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SUPPLEMENTARY MATERIAL TO

QSAR studies for assessing the acute toxicity of nitrobenzenes to *Tetrahymena pyriformis*

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TABLE S-I. Results of the *y*-randomization validation

Model	R^2	Q^2	Model	R^2	Q^2
Random 1	0.1358	–0.2708	Random 51	0.1478	–0.2123
Random 2	0.4068	–0.0344	Random 52	0.238	–0.2097
Random 3	0.1997	–0.245	Random 53	0.2662	–0.0487
Random 4	0.027	–0.4036	Random 54	0.1726	–0.2493
Random 5	0.1244	–0.2722	Random 55	0.113	–0.5259
Random 6	0.0657	–0.4161	Random 56	0.0907	–0.3946
Random 7	0.1167	–0.4297	Random 57	0.1956	–0.2543
Random 8	0.169	–0.206	Random 58	0.1963	–0.3116
Random 9	0.2548	–0.1416	Random 59	0.0217	–0.4579
Random 10	0.0493	–0.5385	Random 60	0.1344	–0.4856
Random 11	0.0859	–0.5537	Random 61	0.1518	–0.2407
Random 12	0.0817	–0.5627	Random 62	0.2178	–0.1744
Random 13	0.1884	–0.3312	Random 63	0.2399	–0.1354
Random 14	0.0783	–0.3652	Random 64	0.0806	–0.4553
Random 15	0.0815	–0.3685	Random 65	0.0867	–0.4405
Random 16	0.1508	–0.1935	Random 66	0.1739	–0.3648
Random 17	0.2424	–0.0816	Random 67	0.1055	–0.4815
Random 18	0.1629	–0.4217	Random 68	0.1838	–0.4349
Random 19	0.0274	–0.4958	Random 69	0.0963	–0.3776
Random 20	0.0737	–0.2858	Random 70	0.2123	–0.1789
Random 21	0.1724	–0.2384	Random 71	0.2245	–0.1861
Random 22	0.1011	–0.4897	Random 72	0.1035	–0.456
Random 23	0.3505	0.0922	Random 73	0.4003	0.1303
Random 24	0.3104	–0.0892	Random 74	0.1107	–0.2842
Random 25	0.1264	–0.3953	Random 75	0.0527	–0.5697
Random 26	0.2193	–0.195	Random 76	0.1486	–0.2057

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TABLE S-I. Continued

Model	R^2	Q^2	Model	R^2	Q^2
Random 27	0.0714	–0.4154	Random 77	0.1269	–0.3869
Random 28	0.1653	–0.3346	Random 78	0.2844	–0.1379
Random 29	0.1001	–0.2356	Random 79	0.3716	0.0884
Random 30	0.0579	–0.448	Random 80	0.1852	–0.2434
Random 31	0.1234	–0.3085	Random 81	0.0795	–0.4541
Random 32	0.1502	–0.1818	Random 82	0.2168	–0.1933
Random 33	0.0663	–0.4397	Random 83	0.0269	–0.5164
Random 34	0.219	–0.298	Random 84	0.0636	–0.4222
Random 35	0.2231	–0.3232	Random 85	0.2222	–0.1293
Random 36	0.285	–0.0902	Random 86	0.2445	–0.1094
Random 37	0.2525	–0.0109	Random 87	0.0223	–0.433
Random 38	0.1614	–0.2618	Random 88	0.1899	–0.4443
Random 39	0.1511	–0.3019	Random 89	0.048	–0.6216
Random 40	0.1492	–0.2454	Random 90	0.0823	–0.4262
Random 41	0.1898	–0.1992	Random 91	0.0766	–0.3398
Random 42	0.1685	–0.3456	Random 92	0.3163	0.0506
Random 43	0.1489	–0.2463	Random 93	0.1601	–0.1501
Random 44	0.1061	–0.3298	Random 94	0.2543	0.0004
Random 45	0.1179	–0.5352	Random 95	0.0845	–0.4744
Random 46	0.1962	–0.1834	Random 96	0.3105	–0.2083
Random 47	0.3078	0.0595	Random 97	0.1234	–0.2445
Random 48	0.2635	–0.0631	Random 98	0.1498	–0.2165
Random 49	0.3353	–0.0816	Random 99	0.1379	–0.2898
Random 50	0.1327	–0.4471	Random 100	0.168	–0.2025
Average value	0.1625	–0.2871			

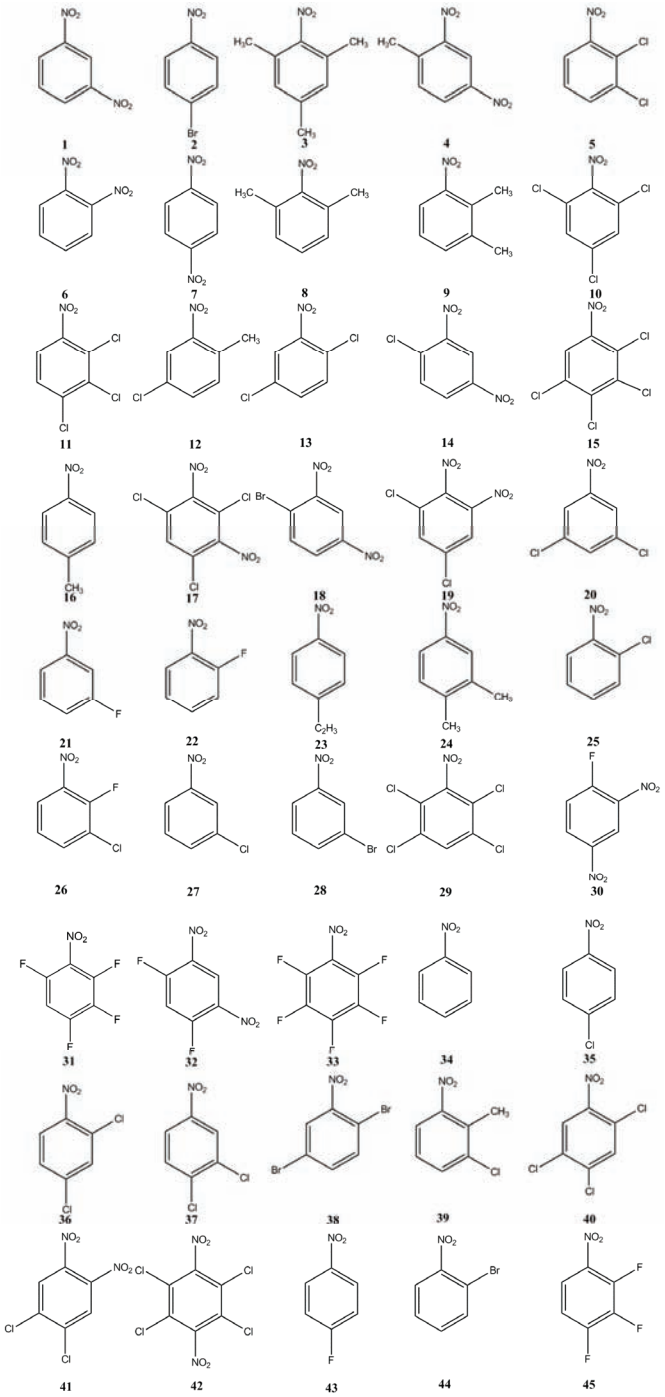

Fig. S-1. Molecular structures of the 45 titled compounds.