

Supramolecular luminescent Pt(II) tweezers. Aggregation studies and $^1\text{O}_2$ production.

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Supporting Information

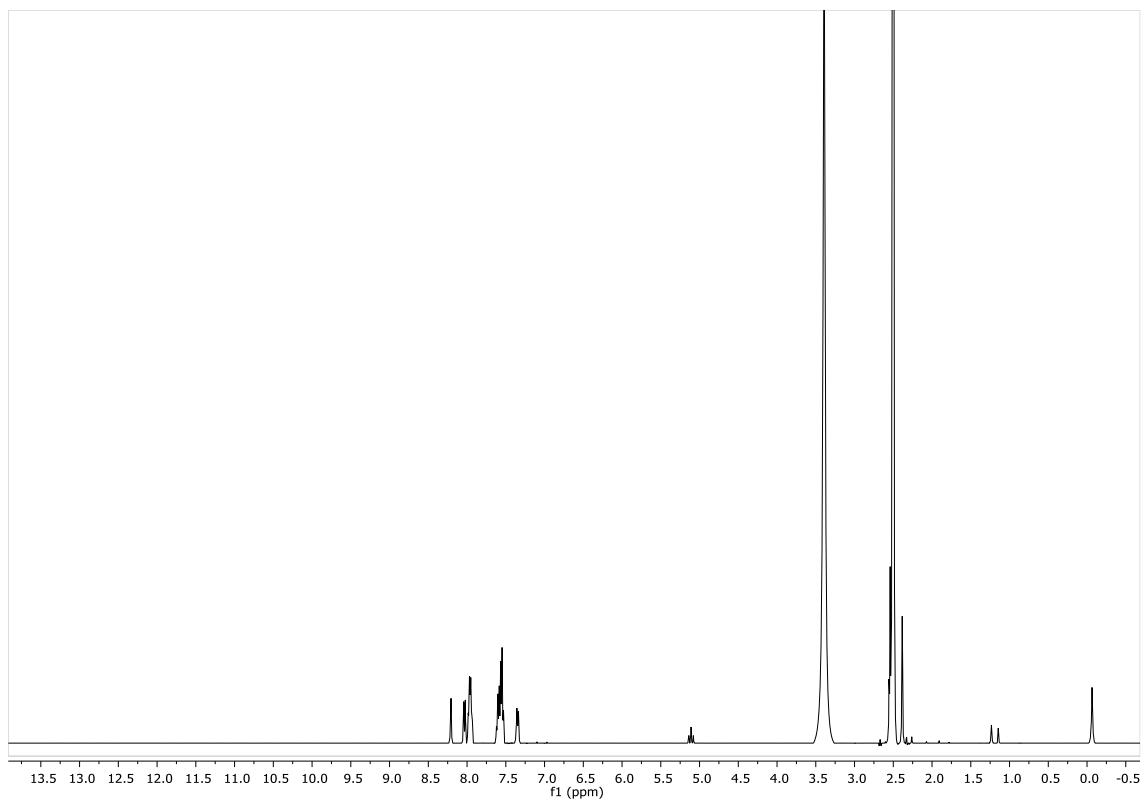


Figure S1. ¹H NMR spectrum of complex **10** in DMSO-d⁶.

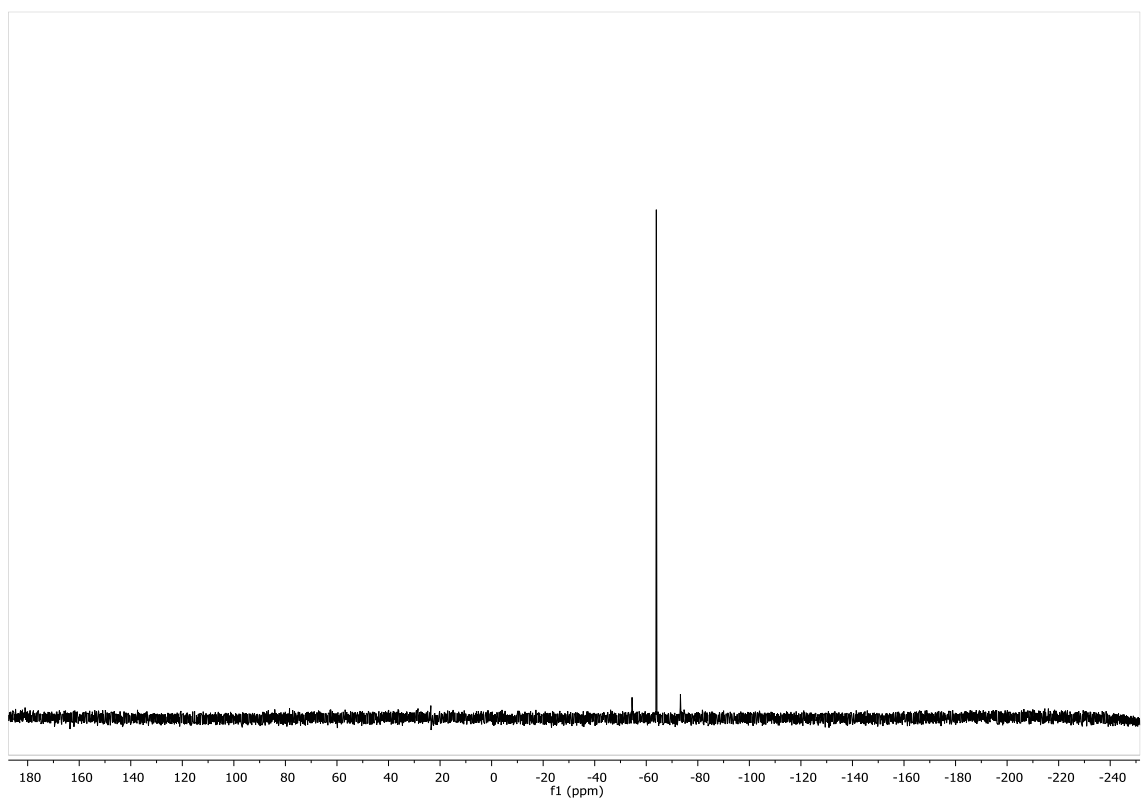


Figure S2. ³¹P NMR spectrum of complex **10** in DMSO-d⁶.

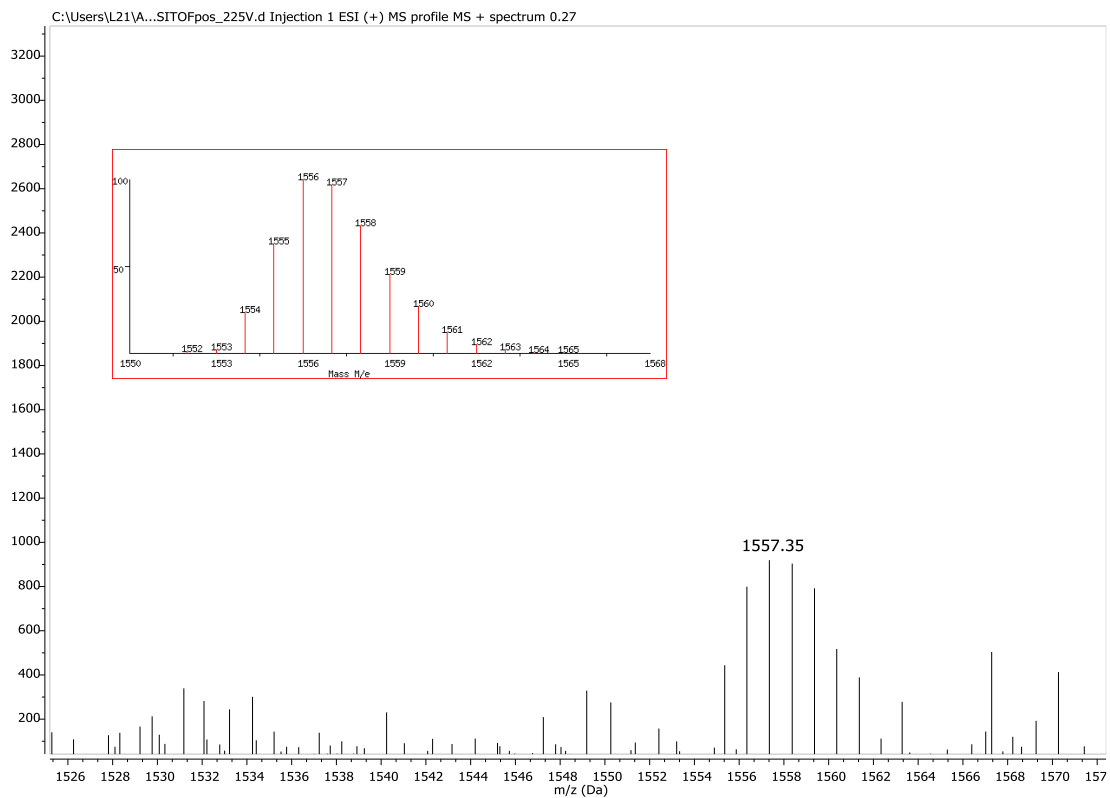


Figure S3. ESI-TOF(+) of complex **10**. Inset: calculated isotopic pattern.

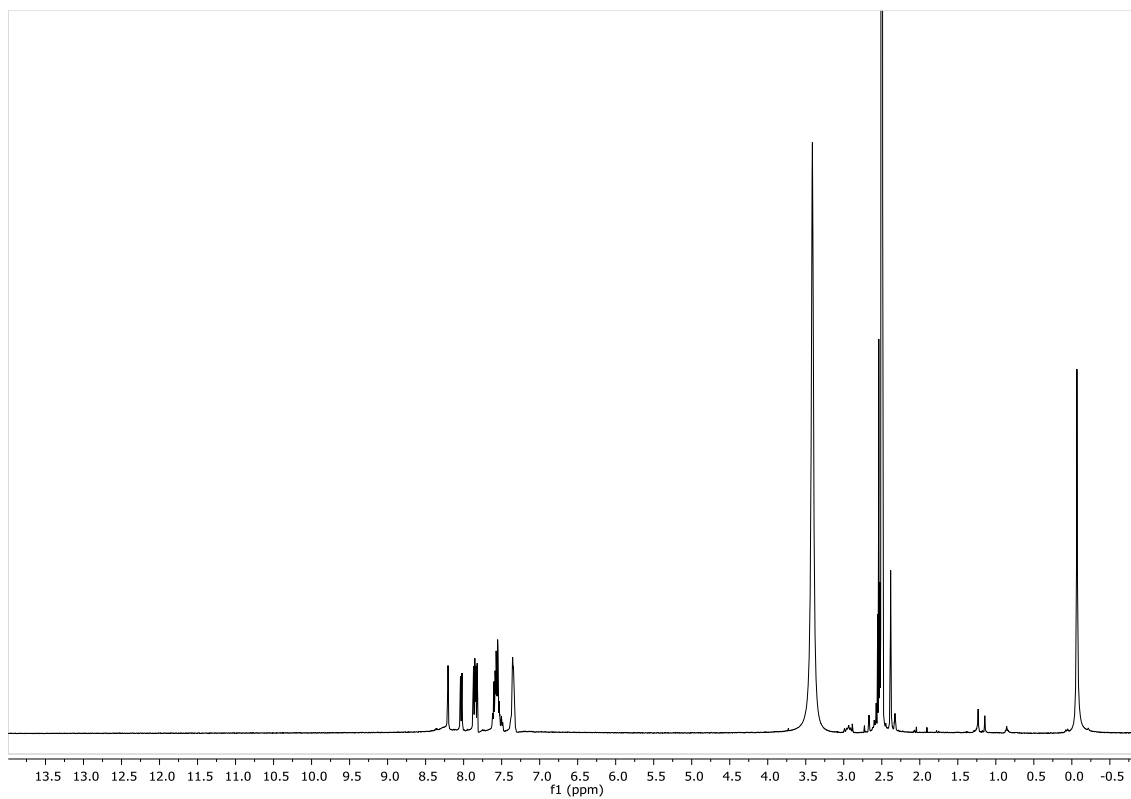


Figure S4. ^1H NMR spectrum of complex **11** in DMSO-d_6 .

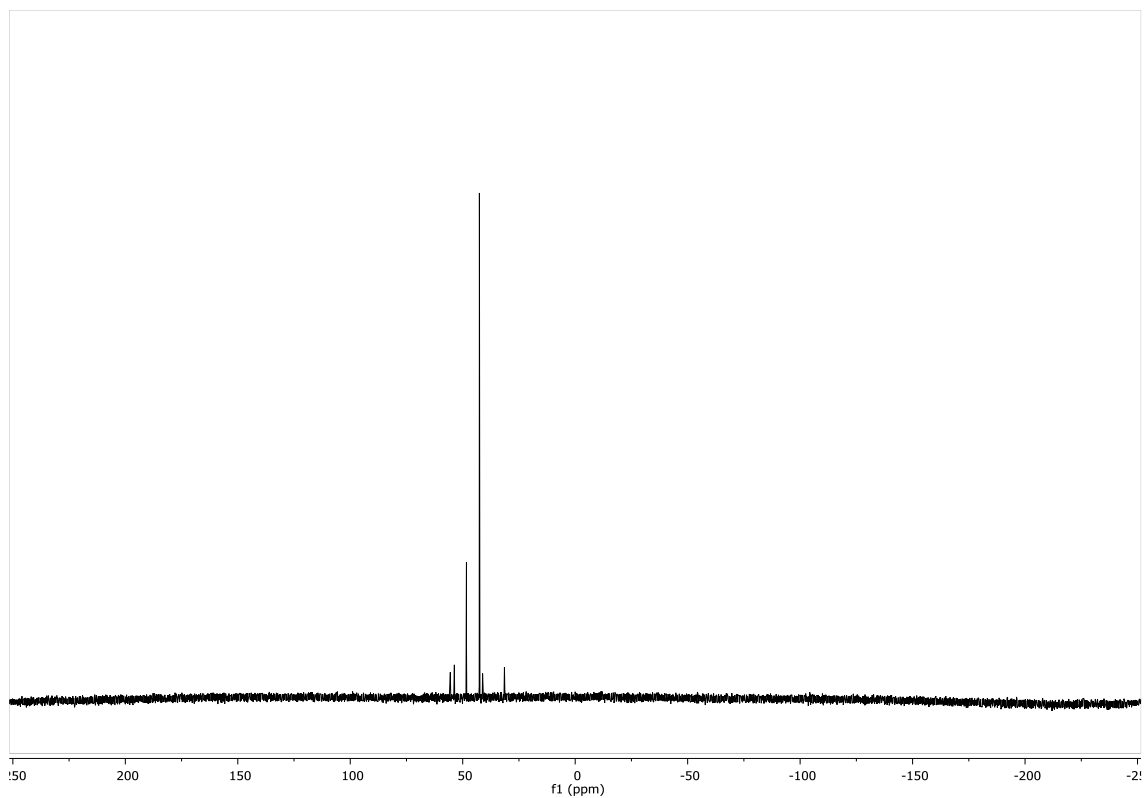


Figure S5. ^{31}P NMR spectrum of complex **11** in DMSO-d_6 .

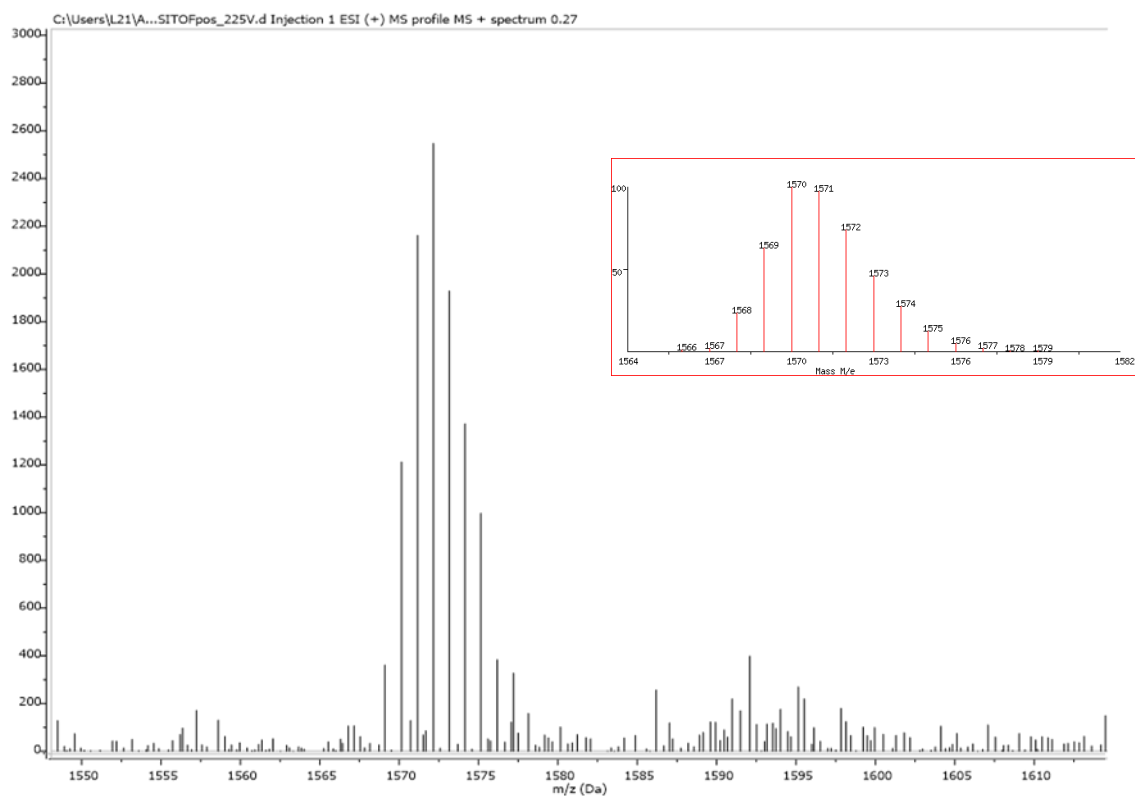


Figure S6. ESI-TOF(+) of complex **11**. Inset: calculated isotopic pattern.

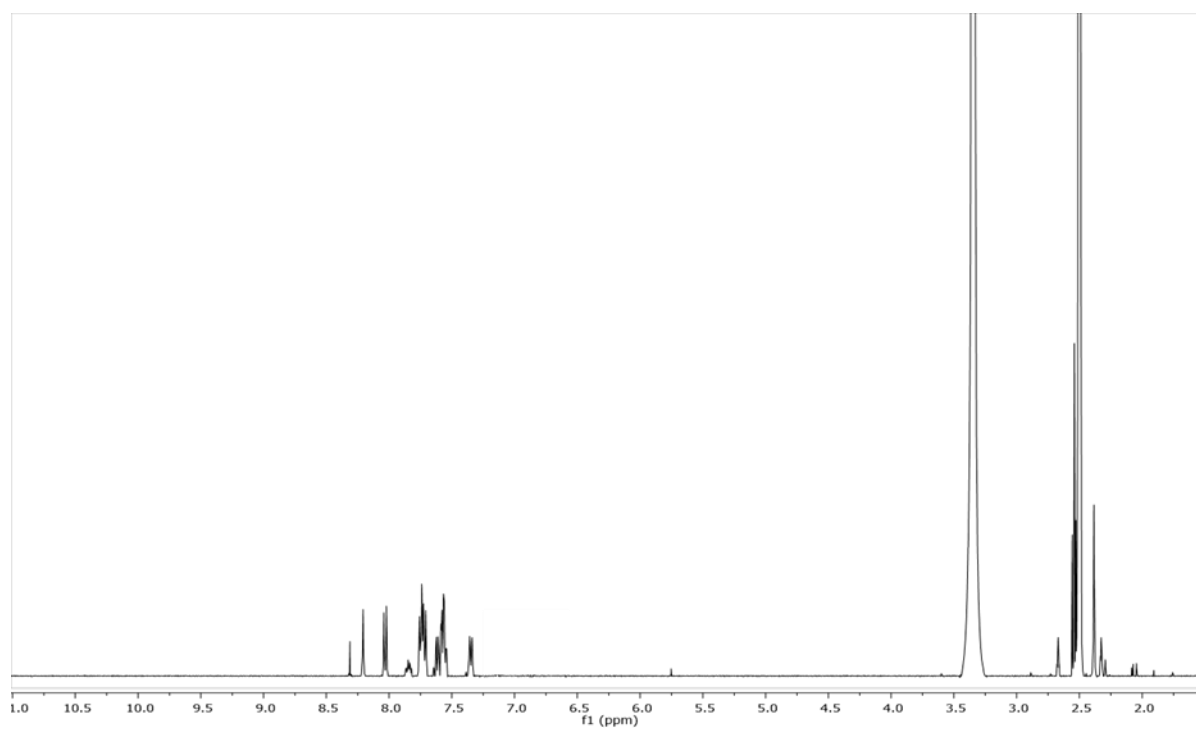


Figure S7. ^1H NMR spectrum of complex **12** in DMSO-d_6 .

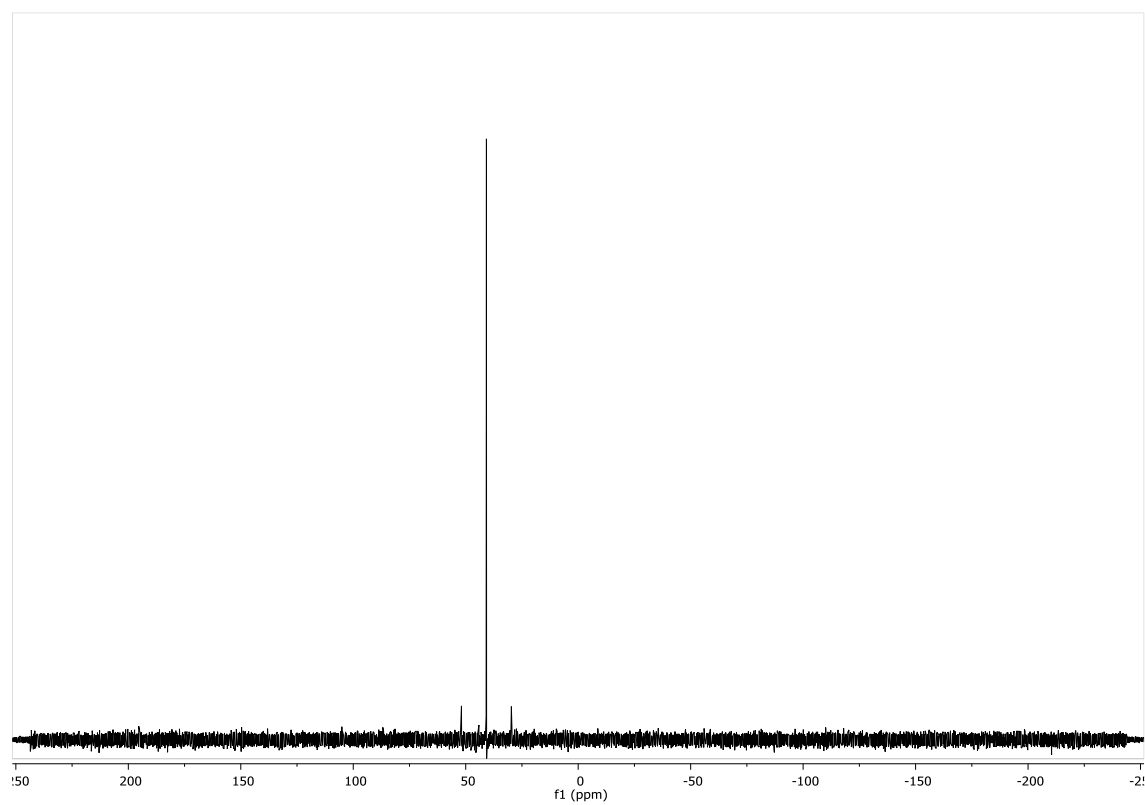


Figure S8. ^{31}P NMR spectrum of complex **12** in DMSO-d_6 .

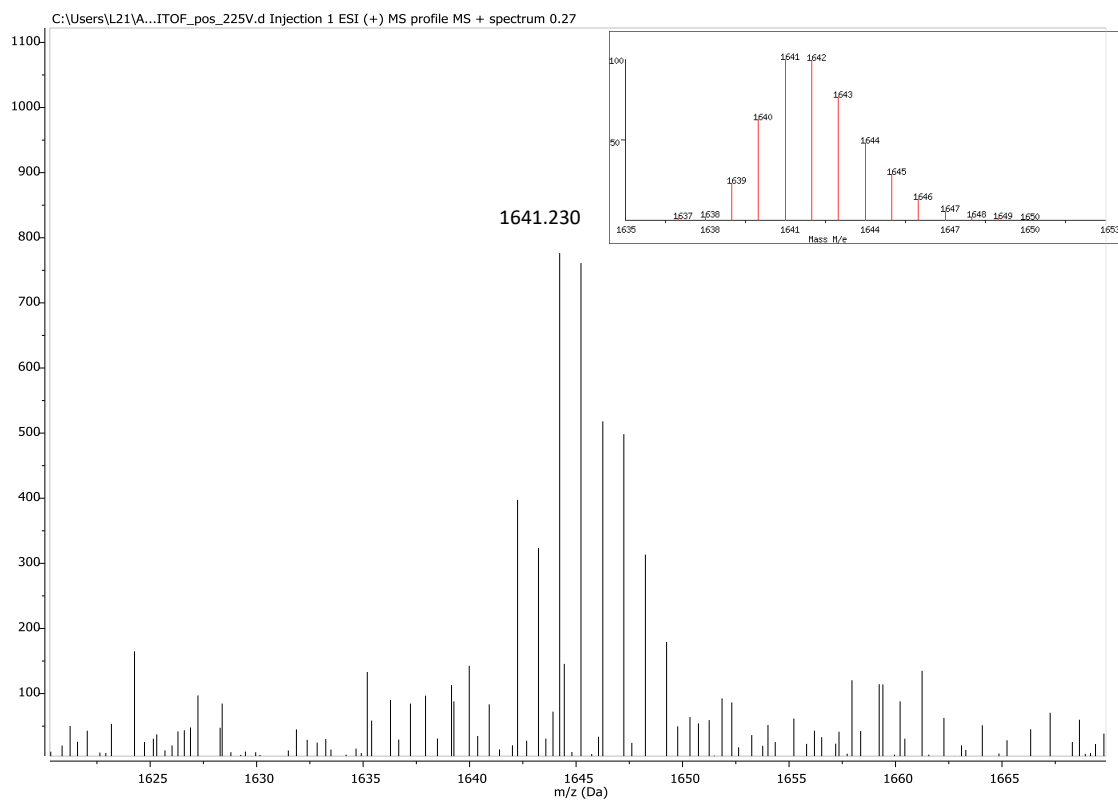


Figure S9. ESI-TOF(+) of complex **12**. Inset: calculated isotopic pattern.

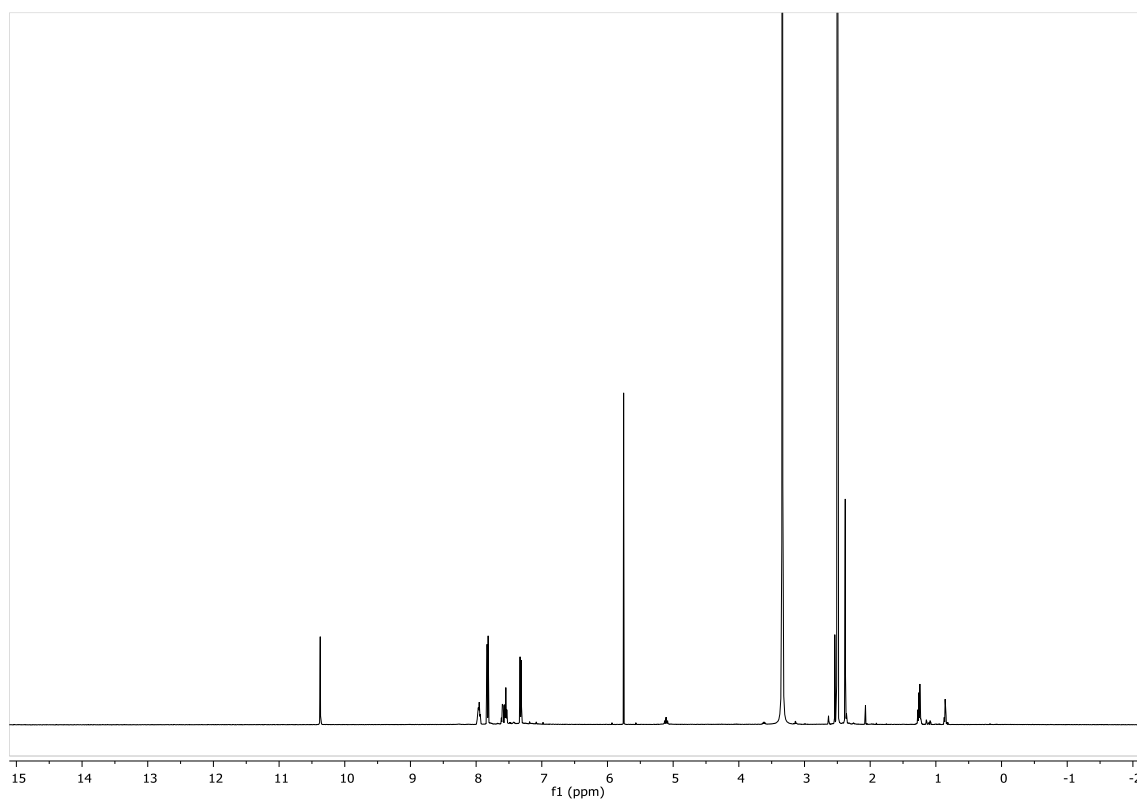


Figure S10. ^1H NMR spectrum of complex **13** in DMSO-d_6 .

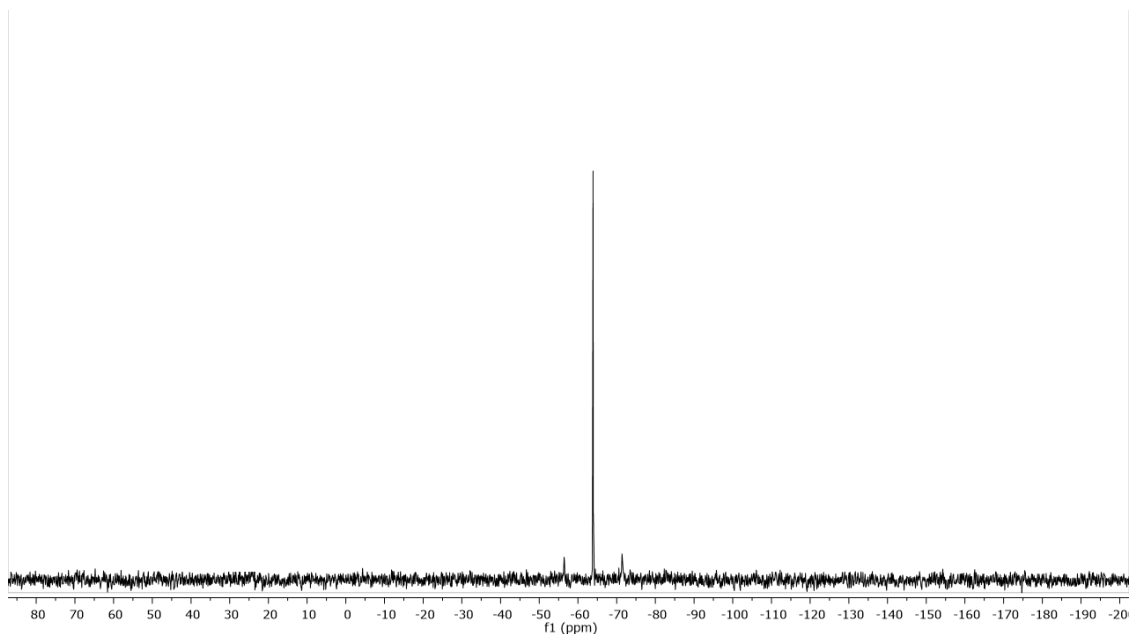


Figure S11. ^{31}P NMR spectrum of complex **13** in DMSO-d_6 .

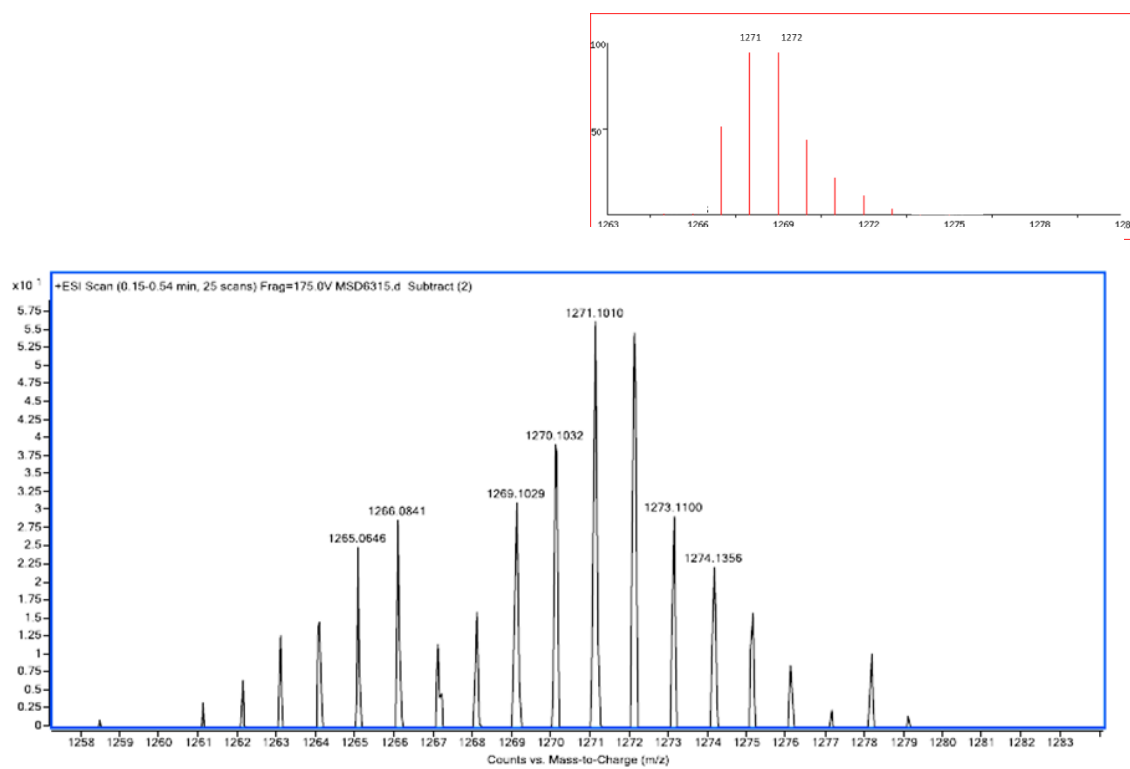


Figure S12. ESI-TOF(+) of complex **13**. Inset: calculated isotopic pattern.

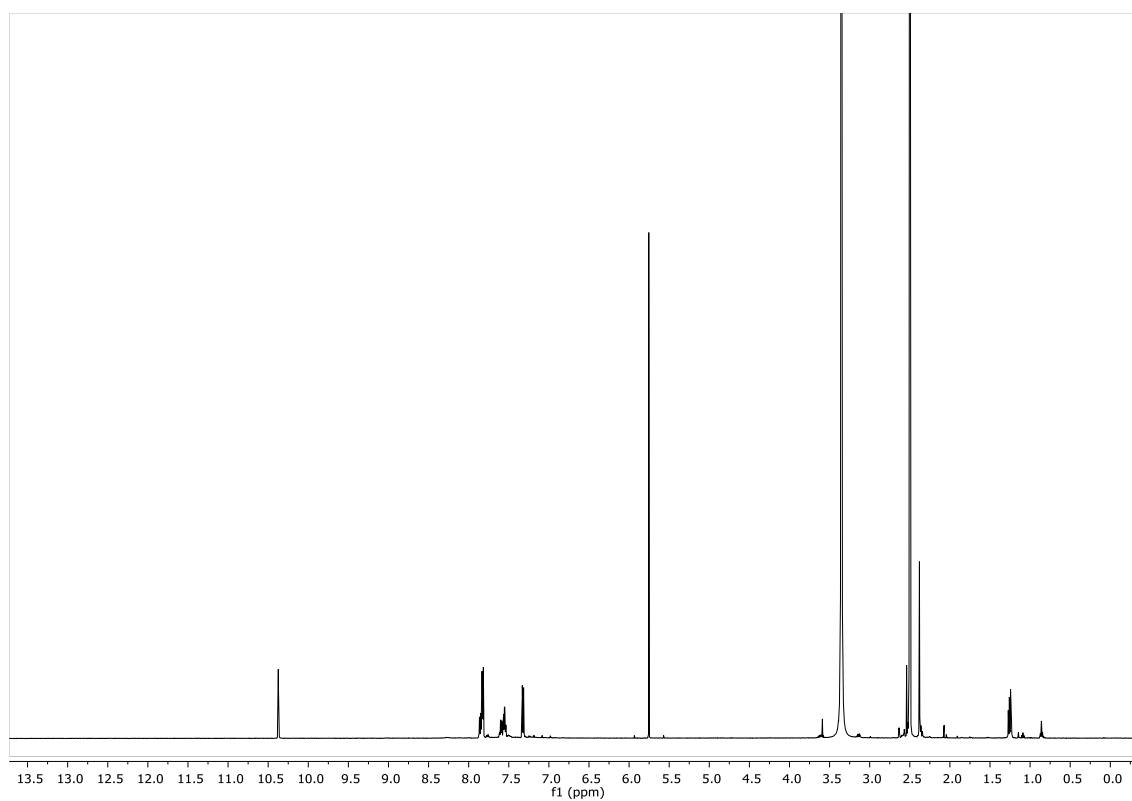


Figure S13. ^1H NMR spectrum of complex **14** in DMSO-d_6 .

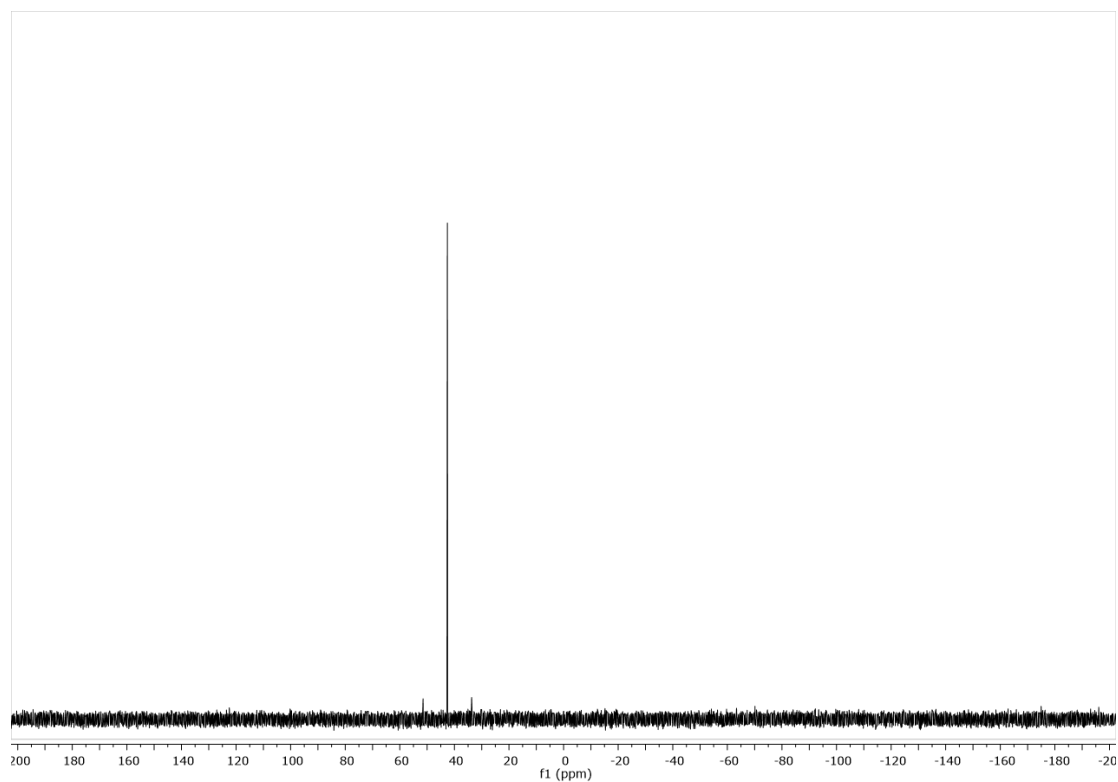


Figure S14. ^{31}P NMR spectrum of complex **14** in DMSO-d_6 .

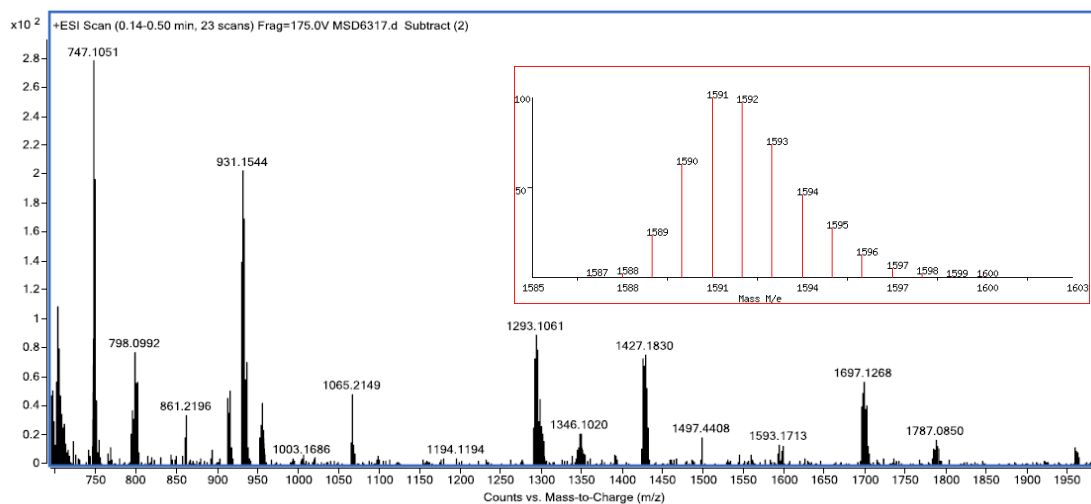


Figure S15. ESI-TOF(+) of complex **14**. Inset: calculated isotopic pattern.

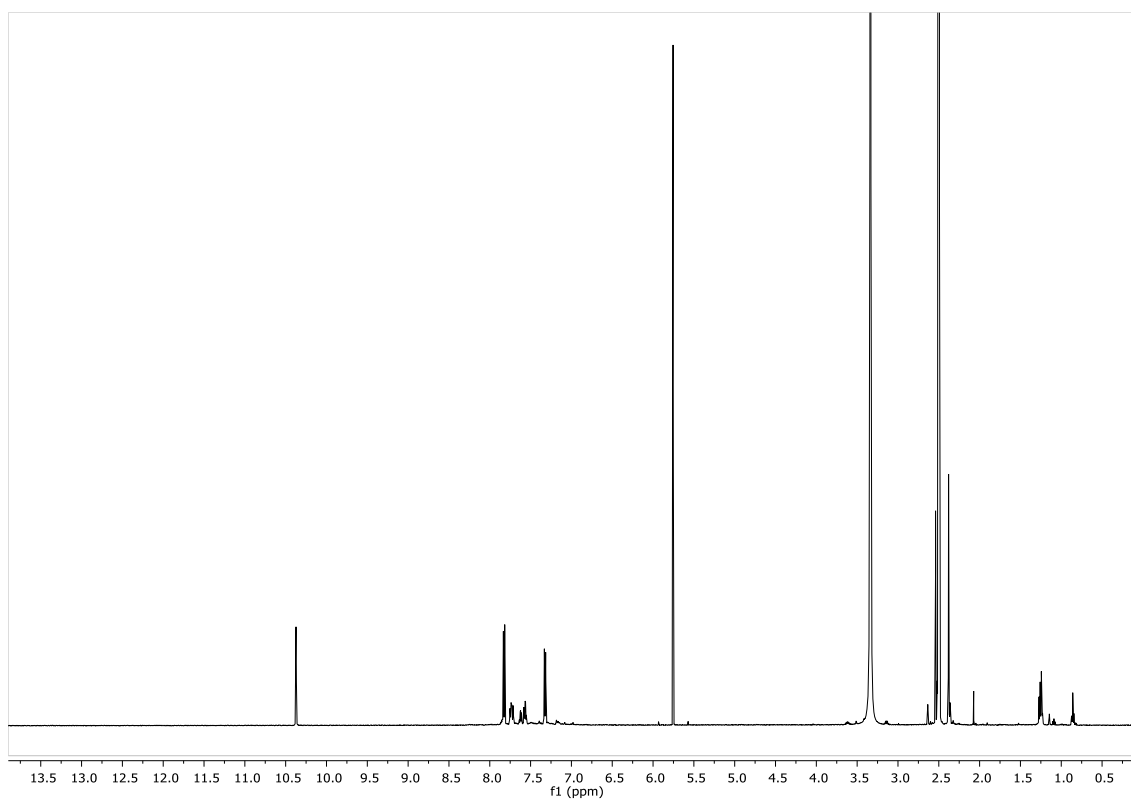


Figure S16. ^1H NMR spectrum of complex **15** in DMSO-d_6 .

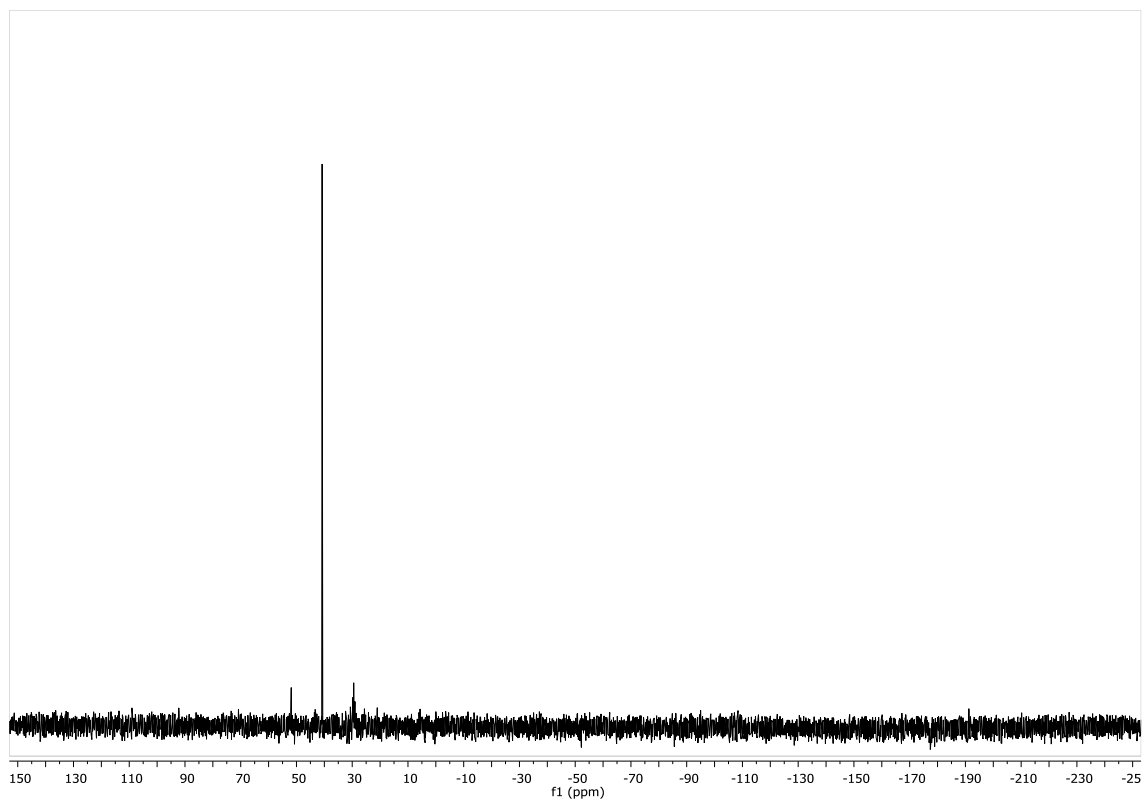


Figure S17. ^{31}P NMR spectrum of complex **15** in DMSO-d_6 .

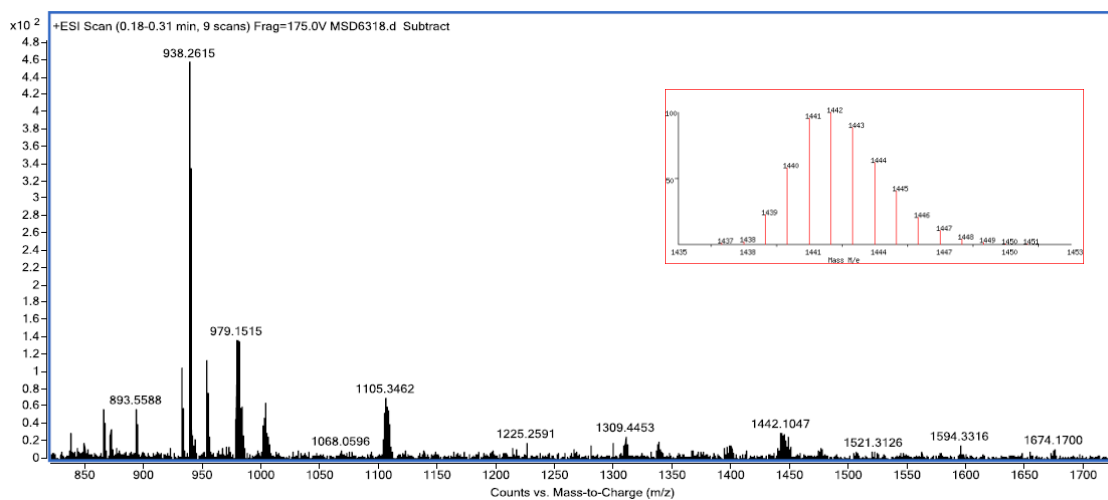


Figure S18. ESI-TOF(+) of complex **15**. Inset: calculated isotopic pattern.

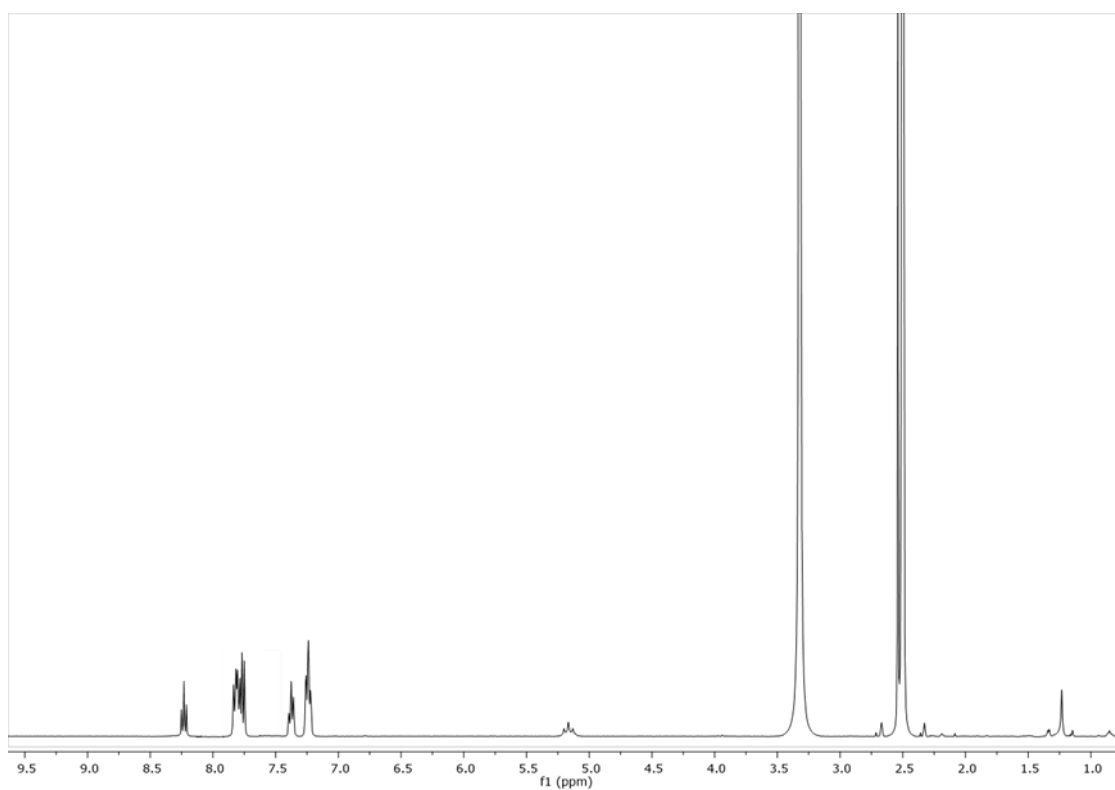


Figure S19. ^1H NMR spectrum of complex **16** in DMSO-d_6 .

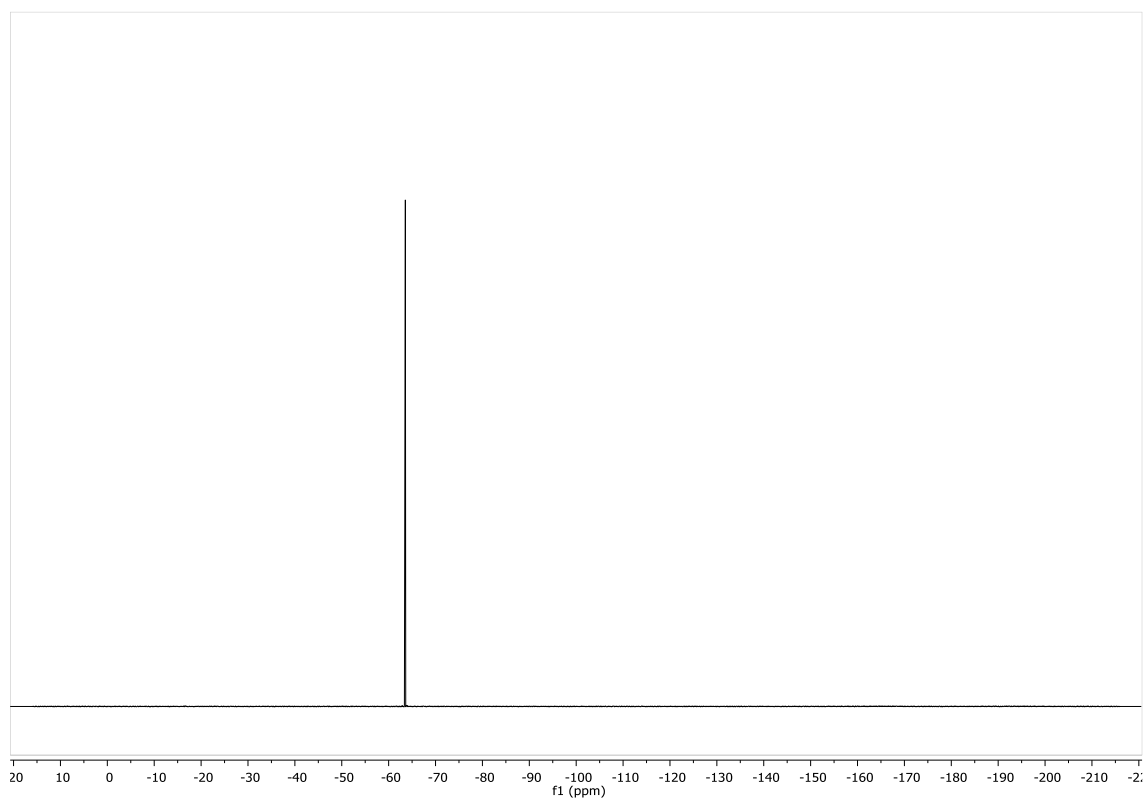


Figure S20. ^{19}F NMR spectrum of complex **16** in DMSO-d_6 .

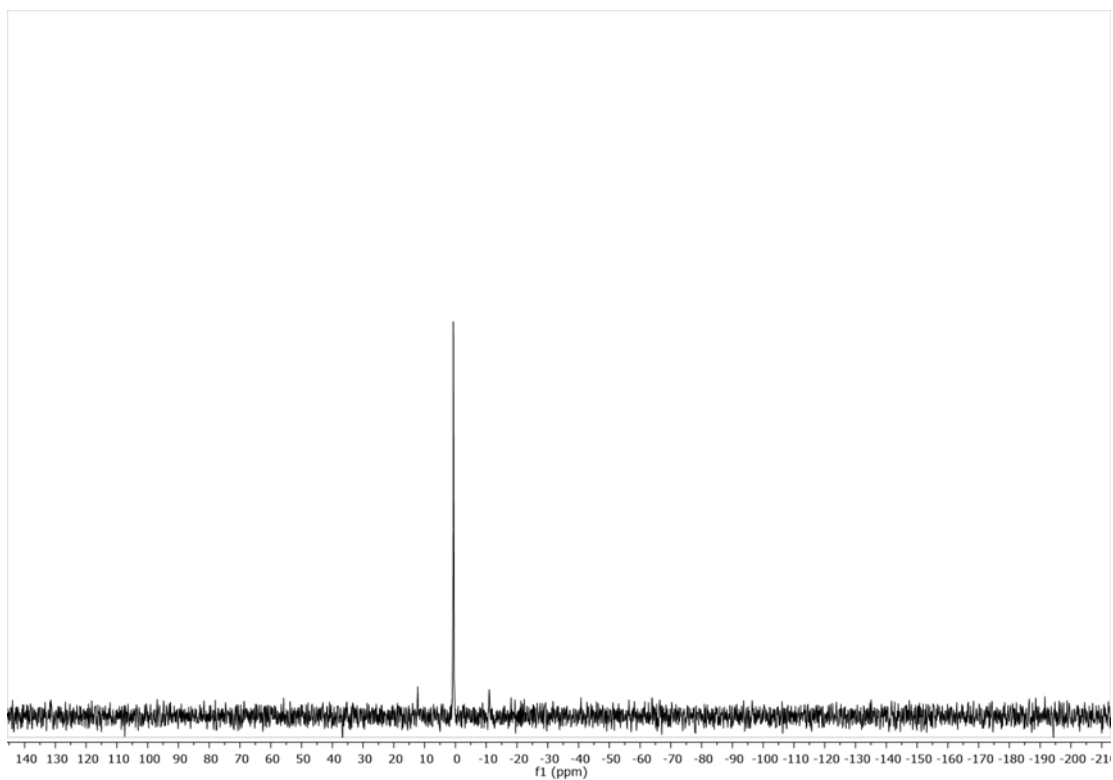


Figure S21. ^{31}P NMR spectrum of complex **16** in DMSO- d_6 .

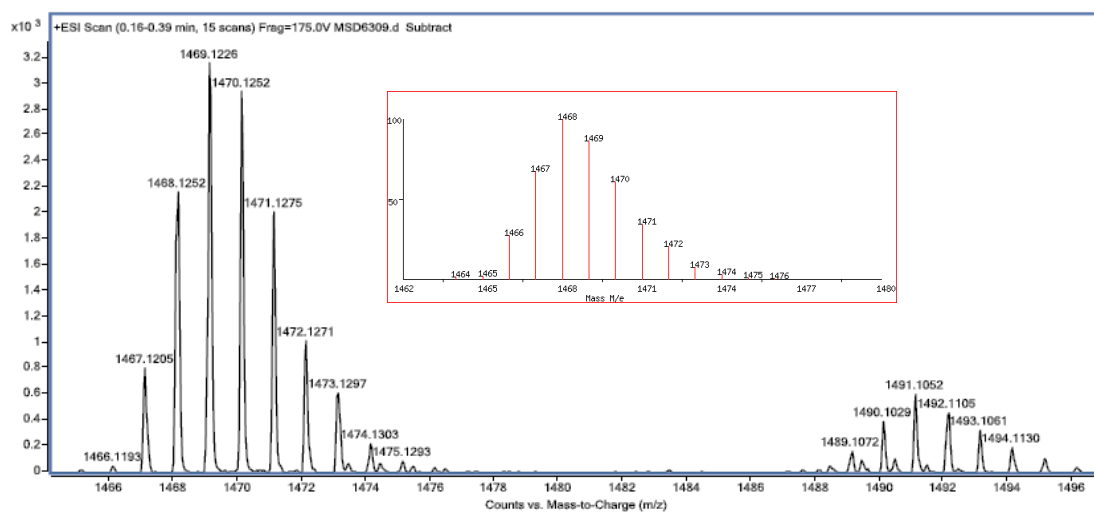


Figure S22. ESI-TOF(+) of complex **16**. Inset: calculated isotopic pattern.

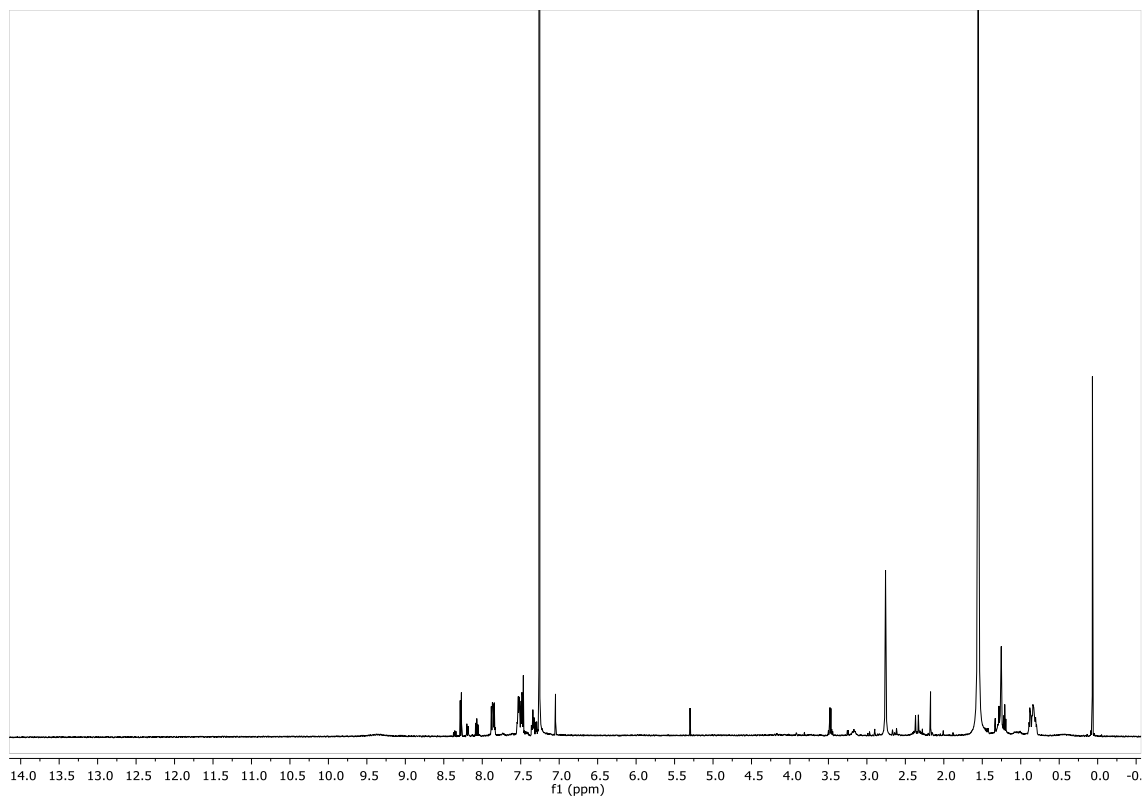


Figure S23. ^1H NMR spectrum of complex **17** in DMSO-d^6 .

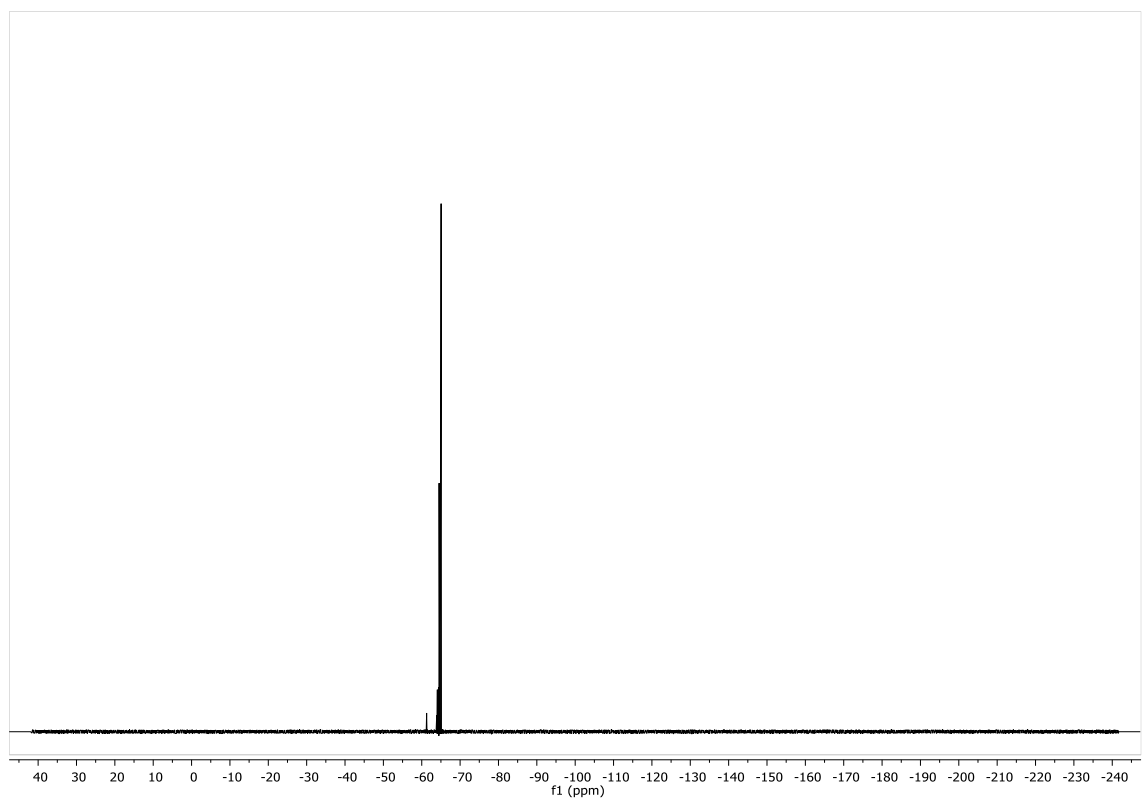


Figure S24. ^{19}F NMR spectrum of complex **17** in DMSO-d^6 .

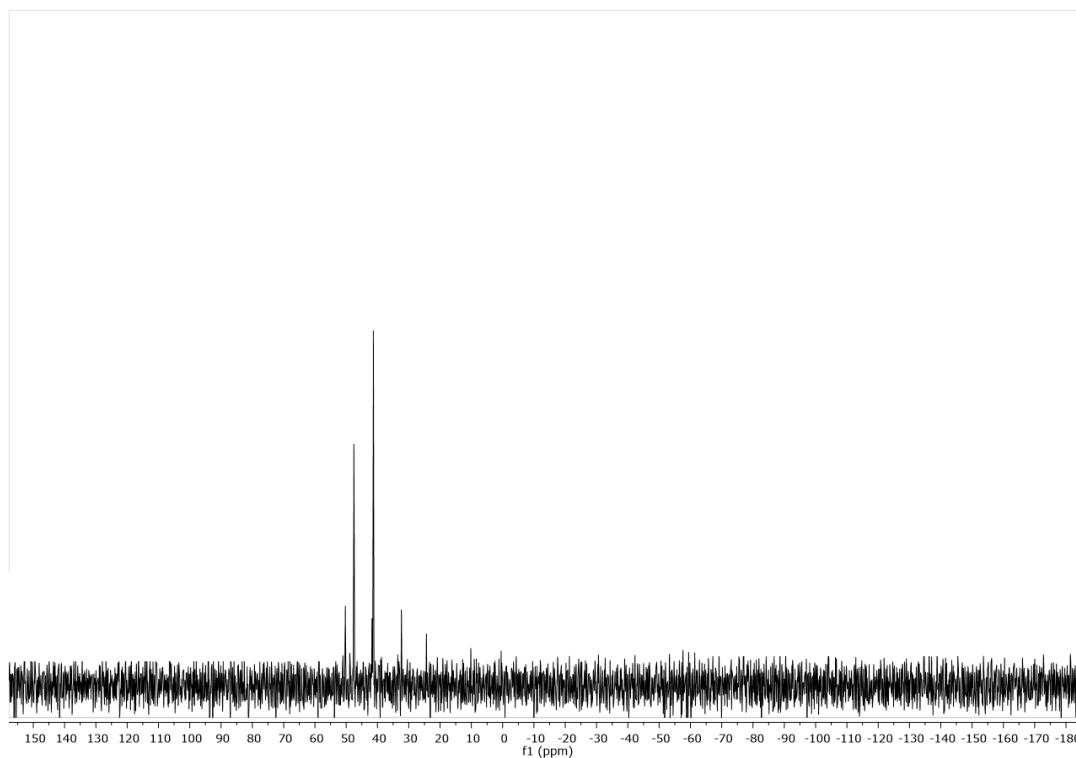


Figure S25. ^{31}P NMR spectrum of complex **17** in DMSO-d^6 .

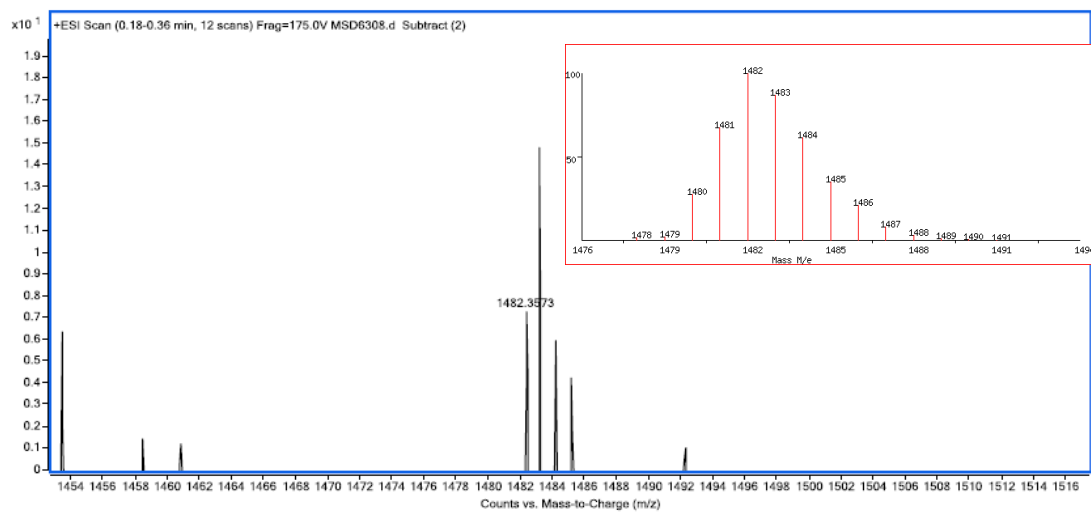


Figure S26. ESI-TOF(+) of complex **17**. Inset: calculated isotopic pattern.

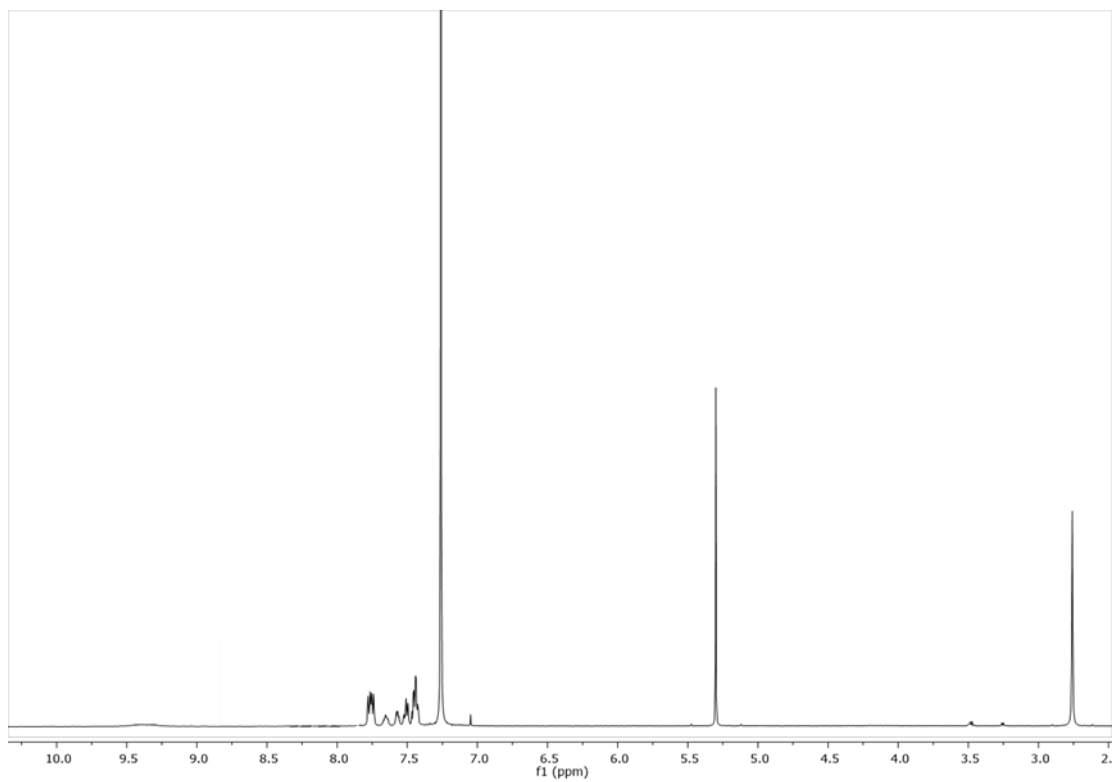


Figure S27. ^1H NMR spectrum of complex **18** in DMSO-d^6 .

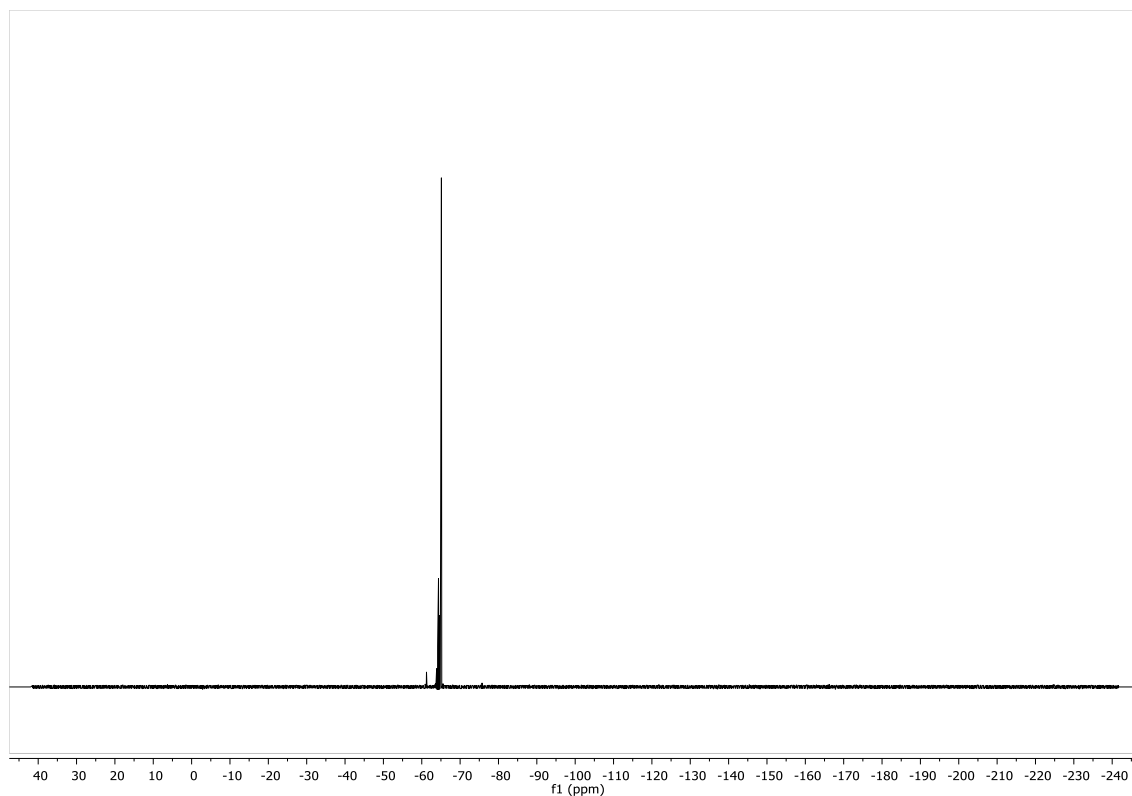


Figure S28. ^{19}F NMR spectrum of complex **18** in DMSO-d^6 .

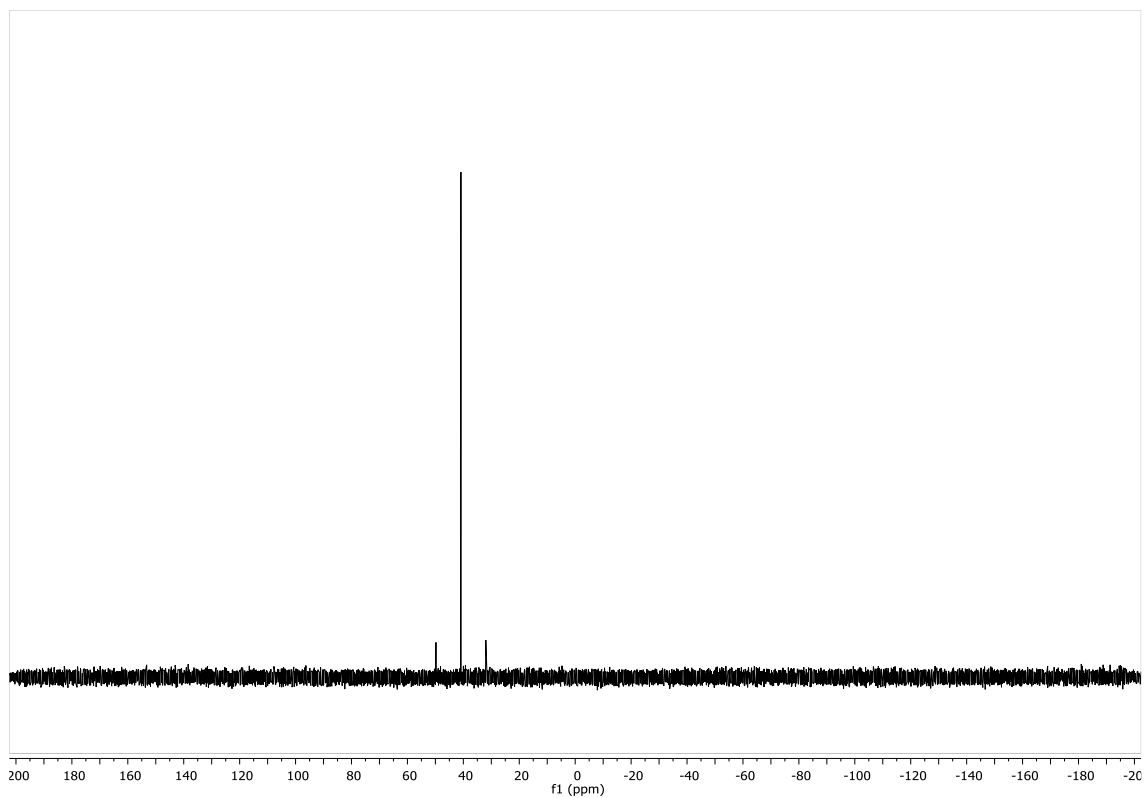


Figure S29. ^{31}P NMR spectrum of complex **18** in DMSO-d_6 .

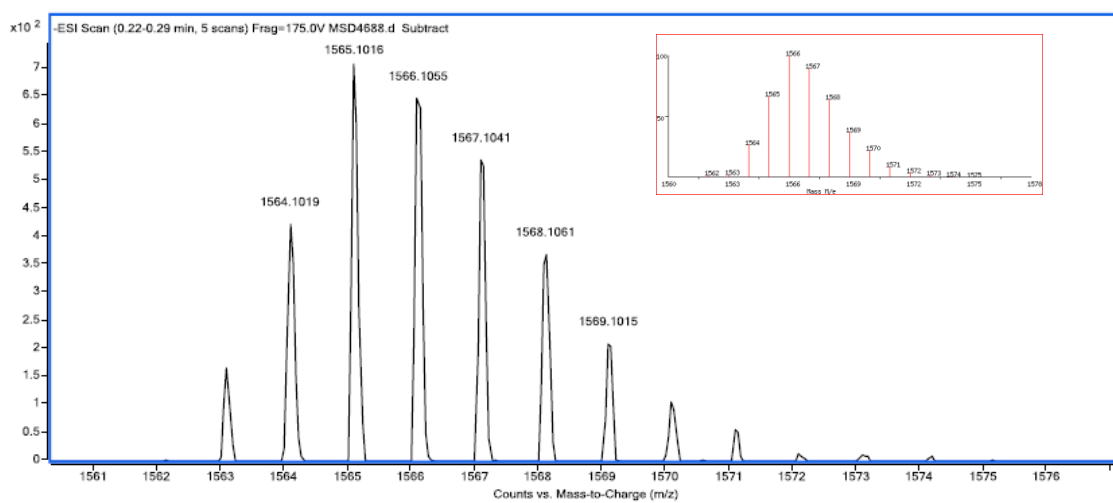


Figure S30. ESI-TOF(+) of complex **18**. Inset: calculated isotopic pattern.

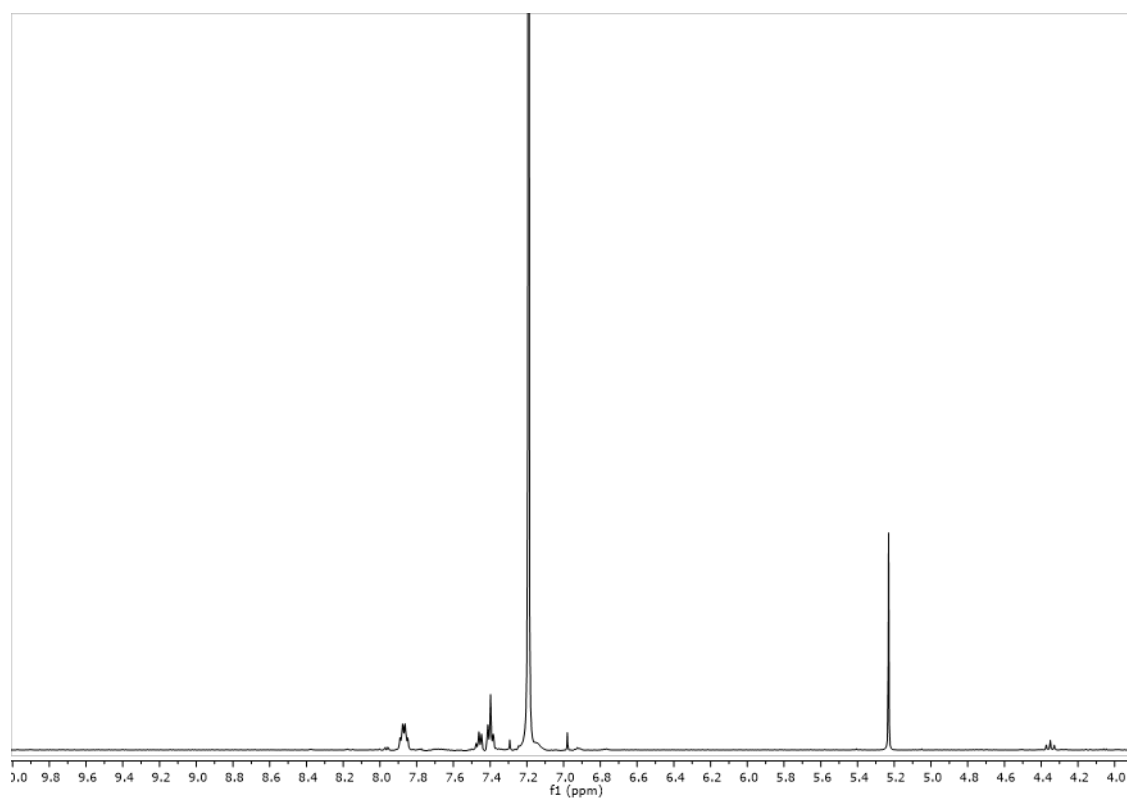


Figure S31. ^1H NMR spectrum of complex **19** in DMSO-d_6 .

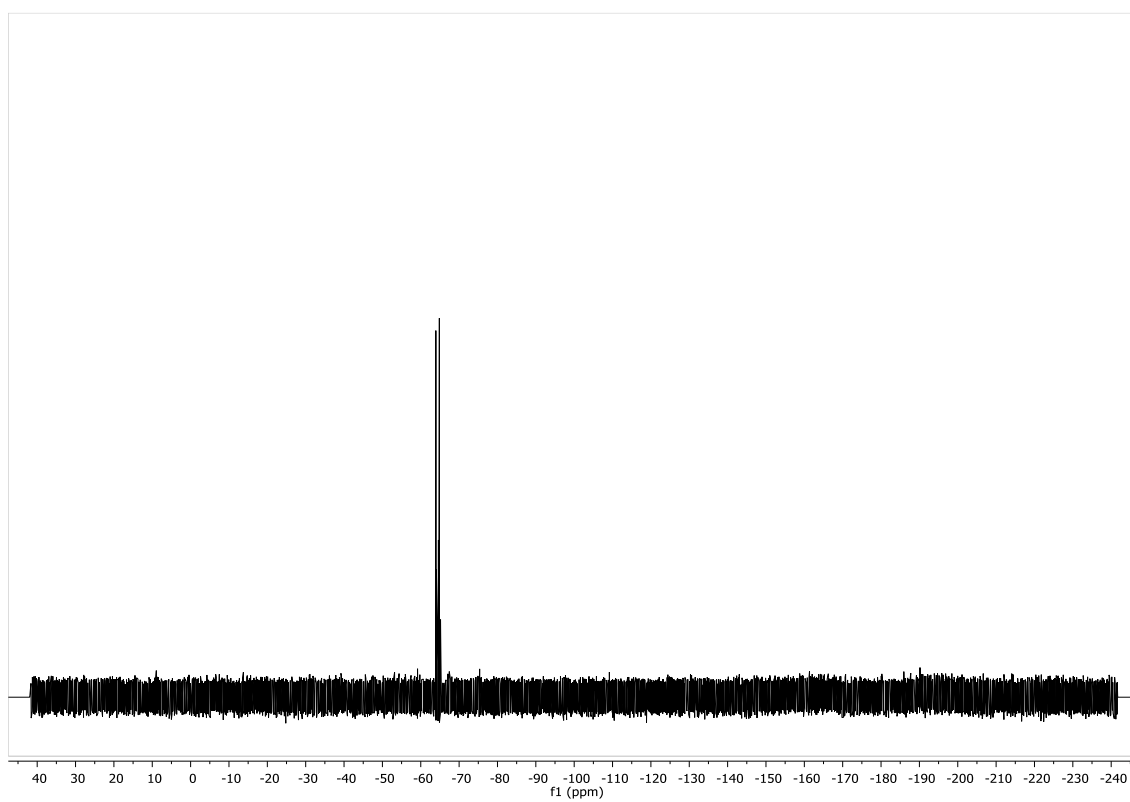


Figure S32. ^{19}F NMR spectrum of complex **19** in DMSO-d_6 .

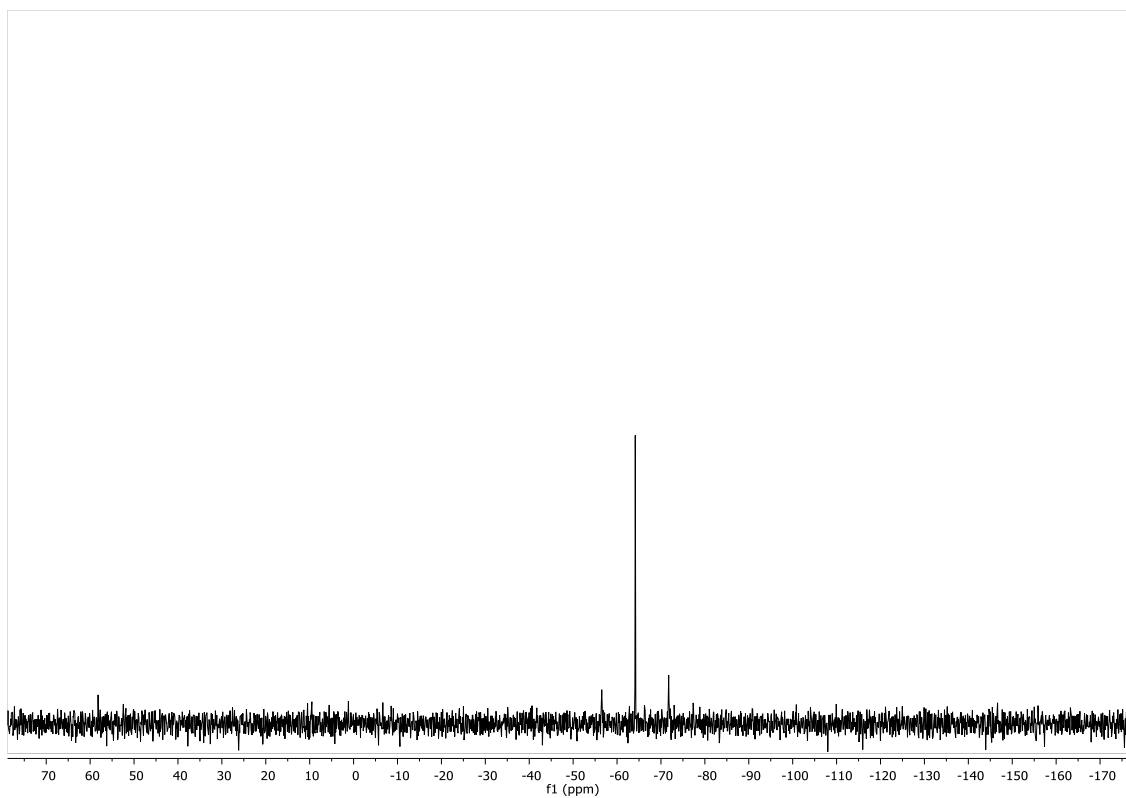


Figure S33. ^{31}P NMR spectrum of complex **19** in DMSO-d_6 .

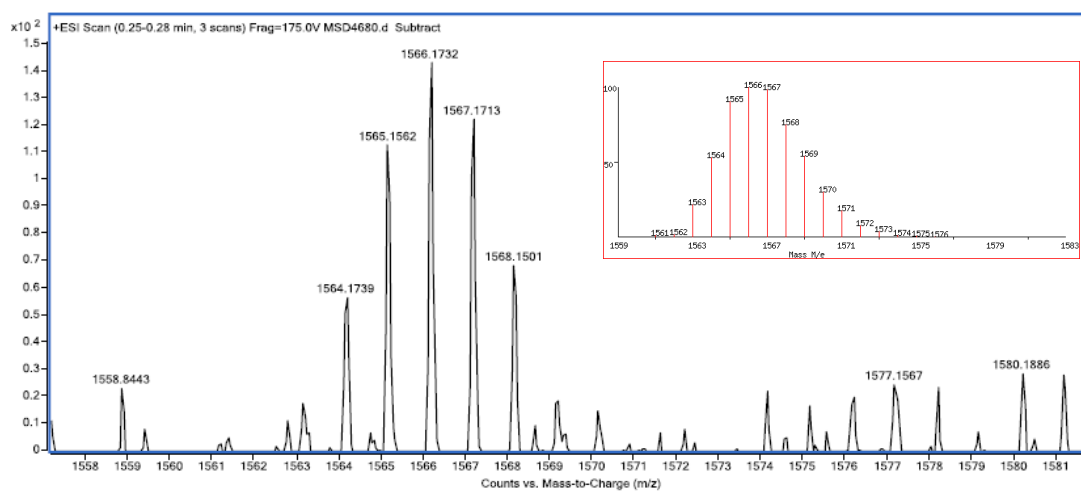


Figure S34. ESI-TOF(+) of complex **19**. Inset: calculated isotopic pattern.

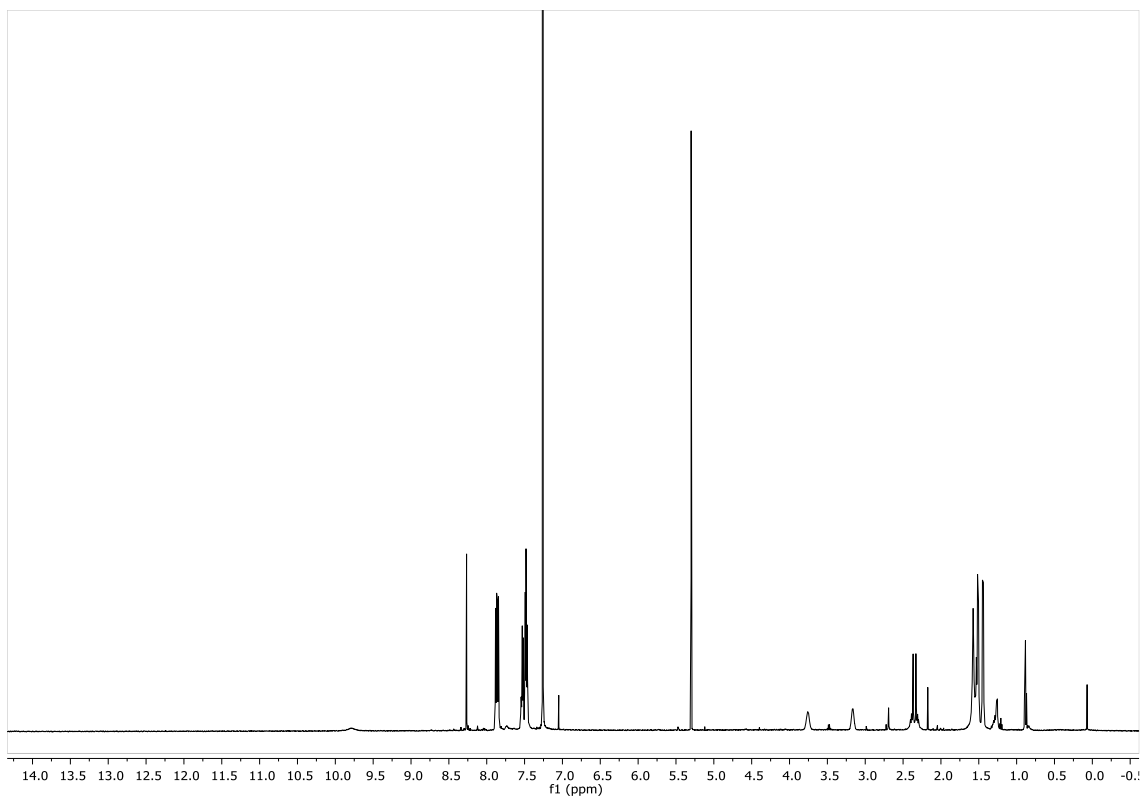


Figure S35. ^1H NMR spectrum of complex **20** in DMSO-d_6 .

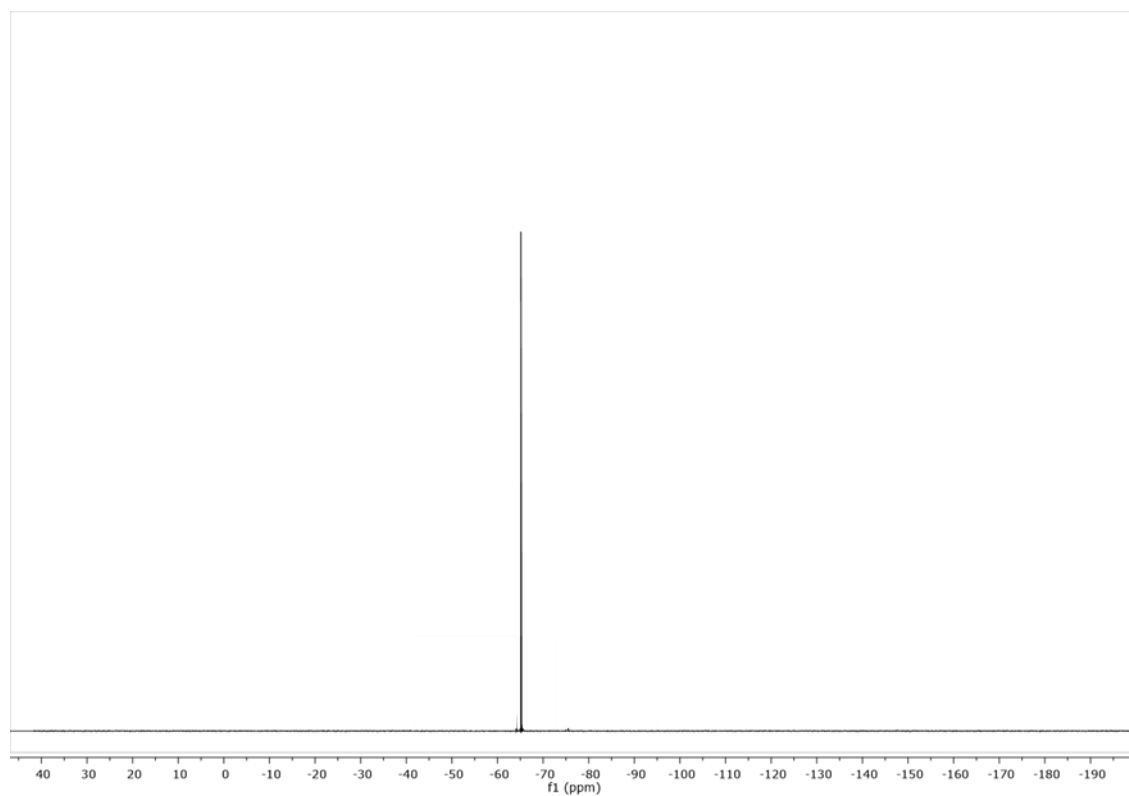


Figure S36. ^{19}F NMR spectrum of complex **20** in DMSO-d_6 .

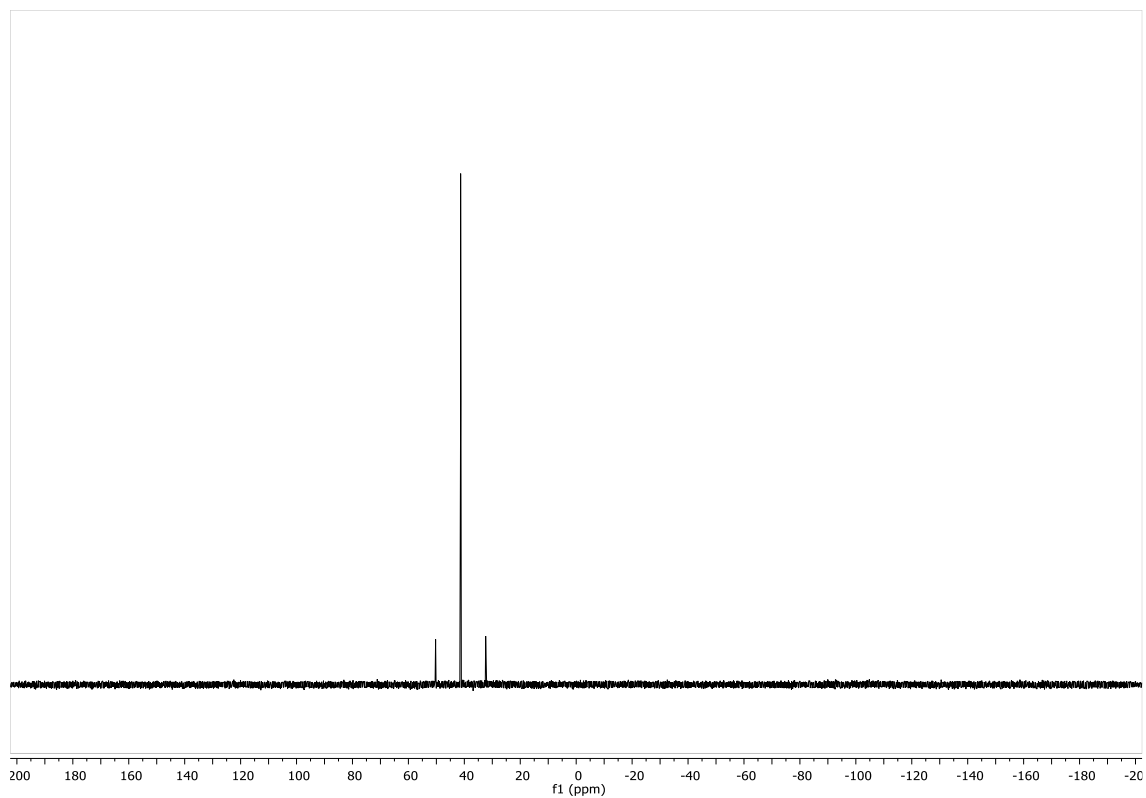


Figure S37. ^{31}P NMR spectrum of complex **20** in DMSO-d_6 .

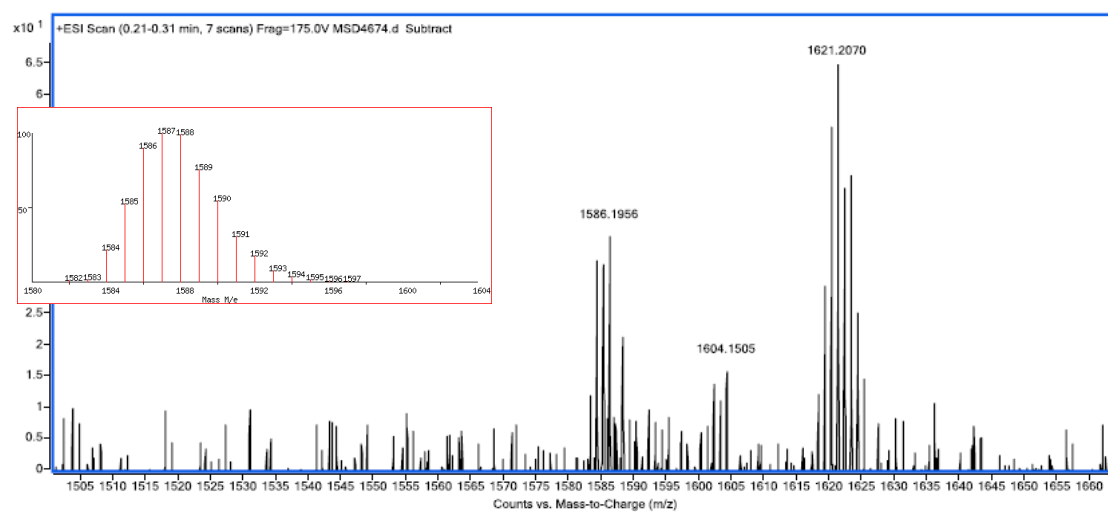


Figure S38. ESI-TOF(+) of complex **20**. Inset: calculated isotopic pattern.

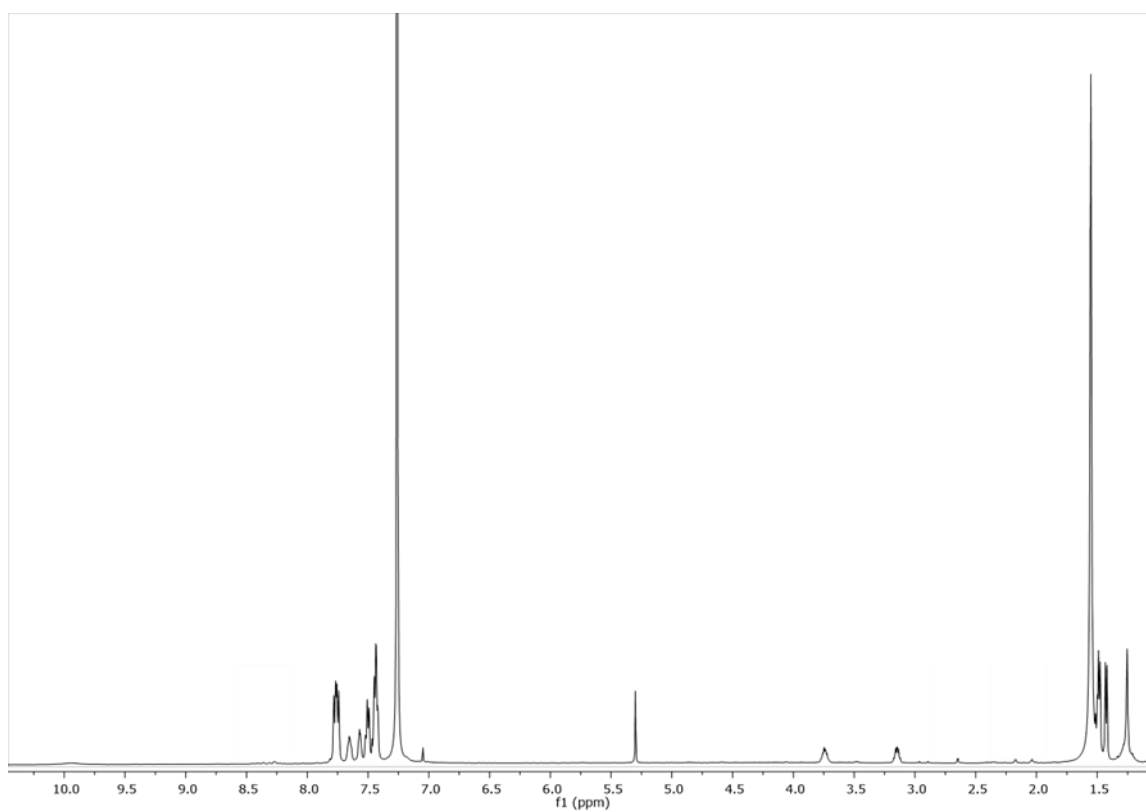


Figure S39. ¹H NMR spectrum of complex **21** in DMSO-d⁶.

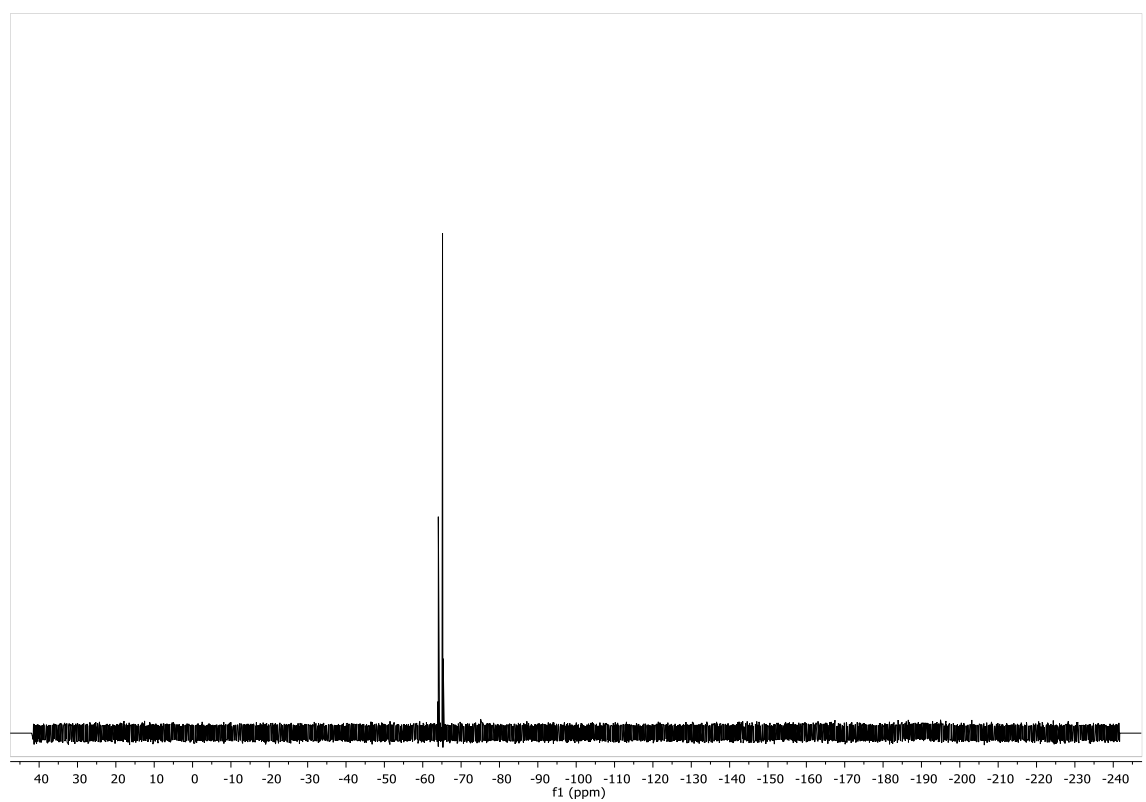


Figure S40. ¹⁹F NMR spectrum of complex **21** in DMSO-d⁶.

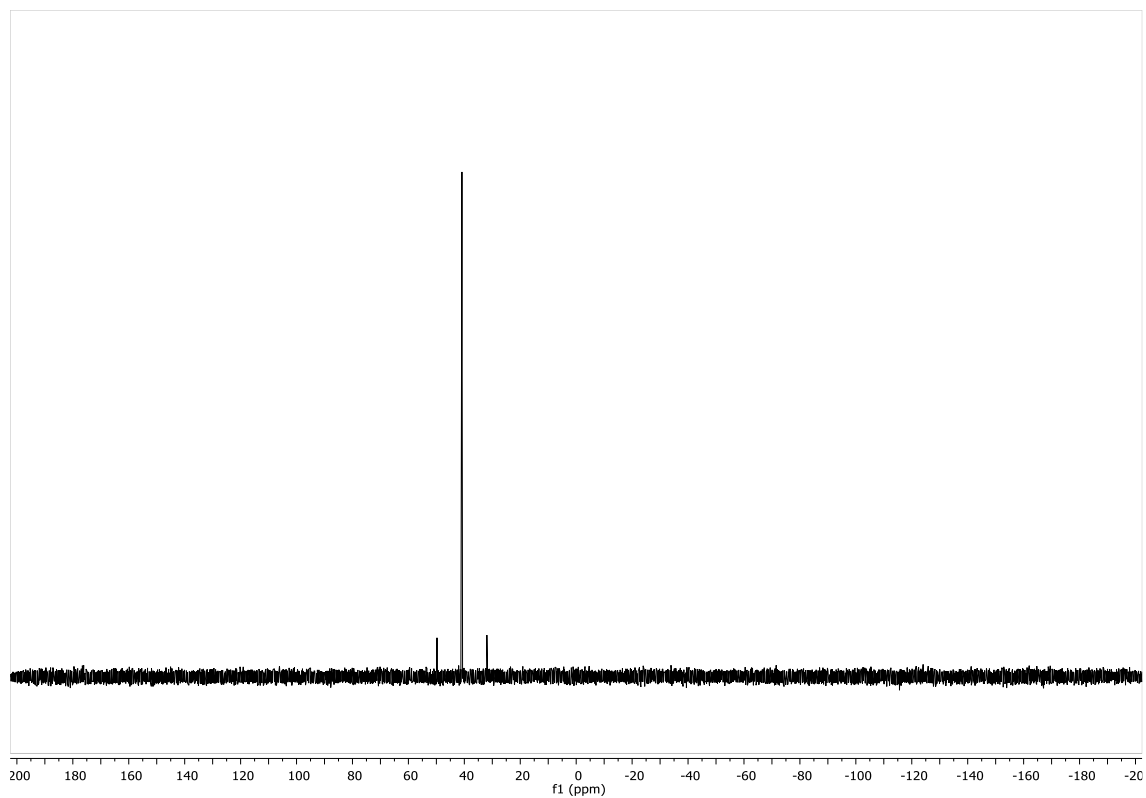


Figure S41. ^{31}P NMR spectrum of complex **21** in DMSO-d_6 .

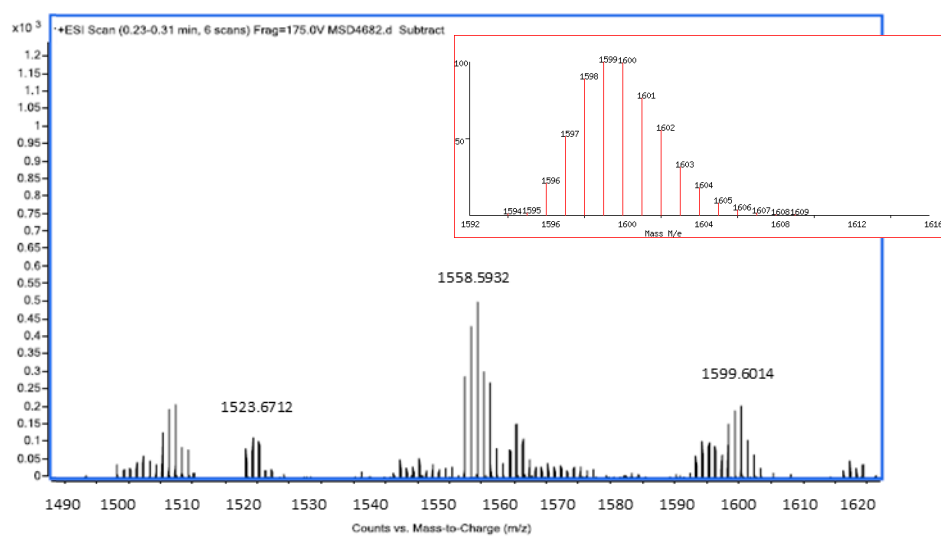


Figure S42. ESI-TOF(+) of complex **21**. Inset: calculated isotopic pattern.

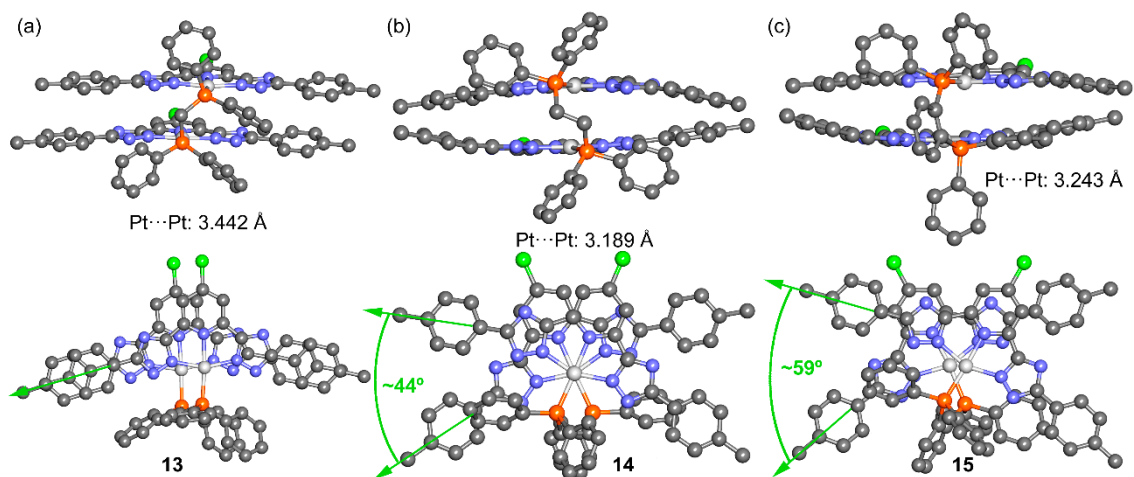


Figure S43. Ball and stick representation of the minimum energy geometries using two orientations calculated for compounds **13-15** at the RI-BP86-D3/def2-TZVP level of theory. The Pt···Pt distance is also indicated.

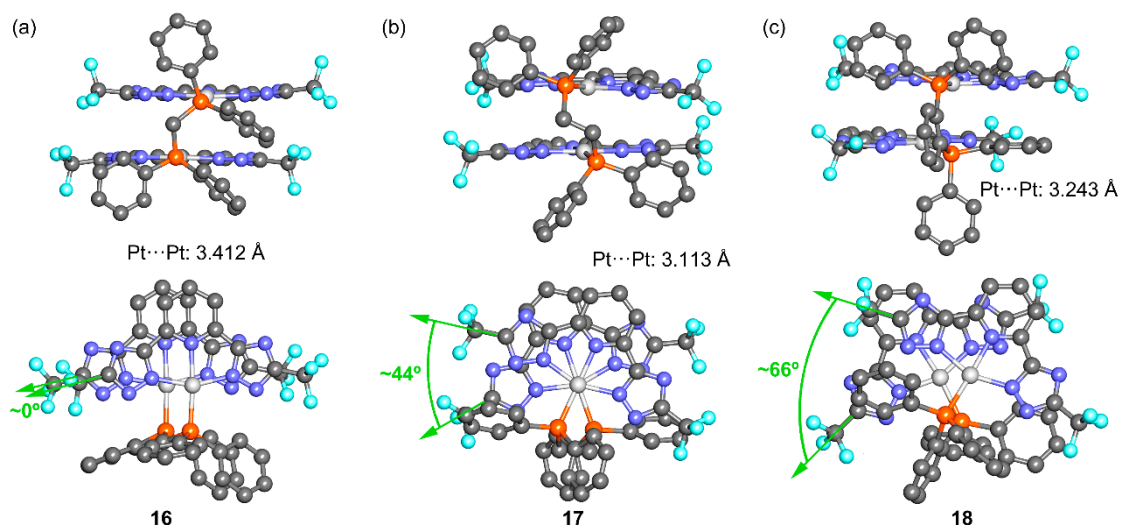


Figure S44. Ball and stick representation of the minimum energy geometries using two orientations calculated for compounds **16-18** at the RI-BP86-D3/def2-TZVP level of theory. The Pt···Pt distance is also indicated.

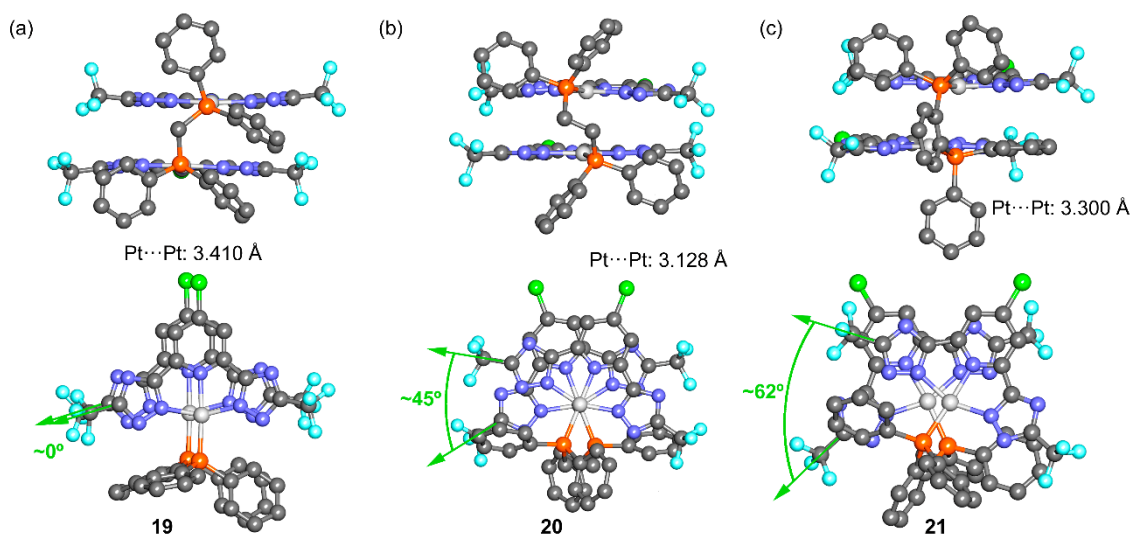


Figure S45. Ball and stick representation of the minimum energy geometries using two orientations calculated for compounds **19-21** at the RI-BP86-D3/def2-TZVP level of theory. The Pt...Pt distance is also indicated.

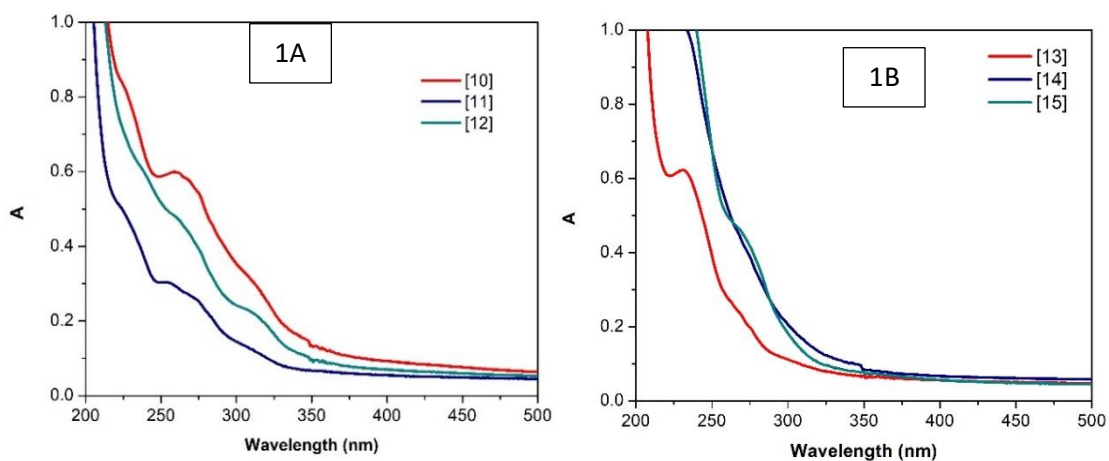


Figure S46. Absorption spectra of 10^{-5} M acetonitrile air-equilibrated solutions of compounds **10-12** (1A) and **13-15** (1B).

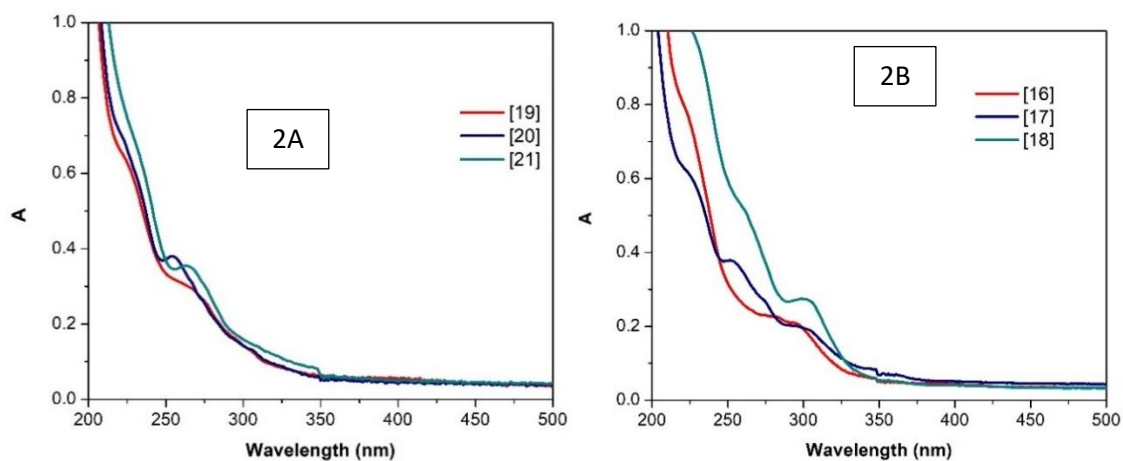


Figure S47. Absorption spectra of 10^{-5} M acetonitrile air-equilibrated solutions of compounds **16-18** (2A) and **19-21** (2B).

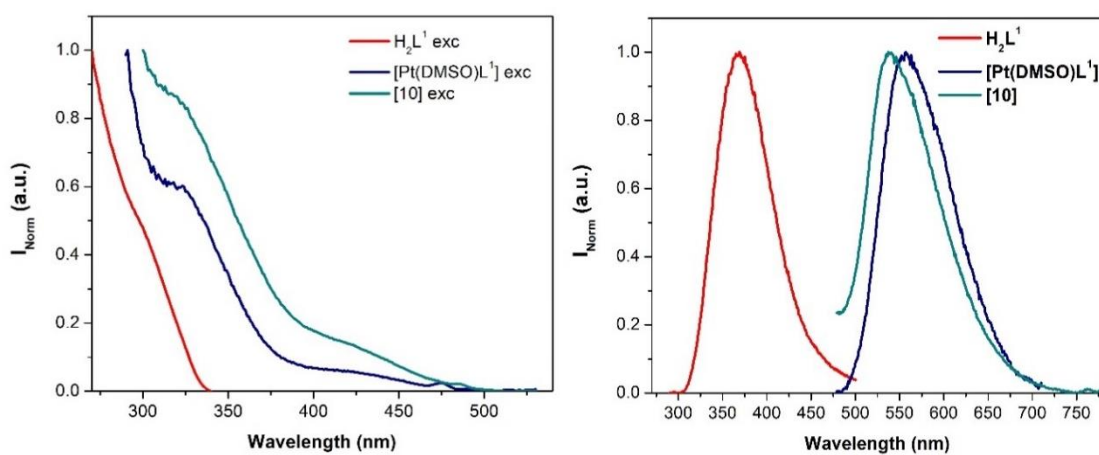


Figure S48. Normalized excitation (5A) and emission (5B) spectra of H_2L^1 , $[\text{Pt}(\text{DMSO})\text{L}^1]$ and **10** compounds in acetonitrile 10^{-5} M air-eq solutions ($\lambda_{\text{exc}} = 280$ and 400 nm respectively).

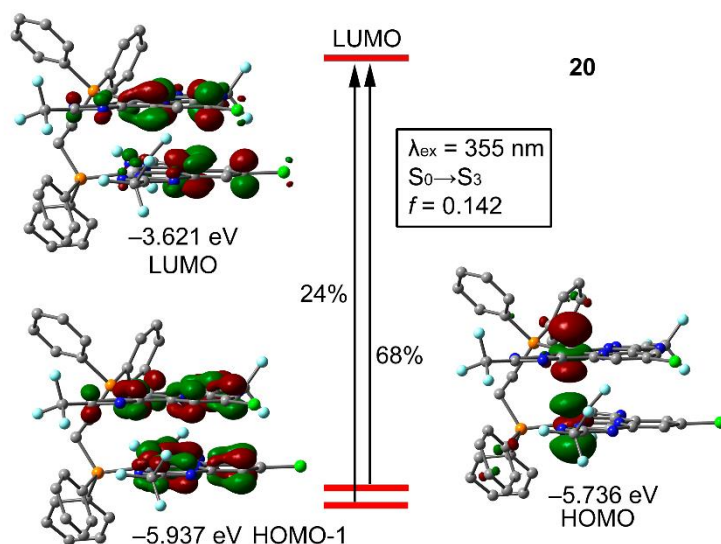


Figure S49. Representation of the MOs involved in the $S_0 \rightarrow S_3$ excitation of compound **20**, with indication of the theoretical λ_{exc} , oscillator strength and relative contribution of each transition.

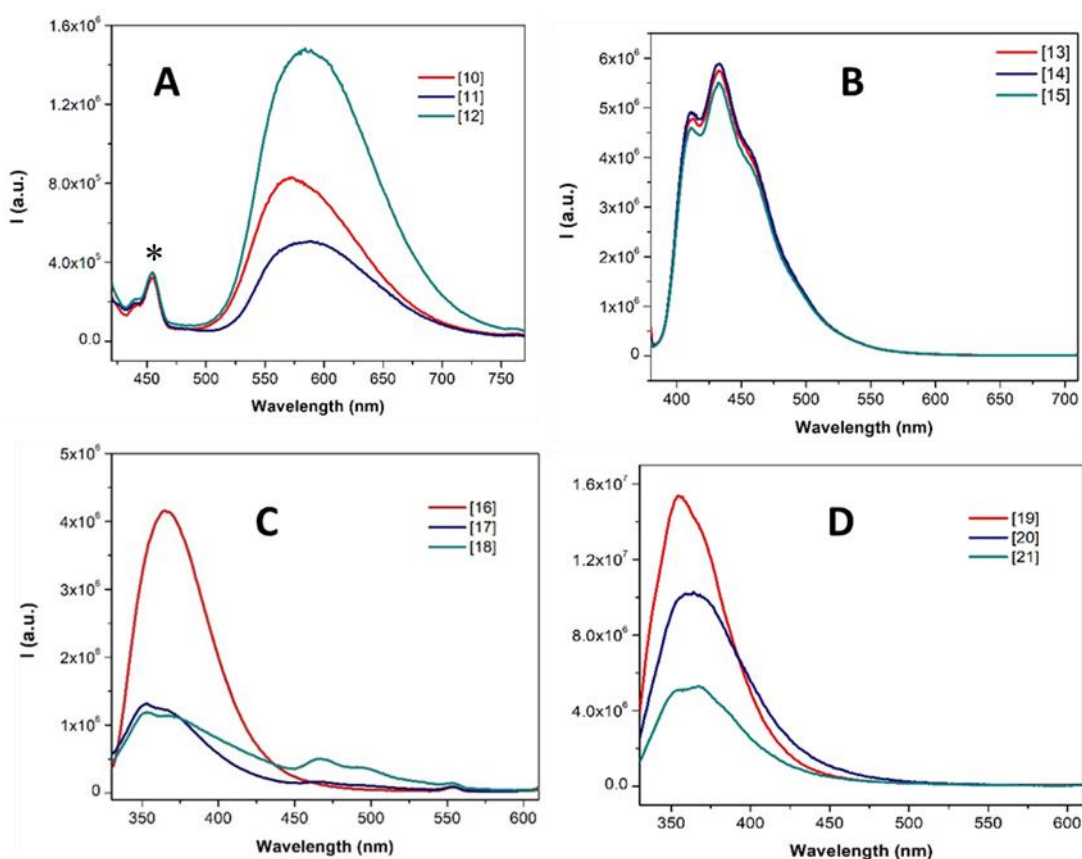


Figure S50. Emission spectra of the compounds in air-equilibrated $1 \cdot 10^{-5} \text{ M}$ acetonitrile solutions. * Indicates residual of the Raman band.

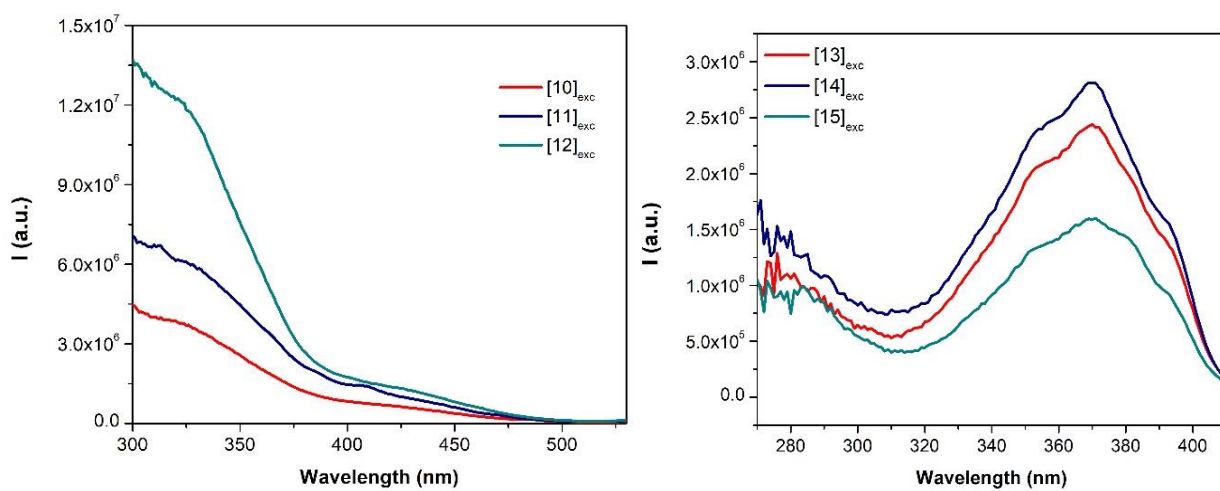


Figure S51. Excitation spectra of compounds **10-15** collected at the emission maxima.

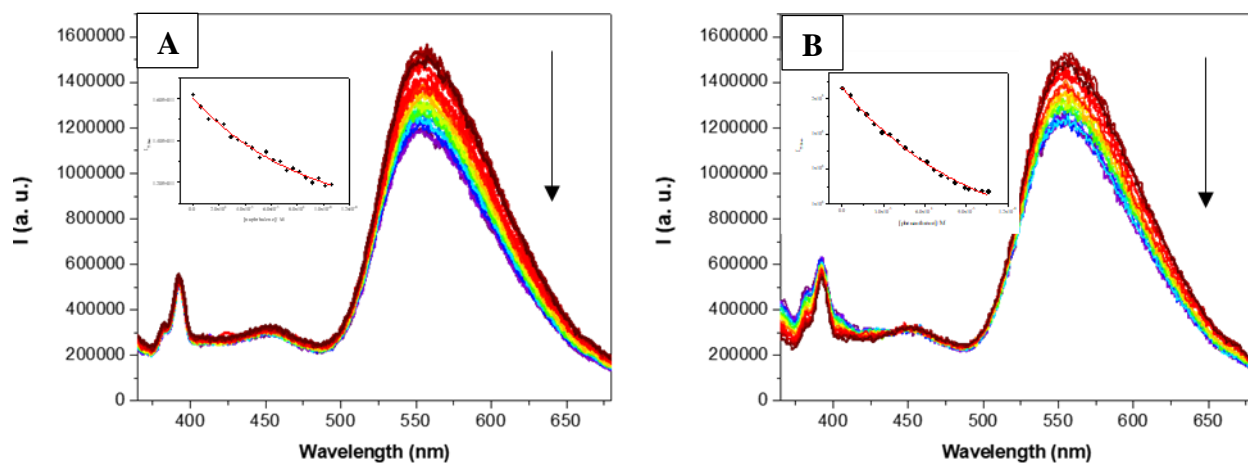


Figure S52. Emission spectra of compound **11** in the presence of different amounts of anthracene (A) and phenanthrene (B) in acetonitrile at room temperature. $\lambda_{\text{exc}} = 350$ nm.

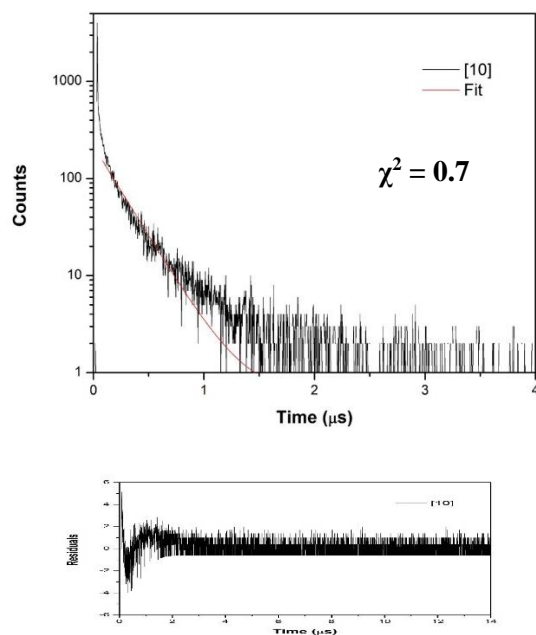


Figure S53. Phosphorescence lifetime and residuals of **10** in acetonitrile solution.

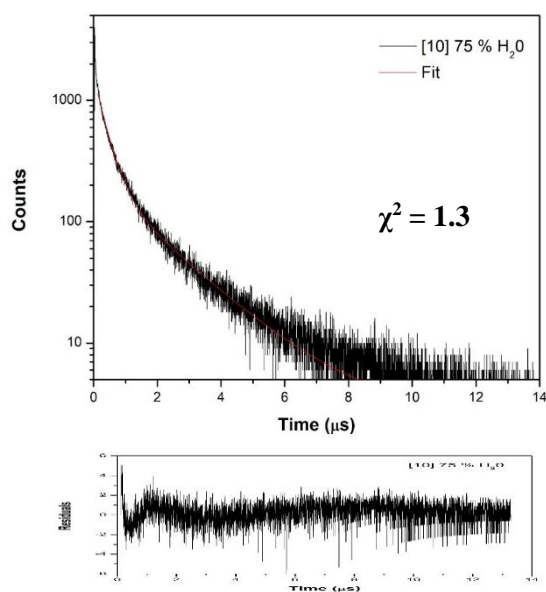


Figure S54. Phosphorescence lifetime and residuals of **10** in 25/75% acetonitrile/water solution.

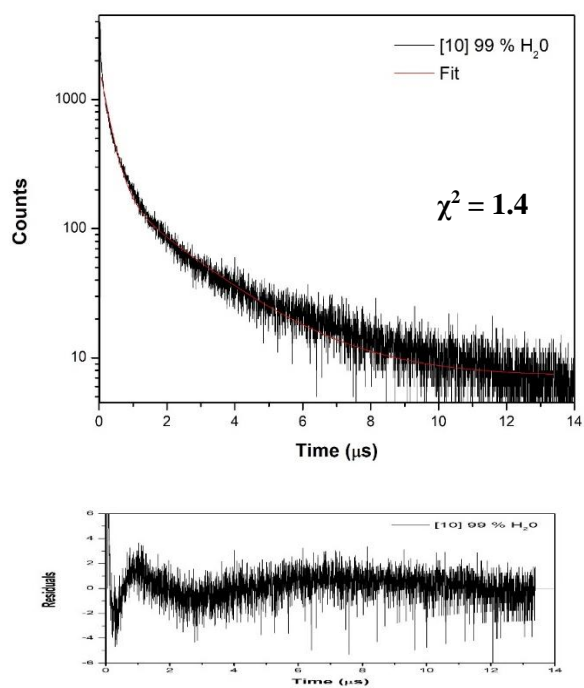


Figure S55. Phosphorescence lifetime and residuals of **10** in 1/99% acetonitrile/water solution.

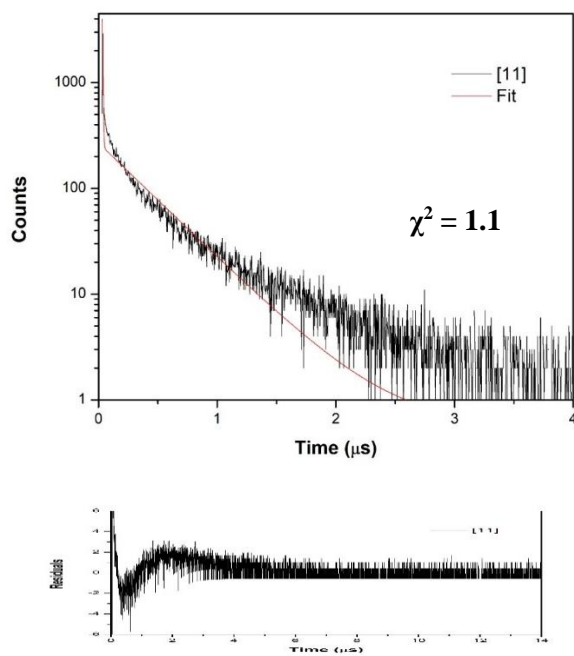


Figure S56. Phosphorescence lifetime and residuals of **11** in acetonitrile solution.

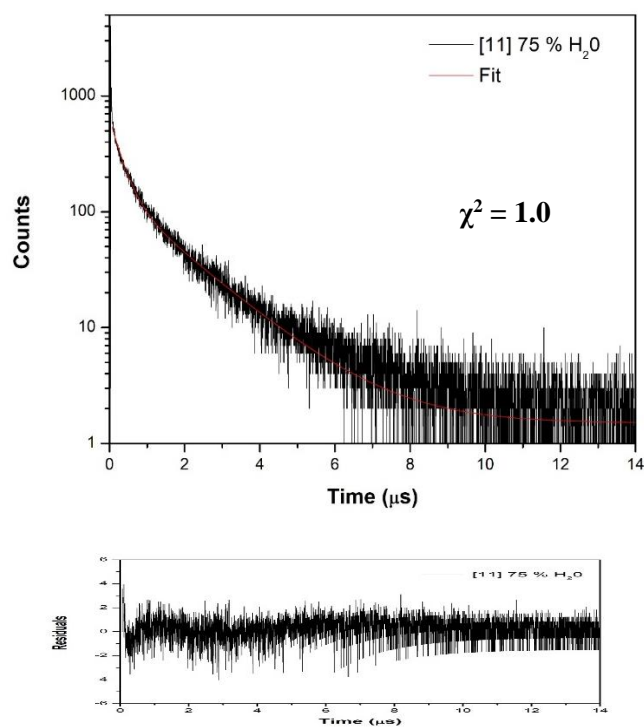


Figure S57. Phosphorescence lifetime and residuals of **11** in 25/75% acetonitrile/water solution.

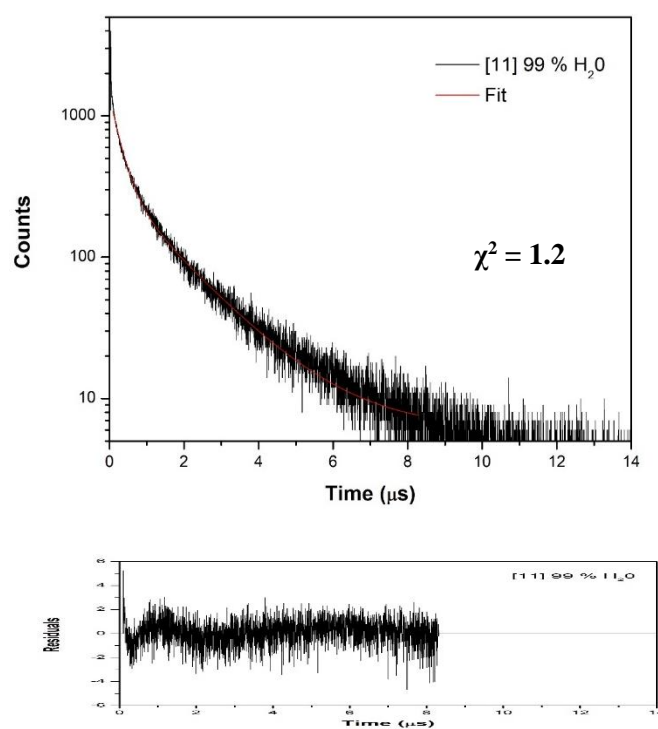


Figure S58. Phosphorescence lifetime and residuals of **11** in 1/99% acetonitrile/water solution.

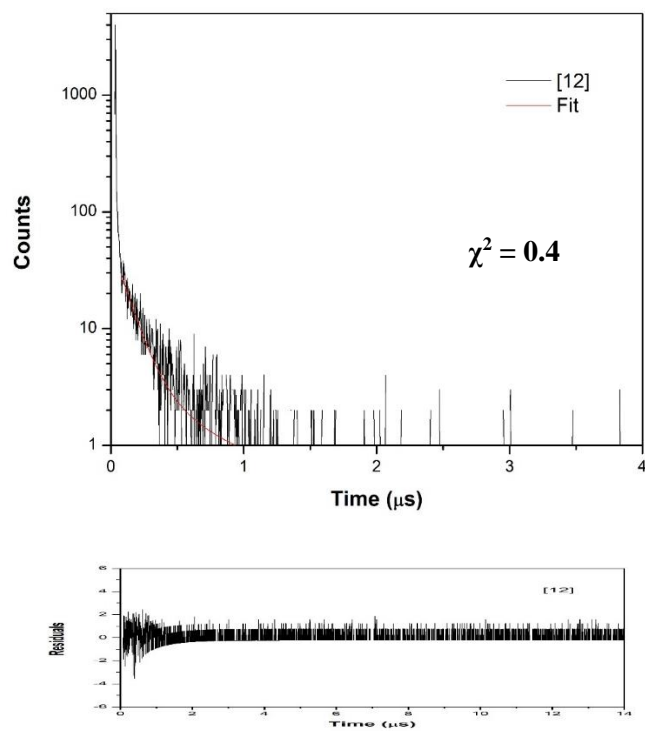


Figure S59. Phosphorescence lifetime and residuals of **12** in acetonitrile solution.

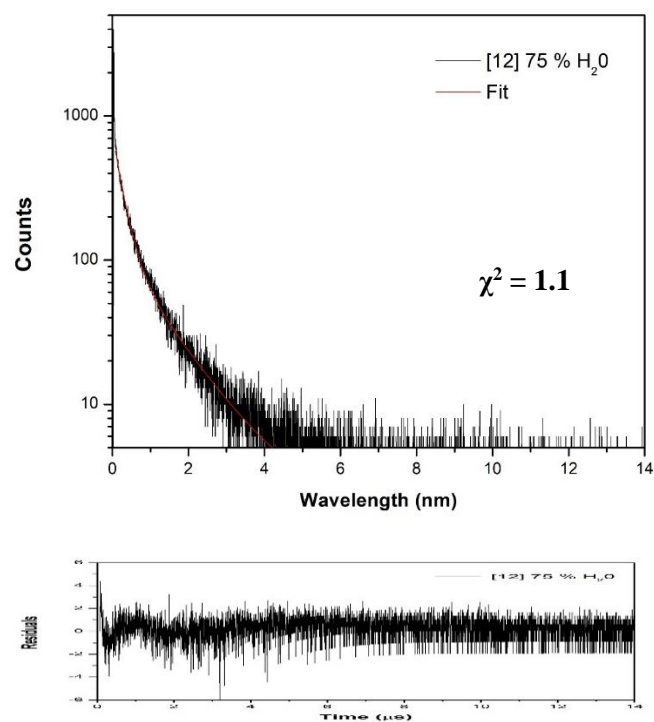


Figure S60. Phosphorescence lifetime and residuals of **12** in 25/75% acetonitrile/water solution.

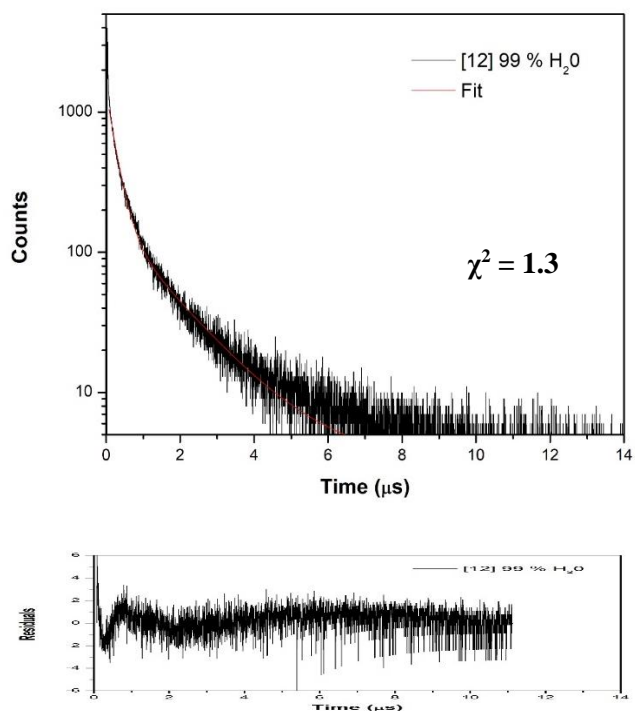


Figure S61. Phosphorescence lifetime and residuals of **12** in 1/99% acetonitrile/water solution.

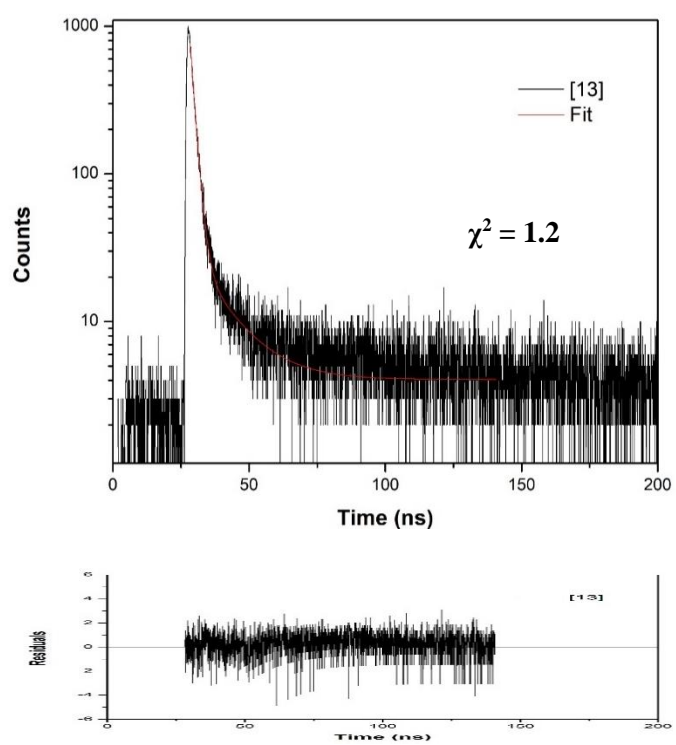


Figure S62. Fluorescence lifetime and residuals of **13** in acetonitrile solution.

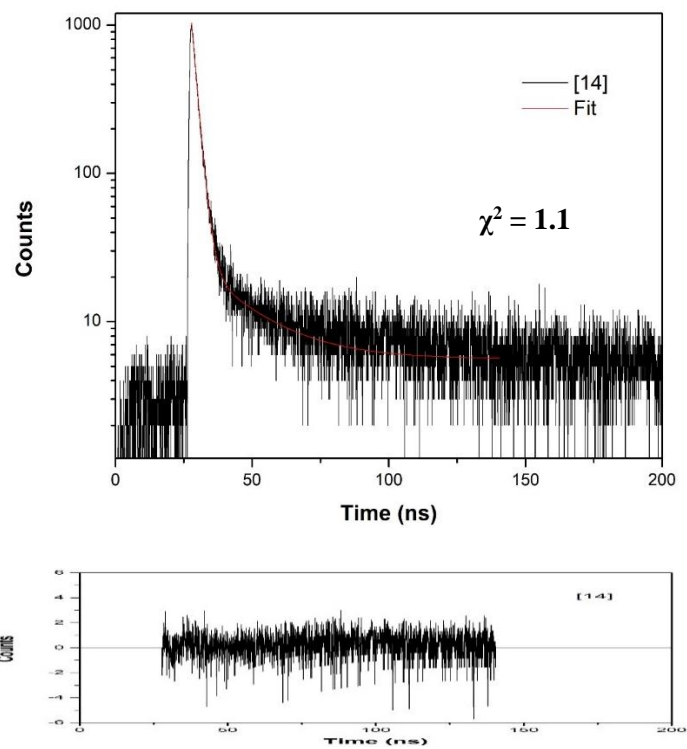


Figure S63. Fluorescence lifetime and residuals of **14** in acetonitrile solution.

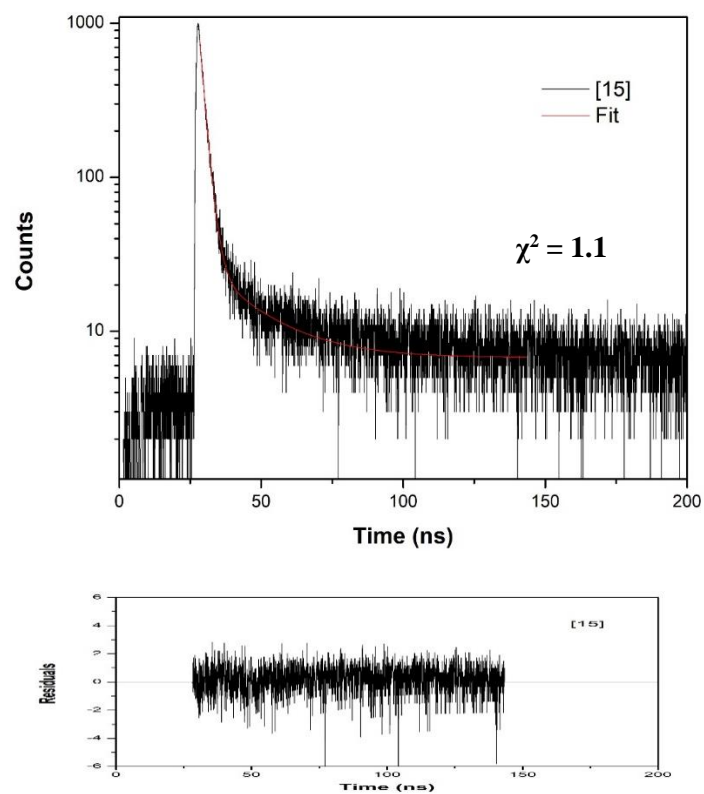


Figure S64. Fluorescence lifetime and residuals of **15** in acetonitrile solution.

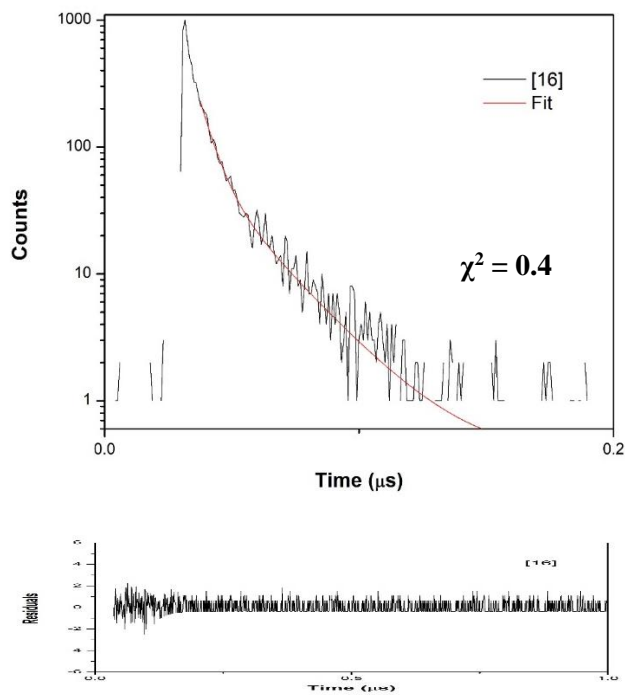


Figure S65. Phosphorescence lifetime and residuals of **16** in acetonitrile solution.

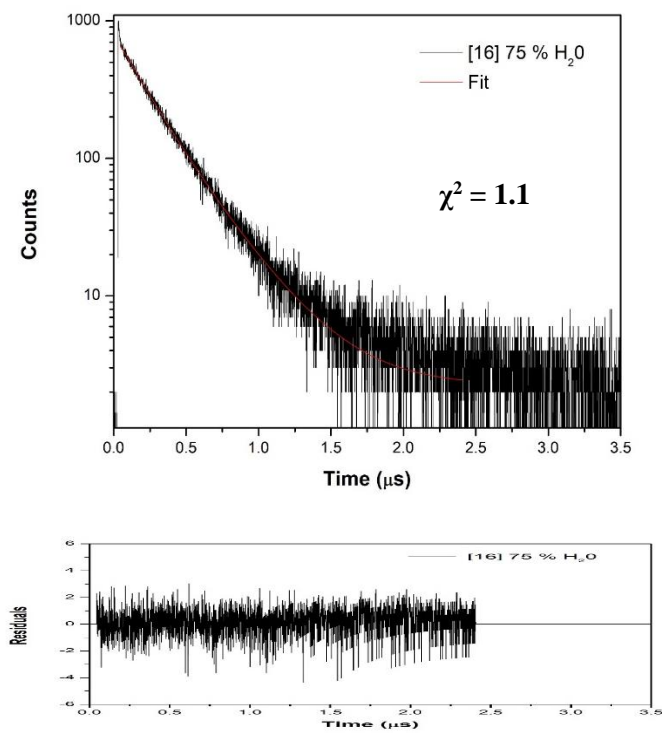


Figure S66. Phosphorescence lifetime and residuals of **16** in 25/75% acetonitrile/water solution.

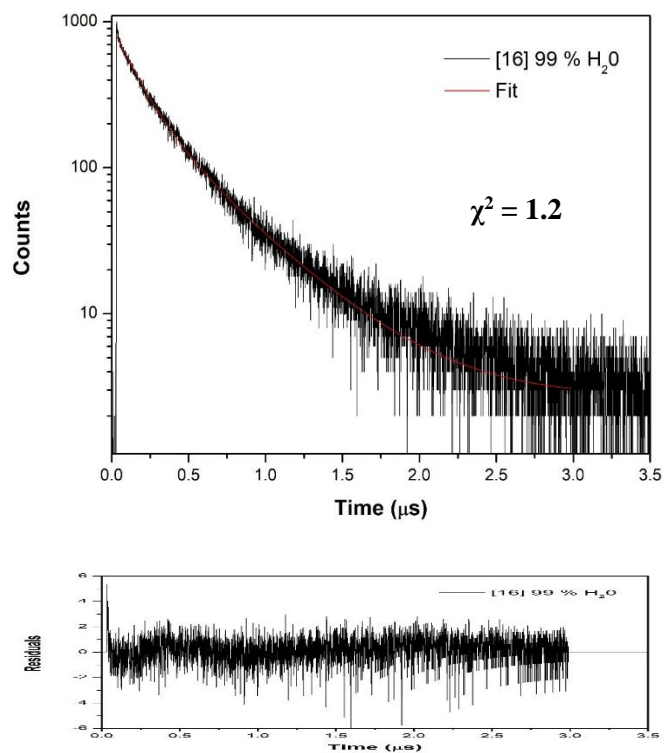


Figure S67. Phosphorescence lifetime and residuals of **16** in 1/99% acetonitrile/water solution.

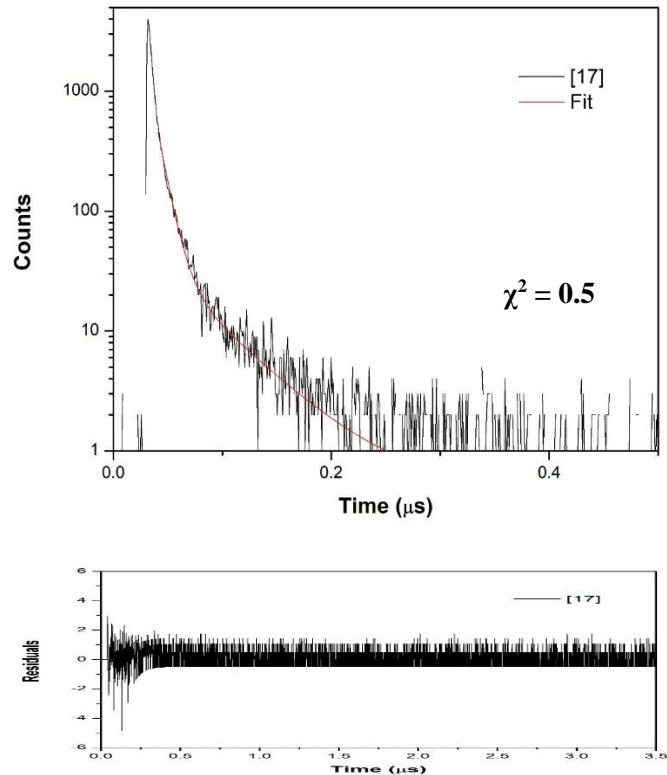


Figure S68. Phosphorescence lifetime and residuals of **17** in acetonitrile solution.

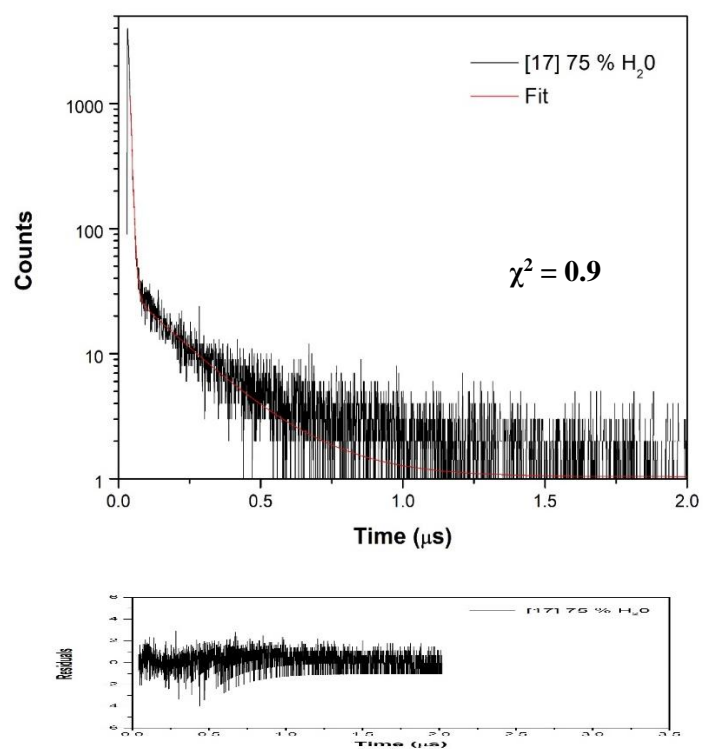


Figure S69. Phosphorescence lifetime and residuals of **17** in 25/75% acetonitrile/water solution.

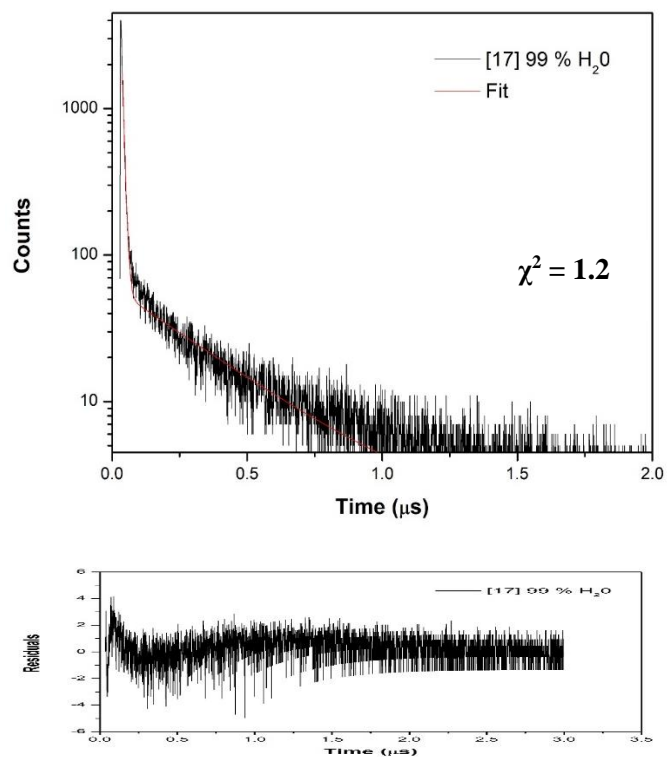


Figure S70. Phosphorescence lifetime and residuals of **17** in 1/99% acetonitrile/water solution.

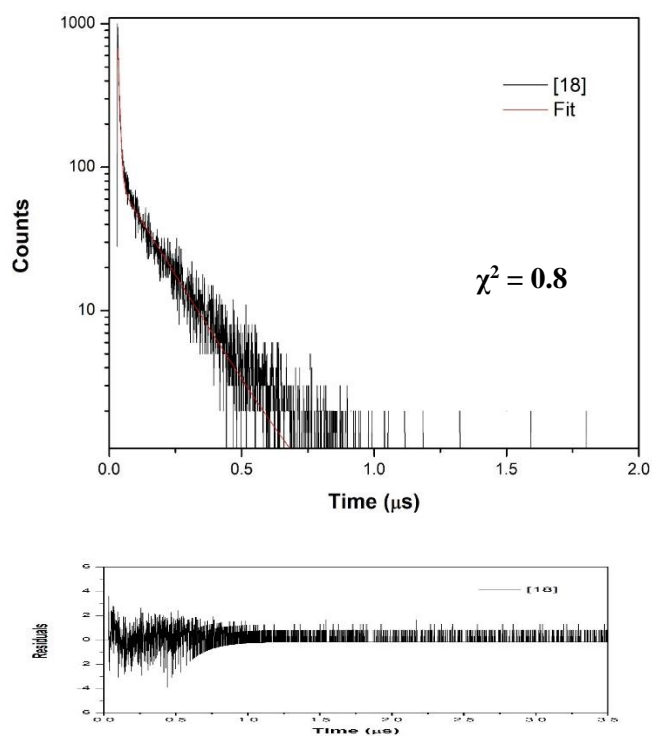


Figure S71. Phosphorescence lifetime and residuals of **18** in acetonitrile solution.

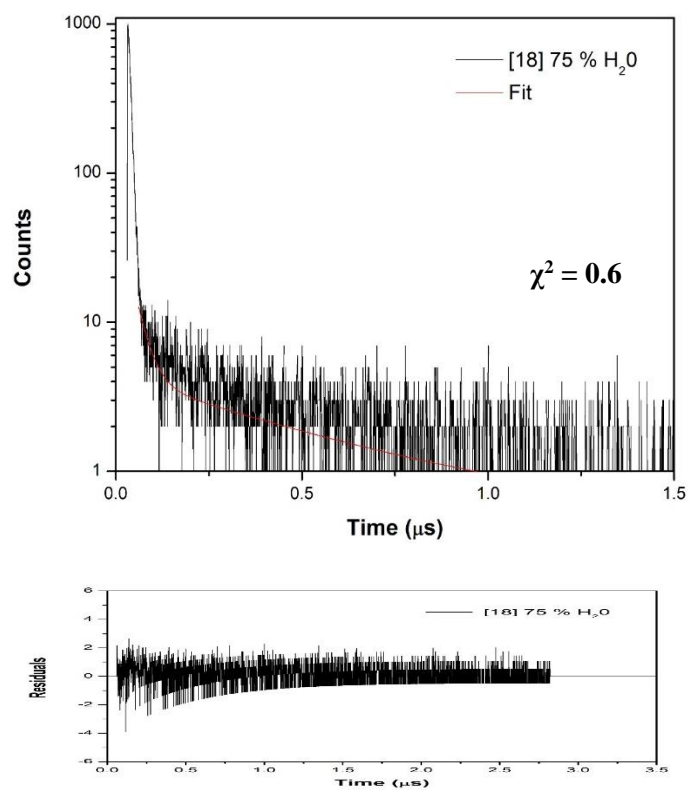


Figure S72. Phosphorescence lifetime and residuals of **18** in 25/75% acetonitrile/water solution.

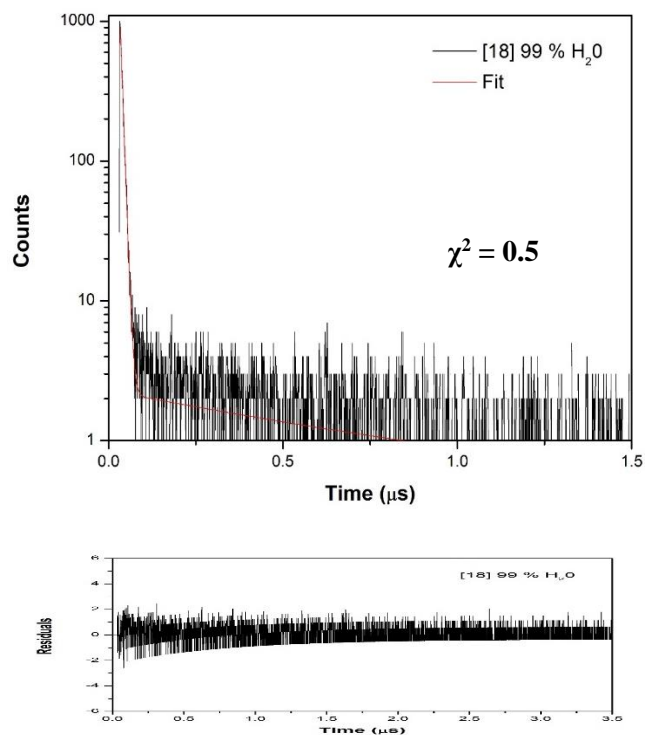


Figure S73. Phosphorescence lifetime and residuals of **18** in 1/99% acetonitrile/water solution.

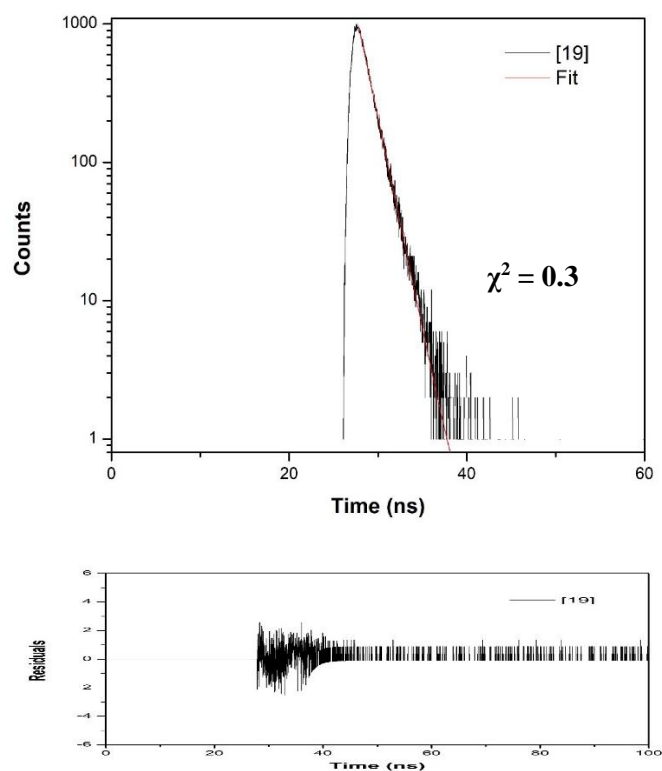


Figure S74. Fluorescence lifetime and residuals of **19** in acetonitrile solution.

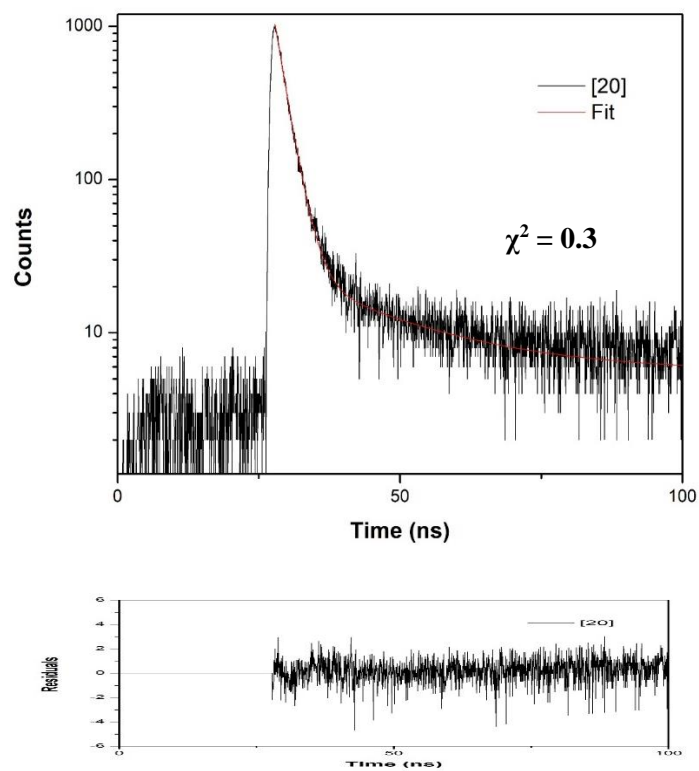


Figure S75. Fluorescence lifetime and residuals of **20** in acetonitrile solution.

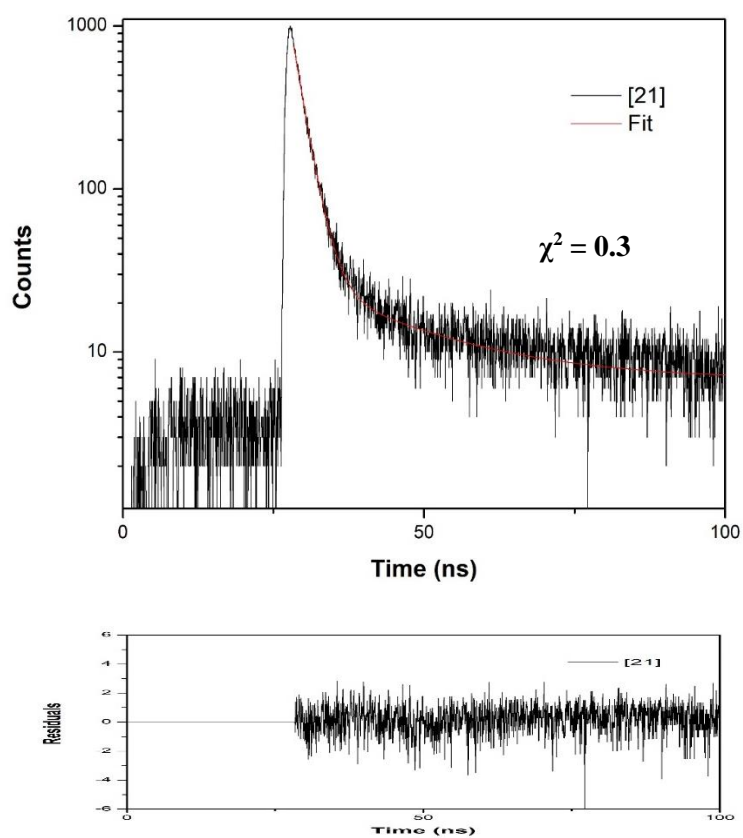


Figure S76. Fluorescence lifetime and residuals of **21** in acetonitrile solution.

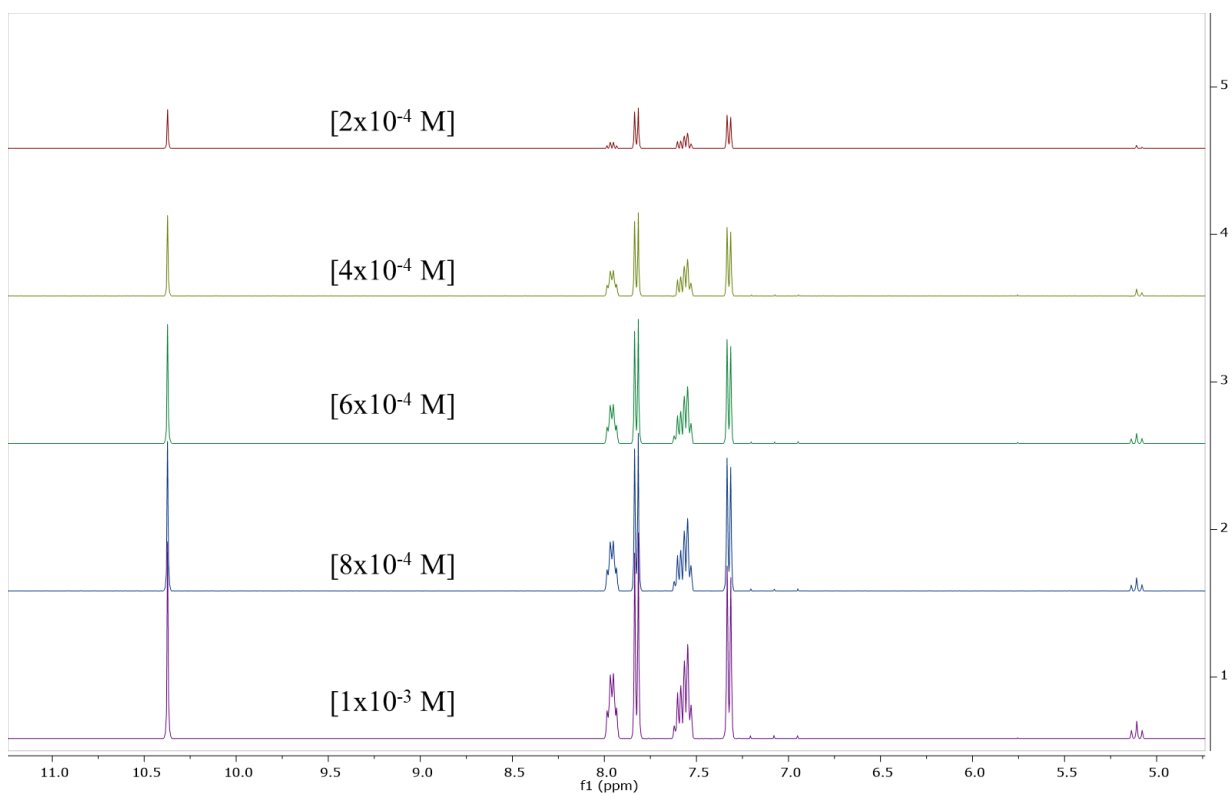


Figure S77. ^1H NMR spectra of complex **13** in DMSO-d_6 at different concentrations.

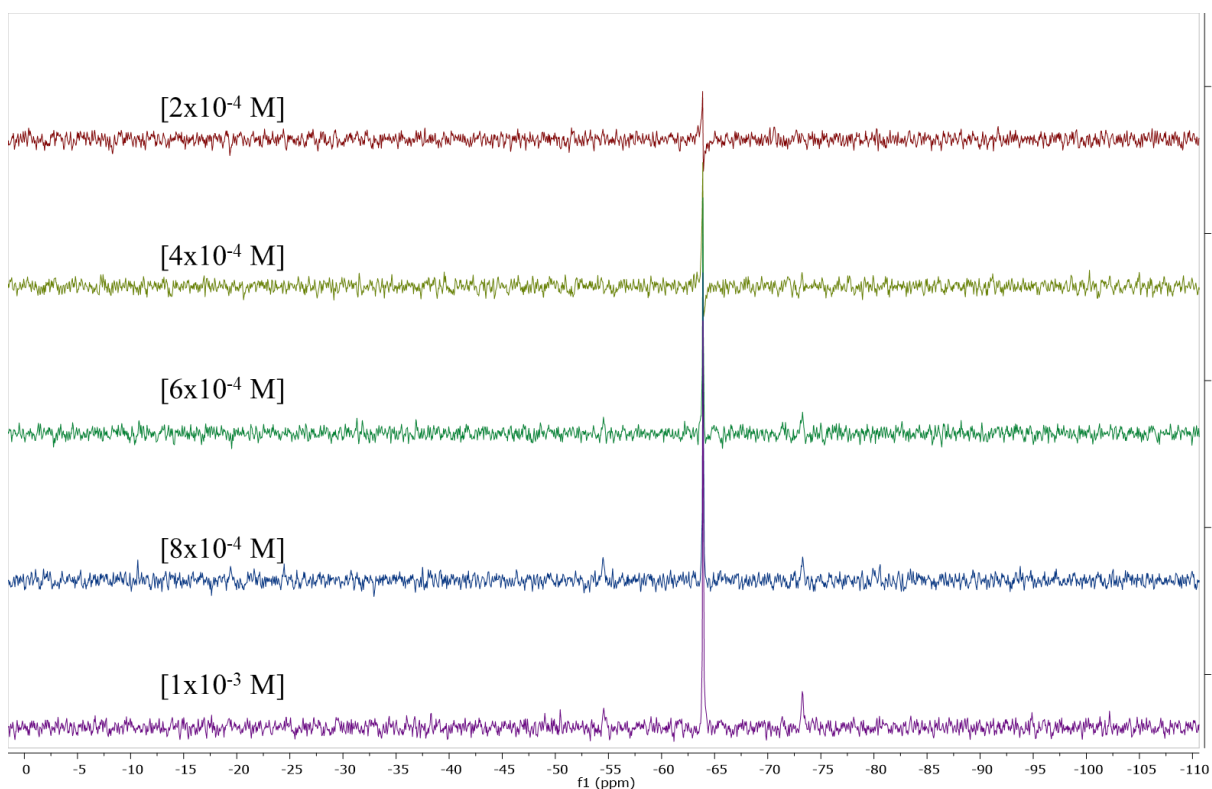


Figure S78. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of complex **13** in DMSO-d_6 at different concentrations.

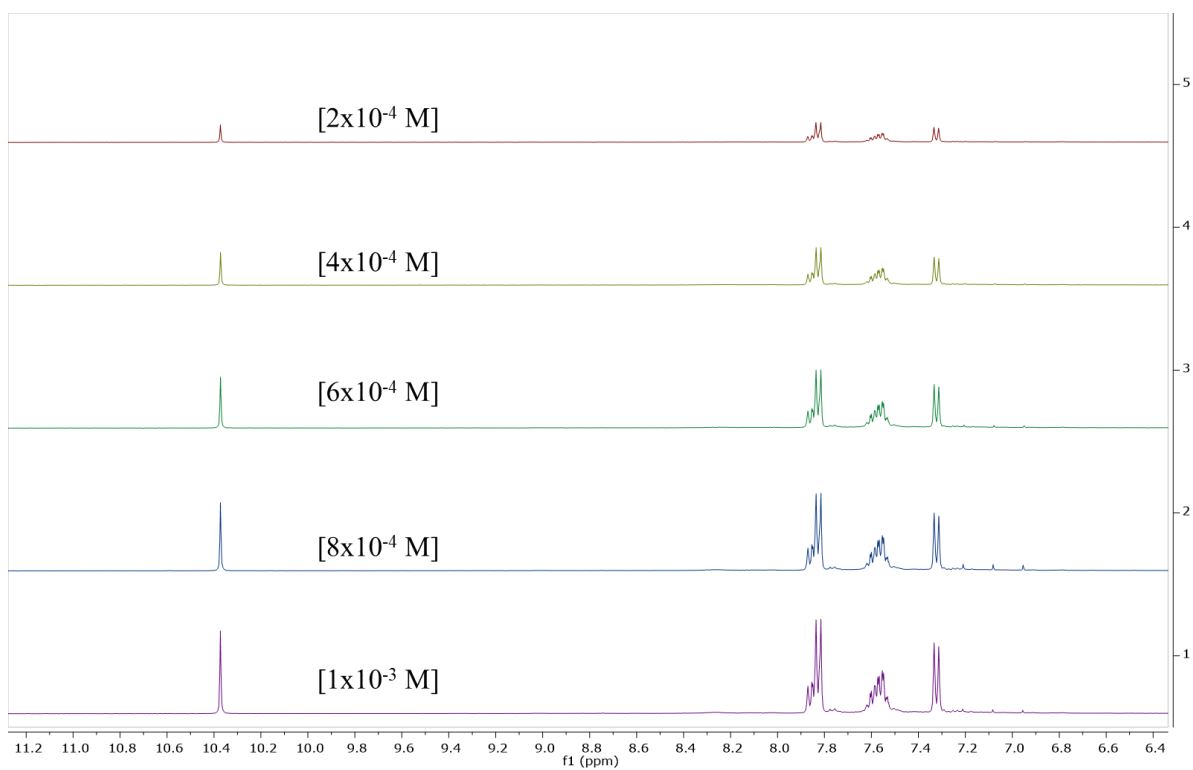


Figure S79. ^1H NMR spectra of complex **14** in DMSO-d_6 at different concentrations.

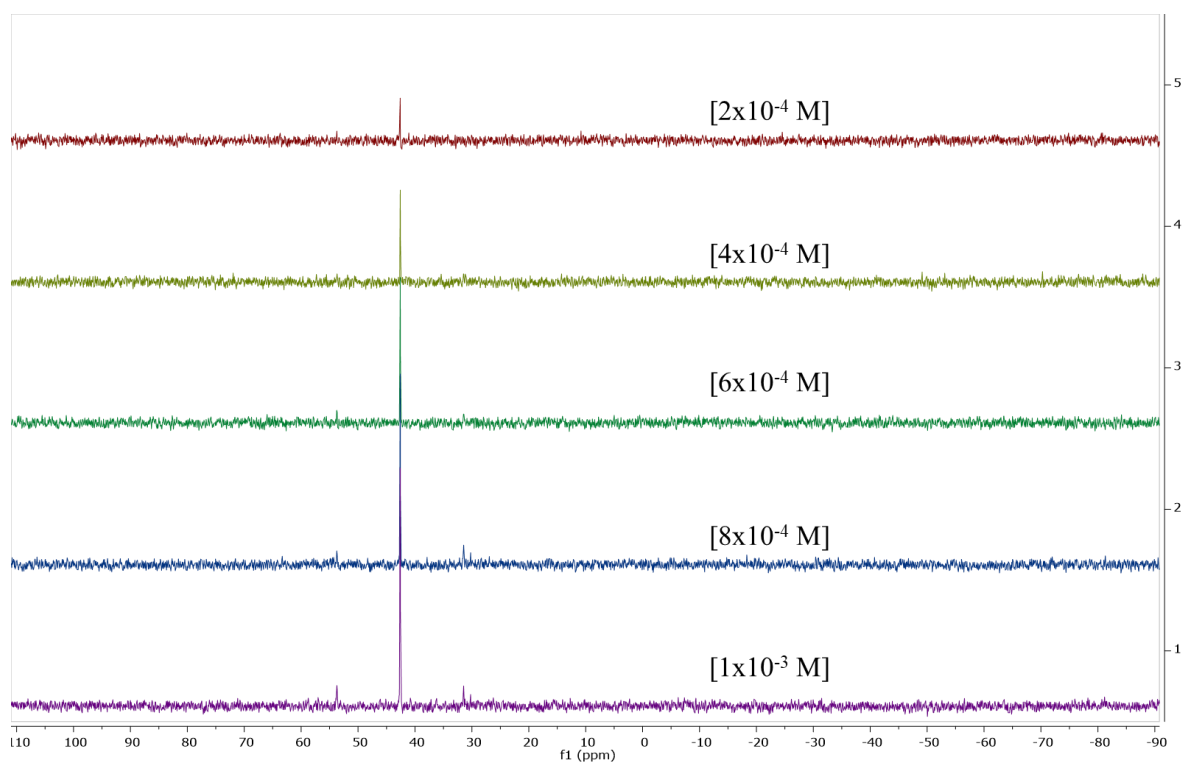


Figure S80. $^{31}\text{P}\{^1\text{H}\}$ spectra of complex **14** in DMSO-d_6 at different concentrations.

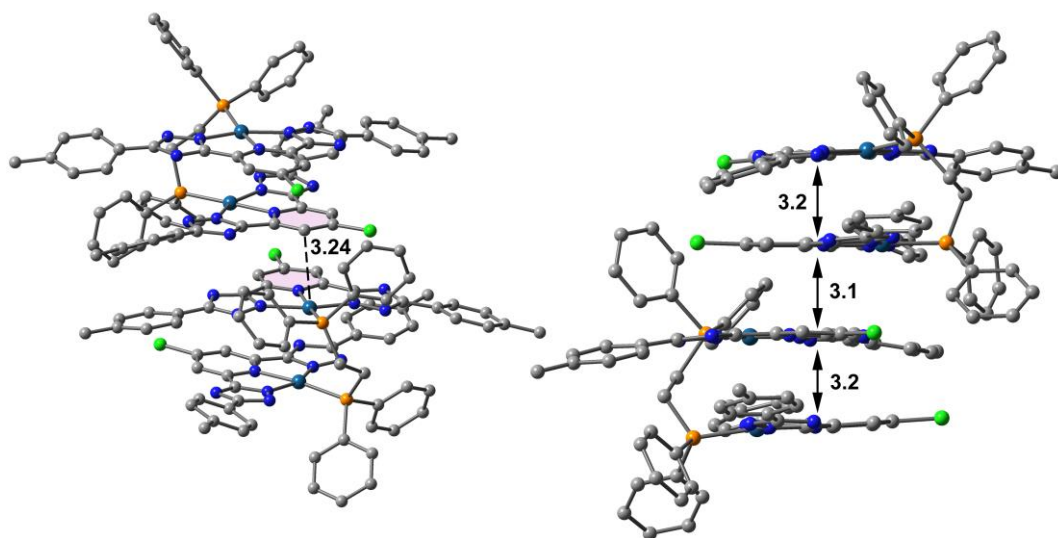


Figure S81. Calculated dimer assembly for compound **14**.

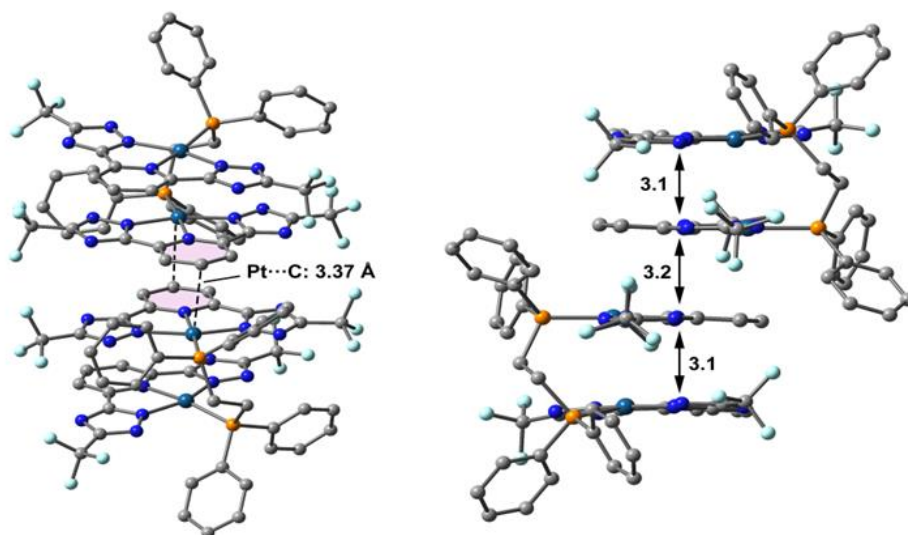


Figure S82. Calculated dimer assembly for compound **17**.

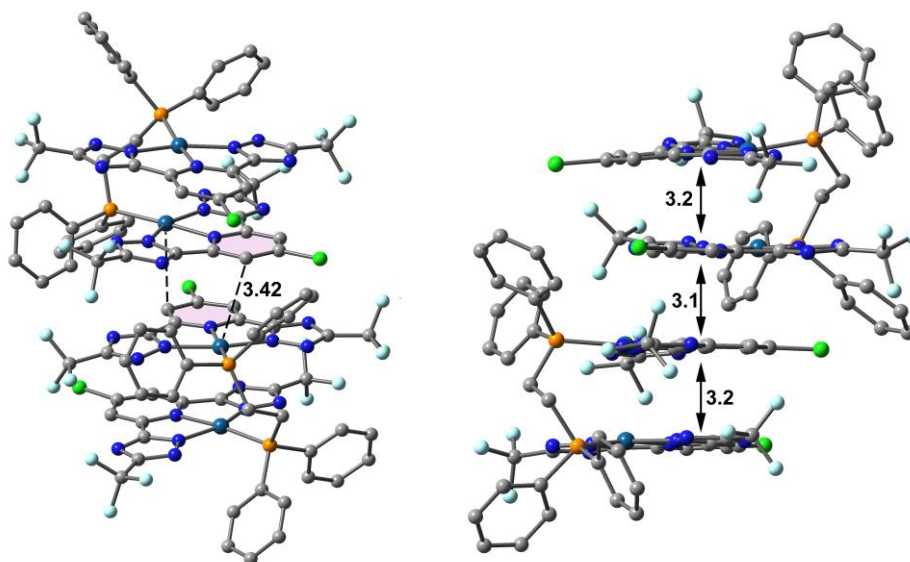


Figure S83. Calculated dimer assembly for compound **20**.

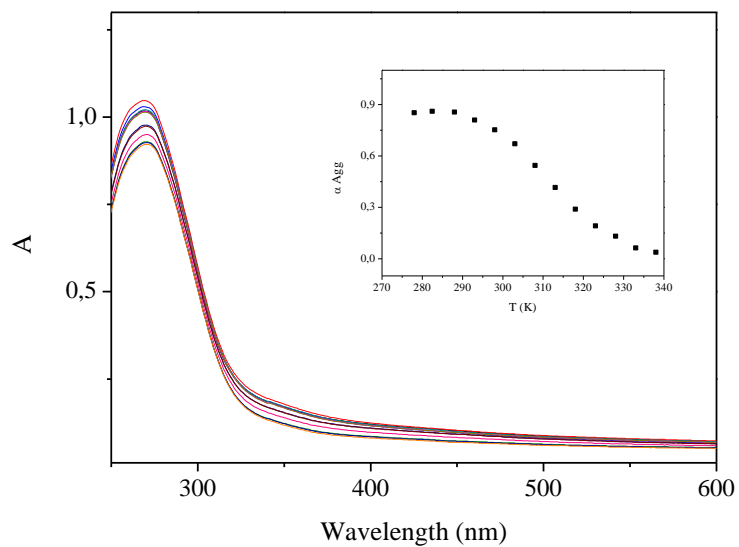


Figure S84. Absorption spectra of compound **11** recorded at different temperatures in acetonitrile. Inset: plot of the variation of the aggregation with temperature.

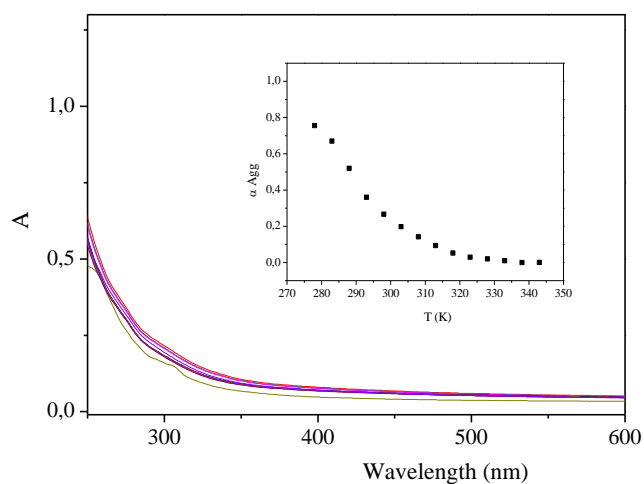


Figure S85. Absorption spectra of compound **14** recorded at different temperatures in acetonitrile. Inset: plot of the variation of the aggregation with temperature.

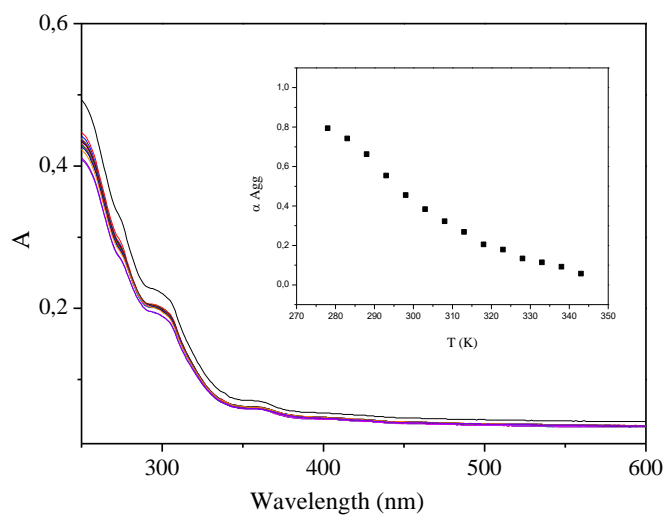


Figure S86. Absorption spectra of compound **17** recorded at different temperatures in acetonitrile. Inset: plot of the variation of the aggregation with temperature.

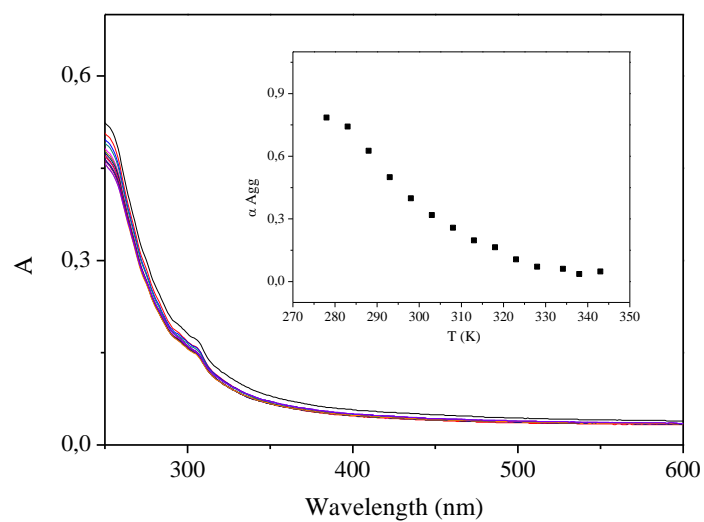


Figure S87. Absorption spectra of compound **20** recorded at different temperatures in acetonitrile. Inset: plot of the variation of the aggregation with temperature.

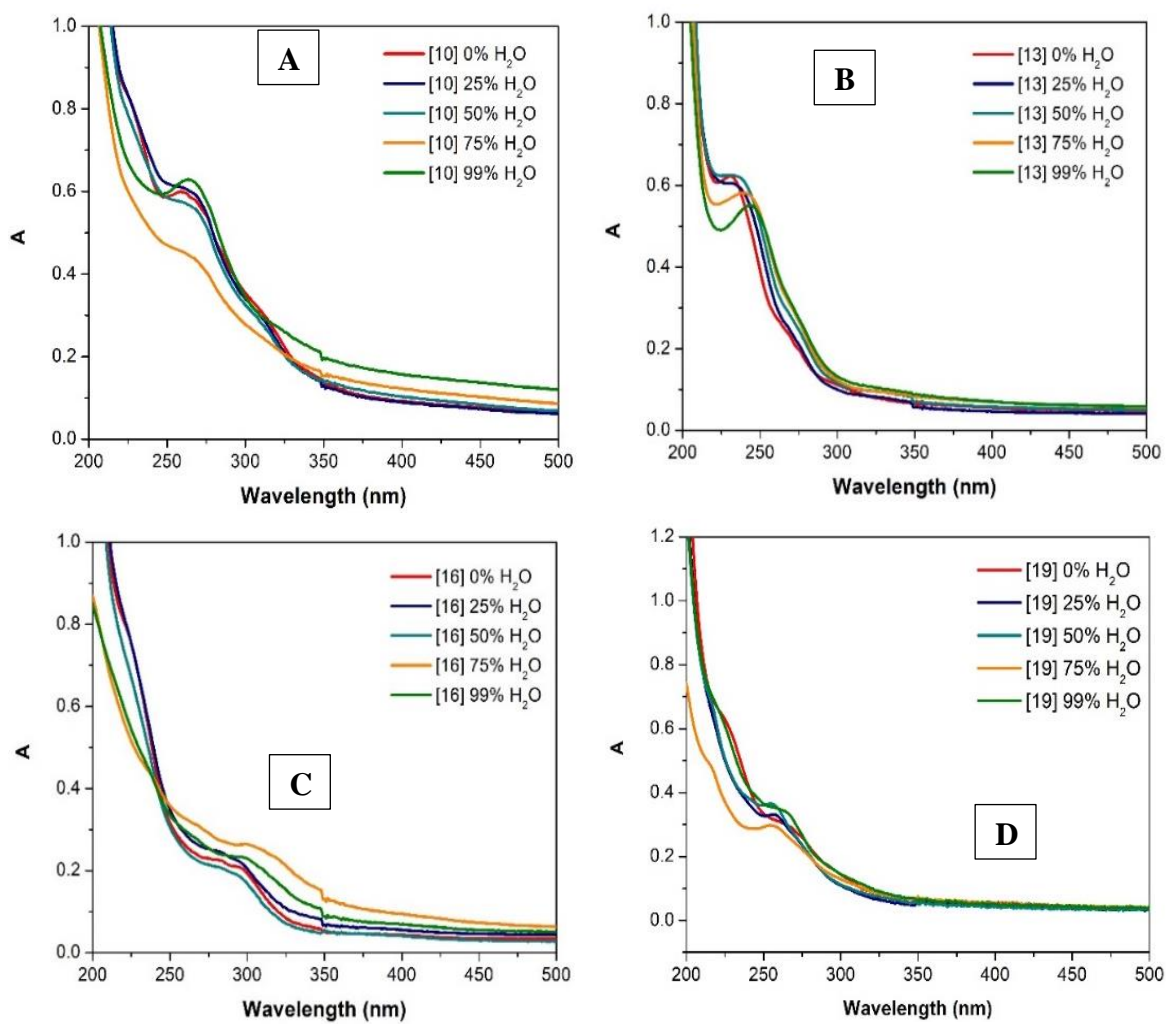


Figure S88.- Absorption spectra of the formed aggregates of **10**(12A), **13**(12B), **16**(12C), and **19**(12D) compounds in the function of the % of water in the samples.

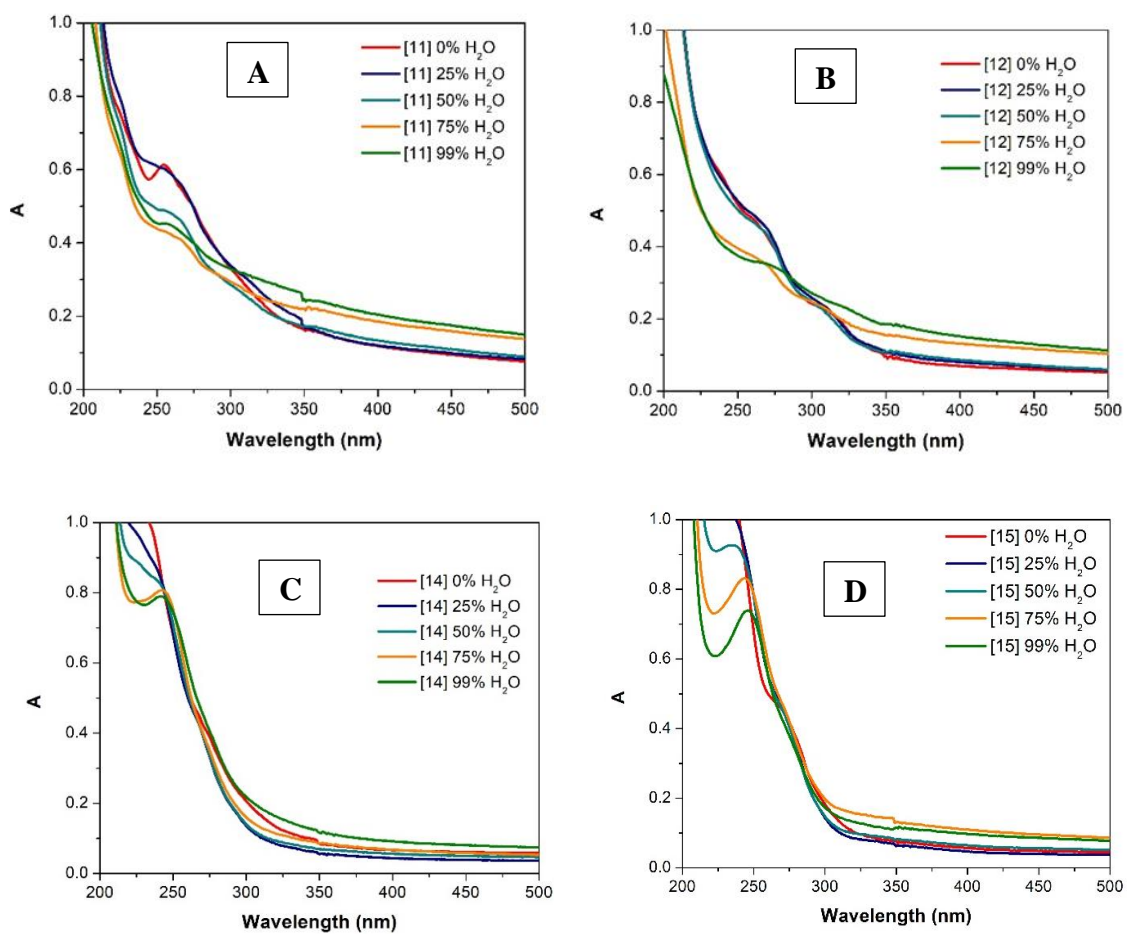


Figure S89.- Absorption spectra of the formed aggregates of **11**(A), **12**(B), **14**(C), **15**(D,) compounds in the function of the % of water in the samples.

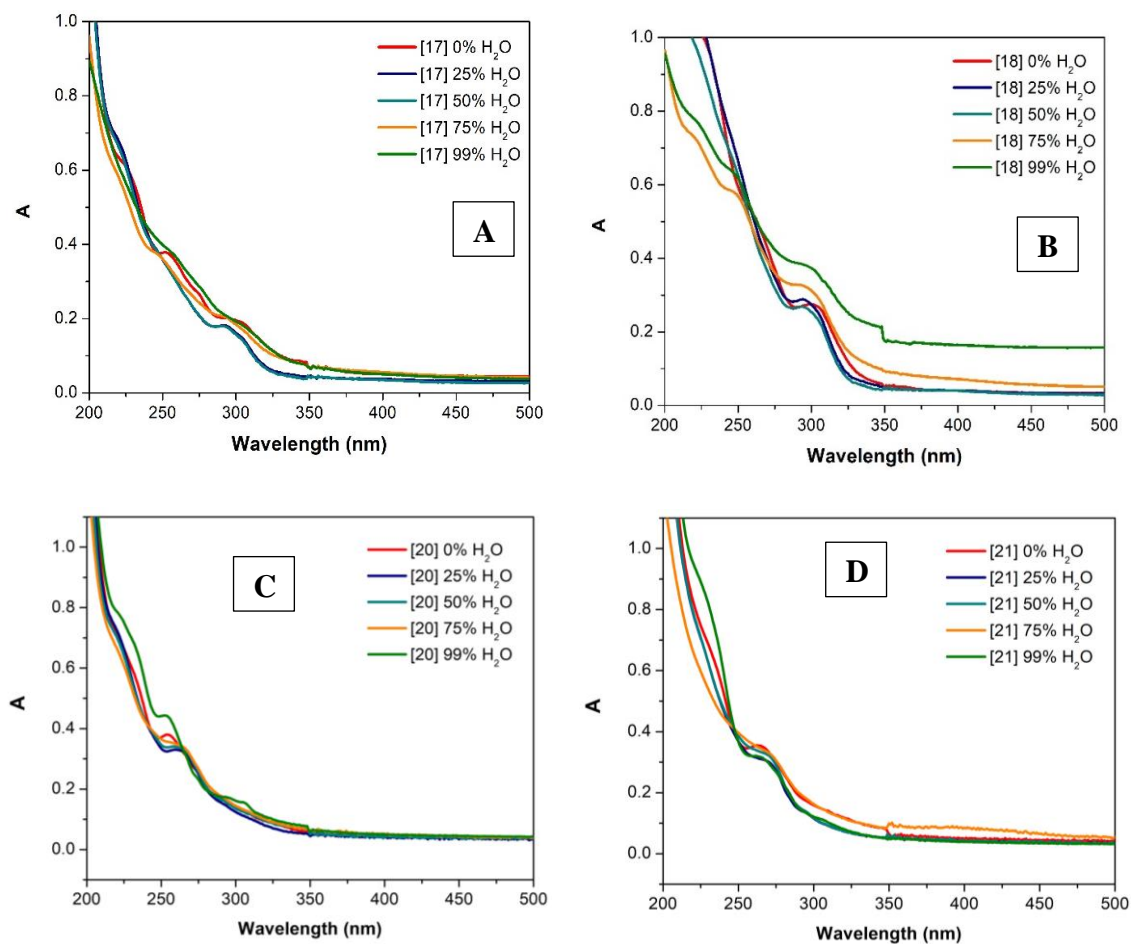


Figure S90.- Absorption spectra of the formed aggregates of **17**(A), **18** (B), **20** (C) and **21**(D) compounds in the function of the % of water in the samples.

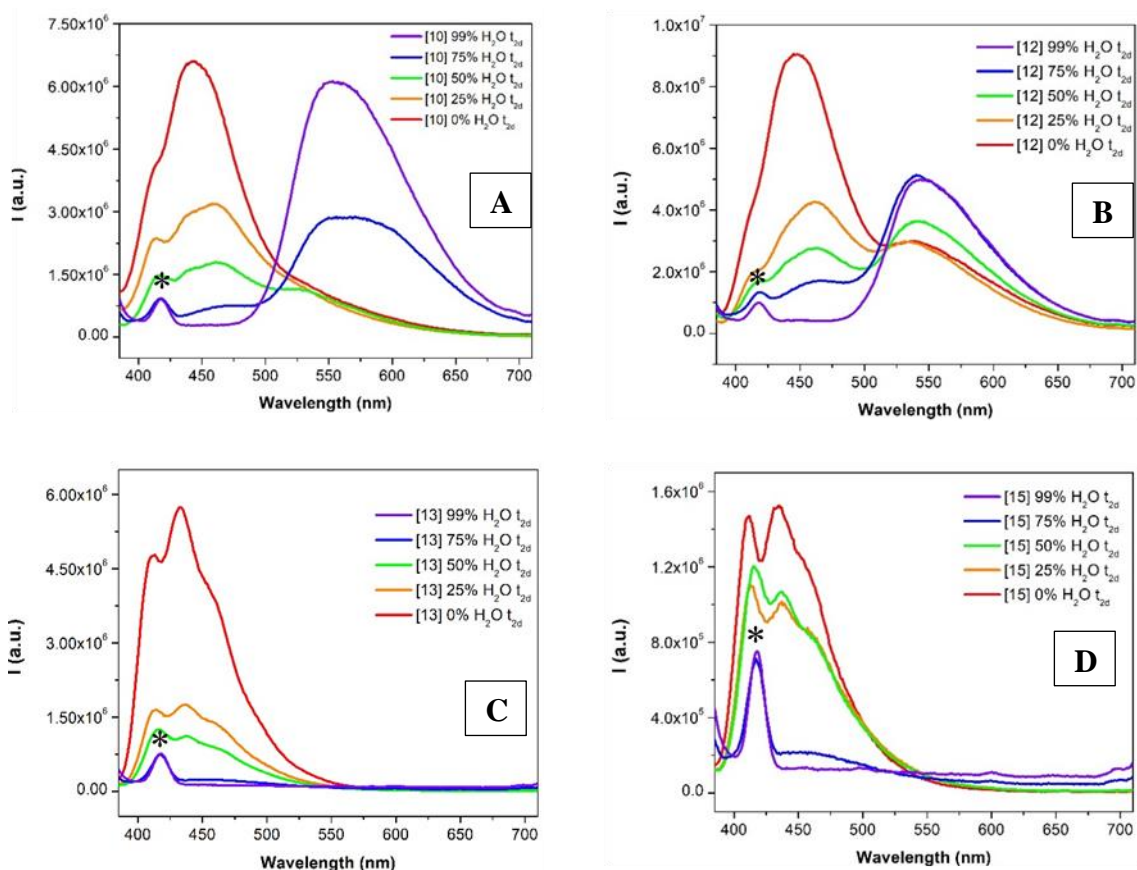


Figure S91. Emission spectra of compounds **11(A)**, **12(B)**, **14(C)**, **15(D)** compounds at different % of water in acetonitrile:water solutions after 2 days ($\lambda_{exc} = 350$ nm). * Indicates residual of the Raman band.

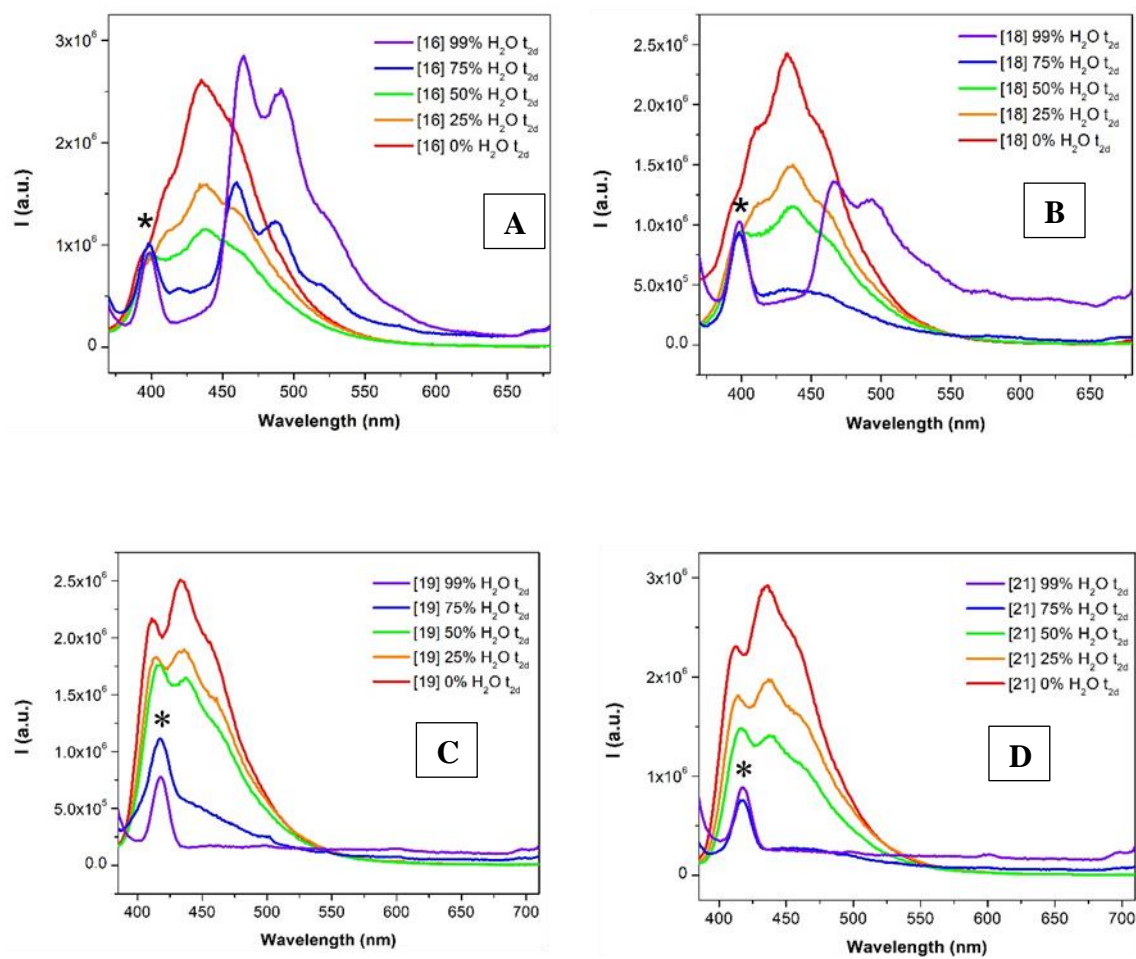


Figure S92. Emission spectra of compounds **16(A)**, **18(B)**, **19(C)**, **21(D)** compounds at different % of water in acetonitrile:water solutions after 2 days ($\lambda_{\text{exc}} = 350$ nm).

* Indicates residual of the Raman band.

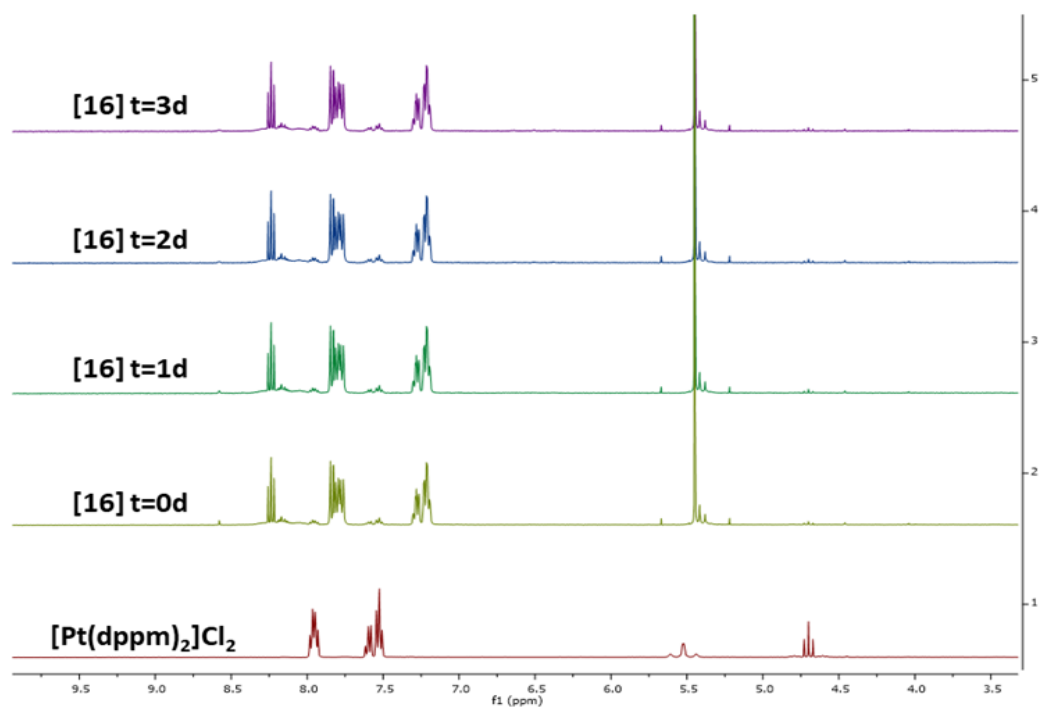


Figure S93. ^1H NMR spectra in CD_3CN of compounds **16** and $[\text{Pt}(\text{dppm})_2]\text{Cl}_2$ at different times

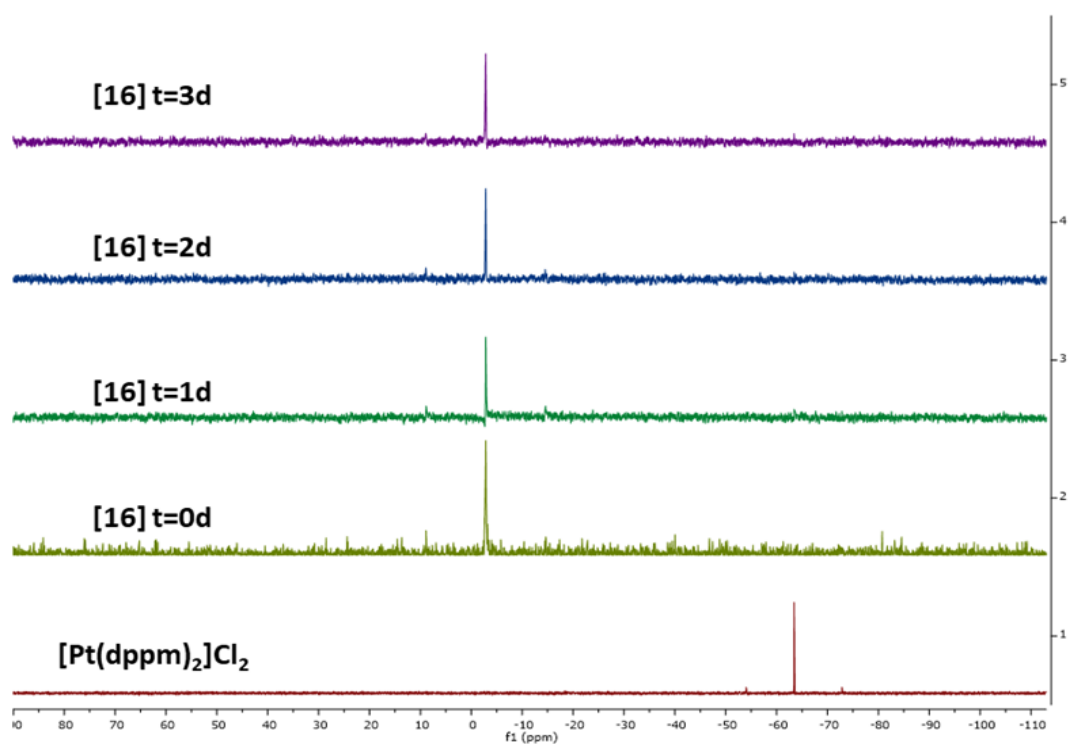


Figure S94. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in CD_3CN of compounds **16** and $[\text{Pt}(\text{dppm})_2]\text{Cl}_2$ at different times.

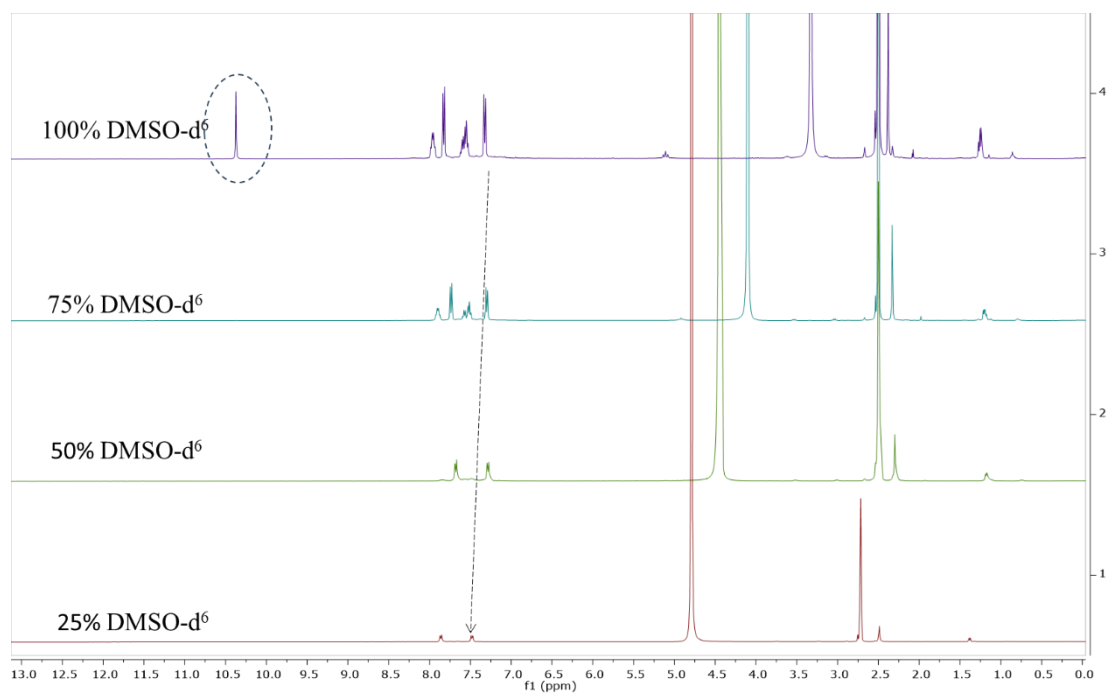


Figure S95. ^1H NMR spectra in DMSO-d_6 of compound **13** at different mixtures $\text{DMSO:D}_2\text{O}$

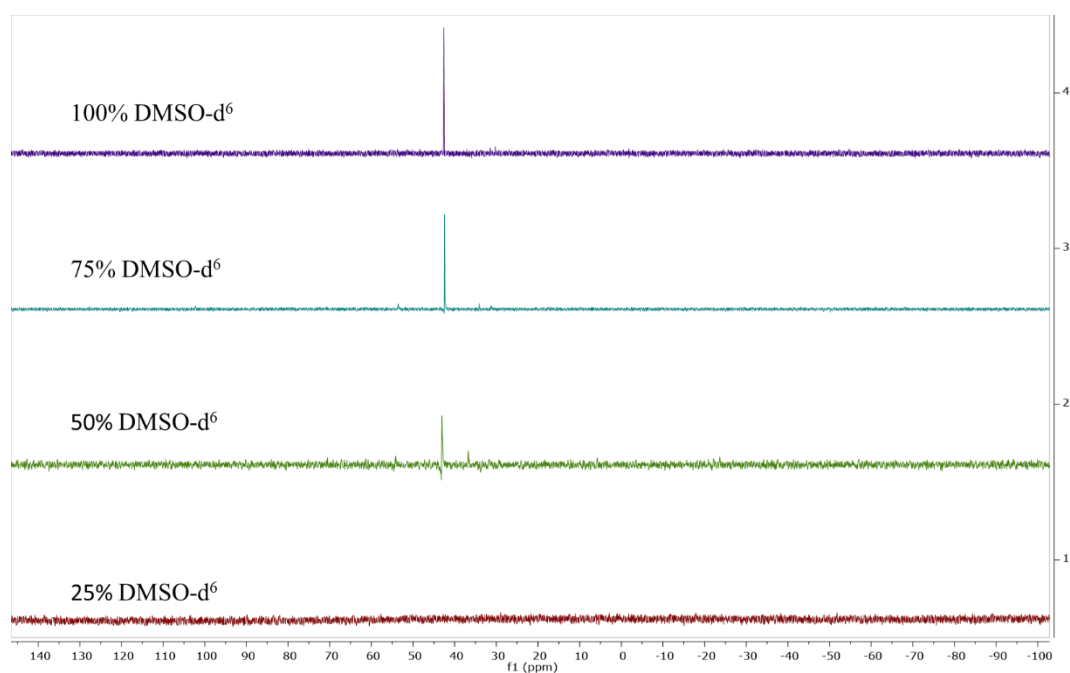


Figure S96. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in DMSO-d_6 of compound **13** at different mixtures $\text{DMSO:D}_2\text{O}$

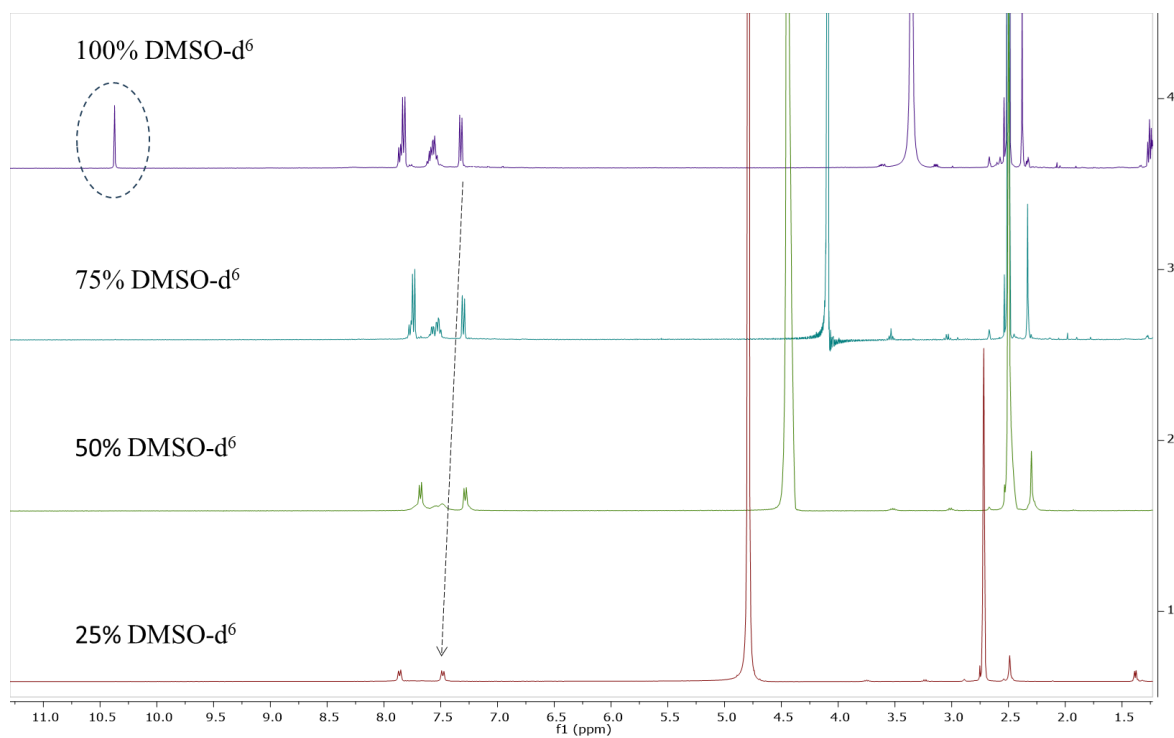


Figure S97. ^1H NMR spectra in DMSO-d^6 of compound **14** at different mixtures $\text{DMSO:D}_2\text{O}$

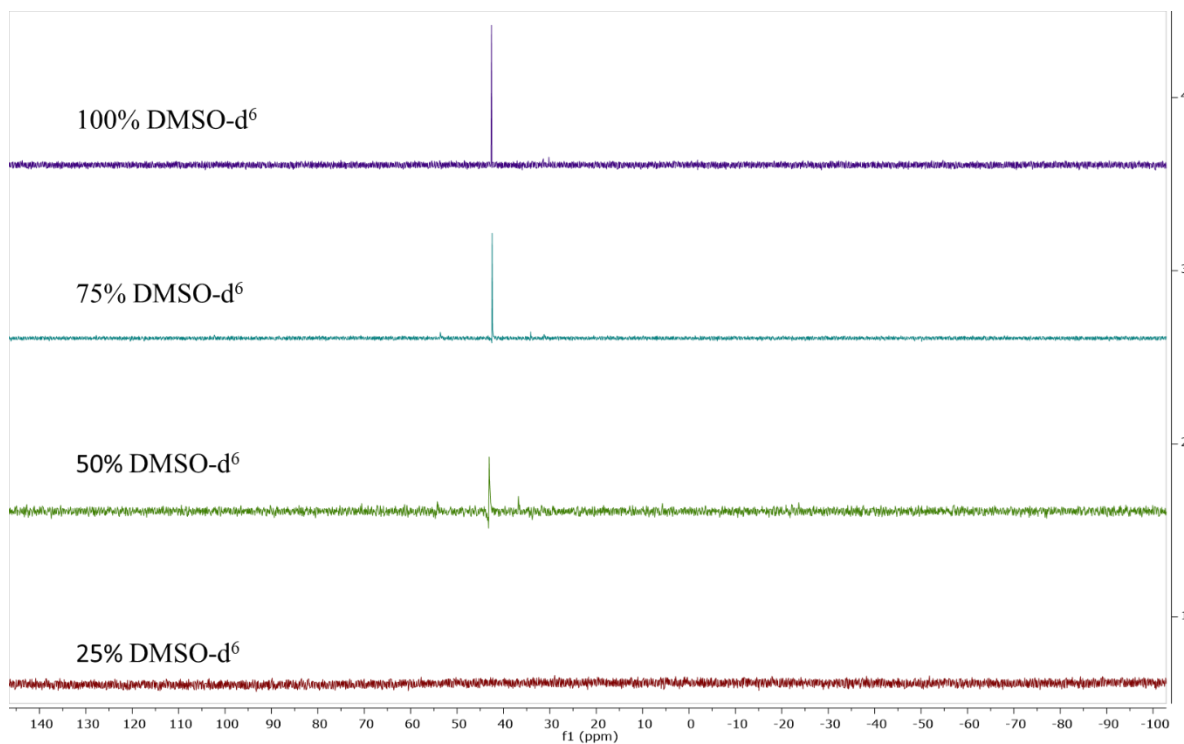


Figure S98. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in DMSO-d^6 of compound **14** at different mixtures $\text{DMSO:D}_2\text{O}$

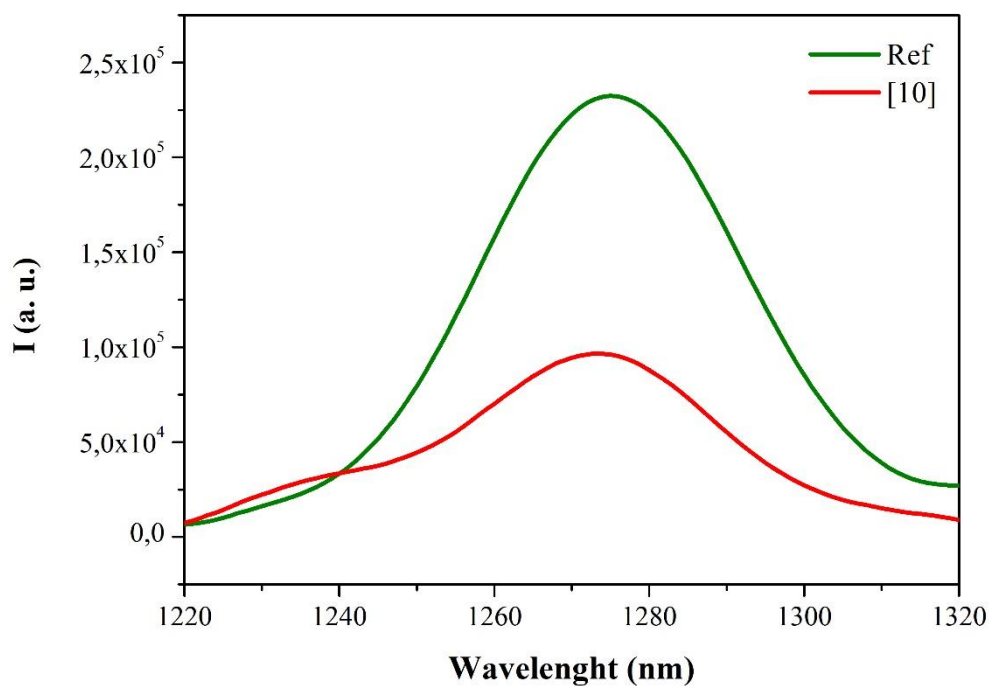


Figure S99. $^1\text{O}_2$ production of complex **10** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330 \text{ nm}$

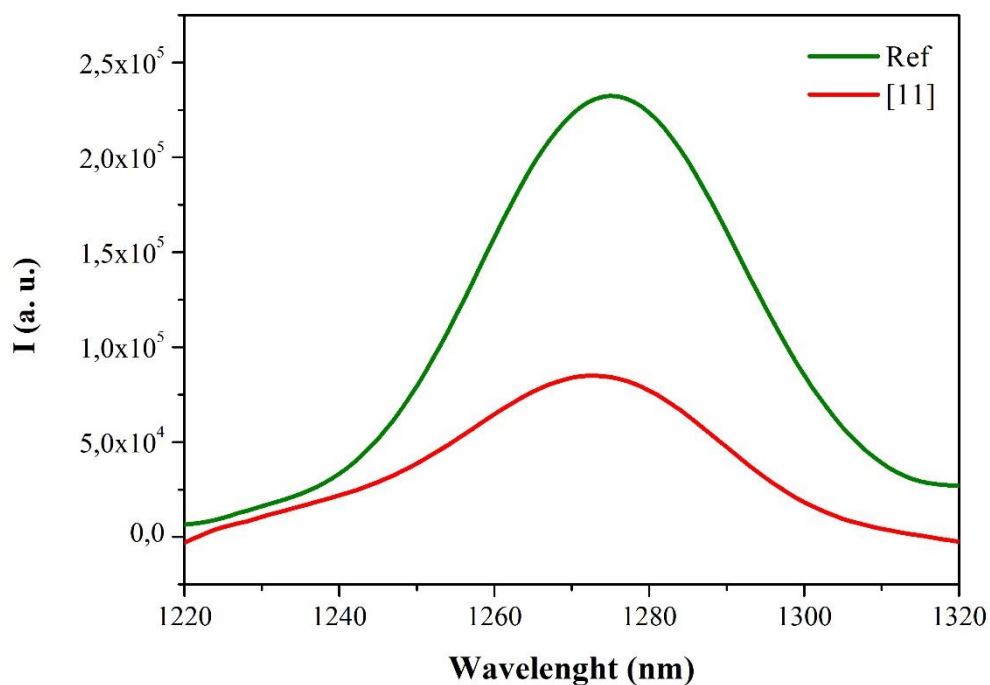


Figure S100. $^1\text{O}_2$ production of complex **11** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330 \text{ nm}$

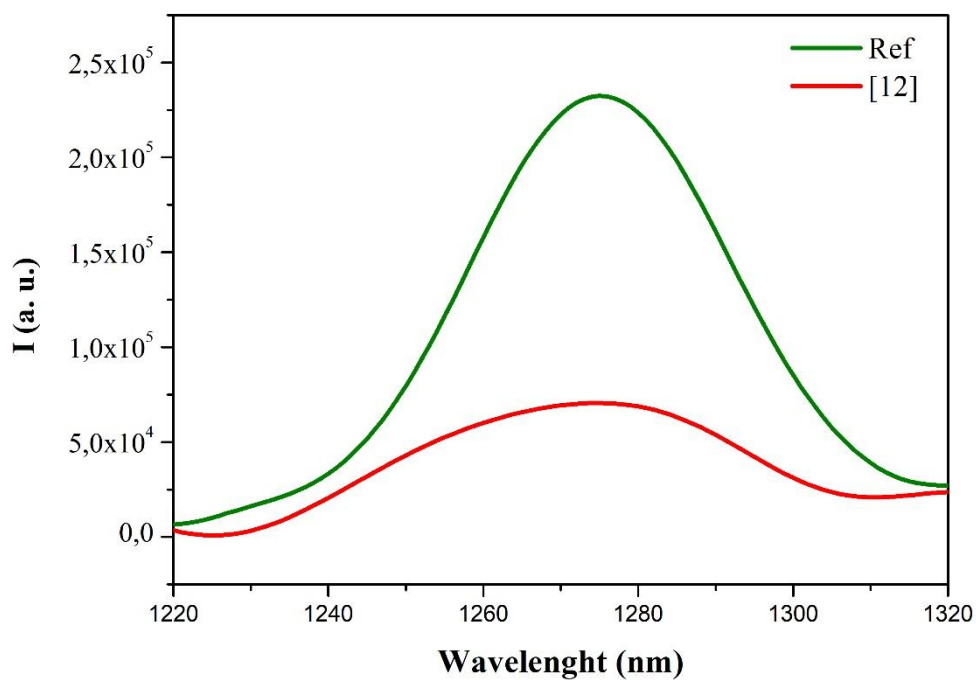


Figure S101. $^1\text{O}_2$ production of complex **12** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$.

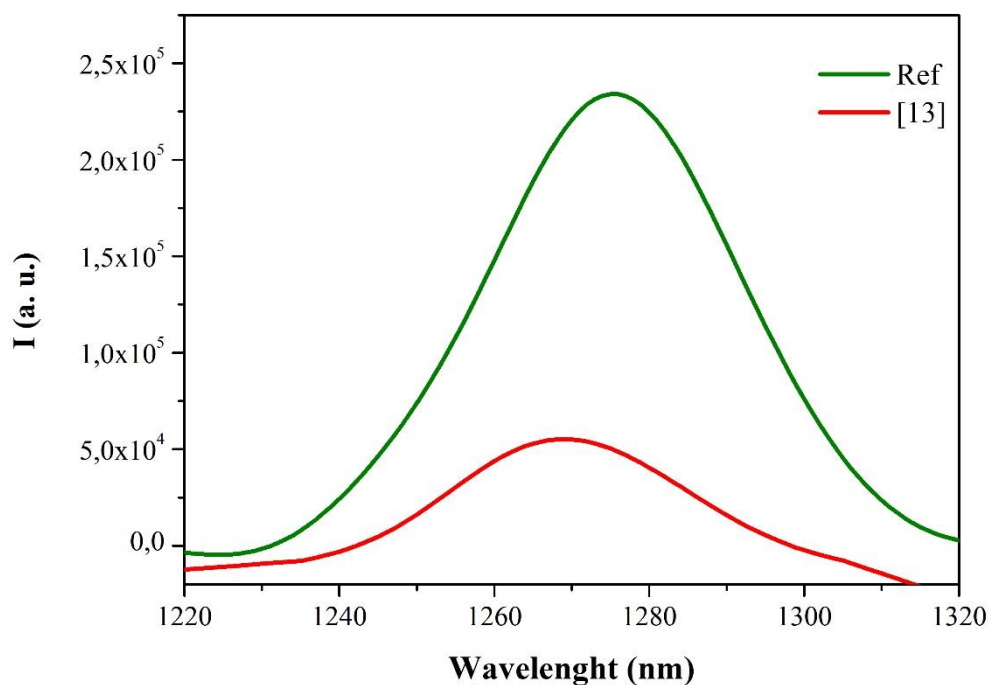


Figure S102. $^1\text{O}_2$ production of complex **13** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$.

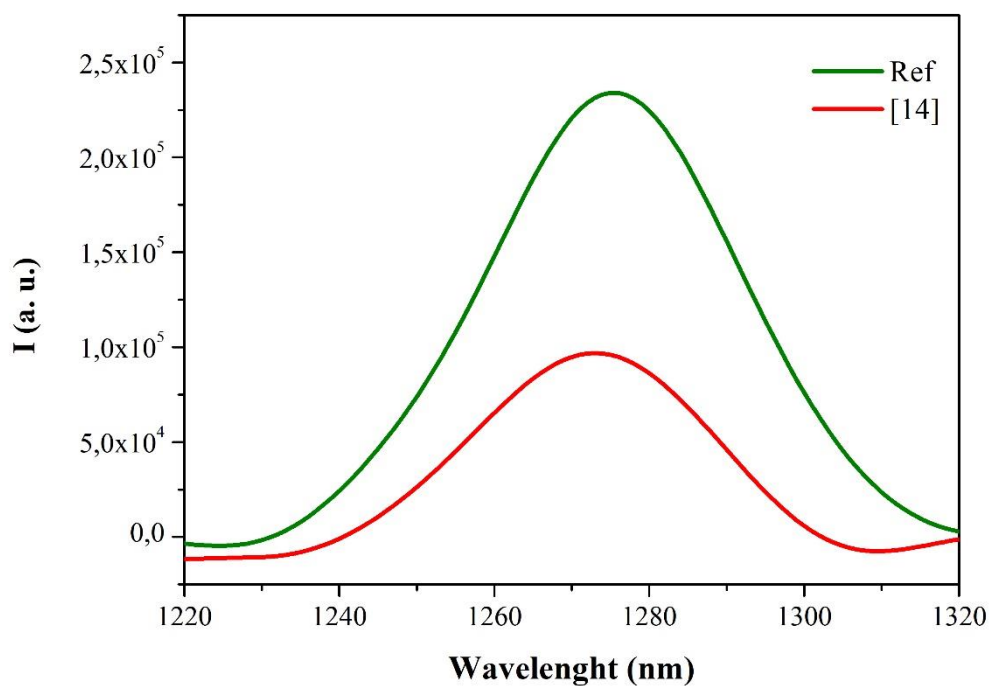


Figure S103. $^1\text{O}_2$ production of complex **14** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$.

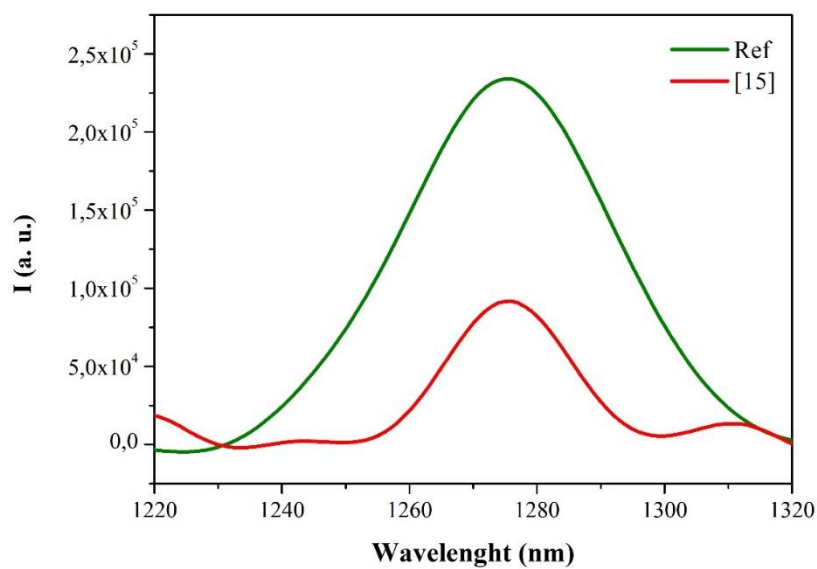


Figure S104. $^1\text{O}_2$ production of complex **15** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$

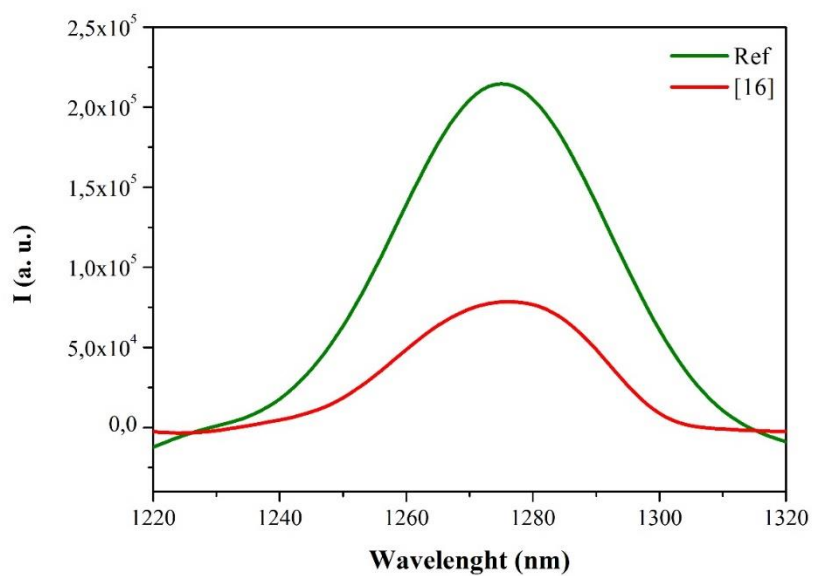


Figure S105. $^1\text{O}_2$ production of complex **16** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$

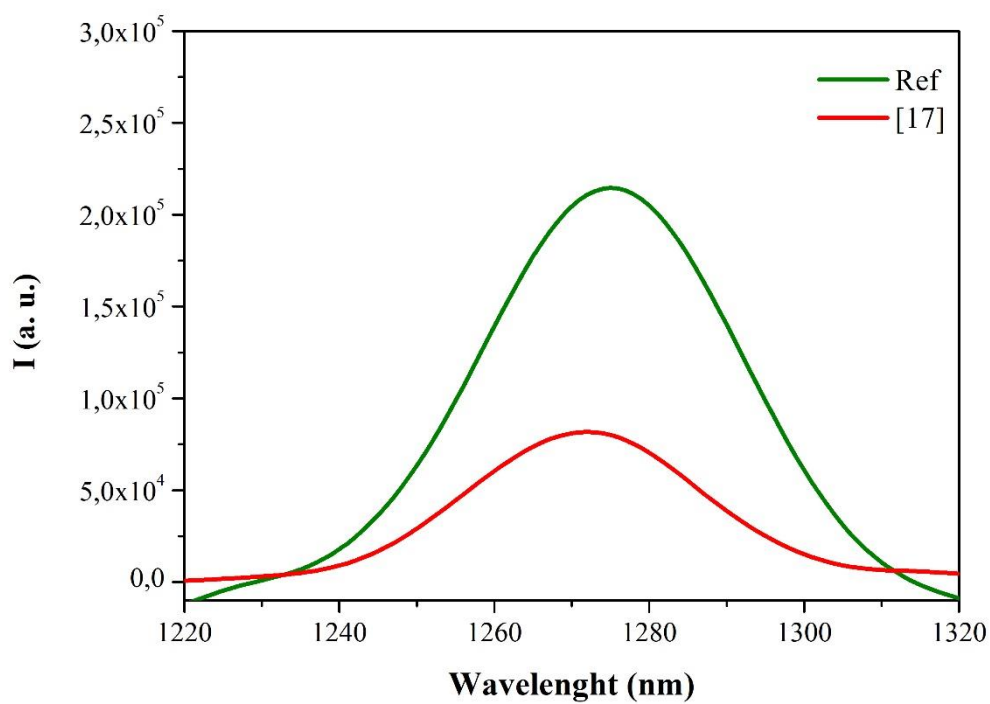


Figure S106. $^1\text{O}_2$ production of complex **17** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$.

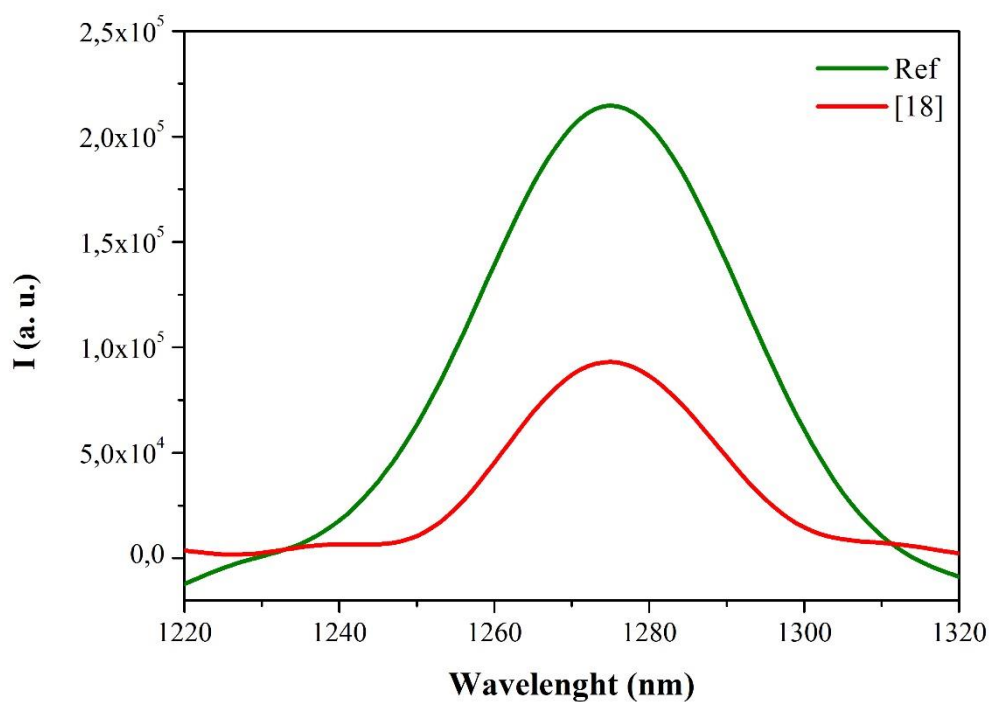


Figure S107. $^1\text{O}_2$ production of complex **18** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$.

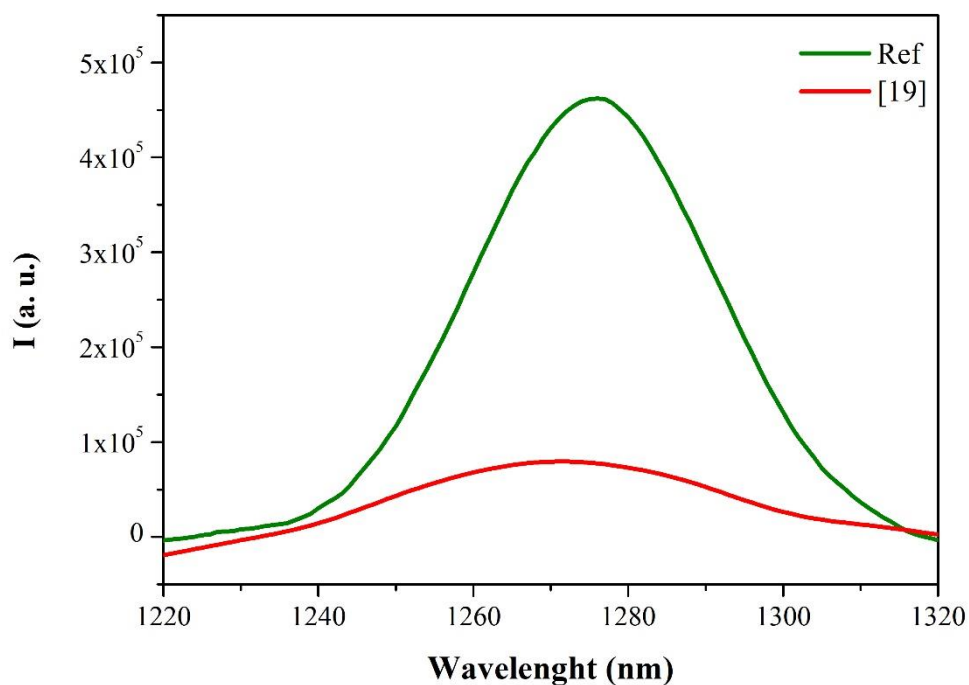


Figure S108. $^1\text{O}_2$ production of complex **19** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$.

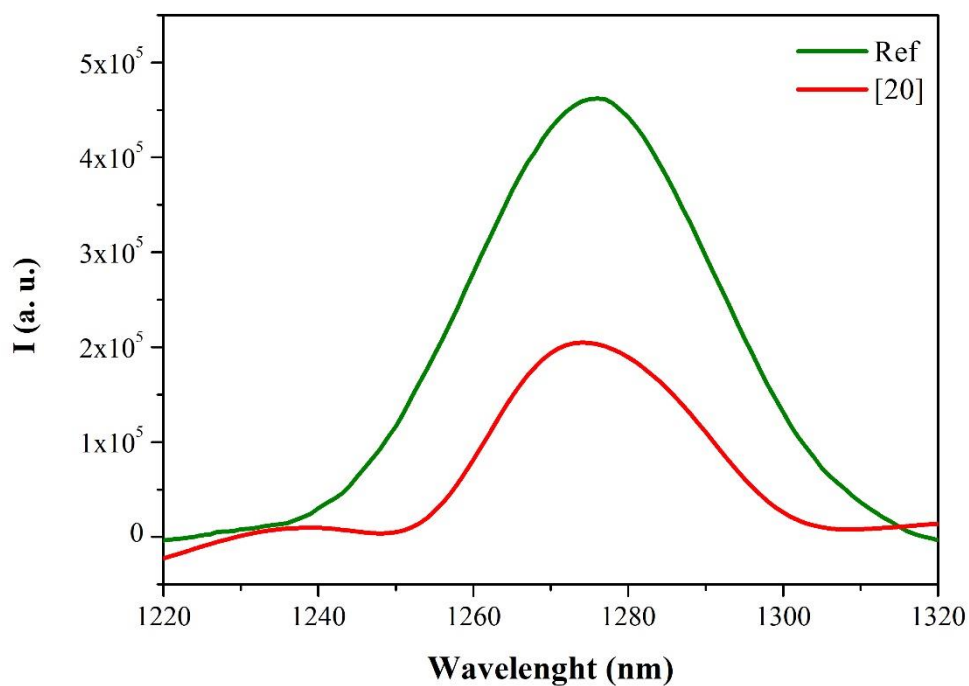


Figure S109. $^1\text{O}_2$ production of complex **20** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$

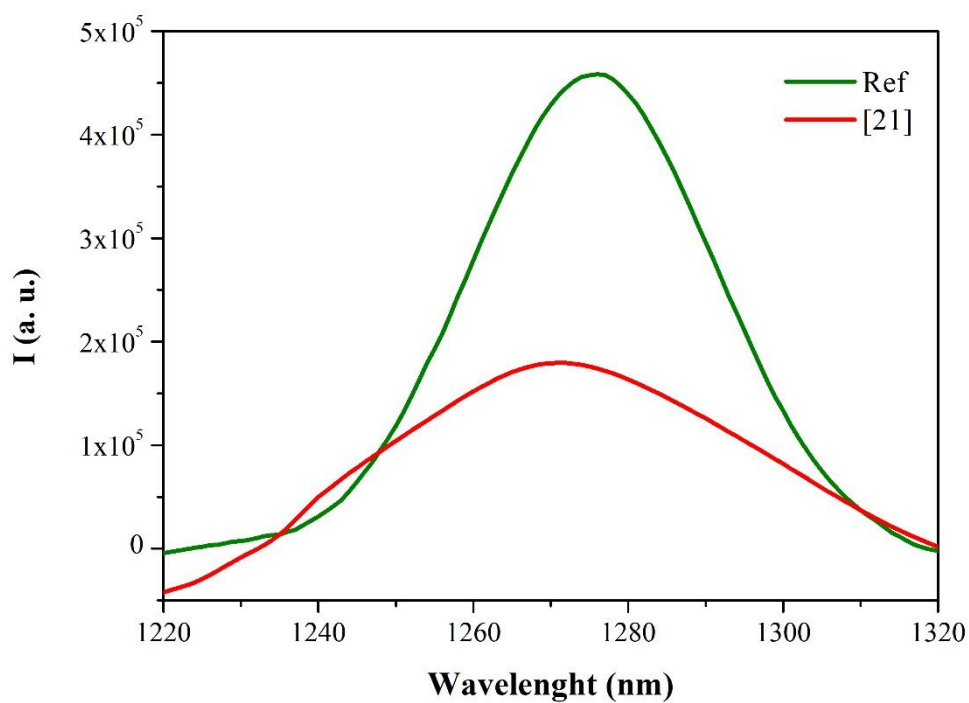


Figure S110. $^1\text{O}_2$ production of complex **21** in acetonitrile air-equilibrated solutions at $\lambda_{\text{exc}} = 330\text{nm}$

Comparison of experimental and geometric parameters of the Pt-complexes retrieved from the CSD.

Figure S111 shows the X-ray and DFT optimized geometries of three Pt-complexes (the CSD reference codes are indicated) that are related to those reported herein. The main difference is that they are mononuclear compounds, but the ligands are very similar. It can be observed a good agreement between the optimized and experimental geometries. The coordination distances and N–Pt–N angle are also in good agreement. The values in red correspond to the optimized geometries without dispersion (D3). It can be observed that the agreement is also acceptable, although the Ph₃P–Pt and N(triazole)–Pt distances are longer than those with D3 and much longer than the experimental ones. Moreover, the dihedral angle between the phenyl and triazole rings in RUDVET is better reproduced if D3 correction is used.

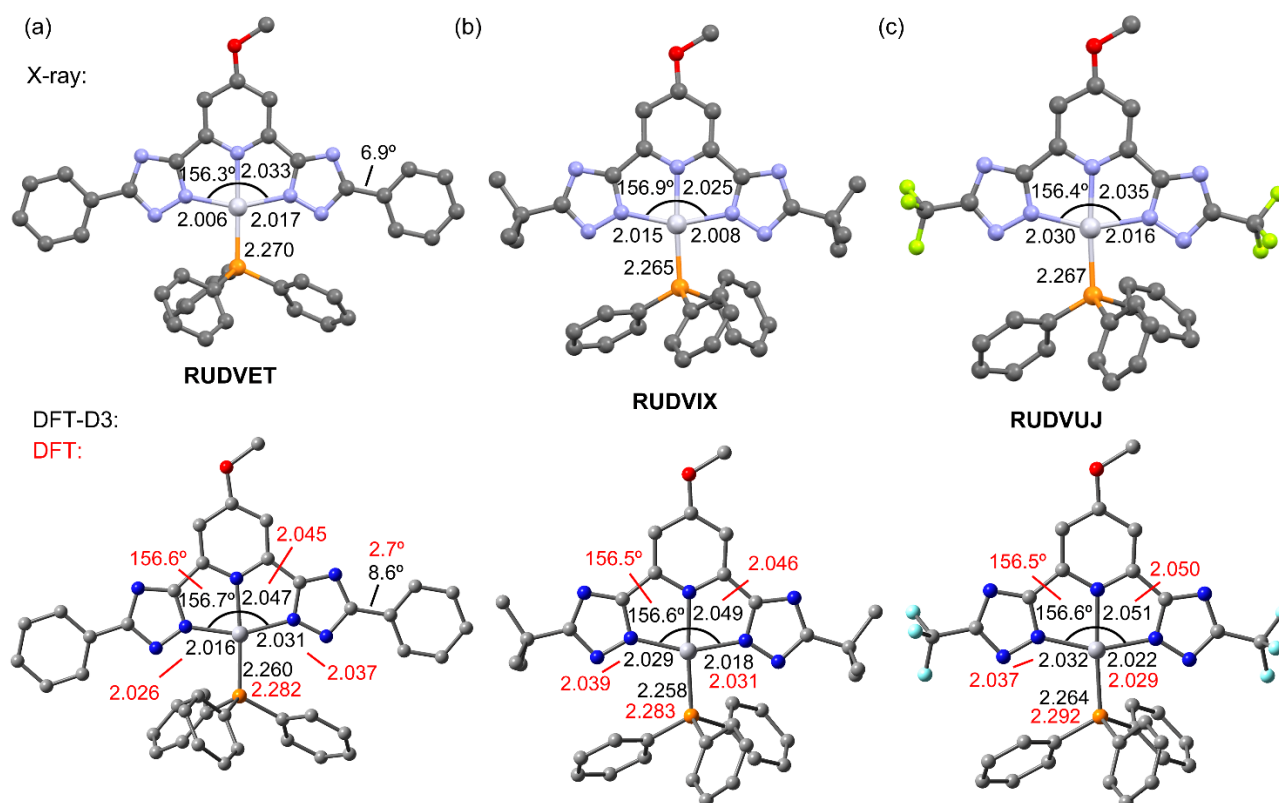


Figure S111. X-ray (top panel) and DFT (low panel) of RUDVET (a), RUDVIX (b) and RUDVUJ (c) structures. Distances are indicated in Å. In the bottom panel the distances indicated in black correspond to RI-PB86-D3/def2-TVP level and those in red to RI-PB86/def2-TVP level of theory.

Table S1. Radiative (k_r) and non-radiative (k_{nr}) constants of the gold(I) complexes **10-21** in acetonitrile solution.

Complex	k_r (air-eq) $\times 10^5 \text{ s}^{-1}$	k_{nr} (air-eq) $\times 10^5 \text{ s}^{-1}$	k_r (N_2 sat) $\times 10^5 \text{ s}^{-1}$	k_{nr} (N_2 sat) $\times 10^5 \text{ s}^{-1}$
10	0.1	10.3	0.2	2.2
11	0.5	15.9	0.2	2.8
12	0.3	13.8	0.4	3.8
13	8.1	2690	6.4	2120
14	6.0	1990	5.6	1880
15	4.26	2120	6.4	2120
16	22.7	2250	12.0	1190
17	17.9	1770	28.2	1380
18	45.5	4500	43.5	4300
19	42.9	7100	50.0	7090
20	42.9	7100	40.0	6630
21	33.3	6630	31.1	6220

Table S2. Lifetime values and amplitudes of compounds **10-21** measured in acetonitrile.

Complex	τ air-eq ns (Amplitude)	τ N ₂ sat, ns (Amplitude)	τ air-eq μ s (Amplitude)	τ N ₂ sat, μ s (Amplitude)
10			$\tau_1 = 0.32$ (52.14)	$\tau_1 = 1.04$ (23.54)
			$\tau_2 = 1.67$ (47.86)	$\tau_2 = 4.92$ (76.46)
11			$\tau_1 = 0.24$ (48.91)	$\tau_1 = 0.58$ (35.75)
			$\tau_2 = 0.98$ (51.09)	$\tau_2 = 4.83$ (64.26)
12			$\tau_1 = 0.30$ (51.57)	$\tau_1 = 0.59$ (37.14)
			$\tau_2 = 1.15$ (48.43)	$\tau_2 = 3.50$ (62.86)
13	$\tau_1 = 1.6$ (79.65)	$\tau_1 = 1.7$ (22.46)		
	$\tau_2 = 12.5$ (20.35)	$\tau_2 = 13.9$ (77.54)		
14	$\tau_1 = 1.9$ (83.29)	$\tau_1 = 2.0$ (77.79)		
	$\tau_2 = 19.8$ (16.71)	$\tau_2 = 17.5$ (22.21)		
15	$\tau_1 = 1.9$ (78.22)	$\tau_1 = 1.9$ (77.62)		
	$\tau_2 = 18.8$ (21.78)	$\tau_2 = 15.8$ (22.38)		
16	$\tau_1 = 2.2$ (61.57)	$\tau_1 = 2.8$ (59.80)		
	$\tau_2 = 8.0$ (38.43)	$\tau_2 = 16.7$ (40.20)		
17	$\tau_1 = 2.4$ (49.08)	$\tau_1 = 3.6$ (69.59)	$\tau_1 = 0.05$ (29.84)	$\tau_1 = 0.01$ (88.17)
	$\tau_2 = 8.7$ (50.92)	$\tau_2 = 14.9$ (30.41)	$\tau_2 = 0.08$ (70.16)	$\tau_2 = 0.15$ (11.83)
18	$\tau_1 = 2.2$ (100)	$\tau_1 = 0.5$ (5.07)	$\tau_1 = 0.01$ (81.30)	$\tau_1 = 0.02$ (58.46)
		$\tau_2 = 2.2$ (94.93)	$\tau_2 = 0.14$ (18.70)	$\tau_2 = 0.30$ (41.54)
19	$\tau_1 = 1.4$ (100)	$\tau_1 = 1.4$ (100)		
20	$\tau_1 = 1.4$ (100)	$\tau_1 = 1.5$ (100)		
21	$\tau_1 = 1.5$ (100)	$\tau_1 = 1.6$ (100)		

Table S3. Photophysical data of aggregates of compounds **10-21** in 10^{-5} M water/acetonitrile solutions.

Compound	% water	ϕ	τ (μ s)	k_r ($\times 10^5$ s $^{-1}$)	k_{nr} ($\times 10^5$ s $^{-1}$)
10	0	0.01	0.23	0.53	42.60
	75	0.04	1.14	0.37	8.40
	99	0.05	1.20	0.43	7.90
11	0	0.02	1.3E-2	232	746
	75	0.02	0.26	0.74	3.77
	99	0.02	0.33	0.46	2.98
12	0	0.01	0.30	0.50	32.8
	75	0.03	0.72	0.35	13.5
	99	0.03	0.85	0.34	11.4
13	0	0.01	3.7E-3	8.1	2690
	75	-	-	-	-
	99	-	-	-	-
14	0	0.01	5.0E-3	6.0	1990
	75	-	-	-	-
	99	-	-	-	-
15	0	0.01	5.8E-3	4.26	2120
	75	-	-	-	-
	99	-	-	-	-
16	0	0.02	1.3E-2	232	746
	75	0.02	0.26	0.74	3.77
	99	0.02	0.33	0.46	2.98
17	0	0.01	2.1E-2	4.57	47.2
	75	0.02	8.2E-2	1.66	12.0
	99	0.02	0.20	0.91	4.91
18	0	0.01	0.11	1.00	89.9
	75	0.02	0.42	0.35	23.5
	99	0.01	6.2E-2	1.55	16.0
19	0	0.01	1.4E-3	42.9	7100
	75	-	-	-	-

	99	-	-	-	-
20	0	0.01	1.4E-3	42.9	7100
	75	-	-	-	-
	99	-	-	-	-
21	0	0.01	1.5E-3	33.3	6630
	75	-	-	-	-
	99	-	-	-	-

Cartesian Coordinates

11

Energy = -4469.034576817

Pt	2.8284727	3.4285429	4.5314759
P	1.3059004	2.8721122	2.9532288
N	2.9578862	5.4413943	4.3234229
N	2.2928673	6.4085652	3.6714218
N	4.3795238	3.8819506	5.7988311
N	3.3006816	1.6060743	5.2557759
N	2.8143831	0.3669627	5.1564137
C	2.9228234	7.5536154	4.0366250
C	3.9573912	6.0361794	5.0582238
C	4.7758650	5.1724100	5.8861301
C	5.8420406	5.5056526	6.7262629
H	6.1350959	6.5483328	6.8294634
C	6.4626616	4.4766332	7.4404514
C	6.0467904	3.1464691	7.3143655
H	6.5213644	2.3341252	7.8608792
C	4.9765534	2.8633258	6.4597572
C	4.3454883	1.5930821	6.1581682
C	3.5884130	-0.3656719	5.9956496
C	1.6206574	3.6830763	1.3387928
C	2.7289555	4.5146935	1.1370874
H	3.4234007	4.6998113	1.9536395
C	2.9424914	5.1101062	-0.1088289
H	3.8052991	5.7616777	-0.2521381
C	2.0554768	4.8771840	-1.1608518
H	2.2223193	5.3459818	-2.1317220
C	0.9567525	4.0317087	-0.9716616
H	0.2693248	3.8319395	-1.7948541
C	0.7435459	3.4341936	0.2694741
H	-0.0991801	2.7519728	0.3995463
C	-0.4306131	3.3238708	3.3459373
C	-0.5310920	4.7841459	3.8284662
C	1.3018782	1.1051620	2.5298135
C	2.5069310	0.5616863	2.0556159
H	3.3814313	1.2045192	1.9391587
C	2.5955555	-0.7972800	1.7685869
H	3.5388687	-1.2166259	1.4168957
C	1.4830071	-1.6259479	1.9543916
H	1.5594142	-2.6945249	1.7487120
C	0.2820880	-1.0898804	2.4211402
H	-0.5849501	-1.7302568	2.5878810
C	0.1899378	0.2750312	2.7085456
H	-0.7439971	0.6684813	3.1040695
Pt	0.6955105	3.5896046	6.8456804
P	-0.7371424	4.8700928	5.6518746
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C	1.1921841	-5.1910885	12.3627462
H	0.2039872	-3.4627069	11.5071101
C	3.1057160	-4.7264516	13.7434463
H	3.6178378	-2.6426509	13.9845462
C	2.2388299	-5.6689069	13.1693205
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H	7.5227377	8.5184291	19.4401275
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H	6.7418470	7.8264620	14.1622941
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C	4.7661912	5.2138771	5.8716825
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H	6.0885211	6.6098800	6.8555717
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H	6.4774169	2.4065726	7.9255123
C	4.9744849	2.9118270	6.4578313
C	4.3575936	1.6361327	6.1547167
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C	2.7203519	4.5349203	1.1058683
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C	2.9282746	5.1195004	-0.1461942
H	3.7865122	5.7753182	-0.2974814
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H	2.2052463	5.3292856	-2.1708294
C	0.9493198	4.0186904	-0.9962543
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C	-0.5291861	4.7841279	3.8349327
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H	3.5798155	-1.1876939	1.4134584
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H	1.6027796	-2.6745496	1.7211127
C	0.3140527	-1.0780913	2.3907545
H	-0.5513951	-1.7228926	2.5477039
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C	2.4189262	0.3072639	8.9875663
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C	-3.2612762	-1.8537158	3.6130344
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C	3.1517565	3.0935125	9.0764372
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C	0.7297850	0.7216401	11.5019266
C	-0.3676793	0.3217280	10.7415981
H	-0.6360824	-0.7284801	10.6681568
C	-1.1237866	1.3258041	10.1334524
C	-0.7768632	2.6813928	10.2147245
H	-1.3575949	3.4627645	9.7326400
C	0.3539657	3.0113483	10.9675421
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C	5.9777745	2.0438659	13.3159432
C	6.1588566	0.7657912	13.8681361
H	5.4816378	0.3919432	14.6304270
C	7.1806557	-0.0668659	13.4105505
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C	8.0364696	0.3607115	12.3936049
H	8.8274796	-0.2958027	12.0287249
C	7.8685101	1.6326819	11.8435516
H	8.5264675	1.9795140	11.0466880
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H	6.5058446	7.4790113	15.2435153
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H	3.0357700	9.3267827	14.7553984
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C	0.4735909	8.5081954	10.9133984
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H	3.4405696	7.9155112	12.4679946
C	0.5081912	9.9020996	10.8968029
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C	-1.9152796	-1.2091031	13.3764250
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C	-2.5205318	-3.8743578	12.6366166
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C	4.0966977	-2.9345025	14.8959241
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H	1.2534180	-3.8377021	13.2672767
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C	3.4813220	-5.2208326	15.4763330
H	1.6964409	-5.9513377	14.5039206
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Energy = -4735.889623077

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F	2.7934350	9.8743940	4.4446347
F	3.1508481	-2.2292418	7.2516572
F	2.3452763	-2.3336034	5.2137223
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C	2.9976454	7.5469706	4.0713557
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C	4.7702025	5.1157620	5.9014349
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C	3.3771904	-1.8803491	5.9510762
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H	2.3300484	5.6725519	-2.0621743
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C	0.7264363	3.7467102	0.2456283
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C	-0.4421403	3.3595157	3.2842745
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C	1.3459225	1.2107554	2.3866878
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H	3.3535470	1.4426381	1.6077191
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H	3.6286858	-0.9710774	1.0989630
C	1.6613255	-1.5068880	1.8228316
H	1.7904782	-2.5710254	1.6223174
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H	-0.6165609	0.6521073	3.1287882
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N	1.9714785	6.4097761	7.4649074
F	-0.9349018	-2.3620263	5.1481473
F	-2.5964846	-1.6303975	6.3637285
F	-2.2674831	-0.8089840	4.3596320
F	4.8297766	8.1775274	8.3471292
F	2.9182820	8.9704070	7.6192577
F	3.2022039	8.5720562	9.7535302
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C	-0.2954869	8.8873740	5.8925136
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N	2.9970719	-0.0228397	5.4753165
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F	3.0752569	9.5461275	5.1206474
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F	2.5898912	-2.7170019	5.6313465
F	4.7679479	-2.9337548	5.5908372
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C	4.1674253	5.6434399	5.7698573
C	5.0285559	4.7119922	6.4763029
C	6.1789536	4.9700015	7.2234708
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C	6.8882128	3.8785111	7.7356665
H	7.7876418	4.0569105	8.3251154
C	6.4699631	2.5639679	7.4997950
H	7.0186770	1.7030904	7.8765053
C	5.2975179	2.3630305	6.7667071
C	4.6398883	1.1215803	6.3983200
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C	3.7311079	-2.2919597	6.2017447
C	1.6626730	3.6488941	2.0514691
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H	3.6307268	4.3231672	2.6316711
C	3.0931901	5.0386796	0.6695143
H	4.0314705	5.5771664	0.5329694
C	2.1171549	5.0619888	-0.3277576
H	2.2897019	5.6188864	-1.2495853
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H	0.1564883	4.3710696	-0.9261607
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H	-0.2366006	3.0995936	1.1511833
C	-0.3636522	3.0707329	4.0467573
C	-0.4814726	4.5243919	4.5485582
C	1.4034547	0.9572724	3.0291966
C	2.5613704	0.5278045	2.3601145
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C	2.7211093	-0.8165424	2.0370458
H	3.6274896	-1.1482329	1.5292338
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H	0.5215841	9.3757156	5.8809471
C	-0.0907223	7.3197265	6.0338284
H	0.3044323	7.0731791	5.0516417
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H	-3.2042245	5.1391436	12.7053226
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C	-2.5217116	2.3998412	13.1475713
C	-3.5689063	0.7997180	12.3219127
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C	-4.5758715	0.0259533	11.5193423
C	0.2021876	-0.6742886	17.3069436
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H	0.4603451	-0.8725270	21.1882258
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H	0.8701846	-2.9053509	19.8041513
C	0.5223638	-1.8887441	17.9368403
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C	-2.5936997	-1.3725292	15.7914350
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C	-3.7531466	-2.0821552	15.4933963
H	-4.6907020	-1.8196514	15.9846951
C	-3.7166962	-3.1168093	14.5528448
H	-4.6289114	-3.6599940	14.3040048
C	-2.5159524	-3.4482667	13.9248570
H	-2.4834262	-4.2455225	13.1830542
C	-1.3490668	-2.7404941	14.2201268
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F	3.0279287	7.0374939	14.2807424
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C	-0.8477899	-3.4835656	10.6048499
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F	2.8184581	9.8596744	4.4549500
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C	6.3810389	4.3198496	7.4940573
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