

Electronic Supplementary Information

Investigation on the antitrypanosomal effects of 2-formyl-8-hydroxyquinoline-derived hydrazones and their antimony(III) and bismuth(III) complexes

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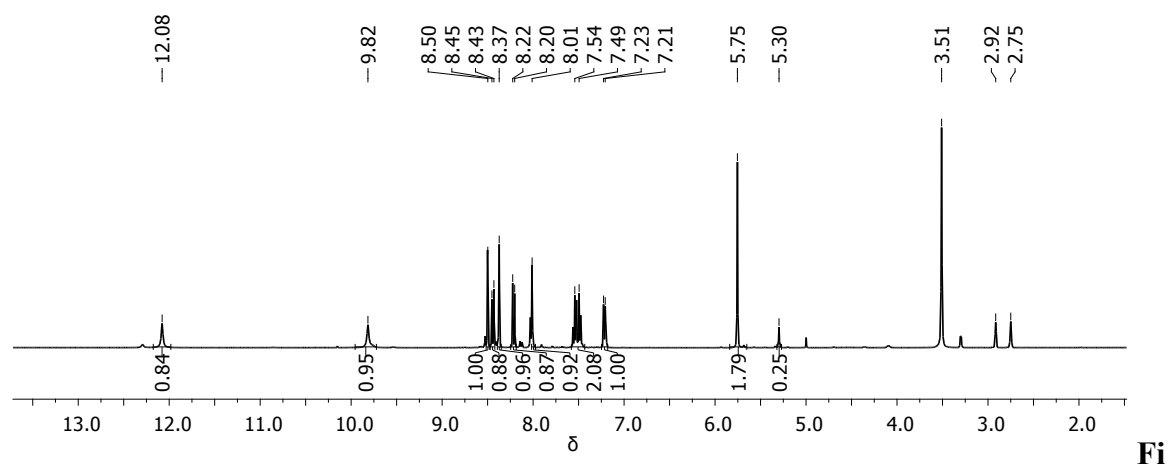
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^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compounds (**1-6**)



g. S1 ^1H NMR spectrum of $\text{H}_2\text{Q}_4\text{NO}_2\text{Im}$ (**H₂La, 1**) in $\text{DMF-}d_7$ (400 MHz) at room temperature

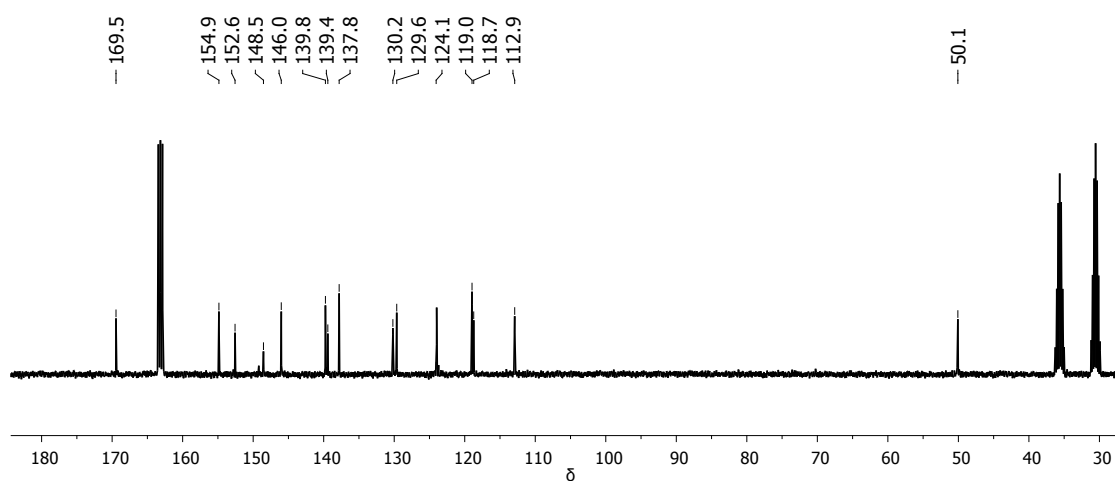


Fig. S2 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{H}_2\text{Q}_4\text{NO}_2\text{Im}$ (**H₂La, 1**) in $\text{DMF-}d_7$ (100 MHz) at room temperature

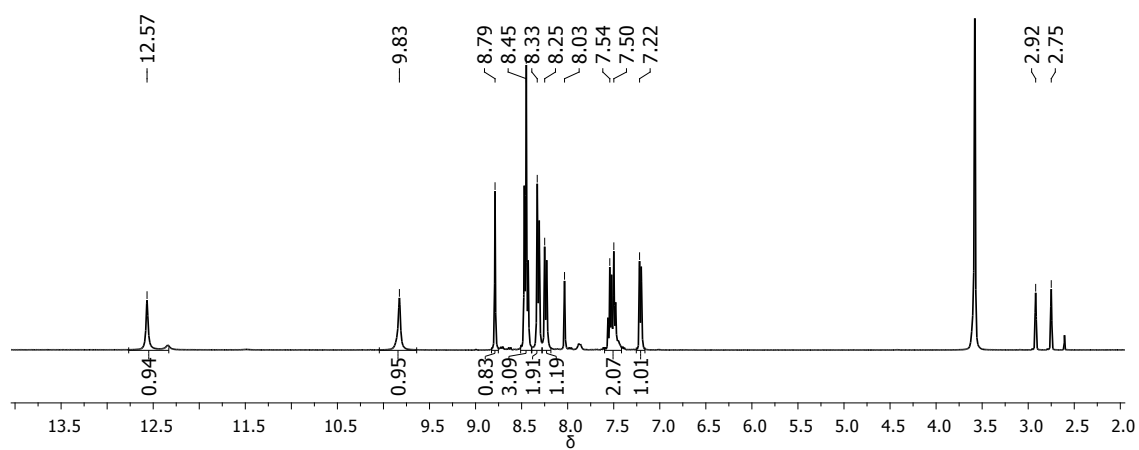


Fig. S3 ^1H NMR spectrum of $\text{H}_2\text{Q}_4\text{NO}_2\text{Ph}$ (**H₂Lb**, **2**) in $\text{DMF-}d_7$ (400 MHz) at room temperature

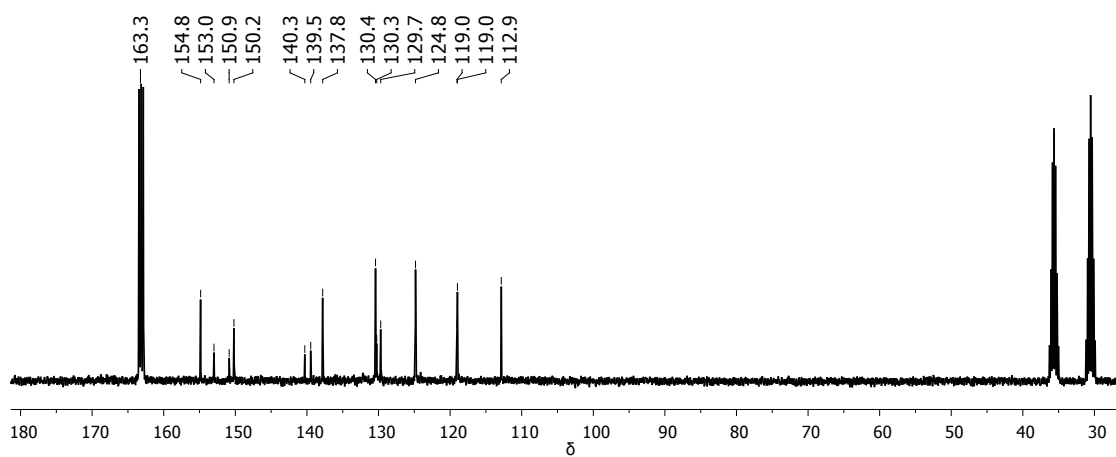


Fig. S4 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{H}_2\text{Q}_4\text{NO}_2\text{Ph}$ (**H₂Lb**, **2**) in $\text{DMF-}d_7$ (100 MHz) at room temperature

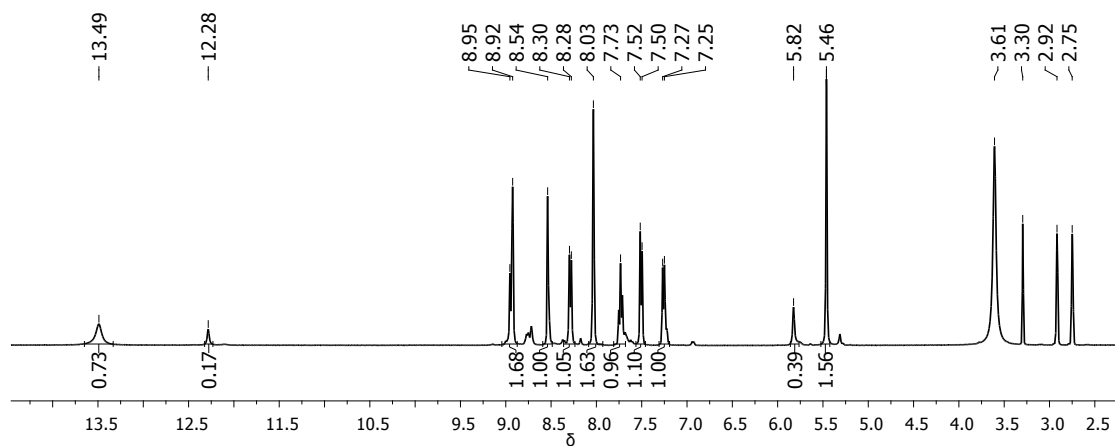


Fig. S5 ^1H NMR spectrum of $[\text{Sb}(\text{HQ4NO}_2\text{Im})\text{Cl}_2]$ (**3**) in $\text{DMF-}d_7$ (400 MHz) at room temperature

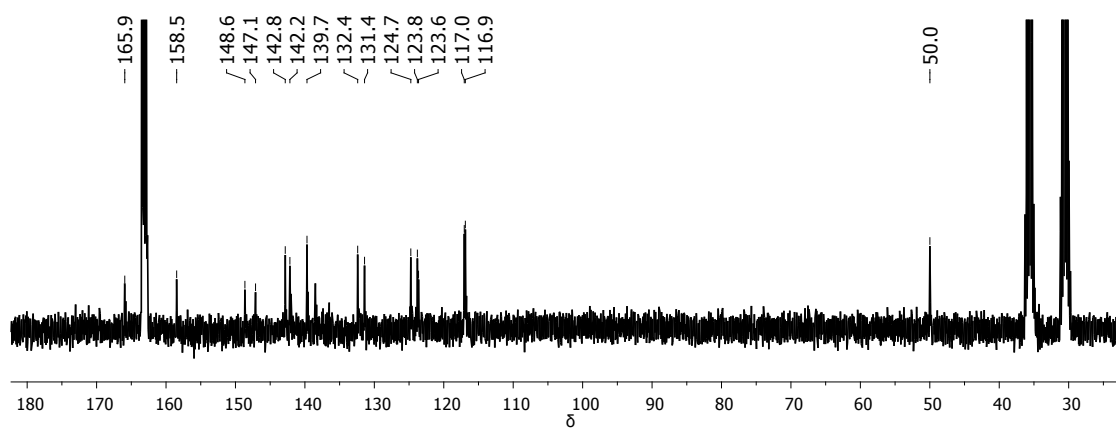


Fig. S6 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Sb}(\text{HQ4NO}_2\text{Im})\text{Cl}_2]$ (**3**) in $\text{DMF-}d_7$ (100 MHz) at room temperature

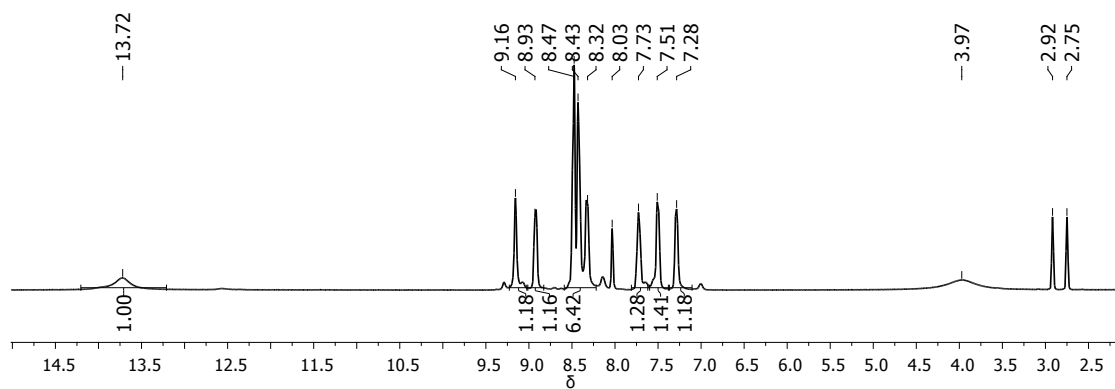


Fig. S7 ^1H NMR spectrum of $[\text{Sb}(\text{HQ4NO}_2\text{Ph})\text{Cl}_2]$ (**4**) in $\text{DMF-}d_7$ (400 MHz) at room temperature

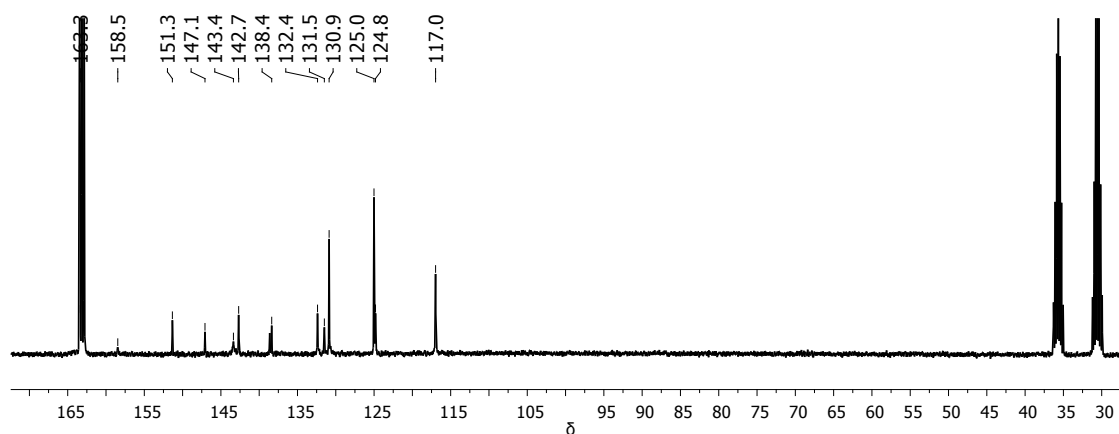


Fig. S8 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Sb}(\text{HQ4NO}_2\text{Ph})\text{Cl}_2]$ (**4**) in $\text{DMF-}d_7$ (100 MHz) at room temperature

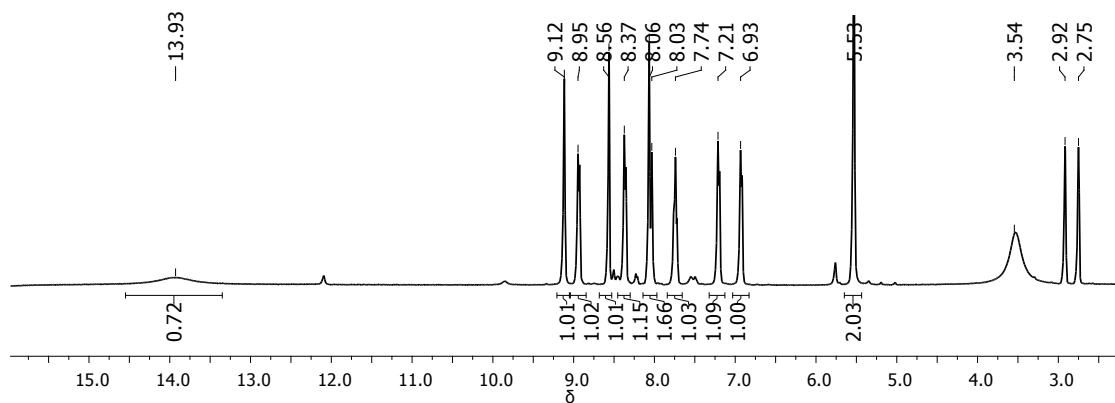


Fig. S9 ^1H NMR spectrum of $[\text{Bi}(\text{HQ4NO}_2\text{Im})\text{Cl}_2]$ (**5**) in $\text{DMF-}d_7$ (400 MHz) at room temperature

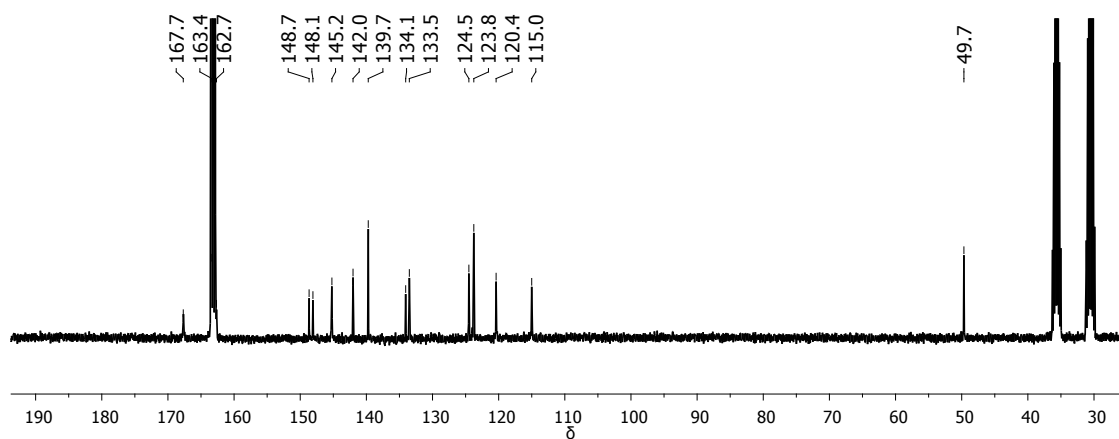


Fig. S10 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Bi}(\text{HQ4NO}_2\text{Im})\text{Cl}_2]$ (**5**) in $\text{DMF-}d_7$ (100 MHz) at room temperature

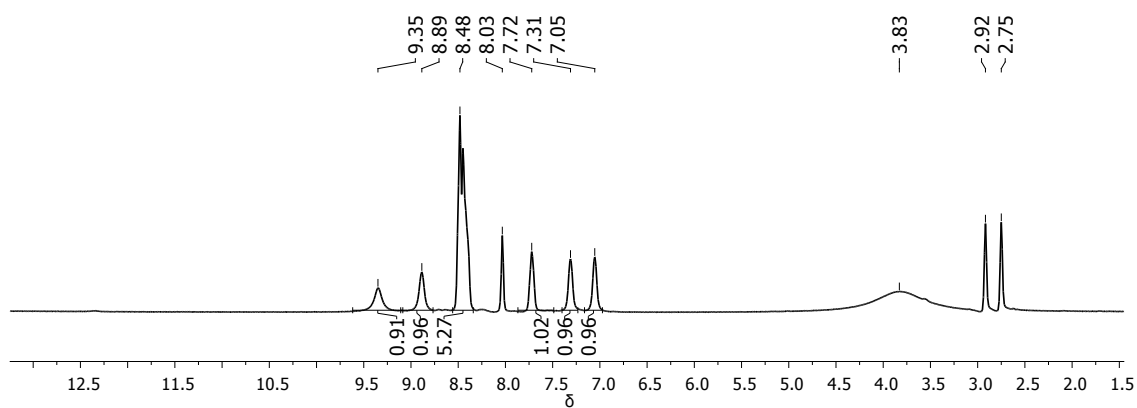


Fig. S11 ^1H NMR spectrum of $[\text{Bi}(\text{HQ4NO}_2\text{Ph})\text{Cl}_2]$ (**6**) in $\text{DMF-}d_7$ (400 MHz) at room temperature

Infrared spectra of compounds (1-6)

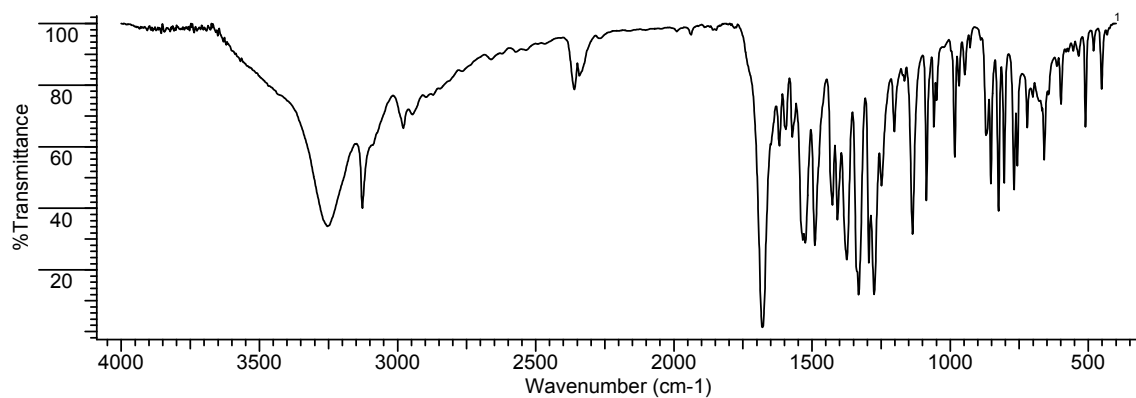


Fig. S12 FT-IR spectrum of H₂Q4NO₂Im (**H₂La, 1**) (ATR technique)

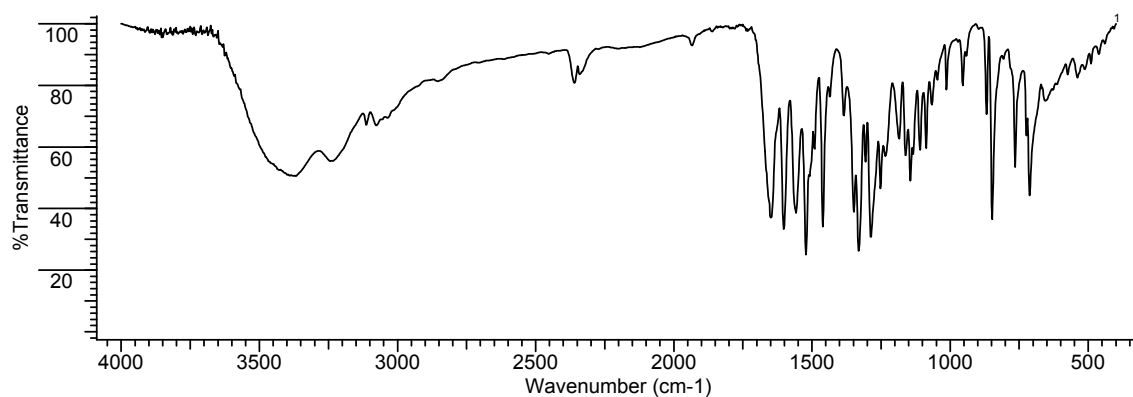


Fig. S13 FT-IR spectrum of H₂Q4NO₂Ph (**H₂Lb, 2**) (ATR technique)

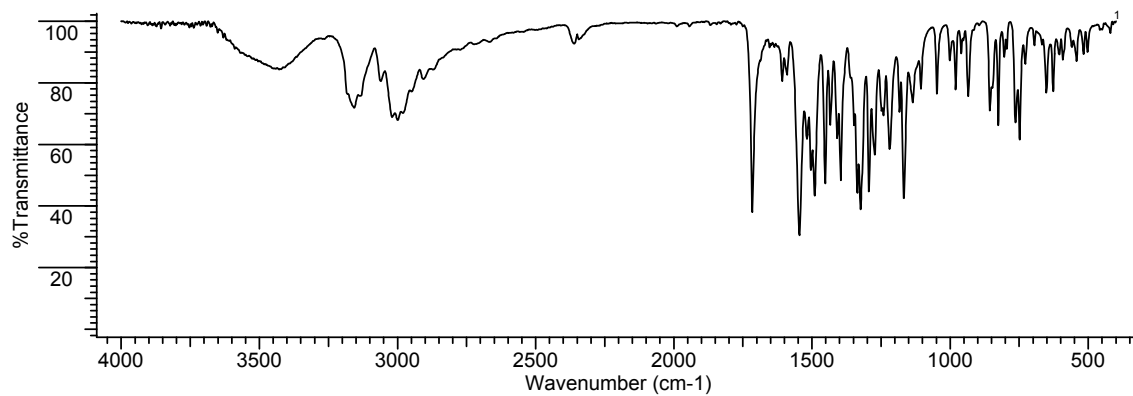


Fig. S14 FT-IR spectrum of [Sb(HQ4NO₂Im)Cl₂] (**3**) (ATR technique)

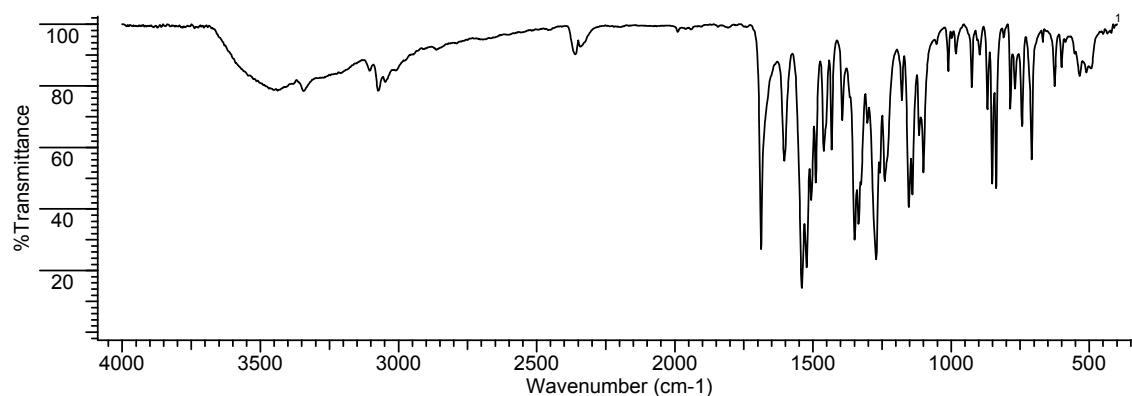


Fig. S15 FT-IR spectrum of [Sb(HQ4NO₂Ph)Cl₂] (**4**) (ATR technique)

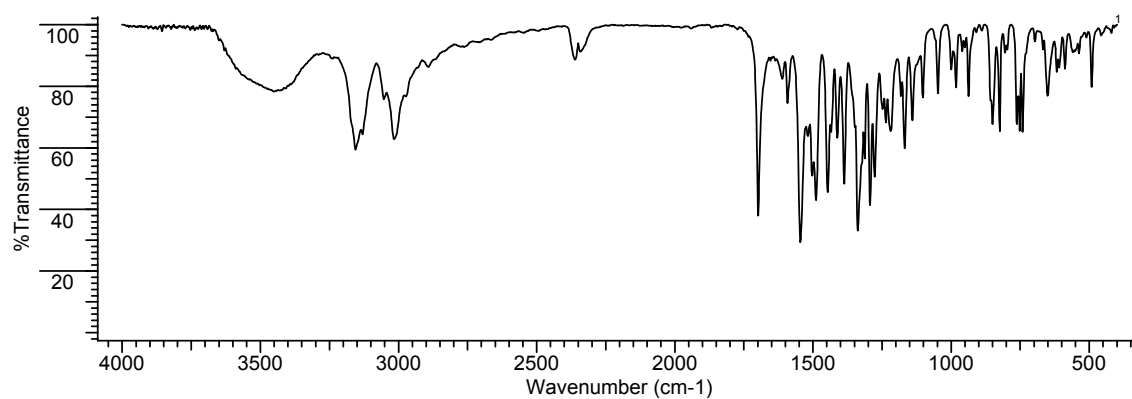


Fig. S16 FT-IR spectrum of [Bi(HQ4NO₂Im)Cl₂] (**5**) (ATR technique)

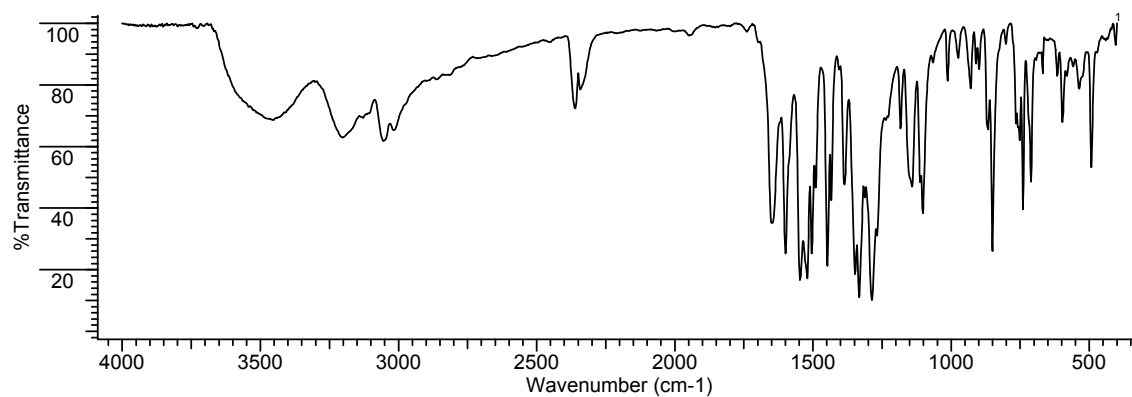


Fig. S17 FT-IR spectrum of [Bi(HQ4NO₂Ph)Cl₂] (**6**) (ATR technique)

Thermogravimetry

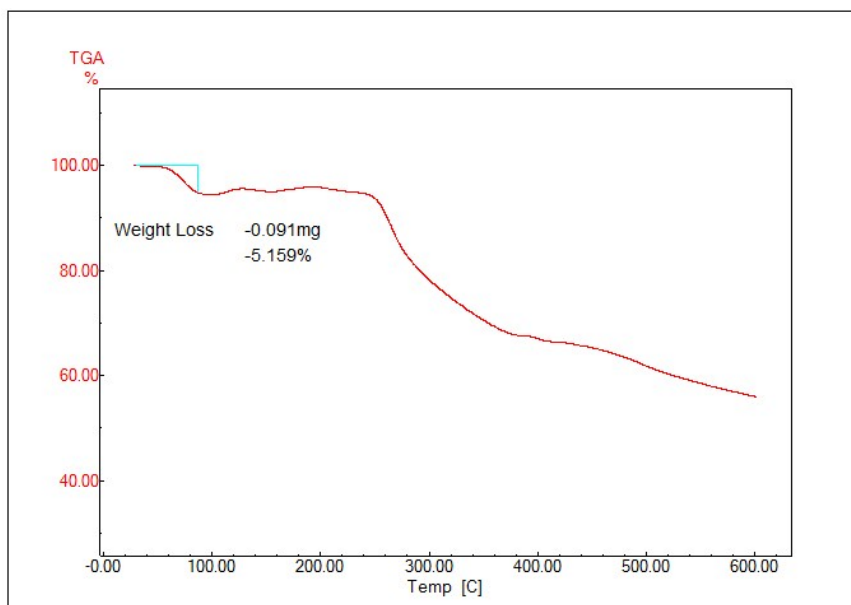


Fig. S18 TG curve of the H₂Q₄NO₂Ph (**H₂Lb**, **2**) at a heating rate of 10°C min⁻¹ under N₂ flow of 50 mL min⁻¹

Crystal packing of [Sb(HQ₄NO₂Ph)(DMF)Cl₂] $\cdot$ 3DMF (**4a**)

The crystal packing of complex (**4a**) shows an intermolecular hydrogen bond involving the hydrazone nitrogen and the oxygen of a DMF molecule [$d(\text{N}3\cdots\text{O}41^i) = 2.737(3) \text{ \AA}$, $\angle(\text{N}3\text{-H}3\text{N}\cdots\text{O}41^i) = 157^\circ$ (symmetry operator: $i = 1-x, -y, 1-z$)]. Non classical C-H $\cdots$ Cl and C-H $\cdots$ O hydrogen intermolecular interactions forming a dimeric arrangement were also observed, Figure S19 and Table S1.

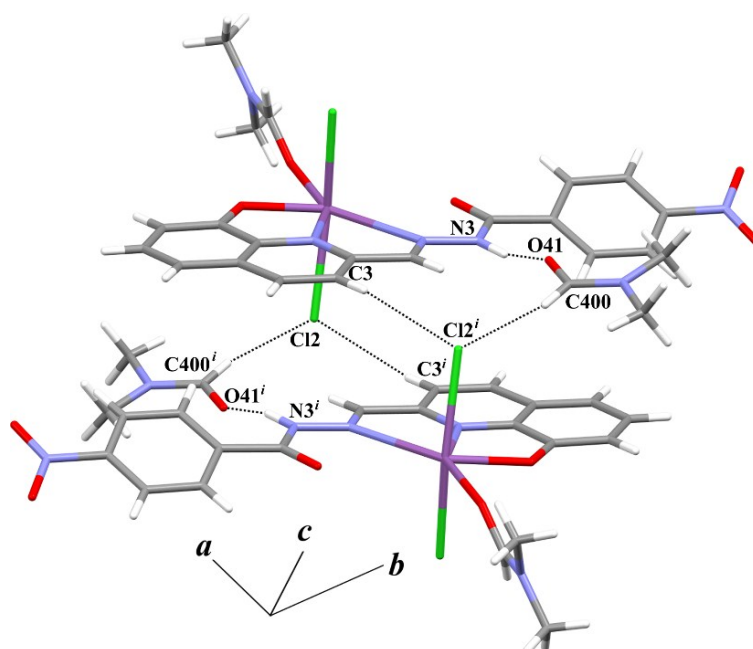


Figure S19. Dimers formed by $\text{NH}\cdots\text{O}$ and $\text{CH}\cdots\text{Cl}$ intermolecular interactions in the crystal packing of complex $[\text{Sb}(\text{HQ4NO}_2\text{Ph})(\text{DMF})\text{Cl}_2]\cdot 3\text{DMF}$ (**4a**). Symmetry code: i ($1 - x, -y, 1 - z$).

Table S1. Geometrical parameters of intermolecular interactions in the structure of $[\text{Sb}(\text{HQ4NO}_2\text{Ph})(\text{DMF})\text{Cl}_2]\cdot 3\text{DMF}$ (**4a**).

H (D-H $\cdots$ A)	d(D-H) / Å	d(H $\cdots$ A) / Å	d(D $\cdots$ A) / Å	D-H $\cdots$ A / °
N3-H3N $\cdots$ O41	0.86	1.93	2.737(3)	157.0
C3--H(3) $\cdots$ Cl2 ^{<i>i</i>}	0.93	2.81	3.692(2)	158.0
C400-H400 $\cdots$ Cl2	0.93	2.62	3.535(3)	167.0

Symmetry code: i ($1 - x, -y, 1 - z$).