

Table S1: The experimentally measured LogP values (MLogP) of 154 drugs vs. the in-silico calculations of LogP with the different methods

Drug	MLogP (BioLoom 5.0)	CLogP (BioLoom 5.0)	CLogP (ChemDraw Ultra 8.0)	ALogP (MOE 2004.03)	KLogP molecular formula
abacavir sulfate	1.22	0.81	0.58	1.09	0.99
acetaminophen	0.51	0.49	0.49	1.35	0.7
acetazolamide	-0.26	-0.98	-1.13	-0.86	-1.58
acetylsalicylic acid	1.19	1.02	1.02	1.31	0.36
acyclovir	-1.56	-2.42	-2.42	-1.46	-1.03
albendazole	2.85	3.46	3.46	3.24	1.06
allopurinol	-0.55	-0.83	0.63	0.06	-0.51
alprazolam	2.12	2.55	2.21	3.58	3.5
amiloride hydrochloride	0.1	0.11	0.11	-1.08	-0.58
amisulpride	1.1	1.8	1.8	1.29	1.32
amitriptyline hydrochloride	4.92	4.85	4.85	4.17	4.47
amlodipine besylate	3.3	3.43	3.43	2.27	2.54
amoxicillin	-1.99	-1.87	-1.87	0.02	0.67
amphetamine (mixed salt)	1.76	1.74	1.29	1.58	1.82
artemether	2.86	3.05	3.05	2.84	1.53
ascorbic acid	-1.64	-1.76	-1.76	-1.41	-1.28
atenolol	0.16	-0.11	-0.11	0.45	1.33
atropine sulfate	1.83	1.3	1.3	1.93	2.38
azathioprine	0.1	0.11	0.51	0.82	-0.91
azithromycin hydrate	4.02	2.64	na	1.9	2.88
azulene sulfonate sodium	3.2	3.32	2.95	2.79	2.42

benznidazole	0.91	0.9	0.9	0.57	0.26
biperiden					
hydrochloride	4.25	4.94	4.94	3.96	4.23
bisoprolol fumarate	1.87	1.83	1.92	2.37	2.13
brotizolam	2.79	2.71	2.36	4.4	2.79
captopril	0.9	0.89	0.89	0.63	0.5
carbamazepine	2.19	2.38	2.38	3.39	2.54
carvedilol	4.11	4.04	4.04	3.74	3.32
cefaclor	-1.79	-1.64	-1.64	0.62	1.55
ceftazidime sodium	-0.6	-1.34	-1.34	-0.73	-0.74
cefroxadine	-2.27	-2.15	-1.95	-0.21	0.67
cefuroxime axetil	0.26	0.23	0.23	-0.54	-0.99
cetirizine					
hydrochloride	1.7	2.08	2.08	3.15	3.69
chloramphenicol	1.14	1.28	1.28	0.37	1.05
chloroquine					
phosphate	4.63	5.06	5.06	4.81	3.98
chlorpheniramine					
maleate	3.17	3.15	3.15	3.82	3.85
chlorpromazine					
hydrochloride	5.35	5.3	5.8	4.89	4.14
cimetidine	0.4	0.38	0.35	0.6	0.51
ciprofloxacin					
hydrochloride	-1.08	-0.73	-1.15	1.37	1.67
citalopram					
hydrobromide	3.41	3.13	3.13	3.67	3.59
clarithromycin	3.16	2.37	na	2.44	2.76
clofazimine	7.48	7.7	7.5	7.96	6.56
clomipramine					
hydrochloride	5.32	5.92	5.92	4.53	4.56
clonidine					
hydrochloride	1.43	1.43	1.43	2.23	2.52

cloxacillin sodium	2.43	2.52	2.52	2.55	2.06
clozapine	3.32	3.71	4.1	3.72	3.71
codeine phosphate	1.14	0.98	0.98	1.5	2.64
colchicine	1.3	1.2	1.2	2.59	2.24
cyclophosphamide	0.63	0.8	0.93	0.81	0.63
dapsone	0.97	0.89	0.89	1.68	1.39
dexamethasone	1.74	1.79	1.79	1.51	2.65
diazepam	2.99	2.96	na	3.15	3.43
diclofenac sodium	4.75	4.73	4.73	4.36	3.47
didanosine	-1.24	-1.92	-1.92	-1.56	-0.49
digoxin	1.67	1.42	na	2.22	3.39
diloxanide furoate	1.78	1.77	1.77	2.16	2.25
diltiazem					
hydrochloride	2.8	3.65	3.65	3.37	2.87
dl-methionine	-1.87	-1.73	-1.73	0.15	-0.01
domperidone					
maleate	4.05	4.27	4.27	4.6	3.44
doxifluridine	-1.16	-1.19	-1.19	-1.18	-0.84
doxycycline					
hydrochloride	-0.02	-0.5	-0.51	-0.35	1.03
epinastine					
hydrochloride	3.1	3.01	3.51	2.47	2.9
erythromycin					
ethylsuccinate	2.54	1.61	na	1.79	2.53
escitalopram oxalate	3.41	3.13	3.13	3.81	3.61
ethinyl estradiol	3.67	3.86	3.86	3.61	3.88
ethosuximide	0.38	0.39	0.4	0.45	0.44
famotidine	-0.64	0.58	-0.61	-0.77	-1.1
finasteride	3.03	3.01	3.01	3.81	3.91
fluconazole	0.5	-0.44	-0.44	0.74	0.57

fluoxetine					
hydrochloride	4.5	4.57	4.57	4.44	3
flurbiprofen	4.16	3.75	3.75	3.68	2.61
fluvastatin sodium	3.8	4.05	4.05	4.63	3.53
furosemide	2.03	1.9	1.9	1.89	0.7
glipizide	1.91	2.57	2.57	2.08	1.67
glyceryl trinitrate	1.62	1.76	na	na	na
griseofulvin	2.18	2.05	1.91	2.81	2.03
haloperidol	4.28	3.85	3.85	4.43	4.37
hydralazine					
hydrochloride	1	1.17	1.02	0.92	0.66
hydrochlorothiazide	-0.07	-0.36	-0.37	-0.35	-0.34
hydroxyzine					
pamoate	3.5	4	4	3.06	4.13
ibuprofen	3.5	3.68	3.68	3.07	2.19
indinavir sulfate	3.49	3.68	3.68	2.87	2.2
isoniazid	-0.7	-0.67	-0.67	-0.31	0.04
isosorbide dinitrate	1.17	0.22	na	na	na
isotretinoin	6.3	6.74	6.74	5.6	3.86
ketoprofen	3.12	2.76	2.76	3.11	2.5
lamivudine	-0.93	-1.46	-1.46	-0.3	-0.35
levamisole					
hydrochloride	1.84	1.84	1.84	2.15	2.05
levodopa	-2.74	-2.82	-2.82	0.05	0.03
levofloxacin	-0.39	-0.51	-0.88	1.6	1.46
levosulpiride	1.23	1.11	1.11	0.56	0.85
linezolid	0.5	0.17	0.53	1.12	0.96
loratadine	5.2	5.05	5.05	4.89	4.4
lorazepam	2.39	2.37	2.37	3.1	3.41
lovastatin	4.26	4.08	4.08	4.2	3.44
mebendazole					
(chewable)	2.83	3.08	3.08	2.97	1.56

methylphenidate					
hydrochloride	1.8	2.56	2.56	2.09	2.12
metoclopramide					
hydrochloride	2.62	2.23	2.23	2	2.12
metoprolol tartrate	1.88	1.49	1.49	1.61	1.87
metronidazole	-0.02	-0.46	-0.46	-0.45	-0.89
morphine sulfate	0.76	0.57	0.57	1.2	2.4
nabumetone	3.08	2.98	2.98	3.37	2.7
nalidixic acid	1.59	1.02	1.34	1.38	0.9
nevirapine	1.81	2.65	2.42	1.68	1.89
niacin	0.66	0.8	0.8	0.78	0.23
nicardipine					
hydrochloride	4.96	5.23	5.23	3.14	2.57
nicotinamide	-0.34	-0.21	-0.21	0.18	0.36
nifedipine	3.27	3.12	3.13	1.64	0.73
nimesulide	2.6	3.21	3.21	2.22	0.28
nitrofurantoin	-0.47	-0.47	-0.47	-0.46	-0.19
nizatidine	-0.2	-0.16	-0.2	0.91	0.43
norethindrone (norethisterone)	2.97	2.97	2.78	3.49	3.87
olanzapine	3	3.01	3.39	3.44	2.85
oxycodone					
hydrochloride	0.21	-0.04	-0.04	1.05	2.19
penicillamine	-1.78	-1.73	-1.73	0.11	-0.01
phenobarbital	1.47	1.37	1.37	0.7	0.9
phenoxymethylpenicillin (penicillin v potassium)	2.09	1.94	1.94	0.7	0.99
phenytoin (chewable)	2.26	2.08	2.09	1.77	2.09
phenytoin sodium	2.26	2.08	2.09	1.77	2.09
pravastatin sodium	2.18	2.05	2.05	2.44	2.29

prednisolone	1.42	1.42	1.42	1.56	2.75
proguanil					
hydrochloride	2.53	2.53	na	2.21	1.69
promethazine					
hydrochloride	4.81	4.4	4.9	4.24	3.48
propranolol					
hydrochloride	2.98	2.75	2.75	2.58	2.6
pseudoephedrine					
hydrochloride	0.93	0.89	0.89	1.33	1.61
pyrazinamide	-0.6	-0.68	-0.68	-0.42	-0.2
pyridoxine					
hydrochloride	-0.72	-0.35	-0.8	0.08	0.23
pyrimethamine	2.69	3	3	2.52	2.27
quinine sulfate	2.64	2.79	2.79	3.17	3.25
ranitidine					
hydrochloride	0.27	0.67	0.63	1.05	0.49
reserpine	3.72	3.86	3.86	3.54	3.2
retinol palmitate	5.68	6.4	na	5.51	4.29
ribavirin	-1.85	-2.85	-2.85	-3.01	-1.62
riboflavin	-1.46	-0.73	-0.73	-1.08	0.09
risperidone	3.04	2.71	2.71	4.36	3.24
saquinavir mesylate	4.7	4.73	4.73	3.09	4.9
simvastatin	4.68	4.48	4.48	4.59	3.67
spironolactone	2.26	2.84	2.25	4.85	3.96
stavudine	-0.64	-0.49	-0.73	-0.28	-0.05
sulfadiazine	-0.09	0.1	0.01	0.86	0.28
sulfamethoxazole	0.89	0.56	0.56	1.37	0.14
sumatriptan					
succinate	0.93	0.74	0.74	1.32	1.52
tegafur	-0.27	-0.07	-0.07	0.49	-0.17
terbinafine					
hydrochloride	6	5.96	5.96	4.88	4.71

theophylline	-0.02	-0.03	-0.03	0.05	-0.49
tosufloxacin tosylate	-0.46	-0.39	0.19	2.34	1.66
tramadol					
hydrochloride	2.63	3.1	3.1	2.63	2.57
trimethoprim	0.91	0.98	0.98	1.26	0.72
ursodeoxycholic					
acid (ursodiol)	4.15	4.51	4.51	4.48	3.87
valproate sodium	2.75	2.76	2.76	2.29	0.97
valproic acid	2.75	2.76	2.76	2.29	0.97
verapamil					
hydrochloride	3.97	4.47	4.47	5.09	3.98
warfarin sodium	2.7	2.9	2.9	3.64	2.78
zidovudine	0.05	0.04	0.04	0.23	-1