

Electronic Supporting Information

Anti-leishmanial activity of Ni(II), Pd(II) and Pt(II) β -oxodithioester complexes

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SI- Ligand synthesis

[HL1]

Yield: (0.252 g, 87%). Anal. Calcd for: C₁₀H₉BrOS₂ (289.21): C 41.53, H 3.14, S 22.13 %. Found: C 41.38, H 3.22, S 21.68 %. IR (KBr, cm⁻¹): ν = 1580 ($\nu_{C=C}$), 1243 ($\nu_{C=S}$), 1181 (ν_{C-OH}). ¹H NMR (300.70 MHz, CDCl₃): δ 14.99 (s, 1H, -C(OH)-), 7.83 (m, 2H, Ar-H), 7.60 (m, 2H, Ar-H), 6.87 (s, 1H, -CH=C-), 2.71 (s, 3H, -SCH₃) ppm. ¹³C{¹H} NMR (75.45 MHz, CDCl₃): δ 217.62 (-C=S), 167.14 (-C(OH)-), 136.41, 134.58, 129.63, 122.95 (Ar-C), 107.89 (-CH=C-), 19.05 (-SCH₃) ppm.

[(HL2)]

Yield: (1.94 g, 85%), Anal. Calcd for C₁₀H₉F₁O₁S₂ (228.31): C 52.61, H 3.97, S 28.03 %. Found: C 52.29, H 4.07, S 27.61 %. IR (KBr, cm⁻¹): ν = 1587 ($\nu_{C=C}$), 1243.36 ($\nu_{C=S}$), 1057 (ν_{C-OH}). ¹H NMR (300.70 MHz, CDCl₃): δ 14.89 (s, 1H, -C(OH)-), 7.86-7.83 (m, 2H, Ar-H), 6.95-6.97 (m, 2H, Ar-H), 6.72 (s, 1H, -CH=C(S)-), 2.66 (s, 3H, -SCH₃) ppm. ¹³C{¹H} NMR (75.45 MHz, CDCl₃): δ 215.02 (-C=S), 167.10 (-C(OH)-), 126.21, 128.68, 137.49, 162.81 (Ar-C), 107.87 (-CH=C(S)-), 18.20 (-SCH₃) ppm.

[(HL3)]

Yield: (1.93g, 74%), Anal. Calcd for; C₁₄H₁₂OS₂ (260.38): C 64.58, H 4.65, S 24.58 %. Found: C 64.13, H 4.81, S 24.15 %. IR (KBr, cm⁻¹): ν = 1593 ($\nu_{C=C}$), 1242.89 ($\nu_{C=S}$), 1107 (ν_{C-OH}). ¹H NMR (300.40 MHz, CDCl₃): δ 15.17 (s, 1H, -C(OH)-), 8.46 (m, 1H, Ar-H), 7.94-7.91 (m, 1H, Ar-H), 7.87-7.84 (m, 2H, Ar-H), 7.58-7.50 (m, 2H, Ar-H), 7.24-7.21 (m, 1H, Ar-H), 7.10 (s, 1H, -CH=C-), 2.68-2.64 (s, 3H, SCH₃) ppm. ¹³C{¹H} NMR (75.45, CDCl₃): δ 218.0 (-C=S-), 169.1 (-C(OH)-), 134.95-122.72 (Ar-C), 108.22 (-CH=C(S)-), 19.7 (-SCH₃) ppm.

[HL4]

Yield: (0.197 g, 82%). Anal. Calcd for: C₁₁H₁₂O₂S₂ (240.34): C 54.97, H 5.03, S 26.63 %. Found: C 54.74, H 5.09, S 26.37 %. IR (KBr, cm⁻¹): ν = 1603 ($\nu_{C=C}$), 1231 ($\nu_{C=S}$), 1179 (ν_{C-OH}). ¹H NMR (300.40 MHz, CDCl₃): δ 15.09 (s, 1H, -C(OH)-), 7.86 (m, 2H, Ar-H), 6.95 (m, 2H, Ar-H), 6.97 (s, 1H, -CH=C-), 3.86 (s, 3H, -OCH₃), 2.64 (s, 3H, -SCH₃) ppm. ¹³C{¹H} NMR (74.45 MHz, CDCl₃): δ 215.62 (-C=S), 169.51 (-C(OH)-), 162.81, 128.68, 126.21, 114.40 (Ar-C), 107.08 (-CH=C(S)-), 55.51 (-OCH₃), 17.96 (-SCH₃) ppm.

SII- Weak Interactions table-

Table-3 Weak Interactions, distances, Å, angles deg. A = acceptor, D = donor

	Contact D-H...A	H...A	D...A	D...A	Symmetry element for A
2	C16-H16B...S31	2.97	150	3.826	-x,-1-y,1z
	C16-H16A...S11	2.98	146	3.811	x,-1+y,z
	C23-H23...F47	2.52	169	3.436	-x,3-y,-z
3	C28-H28... $\pi^{a,b}$	2.87	131	3.546	x, 1.5-y, 1/2+z

	C45-H45... $\pi^{a,c}$	2.88	128	3.524	x, 1/2-y, -1/2+z
	C36-H36A...S11	2.89	151	3.753	1-x,2-y,-z
	C36-H36B...S33	2.92	141	3.723	1-x, 1-y, -z
4	C28-H28...S11	2.99	157	3.888	x,y,1+z
	C16-H16...S11	3.01	168	3.955	-x,1/2+y,-z
8	C28...H28A...S13	2.89	151	3.766	1/2-x, 3/2-y, 1/2-z
	C16...H16C...O27	2.57	132	3.290	1/2-x, y, 1/2-z
11	C16-H16C... $\pi^{a,b}$	2.72	146	3.559	-1+x,y,z
	C48-H48... $\pi^{a,d}$	2.50	147	3.318	2-x,-1/2+y,1/2-z

^a dimensions involve the centre of gravity of the ring, ^bring C44-C49, ^cring C24-C29, ^dring C21, C22, C23, C28, C29, C30