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ELECTRONIC SUPPLEMENTARY INFORMATION FOR:

The effect of incorporation of carboxylic acid functionalities in 2,2'-bipyridine on the biological activity of the complexes formed: Synthesis, structure, DNA/protein interaction, antioxidant activity and cytotoxicity

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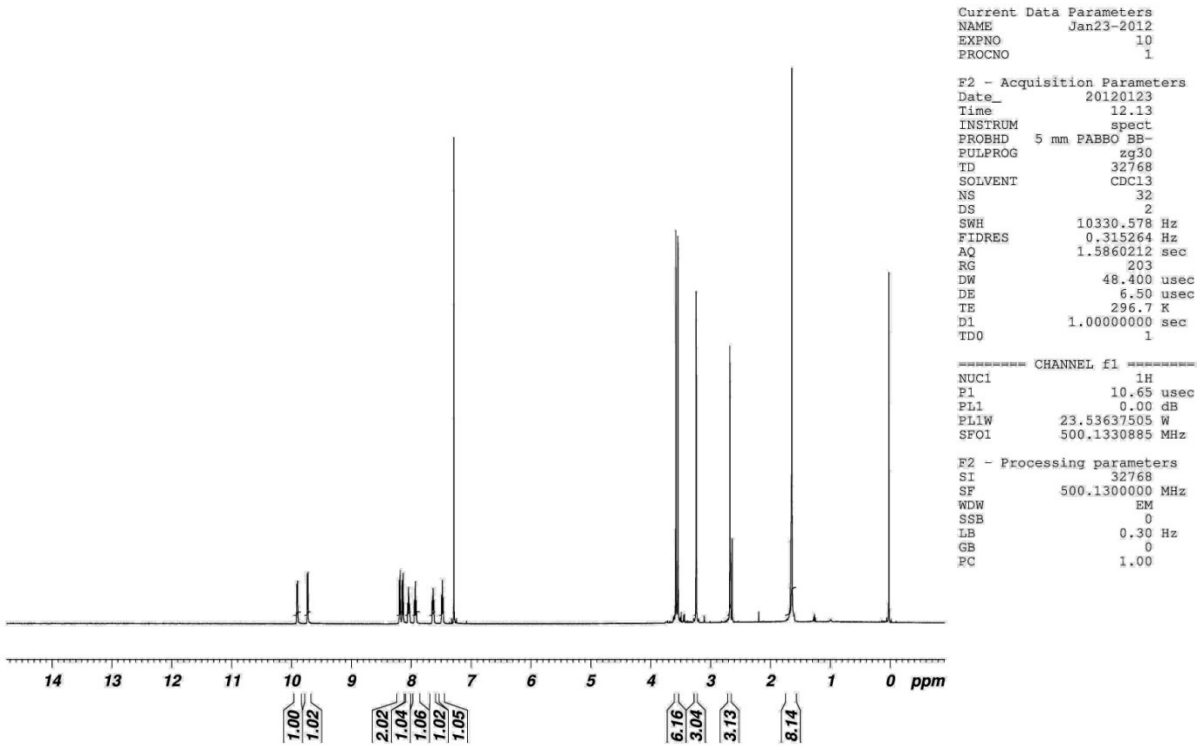
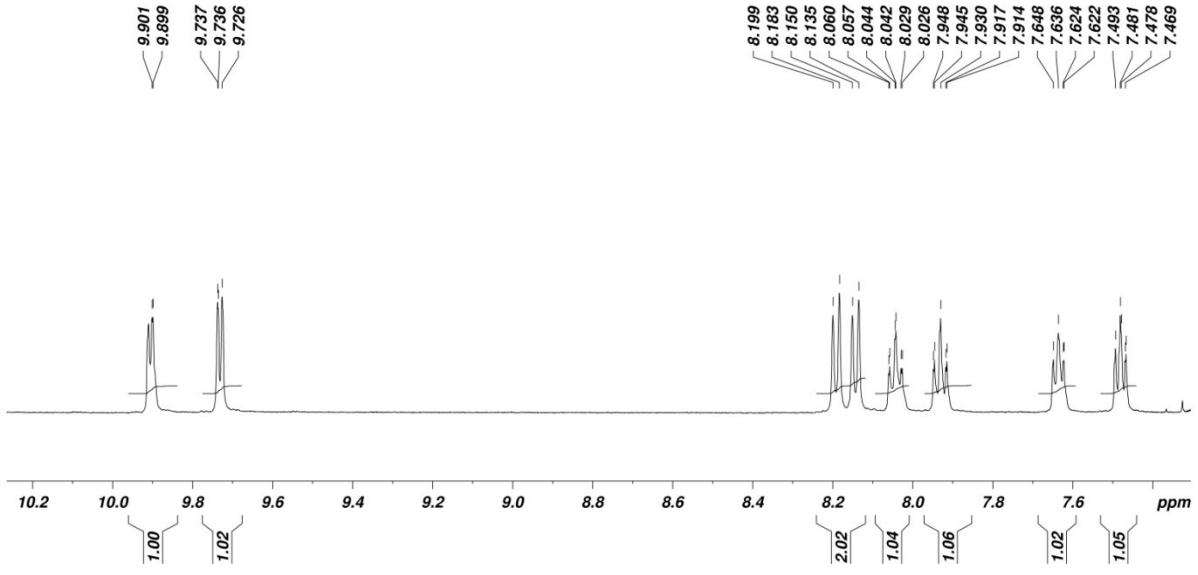
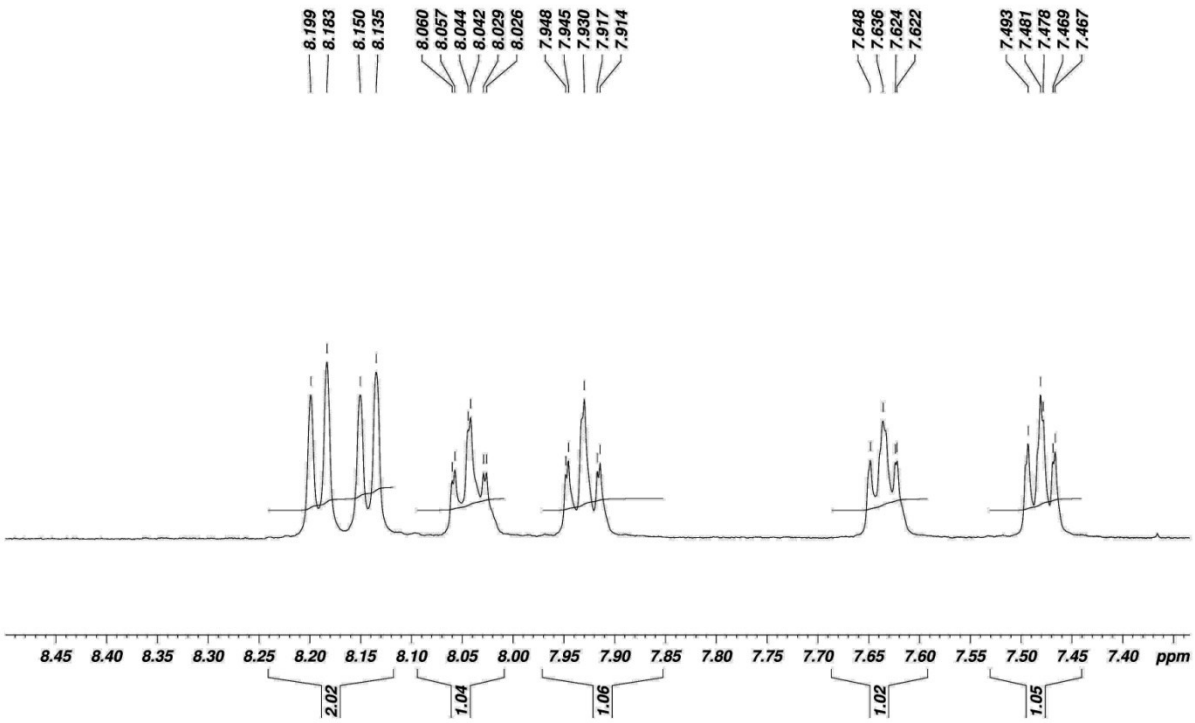
Fig. S1 ^{1}H NMR spectrum of complex **1**






8.199
8.183
8.150
8.135
8.060
8.057
8.044
8.042
8.029
8.026
7.948
7.945
7.930
7.917
7.914
7.648
7.636
7.624
7.622
7.493
7.481
7.478
7.469
7.467
8.45 8.40 8.35 8.30 8.25 8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 ppm
2.02
1.04
1.06
1.02
1.05

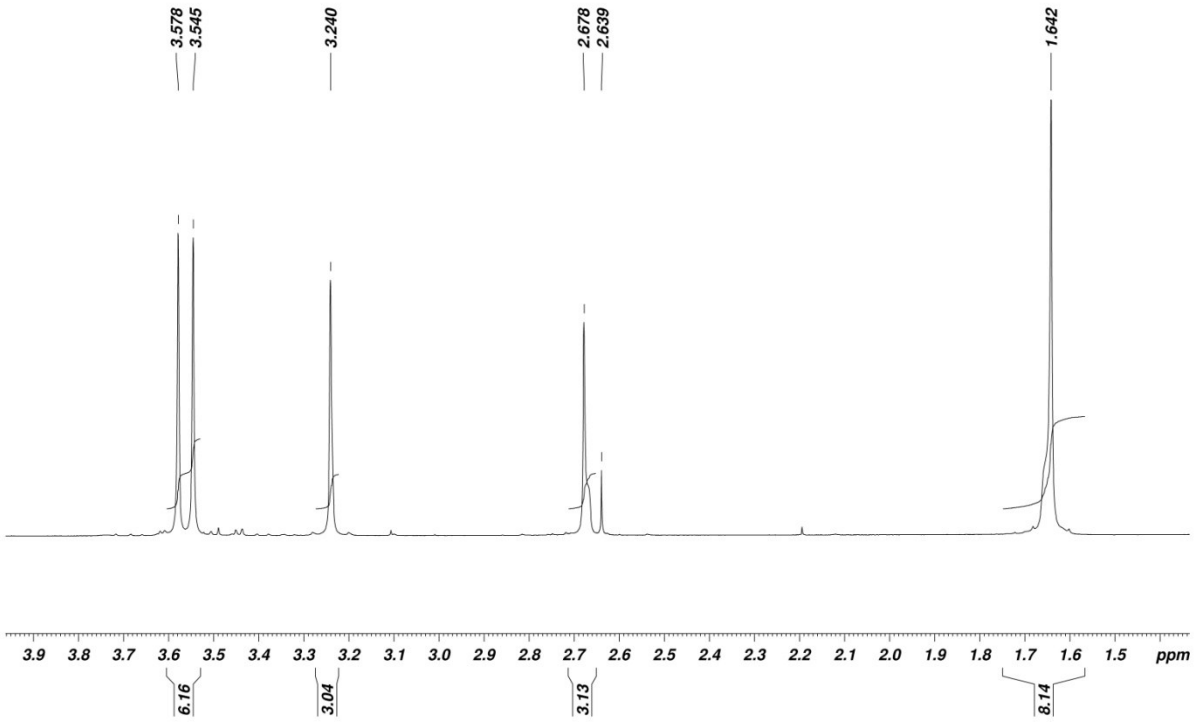

3.578
3.545
3.240
2.678
2.639
1.642
3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 ppm
6.16
3.04
3.13
8.14

Table S1 Selected geometrical parameters for complexes **1** and **3**

Interatomic distances (Å)					
Complex 1				**Complex 3**	
Ru1A–N1A	2.086(3)	Ru1B–N1B	2.081(5)	Ru1–N1	2.076(3)
Ru1A–N2A	2.077(3)	Ru1B–N2B	2.087(5)	Ru1–N2	2.090(3)
Ru1A–S1A	2.2322(15)	Ru1B –S1B	2.2366(15)	Ru1–S1	2.2258(9)
Ru1A–S2A	2.2888(16)	Ru1B–S2B	2.2885(15)	Ru1–S2	2.291(1)
Ru1A–Cl1A	2.42229(14)	Ru1B–Cl1B	2.4209(15)	Ru1–Cl1	2.414(1)
Ru1A–Cl2A	2.4310(15)	Ru1B–Cl2B	2.4309(16)	Ru1–Cl2	2.4289(9)
Bond angles(°)					
N1A-Ru1A-N2A	78.17(19)			N1-Ru1-N2	78.70(1)
N1A-Ru1A-S1A	91.47(14)			N1-Ru1-S1	91.28(8)
N1A-Ru1A-S2A	175.34(14)			N1-Ru1-S2	100.01(8)
N1A-Ru1A-Cl1A	94.10(13)			N1-Ru1-Cl1	170.99(8)
N1A-Ru1A-Cl2A	83.62(14)			N1-Ru1-Cl2	85.58(8)
N2A-Ru1A-S1A	89.28(14)			N2-Ru1-S1	91.35(8)
N2A-Ru1A-S2A	99.74(14)			N2-Ru1-S2	175.55(8)
N2A-Ru1A-Cl1A	171.63(15)			N2-Ru1-Cl1	93.40(8)
N2A-Ru1A-Cl2A	86.66(14)			N2-Ru1-Cl2	85.55(8)
S1A-Ru1A-S2A	92.68(6)			S1-Ru1-S2	92.94(4)
S1A-Ru1A-Cl1A	94.18(5)			S1-Ru1-Cl1	93.22(4)
S1A-Ru1A-Cl2A	174.17(6)			S1-Ru1-Cl2	175.96(4)
S2A-Ru1A-Cl1A	87.73(5)			S2-Ru1-Cl1	87.55(4)
S2A-Ru1A-Cl2A	92.13(5)			S2-Ru1-Cl2	90.11(4)
Cl1A-Ru1A-Cl2A	89.31(5)			Cl-Ru1-Cl2	89.55(4)
C11A-S1A-C12A	96.8(3)			C13-S1-C14	101.10(3)
C11A-S1A-O1A	107.3(3)			C13-S1-O5	104.90(2)
C1BA-S2A-C1CA	99.1(3)			C14-S1-O5	105.6(3)
C1BA-S2A-O3A	105.2(3)			C15-S2-C16	99.50(3)
N1B-Ru1B-N2B	78.84(19)			C15-S2-O6	106.20(2)
N1B-Ru1B-S1B	89.44(14)			C16-S2-O6	104.20(2)
N1B-Ru1B-S2B	98.74(14)				
N1B-Ru1B-Cl1B	172.30(15)				
N1B-Ru1B-Cl2B	86.45(14)				
N2B-Ru1B-S1B	92.47(14)				
N2B-Ru1B-S2B	173.25(14)				
N2B-Ru1B-Cl1B	93.83(14)				
N2B-Ru1B-Cl2B	83.27(14)				
S1B-Ru1B-S2B	93.80(6)				
S1B-Ru1B-Cl1B	93.25(5)				
S1B-Ru1B-Cl2B	174.58(6)				
S2B-Ru1B-Cl1B	88.29(5)				
S2B-Ru1B-Cl2B	90.32(6)				
Cl1B-Ru1B-Cl2B	90.39(5)				
C11B-S1B-C12B	96.6(3)				
C11B-S1B-O1B	107.2(3)				
C1BB-S2B-C1CB	98.4(3)				
C1BB-S2B-O3B	105.9(3)				

Fig. S2 Plot of [DNA]/($\varepsilon_a - \varepsilon_f$) vs [DNA] for the titration of CT-DNA with complexes **1-3** and solid line is linear fitting of the data

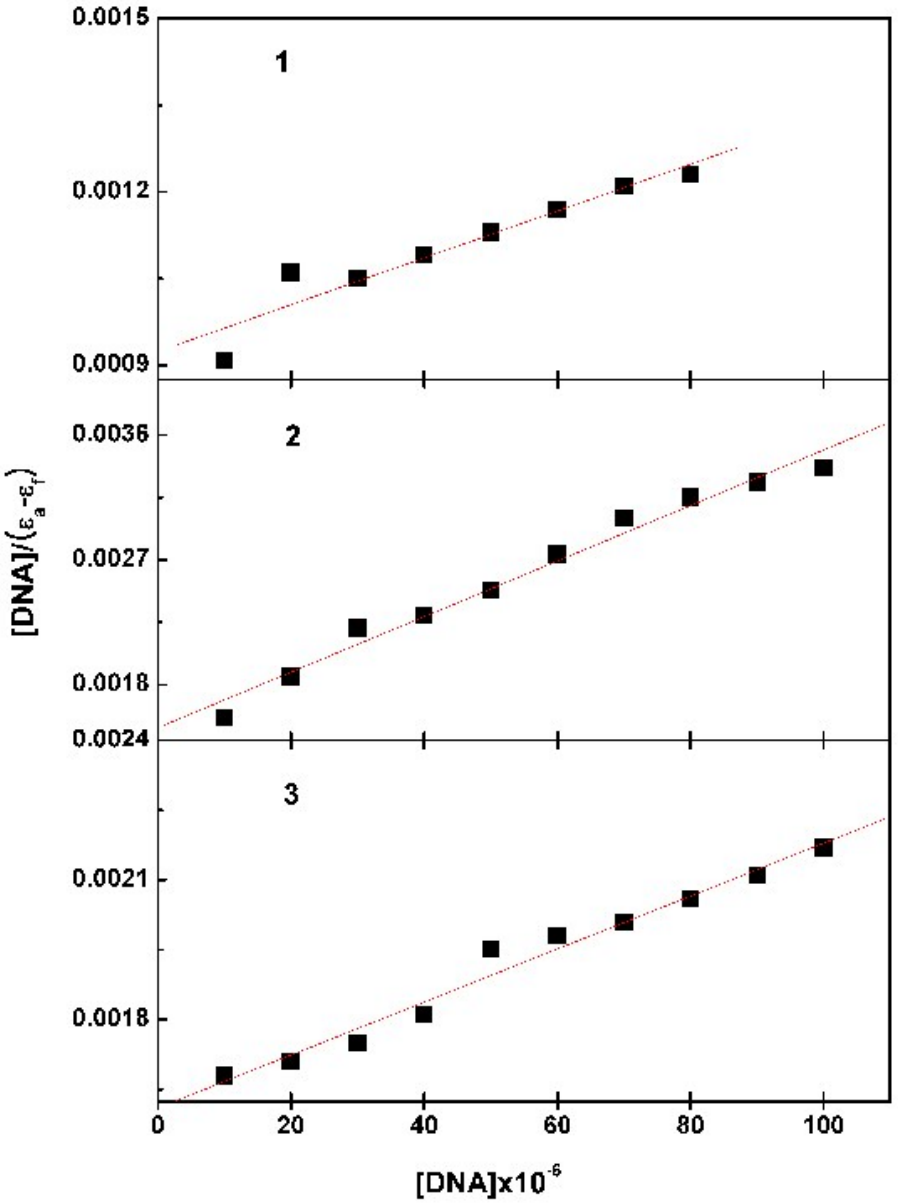


Table S2 Correlation equation and R^2 value of 1-3 for plot of [DNA]/($\varepsilon_a - \varepsilon_f$) vs [DNA]

Complexes	Correlation equation	R^2 value
1	$y = 4 \times 10^{-6} x + 0.0009$	0.913
2	$y = 2 \times 10^{-5} x + 0.0015$	0.967
3	$y = 5 \times 10^{-6} x + 1.0016$	0.974

Table S3 Correlation equation and R^2 value for EB–DNA fluorescence quenching by complexes 1-3

Complexes	Correlation equation	R^2 value
1	y = -2.803 x + 100.33	0.938
2	y = -5.005 x + 100.77	0.979
3	y = -3.592 x + 101.20	0.950

Fig. S3 Stern–Volmer plots for EB–DNA quenching by the ruthenium complexes at different temperatures

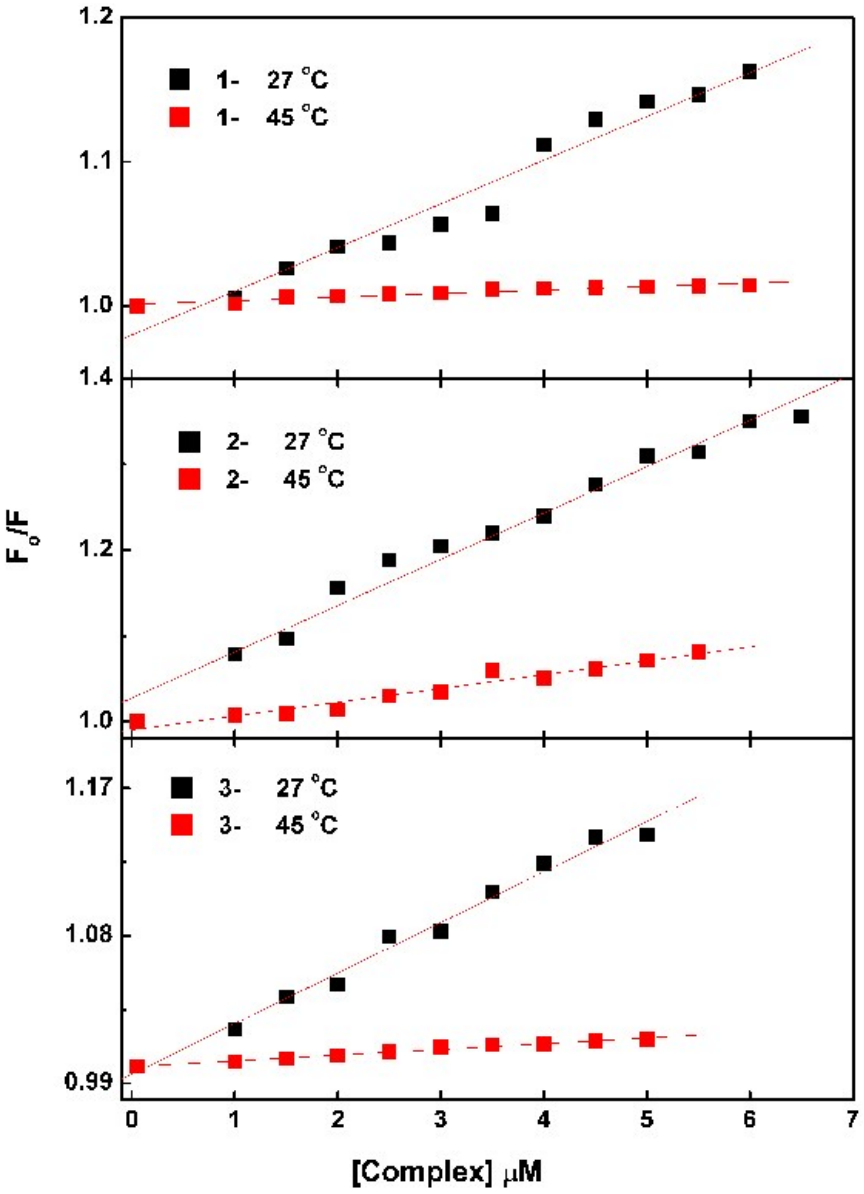


Table S4 Correlation equation and R^2 value of 1-3 for Stern–Volmer plots for EB–DNA quenching by the ruthenium complexes at different temperatures

Complexes	Correlation equation		R^2 value	
	27 °C	45 °C	27 °C	45 °C
1	y = 0.027 x + 0.970	y = 0.001 x + 1.004	0.969	0.460
2	y = 0.051 x + 1.036	y = 0.012 x + 1.002	0.986	0.877
3	y = 0.031 x + 0.992	y = 0.004 x + 0.998	0.987	0.984

Table S5 Correlation equation and R^2 value of the EB and complexes on viscosity of DNA

Complexes	Correlation equation	R^2 value
1	y = 0.049 x + 0.998	0.094
2	y = 0.060 x + 1.005	0.127
3	y = -0.061 x + 1.005	0.134
EB	y = 1.393 x + 1.027	0.887

Fig. S4 UV-Visible absorption spectra of BSA (1 μM) in the absence and presence of the complexes **1-3** (10 μM).

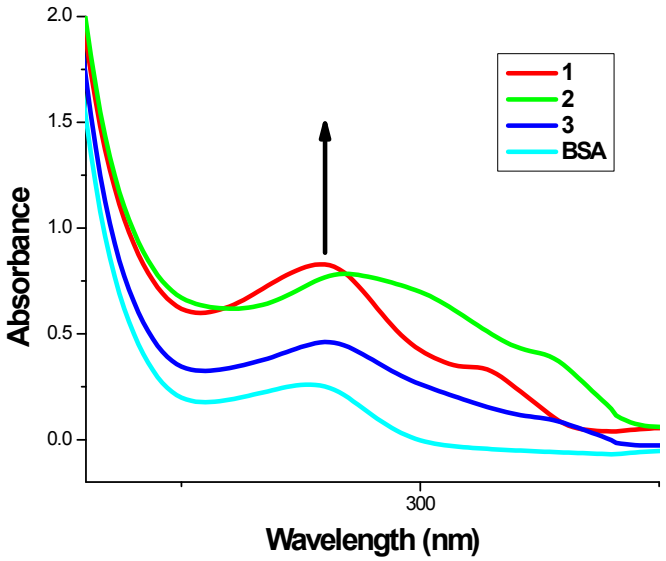


Fig. S5 Plot of I_0/I vs log [Q]

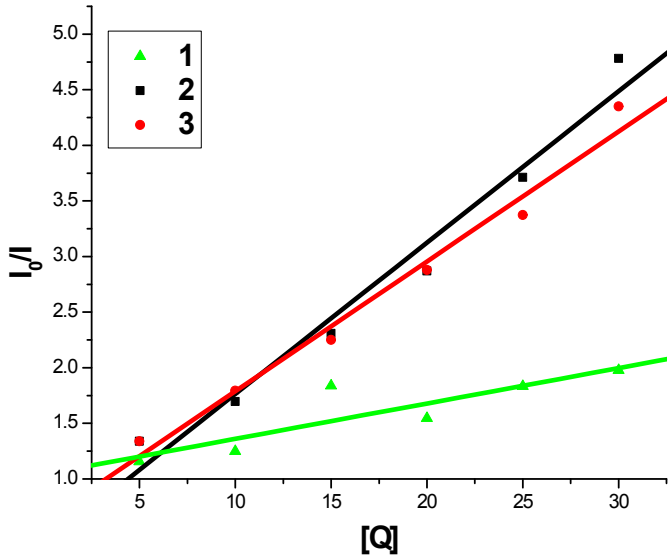


Table S6 Correlation equation and R^2 value of complexes 1-3 for plot of I_0/I vs log [Q]

Complexes	Correlation equation	R^2 value
1	y = 0.136 x + 0.402	0.985
2	y = 0.117 x + 0.622	0.990
3	y = 0.032 x + 1.042	0.876

Fig. S6 Plot of log [(F_0-F)/F] vs log [Q]

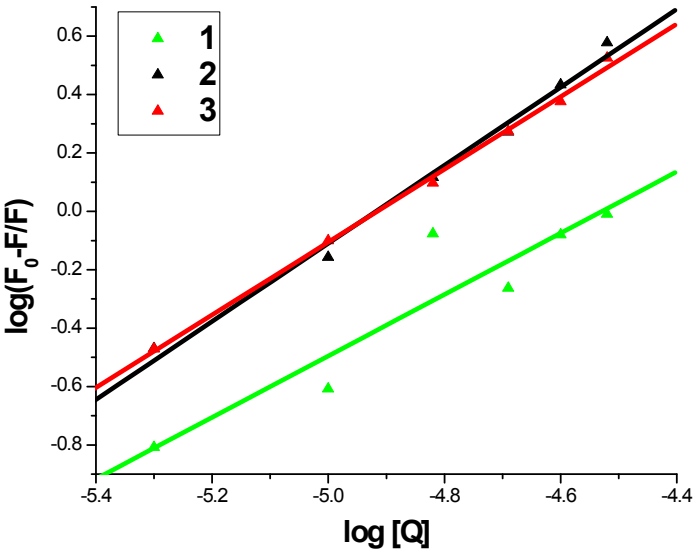


Table S7 Correlation equation and R^2 value of the complexes 1-3 for plot of log [(F_0-F)/F] vs log [Q]

Complexes	Correlation equation	R^2 value
1	y = 1.337 x + 6.577	0.995
2	y = 1.246 x + 6.123	0.998
3	y = 1.052 x + 4.763	0.928

Fig. S7 Synchronous spectra of BSA (1 μM) in the presence of increasing amounts of the complexes **1-3** for a wavelength difference of $\Delta\lambda$ = 15 nm. The arrow shows the emission intensity changes upon increasing concentration of complex

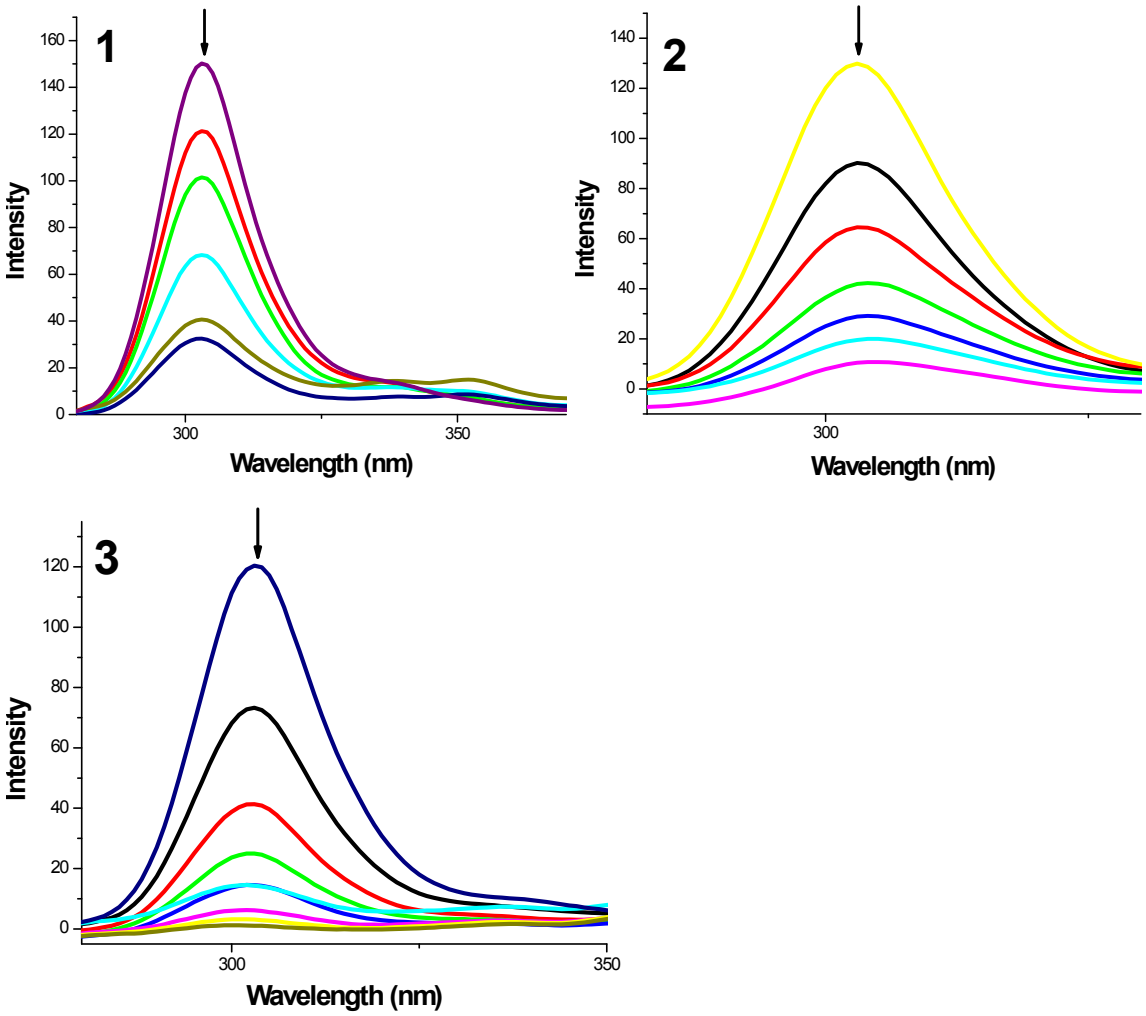


Fig. S8 Synchronous spectra of BSA (1 μM) in the presence of increasing amounts of the complexes **1-3** for a wavelength difference of $\Delta\lambda$ = 60 nm. The arrow shows the emission intensity changes upon increasing concentration of compound

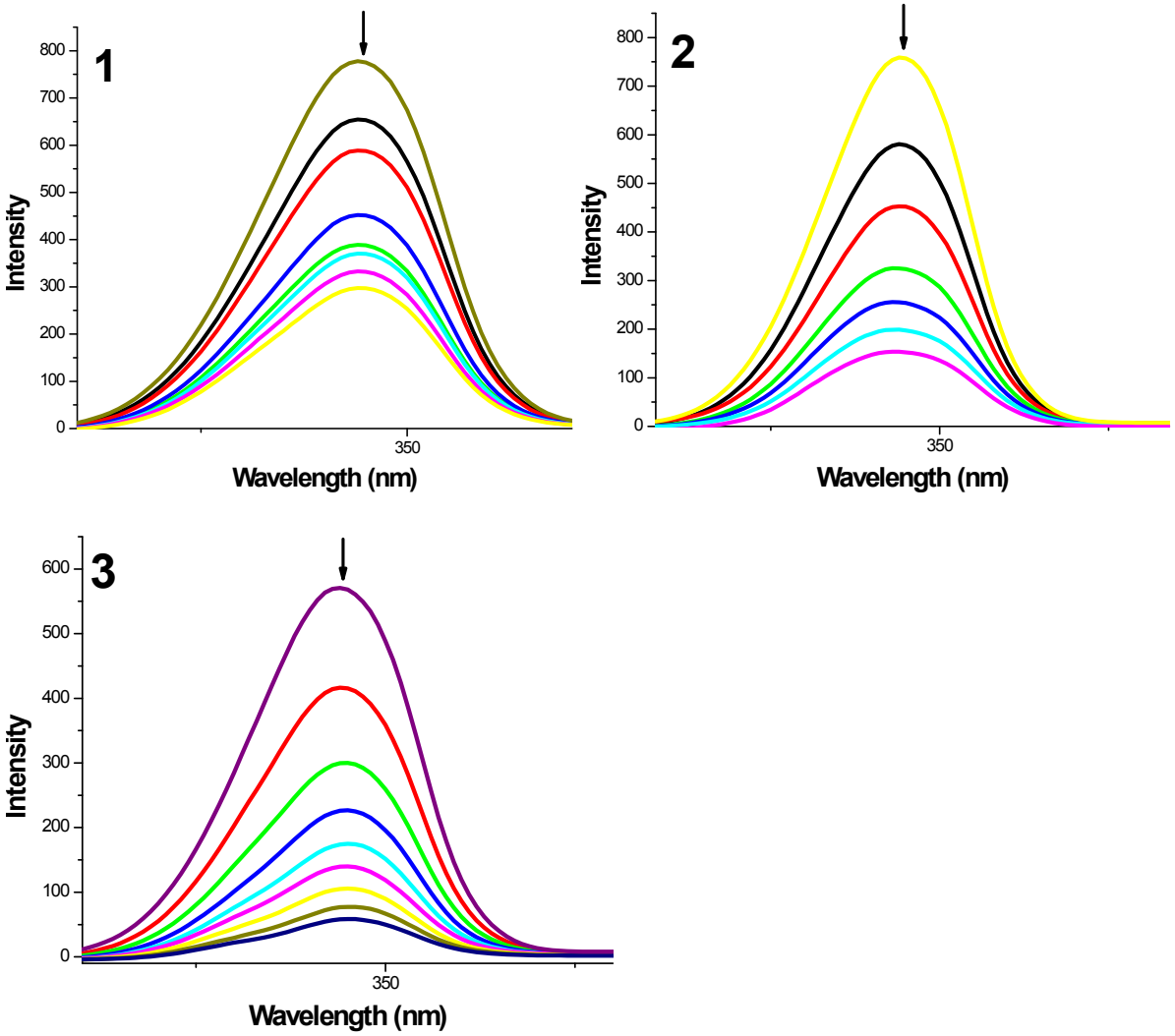


Fig. S9 Plausible mechanisms for DPPH radical scavenging and metal chelating activity for complex **3**