Supporting Information

Multiple Phenyl Rings appended Re-based Complexes for Strong Visible Light Absorption and DNA Binding

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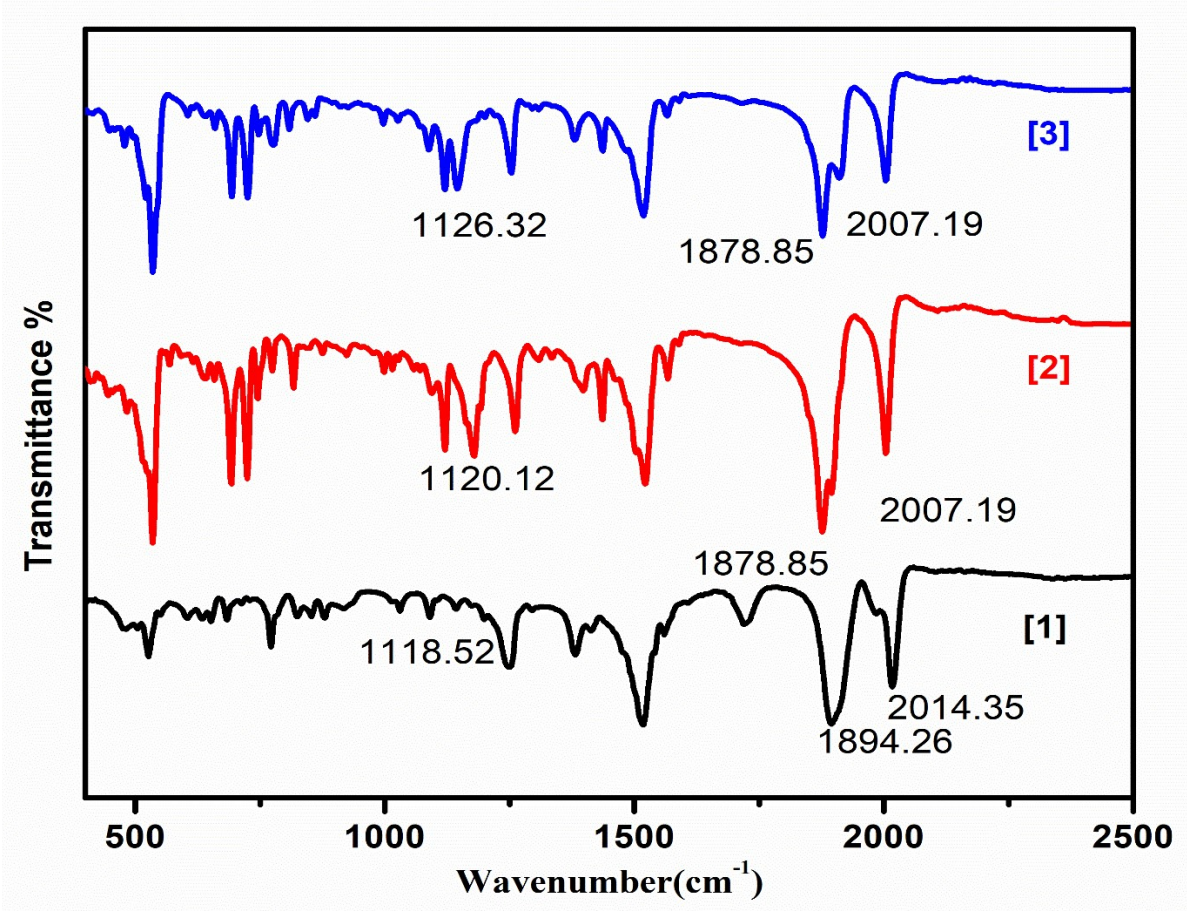

Figure S1: Solid-state FTIR spectra of **1**–**3**.

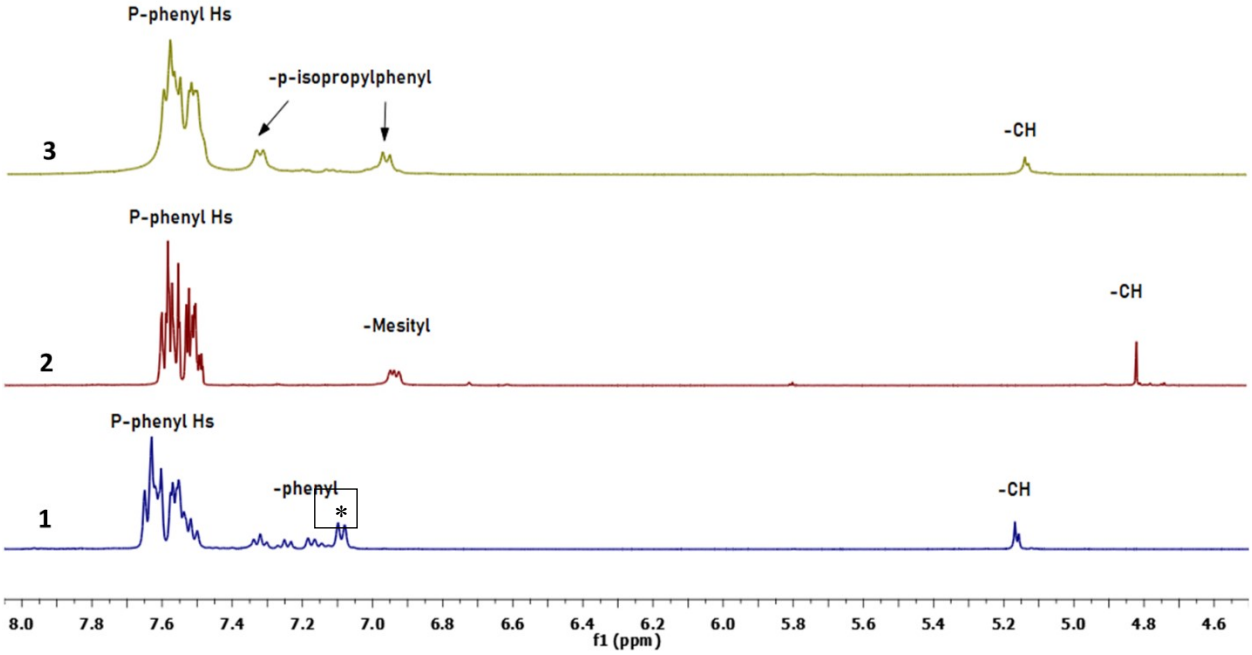

Figure S2: ^{1}H–NMR spectra of **1**–**3** in DMSO-d_6 (300MHz). *indicates signals belonging to reaction solvent (toluene).

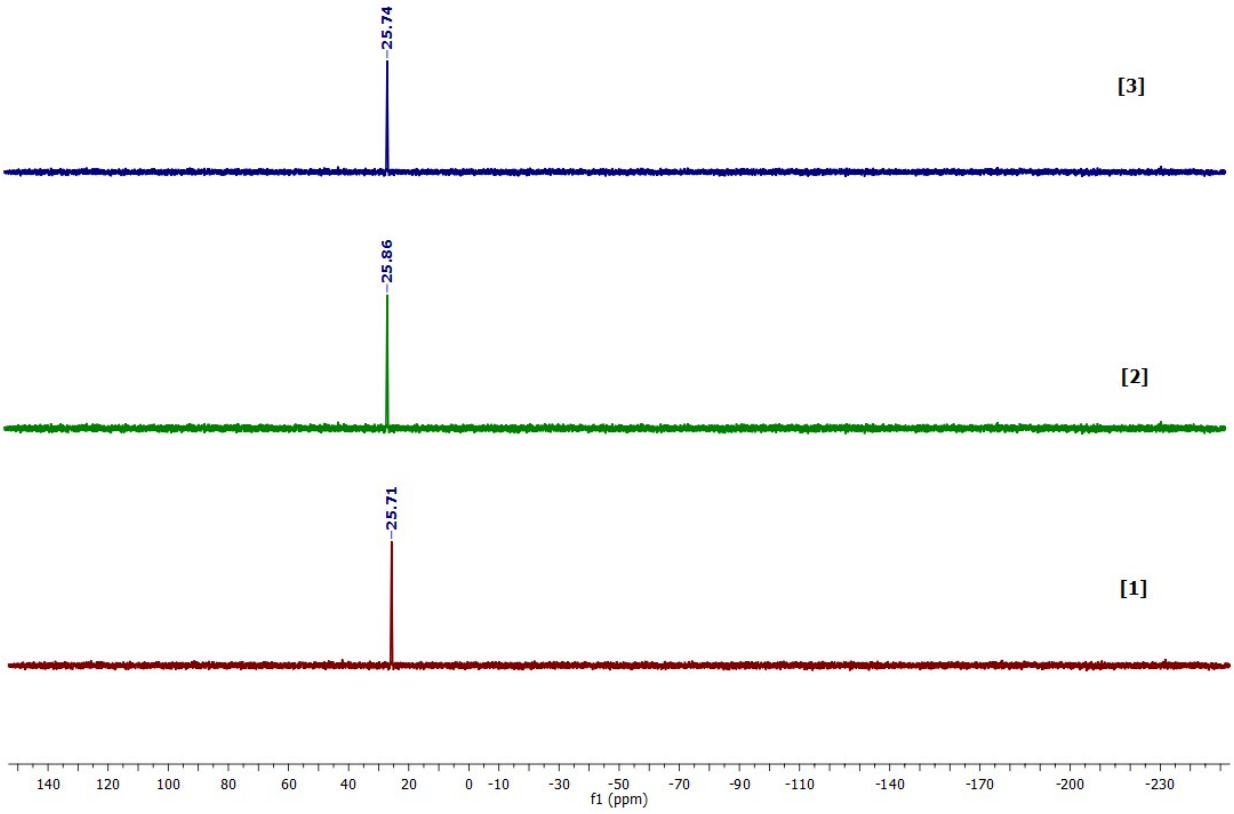

Figure S3: ^{31}P-{^{1}H} NMR spectra of **1**–**3** in DMSO-d_6 (300MHz).

Table: S1 Crystallographic data for crystal structures of **1** and **2**.

Empirical formula	**C_{60} H_{48} N_2 O_{10} P_2 Re_2**	**C_{66} H_{60} N_2 O_{10} P_2 Re_2**
Crystal system	Monoclinic	Triclinic
Space Group	*P 21/n (14)`*	*P -1 (2)`*
a [Å]	13.6091(4)	10.1180(6)
b [Å]	15.1518(5)	10.6093(6)
c [Å]	15.1092(7)	15.8454(7)
V[Å^3]	3103.6(2)	1522.66(15)
Z	2	2
Molecular weight	1385.29	734.72
ρ calc [g/cm^3]	1.482	1.603
Temperature [K]	293(2)	293(2)
Wavelength [MoK$_\alpha$] [Å]	0.71073	0.71073
Monochromator	Graphite	Graphite
Min/Max Bragg angle [°]	3.023-29.783	3.6030-27.5740
hkl range	-17 to 16, -18 to 18, -18 to 18	-12 to 12, -12 to 12, -19 to 19
F(000)	1352	724
μ (mm^{-1})	4.002	4.083
R_{int}	0.1145	0.0383
R_{sigma}	0.0725	0.0310
Refinement	F2	F2
No. of reflections used	23257	16621
Number of parameters	346	374
GoF	1.058	1.002
wR_2	0.2208	0.0637
Δρ/e [Å^{-3}]	2.355/-0.591	0.977/-0.617
Number of parameters	346	374
GoF	1.058	1.002

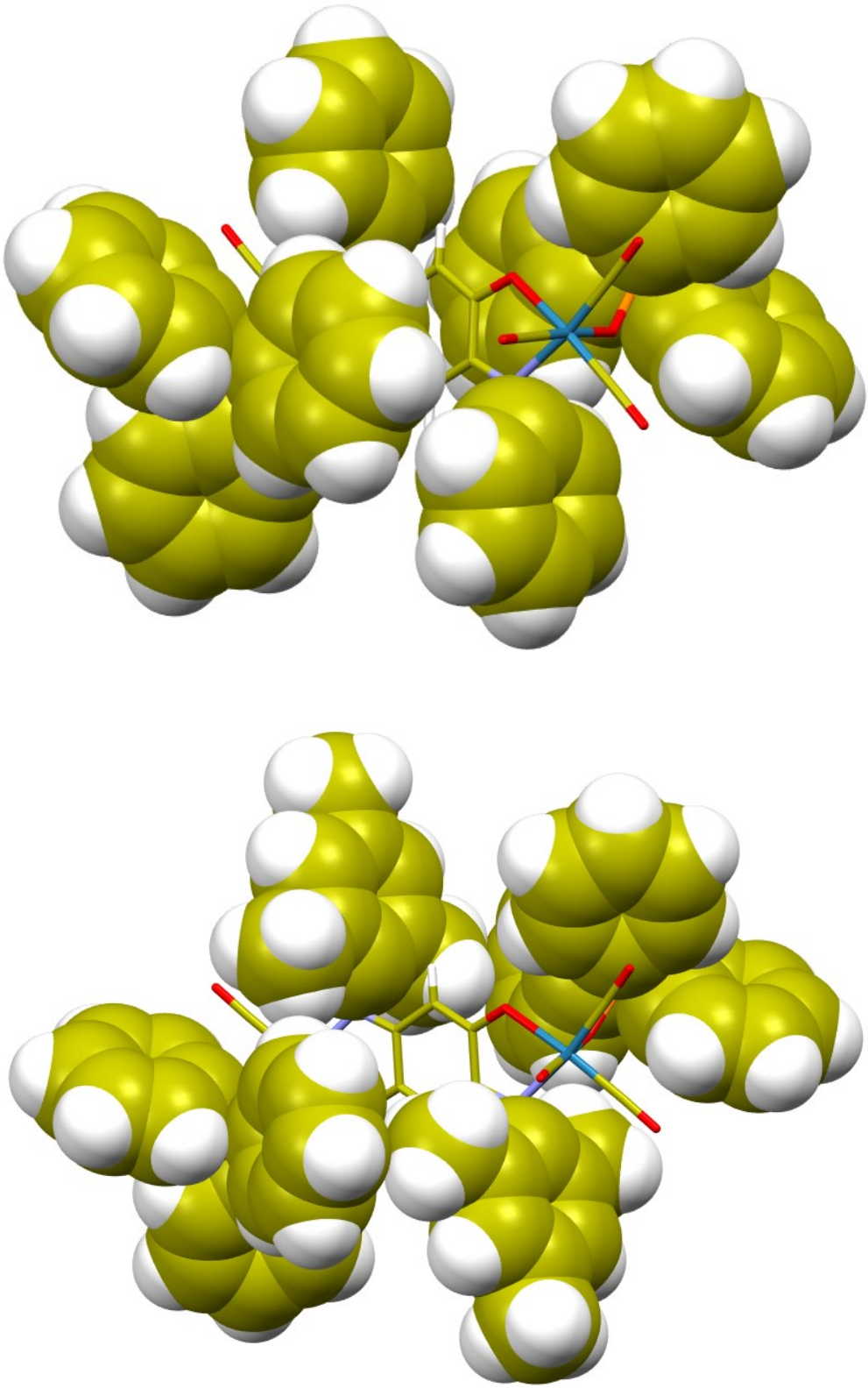

Figure S4: The bunch of aromatic units around Re-(NO)-Re core in **1**(top) and **2**(bottom).

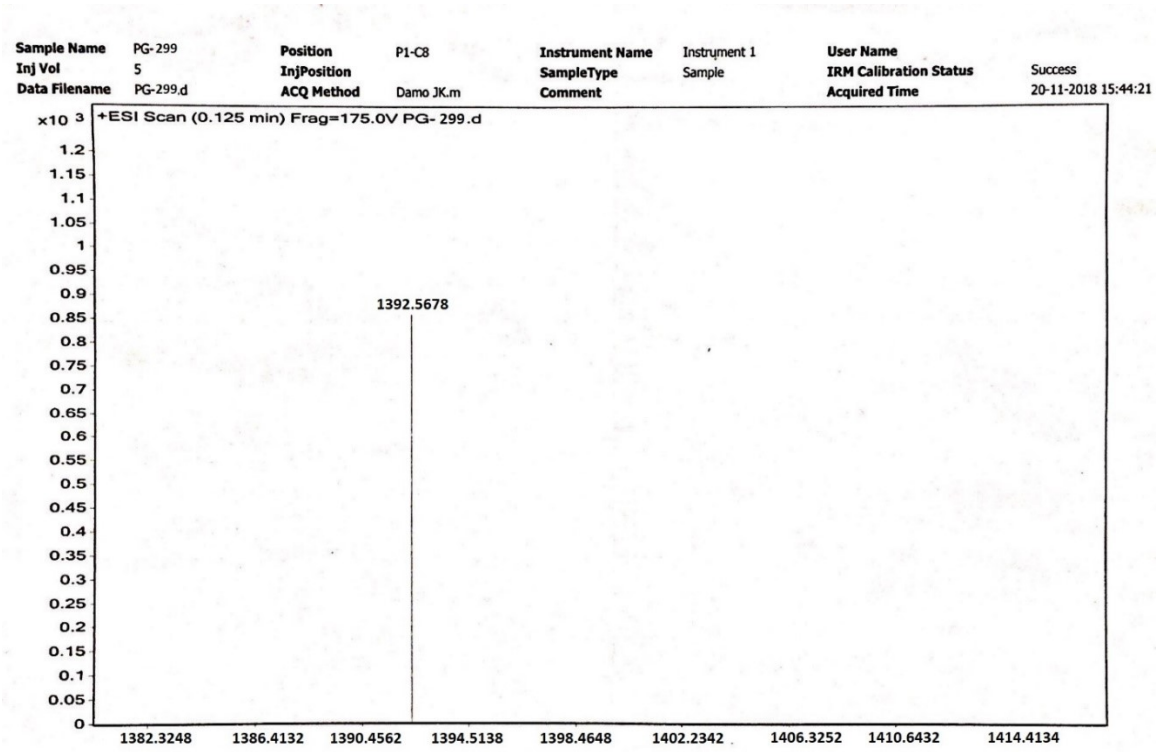

Figure S5: ESI–MS spectra of **1** in acetonitrile.

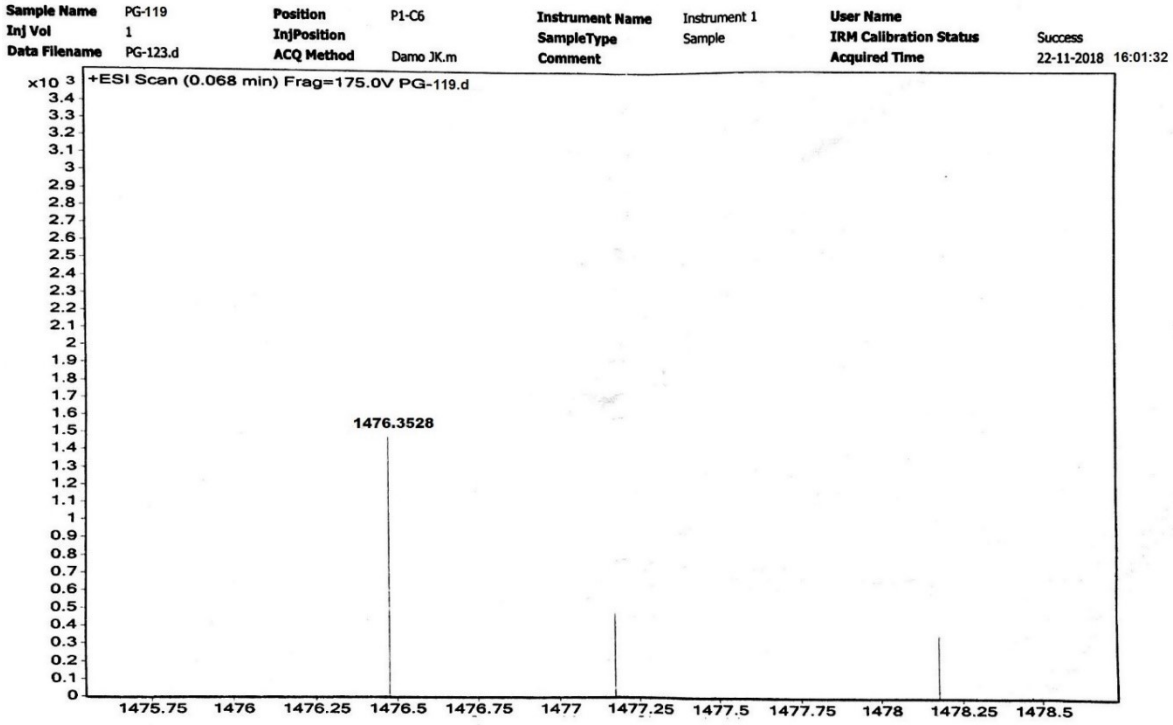

Figure S6: ESI–MS spectra of **2** in acetonitrile.

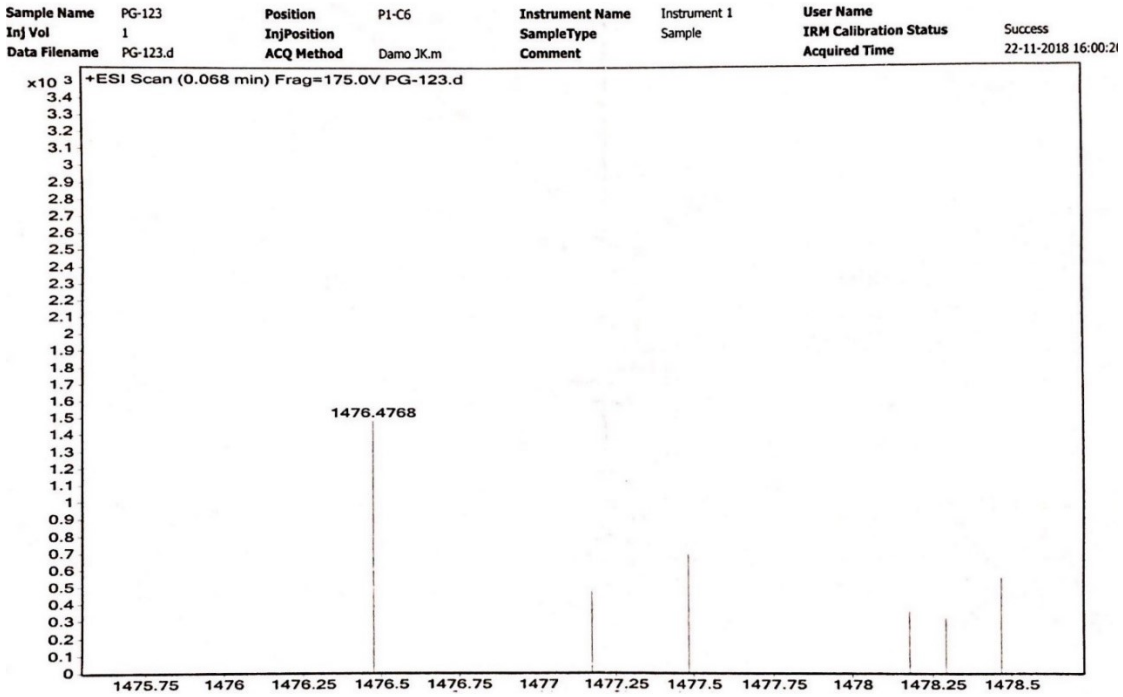

Figure S7: ESI–MS spectra of **3** in acetonitrile.

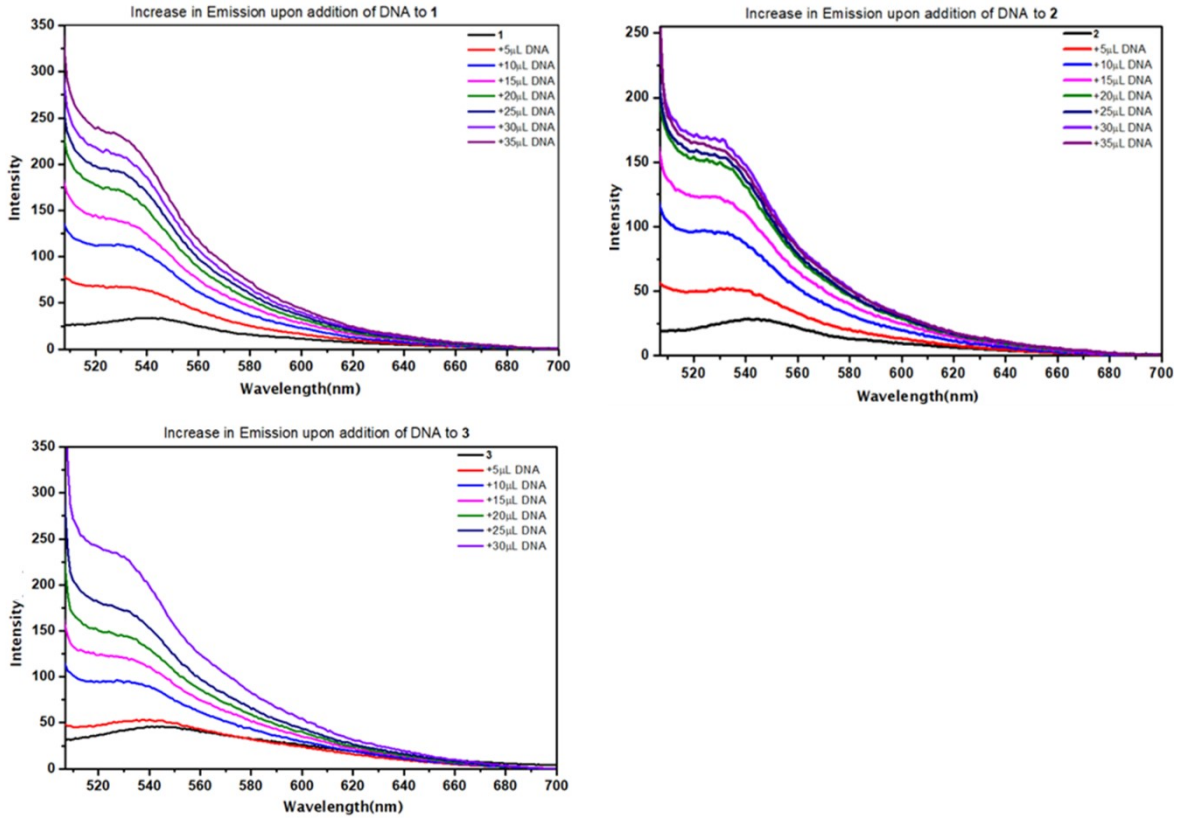

Figure S8: Fluorescence emission spectra of acyclic complexes 1-3 in acetonitrile in absence and presence of different concentrations of (0.2184- 1.5288μM) of ct-DNA in PBS at pH 7.0 at 25^0C. The excitation wavelength (λ_{ex}) was 490 nm.

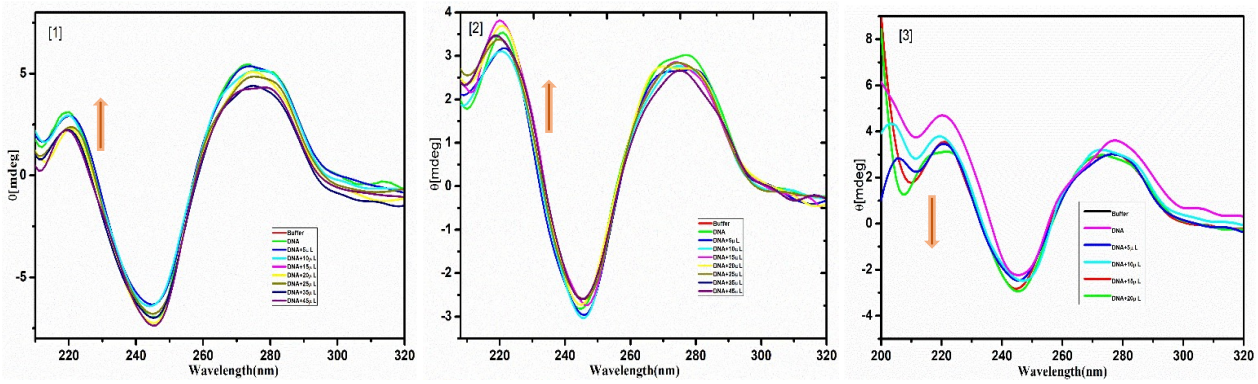

Figure S9: Circular dichroism (CD) spectra of ct−DNA (100 mM) in absence and presence of different concentrations [Q] (0.1654−1.1518 μM) of acyclic complexes **1**−**3** in PBS (pH 7.0) at 25^0C.

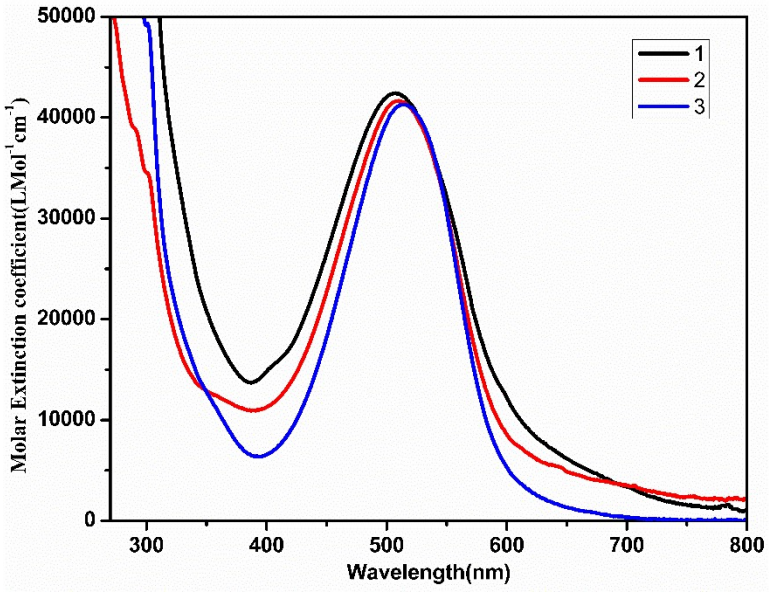

Figure S10: Absorption spectra of complexes **1**−**3** in DCM.

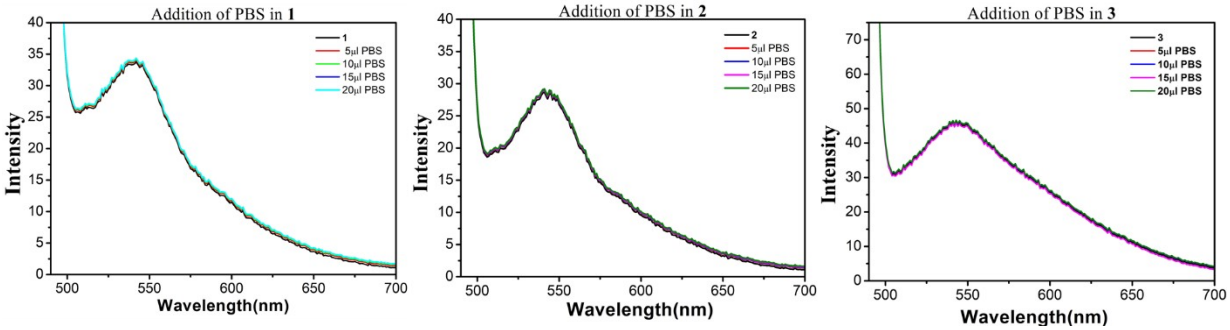

Figure S11: Emission spectra of complexes (1-3) in dry and degassed ACN with successive addition of PBS buffer solution.