

Study of the Lipophilicity and ADMET Parameters of New Anticancer Diquinothiazines with Pharmacophore Substituents

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Table S1. The absorption and metabolism descriptors for compounds **1 – 15**.

No. of Compound	P-glycoprotein Substrate	P-glycoprotein I Inhibitor	P-glycoprotein II Inhibitor	CYP2D6 Substrate	CYP3A4 Substrate	CYP1A2 Inhibitor	CYP2C19 Inhibitor	CYP2C9 Inhibitor	CYP2D6 Inhibitor	CYP3A4 Inhibitor
1	-	+	+	-	+	+	-	-	+	+
2	+	+	+	-	+	+	+	-	+	-
3	+	+	+	-	+	+	-	-	-	+
4	+	+	+	-	+	+	-	-	-	+
5	+	+	+	-	+	+	+	-	+	+
6	+	+	+	-	+	+	-	-	+	+
7	+	+	+	-	+	+	-	-	+	+
8	+	+	+	-	+	+	+	-	+	+
9	+	+	+	-	+	+	+	-	+	+
10	+	+	+	-	+	+	-	-	+	+
11	+	+	+	-	+	+	+	-	+	+
12	+	+	+	-	+	+	-	-	+	+
13	+	+	+	+	+	+	-	-	+	+
14	+	+	+	+	+	+	-	-	+	+
15	+	+	+	-	+	+	+	-	+	+

Table S2. The excretion and toxicity descriptors for compounds **1 – 15**.

No. of Compound	Renal OCT2 Substrate	AMES Toxicity	hERG I Inhibitor	hERG II Inhibitor	Hepatotoxicity	Skin Sensitisation
1	-	+	-	+	+	-
2	-	-	-	+	+	-
3	-	-	-	+	+	-
4	-	+	-	+	+	-
5	-	+	-	+	+	-
6	-	+	-	+	+	-
7	-	+	-	+	+	-
8	+	+	-	+	+	-
9	+	+	-	+	+	-
10	-	-	-	+	+	-
11	-	+	-	+	+	-
12	-	+	-	+	+	-
13	-	+	-	+	+	-
14	-	-	-	+	+	-
15	-	+	-	+	+	-



Figure S1. The bioavailability radars for compounds 1 – 15.

Table S3. The summary formulas, molecular weights, melting points and appearance of the tested diquinothiazines **1-15**.

No. of Compound	Chem. Formula	Mol. wt.	Physical Appearance	Melting Point °C (lit. m.p. [24])
1	C ₂₄ H ₂₄ N ₄ S	400,50	yellow oil	-
2	C ₂₃ H ₂₂ N ₄ S	386,52	yellow solid	129.8 - 130.7 (130 - 131)
3	C ₂₄ H ₂₂ N ₄ S	398,53	yellow oil	-
4	C ₂₅ H ₂₄ N ₄ S	412,56	orange oil	-
5	C ₂₆ H ₂₆ N ₄ S	426,58	yellow solid	144.2 - 145.0 (144 - 145)
6	C ₂₄ H ₂₄ N ₄ S	400,50	yellow oil	-
7	C ₂₃ H ₂₂ N ₄ S	386,52	yellow oil	-
8	C ₂₄ H ₂₂ N ₄ S	398,53	yellow oil	-
9	C ₂₅ H ₂₄ N ₄ S	412,56	orange oil	-
10	C ₂₆ H ₂₆ N ₄ S	426,58	orange oil	-
11	C ₂₄ H ₂₄ N ₄ S	400,50	yellow oil	-
12	C ₂₃ H ₂₂ N ₄ S	386,52	yellow oil	-
13	C ₂₄ H ₂₂ N ₄ S	398,53	yellow oil	-
14	C ₂₅ H ₂₄ N ₄ S	412,56	orange oil	-
15	C ₂₆ H ₂₆ N ₄ S	426,58	orange solid	143.5 – 144.8 (144 - 145)