

Table S4: provisional BCS classifications of 185 drugs with the various in-silico methods

Drug	BCS Classification based on									
	CLogP (BioLoom 5.0) and reference solubility	CLogP (BioLoom 5.0) and <i>in silico</i> solubility using experimental melting point	CLogP (BioLoom 5.0) and <i>in silico</i> solubility using average melting point	CLogP (ChemDraw 8.0) and reference solubility	CLogP (ChemDraw 8.0) and <i>in silico</i> solubility using experimental melting point	AlogP (MOE 2004.03) and reference solubility	AlogP (MOE 2004.03) and <i>in silico</i> solubility using experimental melting point	KlogP (Molecular Formula) and reference solubility	KlogP (Molecular Formula) and <i>in silico</i> solubility using experimental melting point	KlogP (Molecular Formula) and <i>in silico</i> solubility using average melting point
abacavir sulfate	3	3	3	3	3	3	4	3	4	4
aceclofenac	2	2	2	2	2	2	2	2	2	2
acetaminophen <sup>b</sup>	4	3	3	4	3	4	4	4	4	4
acyclovir <sup>a,c</sup>	4	3	3	4	3	4	3	4	3	3
albendazole	2	2	2	2	2	2	2	4	4	4
alibendol	1	1	1	1	1	3	3	3	3	3
alprazolam	1	1	1	1	1	1	1	1	1	1
amiloride hydrochloride	3	3	3	3	3	3	3	3	3	3
anastrozole	3	3	3	3	3	1	1	1	1	1
atenolol	3	3	3	3	3	3	3	3	3	3
atropine sulfate	3	3	3	3	3	1	1	1	1	1
azithromycin hydrate	2	2	2			2	2	2	2	2







imatinib mesylate	2	2	2	2	2	2	2	2	2	2
imidapril hydrochloride	1	1	1	1	1	3	3	3	3	3
indapamide	1	1	1	1	1	1	1	1	1	1
indinavir sulfate	2	2	2	2	2	2	2	2	2	2
irbesartan	2	2	2	2	2	2	2	2	2	2
isoniazid	3	3	3	3	3	3	3	3	3	3
isotretinoin	2	2	2	2	2	2	2	2	2	2
itraconazole	2	2	2	2	2	2	2	2	2	2
ketoprofen	2	2	2	2	2	2	2	2	1	2
ketotifen fumarate	1	1	1	1	1	1	1	1	1	1
lamivudine	3	3	3	3	3	3	3	3	3	3
l-carbocysteine	4	3	3	4	3	4	3	4	3	3
letrozole	3	3	3	3	3	1	1	1	1	1
levamisole hydrochloride	1	1	2	1	1	1	1	1	1	2
levetiracetam	3	3	3	3	3	3	3	3	3	3
levodopa <sup>a,c</sup>	4	3	3	4	3	4	4	4	4	3
levonorgestrel	1	1	1			1	1	1	1	1
levosulpiride	4	3	3	4	3	4	3	4	3	3
limaprost alfadex	1	1	1	1	1	1	1	1	1	1
linezolid <sup>c</sup>	4	3	3	4	3	4	4	4	4	3
lopinavir	2	2	2	2	2	2	2	2	2	2
loratadine	2	2	2	2	2	2	2	2	2	2
lorazepam <sup>a</sup>	1	1	1	1	1	1	2	1	2	2
losartan potassium <sup>d</sup>	1	2	2	1	2	1	2	1	2	2





pyrantel embonate	2	2	2	2	2	2	2	2	2	2
pyrazinamide	3	3	3	3	3	3	3	3	3	3
pyridostigmine bromide	3	3	3	3	3	3	3	3	3	3
pyridoxine hydrochloride	3	3	3	3	3	3	3	3	3	3
pyrimethamine raloxifene hydrochloride	2	2	2	2	2	2	2	2	2	1
ramipril	1	1	1	1	1	1	1	1	1	1
ranitidine hydrochloride	3	3	3	3	3	3	3	3	3	3
ribavirin	3	3	3	3	3	3	3	3	3	3
rizatriptan benzoate	3	3	3	3	3	1	1	1	1	1
rosiglitazone maleate	1	1	2	1	1	1	1	1	1	1
sildenafil citrate <sup>d</sup>	1	2	1	1	2	3	3	3	3	3
simvastatin	2	2	2	2	2	2	2	2	2	2
spironolactone <sup>c</sup>	2	1	1	2	1	2	2	2	2	2
stavudine	3	3	3	3	3	3	3	3	3	3
sulfadiazine	4	4	3	4	4	4	4	4	4	3
sulfamethoxazol e	4	3	3	4	3	4	4	4	3	3
sultamicillin tosilate	2	2	2	2	2	4	3	4	3	3
sumatriptan succinate	3	3	3	3	3	3	3	3	3	3
tacrolimus <sup>a</sup>	2	2	2			2	2	2	2	2



taltirelin hydrate	3	3	3	3	3	3	3	3	3	3
tamoxifen citrate	2	2	2	2	2	2	2	2	2	2
tegafur	3	3	3	3	3	3	3	3	3	3
telmisartan	2	2	2	2	2	2	2	2	2	2
temocapril hydrochloride	1	1	1	1	1	1	1	1	1	1
tenofovir disoproxil fumarate <sup>d</sup>	3	4	3	3	4	1	2	3	3	3
terazosin hydrochloride <sup>d</sup>	1	2	1	3	3	3	3	3	3	3
terbinafine hydrochloride <sup>d</sup>	1	2	2	1	2	1	2	1	2	2
theophylline	4	4	3	4	4	4	4	4	3	3
topiramate	3	3	3	3	3	3	3	3	3	3
toremifene citrate <sup>d</sup>	1	2	2	1	2	1	2	1	2	2
triflusal	2	2	2	2	2	2	2	4	3	3
trimebutin maleate <sup>d</sup>	1	2	2	1	2	1	2	1	1	2
trimethoprim <sup>c</sup>	4	3	3	4	3	4	3	4	3	3
tulobuterol hydrochloride	1	1	1	1	1	1	1	1	1	1
ursodeoxycholic acid (ursodiol)	2	2	2	2	2	2	2	2	2	2
valsartan	2	2	2	2	2	2	2	2	2	2
voglibose	3	3	3	3	3	3	3	3	3	3
warfarin sodium <sup>b</sup>	2	1	1	2	1	2	2	2	1	1

zaltoprofen	2	2	2	2	2	2	2	2	2	2
zidovudine	3	3	3	3	3	3	3	3	3	3
zolmitriptan	3	3	3	3	3	1	1	1	1	1
zolpidem tartrate <sup>d</sup>	1	2	2	1	2	1	2	1	2	2

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