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Supporting information

Correlation between structure, retention and activity of cholic acid derived cis-trans isomeric bis-steroidal tetraoxanes

Sandra Šegan¹, Filip Andrić², Aleksandra Radoičić², Dejan Opsenica¹, Bogdan Šolaja², Mario Zlatović², Dušanka Milojković-Opsenica^{1*}

¹ Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000 Belgrade, Serbia

² Faculty of Chemistry, University of Belgrade, P. O. Box 51, 11158 Belgrade, Serbia

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Table S1. The R_M^0 values of the investigated compounds

Comp.	Chromatographic system used				
	RP-18 stationary phase			CN-silica stationary phase	
	Methanol/water	Acetone/water	Dioxane/water	Methanol/water	Acetone/water
1	11.852 ± 0.492	7.908 ± 0.274	8.125 ± 0.188	4.939 ± 0.210	4.408 ± 0.297
2	12.544 ± 0.568	7.829 ± 0.311	8.014 ± 0.170	5.834 ± 0.406	4.582 ± 0.206
3	6.922 ± 0.226	4.425 ± 0.181	3.548 ± 0.183	3.248 ± 0.275	2.996 ± 0.128
4	8.069 ± 0.245	4.859 ± 0.200	3.970 ± 0.216	3.811 ± 0.337	3.462 ± 0.116
5	8.842 ± 0.219	5.972 ± 0.167	4.876 ± 0.279	4.341 ± 0.196	4.209 ± 0.096
6	10.188 ± 0.340	6.375 ± 0.093	5.081 ± 0.183	4.612 ± 0.448	4.329 ± 0.112
7	6.623 ± 0.371	5.608 ± 0.185	6.047 ± 0.144	3.485 ± 0.182	3.559 ± 0.206
8	7.541 ± 0.425	6.041 ± 0.254	6.602 ± 0.164	4.124 ± 0.164	3.817 ± 0.179
9	7.035 ± 0.310	4.417 ± 0.169	4.093 ± 0.288	3.861 ± 0.364	3.707 ± 0.303
10	8.639 ± 0.276	5.146 ± 0.083	4.227 ± 0.165	4.155 ± 0.505	3.756 ± 0.214
11	14.450 ± 1.155	8.276 ± 0.515	8.050 ± 0.101	6.004 ± 0.585	4.494 ± 0.459
12	16.092 ± 1.140	9.196 ± 0.142	7.997 ± 0.245	6.257 ± 0.478	5.035 ± 0.319
13	10.245 ± 0.420	6.953 ± 0.126	6.793 ± 0.180	3.248 ± 0.275	4.063 ± 0.201
14	11.323 ± 0.498	6.970 ± 0.163	6.915 ± 0.205	5.200 ± 0.478	4.193 ± 0.305

Table S2. Biological activity against Fem-X and HeLa cell lines expressed as $\log IC_{50}$

Biological activity	Compound No.													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Fem-X	<i>l</i> *	1.29	0.49	0.79	1.36	1.97	0.62	0.88	2.03	0.67	1.68	1.93	1.9	2.01
HeLa	<i>l</i> *	1.31	0.57	0.78	1.52	2.22	0.72	0.96	<i>l</i> *	0.56	2.02	<i>l</i> *	1.95	2.08

*The values could not be precisely quantified