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Table 5.Calculated chemical physical parameters of compounds **1-34**

N	MDR-reverting activity (μM; α=0.5)	volume[a] (Å^3)	Van der Waals surface[a] (Å^2)	Connolly surface[a] (Å^2)	logP[b]	MR[b]	MW (base)
1	2.0	361.07	478.068	404.784	4.63	11.95	410.60
2	0.25	377.84	532.233	469.611	5.35	13.50	442.60
3	0.25	392.01	551.199	491.446	5.36	13.96	456.63
4	0.3	398.93	537.997	490.713	6.04	14.25	468.64
5	0.25	365.85	503.941	435.768	5.34	13.40	439.58
6	toxic	380.19	531.441	486.337	5.35	13.86	454.61
7	0.05	392.39	527.560	498.104	6.35	14.37	466.62
8	toxic	390.45	534.961	495.488	6.35	14.37	466.62
9	1.6	n.c.	n.c.	n.c.	4.51	15.87	548.74
10	inactive	375.95	495.792	403.242	4.96	12.42	424.63
11	1.4	389.61	509.707	428.700	5.58	12.88	438.65
12	1	380.67	518.428	450.618	5.62	13.86	454.61
13	2.2	394.47	542.134	483.293	5.67	14.32	468.64
14	2.5	405.51	554.416	497.357	6.64	14.83	480.65
15	0.5	335.18	437.416	396.527	5.29	11.84	384.56
16	2	352.35	478.170	448.219	6.00	13.39	416.56

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17	toxic	366.77	502.087	465.418	6.01	13.85	430.59
18	0.5	371.74	513.192	502.082	6.70	14.14	442.60
19	0.3	339.71	471.613	457.086	5.99	13.28	414.55
20	0.5	365.80	494.296	482.845	7.00	14.25	440.58
21	toxic	364.96	498.286	468.004	7.00	14.25	440.58
22	3	355.40	482.010	460.531	6.28	13.75	428.57
23	2.1	380.67	518.465	499.790	7.29	14.72	454.61
24	0.5	380.65	532.075	463.973	5.77	13.84	452.59
25	0.1	395.69	552.144	475.049	5.78	14.30	466.62
26	1.5	370.79	507.000	449.173	5.76	13.73	450.58
27	2.0	393.71	542.028	502.037	6.77	14.70	476.61
28	0.5	394.52	556.268	464.676	6.77	14.70	476.61
29	0.2	n.c.	n.c.	n.c.	4.94	16.21	558.73
30	0.8	379.76	502.256	400.183	4.88	12.76	434.62
31	1.3	393.88	521.881	421.204	5.50	13.22	448.65
32	0.5	387.15	538.430	440.320	5.54	14.20	464.60
33	toxic	401.98	566.050	469.861	5.59	14.66	478.63
34	toxic	409.81	566.012	498.897	6.56	15.17	490.64

a) Volume, Van der Waals surface and Connolly surface were calculated using the MSI package Insight II (v. 2.3.0/95.0) (MSI, San Diego, CA) implemented on a Risc IBM. The molecules were first generated using the Builder module and minimized with Discover (v. 2.9.7/95.0) using the cvff force-field and the conjugate gradient algorithm. b) The log P and molecular refractivity values of the molecules were calculated using the

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software package ClogP 2.0 (Biobyte Corp., Claremont, CA) implemented on a Pentium 200. This method gives the best approximation to the experimental log P value of verapamil (3.79) calculating a value of 3.71. n.c.) not calculated.