ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

SYNTHESIS, STRUCTURAL COMMENTARY, SUPRAMOLECULAR ARCHITECTURE, AND MOLECULAR DOCKING INVESTIGATIONS OF A NOVEL THIOPHENE-FUSED 1,2,3,4-TETRAHYDROISOQUINOLINE DERIVATIVE AS A POTENT ANTI-CANCER AGENTA.

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NMR Data for the title molecule BDTTIQ

Yellow solid, m.p. 114 - 116 ºC; IR (KBr): 3059, 2929, 2833, 1603, 1561, 1508, 1454, 1267, 1053, 757, 841, 697, 491 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.39 (d, *J* = 8.00 Hz, 2H, Ar-*H*), 7.33 (t, *J* = 8.00 Hz, 3H, Ar-*H*), 7.25 – 7.17 (m, 3H, Ar-*H*), 7.15 – 7.03 (m, 6H, Ar-*H*), 6.90 (t, *J* = 8.00 Hz, 1H, Ar-*H*), 6.77 – 6.76 (m, 2H, Ar-*H*), 6.68 (s, 1H, Ar-*H*), 6.21 (s, 1H, Ar-*H*), 5.83 (s, 1H, -C*H*), 4.13 (AB_q, *J* = 16.00 Hz, 2H, -CH_2), 3.96 (d, *J* = 12.00 Hz, 1H, -CH_2), 3.72 – 3.67 (m, 4H, -CH_2, -OCH_3), 3.54 (s, 3H, -OCH_3), 2.28 (s, 3H, -CH_3) ppm;

^{13}C NMR (100 MHz, $CDCl_3$): δ = 151.1, 147.0, 145.0, 141.8, 141.7, 139.6, 138.0, 137.3, 135.9, 135.8, 135.3, 135.0, 129.6, 129.3, 128.8, 128.7, 128.6, 127.6, 127.2, 127.0, 126.4, 126.1, 126.0, 125.2, 123.6, 121.5, 116.6, 108.1, 65.9, 60.1, 56.1, 56.1, 48.6, 21.6 ppm; HRMS (ESI): calcd. for $C_{38}H_{34}NO_2S$ $[M + H]^+$ 568.2310; found 568.2305.

TABLE S1. Selected structural parameters for compound BDTTIQ

Parameters	X-ray
1	2
Bond lengths (Å)	
C1—N1	1.462(2)
C4—O1	1.365(2)
C5—O2	1.3642(2)
C5—C6	1.370(2)
C9—N1	1.4730(2)
C10—O2	1.410(2)
C11—O1	1.421(2)
C12—C13	1.480(2)
C12—C20	1.488(2)
C18—C19	1.440(2)
C19—C20	1.353(2)
C31—C38	1.509(2)

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Continued Table S1	
1	2
Bond angles(°)	
N1—C1—C2	114.84(11)
O1—C4—C3	125.13(13)
O1—C4—C5	115.68(13)
O2—C5—C6	125.20(13)
O2—C5—C4	115.12(13)
N1—C9—C28	111.03(11)
N1—C9—C8	108.55(11)
N1—C21—C22	113.37(12)
N1—C1—C3	120
O1—C4—C3	119.6
O1—C4—C5	121.50(2)
O2—C5—C6	119.3
O2—C5—C4	117.62(15)
N1—C9—C28	109.5
Torsion angles (°)	
N1—C1—C2—C7	15.44(2)
N1—C1—C2—C3	–166.84(13)
O1—C4—C5—O2	–3.22(19)
O2—C5—C6—C7	179.45(14)
N1—C21—C22—C23	30.1(2)
N1—C21—C22—C27	–152.12(14)
N1—C9—C28—C33	144.69(13)
N1—C9—C28—C29	–39.75(18)
C22—C21—N1—C1	68.60(2)
C22—C21—N1—C9	–163.96(12)
C2—C1—N1—C21	83.3(2)
C2—C1—N1—C9	–44.7(2)
C28—C9—N1—C21	166.76(11)
C8—C9—N1—C21	–65.50(14)
C28—C9—N1—C1	–65.12(14)
C8—C9—N1—C1	62.63(14)
C19—C20—C34A—S1A	40.4(19)
C34B—C20—C34A—S1A	11(27)
C12—C20—C34A—S1A	–152.0(9)
S1A—C35A—C36A—C37A	3.0(13)
S1A—C34A—C37A—C36A	8(2)
C19—C20—C34B—S1B	–132.9(18)
C12—C20—C34B—S1B	37(3)
C34A—C20—C34B—S1B	19(26)
C37B—C35B—C36B—S1B	–0.8(17)
S1B—C34B—C37B—C35B	4(3)
C35B—C36B—S1B—C34B	2.4(17)
C37B—C34B—S1B—C36B	–3(2)

Table S2. Docking score and interactions with distance of ligand BDTTIQ binding with 4FALprotein

Inhibitor	Docking Score	Interactions	Distance (Å)	Category of Bonding	Bonding Type
Thiazole	12`2	SER217 (OG –HG …O2)	3.07	Hydrogen Bond	H-bond
		GLN222 (N1-H1…O1)	2.93	Hydrogen Bond	H-bond
		LYS84 (N…π)	3.29	Electrostatic	Cation- π
		LYS84 (N…π)	3.97	Electrostatic	Cation- π
		TYR24(C21-H21… π)	2.91	Hydrophobic	sigma- π
Dexobrucin	10.8	GLN222(N1-H1…O1)	2.61	Hydrogen Bond	H-bond
		TYR216(O2-H2….O)	3.32	Hydrogen Bond	H-bond
		LYS84(N….H…O2)	3.31	Hydrogen Bond	H-bond
		TYR55(O1-H1…O3)	3.23	Hydrogen Bond	H-bond
		LY584(N… π)	6.72	Hydrophobic	Cation- π