Tripodal gold(I) polypyridyl complexes and their Cu+ and Zn2+ heterometallic derivatives. Effects on luminescence

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Supporting Information

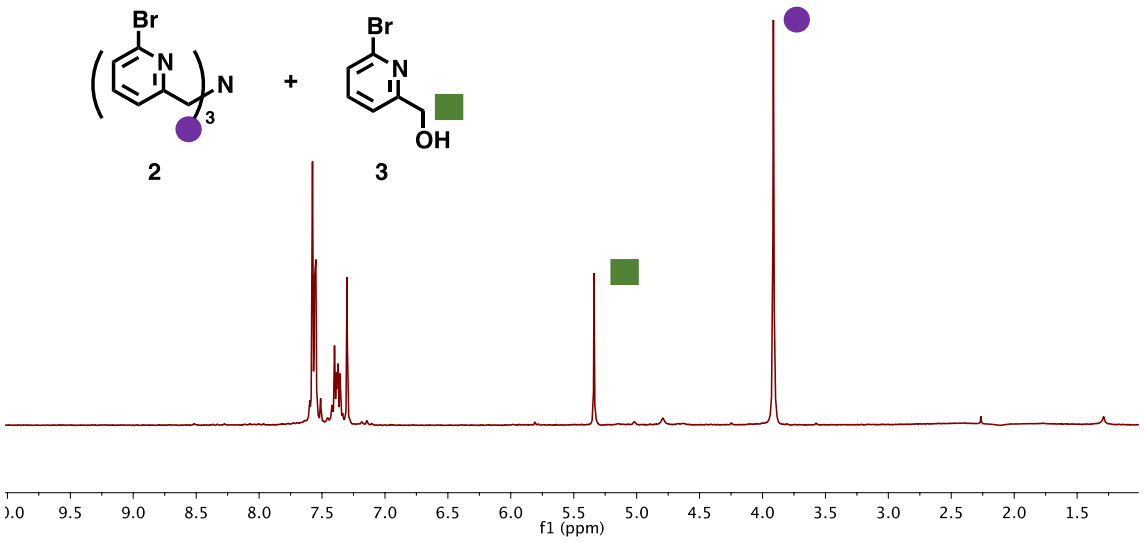


Figure S1. ^{1}H-NMR spectrum of the crude reaction mixture for the synthesis of **L1**.

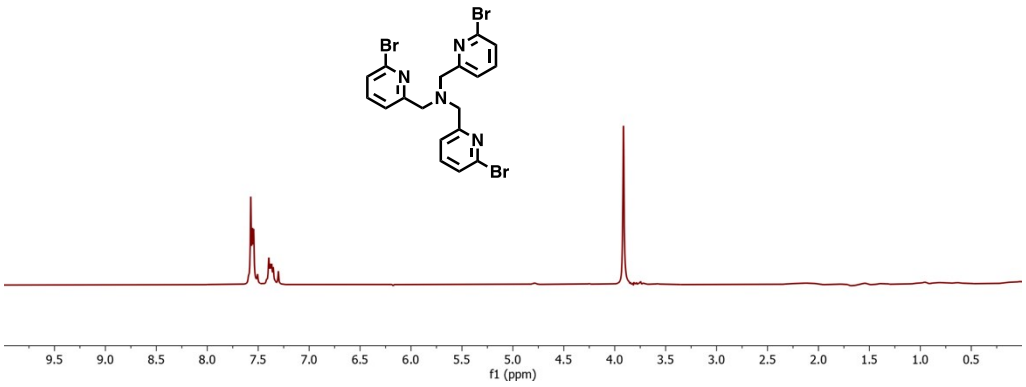


Figure S2. ^{1}H NMR spectrum of **L1** in $CDCl_3$.

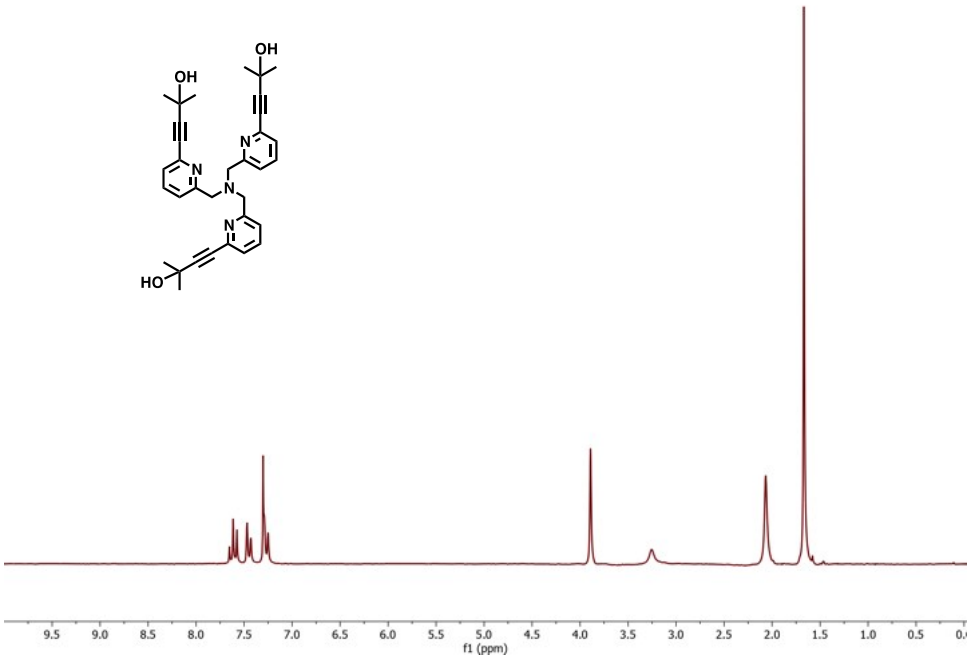


Figure S3. ^{1}H NMR spectrum of protected **L2** in $CDCl_3$.

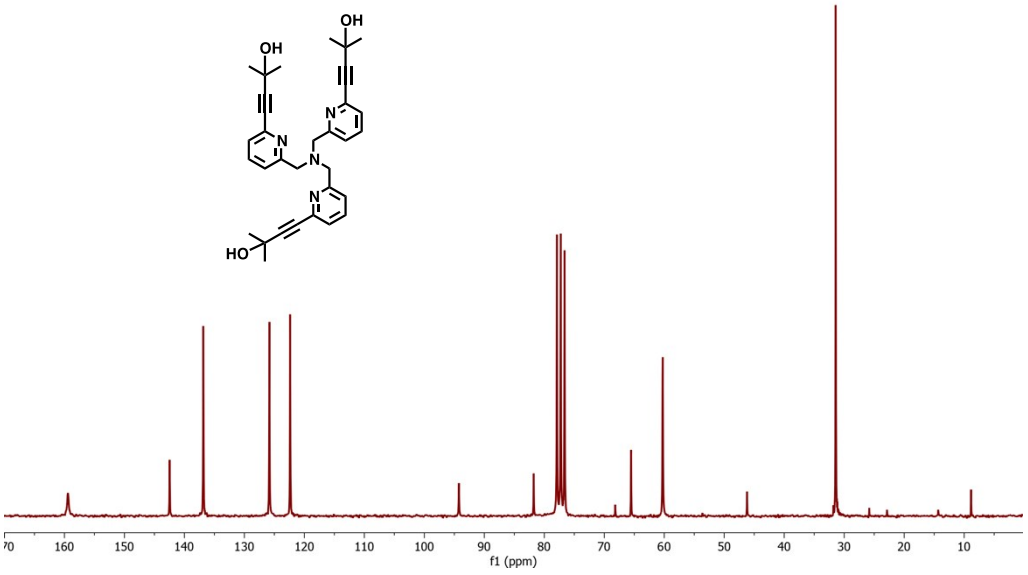


Figure S4. ^{13}C NMR spectrum of protected **L2** in $CDCl_3$.

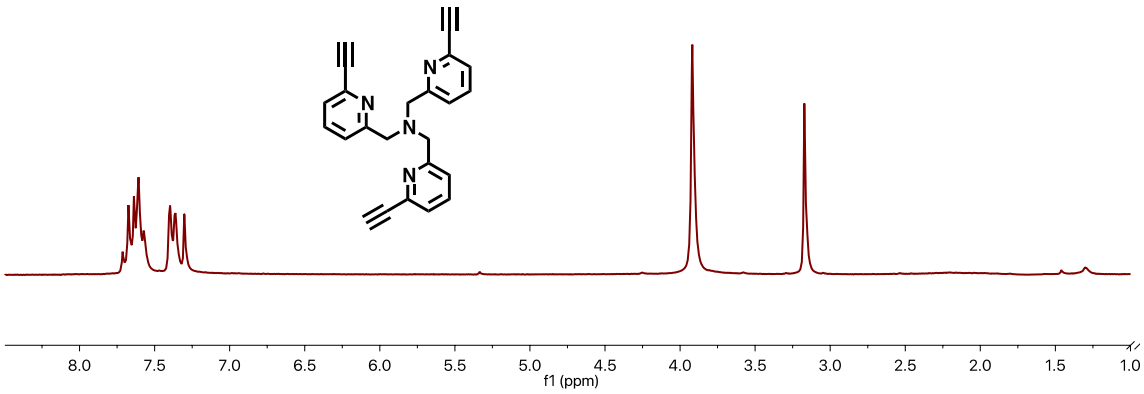


Figure S5. ^{1}H NMR spectrum of **L** in $CDCl_3$

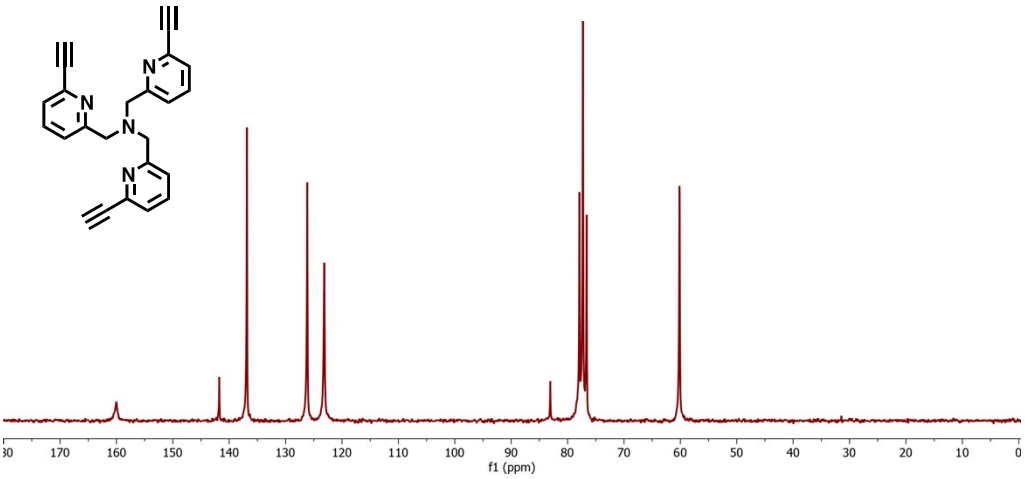


Figure S6. ^{13}C NMR spectrum of **L** in $CDCl_3$.

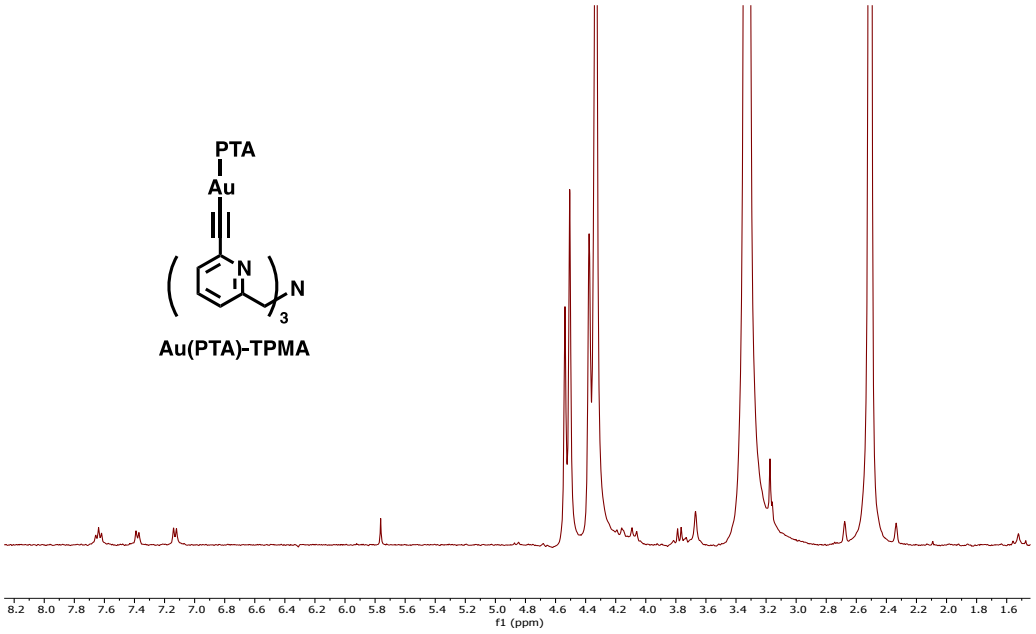


Figure S7. ^{1}H NMR spectrum of **1** in DMSO-d_6

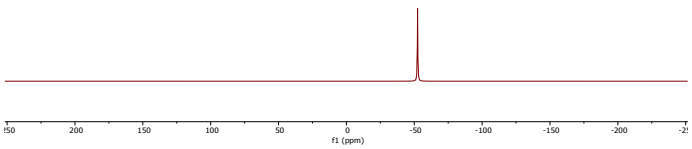


Figure S8. ^{31}P NMR spectrum of **1** in DMSO-d_6

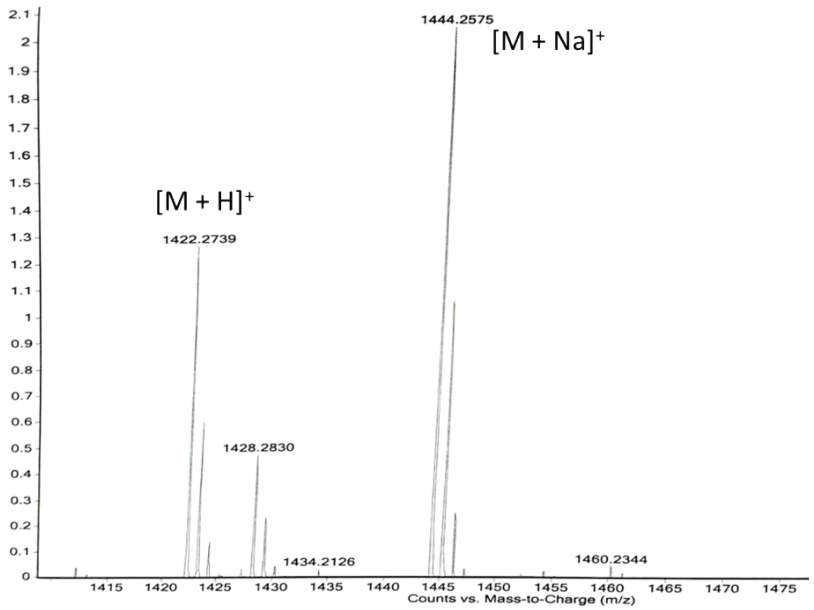


Figure S9. ESI-MS(+) spectrum of **1**.

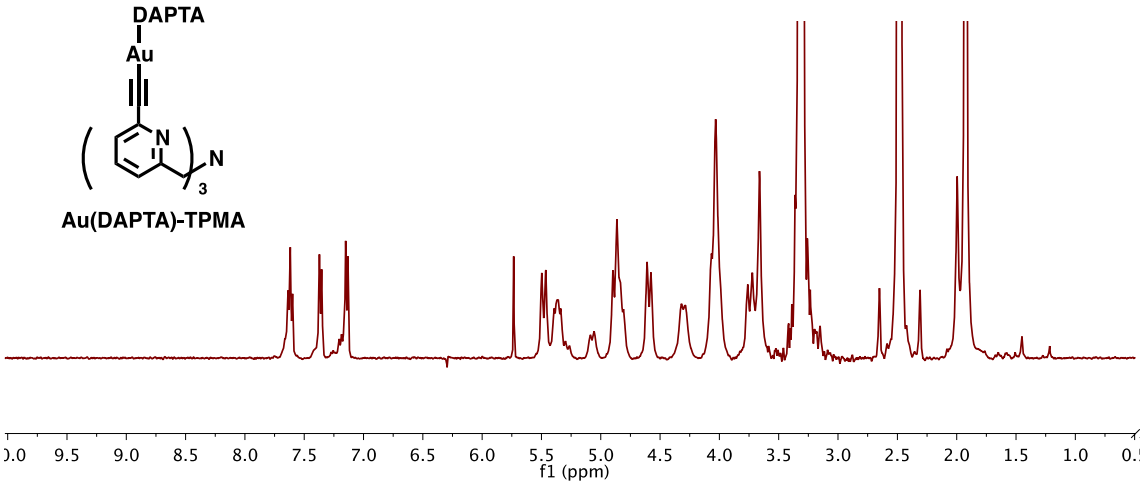


Figure S10. ^{1}H NMR spectrum of **2** in DMSO-d_6

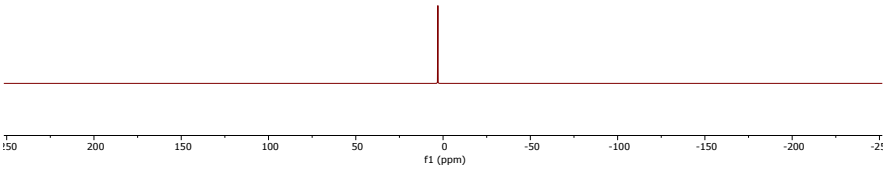


Figure S11. ^{31}P NMR spectrum of **2** in DMSO-d_6

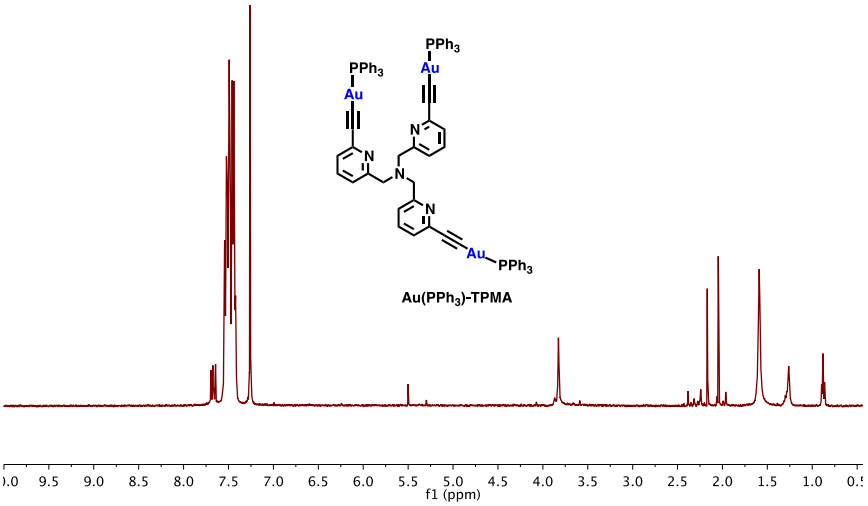


Figure S12. ^{1}H NMR spectrum of **3** in $CDCl_3$

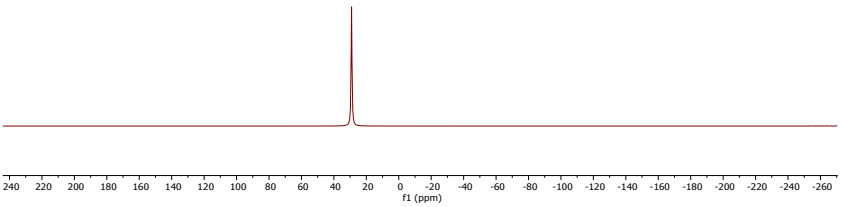


Figure S13. ^{31}P NMR spectrum of **3** in $CDCl_3$

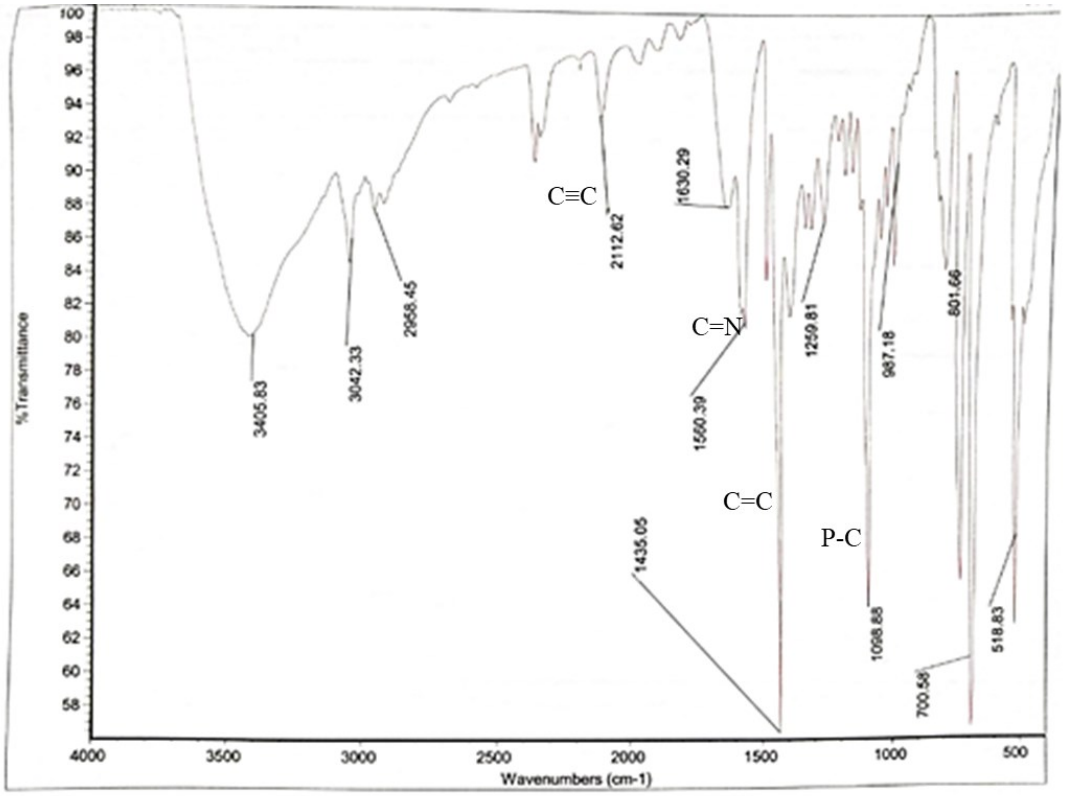


Figure S14. IR spectrum of **4**.

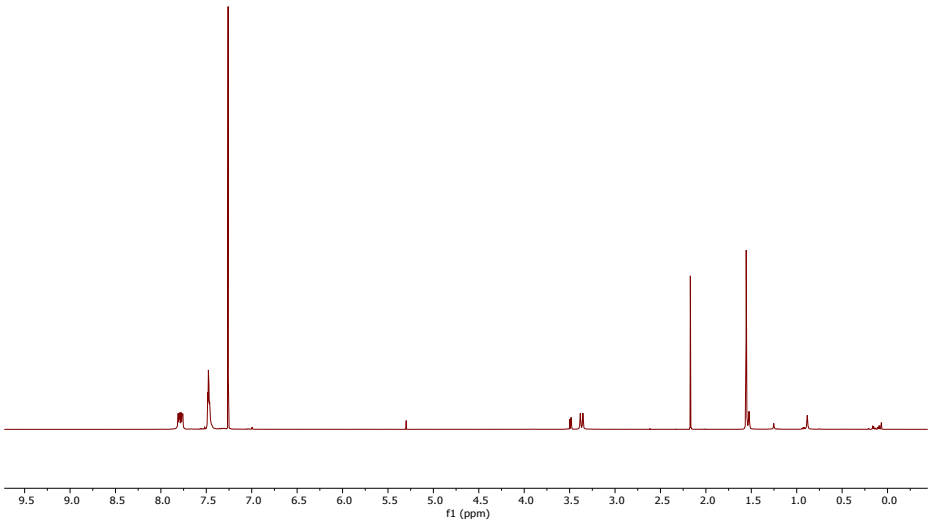


Figure S15. ^{1}H NMR spectrum of **4** in $CDCl_3$.

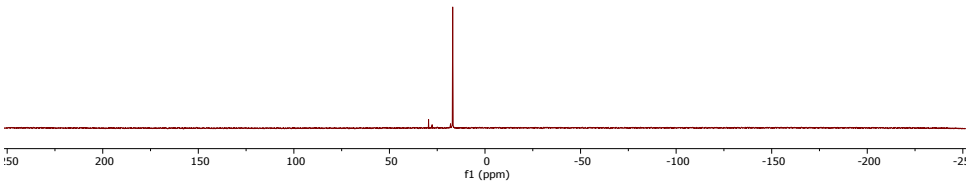


Figure S16. ^{31}P NMR spectrum of **4** in $CDCl_3$

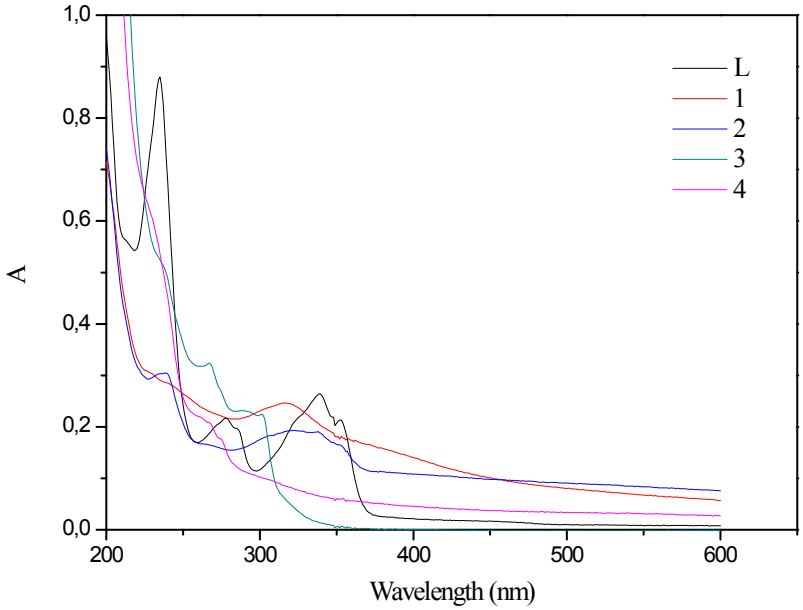


Figure S17. Absorption spectra in in acetonitrile of compounds **L** and **1-4** at *ca*. $1 \cdot 10^{-5}$ M.

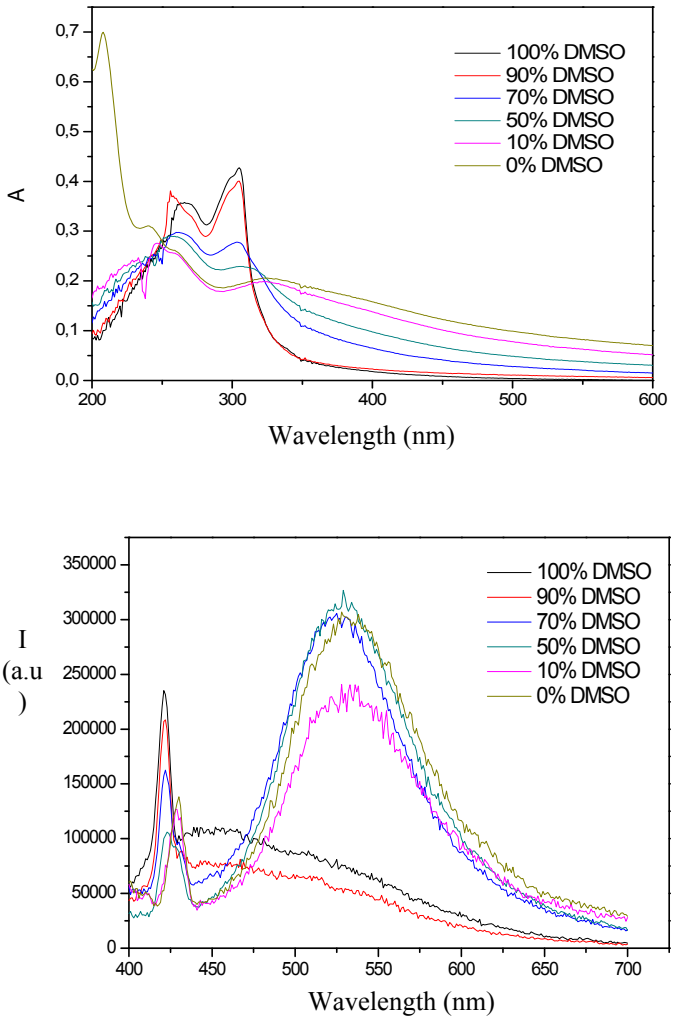


Figure S18. Absorption (above) and emission (below) spectra of **1** at different DMSO-water content.

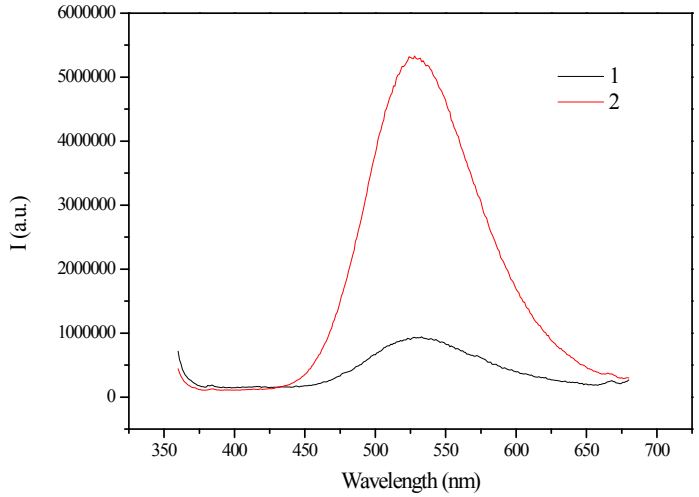


Figure S19. Solid emission spectra of **1** and **2** (λ_{exc} = 350 nm).

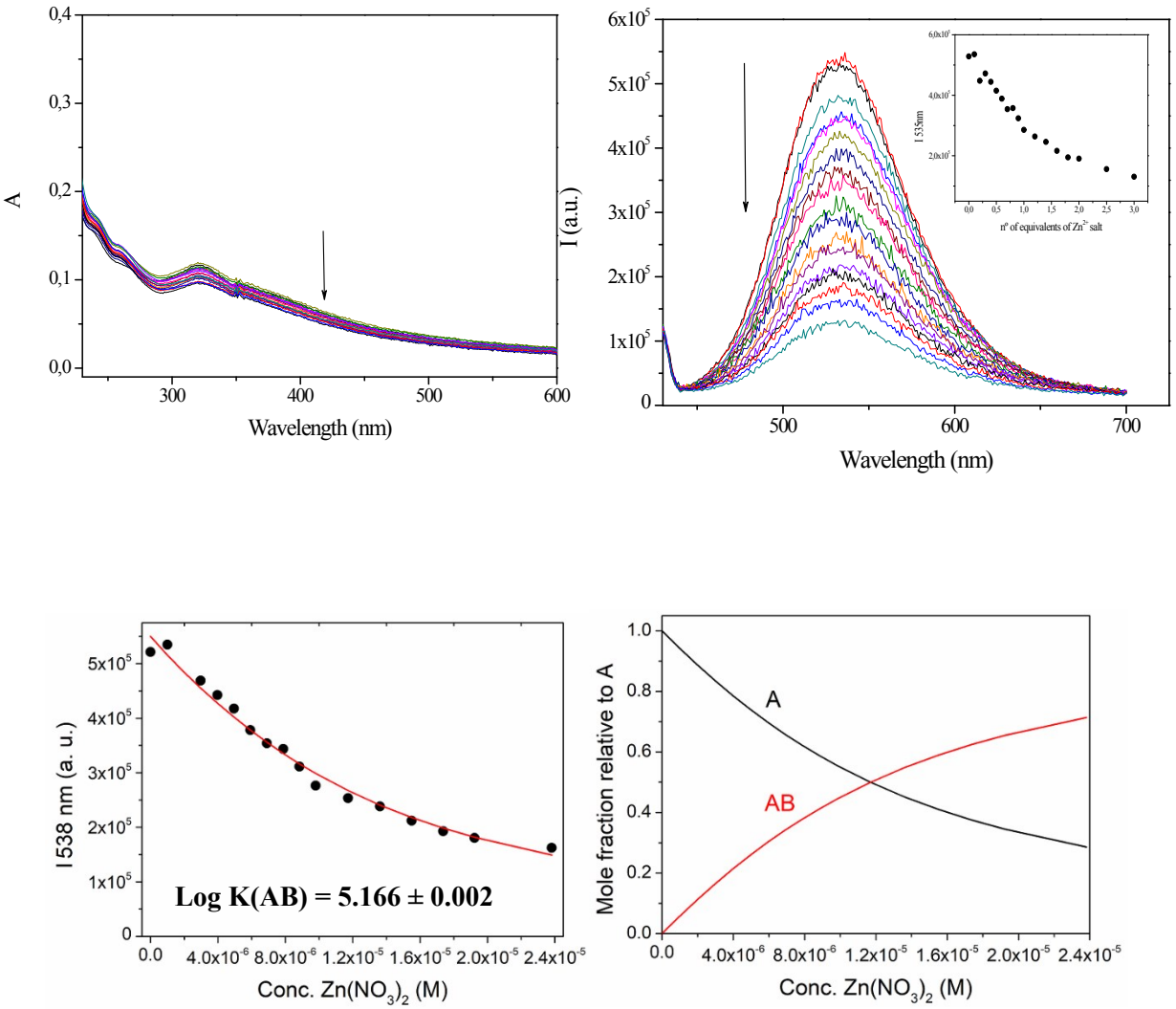
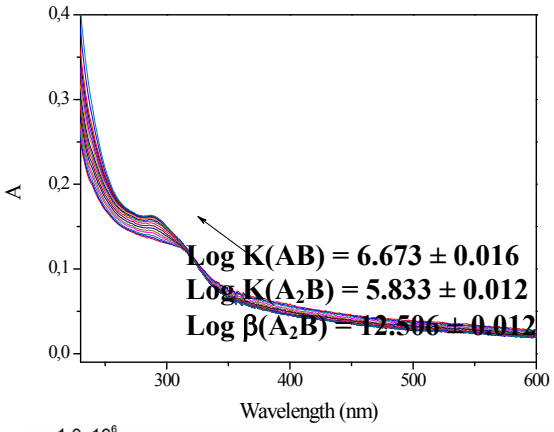
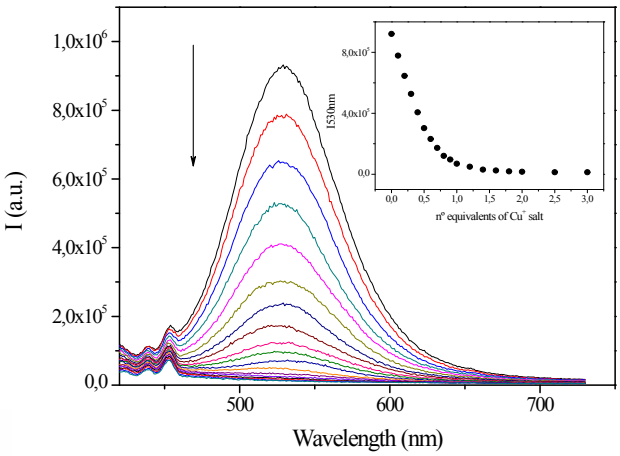
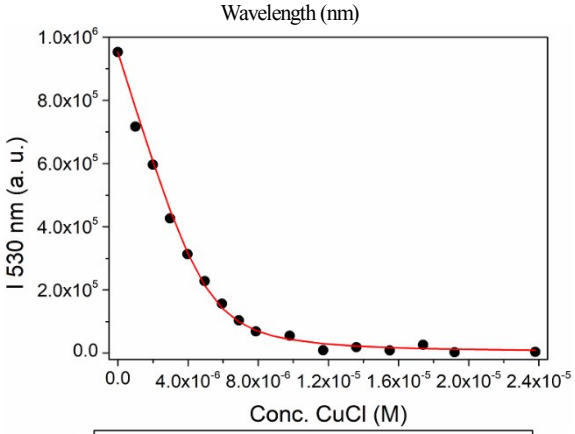
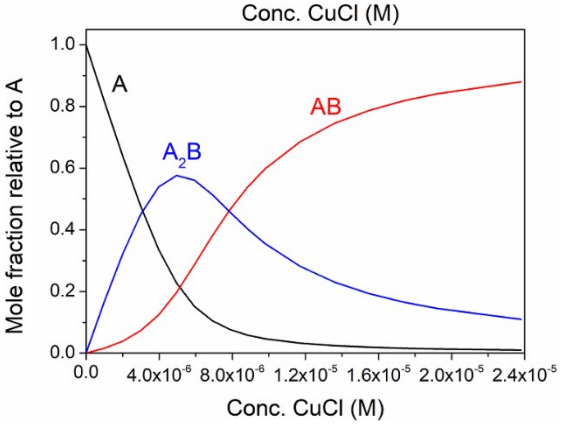


Figure S20. (above) Absorption and emission titrations of **1** with increasing amounts of $Zn(NO_3)_2$ in methanol at $1 \cdot 10^{-5}$M; (below) Left: Variations in the emission maximum of compound **1** ($1 \cdot 10^{-5}$M) upon addition of $Zn(NO_3)_2$ in MeOH. Fitting of the spectral variations with HypSpec program agrees with the formation of the 1:1 complex. Right: Calculated mole fractions of free compound **1** (A) and complex 1:1 (AB) with increasing amounts of $Zn(NO_3)_2$.


A
Wavelength (nm)
Log K(AB) = 6.673 ± 0.016
Log K(A2B) = 5.833 ± 0.012
Log β(A2B) = 12.506 ± 0.012


I (a.u.)
Wavelength (nm)
I530nm
nº equivalents of Cu2+ salt


I 530 nm (a. u.)
Conc. CuCl (M)


Mole fraction relative to A
A
AB
A2B
Conc. CuCl (M)

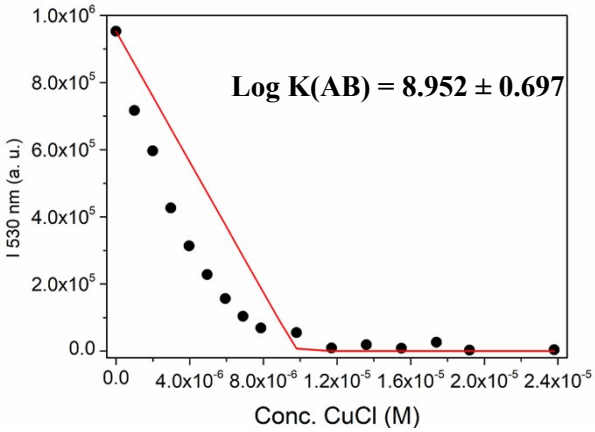
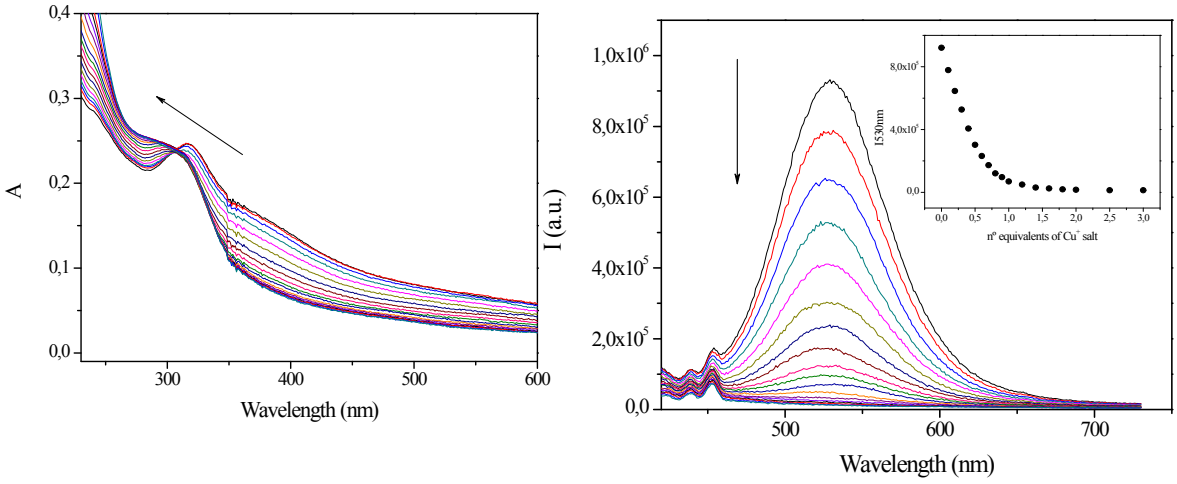
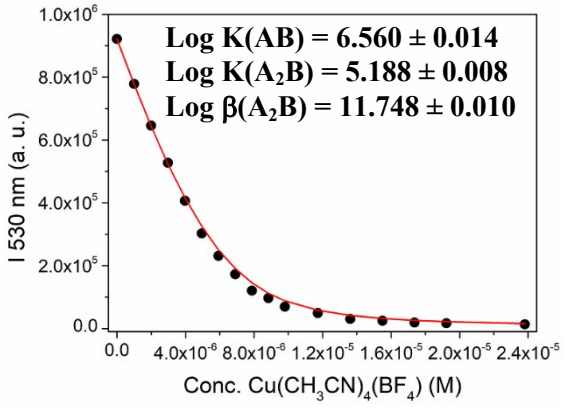
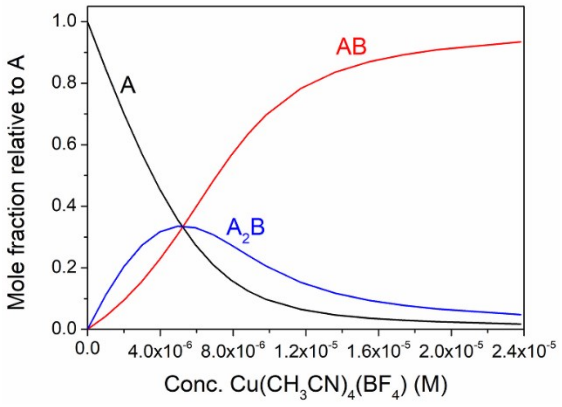

Log K(AB) = 8.952 ± 0.697
I 530 nm (a. u.)
Conc. CuCl (M)

Figure S21. (above) Absorption and emission titrations of **1** with increasing amounts of CuCl in acetonitrile at $1 \cdot 10^{-5}$M; (middle) Left: Variations in the emission maximum of compound **1** ($1 \cdot 10^{-5}$M) upon addition of CuCl in CH_3CN. Fitting of the spectral variations with HypSpec program agrees with the formation of the 1:1 complex (AB) and the intermediate species (A_2B). Right: Calculated mole fractions of free compound **1** (A) and complexes 2:1 (A_2B) and 1:1 (AB) with increasing amounts of CuCl; (below) Best fitting calculated with HypSpec corresponding to the emission titration of compound **1** ($1 \cdot 10^{-5}$M) with increasing amounts of CuCl in CH_3CN, considering only formation of complex 1:1.







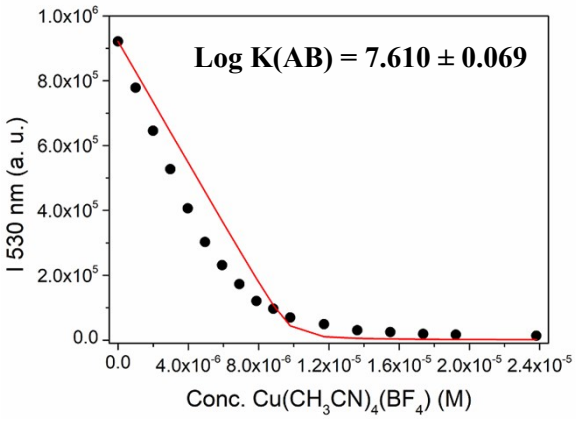
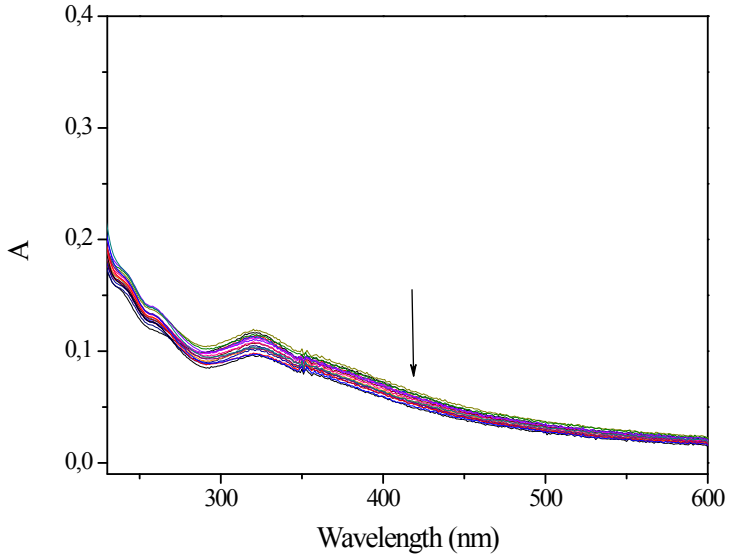


Figure S22. (above) Absorption and emission titrations of **1** with increasing amounts of $[Cu(CH_3CN)_4](BF_4)$ in acetonitrile at $1\cdot10^{-5}$M; (middle) Left: Variations in the emission maximum of compound **1** ($1\cdot10^{-5}$M) upon addition of $Cu(CH_3CN)_4(BF_4)$ in CH_3CN. Fitting of the spectral variations with HypSpec program agrees with the formation of the 1:1 complex (AB) and the intermediate species (A_2B). Right: Calculated mole fractions of free compound **1** (A) and complexes 2:1 (A_2B) and 1:1 (AB) with increasing amounts of $Cu(CH_3CN)_4(BF_4)$; (below) Best fitting calculated with HypSpec corresponding to the emission titration of compound **1** ($1\cdot10^{-5}$M) with increasing amounts of $Cu(CH_3CN)_4(BF_4)$ in CH_3CN, considering only formation of complex 1:1.



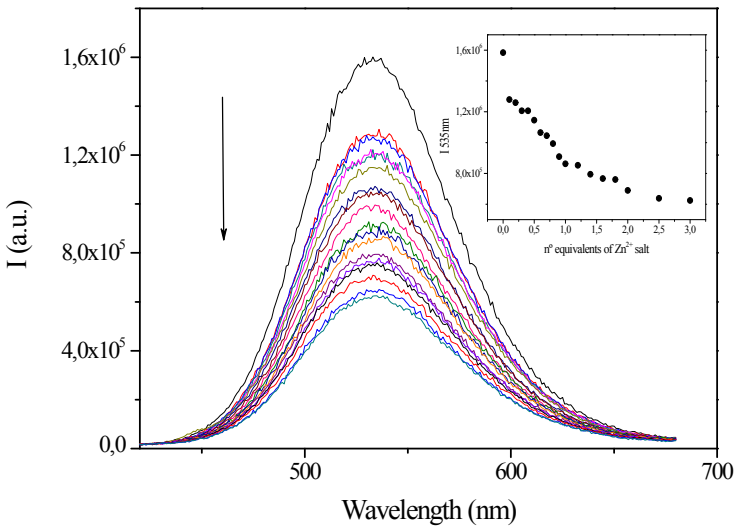


Figure S23. Absorption (above) and emission (below) titrations of **2** with increasing amounts of $Zn(NO_3)_2$ in methanol at $1 \cdot 10^{-5}$M.

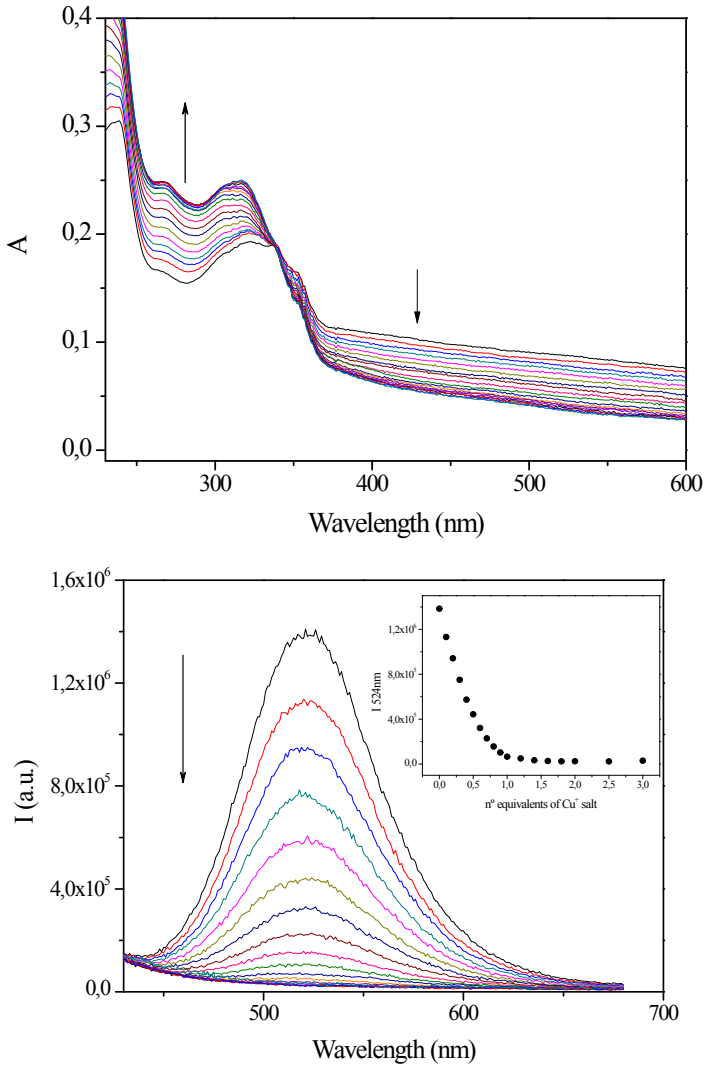


Figure S24. Absorption (above) and emission (below) titrations of **2** with increasing amounts of CuCl in acetonitrile at $1 \cdot 10^{-5}$M.

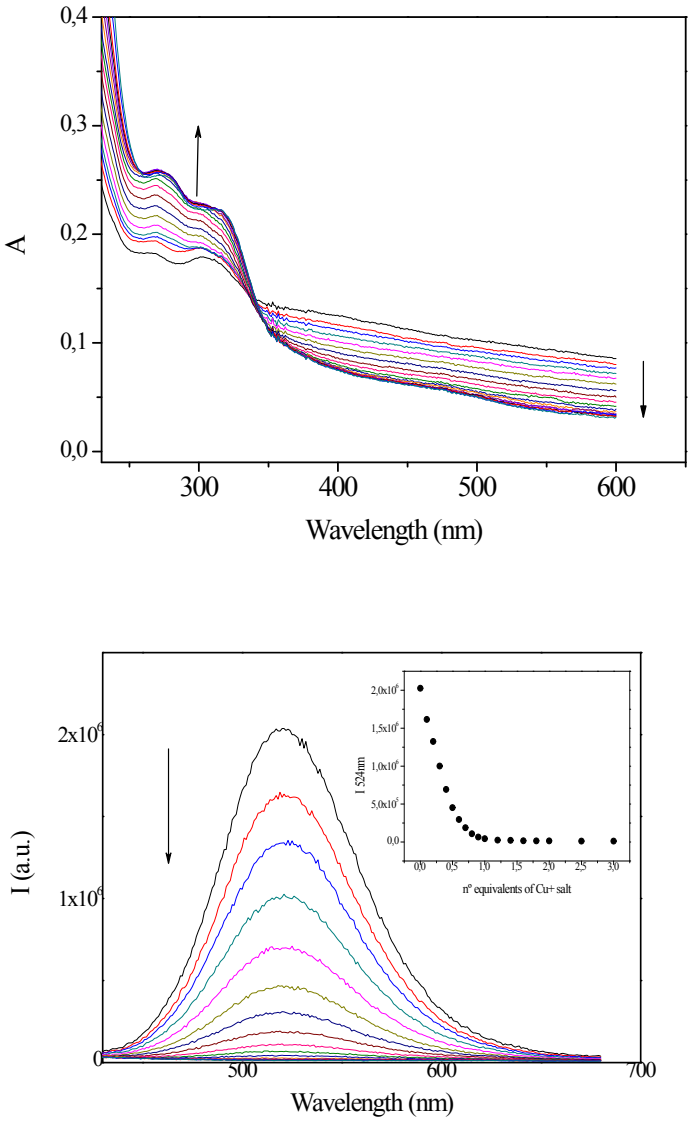


Figure S25. Absorption (above) and emission (below) titrations of **2** with increasing amounts of $[Cu(CH_3CN)_4](BF_4)$ in acetonitrile at $1 \cdot 10^{-5}$M.

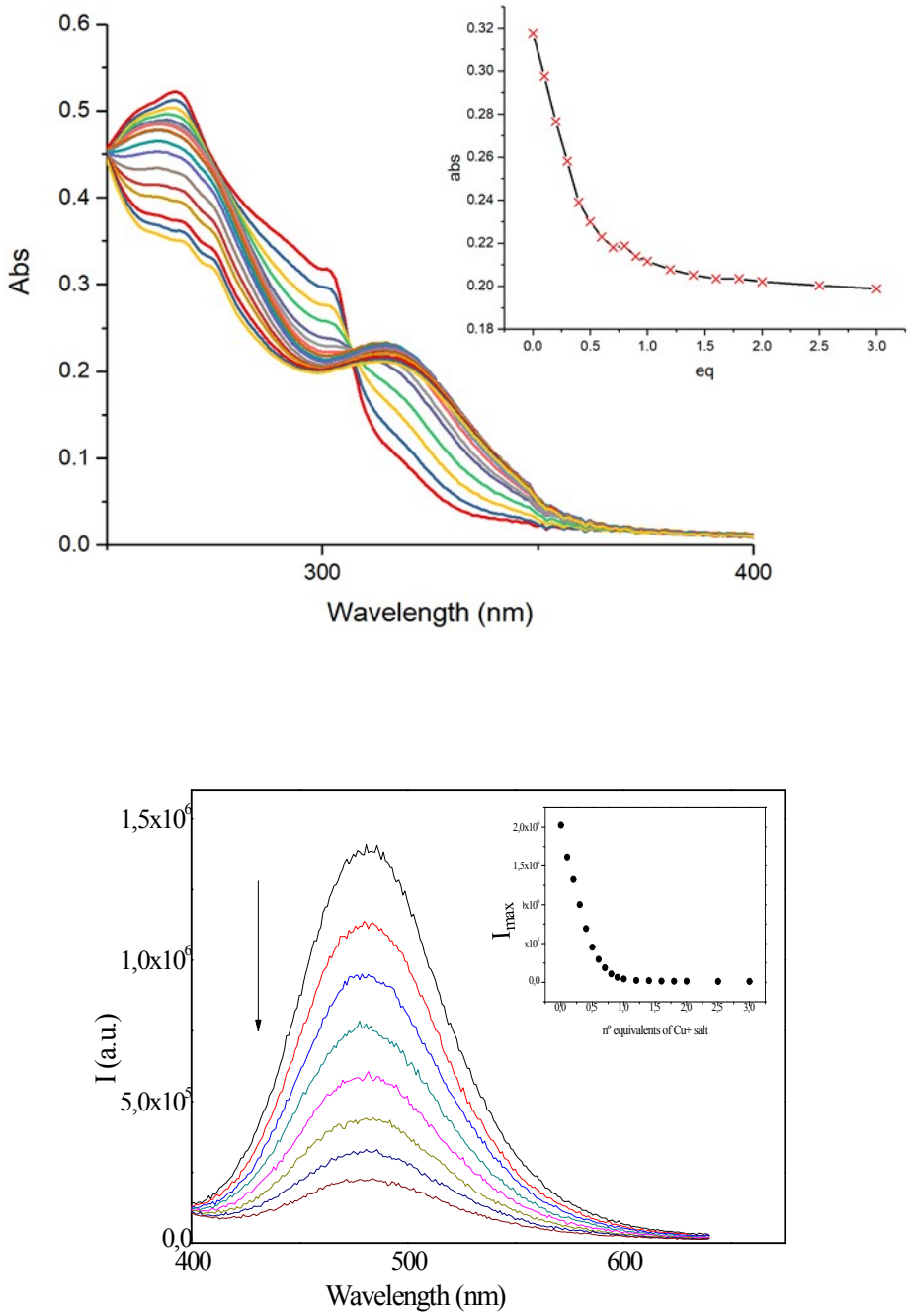
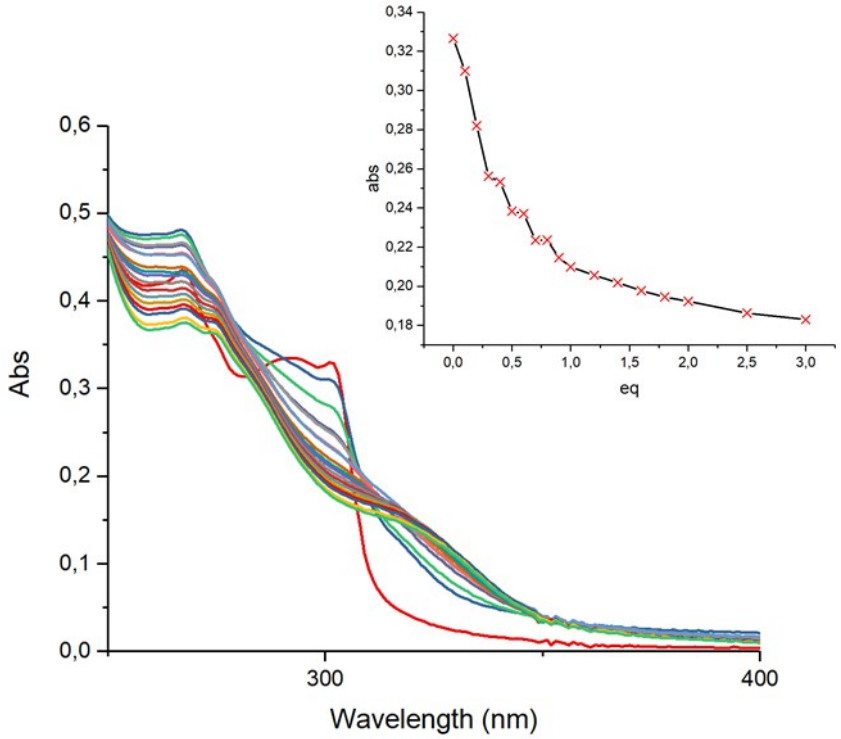


Figure S26. Absorption (above) and emission (below) titrations of **3** with increasing amounts of $Zn(NO_3)_2$ in acetonitrile at $1 \cdot 10^{-5}$M.


Abs
Wavelength (nm)
abs
eq

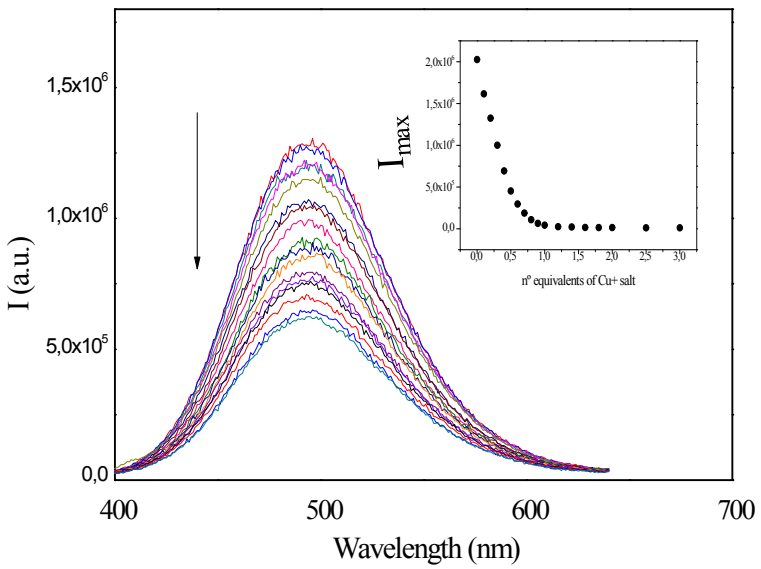

I (a.u.)
Wavelength (nm)
I max
n° equivalents of Cu+ salt

Figure S27. Absorption (above) and emission (below) titrations of **3** with increasing amounts of CuCl in acetonitrile at $1 \cdot 10^{-5}$M.

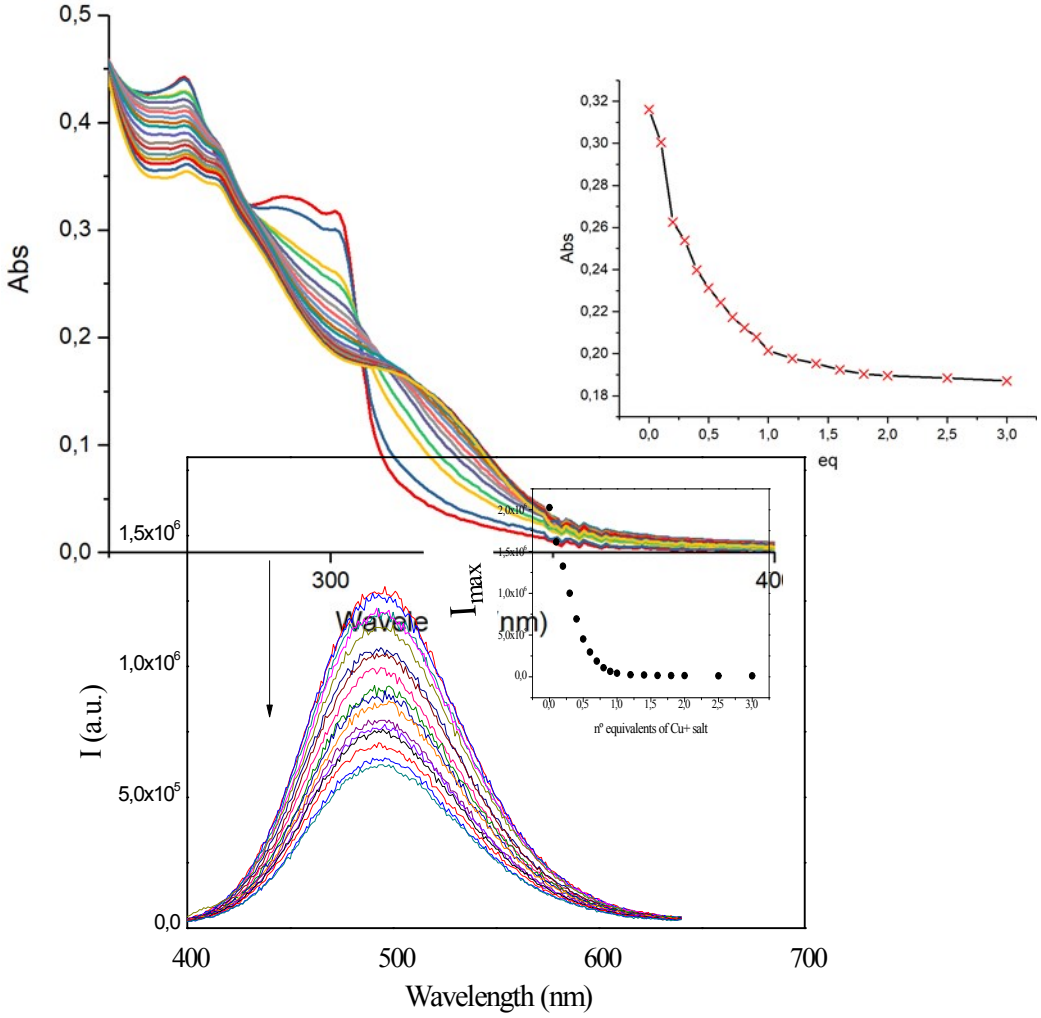


Figure S28. Absorption (above) and emission (below) titrations of **3** with increasing amounts of $[Cu(CH_3CN)_4](BF_4)$ in acetonitrile at $1 \cdot 10^{-5}$M.

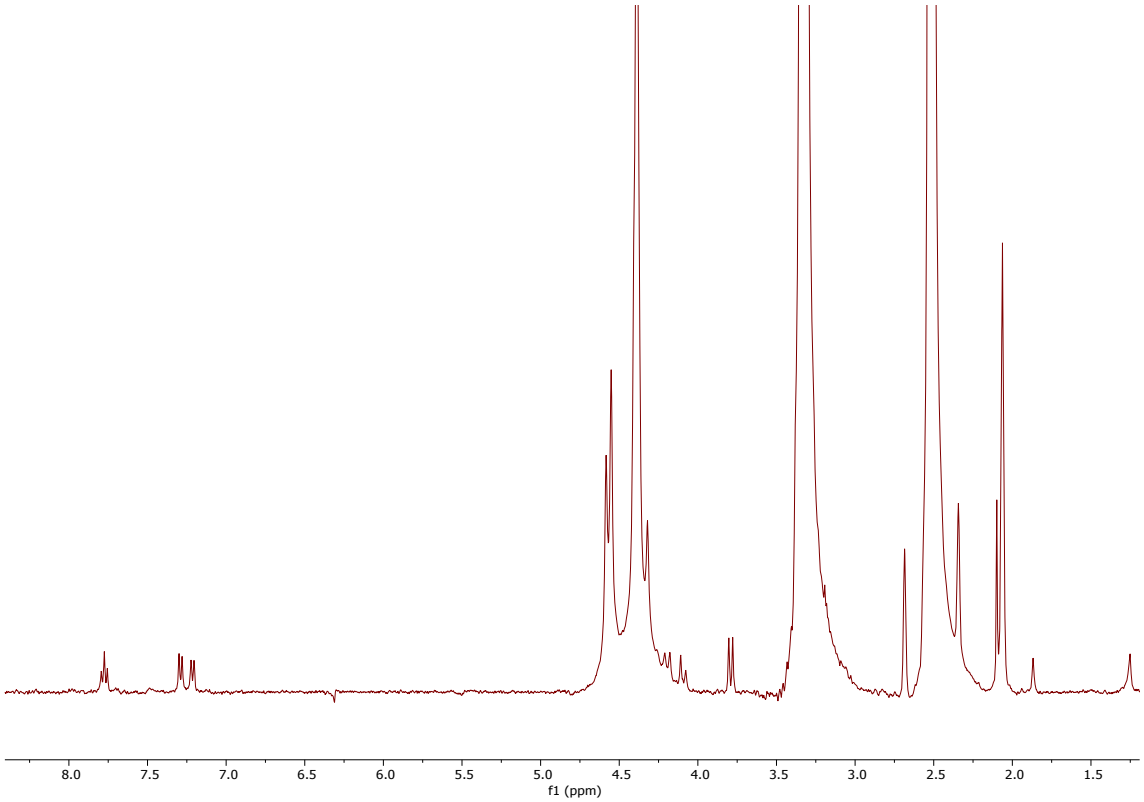


Figure S29. ^{1}H NMR spectrum of **1a** in DMSO-d_6

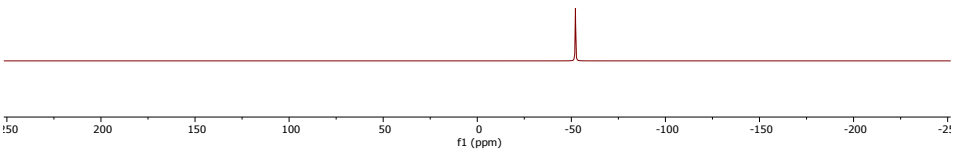


Figure S30. ^{31}P NMR spectrum of **1a** in DMSO-d_6

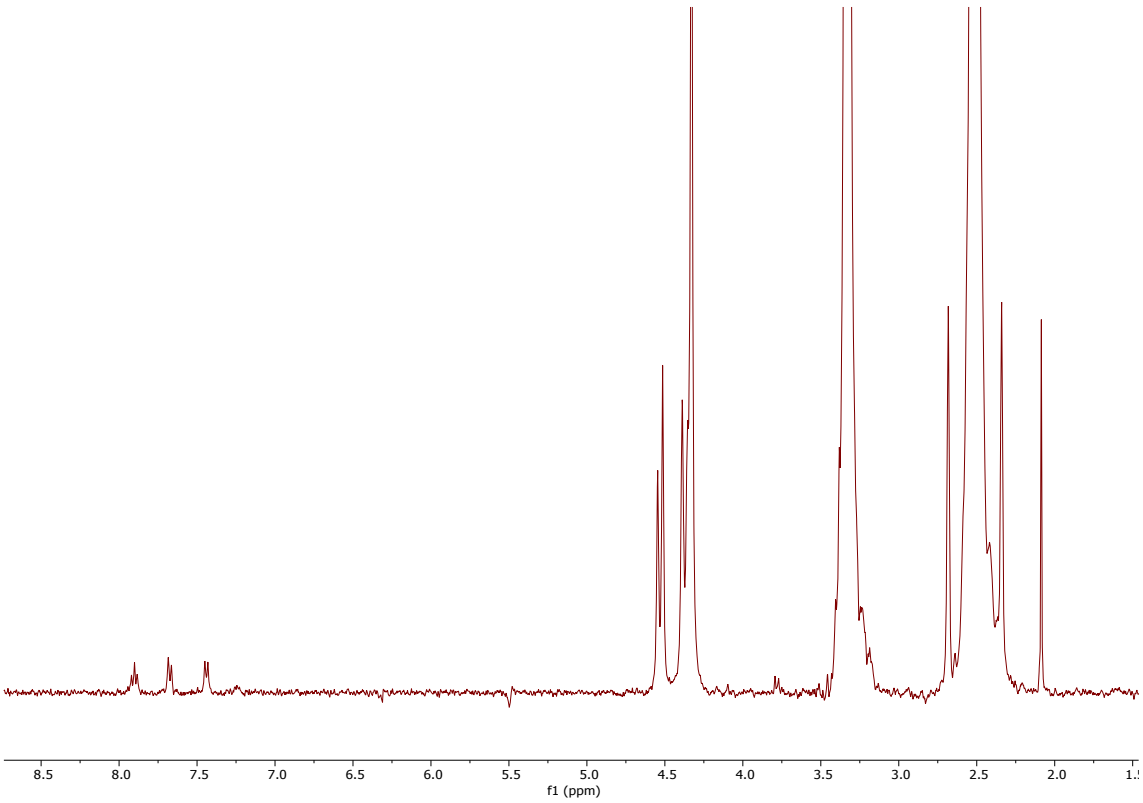


Figure S31. ^{1}H NMR spectrum of **1b** in DMSO-d_6

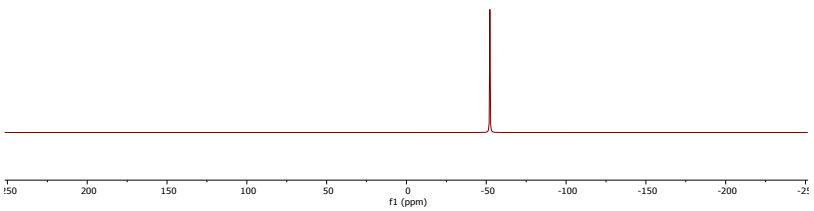


Figure S32. ^{31}P NMR spectrum of **1b** in DMSO-d_6

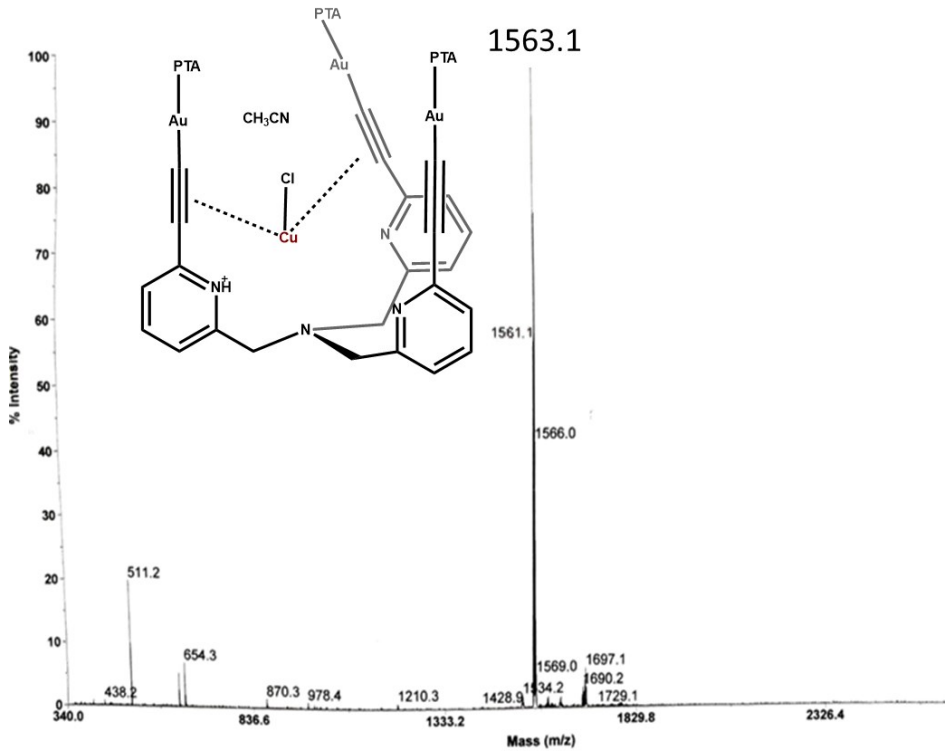


Figure S33. MALDI-TOF(+) mass spectrum of compound **1b**.

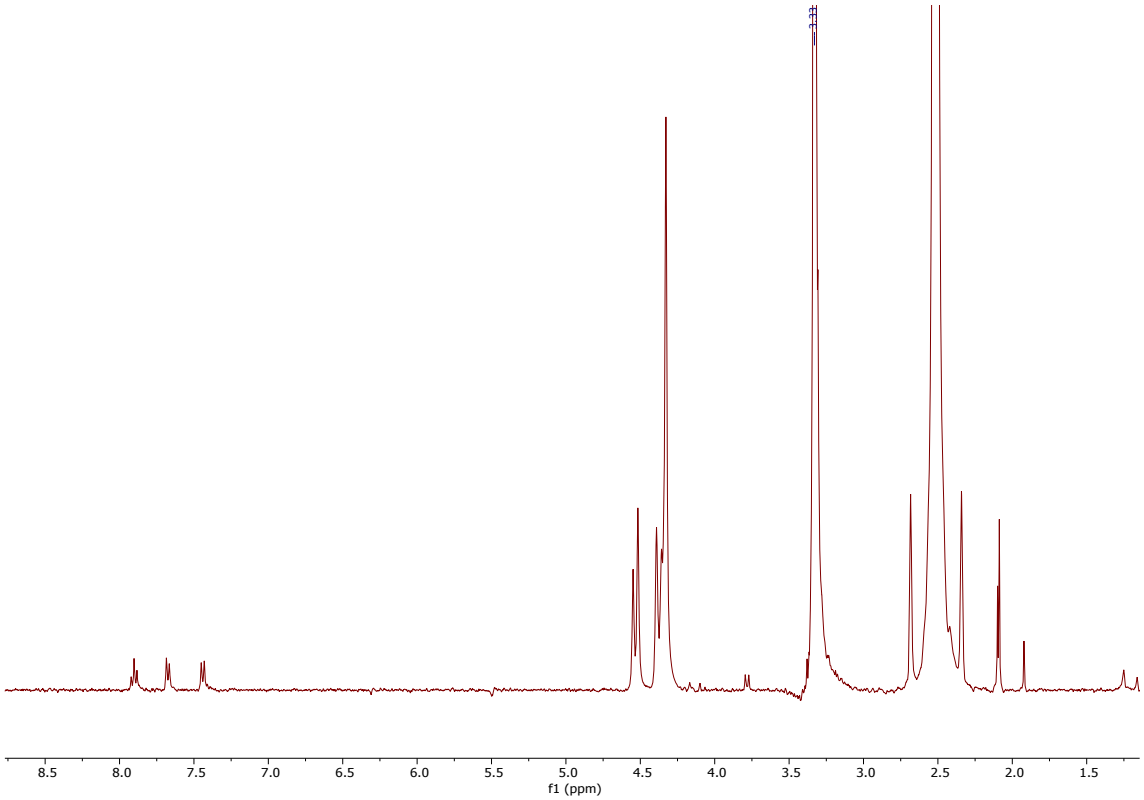


Figure S34. ^{1}H NMR spectrum of **1c** in DMSO-d_6

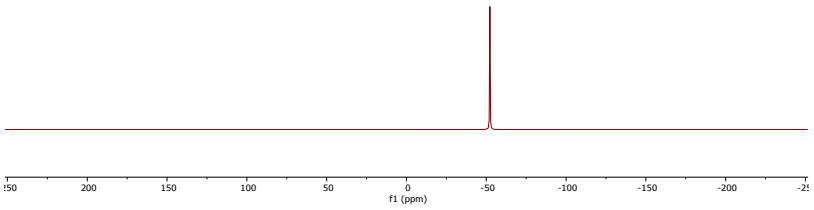


Figure S35. ^{31}P NMR spectrum of **1c** in DMSO-d_6

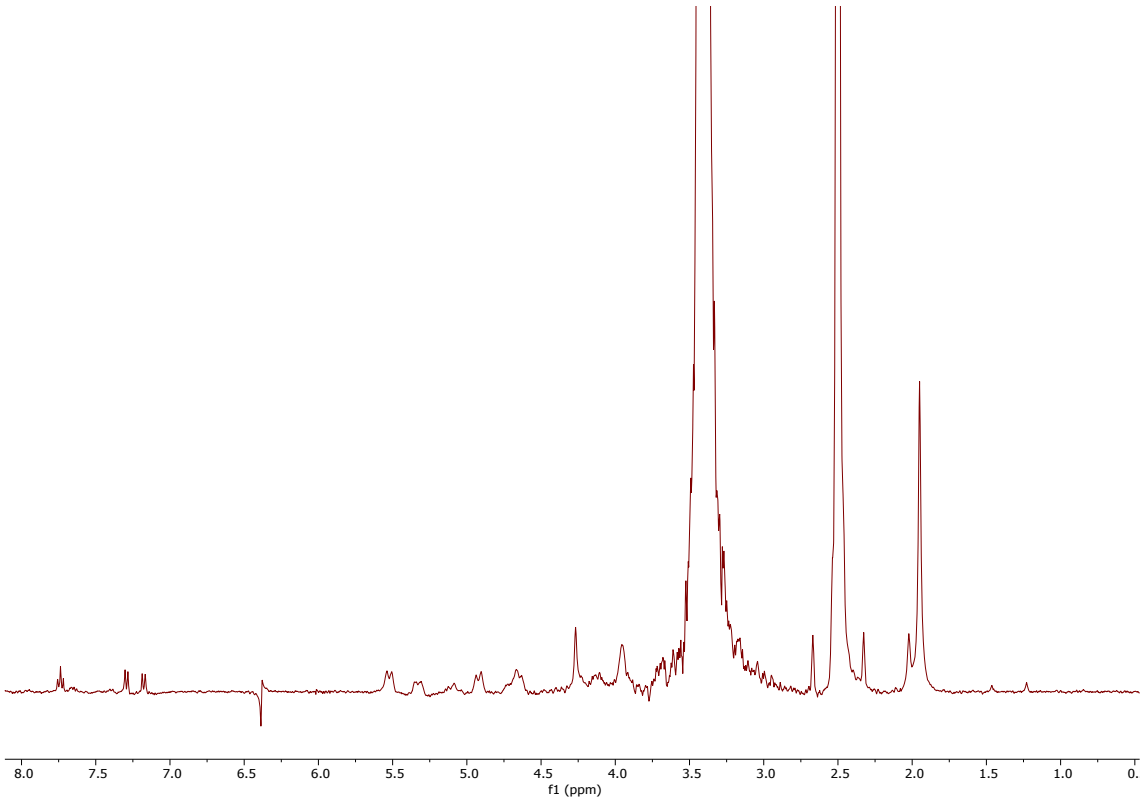


Figure S36. ^{1}H NMR spectrum of **2a** in DMSO-d_6

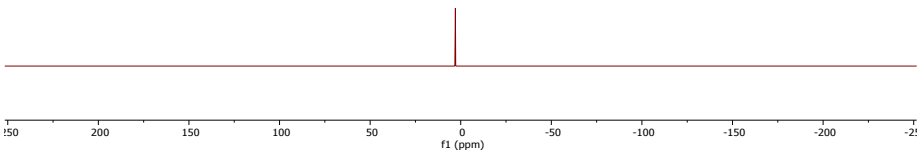


Figure S37. ^{31}P NMR spectrum of **2a** in DMSO-d_6

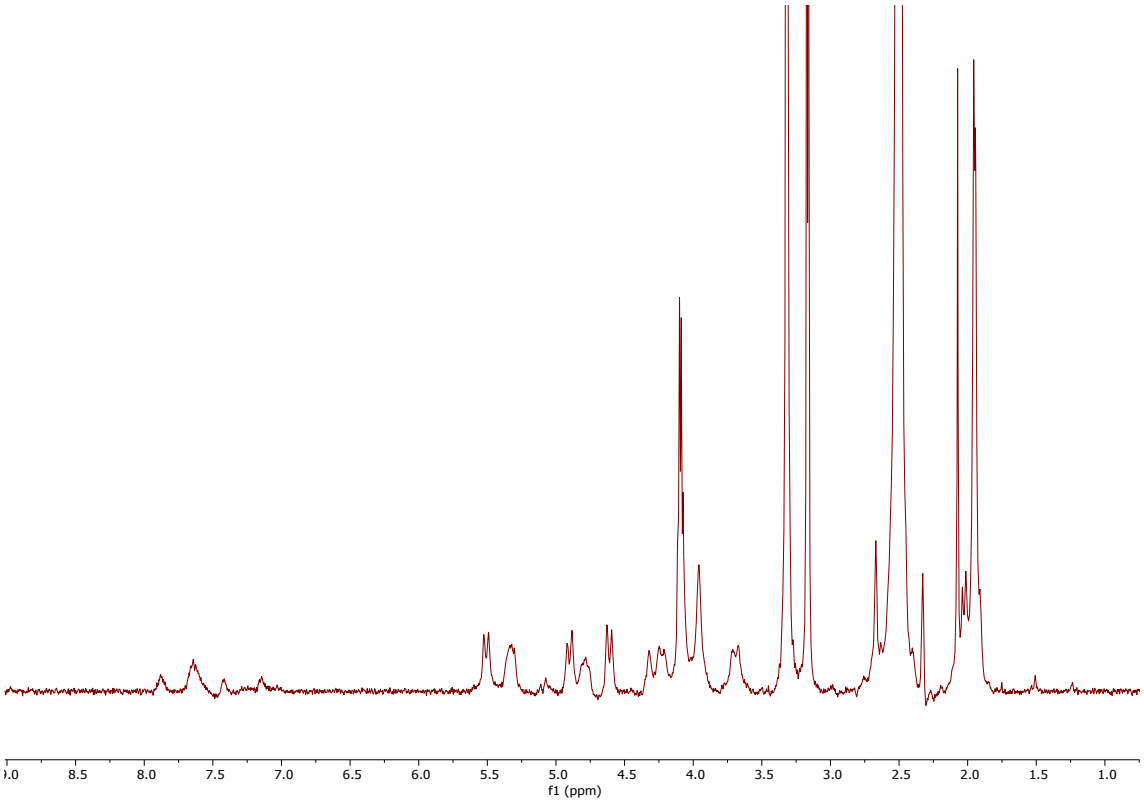


Figure S38. ^{1}H NMR spectrum of **2b** in DMSO-d_6

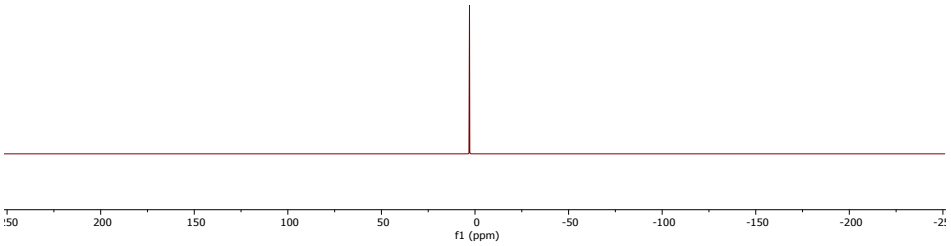


Figure S39. ^{31}P NMR spectrum of **2b** in DMSO-d_6

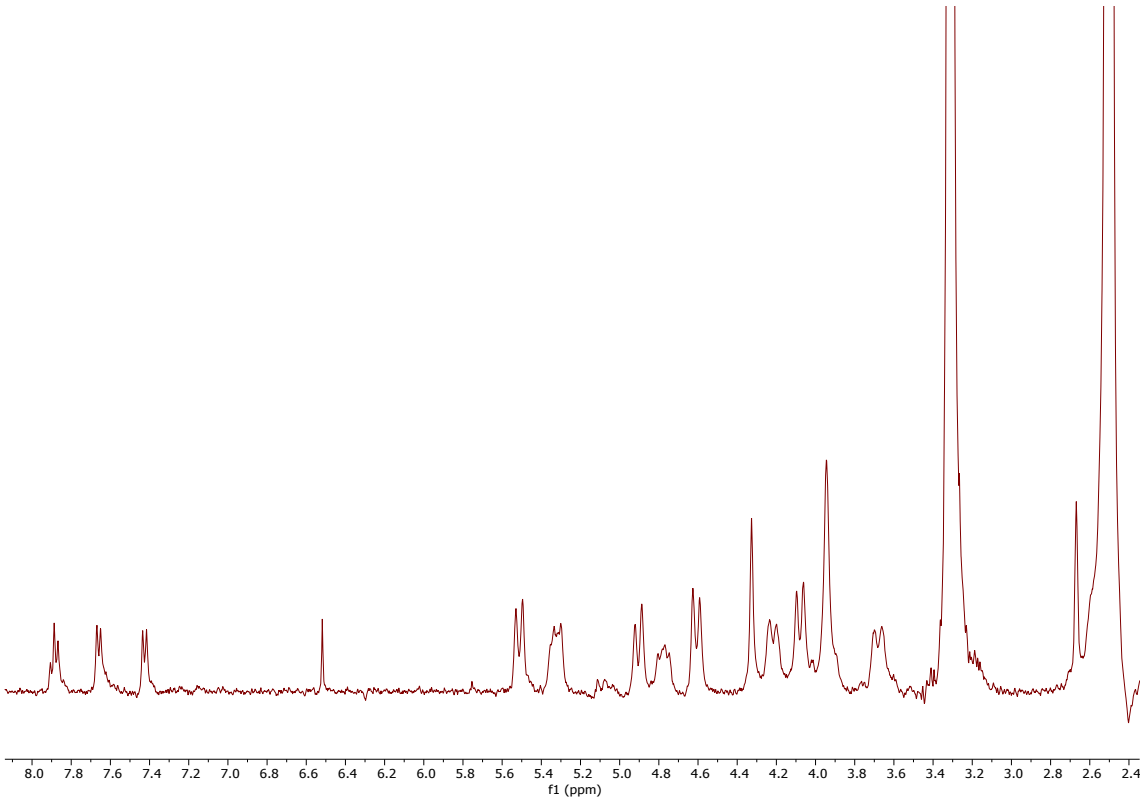


Figure S40. ^{1}H NMR spectrum of **2c** in DMSO-d_6

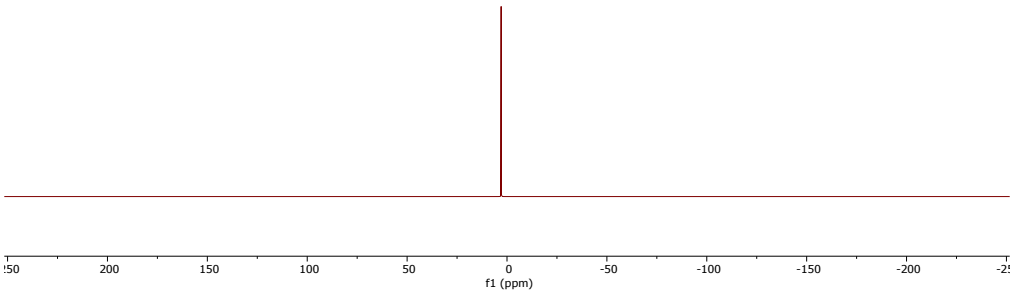


Figure S41. ^{31}P NMR spectrum of **2c** in DMSO-d_6

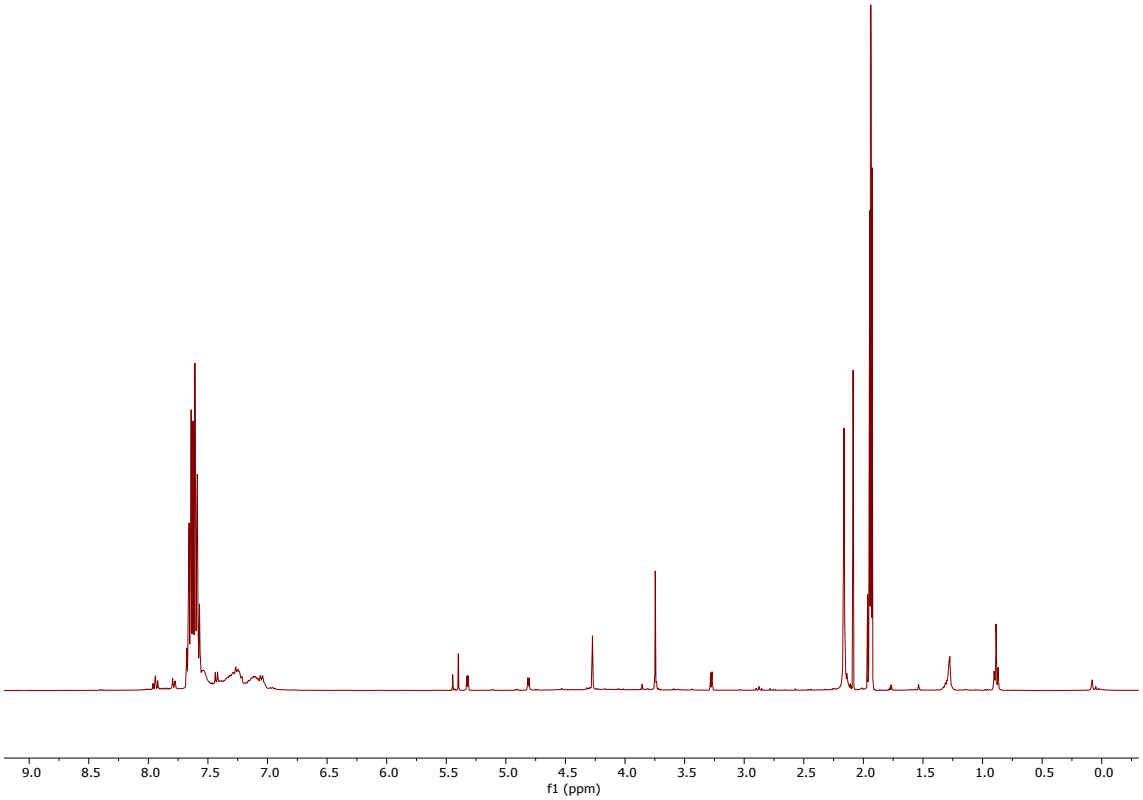


Figure S42. ^{1}H NMR spectrum of **3a** in ACN-d_3

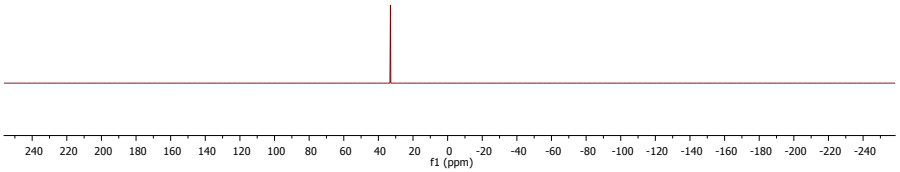


Figure S43. ^{31}P NMR spectrum of **3a** in ACN-d_3

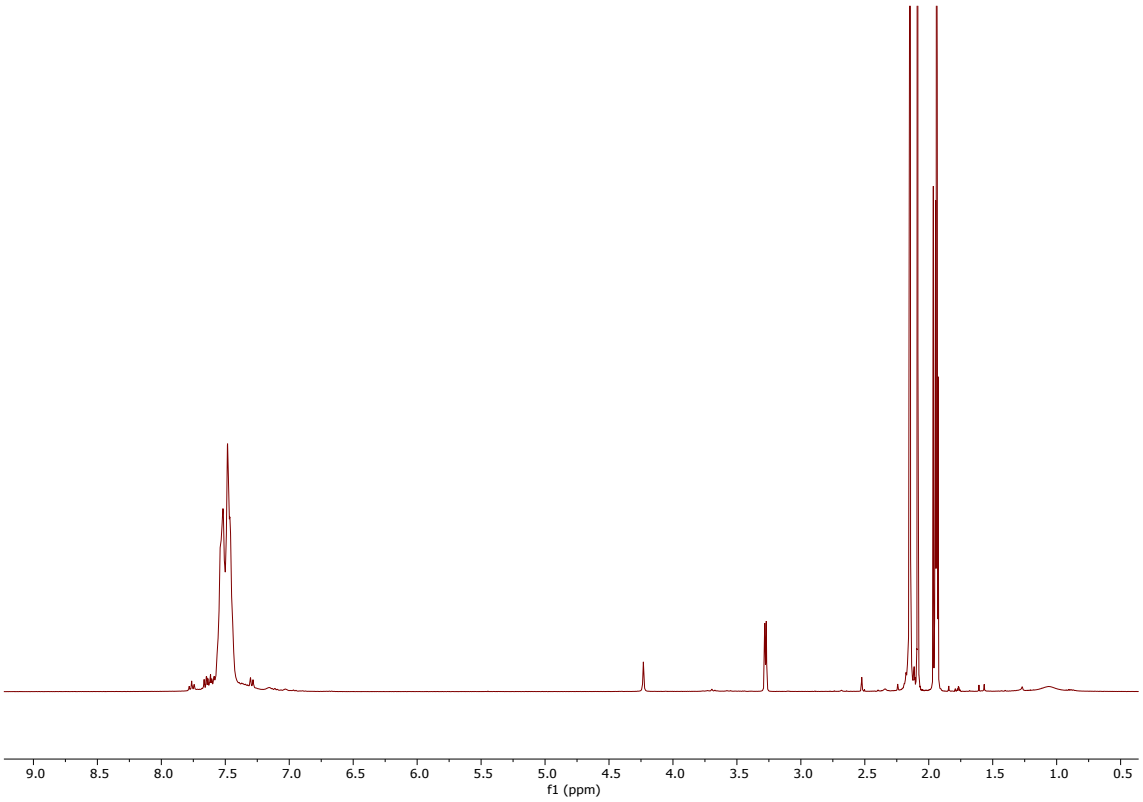


Figure S44. ^{1}H NMR spectrum of **3b** in ACN-d_3

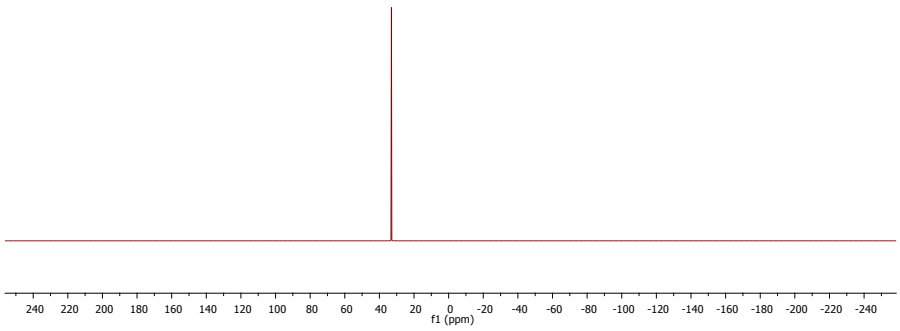


Figure S45. ^{31}P NMR spectrum of **3b** in ACN-d_3

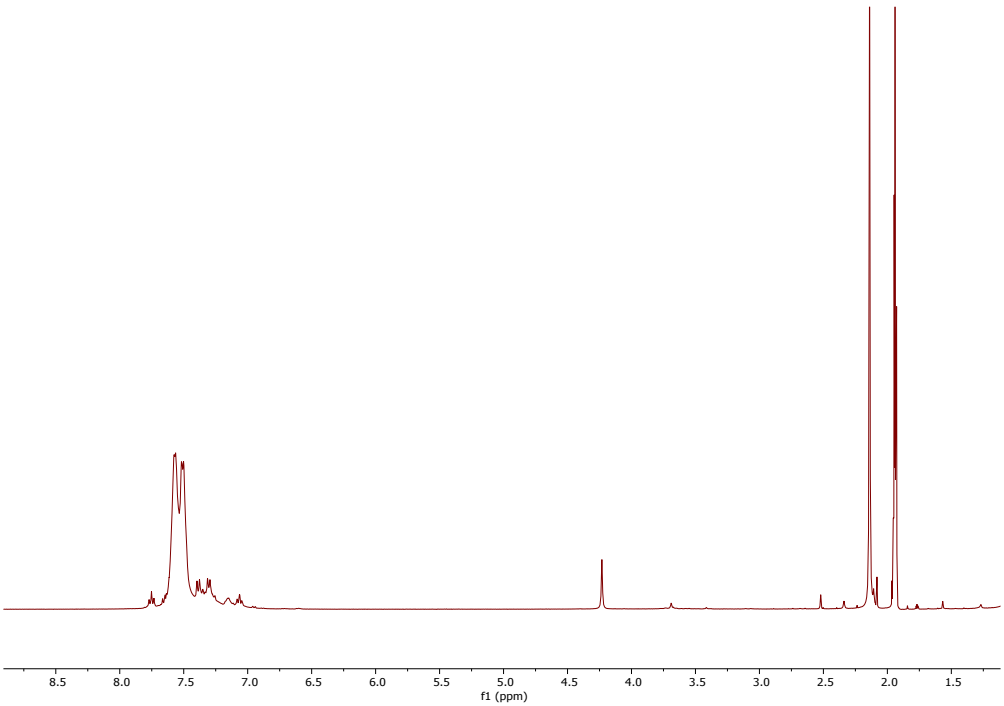


Figure S46. ^{1}H NMR spectrum of **3c** in ACN-d_3

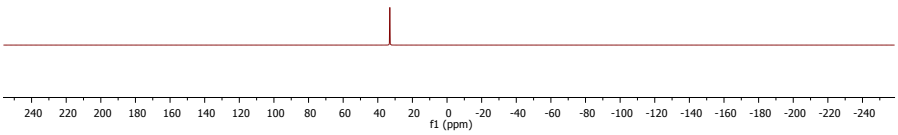


Figure S47. ^{31}P NMR spectrum of **3c** in ACN-d_3

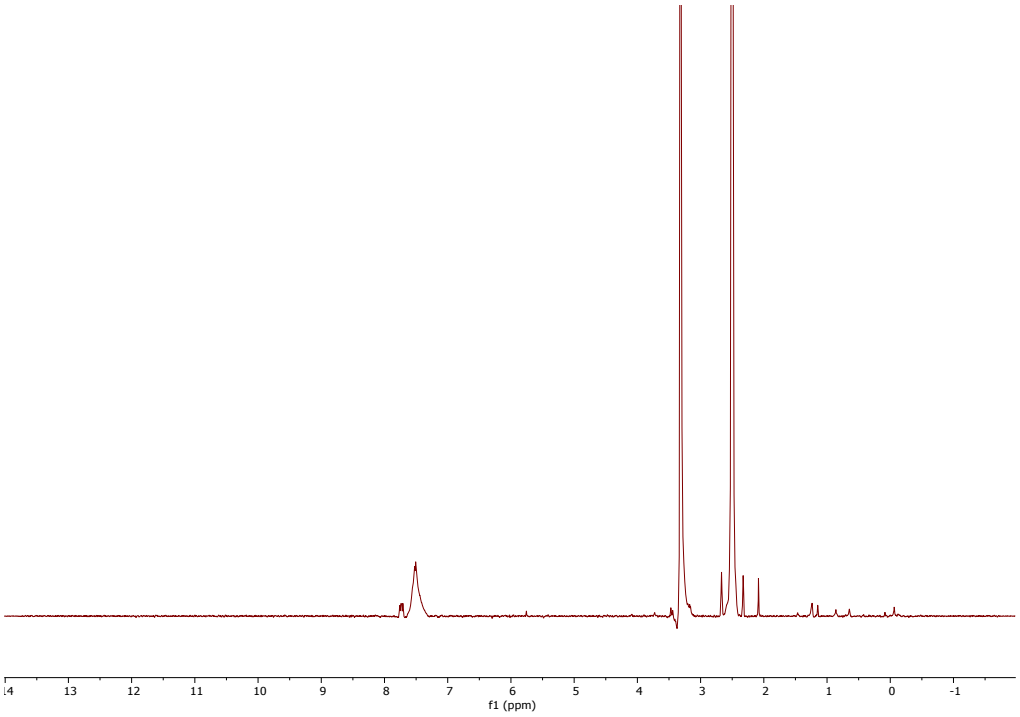


Figure S48. ^{1}H NMR spectrum of **4a** in DMSO-d_6

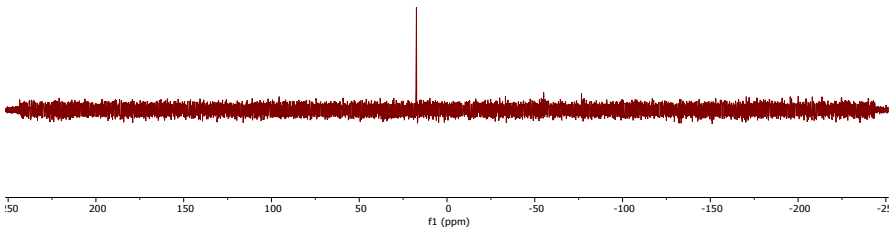


Figure S49. ^{31}P NMR spectrum of **4a** in DMSO-d_6

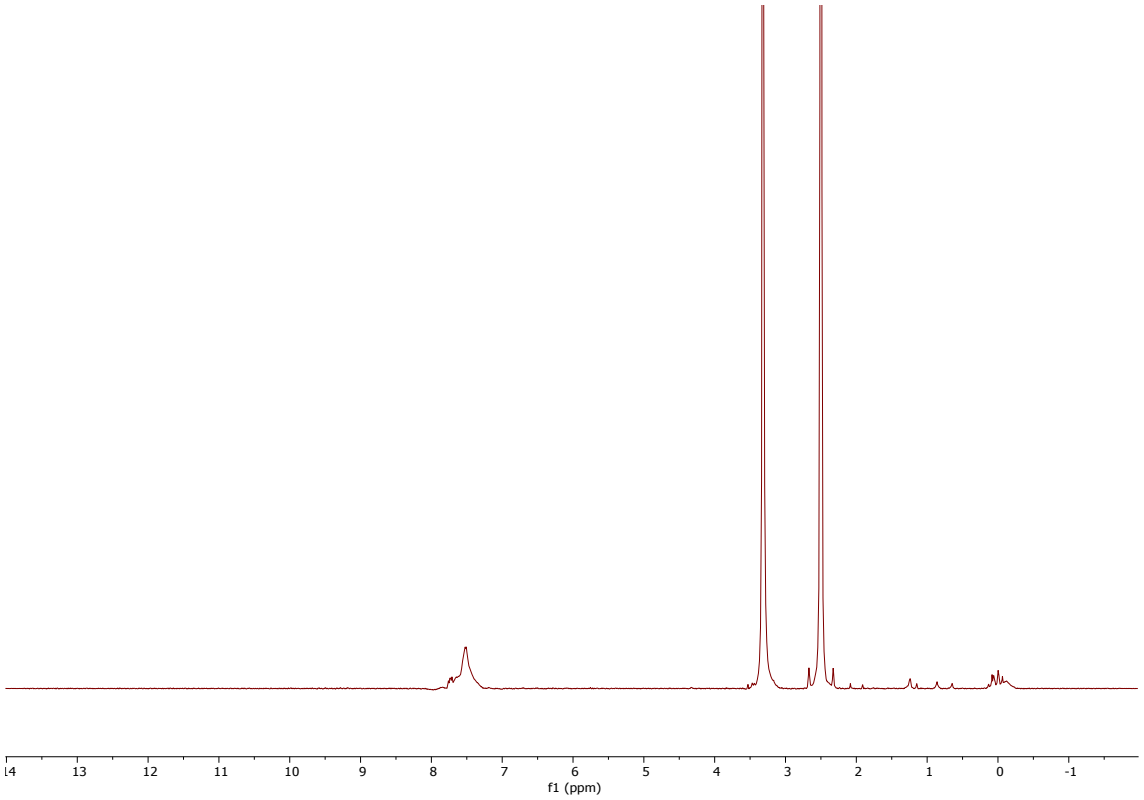


Figure S50. ^{1}H NMR spectrum of **4b** in DMSO-d_6

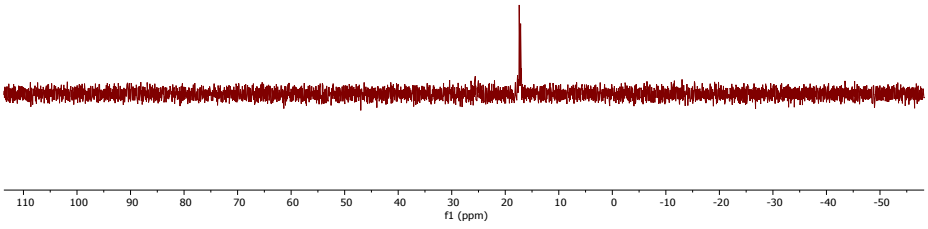


Figure S51. ^{31}P NMR spectrum of **4b** in DMSO-d_6

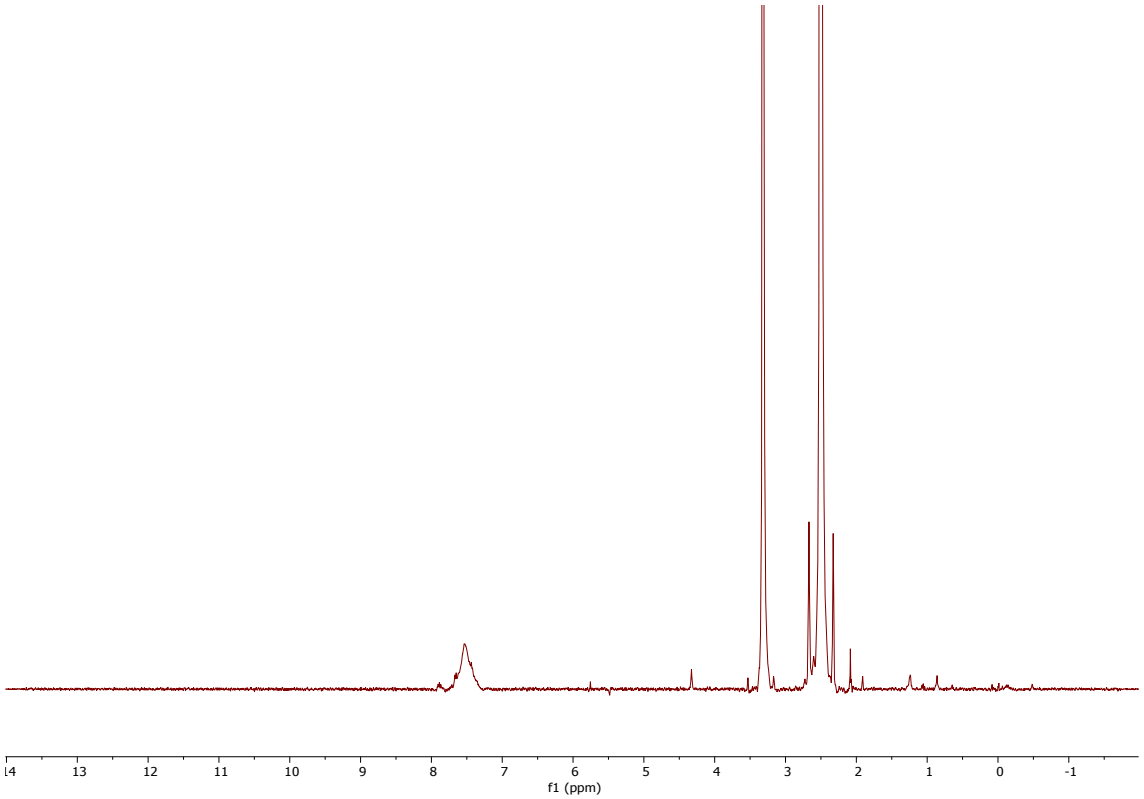


Figure S52. ^{1}H NMR spectrum of **4c** in DMSO-d_6

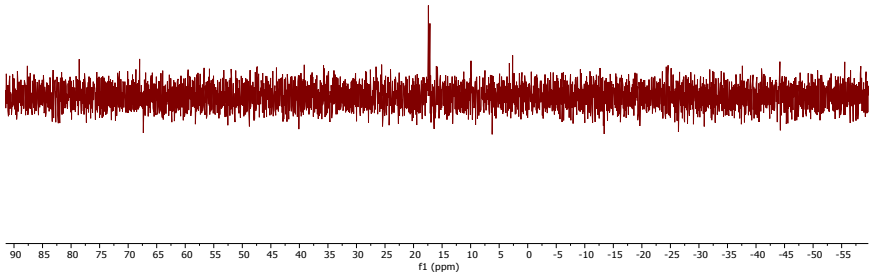


Figure S53. ^{31}P NMR spectrum of **4c** in DMSO-d_6

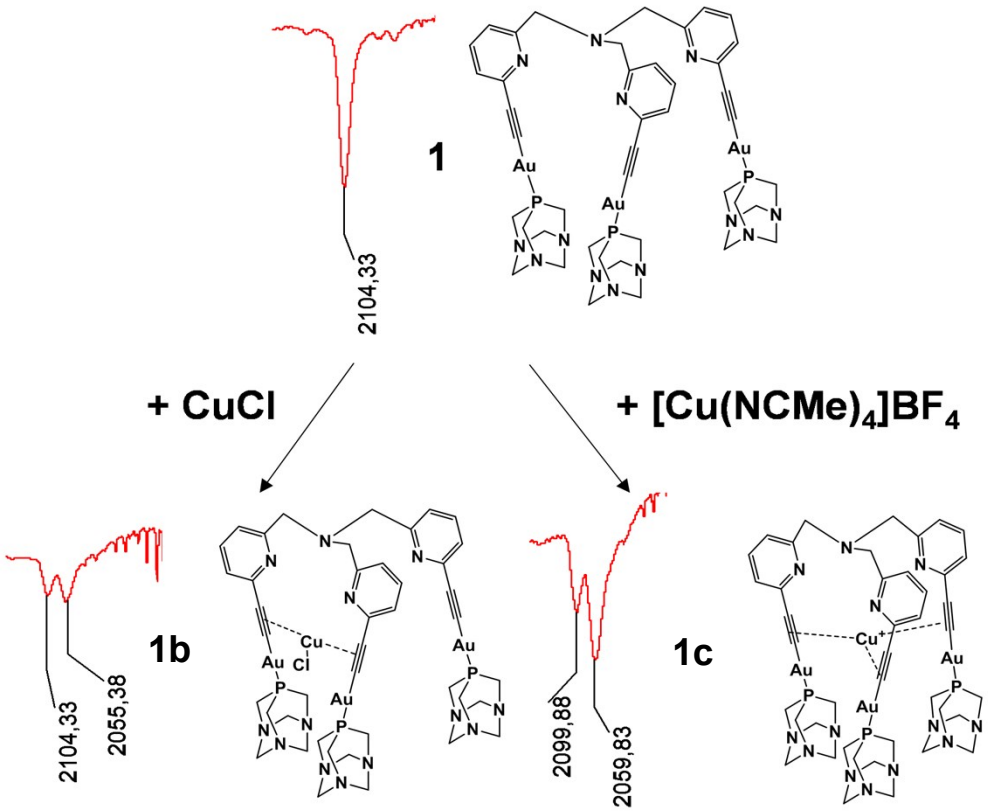


Figure S54. IR spectra of 1 and respective Cu^{+} derivatives of **1**.

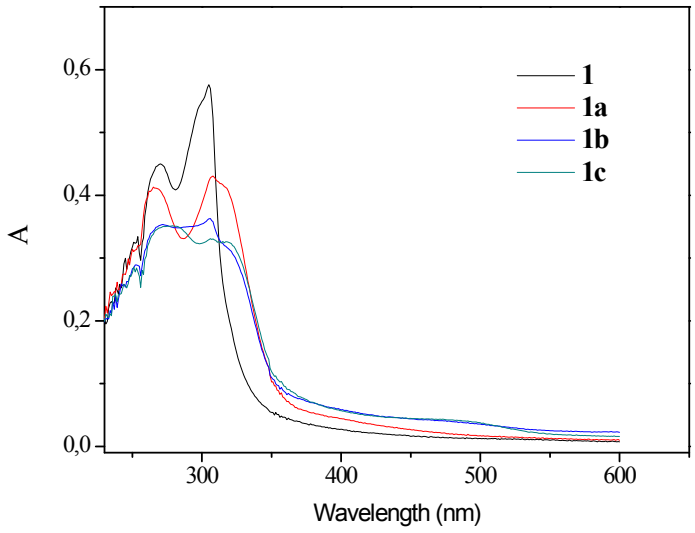


Figure S55. Absorption spectra of **1** and respective heterometallic complexes **1a-c** in DMSO at $1 \cdot 10^{-5}$M.

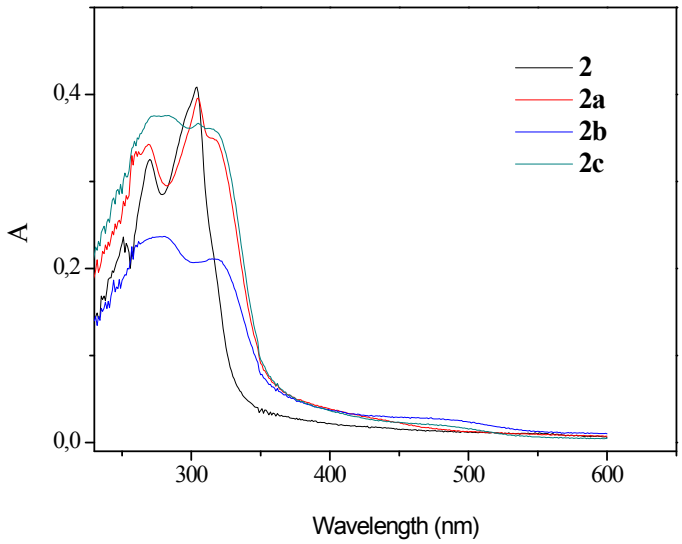


Figure S56. Absorption spectra of **2** and respective heterometallic complexes **1a-c** in DMSO at $1 \cdot 10^{-5}$M.

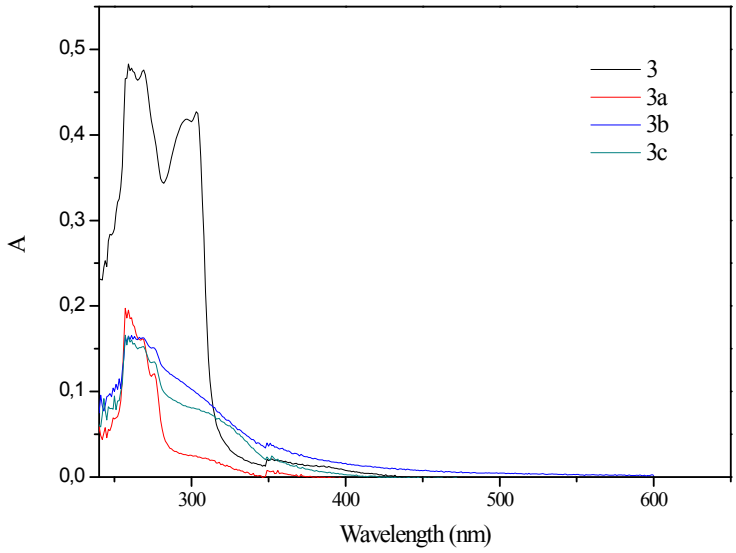


Figure S57. Absorption spectra of **3** and respective heterometallic complexes **3a-c** in DMSO at $1 \cdot 10^{-5}$M.

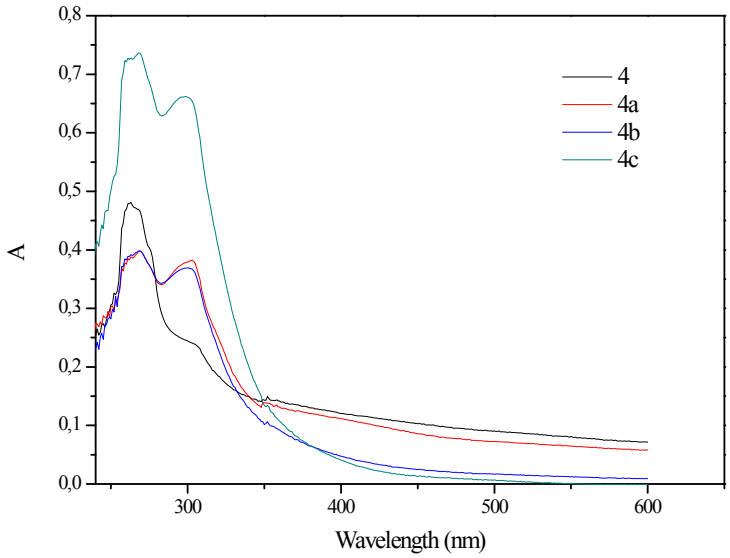


Figure S58. Absorption spectra of **4** and respective heterometallic complexes **4a-c** in DMSO at $1 \cdot 10^{-5}$M.

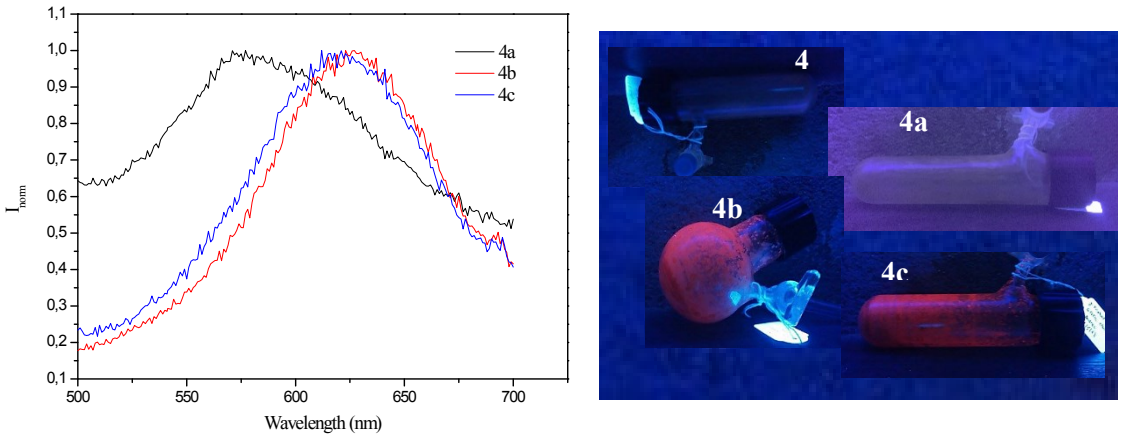
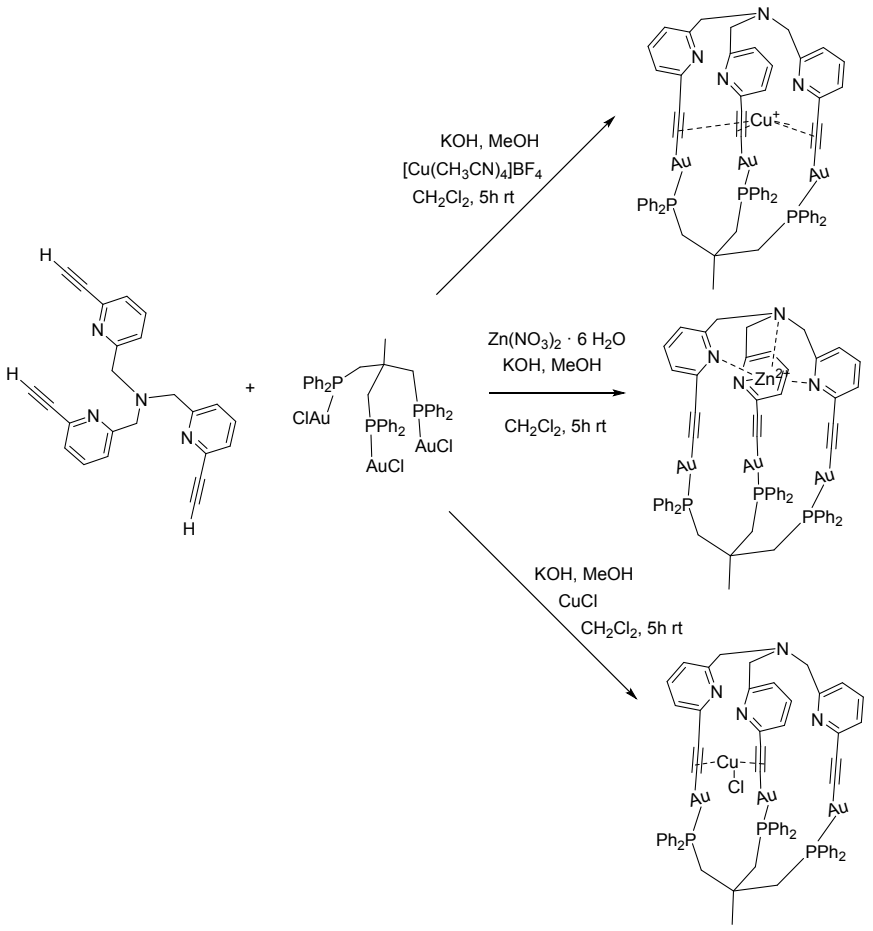


Figure S59. Normalized emission spectra in solid state of compounds **4**, **4a**, **4b** and **4c** (left); image of the solids observed under UV light (right).



Scheme S1. Synthesis of heterometallic complexes **4a-c**.

Coordinates of the minimised structures

1a

2 1

C	-5.90006500	-2.05617700	3.09849800
C	-5.54209200	-1.23910900	2.03818000
N	-4.29669800	-1.24888500	1.53233200
C	-3.35281800	-2.08864600	2.02617700
C	-6.51003700	-0.26720400	1.39608300
N	-6.15157500	-0.02006300	-0.00272700
C	-6.50859500	-1.10974400	-0.91453200
C	-6.51737700	1.31262700	-0.48889100
C	-5.54485300	-1.17623200	-2.08104000
C	-5.90505800	-1.68998700	-3.31648900
C	-4.93818400	-1.74604600	-4.32216200
C	-3.66273600	-1.26242700	-4.08196400
C	-3.36048200	-0.73189900	-2.81990900
N	-4.30073000	-0.72673100	-1.84219500
C	-5.55777600	2.36090000	0.03467400
C	-5.92513400	3.68512300	0.21196400
C	-4.96224700	4.58842400	0.66589900
C	-3.68342000	4.14528600	0.95998500
C	-3.37339300	2.78944400	0.78328000
N	-4.31018600	1.93592000	0.29919800
C	-3.65323300	-2.92114900	3.11352600
C	-4.92992800	-2.89523700	3.64992500
C	-2.11239800	-2.09413400	1.35189600
C	-1.07754000	-2.11958000	0.68820600
C	-2.13004300	2.21673800	1.12929000
C	-1.09263100	1.66231100	1.48781900

C	-2.12134500	-0.13926800	-2.49340000
C	-1.08712600	0.45339600	-2.19139300
H	-6.91349500	-2.04025200	3.48541400
H	-7.54184300	-0.62675200	1.50673500
H	-6.44798300	0.68946000	1.92974100
H	-7.54221800	-1.03070000	-1.27718800
H	-6.44008800	-2.04969800	-0.35271000
H	-6.45214300	1.29698900	-1.58403800
H	-7.55169700	1.58141900	-0.23573800
H	-6.91746400	-2.03833700	-3.49165000
H	-5.19205600	-2.14983800	-5.29753800
H	-2.89995800	-1.26367900	-4.85126300
H	-6.94014800	4.00559300	0.00210100
H	-2.92369700	4.81549200	1.34379000
H	-2.88785700	-3.58388500	3.49906400
H	-5.18220200	-3.54141200	4.48519400
H	-5.22194800	5.63307000	0.80774900
Au	0.46145500	0.63129200	2.17993600
Au	0.47751600	-2.20363600	-0.54923500
Au	0.45959500	1.57734600	-1.64266900
P	2.13414600	-0.63838500	3.12601100
P	2.11489300	3.04708100	-1.00668600
P	2.15614100	-2.38665800	-2.11553000
C	3.49867900	-1.35739600	2.06968100
H	4.05811400	-0.53837300	1.60168700
C	1.56847400	4.55784700	-0.05154800
H	1.04144300	4.23006300	0.85195600
C	3.26536500	-3.89180500	-2.17602600
H	2.64670300	-4.78985900	-2.28141000
C	3.18450300	3.91015700	-2.27552700
H	2.54171200	4.45186300	-2.97813900

H	3.74109700	3.16110800	-2.84990200
C	3.47993200	2.49994800	0.14709000
H	4.04752800	1.69106200	-0.32851400
H	3.01933400	2.09885600	1.05882500
C	1.63498300	-2.37090900	-3.91055700
H	1.08863800	-1.44160700	-4.10902100
H	0.94638500	-3.20465600	-4.08753900
C	3.49036200	-1.08242800	-2.23019500
H	4.04316500	-1.05276200	-1.28342500
H	3.00695100	-0.10716000	-2.36983000
C	1.60318000	-2.22302700	3.96302300
H	1.07691200	-2.84685600	3.23131000
H	0.89434800	-1.98098900	4.76279300
C	3.20660800	0.03893700	4.50087700
H	2.56576600	0.37420800	5.32382700
H	3.75553200	0.91374000	4.13452900
H	3.03791800	-1.95191000	1.27049700
H	3.81109900	-3.97783100	-1.22959900
H	0.85733700	5.12516800	-0.66235400
N	2.74636400	-2.93308000	4.50792600
N	4.39595400	-2.18340300	2.85747000
N	4.13706300	-0.97240500	4.97093600
N	2.78659600	-2.48012100	-4.78803500
N	4.40118400	-1.35446700	-3.32754500
N	4.20029200	-3.79538000	-3.28318200
N	4.10581300	4.82866800	-1.62961200
N	4.36723200	3.60142600	0.47445700
N	2.70400600	5.39290500	0.29661600
C	3.40858800	5.87996800	-0.89026700
C	3.65778500	4.68953000	1.15089600
H	4.40265900	5.41353100	1.49701500

H	3.13436000	4.29215600	2.02761700
H	2.69836900	6.38306300	-1.55461100
H	4.15107300	6.61645100	-0.56625600
C	5.04973500	-1.41379900	3.91927200
C	3.69757300	-3.31691500	3.46768800
H	5.81339700	-2.05100500	4.37688100
H	5.55080000	-0.54351300	3.48204400
H	4.44935600	-3.97236700	3.91935100
H	3.17421100	-3.88293600	2.68909200
C	3.71053600	-1.36112900	-4.61896700
C	5.08477800	-2.63953900	-3.15921900
H	4.46871300	-1.42424600	-5.40636000
H	3.16557200	-0.41891800	-4.74417100
H	5.85510900	-2.71621200	-3.93338100
H	5.58070200	-2.66270900	-2.18290100
Zn	-3.98286000	-0.01135900	-0.00429500
C	3.45050000	-2.14182800	5.51786700
H	2.74189900	-1.82115900	6.28852100
H	4.19973400	-2.78456600	5.99135500
C	3.51936100	-3.72908500	-4.57548700
H	4.27544600	-3.81739100	-5.36237200
H	2.83125700	-4.57563300	-4.66885900
C	5.02070000	4.14388400	-0.71974000
H	5.77752200	4.86416700	-0.39261300
H	5.52999000	3.33514600	-1.25469600

1c

1 1

C	-4.41874600	-3.62660300	-3.19774100
C	-4.38326300	-3.10602500	-1.89937800

N	-3.43315100	-2.26055500	-1.50547400
C	-2.50223000	-1.88354400	-2.38870900
C	-5.42834100	-3.52093300	-0.87875100
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C	-6.64392500	-1.35071200	-0.81734400
C	-6.32263600	-2.64093900	1.25566600
C	-6.23459700	0.02134900	-0.30003400
C	-7.18092700	1.03118300	-0.10087700
C	-6.75359200	2.27262100	0.35991900
C	-5.40590100	2.46979600	0.62893800
C	-4.53389700	1.39544500	0.40891600
N	-4.93966100	0.20825700	-0.05849400
C	-5.24313600	-2.10609100	2.18525300
C	-5.52741100	-1.46537400	3.39422100
C	-4.47336000	-0.93615100	4.13221400
C	-3.17964800	-1.02752100	3.63225100
C	-2.99970300	-1.69785800	2.41771000
N	-4.00421400	-2.25574300	1.73566000
C	-2.44150900	-2.37020300	-3.70115100
C	-3.42507300	-3.26360000	-4.10153800
C	-1.58680400	-0.87237800	-1.92798900
C	-0.83885000	0.11410000	-1.81017600
C	-1.72946000	-1.76889000	1.74197300
C	-0.67593900	-2.02801100	1.13562000
C	-3.13528800	1.48425800	0.70578100
C	-1.93448000	1.47557200	0.97715100
H	-5.21634700	-4.30300500	-3.49104500
H	-6.17905900	-4.14495100	-1.40168200
H	-4.92195600	-4.17185800	-0.15794300
H	-7.74831700	-1.41206900	-0.79338200
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H	-7.27967700	-2.16041600	1.50135700
H	-6.46790200	-3.71165000	1.46137500
H	-8.23213900	0.84261500	-0.29927500
H	-7.46738200	3.07527200	0.52149500
H	-5.03201900	3.41441600	1.00886100
H	-6.55329600	-1.36445300	3.73739100
H	-2.33520400	-0.58504700	4.14948100
H	-1.66197100	-2.03418000	-4.37634300
H	-3.42923700	-3.65961200	-5.11300800
H	-4.66154100	-0.42798300	5.07359800
Au	0.96110600	-2.72997100	0.23957000
Au	0.05293700	1.89618200	-1.71636600
Au	-0.03094700	1.46539000	1.59347400
P	2.81084700	-3.58224600	-0.81342400
P	2.08234900	1.11728700	2.40014300
P	0.85033800	4.03984100	-1.69260700
C	3.36168700	-2.84544700	-2.43920200
H	3.57491400	-1.78021400	-2.29467500
C	2.18749900	-0.02832700	3.87003900
H	1.64821700	-0.95134900	3.62800700
C	1.54174100	4.81788200	-3.24285300
H	0.78908300	4.75829200	-4.03688300
C	3.29170100	2.41272600	2.99152600
H	2.84168900	2.98336400	3.81163100
H	3.50070900	3.11682400	2.17799000
C	3.23912400	0.18716400	1.27386000
H	3.43714100	0.79353200	0.38187900
H	2.72380900	-0.72444200	0.94331400
C	-0.37752300	5.37735200	-1.25630200
H	-0.78659000	5.16946300	-0.26097400
H	-1.21178800	5.33877400	-1.96541600

C	2.20721500	4.56010400	-0.51988800
H	3.10969800	3.97391300	-0.73195200
H	1.88804100	4.32682000	0.50350400
C	2.81587400	-5.37732100	-1.32929700
H	1.97139900	-5.55748400	-2.00378100
H	2.66565800	-6.00453200	-0.44348800
C	4.46772200	-3.55896700	0.05176900
H	4.38384200	-4.11895800	0.99062200
H	4.73282600	-2.52505600	0.30725900
H	2.54004700	-2.91796100	-3.16041800
H	2.41400100	4.24482100	-3.57696700
H	1.68104000	0.43432100	4.72434400
N	4.06516500	-5.72871000	-1.98555600
N	4.54056000	-3.52605700	-2.95143300
N	5.50314800	-4.14857000	-0.78307300
N	0.24347600	6.69228300	-1.28407000
N	2.49948400	5.97952600	-0.63861900
N	1.91431200	6.20491000	-3.01003500
N	4.53066900	1.79307100	3.43939800
N	4.49021100	-0.14907500	1.93918500
N	3.57055400	-0.32380600	4.20921300
C	4.31271100	0.88361000	4.56458400
C	4.26476000	-0.99578800	3.11574900
H	5.24252900	-1.32484000	3.48425300
H	3.69230200	-1.88122500	2.81750100
H	3.78324900	1.41401600	5.36293400
H	5.29280500	0.58085700	4.94866000
C	5.67492900	-3.41332400	-2.03533700
C	4.28288400	-4.94468500	-3.20011500
H	6.55973500	-3.81265000	-2.54280300
H	5.85727000	-2.35646000	-1.81227900

H	5.15306800	-5.36016900	-3.71961700
H	3.41310500	-5.04530400	-3.85801400
C	1.33089000	6.80060900	-0.31505100
C	2.95047700	6.32751400	-1.98751800
H	1.65391500	7.84668500	-0.28213600
H	0.95969200	6.52667400	0.67855800
H	3.28871700	7.36911300	-1.97071800
H	3.80431200	5.69680300	-2.25836900
Cu	-1.51022800	-0.46094800	0.10137400
C	5.21503500	-5.54722300	-1.10139700
H	5.05043600	-6.10420100	-0.17282800
H	6.09490500	-5.96823800	-1.59972600
C	0.76631000	7.01866900	-2.61027800
H	1.08217000	8.06741600	-2.60152600
H	-0.03175800	6.90928600	-3.35206200
C	5.20215700	1.05749000	2.37048700
H	6.18910400	0.75558700	2.73723200
H	5.34611400	1.71898100	1.50909200

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C	7.33762300	1.97893600	1.97178100
C	6.07142200	2.36948100	1.51708100
N	5.01619500	1.56652100	1.55729700
C	5.16749800	0.32095200	2.04605800
C	5.90747700	3.75614600	0.91721000
N	4.54978900	4.18475100	0.69529800
C	3.83309800	4.37366800	1.94419700
C	4.43686900	5.27572900	-0.25108800
C	2.35551600	4.67506800	1.81959700

C	1.85168800	5.88158500	2.31147300
C	0.48458200	6.12720600	2.22806200
C	-0.32848200	5.17525100	1.63857000
C	0.26405000	3.99014800	1.16718100
N	1.57134900	3.73946400	1.27619700
C	3.14853500	5.22168900	-1.05347900
C	2.43117800	6.37411600	-1.38419900
C	1.22998800	6.23186800	-2.07233700
C	0.75591900	4.95615100	-2.35120700
C	1.54565200	3.86485800	-1.97230700
N	2.74118300	4.00508600	-1.39105100
C	6.40262600	-0.16153700	2.50120500
C	7.49943800	0.68985500	2.46108000
C	3.99761000	-0.49853400	2.08513600
C	2.96537700	-1.15985500	2.11141400
C	1.09897100	2.49437900	-2.06418100
C	1.23268800	1.25634300	-2.16091300
C	-0.59971600	3.01532400	0.53989600
C	-1.71311200	2.51656000	0.25851300
H	8.17221600	2.67423900	1.93656100
H	6.49021300	4.46440900	1.54619800
H	6.41376300	3.73733300	-0.05653200
H	4.29466400	5.18112100	2.55029800
H	3.92321400	3.43809000	2.50464100
H	4.53248100	6.27360000	0.22070000
H	5.27186600	5.19334800	-0.95809800
H	2.52472000	6.61209500	2.75060200
H	0.06357200	7.05436200	2.60754100
H	-1.39764700	5.32039600	1.52974100
H	2.79375500	7.35437100	-1.08701500
H	-0.20677400	4.79534100	-2.82504200

H	6.47987600	-1.17395900	2.88270300
H	8.46988200	0.35194100	2.81477400
H	0.64756200	7.10627200	-2.34972300
Au	1.90613000	-0.61764900	-2.12054300
Au	1.15950200	-1.97048600	2.06172300
Au	-3.53646500	1.77253500	-0.05570700
P	2.95689900	-2.62866100	-1.95603600
P	-5.62031100	0.91142600	-0.36506000
P	-0.95961800	-2.82551000	1.89348700
C	3.53389500	-3.51334300	-3.49367800
H	4.19144800	-2.84634900	-4.06278500
C	-5.89425300	-0.30219500	-1.75305400
H	-5.19668300	-1.13829000	-1.63704800
C	-1.58764100	-4.09140100	3.11225400
H	-1.57099100	-3.66152100	4.12034000
C	-7.08427600	2.01501500	-0.70883000
H	-6.89141100	2.59596400	-1.61786600
H	-7.19458300	2.72852000	0.11576100
C	-6.37944500	-0.08874500	1.01278600
H	-6.46951700	0.54898500	1.89994600
H	-5.69863700	-0.91038900	1.27297300
C	-2.42891500	-1.68118000	1.93589200
H	-2.29594000	-0.94626200	1.13386000
H	-2.44867700	-1.15150000	2.89471900
C	-1.38492300	-3.74544400	0.32940500
H	-0.70018300	-4.59340400	0.21292300
H	-1.23750000	-3.05464500	-0.50912800
C	2.14366100	-4.08651900	-1.12734700
H	1.21740800	-4.32949800	-1.66105600
H	1.87428400	-3.79025400	-0.10584000
C	4.56551500	-2.67023600	-1.01631100

H	4.37867500	-2.32041000	0.00592400
H	5.26509900	-1.96532600	-1.47926200
H	2.66830700	-3.73511200	-4.12845900
H	-0.91631000	-4.95779100	3.11714000
H	-5.65149400	0.18399700	-2.70439700
N	3.02188400	-5.25042700	-1.09595600
N	4.24081000	-4.74805600	-3.16954300
N	5.13982600	-4.01167900	-1.00610300
N	-3.67948800	-2.41821500	1.74621000
N	-2.76270100	-4.22177100	0.35166900
N	-2.94341400	-4.52144000	2.78111200
N	-8.31172000	1.24232900	-0.86498700
N	-7.69380100	-0.59985300	0.63782900
N	-7.26964500	-0.78644100	-1.77466200
C	-8.21930900	0.30415000	-1.98348900
C	-7.62033500	-1.47297500	-0.53242300
H	-8.60445200	-1.93612200	-0.67021600
H	-6.89087200	-2.26781800	-0.34312900
H	-7.94541400	0.85156200	-2.89205200
H	-9.21178800	-0.13580900	-2.13545400
C	5.42849900	-4.48909500	-2.35482900
C	3.38405100	-5.68423500	-2.44389900
H	5.98717300	-5.42882700	-2.27009600
H	6.06361300	-3.75852400	-2.86792300
H	3.92301700	-6.63520800	-2.35842200
H	2.47068800	-5.85962200	-3.02363500
C	-3.69932500	-3.10666400	0.45057100
C	-3.00297500	-5.14197000	1.45803400
H	-4.71108800	-3.50384100	0.29675400
H	-3.46783900	-2.38130400	-0.33673800
H	-4.00539200	-5.56885500	1.33340900

H	-2.27535000	-5.95999100	1.41144100
Cu	-0.31720500	1.64158200	-0.91518700
C	4.25244000	-4.97040100	-0.35259500
H	3.99378900	-4.59829200	0.64434500
H	4.79756700	-5.91512400	-0.23983700
C	-3.88758300	-3.40659600	2.80450100
H	-4.89659700	-3.82047200	2.68904200
H	-3.83180800	-2.90656900	3.77783700
C	-8.62920400	0.48397500	0.34467600
H	-9.62533800	0.04537700	0.21358600
H	-8.66685500	1.16839400	1.19938900
Cl	-1.45292000	-0.42282100	-1.22981200

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C	5.35041500	-3.08587700	-2.27890500
C	4.94134100	-2.11369500	-1.35561300
N	3.83307800	-2.23478900	-0.63722800
C	3.05135300	-3.31341900	-0.82684400
C	5.75791700	-0.84430800	-1.19750700
N	5.41935000	-0.04945000	-0.04782100
C	5.78415800	-0.64860400	1.20761800
C	5.78748800	1.33580300	-0.16439100
C	4.99376300	-0.14922400	2.40319700
C	5.42827900	-0.46562100	3.69778100
C	4.65094500	-0.06805100	4.77682300
C	3.47214900	0.63122000	4.54385000
C	3.12487700	0.91652000	3.21732700
N	3.88353100	0.53849500	2.17233300
C	4.97779200	2.12600500	-1.17600200

C	5.40892800	3.40449500	-1.55635700
C	4.61518200	4.14482300	-2.42147000
C	3.42353500	3.59901400	-2.88522600
C	3.08035900	2.30835800	-2.46358000
N	3.85515500	1.58752200	-1.63243800
C	3.37248800	-4.32718900	-1.73826900
C	4.54940600	-4.20361400	-2.46796900
C	1.85497600	-3.34307300	-0.04311200
C	0.85959700	-3.23568200	0.66598600
C	1.86793900	1.66876600	-2.87264300
C	0.85729800	1.02126800	-3.12664600
C	1.92493700	1.61669000	2.87634100
C	0.92393700	2.18250100	2.44854400
H	6.27501900	-2.95875400	-2.83570200
H	6.83627700	-1.10874900	-1.24276400
H	5.55378800	-0.23636400	-2.08676300
H	6.86776200	-0.55719700	1.43596600
H	5.57669500	-1.72238300	1.13025300
H	5.60339400	1.80604200	0.80882600
H	6.86730700	1.48342900	-0.38117800
H	6.35387700	-1.01534500	3.84661200
H	4.95929200	-0.30012100	5.79280900
H	2.83429900	0.96072000	5.35750300
H	6.34462600	3.80398600	-1.17432000
H	2.77264600	4.14272800	-3.56210500
H	2.71654300	-5.18370700	-1.85466600
H	4.83793100	-4.97406900	-3.17811700
H	4.92059900	5.14007900	-2.73347400
Au	-0.45252000	-0.46375600	-3.12035000
Au	-0.42196700	-2.48058700	1.97304400
Au	-0.37514200	2.94867400	1.16542300

P	-1.73482500	-2.33598500	-2.84931400
P	-1.65099800	3.67942400	-0.58456700
P	-1.67146000	-1.29691200	3.47704600
C	-2.74240500	-2.48322200	-1.28665200
H	-3.47374000	-1.66672500	-1.25307300
C	-0.74433700	4.35648900	-2.06760700
H	-0.04093000	3.59024000	-2.41558400
C	-2.98596000	-2.06095400	4.55842300
H	-2.53576900	-2.85273400	5.16809300
C	-2.94508100	5.01468000	-0.43095800
H	-2.47482500	5.93014600	-0.05402800
H	-3.69547800	4.70696900	0.30653200
C	-2.69242900	2.42306500	-1.48794000
H	-3.42906100	2.00152100	-0.79349300
H	-2.03643300	1.60869800	-1.81954700
C	-0.74521400	-0.36573500	4.80123800
H	-0.02504500	0.29948100	4.30956000
H	-0.18332000	-1.07806000	5.41589200
C	-2.67837600	0.13389300	2.83082400
H	-3.42324300	-0.24388000	2.12013100
H	-2.00578400	0.80939400	2.28789000
C	-0.83553400	-3.96464000	-2.71446300
H	-0.11278100	-3.88748500	-1.89311600
H	-0.27776900	-4.14505800	-3.64035000
C	-3.05960900	-2.86220600	-4.05304100
H	-2.61227900	-2.99683200	-5.04454100
H	-3.80708200	-2.06497400	-4.13886200
H	-2.06648500	-2.36665600	-0.43046300
H	-3.74640300	-2.53126500	3.92421200
H	-0.16461900	5.23561700	-1.76436800
N	-1.76370400	-5.06100300	-2.46549400

N	-3.42721100	-3.76790700	-1.20812400
N	-3.70208900	-4.10077200	-3.62758700
N	-1.65550900	0.40916000	5.63605000
N	-3.34185500	0.85496900	3.91041600
N	-3.60828400	-1.06414400	5.42266600
N	-3.58904100	5.28045200	-1.71255800
N	-3.37103400	3.01300400	-2.63559400
N	-1.67122100	4.71004300	-3.13588300
C	-2.62396200	5.73169400	-2.71692700
C	-2.41063800	3.54110700	-3.60907300
H	-2.96905300	3.83305500	-4.50615900
H	-1.70085700	2.75273800	-3.87981700
H	-2.07805800	6.59771300	-2.32605800
H	-3.18780800	6.05315000	-3.60054700
C	-4.35040400	-3.95326900	-2.32466900
C	-2.47371300	-4.88125200	-1.20015200
H	-4.93068300	-4.86393200	-2.13520200
H	-5.04554500	-3.10664400	-2.36355600
H	-3.03363400	-5.80041300	-0.99173200
H	-1.74462600	-4.72625200	-0.39828600
C	-2.36978100	1.41636400	4.85317500
C	-4.26043500	-0.00866400	4.64766900
H	-2.91446200	2.06412500	5.54999900
H	-1.64437400	2.02508800	4.30377100
H	-4.82563000	0.61854800	5.34701800
H	-4.96961800	-0.46419200	3.94690300
C	-2.74201200	-5.20257700	-3.53794800
H	-2.21829500	-5.30072300	-4.49548900
H	-3.30817700	-6.12475600	-3.36168700
C	-2.62988700	-0.43809900	6.31404900
H	-3.18061500	0.18344300	7.02989500

H	-2.10339500	-1.21925600	6.87388200
C	-4.26750800	4.09339500	-2.23256100
H	-4.84607700	4.39786000	-3.11260400
H	-4.96698000	3.71959400	-1.47592100