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SUPPLEMENTARY MATERIAL TO  
**Estimation of the volume of distribution of some  
pharmacologically important compounds from  
their structural descriptors**

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TABLE I-S. Data set and the corresponding observed values as well as MLR and ANN calculated values of  $V_d$  (int and ext denote the internal and external test set, respectively)

No	Name	$\log(V_d)_{\text{EXP}}$	$\log(V_d)_{\text{MLR}}$	Deviation	$\log(V_d)_{\text{ANN}}$	Deviation
1	Acetanilide	-0.797	-0.096	-0.701	-0.663	-0.134
2	Alprazolam	-0.064	0.333	-0.397	0.034	-0.098
3	Amitriptyline	1.025	1.362	-0.337	1.079	-0.053
4	Amobarbital	0.021	-0.489	0.510	-0.027	0.048
5	Amoxicillin	-0.072	-0.578	0.506	-0.096	0.024
6	Amphetamine <sub>int</sub>	0.592	0.520	0.072	1.038	-0.446
7	Ampicillin	-0.214	-0.448	0.235	-0.230	0.016
8	Bromazepam	0.053	0.269	-0.215	0.038	0.016
9	Bupivacaine	0.001	0.625	-0.624	-0.043	0.044
10	Bupropion	1.208	0.645	0.562	1.071	0.137
11	Butorphanol	0.697	0.297	0.400	0.564	0.133
12	Caffeine	-0.259	-0.153	-0.106	-0.327	0.068
13	Carbamazepine	0.078	-0.327	0.405	0.034	0.044
14	Carbenicillin	-0.603	-0.643	0.040	-0.525	-0.077
15	Cefazolin <sub>ext</sub>	-0.769	-0.056	-0.713	-0.497	-0.272
16	Cephalexin	-0.469	-0.501	0.032	-0.582	0.113
17	Cephaloridine	-0.639	-0.201	-0.438	-0.623	-0.017
18	Cephalothin	-0.376	-0.355	-0.021	-0.432	0.056
19	Cephradine	-0.356	-0.327	-0.029	-0.218	-0.138
20	Chloral hydrate <sub>ext</sub>	-0.222	-0.363	0.141	-0.161	-0.061
21	Chloramphenicol	-0.242	0.151	-0.393	-0.238	-0.004
22	Chlordiazepoxide	-0.445	0.171	-0.616	-0.238	-0.207
23	Chloroquine	2.050	0.982	1.068	1.816	0.234
24	Chlorphentermine	0.398	0.678	-0.280	0.609	-0.211
25	Chlortetracycline	0.207	-0.295	0.502	0.098	0.109
26	Clindamycin	0.001	-0.250	0.251	-0.007	0.008

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TABLE I-S. Continued

No	Name	$\log (V_d)_{\text{EXP}}$	$\log (V_d)_{\text{MLR}}$	Deviation	$\log (V_d)_{\text{ANN}}$	Deviation
27	Clobazam	0.049	-0.096	0.145	0.005	0.044
28	Clomipramine	1.232	1.042	0.190	1.423	-0.191
29	Clonazepam	0.495	-0.100	0.595	0.467	0.028
30	Clorazepate	-0.036	-0.222	0.186	0.001	-0.037
31	Cloxacillin	-0.826	-0.299	-0.527	-0.789	-0.037
32	Cyclacillin	-0.396	-0.473	0.077	-0.238	-0.158
33	Demeclocycline <sub>ext</sub>	0.252	0.265	-0.013	0.378	-0.126
34	Desipramine <sub>ext</sub>	1.479	0.986	0.493	1.059	0.420
35	Diazepam <sub>ext</sub>	0.284	0.135	0.149	-0.068	0.352
36	Dicloxacillin	-0.886	-0.493	-0.393	-0.935	0.048
37	Doxepine <sub>ext</sub>	1.102	1.172	-0.070	1.059	0.044
38	Doxycycline <sub>ext</sub>	-0.129	0.054	-0.183	0.163	-0.292
39	Ethambutol	0.126	0.058	0.068	0.127	-0.001
40	Ethchlorvynol	0.398	0.508	-0.110	0.427	-0.029
41	Ethosuximide	-0.173	-0.558	0.384	-0.104	-0.069
42	Etidocaine	0.300	0.556	-0.256	0.240	0.060
43	Fentanyl 3.60e	0.556	0.188	0.368	0.714	-0.159
44	Flunitrazepam	0.600	-0.116	0.716	0.670	-0.070
45	Fluoxetine <sub>int</sub>	1.649	0.738	0.911	1.362	0.287
46	Gentamycin	-0.554	-0.412	-0.142	-0.615	0.060
47	Glutethimide	0.495	-0.068	0.562	0.508	-0.013
48	Griseofulvin	0.240	0.175	0.064	0.228	0.012
49	Haloperidol	1.200	0.609	0.591	1.302	-0.102
50	Hetacillin	-0.396	-0.493	0.097	-0.331	-0.065
51	Ibuprofen	-1.000	-0.169	-0.831	-0.991	-0.008
52	Imipramine	1.216	10.156	0.060	1.071	0.145
53	Indomethacin	-0.024	0.192	-0.215	-0.007	-0.017
54	Isoniazid	-0.194	-0.250	0.056	-0.153	-0.041
55	Kanamycin <sub>int</sub>	-0.720	-0.197	-0.523	-0.874	0.154
56	Ketamine	0.600	0.313	0.287	0.662	-0.061
57	Lidocaine <sub>ext</sub>	0.151	0.309	-0.159	0.244	-0.094
58	Lincomycin	-0.481	-1.048	0.567	-0.380	-0.102
59	Lorazepam	0.078	-0.043	0.121	0.078	-0.001
60	Maprotiline <sub>ext</sub>	1.321	0.860	0.461	1.516	-0.195
61	Meprobamate	-0.153	0.054	-0.207	-0.173	0.020
62	Meptazinol	0.738	0.544	0.194	0.819	-0.082
63	Methacycline	-0.011	-0.282	0.271	-0.092	0.081
64	Methadone	0.531	0.212	0.319	0.483	0.048
65	Methaqualone <sub>int</sub>	0.778	0.933	-0.155	1.059	-0.280
66	Meticillin	-0.445	-0.509	0.064	-0.424	-0.021
67	Metoclopramide	0.479	0.094	0.384	0.467	0.012
68	Midazolam <sub>int</sub>	0.114	0.439	-0.325	0.471	-0.357
69	Minocycline	-0.125	-0.072	-0.053	-0.124	0.000
70	Moclobemide	0.110	0.528	-0.418	0.127	-0.017
71	Morphine	0.458	0.439	0.020	0.341	0.117
72	Nafcillin	-0.538	-0.473	-0.065	-0.534	-0.004

TABLE I-S. Continued

No	Name	$\log (V_d)_{\text{EXP}}$	$\log (V_d)_{\text{MLR}}$	Deviation	$\log (V_d)_{\text{ANN}}$	Deviation
73	Naloxone	0.479	0.678	-0.199	0.528	-0.049
74	Neomycin(a)	-2.000	-0.343	-1.657	-1.749	-0.251
75	Nitrazepam <sub>int</sub>	0.349	-0.108	0.457	0.973	-0.624
76	Nitrofurantoin	-0.493	-0.258	-0.235	-0.254	-0.239
77	Nortriptyline	1.313	1.289	0.023	1.249	0.064
78	Oxacillin	-0.538	-0.242	-0.296	-0.785	0.247
79	Oxazepam	-0.003	0.155	-0.158	-0.254	0.251
80	Oxyphenbutazone	-0.959	-0.315	-0.644	-0.906	-0.053
81	Oxytetracycline	0.276	-0.080	0.356	0.090	0.186
82	Paracetamol	0.082	-0.096	0.178	-0.019	0.101
83	Paroxetine	1.366	0.629	0.736	1.281	0.084
84	PAS	-0.639	-0.339	-0.300	-0.505	-0.134
85	Penicillin G	-0.169	-0.566	0.397	-0.189	0.020
86	Penicillin V	-0.153	-0.659	0.506	-0.201	0.048
87	Pethidine	0.701	0.107	0.595	0.625	0.076
88	Phenacetin	0.118	0.269	-0.150	0.082	0.036
89	Phenazone	-0.003	-0.197	0.194	-0.080	0.076
90	Phencyclidine	0.778	0.256	0.522	0.791	-0.013
91	Phenethicillin K	-0.457	-0.469	0.012	-0.286	-0.171
92	Phenobarbital <sub>int</sub>	-0.097	-0.380	0.283	-0.797	0.700
93	Phenylbutazone <sub>ext</sub>	-0.826	-0.274	-0.551	-0.444	-0.381
94	Phenytoin	-0.222	0.143	-0.365	-0.153	-0.069
95	Prazepam	0.175	0.204	-0.029	0.297	-0.122
96	Primidone	-0.003	-0.068	0.064	-0.242	0.239
97	Propofol	0.543	0.220	0.323	0.601	-0.057
98	Protriptyline	1.167	1.127	0.040	1.111	0.056
99	Pyrimethamine	0.341	0.236	0.105	0.390	-0.049
100	Quinine sulfate <sub>int</sub>	0.211	0.297	-0.086	-0.068	0.279
101	Rolietracycline	-0.238	-0.367	0.129	-0.323	0.085
102	Salicylamide <sub>int</sub>	-0.826	-0.380	-0.446	-1.012	0.186
103	Sertraline	1.301	0.828	0.473	1.298	0.003
104	Spectinomycin	-0.923	-0.112	-0.810	-0.971	0.048
105	Sulbenicillin	-0.700	-0.598	-0.102	-0.671	-0.029
106	Sulfadiazine	-0.036	-0.420	0.384	-0.100	0.064
107	Sulfadimethoxine <sub>ext</sub>	-0.388	-0.286	-0.102	-0.704	0.316
108	Sulfadoxine	-0.923	-0.440	-0.482	-0.813	-0.110
109	Sulfaethidole <sub>int</sub>	-0.745	-0.517	-0.227	-0.817	0.073
110	Sulfamerazine <sub>ext</sub>	-0.408	-0.367	-0.041	-0.469	0.060
111	Sulfameter	-0.587	-0.238	-0.349	-0.550	-0.037
112	Sulfamethazine	-0.214	-0.339	0.125	-0.234	0.020
113	Sulfamethizole <sub>int</sub>	-0.457	0.123	-0.580	-1.080	0.623
114	Sulfamethopyrazine	-0.659	-0.359	-0.300	-0.590	-0.069
115	Sulfamethoxazole	-0.659	-0.254	-0.405	-0.505	-0.154
116	Sulfamethoxypyridazine	-0.720	-0.845	0.125	-0.732	0.012
117	Sulfinpyrazone	-1.000	0.293	-1.293	-1.016	0.016
118	Sulfisomidine	-0.493	-0.307	-0.187	-0.752	0.259

TABLE I-S. Continued

No	Name	$\log (V_d)_{EXP}$	$\log (V_d)_{MLR}$	Deviation	$\log (V_d)_{ANN}$	Deviation
119	Sulfisoxazole <sub>int</sub>	-0.769	-0.436	-0.332	-0.833	0.065
120	Sulfisoxazole acetyl	0.074	-0.222	0.295	-0.534	0.607
121	Temazepam	-0.007	0.192	-0.199	-0.112	0.105
122	Tetracycline	0.147	0.017	0.129	0.167	-0.021
123	Theobromine	-0.125	-0.120	-0.005	0.090	-0.215
124	Tinidazole	-0.408	-0.323	-0.085	-0.335	-0.073
125	Tramadol <sub>int</sub>	0.479	0.406	0.072	-0.169	0.648
126	Triazolam	0.041	0.394	-0.353	0.038	0.004
127	Trimethoprim <sub>ext</sub>	0.381	0.204	0.178	-0.303	0.684
128	Valproic acid	-0.769	-1.020	0.251	-0.744	-0.025
129	Viloxazine	0.001	0.159	-0.158	0.026	-0.025