DEVELOPMENT OF A DYNAMIC PHYSIOLOGICALLY-BASED MECHANISTIC KIDNEY MODEL TO PREDICT RENAL CLEARANCE
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Table S2. Summary of physicochemical and pharmacokinetic properties of 46 test drugs

Drug	Chem	pKa (acid)	pKa (base)	fu,p	Observed CLr (mL/min)	Mean predicted CLr (mL/min)	Net reabsorbed (R) or secreted (S)	Irvine 1998[g]	Irvine 1998	Di 2001[g]	Scotcher 2016	Alsenz 2003	Li 2007	Yazdanian 1998	Artursson 1991	Yee 1997	Gres 1998	Hovgaard 1995	Yamashita 2000
Acetaminophen	Neutral			0.81[a]	11.5[a]	14.11	R	35	100	-	-	-	-	-	-	-	-	-	23.7
Betamethasone	Neutral			0.36[a]	9.5[a]	9.42	R	-	-	-	26.5	-	-	-	-	-	-	-	-
Dapsone	Neutral			0.27[a]	5.5[a]	3.24	R	-	-	-	49.7	-	-	-	-	-	-	-	-
Dexamethasone	Neutral			0.32[b]	6.3[b]	13.37	R	20	40	-	-	-	12.5	12.2	12.50	23.40	-	-	12.1
Fluconazole	Neutral			0.86[a]	15.7[a]	17.29	R	-	-	-	36.3	-	-	-	-	29.80	-	-	-
Levetiracetam	Neutral			0.9[a]	39.4[a]	38.72	R	-	-	-	15.7	-	-	-	-	-			
Linezolid	Neutral			0.78[a]	39.5[a]	13.85	R	-	-	-	36.1	-	-	-	-	-	-	-	-
Metronidazole	Neutral			0.98[a]	9.6[a]	8.04	R	-	-	-	64.7	-	-	-	-	-	-	-	-
Ribavirin	Neutral			1[a]	109.9[a]	106.44	R	-	-	-	1.55	-	-	-	-	-	-	-	-
Topiramate	Neutral			0.87[a]	15.1[a]	11.19	R	-	-	-	46.2	-	-	-	-	-	-	-	-
Voriconazole	Neutral			0.42[a]	1.57[a]	2.12	R	-	-	-	96.5	-	-	-	-	-	-	-	-
Atenolol	Base		9.67	0.97[a]	145.3[a]	114.33	S	1.8	3.3	1.31	0.256	1.73	1.6	0.53	0.20	-	1.16	-	0.4
Betaxolol	Base		9.67	0.45[a]	49.6[a]	26.31	R	-	-	-	20	-	-	-	-	-	-	48.50	-
Desipramine	Base		10.02	0.13[a]	28.6[a]	9.37	S	-	-	-	-	43	-	24.4	-	21.60	-	-	-
Imipramine	Base		9.17	0.13[a]	6.8[a]	5.41	R	-	-	-	33.4	-	-	-	-	14.10	-	-	-
Lamotrigine	Base		5.87	0.45[a]	2.5[a]	2.83	R	88	110	-	-	-	-	-	-	-	-	-	-
Metoprolol	Base		9.7	0.87[a]	109.6[a]	69.96	S	150	140	24.6	17	31.77	33.2	23.7	27.00	-	18.00	-	-
Midazolam	Base		6.57	0.05[e]	0.55[c]	0.79	R	-	-	-	-	-	-	-	-	-	-	-	69.9
Nadolol	Base		9.76	0.7[f]	126[d]	82.77	S	1.4	0.39	0.83	-	-	0.6	3.88	-	-	-	-	0.33
Ondansetron	Base		7.34	0.27[b]	20.7[b]	7.05	R	110	110	-	-	-	-	-	-	-	-	-	-
Oxprenolol	Base		9.67	0.14[a]	9.35[a]	6.71	R	130	160	-	30	-	-	-	-	-	-	65.50	-
Trimethoprim	Base		7.16	0.49[a]	78.2[a]	21.93	S	52	87	17.9	-	-	-	-	-	-	-	-	-
Verapamil	Base		9.68	0.16[a]	25.6[a]	9.58	S	-	-	7.48	20.9	44.67	45.7	-	-	-	-	-	-
Acetylsalicylic Acid	Acid	3.41		0.51[b]	9.1[b]	18.03	R	7.4	2.2	-	-	-	-	9.09	2.4	30.7	-	-	-
Cefuroxime	Acid	3.15		0.67[b]	127.4[b]	73.30	S	0.16	0.38	-	-	-	-	-	-	-	-	-	-
Chloramphenicol	Acid	7.49		0.34[b]	16.8[b]	11.70	R	-	-	-	-	-	-	-	-	20.60	-	-	-
Chlorpropamide	Acid	4.33		0.05[a]	0.6[a]	0.36	R	-	-	-	88.1	-	-	-	-	-	-	-	-
Ibuprofen	Acid	4.85		0.01[e]	0.574[d]	0.23	R	-	-	-	-	-	-	-	-	52.50	-	-	-
Probenecid	Acid	3.53		0.09[a]	0.5[a]	0.70	R	-	-	-	84.5	-	-	-	-	-	-	-	-
Propylthiouracil	Acid	8.09		0.16[a]	3.2[a]	1.15	R	41	96	-	80.8	-	-	-	-	-	-	-	-
Sulfamethoxazole	Acid	6.16		0.35[a]	4.5[a]	7.54	R	-	-	-	41.7	-	-	-	-	-	-	-	-
Theophylline	Acid	7.82		0.52[a]	5.5[a]	9.18	R	-	-	23.1	65.1	-	22.6	-	-	-	-	-	25
Amoxicillin	Zwitterion	3.23	7.43	0.83[a]	167[a]	97.75	S	0.24	0.021	-	-	0.01	-	-	-	-	0.33	-	-
Ampicillin	Zwitterion	3.24	7.44	0.8[a]	163.6[a]	95.03	S	-	-	-	-	-	-	-	-	-	-	-	0.081
Difloxacin	Zwitterion	5.81	7.39	0.62[a]	4.5[a]	3.32	R	-	-	-	74.6	-	-	-	-	-	-	-	-
Enalaprilat	Zwitterion	3.13	7.83	0.61[b]	112[b]	61.17	S	-	-	-	-	1.85	-	-	-	-	-	-	-
Gabapentin	Zwitterion	4.63	9.91	0.97[a]	95.1[a]	113.30	R	0.36	0.01	-	0.67	-	-	-	-	-	-	-	-
Labetalol	Zwitterion	8.1	9.8	0.49[b]	64.4[b]	43.06	S	25	76	7.34	-	-	-	9.31	-	-	-	-	-
Lisinopril	Zwitterion	3.17	10.2	0.99[b]	84[b]	114.55	R	0.18	0.22	0.23	-	1.27	-	-	-	-	-	-	-
Melagatran	Zwitterion	2.12	11.62	0.93[a]	113.7[a]	110.34	S	-	-	-	0.145	-	-	-	-	-	-	-	-
Methyldopa	Zwitterion	1.73	9.85	0.84[b]	147[b]	99.62	S	-	-	-	-	-	0.15	-	-	-	-	-	-
Oxytetracycline	Zwitterion	0.24	7.75	0.77[a]	90.8[a]	86.67	R	-	-	-	0.85	-	-	-	-	-	-	-	-
Pefloxacin	Zwitterion	5.66	6.47	0.75[a]	12.9[a]	6.34	R	-	-	-	63.7	-	-	-	-	-	-	-	-
Terbutaline	Zwitterion	8.86	9.76	0.74[b]	154[b]	87.86	S	1	0.41	-	-	1.71	0.8	0.47	0.38	-	1.04	-	0.12
Tetracycline	Zwitterion	-2.2	8.24	0.76[a]	86.4[a]	83.83	R	-	-	-	1.1	-	-	-	-	-	-	-	-
Trovafloxacin	Zwitterion	5.41	9.44	0.31[a]	12.6[a]	6.79	R	-	-	-	-	-	-	-	-	30.23	-	-	-

Reported apparent permeability value of each drug from individual primary sources (10^{-6} cm/s)

[a]CLr value is obtained from Scotcher 2016; [b]CLr value is obtained from Ito 2013; [c]CLr value is obtained from Bjelland 2012; [d]CLr value is obtained from Varma 2009; [e]Data is obtained from Zhang 2012; [f]Data is obtained from FDA drug label;

[g]Permeability value is obtained from MDCK cell line; otherwise Caco-2 cell line

Drug is defined as net reabsorbed (R) when observed CLr < unbound filtration, net secreted (S) when observed CLr > unbound filtration