Evaluation of the Lipophilicity of Angularly Condensed Diquino- and Quinonaphthothiazines as Potential Candidates for New Drugs

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Table S1. Obtained linear correlations between theoretical and chromatographic parameters of lipophilicity of the tested compounds **1–21**. (r - correlation coefficient; s - standard error of estimation; p - significance level; F- ratio).

Compounds	Lipophilicity parameter	Equation	r	p-value	s	F-ratio
1-21	AClogP	AClogP = 0.8996logP_{TLC} + 0.7407	0.670	0.000	0.488	18.22
1-21	MLOGP	MLOGP = 0.7383logP_{TLC} – 0.1778	0.563	0.008	0.574	8.84
1-21	XLOGP2	XLOGP2 = 0.7824logP_{TLC} + 1.3324	0.578	0.006	0.586	9.53
1-21	XLOGP3	XLOGP3 = 0.6477logP_{TLC} + 1.6152	0.570	0.007	0.495	9.16
1-21	LogP	LogP = 0.6969logP_{TLC} + 1.5062	0.616	0.003	0.472	11.64
1-21	ClogP	ClogP = 0.5503logP_{TLC} + 2.7581	0.450	0.041	0.579	4.83

Table S2. The molecular descriptors for compounds **1–21**.

Compounds	Molar mass (M)	Molar volume (V_M)	Molar refractivity (Ref_M)
1	301.37	254.81	87.58
2	315.39	271.91	92.58
3	341.43	299.73	102.03
4	339.11	294.25	100.16
5	301.37	254.81	87.58
6	315.39	271.75	92.58
7	341.43	299.73	102.03
8	339.11	294.25	100.16
9	301.37	254.81	87.58
10	315.39	271.75	92.58
11	301.37	254.81	87.58
12	315.39	271.75	92.58
13	341.43	299.73	102.03
14	300.38	258.97	90.06
15	314.40	275.91	95.06
16	340.44	303.88	104.51
17	338.43	298.41	102.65
18	300.38	258.97	90.06
19	314.40	275.91	95.06
20	340.44	303.88	104.51
21	338.43	298.41	102.65

Table S3. The correlation of the $logP_{TLC}$ values with the molecular descriptors and predicted ADME activities for compounds **1–21**. (r - correlation coefficient; s - standard error of estimation; p - significance level; F- ratio).

Compounds	Molecular Descriptor and ADME Activities	Equation	r	p-value	s	F-ratio
1-21	Molar volume	$V_M = 15.62logP_{TLC} + 194.72$	0.428	0.053	17.481	4.27
1-21	Molar refractivity	$Ref_M = 5.3645logP_{TLC} + 66.692$	0.445	0.043	5.734	4.68
1-21	Caco-2	$Caco\text{-}2 = -42.984logP_{TLC} + 421.64$	0.451	0.040	45.196	4.84
1-21	P-gp	$P\text{-}gp = 0.0411logP_{TLC} + 0.1211$	0.584	0.005	0.030	9.86
1-21	CYP2C9	$CYP2C9 = -0.0387logP_{TLC} + 0.5331$	0.417	0.062	0.045	3.99
1-21	CYP2C19	$CYP2C19 = 0.0209logP_{TLC} + 0.4000$	0.459	0.036	0.021	5.08
1-21	CYP3A4	$CYP3A4 = -0.0212logP_{TLC} + 0.6513$	0.439	0.046	0.023	4.54

Table S4. The parameters of Lipinski's. Ghose's. Veber's and Egan's rules for compounds **1–21**.

Compounds	H-Bond Acceptors	H-Bond Donors	Rotatable Bonds	TPSA [Å²]	Lipinski's Rules	Ghose's Rules	Veber's Rules	Egan's Rules
1	2	1	0	63.11	+	+	+	+
2	2	0	0	54.32	+	+	+	+
3	2	0	2	54.32	+	+	+	+
4	2	0	1	54.32	+	+	+	+
5	2	1	0	63.11	+	+	+	+
6	2	0	0	54.32	+	+	+	+
7	2	0	2	54.32	+	+	+	+
8	2	0	1	54.32	+	+	+	+
9	2	1	0	63.11	+	+	+	+
10	2	1	0	63.11	+	+	+	+
11	2	1	0	63.11	+	+	+	+
12	2	0	0	54.32	+	+	+	+
13	2	0	0	54.32	+	+	+	+
14	1	1	0	50.22	+	+	+	+
15	1	0	0	41.43	+	+	+	+
16	1	0	2	41.43	+	-	+	+
17	1	0	1	41.43	+	+	+	+
18	1	1	0	50.22	+	+	+	+
19	1	0	0	41.43	+	+	+	+
20	1	0	2	41.43	+	-	+	+
21	1	0	1	41.43	+	+	+	+