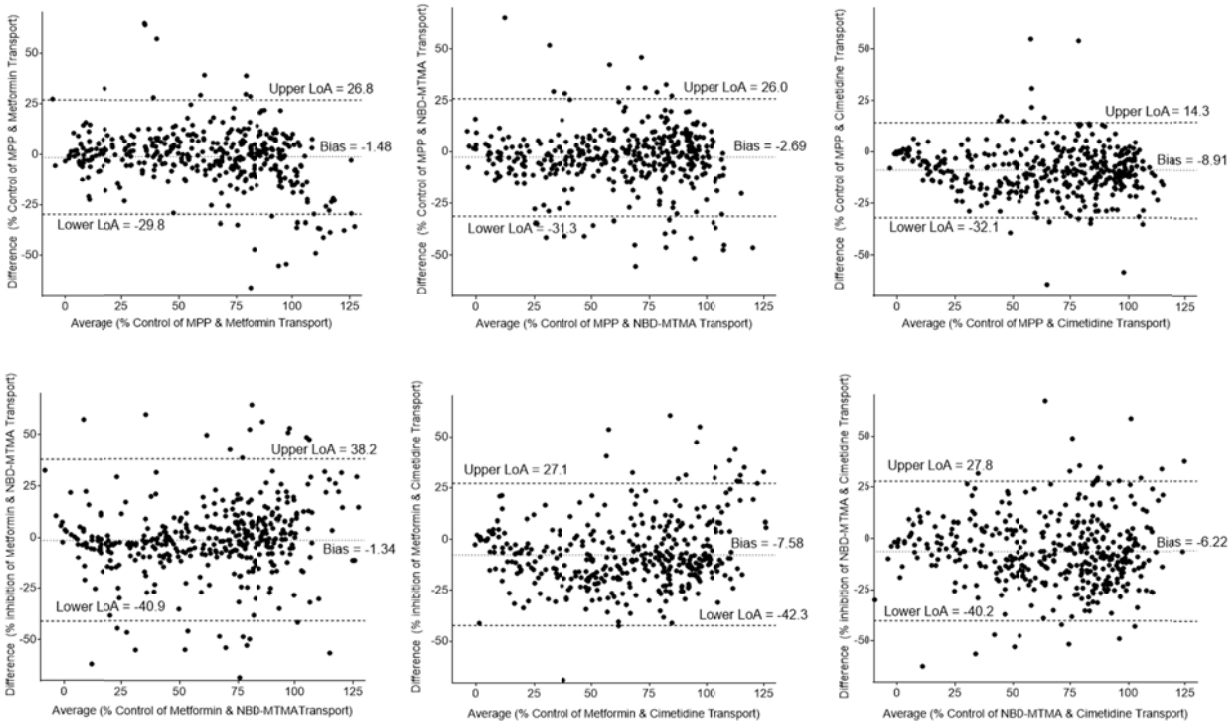
Lack of Influence of Substrate on Ligand Interaction with the Human Multidrug And Toxin Extruder, MATE1

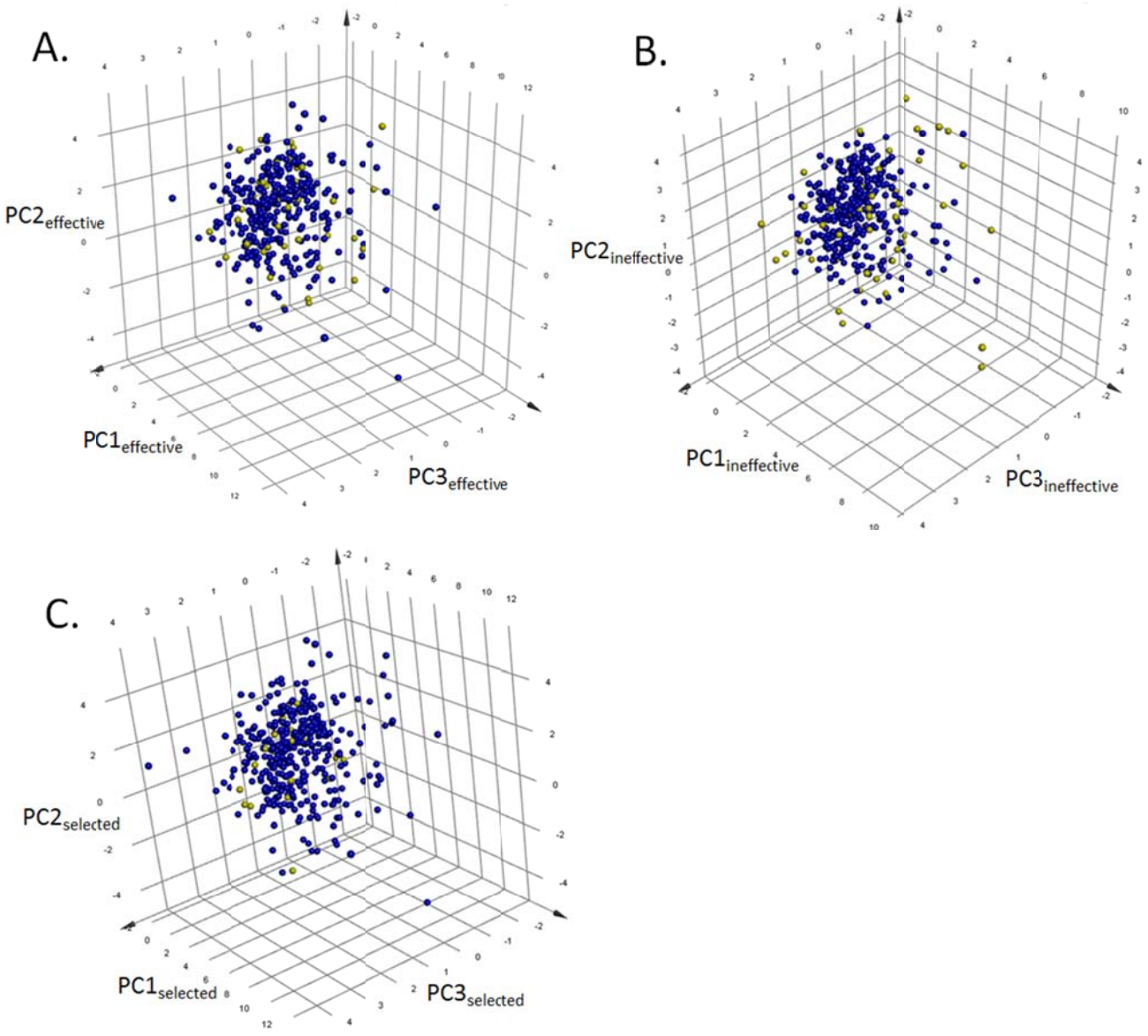
Authors:

Lucy J Martínez-Guerrero, Mark Morales, Sean Ekins and Stephen H Wright

Supplemental Figures and Tables



Supplemental Figure 1. Bland-Altman plots for the pair-wise comparisons of the inhibition of MATE1-mediated transport of MPP, NBD-MTMA, cimetidine and metformin produced by 50 µM concentrations of the 400 test compounds from the NCC. *Average* of the % of control uptake of two test substrates measured for each test inhibitor is plotted against the *Difference* between these measured uptakes. The dotted lines indicate calculated bias (in no case did calculated bias differ significantly from 0 on the basis of a 1-sample t-test); dashed lines indicate 95% upper and lower limits of agreement (LoA).


A.
PC2effective
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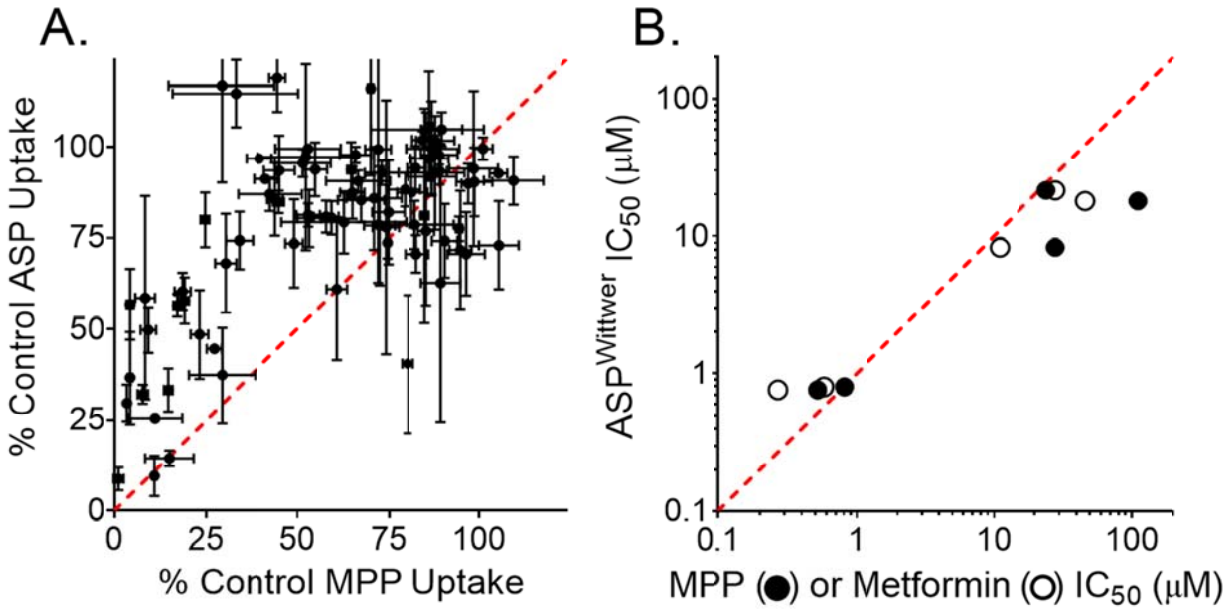
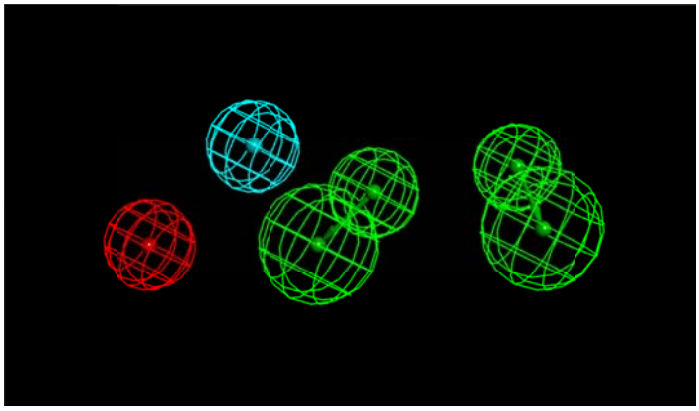


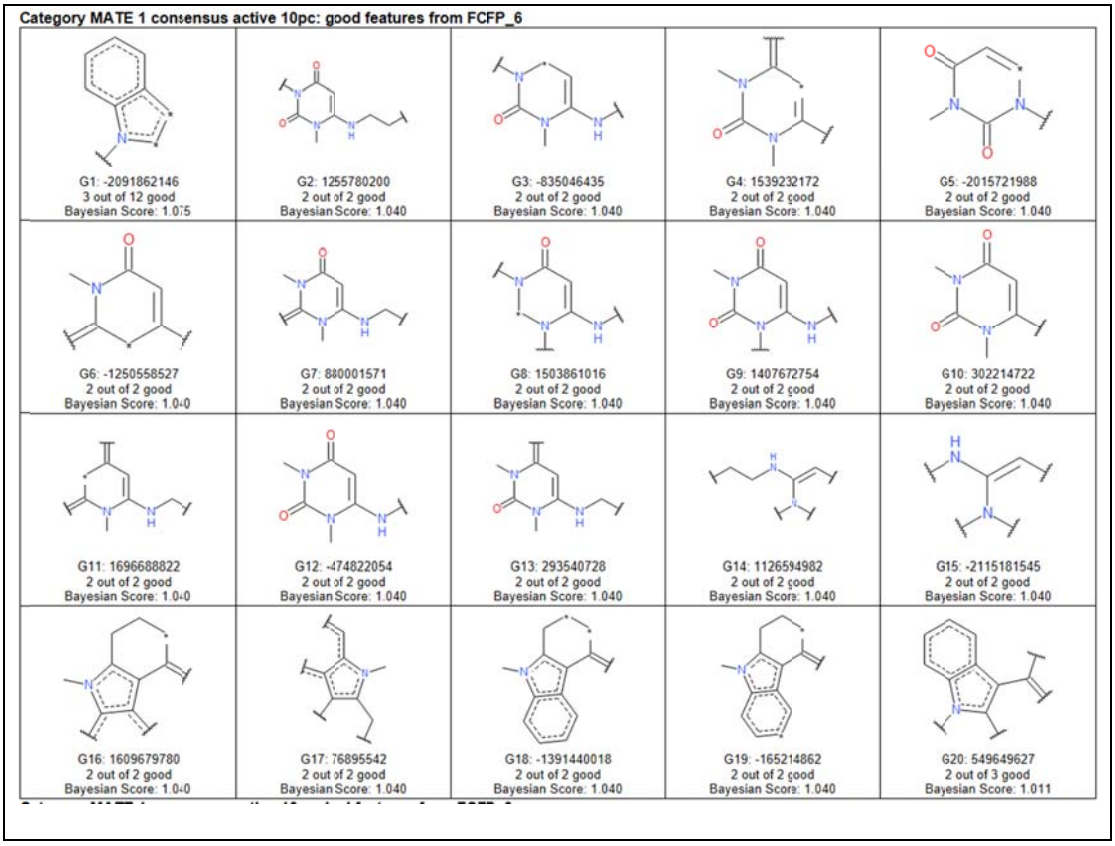
Supplemental Figure 3 (A) Comparison of the inhibition of MATE1-mediated transport of [^{3}H]MPP resulting from exposure to a 50 μM concentration of 86 compounds from the NCC, determined in the present study, to the inhibition of MATE1-mediated ASP transport that resulted from exposure to a 20 μM concentration of the same compounds as reported in the study of Wittwer et al. (J Med Chem, 56, 781, 2013). (B) Comparison of IC_{50} values for five compounds for inhibition of MATE1-mediated transport of MPP (solid circles) or metformin (open circles) determined in the present study, to those reported for inhibition of MATE1-mediated ASP transport by Wittwer et al. (J Med Chem, 56, 781, 2013).



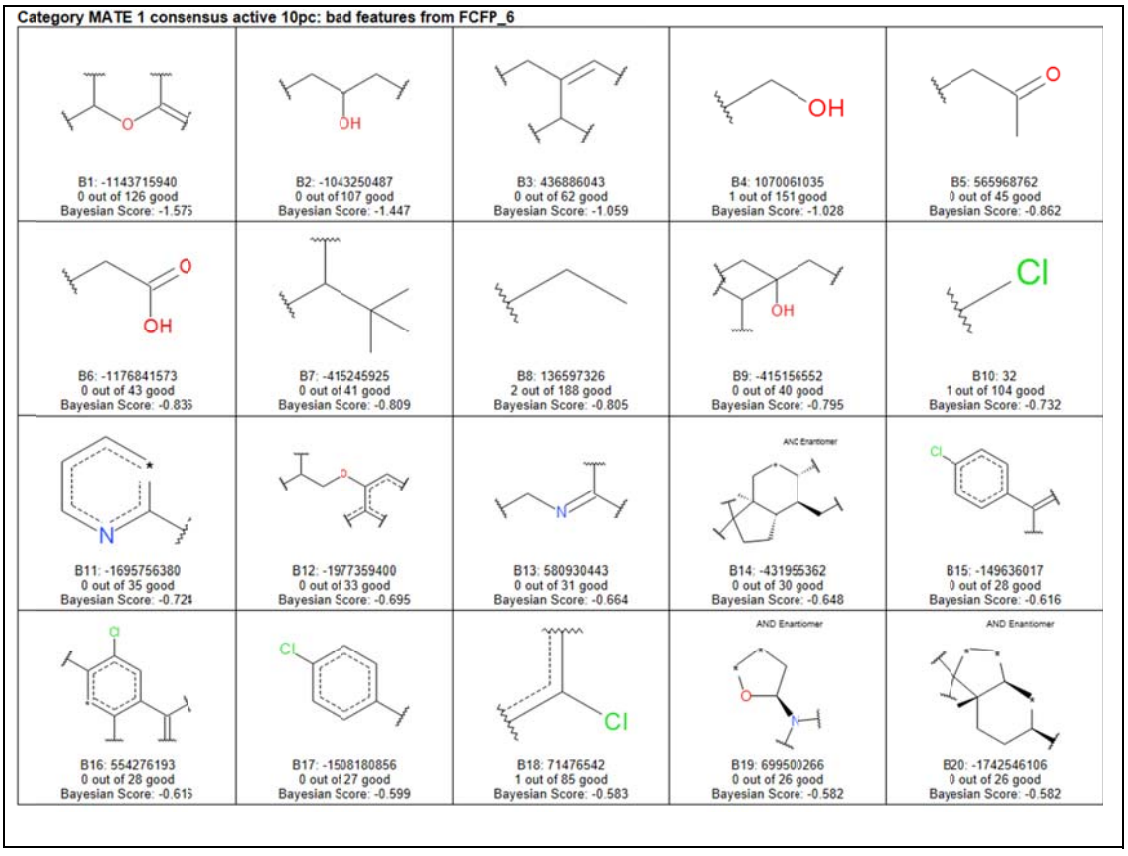
Supplemental Figure 4. N32 Pharmacophore for MPP

Supplemental Figure 5. A. Good features in the consensus MATE1 Bayesian model. B. Bad features in the consensus MATE1 Bayesian model.

A.



B.



Supplemental Table 1. Pharmacophore predictions

Test Molecules	Measured IC_{50} against MPP (μM)	Cimetidine IC_{50} prediction (μM)	Metformin IC_{50} prediction (μM)	MPP IC_{50} prediction (μM)	NBD-MTMA IC_{50} prediction (μM)
BMIM	179	256	312	247	340
NBuPY	26.5	1,514	312	821	2,056
alosetron	0.1	259	12.7	121	343
levofloxacin	51.6	256	254	119	208
nifekalant	2.9	106	52.1	31.3	70.8
terbinafine	1,209	369	14.7	307	501

Supplemental Table 2. Bayesian models statistics using Discovery Studio and CDD Models for the 400 molecules.

	ROC 5 fold	Sensitivity	Specificity	Concordance	CDD Bayesian 3 fold ROC FCFP6 only
MPP	0.697	1.00	0.358	0.403	0.69
NBD-MTMA	0.633	0.957	0.875	0.880	0.65
Cimetidine	0.652	1.00	0.485	0.512	0.65
Metformin	0.655	0.909	0.765	0.772	0.63
Consensus	***0.761***	***1.00***	***0.68***	***0.69***	***0.82***

Bayesian models were generated with the complete 400 molecules for each substrate probes. The 5 fold cross validation ROC values were MPP (0.70), NBD-MTMA (0.63), cimetidine (0.65), Metformin (0.65). These models also enable the determination of good and bad features in the molecules (Supp Fig 5). A consensus model was created using 12 molecules out of the 400 that were considered active across all 4 substrate probes. This model had a 5 fold cross validation ROC = 0.76 (Supp Fig. 5). The good features in the 12 active compounds mainly consisted of nitrogen containing heterocycles (Supp Figure 5). The 26 molecules with IC_{50} data for each probe were also used to build Bayesian models with actives classed as $IC_{50} < 50$ μM MPP (0.60), NBD-MTMA (0.67), cimetidine (0.79), Metformin (0.60). Ideally these ROC values should be 0.75 or preferably higher to be useful for predictions.

Supplemental Table 3. Bayesian models statistics using Discovery Studio for the 26 molecules.

	ROC 5 fold	Sensitivity	Specificity	Concordance
MPP	0.597	1.00	0.818	0.920
NBD-MTMA	0.667	0.833	0.923	0.880
Cimetidine	0.673	0.923	0.917	0.920
Metformin	0.597	0.875	0.778	0.840

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Molecular Pharmacology

Inhibition by 50 uM of each NCC compound (as percent control, i.e., transport in the absence of inhibitor)

NCC Plate 1-5 (NGP-105-01-05) - Single Concentration (50 uM) Inhibition Summary

				MPP				NBD-MTMA				CIMETIDINE				METFORMIN			
Compounds highlighted in yellow also list IC50 values				***Mean***	***SE***	***IC50***	***SE***	***Mean***	***SE***	***IC50***	***SE***	***Mean***	***SE***	***IC50***	***SE***	***Mean***	***SE***	***IC50***	***SE***
Plate row	**Plate 1**	SMILES	Plate column	***100.0***	***0.0***			***100.0***	***0.0***			***100.0***	***0.0***			***100.0***	***0.0***		
A	BUPROPION HYDROCHLORIDE	CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1.Cl	**2**	***54.8***	***3.3***			***56.8***	***9.5***			***39.7***	***1.7***			***60.9***	***4.3***		
	PAZUFLOXACIN	C[C@H]1COc2c(c(F)cc3c(=O)c(cn1c23)C(=O)O)C4(N)CC4	**3**	***86.0***	***3.4***			***85.7***	***3.0***			***92.5***	***7.9***			***85.3***	***3.0***		
	TOPOTECAN HYDROCHLORIDE	CC[C@@]1(O)C(=O)OCc2c1cc3-c4nc5ccc(O)c(CN(C)C)c5cc4Cn3c2=O.Cl	**4**	***9.2***	***2.1***			***9.5***	***5.2***			***9.6***	***0.4***			***6.0***	***0.7***		
	NAFTOPIDIL	COc1ccccc1N2CCN(CC(O)COc3ccccc4ccccc34)CC2	**5**	***66.5***	***8.7***			***65.8***	***11.6***			***71.2***	***17.0***			***65.5***	***3.4***		
	ROSIGLITAZONE MALEATE	CN(CCOc1ccc(CC2SC(=O)NC2=O)cc1)c3ccccn3.OC(=O)/C=C\C(=O)O	**6**	***1.2***	***2.9***			***-8.9***	***6.1***			***0.9***	***3.1***			***1.8***	***0.3***		
	BICALUTAMIDE	CC(O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc2ccc(C#N)c(c2)C(F)(F)F	**7**	***82.7***	***16.9***			***83.5***	***16.5***			***90.3***	***3.8***			***90.1***	***6.3***		
		Fc1cn(C2CCCO2)c(=O)[nH]c1=O	**8**	***95.9***	***2.9***			***85.7***	***4.2***			***100.8***	***5.9***			***89.4***	***5.1***		
	ISOQUERCITRIN	OC[C@H]1O[C@@H](Oc2c(oc3cc(O)cc(O)c3c2=O)c4ccc(O)c(O)c4)[C@H](O)[C@@H](O)[C@@H]1O	**9**	***98.8***	***7.6***			***65.9***	***3.3***			***89.9***	***6.0***			***59.9***	***9.6***		
	DOXORUBICIN HYDROCHLORIDE	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO.Cl	**10**	***49.1***	***2.4***			***44.1***	***8.8***			***83.0***	***3.4***			***40.6***	***3.7***		
	MIDAZOLAM HYDROCHLORIDE	Cc1ncc2CN=C(c3ccccc3F)c4cc(Cl)ccc4-n12.Cl	**11**	***5.9***	***4.3***			***2.2***	***3.7***			***4.2***	***6.5***			***3.7***	***0.3***		
B	IRSOGLADINE MALEATE	Nc1nc(N)nc(n1)c2cc(Cl)ccc2Cl.OC(=O)/C=C\C(=O)O	**2**	***89.9***	***6.3***			***84.9***	***3.5***			***76.9***	***30.2***			***95.7***	***4.6***		
	MIGLITOL	OCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	**3**	***94.5***	***0.1***			***95.2***	***4.2***			***106.6***	***4.4***			***94.3***	***3.9***		

	LEVETIRACETAM	CC[C@H](N1CCCC1=O)C(=O)N	4	95.1	4.9			89.7	5.9			97.3	2.7			87.4	5.9		
	NOBILETIN	COc1ccc(cc1OC)c2cc(=O)c3c(OC)c(OC)c(OC)c(OC)c3o2	5	13.7	0.5			11.9	4.3			37.6	16.0			7.3	0.5		
	ESCITALOPRAM OXALATE	CN(C)CCC[C@]1(OCc2cc(C#N)ccc21)c3ccc(F)cc3.OC(=O)C(=O)O	6	47.8	2.3			51.4	1.6			55.6	1.2			40.1	4.1		
	BENIDIPINE HCL	CO/C(=C\1/[C@H](C(=C(C)N=C1C)C(=O)O[C@@H]2CCCN(Cc3ccccc3)C2)c4cccc(c4)[N+](=O)[O-])/O.Cl	7	62.2	3.3			53.1	2.1			75.6	10.7			68.0	8.0		
	OLIGOMYCIN C	CC[C@H]1CC[C@H]2O[C@@]3(CC[C@@H](C)[C@@H](C[C@H](C)O)O3)[C@H](C)[C@@H](OC(=O)C=C[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@@H](C)[C@H](O)[C@@H](C)C(=O)[C@H](C)[C@H](O)[C@@H](C)CC=CC=C1)[C@H]2C	8	101.9	11.0			94.8	3.9			110.0	6.4			94.0	0.9		
		CCOC(=O)c1ncn-2c1CN(C)C(=O)c3cc(F)ccc32	9	76.1	2.6			77.5	5.9			96.8	9.7			71.2	1.7		
	MOXONIDINE HCL	COc1nc(C)nc(Cl)c1NC2=NCCN2.Cl	10	74.8	4.4			71.9	2.1			97.4	9.0			66.9	6.1		
	LAMIVUDINE	Nc1ccn([C@@H]2CS[C@H](CO)O2)c(=O)n1	11	85.1	1.1			85.4	7.0			86.7	2.8			82.7	3.0		
C	ACARBOSE	C[C@H]1O[C@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O[C@H]3[C@H](O)[C@@H](O)C(O)O[C@@H]3CO)O[C@@H]2CO)[C@H](O)[C@@H](O)[C@@H]1N[C@H]4C=C(CO)[C@@H](O)[C@H](O)[C@H]4O	2	95.1	5.6			86.4	5.9			111.7	10.5			93.0	4.1		
		COc1ccc(/C=C/C(=O)Nc2ccccc2C(=O)O)cc1OC	3	87.5	1.8			89.5	2.0			106.0	12.4			86.7	0.5		
	PRAMIPEXOLE HCL	CCCN[C@H]1CCc2nc(N)sc2C1.Cl	4	61.6	8.9			50.7	5.9			69.7	0.1			55.3	0.4		
	FINASTERIDE	CC(C)(C)NC(=O)[C@H]1CC[C@H]2[C@@H]3CC[C@H]4NC(=O)C=C[C@]4(C)[C@H]3CC[C@]12C	5	8.4	2.7			12.4	2.5			22.5	2.8			11.2	2.2		
		CC1CCC[C@H](O)CCCCCc2cc(O)cc(O)c2C(=O)O1	6	62.3	12.4			56.6	11.3			94.9	6.0			73.0	1.7		
	AMLEXANOX	CC(C)c1ccc2oc3nc(N)c(cc3c(=O)c2c1)C(=O)O	7	66.5	0.3			65.6	9.2			101.1	3.8			83.9	5.5		

	BENAZEPRIL HYDROCHLORIDE	CCOC(=O)[C@H](CCc1ccccc1)N[C@H]2CCc3ccccc3N(CC(=O)O)C2=O.Cl	8	88.7	9.6			97.3	8.2			123.6	7.7			99.8	3.6		
		OC(=O)/C=C/c1ccc(Cn2ccnc2)cc1.Cl	9	64.3	2.4			62.7	1.8			73.6	0.5			57.2	2.5		
		[O-][N+](=O)c1ccc2NC(=O)CN=C(c3ccccc3)c2c1	10	63.1	8.6			56.2	3.3			85.0	9.0			48.7	0.1		
	366-70-1	CNNCc1ccc(cc1)C(=O)NC(C)C.Cl	11	72.7	1.7			74.8	4.2			101.5	3.7			76.1	2.9		
D	BENPROPERINE PHOSPHATE	CC(COc1ccccc1Cc2ccccc2)N3CCCCC3.OP(=O)(O)O	2	29.4	4.1			23.9	0.9			26.0	6.5			21.2	1.2		
	OLANZAPINE	CN1CCN(CC1)C2=Nc3ccccc3Nc4sc(C)cc24	3	29.3	14.5			47.8	1.8			68.4	1.9			39.0	0.1		
	RISPERIDONE	Cc1nc2CCCCn2c(=O)c1CCN3CCC(CC3)c4noc5cc(F)ccc45	4	5.5	1.5			5.9	6.2			4.8	1.0			5.2	2.7		
	ZOLPIDEM TARTRATE	CN(C)C(=O)Cc1c(nc2ccc(C)cn12)c3ccc(C)cc3.OC(C(O)C(=O)O)C(=O)O	5	41.3	3.3			48.0	6.2			60.9	1.6			35.8	1.7		
	LATANOPROST	CC(C)OC(=O)CCC/C=C\C[C@H]1[C@@H](O)C[C@@H](O)[C@@H]1CC[C@@H](O)CCc2ccccc2	6	49.2	5.2			53.0	9.9			49.0	12.9			53.1	2.5		
	CERIVASTATIN SODIUM	COCc1c(nc(C(C)C)c(/C=C/[C@@H](O)C[C@@H](O)CC(=O)[O-])c1c2ccc(F)cc2)C(C)C.[Na+]	7	88.0	8.0	249	55.9	80.3	9.9	170	47.3	100.6	8.2	204	58.6	86.6	6.7	241	50.4
		C[C@]1(O)CC[C@H]2[C@@H]3CC[C@H]4CC(=C(C[C@]4(C)[C@H]3CC[C@@]21C)C=O)O	8	85.3	31.1			130.3	21.2			71.8	6.8			119.1	11.3		
	HYPEROSIDE	OC[C@H]1O[C@@H](Oc2c(oc3cc(O)cc(O)c3c2=O)c4ccc(O)c(O)c4)[C@H](O)[C@@H](O)[C@H]1O	9	85.3	5.0			77.6	5.4			103.5	2.6			80.7	11.6		
	PEFLOXACIN MESYLATE	CCn1cc(C(=O)O)c(=O)c2cc(F)c(cc12)N3CCN(C)CC3.CS(=O)(=O)O	10	45.1	1.6			42.0	0.8			74.8	2.3			39.1	1.0		
	ESOMEPRAZOLE MG	COc1ccc2n([Mg]n3c(nc4cc(OC)ccc34)S(=O)Cc5ncc(C)c(OC)c5C)c(nc2c1)S(=O)Cc6ncc(C)c(OC)c6C	11	23.4	6.4			17.3	3.6			40.7	2.7			14.2	2.2		
E		NC(=O)OCCCc1ccccc1	2	76.6	5.6			77.0	5.9			94.4	11.1			79.1	2.5		
	NEFAZODONE	CCc1nn(CCCN2CCN(CC2)c3cccc(Cl)c3)c(=O)n1CCOc4ccccc4.Cl	3	42.5	8.8			50.7	8.9			48.7	22.1			51.1	3.5		
	PIOGLITAZONE HYDROCHLORIDE	CCc1ccc(CCOc2ccc(CC3SC(=O)NC3=O)cc2)nc1.Cl	4	76.2	6.2			85.3	4.9			104.9	13.4			86.6	1.5		

	VIRAMUNE	Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	5	68.6	0.9			68.5	7.2			92.5	19.0			66.6	0.8		
		OC[C@@H]1CC[C@@H](O1)n2cnc3c(O)ncnc23	6	84.2	5.5			92.7	6.1			94.3	18.1			84.7	0.9		
	ICARIIN	COc1ccc(cc1)c2oc3c(CC=C(C)C)c(O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)cc(O)c3c(=O)c2O[C@@H]5O[C@@H](C)[C@H](O)[C@@H](O)[C@H]5O	7	58.2	9.7			50.2	8.2			85.4	15.2			93.0	22.0		
	35212-22-7	CC(C)Oc1ccc2c(=O)c(coc2c1)c3ccccc3	8	88.7	7.8			89.2	2.6			104.7	8.7			88.7	4.5		
	RIFABUTIN	CO[C@H]1C=CO[C@@]2(C)Oc3c(C2=O)c4c5=NC6(CCN(CC(C)C)CC6)N=c5c(NC(=O)C(=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)C)c(O)c4c(O)c3C	9	65.8	4.3			77.7	4.6			80.7	11.3			75.1	11.6		
	VENLAFAXINE HYDROCHLORIDE	COc1ccc(cc1)C(CN(C)C)C2(O)CCCCC2.Cl	10	75.9	5.8	366	55.0	88.1	13.2	332	34.4	68.7	4.9	303	33.6	86.9	26.0	168	25.8
	SULFASALAZINE	OC(=O)c1cc(N=Nc2ccc(cc2)S(=O)(=O)Nc3ccccn3)ccc1O	11	53.0	3.2			46.1	12.5			68.6	7.3			55.2	2.8		
F		C[C@@]1(C[C@@H]2C[C@]3(C)C1)C[C@](N)(C2)C3.Cl	2	53.5	3.5			59.0	6.6			36.2	6.5			53.9	5.5		
	MOXIFLOXACIN HYDROCHLORIDE	COc1c(N2C[C@@H]3CCCN[C@@H]3C2)c(F)cc4c(=O)c(cn(C5CC5)c14)C(=O)O.Cl	3	41.5	3.5			36.6	0.7			57.0	6.6			33.8	2.0		
	CILASTATIN SODIUM	CC1(C)C[C@@H]1C(=O)N/C(=C\CCCCSC[C@H](N)C(=O)O)/C(=O)[O-].[Na+]	4	90.6	6.8			96.0	0.9			101.3	4.7			91.8	2.2		
	TOPIRAMATE	CC1(C)O[C@@H]2CO[C@@]3(COS(=O)(=O)N)OC(C)(C)O[C@H]3[C@@H]2O1	5	81.5	4.4			95.9	4.9			79.6	16.5			84.0	2.2		
	SERTRALINE	CN[C@H]1CC[C@@H](c2ccc(Cl)c(Cl)c2)c3ccccc13.Cl	6	51.5	7.6			54.9	2.1			62.5	4.4			48.0	1.8		
	METHYLANDROSTENEDIOL	C[C@]1(O)CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C	7	77.8	6.3			84.8	8.4			94.2	13.0			87.6	6.1		
	OXAPROZIN	OC(=O)CCc1nc(c(o1)c2ccccc2)c3ccccc3	8	89.8	5.6			97.2	11.5			111.5	0.4			98.8	1.0		
	ESMOLOL HYDROCHLORIDE	COC(=O)CCc1ccc(OCC(O)CNC(C)C)cc1.Cl	9	30.5	2.8	16.2	0.9	37.0	4.0	24.5	2.9	30.4	5.1	12.7	1.6	35.0	2.9	11	1.0
	PANTOPRAZOLE SODIUM	COc1ccnc(CS(=O)c2nc3cc(OC(F)F)ccc3[n-]2)c1OC.[Na+]	10	22.8	1.8			22.7	4.5			36.2	6.1			19.6	3.5		
	TORASEMIDE	CC(C)NC(=O)NS(=O)(=O)c1ccccc1Nc2cccc(C)c2	11	93.8	6.0			97.3	9.4			95.3	19.8			83.9	17.2		

G	CARVEDILOL	COc1ccccc1OCCNCC(O)COc2ccc c3[nH]c4ccccc4c23	**2**	***62.7***	***17.0***			***56.3***	***10.4***			***47.8***	***13.4***			***44.8***	***1.0***		
	NELFINAVIR MESYLATE	Cc1c(O)cccc1C(=O)N[C@@H](C Sc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)N C(C)(C)C.CS(=O)(=O)O	**3**	***33.1***	***17.2***			***68.6***	***2.8***			***97.3***	***0.3***			***62.2***	***0.9***		
	ARGATROBAN	C[C@@H]1CCN([C@H](C1)C(= O)O)C(=O)[C@H](CCCN=C(N)N) NS(=O)(=O)c2cccc3CC(C)CNc23	**4**	***71.5***	***7.9***			***78.1***	***0.3***			***100.4***	***4.5***			***77.8***	***7.9***		
	VORICONAZOLE	C[C@@H](c1ncncc1F)[C@](O)(Cn2cncn2)c3ccc(F)cc3F	**5**	***91.3***	***11.9***			***80.1***	***2.9***			***100.7***	***3.0***			***77.3***	***5.4***		
	CALCIPOTRIOL	C[C@H](/C=C/[C@@H](O)C1CC 1)[C@H]2CC[C@H]3\C(=C\C=C/ 4\C[C@@H](O)C[C@H](O)C4=C)\CCC[C@]23C	**6**	***29.7***	***2.8***			***36.5***	***7.6***			***47.6***	***0.9***			***28.5***	***4.0***		
	TRIPTOLIDE	CC(C)[C@@]12O[C@H]2[C@@ H]3O[C@]34[C@]5(O[C@H]5C[C@H]6C7=C(CC[C@@]64C)C(= O)OC7)[C@@H]1O	**7**	***81.1***	***5.2***			***86.1***	***7.2***			***109.3***	***0.7***			***82.8***	***5.8***		
	ROLIPRAM	COc1ccc(cc1OC2CCCC2)C3CNC(=O)C3	**8**	***59.0***	***1.6***	***147***	***12.9***	***62.7***	***2.2***	***183***	***40.8***	***73.3***	***1.1***	***111***	***11.4***	***62.4***	***1.4***	***124***	***11.0***
	TADALAFIL	CN1CC(=O)N2[C@@H](c3[nH]c 4ccccc4c3C[C@@H]2C1=O)c5c cc6OCOc6c5	**9**	***59.5***	***10.4***			***74.3***	***21.3***			***90.8***	***2.0***			***106.5***	***2.4***		
	FLUTICASONE PROPIONATE	CCC(=O)O[C@@]1([C@H](C)C[C@H]2[C@@H]3C[C@H](F)C4= CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C)C(=O)S CF	**10**	***92.1***	***7.7***			***71.6***	***11.6***			***120.6***	***12.1***			***89.7***	***1.1***		
	TROPISETRONÂ HYDROC HLORIDE	CN1[C@H]2CC[C@@H]1C[C@ @H](C2)OC(=O)c3c[nH]c4ccccc 34.Cl	**11**	***1.6***	***1.1***			***-1.6***	***4.6***			***2.1***	***1.5***			***2.2***	***0.2***		
H	LOMIFYLLINE	CC(=O)CCCCn1cnc2n(C)c(=O)n(C)c(=O)c12	**2**	***50.0***	***4.6***			***47.3***	***4.3***			***72.1***	***6.4***			***45.7***	***4.9***		
	PRAVASTATIN SODIUM	CC[C@H](C)C(=O)O[C@H]1C[C @H](O)C=C2C=C[C@H](C)[C@H](CC[C@@H](O)C[C@@H](O)C C(=O)[O-])[C@@H]12.[Na+]	**3**	***105.3***	***5.4***			***91.9***	***3.9***			***117.1***	***7.2***			***99.6***	***4.9***		
	VALDECOXIB	Cc1onc(c1c2ccc(cc2)S(=O)(=O) N)c3ccccc3	**4**	***79.1***	***8.0***			***36.7***	***21.2***			***107.1***	***5.9***			***86.6***	***1.2***		
	FENOLDOPAM MESYLATE	Oc1ccc(cc1)C2CNCCc3c(Cl)c(O) c(O)cc23.CS(=O)(=O)O	**5**	***12.5***	***2.5***			***15.5***	***6.8***			***20.8***	***4.7***			***9.9***	***0.2***		

	EPIRUBICIN HYDROCHLORIDE	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO.Cl	6	16.6	0.5			22.8	6.9			45.6	11.8			16.3	1.0		
	ROSIGLITAZONE HCL	CN(CCOc1ccc(CC2SC(=O)NC2=O)cc1)c3ccccn3.Cl	7	0.5	0.9			-0.7	3.7			1.2	0.3			2.4	2.1		
	MOSAPRIDE CITRATE	CCOc1cc(N)c(Cl)cc1C(=O)NCC2CN(Cc3ccc(F)cc3)CCO2.OC(=O)CC(O)(CC(=O)O)C(=O)O	8	72.8	29.5			66.8	18.3			98.8	15.0			85.4	0.5		
		NC(=O)CS(=O)C(c1ccccc1)c2ccccc2	9	88.8	2.8			95.0	5.2			120.3	13.9			101.1	10.4		
	INDINAVIR SULFATE	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45.OS(=O)(=O)O	10	7.7	1.4			10.9	3.2			18.8	3.4			8.0	1.6		
	RANOLAZINE DIHYDROCHLORIDE	COc1ccccc1OCC(O)CN2CCN(CC(=O)Nc3c(C)cccc3C)CC2.Cl	11	28.1	2.5			36.5	4.0			44.0	9.7			25.5	1.5		
	PLATE 2																		
A		CC1=C(N2[C@H](SC1)[C@H](NC(=O)[C@H](N)c3ccccc3)C2=O)C(=O)O	2	103.0	3.1			88.3	9.1			101.3	0.5			98.5	4.9		
	TROXIPIDE	COc1cc(cc(OC)c1OC)C(=O)NC2CCCNC2	3	19.1	1.5			21.7	11.0			31.9	3.3			17.2	1.8		
	LEVOSULPIRIDE	CCN1CCC[C@H]1CNC(=O)c2cc(ccc2OC)S(=O)(=O)N	4	17.1	1.3			17.9	2.9			26.6	3.3			11.8	1.3		
		Cc1nnc2CN=C(c3ccccc3)c4cc(Cl)ccc4-n12	5	55.5	5.3			63.9	7.8			63.0	1.8			41.5	4.5		
	DOCETAXEL	CC(=O)O[C@]12CO[C@@H]2C[C@H](O)[C@]3(C)[C@@H]1[C@H](OC(=O)c4ccccc4)[C@@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)OC(C)(C)C)c6ccccc6)C(=C([C@@H](O)C3=O)C5(C)C)C	6	67.4	7.8			80.0	10.5			88.9	0.0			2.7	0.1		
		C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C	7	59.7	6.8			55.1	4.0			69.0	10.4			50.2	3.4		
	4-CHLORO-N-(2-MORPHOLIN-4-YL-ETHYL)-BENZAMIDE	Clc1ccc(cc1)C(=O)NCCN2CCOCC2	8	83.4	1.1			77.1	4.8			89.6	3.9			73.9	3.2		
	FLUBENDAZOLE	COC(=O)Nc1nc2cc(ccc2[nH]1)C(=O)c3ccc(F)cc3	9	90.8	1.5			81.3	2.0			102.8	5.0			81.0	0.5		

	PICEID	OC[C@H]1O[C@@H](Oc2cc(O)cc(/C=C/c3ccc(O)cc3)c2)[C@H](O)[C@@H](O)[C@@H]1O	10	81.7	0.5			50.3	18.2			92.4	2.7			69.8	2.4		
	GABEXATE	CCOC(=O)c1ccc(OC(=O)CCCCCN=C(N)N)cc1.CS(=O)(=O)O	11	7.7	1.6	0.7	0.1	-8.3	12.2	0.7	0.1	10.6	3.2	0.6	0.1	13.7	3.1	0.58	0.1
B	PIDOTIMOD	OC(=O)[C@@H]1CSCN1C(=O)[C@@H]2CCC(=O)N2	2	76.4	0.2			82.6	12.1			82.9	0.3			91.9	0.3		
	ACTARIT	CC(=O)Nc1ccc(CC(=O)O)cc1	3	96.9	3.8			96.1	1.9			114.4	6.4			105.2	6.4		
		NC1=NC(=O)C(O1)c2ccccc2	4	93.8	0.6			84.5	4.2			105.9	0.2			96.4	7.3		
		Nc1nnc(c(N)n1)c2cccc(Cl)c2Cl	5	47.7	0.4			40.1	15.0			53.3	0.3			45.5	1.7		
	HONOKIOL	Oc1ccc(cc1CC=C)c2cc(CC=C)ccc2O	6	80.4	3.0			78.8	3.2			92.5	1.8			74.9	6.5		
	TOSUFLOXACIN TOSILATE	NC1CCN(C1)c2nc3n(cc(C(=O)O)c(=O)c3cc2F)c4ccc(F)cc4F.Cc1ccc(cc1)S(=O)(=O)O	7	67.6	7.1			69.3	15.0			100.3	3.8			62.1	11.3		
	HALOMETASONE MONOHYDRATE	C[C@@H]1C[C@H]2[C@@H]3C[C@H](F)C4=CC(=O)C(=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO)Cl	8	36.6	7.1			34.4	9.0			51.1	13.4			35.2	3.5		
	TACROLIMUS	CO[C@@H]1C[C@@H](CC[C@H]1O)/C=C(\C)/[C@H]2OC(=O)[C@@H]3CCCCN3C(=O)C(=O)[C@]4(O)O[C@@H]([C@H](C[C@H]4C)OC)[C@H](C[C@@H](C)CC(=C[C@@H](CC=C)C(=O)C[C@H](O)[C@H]2C)C)OC	9	26.1	3.9			37.0	0.8			51.1	1.6			31.9	0.3		
	1-(2-METHYL-5-NITRO-IMIDAZOL-1-YL)-PROPAN-2-OL	CC(O)Cn1c(C)ncc1[N+](=O)[O-]	10	96.2	4.5			88.7	4.4			110.6	2.9			97.1	5.6		
	OXICONAZOLE NITRATE	Clc1ccc(CON=C(Cn2ccnc2)c3ccc(Cl)cc3Cl)c(Cl)c1.O[N+](=O)[O-]	11	94.3	2.1			74.4	17.9			110.9	6.2			100.9	5.7		
C	RAMIPRIL	CCOC(=O)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N2[C@@H](C[C@@H]3CCC[C@@H]32)C(=O)O	2	89.5	6.6			81.4	6.1			106.6	1.5			95.4	3.8		
	AZELASTINE HYDROCHLORIDE	CN1CCCC(CC1)n2nc(Cc3ccc(Cl)cc3)c4ccccc4c2=O.Cl	3	13.9	0.4			18.7	0.2			23.5	4.5			19.6	1.7		
	LETROZOLE	N#Cc1ccc(cc1)C(c2ccc(C#N)cc2)n3cncn3	4	53.2	3.9			45.3	0.0			54.8	0.9			45.5	2.1		
	N-ETHYL-O-CROTONOTOLUIDIDE	CCN(C(=O)/C=C/C)c1ccccc1C	5	89.1	4.9			74.5	1.2			89.9	2.8			96.2	5.4		

	TOLTERODINE TARTRATE	CC(C)N(CC[C@H](c1ccccc1)c2cc(C)ccc2O)C(C)C.OC(C(O)C(=O)O)C(=O)O	6	49.8	9.3			46.9	2.2			62.7	3.4			49.6	9.7		
	MECILLINAM	CC1(C)S[C@@H]2[C@H](N=CN3CCCCCC3)C(=O)N2[C@H]1C(=O)O	7	77.8	6.0			80.0	10.1			84.3	2.6			89.1	5.1		
	TRICLABENDAZOLE	CSc1nc2cc(Cl)c(Oc3cccc(Cl)c3Cl)cc2[nH]1	8	92.5	7.4			95.4	9.4			102.4	2.8			106.2	4.2		
	VALACICLOVIR HYDROCHLORIDE	CC(C)[C@H](N)C(=O)OCCOCn1cnc2c(O)nc(N)nc12.Cl	9	46.4	4.7			46.1	4.1			65.8	3.5			45.5	5.5		
	NIFEKALANT HYDROCHLORIDE	Cn1c(NCCN(CCO)CCCc2ccc(cc2)[N+](=O)[O-])cc(=O)n(C)c1=O.Cl	10	4.3	0.7	2.9	0.1	6.0	3.9			9.1	1.6			10.3	0.1		
	KITASAMYCIN	CO[C@H]1[C@@H](CC(=O)O[C@H](C)CC=CC=C[C@H](O)[C@H](C)C[C@H](CC=O)[C@@H]1O[C@@H]2O[C@H](C)[C@@H](O[C@H]3C[C@@](C)(OC(=O)CC(C)C)[C@@H](O)[C@H](C)O3)[C@@H]([C@H]2O)N(C)C)OC(=O)C	11	27.2	2.4			31.2	0.5			44.8	5.5			27.5	0.2		
D	FENPIVERINIUM BROMIDE	C[N+]1(CCC(C(=O)N)(c2ccccc2)c3ccccc3)CCCCC1.[Br-]	2	48.6	6.5			52.6	3.4			74.0	3.6			45.8	3.8		
	TOCAINIDE	CC(N)C(=O)Nc1c(C)cccc1C	3	89.2	2.4			81.3	7.8			103.5	1.5			86.0	4.0		
	MEROPENEM	C[C@@H](O)[C@@H]1[C@H]2[C@@H](C)C(=C(N2C1=O)C(=O)O)S[C@@H]3CN[C@@H](C3)C(=O)N(C)C	4	72.0	4.3			102.0	8.7			86.8	0.3			77.1	5.0		
	AMFEBUTAMONE	CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1	5	52.9	3.5			51.1	6.3			46.8	1.0			45.8	0.8		
	CARMOFUR	CCCCCCNC(=O)n1cc(F)c(=O)[nH]c1=O	6	90.7	5.7			74.9	6.0			97.7	0.8			85.6	2.9		
	ATOMOXETINE HYDROCHLORIDE	CNCC[C@@H](Oc1ccccc1C)c2ccccc2.Cl	7	69.8	5.4			75.3	3.0			77.7	4.4			68.1	7.2		
	ROFECOXIB	CS(=O)(=O)c1ccc(cc1)C2=C(C(=O)OC2)c3ccccc3	8	48.0	1.1			18.5	6.5			65.5	1.3			35.5	0.4		
	CLARITHROMYCIN	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@@H]([C@H]3O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC	9	86.5	6.4			89.1	10.1			93.5	1.8			73.9	1.4		

	NATEGLINIDE	CC(C)[C@H]1CC[C@@H](CC1)C(=O)N[C@H](Cc2ccccc2)C(=O)O	10	89.1	6.1			77.5	7.0			102.0	4.9			84.8	2.3		
	FAMCICLOVIR	CC(=O)OCC(CCn1cnc2cnc(N)nc12)COC(=O)C	11	82.7	4.3			79.0	7.1			103.7	7.6			80.0	3.6		
E	19-NORTESTOSTERONE	C[C@@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]2CC[C@@H]1O	2	17.2	2.3			24.4	0.8			22.1	2.1			17.0	0.2		
	TAXIFOLIN-(+/-)	O[C@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c3ccc(O)c(O)c3	3	53.8	3.4			58.1	5.7			72.4	1.8			62.2	1.2		
	ORLISTAT	CCCCCCCCCCC[C@@H](C[C@@H]1OC(=O)[C@H]1CCCCCC)OC(=O)[C@H](CC(C)C)NC=O	4	82.8	4.2			78.7	0.4			85.6	1.1			79.7	0.9		
	ALFUZOSIN	COc1cc2nc(nc(N)c2cc1OC)N(C)CCCNC(=O)C3CCCO3	5	18.7	4.1			19.7	1.5			30.6	3.1			16.7	1.8		
	PAROXETINE	CN1CC[C@H]([C@H](COc2ccc3OCOc3c2)C1)c4ccc(F)cc4	6	56.3	6.8			56.8	3.6			69.2	2.9			66.8	8.7		
	ARTESUNATE	C[C@@H]1CC[C@H]2[C@@H](C)[C@@H](OC(=O)CCC(=O)O)O[C@@H]3O[C@@]4(C)CC[C@@H]1[C@@]23OO4	7	74.9	1.1			88.2	3.0			84.8	1.9			76.8	2.9		
	BISOPROLOL FUMARATE	CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1.OC(=O)/C=C/C(=O)O	8	40.4	6.5			40.8	1.5			55.0	3.4			36.5	2.8		
	ARIPIPRAZOLE	Clc1cccc(N2CCN(CCCCOc3ccc4CCC(=O)Nc4c3)CC2)c1Cl	9	44.9	6.9			29.3	10.7			76.9	6.1			50.3	14.2		
		CC(=O)O[C@@]1(CC[C@H]2[C@@H]3C=C(C)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C)C(=O)C	10	50.2	12.5			68.8	7.6			71.7	2.0			55.4	4.7		
		CC(C)NCC(O)c1ccc(NS(=O)(=O)C)cc1.Cl	11	75.0	5.6			71.8	6.6			88.4	2.8			78.0	6.4		
F		CN/C(=C\[N+](=O)[O-])/NCCSCc1csc(CN(C)C)n1	2	36.0	4.7			42.3	3.9			52.6	5.6			36.9	2.5		
	LEVOFLOXACIN	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc4c(=O)c(cn1c24)C(=O)O	3	34.0	4.5	71.5	10.5	33.5	0.2	35.0	9.9	54.0	4.9	90.5	10.9	24.5	2.3	45.8	2.9
		Cc1nccn1CC2CCc3c(C2=O)c4ccccc4n3C.Cl	4	-1.7	1.2			-4.4	13.3			-0.7	0.7			1.5	1.8		
	AMISULPRIDE	CCN1CCCC1CNC(=O)c2cc(c(N)cc2OC)S(=O)(=O)CC	5	4.8	1.2			-4.6	10.3			9.0	3.1			3.0	0.2		
	OLMESARTAN MEDOXOMIL	CCCc1nc(c(C(=O)O)n1Cc2ccc(cc2)c3ccccc3c4nn[nH]n4)C(C)(C)O	6	66.7	3.8			76.7	1.6			83.0	0.2			70.6	1.2		

		CCC(C)n1ncn(c2ccc(cc2)N3CCN(CC3)c4ccc(OCC5COC(Cn6cncn6)(O5)c7ccc(Cl)cc7Cl)cc4)c1=O	7	73.3	5.1			80.2	13.2			82.7	7.5			76.0	7.3		
	EZETIMIBE	O[C@@H](CC[C@@H]1[C@H](N(C1=O)c2ccc(F)cc2)c3ccc(O)cc3)c4ccc(F)cc4	8	54.2	1.4			48.7	3.9			62.4	4.8			40.8	1.5		
	TRIMEBUTINE MALEATE	CCC(COC(=O)c1cc(OC)c(OC)c(OC)c1)(N(C)C)c2ccccc2.OC(=O)/C=C\C(=O)O	9	28.4	4.7			39.2	9.9			35.9	8.0			29.8	6.1		
	ORMETOPRIM	COc1cc(C)c(Cc2cnc(N)nc2N)cc1OC	10	3.9	0.7			-24.7	6.3			5.4	0.5			8.1	13.5		
	RUFLOXACIN MONOHYDROCHLORIDE	CN1CCN(CC1)c2c(F)cc3c(=O)c(cn4CCSc2c43)C(=O)O	11	30.9	3.9			33.2	7.6			52.8	6.3			29.4	4.4		
G		Nc1nc(O)ncc1F	2	96.3	5.1			86.9	6.8			97.1	4.3			88.9	1.6		
	CEFATRIZINE PROPYLENE GLYCOL	N[C@@H](C(=O)N[C@H]1[C@H]2SCC(=C(N2C1=O)C(=O)O)CSc3c[nH]nn3)c4ccc(O)cc4.CC(O)CO	3	94.4	1.9			93.9	8.0			103.2	12.1			86.2	0.9		
		CC[C@@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]2CC[C@@]1(O)C#C	4	88.9	0.8			89.6	0.9			88.8	2.2			73.0	1.5		
	LOFEPRAMINE	CN(CCCN1c2ccccc2CCc3ccccc13)CC(=O)c4ccc(Cl)cc4.Cl	5	34.7	6.8			29.4	12.8			42.5	11.9			26.0	6.0		
	LOSARTAN POTASSIUM	CCCCc1nc(Cl)c(CO)n1Cc2ccc(cc2)c3ccccc3c4nnn[n-]4.[K+]	6	79.4	5.6			64.6	0.7			91.9	0.9			74.7	3.4		
	CEFPODOXIME PROXETIL	COCC1=C(N2[C@H](SC1)[C@H](NC(=O)C(=NOC)c3csc(N)n3)C2=O)C(=O)OC(C)OC(=O)OC(C)C	7	45.1	5.1			44.0	5.0			60.4	0.7			44.4	9.6		
	TIAGABINE HCL	Cc1ccsc1C(=CCCN2CCC[C@H](C2)C(=O)O)c3sccc3C.Cl	8	77.5	1.4			75.8	13.0			91.6	4.8			66.6	1.9		
		C[C@]1(O)CC[C@H]2[C@@H]3CC[C@H]4CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C	9	69.0	0.4			63.3	3.6			90.8	4.7			76.2	4.8		
	ZILEUTON	CC(N(O)C(=O)N)c1cc2ccccc2s1	10	98.7	6.0			92.1	12.0			102.3	1.1			76.9	9.6		
	TAXIFOLIN-(+)	O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c3ccc(O)c(O)c3	11	71.8	2.8			63.6	3.5			83.0	5.8			55.6	2.0		
H		NC(=O)N1c2ccccc2CC(=O)c3ccccc13	2	89.3	0.0			85.2	1.7			89.3	8.6			80.3	5.0		
	IDEBENONE	COC1=C(OC)C(=O)C(=C(C)C1=O)CCCCCCCCCCO	3	29.3	11.0			31.0	12.3			31.9	6.8			28.3	8.6		

	CETRAXATE HCL	NC[C@H]1CC[C@@H](CC1)C(=O)Oc2ccc(CCC(=O)O)cc2.Cl	4	101.0	3.1			98.4	4.2			104.1	1.6			91.0	1.1		
	PEROSPIRONE HCL	O=C1[C@H]2CCCC[C@H]2C(=O)N1CCCCN3CCN(CC3)c4nsc5ccccc45.Cl	5	3.4	0.4			7.5	4.5			4.7	1.1			4.2	0.2		
	TEMOZOLOMIDE	Cn1nnc2c(ncn2c1=O)C(=O)N	6	112.3	4.6			100.1	1.8			106.4	3.7			105.0	5.5		
	BUFLOMEDIL HCL	COc1cc(OC)c(C(=O)CCCN2CCCC2)c(OC)c1.Cl	7	18.6	2.8			23.0	1.0			28.3	4.1			16.3	0.0		
	IDARUBICIN HYDROCHLORIDE	C[C@@H]1O[C@H](C[C@H](N)[C@@H]1O)O[C@H]2C[C@@](O)(Cc3c(O)c4C(=O)c5ccccc5C(=O)c4c(O)c23)C(=O)C.Cl	8	39.5	4.2			39.9	8.8			58.8	11.1			39.8	8.1		
	NISOLDIPINE	CO/C(=C\1/C(C(=C(C)N=C1C)C(=O)OCC(C)C)c2ccccc2[N+](=O)[O-])/O	9	43.9	2.5			50.3	5.8			59.3	0.8			36.0	5.1		
		Cc1cn([C@@H]2O[C@H](CO)C=C2)c(=O)[nH]c1=O	10	98.7	2.6			91.2	4.2			99.6	6.8			86.5	1.4		
	ALOSETRON MONOHYDROCHLORIDE	Cc1[nH]cnc1CN2CCc3c(C2=O)c4ccccc4n3C.Cl	11	-7.2	6.1	0.1	0.0	0.4	4.6			0.8	0.0			-1.7	4.8		
	PLATE 3																		
A	BESTATIN	CC(C)C[C@H](NC(=O)[C@@H](O)[C@H](N)Cc1ccccc1)C(=O)O	2	93.7	5.7			104.3	0.2			99.3	0.9			130.4	2.1		
	16502-01-5 (TRYPTOLINE)	C1Cc2c(CN1)[nH]c3ccccc23	3	33.6	3.6	103	10.4	39.3	1.9	143	27.5	27.4	1.3	110	13.6	1.1	0.0	95.6	11.7
		COc1cc(C)nn1c2nc(C)cc(OC)n2	4	93.0	5.4			63.7	2.0			99.0	1.4			134.0	3.3		
	HOMOVERATRYLAMINE	COc1ccc(CCN)cc1OC	5	51.5	1.2			53.9	0.6			36.2	1.8			76.8	4.6		
		C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@H]3[C@H](CC(=O)[C@]12C)[C@@]4(C)CCC(=O)C[C@H]4CC3=O	6	88.8	1.4			71.5	1.9			98.3	3.8			122.6	5.4		
		C[C@H]1C[C@H]2[C@@H]3CC[C@](O)(C(=O)C)[C@@]3(C)CC[C@@H]2[C@@]4(C)CCC(=O)C=C14	7	59.0	14.1			79.2	2.0			65.0	8.2			72.0	5.0		
	NAFADOTRIDE	CCCCN1CCCC1CNC(=O)c2cc(C#N)c3ccccc3c2OC	8	16.0	4.4	11.5	1.0	19.4	1.8	10.4	2.0	18.8	3.8	19.9	1.4	30.7	13.0	7.3	0.6

	METHANESULFONAMIDE, N-[4-[[1-[2-(6-METHYL-2-PYRIDINYL)ETHYL]-4-PIPERIDINYL]CARBONYL]PHENYL]-, DIHYDROCHLORIDE [CAS]	Cc1cccc(CCN2CCC(CC2)C(=O)c3ccc(NS(=O)(=O)C)cc3)n1.Cl	9	*16.7*	*2.8*			*45.6*	*5.5*			*21.4*	*0.2*			*1.0*	*0.4*		
	TRAMADOL	COc1cccc(c1)[C@@]2(O)CCCC[C@@H]2CN(C)C.Cl	10	*70.9*	*9.2*			*68.8*	*0.1*			*82.1*	*4.0*			*73.2*	*5.8*		
	CORTISONE	C[C@@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]2CC[C@]1(O)C(=O)CO	11	*49.2*	*5.4*	*56.9*	*6.5*	*49.0*	*2.5*	*77.4*	*11.2*	*55.6*	*1.2*	*131*	*13.3*	*45.8*	*3.3*	*28.5*	*2.8*
B	TOREMIFENE CITRATE	CN(C)CCOc1ccc(cc1)/C(=C(/CCCl)\c2ccccc2)/c3ccccc3.OC(=O)CC(O)(CC(=O)O)C(=O)O	2	*68.7*	*7.5*			*80.2*	*2.2*			*79.3*	*5.5*			*87.7*	*1.6*		
		OCCN1CCN(CCCN2c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1.Cl	3	*10.1*	*2.5*			*10.9*	*2.9*			*15.4*	*2.6*			*1.1*	*0.1*		
		OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n2ncc(=O)[nH]c2=O	4	*93.3*	*1.1*			*90.6*	*2.6*			*104.9*	*0.6*			*108.6*	*14.8*		
		CCS(=O)(=O)CCn1c(C)ncc1[N+](=O)[O-]	5	*94.7*	*2.4*			*92.7*	*0.7*			*88.7*	*1.5*			*118.5*	*11.7*		
		N[C@@H](C(=O)N[C@H]1[C@H]2SCC(=C(N2C1=O)C(=O)O)Cl)c3ccccc3	6	*95.1*	*8.5*			*89.7*	*0.1*			*101.1*	*0.2*			*109.2*	*6.0*		
	PINACIDIL MONOHYDRATE	CC(N=C(NC#N)Nc1ccncc1)C(C)(C)C.O	7	*73.9*	*0.9*			*71.2*	*2.9*			*76.5*	*2.5*			*82.8*	*11.3*		
		C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@H]1C(=O)CO	8	*40.3*	*4.8*			*42.8*	*2.5*			*55.9*	*3.0*			*45.3*	*9.4*		
	2H-INDOL-2-ONE, 1,3-DIHYDRO-1-PHENYL-3,3-BIS(4-PYRIDINYLMETHYL)-[CAS]	O=C1N(c2ccccc2C1(Cc3ccncc3)Cc4ccncc4)c5ccccc5.O.Cl	9	*37.0*	*2.2*			*36.9*	*1.7*			*52.3*	*1.1*			*34.5*	*8.1*		
	CHLORDIAZEPOXIDE	CNC1=Nc2ccc(Cl)cc2C(=[N+]([O-])C1)c3ccccc3	10	*72.9*	*5.7*			*81.8*	*2.6*			*78.8*	*7.3*			*90.0*	*10.8*		
		CN1CCC(=C2c3ccccc3C=Cc4ccccc24)CC1.Cl	11	*69.9*	*11.1*			*89.6*	*0.6*			*68.2*	*6.2*			*76.1*	*4.8*		

C	GOSERELIN ACETATE	CC(C)CC(NC(=O)C(COC(C)(C)C)NC(=O)C(Cc1ccc(O)cc1)NC(=O)C(CO)NC(=O)C(Cc2c[nH]c3ccccc23)NC(=O)C(Cc4c[nH]cn4)NC(=O)C5CCC(=O)N5)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N6CCCC6C(=O)NNC(=O)N.CC(=O)O	2	67.9	2.3			65.3	0.4			94.7	2.6			69.5	8.0		
	PALONOSETRON HYDROCHLORIDE	O=C1N(C[C@H]2CCCc3cccc1c23)[C@@H]4CN5CCC4CC5.Cl	3	10.2	6.0			2.6	0.2			3.8	1.0			18.6	11.4		
	REICHSTEINS SUBSTANCE S	CC12CCC3C(CCC4=CC(=O)CCC34C)C2CCC1(O)C(=O)CO	4	48.5	3.2			44.1	0.7			54.7	1.4			44.9	7.3		
	XANTHINOL NICOTINATE	CN(CCO)CC(O)Cn1cnc2n(C)c(=O)n(C)c(=O)c12.OC(=O)c1cccnc1	5	81.2	0.1			71.4	1.1			84.3	3.0			74.2	7.3		
		C(c1ccccc1)n2ccnc2	6	41.6	0.6			41.4	0.4			35.4	0.3			46.3	5.1		
		[O-][N+](=O)c1cccc2c[nH]nc12	7	101.7	3.1			113.2	7.3			99.3	1.4			127.6	11.8		
	DEXCHLORPHENIRAMINE MALEATE	CN(C)CC[C@@H](c1ccc(Cl)cc1)c2ccccn2.OC(=O)/C=C\C(=O)O	8	70.0	1.0			59.5	5.8			65.7	2.1			77.4	6.8		
	BECLOMETHASONE	CC1CC2C3CCC4=CC(=O)C=CC4(C)[C@@]3(Cl)C(O)CC2(C)C1(O)C(=O)CO	9	57.8	4.2			62.1	0.0			70.3	5.0			58.6	7.6		
	CEFIXIME TRIHYDRATE	Nc1nc(cs1)C(=NOCC(=O)O)C(=O)N[C@H]2[C@H]3SCC(=C(N3C2=O)C(=O)O)C=C.O	10	105.2	2.9			100.7	0.9			100.7	4.1			128.8	17.2		
	HOMOHARRINGTONINE	COC(=O)C[C@](O)(CCCC(C)(C)O)C(=O)O[C@H]1[C@H]2c3cc4OCOc4cc3CCN5CCC[C@]25C=C1OC	11	89.0	0.5			101.7	2.4			99.9	2.0			96.7	18.8		
D	SECOISOLARICIRESINOL	COc1cc(C[C@@H](CO)[C@H](CO)Cc2ccc(O)c(OC)c2)ccc1O	2	72.5	0.7			64.5	1.3			81.1	0.1			81.5	6.9		
	NAPROXEN SODIUM	COc1ccc2cc(ccc2c1)[C@H](C)C(=O)[O-].[Na+]	3	96.5	6.3			85.3	0.1			98.2	0.1			107.4	8.9		
	3-PYRIDINEMETHANOL	OCc1cccnc1	4	92.3	2.8			103.5	1.4			114.0	2.0			107.8	3.8		
	SYNEPHRINE	CNCC(O)c1ccc(O)cc1	5	97.4	3.7			88.4	2.5			97.0	2.5			105.2	16.7		
	DULOXETINE HYDROCHLORIDE	CNCC[C@H](Oc1cccc2ccccc12)c3cccs3.Cl	6	80.3	4.2			76.3	0.1			88.3	12.0			74.6	1.0		
		COc1ccc2[nH]cc(CCN)c2c1	7	57.4	4.4			5.6	2.8			62.0	3.4			65.6	17.4		
	GUANIDINE	CCC(C)(C)NC(=NC#N)Nc1cccnc1	8	97.5	2.6			95.0	2.6			101.5	1.0			106.6	9.8		
	73590-58-6 (OMEPRAZOLE)	COc1ccc2[nH]c(nc2c1)S(=O)Cc3ncc(C)c(OC)c3C	9	38.5	2.2	19.8	2.9	49.5	1.9	17.2	2.7	45.1	3.0	23.5	2.5	52.1	4.9	16.1	1.1

		Nc1nc(cs1)C(=NO)C(=O)N[C@H]2[C@H]3SCC(=C(N3C2=O)C(=O)O)C=C	10	111.0	9.5			102.3	0.7			121.2	3.9			140.4	12.5		
	50-22-6	C[C@@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]2CC[C@@H]1C(=O)CO	11	53.6	4.8			52.3	2.4			59.9	0.0			55.2	16.5		
E	RALTITREXED	CN(Cc1ccc2nc(C)nc(O)c2c1)c3ccc(s3)C(=O)N[C@@H](CCC(=O)O)C(=O)O	2	49.9	1.1			43.0	0.1			61.1	3.1			52.3	5.4		
		CN1CCCCC1C(=O)Nc2c(C)cccc2C.Cl	3	83.2	6.0			65.8	2.4			81.5	2.1			79.4	9.6		
	HALOPERIDOL	OC1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c3ccc(Cl)cc3.Cl	4	46.2	5.3			47.2	2.6			47.0	3.9			58.8	4.3		
	501-36-0	Oc1ccc(/C=C/c2cc(O)cc(O)c2)cc1	5	88.9	13.2			57.6	1.5			80.2	2.0			96.3	21.1		
	VARDENAFIL CITRATE	CCCc1nc(C)c2c(O)nc(nn12)c3cc(ccc3OCC)S(=O)(=O)N4CCN(CC)CC4.OC(=O)CC(O)(CC(=O)O)C(=O)O	6	74.0	7.3			54.1	0.2			43.0	9.6			44.7	8.3		
	92-84-2	N1c2ccccc2Sc3ccccc13	7	93.1	9.5			80.6	1.3			91.0	3.9			129.4	27.3		
	L-694,247	CS(=O)(=O)Nc1ccc(Cc2noc(n2)c3ccc4[nH]cc(CCN)c4c3)cc1.O	8	-0.4	0.5			-2.0	1.9			-0.3	0.0			20.6	13.9		
	DOLASETRON MESYLATE	O=C(O[C@H]1C[C@H]2C[C@H]3C[C@@H](C1)N2CC3=O)c4c[nH]c5ccccc45.CS(=O)(=O)O	9	22.0	4.7			49.5	0.7			37.1	7.1			22.4	2.7		
	LOFEXIDINE HYDROCHLORIDE	CC(Oc1c(Cl)cccc1Cl)C2=NCCN2.Cl	10	6.7	2.0			4.0	0.3			13.3	3.4			9.3	0.7		
	VECURONIUM BROMIDE	CC(=O)O[C@H]1[C@H](C[C@H]2[C@@H]3CC[C@H]4C[C@H](OC(=O)C)[C@H](C[C@]4(C)[C@H]3CC[C@]12C)N5CCCCC5)[N+]6(C)CCCCC6.[Br-]	11	15.0	8.1			25.9	2.3			32.2	1.1			0.7	0.0		
F	DOXAPRAM HYDROCHLORIDE	CCN1CC(CCN2CCOCC2)C(C1=O)(c3ccccc3)c4ccccc4.Cl	2	74.1	4.4			49.7	0.7			64.7	2.7			55.9	5.3		
	3-[3,5-DIBROMO-4-HYDROXYBENZOYL]-2-ETHYLBENZOFURAN	CCc1oc2ccccc2c1C(=O)c3cc(Br)c(O)c(Br)c3	3	71.0	3.6			59.7	0.5			68.5	1.5			70.9	3.3		
	STIRIPENTOL	CC(C)(C)C(O)/C=C/c1ccc2OCOc2c1	4	83.9	6.6	201	28.7	131.2	0.3	194	79.5	97.5	4.1	331	84.3	120.0	15.8	170	49.8
	118-71-8	Cc1occc(=O)c1O	5	102.1	6.3			82.2	1.6			110.7	1.0			130.0	29.8		
	ROPIVACAINE HYDROCHLORIDE	CCCN1CCCC[C@H]1C(=O)Nc2c(C)cccc2C.Cl	6	94.6	4.3			48.6	0.2			100.3	1.0			113.4	19.4		

		Nc1nc(Cl)nc2n(cnc12)[C@H]3C[C@H](O)[C@@H](CO)O3	7	89.2	8.9			85.5	1.4			105.0	6.3			99.5	8.3		
	AM-251	Cc1c(nn(c1c2ccc(I)cc2)c3ccc(Cl)cc3Cl)C(=O)NN4CCCCC4	8	96.7	0.4			99.5	0.3			108.3	2.6			112.2	6.1		
	ZOLMITRIPTAN	CN(C)CCc1c[nH]c2ccc(C[C@H]3COC(=O)N3)cc12	9	44.9	1.8			-20.3	1.9			42.2	1.0			37.0	6.6		
	BALSALAZIDE	OC(=O)CCNC(=O)c1ccc(N=Nc2ccc(O)c(c2)C(=O)O)cc1	10	109.3	10.0			84.6	3.0			113.1	4.7			144.9	28.5		
	TIBOLONE	C[C@@H]1CC2=C(CCC(=O)C2)[C@H]3CC[C@@]4(C)[C@@H](CC[C@@]4(O)C#C)[C@H]13	11	60.8	3.5			54.7	0.1			56.2	3.5			59.8	13.3		
G	RU 24969	COc1ccc2[nH]cc(C3=CCNCC3)c2c1.OC(=O)CCC(=O)O	2	17.5	0.7			10.2	2.8			23.2	0.6			21.1	5.4		
		COCCO/C(=C\1/C(C(=C(C)N=C1C)C(=O)OC(C)C)c2cccc(c2)[N+](=O)[O-])/O	3	38.0	10.3			40.7	2.3			58.2	12.1			39.6	1.9		
	FLUPERLAPINE	CN1CCN(CC1)C2=Nc3cc(F)ccc3Cc4ccccc24	4	60.5	4.2	37.1	5.7	60.8	3.2	53.4	14.5	66.9	2.1	41.2	6.1	66.2	0.9	32.6	4.9
		Nc1ccc2c[nH]nc2c1	5	100.8	3.8			87.0	0.9			120.7	0.2			106.6	3.0		
	ANASTROZOLE	CC(C)(C#N)c1cc(Cn2cncn2)cc(c1)C(C)(C)C#N	6	90.6	4.3			74.0	2.0			97.9	2.8			85.1	2.4		
	GRANISETRONÂ HYDROCHLORIDE	CN1[C@H]2CCC[C@@H]1C[C@@H](C2)NC(=O)c3nn(C)c4ccccc34.Cl	7	14.7	1.5			8.4	1.3			21.3	3.1			37.8	21.8		
	HTMT	CC(CCCCC(=O)Nc1ccc(cc1)C(F)(F)F)NCCc2c[nH]cn2.OC(=O)/C=C\C(=O)O	8	5.7	7.7			6.7	3.3			4.9	1.5			9.8	2.2		
	TREMULACIN	OC[C@H]1O[C@@H](Oc2ccccc2COC(=O)C3(O)C=CCCC3=O)[C@H](OC(=O)c4ccccc4)[C@@H](O)[C@@H]1O	9	85.2	5.0			102.8	0.8			102.7	2.1			90.5	9.3		
	OLOPATADINE HYDROCHLORIDE	CN(C)CC/C=C\1/c2ccccc2COc3ccc(CC(=O)O)cc13.Cl	10	100.7	1.4			81.2	1.8			124.2	0.4			107.0	5.8		
	98-92-0	NC(=O)c1cccnc1	11	106.8	5.1			96.8	2.2			122.9	6.2			128.7	25.4		
H	BRUCINE	COc1cc2N3[C@H]4[C@H]5[C@H]6C[C@@H]7N(CC[C@@]74c2cc1OC)CC6=CCO[C@H]5CC3=O	2	40.8	1.3			40.7	1.0			65.0	4.3			40.2	3.1		
		CN(C)[C@H]1C2CC3C(=C(O)[C@]2(O)C(=C(C(=O)NCN4CCCC4)C1=O)O)C(=O)c5c(O)cccc5[C@@]3(C)O	3	105.6	7.8			100.4	1.7			51.6	5.5			84.0	8.6		
		CC[N+](C)(C)CCOC(=O)C(O)(C1CCCCC1)c2ccccc2.[Br-]	4	52.8	1.4			24.2	1.1			77.1	1.8			55.8	8.1		

	ENROFLOXACIN	CCN1CCN(CC1)c2cc3n(cc(C(=O)O)c(=O)c3cc2F)C4CC4	5	58.1	2.8			72.7	1.3			77.0	4.0			45.8	3.2		
	KETOTIFEN FUMARATE	CN1CCC(=C2c3ccsc3C(=O)Cc4ccccc24)CC1.OC(=O)/C=C/C(=O)O	6	30.3	3.5	22.3	3.1	31.3	0.1	24.3	2.6	31.9	5.7	27.0	1.7	26.3	2.4	12.7	1.3
	RIMCAZOLE	C[C@H]1CN(CCCn2c3ccccc3c4ccccc24)C[C@@H](C)N1.O.Cl	7	29.5	3.7			25.5	1.0			31.7	8.4			23.2	0.8		
	BENZO[A]PHENANTHRIDINE-10,11-DIOL, 5,6,6A,7,8,12B-HEXAHYDRO-, TRANS-[CAS]	Oc1cc2CC[C@H]3NCc4ccccc4[C@@H]3c2cc1O.O.Cl	8	15.8	7.2			5.3	1.1			10.9	3.1			4.6	1.0		
	DACTINOMYCIN	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)c2ccc(C)c3oc4c(C)c(=O)c(N)c(C(=O)N[C@H]5[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]6CCCN6C(=O)[C@H](NC5=O)C(C)C)c4nc23)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C	9	85.6	2.7			97.9	0.2			30.7	26.5			84.3	6.8		
	ITAVASTATIN CA	O[C@H](C[C@H](O)/C=C/c1c(nc2ccccc2c1c3ccc(F)cc3)C4CC4)CC(=O)O[Ca]OC(=O)C[C@H](O)C[C@H](O)/C=C/c5c(nc6ccccc6c5c7ccc(F)cc7)C8CC8	10	94.0	1.5			88.5	1.9			105.3	4.3			64.3	1.9		
		O=C(CCNNC(=O)c1ccncc1)NCc2ccccc2	11	104.8	4.8			108.6	2.0			115.2	0.0			106.0	9.1		
	PLATE 4																		
A		Nc1nc(Cl)nc2n(cnc12)[C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O	2	95.2	0.3			100.6	2.1			112.6	0.1			97.1	3.6		
	ALTANSERIN	Fc1ccc(cc1)C(=O)C2CCN(CCn3c(=O)c4ccccc4[nH]c3=S)CC2.O.Cl	3	36.8	7.2			40.9	6.9			59.5	3.2			42.5	5.2		
		CCO/C(=C\1/C(C(=C(C)N=C1C)C(=O)OC)c2cccc(c2)[N+](=O)[O-])/O	4	52.6	21.6			45.9	23.5			63.8	27.3			42.5	23.9		
	RUTIN	C[C@@H]1O[C@@H](OC[C@H]2O[C@@H](Oc3c(oc4cc(O)cc(O)c4c3=O)c5ccc(O)c(O)c5)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	5	87.0	3.9			79.7	2.7			102.2	2.4			94.6	0.3		

	RITONAVIR	CC(C)[C@H](NC(=O)N(C)Cc1csc(n1)C(C)C)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	6	*10.9*	*0.6*			*19.5*	*2.5*			*7.2*	*8.5*			*12.1*	*16.0*		
		COc1cc(OC)cc(/C=C/c2ccc(O)cc2)c1	7	*124.0*	*11.7*			*93.2*	*3.1*			*102.9*	*0.3*			*127.2*	*7.3*		
	TICLOPIDINE HYDROCHLORIDE	Clc1ccccc1CN2CCc3sccc3C2.Cl	8	*84.6*	*2.9*	*678*	*98.3*	*96.3*	*4.4*	*444*	*67.3*	*79.2*	*13.6*	*692*	*110*	*72.0*	*25.7*	*442*	*56.1*
	PHYSOSTIGMINE	CNC(=O)Oc1ccc2N(C)C3N(C)CC[C@@]3(C)c2c1.OS(=O)(=O)O	9	*64.5*	*6.8*			*69.6*	*3.5*			*59.2*	*4.4*			*80.1*	*3.4*		
	RIZATRIPTAN BENZOATE	CN(C)CCc1c[nH]c2ccc(Cn3cncn3)cc12.OC(=O)c1ccccc1	10	*24.2*	*2.3*			*32.9*	*3.0*			*39.1*	*0.1*			*30.0*	*0.4*		
	ITOPRIDE HCL	COc1ccc(cc1OC)C(=O)NCc2ccc(OCCN(C)C)cc2.Cl	11	*24.6*	*1.2*			*30.8*	*3.9*			*36.0*	*1.7*			*17.3*	*3.9*		
B		Cc1ncc([N+](=O)[O-])n1CC(O)CCl	2	*90.3*	*1.0*			*97.3*	*4.4*			*102.9*	*1.1*			*99.5*	*1.3*		
	ACETAMIDE, 2-AMINO-N-(1-METHYL-1,2-DIPHENYLETHYL)-, (+/-)- [CAS]	CC(Cc1ccccc1)(NC(=O)CN)c2ccccc2.Cl	3	*83.9*	*2.1*			*78.6*	*4.0*			*92.8*	*1.1*			*83.7*	*1.0*		
	SAQUINAVIR MESYLATE	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4.CS(=O)(=O)O	4	*9.3*	*3.1*			*11.5*	*7.6*			*14.2*	*2.6*			*12.0*	*2.8*		
	PENCICLOVIR	Nc1nc(O)c2ncn(CCC(CO)CO)c2n1	5	*94.5*	*0.9*			*96.4*	*4.3*			*102.3*	*0.7*			*95.6*	*1.3*		
	VINORELBINEÂ TARTRATE	CCC1=C[C@H]2CN(C1)Cc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@@H]7[C@@]86CCN9CC=C[C@](CC)([C@H]98)[C@@H](OC(=O)C)[C@]7(O)C(=O)OC.OC(C(O)C(=O)O)C(=O)O	6	*65.0*	*3.3*			*72.1*	*2.9*			*93.4*	*0.3*			*70.9*	*3.6*		
	ROXATIDINE ACETATEÂ HYDROCHLORIDE	CC(=O)OCC(=O)NCCCOc1cccc(CN2CCCCC2)c1.Cl	7	*24.0*	*2.2*			*29.5*	*6.0*			*41.4*	*1.8*			*27.0*	*1.4*		
	SODIUMÂ LOXOPROFEN	CC(C(=O)[O-])c1ccc(CC2CCCC2=O)cc1.[Na+]	8	*99.3*	*2.4*			*102.1*	*6.0*			*103.8*	*3.4*			*94.0*	*2.1*		

	1H-INDOLE-2-PROPANOIC ACID, 1-[(4-CHLOROPHENYL)METHYL]-3-[(1,1-DIMETHYLETHYL)THIO]-ALPHA,ALPHA-DIMETHYL-5-(1-METHYLETHYL)-[CAS]	CC(C)c1ccc2n(Cc3ccc(Cl)cc3)c(CC(C)(C)C(=O)O)c(SC(C)(C)C)c2c1	9	75.8	6.3			70.3	10.4			90.7	3.6			77.5	1.9		
	RIFAPENTINE	CO[C@H]1C=CO[C@@]2(C)Oc3c(C2=O)c4c(O)c(C=NN5CCN(CC5)C6CCCC6)c(NC(=O)C(=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)C)c(O)c4c(O)c3C	10	64.7	2.1			73.4	2.0			80.6	2.6			69.9	3.3		
	RIFAXIMIN	CO[C@H]1C=CO[C@@]2(C)Oc3c(C2=O)c4c5nc6cc(C)ccn6c5c(NC(=O)C(=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)C)c(O)c4c(O)c3C	11	82.2	2.5			78.3	3.1			82.8	5.4			84.3	6.2		
C	1,1-DIMETHYL-4-PHENYLPIPERAZINIUM IODIDE	C[N+]1(C)CCN(CC1)c2ccccc2.[I-]	2	81.8	1.7			84.5	0.3			94.1	3.0			81.6	2.2		
		CC(C)NCC(O)COc1ccc(CCOCC2CC2)cc1.Cl	3	32.7	3.7			38.7	1.5			34.8	3.3			37.2	2.1		
	60628-96-8	c1cn(cn1)C(c2ccccc2)c3ccc(cc3)c4ccccc4	4	85.9	8.3			85.3	9.5			85.6	19.1			85.6	11.2		
	CALCITRIOL	C[C@H](CCCC(C)(C)O)[C@H]1CC[C@H]2/C(=C/C=C\3/C[C@@H](O)C[C@H](O)C3=C)/CCC[C@]12C	5	44.6	2.2			45.6	7.0			63.9	0.0			44.9	3.4		
	LINEZOLID	CC(=O)NC[C@H]1CN(C(=O)O1)c2ccc(N3CCOCC3)c(F)c2	6	86.4	0.9			86.4	0.2			95.0	1.9			84.9	2.7		
	DEXBROMPHENIRAMINE MALEATE	CN(C)CC[C@@H](c1ccc(Br)cc1)c2ccccn2.OC(=O)/C=C\C(=O)O	7	64.7	1.1			65.2	1.6			62.0	6.0			56.8	0.8		
	ZAFIRLUKAST	COc1cc(ccc1Cc2cn(C)c3ccc(NC(=O)OC4CCCC4)cc23)C(=O)NS(=O)(=O)c5ccccc5C	8	23.1	2.4			20.3	6.4			49.3	0.2			18.8	6.7		
	562-10-7	CN(C)CCOC(C)(c1ccccc1)c2ccccn2.OC(=O)CCC(=O)O	9	40.1	3.2			44.5	3.2			53.0	1.2			43.2	1.4		
	LOTEPREDNOL ETABONATE	CCOC(=O)O[C@@]1(CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C)C(=O)OCCl	10	75.9	3.3			73.7	0.9			86.5	0.9			74.5	3.9		

	MONTELUKAST SODIUM	CC(C)(O)c1ccccc1CC[C@@H](SCC2(CC(=O)[O-])CC2)c3cccc(/C=C/c4ccc5ccc(Cl)cc5n4)c3.[Na+]	11	59.9	7.6			62.3	4.6			79.6	1.7			67.2	7.9		
D		Cc1nc2ccccn2c(=O)c1CCN3CCC(CC3)C(=O)c4ccc(F)cc4	2	4.2	0.8			16.3	4.4			18.1	2.7			15.5	2.4		
		Oc1[nH]c2ccccc2c1C3=Nc4ccccc4C3=O	3	92.4	0.7			91.8	3.1			103.2	0.6			90.6	0.0		
	SUMATRIPTAN SUCCINATE	CNS(=O)(=O)Cc1ccc2[nH]cc(CCN(C)C)c2c1.OC(=O)CCC(=O)O	4	41.7	1.8			48.1	1.4			57.9	4.7			38.2	0.8		
	DIPHENOXYLATE	CCOC(=O)C1(CCN(CCC(C#N)(c2ccccc2)c3ccccc3)CC1)c4ccccc4.Cl	5	99.9	0.4			111.9	20.5			107.0	1.0			95.2	4.9		
	LOMERIZINE DIHCL	COc1ccc(CN2CCN(CC2)C(c3ccc(F)cc3)c4ccc(F)cc4)c(OC)c1OC.Cl	6	87.1	7.5			81.8	8.6			96.5	4.9			103.7	0.4		
	ANAGRELIDE HYDROCHLORIDE	Clc1ccc2N=C3NC(=O)CN3Cc2c1Cl.Cl	7	67.1	8.9			71.4	4.1			76.9	1.4			70.1	11.6		
	TERBINAFINE HYDROCHLORIDE	CN(C/C=C/C#CC(C)(C)C)Cc1ccccc2ccccc12.Cl	8	93.3	0.2	####	###	93.3	3.7			104.3	0.4			95.2	0.4		
	MILNACIPRAN	CCN(CC)C(=O)[C@@]1(C[C@@H]1CN)c2ccccc2.Cl	9	69.4	0.6			72.9	0.4			78.3	1.3			66.7	3.4		
	ENALAPRILAT	C[C@H](N[C@@H](CCc1ccccc1)C(=O)O)C(=O)N2CCC[C@H]2C(=O)O	10	100.5	3.6			93.1	1.0			104.8	0.3			96.8	2.5		
	2',3'-DIDEOXYCYTIDINE	Nc1ccn([C@H]2CC[C@@H](CO)O2)c(=O)n1	11	101.8	10.1			88.4	0.4			103.0	1.2			92.8	2.7		
E	72-33-3	COc1ccc2[C@H]3CC[C@@]4(C)[C@@H](CC[C@@]4(O)C#C)[C@@H]3CCc2c1	2	95.4	1.5			94.8	3.6			105.6	1.4			96.8	1.0		
	AZASETRON	CN1C(=O)COc2c(cc(Cl)cc12)C(=O)NC3CN4CCC3CC4.Cl	3	3.8	1.4			14.1	2.5			6.0	0.1			8.8	0.4		
	EXEMESTANE	C[C@@]12CC[C@H]3[C@@H](CC(=C)C4=CC(=O)C=C[C@]34C)[C@@H]2CCC1=O	4	8.8	0.6			19.3	3.6			13.4	0.6			-1.7	2.1		
	FELBAMATE	NC(=O)OCC(COC(=O)N)c1ccccc1.O	5	92.4	4.6			92.4	1.1			103.2	1.4			89.7	0.2		
	EFAVIRENZ	FC(F)(F)[C@]1(OC(=O)Nc2ccc(Cl)cc21)C#CC3CC3	6	87.1	6.8			82.1	12.0			100.7	1.2			86.0	12.0		
	TEGASEROD MALEATE	CCCCCN=C(N)NN=Cc1c[nH]c2ccc(OC)cc12.OC(=O)/C=C\C(=O)O	7	-0.7	10.8			9.7	2.1			0.5	2.4			21.7	8.5		
	ISRADIPINE	CO/C(=C\1/C(C(=C(C)N=C1C)C(=O)OC(C)C)c2cccc3nonc23)/O	8	43.8	16.5			45.9	10.1			61.0	9.5			37.0	8.1		
	5-FLUORO-2-PYRIMIDONE	Oc1ncc(F)cn1	9	103.3	3.1	1444	315	100.7	8.1	1587	384	103.9	1.4			95.3	2.5	5138	2114

	DONEPEZIL	COc1cc2CC(CC3CCN(Cc4ccccc4)CC3)C(=O)c2cc1OC.Cl	**10**	***4.3***	***1.0***	***1.2***	***0.2***	***10.3***	***2.3***	***1.5***	***0.2***	***3.5***	***1.0***	***1.3***	***0.1***	***7.6***	***0.2***	***0.78***	***0.1***
	1H-IMIDAZOL-2-AMINE, N-(2,6-DICHLOROPHENYL)-4,5-DIHYDRO- [CAS]	Clc1cccc(Cl)c1NC2=NCCN2.Cl	**11**	***37.1***	***7.9***			***35.0***	***9.2***			***38.1***	***2.1***			***33.6***	***2.8***		
F	BENACTYZINE HYDROCHLORIDE	CCN(CC)CCOC(=O)C(O)(c1ccccc1)c2ccccc2.Cl	**2**	***29.9***	***5.9***			***34.2***	***8.0***			***58.9***	***2.5***			***38.5***	***3.6***		
	GR 89696	COC(=O)N1CCN(C(CN2CCCC2)C1)C(=O)Cc3ccc(Cl)c(Cl)c3.OC(=O)/C=C/C(=O)O	**3**	***51.5***	***4.0***			***57.7***	***4.2***			***71.2***	***0.1***			***51.9***	***2.9***		
	NITAZOXANIDE	CC(=O)Oc1ccccc1C(=O)Nc2ncc(s2)[N+](=O)[O-]	**4**	***66.3***	***0.6***			***104.9***	***20.9***			***78.4***	***1.1***			***55.1***	***9.0***		
		Oc1nc2ccccc2n1C3=CCN(CCCC(=O)c4ccc(F)cc4)CC3	**5**	***10.3***	***2.8***			***18.2***	***3.9***			***16.8***	***6.2***			***12.5***	***3.0***		
	IRBESARTAN	CCCCC1=NC2(CCCC2)C(=O)N1Cc3ccc(cc3)c4ccccc4c5nn[nH]n5	**6**	***87.6***	***1.1***			***84.4***	***4.4***			***92.7***	***0.0***			***90.3***	***1.2***		
	MILRINONE	Cc1nc(O)c(C#N)cc1c2ccncc2	**7**	***74.5***	***0.2***			***79.9***	***6.5***			***74.3***	***0.1***			***71.3***	***4.1***		
	VALSARTAN	CCCCC(=O)N(Cc1ccc(cc1)c2ccccc2c3nn[nH]n3)[C@@H](C(C)C)C(=O)O	**8**	***94.9***	***3.0***			***87.8***	***0.7***			***106.4***	***2.7***			***96.6***	***2.4***		
	CHLORPHENIRAMINE	CN(C)CCC(c1ccc(Cl)cc1)c2ccccn2.OC(=O)/C=C\C(=O)O	**9**	***52.3***	***13.3***			***67.1***	***12.4***			***69.1***	***3.5***			***59.3***	***1.7***		
		CN1C(=O)CN=C(c2ccccc2)c3cc(ccc13)[N+](=O)[O-]	**10**	***65.0***	***5.8***			***64.6***	***1.8***			***72.1***	***2.4***			***68.6***	***3.8***		
	6H-PYRIDO[2,3-B][1,4]BENZODIAZEPIN-6-ONE, 11-[[2-[(DIETHYLAMINO)METHYL]-1-PIPERIDINYL]ACETYL]-5,11-DIHYDRO- [CAS]	CCN(CC)CC1CCCCN1CC(=O)N2c3ccccc3C(=O)Nc4cccnc24	**11**	***58.7***	***0.0***			***68.5***	***3.7***			***81.2***	***3.4***			***49.1***	***7.0***		
G		NCCc1ccccn1	**2**	***82.1***	***2.8***			***89.0***	***6.4***			***89.1***	***2.2***			***80.8***	***1.4***		
	DELTA1-HYDROCORTISONE 21-HEMISUCCINATE SODIUM SALT	C[C@@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]2CC[C@]1(O)C(=O)COC(=O)CCC(=O)[O-].[Na+]	**3**	***69.7***	***4.5***	***66.7***	***7.4***	***75.9***	***3.5***	***57.3***	***11.7***	***87.2***	***3.3***	####	***18.2***	***69.3***	***2.9***	***64.1***	***9.2***
		CN1C(=O)CN=C(c2ccccc2)c3cc(Cl)ccc13	**4**	***46.3***	***4.3***			***50.1***	***2.2***			***59.0***	***2.2***			***41.3***	***1.1***		
		CC(=O)CCCCn1c(=O)n(C)c2ncn(C)c2c1=O	**5**	***76.7***	***1.6***			***85.2***	***7.7***			***80.4***	***5.8***			***66.2***	***1.3***		
		CCOc1cc(CC(=O)N[C@@H](CC(C)C)c2ccccc2N3CCCCC3)ccc1C(=O)O	**6**	***85.4***	***4.5***			***94.3***	***13.1***			***98.3***	***0.5***			***86.5***	***5.2***		
	LEVOCETIRIZINE	OC(=O)COCCN1CCN(CC1)[C@H](c2ccccc2)c3ccc(Cl)cc3	**7**	***81.6***	***2.6***			***85.3***	***0.5***			***83.2***	***0.8***			***75.5***	***7.1***		

	PIROXICAM	CN1C(=C(O)c2ccccc2S1(=O)=O)C(=O)Nc3ccccn3.O	8	98.5	6.6			71.0	22.1			102.4	0.4			87.8	12.3		
	DOFETILIDE	CN(CCOc1ccc(NS(=O)(=O)C)cc1)CCc2ccc(NS(=O)(=O)C)cc2	9	12.9	0.6			28.3	6.5			20.3	0.8			13.4	3.7		
		[O-][N+](=O)OCCNC(=O)c1cccnc1	10	79.0	7.1			85.5	2.0			93.4	4.5			66.7	11.2		
	3'-DEOXYDENOSINE	Nc1ncnc2n(cnc12)[C@@H]3O[C@H](CO)C[C@@H]3O.O	11	79.6	2.3			83.6	2.0			92.7	0.2			73.8	0.2		
H	79-43-6	OC(=O)C(Cl)Cl	2	105.2	4.8			99.3	4.7			112.8	0.4			101.2	0.3		
		CC1=NS(=O)(=O)c2cc(Cl)ccc2N1	3	80.3	11.0			74.0	12.1			96.6	4.7			80.7	14.9		
	QUETIAPINE HEMIFUMARATE	OCCOCCN1CCN(CC1)C2=Nc3ccccc3Sc4ccccc24.OC(=O)/C=C/C(=O)O	4	16.7	3.6			23.5	12.0			30.6	2.7			19.8	17.3		
	1H-IMIDAZOLE-5-CARBOXYLIC ACID, 1-(1-PHENYLETHYL)-, ETHYL ESTER, (R)- [CAS]	CCOC(=O)c1cncn1[C@H](C)c2ccccc2	5	70.2	8.0			88.2	25.2			79.9	0.5			76.4	11.8		
		CC[C@]1(O)CC[C@H]2[C@@H]3CCC4=CCCC[C@@H]4[C@H]3CC[C@@]21C	6	82.4	5.8			72.4	0.7			87.5	5.0			80.2	6.7		
	CITALOPRAM	CN(C)CCCC1(OCc2cc(C#N)ccc21)c3ccc(F)cc3.Br	7	53.1	4.1			56.5	2.3			67.7	0.1			54.9	0.8		
		C[N+]1(C)CCC(C1)OC(=O)C(O)(C2CCCC2)c3ccccc3.[Br-]	8	65.5	1.5			66.4	6.4			82.7	4.8			63.0	6.2		
	FORMOTEROL FUMARATE DIHYDRATE	COc1ccc(C[C@H](C)NC[C@@H](O)c2ccc(O)c(NC=O)c2)cc1.O.OC(=O)/C=C/C(=O)O	9	27.5	0.9			52.4	14.3			48.4	1.8			25.7	2.7		
		CCCc1nc2c(C)cc(cc2n1Cc3ccc(cc3)c4ccccc4C(=O)O)c5nc6ccccc6n5C	10	14.8	0.6			26.2	4.6			25.1	2.5			11.9	1.6		
	IFENPRODIL	CC(C(O)c1ccc(O)cc1)N2CCC(Cc3ccccc3)CC2.O.OC(C(O)C(=O)O)C(=O)O	11	35.2	2.0			45.3	1.8			42.7	1.8			43.2	4.2		
	PLATE 5																		
A	5-AMINO-2-HYDROXY-BENZOIC ACID	Nc1ccc(O)c(c1)C(=O)O	2	110.0	9.1			118.3	6.1			95.0	9.6			107.1	9.3		
	ZACOPRIDE	COc1cc(N)c(Cl)cc1C(=O)NC2CN3CCC2CC3.O.Cl	3	3.2	2.2			15.8	15.7			2.0	0.3			1.6	0.0		
	LOXAPINE	CN1CCN(CC1)C2=Nc3ccccc3Oc4ccc(Cl)cc24.OC(=O)CCC(=O)O	4	62.0	1.1			101.5	25.3			72.1	9.5			52.9	2.0		

	PANCURONIUM	CC(=O)OC1C(C[C@H]2C3CC[C@H]4C[C@H](OC(=O)C)C(CC4(C)[C@H]3CCC12C)[N+]5(C)CCCCC5)[N+]6(C)CCCCC6.[Br-]	5	88.1	5.2			111.4	5.0			90.9	7.3			101.7	16.3		
	PICROTIN - PICROTOXININ	CC(C)(O)[C@@H]1[C@H]2OC(=O)[C@@H]1[C@]3(O)C[C@H]4O[C@]45C(=O)O[C@H]2[C@@]53C.[C@]12([C@@]3(O1)[H])[C@](C)([C@H](OC2=O)[C@H](OC4=O)[C@H]([C@H]45)C(C)=C)[C@]5(C3)O	6	68.8	27.6			120.4	14.0			127.1	11.4			11.9	55.0		
	CLOTRIMAZOLE	Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4	7	85.6	15.6			122.3	19.2			98.3	7.0			90.5	7.0		
	CINANSERIN	CN(C)CCCSc1ccccc1NC(=O)/C=C/c2ccccc2.O.Cl	8	20.2	1.2			17.6	38.5			20.2	0.6			13.1	15.0		
	FLUVOXAMINE	COCCCCC(=NOCCN)c1ccc(cc1)C(F)(F)F.OC(=O)/C=C\C(=O)O	9	73.0	20.7			97.7	23.5			71.7	7.5			67.7	1.0		
	N,N'-DIACETYL-1,6-DIAMINOHEXANE	CC(=O)NCCCCCCNC(=O)C	10	105.1	3.9			125.3	7.0			104.3	9.2			95.1	4.6		
	PYRAZINECARBOXAMIDE, 3,5-DIAMINO-N-(AMINOIMINOMETHYL)-6-CHLORO- [CAS]	NC(=N)NC(=O)c1nc(Cl)c(N)nc1N.O.Cl	11	18.0	1.3			58.7	33.6			37.1	11.2			3.5	3.7		
B	PAROXETINE	Fc1ccc(cc1)[C@@H]2CCNC[C@H]2COc3ccc4OCOc4c3.OC(=O)/C=C\C(=O)O	2	69.4	11.2			71.7	0.7			47.6	11.7			64.1	7.7		
	SKF 83566	CN1CCc2cc(Br)c(O)cc2C(C1)c3ccccc3.Br	3	38.4	7.0			44.9	0.2			40.1	10.9			26.2	5.0		
	D-3-METHOXY-N-METHYLMORPHINAN HYDROBROMIDE	COc1ccc2C[C@H]3[C@H]4CCCC[C@@]4(CCN3C)c2c1.O.Br	4	18.6	2.7			30.1	3.7			22.4	7.2			15.7	0.6		
	443-48-1	Cc1ncc([N+](=O)[O-])n1CCO	5	95.3	2.2			114.3	16.2			101.2	10.2			117.7	9.6		
	TERAZOSIN	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4CCCO4.O.Cl	6	32.7	2.3			50.9	13.0			52.5	2.4			27.9	32.8		
	79794-75-5	CCOC(=O)N1CCC(=C2c3ccc(Cl)cc3CCc4cccnc24)CC1	7	16.6	8.5			14.3	32.2			35.8	13.4			14.4	4.6		
	CISAPRIDE	CO[C@H]1CN(CCCOc2ccc(F)cc2)CC[C@H]1NC(=O)c3cc(Cl)c(N)cc3OC.O	8	46.3	6.0			91.3	23.2			58.6	14.9			59.6	15.2		
	DOXEPIN	CN(C)CC/C=C\1/c2ccccc2COc3ccccc13.Cl	9	52.9	8.9			79.9	6.2			53.6	12.4			24.8	24.0		
	147-24-0	CN(C)CCOC(c1ccccc1)c2ccccc2.Cl	10	61.2	3.2			74.4	2.3			65.6	22.2			51.1	9.1		

	9-AMINO-1,2,3,4-TETRAHYDROACRIDINE HYDROCHLORIDE	Nc1c2CCCCc2nc3ccccc13.Cl	11	9.3	0.2			50.7	5.7			19.1	5.7			4.1	4.4		
C	LOBELINE HYDROCHLORIDE	CN1[C@H](C[C@H](O)c2ccccc2)CCC[C@@H]1CC(=O)c3ccccc3.Cl	2	41.0	5.0			50.8	4.4			42.4	8.8			40.0	1.7		
	AM 404	CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)Nc1ccc(O)cc1	3	76.9	9.0			70.7	13.0			75.8	12.1			61.2	5.5		
	DULOXETINE	CNCC[C@H](Oc1cccc2ccccc12)c3cccs3	4	69.8	6.4			80.2	3.4			72.1	12.0			81.5	5.0		
	BENZENEACETIC ACID, ALPHA-(HYDROXYMETHYL)-, 9-METHYL-3-OXA-9-AZATRICYCLO[3.3.1.02,4]NON-7-YL ESTER, [7(S)-(1ALPHA,2 ,4 ,5ALPHA,7)]- [CAS]	CN1[C@H]2CC(C[C@@H]1[C@H]3O[C@H]32)OC(=O)[C@H](CO)c4ccccc4.O.Br	5	58.6	2.8			77.3	0.2			82.1	8.5			84.2	11.4		
	DIPHENYLCYCLOPROPENONE	O=c1c(c1c2ccccc2)c3ccccc3	6	43.1	26.9			76.5	10.7			64.8	17.2			30.6	8.2		
	PHENELZINE SULFATE	NNCCc1ccccc1.OS(=O)(=O)O	7	82.4	10.7			87.9	17.2			97.7	6.7			71.2	5.9		
	INDATRALINE	CN[C@@H]1C[C@H](c2ccccc12)c3ccc(Cl)c(Cl)c3.Cl	8	26.6	10.2			67.3	0.4			44.8	9.4			32.1	23.3		
		CN1CCN(CCCN2c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1.Cl	9	23.5	0.9			36.0	8.3			26.8	3.5			11.3	6.5		
	GALANTHAMINE	COc1ccc2CN(C)CC[C@]34C=C[C@H](O)C[C@@H]4Oc1c23.Br	10	64.0	1.7			69.6	0.1			72.7	19.0			67.8	12.0		
	ETHYNYLESTRADIOL	C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]2CC[C@@]1(O)C#C	11	80.2	1.7			80.7	19.7			74.5	4.8			75.3	8.7		
D	L-ORNITHINE, N5-[IMINO(METHYLAMINO)METHYL]-[CAS]	CN=C(N)NCCC[C@H](N)C(=O)O.CC(=O)O	2	90.8	1.9			94.6	8.3			88.1	9.2			102.8	0.0		
	NALBUPHINE	OC1CC[C@@]2(O)[C@H]3Cc4ccc(O)c5OC1[C@]2(CCN3CC6CCC6)c54.Cl	3	95.4	4.2			91.2	14.0			82.2	23.0			66.8	26.1		
	GLYCINE, N-[2-[(ACETYLTHIO)METHYL]-1-OXO-3-PHENYLPROPYL]-,PHENYLMETHYL ESTER [CAS]	CC(=O)SCC(Cc1ccccc1)C(=O)NCC(=O)OCc2ccccc2	4	71.6	17.3			98.7	42.6			71.7	3.3			81.9	16.4		

	BENZENEACETONITRILE, ALPHA-[3-[[2-(3,4-DIMETHOXYPHENYL)ETHYL]METHYLAMINO]PROPYL]-3,4-DIMETHOXY-ALPHA-(1-METHYLETHYL)-, (R)- [CAS]	COc1ccc(CCN(C)CCCC(C#N)(C(C)C)c2ccc(OC)c(OC)c2)cc1OC.O.Cl	5	45.0	11.0			57.0	8.6			51.2	19.4			50.9	7.8		
	4-THIAZOLIDINECARBOXYLIC ACID, 2-OXO-, (R)- [CAS]	OC(=O)[C@@H]1CSC(=O)N1	6	90.8	6.2			97.5	14.3			102.1	5.8			109.9	21.4		
	RILUZOLE	Nc1nc2ccc(OC(F)(F)F)cc2s1.Cl	7	97.0	1.8			143.3	6.8			105.7	6.6			86.6	18.0		
	25332-39-2	Clc1cccc(c1)N2CCN(CCCn3nc4ccccn4c3=O)CC2.Cl	8	11.2	1.1			39.0	0.6			25.8	4.2			9.3	1.0		
	(+)-3-HYDROXY-N-METHYLMORPHINAN D-TARTRATE	CN1CC[C@]23CCCC[C@@H]3[C@@H]1Cc4ccc(O)cc42.OC(C(O)C(=O)O)C(=O)O	9	9.9	0.3			25.1	8.2			14.6	1.1			8.2	8.5		
	INDOMETHACIN	COc1ccc2n(C(=O)c3ccc(Cl)cc3)c(C)c(CC(=O)O)c2c1.O	10	82.7	2.8			75.7	1.0			73.7	21.0			79.6	6.0		
	2(1H)-PYRIMIDINONE, 4-AMINO-1-Y-D-ARABINOFURANOSYL- [CAS]	Nc1ccn([C@@H]2O[C@H](CO)[C@@H](O)[C@@H]2O)c(=O)n1	11	90.0	0.3			92.1	6.7			85.0	13.5			91.5	3.8		
E		OC(=O)C1CCn2c(ccc12)C(=O)c3ccccc3.NC(CO)(CO)CO	2	79.9	2.6			90.1	4.7			79.4	20.1			85.9	0.9		
	PILOCARPINE HYDROCHLORIDE	CC[C@H]1[C@@H](Cc2cncn2C)COC1=O.Cl	3	59.3	0.3			68.7	3.8			62.1	12.5			72.2	5.6		
	BENZENEACETIC ACID, 2-[(2,6-DICHLOROPHENYL)AMINO]-, MONOSODIUM SALT [CAS]	[Na]OC(=O)Cc1ccccc1Nc2c(Cl)cccc2Cl	4	96.2	7.3			102.6	23.5			83.7	14.7			75.6	18.9		
		C[C@H](Cc1ccccc1)N(C)CC#C.Cl	5	30.0	2.8			38.8	1.3			33.9	6.0			38.2	13.5		
	MESORIDAZINE	CN1CCCCC1CCN2c3ccccc3Sc4ccc(cc24)S(=O)C.OS(=O)(=O)c1ccccc1	6	14.9	3.2			26.0	5.9			21.2	6.0			14.8	3.6		
	NALTRINDOLE	Oc1ccc2CC3N(CC4CC4)CC[C@]5([C@H]6Oc1c25)[C@@]3(O)Cc7c6[nH]c8ccccc78.O.Cl	7	58.7	2.8			70.8	27.6			88.6	1.7			78.1	4.4		
	PRAZOSIN	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)c4ccco4.O.Cl	8	11.1	7.4			22.6	17.9			26.0	7.6			19.1	7.2		

	LY 171883	CCCc1c(O)c(ccc1OCCCCc2nn[nH]n2)C(=O)C	9	72.1	4.1			113.8	9.3			87.7	1.6			85.5	11.7		
	TETRAETHYLTHIURAM DISULFIDE	CCN(CC)C(=S)SSC(=S)N(CC)CC	10	90.0	0.2			92.6	9.9			76.2	23.2			87.8	9.0		
	L-GLUTAMIC ACID, N-[4-[[(2,4-DIAMINO-6-PTERIDINYL)METHYL]METHYLAMINO]BENZOYL]- [CAS]	CN(Cc1cnc2nc(N)nc(N)c2n1)c3ccc(cc3)C(=O)N[C@@H](CCC(=O)O)C(=O)O.O	11	82.5	3.5			82.3	11.9			74.4	26.2			64.5	17.1		
F	OXIRANECARBOXYLIC ACID, 2-[6-(4-CHLOROPHENOXY)HEXYL]-, ETHYL ESTER- [CAS]	CCOC(=O)C1(CCCCCCOc2ccc(Cl)cc2)CO1	2	86.3	0.8			84.0	13.3			72.8	14.8			102.3	4.6		
		CO/C(=C\1/C(C(=C(C)N=C1C)C(=O)OC)c2ccccc2[N+](=O)[O-])/O	3	69.6	4.3			73.2	7.1			60.5	18.5			77.4	3.6		
		CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	4	41.4	19.1			96.8	28.9			61.4	25.2			42.8	0.2		
	ZUCAPSAICIN	COc1cc(CNC(=O)CCCC/C=C\C(C)C)ccc1O	5	53.5	0.6			27.9	8.2			65.0	1.0			47.7	1.0		
	3(2H)-PYRIDAZINONE, 6-[4-(DIFLUOROMETHOXY)-3-METHOXYPHENYL]- [CAS]	COc1cc(ccc1OC(F)F)c2ccc(O)nn2	6	91.6	7.9			122.0	8.4			103.6	3.1			80.3	3.1		
	NORNICOTINE	C1CNC(C1)c2cccnc2	7	99.3	3.8			101	101			97.8	8.9			113.3	0.9		
	URAPIDIL HYDROCHLORIDE	COc1ccccc1N2CCN(CCCNc3cc(=O)n(C)c(=O)n3C)CC2.Cl	8	33.5	0.5			41.9	11.5			52.0	7.1			44.8	3.6		
	MAPROTILINE HYDROCHLORIDE	CNCCCC1(CCC2c3ccccc31)c4ccccc24.Cl	9	67.2	7.2			100.1	35.5			72.1	6.9			3.4	16.1		
	PIRIBEDIL	C(N1CCN(CC1)c2ncccn2)c3ccc4OCOc4c3.O.Cl	10	59.1	14.6			105.3	6.3			70.7	4.0			52.3	8.0		
	TFMPP	FC(F)(F)c1cccc(c1)N2CCNCC2.Cl	11	85.4	10.0			100.9	26.2			72.7	8.3			62.7	16.8		
G	EPIGALLOCATECHIN GALLATE	Oc1cc(O)c2C[C@@H](OC(=O)c3cc(O)c(O)c(O)c3)[C@H](Oc2c1)c4cc(O)c(O)c(O)c4	2	70.3	5.9			71.1	0.6			69.5	21.7			124.3	22.8		
	FLURBIPROFEN	CC(C(=O)O)c1ccc(c(F)c1)c2ccccc2	3	72.3	4.2			68.3	4.2			55.6	14.5			79.1	4.3		
	FAMOTIDINE	NC(=N)Nc1nc(CSCCC(=N)NS(=O)(=O)N)cs1	4	1.2	1.4	0.3	0.1	15.1	13.4	1.7	0.8	4.6	0.4	0.5	0.1	13.6	3.5	0.27	0.0
	SALBUTAMOL SULFATE	CC(C)(C)NCC(O)c1ccc(O)c(CO)c1.OS(=O)(=O)O	5	85.8	2.5			120.1	16.9			90.7	14.1			134.5	6.4		
	PROCHLORPERAZINE	CN1CCN(CCCN2c3ccccc3Sc4ccc(Cl)cc24)CC1.OC(=O)/C=C\C(=O)O	6	15.9	3.4	10.6	1.8	41.9	14.7	14.1	6.3	40.1	6.7	15.3	2.2	32.6	11.6	7.89	0.8

	BIFEMELANE	CNCCCCOc1ccccc1Cc2ccccc2.Cl	7	67.5	4.8			91.4	16.0			71.7	5.7			42.9	15.3		
	(-)-COTININE	CN1[C@@H](CCC1=O)c2cccnc2	8	96.5	5.5			111.0	31.2			94.2	17.2			94.8	47.7		
	PIZOTYLINE	CN1CCC(=C2c3ccsc3CCc4ccccc24)CC1.OC(=O)/C=C\C(=O)O	9	56.9	0.9			46.1	3.0			55.7	15.8			54.2	9.5		
		CC(=O)N1CCN(CC1)c2ccc(OC[C@H]3CO[C@@](Cn4ccnc4)(O3)c5ccc(Cl)cc5Cl)cc2	10	8.1	11.4			42.7	67.7			21.9	4.8			-19.2	41.5		
	PRAMIPEXOLE	CCCN[C@H]1CCc2nc(N)sc2C1	11	51.0	5.3			64.4	41.9			61.6	18.0			85.2	36.2		
H	RACLOPRIDE	CCN1CCC[C@H]1CNC(=O)c2c(O)c(Cl)cc(Cl)c2OC	2	75.6	5.8			53.8	8.6			75.2	5.9			106.4	20.9		
	3-HYDROXY-1,2-DIMETHYL-4(1H)-PYRIDONE	Cc1c(O)c(=O)ccn1C	3	103.7	0.9			111.8	40.0			108.5	7.9			141.2	27.6		
	SR 57227A	NC1CCN(CC1)c2cccc(Cl)n2.Cl	4	80.7	12.7			110.0	15.8			82.0	7.6			41.5	32.5		
	(+/-)-VESAMICOL HYDROCHLORIDE	O[C@@H]1CCCC[C@H]1N2CCC(CC2)c3ccccc3.Cl	5	66.5	3.1	49.8	8.9	92.2	3.0	74.6	20.0	86.5	7.2	83.8	23.0	121.5	6.8	39.3	7.0
	1H-CYCLOPENTA[B]QUINOLIN-9-AMINE, 2,3,5,6,7,8-HEXAHYDRO-, MONOHYDROCHLORIDE-[CAS]	Nc1c2CCCc2nc3CCCCc13	6	8.7	4.0			43.4	31.8			16.9	1.6			26.7	5.6		
	CGS 15943	Nc1nc2ccc(Cl)cc2c3nc(nn13)c4ccco4	7	97.4	13.1			110.7	4.9			105.1	4.3			75.8	27.9		
	D-CYCLOSERINE	N[C@@H]1CONC1=O	8	97.2	9.9			104.3	16.9			108.6	3.3			135.7	1.0		
	BETA-ESTRADIOL	C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]2CC[C@@H]1O	9	94.6	9.8			102.4	21.1			105.4	7.3			124.2	38.4		
		CN(C)CCN(Cc1ccccc1)c2ccccn2.Cl	10	48.4	2.9			57.8	6.0			53.8	0.5			114.2	69.5		
		CCN(CC)CC(=O)Nc1c(C)cccc1C	11	106.9	2.9			107.7	14.8			121.4	2.1			129.7	15.5		
	TRIMETHOPRIM	O[C@@H]1CCCC[C@H]1N2CCC(CC2)c3ccccc3.Cl				1.4	0.1			1.5	0.2			1.61	0.1			0.75	0.1

RANITIDINE	[O-][N+](=O)\C=C(\NC)NCCSCc1ccc (CN(C)C)o1				***13.4***	***1.2***			***13.1***	***3.5***			***22.3***	***3.0***			***11***	***1.2***
BMIM	CCCCn1cc[n+](C)c1				***179***	***12.7***												
NBUPY	CCCC[n+]1ccccc1				***26.5***	***3.8***												