Supporting Information

Structure-activity relationship of anticancer and antiplasmodial gold bis(dithiolene) complexes

Constantin Vitré[1], Yann Le Gal[1], Antoine Vacher[1], Thierry Roisnel[1],Dominique Lorcy[1]*, Sofia Santana[2], Miguel Prudêncio[2], Teresa Pinheiro[3,4], Fernanda Marques[4,5]*

Table of content

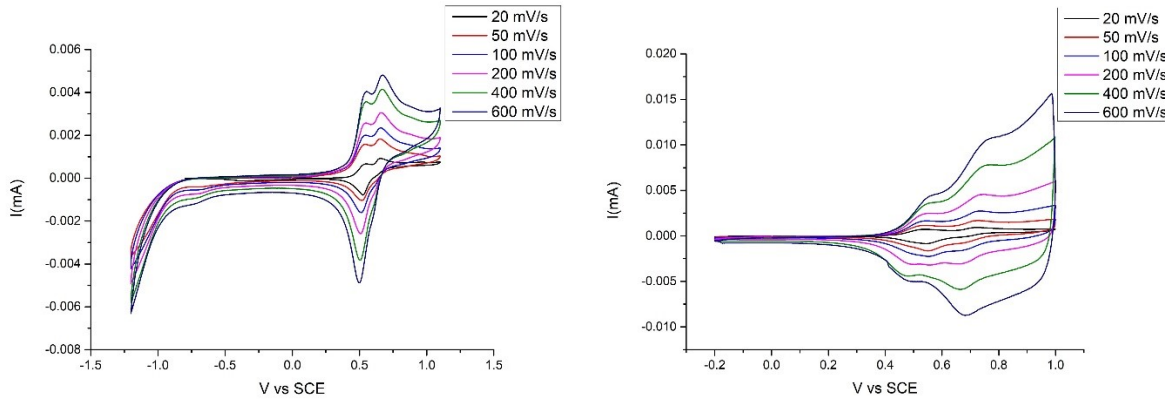


Fig. S1 : CVs of **AuN-PEG** (left) and **AuN-C_8** (right) in 0.1M $[CH_2Cl_2][Bu_4NPF_6]$ at different scan rate from 20 to 600 mVs^{-1}

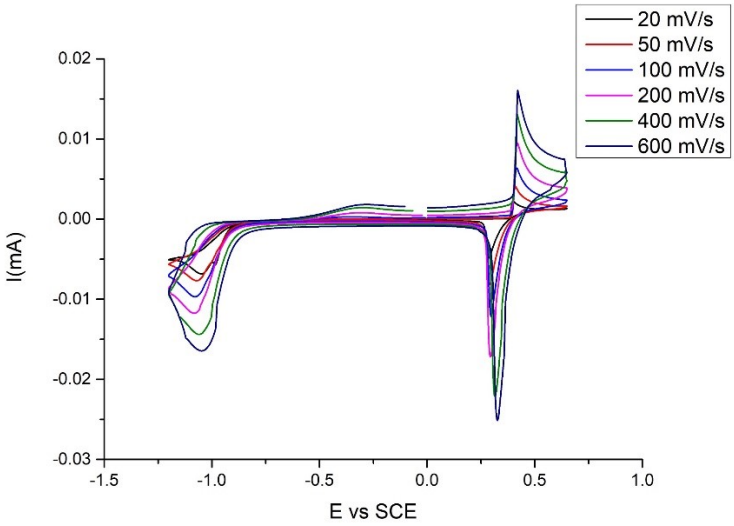


Fig. S2 : CVs of **AuS-EtOH** in 0.1M $[CH_2Cl_2][Bu_4NPF_6]$ at different scan rate from 20 to 600 mVs^{-1}

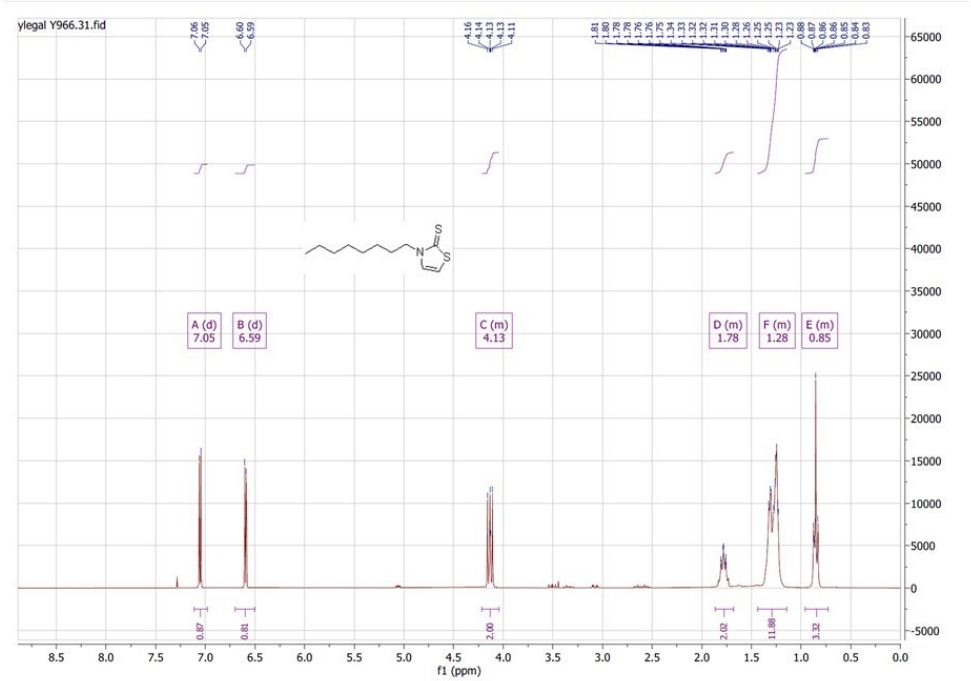


Fig. S3: ^{1}H NMR of **2a**

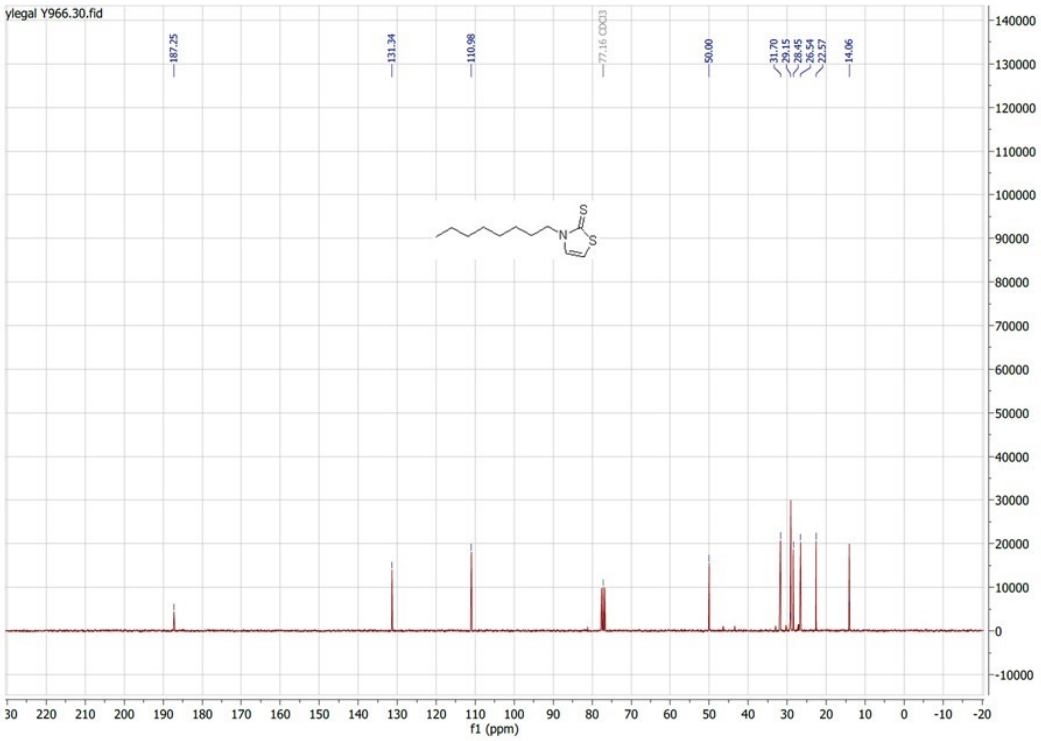


Fig. S4: ^{13}C NMR of **2a**

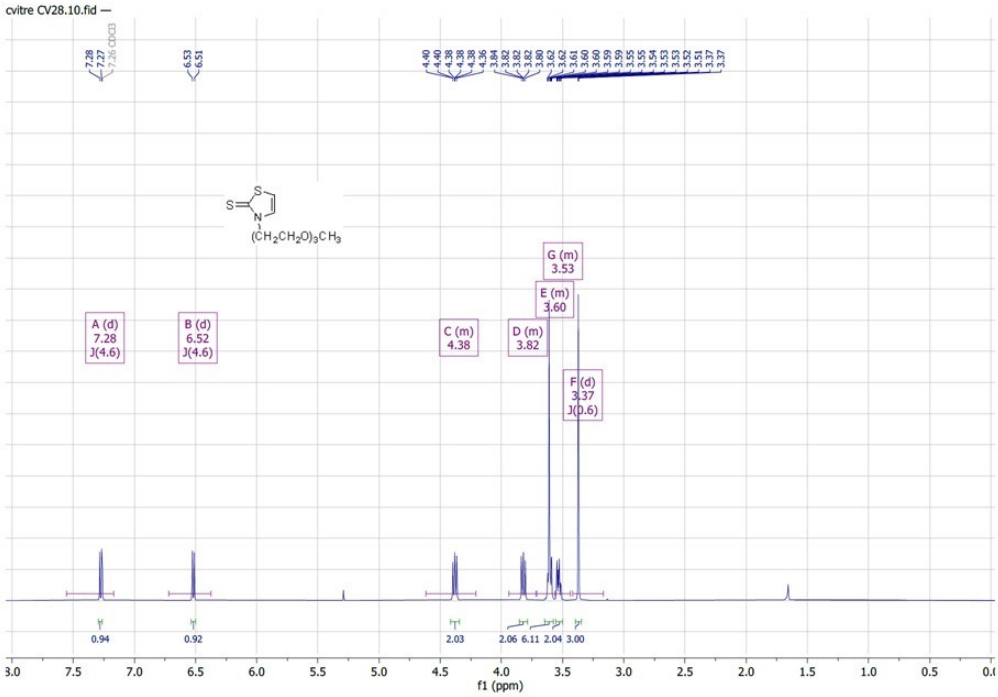


Fig. S5: ^{1}H NMR of **2b**

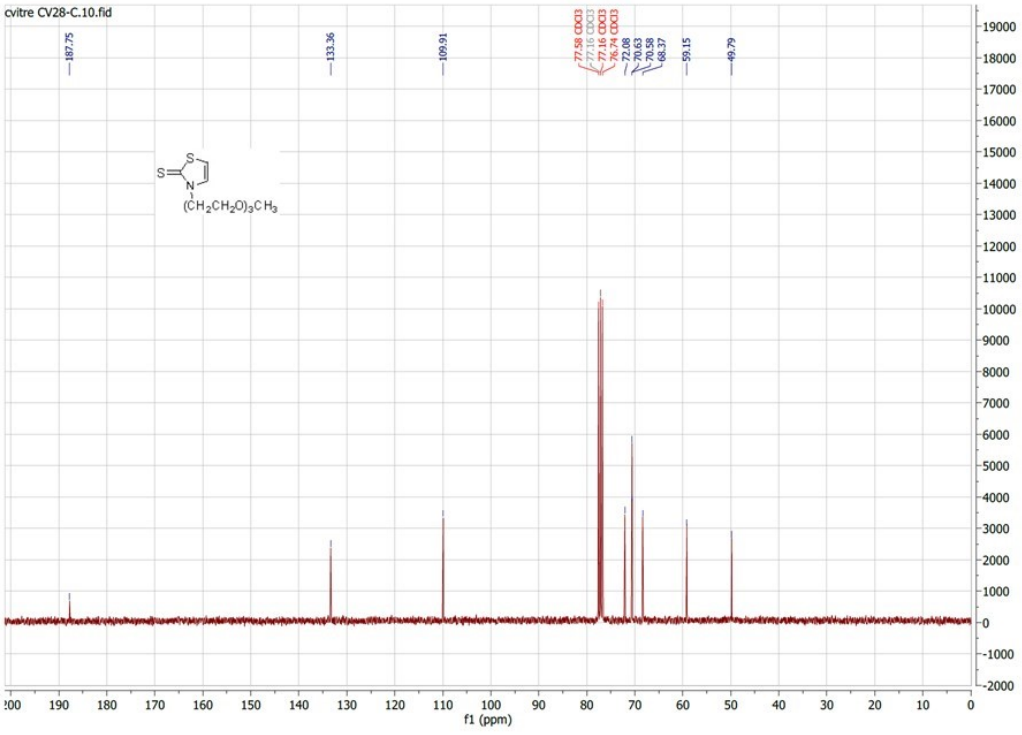


Fig. S6: ^{13}C NMR of **2b**

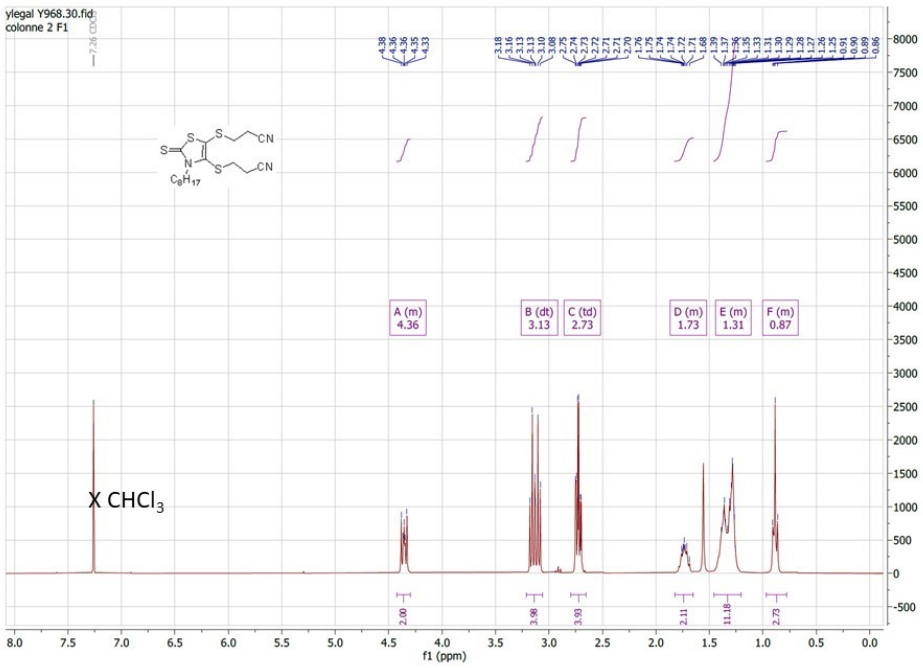


Fig. S7: ^{1}H NMR of **3**

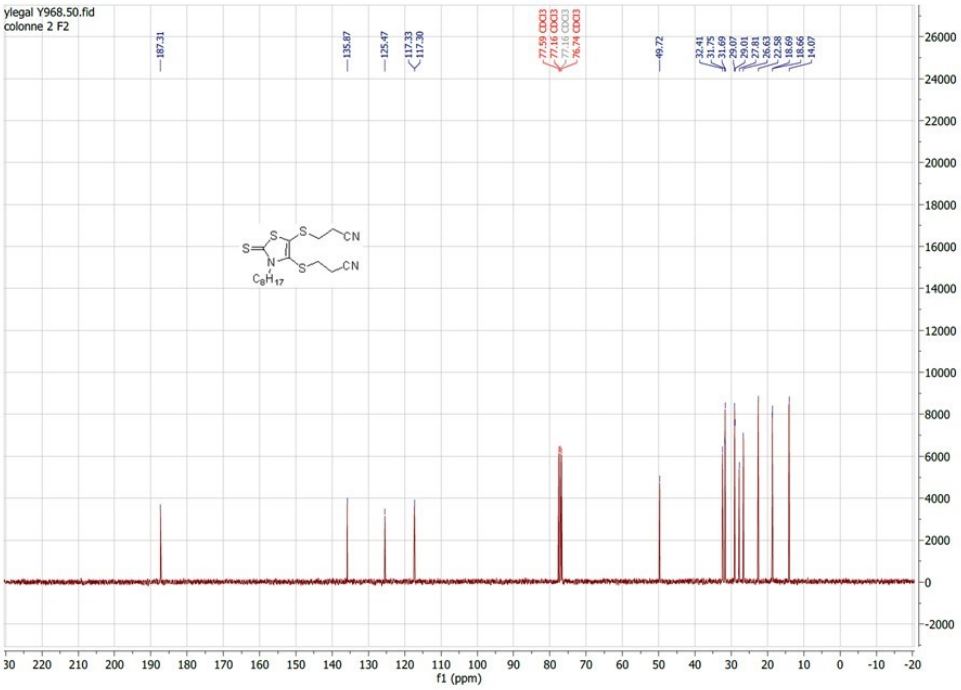


Fig. S8: ^{13}C NMR of **3**

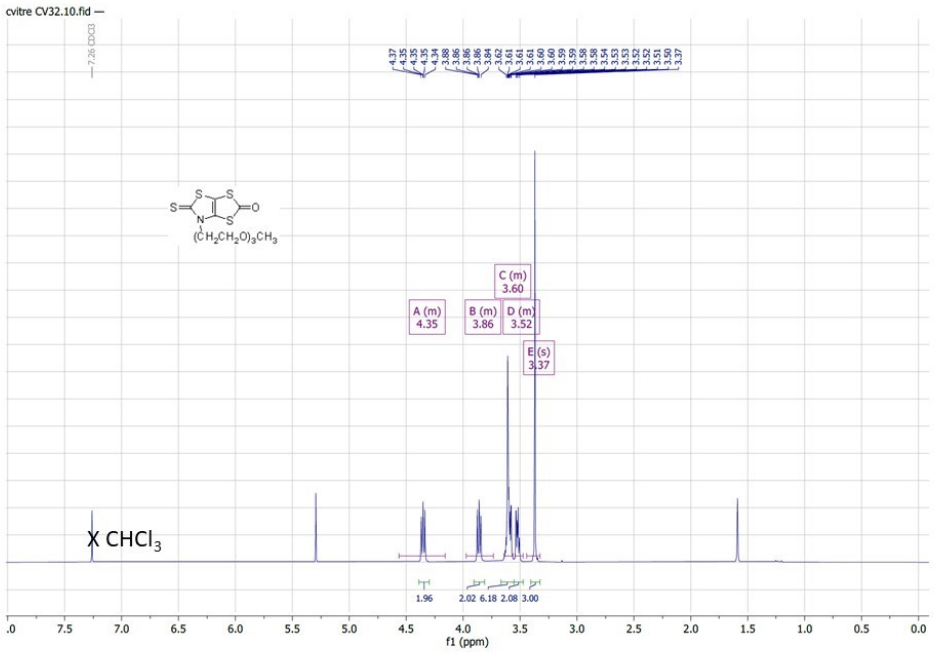


Fig. S9: ^{1}H NMR of **4**

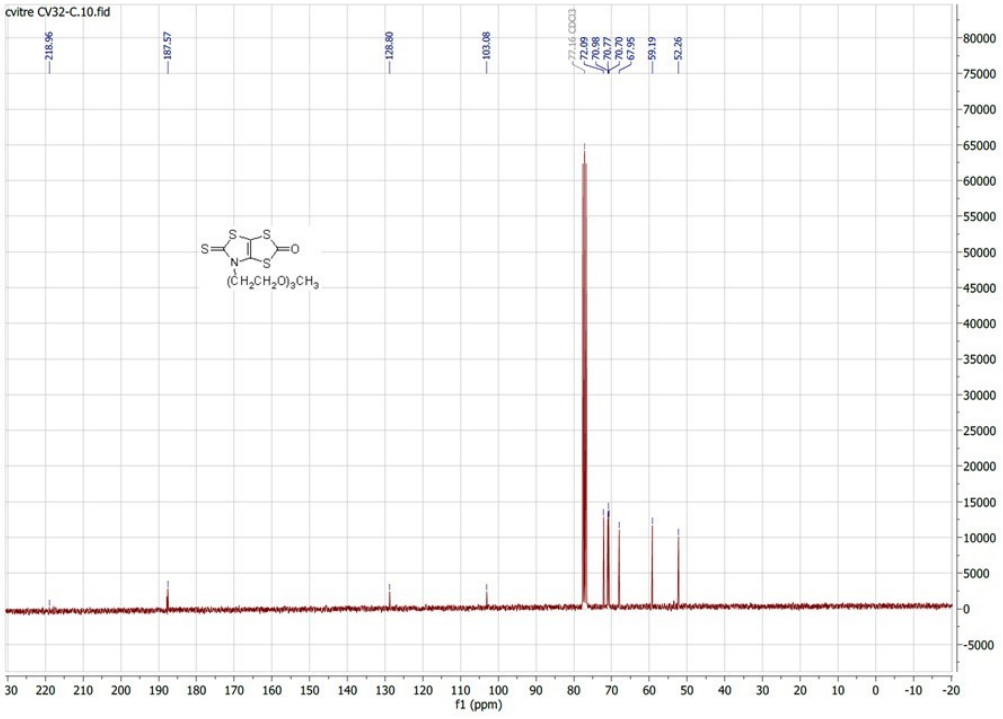


Fig. S10: ^{13}C NMR of **4**

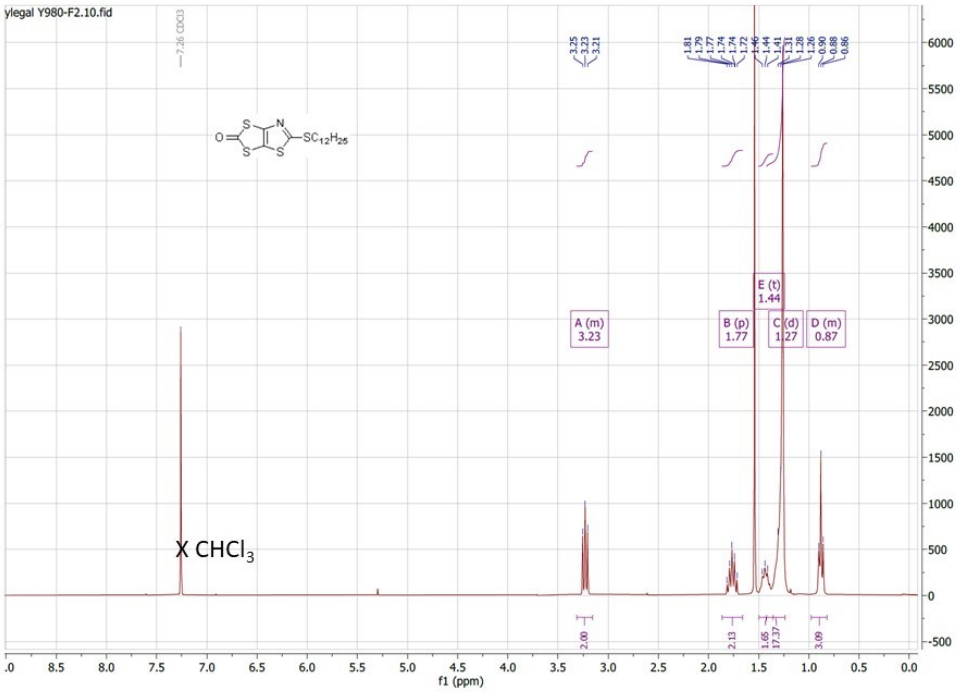


Fig. S11: ^{1}H NMR of **6a**

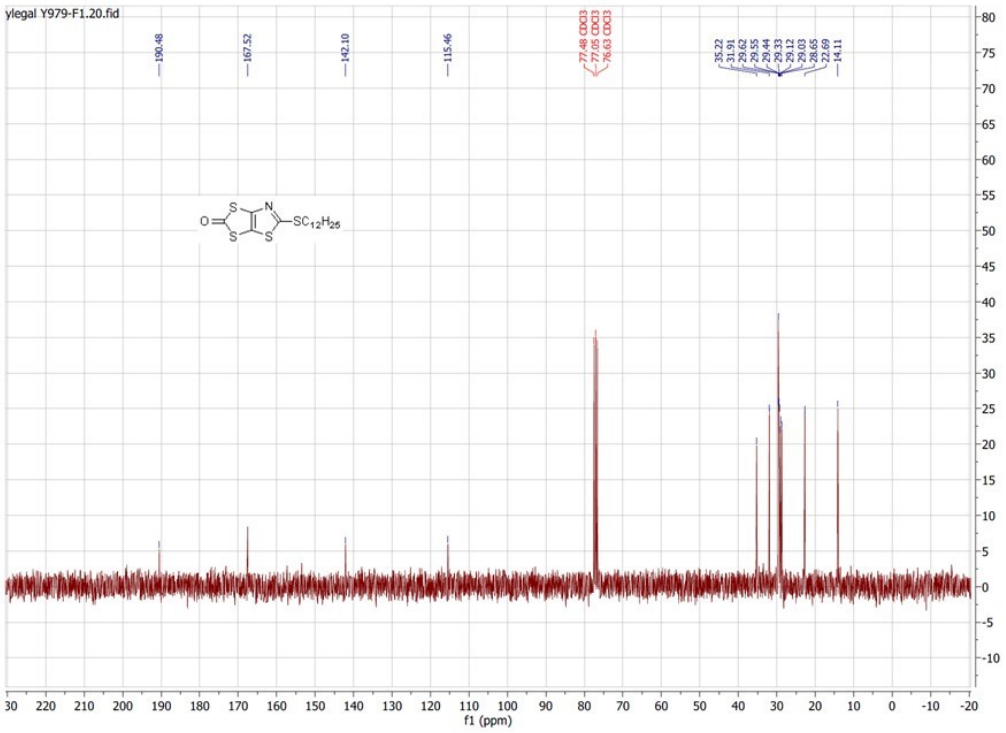


Fig. S12: ^{13}C NMR of **6a**

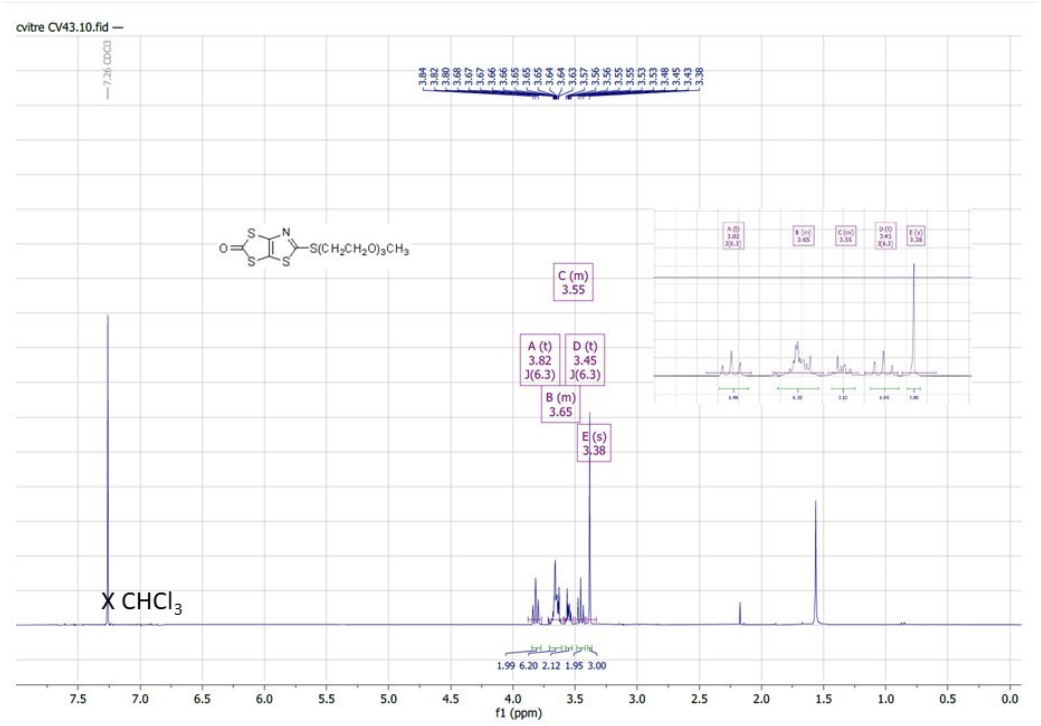


Fig. S13: ^{1}H NMR of **6b**

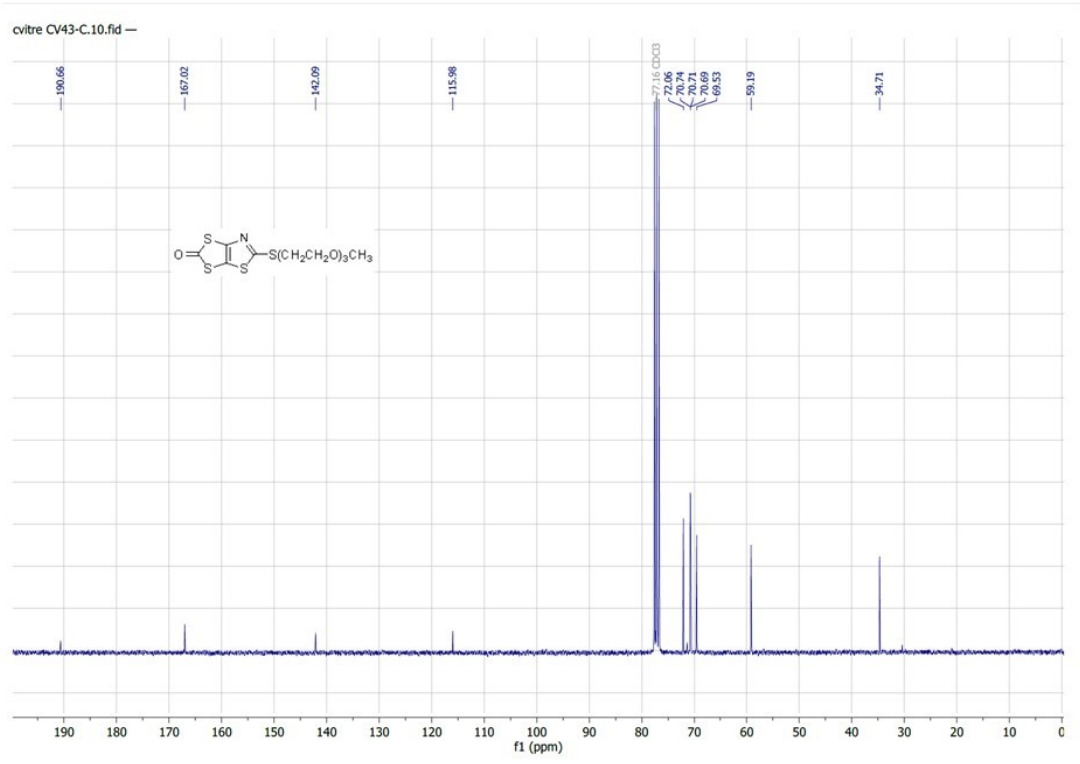


Fig. S14: ^{13}C NMR of **6b**

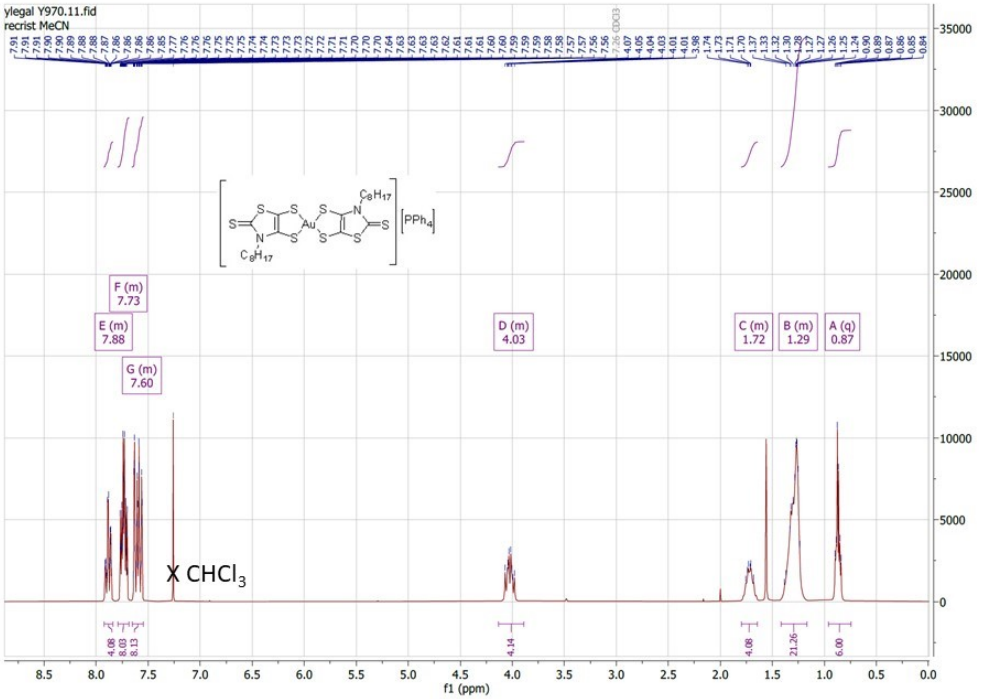


Fig. S15: ^{1}H NMR of **AuN-C$_8$**

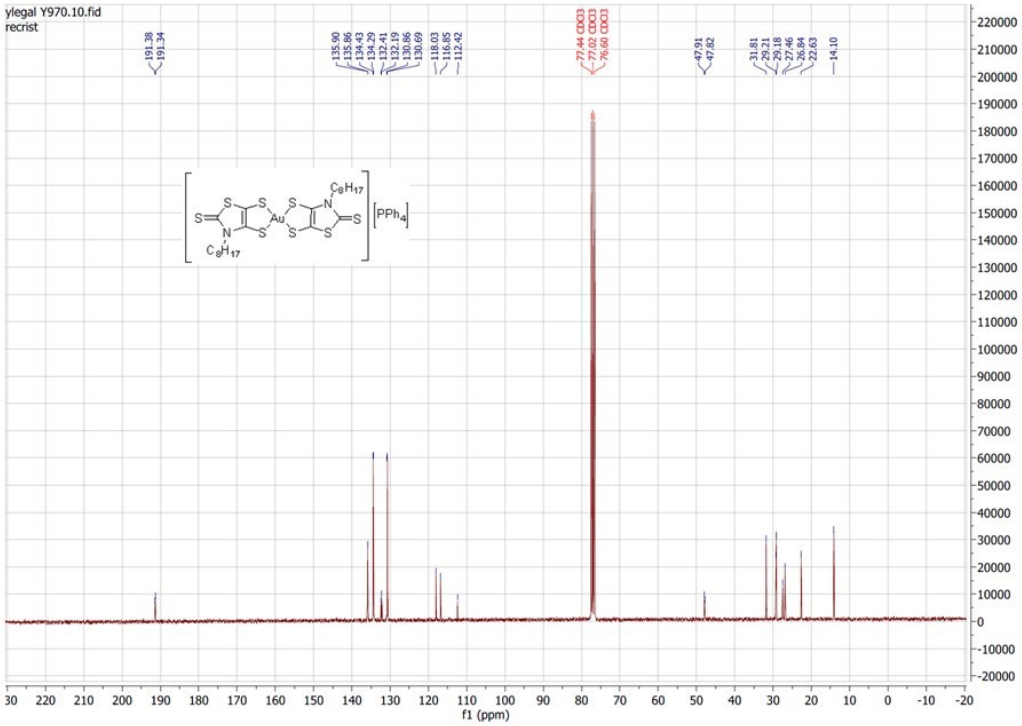


Fig. S16: ^{13}C NMR of **AuN-C$_8$**

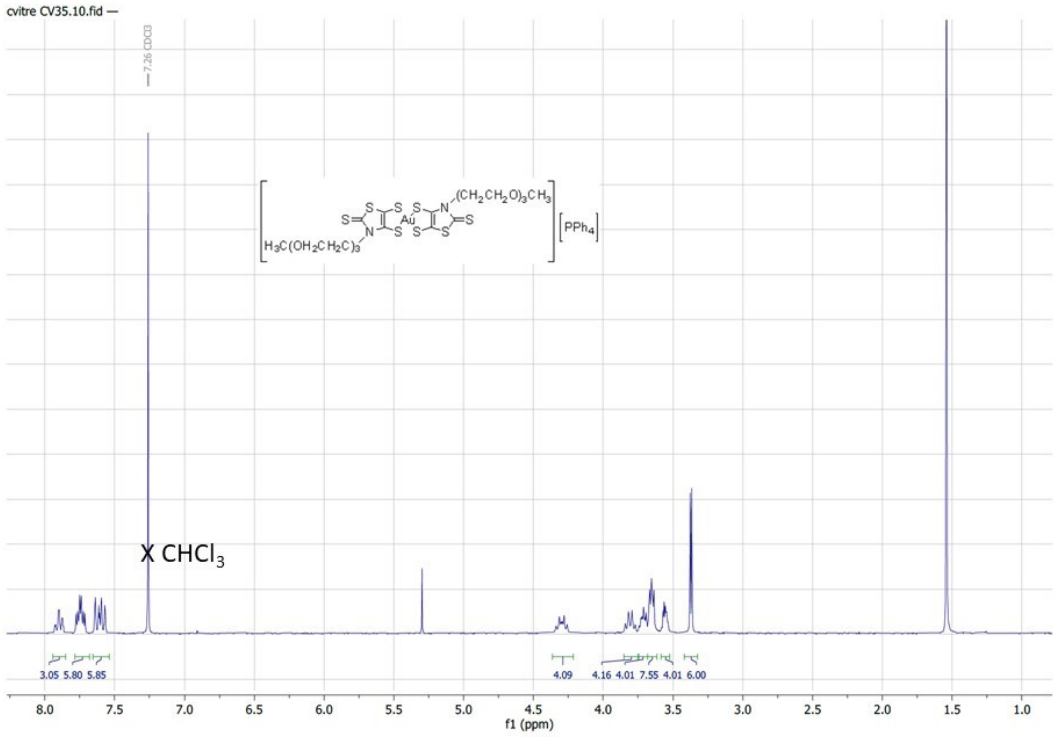


Fig. S17: ^{1}H NMR of **AuN-PEG**

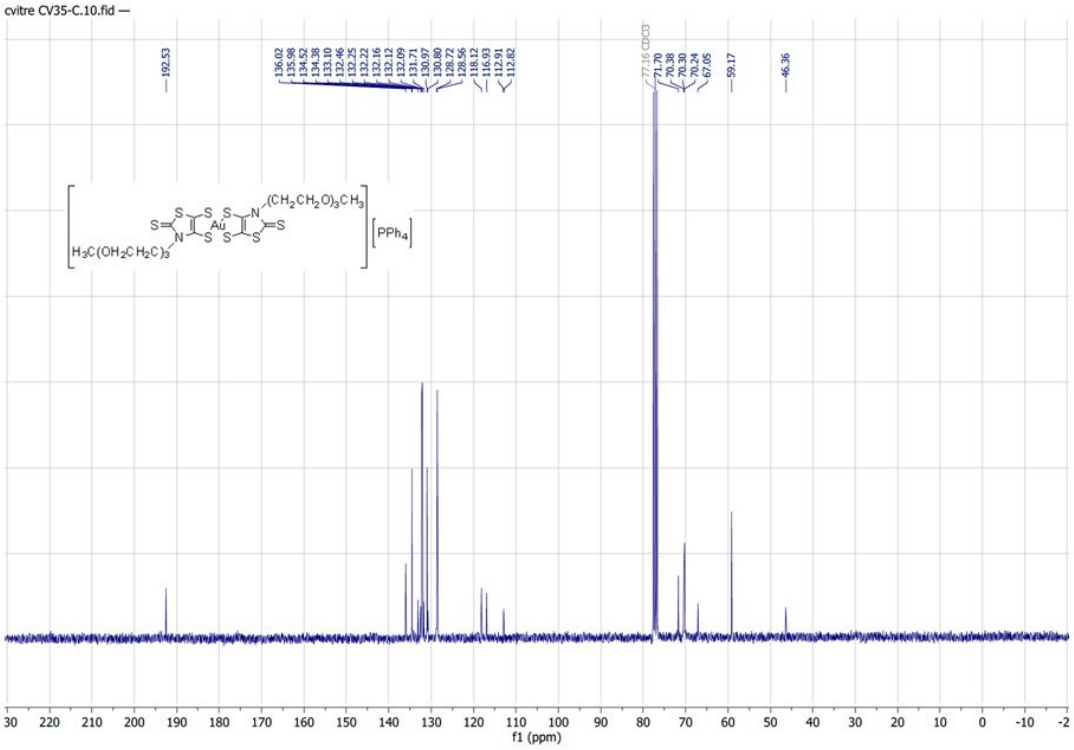


Fig. S18: ^{13}C NMR of **AuN-PEG**

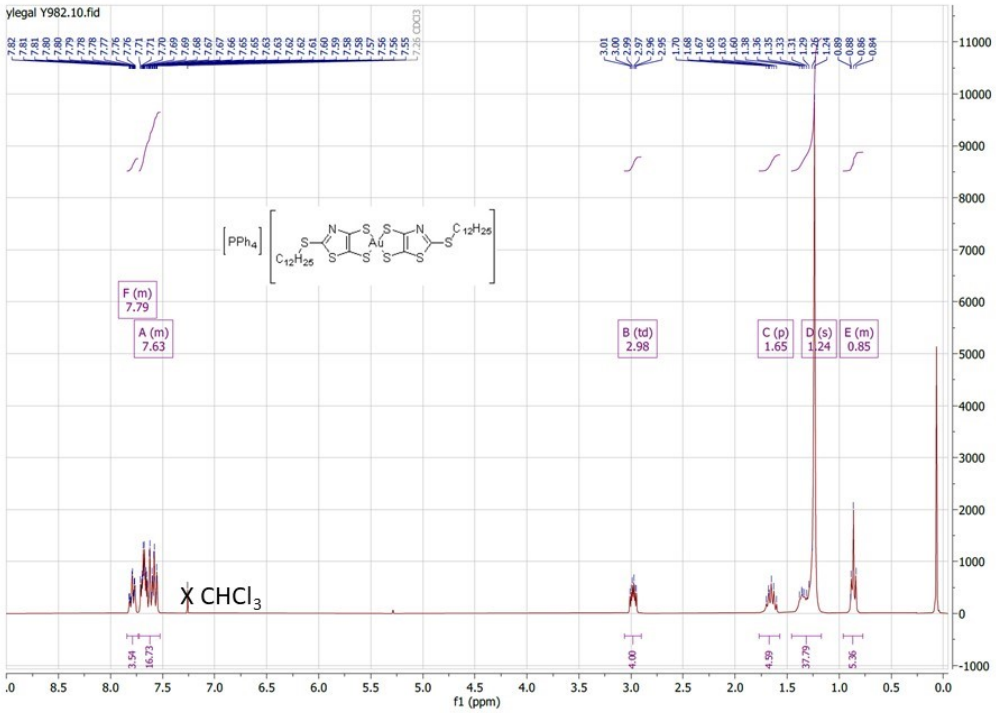


Fig. S19: ^{1}H NMR of **AuS- C_{12}**

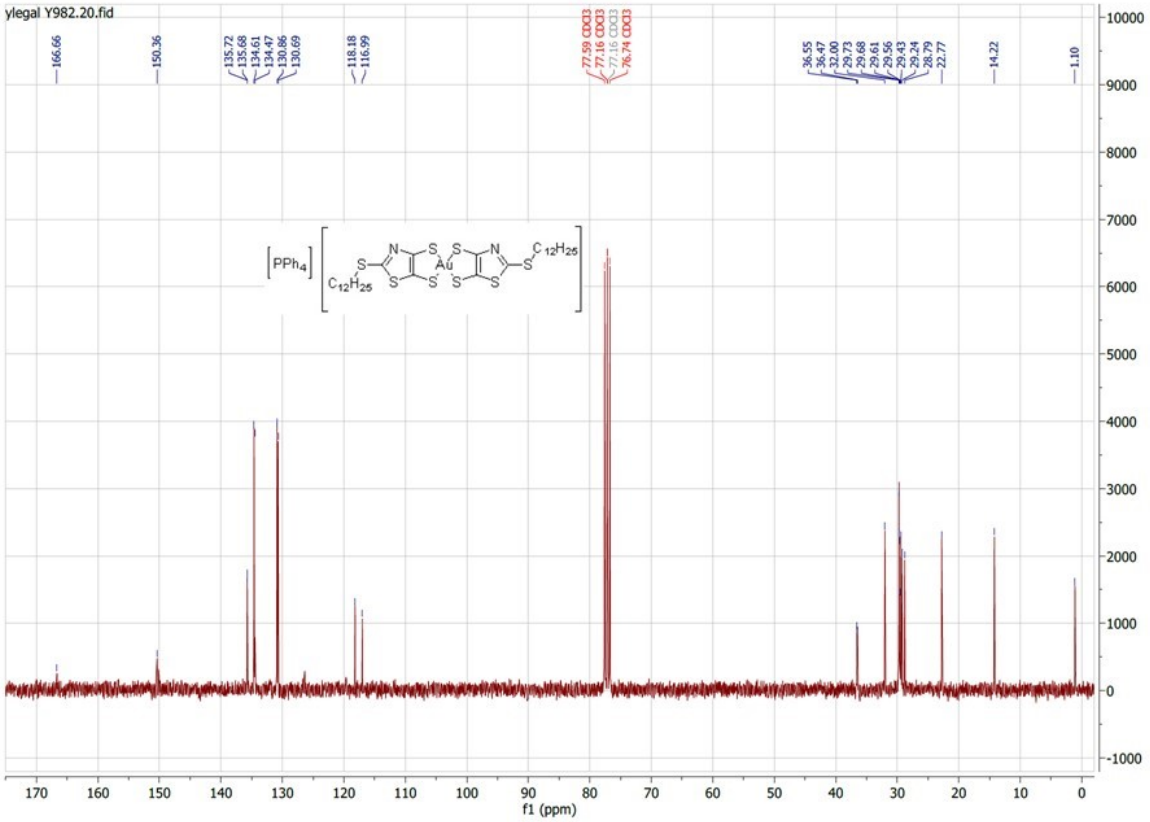


Fig. S20: ^{13}C NMR of **AuS-C_{12}**

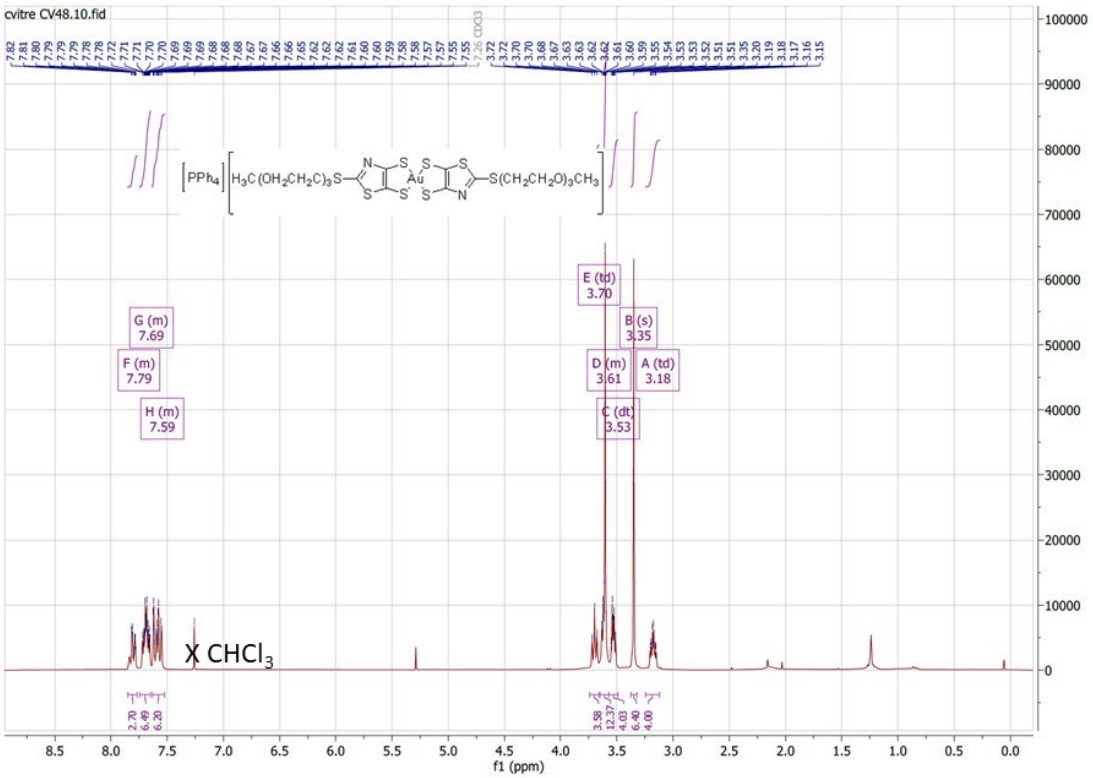


Fig. S21: ^{1}H NMR of **AuS-PEG**

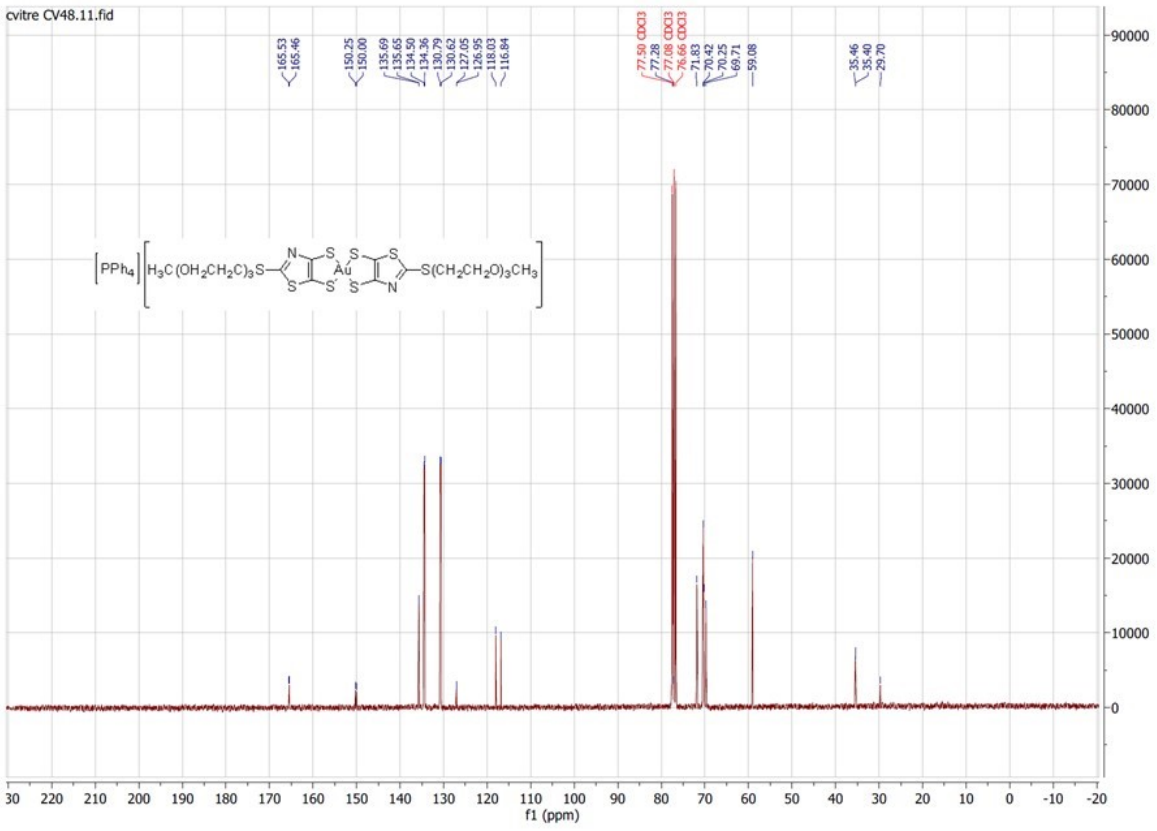


Fig. S22: ^{13}C NMR of **AuS-PEG**

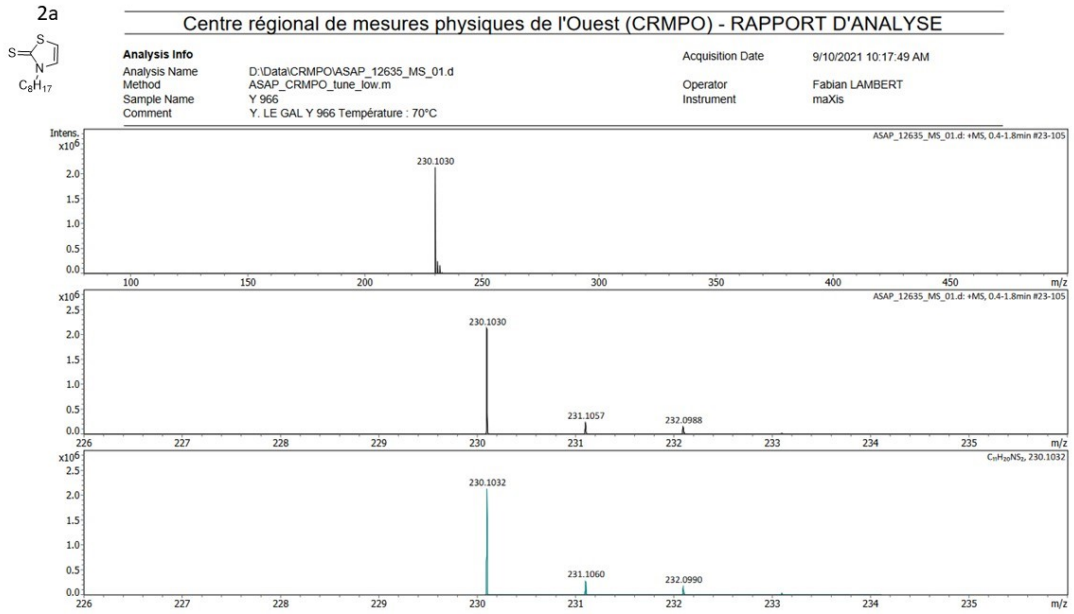


Fig. S23: HRMS of 2a

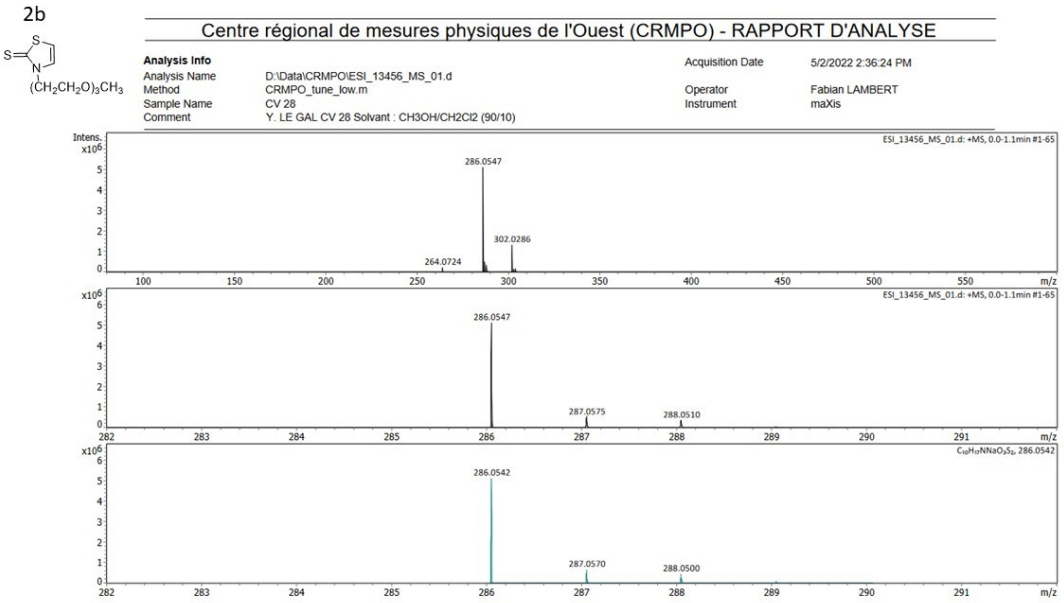


Fig. S24: HRMS of 2b

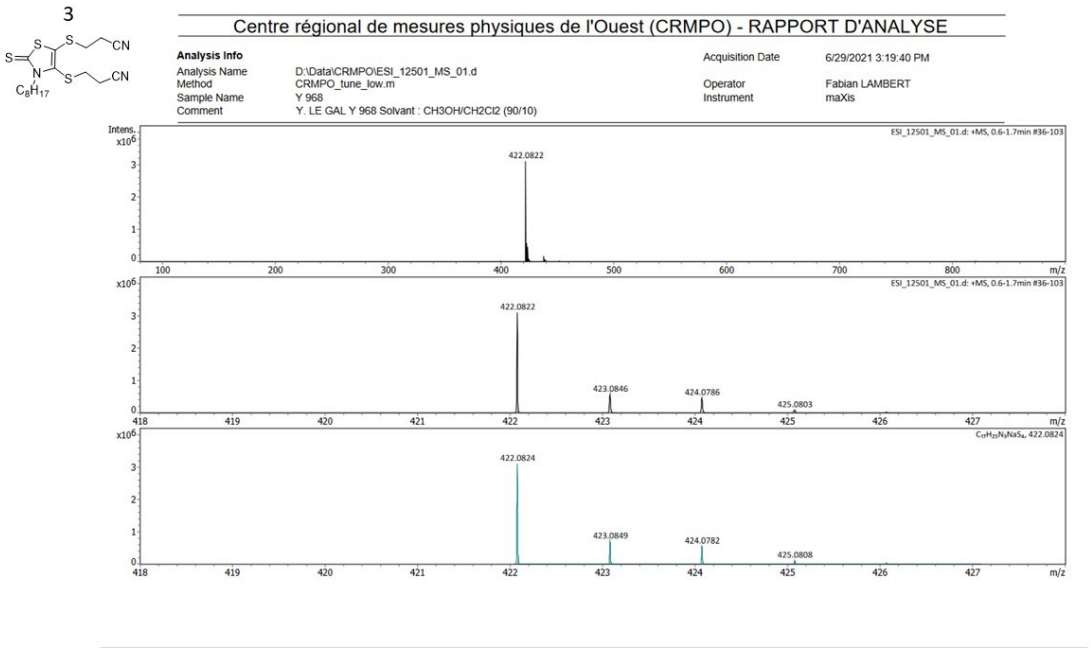


Fig. S25: HRMS of 3

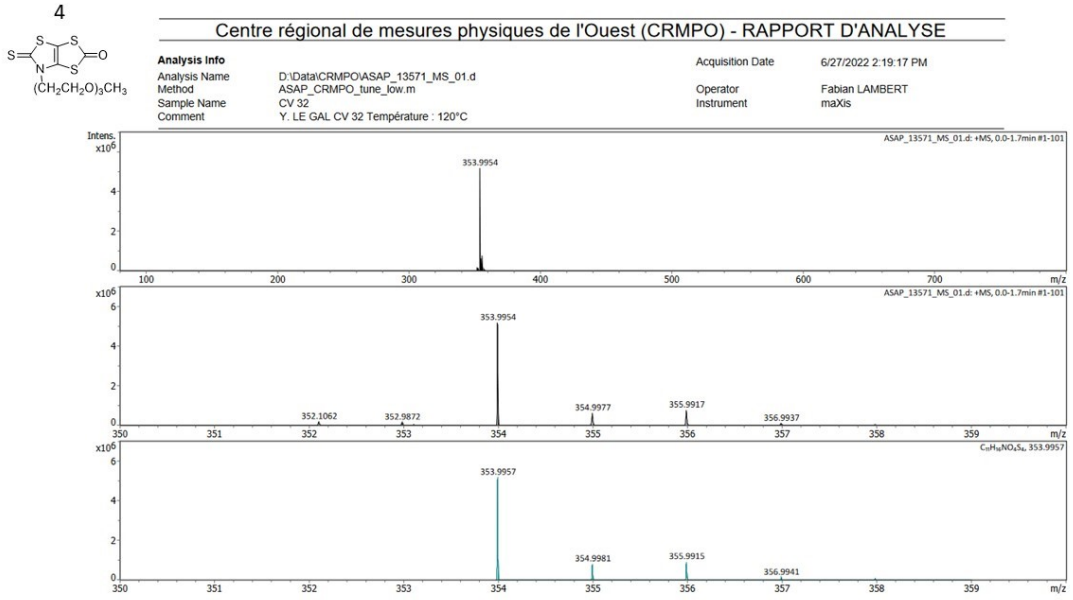


Fig. S26: HRMS of 4

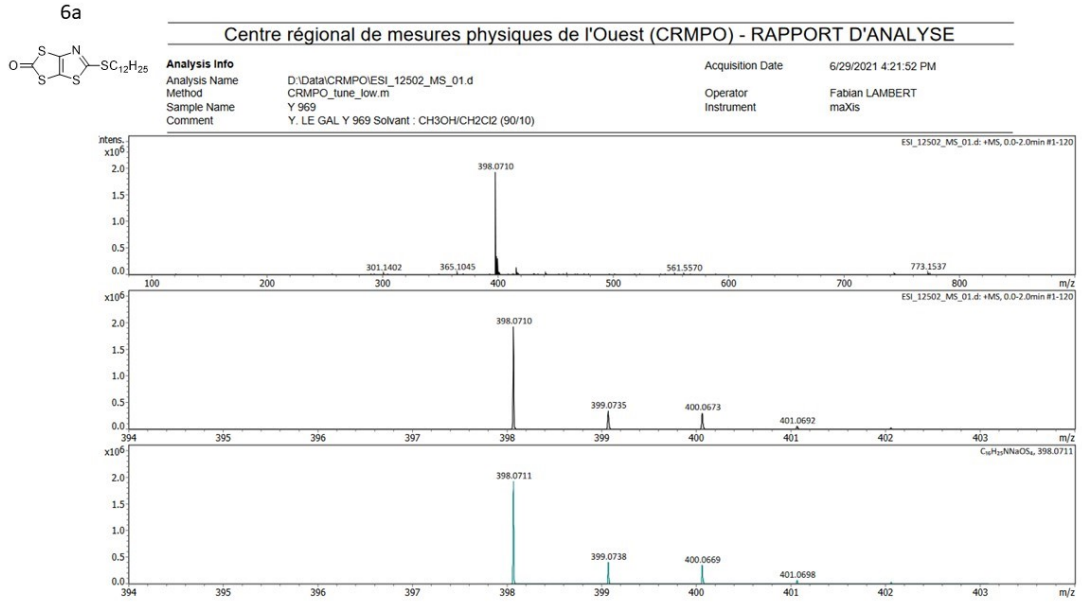


Fig. S27: HRMS of 6a

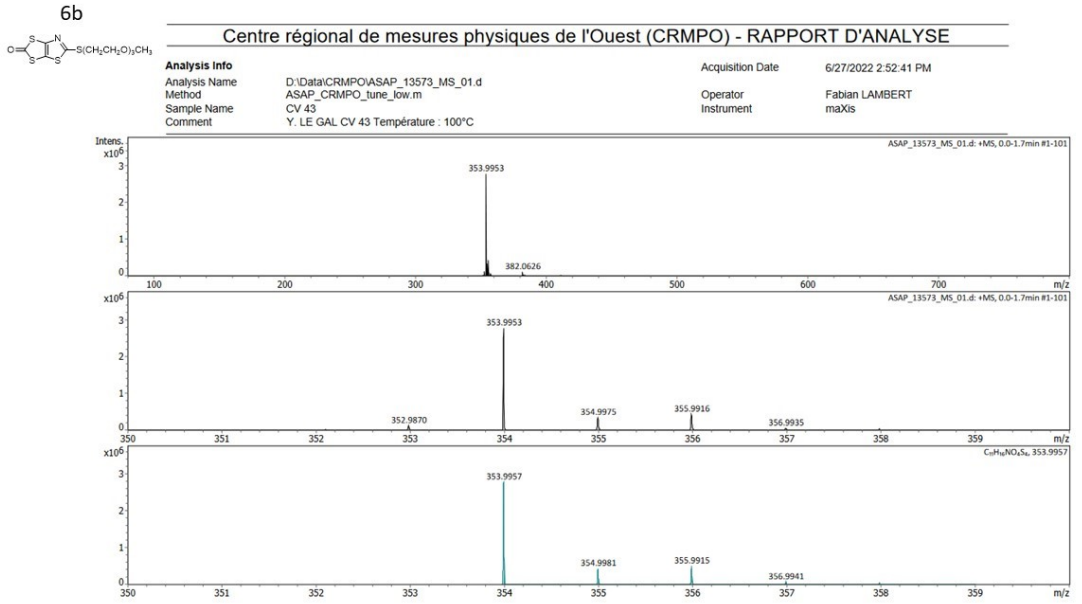


Fig. S28: HRMS of 6b

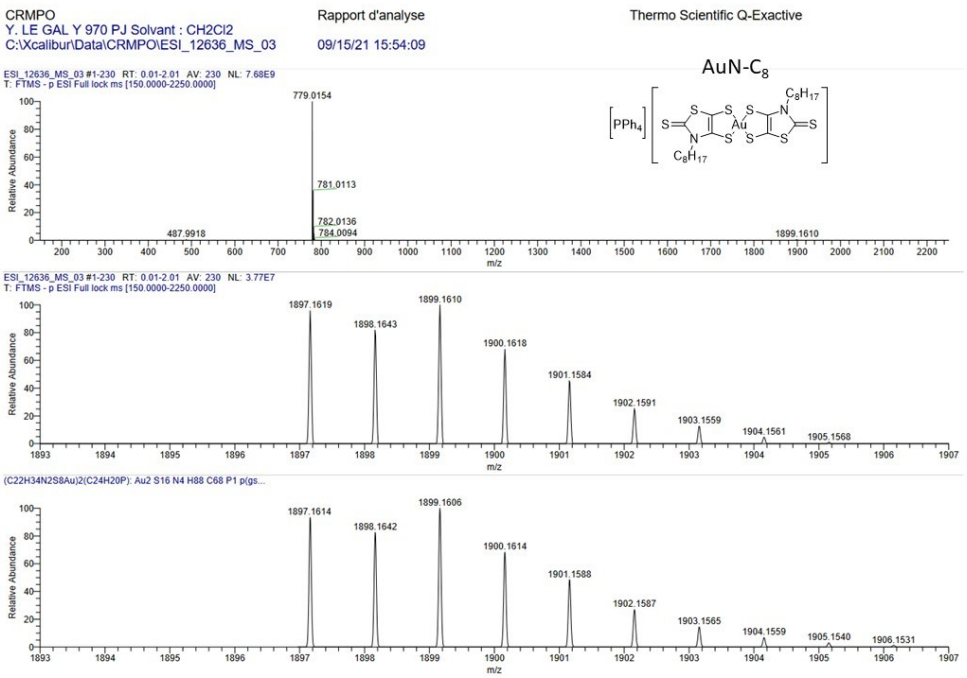


Fig. S29: HRMS of AuN-C_8

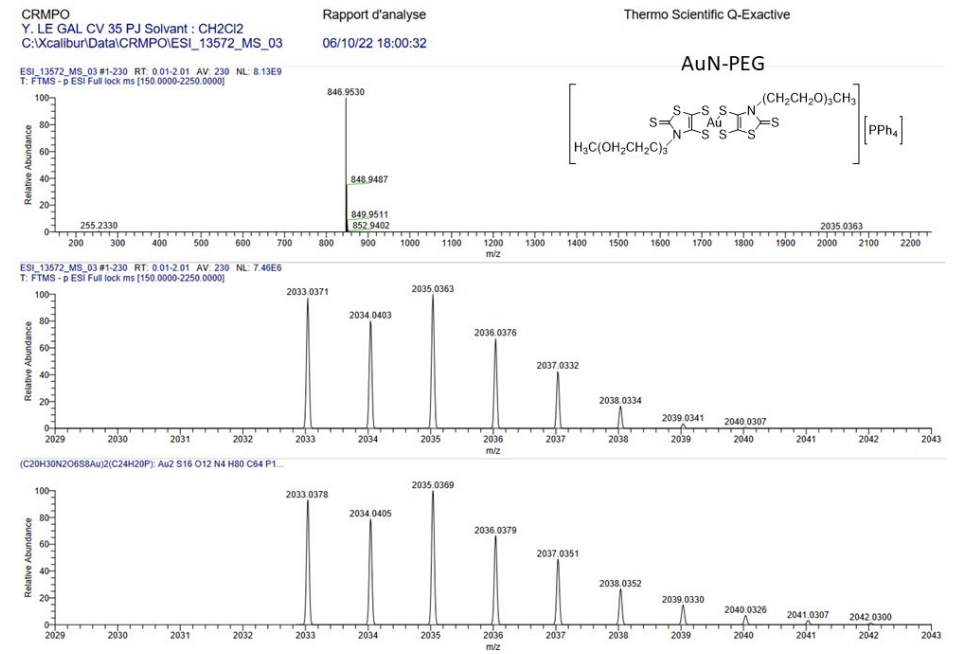


Fig. S30: HRMS of AuN-PEG

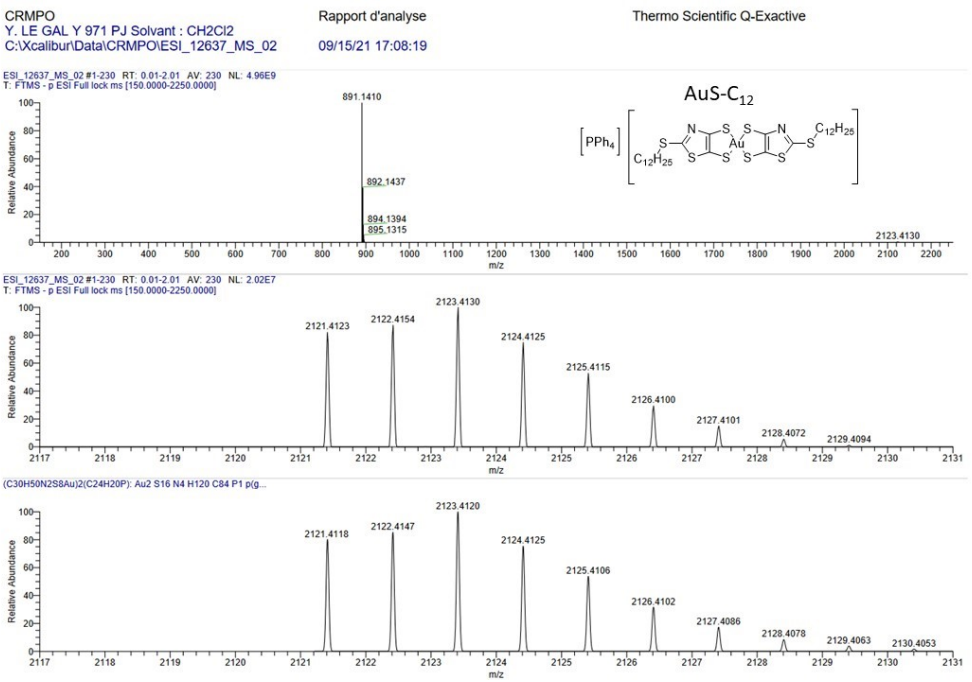


Fig. S31: HRMS of AuS-C_{12}

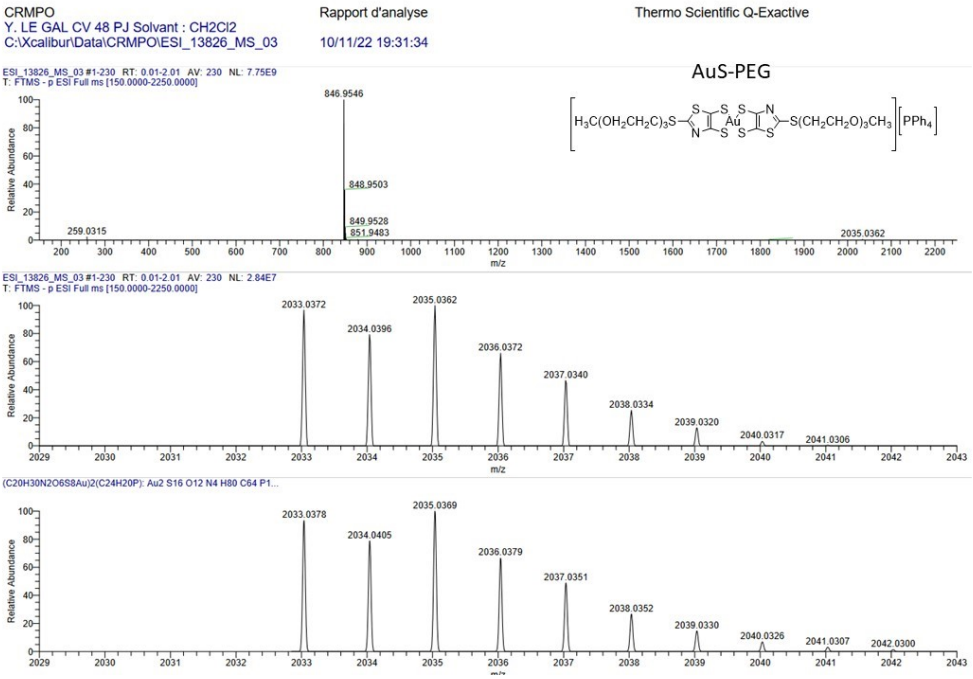
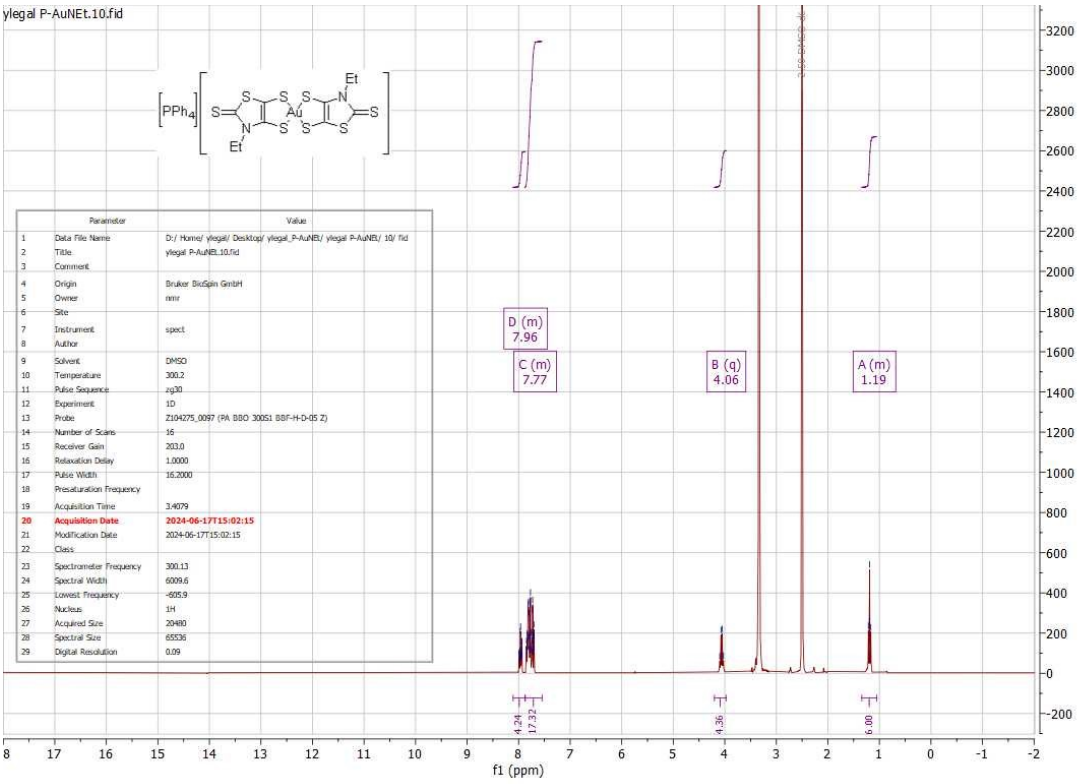
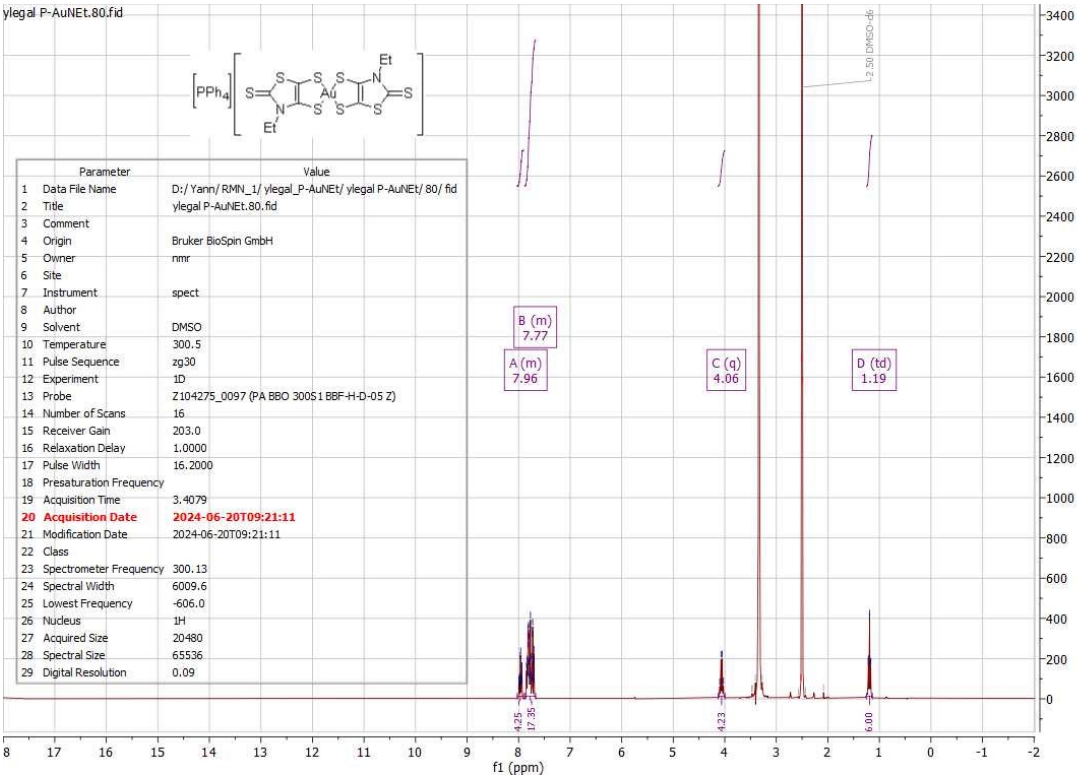


Fig. S32: HRMS of AuS-PEG

Table S1. Redox potentials (E in V *vs.* SCE) and absorption maxima λ_{max} (nm) for the NIR absorptions of the investigated monoanionic gold complexes.

				λmax (nm)	
	E_{pc}[1]	**$E_{pa/pc}$[2]**	**$E_{pa/pc}$[3]**	**Neutral**	**Monocation**
AuN-C_8	-1.10*	0.54/0.49	0.77/0.59	2080	-
AuN-PEG	-0.94*	0.54/0.53 [a]	0.68/0.58 [a]	2030	-
AuN-Et	-0.90*	0.55/0.49 [a]	0.71/0.61 [a]	-	-
AuN-EtOH	-0.99*	0.47/0.35 [a]	0.67/0.46 [a]	-	-
AuS-C_{12}	-1.01*	0.51/0.36	1.10/0.91	1734	1030
AuS-PEG	-1.10*	0.52/0.46	1.00/0.93	1700	1050
AuS-Et	-1.04*	0.48/0.44 [a]	-	-	-
AuS-EtOH	-1.12*	0.45/0.28 [a]	-	-	-
AuS-*t*BuS[13]	-1.18*	0.58/0.42	1.05/0.98	1614	1038





Parameter	Value
1 Data File Name	D:/ Yann/ RMN_1/ ylegal_P-AuNEt/ ylegal P-AuNEt/ 80/ fid
2 Title	ylegal P-AuNEt.80.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	DMSO
10 Temperature	300.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z104275_0097 (PA BBO 300S1 BBF-H-D-05 Z)
14 Number of Scans	16
15 Receiver Gain	203.0
16 Relaxation Delay	1.0000
17 Pulse Width	16.2000
18 Presaturation Frequency	
19 Acquisition Time	3.4079
20 Acquisition Date	**2024-06-20T09:21:11**
21 Modification Date	2024-06-20T09:21:11
22 Class	
23 Spectrometer Frequency	300.13
24 Spectral Width	6009.6
25 Lowest Frequency	-606.0
26 Nucleus	1H
27 Acquired Size	20480
28 Spectral Size	65536
29 Digital Resolution	0.09

Figure S33 - ^{1}NMR spectra of complex **AuN-Et** in DMSO solution at T0 (top) and the same tube analyzed 66h later (bottom).