Supplementary Material (ESI) for Dalton Transactions

Anaerobic DNA cleavage activity in red light and photocytotoxicity of (pyridine-2-thiol)cobalt(III) complexes of phenanthroline bases

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Electronic Supplementary Information

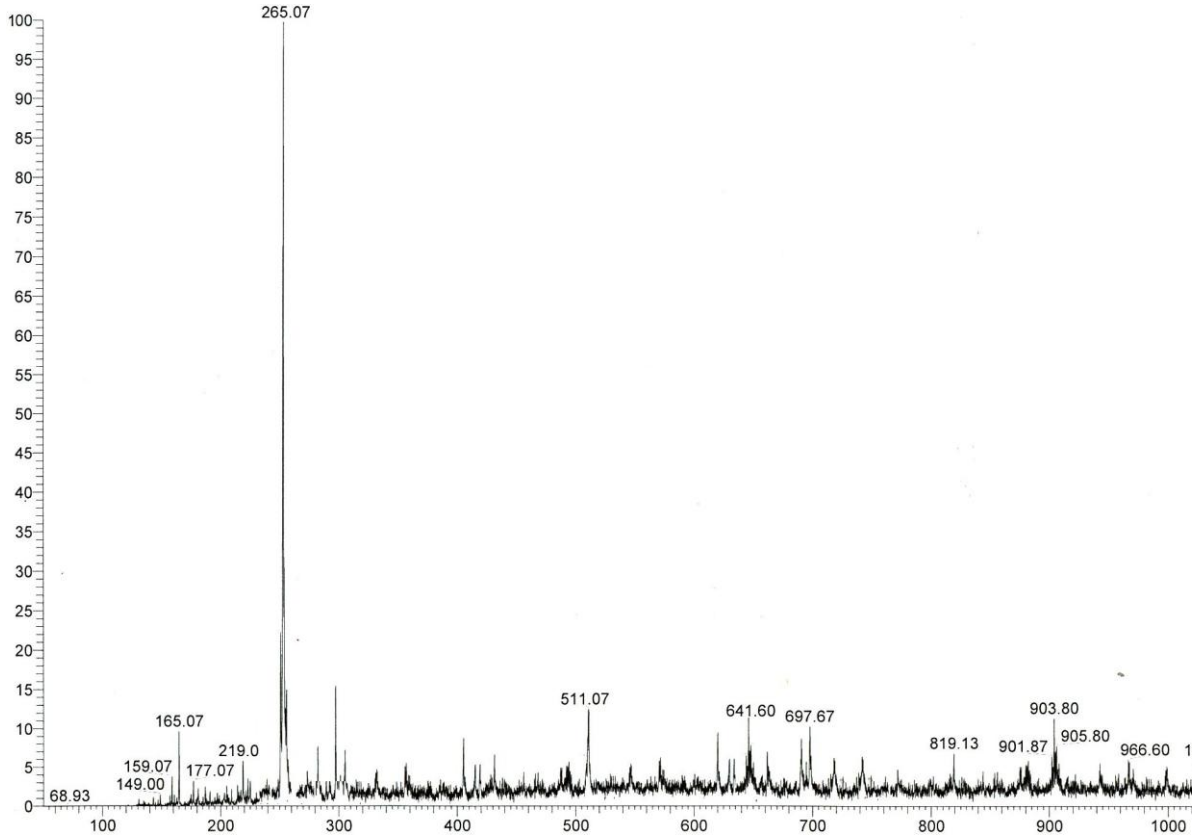

Fig. S1 Mass spectrum of complex **1** in aqueous DMF (1:1 v/v) showing the parent ion peak at 265.07 m/z.

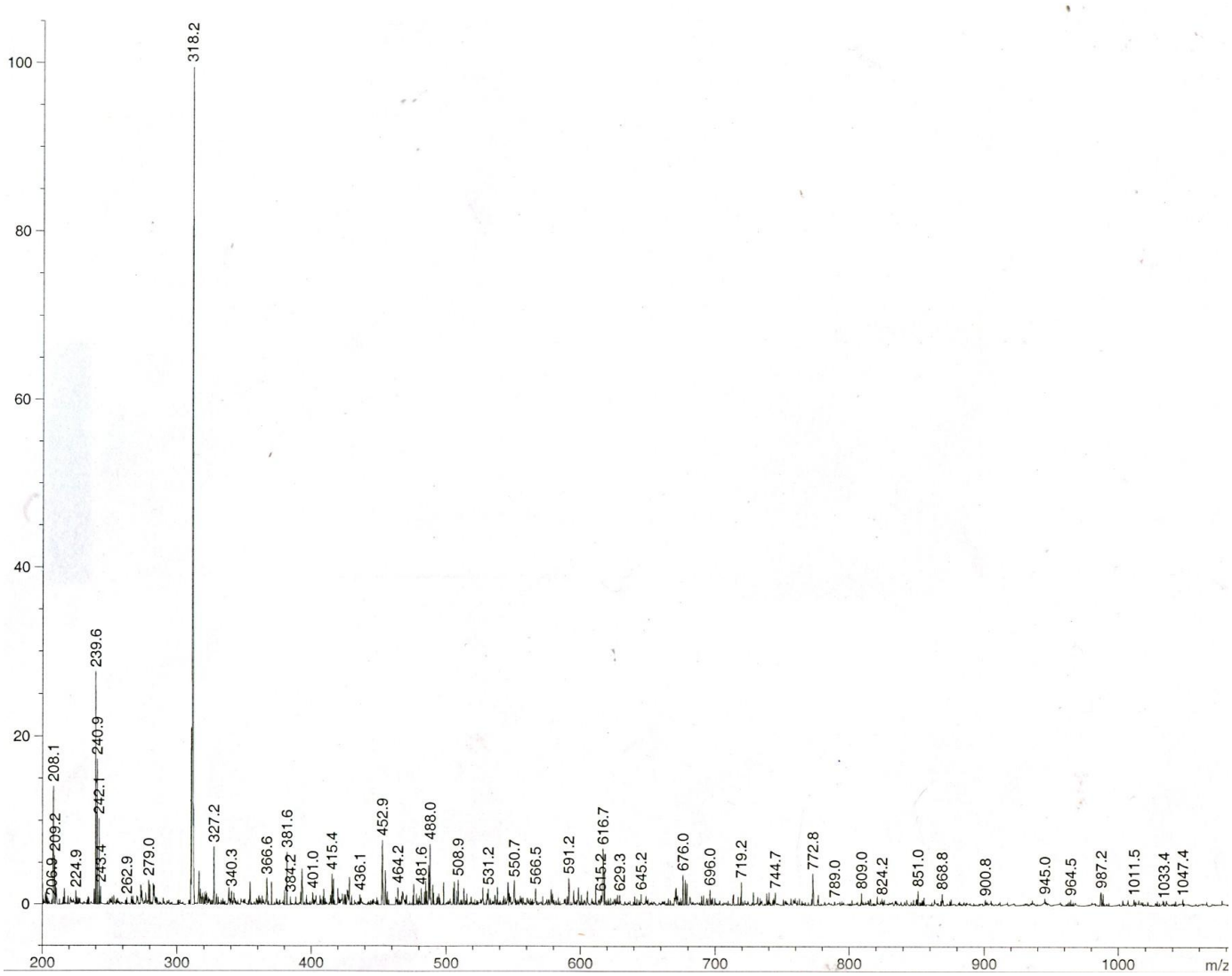

Fig. S2 Mass spectrum of complex **2** in aqueous DMF (1:1 v/v) showing the parent ion peak at 318.20 m/z.

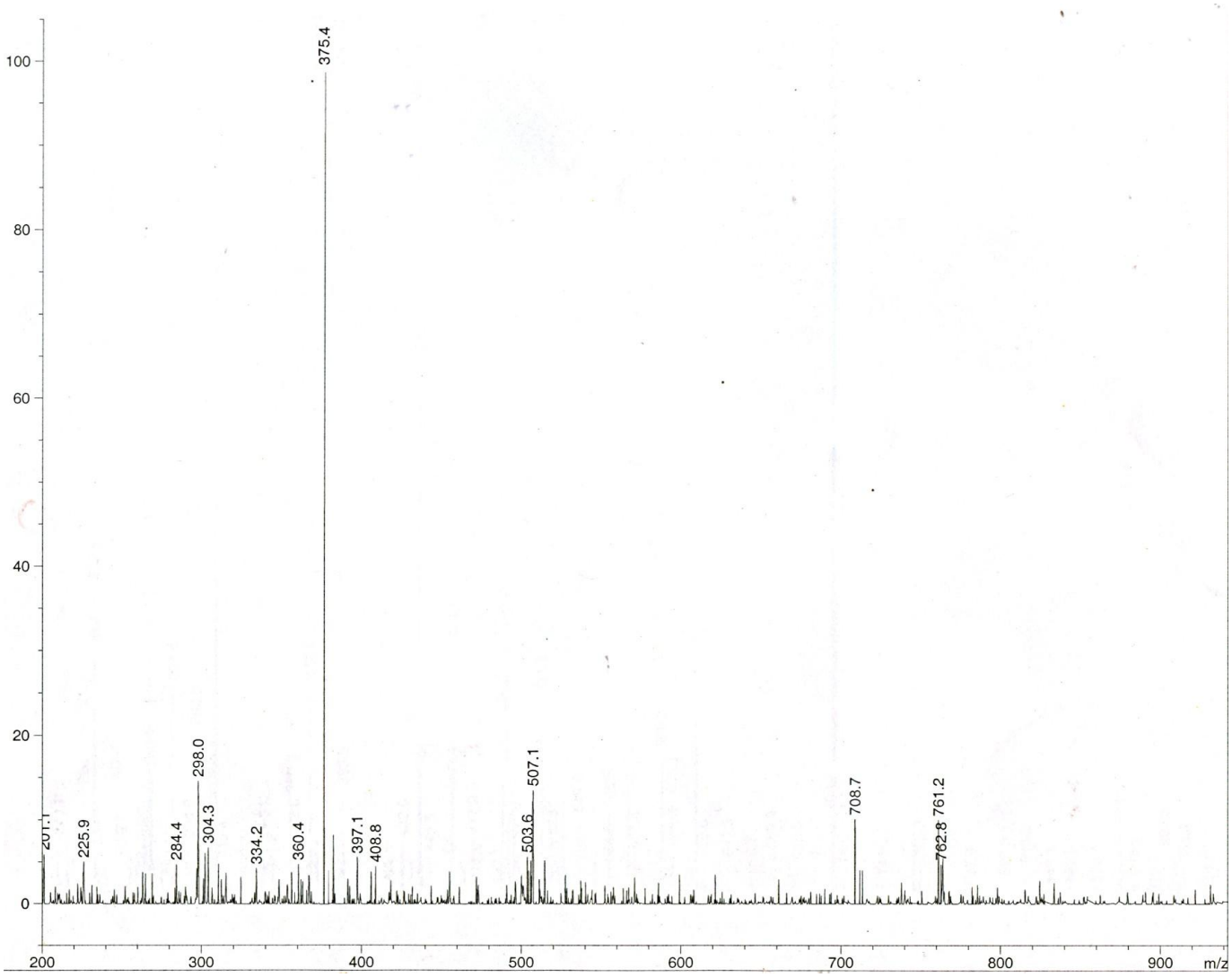

Fig. S3 Mass spectrum of complex **3** in aqueous DMF (1:1 v/v) showing the parent ion peak at 375.47 m/z.

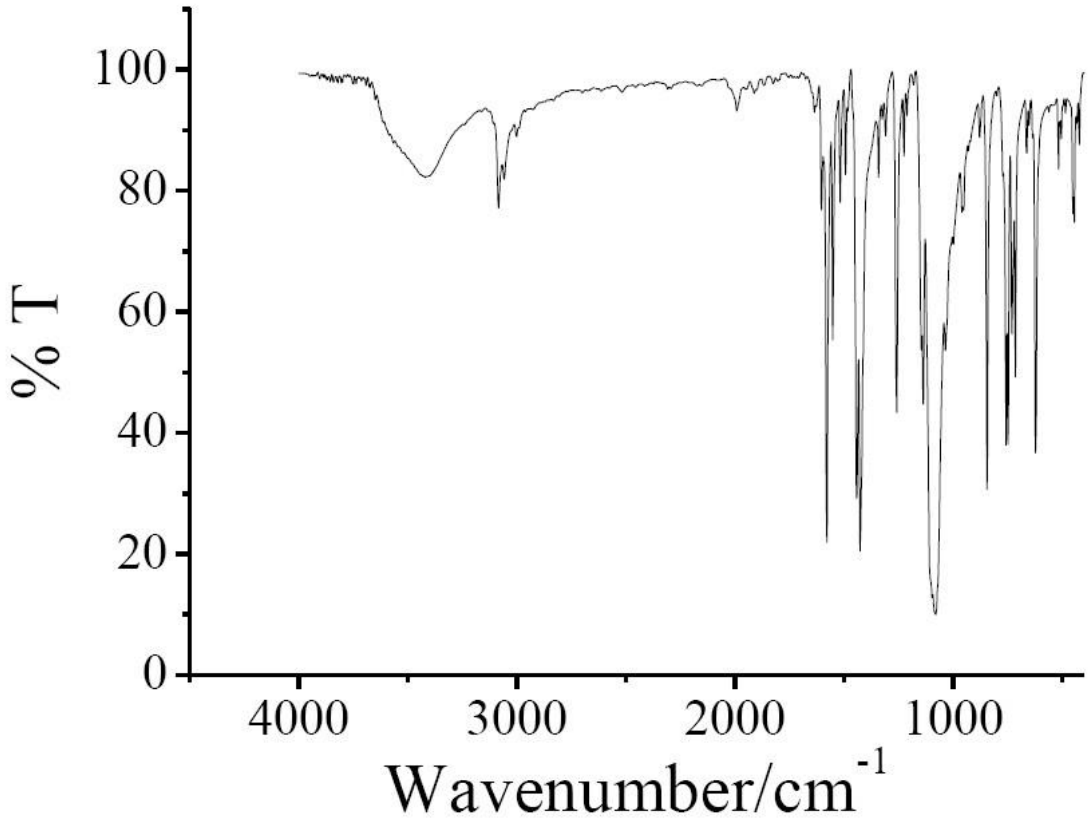

Fig. S4 IR spectrum of complex **1** in solid KBr matrix.

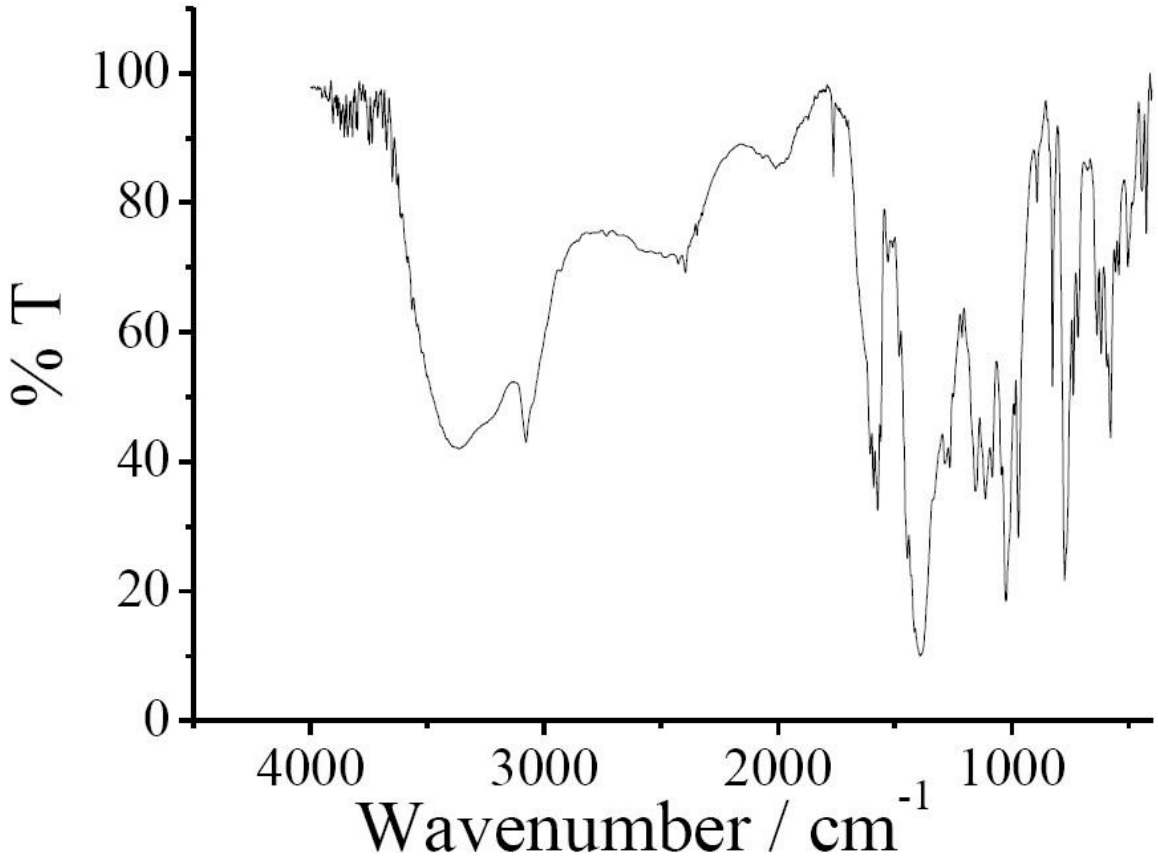

Fig. S5 IR spectrum of complex **2** in solid KBr matrix.

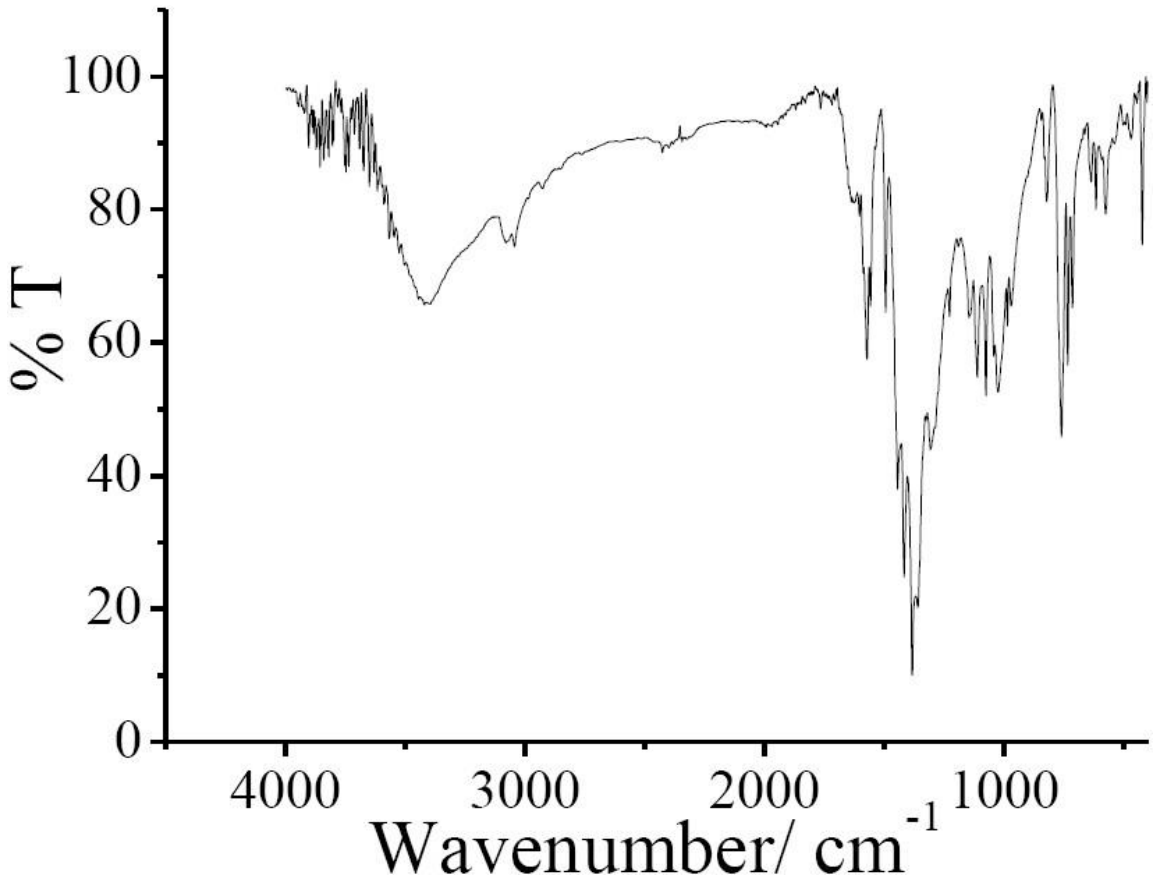

Fig. S6 IR spectrum of complex **3** in solid KBr matrix.

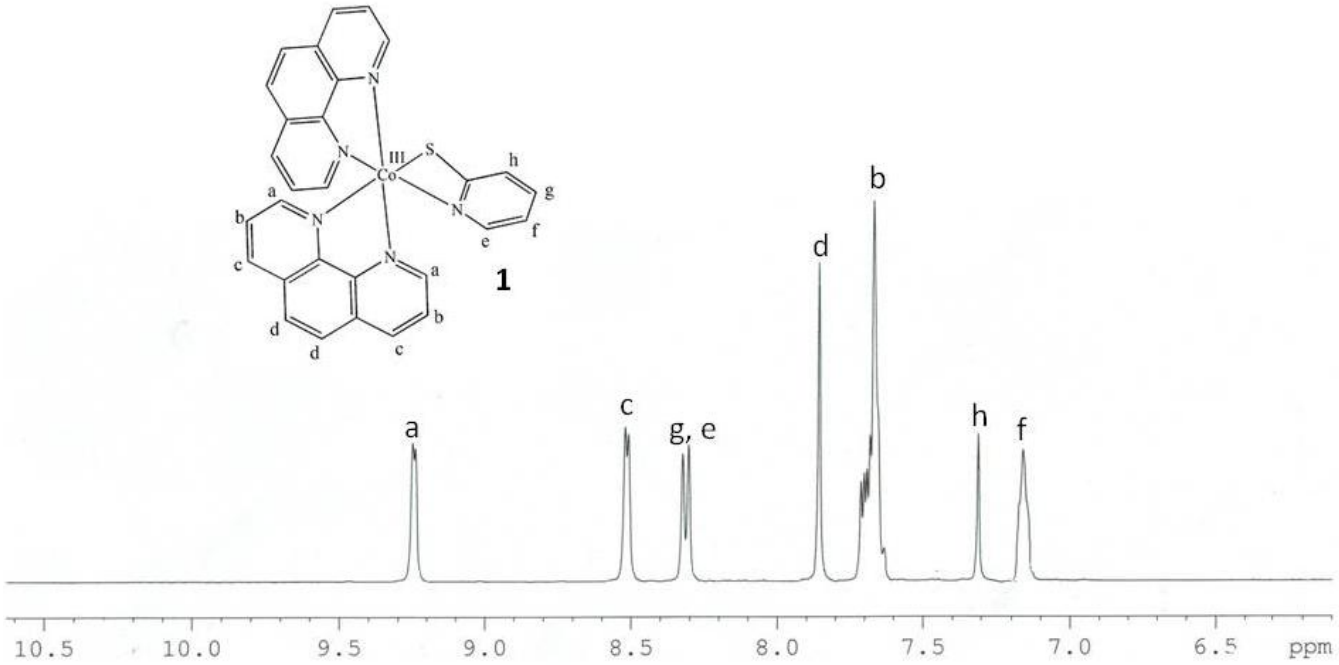

Fig. S7 NMR spectrum of complex **1** in DMSO-d_6 showing the peak assignments.

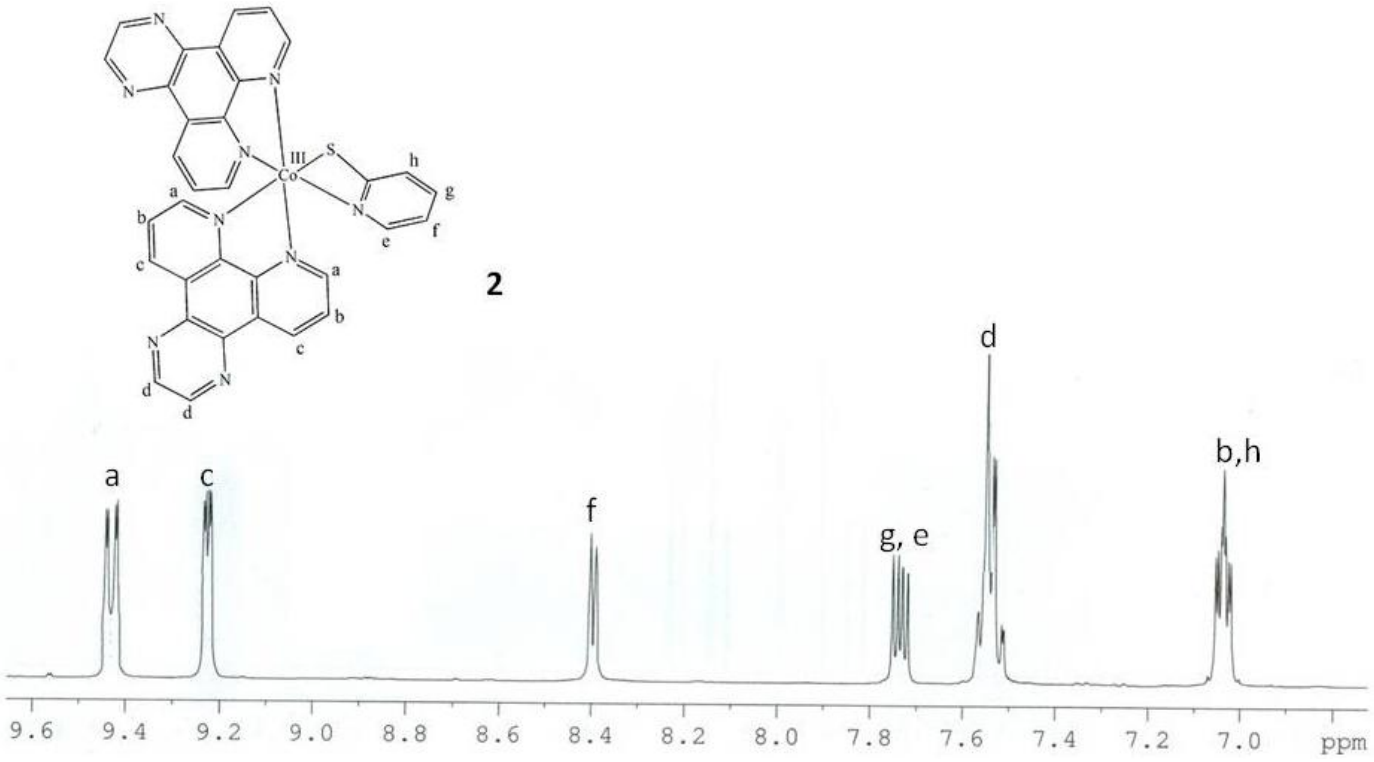

Fig. S8 NMR spectrum of complex **2** in DMSO-d_6 showing the peak assignments.

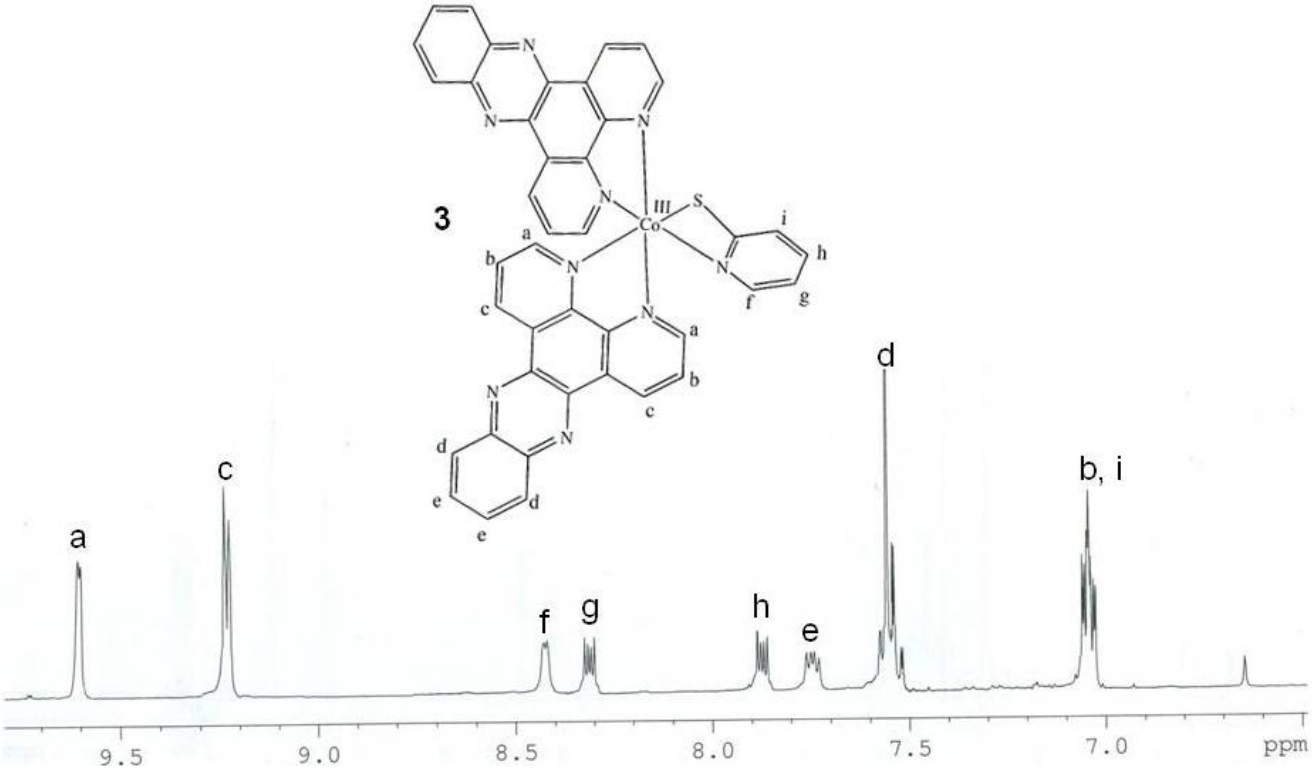

Fig. S9 NMR spectrum of complex **3** in DMSO-d_6 showing the peak assignments.

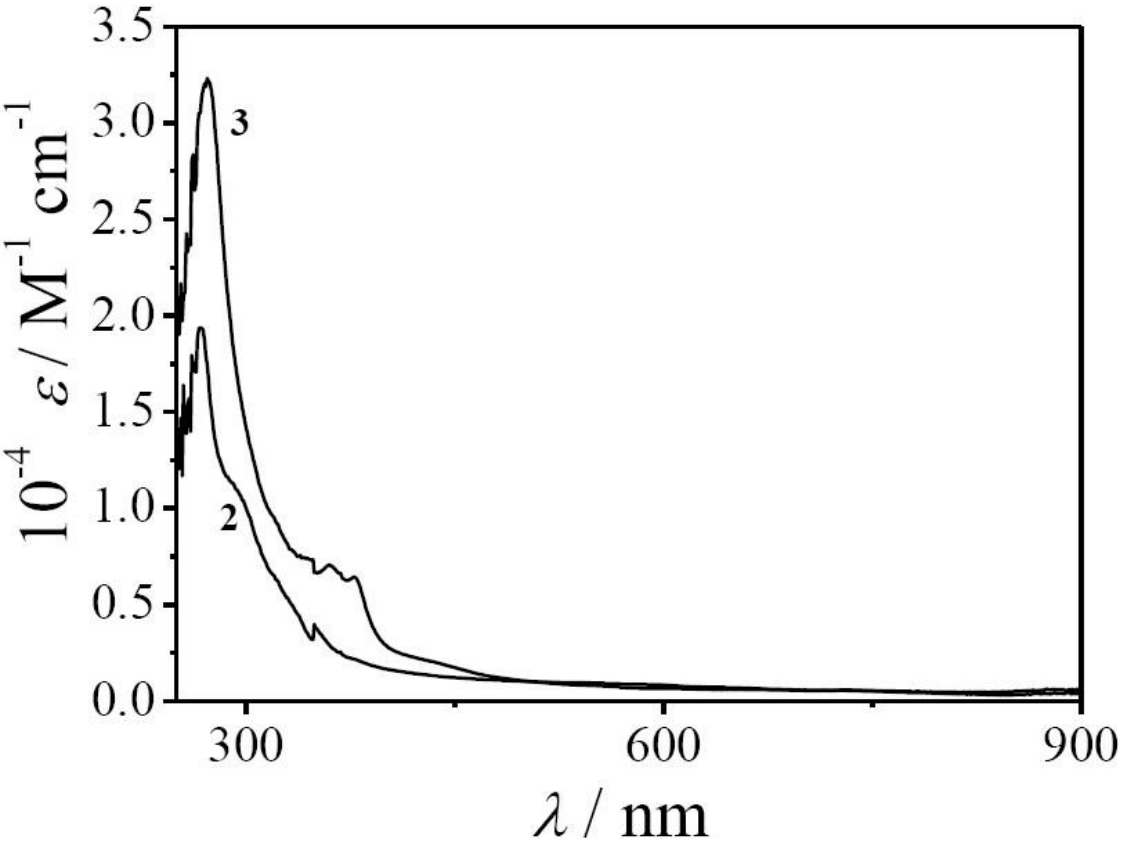

Fig. S10 Electronic spectra of $[Co(pnt)(dpq)_2](NO_3)_2$ (**2**) and $[Co(pnt)(dppz)_2](NO_3)_2$ (**3**) in aqueous DMF (1:1 v/v).

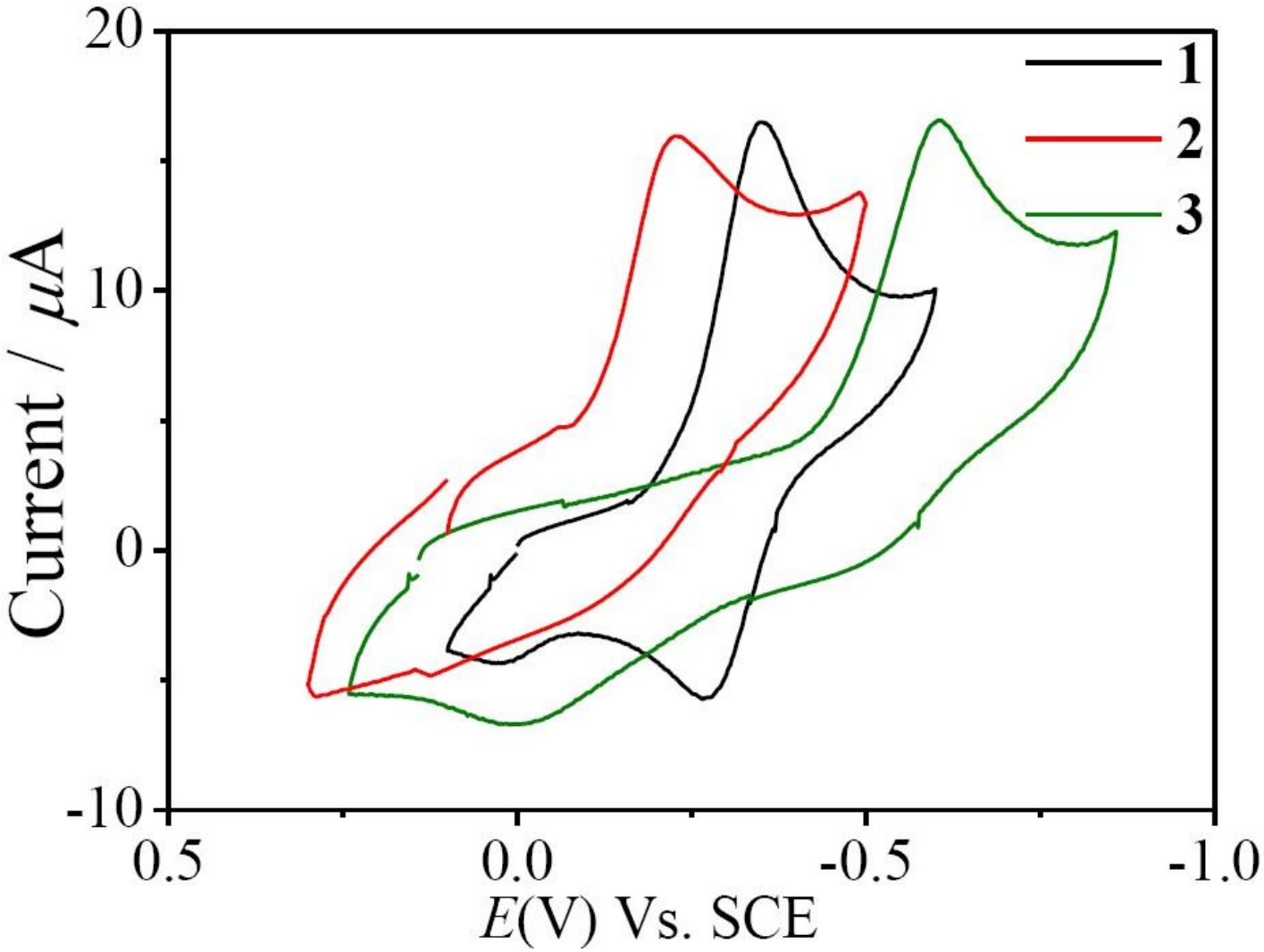

Fig. S11 Cyclic voltammetric responses for the complexes **1** (black), **2** (red), **3** (green) in DMF using TBAP (0.1 M) as the supporting electrolyte with a scan rate of 50 mV s^{-1}.

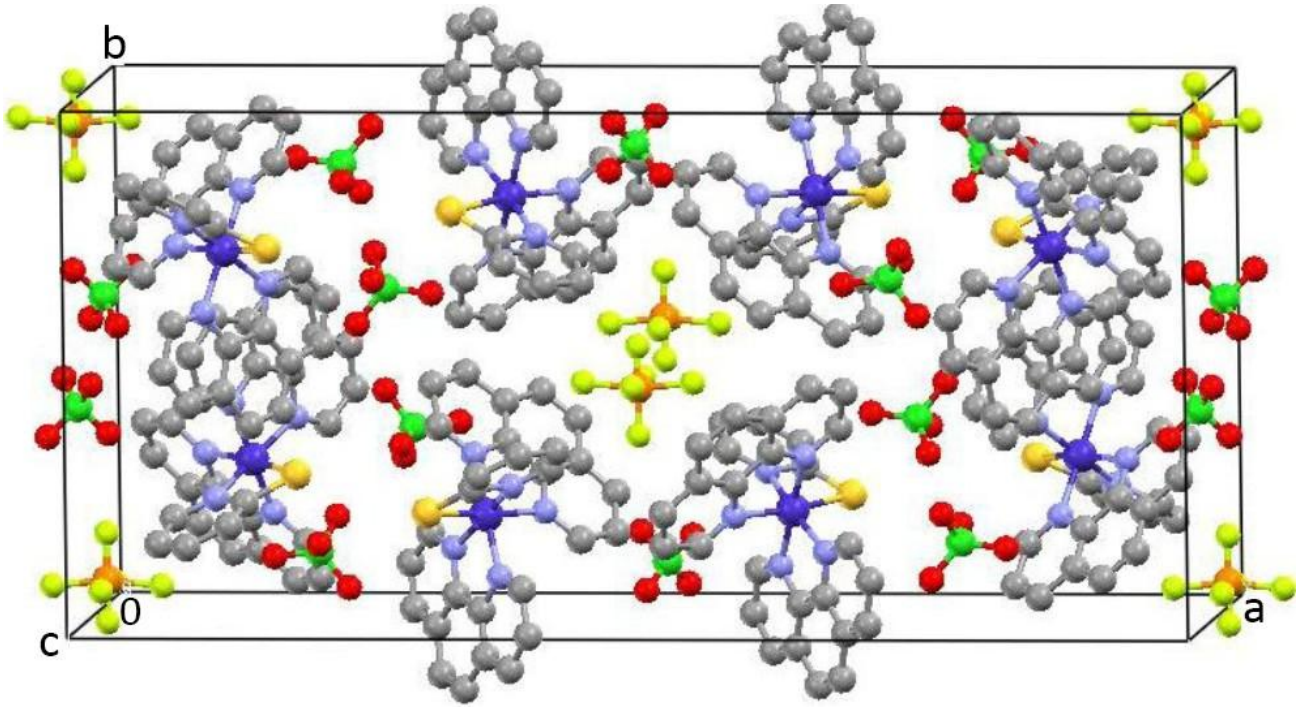

Fig. S12 Unit cell packing diagram of complex **1a** in the orthorhombic space group *P*bcn. One ClO_4 and the PF_6 anions have half occupancies.

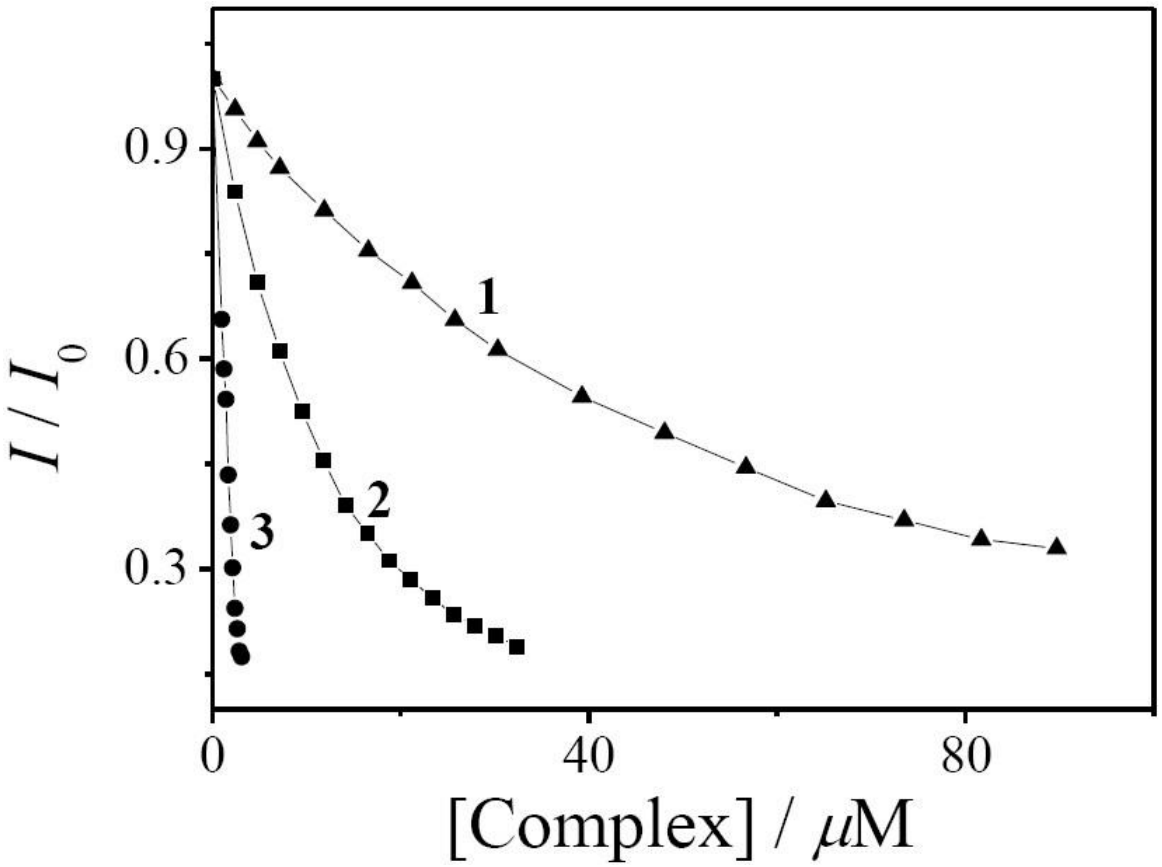

Fig. S13 Effect of addition of $[Co(pnt)(B)_2](NO_3)_2$ (**1**-**3**) [B = phen (**1**); dpq (**2**); dppz (**3**) on the emission intensity of ethidium bromide bound to CT-DNA.

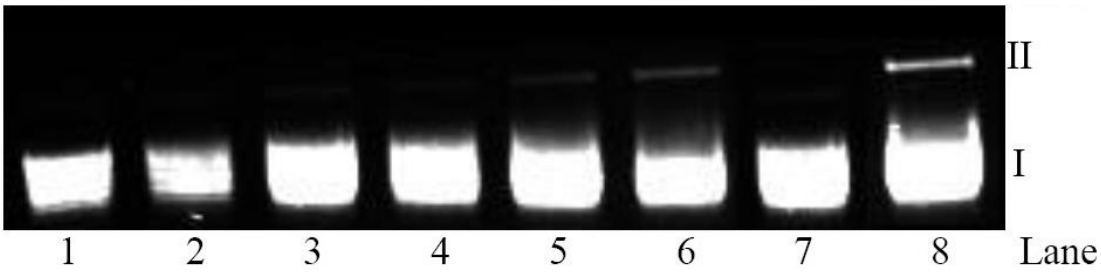

Fig. S14 Cleavage of SC pUC19 DNA (0.2 μg, 30 μM) by the complexes **1**-**3** (5 μM) in 50 mM Tris-HCl/NaCl buffer (pH, 7.2) in presence of 3-mercaptopropionic acid for 1 h incubation time. Form I and II are supercoiled and nicked circular forms of DNA, respectively.

Lane No.	Conditions	Atmosphere	%SC	%NC
1.	DNA control	air	96	4
2.	DNA + MPA (200 μM)	air	94	6
3.	DNA + **1** (in dark)	air	95	5
4.	DNA + **2** (in dark)	air	93	7
5.	DNA + **3** (in dark)	air	91	9
6.	DNA + MPA + **1** (in dark)	air	89	11
7.	DNA + MPA + **2** (in dark)	air	92	8
8.	DNA + MPA + **3** (in dark)	air	85	15

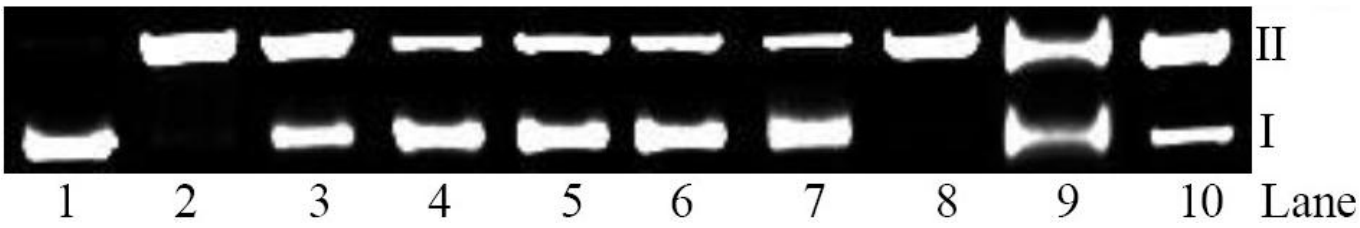

Fig. S15 Cleavage of SC pUC19 DNA (0.2 μg, 30 μM) by the complex **3** (10 μM, 2 h) in the presence of various additives on photo-irradiation at 365 nm in 50 mM Tris-HCl/NaCl buffer (pH, 7.2) for 1 h incubation time [NaN_3, 200 μM; catalase, 4 units; DMSO, 4 μL; SOD, 4 units, DABCO, 500 μM; KI, 200 μM; TEMP, 500 μM]. Form I and II are supercoiled and nicked circular forms of DNA, respectively.

Lane No.	Conditions	Atmosphere	%SC	%NC
1.	DNA control	air	96	4
2.	DNA + **3**	air	14	86
3.	DNA + NaN_3 + **3**	air	46	54
4.	DNA + TEMP + **3**	air	67	33
5.	DNA + DABCO + **3**	air	62	38
6.	DNA + KI + **3**	air	65	35
7.	DNA + DMSO + **3**	air	69	31
8.	DNA + D_2O + **3**	air	5	95
9.	DNA + catalase + **3**	air	46	54
10.	DNA + SOD + **3**	air	22	78

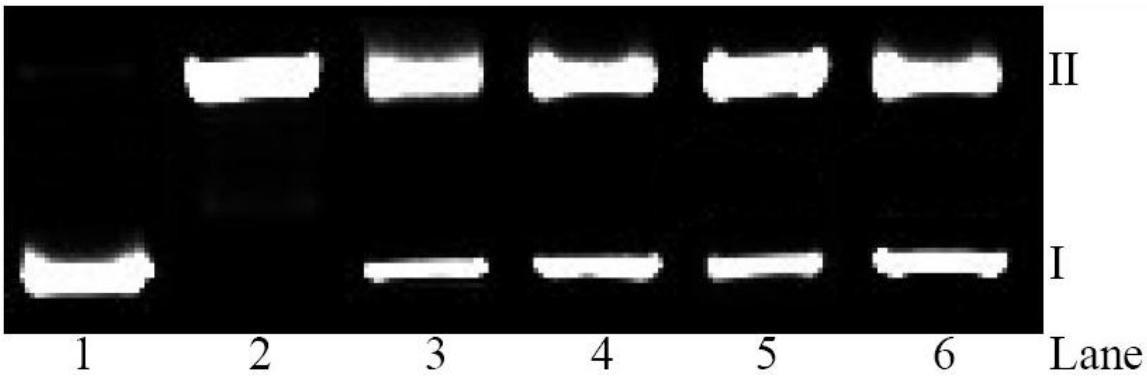

Fig. S16 Cleavage of SC pUC19 DNA (0.2 μg, 30 μM) by the complex **3** (20 μM, 2 h) in the presence of various additives on photo-irradiation at 647.1 nm under argon atmosphere in 50 mM Tris-HCl/NaCl buffer (pH, 7.2) for 1 h incubation time [NaN_3, 200 μM; catalase, 4 units; DMSO, 4 μL]. Form I and II are supercoiled and nicked circular forms of DNA, respectively.

Lane No.	Conditions	Atmosphere	%SC	%NC
1.	DNA control	air	96	4
2.	DNA + **3**	air	18	82
3.	DNA + **3**	argon	29	71
4.	DNA + NaN_3 + **3**	argon	35	65
5.	DNA + DMSO + **3**	argon	32	68
6.	DNA + catalase + **3**	argon	38	62

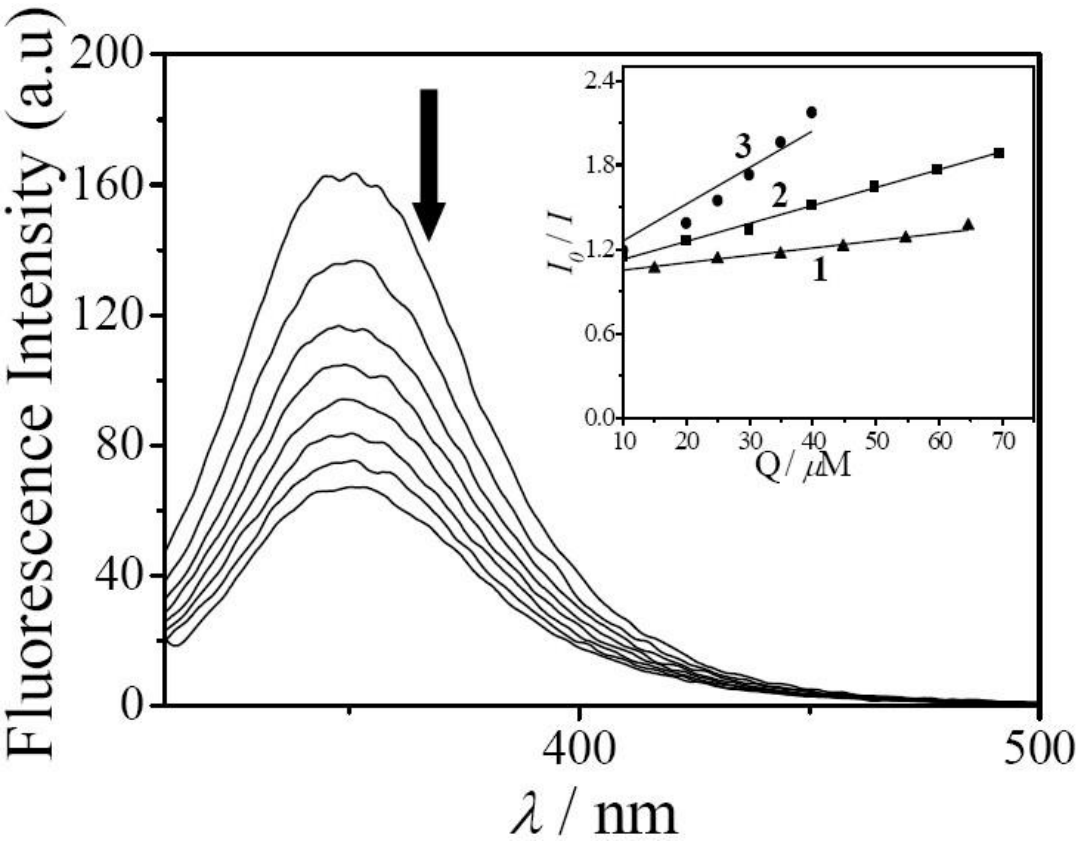

Fig. S17 Effect of addition of $[Co(pnt)(B)_2](NO_3)_2$ (**1**-**3**) [B = phen (**1**); dpq (**2**); dppz (**3**) on the emission intensity of ethidium bromide bound to bovine serum albumin (BSA) protein. The inset shows the Stern-Volmer plots for the BSA binding propensities of the complexes **1**-**3**.

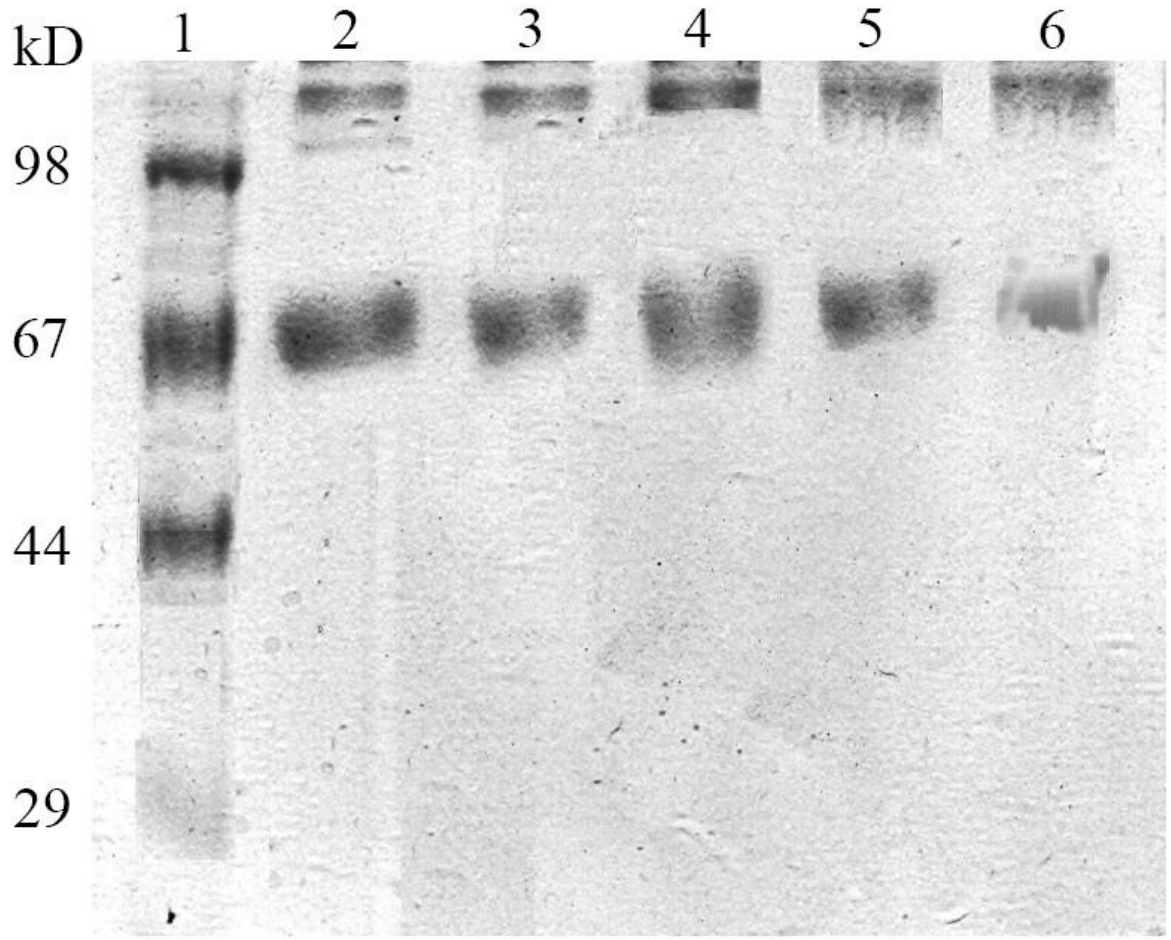

Fig. S18 12.5% SDS-PAGE diagram showing the photocleavage of bovine serum albumin (BSA, 5 μM) protein in UV-A light of 365 nm by the complexes $[Co(pnt)(phen)_2](NO_3)_2$ (**1**) and $[Co(pnt)(dpq)_2](NO_3)_2$ (**2**) in 50 mM Tris-HCl buffer having 0.6% DMF (pH 7.2). (a) lane 1, molecular marker; lane 2, BSA control; lane 3, BSA + complex **1** (200 μM, 1 h, in dark); lane 4, BSA + complex **2** (200 μM, 1 h, in dark); lane 5, BSA + complex **1** (200 μM, 1 h); lane 6, BSA + complex **2** (200 μM, 1 h).