Supporting Information

Discovery of half-sandwich Iridium complexes containing lidocaine and (Pyren-1-yl)ethynyl derivatives of phenylcyanamide ligands for photodynamic therapy

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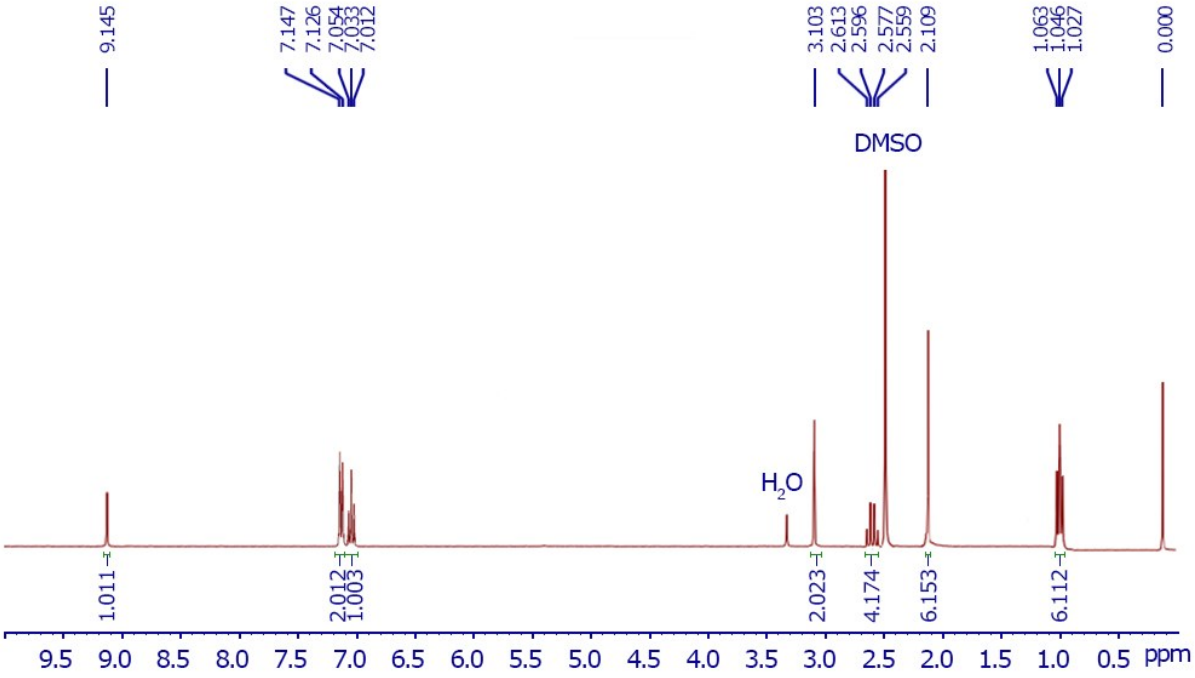

Fig. S1. ^{1}H NMR spectrum of ligand LC (DMSO-d_6).

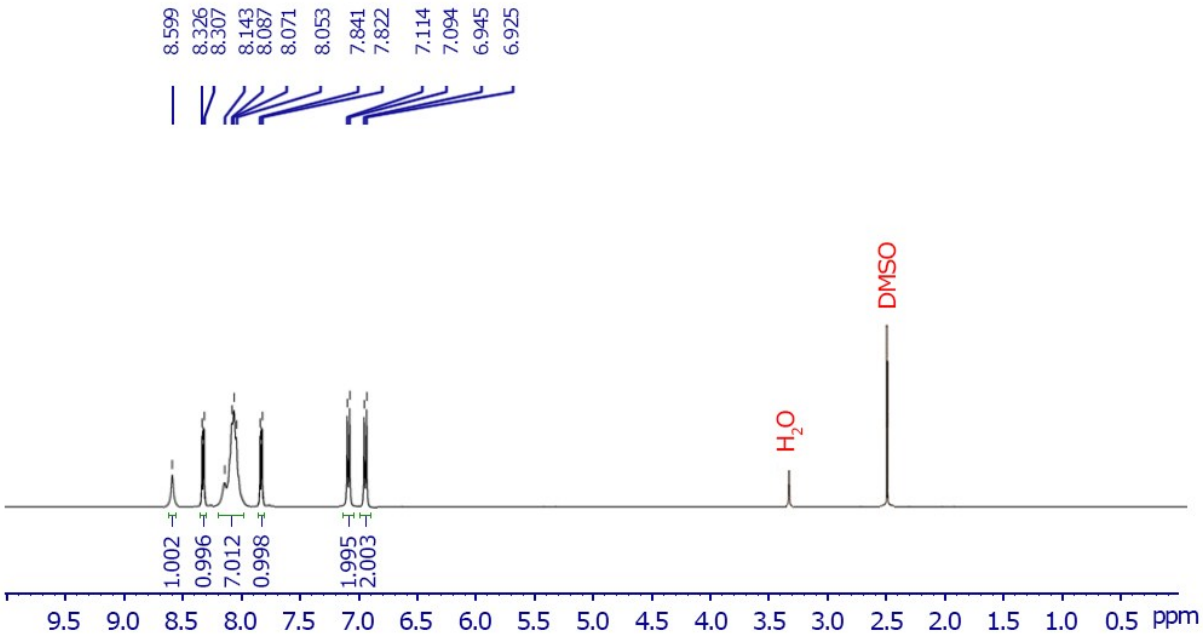

Fig. S2. ^{1}H NMR spectrum of ligand L1 (DMSO-d_6).

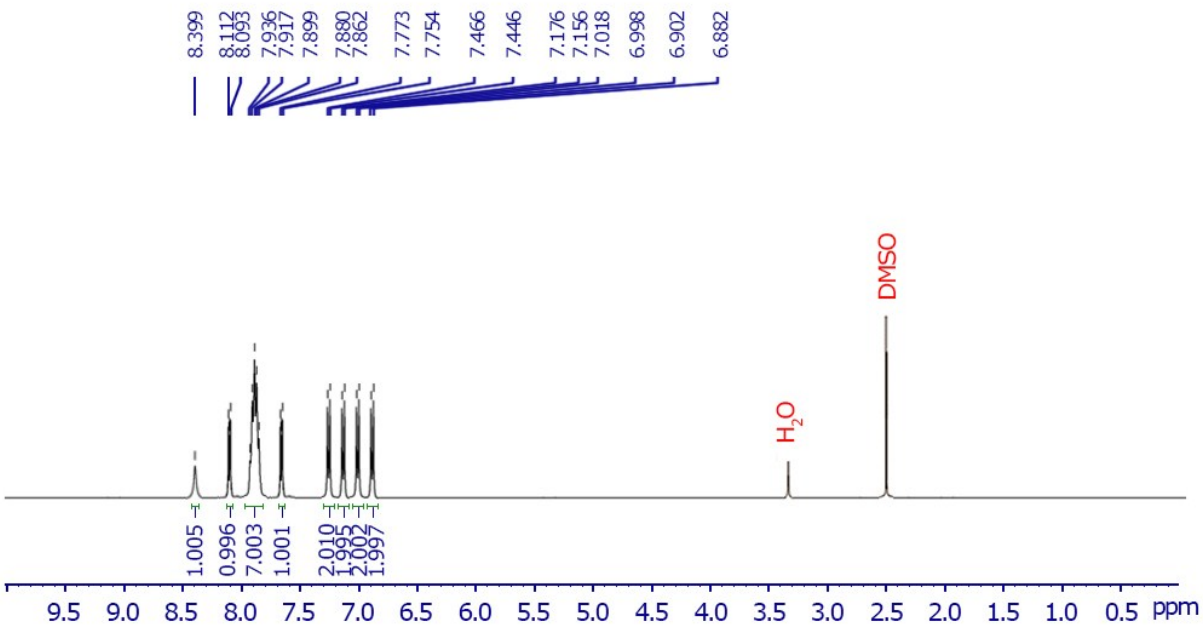

Fig. S3. ^{1}H NMR spectrum of ligand L2 (DMSO-d_6).

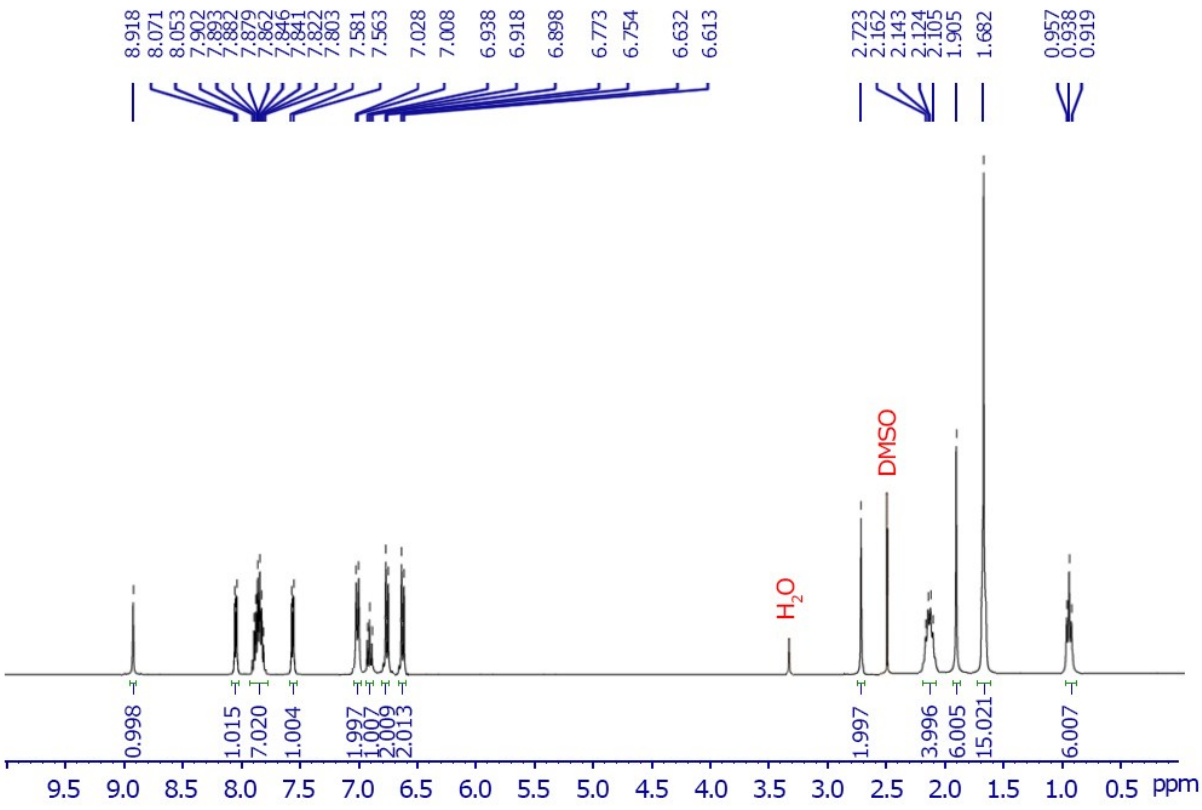

Fig. S4. ^{1}H NMR spectrum of complex **1** (DMSO-d_6).

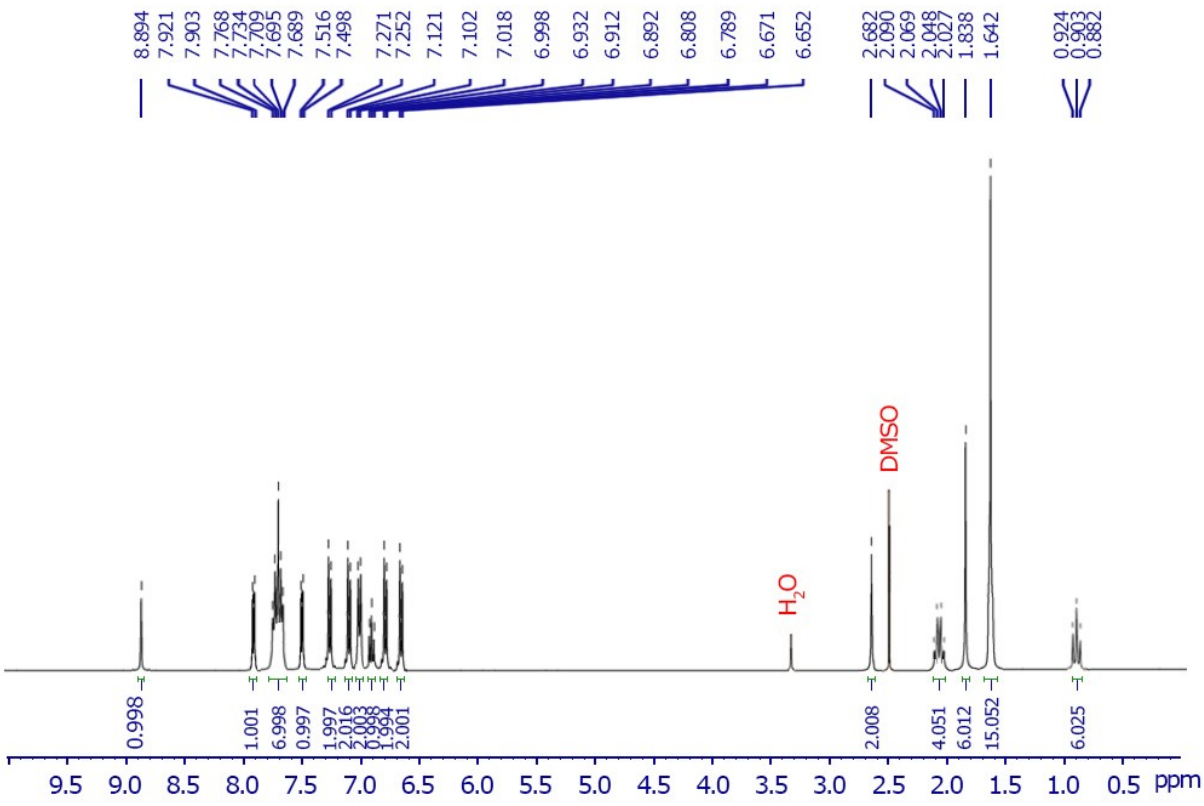

Fig. S5. ^{1}H NMR spectrum of complex **2** (DMSO-d_6).

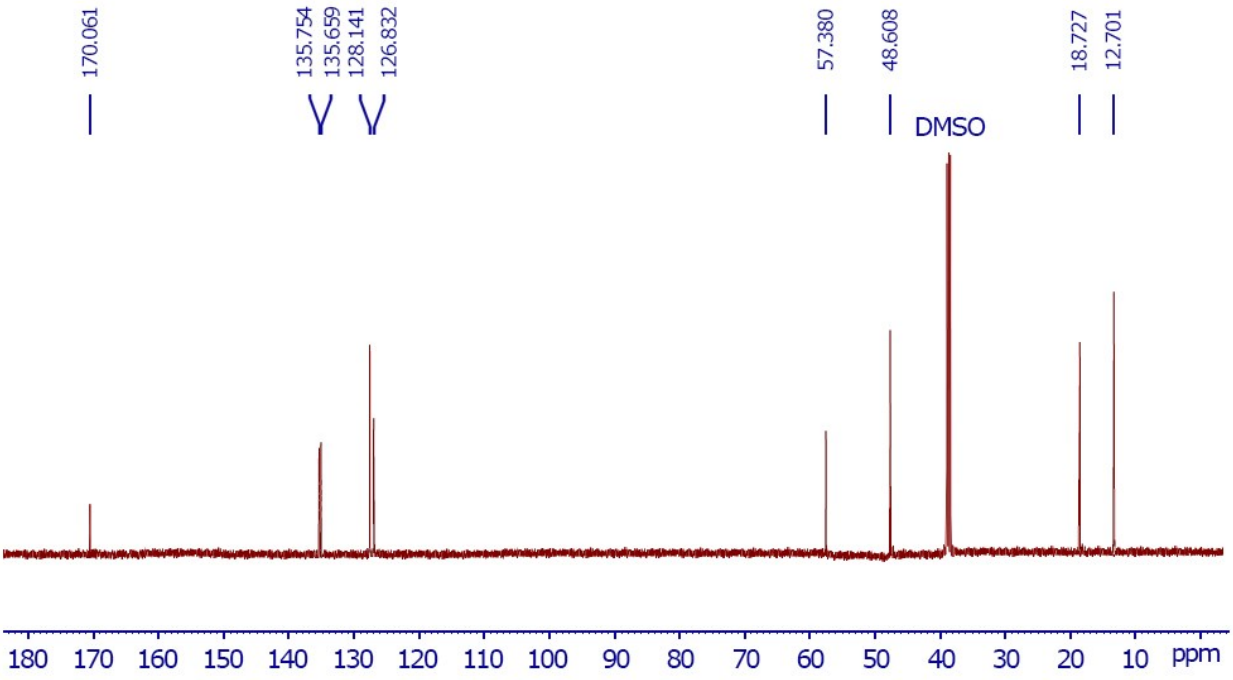

Fig. S6. ^{13}C NMR spectrum of ligand LC (DMSO-d_6).

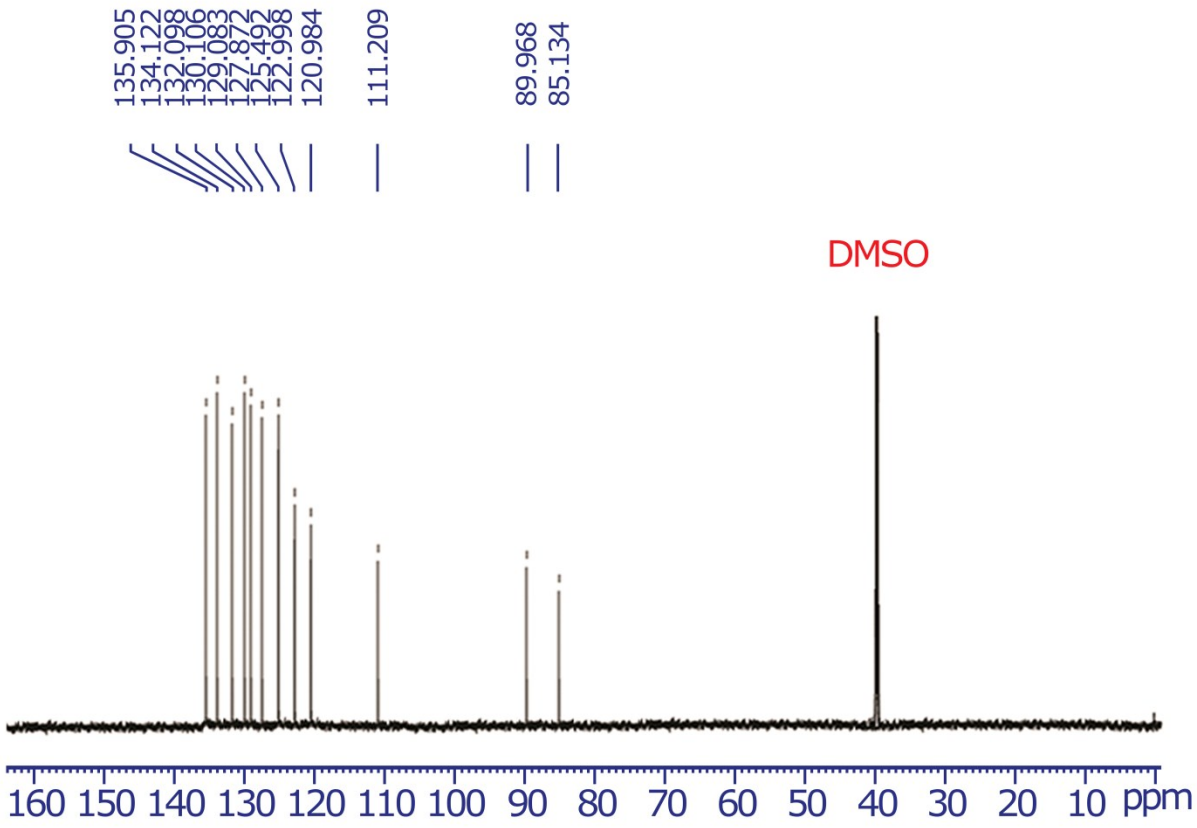

Fig. S7. ^{13}C NMR spectrum of ligand L1 (DMSO-d_6).

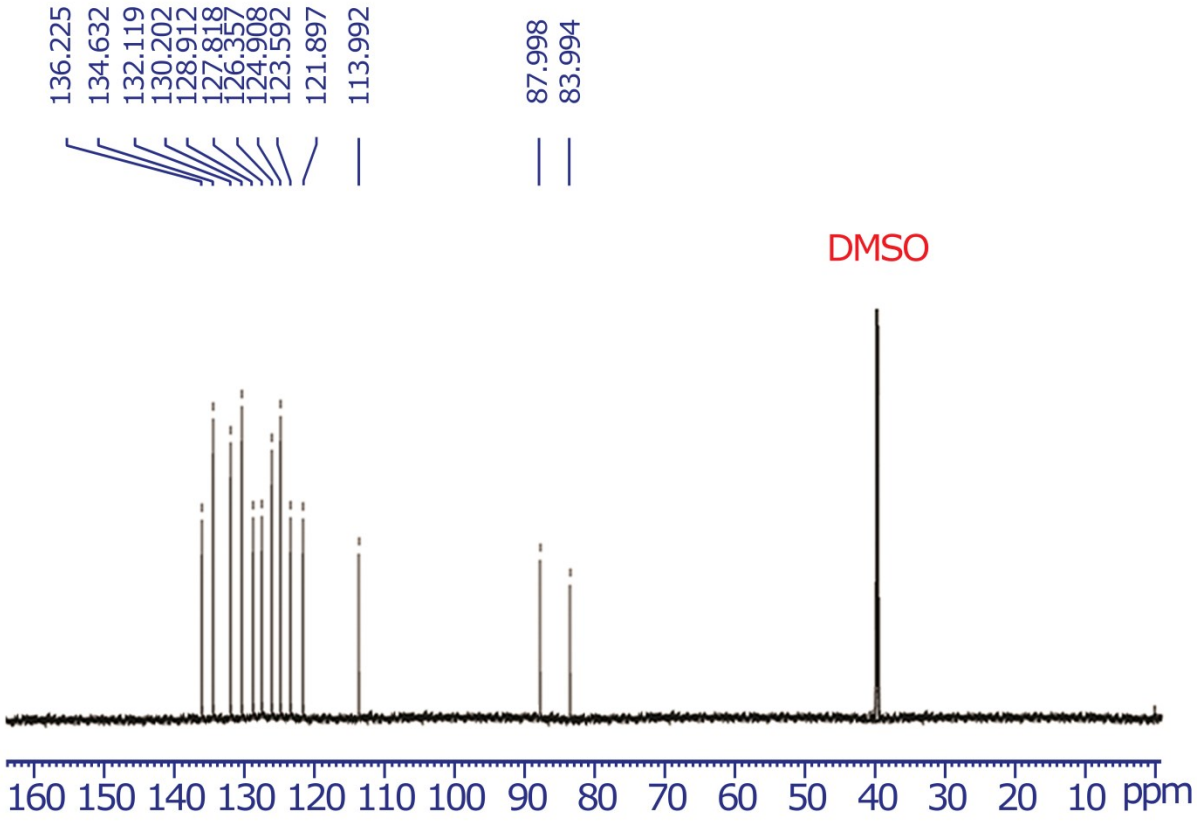

Fig. S8. ^{13}C NMR spectrum of ligand L2 (DMSO-d_6).

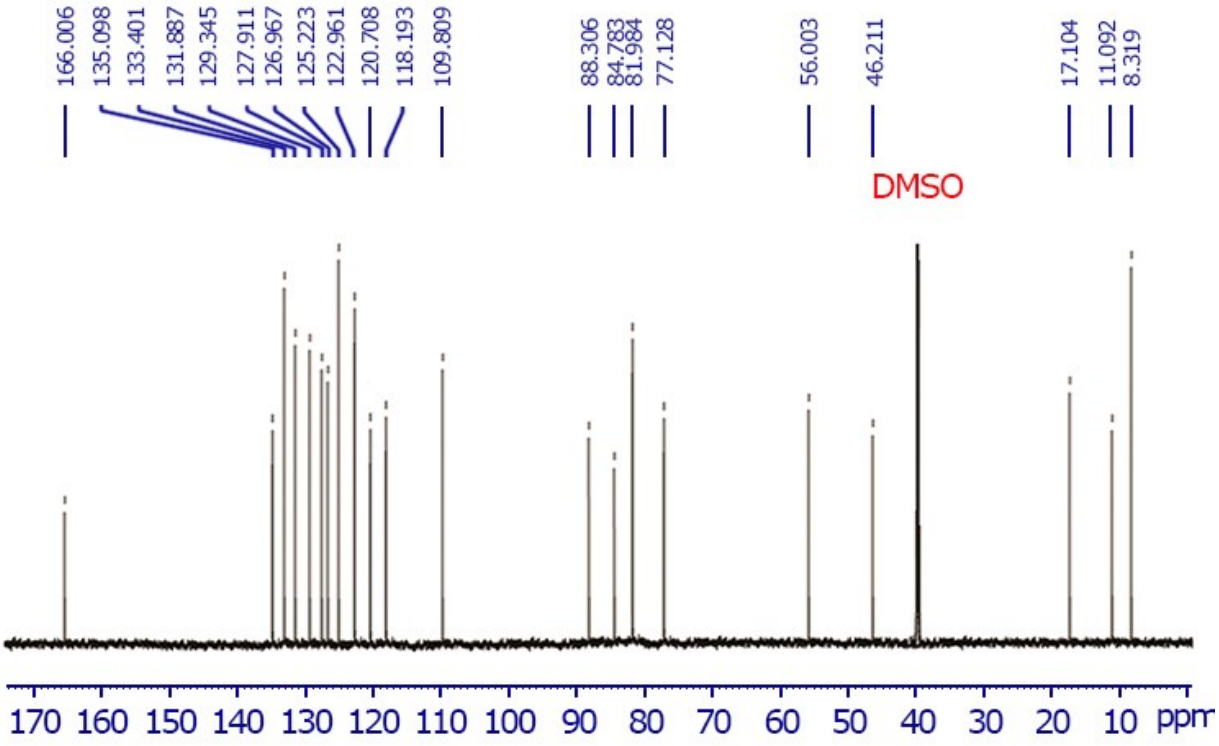

Fig. S9. ^{13}C NMR spectrum of complex **1** (DMSO-d_6).

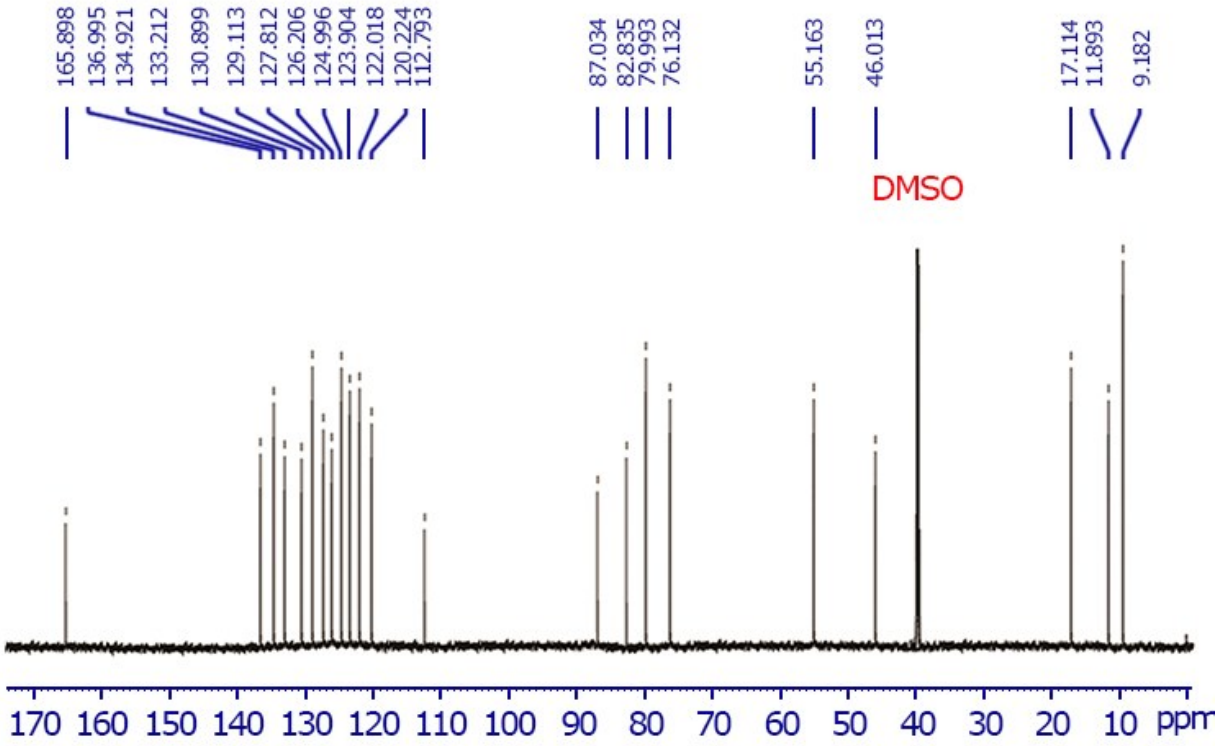

Fig. S10. ^{13}C NMR spectrum of complex **2** (DMSO-d_6).

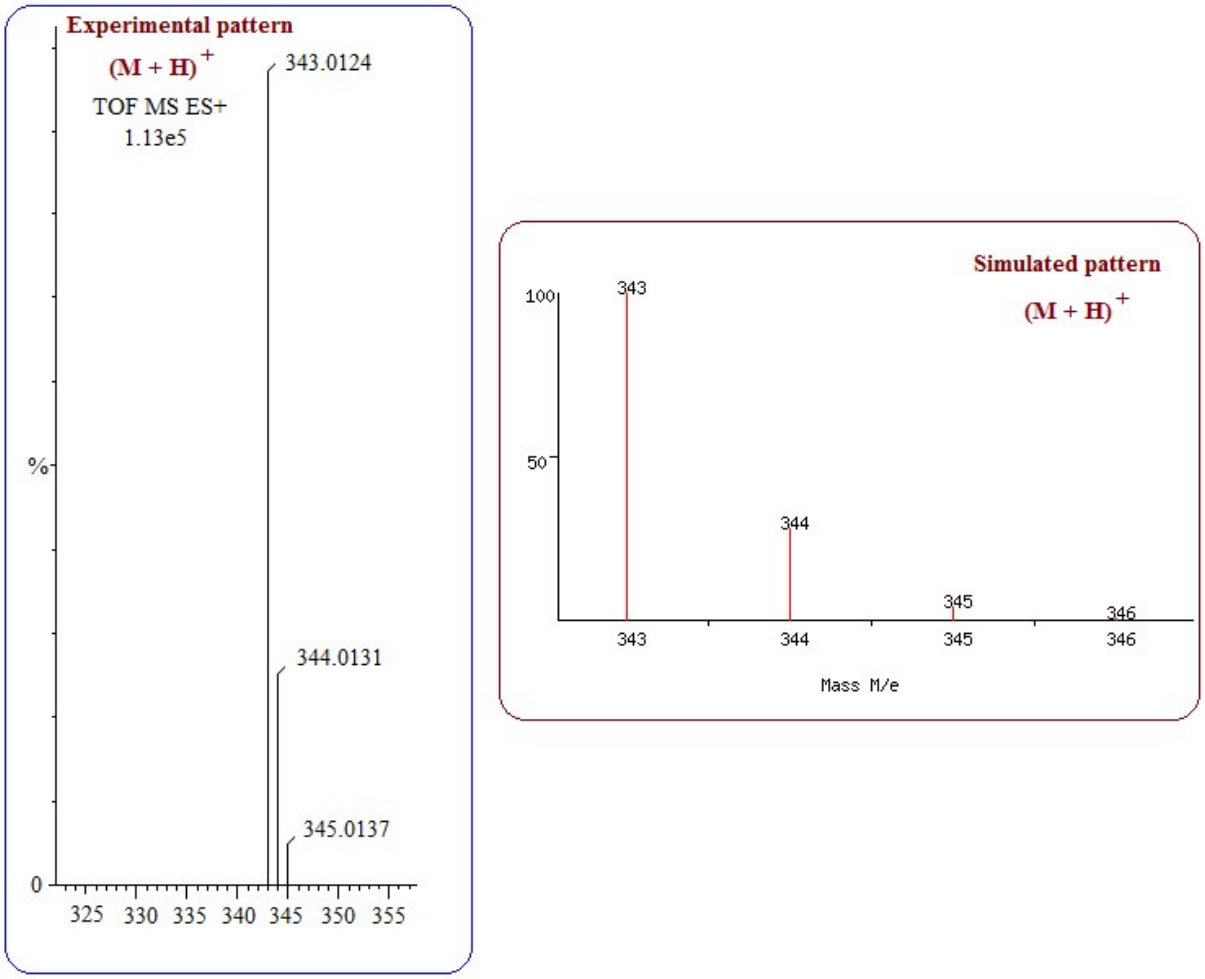

Fig. S11. TOF MS spectrum of ligand L1.

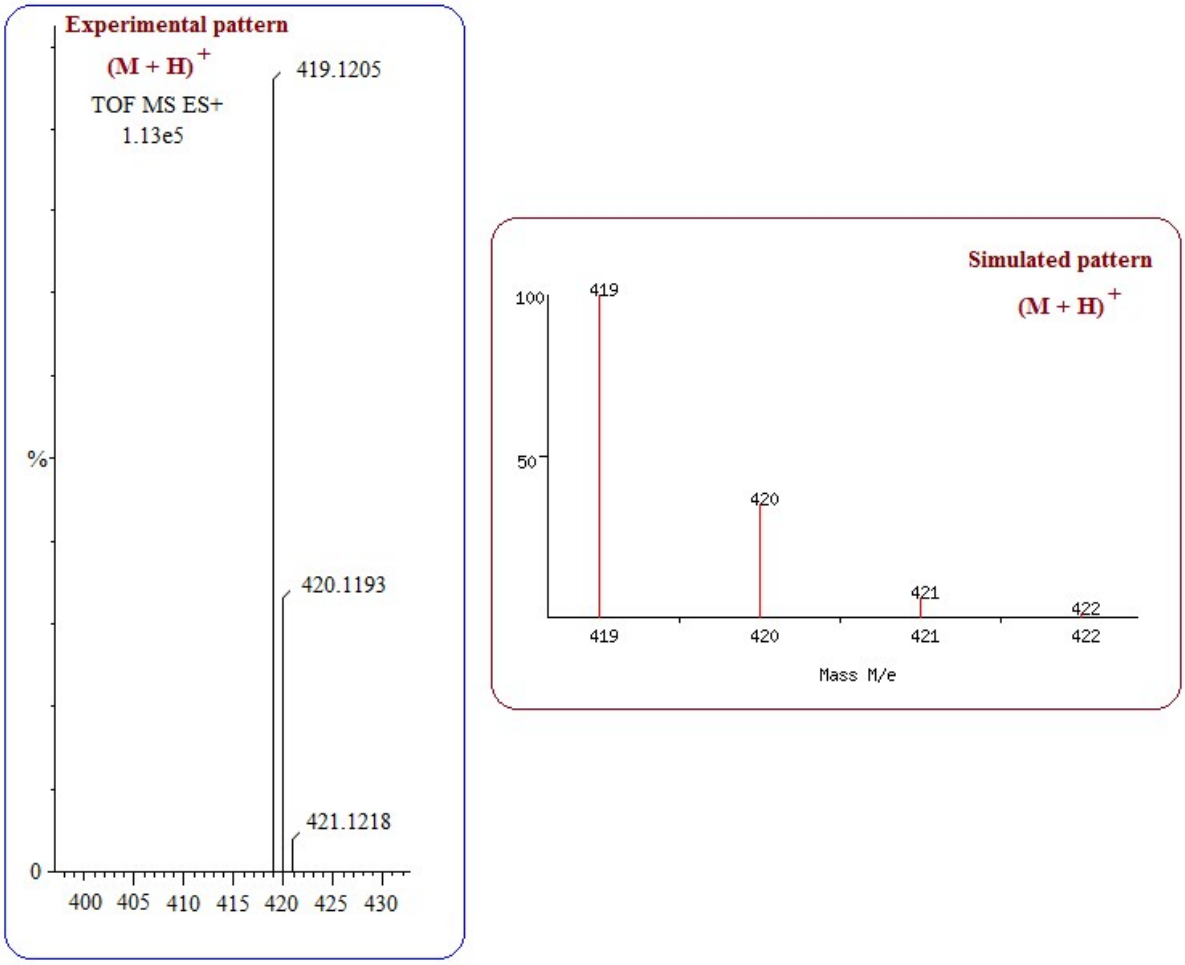

Fig. S12. TOF MS spectrum of ligand L2.

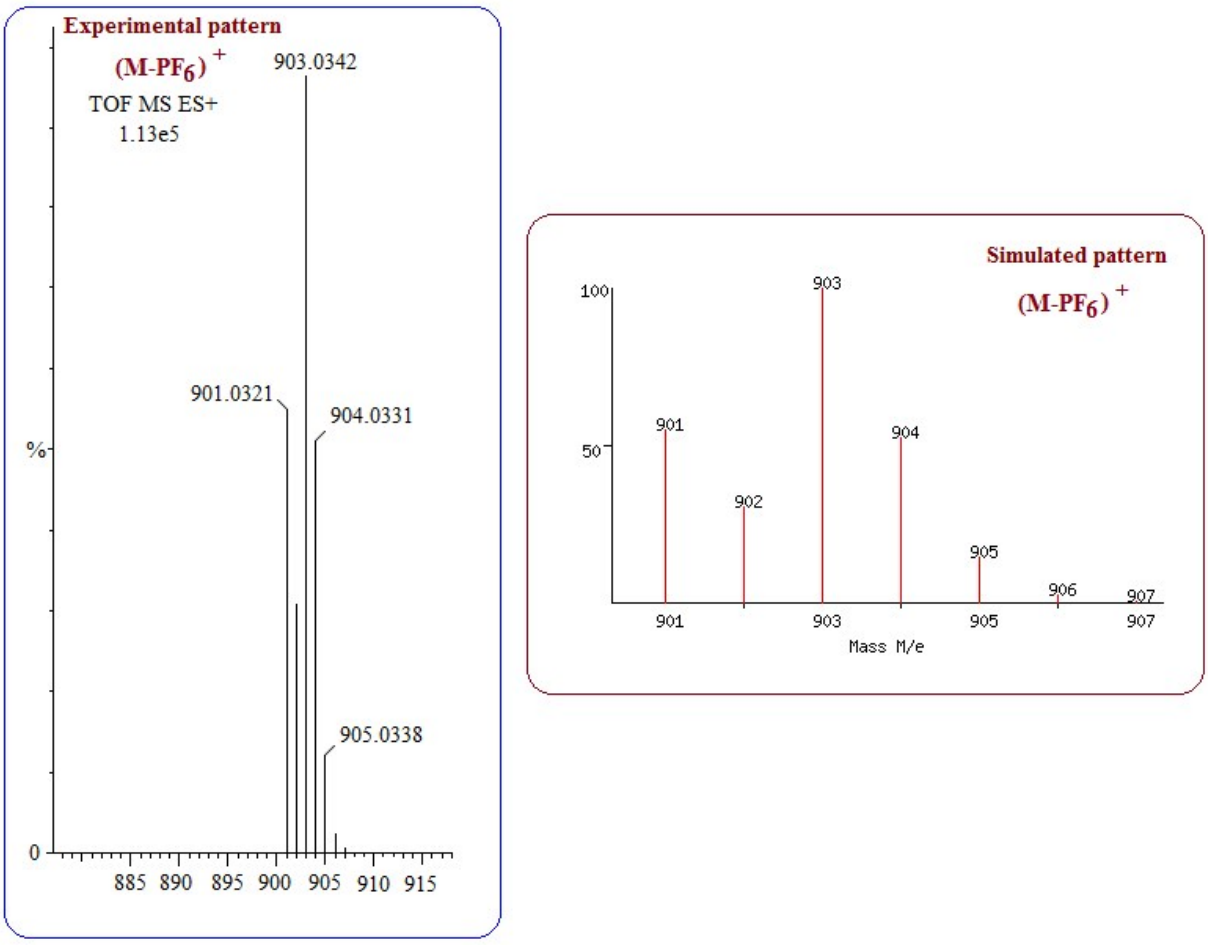

Fig. S13. TOF MS spectrum of complex **1**.

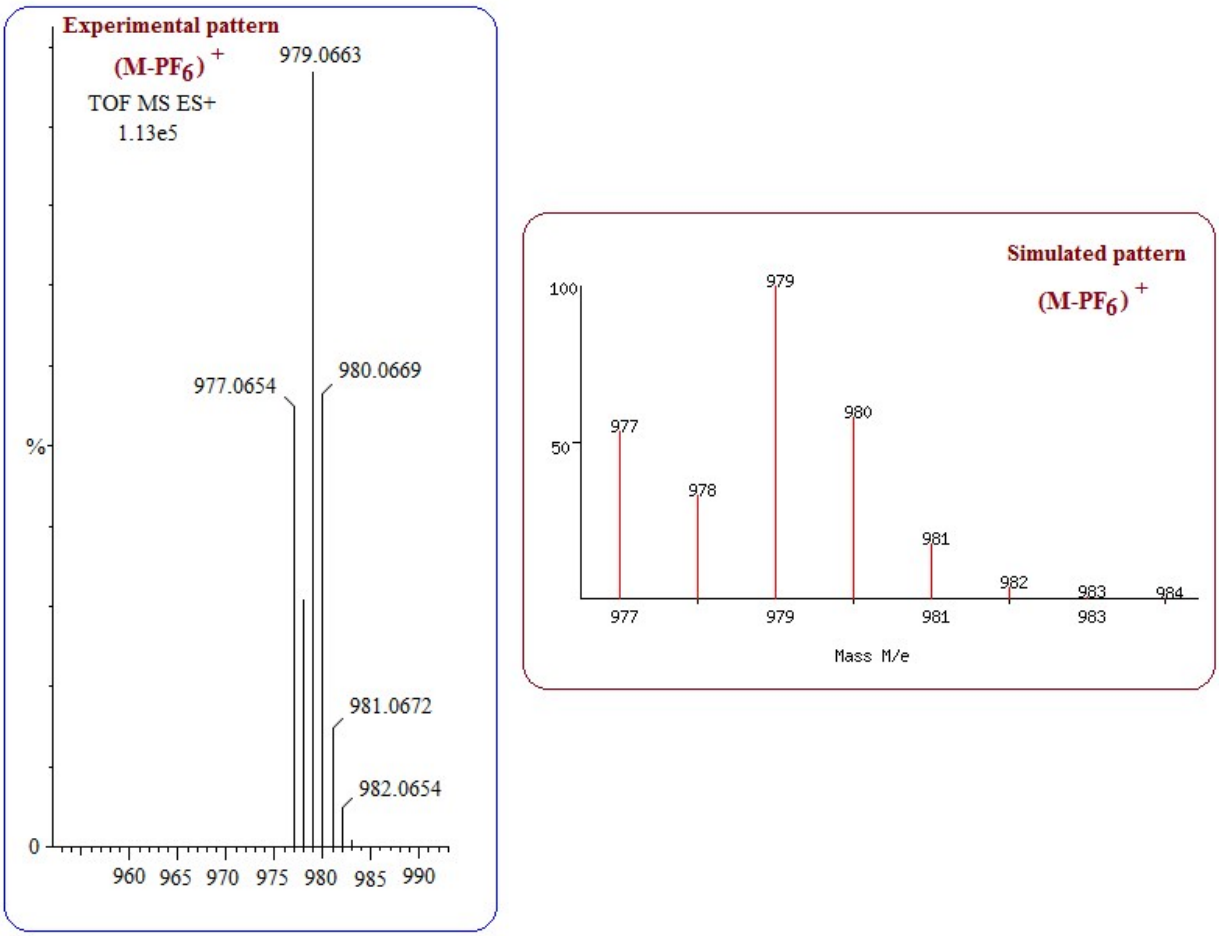

Fig. S14. TOF MS spectrum of complex **2**.

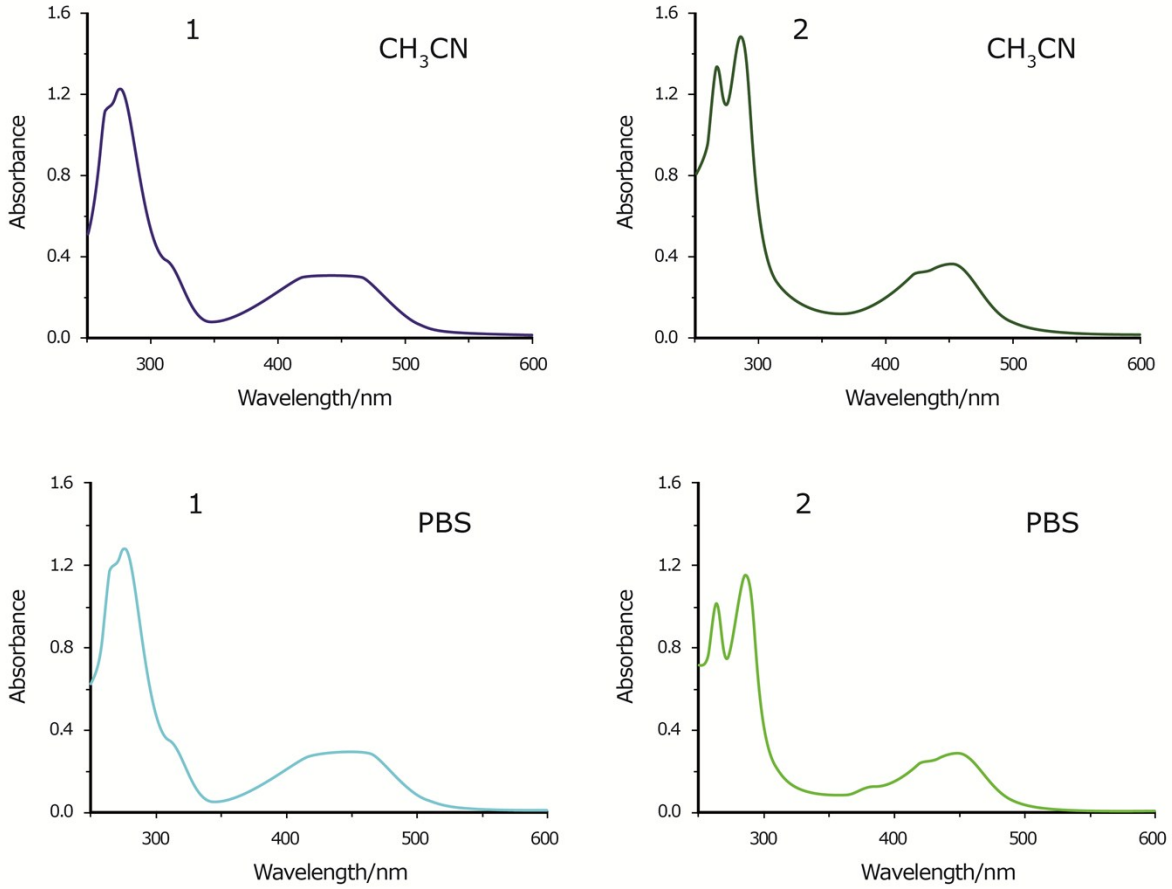

Fig. S15. UV/Vis spectra of complexes **1** and **2** in CH_3CN and PBS at 298 K.

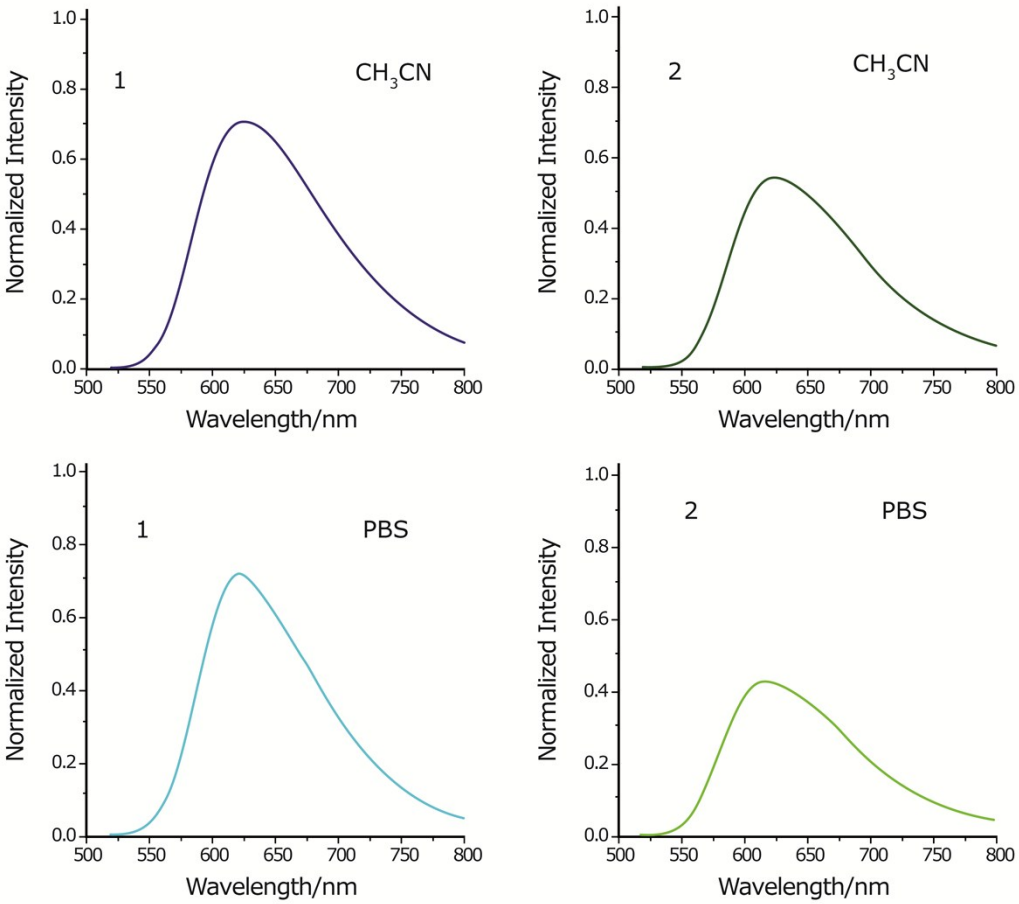

Fig. S16. Emission spectra of complexes **1** and **2** in CH_3CN and PBS at 298 K.

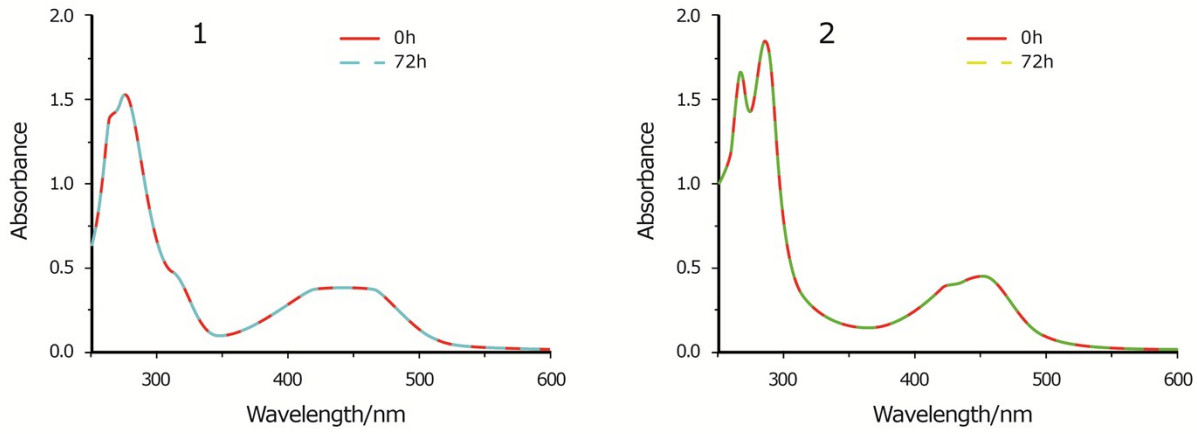

Fig. S17. Photostability of **1** and **2** (10 μM) detected by UV-Vis spectra in Tris-HCl buffer (5 mM Tris, 50 mM NaCl, pH = 7.4).

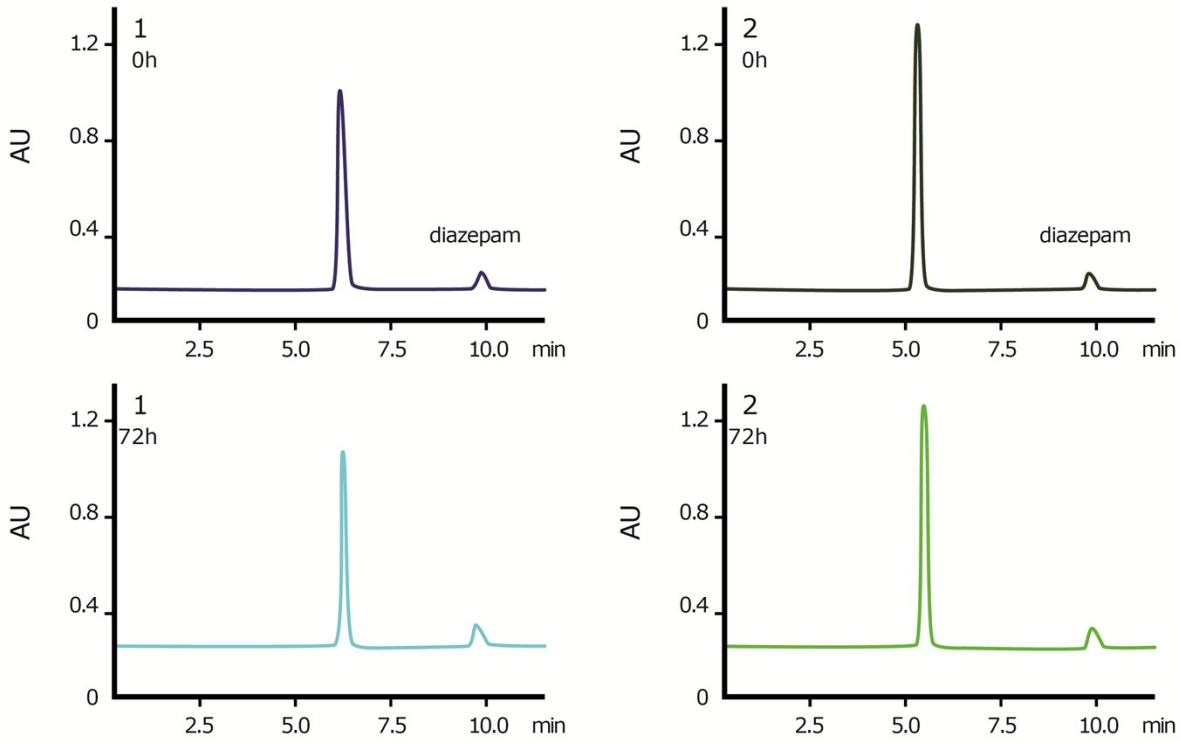

Fig. S18. LC-UV traces of plasma incubated with complexes **1** and **2** (20 μM, 37 ˚C) at t = 0 and 72 h. (Diazepam was used as internal standard).

Table S1. Photophysical data of complexes **1** and **2**.

Complex	UV/Vis λ [nm]	Emission[a] λ [nm]	(Φ_{em}) [b]	Lifetimes [ns][c]
1	ACN: 265 sh, 279, 435	ACN: 623	0.93	910
	PBS: 269 sh, 282, 450	PBS: 626		
2	ACN: 262, 283, 449	ACN: 612	1.05	985
	PBS: 265, 286, 453	PBS: 624		

[a] Emission spectra recorded in ACN (acetonitrile).
[b] Φ_{em} refers to the luminescence quantum yield and were calculated according to literature procedures. [1]
[c] Lifetimes evaluated ACN (acetonitrile).

Table S2. Singlet oxygen quantum yields upon irradiation at 450 nm.

	1	**2**
PBS (indirect)	3%	5%
ACN (direct)	85%	97%
ACN (indirect)	73%	92%

Table S3. Ratio of peak areas of complex/diazepam

	1	**2**
t = 0 h	9.22	8.98
t = 72 h	9.18	8.92

References

1. G. A. Crosby and J. N. Demas, *J. Phys. Chem.*, 1971, **75**, 991-1024.