Electronic Supplementary Material (ESI) for Dalton Transactions.

Aggregation of gold(I) complexes: phosphorescence *vs* singlet oxygen production

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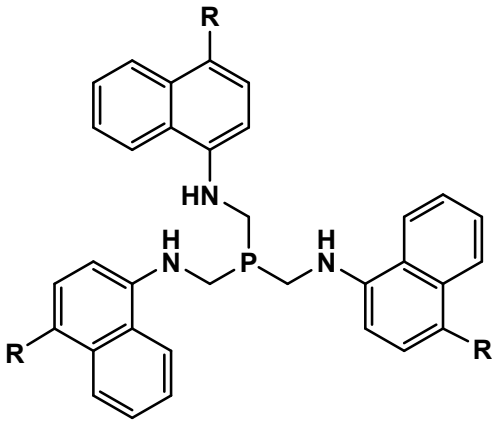
Supporting Information



R = H (P1), Cl (P2), Br (P3)

Figure S1. Chemical structure of P{CH_2-1-N(H)naphthyl}$_3$ phosphane.

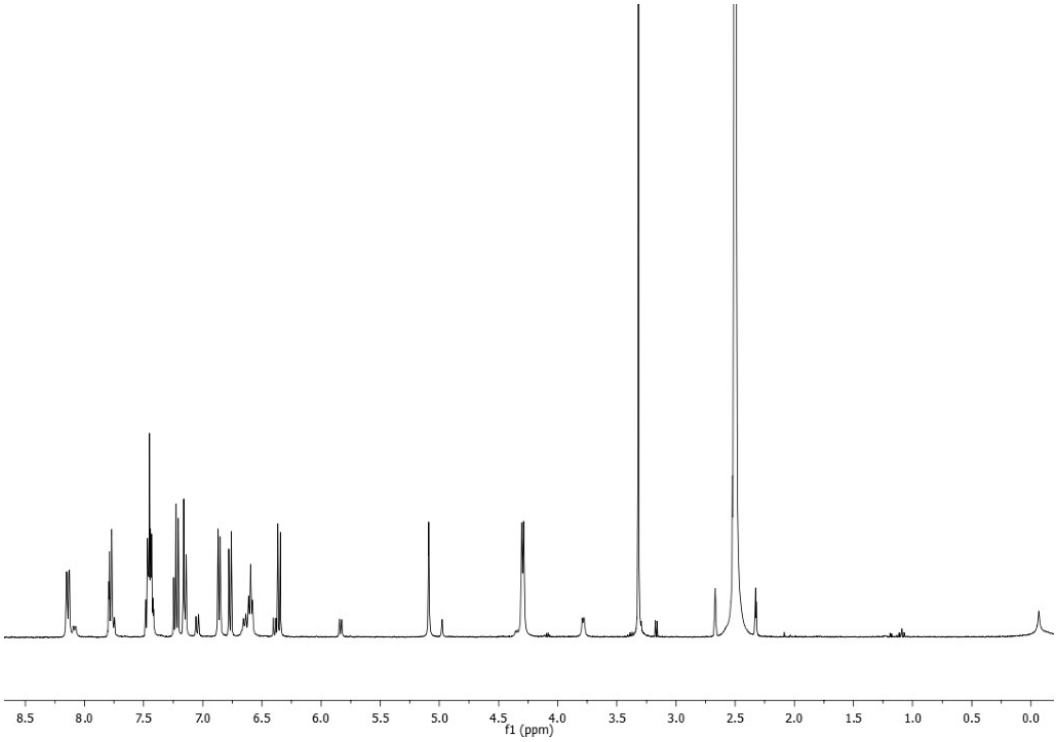


Figure S2. ^{1}H-NMR spectra of **1** in DMSO-d_6

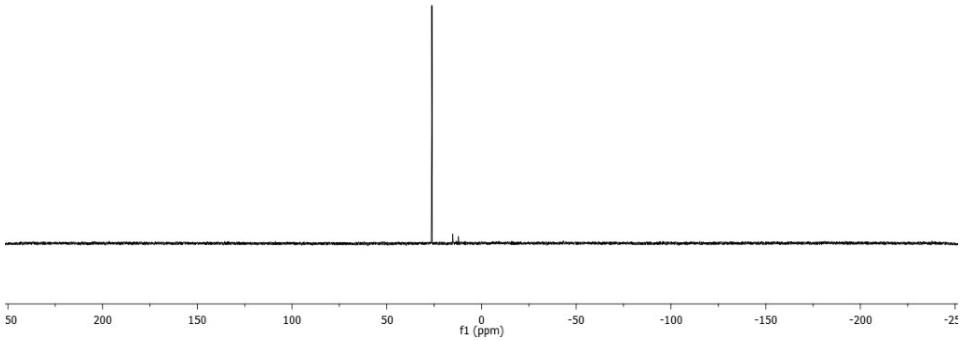


Figure S3. ^{31}P-NMR spectra of **1** in DMSO-d_6.

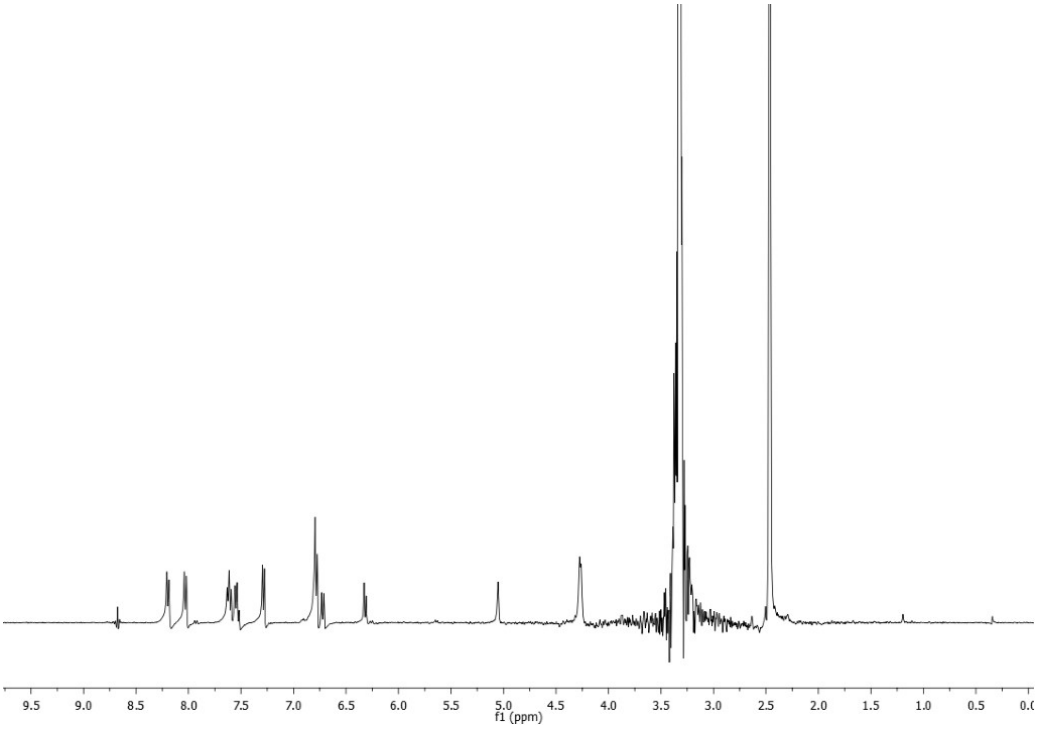


Figure S4. ^{1}H-NMR spectra of **2** in DMSO-d_6.

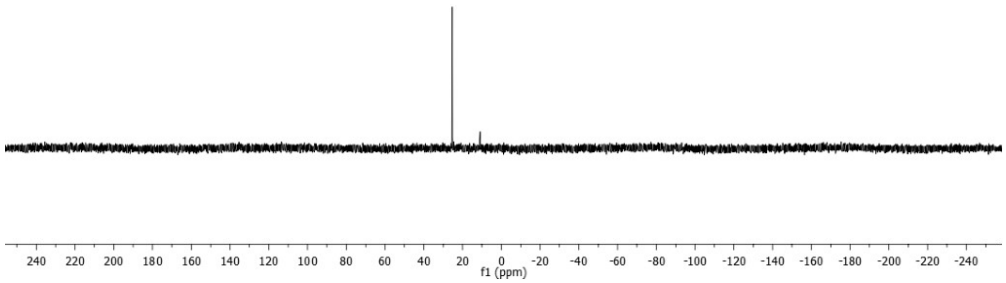


Figure S5. ^{31}P-NMR spectra of **2** in DMSO-d_6.

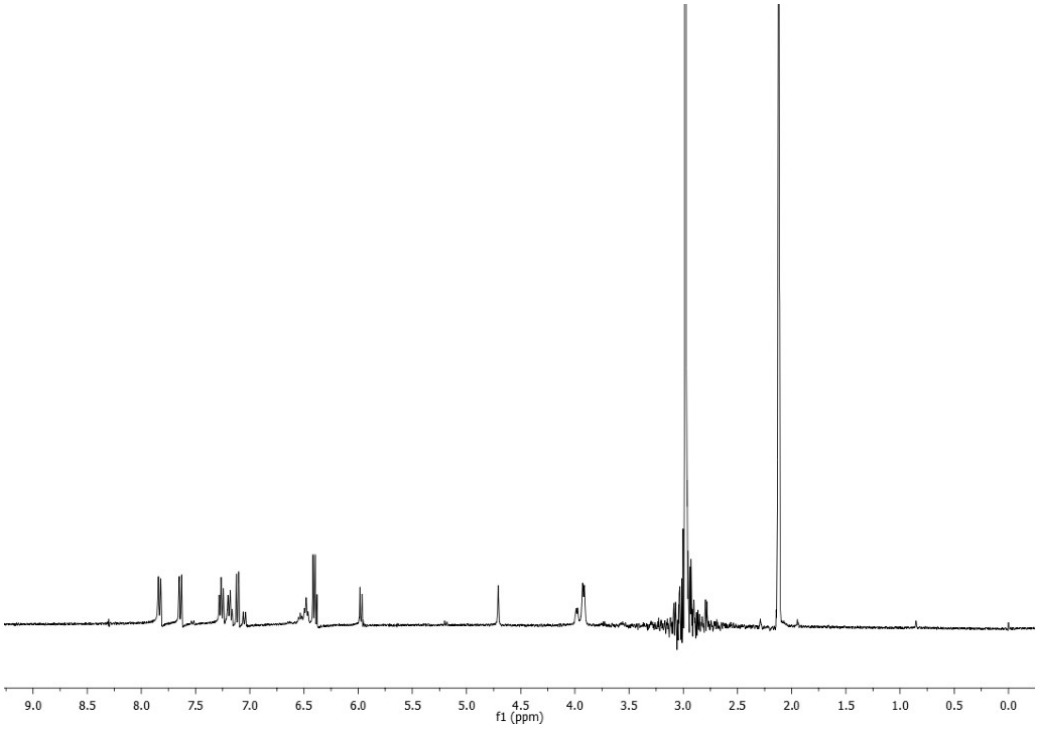


Figure S6. ^{1}H-NMR spectra of **3** in DMSO-d_6.

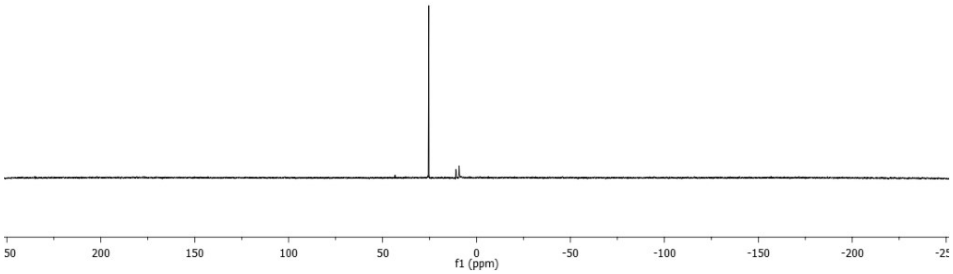


Figure S7. ^{31}P-NMR spectra of **3** in DMSO-d_6.

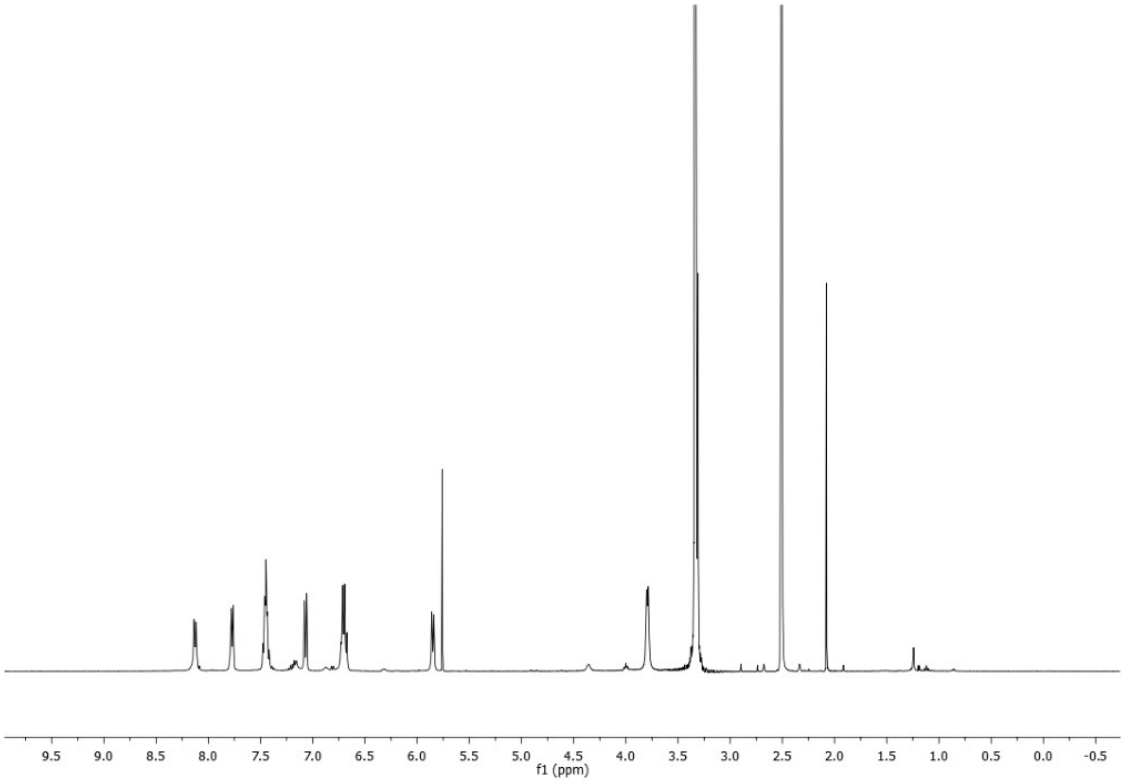


Figure S8. ^{1}H-NMR spectra of **4** in DMSO-d_6.

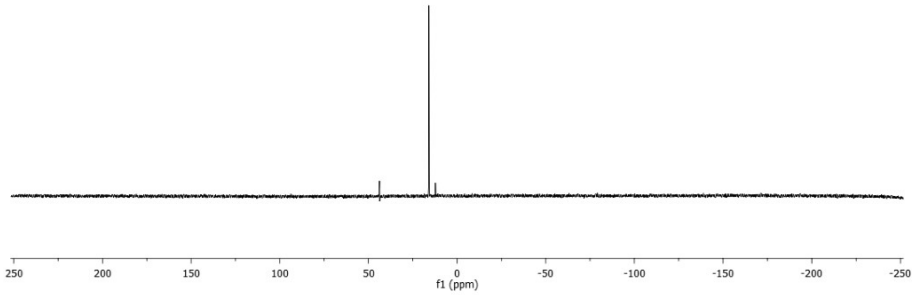


Figure S9. ^{31}P-NMR spectra of **4** in DMSO-d_6.

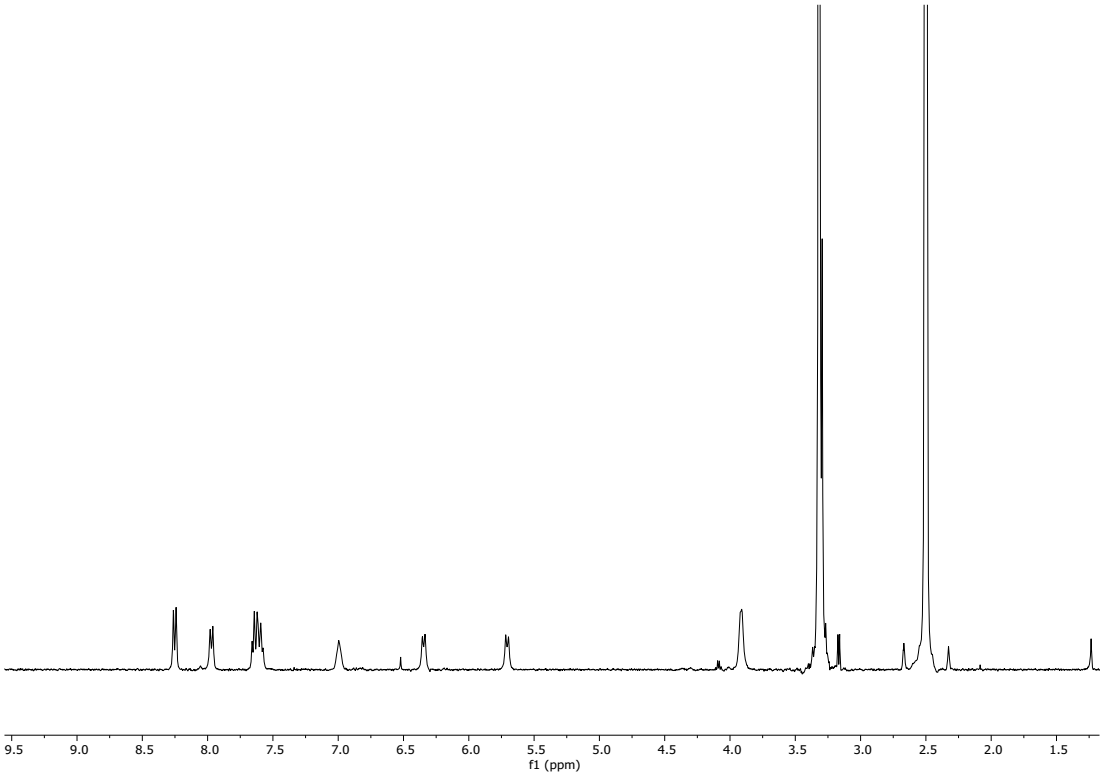


Figure S10. ^{1}H-NMR spectra of **5** in DMSO-d_6.

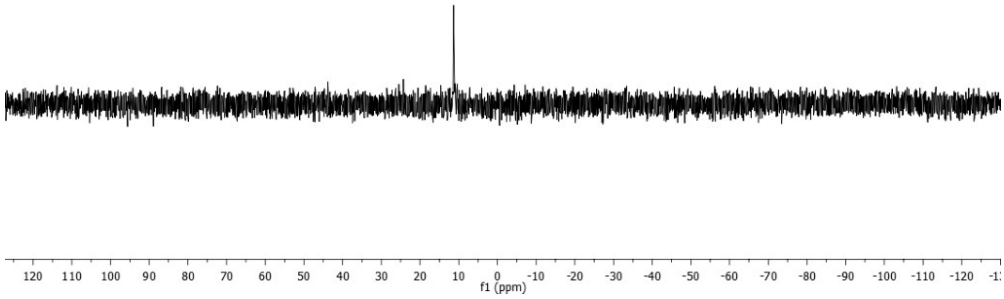


Figure S11. ^{31}P-NMR spectra of **5** in DMSO-d_6.

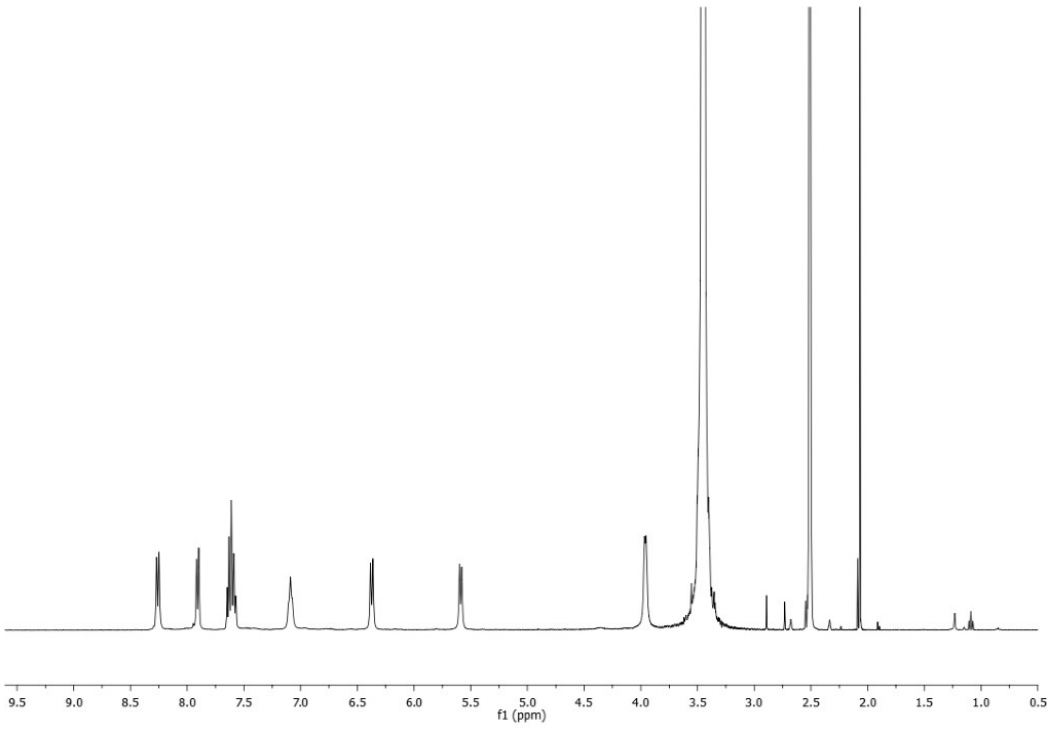


Figure S12. ^{1}H-NMR spectra of **6** in DMSO-d_6.

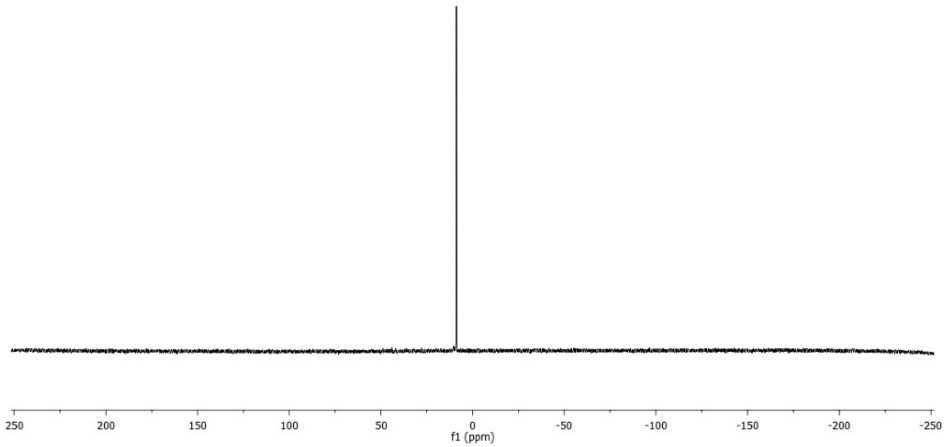


Figure S13. ^{31}P-NMR spectra of **6** in DMSO-d_6.

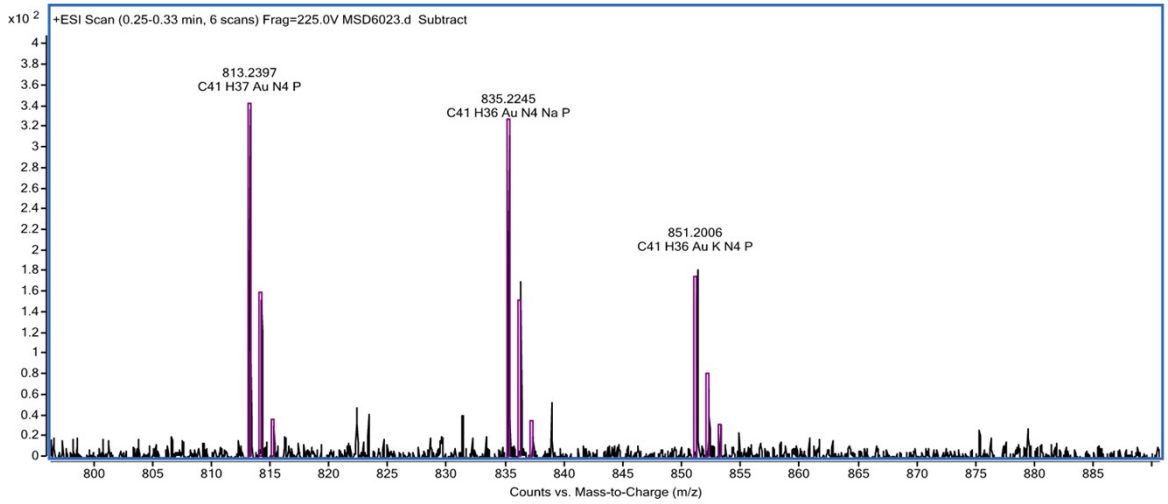


Figure S14. Mass spectra of **1**.

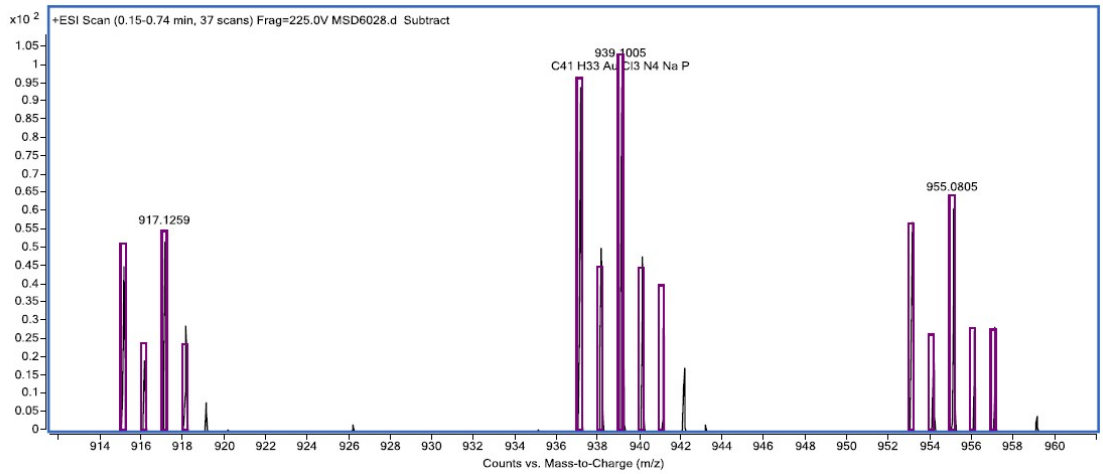


Figure S15. Mass spectra of **2**.

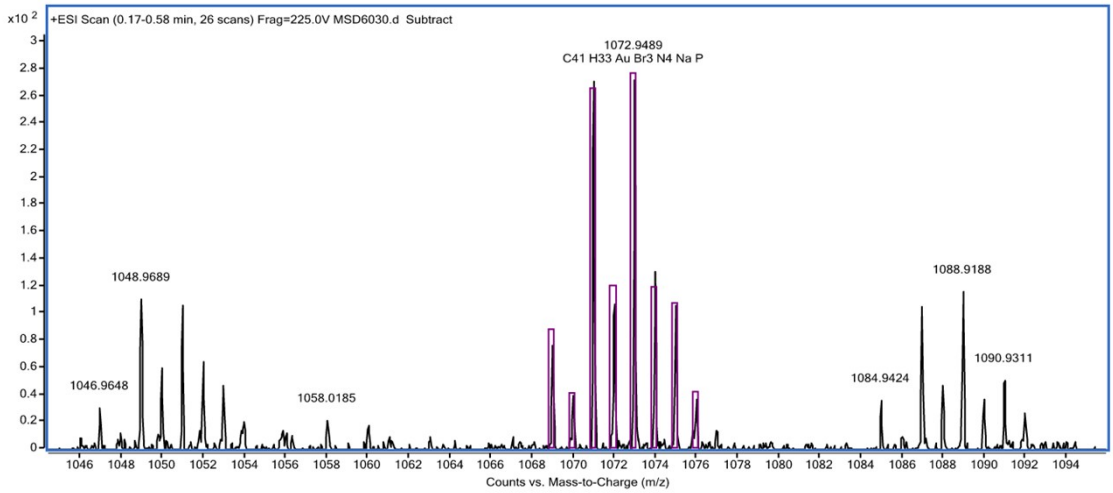


Figure S16. Mass spectra of **3**.

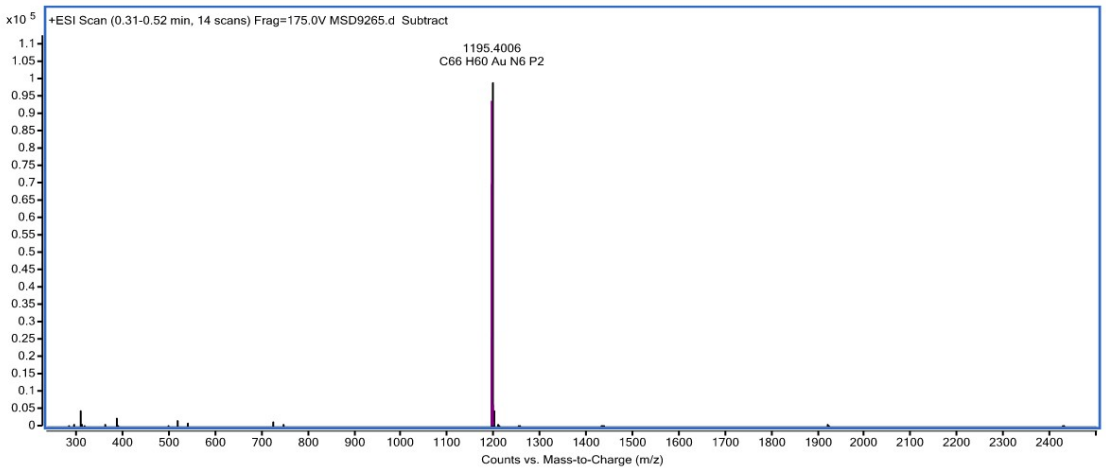


Figure S17. Mass spectra of **4**.

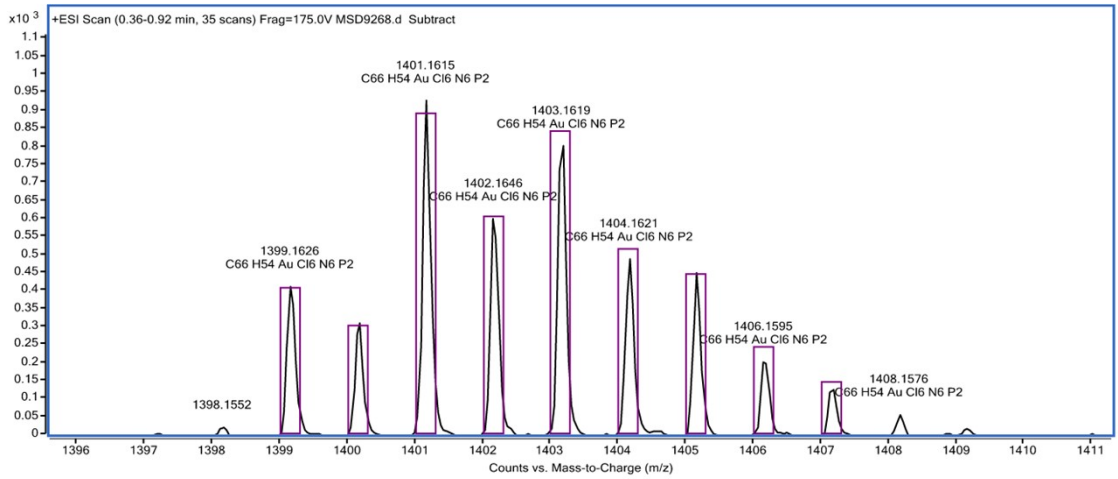


Figure S18. Mass spectra of **5**.

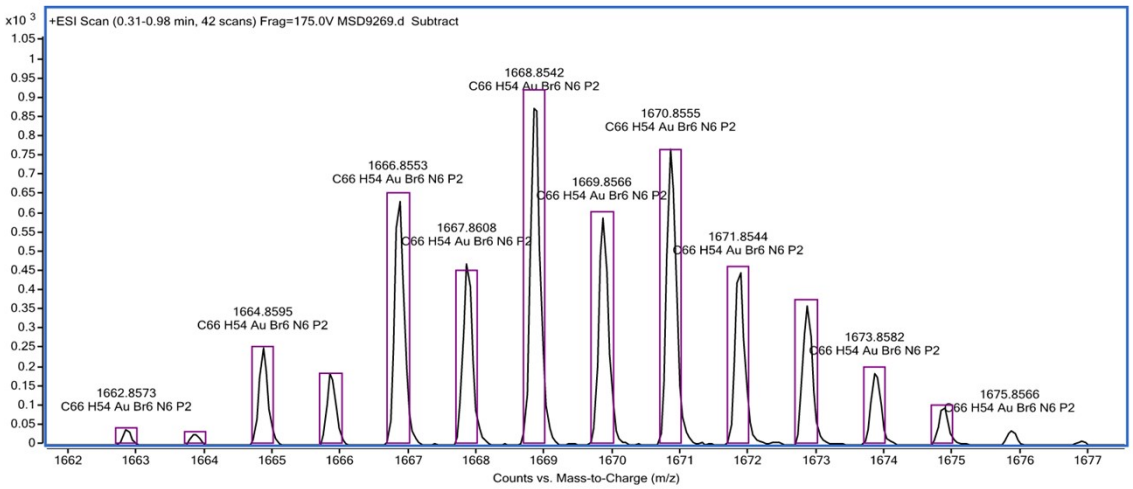


Figure S19. Mass spectra of **6**.

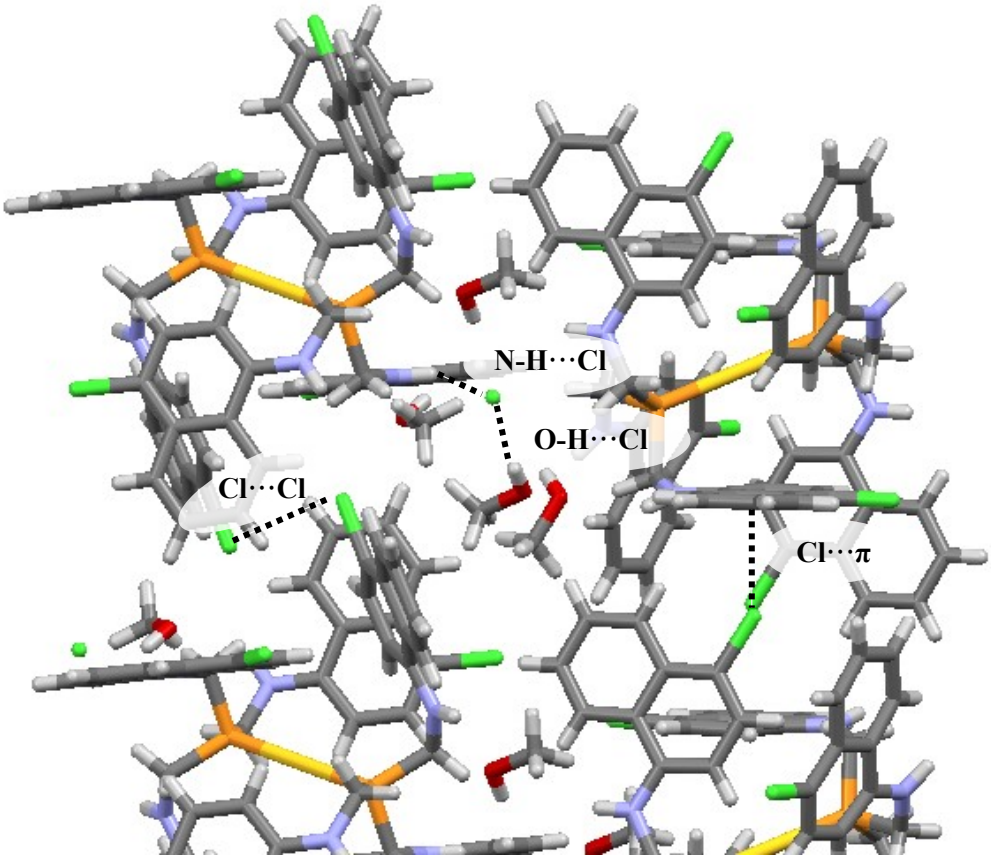


Figure S20. Representation of the packing of **5** showing the short contacts.

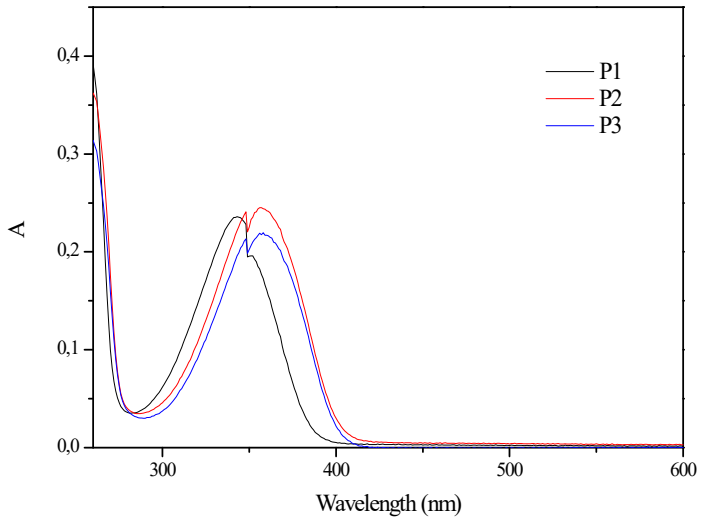


Figure S21. Absorption spectra of phosphanes **P1-3**.

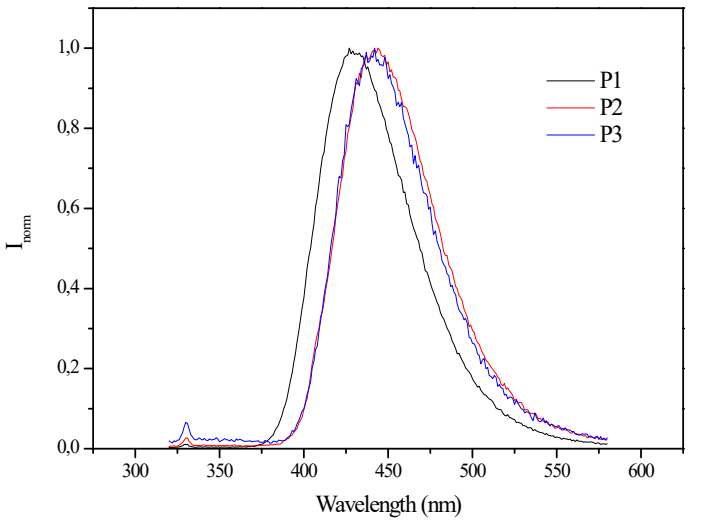


Figure S22. Emission spectra of phosphanes **P1-3**.

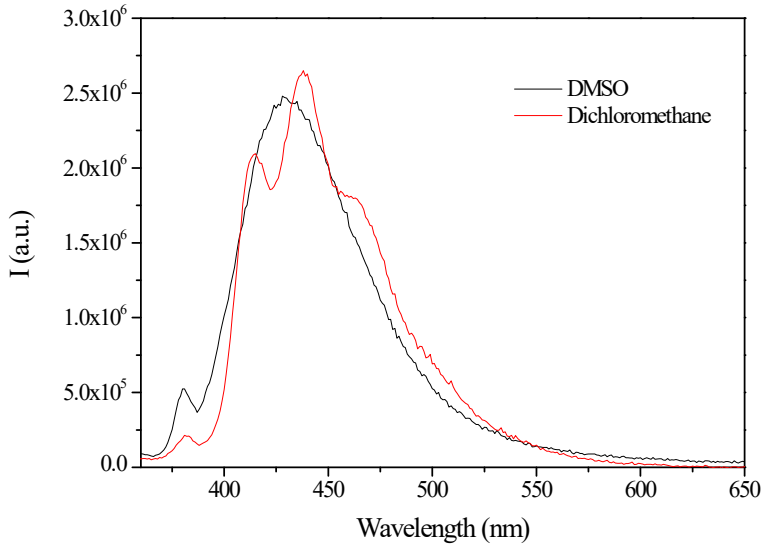


Figure S23. Emission spectra of **4** in different solvents.

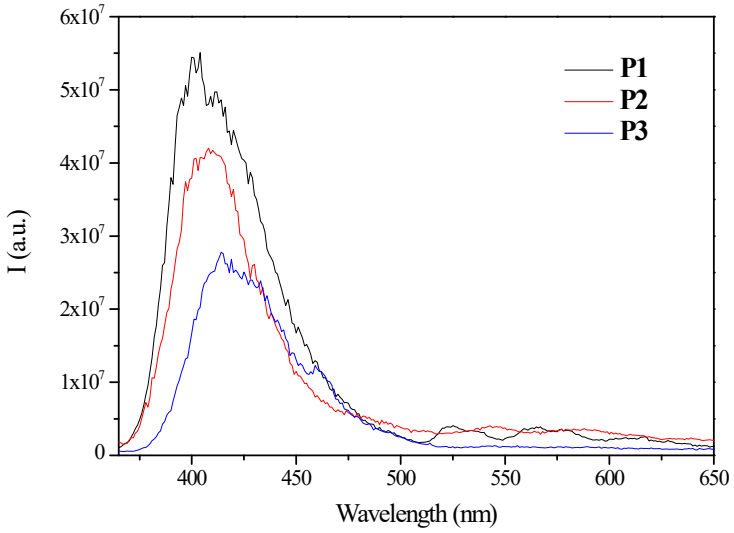


Figure S24. Emission spectra of phosphanes **P1-3** at 77K.

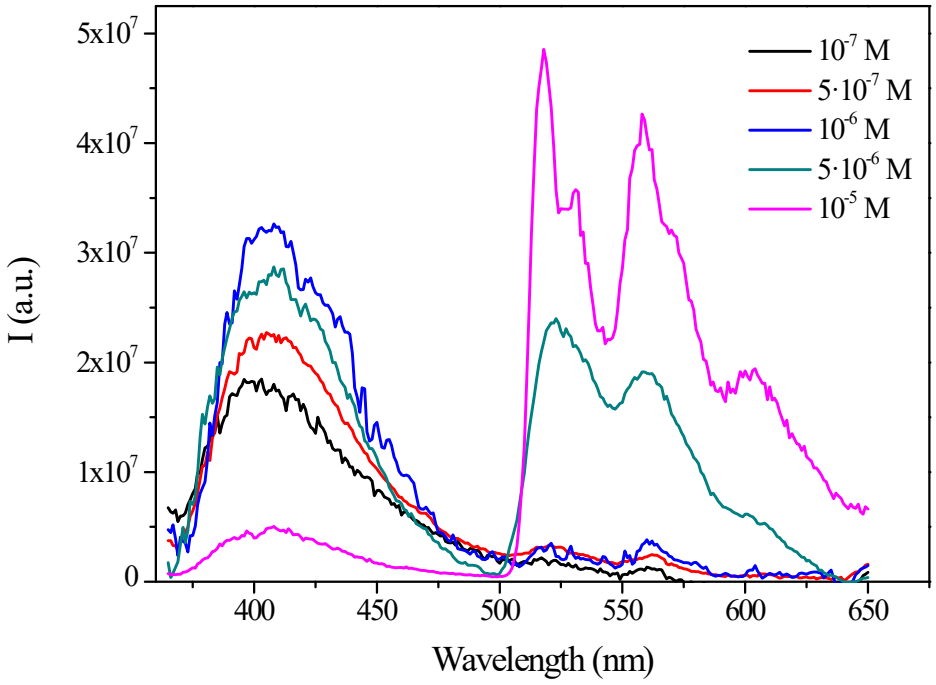


Figure S25. Emission spectra of **4** in different concentrations at 77K.

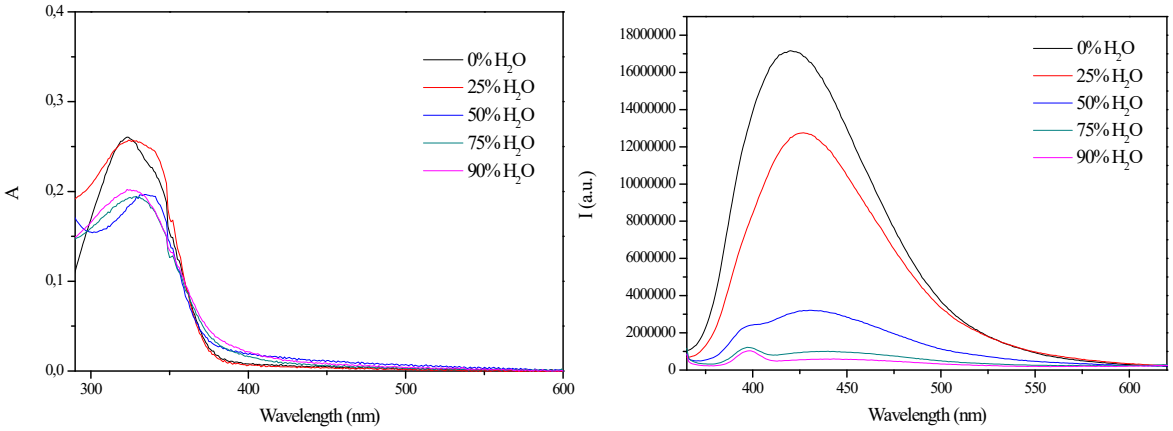
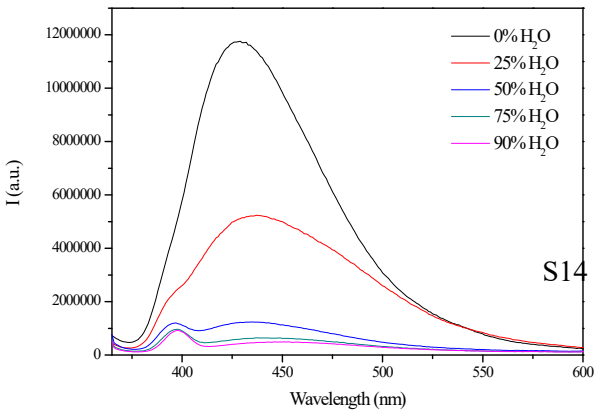


Figure S26. Absorption (left) and emission (right) spectra of complex **1** in DMSO:water mixtures.



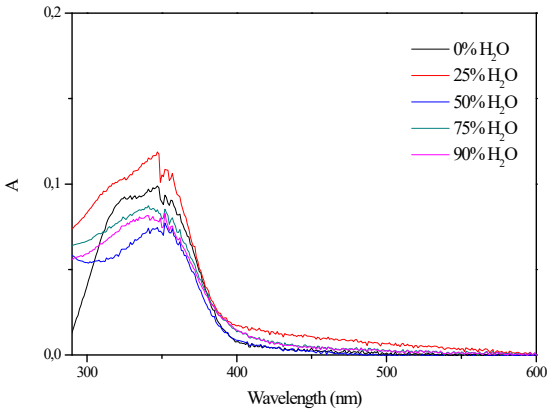


Figure S27. Absorption (left) and emission (right) spectra of complex **3** in DMSO:water mixtures.

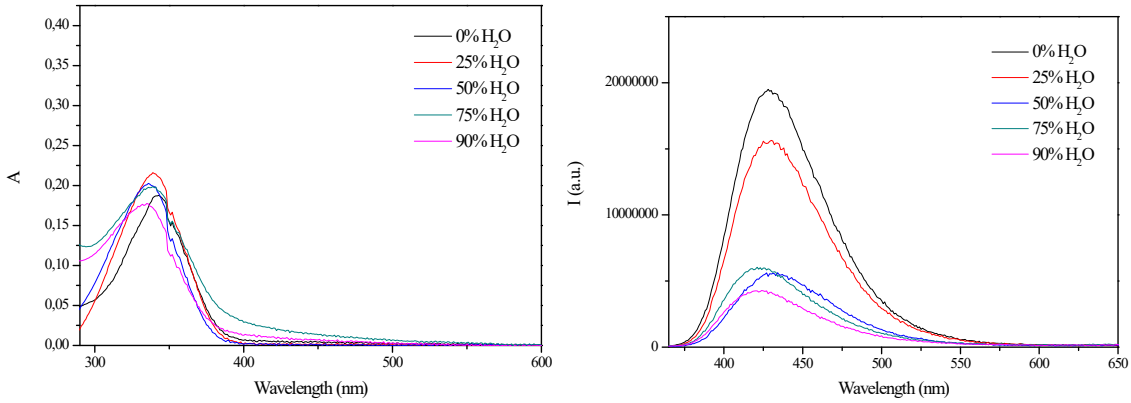


Figure S28. Absorption (left) and emission (right) spectra of complex **P1** in DMSO:water mixtures.

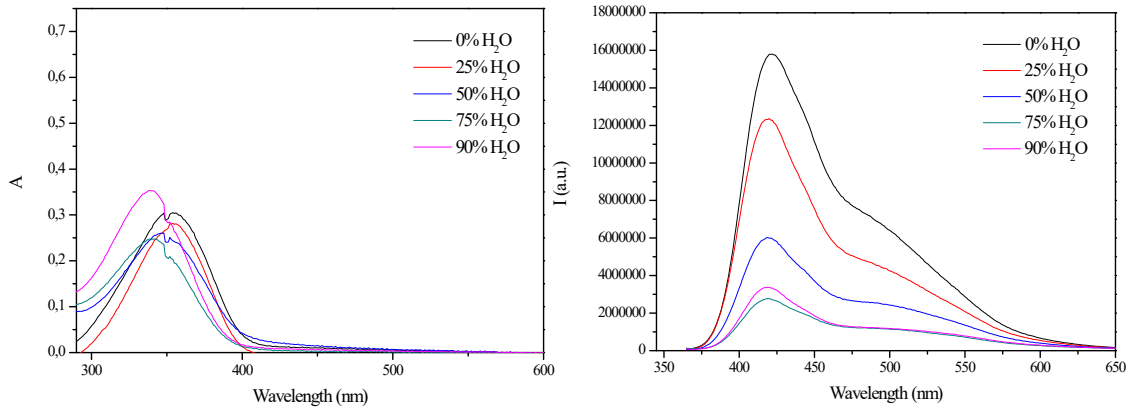


Figure S29. Absorption (left) and emission (right) spectra of complex **P2** in DMSO:water mixtures.

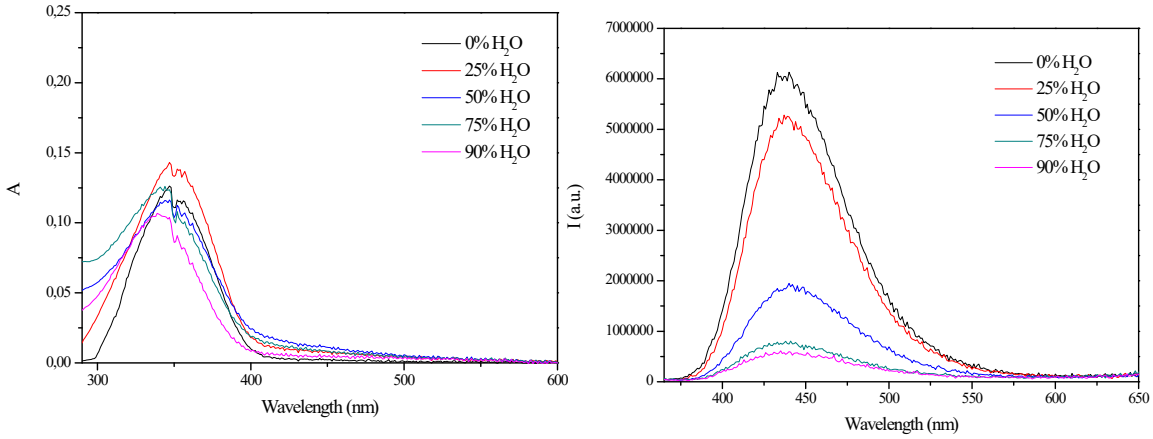


Figure S30. Absorption (left) and emission (right) spectra of complex **P3** in DMSO:water mixtures.

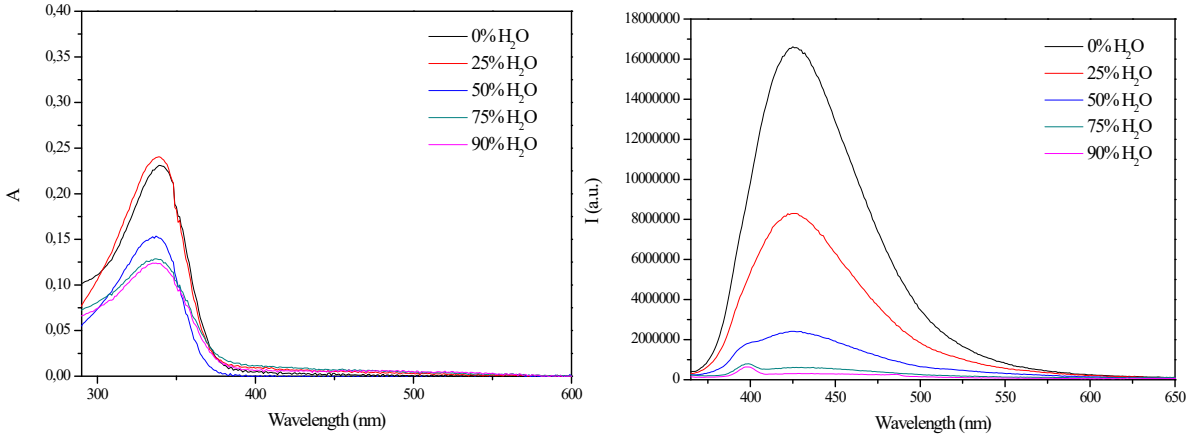


Figure S31. Absorption (left) and emission (right) spectra of complex **4** in DMSO:water mixtures.

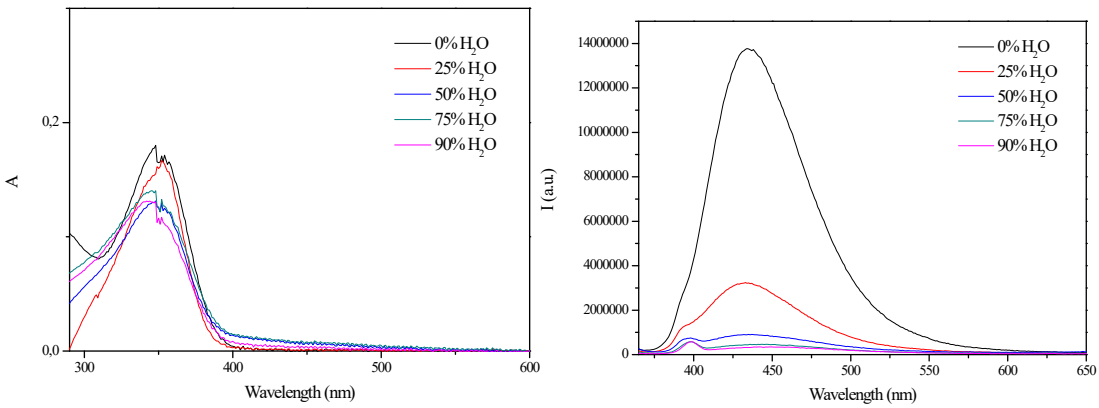


Figure S32. Absorption (left) and emission (right) spectra of complex **6** in DMSO:water mixtures.

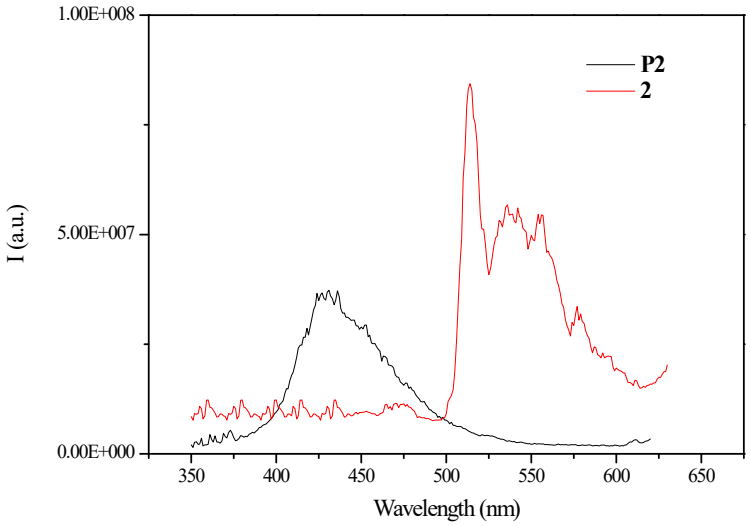


Figure S33. Emission spectra of phosphanes **P2** and gold(I) complexes **2** at 77 K in DMSO/water mixture (10:90).

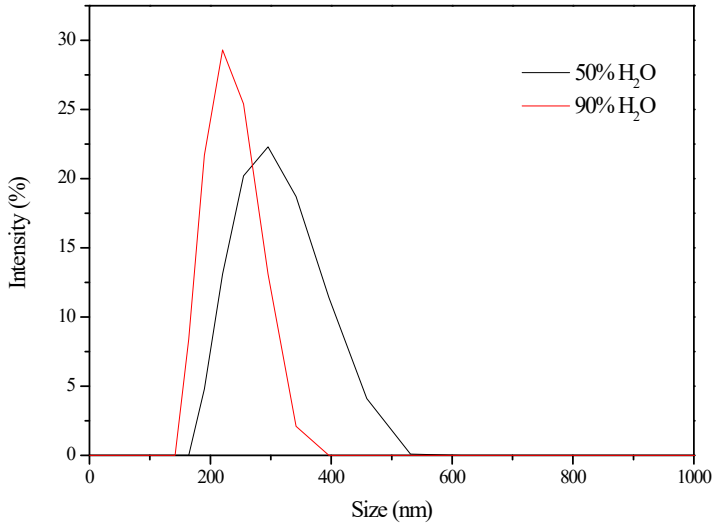


Figure S34. Dynamic light scattering (DLS) of **P1**.

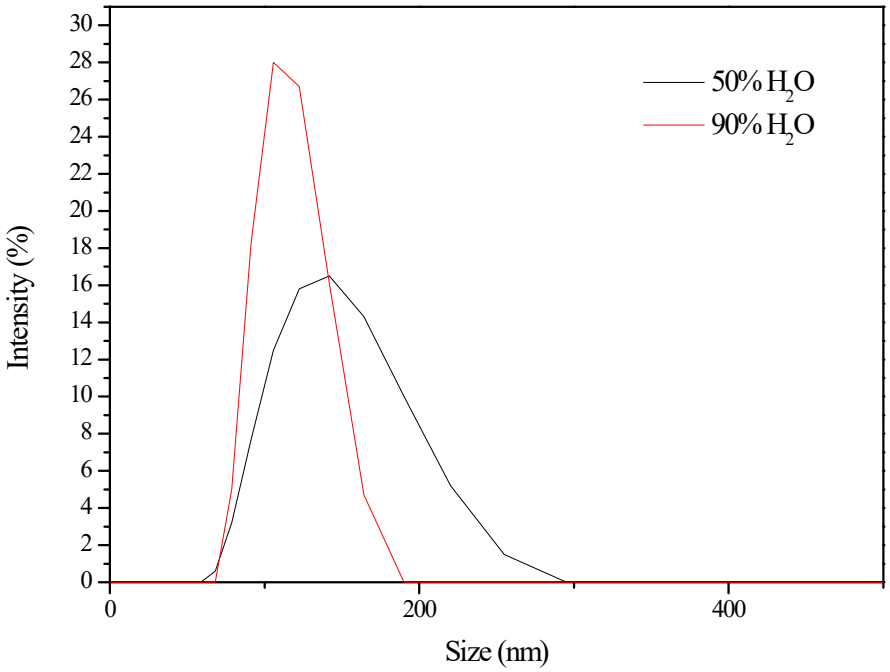


Figure S35. Dynamic light scattering (DLS) of **P2**.

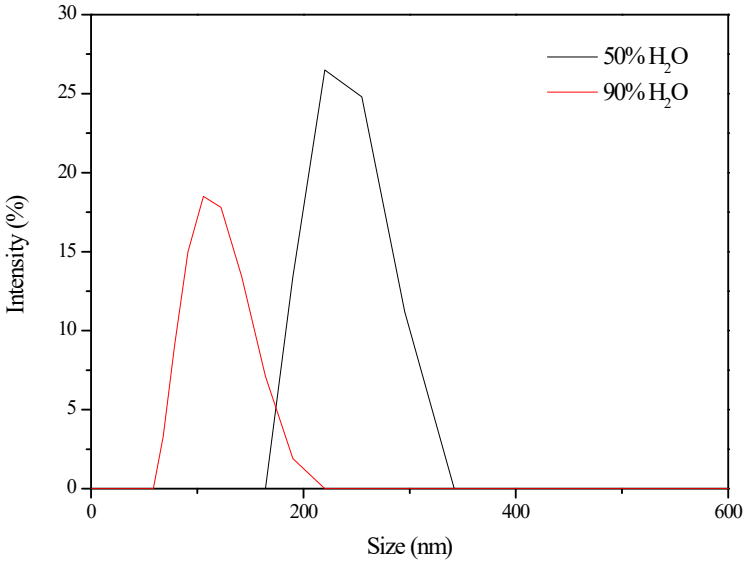


Figure S36. Dynamic light scattering (DLS) of **P3**.

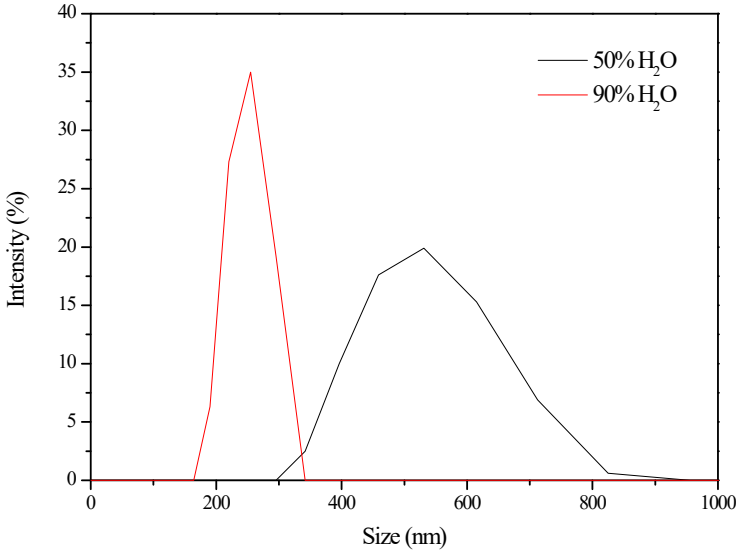


Figure S37. Dynamic light scattering (DLS) of **1**.

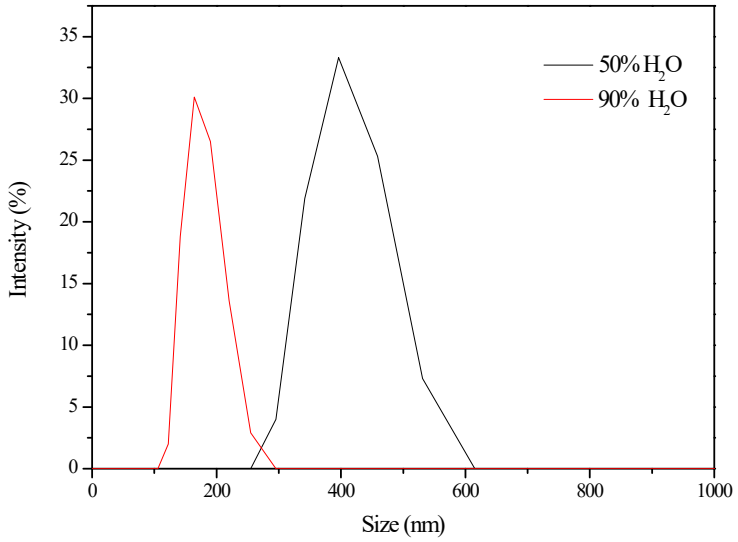


Figure S38. Dynamic light scattering (DLS) of **2**.

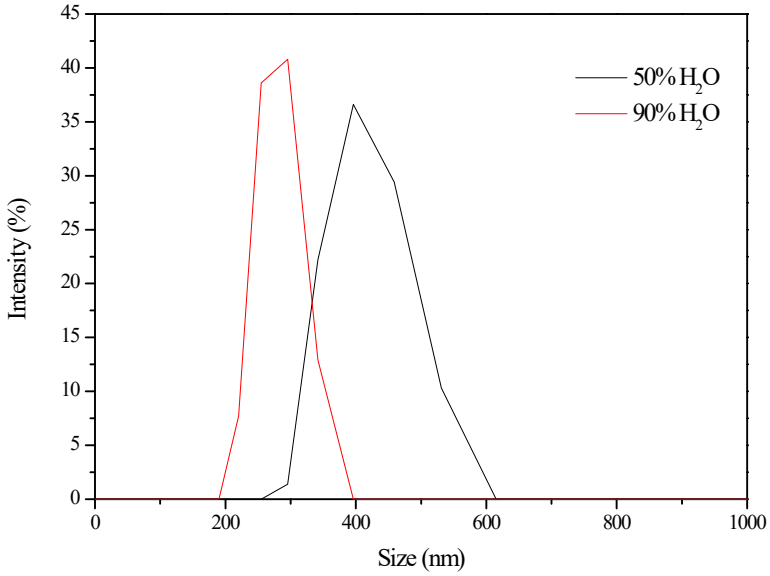


Figure S39. Dynamic light scattering (DLS) of **3**.

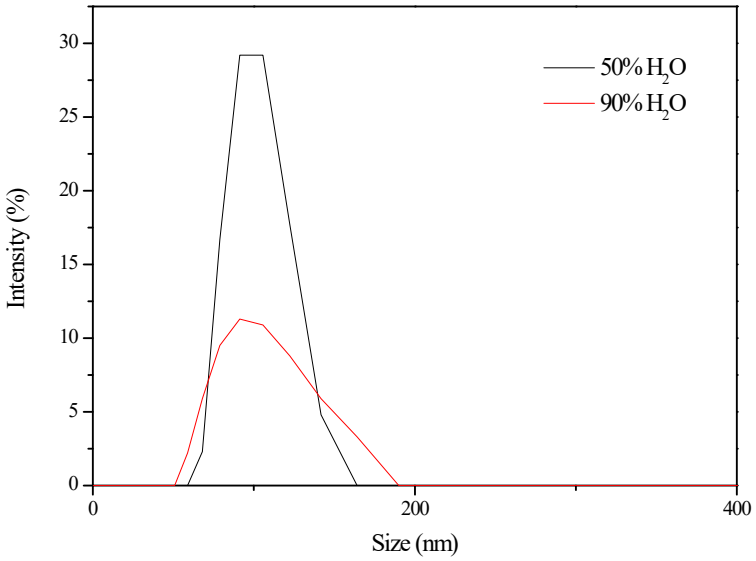


Figure S40. Dynamic light scattering (DLS) of **4**.

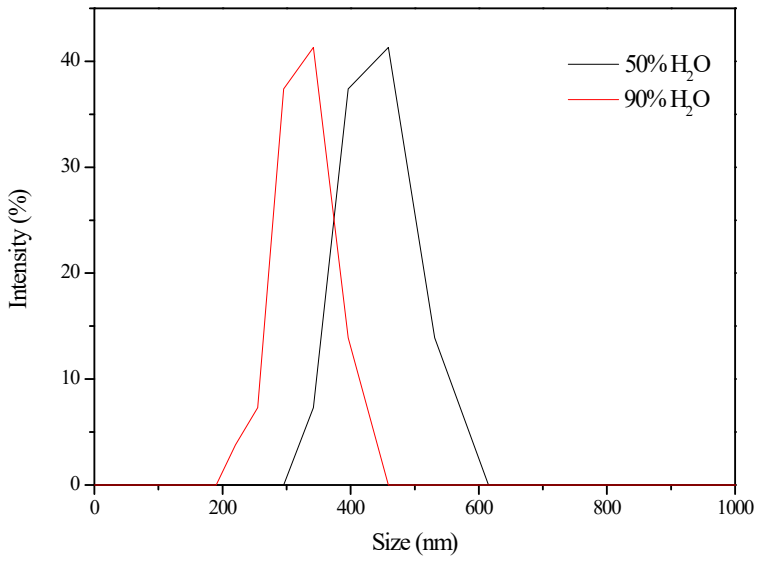


Figure S41. Dynamic light scattering (DLS) of **5**.

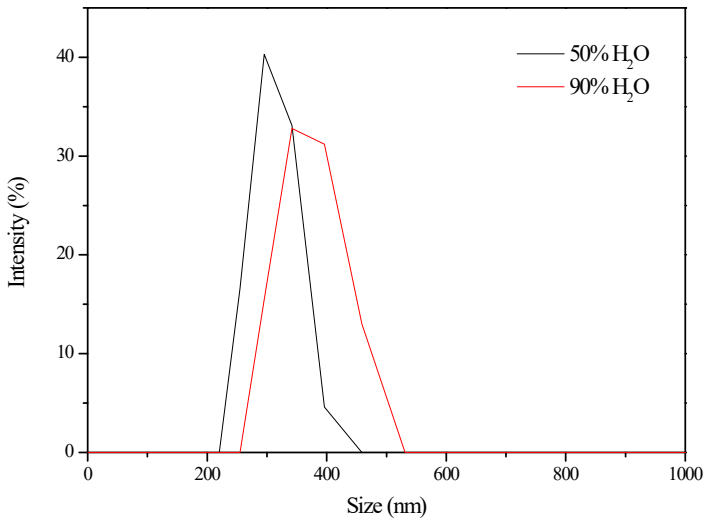


Figure S42. Dynamic light scattering (DLS) of **6**.

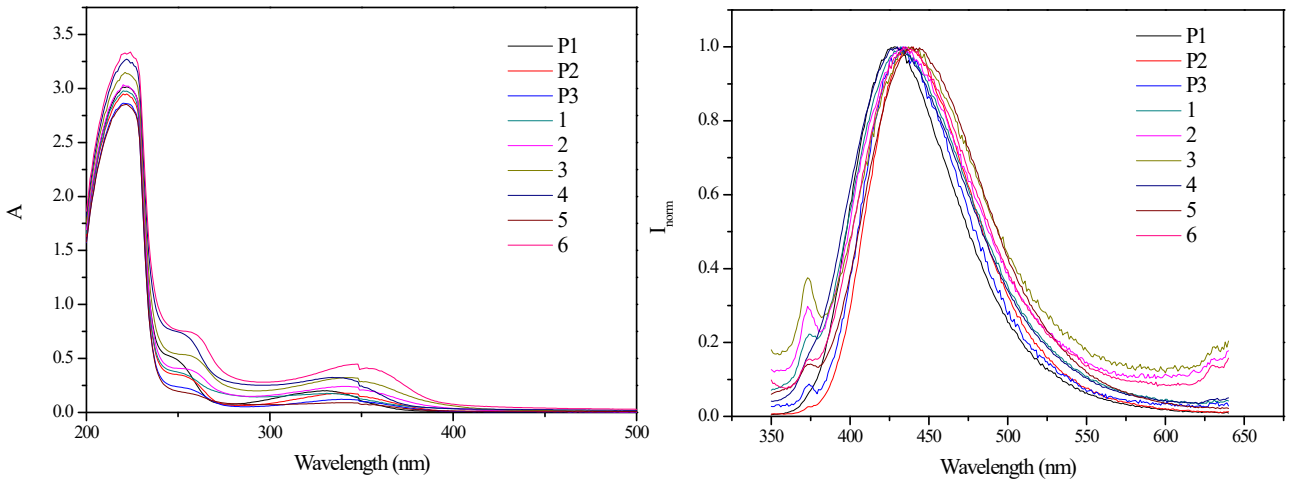


Figure S43. Absorption and emission spectra of phosphanes **P1-3** and gold(I) complexes **1-6** in SDS solutions.

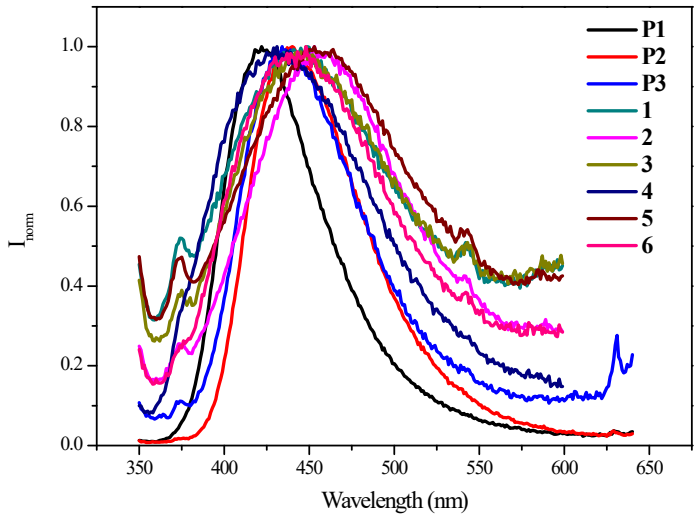


Figure S44. Emission spectra of phosphanes **P1-3** and gold(I) complexes **1-6** in alginate.

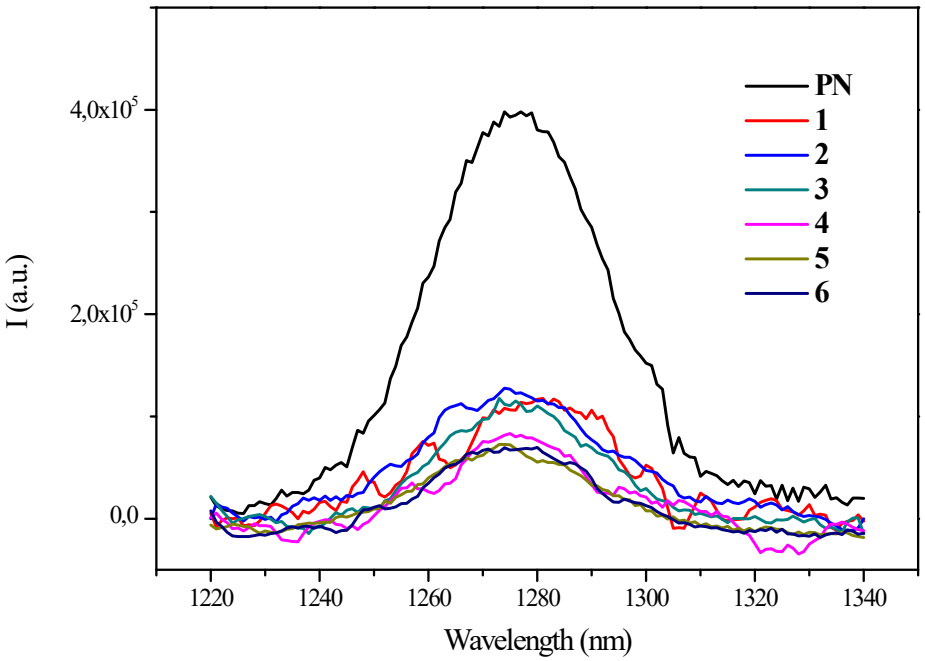


Figure S45. Singlet oxygen spectra for 1H-phenal-1-one (**PN**) and gold(I) complexes **1-6** in dichloromethane upon excitation on the absorption maxima.

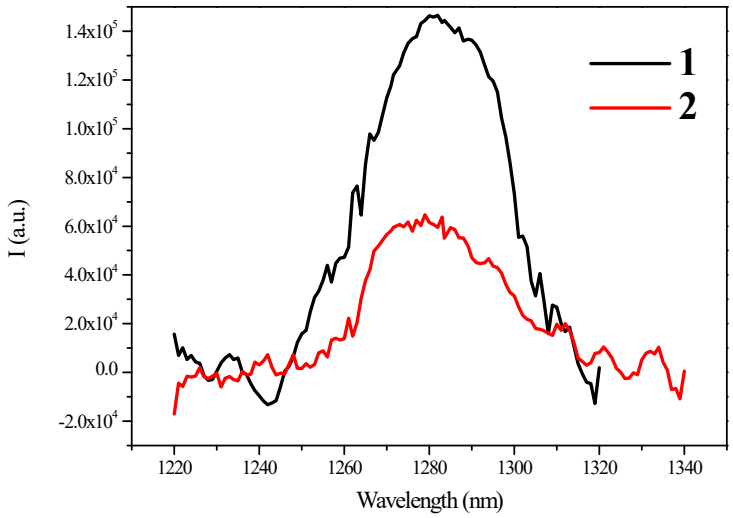


Figure S46. Singlet oxygen spectra for gold(I) complexes **1** and **2** in alginate matrixes upon excitation on the absorption maxima.

Table S1. Crystal data and structure for ***5***

Compound	**5**
Formula	$C_{70}H_{70}AuCl_7N_6O_4P_2$
Crystal size, nm	0.4 x 0.34 x 0.12
Fw	1566.37
Temp., K	170
Wavelength, Å	0.71073
Crystal system	Monoclinic
Space group	C 1 2/c 1
a, Å	20.0915(6)
b, Å	14.5770(4)
c, Å	24.3861(7)
α, º	90
β, º	107.1290(10)
γ, º	90
Volume, Å^3	6825.3(3)
Z	4
D_{calc}, mg m^{-3}	1.524
Abs. coef., mm^{-1}	2.530
F(000)	3168
θ range for data coll, º	1.748 to 28.282
Reflns coll./independent	16013/8486

Data/restraint/parameters	8486/150/412
GOF on F^2	1.278
Final R index ($I > 2\sigma(I)$)	$R_1 = 0.0465$ $wR_2 = 0.1200$
R index (all data)	$R_1 = 0.0569$ $wR_2 = 0.1244$
Peak and hole, e $Å^{-3}$	1.319 and -1.140
CCDC	2165920

Table S2. Phosphorescent quantum yield, lifetime, radiative and non-radiative rate constants for gold(I) **1-6** in dimethyl sulfoxide at 77K.

Compound	Φ_{Ph}	τ_{Ph} (ms)	k_r (ms^{-1})	k_{nr} (ms^{-1})
1	0.41	2.3	0.178	0.256
2	0.22	2.6	0.084	0.300
3	0.10	1.9	0.052	0.473
4	0.53	3.1	0.170	0.151
5	0.56	2.6	0.215	0.169
6	0.17	1.9	0.089	0.436

Table S3. Emission maxima of phosphanes **P1-3** and gold(I) complexes **1-6** in DMSO, PBS, alginate and SDS.

Compound	Emission spectra (DMSO)	Emission spectra (alginate)	Emission spectra (SDS)
P1	430	422	428
P2	446	440	440

P3	446	434	433
1	420	449	432
2	431	453	434
3	428	448	437
4	426	431	430
5	439	453	439
6	437	448	434