

Fragmental Method KowWIN as the Powerful Tool for Prediction of Chromatographic Behavior of Novel Bioactive Urea Derivatives

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Table S1. Structural parameters

No.	HOMO / eV	LUMO / eV	Molar mass	Area 3D	TPSA 2D	VDW surface donor 2D	VDW surface acceptor 2D	Dipole moment D	Molar Vol. 3D	Polarizability	Molar refract.	BBB	log S
1	-8.9	-0.20	342.8	367.2	56.7	11.3	19.2	4.78	329.2	40.25	97.9	0.1	-4.64
2	-9.0	0.34	322.4	374.6	56.7	11.3	19.2	3.12	332.3	43.77	94.7	-0.2	-3.62
3	-9.2	-0.49	366.4	405.6	83.0	11.3	32.8	4.13	358.5	46.32	103.1	-0.6	-3.82
4	-9.0	0.05	322.4	373.4	56.7	11.3	19.2	2.64	332.2	43.77	95.0	-0.1	-3.92
5	-9.0	0.32	336.4	398.0	56.7	11.3	19.2	2.68	349.2	45.60	99.7	0.0	-4.08
6	-9.1	-0.48	380.4	428.2	83.0	11.3	32.8	3.87	375.3	48.16	108.2	-0.5	-4.26
7	-9.0	0.52	286.3	332.0	56.7	11.3	19.2	3.47	293.3	35.57	81.7	-0.3	-3.39
8	-9.1	-0.49	350.4	393.8	73.8	11.3	32.8	3.17	350.0	45.69	102.3	-0.5	-3.94
9	-8.9	0.48	300.4	353.7	56.7	11.3	19.2	3.05	311.0	37.41	86.8	-0.2	-3.87
10	-9.1	-0.46	350.4	390.8	73.8	11.3	32.8	3.09	348.0	45.69	102.0	-0.5	-3.70
11	-9.0	0.51	300.4	353.5	56.7	11.3	19.2	3.39	313.2	37.41	86.5	-0.2	-3.63
12	-9.2	-0.45	380.4	426.4	83.0	11.3	32.8	2.14	375.5	48.16	107.9	-0.5	-4.02
13	-9.1	-1.11	319.4	330.5	92.3	11.3	45.6	5.13	288.1	39.79	86.0	-	-
14	-9.1	-1.30	333.3	325.4	109.4	11.3	59.2	6.25	290.7	39.87	88.6	-	-
15	-9.0	-1.07	444.5	458.9	108.3	5.6	64.8	3.58	408.5	52.00	114.8	-	-4.08
16	-9.0	-0.96	474.5	495.8	117.6	5.6	67.3	5.25	435.2	54.47	121.2	-	-4.07
17	-8.9	-1.06	474.5	488.7	117.6	5.6	67.3	5.58	436.7	54.47	121.2	-	-4.02
18	-9.2	-1.07	472.5	492.5	108.3	5.6	64.8	5.64	442.6	55.67	124.8	-	-4.99
19	-9.1	-1.08	478.9	480.2	108.3	5.6	64.8	6.68	424.2	53.97	119.6	-	-4.76
20	-9.3	-1.21	464.2	457.9	108.38	5.68	64.83	4.35	405.7	52.13	114.5	-	-4.32

HOMO: Highest occupied molecular orbital; LUMO: lowest unoccupied molecular orbital; TPSA: topological polar surface area; BBB: blood-brain barrier permeation; log S: solubility; VDW: van der Waals.

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Table S2. Distribution, log *D* at different pH

No.	pH				
	1.7 (stomach)	4.6 (duodenum)	6.5 (jejunum and ileum)	7.4 (blood)	8 (colon)
1	0.62	0.69	1.79	2.64	3.14
2	-0.24	0.10	1.71	2.43	2.71
3	-0.37	0.37	2.08	2.57	2.68
4	0.05	0.48	2.14	2.81	3.04
5	0.22	0.56	2.17	2.89	3.17
6	0.11	0.86	2.57	3.05	3.17
7	-0.93	-0.64	0.92	1.67	1.98
8	-0.39	0.36	2.07	2.56	2.67
9	-0.49	-0.21	1.35	2.11	2.42
10	-0.49	0.26	1.96	2.45	2.56
11	-0.57	-0.29	1.27	2.03	2.34
12	-0.11	0.64	2.35	2.84	2.95
13	2.03	2.03	2.03	2.03	2.03
14	1.97	1.97	1.97	1.97	1.97
15	-1.90	0.24	1.07	1.10	1.10
16	-1.64	0.50	1.32	1.35	1.36
17	-1.58	0.50	1.40	1.43	1.44
18	-0.82	1.32	2.15	2.18	2.18
19	-1.37	0.81	1.59	1.61	1.61
20	-1.58	0.64	1.36	1.38	1.39