Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Exploiting Click–Chemistry: Backbone Post–functionalisation of Homoleptic Gold(I) 1,2,3–triazole–5–ylidene Complexes

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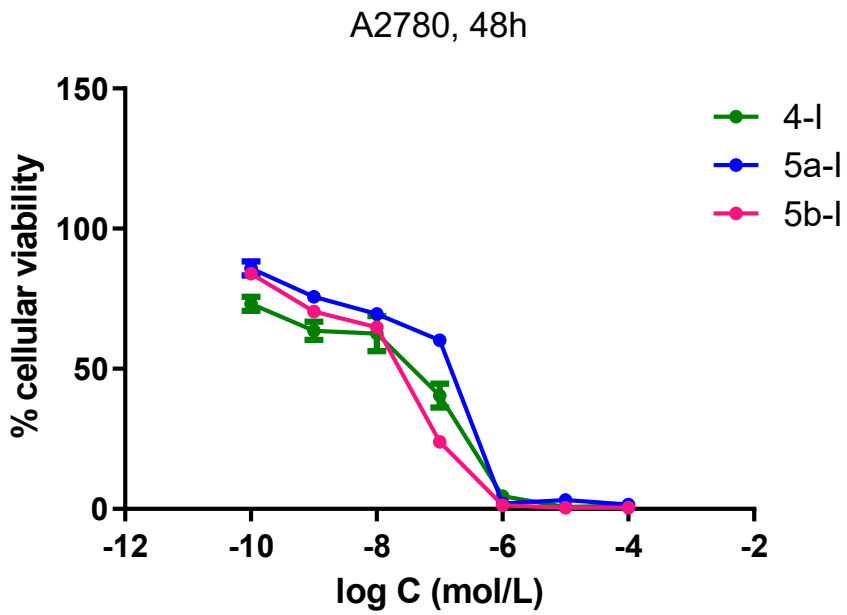

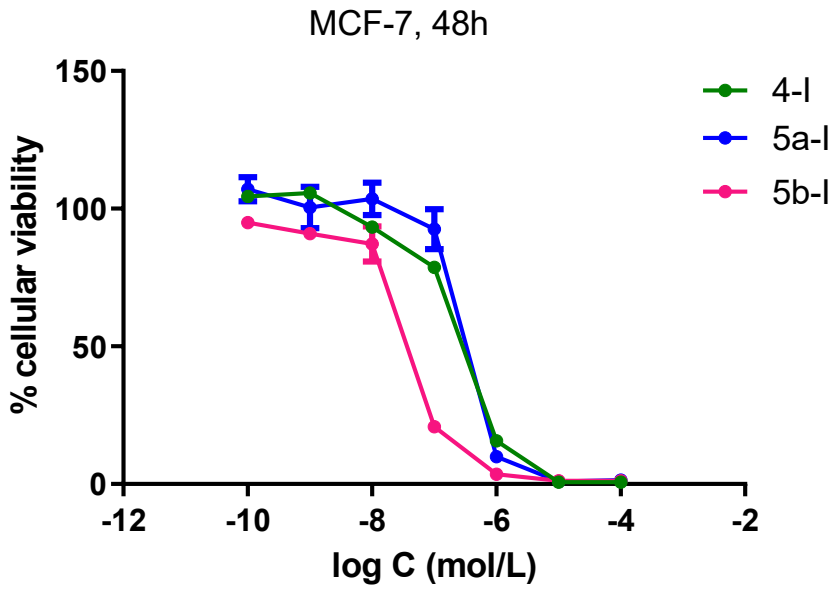

Analytical Data

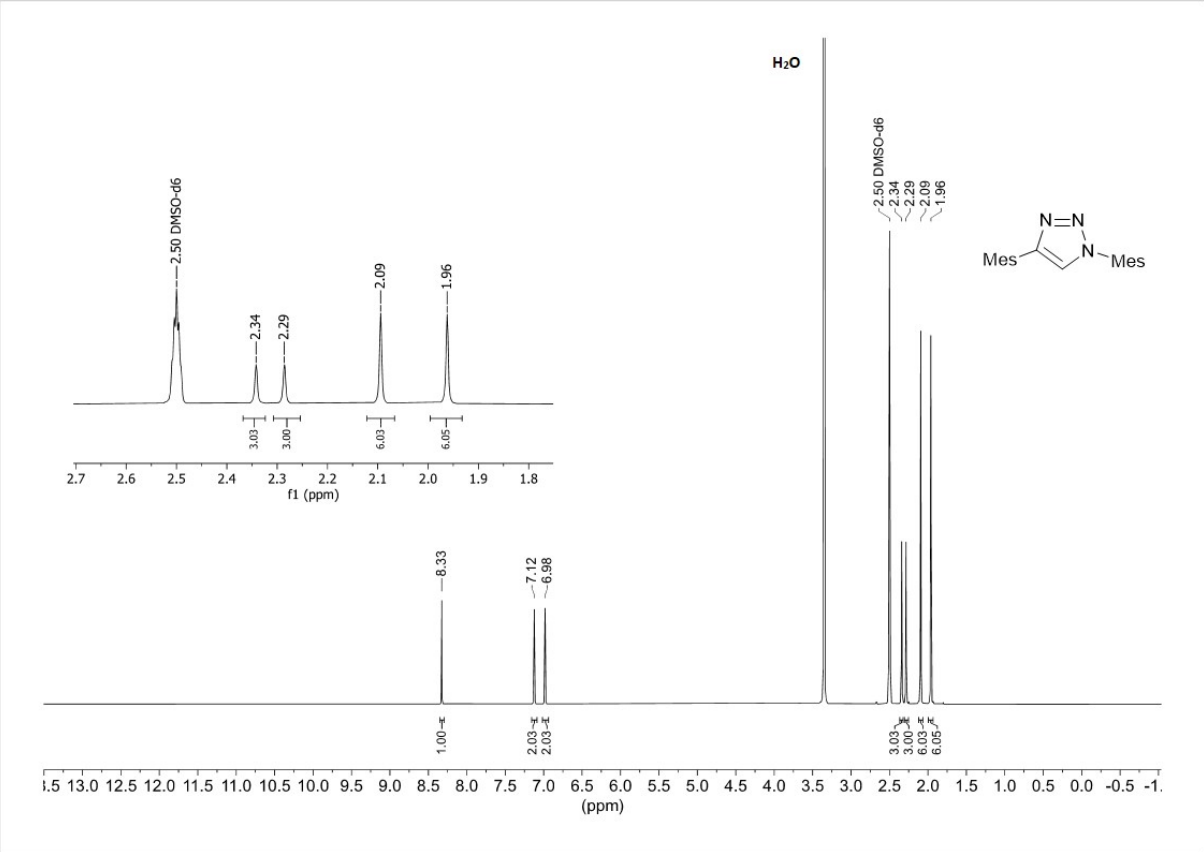

Figure 1: ^{1}H-NMR spectrum of **1** in DMSO-d_6.

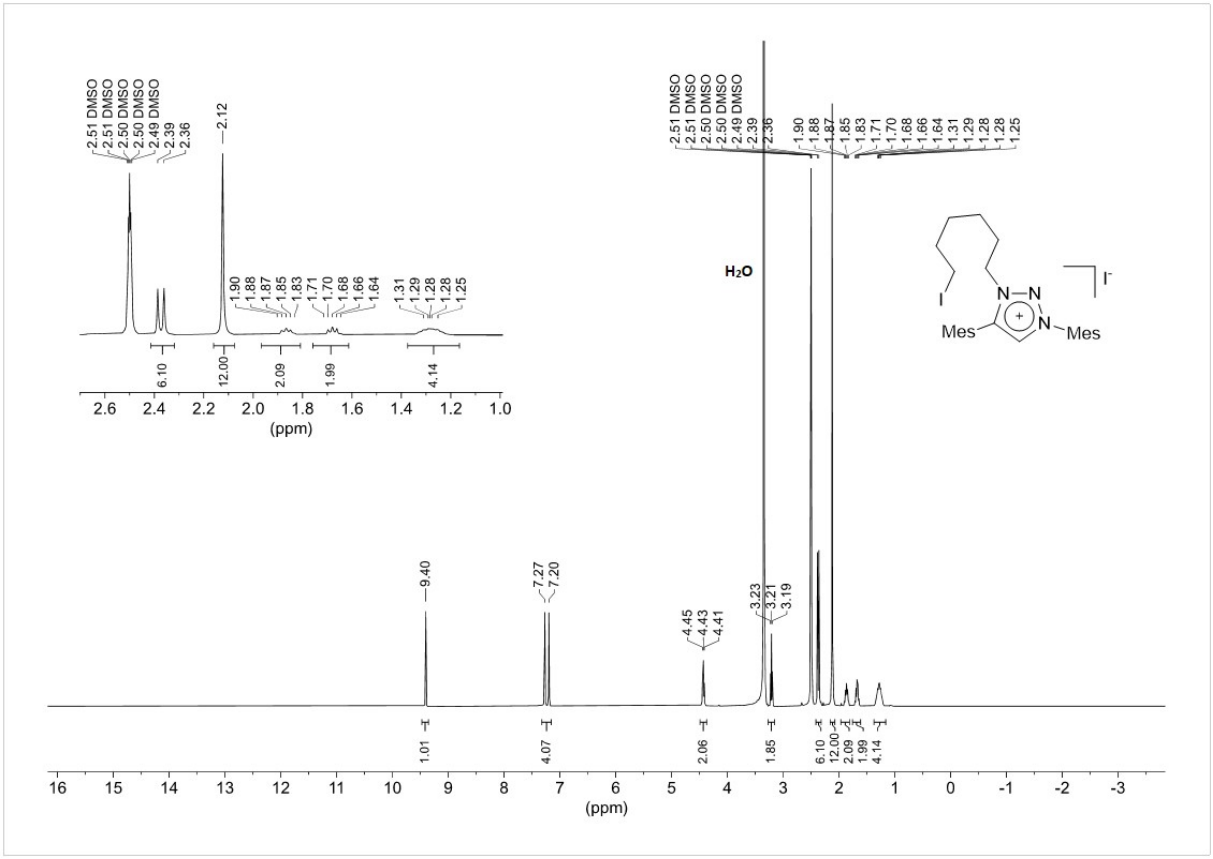

Figure 2: ^{1}H-NMR spectrum of **2** in DMSO-d_6.

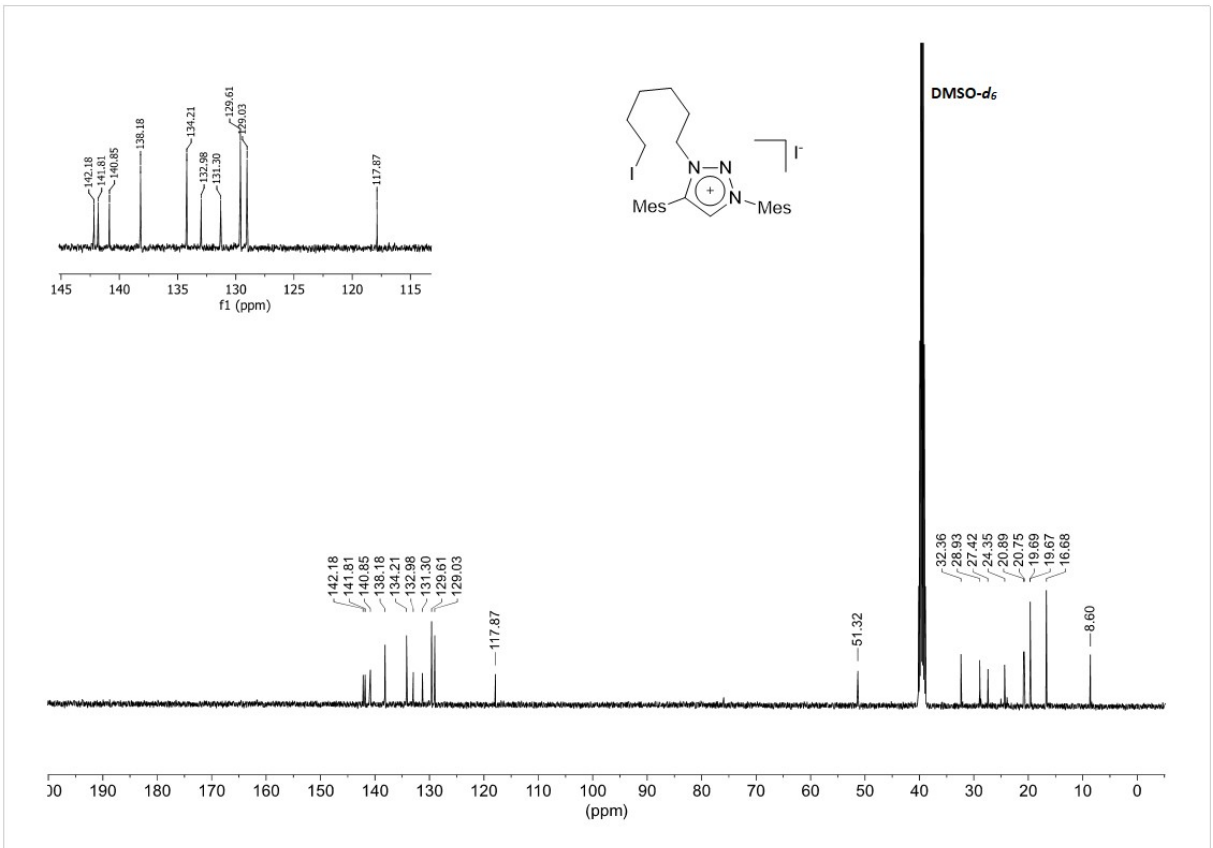

Figure 3: ^{13}C-NMR spectrum of **2** in DMSO-d_6.

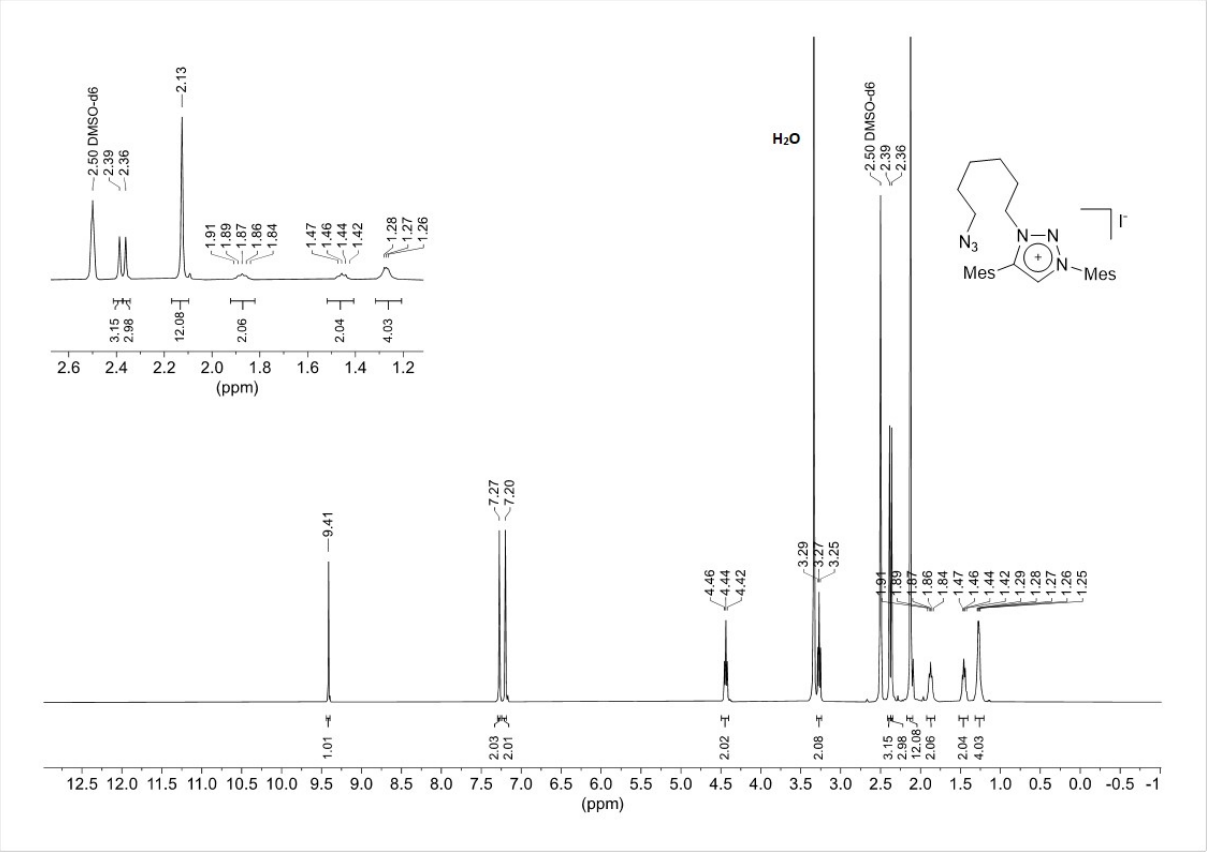

Figure 4: ^{1}H-NMR spectrum of **3** in DMSO-d_6.

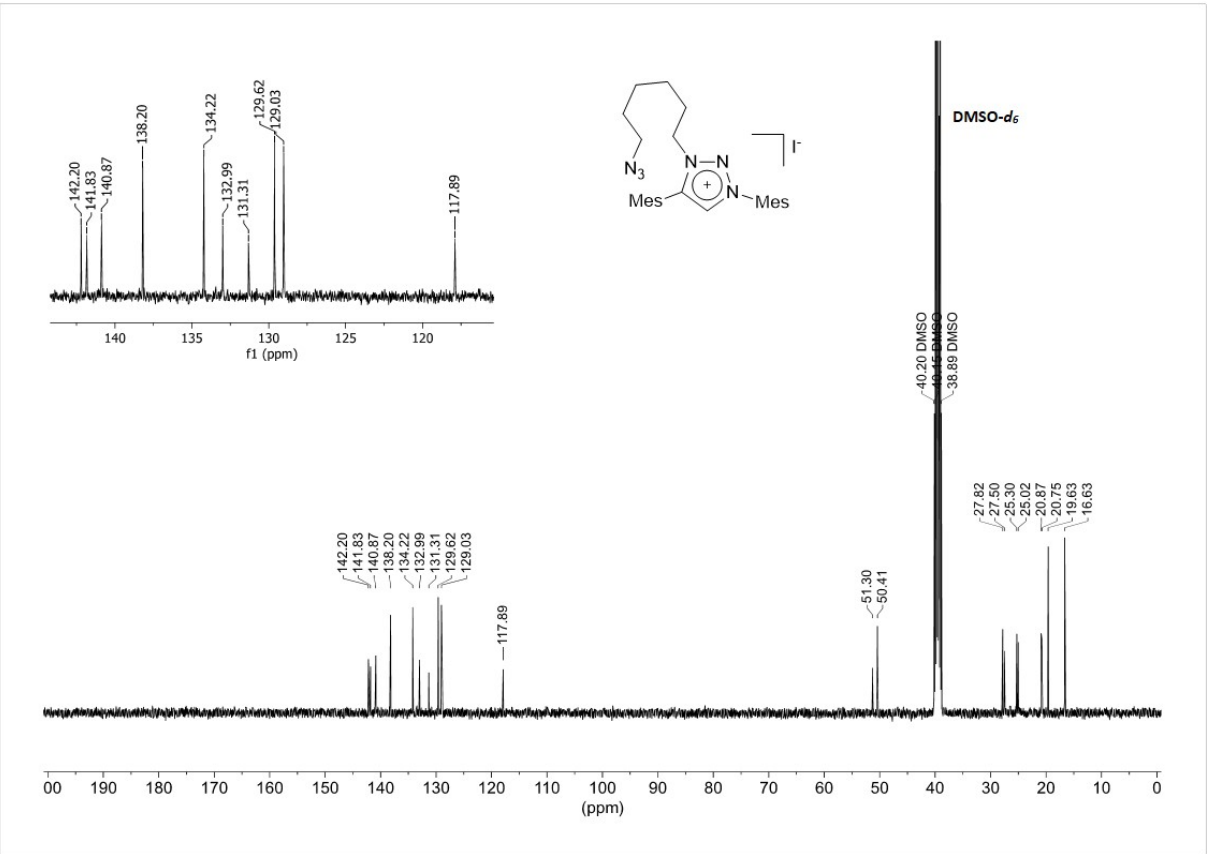

Figure 5: ^{13}C-NMR spectrum of **3** in DMSO-d_6.

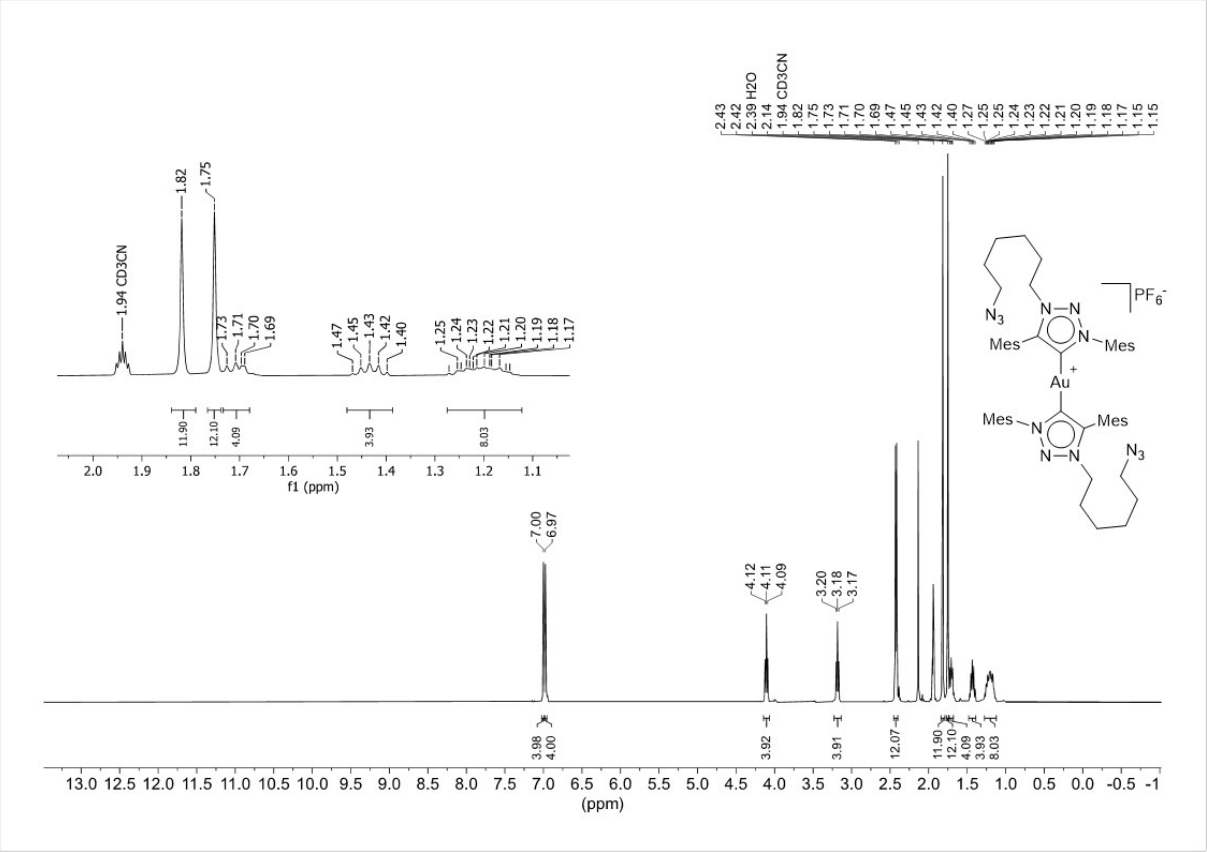

Figure 6: ^{1}H-NMR spectrum of **4** in CD_3CN.

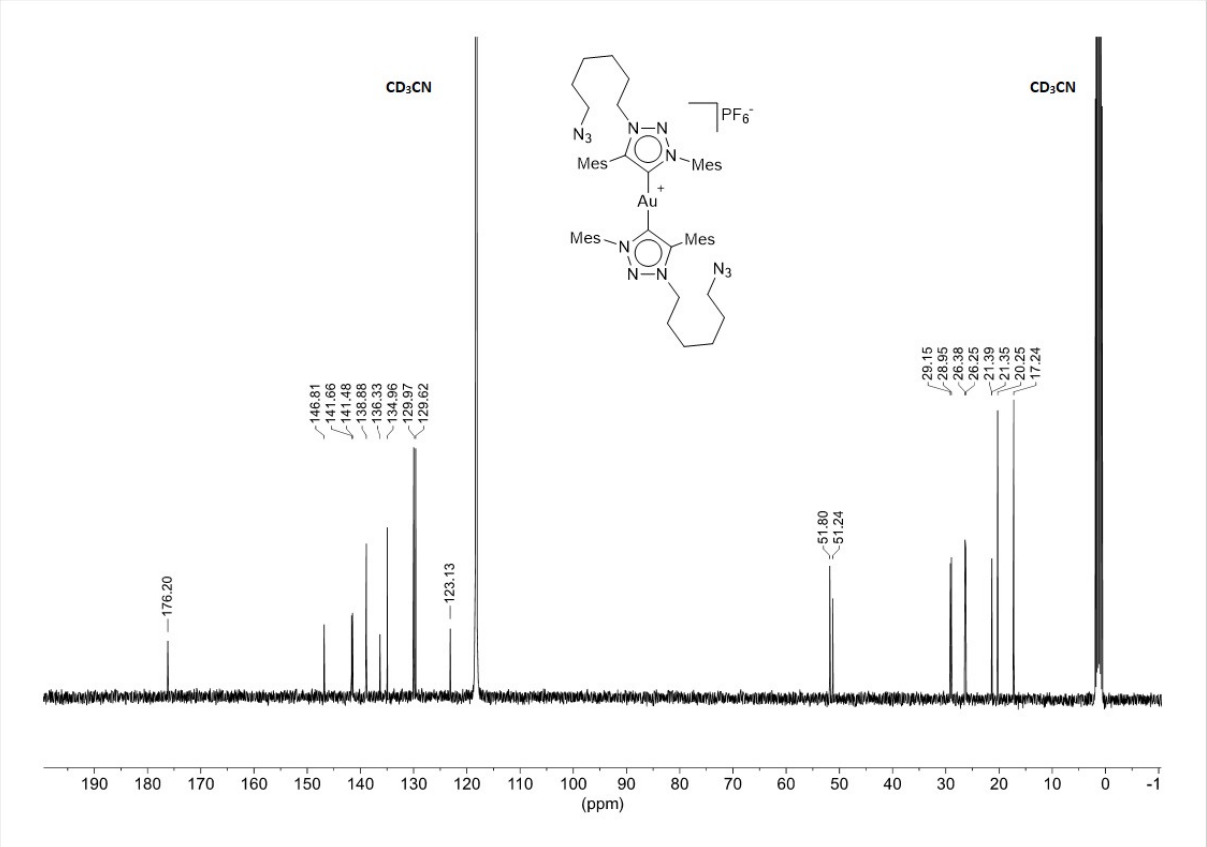

Figure 7: ^{13}C-NMR spectrum of **4** in CD_3CN.

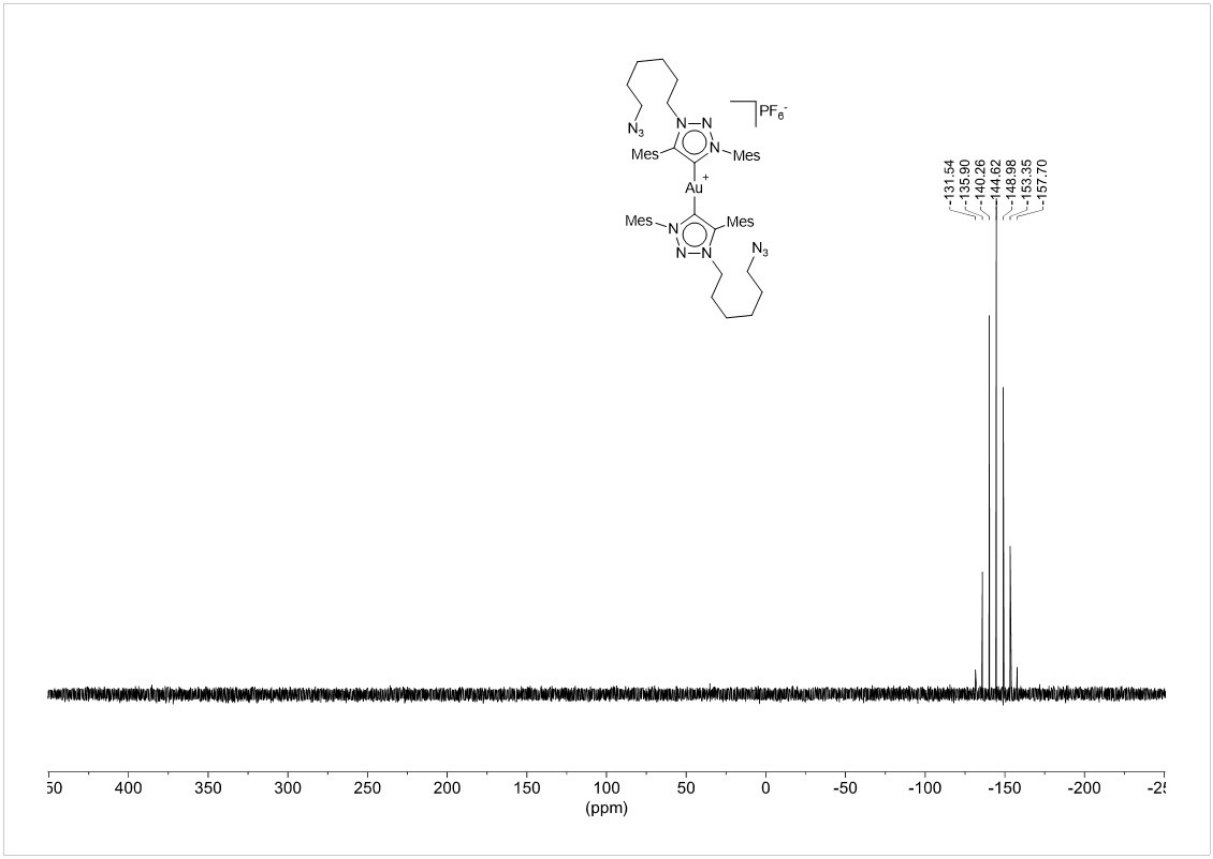

Figure 8: ^{31}P-NMR spectrum of **4-PF$_6$** in CD_3CN.

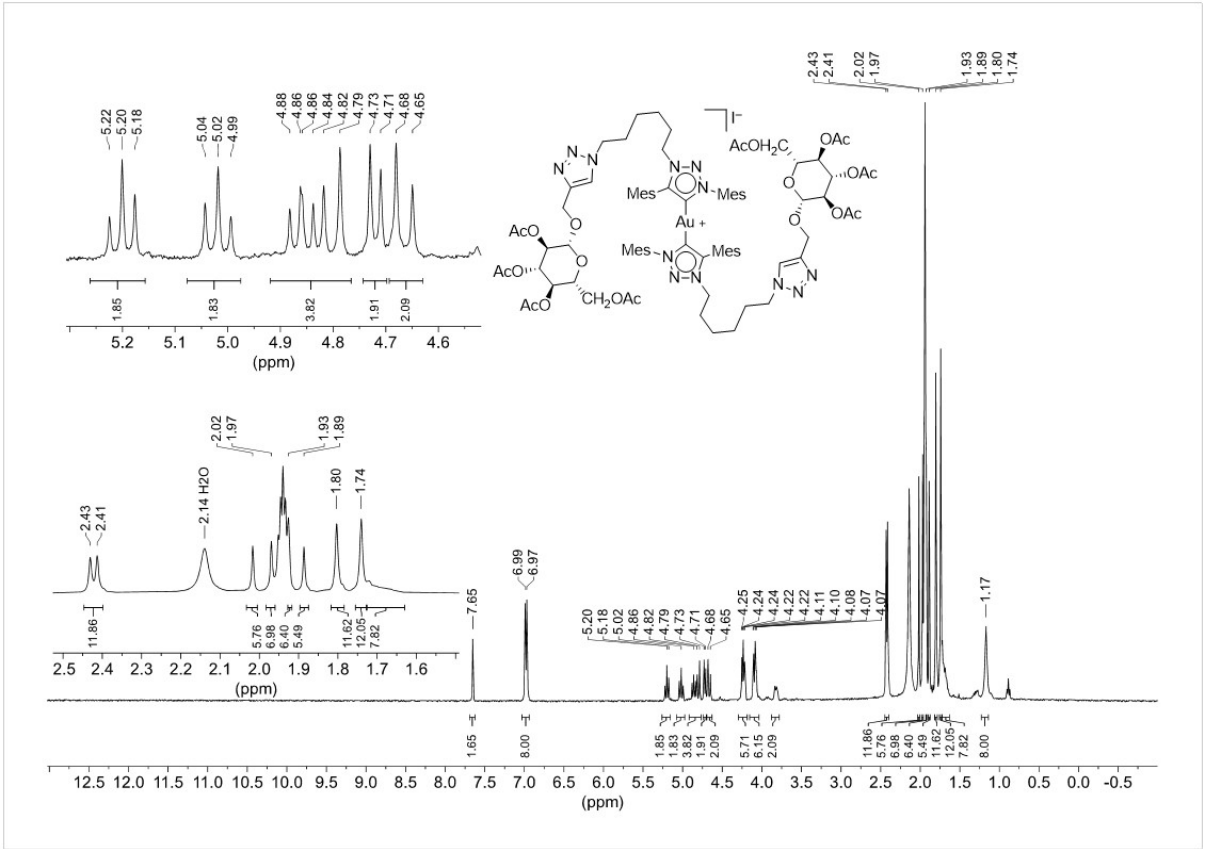

Figure 9: ^{1}H-NMR spectrum of **5a–l** in CD_3CN.

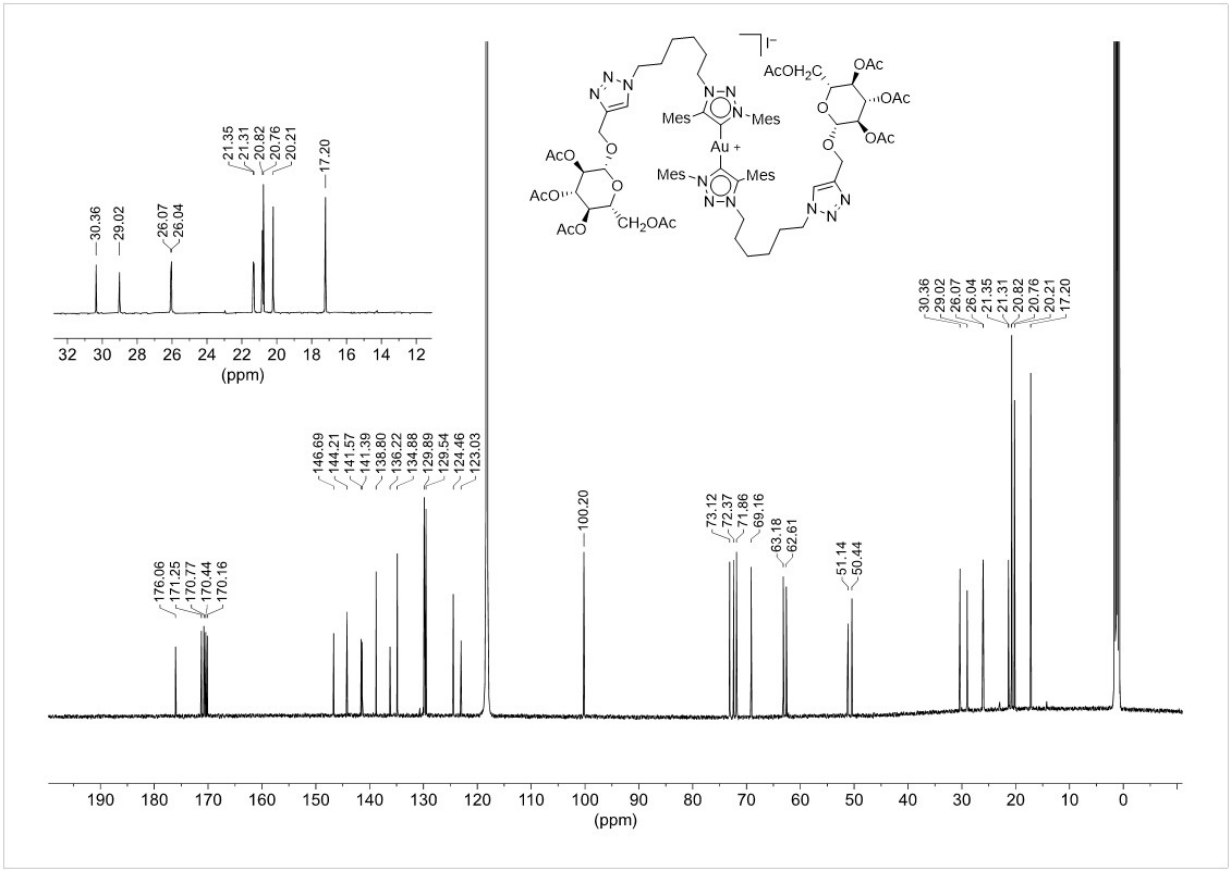

Figure 10: ^{13}C-NMR spectrum of **5a–l** in CD_3CN.

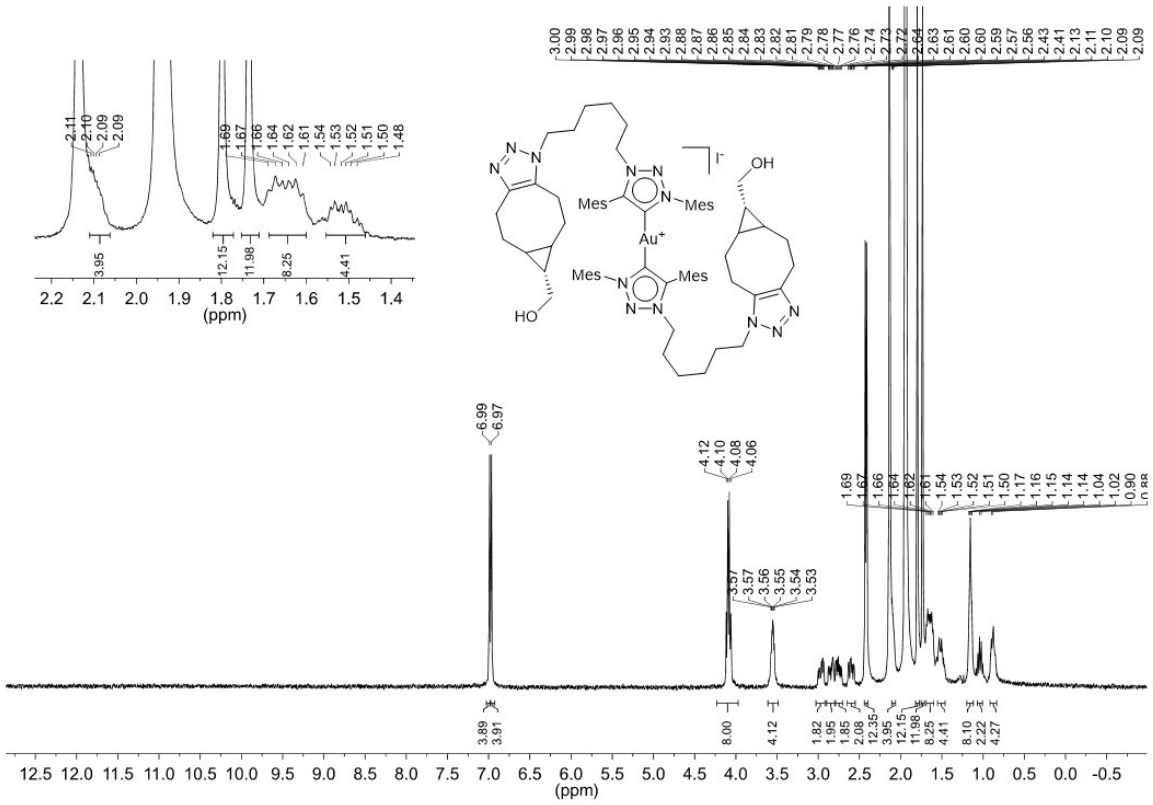

Figure 11: ^{1}H-NMR spectrum of **5b–l** in CD_3CN.

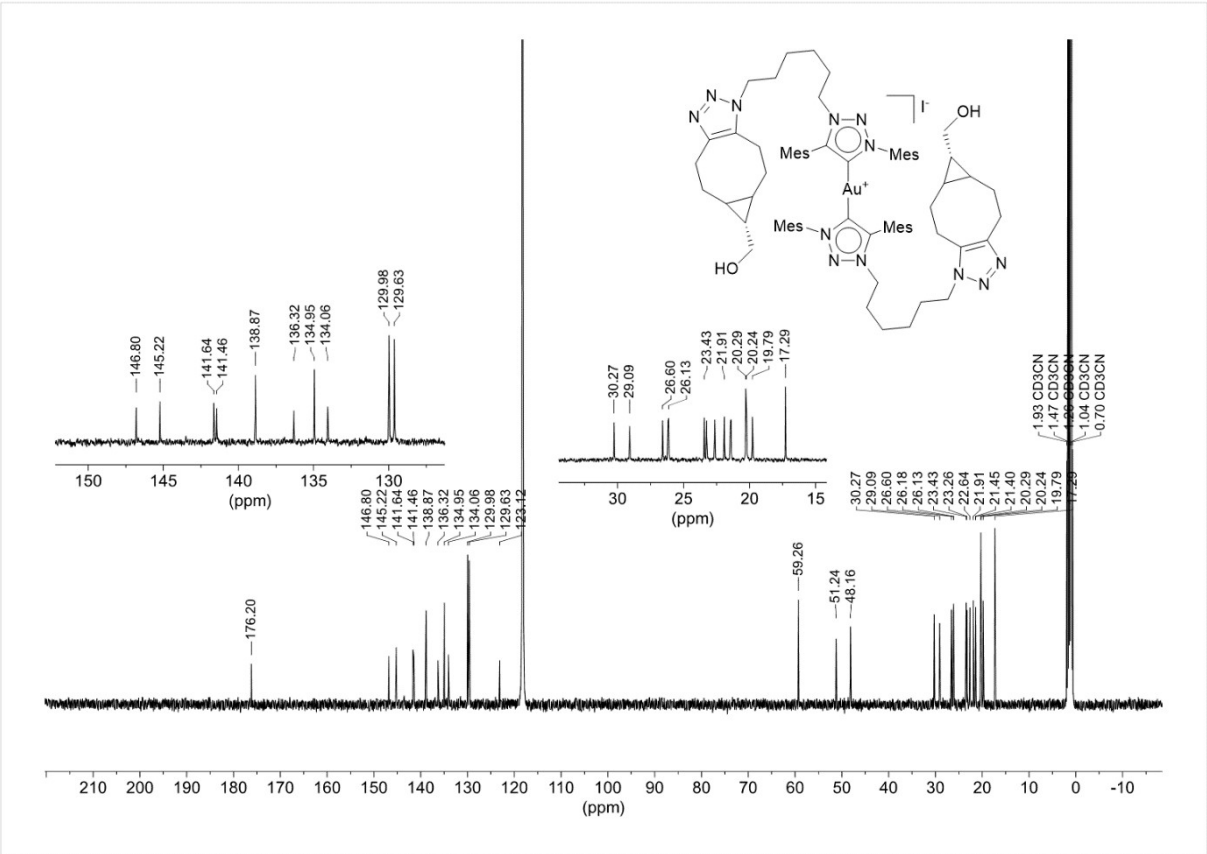

Figure 12: ^{13}C-NMR spectrum of **5b–I** in CD_3CN.

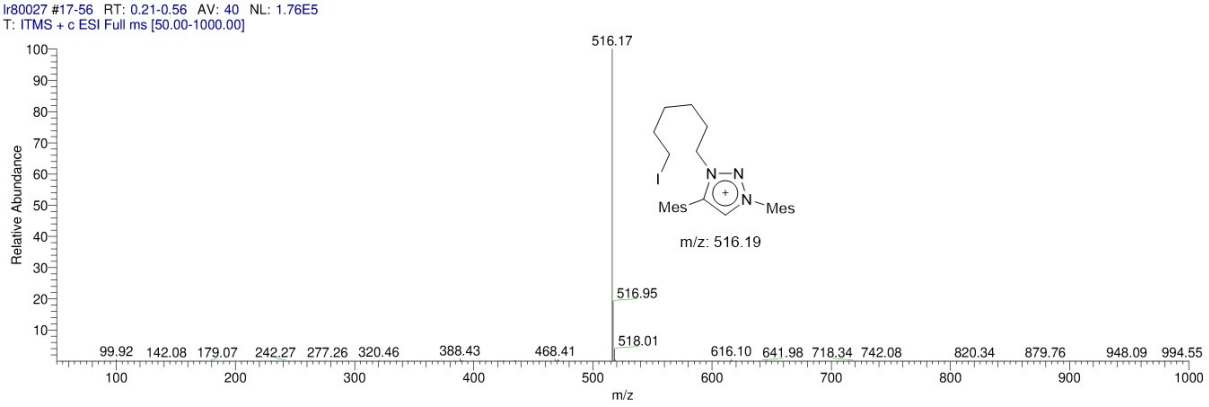

Figure 13: ESI-MS spectrum of **2.**

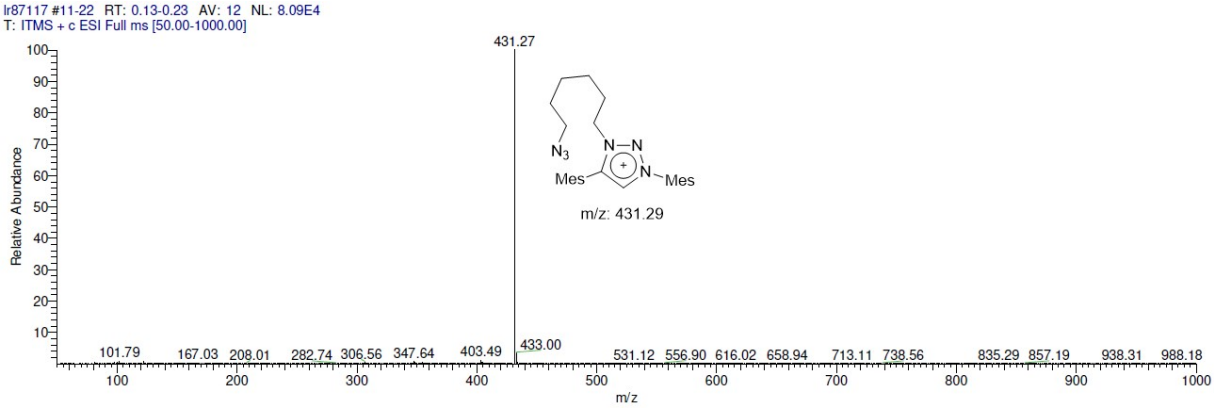

Figure 14: ESI-MS spectrum of **3**.

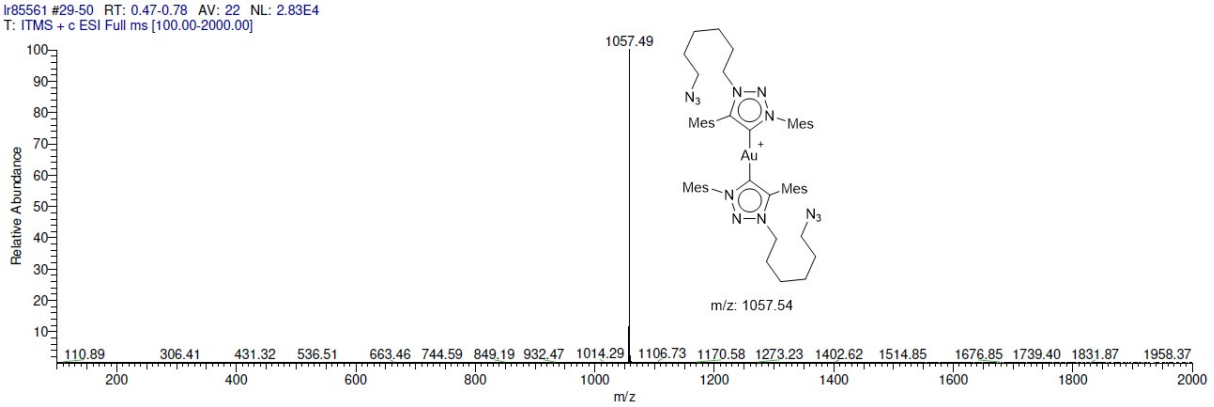

Figure 15: ESI-MS spectrum of **4–I**.

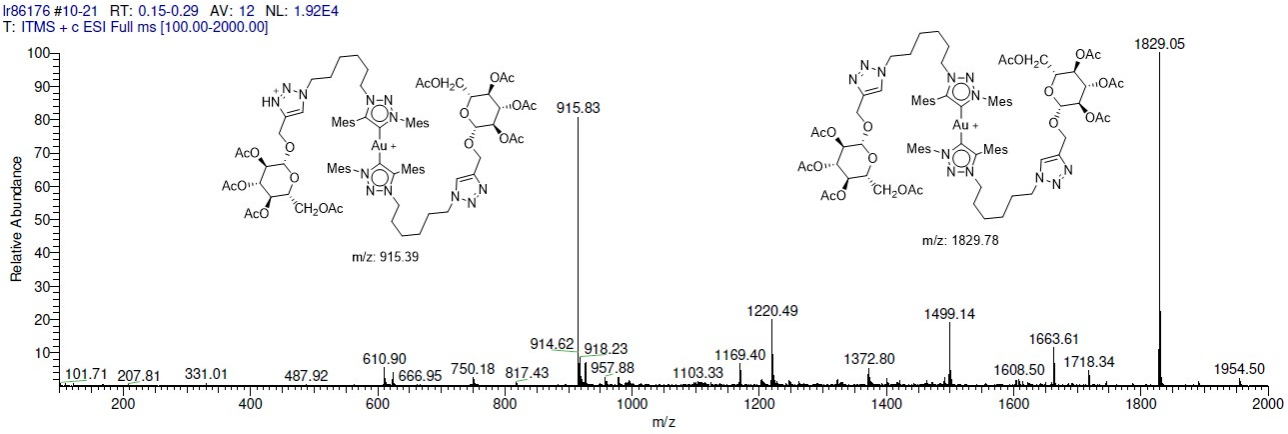

Figure 16: ESI-MS spectrum of **5a-I.**

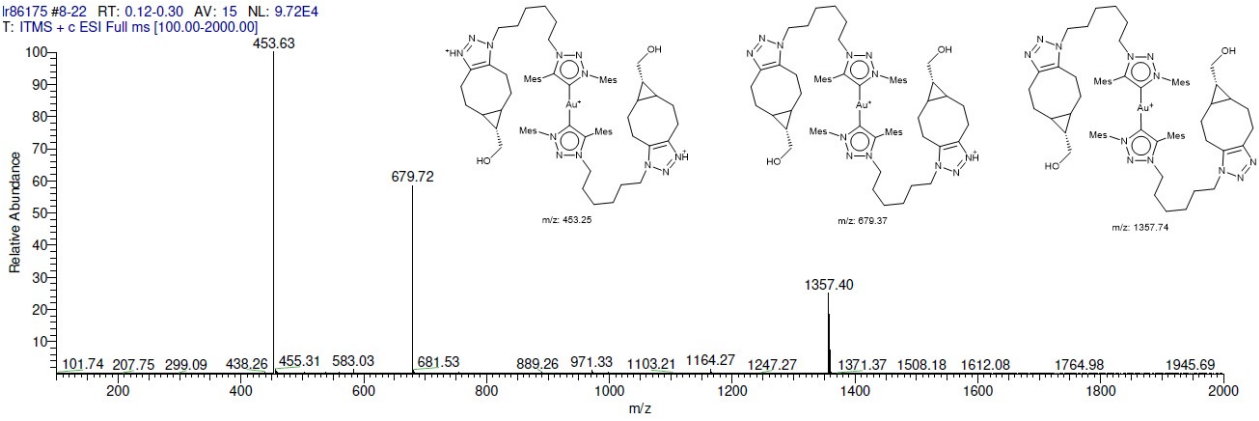

Figure 17: ESI-MS spectrum of **5b-I.**

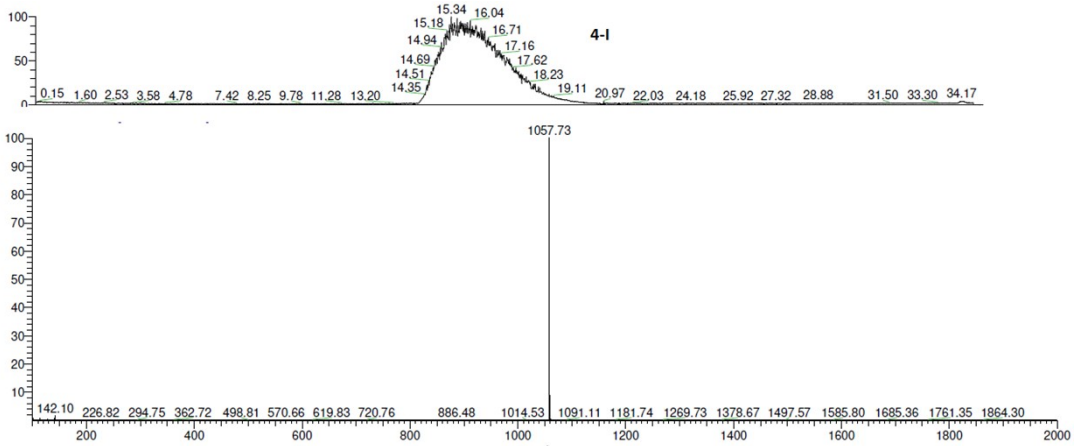

Figure 18 Analytical RP-HPLC of **4-I**(85-100% MeCN/H2O with 0.1% formic acid, 25 min).

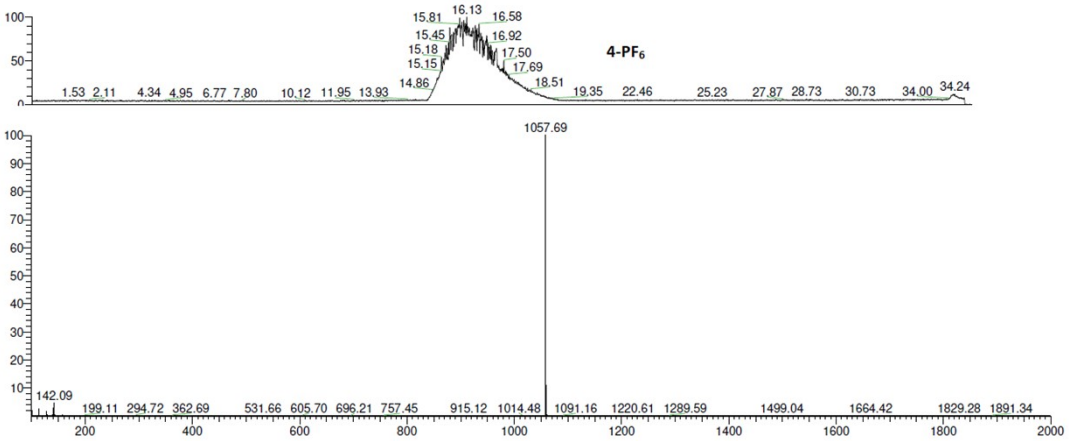

Figure 19 Analytical RP-HPLC of **4-PF_6** (85-100% MeCN/H2O with 0.1% formic acid, 25 min).

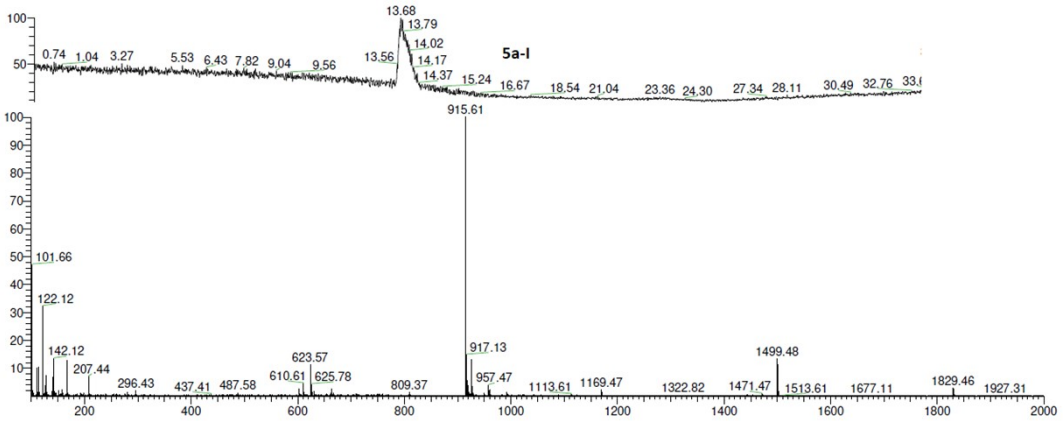

Figure 20 Analytical RP-HPLC of **5a-I** (50-100% MeCN/H2O with 0.1% formic acid, 25 min).

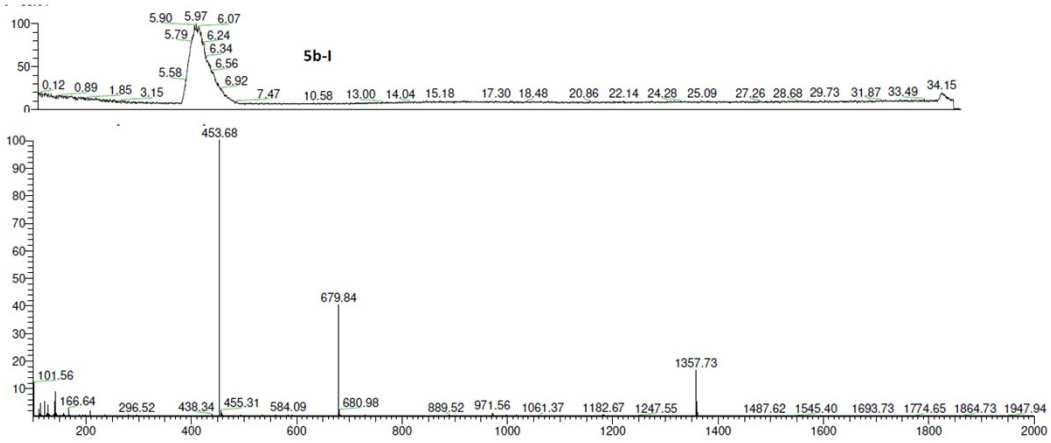

Figure 21 Analytical RP-HPLC of **5b-I** (85-100% MeCN/H2O with 0.1% formic acid, 25 min).

Table 1: Crystallographic data of compound 4-I; CCDC: 2268759.

Chemical formula	**$C_{52}H_{68}AuIN_{12}$**	
Formula weight	1185.06	
Wavelength	0.71073 Å	
Crystal size	0.021 x 0.136 x 0.154 mm	
Crystal system	triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 11.6459(8) Å	*α* = 106.185(2)°
	b = 15.3742(9) Å	*β* = 100.478(2)°
	c = 15.6241(9) Å	*γ* = 91.602(2)°
Volume	2632.6(3) $Å^3$	
Z	2	
Density (calculated)	1.495 g/cm^3	
Absorption coefficient	3.427 mm^{-1}	
F(000)	1192	

Table 2: Data Collection and Structure Refinement of Compound 4-I

Diffractometer	Bruker Photon II
Radiation source	IμS microfocus source (Mo)

Theta range for data collection	2.03 to 25.68°	
Index ranges	-14≤h≤14, -18≤k≤18, -19≤l≤19	
Reflections collected	57455	
Independent reflections	9993 [R(int) = 0.0292]	
Coverage of independent reflections	99.9%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.7457 and 0.6177	
Structure solution technique	direct methods	
Structure solution program	SHELXT (Sheldrick, 2015)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL (Sheldrick, 2017), SHELXLE (Huebschle, 2011)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	9993 / 0 / 607	
Goodness-of-fit on F2	1.140	
Δ/σ_{max}	0.003	
Final R indices	9538 data; I>2σ(I)	R_1 = 0.0256, wR_2 = 0.0546
	all data	R_1 = 0.0276, wR_2 = 0.0553
Weighting scheme	$w=1/[\Sigma^2(F_o^2)+(0.0108P)^2+6.5216P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.665 and -1.032 eÅ^{-3}	
R.M.S. deviation from mean	0.080 eÅ^{-3}	

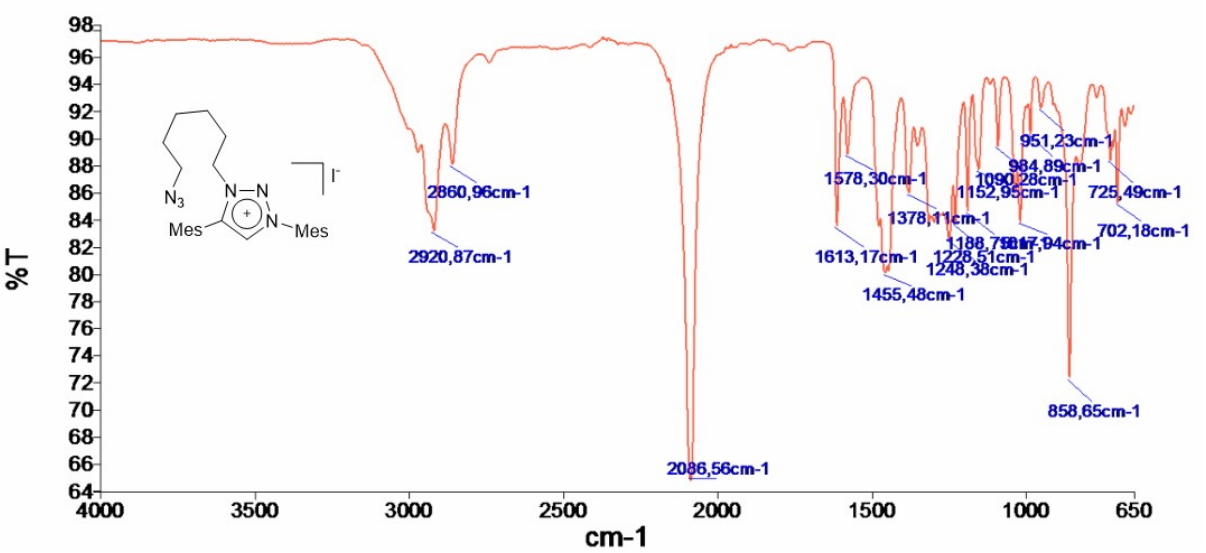

Figure 22: FT-IR spectrum of **3**.

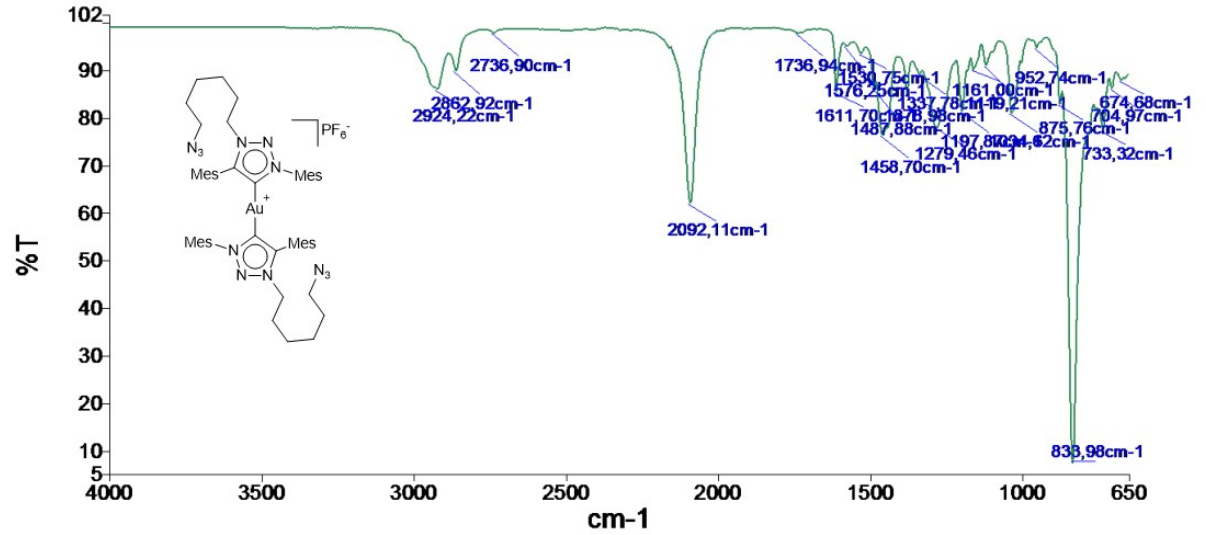

Figure 23: FT-IR spectrum of **4**.

References

[1] Bruker AXS, **n.d.**

[2] C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Crystallogr.* **2011**, *44*, 1281–1284.

[3] G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 3–8.

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