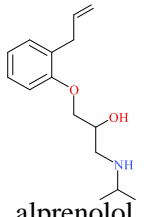
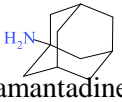
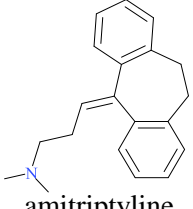
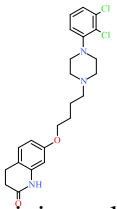
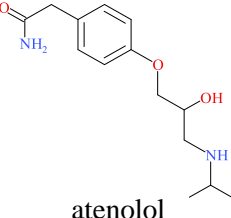
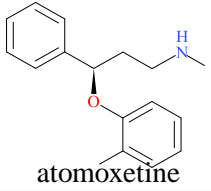
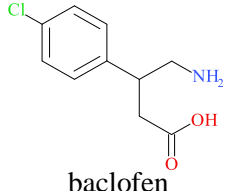
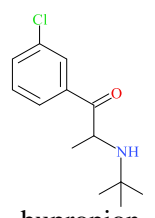
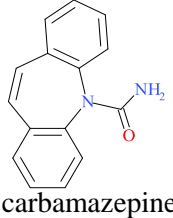
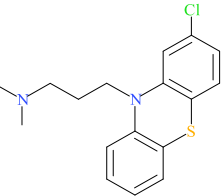
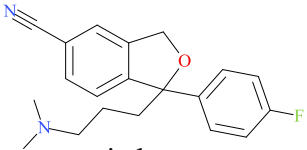
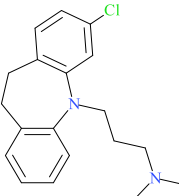
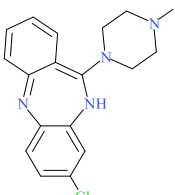
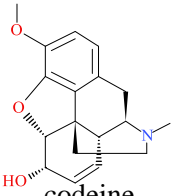
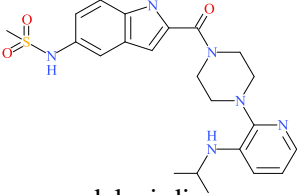
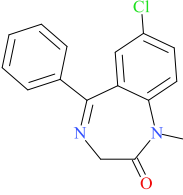
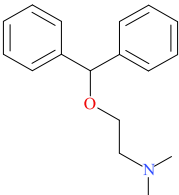
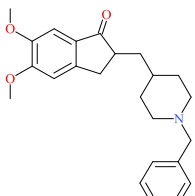
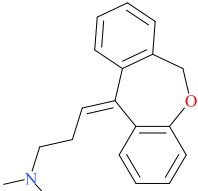
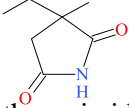
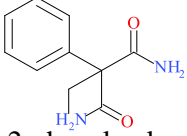
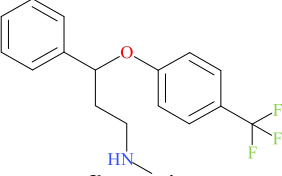
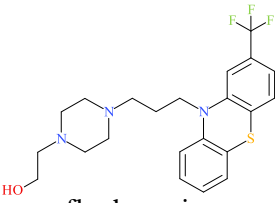
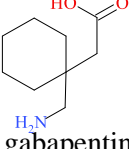
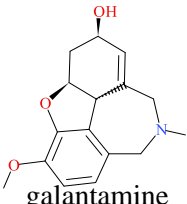
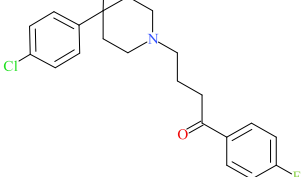
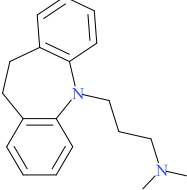
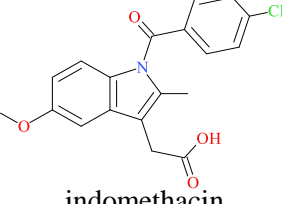
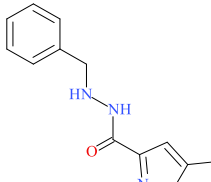
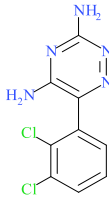
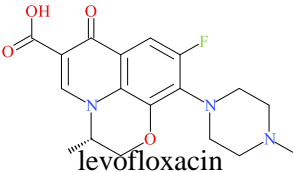
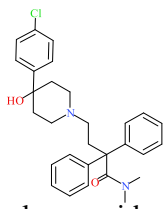
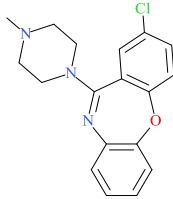
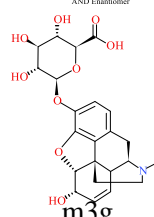
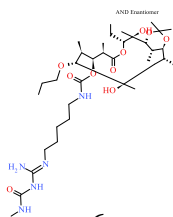
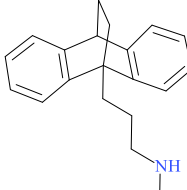
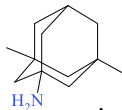
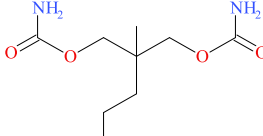


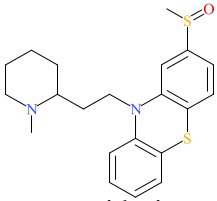
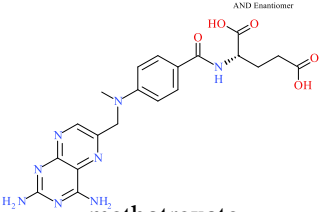
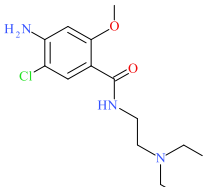
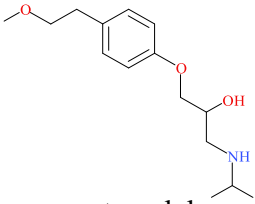
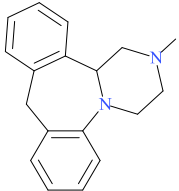
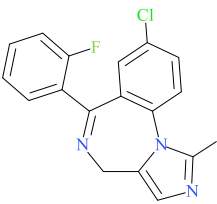
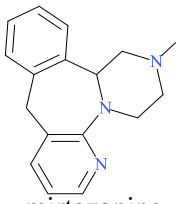
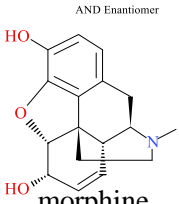
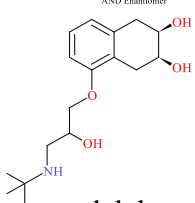
Supplementary Table1 Market drug compounds

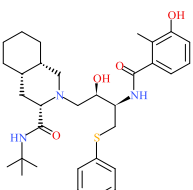
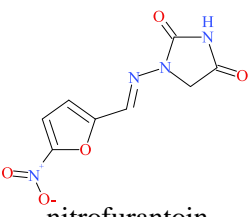
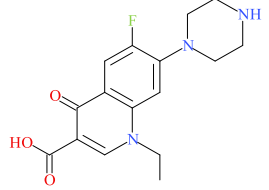
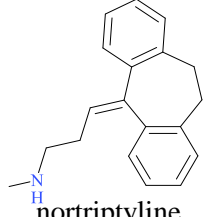
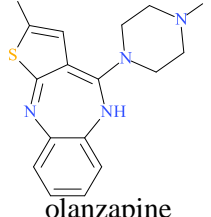
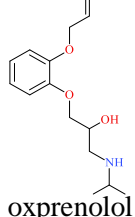
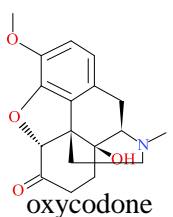
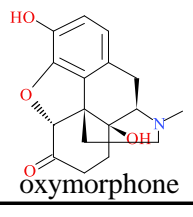
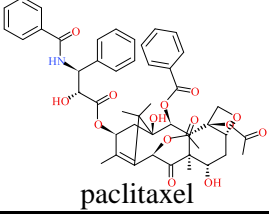
Name	Structures	K _{p,uu,brain}	WPSA	dipole	# rotor	LogBB
alprenolol	 alprenolol	0.38	0	1.91	9	0.34760033
amantadine	 amantadine	3	0	1.214	1	0.39513311
amitriptyline	 amitriptyline	1.03	0	0.913	3	0.59572605
aripiprazole	 aripiprazole	1.64	108.619	4.802	6	0.11766015
atenolol	 atenolol	0.026	0	4.842	9	-0.7992473
atomoxetine	AND Enantiomer  atomoxetine	2.13	0	1.479	6	0.74835506
baclofen	 baclofen	0.02	71.498	5.876	5	-0.7189156
bupropion	 bupropion	4.535	71.501	5.316	4	0.78605775
carbamazepine	 carbamazepine	0.76	0	5.736	0	-0.1812232

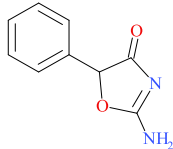
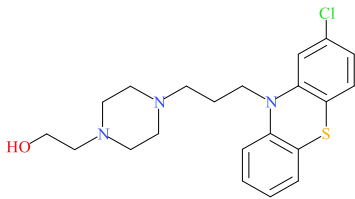
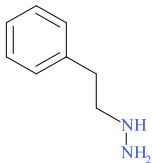
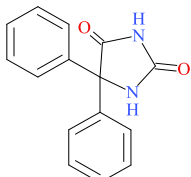
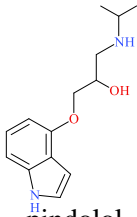
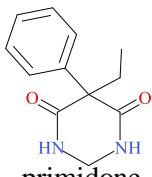
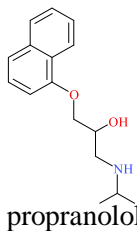
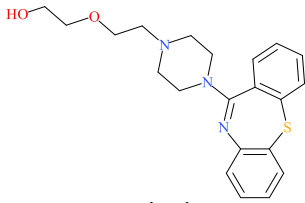
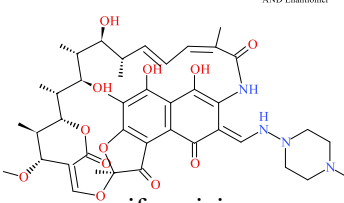
chlorpromazine	 chlorpromazine	4.27	107.457	3.204	4	1.00990209
citalopram	 citalopram	1.3	46.815	3.882	5	0.41956006
clomipramine	 clomipramine	2.77	69.46	2.875	4	1.0175532
clozapine	 clozapine	4.26	71.631	5.308	0	1.01140987
codeine	AND Enantiomer  codeine	0.89	0	3.741	2	0.29701676
delavirdine	 delavirdine	0.043	0	3.35	5	-1.0515182
diazepam	 diazepam	1.015	71.287	4.579	0	0.26791337
diphenhydramine	 diphenhydramine	1.05	0	0.935	6	0.65291433
donepezil	 donepezil	2.36	0	2.35	6	0.44779015

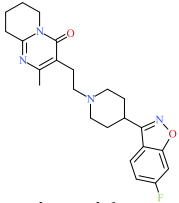
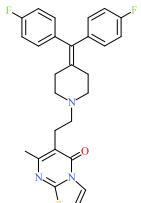
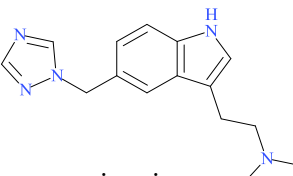
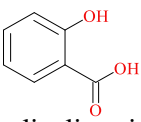
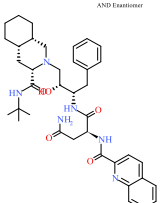
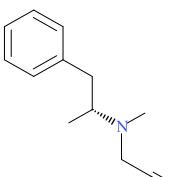
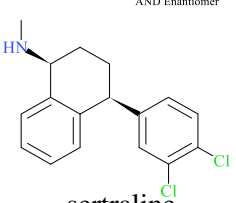
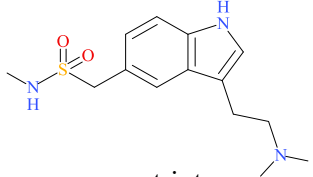
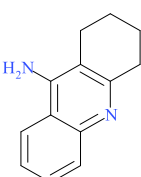
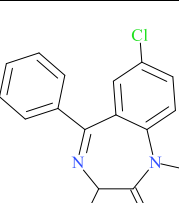
doxepin	 doxepin	3.11	0	2.223	3	0.61422799
ethosuximide	 ethosuximide	1.5	0	2.482	1	-0.0702309
ethyl-2-phenylmalonamide	 ethyl-2-phenylmalonamide	1.25	0	9.297	4	-0.5117463
fluoxetine	 fluoxetine	5.23	117.519	3.658	6	1.00327459
fluphenazine	 fluphenazine	1.58	150.359	4.997	7	0.85964035
gabapentin	 gabapentin	0.14	0	6.829	4	-0.7197993
galantamine	 galantamine	1.16	0	2.39	2	0.2868085
haloperidol	 haloperidol	2.09	118.337	3.744	6	0.66582063
imipramine	 imipramine	3.42	0	1.635	4	0.83201458
indomethacin	 indomethacin	0.11	71.504	3.516	4	-1.0500256

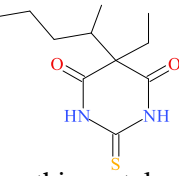
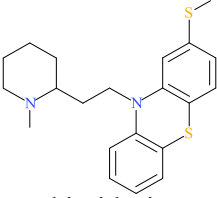
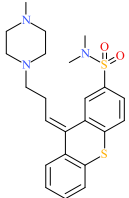
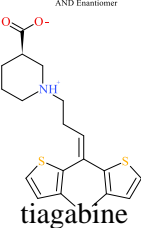
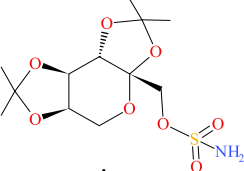
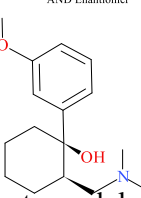
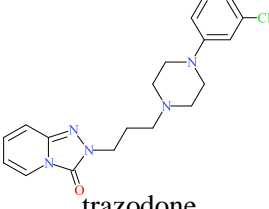
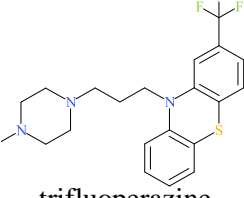
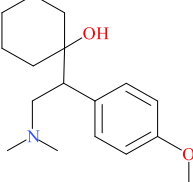
isocarboxazid	 isocarboxazid	0.18	0	9.11	4	-0.53929
lamotrigine	 lamotrigine	2.47	111.544	5.344	3	-0.1783553
levofloxacin	<small>AND Enantiomer</small>  levofloxacin	0.12	26.549	13.051	1	-0.5586958
loperamide	 loperamide	0.007	71.534	6.368	7	0.03208363
loxapine	 loxapine	2.95	71.33	0.911	0	0.9298662
m3g	<small>AND Enantiomer</small>  m3g	0.011	0	10.781	7	-1.3422003
m6g	<small>AND Enantiomer</small>  m6g	0.008	0	4.449	14	-1.1482171
maprotiline	 maprotiline	0.98	0	1.471	4	0.63921931
memantine	 memantine	6.06	0	1.194	1	0.6676614
meprobamate	 meprobamate	0.77	0	6.241	6	-0.6217643

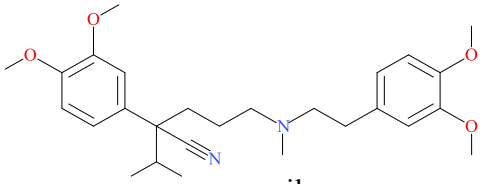
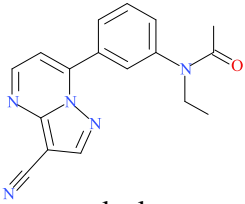
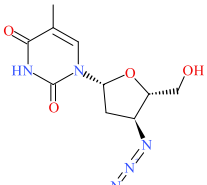
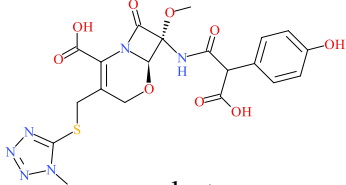
mesoridazine	 mesoridazine	0.1	59.306	8.03	4	0.29048901
methotrexate	 methotrexate	0.006	0	17.739	11	-1.7772972
metoclopramide	 metoclopramide	0.4	66.514	4.991	8	0.16993975
metoprolol	 metoprolol	0.64	0	1.356	10	0.21232817
mianserin	 mianserin	3.15	0	1.152	0	0.59744578
midazolam	 midazolam	1.08	106.25	4.774	0	0.183787
mirtazapine	 mirtazapine	3.83	0	2.236	0	0.42853391
morphine	 morphine	0.21	0	4.249	2	0.06117434
nadolol	 nadolol	0.037	0	4.144	9	-0.5066006

nelfinavir	<div><div>AND Enantiomer</div><div>nelfinavir</div></div>	0.019	21.525	8.952	12	-0.2654292
nitrofurantoin	<div><div>nitrofurantoin</div></div>	0.011	0	4.491	4	-0.742793
norfloxacin	<div><div>norfloxacin</div></div>	0.028	31.195	13.351	2	-0.4740454
nortriptyline	<div><div>nortriptyline</div></div>	1.65	0	1.556	3	0.53894907
olanzapine	<div><div>olanzapine</div></div>	2.14	44.776	5.724	0	0.86978876
oxprenolol	<div><div>oxprenolol</div></div>	0.2	0	2.455	10	0.34821367
oxycodone	<div><div>AND Enantiomer</div><div>oxycodone</div></div>	1.03	0	5.224	2	0.10833084
oxymorphone	<div><div>AND Enantiomer</div><div>oxymorphone</div></div>	0.79	0	5.745	2	-0.012727
paclitaxel	<div><div>AND Enantiomer</div><div>paclitaxel</div></div>	0.007	0	12.163	13	-1.2512715

pemoline	 pemoline	0.55	0	8.077	1	-0.6122243
perphenazine	 perphenazine	7.12	106.383	3.544	7	0.54538535
phenelzine	 phenelzine	1.48	0	2.906	4	0.04047784
phenytoin	 phenytoin	0.66	0	3.934	0	-0.0565406
pindolol	 pindolol	0.5	0	3.601	7	-0.238271
primidone	 primidone	0.38	0	5.953	1	-0.0838313
propranolol	 propranolol	0.61	0	2.028	7	0.57460664
quetiapine	 quetiapine	1.38	27.449	3.017	6	0.0956801
rifampicin	<small>AND Enantiomer</small>  rifampicin	0.035	0	5.211	24	-0.7039848

risperidone	 risperidone	0.21	46.707	8.399	3	-0.2785065
ritanserin	 ritanserin	0.33	148.335	4.139	5	0.56380695
rizatriptan	 rizatriptan	0.04	0	5.327	5	-0.5073632
salicylic acid	 salicylic acid	0.19	0	7.816	2	-0.3794421
saquinavir	<small>AND Enantiomer</small>  saquinavir	0.055	0	2.82	14	-0.8698122
selegiline	<small>AND Enantiomer</small>  selegiline	1.08	0	0.927	5	0.30193082
sertraline	<small>AND Enantiomer</small>  sertraline	2.67	129.894	4.867	1	0.93678274
sumatriptan	 sumatriptan	0.04	0	8.277	6	-0.8489241
tacrine	 tacrine	1.195	0	4.225	1	0.16689372
temazepam	 temazepam	0.8	71.315	3.974	1	0.146207

thiopental	 thiopental	1.53	80.691	2.219	4	-0.1001955
thioridazine	 thioridazine	1.64	78.035	4.258	4	0.93619327
thiothixene	 thiothixene	0.13	37.255	6.16	6	0.14248027
tiagabine	 tiagabine	0.62	46.703	7.694	6	-0.6151577
topimarate	 topimarate	0.33	1.407	2.92	4	-1.4149217
tramadol	 tramadol	1.46	0	0.858	4	0.45758082
trazodone	 trazodone	1.49	71.543	3.82	4	0.43306715
trifluoperazine	 trifluoperazine	3.34	147.568	3.617	4	1.21205563
venlafaxine	 venlafaxine	1.91	0	2.302	6	0.44549143

verapamil	<div> verapamil</div>	0.053	0	6.054	14	-0.353849
zaleplon	<div> zaleplon</div>	0.59	0	6.449	4	-1.0751168
zidovudine	<div>AND Enantiomer  zidovudine</div>	0.09	0	4.64	3	-1.0788293
moxalactam	<div>AND Enantiomer  moxalactam</div>	0.019	33.924	10.5	10	-1.7377688