Supporting Information

Nickel(II) complexes with flexible piperazinyl moiety : studies on DNA and protein binding and catecholase like properties

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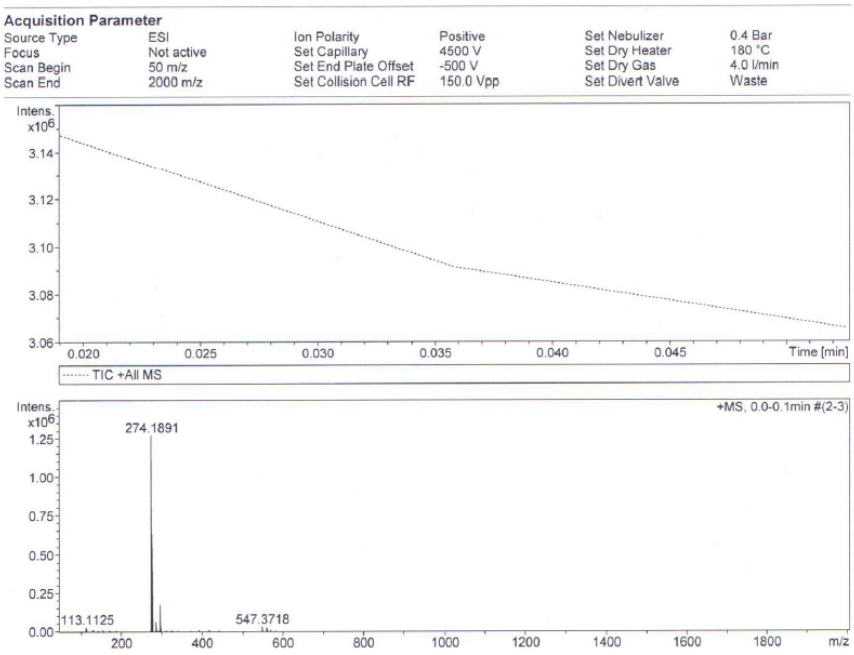
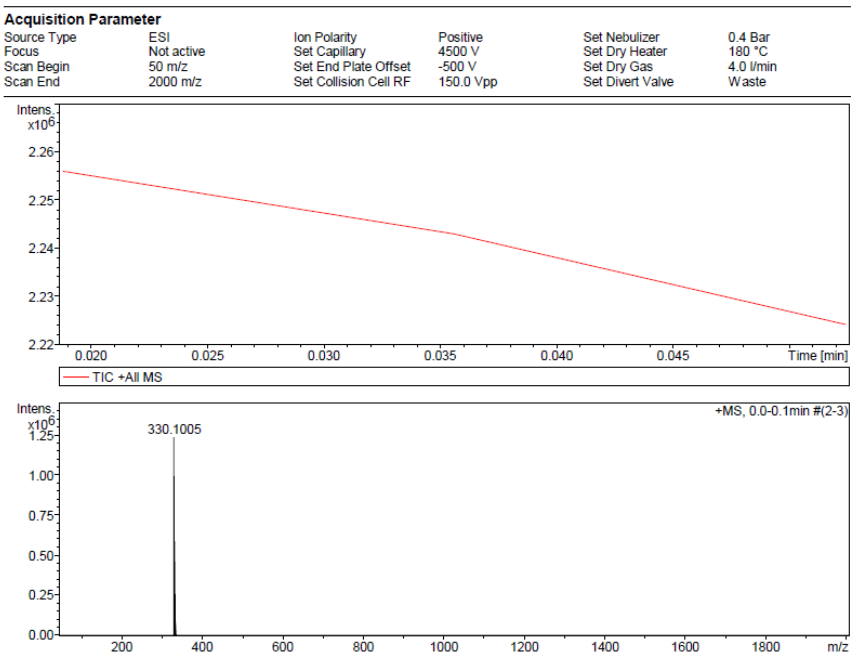


Figure S1: ESI- Mass spectrum of HL[1].



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16 Fig S2: ESI-Mass spectrum of **1a**.

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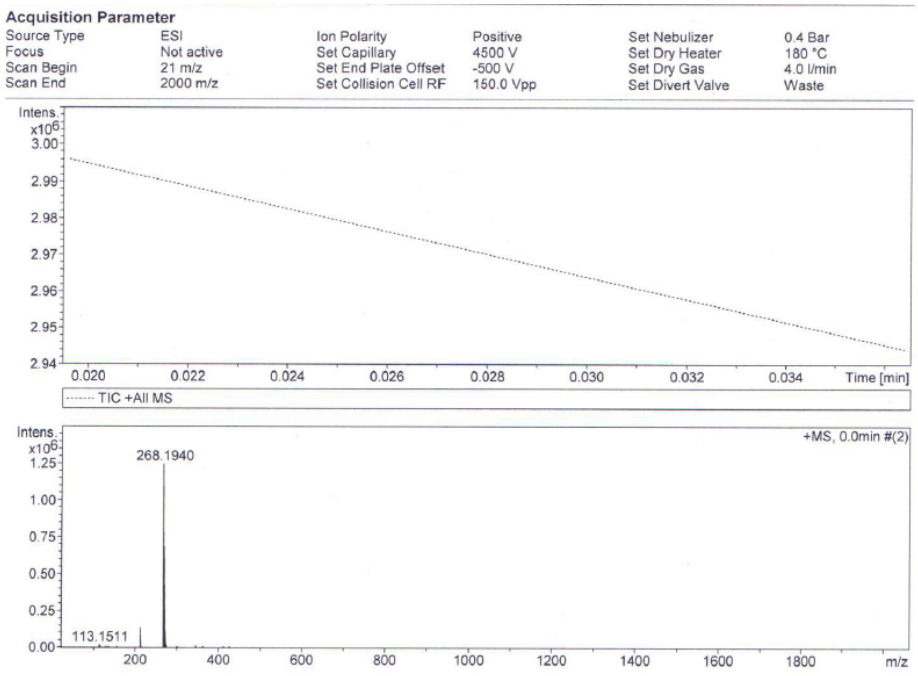

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19 Fig S3: ESI-Mass spectrum of **1b**.

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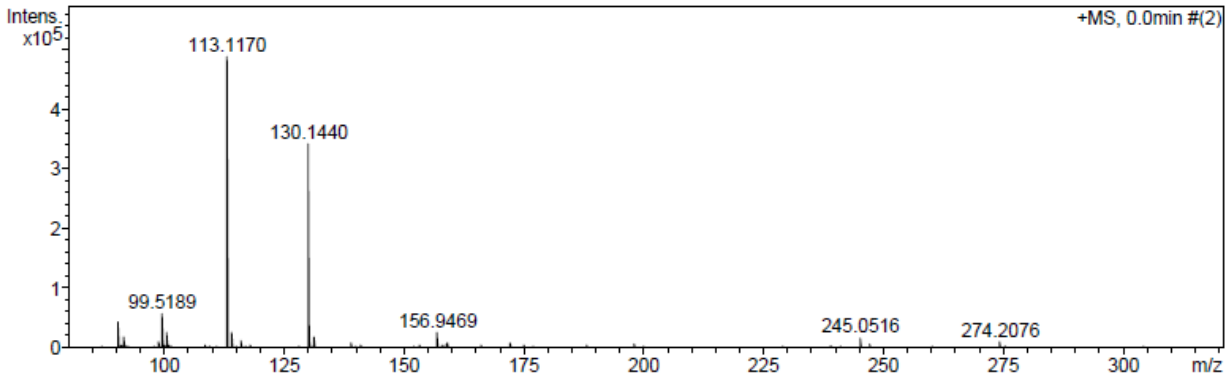


Fig S4: ESI-Mass spectrum of **2a**.

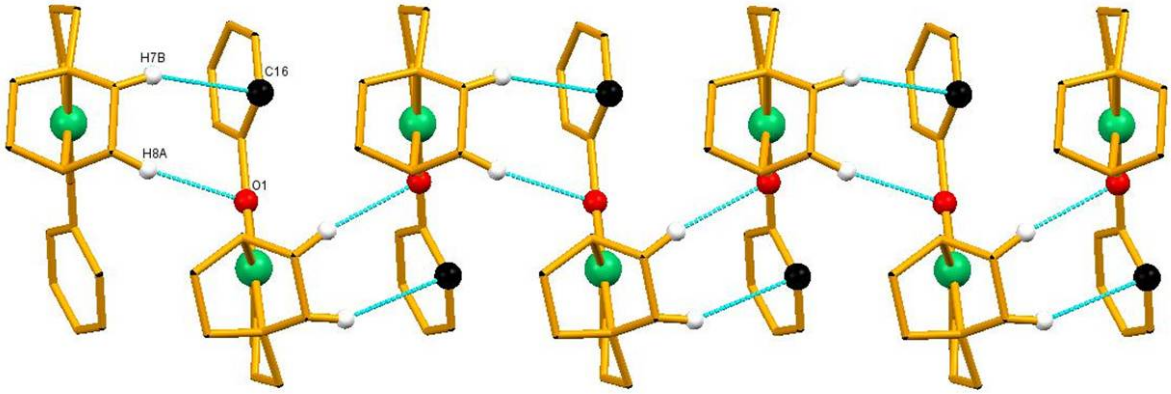


Fig S5: 1D Chain like network of complex **1a**.

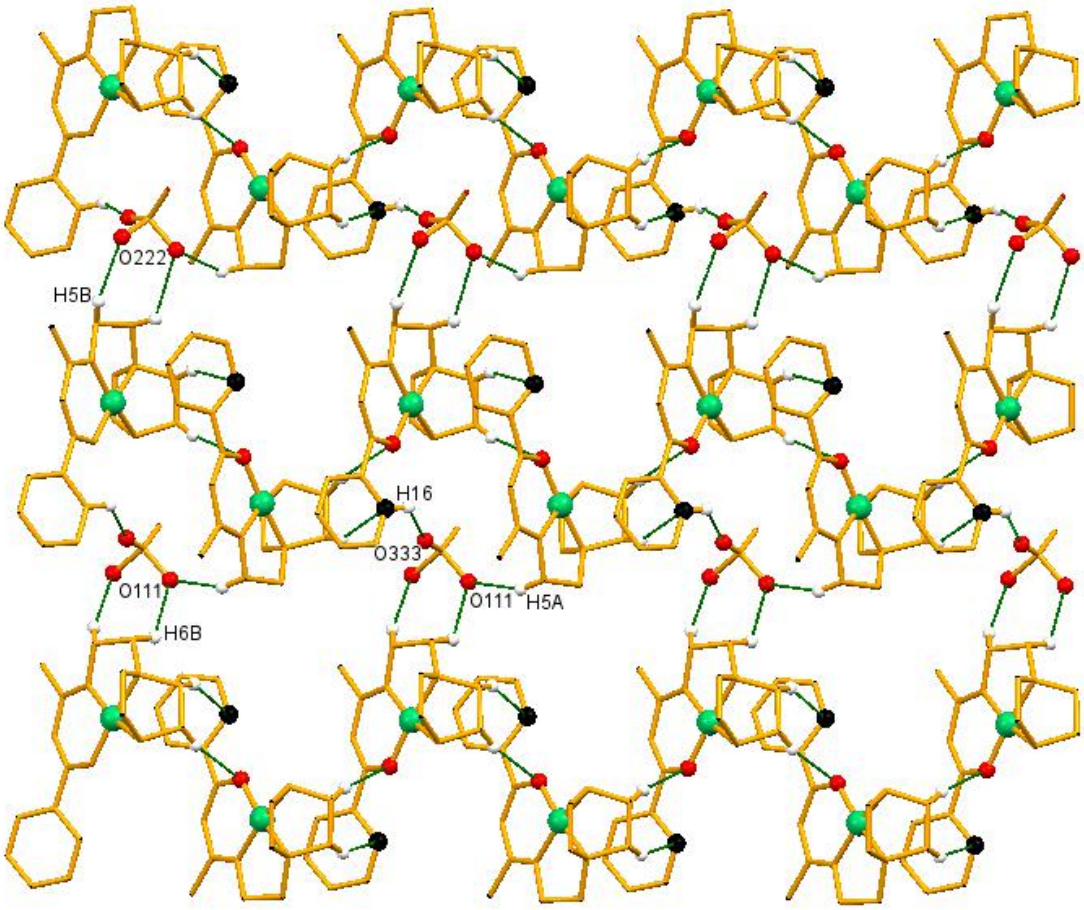


Fig S6: 2D hydrogen bonded sheet of complex **1a**.

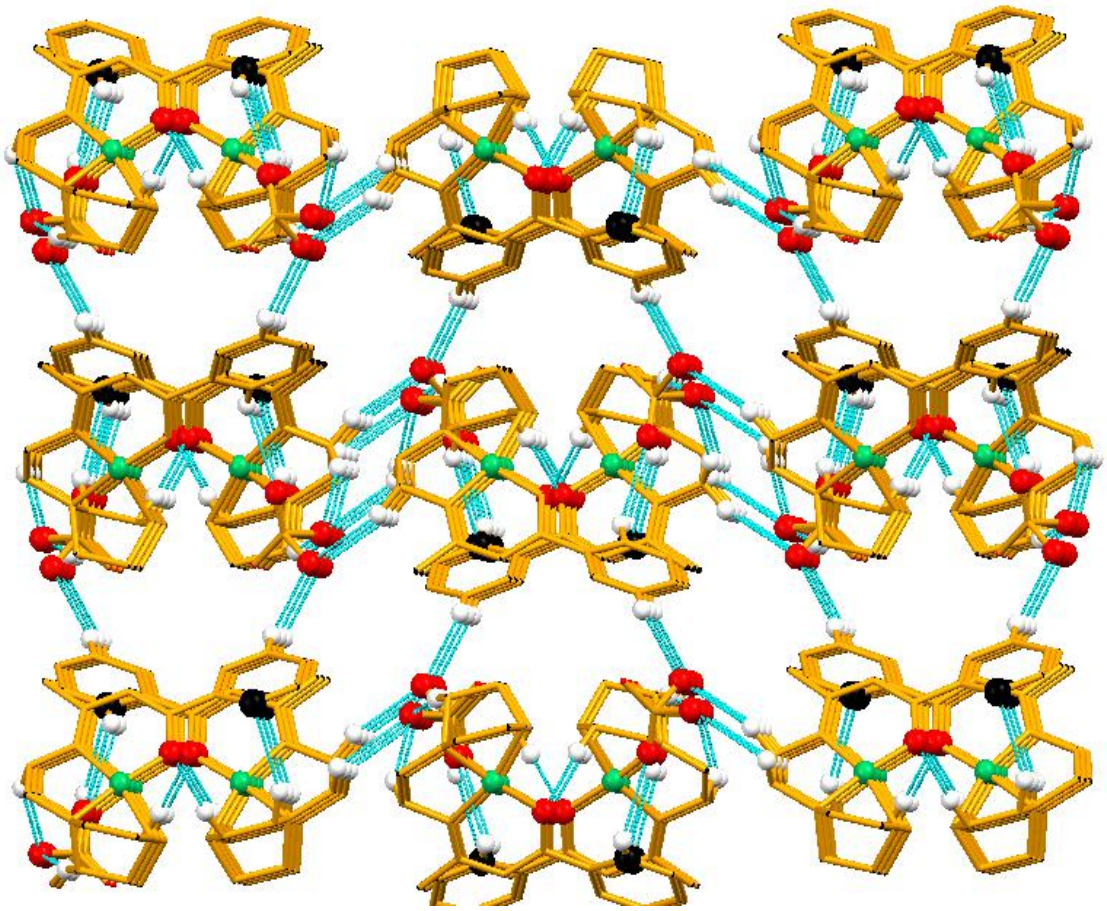


Fig S7: 3D Non-Covalent polymeric network of complex **1a**.

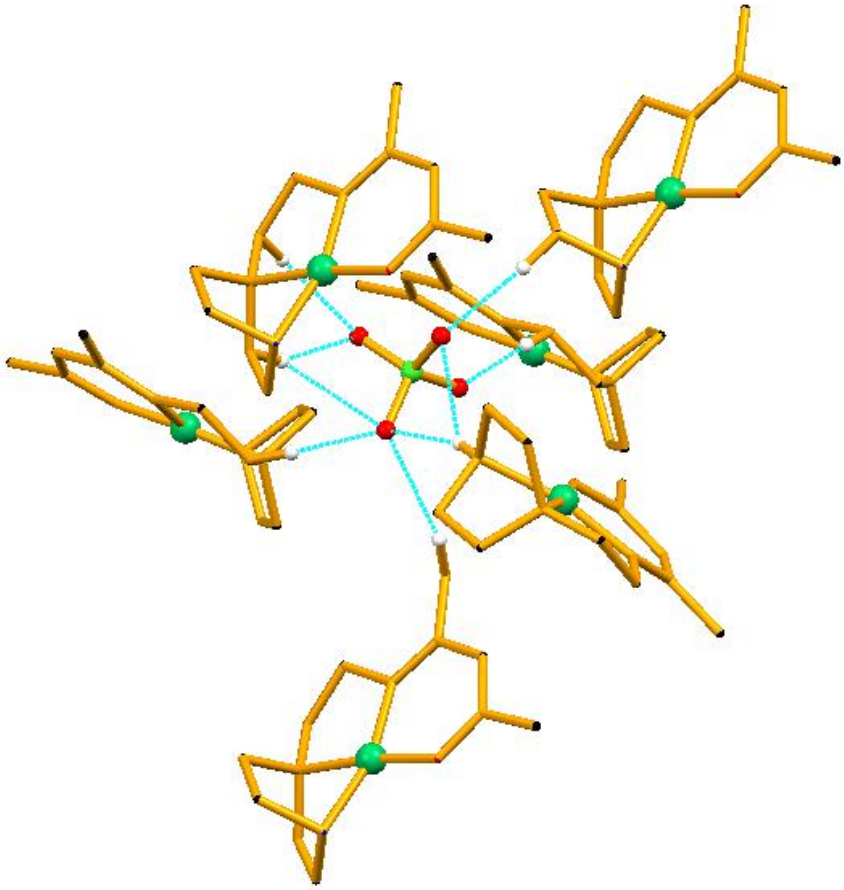


Fig S8: Figure of complex **1b** showing the hydrogen-bonded connection between one perchlorate ion and six surrounding molecules.

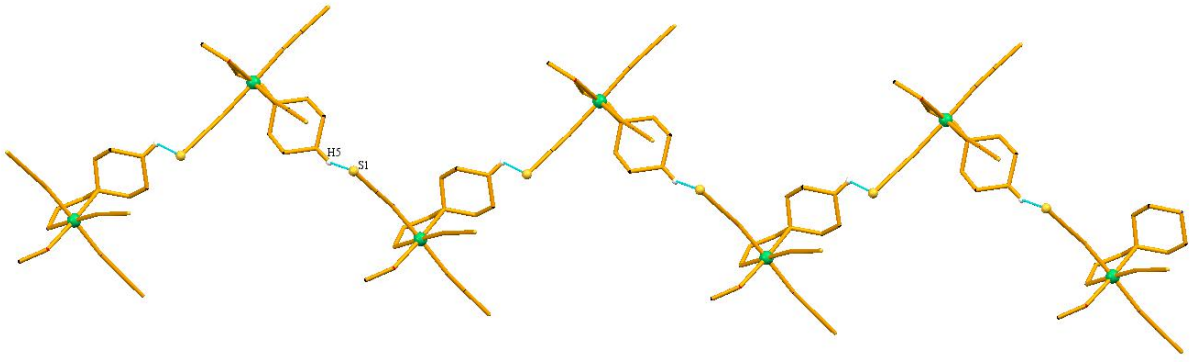


Fig S9: 1D chain like structure complex **2a**.

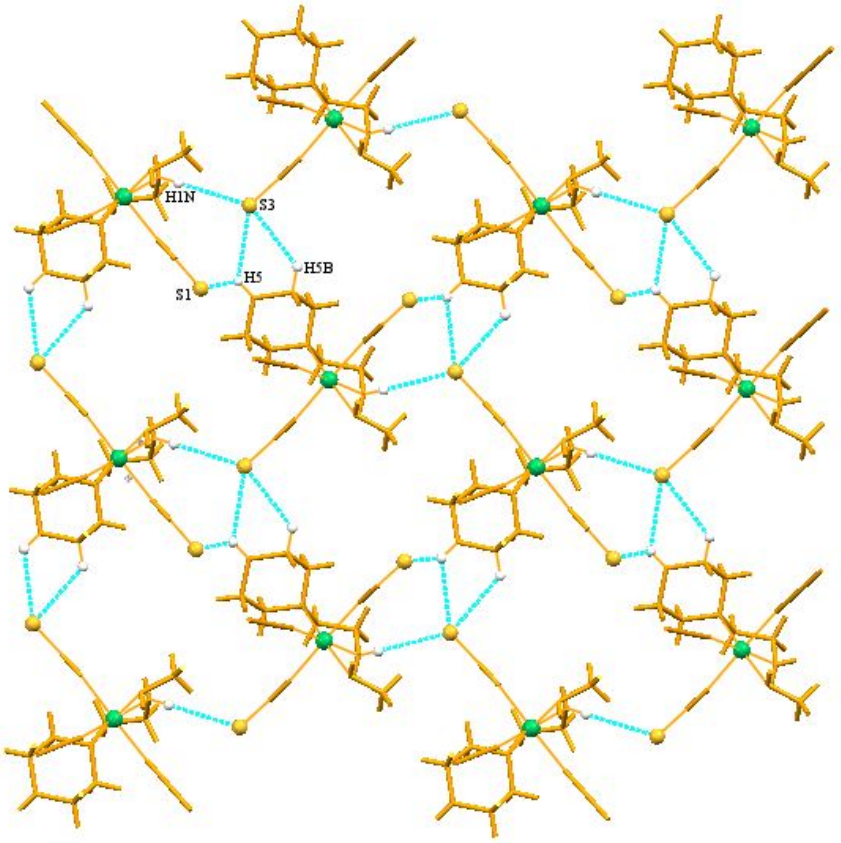


Fig S10: 2D hydrogen bonded sheet like network of complex **2a**.

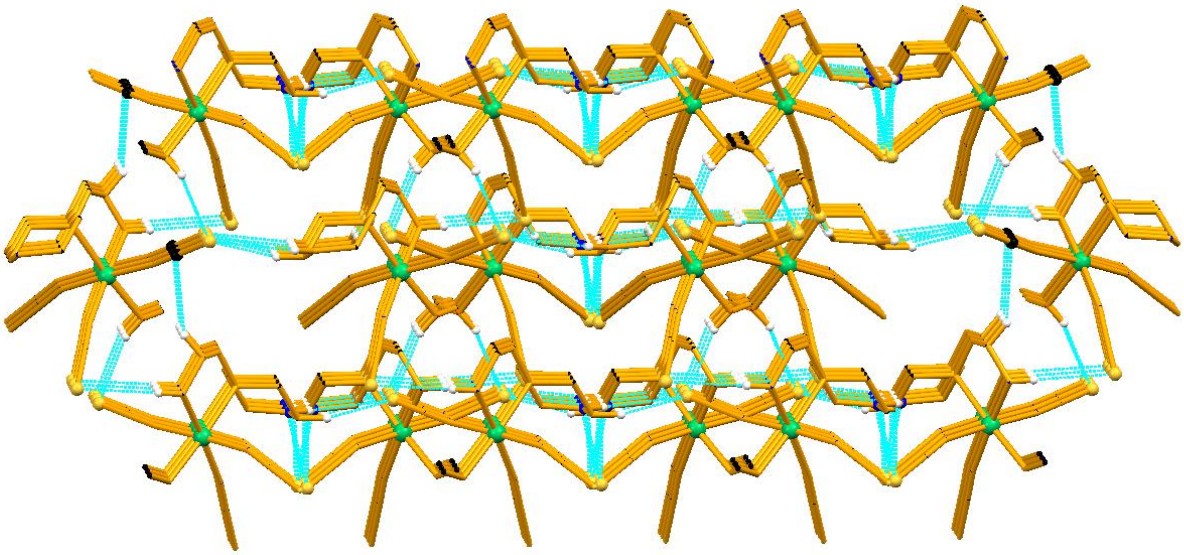


Fig S11: 3D hydrogen bonding network of complex **2a**.

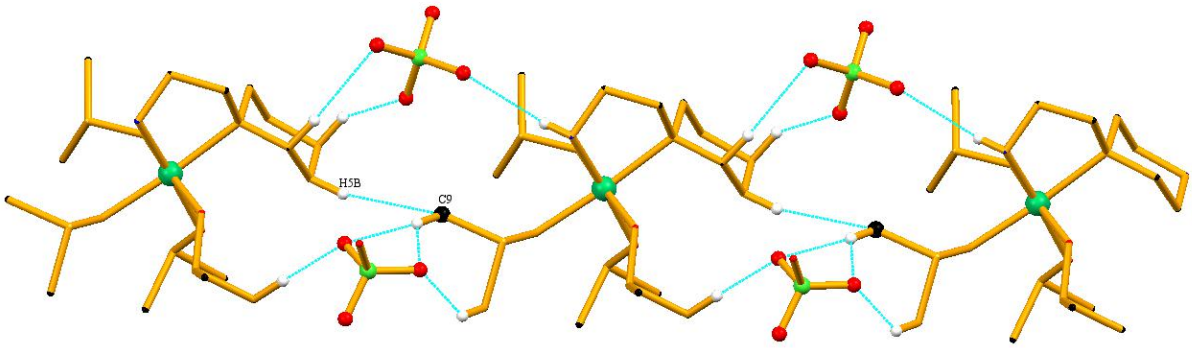


Fig S12: 1D chain like structure of complex **2b**.

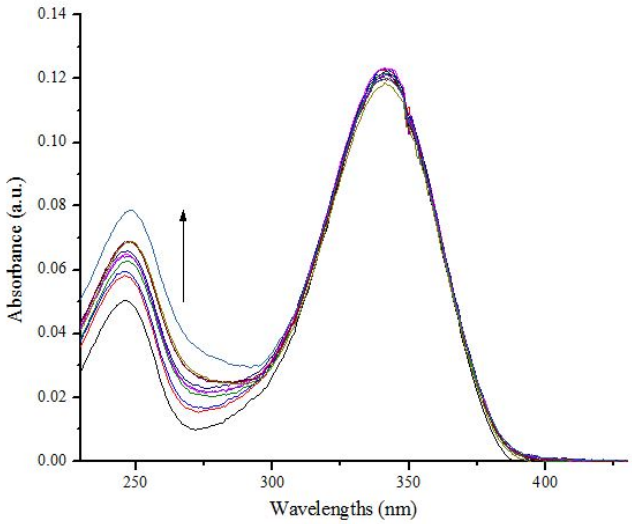


Fig 13A: Absorption titration spectra of fixed concentration (10 μM) of complexes **1a** with increasing concentrations (0–200 μM) of CT-DNA (Tris-HCl buffer, pH 7.4).

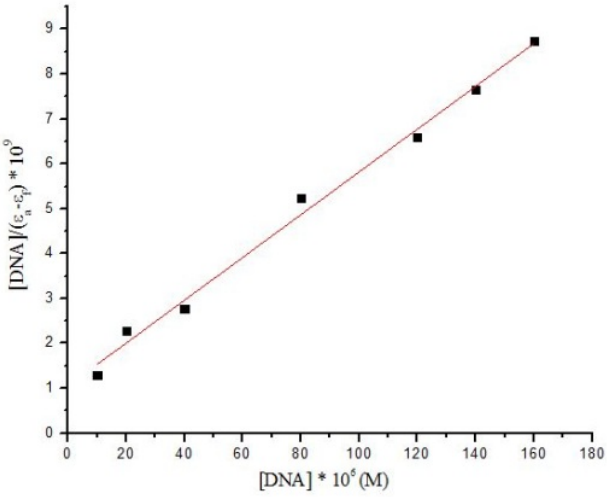


Fig 13B: Binding isotherms of complex **1a**.

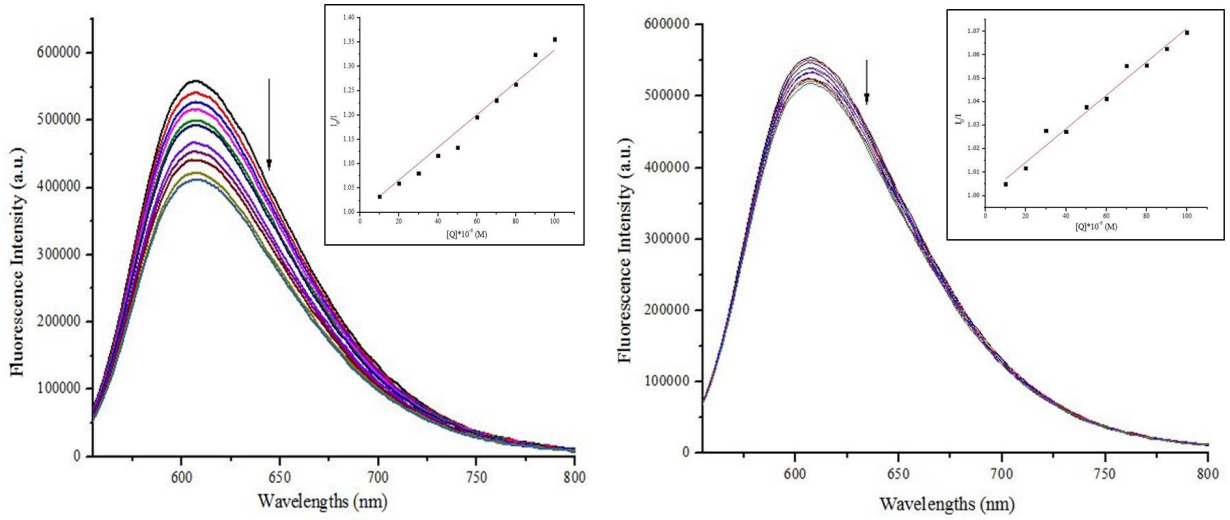


Fig S14: ETBr displacement assay by change in fluorescent intensity of EB with respect to conc. of complex **1a** (left) and complex **1b** (right). Corresponding stern-volmer plot is in inset.

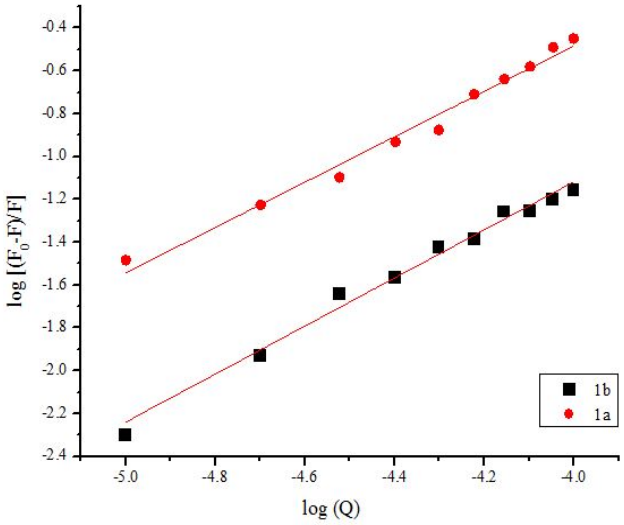


Fig S15: Scatchard plot for determination of K_b for CT-DNA of **1a** and **1b**.

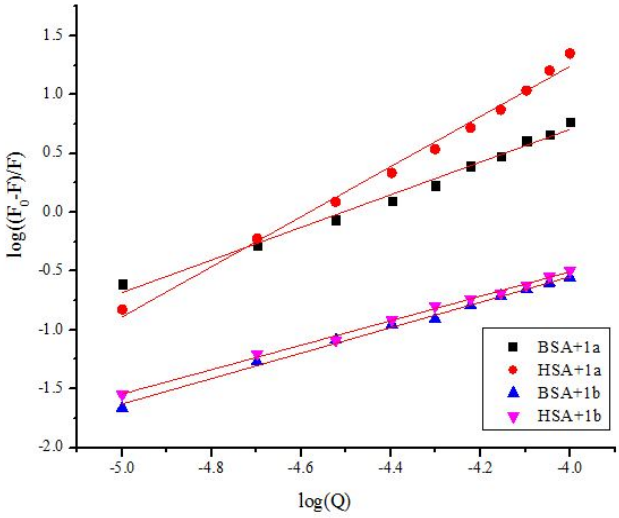


Fig S16: Scatchard plot for various system of fluorescence quenching.

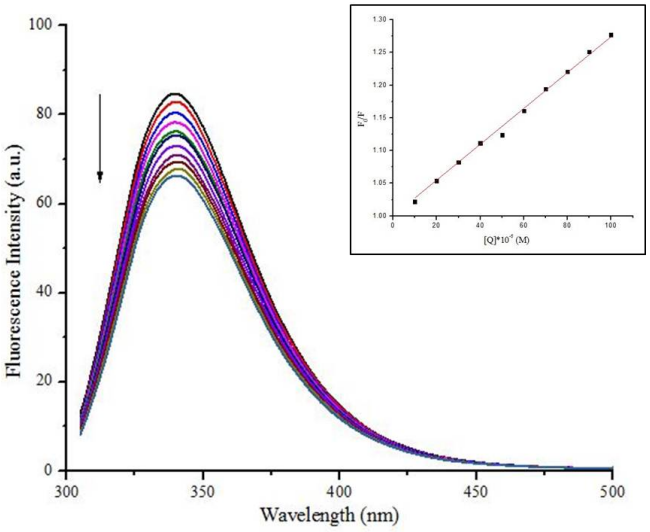


Fig S17: Fluorescence quenching of BSA by **1b**. Stern-Volmer plot is in Inset.

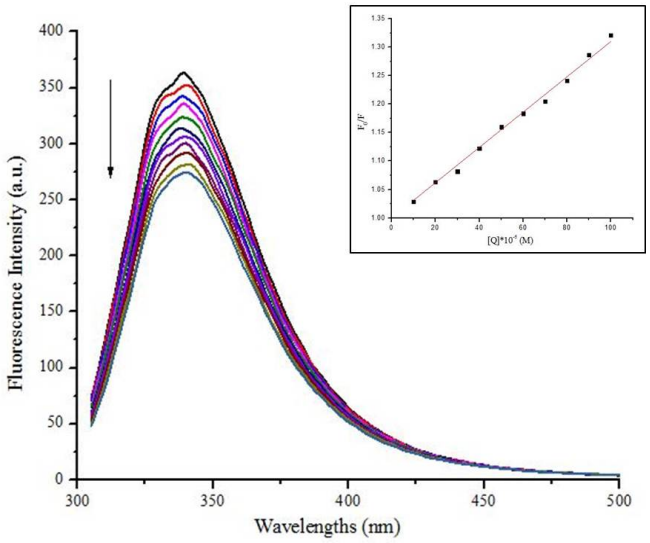


Fig S18: Fluorescence quenching of HSA by **1b**. Stern-Volmer plot is in Inset.

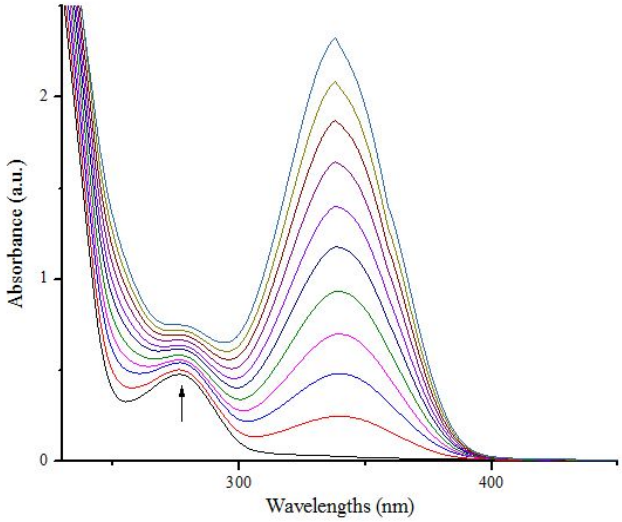


Fig S19A : UV-VIS Absorption titration of BSA (10μM) by successive addition of **1a**.

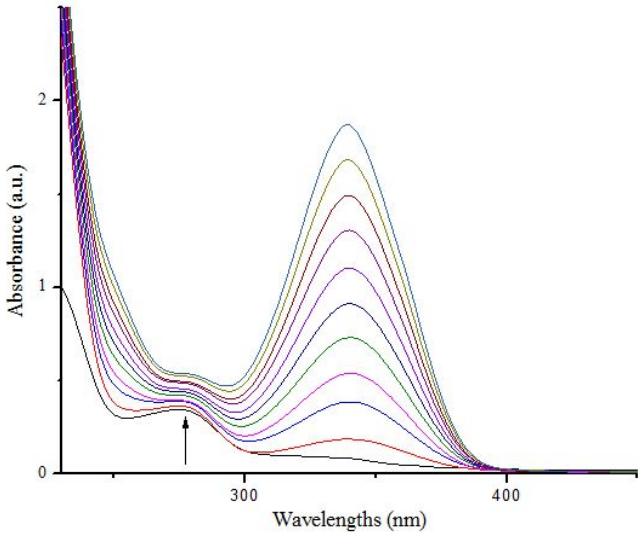
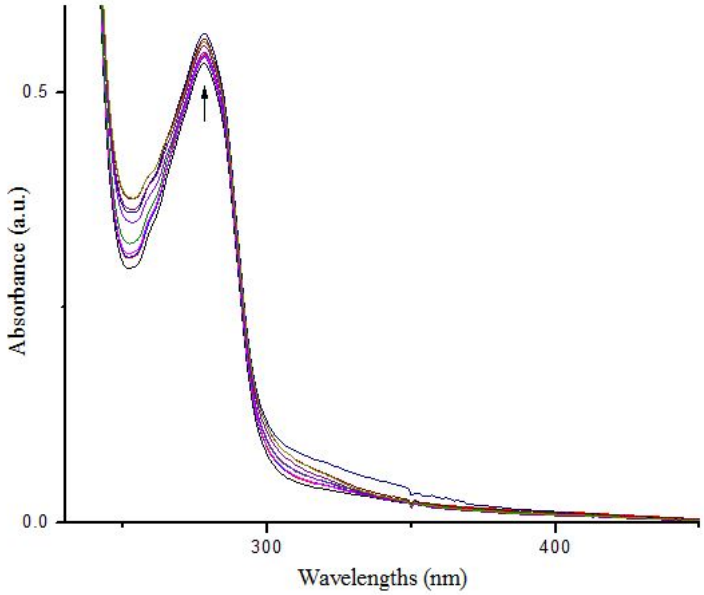


Fig S19B : UV-VIS Absorption titration of HSA (10μM) by successive addition of **1a**.



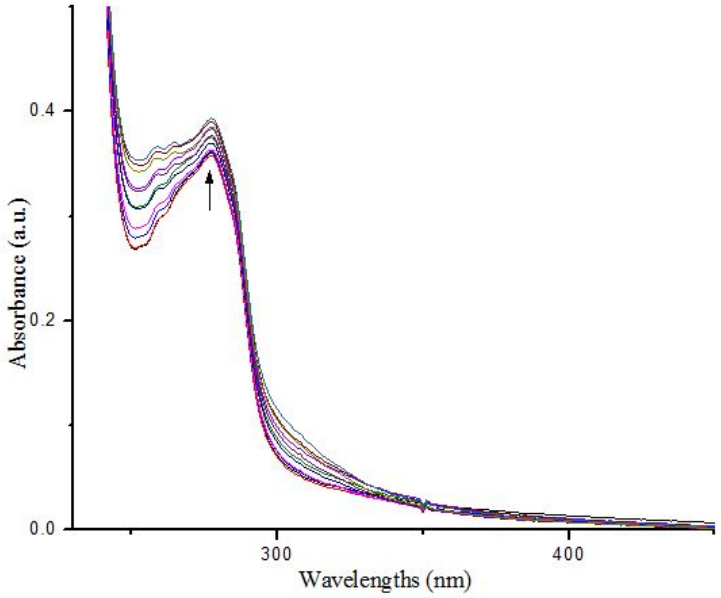


Fig S20A and Fig S20B : UV-VIS Absorption titration of BSA (10μM) (above) and HSA (10μM) (below) by successive addition of **1b**.

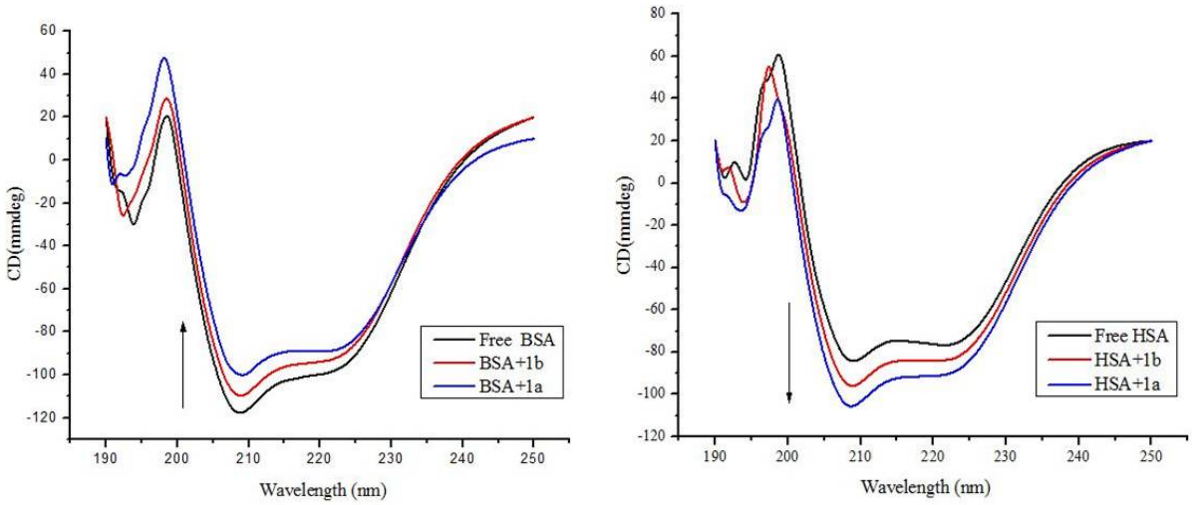


Fig S21: Changes of CD spectra of BSA (left) and HAS (right) by **1a** and **1b**.

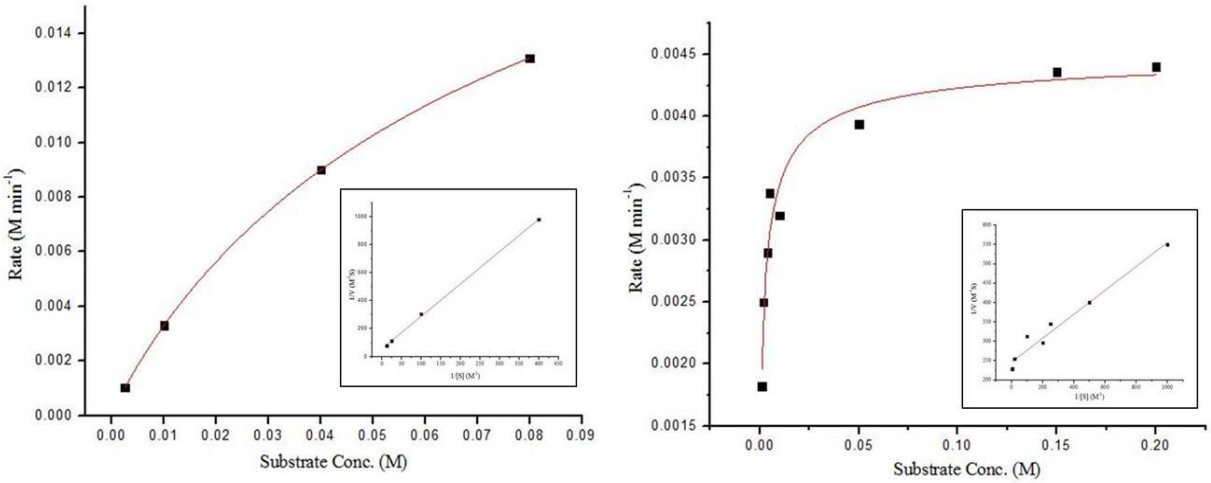


Fig S22: Michael-menten plot for **1a** (left) and **1b** (right). Inset- lineweaver burk plot.

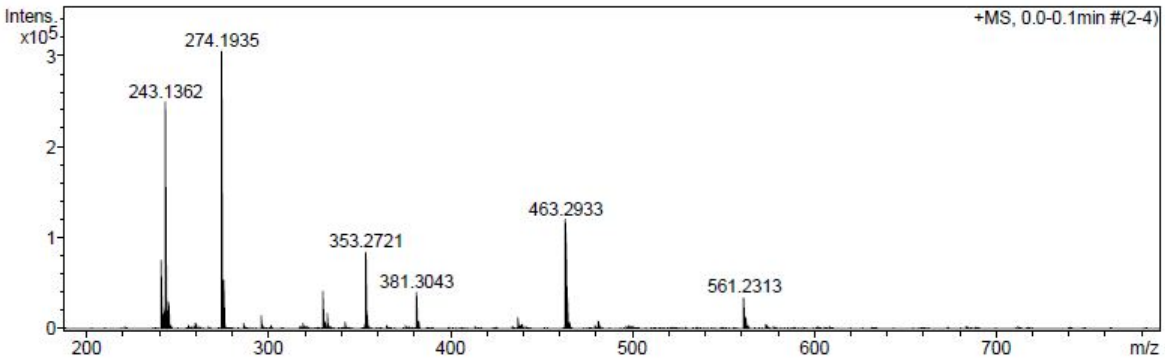


Fig S23A: Electrospray mass spectrum (ESI-MS positive) of a 1:100 **1a**/3,5-DTBC mixture in methanol, recorded within 10 min of mixing.

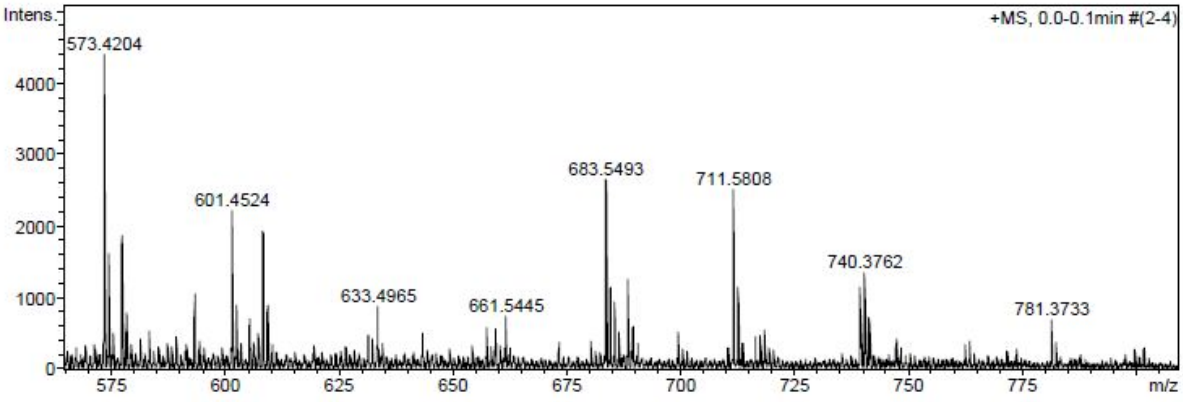


Fig S23B: Electrospray mass spectrum (ESI-MS positive) of a 1:100 **1a**/3,5-DTBC mixture in methanol, recorded within 10 min of mixing (Expanded Zoomed spectra).

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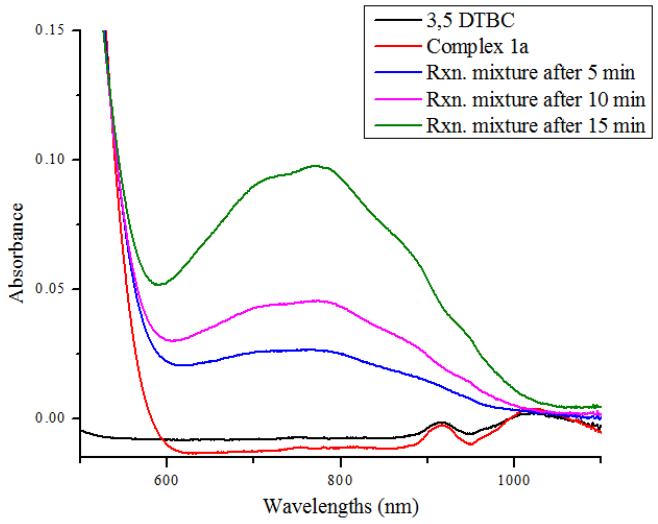
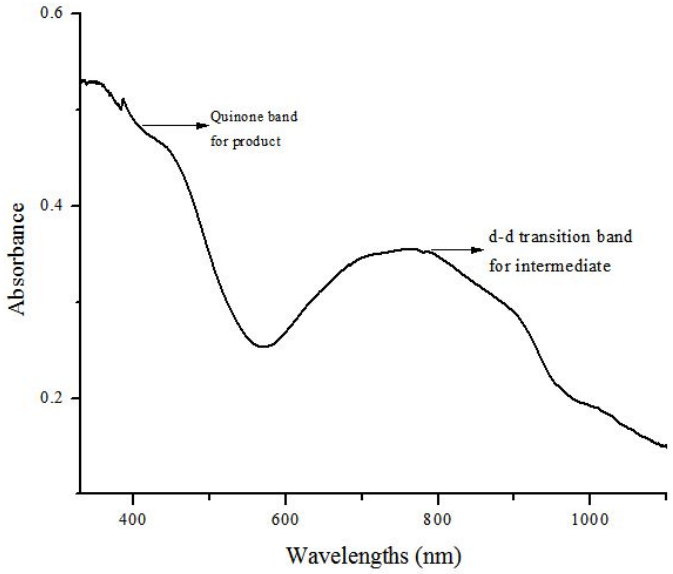


122

123 Fig S24A: Change in d-d transition band of Ni(II) with time upon reaction with 3,5 DTBC.



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125 Fig S24B: After 35min of reaction showing both species (1. Quinone band ≈ 400nm for product

126 and 2. d-d transition band for complex-substrate aggregate) in solutions.

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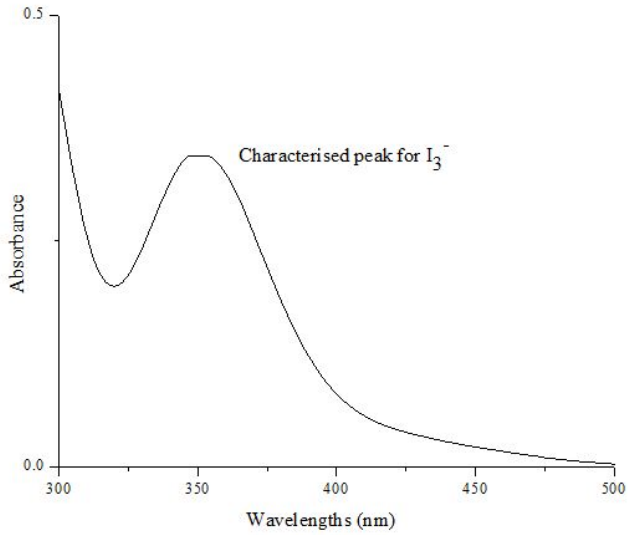


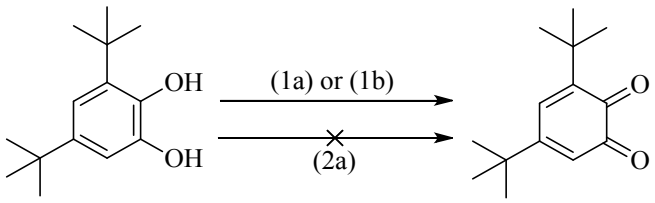
Fig S25: Characterized peak for I_3^- for qualitative detection of H_2O_2 during catalytic oxidation process.

Table S1 : Hydrogen bonding interactions of all complexes.

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	*d*(D–H···A) (°)
1a				
C8–H8A···O1	0.990	2.457	3.434	168.62
C7–H7B···C16	0.991	2.826	3.151	155.81
C9–H9A···O111	0.990	2.646	3.343	170.50
C5–H5A···O111	0.990	2.491	3.403	153.08
C16–H16···O333	0.949	2.610	3.304	130.24
C6–H6B···O111	0.990	2.646	3.343	128.55
C5–H5B···O222	0.989	2.510	3.446	157.92
C13–H13···O222	0.950	2.484	3.313	145.74
1b				
C5–H5C···O333	0.979	2.590	3.484	151.75
C8–H8A···O333	0.991	2.688	3.567	148.01
C8–H8A···O222	0.991	2.643	3.584	158.47
C7–H7A···O222	0.990	2.552	3.510	162.81

N3–H3N···O444	0.766	2.635	3.279	142.80
N3–H3N···O333	0.766	2.388	3.133	164.23
C7–H7B···O333	0.980	2.671	3.641	166.62
C6–H6B···O111	0.990	2.604	3.591	174.88
C10–H10B···O444	0.990	2.562	3.375	139.41
2a				
N5–H5···S1	0.879	2.942	3.283	105.14
N6–H1N···S3	0.794	2.838	3.626	171.66
N5–H5···S3	0.879	2.914	3.523	127.77
C5–H5B···S3	0.990	2.990	3.702	129.71
O111–H101···S3	0.797	2.504	3.261	159.03
N6–H2N···S2	0.817	2.782	3.576	164.28
2b				
C6–H6A···O555	0.990	2.563	3.545	171.53
N1–H1N···O555	1.041	2.342	3.186	137.29
N3–H3N···O101	0.903	2.427	2.998	121.32
C12–H12B···O101	0.980	2.682	3.563	149.82
N3–H3N···O333	0.903	2.172	2.987	149.74
C10–H10B···O444	0.980	2.600	3.405	139.47
C5–H5B···C9	0.990	2.888	2.852	164.70
C14–H14C···O222	0.981	2.463	3.413	162.94
C9–H9B···O222	0.980	2.552	3.528	173.98
N1–N2H···O777	0.823	2.487	3.275	160.80
C9–H9B···O444	0.980	2.709	3.485	136.47

Schemes :



Scheme S1: Schematic representation of catecholase activity.