

Supporting Information

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

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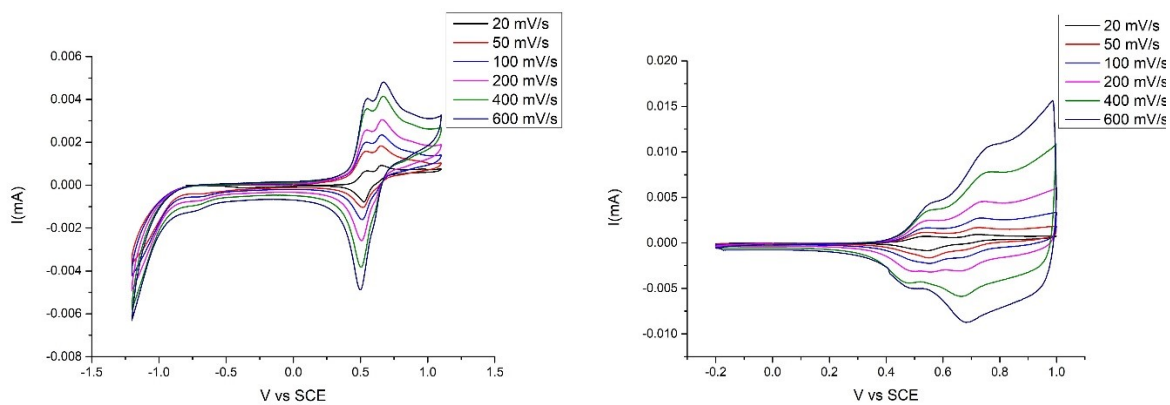


Fig. S1 : CVs of AuN-PEG (left) and AuN-C₈ (right) in 0.1M [CH₂Cl₂][Bu₄NPF₆] at different scan rate from 20 to 600 mV s⁻¹

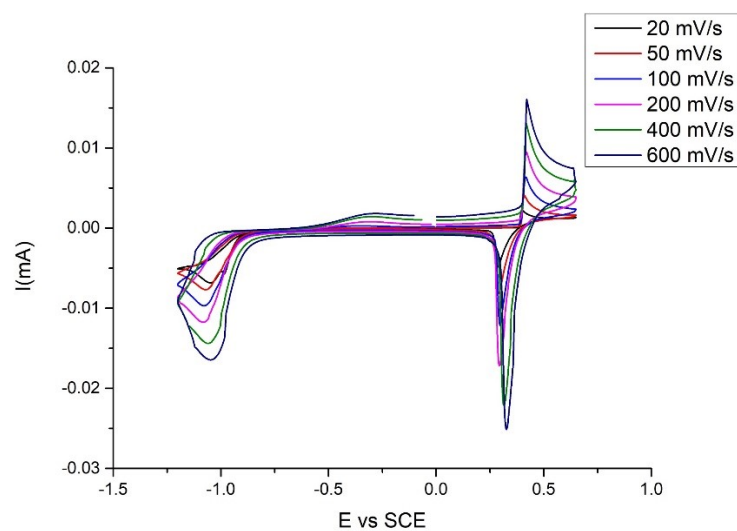


Fig. S2 : CVs of AuS-EtOH in 0.1M [CH₂Cl₂][Bu₄NPF₆] at different scan rate from 20 to 600 mV s⁻¹

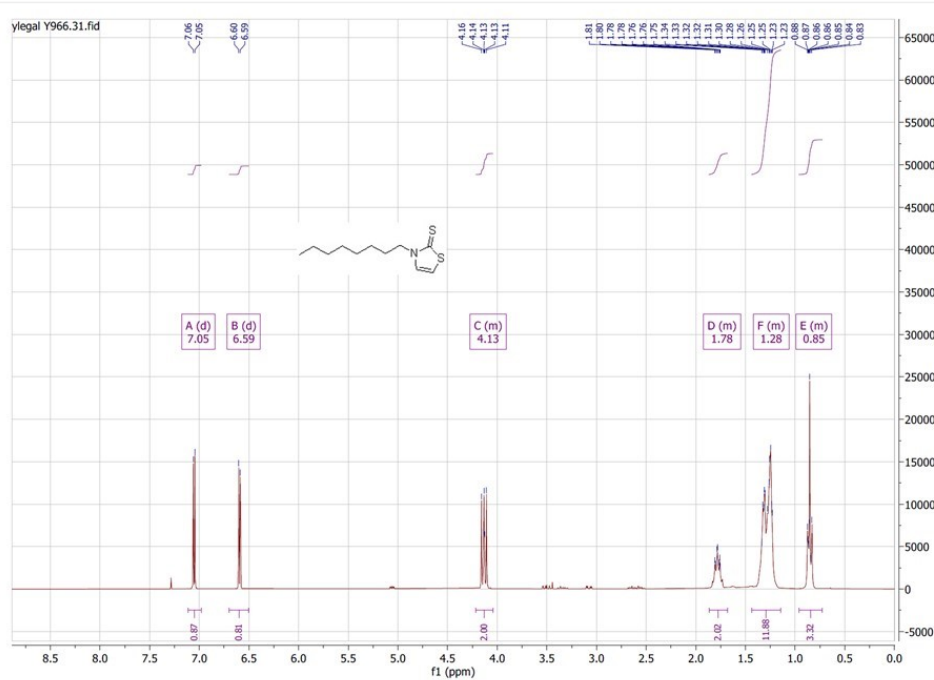


Fig. S3: ^1H NMR of 2a

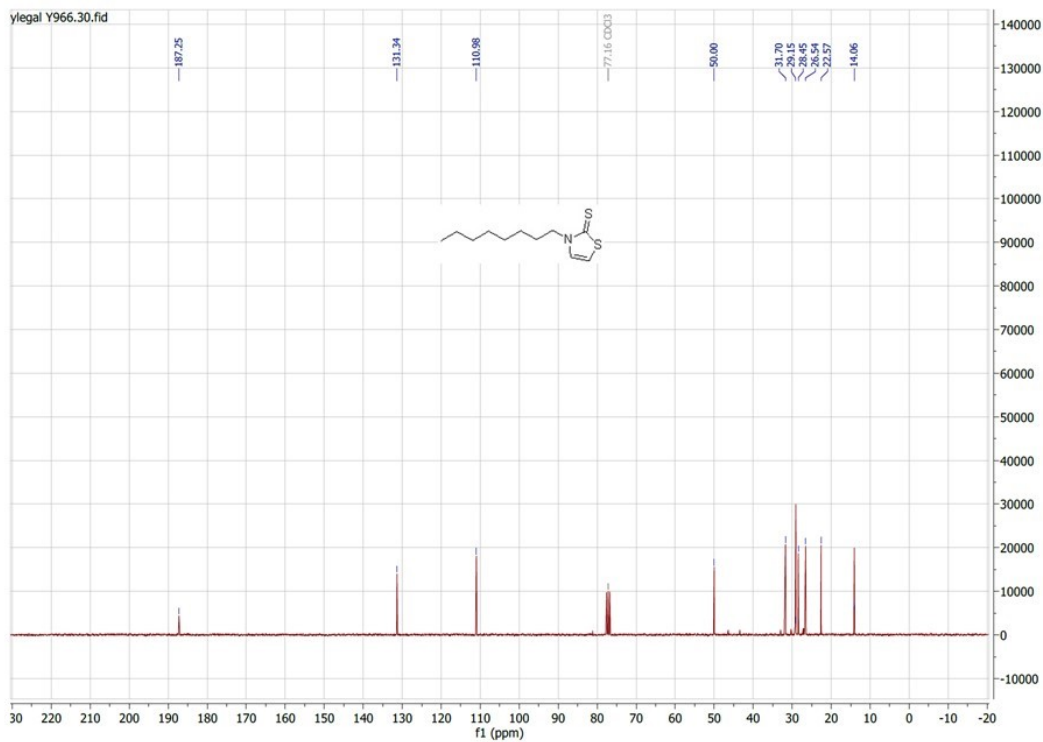


Fig. S4: ^{13}C NMR of 2a

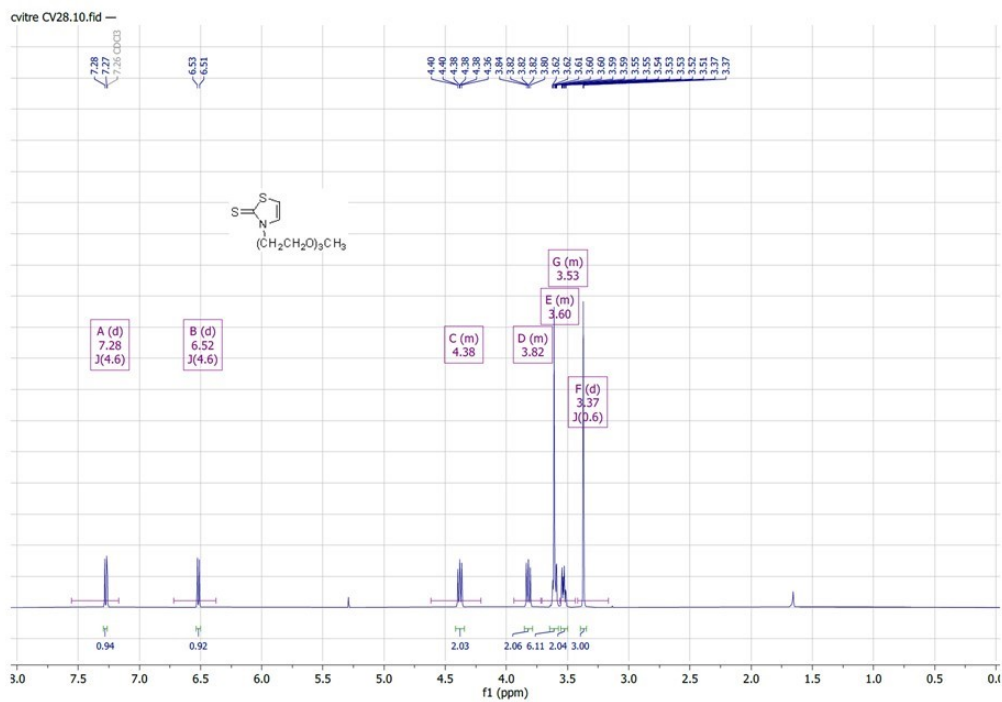


Fig. S5: ^1H NMR of 2b

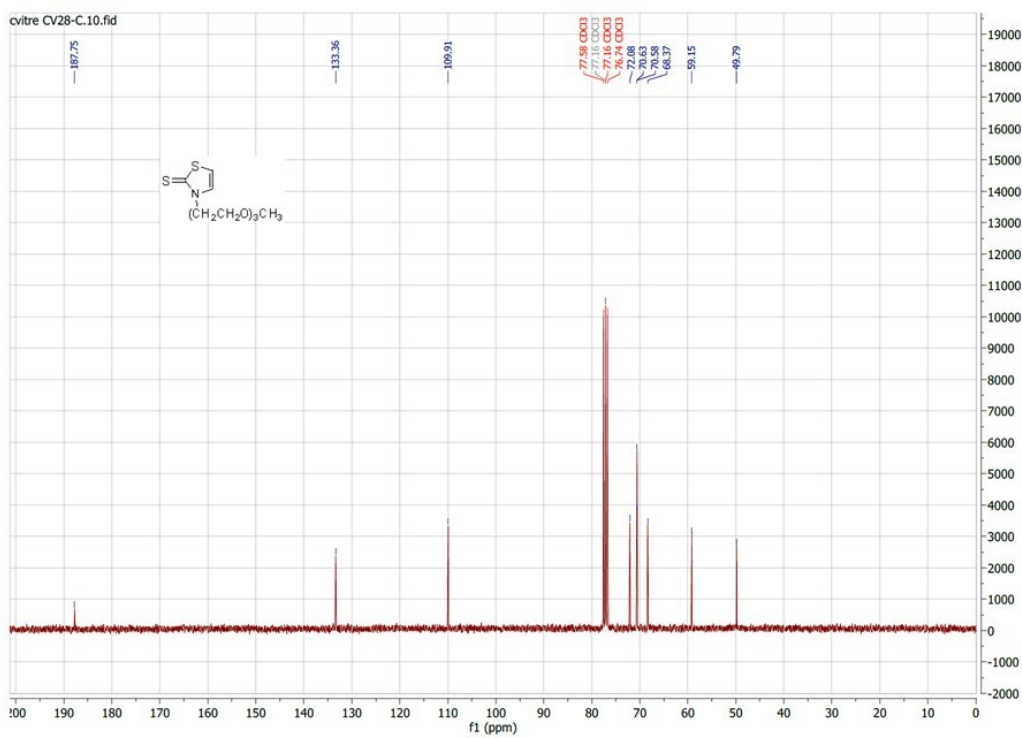


Fig. S6: ^{13}C NMR of 2b

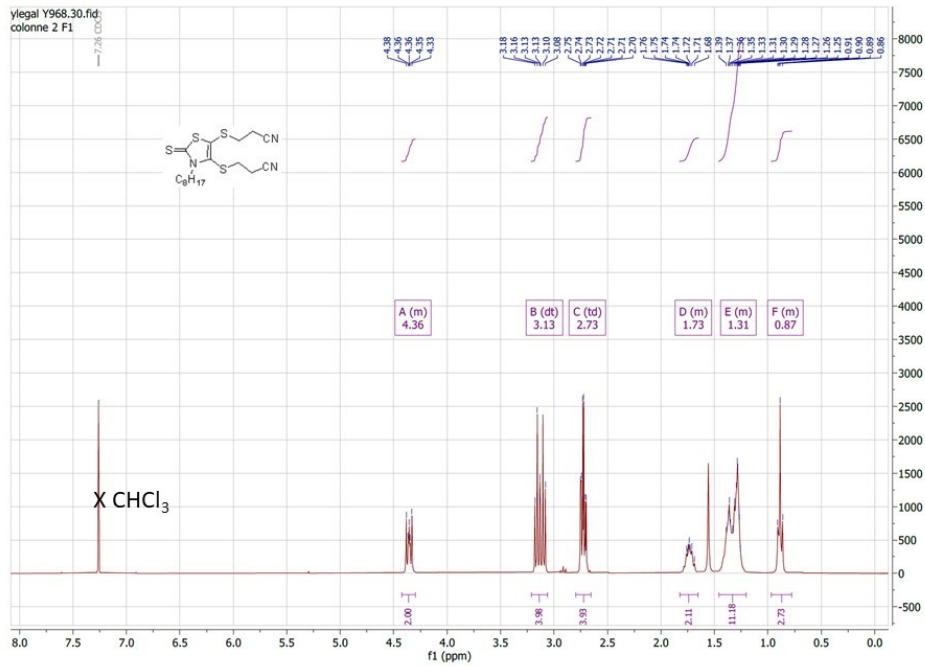


Fig. S7: ¹H NMR of 3

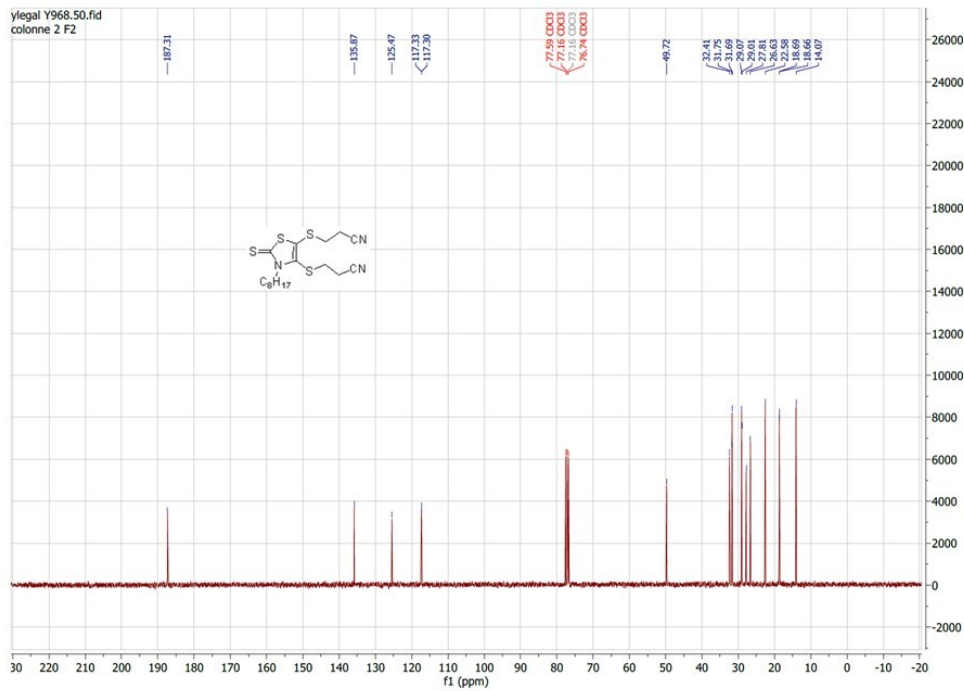


Fig. S8: ¹³C NMR of 3

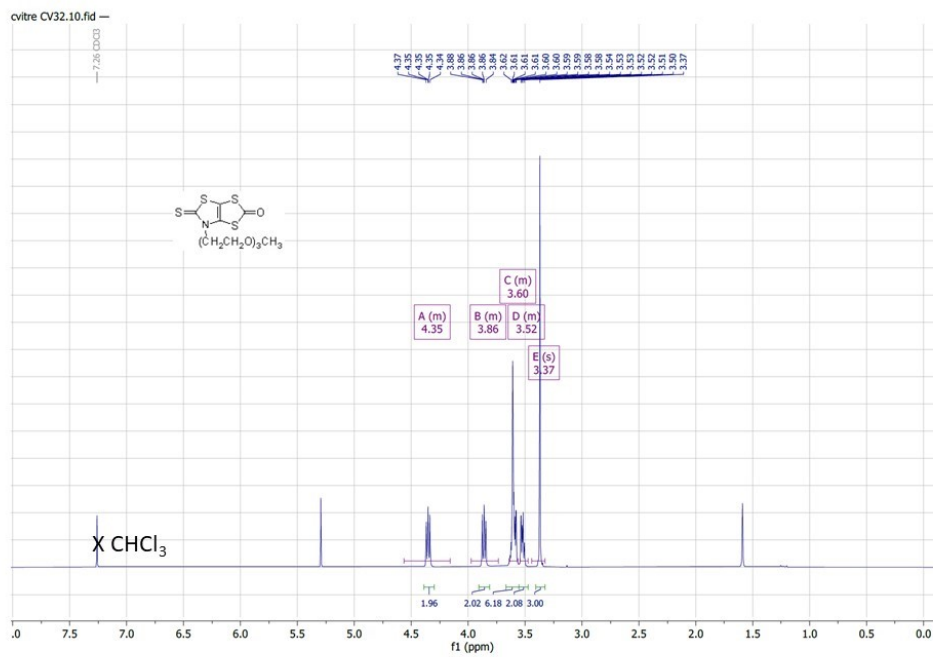


Fig. S9: ¹H NMR of 4

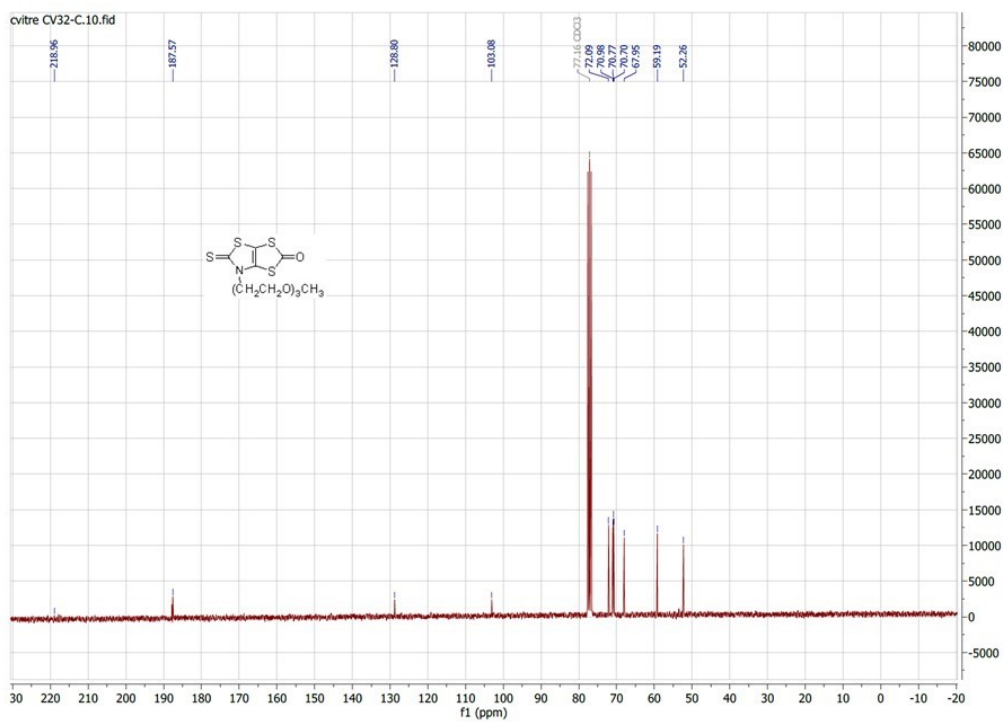


Fig. S10: ¹³C NMR of 4

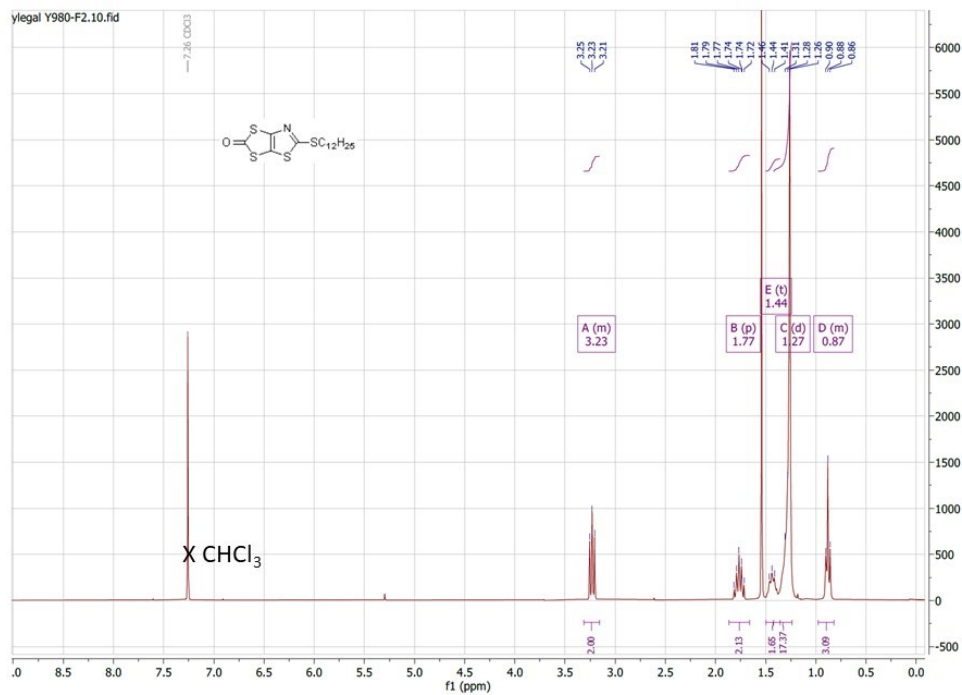


Fig. S11: ¹H NMR of 6a

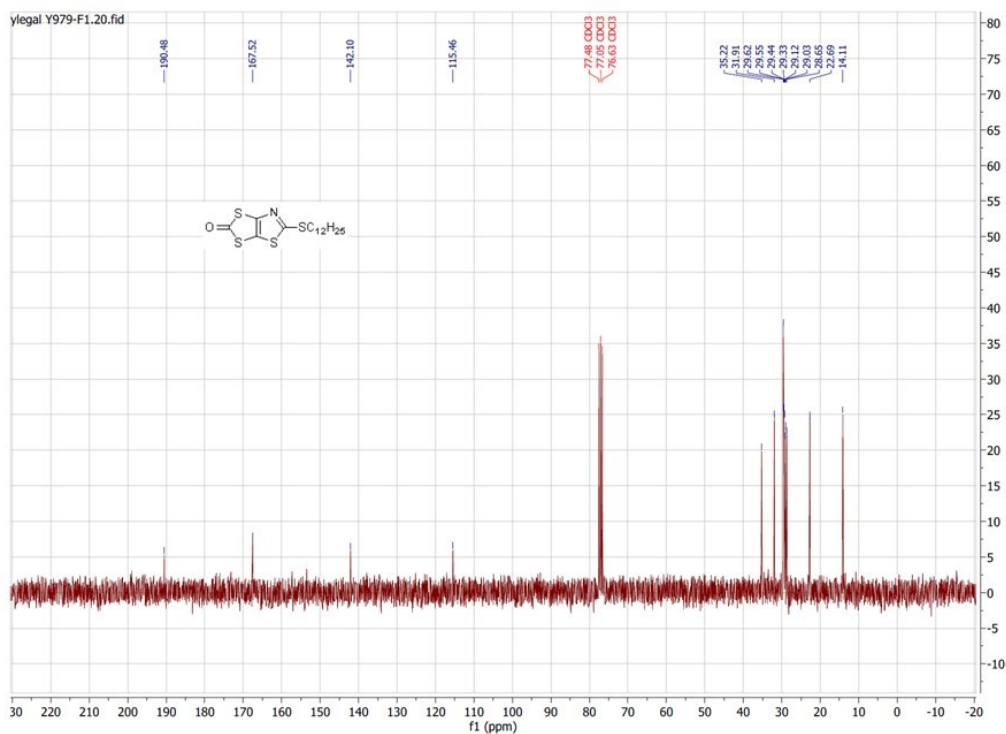


Fig. S12: ¹³C NMR of 6a

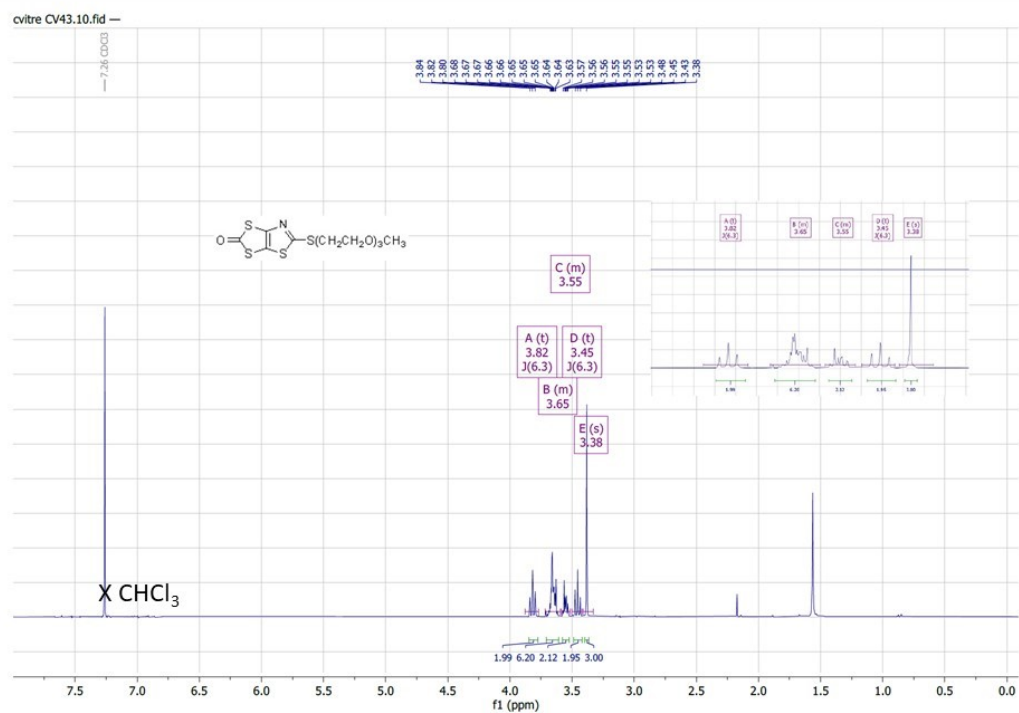


Fig. S13: ¹H NMR of 6b

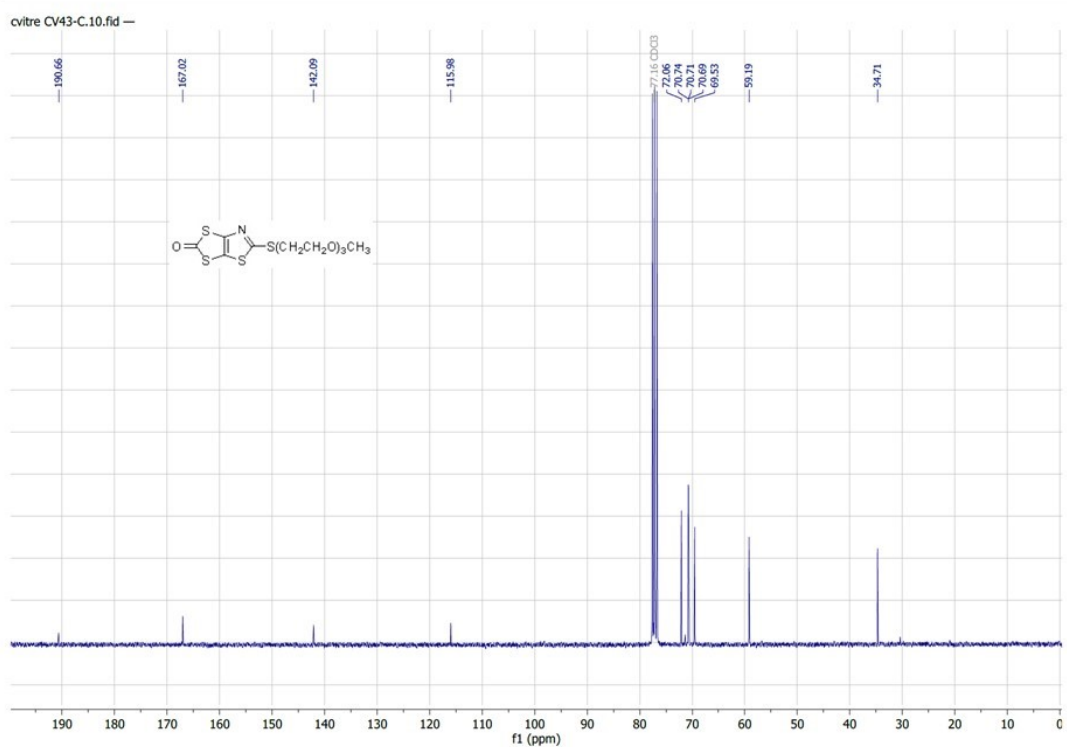


Fig. S14: ¹³C NMR of 6b

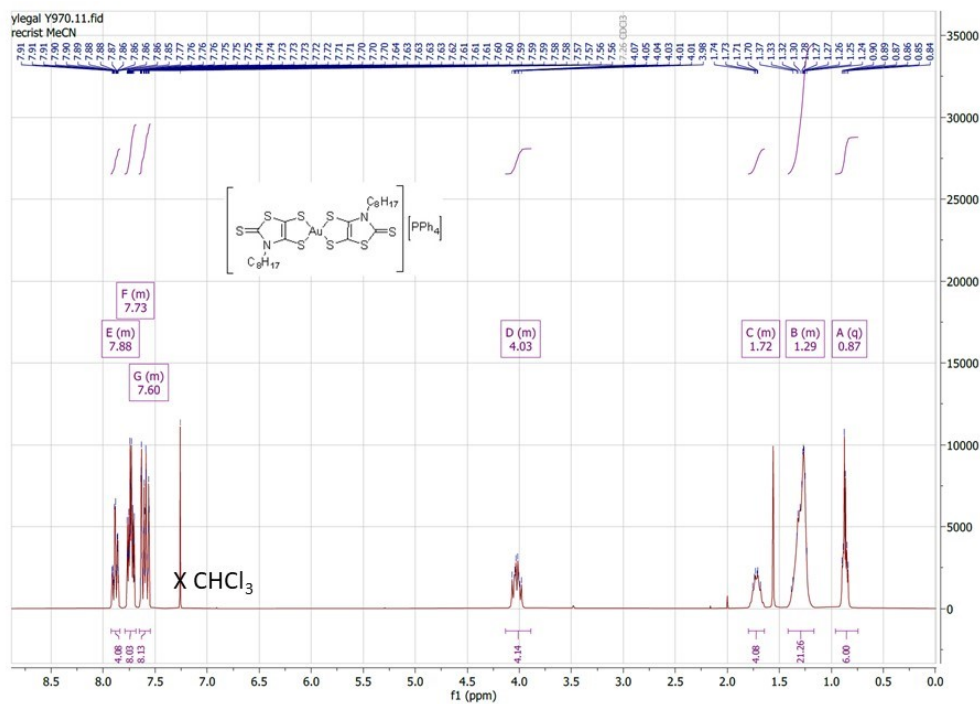


Fig. S15: ¹H NMR of AuN-C₈

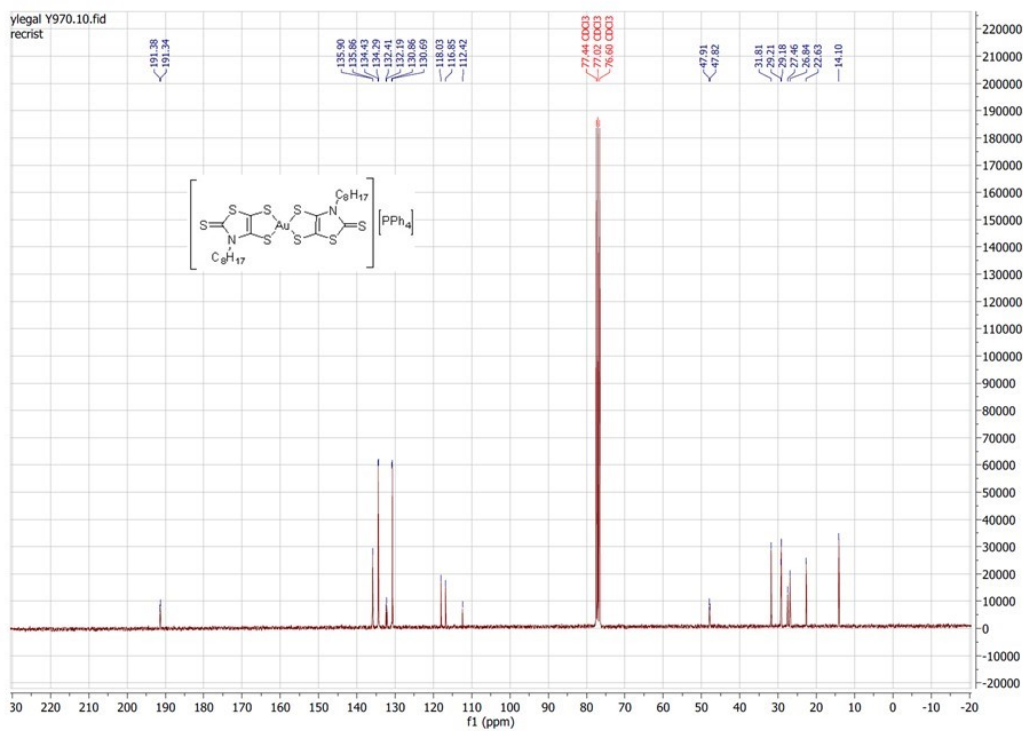


Fig. S16: ¹³C NMR of AuN-C₈

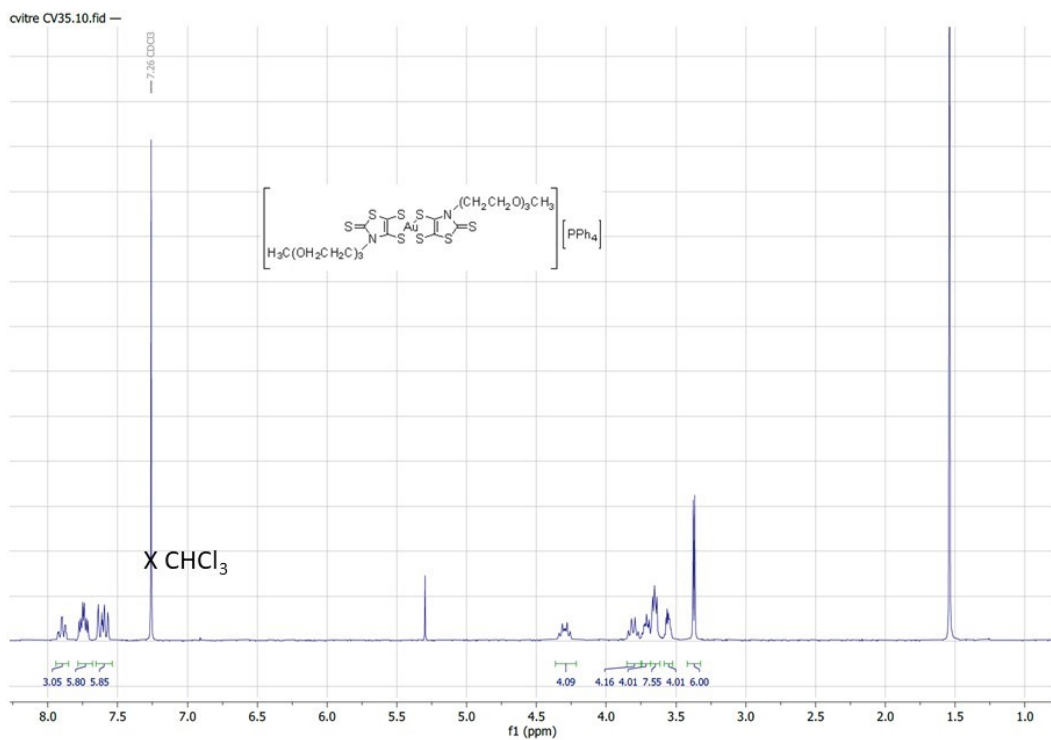


Fig. S17: ¹H NMR of AuN-PEG

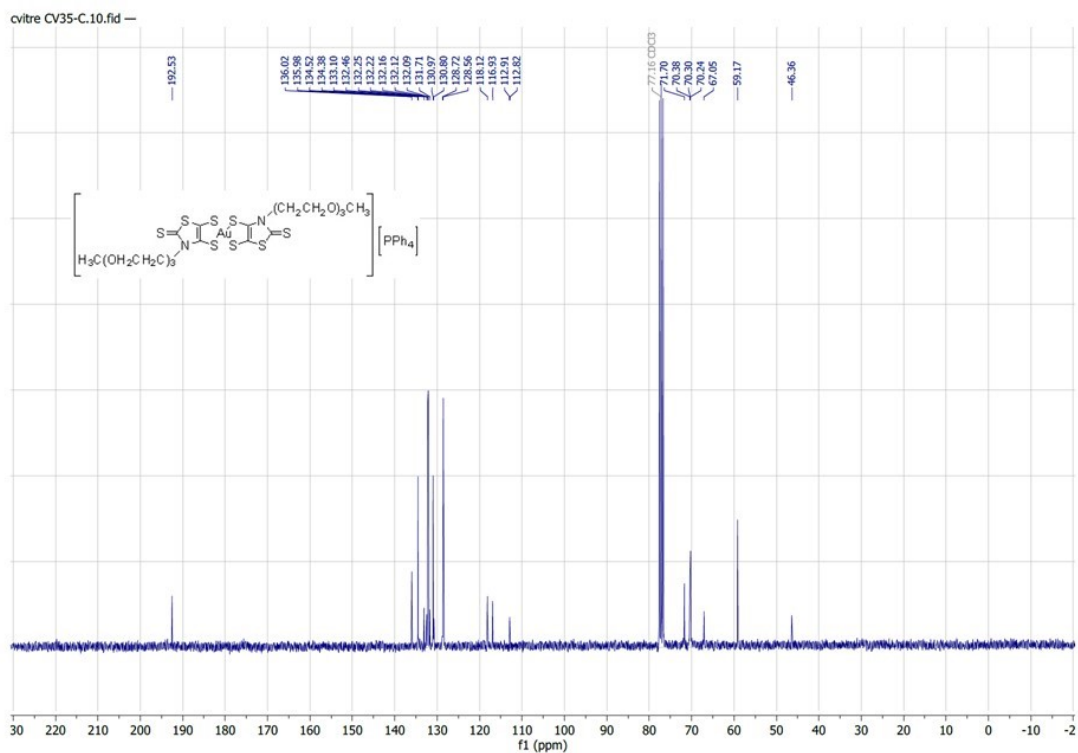


Fig. S18: ¹³C NMR of AuN-PEG

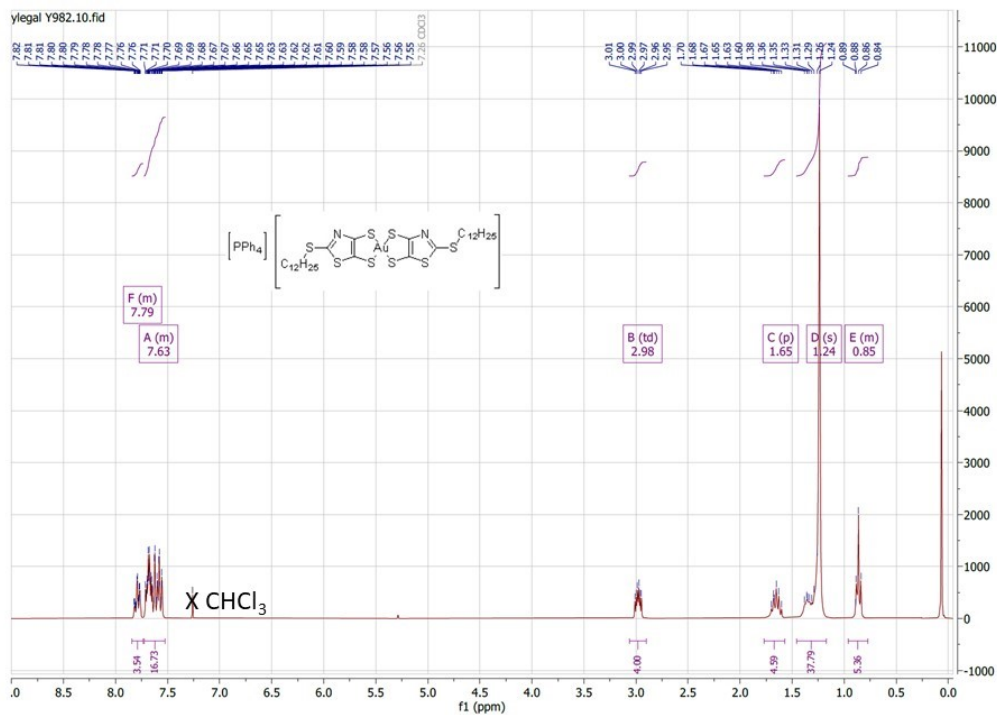


Fig. S19: ^1H NMR of AuS- C₁₂

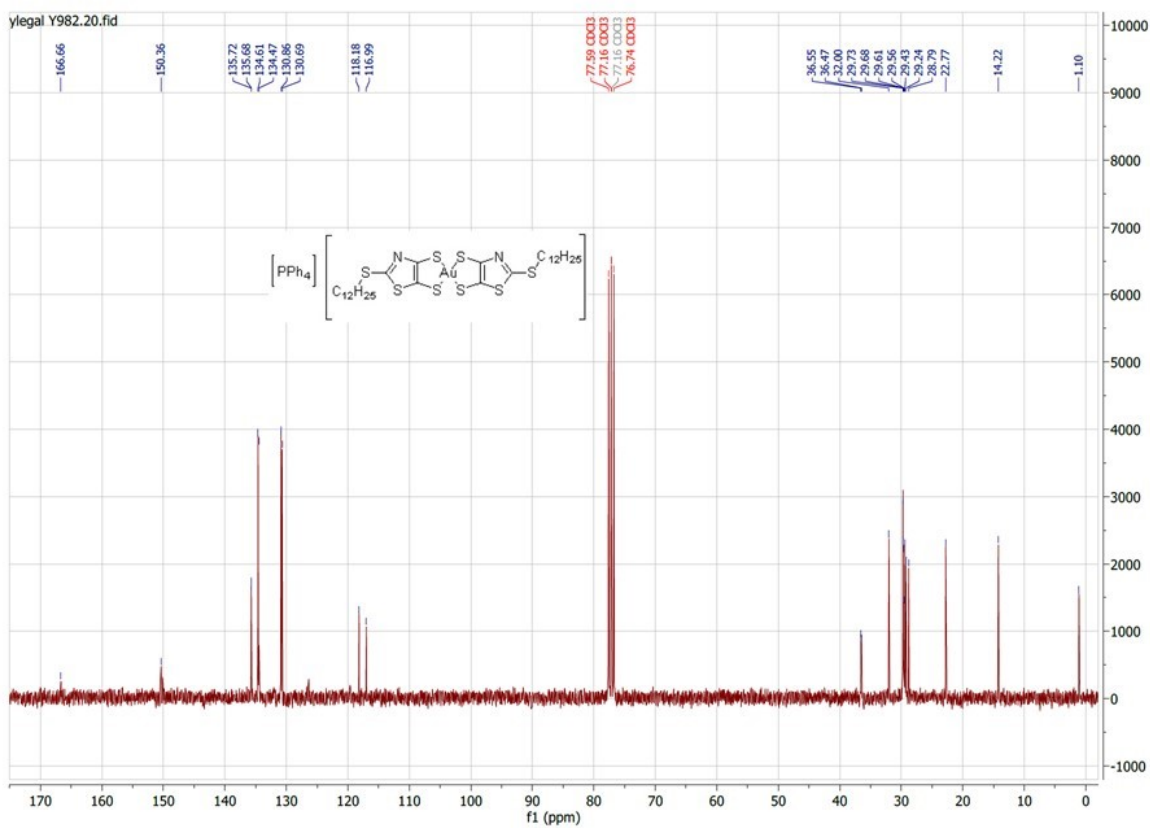


Fig. S20: ^{13}C NMR of AuS-C₁₂

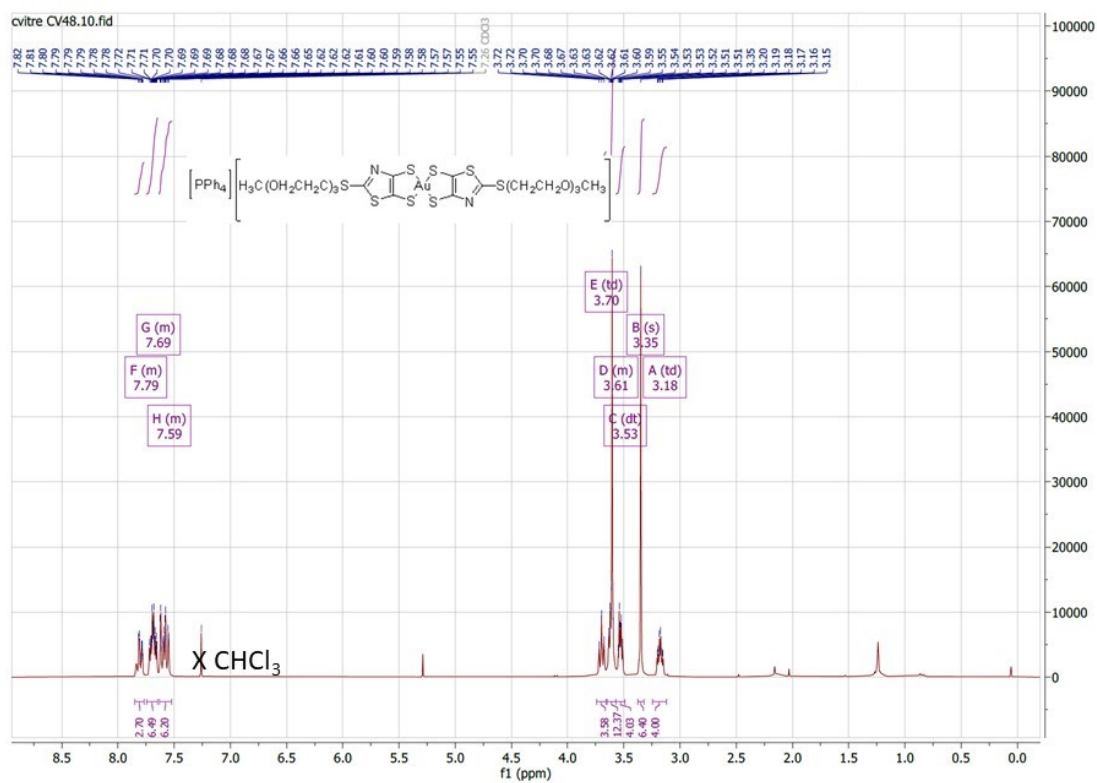


Fig. S21: 1H NMR of AuS-PEG

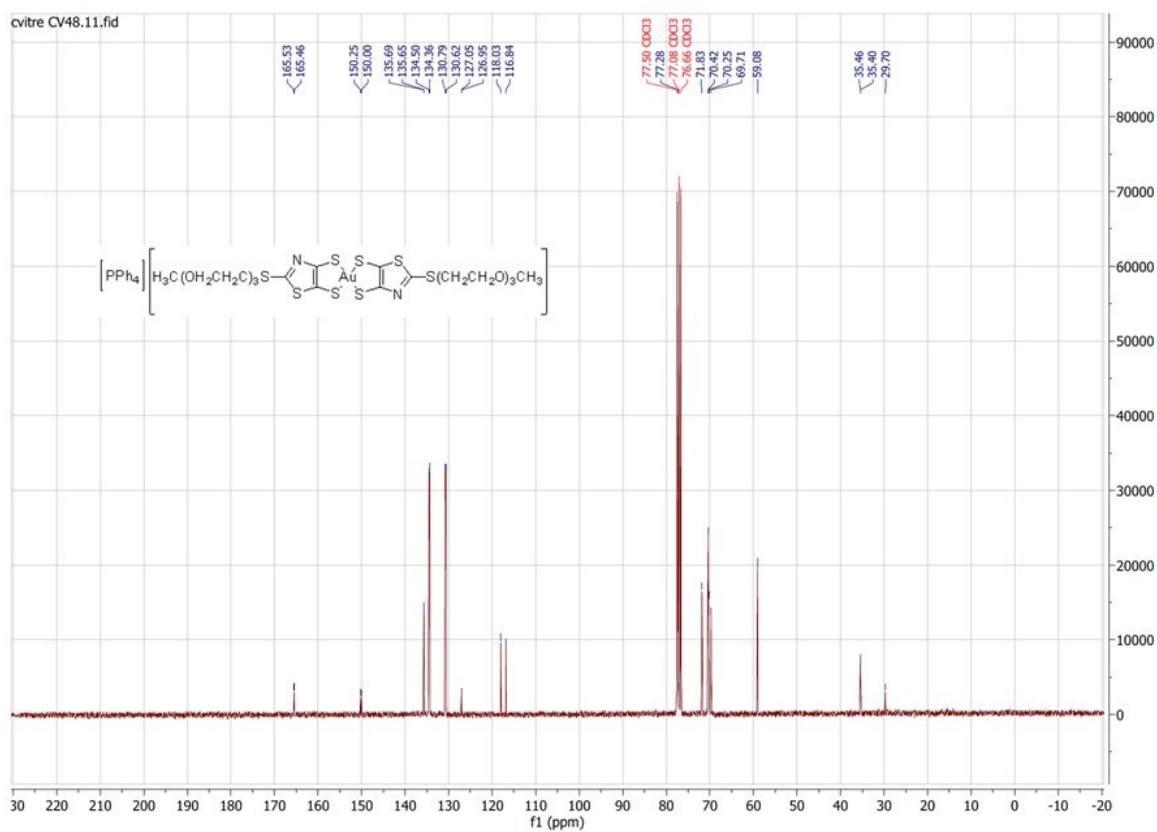


Fig. S22: ^{13}C NMR of AuS-PEG



Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
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 Method ASAP_CRMPO_tune_low.m
 Sample Name Y 966
 Comment Y. LE GAL Y 966 Température : 70°C

Acquisition Date 9/10/2021 10:17:49 AM
 Operator Fabian LAMBERT
 Instrument maXis

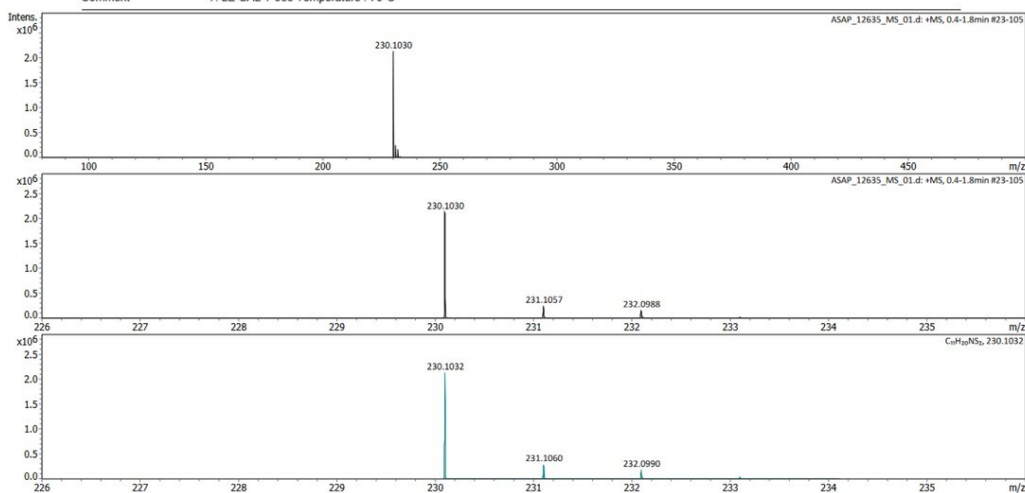
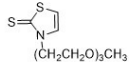


Fig. S23: HRMS of 2a

2b



Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
 Analysis Name D:\Data\CRMPO\ESI_13456_MS_01.d
 Method CRMPO_tune_low.m
 Sample Name CV 28
 Comment Y. LE GAL CV 28 Solvant : CH3OH/CH2Cl2 (90/10)

Acquisition Date 5/2/2022 2:36:24 PM
 Operator Fabian LAMBERT
 Instrument maXis

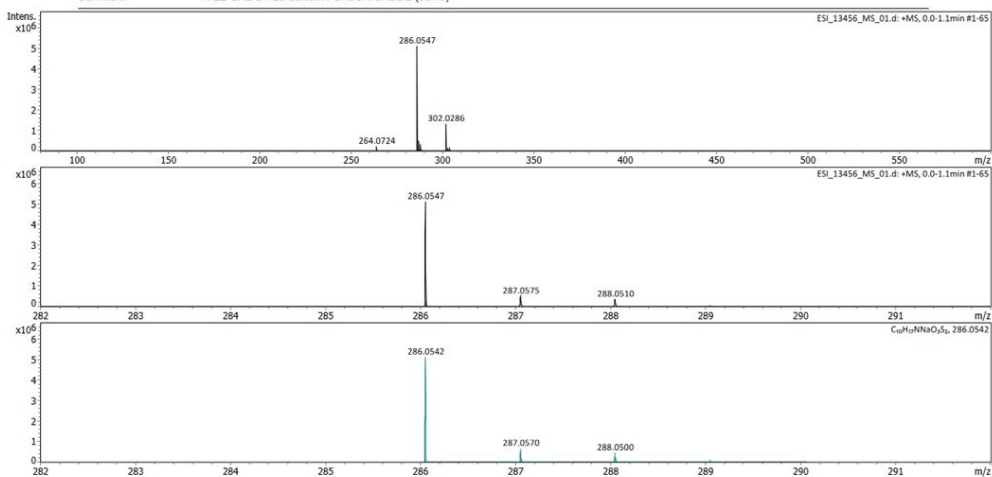
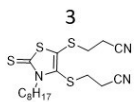


Fig. S24: HRMS of 2b



Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
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 Method: CRMPO_tune_low.m
 Sample Name: Y 968
 Comment: Y. LE GAL Y 968 Solvant : CH3OH/CH2Cl2 (90/10)

Acquisition Date: 6/29/2021 3:19:40 PM
 Operator: Fabian LAMBERT
 Instrument: maXis

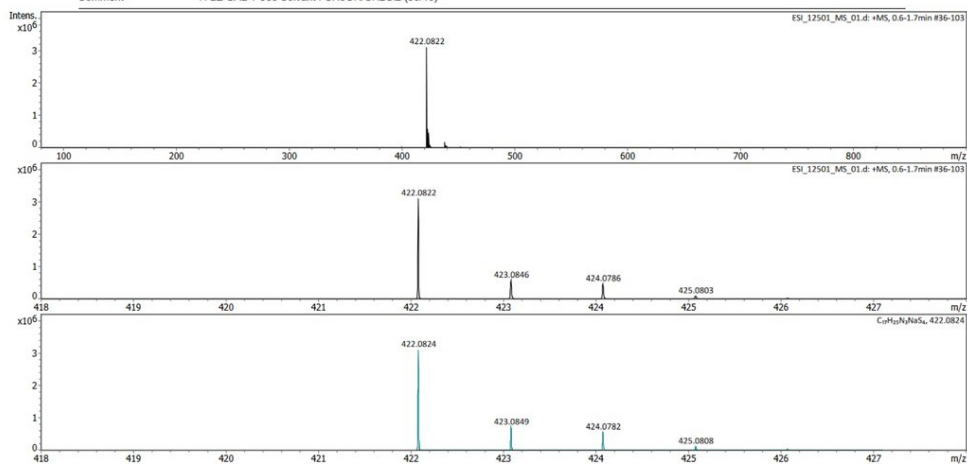
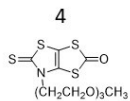


Fig. S25: HRMS of 3



Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
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 Method: ASAP_CRMPO_tune_low.m
 Sample Name: CV 32
 Comment: Y. LE GAL CV 32 Température : 120°C

Acquisition Date: 6/27/2022 2:19:17 PM
 Operator: Fabian LAMBERT
 Instrument: maXis

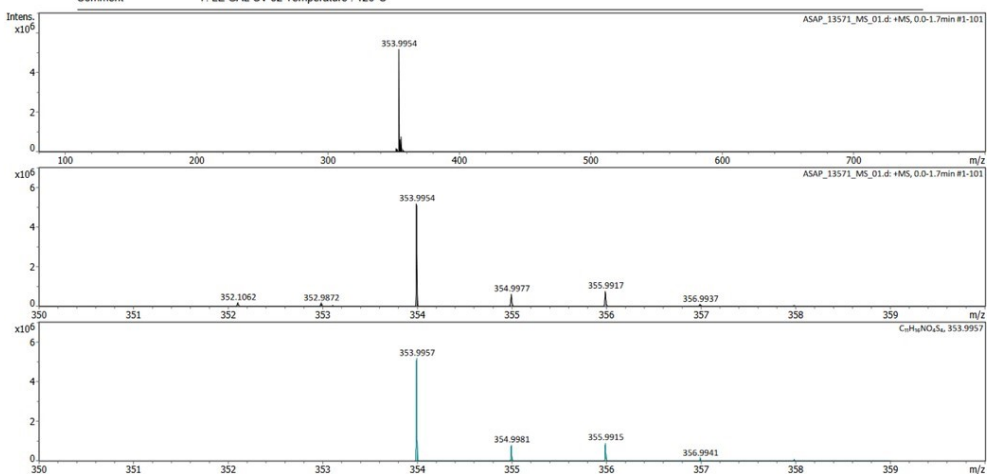
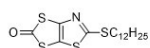


Fig. S26: HRMS of 4

6a



Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
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 Sample Name Y 969
 Comment Y. LE GAL Y 969 Solvant : CH3OH/CH2Cl2 (90/10)

Acquisition Date 6/29/2021 4:21:52 PM
 Operator Fabian LAMBERT
 Instrument maXis

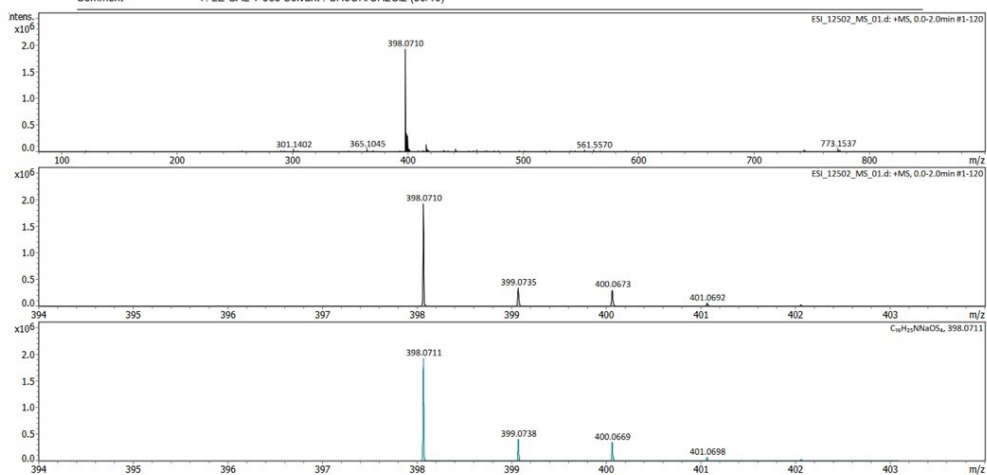
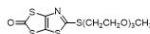


Fig. S27: HRMS of 6a

6b



Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
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 Sample Name CV 43
 Comment Y. LE GAL CV 43 Température : 100°C

Acquisition Date 6/27/2022 2:52:41 PM
 Operator Fabian LAMBERT
 Instrument maXis

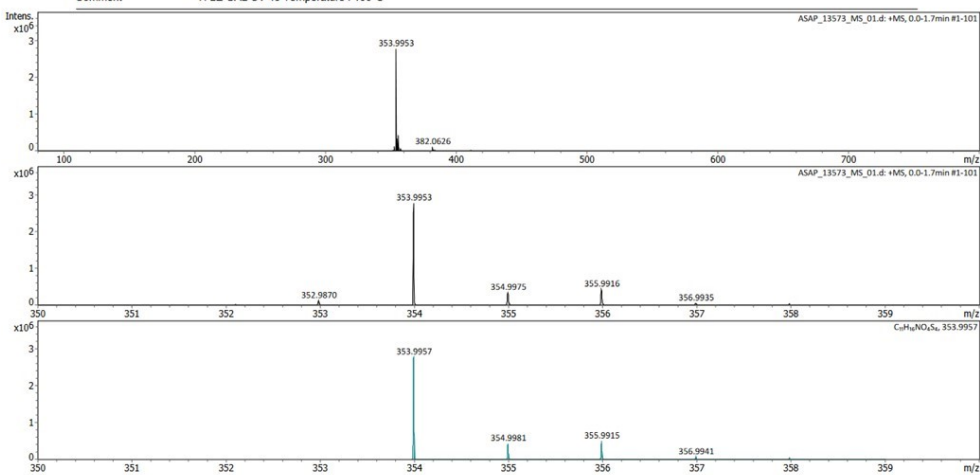


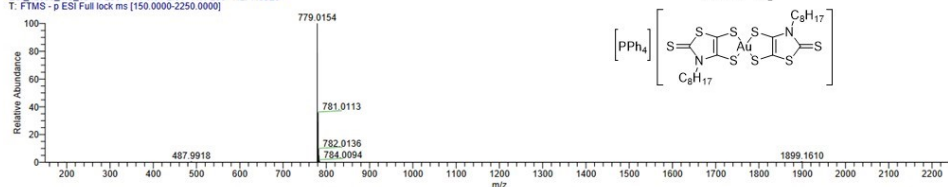
Fig. S28: HRMS of 6b

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Y. LE GAL Y 970 PJ Solvant : CH2Cl2
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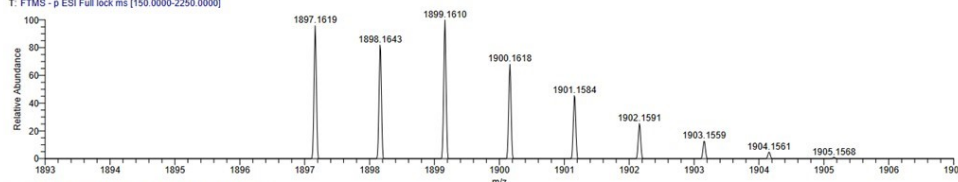
Rapport d'analyse
09/15/21 15:54:09

Thermo Scientific Q-Exactive

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(C22H34N2S8Au)2(C24H20P) Au2 S16 N4 H88 C68 P1 p(g.s.)

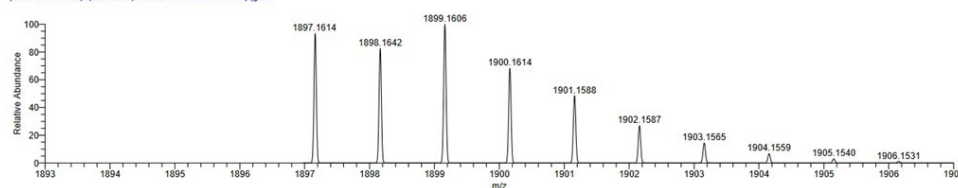


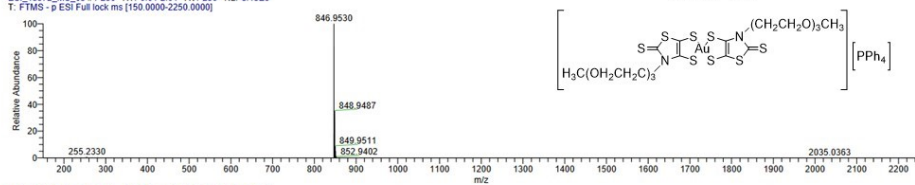
Fig. S29: HRMS of AuN-C₈

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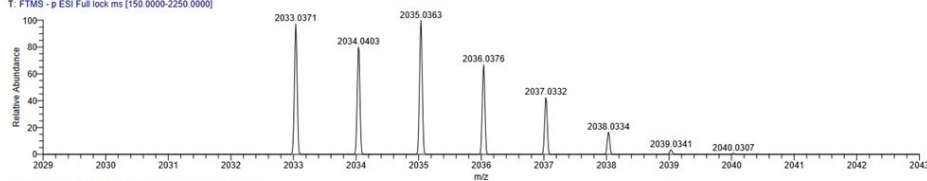
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06/10/22 18:00:32

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(C20H30N2O6S8Au)2(C24H20P) Au2 S16 O12 N4 H80 C64 P1

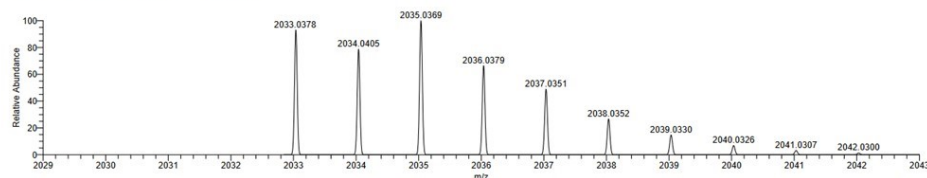


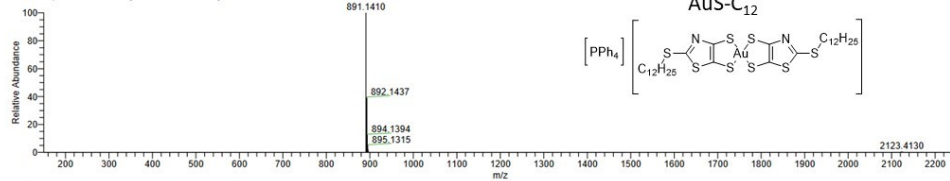
Fig. S30: HRMS of AuN-PEG

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Y. LE GAL Y 971 PJ Solvant : CH2Cl2
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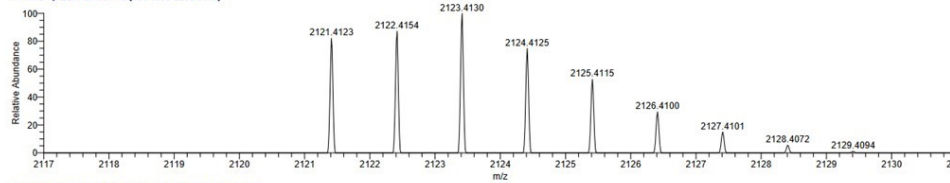
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09/15/21 17:08:19

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(C30H50N2S8Au)2(C24H20P): Au2 S16 N4 H120 C84 P1 p/g...

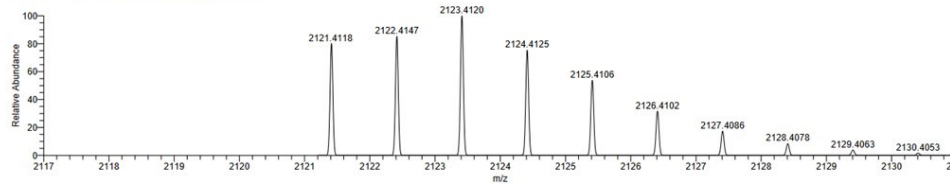


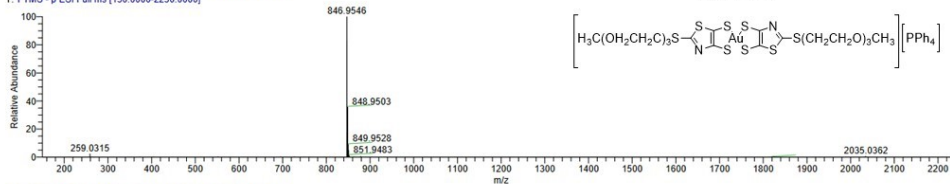
Fig. S31: HRMS of AuS-C₁₂

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Y. LE GAL CV 48 PJ Solvant : CH2Cl2
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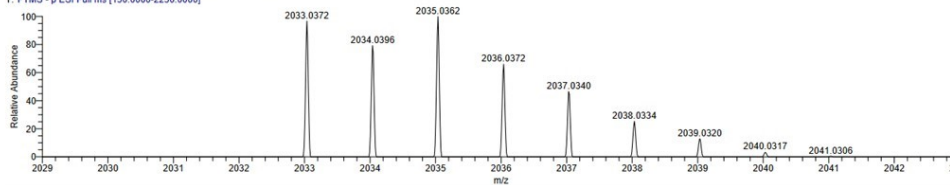
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10/11/22 19:31:34

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(C20H30N2O6S8Au)2(C24H20P): Au2 S16 O12 N4 H80 C84 P1...

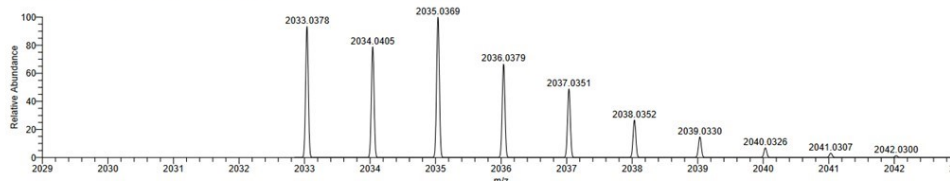


Fig. S32: HRMS of AuS-PEG

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.

	E_{pc}^1	$E_{\text{pa/pc}}^2$	$E_{\text{pa/pc}}^3$	λ_{max} (nm)	
				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- <i>t</i> BuS ¹³	-1.18*	0.58/0.42	1.05/0.98	1614	1038

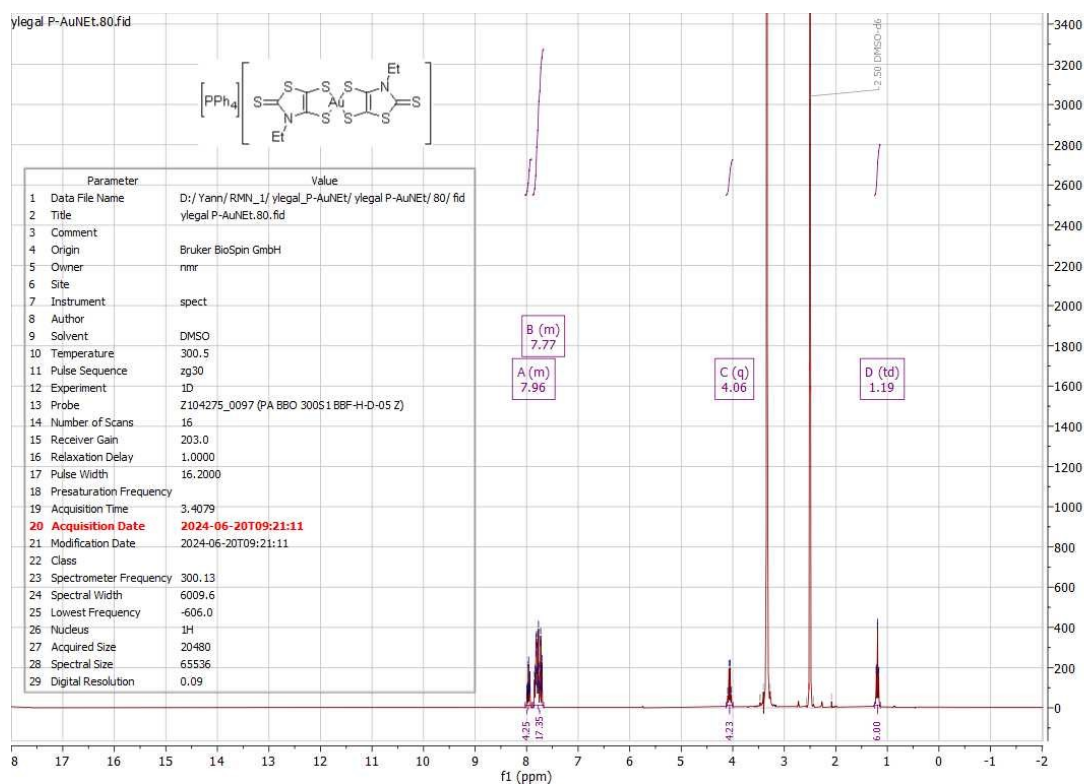
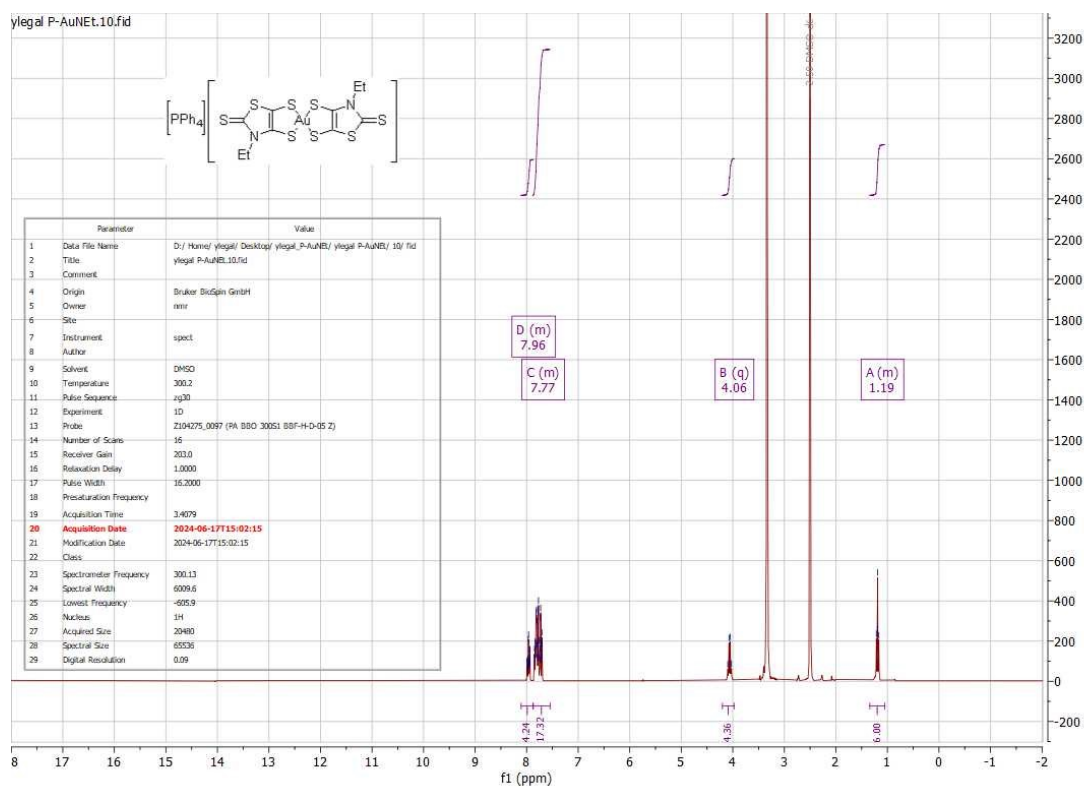


Figure S33 - ^1H NMR spectra of complex AuN-Et in DMSO solution at T0 (top) and the same tube analyzed 66h later (bottom).