC1)CCN2CCNC2=S)1)c1ccc(F)cc1	1	6.2	ref 24
sertindole11	OC(CCC[N+]1CCC(CC1)C(O)(c1ccccc1)c1ccccc1)c1ccc(cc1)C(O)(C)C	0	460	ref 24
sertindole13	Fc1ccc([nH0]2cc(c3ccccc23)[C@H](CC[N+](CC2)CCN3CCNC3=O)2)cc1	1	23.5	ref 24
sertindole14	Clc1ccc2[nH0](cc(c2c1)[C@H](CC[N+]CC1)1)c1ccc(F)cc1	0	204	ref 24
sertindole15	Clc1ccc2[nH0](cc(C[N+](C)C)c2c1)c1ccc(F)cc1	1	11	ref 24
sertindole16	Clc1ccc2[nH0](cc(CCC)c2c1)c1ccc(F)cc1	0	26000	ref 24
sertindole17	Clc1ccc2[nH0](cc(c2c1)[C@@H](CC)CC)c1ccc(F)cc1	0	1480	ref 24
sertindole18	Clc1ccc2[nH0](cc(c2c1)[C@@H](O)C)c1ccc(F)cc1	0	4550	ref 24
sertindole19	Clc1ccc2[nH0](cc(c2c1)C(=O)CC)c1ccc(F)cc1	0	1947	ref 24
sertindole21	Clc1ccc2[nH0](cc(c2c1)[C@@H](O)CC)c1ccc(F)cc1	0	2200	ref 24
sertindole22	Clc1ccc2[nH0](cc(CC)c2c1)c1ccc(F)cc1	0	3500	ref 24

josamycin	O=CCC1CC(C)C(O)C=CC=CCC(OC(=O)CC(OC(=O)C)C(OC)C1OC1OC(C)C(OC2OC(C)C(OC(=O)CC(C)C)C(O)(C)C2)C([N+](C)C)C1O)C	0	102	ref 20
canrenoic	O=C1C=C2C=CC3C4CCC(O)(CCC(=O)[O-])C4(C)CCC3C2(C)CC1	0	104	ref 37
erythromycin	O=C1OC(CC)C(O)(C)C(O)C(C)C(=O)C(C)CC(O)(C)C(OC2OC(C)CC([N+](C)C)C2O)C(C)C(OC2OC(C)C(O)C(OC)(C)C2)C1C	0	72	ref 20
N-desmethylerythromycin	O=C1OC(CC)C(O)(C)C(O)C(C)C(=O)C(C)CC(O)(C)C(OC2OC(C)CC([N+](C)C)C2O)C(C)C(OC2OC(C)C(O)C(O)(C)C2)C1C	0	147	ref 20
oleandomycin	O=C1OC(C)C(C)C(O)C(C)C(=O)C2(OC2)CC(C)C(OC2OC(C)CC([N+](C)C)C2O)C(C)C(OC2OC(C)C(O)C(OC)C2)C1C	0	309	ref 20
lumefantrine	Clc1ccc(cc1)/C=C/1\c2cc(Cl)ccc2c2c\1cc(Cl)cc2C(O)C[N+](CCCC)CCCC	1	8.1	ref 20
pilsicainide	O=C(Nc1c(C)cccc1C)CC12[N+](CCC1)CCC2	1	20.4	ref 20
tadafil	O=C1N2C(Cc3c4ccccc4[nH]c3C2c2ccc3OCOc3c2)C(=O)N(C)C1	0	100	ref 16
vardenafil	[S+2]([O-])([O-])(N1CC[N+](CC1)CC)c1ccc(OCC)c(c1)C1=NC(=O)c2[nH0](N1)c([nH0]c2C)CCC	1	12.8	ref 20
Wombat 01	s1ccc(c1)c1[nH]c2cc(F)ccc2c1C1C[N+]CCC1F	1	1.5	ref 39
Wombat 02	[nH]1c2ccccc2c(c1c1ccccc1)C1[N+](C)CCCC1	1	7	ref 39
Wombat 03	[nH]1c2ccccc2c(c1c1ccccc1)C1C[N+](CCC1)Cc1ccccc1	1	0.29	ref 39
Wombat 04	[nH]1c2ccccc2c(c1c1ccccc1)C1C[N+](CCC1)CCc1ccccc1	1	0.53	ref 39
Wombat 05	[nH]1c2ccccc2c(c1c1ccccc1)C1C[N+](C)CCC1	1	9.6	ref 39
Wombat 06	[nH]1c2ccccc2c(c1c1ccccc1)C1CCN(CC1)c1ccccc1	1	0.08	ref 39
Wombat 07	[nH]1c2ccccc2c(c1c1ccccc1)C1CC2N(c3ccccc3)C(C1)CC2	1	0.018	ref 39
Wombat 08	[S+2]([O-])([O-])(NCC1CCC(CC1)c1[nH0]c(c[nH]1)c1cccc(c1)C(F)(F)F)c1ccccc1	1	<1	ref 39
Wombat 09	[S+2]([O-])([O-])([N-]C(=O)C1CCC(CC1)c1[nH0]c(c[nH]1)c1cccc(c1)C(F)(F)F)c1ccccc1	0		ref 39
Wombat 10	[S+2]([O-])([O-])(N(C)CC1CCC(CC1)c1[nH0]c(c[nH]1)c1cccc(c1)C(F)(F)F)c1ccccc1	1	<1	ref 39
Wombat 11	[S-]c1[nH0]cccc1C(=O)N1CCC([N+]Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	11	ref 39
Wombat 12	S1C(=CNC1C(O)(C)C)[C@H](c1cc[nH0+]([O-])cc1)c1ccc(OC(F)F)c(OC(C)(C)C)c1	0	58.40	ref 39
Wombat 13	S1C(=CNC1C(O)(C(F)(F)F)C(F)(F)F)[C@H](c1c[nH0+]([O-])ccc1)c1ccc(OC(F)F)c(OC(C)C)c1	1	38.10	ref 39
Wombat 14	S1C(=CNC1C(O)(C(F)(F)F)C(F)(F)F)C(c1cc[nH0+]([O-])cc1)c1ccc(OC(F)F)c(OC(C)C)c1	1	21	ref 39
Wombat 15	S1C(=CNC1C(O)(C(F)(F)F)C(F)(F)F)C(c1cc[nH0+]([O-])cc1)c1ccc(OC(F)F)c(OC(C)(C)C)c1	0	61.40	ref 39
Wombat 16	S1C(=CNC1C(O)(C(F)(F)F)C(F)(F)F)C(c1c[nH0+]([O-])ccc1)c1ccc(OC(F)F)c(OC(C)C)c1	1	39	ref 39
Wombat 17	S(CC)c1[nH0]cccc1C(=O)N1CCC([N+]Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	14	ref 39
Wombat 18	S(C)c1[nH0]cccc1C(=O)N1CCC([N+]Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	7.8	ref 39
Wombat 19	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)c1cccc2[nH0]cccc21	1	8.2	ref 39
Wombat 20	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)c1cc[nH0]cc1	1	3.2	ref 39
Wombat 21	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)Cc1ccccc1	1	7.2	ref 39
Wombat 22	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)C(=O)c1ccc[nH0]c1OC	1	21	ref 39
Wombat 23	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)C(=O)c1ccc[nH0]c1[O-]	0	50	ref 39
Wombat 24	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)C(=O)c1ccc[nH0]c1N	0	50	ref 39
Wombat 25	O=C1N(CCC1[N+]Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)C(=O)c1ccc[nH0]c1C	1	10	ref 39
Wombat 26	O=C1N(CCC1[N+]CCc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)c1ccccc1	1	0.15	ref 39

Wombat 27	O=C1N(CCC1[N+](Cc1c[nH0]ccc1)Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)Cc1ccccc1	1	0.87	ref 39
Wombat 28	O=C1N(CCC1[N+](CCCC)Cc1[nH0](c[nH0]c1)Cc1ccc(C#N)cc1)Cc1ccccc1	1	0.19	ref 39
Wombat 29	[nH]1c2ccccc2c(c1c1ccccc1)C1C[N+]CCC1	1	4.9	ref 39
Wombat 30	[nH]1c2ccccc2c(c1c1ccccc1)C1CC[N+]CC1	1	5.7	ref 39
Wombat 31	Fc1cccc2c1[nH]c(c1ccccc1)c2C1C[N+]CCC1F	1	3	ref 39
Wombat 32	Fc1ccc2c([nH]c(c3ccccc3)c2C2C[N+]CCC2F)c1	1	4	ref 39
Wombat 33	Fc1ccc2c([nH]c(c3cccc4ccccc43)c2C2C[N+]CCC2F)c1	1	0.11	ref 39
Wombat 34	Fc1ccc2c([nH]c(c3ccc4ccccc4c3)c2C2C[N+]CCC2F)c1	1	0.5	ref 39
Wombat 35	Fc1ccc2c([nH]c(c2C2C[N+]CC[C@H](F)2)C(=O)OC)c1	1	8.2	ref 39
Wombat 36	Fc1ccc2c([nH]c(c2C2C[N+]CC[C@H](F)2)C(=O)Nc2ccccc2)c1	1	0.93	ref 39
Wombat 37	Fc1ccc2c([nH]c(c2C2C[N+]CCC2F)C2CCCCCC2)c1	1	5.4	ref 39
Wombat 38	Fc1ccc2c([nH]c(C3=CNC=CC3)c2C2C[N+]CCC2F)c1	1	2.5	ref 39
Wombat 39	Fc1ccc2[nH]c(c3ccccc3)c(c2c1)C1C[N+]CCC1F	1	7	ref 39
Wombat 40	Fc1ccc(cc1)c1[nH]c2cc(F)ccc2c1C1C[N+]CC[C@H](F)1	1	1.6	ref 39
Wombat 41	Fc1ccc(cc1)c1[nH]c2cc(F)ccc2c1C1C[N+]CCC1	1	1.3	ref 39
Wombat 42	FC1CC[N+]CC1c1c2ccccc2[nH]c1c1ccccc1	1	1.1	ref 39
Wombat 43	FC(F)Oc1ccc(cc1OC1CCC1)C(C1=CNC(C=C1)C(O)(C)C)c1cc[nH0+](O)cc1	1	22.4	ref 39
Wombat 44	FC(F)Oc1ccc(cc1OC(F)F)[C@H](C1=CNC(C=C1)C(O)(C)C)c1cc[nH0+]([O-])cc1	1	22.7	ref 39
Wombat 45	FC(F)Oc1ccc(cc1OC(F)F)[C@@H](C1=CNC(C=C1)C(O)(C)C)c1cc[nH0+]([O-])cc1	1	25.4	ref 39
Wombat 46	FC(F)Oc1ccc(cc1OC(F)F)C(C1=CNC(C=C1)C(O)(C)c1ccccc1)c1cc[nH0+](O)cc1	1	1.18	ref 39
Wombat 47	FC(F)Oc1ccc(cc1OC(C)C)[C@H](C1=CNC(C=C1)C(O)(C)C)c1cc[nH0+]([O-])cc1	0	41.5	ref 39
Wombat 48	FC(F)Oc1ccc(cc1OC(C)C)[C@H](C1=CNC(C=C1)C(O)(C)C)c1c[nH0+]([O-])ccc1	0	42.2	ref 39
Wombat 49	FC(F)Oc1ccc(cc1OC(C)C)[C@H](C1=CNC(C=C1)C(O)(C)C)C=1C=NC(=O)CC=1	0	55.9	ref 39
Wombat 50	FC(F)Oc1ccc(cc1OC(C)C)[C@@H](C1=CNC(C=C1)C(O)(C)C)c1c[nH0+]([O-])ccc1	0	44.7	ref 39
Wombat 51	FC(F)Oc1ccc(cc1OC(C)(C)C)[C@H](C1=CNC(C=C1)C(O)(C)C)c1cc[nH0+]([O-])cc1	1	25	ref 39
Wombat 52	FC(F)(F)c1cccc(c1)c1[nH0]c([nH]c1)C1CCC(CC1)C(=O)NNC(=O)C	0		ref 39
Wombat 53	FC(F)(F)c1cccc(c1)c1[nH0]c([nH]c1)C1CCC(CC1)C(=O)NCCO	1	<1	ref 39
Wombat 54	FC(F)(F)c1cccc(c1)c1[nH0]c([nH]c1)C1CCC(CC1)C(=O)NC(C)(C)CO	0		ref 39
Wombat 55	Clc1cccc2c1[nH]c(c1ccccc1)c2C1C[N+]CCC1F	1	2.1	ref 39
Wombat 56	Clc1cccc(c1)CN1CCC([N+]Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	0.44	ref 39
Wombat 57	Clc1cccc(c1)CN1CCC([N+](CC[N+]2CCOCC2)Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	0.19	ref 39
Wombat 58	Clc1cccc(c1)CN1CCC([N+](CC[N+]2CC[N+]CC2)Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	1.1	ref 39
Wombat 59	Clc1cccc(c1)CN1CCC([N+](CCCc2ccccc2)Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	0.024	ref 39
Wombat 60	Clc1cccc(c1)CN1CCC([N+](CCCNC(=O)OC(C)(C)C)Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	0.11	ref 39
Wombat 61	Clc1cccc(c1)CN1CCC([N+](CCC[N+])Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	0.48	ref 39
Wombat 62	Clc1cccc(c1)C(=O)N1CCC([N+]Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	5.8	ref 39

Wombat 63	Clc1ccc2c([nH]c(c3ccccc3)c2C2C[N+]CCC2F)c1	1	1.4	ref 39
Wombat 64	Clc1ccc2[nH]c(c3ccccc3)c(c2c1)C1C[N+]CCC1F	1	7	ref 39
Wombat 65	Brc1cccc(c1)c1[nH0]c([nH]c1)C1CCC(CC1)C(=O)NC(=O)C	1	<1	ref 39
Wombat 66	Brc1c[nH0]cc(c1)C(=O)N1CCC([N+]Cc2[nH0](c[nH0]c2)Cc2ccc(C#N)cc2)C1=O	1	6	ref 39