

Article Title: Evaluation of Tissue Binding in 3 Tissues Across 5 Species, and Prediction of Volume of Distribution from Plasma Protein and Tissue Binding with an Existing Model

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Journal: Drug Metabolism and Disposition

Manuscript Number: DMD-AR-2020-000337

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Table S1. Human V_d dataset for marketed drugs

Compound Name	c_pKa_MA	c_pKa_MB	fup	fumic(1mg/mL)	VDss	VDss predicted (LKL Model)	Species	a	b
Dronedarone	8.24	9.64	0.001	0.002	20	10.03	H	20	0.76
Glyburide	5.26	0.00	0.0013	0.600	0.08	0.13	H	20	0.76
Tolcapone	4.51	0.00	0.003	0.193	0.12	0.36	H	20	0.76
Mifepristone	14.00	4.51	0.0032	0.117	0.45	0.59	H	20	0.76
Nefazodone	14.00	6.87	0.0042	0.115	0.51	0.76	H	20	0.76
Rosiglitazone	6.16	5.35	0.0066	0.653	0.2	0.19	H	20	0.76
Ibuprofen	4.36	0.00	0.011	0.910	0.15	0.14	H	20	0.76
Furosemide	3.64	0	0.012	0.942	0.12	0.14	H	20	0.76
Sulfapyridine	2.93	0.00	0.016	0.781	0.12	0.22	H	20	0.76
Warfarin	4.94	0.00	0.023	0.685	0.13	0.35	H	20	0.76
Midazolam	14.00	5.92	0.0342	0.553	1.1	0.70	H	20	0.76
Nifedipine	14.00	3.37	0.035	0.460	0.79	0.97	H	20	0.76
Clomipramine hydrochloride	14.00	9.07	0.039	0.124	13	5.65	H	20	0.76
Chlorpromazine	14.00	9.07	0.044	0.040	10	21.53	H	20	0.76
Trazodone hydrochloride	14.00	6.87	0.053	0.818	0.52	0.41	H	20	0.76
Oxazepam	14.00	2.06	0.065	0.619	0.59	0.99	H	20	0.76
Cefoperazone	2.59	0.00	0.07	0.980	0.17	0.22	H	20	0.76
Zolpidem	14.00	4.94	0.074	0.817	0.54	0.53	H	20	0.76
Promethazine	14.00	9.03	0.096	0.242	14	6.20	H	20	0.76
Erythromycin	14.00	8.47	0.1	0.905	0.95	0.41	H	20	0.76
Amitriptyline·HCl	14.00	8.83	0.12	0.250	8.7	7.43	H	20	0.76
Paroxetine	14.00	9.82	0.12	0.143	18	14.63	H	20	0.76
Imatinib	14.00	8.44	0.1251	0.523	3.9	2.51	H	20	0.76
Tolterodine	14.00	9.25	0.13	0.550	1.5	2.36	H	20	0.76
Tamsulosin	14.00	8.22	0.1461	0.887	0.21	0.63	H	20	0.76
Clonazepam	14.00	0.00	0.15	0.653	2.9	1.89	H	20	0.76
Desipramine	14.00	9.91	0.16	0.245	15	10.12	H	20	0.76
Cefazolin	2.23	0	0.18	0.980	0.12	0.41	H	20	0.76
Quinidine	14.00	9.18	0.19	0.712	2.9	1.85	H	20	0.76
Citalopram	14.00	9.77	0.2	0.706	12	1.99	H	20	0.76
Imipramine	14.00	9.07	0.2	0.365	12	7.28	H	20	0.76
Propranolol	14.00	9.18	0.21	0.925	3.1	0.68	H	20	0.76
Quinacrine	14.00	10.09	0.24	0.504	45	5.11	H	20	0.76
Verapamil	14.00	8.55	0.28	0.642	3.7	3.55	H	20	0.76
Quinine	14.00	8.19	0.3	0.792	1.8	2.03	H	20	0.76
Dexamethasone	14.00	0.00	0.32	0.665	0.94	3.73	H	20	0.76
Lidocaine	14.00	0.00	0.33	0.881	1.8	1.41	H	20	0.76
Indinavir	14.00	6.49	0.36	0.506	0.82	7.59	H	20	0.76
Diphenhydramine	14.00	8.43	0.38	0.818	6.5	2.25	H	20	0.76
Moxalactam	2.87	0	0.39	0.980	0.17	0.75	H	20	0.76
Telithromycin	14.00	8.47	0.44	1.000	3	0.64	H	20	0.76
Acetaminophen	14.00	0.00	0.52	0.959	1	1.21	H	20	0.76
Nevirapine	14.00	5.55	0.52	1.000	1.3	0.76	H	20	0.76
Tacrine	14.00	9.81	0.55	0.923	11	1.70	H	20	0.76
Almotriptan	14.00	9.09	0.6	0.887	2.2	2.38	H	20	0.76
Moxifloxacin	6.19	8.53	0.6	0.905	1.4	2.12	H	20	0.76
Atropine	14.00	9.36	0.61	0.961	3.3	1.36	H	20	0.76
Theophylline	14.00	0.00	0.61	0.965	0.51	1.32	H	20	0.76
Caffeine	14.00	0.00	0.64	1.000	0.63	0.91	H	20	0.76
Bisoprolol	14.00	9.18	0.66	0.852	2.4	3.22	H	20	0.76
Ciprofloxacin	6.13	8.61	0.7	0.835	2.1	3.75	H	20	0.76
Codeine	14.00	8.48	0.7	0.925	3.5	2.11	H	20	0.76
Venlafaxine	14.00	9.18	0.73	0.855	4.4	3.48	H	20	0.76
Zidovudine	14.00	0.00	0.8	0.825	1.8	4.51	H	20	0.76
Famotidine	14.00	6.88	0.84	1.000	1.2	1.16	H	20	0.76
Acyclovir	8.75	2.86	0.85	1.000	0.71	1.17	H	20	0.76
Metoprolol	14.00	9.18	0.88	0.898	3.1	3.21	H	20	0.76

Antipyrine	14.00	0.00	0.93	1.000	0.77	1.27	H	20	0.76
Cyclophosphamide	14.00	10.33	0.93	0.955	0.73	2.15	H	20	0.76
Atenolol	14.00	9.18	0.94	0.980	0.95	1.66	H	20	0.76

Table S2. Cynomolgus, Dog, Rat, Mouse V_d dataset for internal compounds

Compound #	Calc pKa_M A	Calc pKa_M B	fup	fubrain	fulung	fumic or Predicted fumic(1mg/mL)	VDss	VDss predicted (LKL Model)	Species	Tissue	A	B
1	14	3.4	0.48	N/A	N/A	0.9231	1.2	1.54	C	Liver Microsome	20	0.76
2	14	2.7	0.53	N/A	N/A	0.8692	1.3	2.41	C	Liver Microsome	20	0.76
3	14	2.7	0.2	N/A	N/A	0.6529	1.1	2.50	C	Liver Microsome	20	0.76
4	6.5	0	0.11	N/A	N/A	0.8182	0.59	0.75	C	Liver Microsome	20	0.76
5	14	2.7	0.21	N/A	N/A	0.8018	2	1.43	C	Liver Microsome	20	0.76
6	14	2.8	0.23	N/A	N/A	0.7241	1.7	2.17	C	Liver Microsome	20	0.76
7	14	6.3	0.12	N/A	N/A	0.4815	1.9	2.86	C	Liver Microsome	20	0.76
8	14	6.3	0.13	N/A	N/A	0.4184	1.7	3.90	C	Liver Microsome	20	0.76
9	14	6.3	0.1	N/A	N/A	0.3986	2.6	3.26	C	Liver Microsome	20	0.76
10	14	5.9	0.002	N/A	N/A	0.0438	0.43	0.99	C	Liver Microsome	20	0.76
11	14	6.7	0.08	N/A	N/A	0.7699	0.71	0.70	C	Liver Microsome	20	0.76
12	6.7	8	0.11	N/A	N/A	0.9802	0.18	0.30	C	Liver Microsome	20	0.76
13	14	6.7	0.14	N/A	N/A	0.8182	0.87	0.92	C	Liver Microsome	20	0.76
14	6.5	8	0.087	N/A	N/A	1.0000	0.27	0.23	C	Liver Microsome	20	0.76
15	14	6.7	0.19	N/A	N/A	1.0000	0.77	0.37	C	Liver Microsome	20	0.76
16	14	6.7	0.29	N/A	N/A	0.6807	0.92	3.22	C	Liver Microsome	20	0.76
17	14	6.4	0.33	N/A	N/A	0.8692	0.9	1.54	C	Liver Microsome	20	0.76
18	14	3.4	0.41	N/A	N/A	0.9231	0.99	1.29	D	Liver Microsome	20	0.76
19	14	0	0.26	N/A	N/A	0.8182	2.3	1.58	D	Liver Microsome	20	0.76
20	14	2.7	0.48	N/A	N/A	0.8692	0.78	2.14	D	Liver Microsome	20	0.76

21	14	2.7	0.22	N/A	N/A	0.6529	0.81	2.72	D	Liver Micros ome	20	0.76
22	6.3	8.1	0.015	N/A	N/A	0.3889	0.44	0.60	D	Liver Micros ome	20	0.76
23	6.5	0	0.13	N/A	N/A	0.8182	0.45	0.85	D	Liver Micros ome	20	0.76
24	14	2.7	0.2	N/A	N/A	0.8018	1.2	1.34	D	Liver Micros ome	20	0.76
25	14	2.8	0.23	N/A	N/A	0.7241	1.2	2.14	D	Liver Micros ome	20	0.76
26	14	6.3	0.14	N/A	N/A	0.4815	2.2	3.30	D	Liver Micros ome	20	0.76
27	14	6.3	0.072	N/A	N/A	0.4184	2.2	2.20	D	Liver Micros ome	20	0.76
28	14	6.3	0.067	N/A	N/A	0.3986	2	2.21	D	Liver Micros ome	20	0.76
29	14	6.7	0.15	N/A	N/A	0.7699	1.5	1.19	D	Liver Micros ome	20	0.76
30	6.2	9.9	0.08	N/A	N/A	0.6949	1.4	0.91	D	Liver Micros ome	20	0.76
31	6.7	8	0.17	N/A	N/A	0.9802	0.67	0.39	D	Liver Micros ome	20	0.76
32	14	6.7	0.08	N/A	N/A	0.8182	0.49	0.56	D	Liver Micros ome	20	0.76
33	6.5	8	0.15	N/A	N/A	1.0000	0.9	0.29	D	Liver Micros ome	20	0.76
34	14	6.7	0.06	N/A	N/A	1.0000	0.44	0.18	D	Liver Micros ome	20	0.76
35	14	6.7	0.14	N/A	N/A	1.0000	0.56	0.28	D	Liver Micros ome	20	0.76
36	14	6.7	0.22	N/A	N/A	0.6807	0.51	2.44	D	Liver Micros ome	20	0.76
37	14	6.4	0.24	N/A	N/A	0.8692	0.93	1.13	D	Liver Micros ome	20	0.76
38	14	9.1	0.031	N/A	N/A	0.0753	9.4	7.74	M	Liver Micros ome	20	0.76
39	8.8	8.5	0.19	N/A	N/A	0.8868	11	0.83	M	Liver Micros ome	20	0.76
40	14	4.8	0.052	N/A	N/A	0.8868	0.91	0.33	M	Liver Micros ome	20	0.76
41	14	3.4	0.39	N/A	N/A	0.9231	2.8	1.29	M	Liver Micros ome	20	0.76
42	6.8	9.2	0.049	N/A	N/A	0.1976	5.2	4.17	M	Liver Micros ome	20	0.76
43	5.2	0	0.012	N/A	N/A	0.8868	0.69	0.17	M	Liver Micros ome	20	0.76

44	14	8.2	0.09	N/A	N/A	0.6393	1.8	1.22	M	Liver Micros ome	20	0.76
45	14	2.7	0.61	N/A	N/A	0.8692	0.93	2.77	M	Liver Micros ome	20	0.76
46	6.3	9.2	0.051	N/A	N/A	0.4286	1.8	1.55	M	Liver Micros ome	20	0.76
47	14	2.7	0.25	N/A	N/A	0.6529	2.3	3.11	M	Liver Micros ome	20	0.76
48	6.3	8.1	0.029	N/A	N/A	0.3889	1.1	1.07	M	Liver Micros ome	20	0.76
49	14	5.3	0.014	N/A	N/A	0.1429	0.95	1.82	M	Liver Micros ome	20	0.76
50	6.5	0	0.15	N/A	N/A	0.8182	2	0.99	M	Liver Micros ome	20	0.76
51	6.3	4.3	0.002	N/A	N/A	0.2346	0.33	0.26	M	Liver Micros ome	20	0.76
52	6.3	8.1	0.004 3	N/A	N/A	0.1299	0.82	0.71	M	Liver Micros ome	20	0.76
53	14	2.7	0.033	N/A	N/A	0.8018	0.76	0.33	M	Liver Micros ome	20	0.76
54	14	2.8	0.21	N/A	N/A	0.7241	1.9	2.00	M	Liver Micros ome	20	0.76
55	14	6.3	0.087	N/A	N/A	0.4815	1.8	2.11	M	Liver Micros ome	20	0.76
56	6.7	0	0.024	N/A	N/A	0.9608	0.28	0.18	M	Liver Micros ome	20	0.76
57	6.7	0	0.015	N/A	N/A	0.9048	0.3	0.18	M	Liver Micros ome	20	0.76
58	14	6.3	0.032	N/A	N/A	0.4184	1.8	1.06	M	Liver Micros ome	20	0.76
59	14	6.3	0.004 5	N/A	N/A	0.3986	0.44	0.27	M	Liver Micros ome	20	0.76
60	6.6	5.9	0.008 3	N/A	N/A	0.8182	0.49	0.17	M	Liver Micros ome	20	0.76
61	6.3	9.9	0.029	N/A	N/A	0.5385	1.1	0.66	M	Liver Micros ome	20	0.76
62	14	5.9	0.001 6	N/A	N/A	0.0438	1.1	0.82	M	Liver Micros ome	20	0.76
63	14	6.7	0.078	N/A	N/A	0.7699	1.2	0.69	M	Liver Micros ome	20	0.76
64	6.2	9.9	0.043	N/A	N/A	0.6949	0.32	0.56	M	Liver Micros ome	20	0.76
65	5.8	8.2	0.015	N/A	N/A	0.3986	0.51	0.60	M	Liver Micros ome	20	0.76
66	6.6	2.3	0.003 8	N/A	N/A	0.0526	1.8	1.50	M	Liver Micros ome	20	0.76

67	5.4	8.2	0.016	N/A	N/A	0.4184	0.61	0.59	M	Liver Micros ome	20	0.76
68	14	6.7	0.06	N/A	N/A	0.4599	0.87	1.61	M	Liver Micros ome	20	0.76
69	6.1	8.2	0.007 4	N/A	N/A	0.2195	0.65	0.66	M	Liver Micros ome	20	0.76
70	6.3	8.3	0.016	N/A	N/A	0.2903	0.93	0.93	M	Liver Micros ome	20	0.76
71	6.6	8.1	0.008 2	N/A	N/A	0.7391	0.5	0.19	M	Liver Micros ome	20	0.76
72	6.6	9.9	0.022	N/A	N/A	0.6529	0.25	0.39	M	Liver Micros ome	20	0.76
73	6.4	8.1	0.018	N/A	N/A	0.6529	0.21	0.34	M	Liver Micros ome	20	0.76
74	6.7	9.9	0.025	N/A	N/A	0.6667	0.56	0.41	M	Liver Micros ome	20	0.76
75	6.6	2.3	0.05	N/A	N/A	0.9231	1.4	0.27	M	Liver Micros ome	20	0.76
76	6.7	0	0.018	N/A	N/A	0.9608	0.41	0.16	M	Liver Micros ome	20	0.76
77	6.7	8	0.036	N/A	N/A	0.9802	0.72	0.19	M	Liver Micros ome	20	0.76
78	14	3.8	0.013	N/A	N/A	0.1364	0.5	1.79	M	Liver Micros ome	20	0.76
79	5.8	8.1	0.007 3	N/A	N/A	0.2821	0.38	0.51	M	Liver Micros ome	20	0.76
80	14	6.7	0.12	N/A	N/A	0.9802	0.56	0.33	M	Liver Micros ome	20	0.76
81	14	9	0.21	N/A	N/A	0.8519	0.52	1.10	M	Liver Micros ome	20	0.76
82	14	6.7	0.1	N/A	N/A	0.9608	0.99	0.34	M	Liver Micros ome	20	0.76
83	14	9.1	0.014	N/A	N/A	0.2500	0.81	0.94	M	Liver Micros ome	20	0.76
84	6.3	8.2	0.043	N/A	N/A	0.3699	0.43	1.65	M	Liver Micros ome	20	0.76
85	14	9.9	0.061	N/A	N/A	0.4706	2.4	1.54	M	Liver Micros ome	20	0.76
86	6.8	8.1	0.034	N/A	N/A	0.5152	0.74	0.81	M	Liver Micros ome	20	0.76
87	14	9.1	0.006 1	N/A	N/A	0.3605	0.58	0.31	M	Liver Micros ome	20	0.76
88	4.4	2.2	0.013	N/A	N/A	0.5748	0.58	0.33	M	Liver Micros ome	20	0.76
89	6.4	4.3	0.002 9	N/A	N/A	0.0482	0.56	1.27	M	Liver Micros ome	20	0.76

90	14	3.8	0.007	N/A	N/A	0.0929	0.7	1.50	M	Liver Micros ome	20	0.76
91	14	6.8	0.81	N/A	N/A	1.0000	0.74	1.20	M	Liver Micros ome	20	0.76
92	14	5.8	0.12	N/A	N/A	0.6393	0.32	1.64	M	Liver Micros ome	20	0.76
93	4.8	2.3	0.92	N/A	N/A	0.9802	0.87	1.72	M	Liver Micros ome	20	0.76
94	14	6.7	0.068	N/A	N/A	1.0000	0.72	0.21	M	Liver Micros ome	20	0.76
95	14	4.5	0.34	N/A	N/A	0.9231	0.72	1.14	M	Liver Micros ome	20	0.76
96	14	4.5	0.043	N/A	N/A	0.3423	0.54	1.83	M	Liver Micros ome	20	0.76
97	8.1	10.5	0.012	N/A	N/A	0.0811	2.5	2.82	M	Liver Micros ome	20	0.76
98	8.2	9.9	0.004 2	N/A	N/A	0.1976	0.99	0.43	M	Liver Micros ome	20	0.76
99	6.6	2.3	0.004 2	N/A	N/A	0.2270	0.96	0.42	M	Liver Micros ome	20	0.76
100	6.6	2.3	0.005 4	N/A	N/A	0.1561	1.7	0.72	M	Liver Micros ome	20	0.76
101	6.2	8.4	0.02	N/A	N/A	0.6949	0.32	0.33	M	Liver Micros ome	20	0.76
102	6.3	8.8	0.046	N/A	N/A	0.5385	1	0.97	M	Liver Micros ome	20	0.76
103	8	9.9	0.052	N/A	N/A	0.5873	1.3	0.89	M	Liver Micros ome	20	0.76
104	6.6	2.3	0.001 7	N/A	N/A	0.0267	3.4	1.37	M	Liver Micros ome	20	0.76
105	3.9	3.3	0.011	N/A	N/A	1.0000	0.42	0.14	M	Liver Micros ome	20	0.76
106	4	0	0.009 7	N/A	N/A	0.2500	5.1	0.72	M	Liver Micros ome	20	0.76
107	14	6.5	0.042	N/A	N/A	0.7391	0.67	0.48	M	Liver Micros ome	20	0.76
108	14	6.5	0.031	N/A	N/A	0.9048	0.26	0.23	M	Liver Micros ome	20	0.76
109	14	6.7	0.039	N/A	N/A	0.7544	2.1	0.43	M	Liver Micros ome	20	0.76
110	14	6.7	0.057	N/A	N/A	0.8182	0.7	0.45	M	Liver Micros ome	20	0.76
111	14	9.9	0.017	N/A	N/A	0.2422	1.7	1.17	M	Liver Micros ome	20	0.76
112	14	6.7	0.087	N/A	N/A	0.8692	0.67	0.50	M	Liver Micros ome	20	0.76

113	14	8.6	0.55	N/A	N/A	0.9231	2.4	1.75	M	Liver Microsome	20	0.76
114	5.8	8.7	0.011	N/A	N/A	0.1561	0.85	1.33	M	Liver Microsome	20	0.76
115	4	0	0.14	N/A	N/A	0.9608	1.1	0.42	M	Liver Microsome	20	0.76
116	6.6	2.3	0.0049	N/A	N/A	0.1765	1.9	0.59	M	Liver Microsome	20	0.76
117	14	5.8	0.034	N/A	N/A	0.1494	0.52	4.04	M	Liver Microsome	20	0.76
118	6.3	8.8	0.0077	N/A	N/A	0.1765	1.4	0.85	M	Liver Microsome	20	0.76
119	14	9.9	0.0079	N/A	N/A	0.1236	0.74	1.21	M	Liver Microsome	20	0.76
120	14	4.5	0.067	N/A	N/A	0.4925	0.76	1.59	M	Liver Microsome	20	0.76
121	6.8	8.4	0.093	N/A	N/A	0.6667	0.62	1.18	M	Liver Microsome	20	0.76
122	5.3	6	0.0096	N/A	N/A	0.0989	1.4	1.89	M	Liver Microsome	20	0.76
123	6.5	0	0.0078	N/A	N/A	1.0000	0.38	0.13	M	Liver Microsome	20	0.76
124	14	6.4	0.31	N/A	N/A	0.7699	0.79	2.39	M	Liver Microsome	20	0.76
125	8	9.9	0.22	N/A	N/A	0.6260	2.6	3.01	M	Liver Microsome	20	0.76
126	6.5	8	0.046	N/A	N/A	1.0000	0.5	0.19	M	Liver Microsome	20	0.76
127	6.5	4.2	0.39	N/A	N/A	1.0000	0.41	0.64	M	Liver Microsome	20	0.76
128	14	6.7	0.12	N/A	N/A	0.7544	0.7	1.06	M	Liver Microsome	20	0.76
129	14	9.9	0.045	N/A	N/A	0.4085	2.3	1.45	M	Liver Microsome	20	0.76
130	8.1	9.9	0.1	N/A	N/A	0.6129	1.4	1.48	M	Liver Microsome	20	0.76
131	14	6.7	0.058	N/A	N/A	0.9802	0.7	0.22	M	Liver Microsome	20	0.76
132	14	6.7	0.14	N/A	N/A	1.0000	0.51	0.31	M	Liver Microsome	20	0.76
133	4.3	3.6	0.0065	N/A	N/A	0.6393	0.32	0.21	M	Liver Microsome	20	0.76
134	14	6.7	0.14	N/A	N/A	0.9417	0.58	0.48	M	Liver Microsome	20	0.76
135	14	6.7	0.069	N/A	N/A	1.0000	0.44	0.22	M	Liver Microsome	20	0.76

136	14	6.7	0.081	N/A	N/A	0.8519	0.49	0.51	M	Liver Micros ome	20	0.76
137	14	0	0.002 3	N/A	N/A	0.0293	2.4	1.65	M	Liver Micros ome	20	0.76
138	5.2	4.2	0.029	N/A	N/A	0.7241	0.48	0.38	M	Liver Micros ome	20	0.76
139	14	6.4	0.067	N/A	N/A	1.0000	0.74	0.21	M	Liver Micros ome	20	0.76
140	14	6.4	0.12	N/A	N/A	0.8692	0.6	0.64	M	Liver Micros ome	20	0.76
141	14	8.2	0.062	N/A	N/A	0.1976	3	5.20	M	Liver Micros ome	20	0.76
142	14	8.1	0.12	N/A	N/A	0.3333	5.2	5.05	M	Liver Micros ome	20	0.76
143	4.3	3.7	0.03	N/A	N/A	0.9231	0.54	0.21	M	Liver Micros ome	20	0.76
144	14	6.7	0.21	N/A	N/A	0.6807	0.56	2.37	M	Liver Micros ome	20	0.76
145	4.2	3.5	0.003	N/A	N/A	0.1494	0.43	0.47	M	Liver Micros ome	20	0.76
146	14	3.3	0.22	N/A	N/A	1.0000	2.9	0.42	M	Liver Micros ome	20	0.76
147	14	6.4	0.12	N/A	N/A	0.8692	0.49	0.64	M	Liver Micros ome	20	0.76
148	8.8	8.5	0.35	N/A	N/A	0.8868	14	1.43	R	Liver Micros ome	20	0.76
149	6.8	9.2	0.05	N/A	N/A	0.1976	8.7	4.23	R	Liver Micros ome	20	0.76
150	14	0	0.13	N/A	N/A	0.8182	1	0.85	R	Liver Micros ome	20	0.76
151	6.3	9.2	0.022	N/A	N/A	0.4286	1.4	0.72	R	Liver Micros ome	20	0.76
152	6.3	8.1	0.003 5	N/A	N/A	0.3889	0.39	0.22	R	Liver Micros ome	20	0.76
153	6.5	0	0.093	N/A	N/A	0.8182	1	0.64	R	Liver Micros ome	20	0.76
154	5.9	0	0.006 3	N/A	N/A	0.0870	0.86	1.43	R	Liver Micros ome	20	0.76
155	14	3.5	0.26	N/A	N/A	0.7094	5.5	2.57	R	Liver Micros ome	20	0.76
156	14	6.3	0.1	N/A	N/A	0.4815	2.2	2.39	R	Liver Micros ome	20	0.76
157	6.7	0	0.021	N/A	N/A	0.9608	0.24	0.15	R	Liver Micros ome	20	0.76
158	14	6.3	0.025	N/A	N/A	0.5873	1.3	0.49	R	Liver Micros ome	20	0.76

159	14	6.3	0.014	N/A	N/A	0.3986	1.2	0.54	R	Liver Micros ome	20	0.76
160	6.6	5.9	0.005 2	N/A	N/A	0.8182	0.39	0.13	R	Liver Micros ome	20	0.76
161	14	5.9	0.009 5	N/A	N/A	0.0438	1.4	4.26	R	Liver Micros ome	20	0.76
162	14	6.7	0.048	N/A	N/A	0.7699	0.39	0.45	R	Liver Micros ome	20	0.76
163	6.2	9.9	0.015	N/A	N/A	0.6949	0.22	0.25	R	Liver Micros ome	20	0.76
164	14	6.7	0.048	N/A	N/A	0.4599	2.4	1.29	R	Liver Micros ome	20	0.76
165	6.3	8.3	0.007 4	N/A	N/A	0.2903	0.8	0.47	R	Liver Micros ome	20	0.76
166	6.7	0	0.036	N/A	N/A	0.9608	0.26	0.18	R	Liver Micros ome	20	0.76
167	6.7	8	0.086	N/A	N/A	0.9802	0.29	0.25	R	Liver Micros ome	20	0.76
168	14	6.3	0.13	N/A	N/A	0.6807	2.3	1.49	R	Liver Micros ome	20	0.76
169	14	6.3	0.078	N/A	N/A	0.8692	2	0.44	R	Liver Micros ome	20	0.76
170	14	6.7	0.025	N/A	N/A	0.4286	0.98	0.80	R	Liver Micros ome	20	0.76
171	14	6.3	0.06	N/A	N/A	0.7544	1.8	0.57	R	Liver Micros ome	20	0.76
172	4.4	2.2	0.008 5	N/A	N/A	0.5748	1.2	0.24	R	Liver Micros ome	20	0.76
173	14	6.7	0.035	N/A	N/A	0.6393	0.6	0.54	R	Liver Micros ome	20	0.76
174	14	6.7	0.013	N/A	N/A	0.5625	0.53	0.32	R	Liver Micros ome	20	0.76
175	14	6.7	0.05	N/A	N/A	0.6529	2.1	0.70	R	Liver Micros ome	20	0.76
176	14	6.7	0.069	N/A	N/A	0.7391	2.6	0.68	R	Liver Micros ome	20	0.76
177	14	6.7	0.038	N/A	N/A	0.6667	0.73	0.53	R	Liver Micros ome	20	0.76
178	14	6.7	0.036	N/A	N/A	0.4925	2.3	0.89	R	Liver Micros ome	20	0.76
179	14	3.9	0.092	N/A	N/A	0.7544	1.2	0.82	R	Liver Micros ome	20	0.76
180	14	6.3	0.032	N/A	N/A	0.4706	2	0.86	R	Liver Micros ome	20	0.76
181	14	6.7	0.037	N/A	N/A	0.5873	1.1	0.67	R	Liver Micros ome	20	0.76

182	14	6.7	0.071	N/A	N/A	0.5873	1.1	1.19	R	Liver Micros ome	20	0.76
183	6.5	0	0.025	N/A	N/A	1.0000	0.29	0.13	R	Liver Micros ome	20	0.76
184	14	3.9	0.095	N/A	N/A	0.6529	1.3	1.24	R	Liver Micros ome	20	0.76
185	14	6.3	0.074	N/A	N/A	0.7094	1.6	0.81	R	Liver Micros ome	20	0.76
186	14	8.6	0.0068	N/A	N/A	0.0096	6.1	14.12	R	Liver Micros ome	20	0.76
187	14	6.5	0.0041	N/A	N/A	0.9048	0.22	0.12	R	Liver Micros ome	20	0.76
188	14	8	0.19	N/A	N/A	0.9048	0.91	0.72	R	Liver Micros ome	20	0.76
189	14	6.7	0.071	N/A	N/A	0.8182	0.65	0.51	R	Liver Micros ome	20	0.76
190	14	8.6	0.43	N/A	N/A	0.9231	4	1.36	R	Liver Micros ome	20	0.76
191	5.3	9.3	0.19	N/A	N/A	0.3793	3.3	6.57	R	Liver Micros ome	20	0.76
192	14	6.3	0.1	N/A	N/A	0.8018	2.3	0.73	R	Liver Micros ome	20	0.76
193	5.3	8.9	0.41	N/A	N/A	0.2195	0.57	29.79	R	Liver Micros ome	20	0.76
194	5	9.1	0.27	N/A	N/A	0.9608	1.3	0.67	R	Liver Micros ome	20	0.76
195	5	9.1	0.22	N/A	N/A	0.7544	1.4	1.82	R	Liver Micros ome	20	0.76
196	14	0	0.024	N/A	N/A	0.2121	3.5	1.92	R	Liver Micros ome	20	0.76
197	14	5.8	0.021	N/A	N/A	0.1494	9.1	2.52	R	Liver Micros ome	20	0.76
198	5	8	0.13	N/A	N/A	0.8182	1.1	0.85	R	Liver Micros ome	20	0.76
199	5	10	0.46	N/A	N/A	1.0000	2.7	0.70	R	Liver Micros ome	20	0.76
200	5	10.1	0.54	N/A	N/A	0.9231	3.1	1.71	R	Liver Micros ome	20	0.76
201	14	4.5	0.037	N/A	N/A	0.4925	2.5	0.91	R	Liver Micros ome	20	0.76
202	14	4.5	0.037	N/A	N/A	0.2903	6.7	1.96	R	Liver Micros ome	20	0.76
203	14	6.3	0.13	N/A	N/A	0.8349	1.9	0.79	R	Liver Micros ome	20	0.76
204	6.5	8	0.12	N/A	N/A	1.0000	0.89	0.26	R	Liver Micros ome	20	0.76

205	14	6.7	0.16	N/A	N/A	0.7544	0.72	1.35	R	Liver Micros ome	20	0.76
206	14	6.7	0.11	N/A	N/A	1.0000	0.59	0.25	R	Liver Micros ome	20	0.76
207	14	4.4	0.001	N/A	N/A	0.0045	5.2	4.51	R	Liver Micros ome	20	0.76
208	14	4.6	0.0045	N/A	N/A	0.0262	4.3	3.46	R	Liver Micros ome	20	0.76
209	14	4.7	0.005	N/A	N/A	0.0277	3.1	3.61	R	Liver Micros ome	20	0.76
210	14	6.7	0.09	N/A	N/A	1.0000	0.55	0.22	R	Liver Micros ome	20	0.76
211	14	6.4	0.34	N/A	N/A	0.9802	0.89	0.68	R	Liver Micros ome	20	0.76
212	14	3.8	0.24	N/A	N/A	0.8692	1.5	1.14	R	Liver Micros ome	20	0.76
213	14	3.8	0.48	N/A	N/A	1.0000	1.5	0.73	R	Liver Micros ome	20	0.76
214	14	0	0.0028	N/A	N/A	0.0293	4.9	1.96	R	Liver Micros ome	20	0.76
215	14	0	0.0075	N/A	N/A	0.9608	1.2	0.12	R	Liver Micros ome	20	0.76
216	14	3.8	0.27	N/A	N/A	0.7857	1.6	1.93	R	Liver Micros ome	20	0.76
217	14	3.8	0.33	N/A	N/A	0.9802	1.8	0.67	R	Liver Micros ome	20	0.76
218	14	6.4	0.096	N/A	N/A	1.0000	0.64	0.23	R	Liver Micros ome	20	0.76
219	14	0	0.73	N/A	N/A	0.8349	0.87	3.94	R	Liver Micros ome	20	0.76
220	14	6.2	0.29	N/A	N/A	1.0000	2.6	0.48	R	Liver Micros ome	20	0.76
221	3.3	8.1	0.038	N/A	N/A	0.8692	5.6	0.27	R	Liver Micros ome	20	0.76
222	14	6.4	0.16	N/A	N/A	0.8692	0.76	0.79	R	Liver Micros ome	20	0.76
223	14	0	0.025	N/A	N/A	0.8519	0.62	0.22	R	Liver Micros ome	20	0.76
224	14	6.7	0.38	N/A	N/A	0.7857	0.92	2.67	R	Liver Micros ome	20	0.76
225	14	6.7	0.074	N/A	N/A	0.6529	0.52	0.99	R	Liver Micros ome	20	0.76
226	14	6.7	0.077	N/A	N/A	0.6807	0.95	0.93	R	Liver Micros ome	20	0.76
227	14	6.7	0.087	N/A	N/A	0.8868	0.72	0.44	R	Liver Micros ome	20	0.76

228	14	8.2	0.047	N/A	N/A	0.3245	2.9	2.08	R	Liver Micros ome	20	0.76
229	14	6.7	0.073	N/A	N/A	0.6260	0.39	1.07	R	Liver Micros ome	20	0.76
230	14	6.7	0.088	N/A	N/A	0.8519	0.54	0.52	R	Liver Micros ome	20	0.76
231	14	6.7	0.22	N/A	N/A	0.9608	0.49	0.57	R	Liver Micros ome	20	0.76
232	14	6.7	0.12	N/A	N/A	0.8349	0.65	0.73	R	Liver Micros ome	20	0.76
233	14	6.7	0.067	N/A	N/A	0.7391	0.49	0.66	R	Liver Micros ome	20	0.76
234	14	6.7	0.063	N/A	N/A	0.7699	0.52	0.56	R	Liver Micros ome	20	0.76
235	14	6.7	0.052	N/A	N/A	0.6129	0.45	0.83	R	Liver Micros ome	20	0.76
236	14	6.7	0.19	N/A	N/A	0.6393	0.7	2.49	R	Liver Micros ome	20	0.76
237	14	6.1	0.12	N/A	N/A	0.6393	2.5	1.61	R	Liver Micros ome	20	0.76
238	14	8.1	0.1	N/A	N/A	0.3333	6.2	4.20	R	Liver Micros ome	20	0.76
239	14	6.1	0.13	N/A	N/A	0.6667	2.6	1.57	R	Liver Micros ome	20	0.76
240	14	6.4	0.41	N/A	N/A	1.0000	0.86	0.64	R	Liver Micros ome	20	0.76
241	14	0	0.002 3	N/A	N/A	0.0320	2.5	1.50	R	Liver Micros ome	20	0.76
242	14	6.7	0.059	N/A	N/A	0.4493	0.57	1.63	R	Liver Micros ome	20	0.76
243	14	6.4	0.35	N/A	N/A	1.0000	0.92	0.56	R	Liver Micros ome	20	0.76
244	4.3	3.7	0.027	N/A	N/A	0.9231	1.1	0.18	R	Liver Micros ome	20	0.76
245	14	0	0.77	N/A	N/A	1.0000	0.93	1.11	R	Liver Micros ome	20	0.76
246	14	6.7	0.21	N/A	N/A	0.6807	0.95	2.35	R	Liver Micros ome	20	0.76
247	14	6.7	0.055	N/A	N/A	0.6000	0.41	0.91	R	Liver Micros ome	20	0.76
248	14	8.1	0.62	N/A	N/A	0.6667	4.8	7.10	R	Liver Micros ome	20	0.76
249	14	0	0.7	N/A	N/A	1.0000	0.91	1.01	R	Liver Micros ome	20	0.76
250	14	6.7	0.056	N/A	N/A	0.6529	0.38	0.77	R	Liver Micros ome	20	0.76

251	14	6.4	0.23	N/A	N/A	0.9231	1	0.79	R	Liver Micros ome	20	0.76
252	14	6.1	0.24	N/A	N/A	0.7857	2.9	1.72	R	Liver Micros ome	20	0.76
253	14	6.4	0.052	N/A	N/A	0.8868	0.44	0.30	R	Liver Micros ome	20	0.76
254	14	6.3	0.073	N/A	N/A	0.6949	0.78	0.84	R	Liver Micros ome	20	0.76
255	14	6.4	0.16	N/A	N/A	0.9802	1	0.38	R	Liver Micros ome	20	0.76
256	14	6.4	0.31	N/A	N/A	1.0000	1.2	0.51	R	Liver Micros ome	20	0.76
257	4.2	3.5	0.001 4	N/A	N/A	0.1494	0.34	0.26	R	Liver Micros ome	20	0.76
258	14	8.6	0.16	N/A	N/A	0.4388	5.1	4.37	R	Liver Micros ome	20	0.76
259	14	0	0.85	N/A	N/A	1.0000	0.86	1.21	R	Liver Micros ome	20	0.76
260	14	0	0.69	N/A	N/A	0.9048	1.2	2.45	R	Liver Micros ome	20	0.76
261	14	2.3	0.66	N/A	N/A	1.0000	1.7	0.96	R	Liver Micros ome	20	0.76
262	14	6.3	0.11	N/A	N/A	0.9231	0.59	0.43	R	Liver Micros ome	20	0.76
263	14	6.4	0.3	N/A	N/A	0.9608	0.97	0.74	R	Liver Micros ome	20	0.76
264	14	6.4	0.1	N/A	N/A	0.8519	0.94	0.58	R	Liver Micros ome	20	0.76
265	14	8.2	0.39	N/A	N/A	0.5748	7.8	6.36	R	Liver Micros ome	20	0.76
266	14	0	0.77	N/A	N/A	0.9802	0.83	1.42	R	Liver Micros ome	20	0.76
267	14	6.4	0.14	N/A	N/A	0.8692	0.97	0.71	R	Liver Micros ome	20	0.76
268	14	6.7	0.11	N/A	N/A	0.7391	0.79	1.02	R	Liver Micros ome	20	0.76
269	14	6.4	0.12	N/A	N/A	0.8018	0.92	0.85	R	Liver Micros ome	20	0.76
270	14	9	0.29	N/A	N/A	0.9608	1.3	0.69	R	Liver Micros ome	20	0.76
271	14	6.5	0.45	N/A	N/A	0.7857	2.6	3.14	R	Liver Micros ome	20	0.76
272	14	6.7	0.18	N/A	N/A	0.9417	0.63	0.56	R	Liver Micros ome	20	0.76
273	14	0	0.72	N/A	N/A	1.0000	0.93	1.04	R	Liver Micros ome	20	0.76

274	14	6.4	0.36	N/A	N/A	0.9231	0.82	1.17	R	Liver Micros ome	20	0.76
275	14	6.4	0.31	N/A	N/A	0.8349	1	1.73	R	Liver Micros ome	20	0.76
276	8.9	6.3	0.31	N/A	N/A	1.0000	1.1	0.51	R	Liver Micros ome	20	0.76
277	14	6.4	0.16	N/A	N/A	0.6949	0.54	1.72	R	Liver Micros ome	20	0.76
278	14	8.8	0.163 7	0.008	N/A	0.2424	16.6	10.53	C	Brain	20	0.76
279	14	8.8	0.185 9	0.011	N/A	0.3062	23.8	8.75	C	Brain	20	0.76
280	14	8.8	0.222 1	0.006	N/A	0.1932	19.2	18.92	C	Brain	20	0.76
281	14	8.9	0.222 5	0.018	N/A	0.4211	31.7	6.49	C	Brain	20	0.76
282	14	8.4	0.191	0.068	N/A	0.7433	4.997 5	1.65	C	Brain	20	0.76
283	14	5.5	0.458	0.107	N/A	0.8262	1.11	2.64	C	Brain	20	0.76
284	14	4.8	0.443 2	0.133	N/A	0.8589	4.24	2.15	C	Brain	20	0.76
285	14	3.4	0.534	0.237	N/A	0.9250	1.2	1.68	C	Brain	20	0.76
286	14	2.9	0.545	0.325	N/A	0.9503	0.865	1.40	C	Brain	20	0.76
287	14	8.9	0.349	0.018	N/A	0.4211	34.3	10.11	D	Brain	20	0.76
288	14	8.8	0.370 5	0.011	N/A	0.3062	25.5	17.33	D	Brain	20	0.76
289	14	8.9	0.13	0.005	N/A	0.1663	20.5	13.28	D	Brain	20	0.76
290	14	5.5	0.432	0.107	N/A	0.8262	0.684	2.45	D	Brain	20	0.76
291	14	4.8	0.683 6	0.133	N/A	0.8589	2.286 7	3.19	D	Brain	20	0.76
292	14	4.1	0.164 2	0.019	N/A	0.4346	1.265	4.58	D	Brain	20	0.76
293	14	2.5	0.1	0.058	N/A	0.7179	2.57	1.04	M	Brain	20	0.76
294	14	8.3	0.109	0.024	N/A	0.5040	3.17	2.38	M	Brain	20	0.76
295	14	8.8	0.130 7	0.011	N/A	0.3149	6.92	5.95	M	Brain	20	0.76
296	14	8.8	0.184 6	0.044	N/A	0.6554	4.05	2.28	M	Brain	20	0.76
297	14	8.6	0.206	0.055	N/A	0.7063	9.52	2.08	M	Brain	20	0.76
298	14	8.4	0.132	0.068	N/A	0.7509	5.22	1.14	M	Brain	20	0.76
299	14	8.4	0.104 01	0.0290	N/A	0.5524	4.66	1.91	M	Brain	20	0.76
300	14	5.7	0.334 1	0.2402 9	N/A	0.9289	2.26	1.08	M	Brain	20	0.76
301	14	9	0.354 5	0.0458 06	N/A	0.6648	0.432 2	4.14	M	Brain	20	0.76
302	14	5.8	0.282	0.124	N/A	0.8540	1.4	1.46	M	Brain	20	0.76
303	14	4.2	0.102 4	0.05	N/A	0.6850	1.8	1.20	M	Brain	20	0.76
304	14	4.8	0.383 7	0.133	N/A	0.8637	1.771 4	1.84	M	Brain	20	0.76
305	14	2.9	0.455	0.202	N/A	0.9127	1.210 3	1.60	M	Brain	20	0.76
306	14	4	0.474	0.4115 26	N/A	0.9666	6.129 1	1.08	M	Brain	20	0.76
307	14	2.9	0.526	0.325	N/A	0.9521	1.309	1.35	M	Brain	20	0.76
308	14	0	0.702	0.6177	N/A	0.9852	0.990 2	1.27	M	Brain	20	0.76
309	14	8.9	0.100 8	0.018	N/A	0.4135	6.48	3.06	R	Brain	20	0.76
310	14	8.9	0.112 5	0.036	N/A	0.5895	6.35	1.78	R	Brain	20	0.76
311	14	8.3	0.135 7	0.024	N/A	0.4861	8.91	3.11	R	Brain	20	0.76

312	14	8.8	0.1386	0.012	N/A	0.3184	42	6.18	R	Brain	20	0.76
313	14	8.6	0.1727	0.055	N/A	0.6912	20.5	1.84	R	Brain	20	0.76
314	14	8.8	0.1788	0.044	N/A	0.6390	19.7	2.32	R	Brain	20	0.76
315	14	8.3	0.1848	0.018	N/A	0.4135	71	5.55	R	Brain	20	0.76
316	14	5.5	0.1411	0.026	N/A	0.5066	2.2	3.03	R	Brain	20	0.76
317	14	5.7	0.3652	0.24029	N/A	0.9240	2.36	1.18	R	Brain	20	0.76
318	14	5.5	0.1111	0.107	N/A	0.8217	1.79	0.73	R	Brain	20	0.76
319	14	0	0.196	0.035	N/A	0.5825	2.45	3.17	R	Brain	20	0.76
320	14	5.8	0.356	0.124	N/A	0.8448	2.725	1.87	R	Brain	20	0.76
321	14	4.1	0.5099	0.709	N/A	0.9894	1.57	0.88	R	Brain	20	0.76
322	14	4.8	0.3053	0.133	N/A	0.8551	1.7315	1.54	R	Brain	20	0.76
323	14	0	0.1031	0.04	N/A	0.6158	3.81	1.52	R	Brain	20	0.76
324	14	0	0.1131	0.252	N/A	0.9284	0.405	0.42	R	Brain	20	0.76
325	14	0	0.1162	0.057	N/A	0.6992	1.83	1.25	R	Brain	20	0.76
326	14	0	0.1172	0.076	N/A	0.7598	0.686	1.00	R	Brain	20	0.76
327	14	0	0.1213	0.09	N/A	0.7918	0.477	0.90	R	Brain	20	0.76
328	14	0	0.125	0.121	N/A	0.8411	0.86	0.74	R	Brain	20	0.76
329	14	0	0.135	0.082	N/A	0.7745	2.49	1.06	R	Brain	20	0.76
330	14	4.7	0.1634	0.06	N/A	0.7106	2.75	1.65	R	Brain	20	0.76
331	14	0	0.1649	0.117	N/A	0.8360	1.65	0.96	R	Brain	20	0.76
332	14	0	0.1821	0.067	N/A	0.7342	1.12	1.66	R	Brain	20	0.76
333	14	0	0.1904	0.128	N/A	0.8495	1.17	1.02	R	Brain	20	0.76
334	14	0	0.193	0.06309	N/A	0.7214	1.94	1.84	R	Brain	20	0.76
335	14	0	0.208	0.145	N/A	0.8671	1.51	1.01	R	Brain	20	0.76
336	14	0	0.248	0.199	N/A	0.9053	1.96	0.94	R	Brain	20	0.76
337	14	0	0.2496	0.1	N/A	0.8104	2.38	1.60	R	Brain	20	0.76
338	14	0	0.2518	0.162	N/A	0.8815	1.41	1.11	R	Brain	20	0.76
339	14	0	0.2519	0.118	N/A	0.8373	1.9	1.41	R	Brain	20	0.76
340	14	0	0.2539	0.191	N/A	0.9008	0.5247	0.99	R	Brain	20	0.76
341	14	0	0.255	0.054	N/A	0.6871	3.815	2.76	R	Brain	20	0.76
342	14	0	0.2565	0.102	N/A	0.8137	2.14	1.61	R	Brain	20	0.76
343	14	0	0.264	0.614	N/A	0.9839	0.551	0.53	R	Brain	20	0.76
344	14	0	0.2759	0.151	N/A	0.8725	0.859	1.27	R	Brain	20	0.76
345	14	0	0.2855	0.288	N/A	0.9396	1.115	0.84	R	Brain	20	0.76
346	14	0	0.2885	0.098	N/A	0.8069	2.38	1.86	R	Brain	20	0.76
347	14	0	0.2902	0.195	N/A	0.9031	0.6345	1.10	R	Brain	20	0.76
348	14	0	0.3017	0.111	N/A	0.8277	2.5	1.75	R	Brain	20	0.76
349	14	0	0.306	0.148	N/A	0.8698	0.997	1.42	R	Brain	20	0.76

350	14	0	0.307 5	0.168	N/A	0.8859	2.16	1.29	R	Brain	20	0.76
351	14	0	0.310 5	0.265	N/A	0.9327	1.175	0.95	R	Brain	20	0.76
352	14	0	0.332 9	0.087	N/A	0.7856	3.183 1	2.35	R	Brain	20	0.76
353	14	2.9	0.344	0.202	N/A	0.9069	1.65	1.26	R	Brain	20	0.76
354	14	2.6	0.345 7	0.138	N/A	0.8603	1.33	1.68	R	Brain	20	0.76
355	14	0	0.348 6	0.209	N/A	0.9104	1.34	1.24	R	Brain	20	0.76
356	14	0	0.350 3	0.259	N/A	0.9308	1.19	1.08	R	Brain	20	0.76
357	14	0	0.366 6	0.348	N/A	0.9536	1.055 5	0.94	R	Brain	20	0.76
358	14	3.4	0.407	0.237	N/A	0.9228	3	1.31	R	Brain	20	0.76
359	14	0	0.412	0.306	N/A	0.9443	2.85	1.13	R	Brain	20	0.76
360	14	0	0.443 8	0.2415 73	N/A	0.9245	1.51	1.41	R	Brain	20	0.76
361	14	0	0.444 1	0.378	N/A	0.9590	1.41	1.06	R	Brain	20	0.76
362	14	0	0.468	0.324	N/A	0.9485	1.6	1.22	R	Brain	20	0.76
363	14	4.7	0.480 6	0.944	N/A	0.9985	1.08	0.74	R	Brain	20	0.76
364	14	2.9	0.482	0.325	N/A	0.9488	2.055	1.25	R	Brain	20	0.76
365	14	4	0.484	0.4115 26	N/A	0.9642	1.09	1.09	R	Brain	20	0.76
366	14	0	0.491 8	0.34	N/A	0.9520	1.32	1.24	R	Brain	20	0.76
367	14	0	0.495 5	0.613	N/A	0.9839	0.896	0.91	R	Brain	20	0.76
368	14	4.7	0.502 3	0.421	N/A	0.9655	1.24	1.12	R	Brain	20	0.76
369	14	0	0.527 9	0.426	N/A	0.9662	0.529	1.16	R	Brain	20	0.76
370	14	0	0.532 4	0.385	N/A	0.9601	0.597	1.24	R	Brain	20	0.76
371	14	2.7	0.552 3	0.41	N/A	0.9639	1.87	1.24	R	Brain	20	0.76
372	14	0	0.561 7	0.391	N/A	0.9611	1.29	1.29	R	Brain	20	0.76
373	14	0	0.587	0.091	N/A	0.7938	2.43	3.92	R	Brain	20	0.76
374	14	0	0.612 1	0.275	N/A	0.9359	1.38	1.74	R	Brain	20	0.76
375	14	0	0.662 1	0.722	N/A	0.9901	1.42	1.10	R	Brain	20	0.76
376	14	0	0.763 6	0.771	N/A	0.9923	0.665 5	1.22	R	Brain	20	0.76
377	14	0	0.843 4	0.293	N/A	0.9410	1.15	2.26	R	Brain	20	0.76
378	14	3.1	0.129 3	0.049	N/A	0.6646	3.2	1.58	R	Brain	20	0.76
379	14	2.2	0.147 7	0.021	N/A	0.4521	4.09	3.88	R	Brain	20	0.76
380	14	2.5	0.211 1	0.165	N/A	0.8837	1.21	0.93	R	Brain	20	0.76
381	14	2.2	0.350 6	0.097	N/A	0.8051	2.47	2.26	R	Brain	20	0.76
382	14	9.5	0.294 8	0.6317 15	N/A	0.9851	2.725	0.55	R	Brain	20	0.76
383	14	2.7	0.204 5	N/A	0.075	0.8528	1.13	1.09	C	Lung	20	0.76
384	14	2.7	0.509 2	N/A	0.2252	0.9540	1.27	1.27	C	Lung	20	0.76
385	14	2.7	0.215 3	N/A	0.075	0.8528	0.809	1.12	D	Lung	20	0.76
386	14	2.7	0.465 6	N/A	0.2252	0.9540	0.78	1.12	D	Lung	20	0.76

387	14	8.4	0.085 2	N/A	0.018	0.5670	0.539	1.50	M	Lung	20	0.76
388	14	8.4	0.123 7	N/A	0.028	0.6729	1.5	1.45	M	Lung	20	0.76
389	14	8.4	0.136 6	N/A	0.039	0.7435	1.79	1.21	M	Lung	20	0.76
390	14	8.4	0.157 9	N/A	0.041	0.7533	0.61	1.33	M	Lung	20	0.76
391	14	2.7	0.201 9	N/A	0.075	0.8528	2.29	1.09	M	Lung	20	0.76
392	14	2.7	0.425 5	N/A	0.2252	0.9540	0.934	1.10	M	Lung	20	0.76
393	14	2.7	0.184 8	N/A	0.075	0.8528	2.12	0.98	R	Lung	20	0.76
394	14	8.4	0.215 3	N/A	0.041	0.7533	5.99	1.76	R	Lung	20	0.76
395	8.8	8.5	0.265 4	N/A	0.0634	0.8286	14	1.52	R	Lung	20	0.76
396	14	2.7	0.394 6	N/A	0.2252	0.9540	1.62	1.00	R	Lung	20	0.76

Table S3. Calculated f_{mic} from physiochemical properties for V_d predictions

Compound Name	c_pKa_MA	c_pKa_MB	fup	Expfomic (1mg/mL)	Calcfomic (1mg/mL)	VDss	VDss predicted (expfomic)	VDss predicted (calcfomic)	Species	a	b
1	14	6.7	0.14	0.8182	0.6129	0.87	0.92	2.07	C	20	0.76
2	14	6.7	0.19	1.0000	0.6807	0.77	0.37	2.15	C	20	0.76
3	14	6.4	0.33	0.8692	0.7241	0.9	1.54	3.06	C	20	0.76
4	14	6.7	0.29	0.6807	0.7699	0.92	3.22	2.23	C	20	0.76
5	6.5	8	0.087	1.0000	0.8692	0.27	0.23	0.49	C	20	0.76
6	14	3.4	0.48	0.9231	0.9048	1.2	1.54	1.75	C	20	0.76
7	14	6.7	0.08	0.8182	0.6129	0.49	0.56	1.22	D	20	0.76
8	14	6.7	0.14	1.0000	0.6807	0.56	0.28	1.59	D	20	0.76
9	14	6.7	0.06	1.0000	0.7094	0.44	0.18	0.68	D	20	0.76
10	14	6.4	0.24	0.8692	0.7241	0.93	1.13	2.23	D	20	0.76
11	14	6.7	0.22	0.6807	0.7699	0.51	2.44	1.69	D	20	0.76
12	6.5	8	0.15	1.0000	0.8692	0.9	0.29	0.74	D	20	0.76
13	14	3.4	0.41	0.9231	0.9048	0.99	1.29	1.47	D	20	0.76
14	14	5.3	0.014	0.1429	0.0417	0.95	1.82	6.58	M	20	0.76
15	6.6	2.3	0.0017	0.0267	0.0526	3.4	1.37	0.74	M	20	0.76
16	14	9.9	0.045	0.4085	0.0989	2.3	1.45	8.34	M	20	0.76
17	4.2	3.5	0.003	0.1494	0.1561	0.43	0.47	0.45	M	20	0.76
18	14	9.9	0.0079	0.1236	0.1628	0.74	1.21	0.91	M	20	0.76
19	6.6	2.3	0.0054	0.1561	0.2195	1.7	0.72	0.52	M	20	0.76
20	4	0	0.0097	0.2500	0.2270	5.1	0.72	0.80	M	20	0.76
21	6.6	2.3	0.0049	0.1765	0.2500	1.9	0.59	0.42	M	20	0.76
22	6.3	4.3	0.002	0.2346	0.2579	0.33	0.26	0.24	M	20	0.76
23	14	6.4	0.31	0.7699	0.2821	0.79	2.39	16.32	M	20	0.76
24	8.1	9.9	0.1	0.6129	0.2903	1.4	1.48	5.11	M	20	0.76
25	6.3	8.8	0.0077	0.1765	0.3072	1.4	0.85	0.48	M	20	0.76
26	8	9.9	0.22	0.6260	0.3333	2.6	3.01	9.18	M	20	0.76
27	14	9.9	0.017	0.2422	0.3514	1.7	1.17	0.73	M	20	0.76
28	5.3	6	0.0096	0.0989	0.3605	1.4	1.89	0.48	M	20	0.76
29	14	5.8	0.034	0.1494	0.3605	0.52	4.04	1.38	M	20	0.76
30	5.8	8.7	0.011	0.1561	0.3889	0.85	1.33	0.48	M	20	0.76
31	6.2	8.4	0.02	0.6949	0.4085	0.32	0.33	0.73	M	20	0.76
32	4.3	3.7	0.03	0.9231	0.4493	0.54	0.21	0.90	M	20	0.76
33	6.8	8.4	0.093	0.6667	0.4493	0.62	1.18	2.53	M	20	0.76
34	8	9.9	0.052	0.5873	0.4599	1.3	0.89	1.38	M	20	0.76
35	14	9.1	0.031	0.0753	0.4706	9.4	7.74	0.82	M	20	0.76
36	14	6.4	0.067	1.0000	0.4925	0.74	0.21	1.59	M	20	0.76
37	14	6.7	0.039	0.7544	0.5038	2.1	0.43	0.94	M	20	0.76
38	3.9	3.3	0.011	1.0000	0.5504	0.42	0.14	0.32	M	20	0.76
39	14	6.5	0.031	0.9048	0.5748	0.26	0.23	0.62	M	20	0.76
40	14	6.5	0.042	0.7391	0.5748	0.67	0.48	0.80	M	20	0.76
41	14	6.7	0.058	0.9802	0.6000	0.7	0.22	0.97	M	20	0.76
42	14	6.7	0.057	0.8182	0.6129	0.7	0.45	0.92	M	20	0.76
43	6.5	0	0.0078	1.0000	0.6260	0.38	0.13	0.23	M	20	0.76
44	6.3	8.8	0.046	0.5385	0.6260	1	0.97	0.73	M	20	0.76
45	14	4.5	0.067	0.4925	0.6260	0.76	1.59	1.01	M	20	0.76
46	14	6.7	0.12	0.7544	0.6260	0.7	1.06	1.72	M	20	0.76
47	14	8.6	0.55	0.9231	0.6529	2.4	1.75	6.68	M	20	0.76
48	8.8	8.5	0.19	0.8868	0.6667	11	0.83	2.24	M	20	0.76
49	14	6.7	0.069	1.0000	0.6807	0.44	0.22	0.86	M	20	0.76
50	14	6.7	0.14	1.0000	0.7094	0.51	0.31	1.46	M	20	0.76
51	4.3	3.6	0.0065	0.6393	0.7241	0.32	0.21	0.18	M	20	0.76
52	14	6.4	0.12	0.8692	0.7241	0.49	0.64	1.20	M	20	0.76
53	14	6.4	0.12	0.8692	0.7241	0.6	0.64	1.20	M	20	0.76
54	14	6.7	0.21	0.6807	0.7699	0.56	2.37	1.66	M	20	0.76
55	14	6.7	0.081	0.8519	0.7857	0.49	0.51	0.67	M	20	0.76
56	5.2	4.2	0.029	0.7241	0.8018	0.48	0.38	0.31	M	20	0.76
57	14	8.2	0.062	0.1976	0.8018	3	5.20	0.47	M	20	0.76
58	4	0	0.14	0.9608	0.8018	1.1	0.42	1.00	M	20	0.76
59	14	3.3	0.22	1.0000	0.8018	2.9	0.42	1.50	M	20	0.76
60	14	6.7	0.087	0.8692	0.8349	0.67	0.50	0.58	M	20	0.76

61	14	8.1	0.12	0.3333	0.8349	5.2	5.05	0.72	M	20	0.76
62	14	6.7	0.14	0.9417	0.8519	0.58	0.48	0.80	M	20	0.76
63	6.5	8	0.046	1.0000	0.8692	0.5	0.19	0.32	M	20	0.76
64	6.6	2.3	0.05	0.9231	0.8692	1.4	0.27	0.34	M	20	0.76
65	14	3.4	0.39	0.9231	0.9048	2.8	1.29	1.46	M	20	0.76
66	6.5	4.2	0.39	1.0000	0.9417	0.41	0.64	1.12	M	20	0.76
67	14	0	0.0023	0.0320	0.0050	2.5	1.50	9.21	R	20	0.76
68	14	8.6	0.0068	0.0096	0.0050	6.1	14.12	27.00	R	20	0.76
69	14	4.4	0.001	0.0045	0.0582	5.2	4.51	0.43	R	20	0.76
70	14	4.7	0.005	0.0277	0.0811	3.1	3.61	1.24	R	20	0.76
71	14	4.6	0.0045	0.0262	0.0929	4.3	3.46	0.99	R	20	0.76
72	4.2	3.5	0.0014	0.1494	0.1561	0.34	0.26	0.26	R	20	0.76
73	14	4.5	0.037	0.2903	0.1976	6.7	1.96	3.16	R	20	0.76
74	14	0	0.024	0.2121	0.2422	3.5	1.92	1.64	R	20	0.76
75	8.9	6.3	0.31	1.0000	0.3245	1.1	0.51	13.41	R	20	0.76
76	14	5.8	0.021	0.1494	0.3605	9.1	2.52	0.87	R	20	0.76
77	14	8.6	0.16	0.4388	0.3986	5.1	4.37	5.11	R	20	0.76
78	14	0	0.0075	0.9608	0.4184	1.2	0.12	0.32	R	20	0.76
79	4.3	3.7	0.027	0.9231	0.4493	1.1	0.18	0.80	R	20	0.76
80	14	6.3	0.074	0.7094	0.4706	1.6	0.81	1.86	R	20	0.76
81	14	3.9	0.095	0.6529	0.4925	1.3	1.24	2.18	R	20	0.76
82	14	6.4	0.096	1.0000	0.4925	0.64	0.23	2.21	R	20	0.76
83	14	6.3	0.1	0.8018	0.4925	2.3	0.73	2.29	R	20	0.76
84	14	6.4	0.16	0.9802	0.4925	1	0.38	3.61	R	20	0.76
85	14	8.2	0.047	0.3245	0.5267	2.9	2.08	0.97	R	20	0.76
86	14	6.3	0.073	0.6949	0.5267	0.78	0.84	1.51	R	20	0.76
87	14	6.1	0.12	0.6393	0.5504	2.5	1.61	2.22	R	20	0.76
88	14	6.5	0.0041	0.9048	0.5748	0.22	0.12	0.17	R	20	0.76
89	14	6.3	0.11	0.9231	0.6000	0.59	0.43	1.71	R	20	0.76
90	14	6.1	0.24	0.7857	0.6000	2.9	1.72	3.62	R	20	0.76
91	14	6.7	0.071	0.8182	0.6129	0.65	0.51	1.09	R	20	0.76
92	5	10.1	0.54	0.9231	0.6129	3.1	1.71	7.63	R	20	0.76
93	14	4.5	0.037	0.4925	0.6260	2.5	0.91	0.59	R	20	0.76
94	14	6.7	0.16	0.7544	0.6260	0.72	1.35	2.22	R	20	0.76
95	14	6.4	0.31	1.0000	0.6260	1.2	0.51	4.21	R	20	0.76
96	14	6.7	0.11	0.7391	0.6393	0.79	1.02	1.49	R	20	0.76
97	14	6.7	0.077	0.6807	0.6529	0.95	0.93	1.02	R	20	0.76
98	14	6.3	0.13	0.8349	0.6529	1.9	0.79	1.65	R	20	0.76
99	14	6.4	0.35	1.0000	0.6529	0.92	0.56	4.28	R	20	0.76
100	14	8.6	0.43	0.9231	0.6529	4	1.36	5.21	R	20	0.76
101	14	6.7	0.055	0.6000	0.6667	0.41	0.91	0.72	R	20	0.76
102	14	6.7	0.059	0.4493	0.6667	0.57	1.63	0.77	R	20	0.76
103	14	6.4	0.1	0.8519	0.6667	0.94	0.58	1.23	R	20	0.76
104	14	6.1	0.13	0.6667	0.6667	2.6	1.57	1.57	R	20	0.76
105	5	9.1	0.22	0.7544	0.6667	1.4	1.82	2.59	R	20	0.76
106	8.8	8.5	0.35	0.8868	0.6667	14	1.43	4.03	R	20	0.76
107	14	6.7	0.09	1.0000	0.6807	0.55	0.22	1.06	R	20	0.76
108	5	10	0.46	1.0000	0.6807	2.7	0.70	5.02	R	20	0.76
109	14	0	0.025	0.8519	0.7094	0.62	0.22	0.34	R	20	0.76
110	14	6.7	0.11	1.0000	0.7094	0.59	0.25	1.15	R	20	0.76
111	14	6.4	0.14	0.8692	0.7241	0.97	0.71	1.35	R	20	0.76
112	14	6.4	0.16	0.8692	0.7241	0.76	0.79	1.53	R	20	0.76
113	5.3	8.9	0.41	0.2195	0.7391	0.57	29.79	3.53	R	20	0.76
114	14	6.7	0.074	0.6529	0.7544	0.52	0.99	0.68	R	20	0.76
115	5	8	0.13	0.8182	0.7544	1.1	0.85	1.12	R	20	0.76
116	5.3	9.3	0.19	0.3793	0.7544	3.3	6.57	1.59	R	20	0.76
117	5	9.1	0.27	0.9608	0.7544	1.3	0.67	2.21	R	20	0.76
118	14	6.4	0.3	0.9608	0.7544	0.97	0.74	2.45	R	20	0.76
119	14	6.7	0.052	0.6129	0.7699	0.45	0.83	0.48	R	20	0.76
120	14	6.7	0.063	0.7699	0.7699	0.52	0.56	0.56	R	20	0.76
121	14	6.7	0.19	0.6393	0.7699	0.7	2.49	1.49	R	20	0.76
122	14	6.7	0.21	0.6807	0.7699	0.95	2.35	1.63	R	20	0.76
123	14	6.4	0.34	0.9802	0.7699	0.89	0.68	2.58	R	20	0.76
124	14	6.7	0.056	0.6529	0.7857	0.38	0.77	0.48	R	20	0.76
125	14	6.4	0.052	0.8868	0.8018	0.44	0.30	0.43	R	20	0.76
126	14	6.7	0.067	0.7391	0.8018	0.49	0.66	0.52	R	20	0.76

127	14	6.4	0.23	0.9231	0.8018	1	0.79	1.54	R	20	0.76
128	14	3.8	0.24	0.8692	0.8018	1.5	1.14	1.60	R	20	0.76
129	14	6.7	0.087	0.8868	0.8182	0.72	0.44	0.60	R	20	0.76
130	14	6.7	0.12	0.8349	0.8182	0.65	0.73	0.79	R	20	0.76
131	14	3.8	0.33	0.9802	0.8182	1.8	0.67	2.00	R	20	0.76
132	14	0	0.73	0.8349	0.8182	0.87	3.94	4.30	R	20	0.76
133	14	8.1	0.1	0.3333	0.8349	6.2	4.20	0.59	R	20	0.76
134	14	6.4	0.31	0.8349	0.8349	1	1.73	1.73	R	20	0.76
135	14	6.4	0.36	0.9231	0.8349	0.82	1.17	2.00	R	20	0.76
136	14	6.7	0.38	0.7857	0.8349	0.92	2.67	2.10	R	20	0.76
137	14	6.4	0.41	1.0000	0.8349	0.86	0.64	2.26	R	20	0.76
138	14	6.4	0.12	0.8018	0.8519	0.92	0.85	0.68	R	20	0.76
139	14	9	0.29	0.9608	0.8519	1.3	0.69	1.46	R	20	0.76
140	14	6.2	0.29	1.0000	0.8519	2.6	0.48	1.49	R	20	0.76
141	14	6.7	0.073	0.6260	0.8692	0.39	1.07	0.42	R	20	0.76
142	14	6.7	0.088	0.8519	0.8692	0.54	0.52	0.48	R	20	0.76
143	6.5	8	0.12	1.0000	0.8692	0.89	0.26	0.62	R	20	0.76
144	14	6.7	0.18	0.9417	0.8692	0.63	0.56	0.88	R	20	0.76
145	14	0	0.72	1.0000	0.8692	0.93	1.04	3.21	R	20	0.76
146	14	8	0.19	0.9048	0.8868	0.91	0.72	0.80	R	20	0.76
147	14	3.8	0.27	0.7857	0.8868	1.6	1.93	1.14	R	20	0.76
148	14	3.8	0.48	1.0000	0.8868	1.5	0.73	1.95	R	20	0.76
149	14	0	0.77	0.9802	0.8868	0.83	1.42	3.07	R	20	0.76
150	3.3	8.1	0.038	0.8692	0.9048	5.6	0.27	0.23	R	20	0.76
151	14	0	0.85	1.0000	0.9231	0.86	1.21	2.63	R	20	0.76
152	14	6.4	0.16	0.6949	0.9417	0.54	1.72	0.51	R	20	0.76
153	14	6.7	0.22	0.9608	0.9417	0.49	0.57	0.66	R	20	0.76
154	14	8.2	0.39	0.5748	0.9417	7.8	6.36	1.07	R	20	0.76
155	14	6.5	0.45	0.7857	0.9417	2.6	3.14	1.25	R	20	0.76
156	14	2.3	0.66	1.0000	0.9417	1.7	0.96	1.78	R	20	0.76
157	14	0	0.69	0.9048	0.9417	1.2	2.45	1.85	R	20	0.76
158	14	0	0.7	1.0000	0.9417	0.91	1.01	1.88	R	20	0.76
159	14	0	0.77	1.0000	0.9417	0.93	1.11	2.06	R	20	0.76
160	14	8.1	0.62	0.6667	1.0000	4.8	7.10	0.90	R	20	0.76