Supplementary materials

Assessment of Bioavailability Parameters of Mono- and Bistriazole Derivatives of Propynoylbetulin

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Table S1: The theoretical value of lipophilicity of compounds **3-18**.

Compound	ALOGPs	AClogP	miLogP	XLOGP2	XLOGP3	$logP_{calc}$
3	7.32	7.05	7.41	7.12	7.08	7.20
4	7.32	7.07	7.46	7.35	7.14	7.49
5	7.14	6.96	7.31	6.97	6.92	6.66
6	7.39	8.01	7.56	7.34	7.45	6.70
7	4.78	5.49	4.73	5.14	4.86	4.83
8	5.70	5.80	5.84	5.46	5.64	6.24
9	6.07	6.28	6.19	6.04	5.93	5.98
10	6.47	6.29	6.63	6.29	6.38	6.15
11	8.13	7.55	7.89	8.20	8.20	8.44
12	8.19	7.60	7.95	8.37	8.32	8.95
13	8.14	7.38	7.79	7.91	7.88	7.36
14	8.30	9.48	8.05	8.64	8.94	7.45
15	3.51	4.43	3.20	4.24	3.76	3.70
16	5.37	5.07	5.41	4.88	5.32	7.00
17	5.88	6.02	6.10	6.04	5.89	6.01
18	6.81	6.04	6.98	6.54	6.80	6.35

Table S2: The similarity parameter (ED) for the theoretical and experimental lipophilicity for compounds **3-18**.

Compound	ED	Compound	ED
3	0.94	**11**	0.95
4	0.94	**12**	0.95
5	0.89	**13**	0.83
6	0.66	**14**	0.66
7	0.66	**15**	0.00
8	0.79	**16**	0.66
9	0.92	**17**	0.93
10	0.79	**18**	0.79