

**Table S2.** Physicochemical properties comparison between different kinds of 5-Nitroimidazole derivatives.

5-nitroimidazole scaffolds	Compound	Molecular Weight	Properties	
			cLogP (Conc_Octanol/ Conc_Water)	# sp3 atoms
Quinoline-based 5-nitroimidazole	1, 2	360.3 ±40.3	1.37 ± 0.21	6.0 ± 2.8
5-Nitroimidazole-3-carbaldehyde	3a - 5	306.1 ± 31.94	0.92 ± 0.79	3.8 ± 1.2
Nitroimidazopyridazines	6 - 24	397.5 ± 115.3	1.17 ± 1.25	7.7 ± 2.6
2-Pyrazoline spacer	25 - 28	452.1 ± 9.4	1.90 ± 0.44	5.5 ± 0.5
Metronidazole hybridized	29 - 50	429.5 ± 54.0	0.89 ± 0.78	8.5 ± 1.2
Fexinidazole based	51 - 53	295.3 ± 16.0	0.28 ± 0.74	6 ± 0.0
2-(1-methyl-5-nitro-1H-imidazol-2-yl)-1,3,4-thiadiazole based	54a - 54g	329.1 ± 42.0	0.34 ± 0.78	6.8 ± 0.5
Metronidazole based	55a - 62; 72a - 73	363.9 ± 79.7	0.53 ± 1.10	10.2 ± 2.4
Quinoline–metronidazole based	63a - 63m	480.5 ± 48.1	4.82 ± 0.90	5.2 ± 0.4
Nitroimidazolyl-benzofuranone hybrids	64a - 65	306.1 ± 31.8	0.99 ± 0.77	3.9 ± 1.1
3-Nitroimidazopyridines	66a - 70k	450.8 ± 75.8	2.47 ± 1.05	4.4 ± 1.6
Megazol based	71a - 71d	250.2 ± 43.54	0.64 ± 0.58	2.5 ± 0.5