

Supporting Information
for
Synthesis and reactivity of N-heterocyclic carbene (NHC)
gold-fluoroalkoxide complexes

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^b Separation and Conversion Technology, VITO (Flemish Institute for Technological Research),
Boeretang 200, 2400 Mol, Belgium.

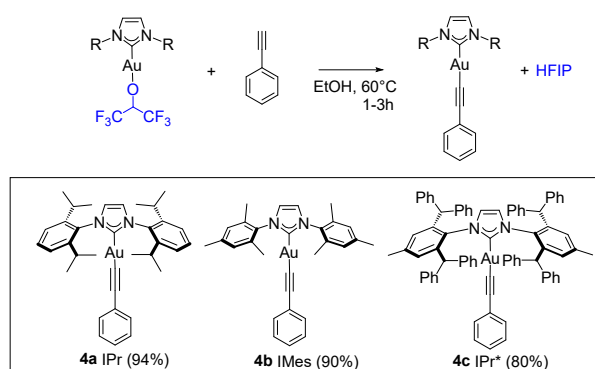
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General information

All reactions were performed in glass vials in air. Ethanol was dried on molecular sieves before use for 16 hours. K_2CO_3 was finely grinded with a mortar and pestle, and dried under high vacuum before use. All other reagents and solvents were purchased and used as received without any additional purification. 1H and ^{13}C - $\{^1H\}$ apt and ^{19}F NMR spectra were recorded in C_6D_6 or $CDCl_3$ using Bruker 300, 400 and 500 MHz spectrometers. Chemical shifts (ppm) in 1H and ^{13}C NMR spectra are referenced to the residual solvent peak (C_6D_6 : $\delta H=7.16$ ppm, $\delta C=128.06$ ppm); ($CDCl_3$: $\delta H=7.26$ ppm, $\delta C=77.16$ ppm). 1H NMR splitting patterns are abbreviated as follows: broad signal (br), singlet (s), doublet (d), triplet (t), doublet of doublets (dd), doublet of triplets (dt), triplet of triplets (tt), quartet (q), quintet (quint), heptet (hept), multiplet (m). All compounds were synthesized according to the procedures described in the literature and the present article. All HRMS experiments (TOF for complex **1f**, and ORBITRAP for complexes **1b,1c, 1d, 1g, 1h, 1i, 1j, 2a**) were performed at Ghent University.

Optimization of the synthesis of gold-acetylide complexes from gold-fluoroalkoxides

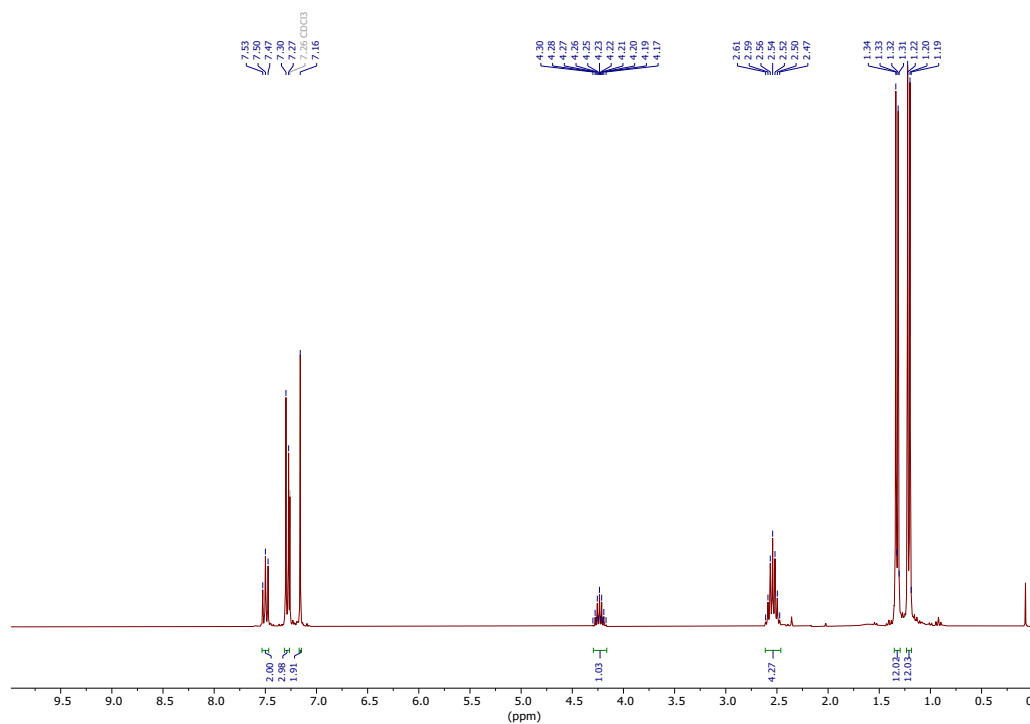


Product	Alkyne (eq)	Temp (°C)	Time (h)	Solvent	Yield (%)
4a	1	60	1	EtOH	94
4a	2	25	6	EtOH	75
4a	3	25	1	Toluene	77
4a	3	25	1	THF	72
4b	1	60	1	EtOH	90
4c	1	60	3	EtOH	80
4c	3	60	3	EtOH	85

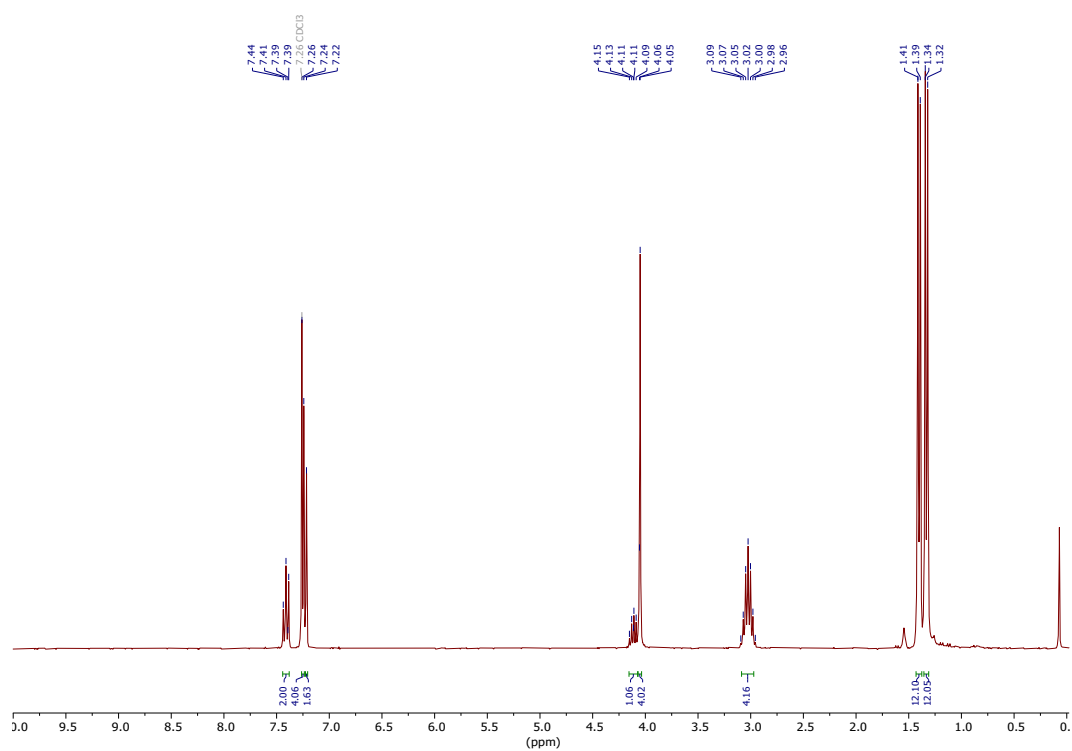
Table S1. Optimization of gold-acetylides synthesis.

NMR Data

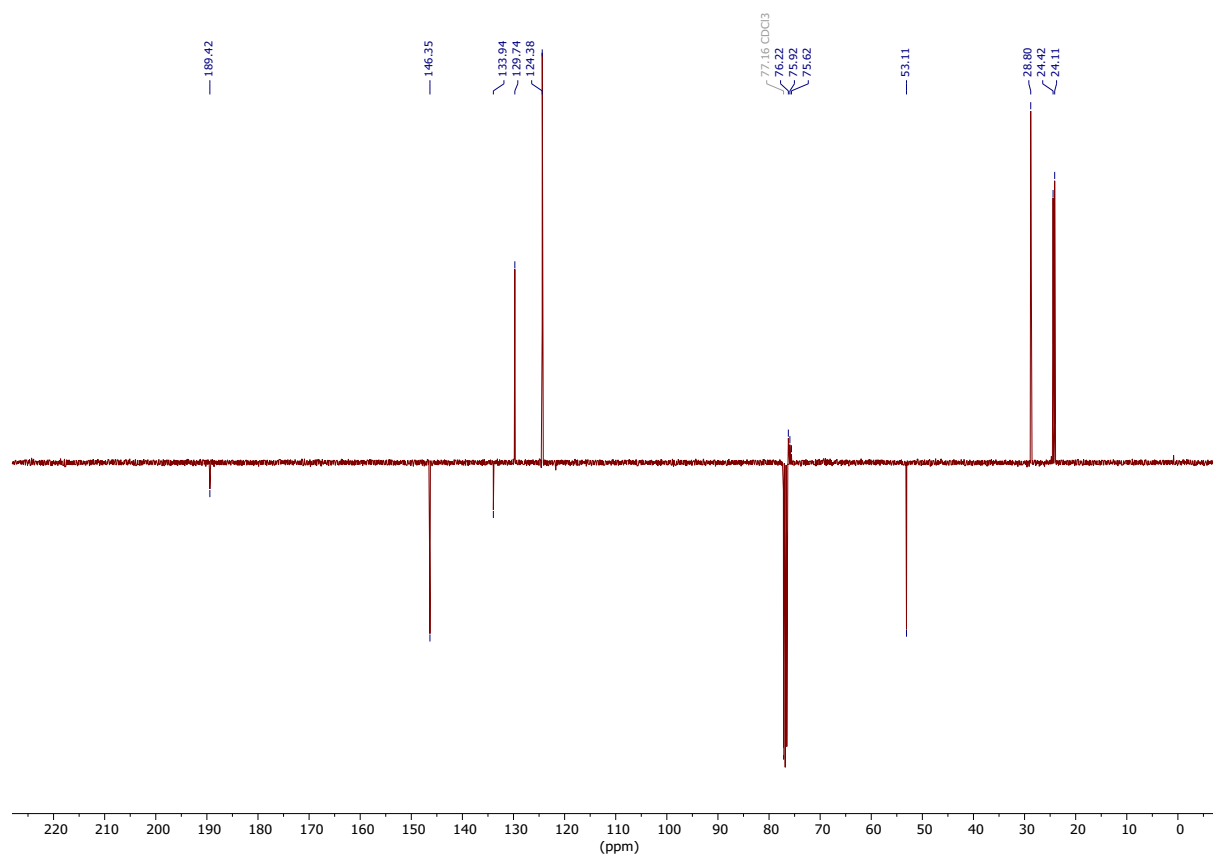
^1H NMR Spectra of $[\text{Au}(\text{IPr})(\text{OCH}(\text{CF}_3)_2)]$ (1a)



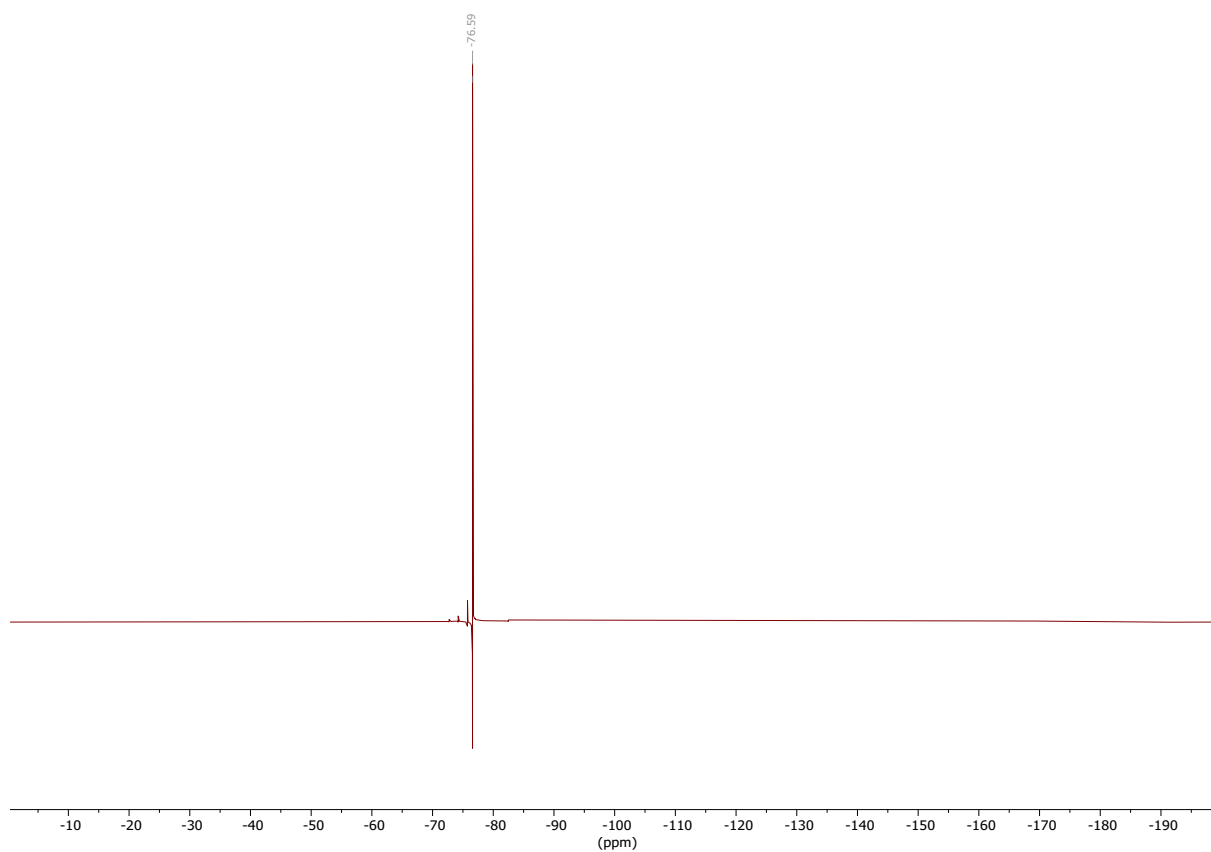
^1H NMR of $[\text{Au}(\text{SIPr})(\text{OCH}(\text{CF}_3)_2)]$ (1b)



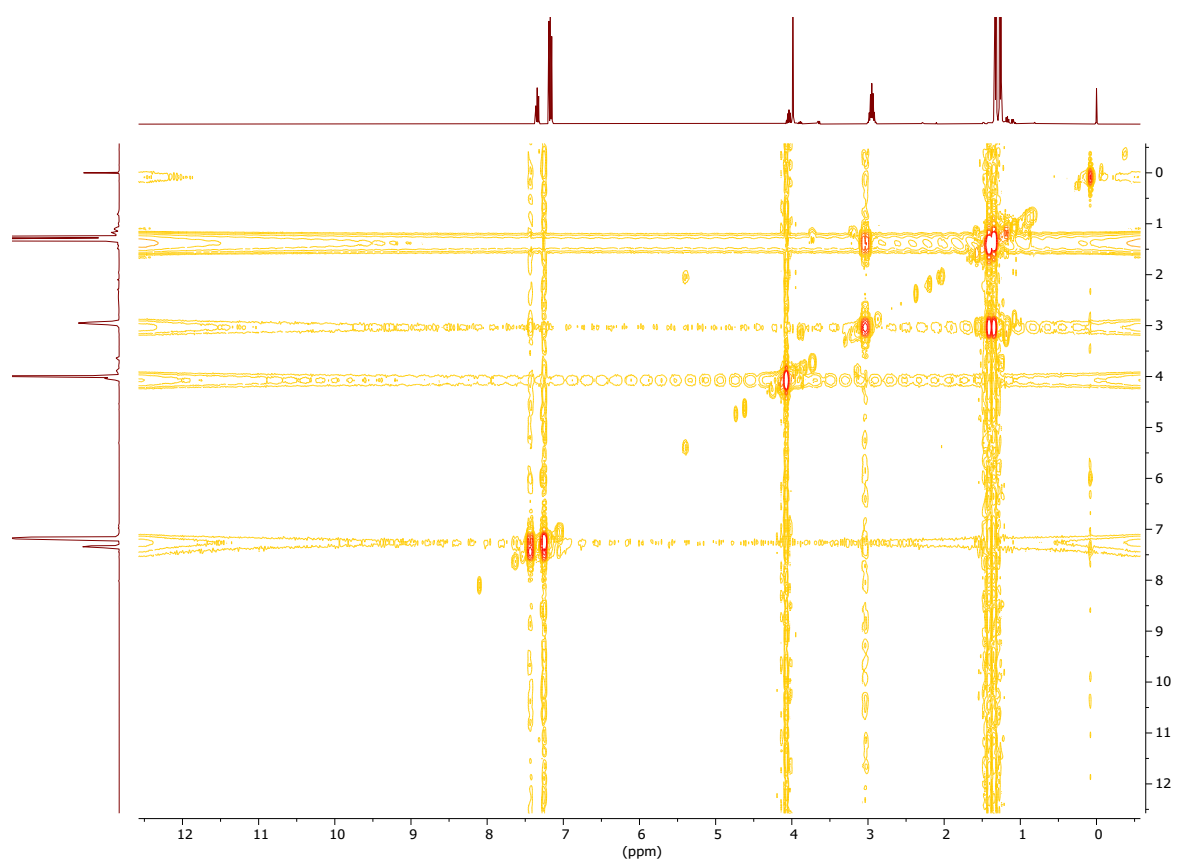
¹³C NMR of 1b



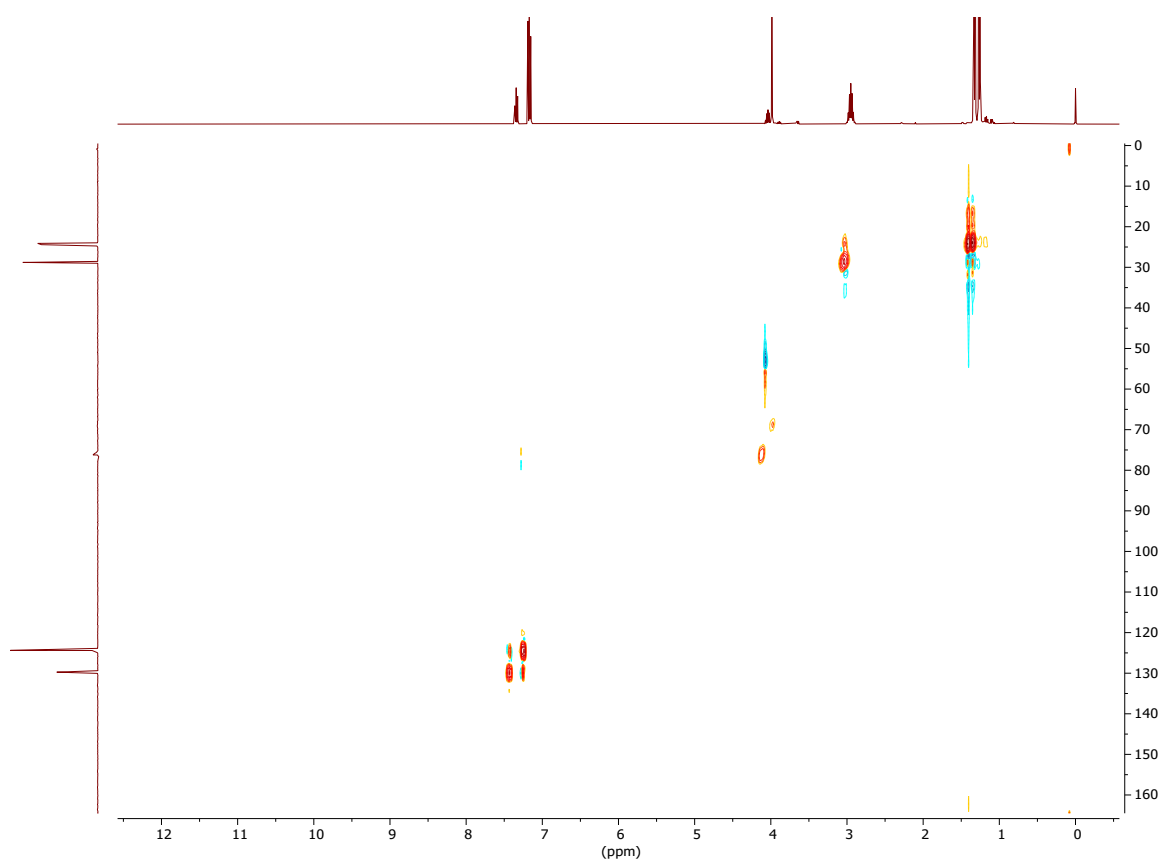
^{19}F NMR of 1b



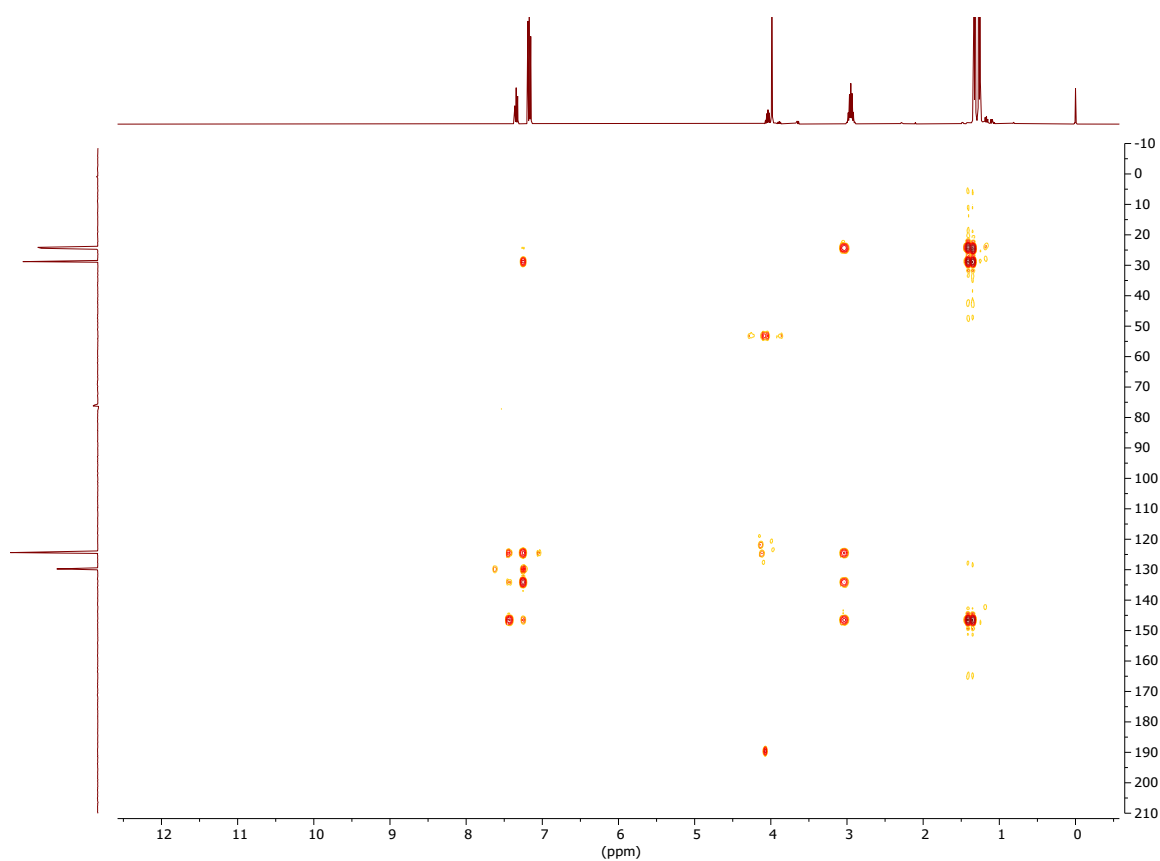
COSY NMR of 1b



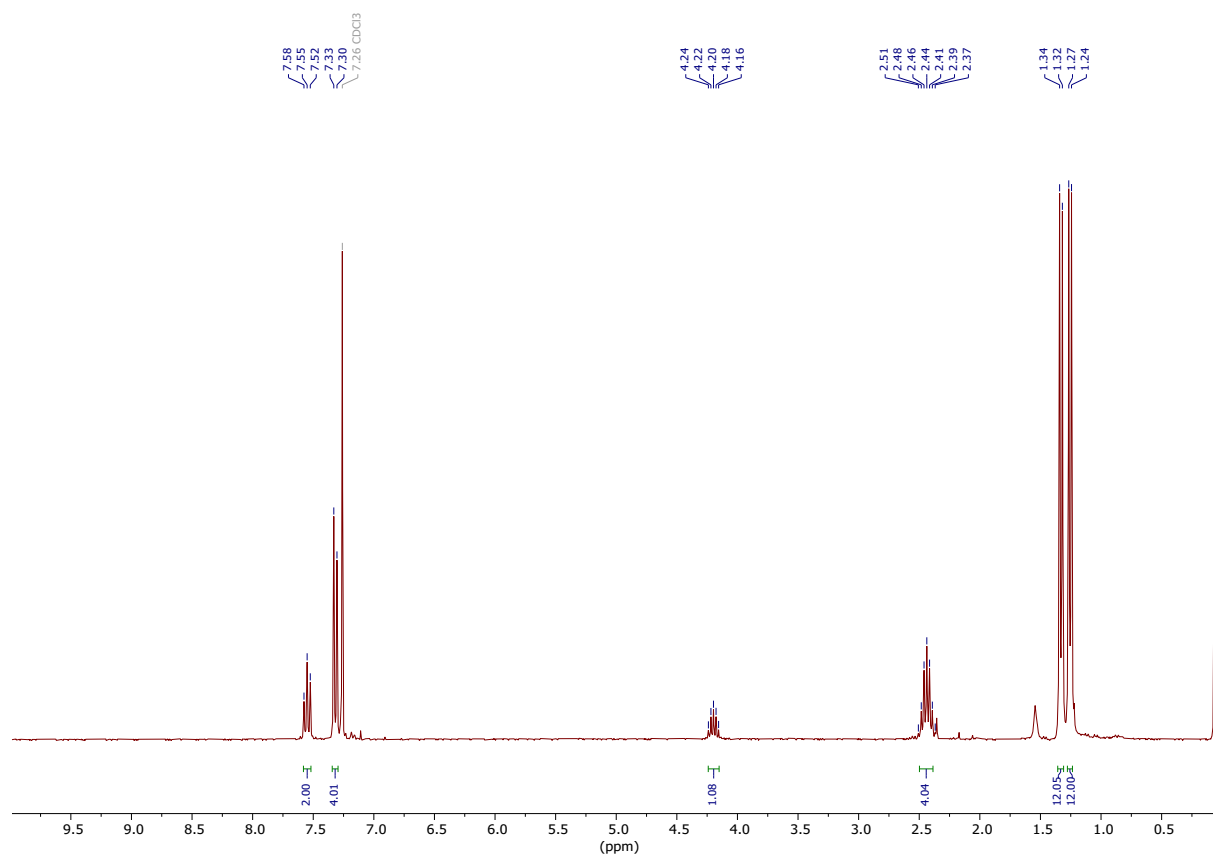
HSQC NMR of 1b



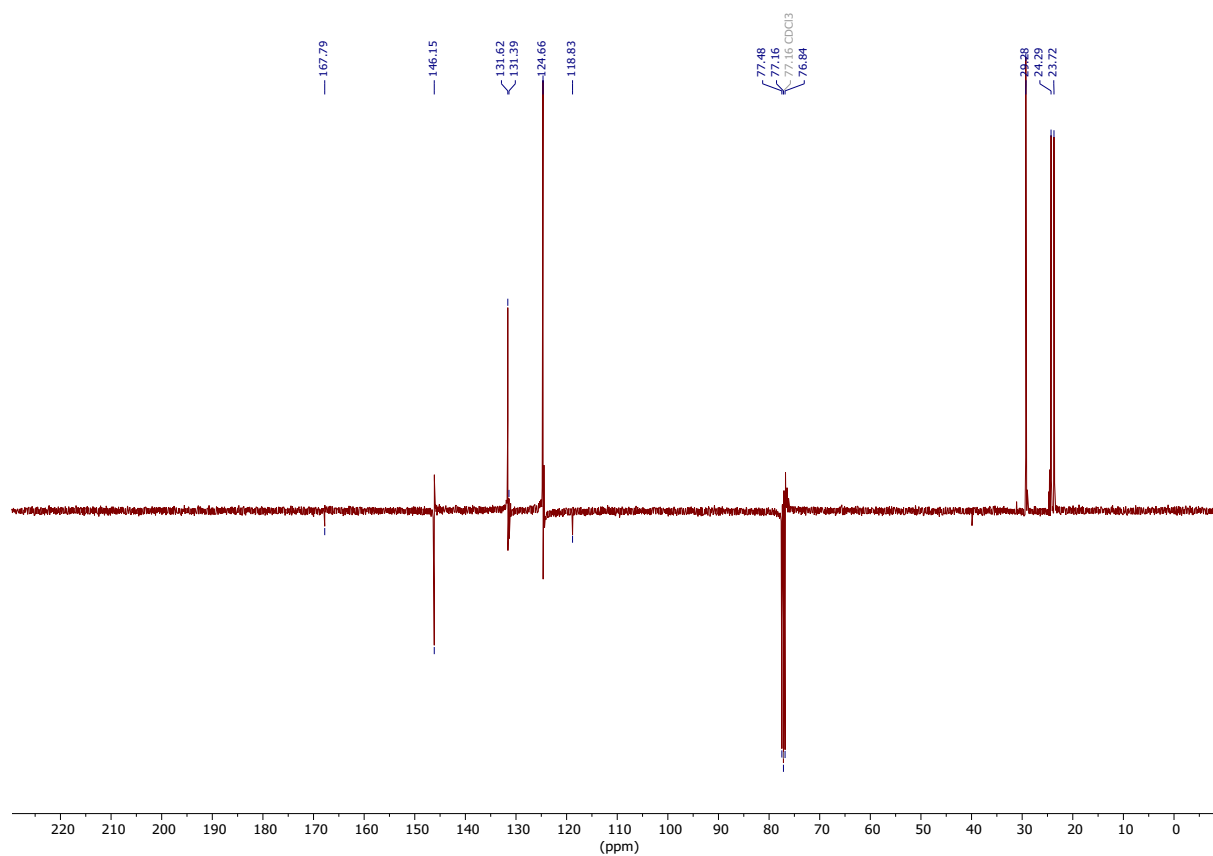
HMBC NMR of 1b



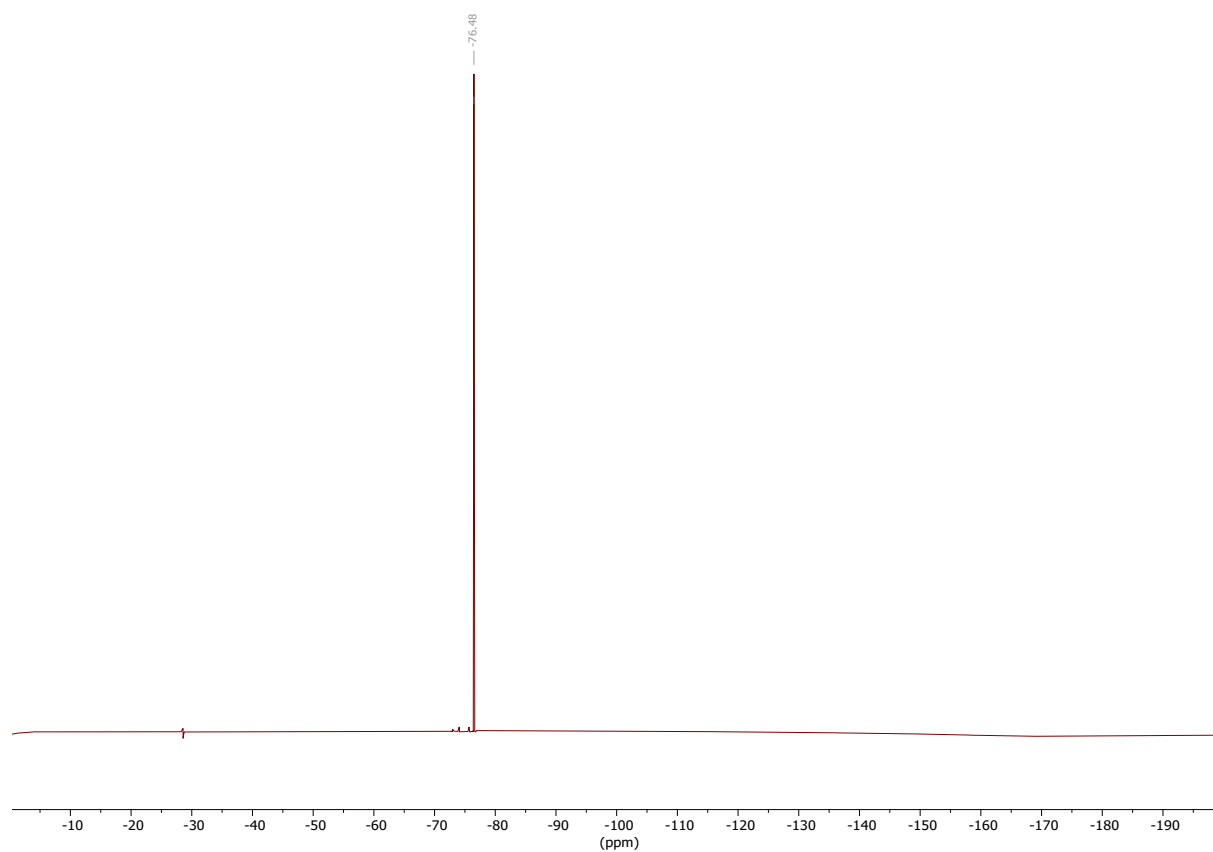
^1H NMR of $[\text{Au}(\text{IPr}^{\text{Cl}})(\text{OCH}(\text{CF}_3)_2)]$ (**1c**)



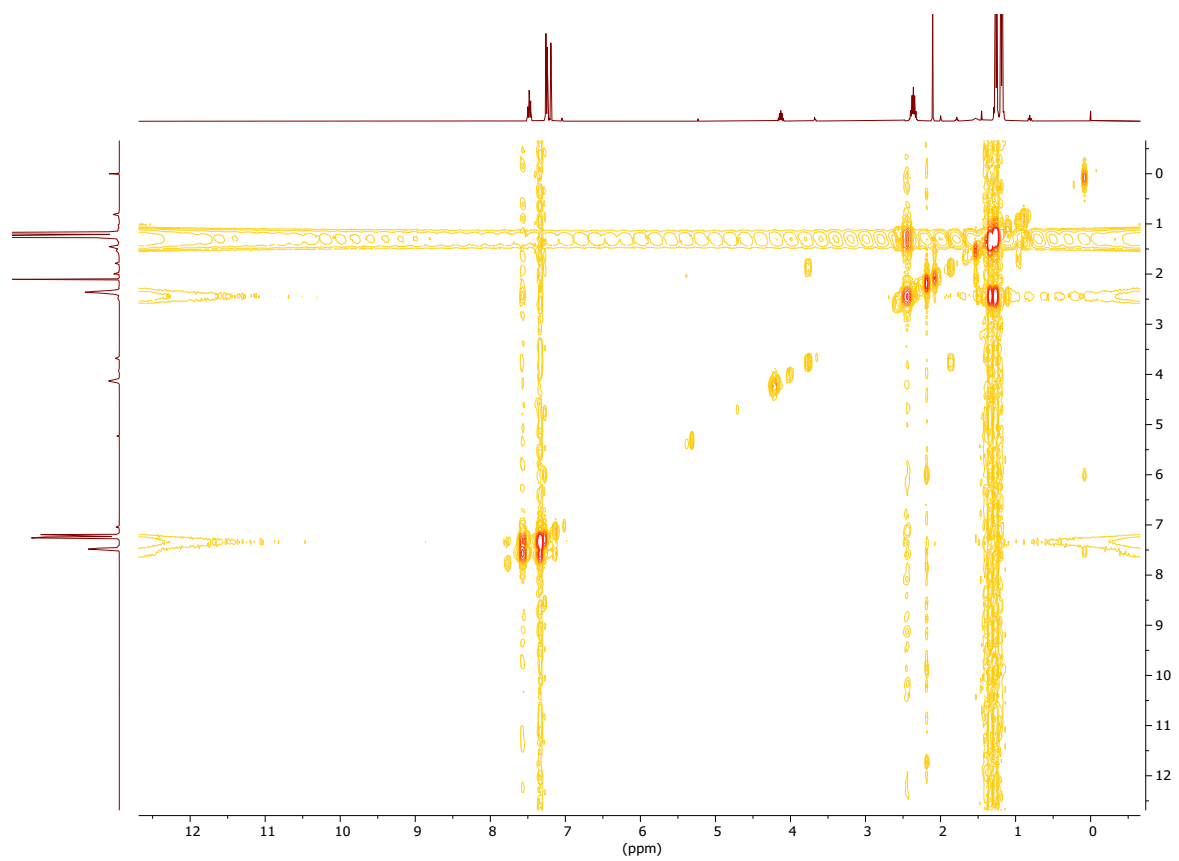
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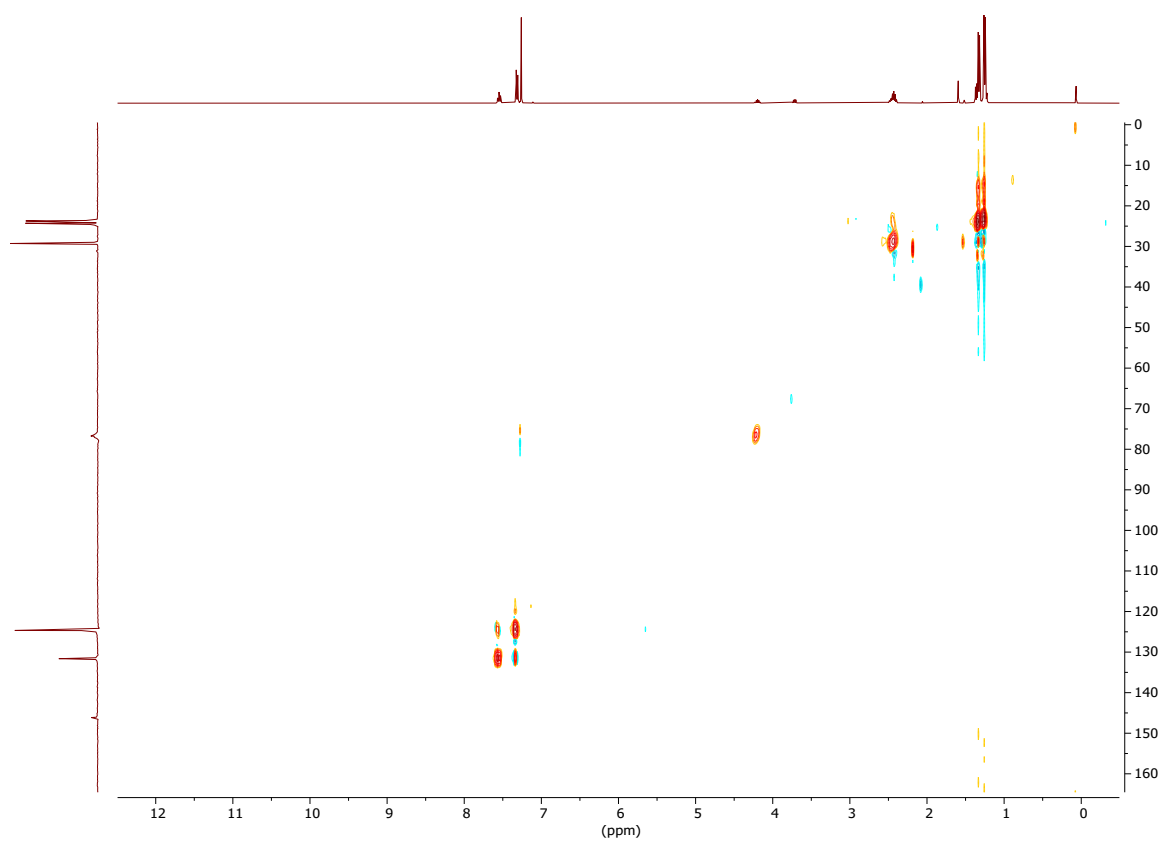
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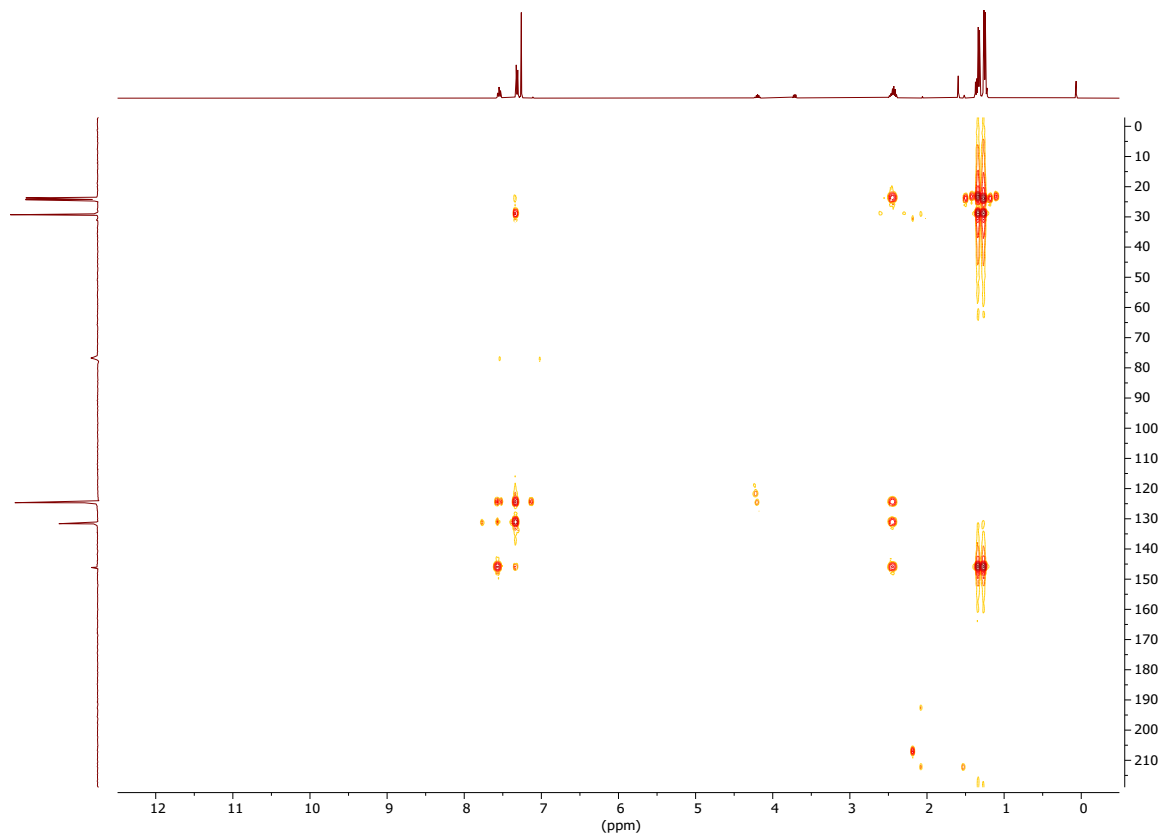
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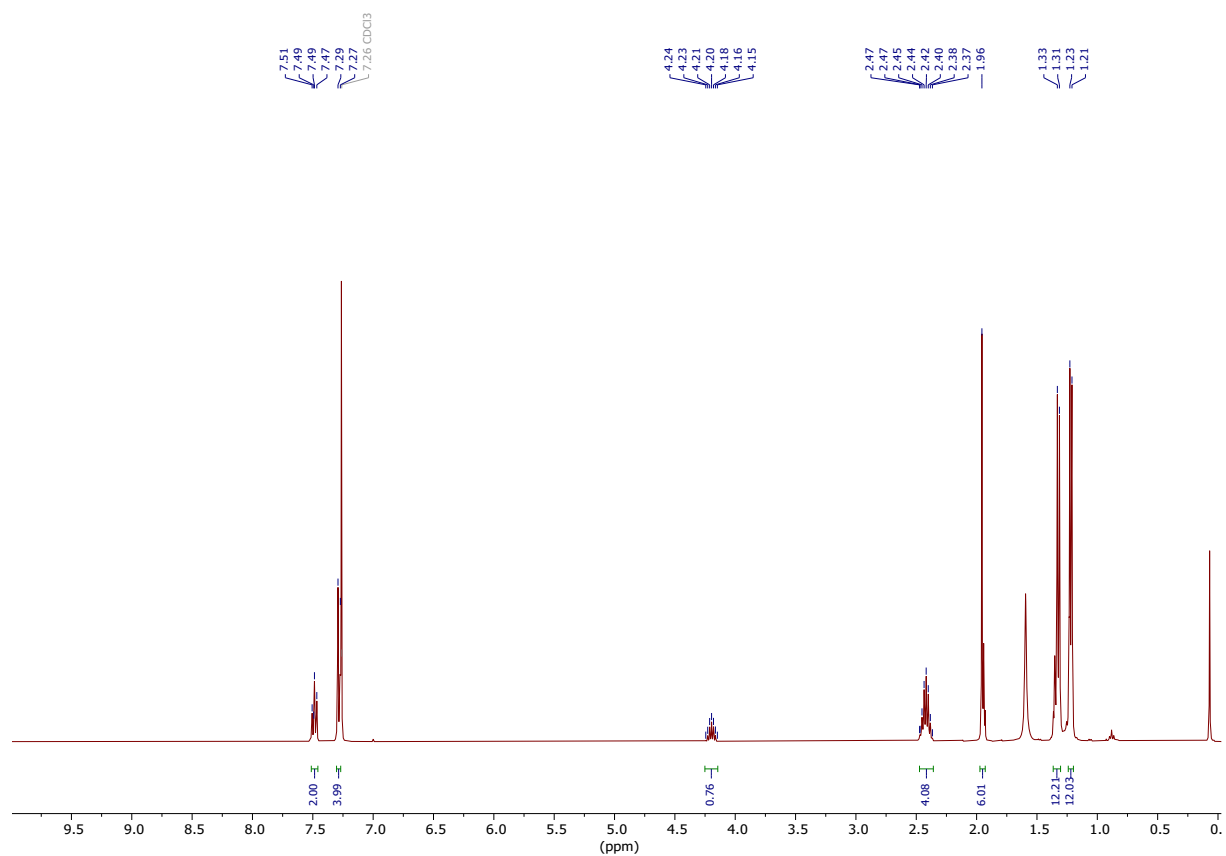
HSQC NMR of 1c



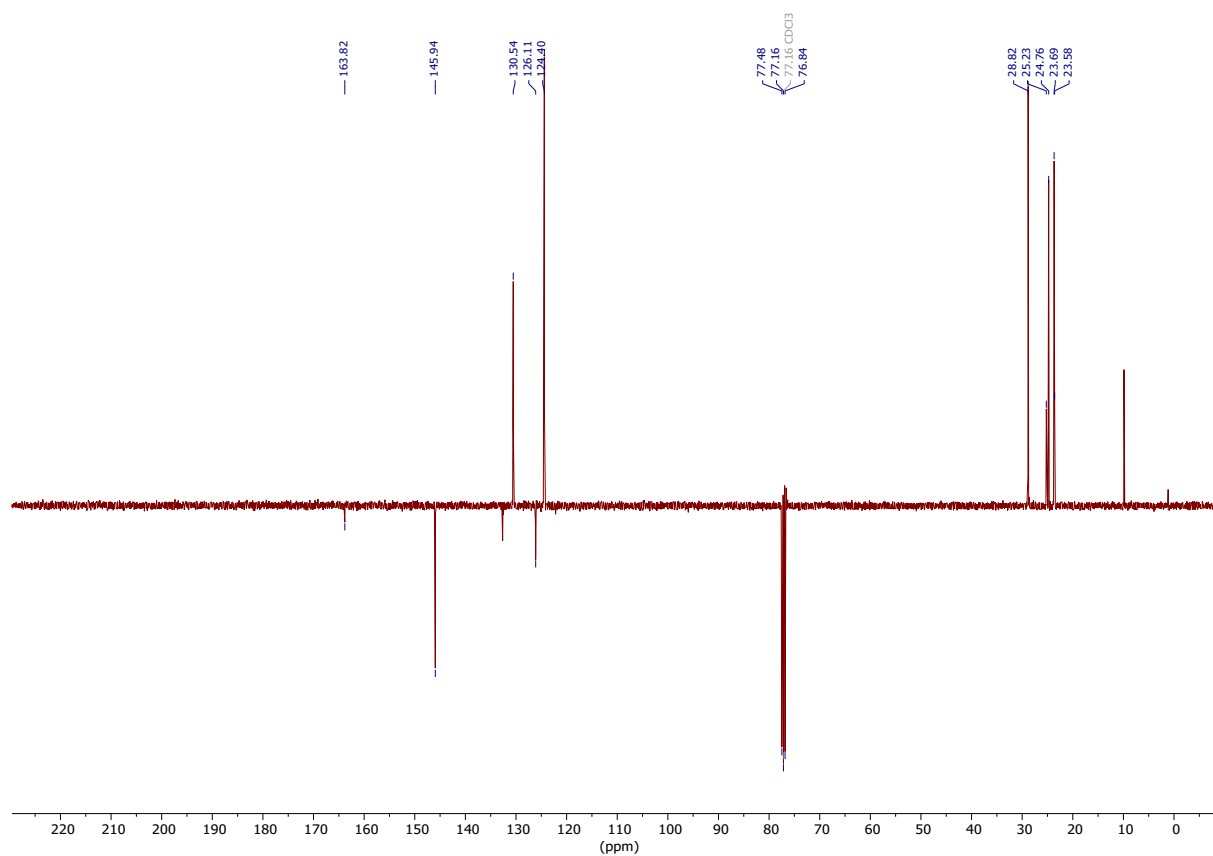
HMBC NMR of 1c



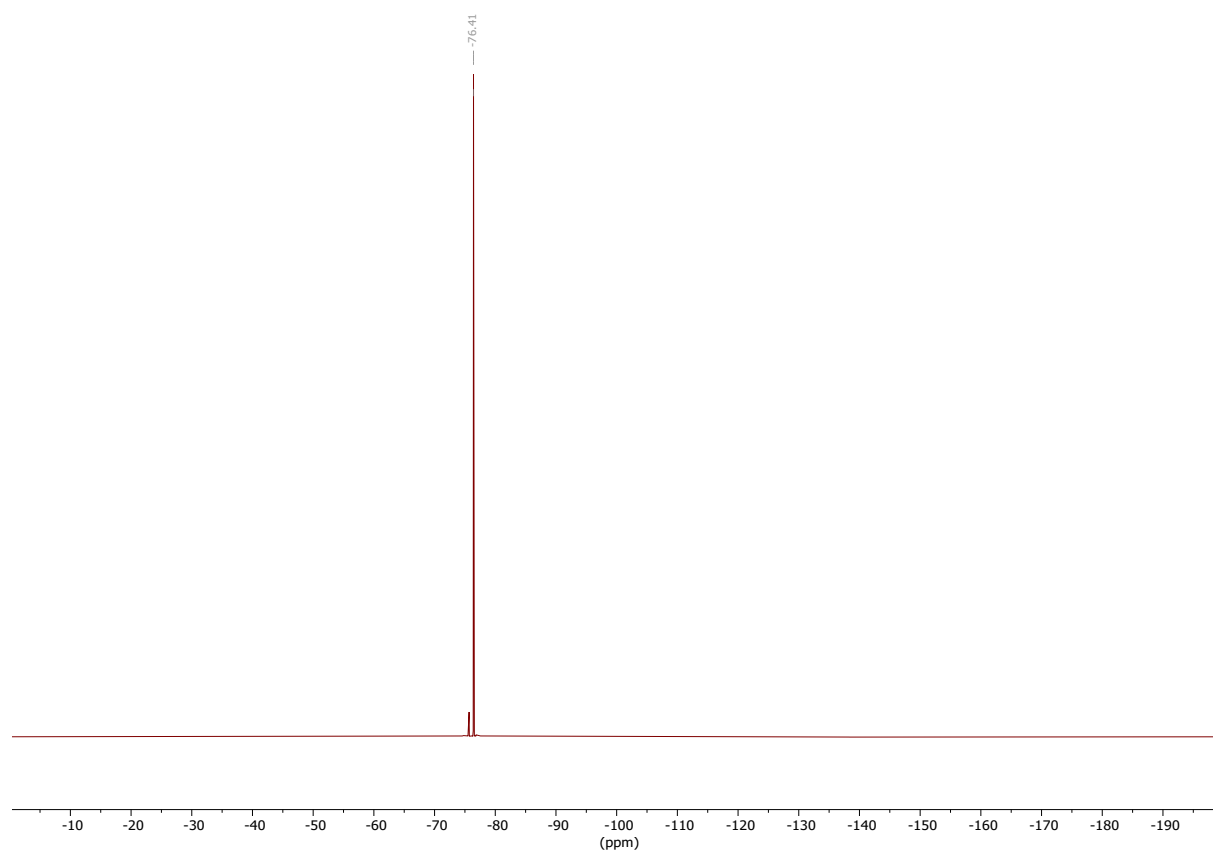
^1H NMR of $[\text{Au}(\text{IPr}^{\text{Me}})(\text{OCH}(\text{CF}_3)_2)]$ (1d)



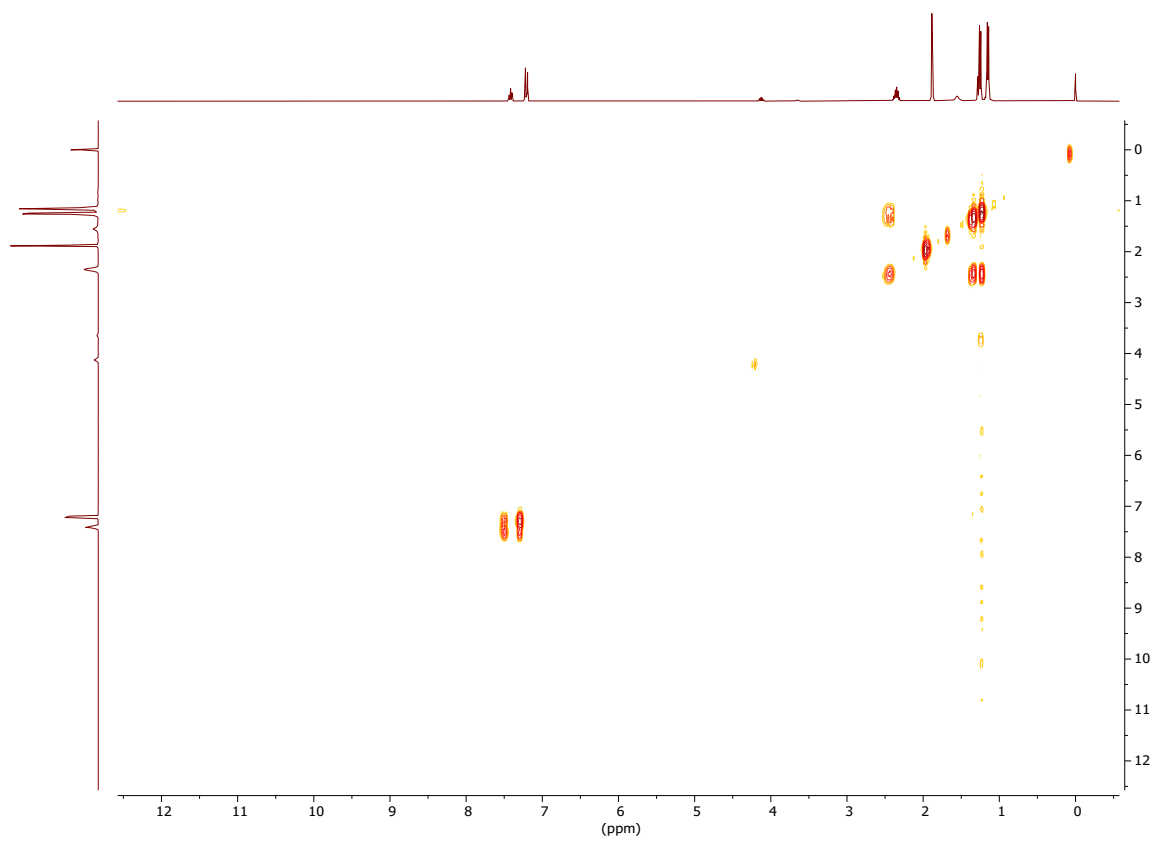
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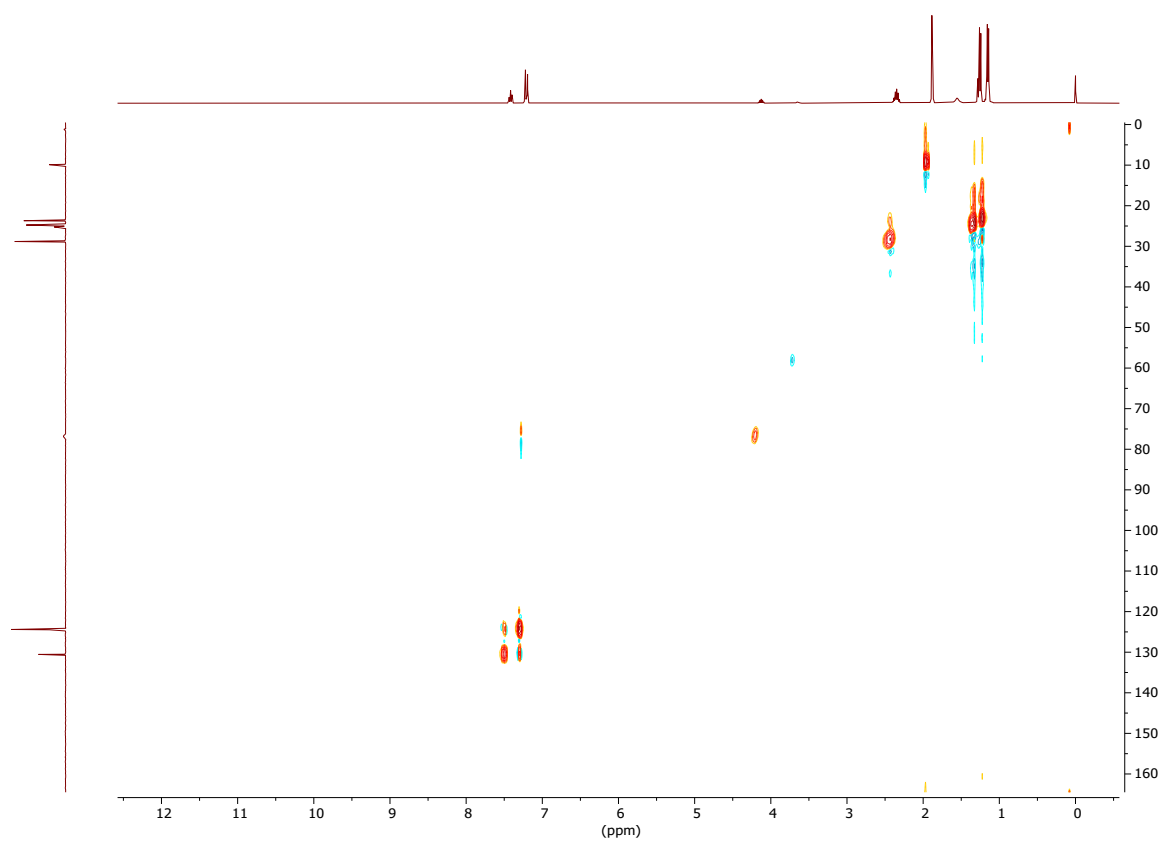
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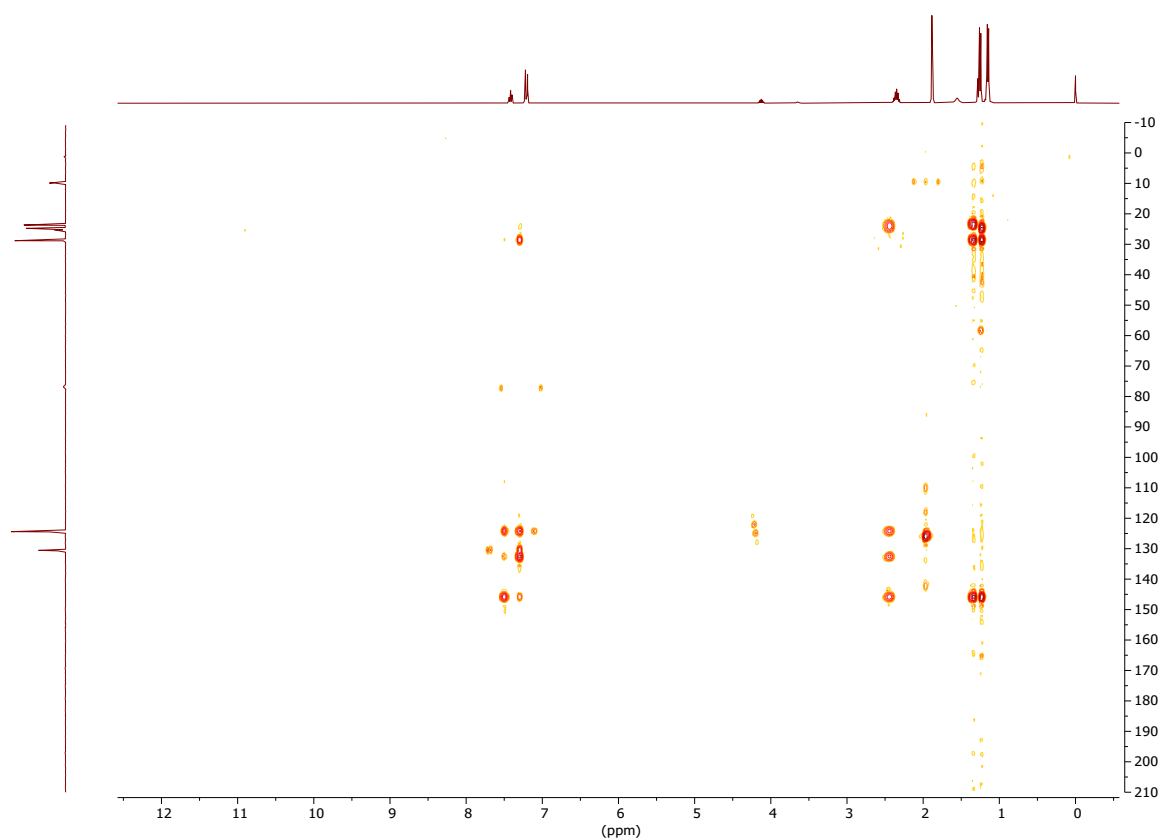
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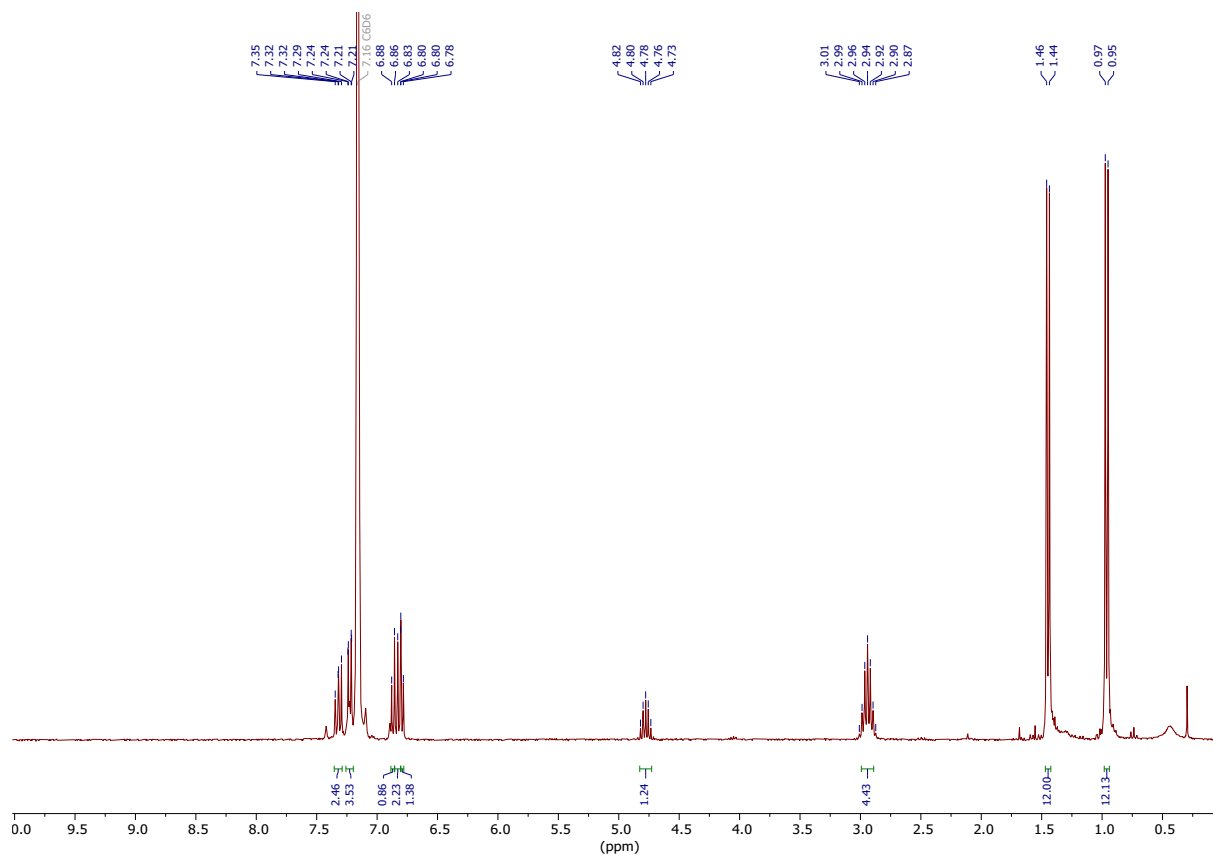
HSQC NMR of 1d



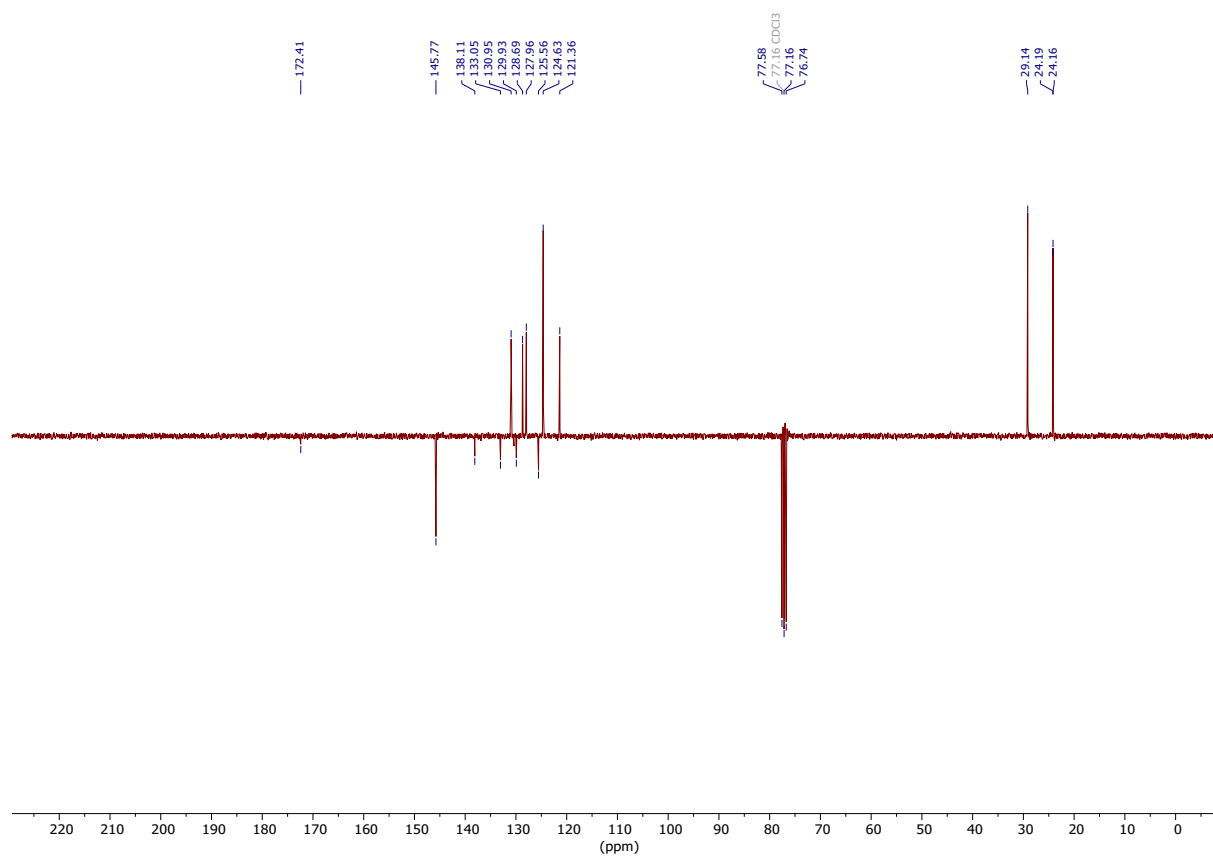
HMBC NMR of 1d



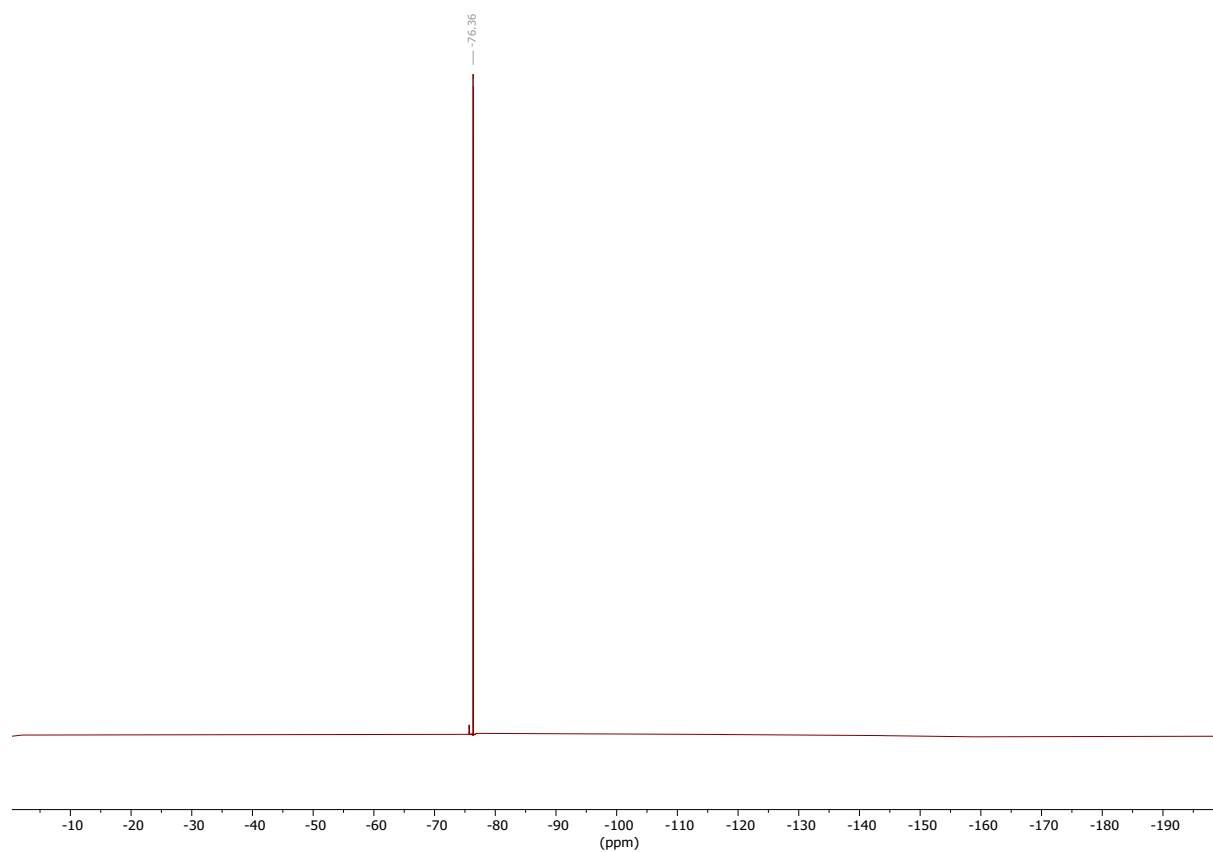
^1H NMR of $[\text{Au}(\text{BIAN-IPr})(\text{OCH}(\text{CF}_3)_2)]$ (1e)



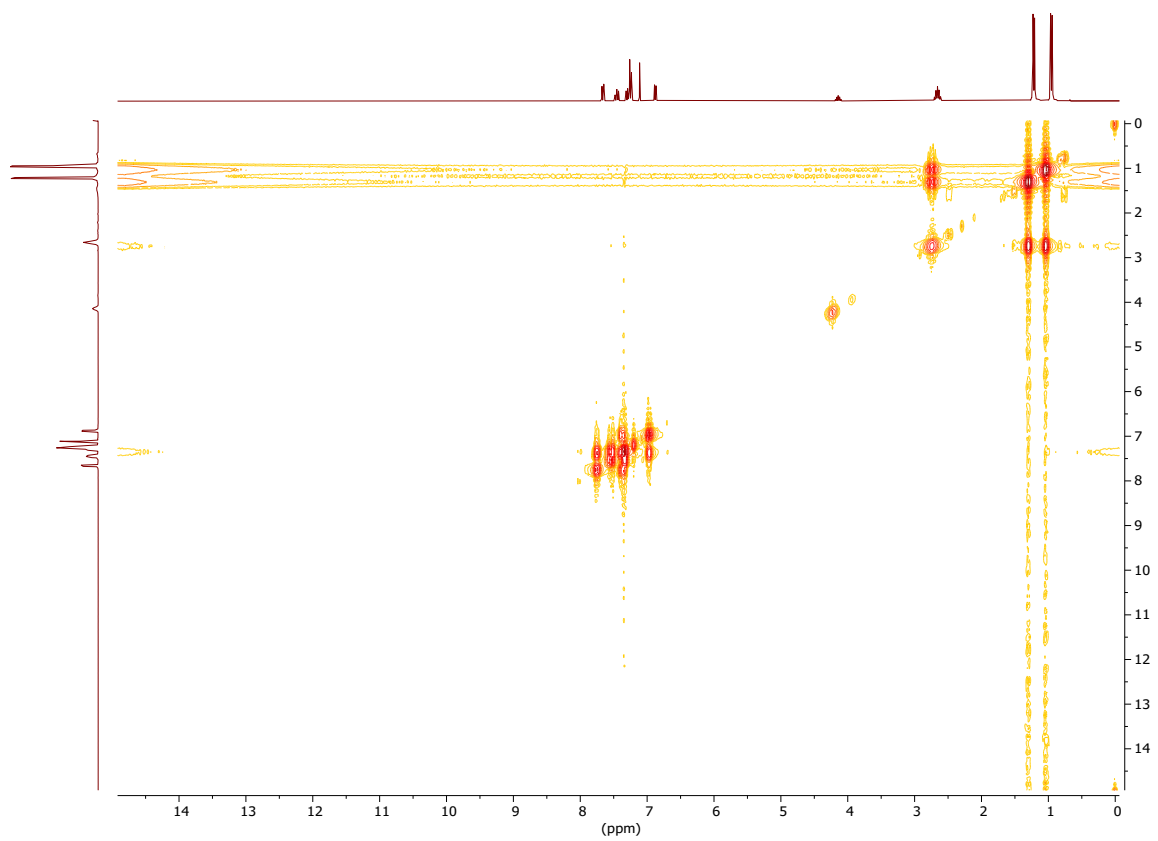
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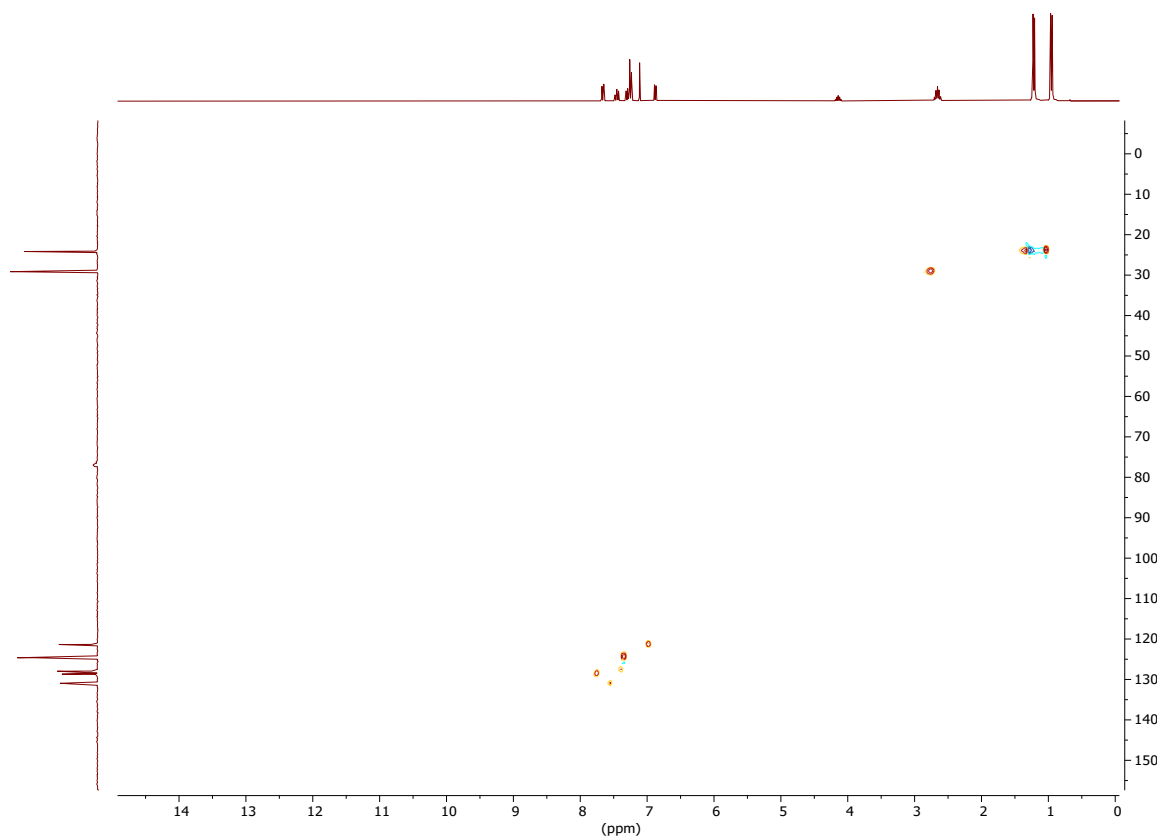
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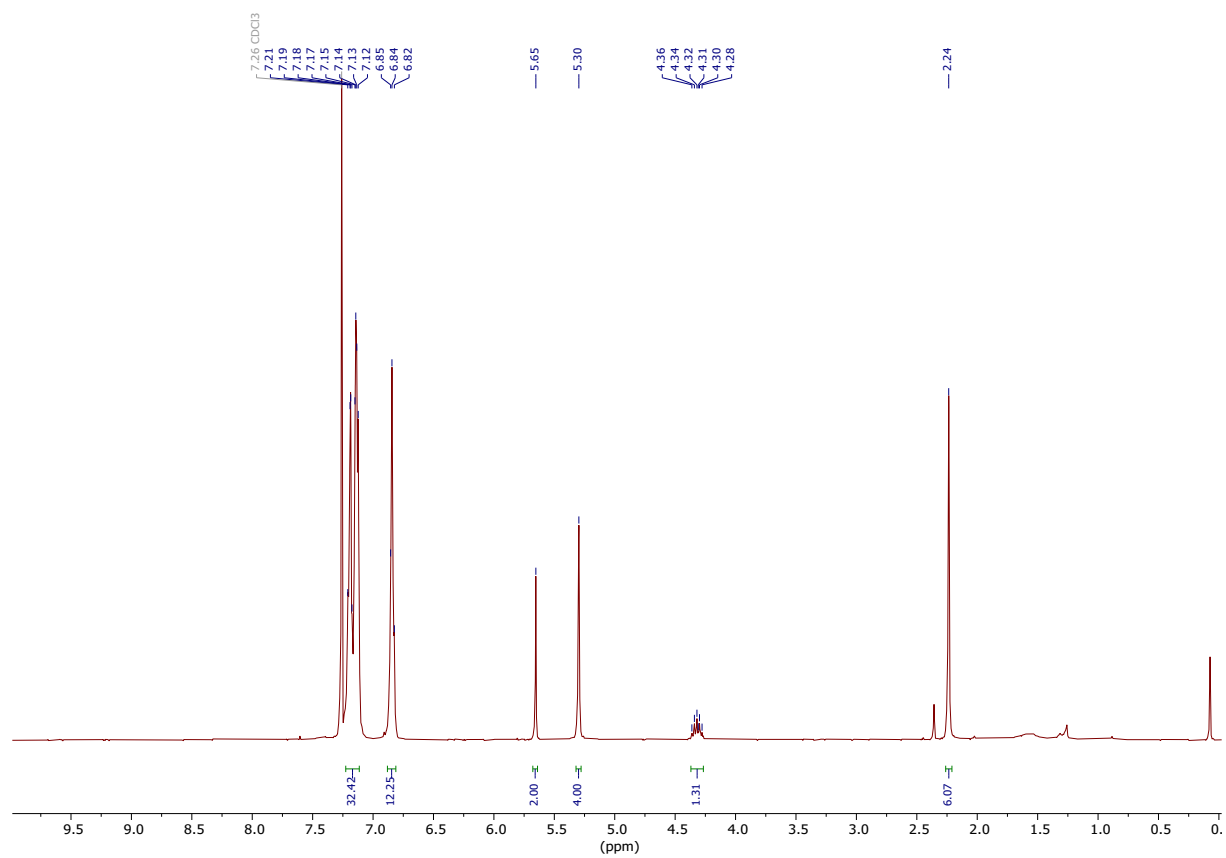
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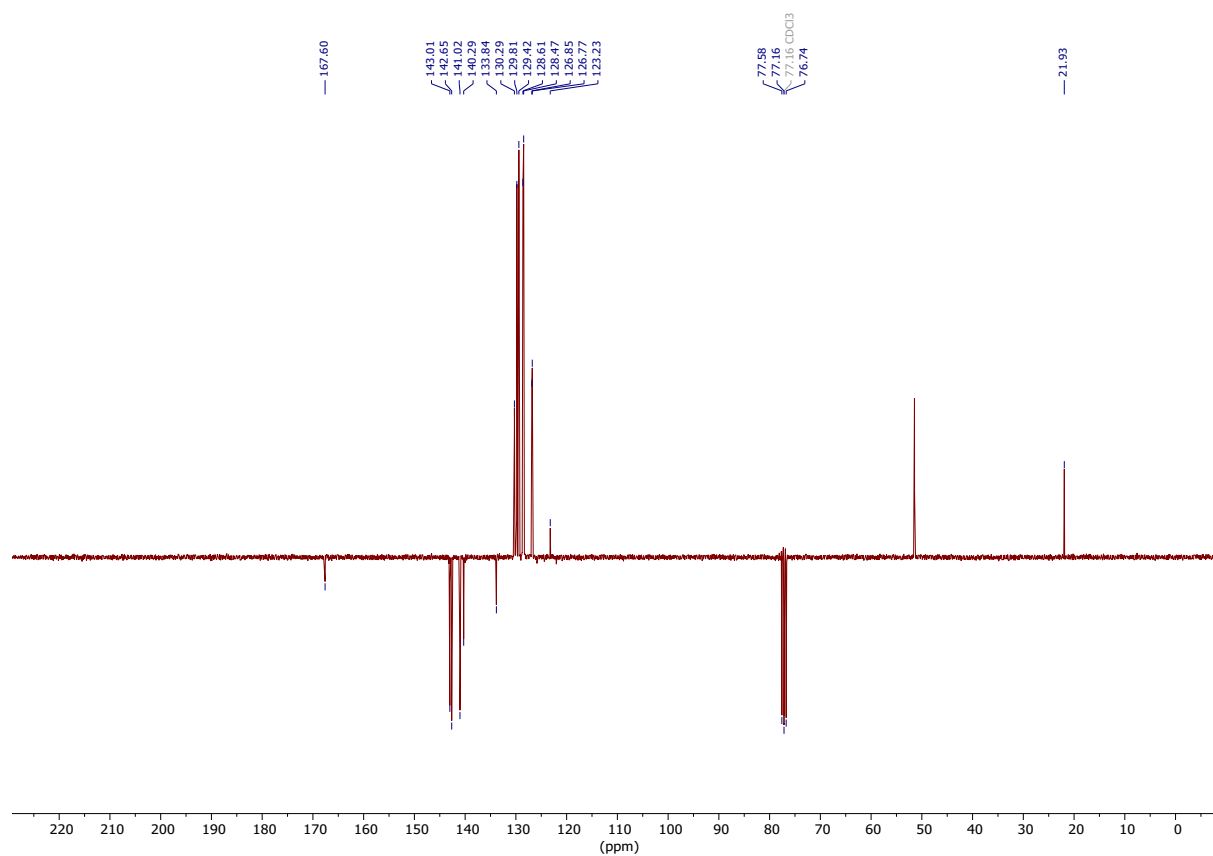
HSQC NMR of 1e



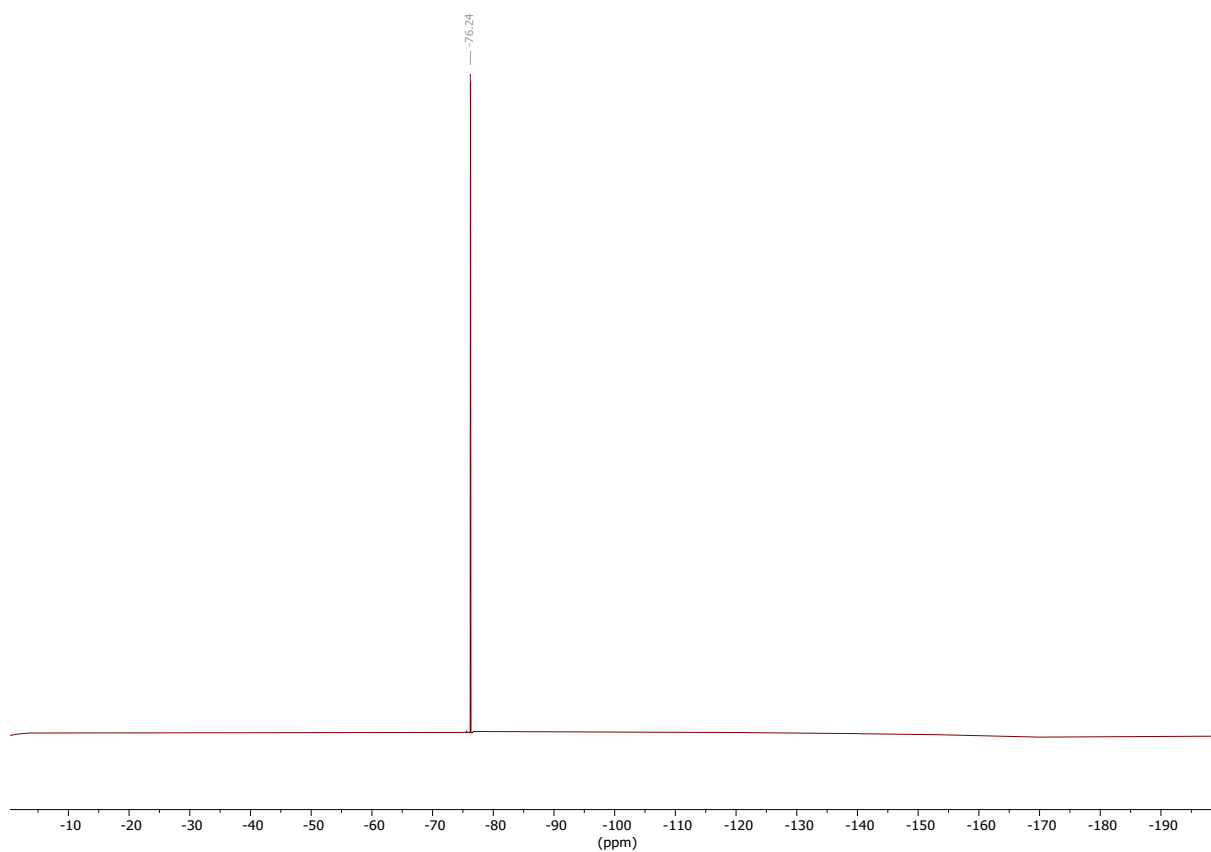
^1H NMR of $[\text{Au}(\text{IPr}^*)(\text{OCH}(\text{CF}_3)_2)]$ (**1f**)



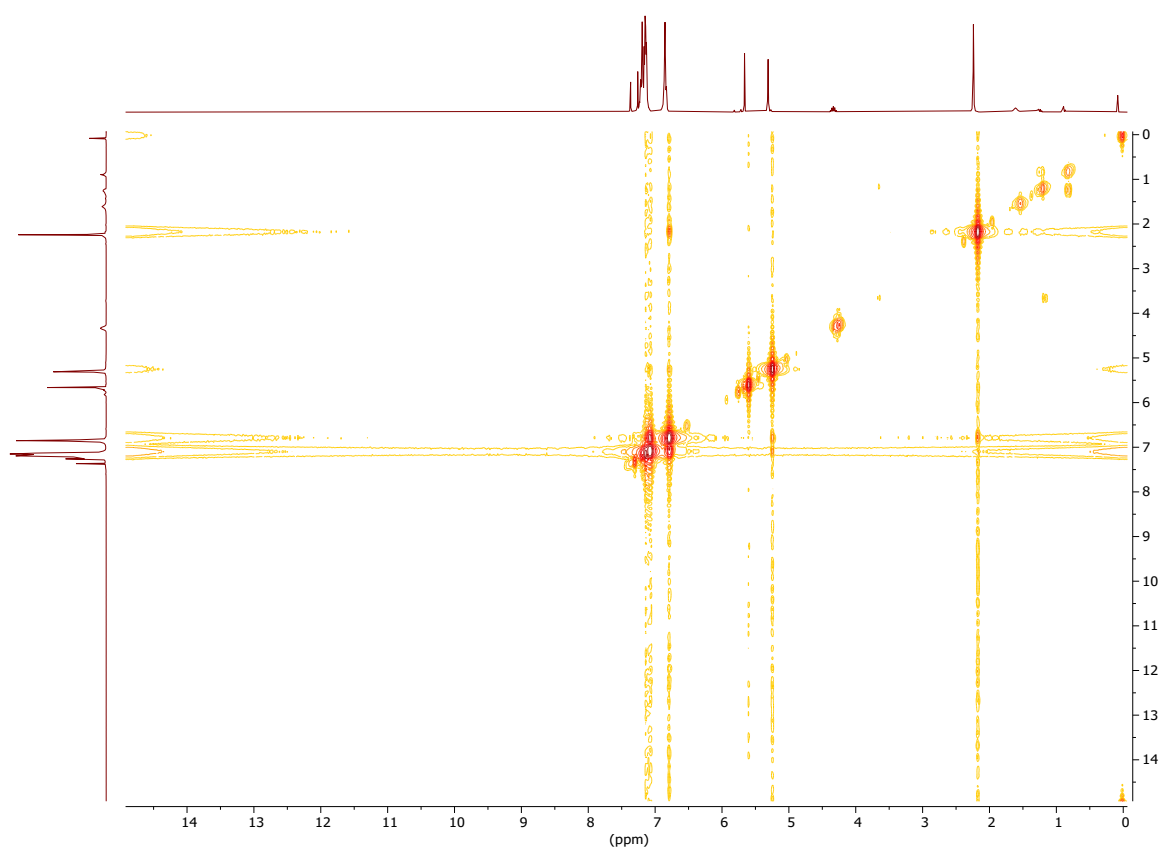
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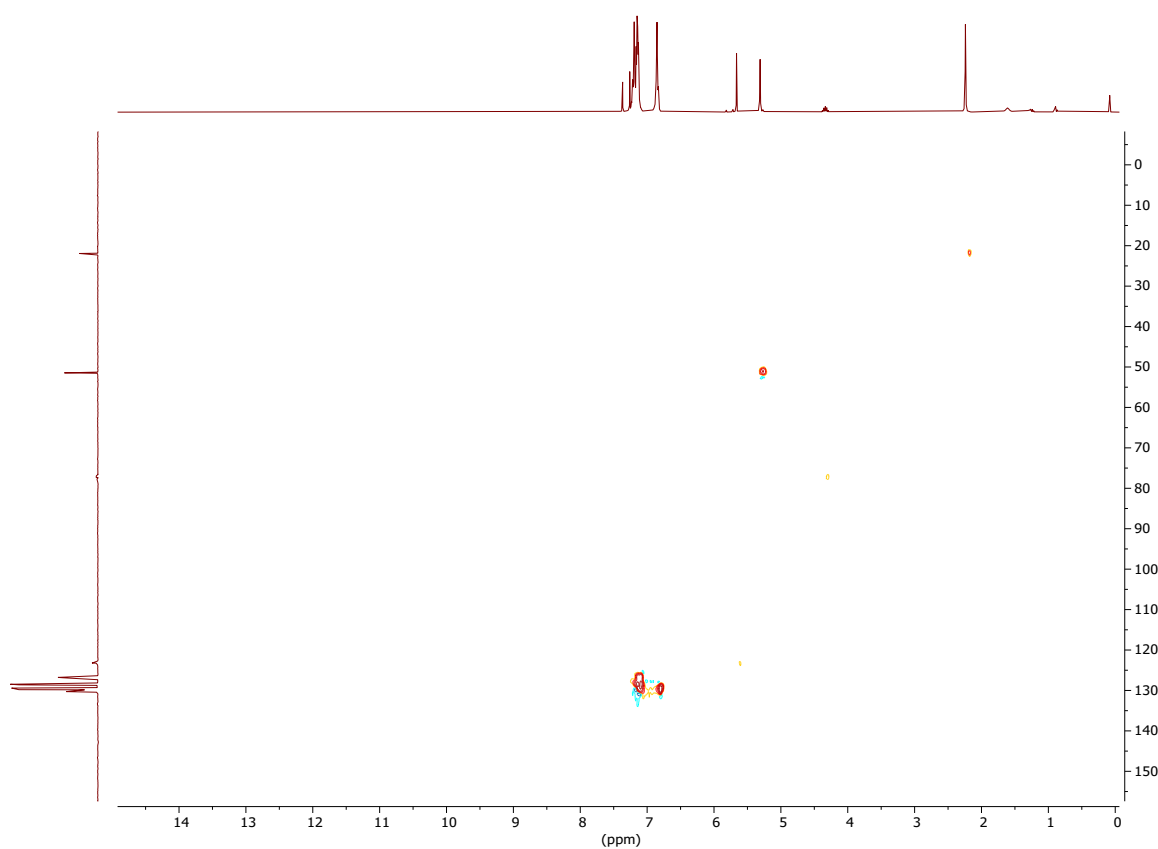
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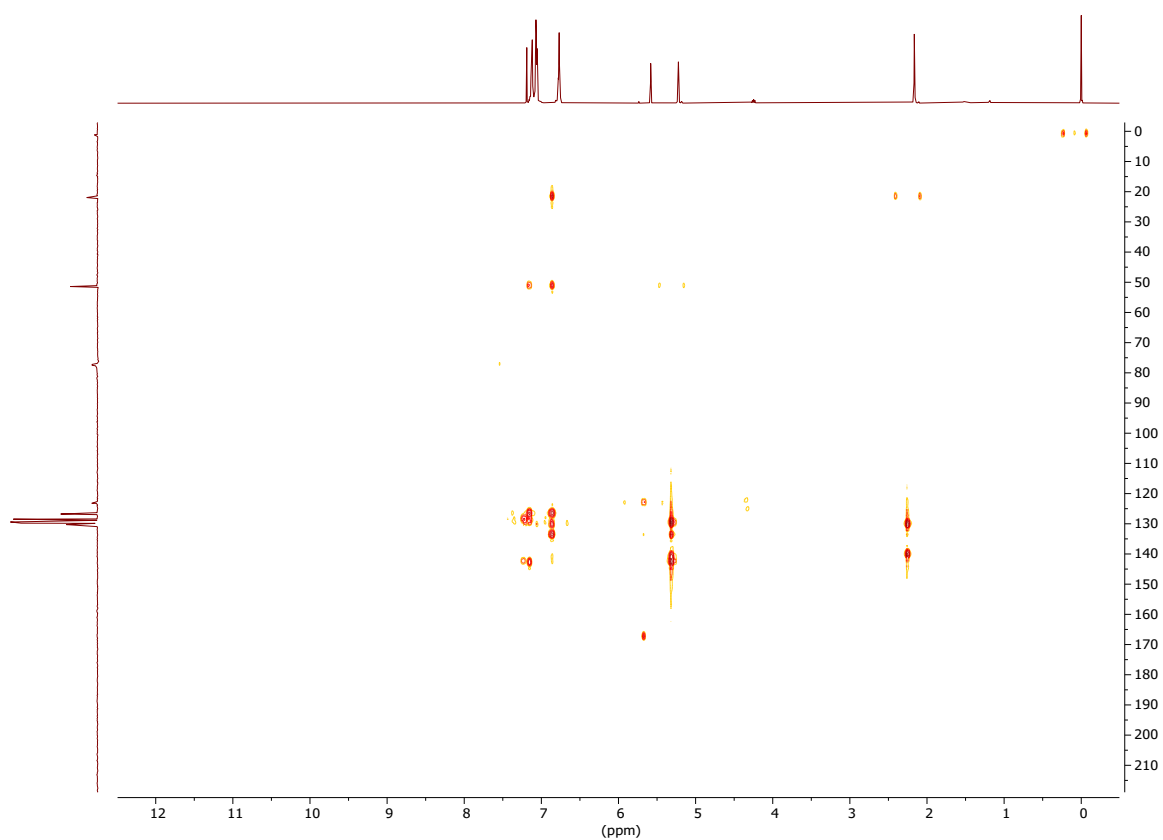
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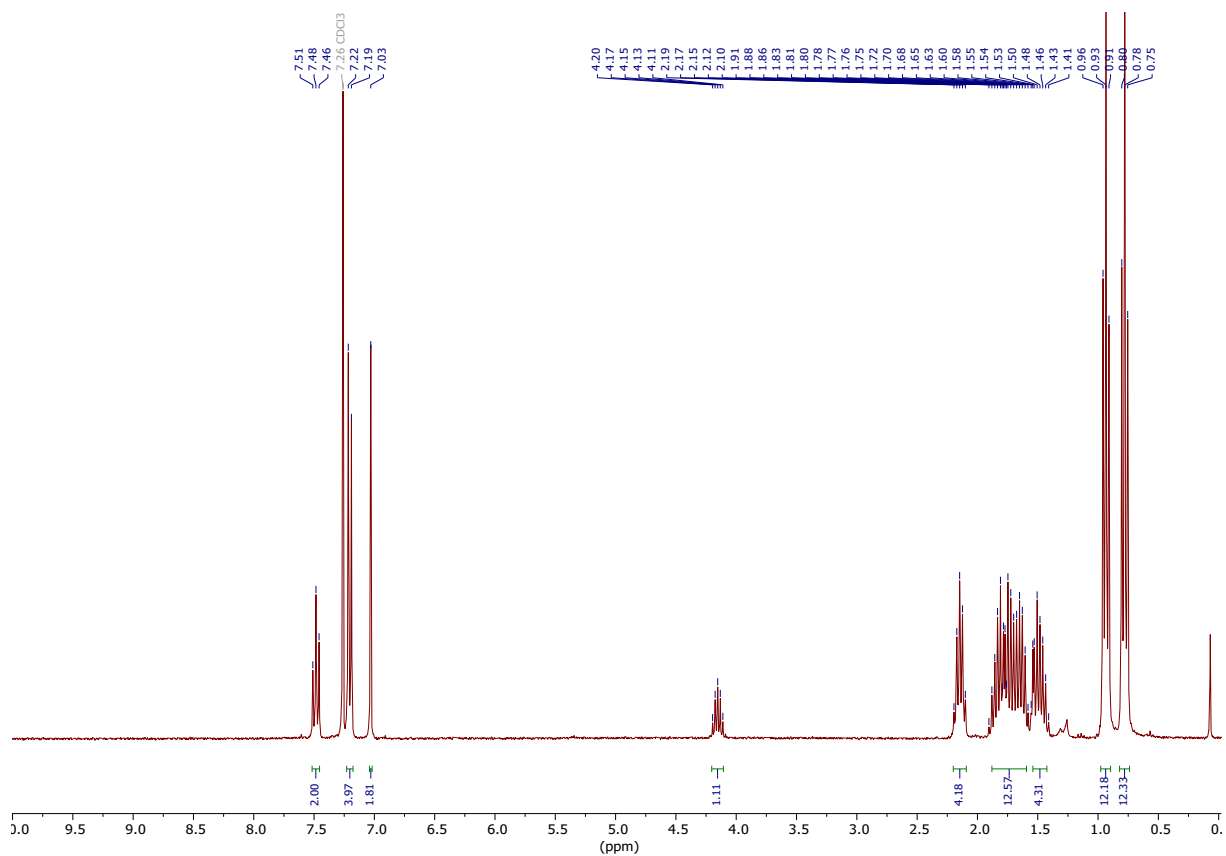
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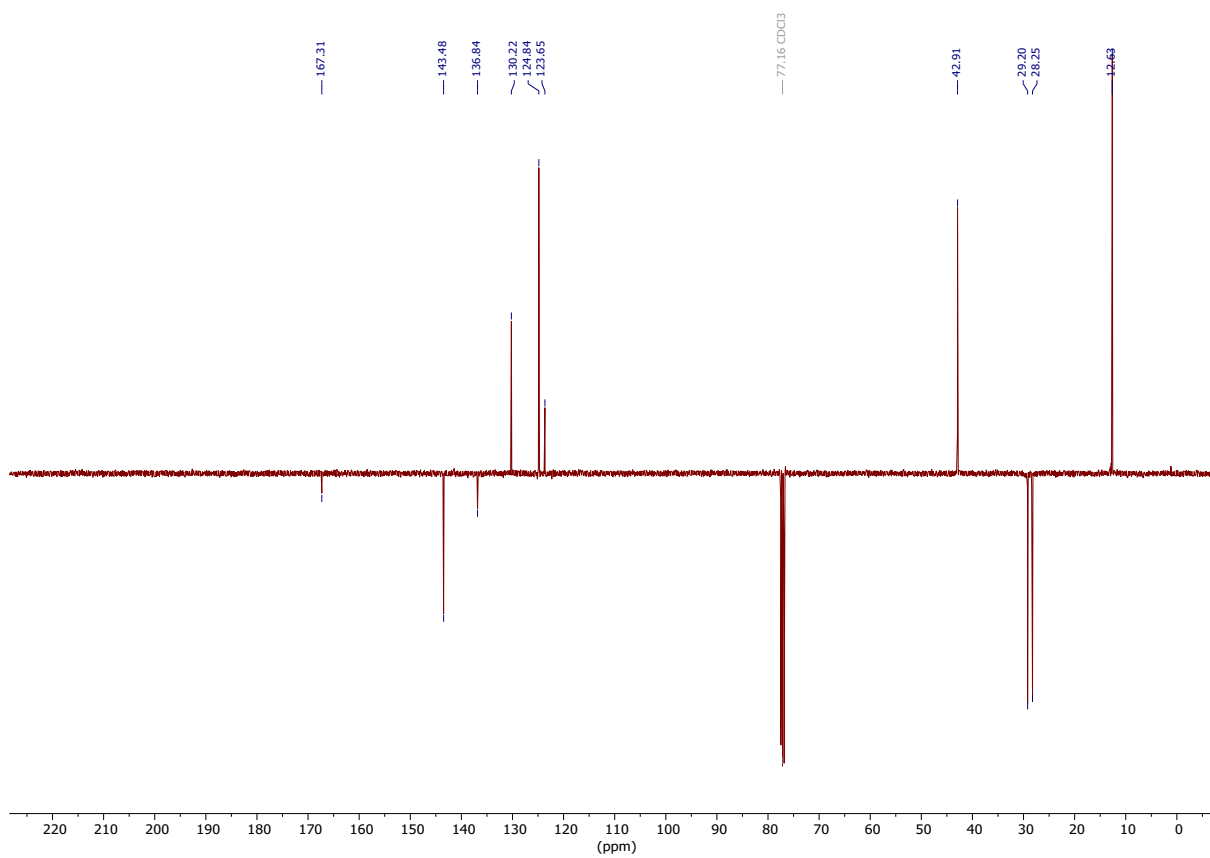
HMBC NMR of 1f



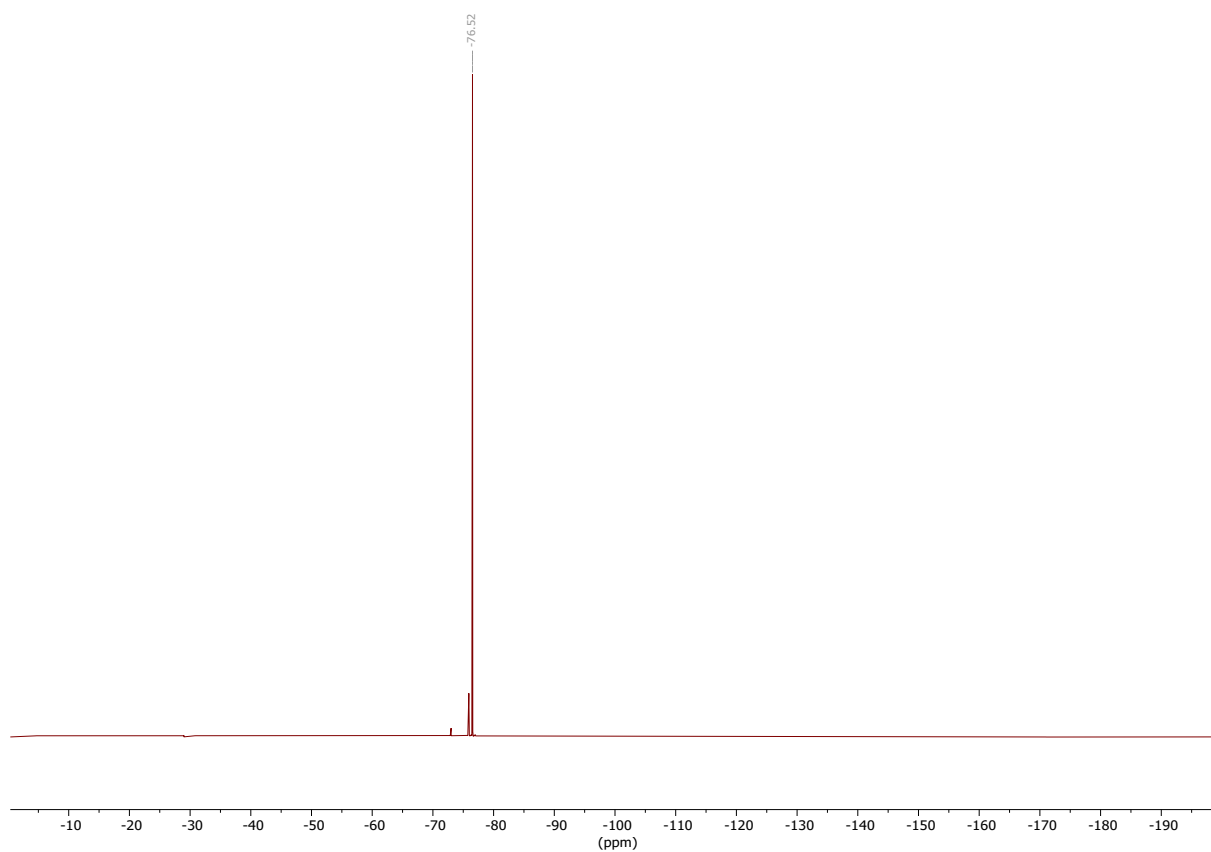
¹H NMR of [Au(IPent)(OCH(CF₃)₂)] (1g)



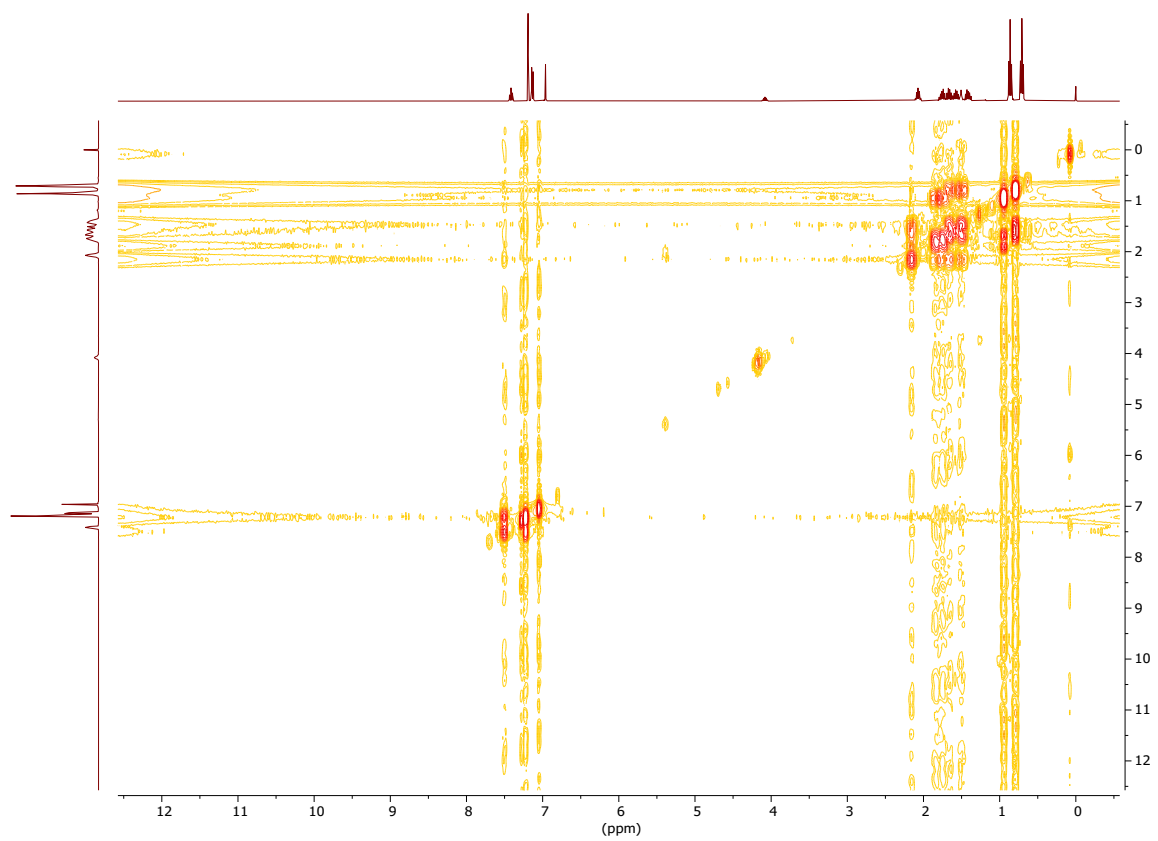
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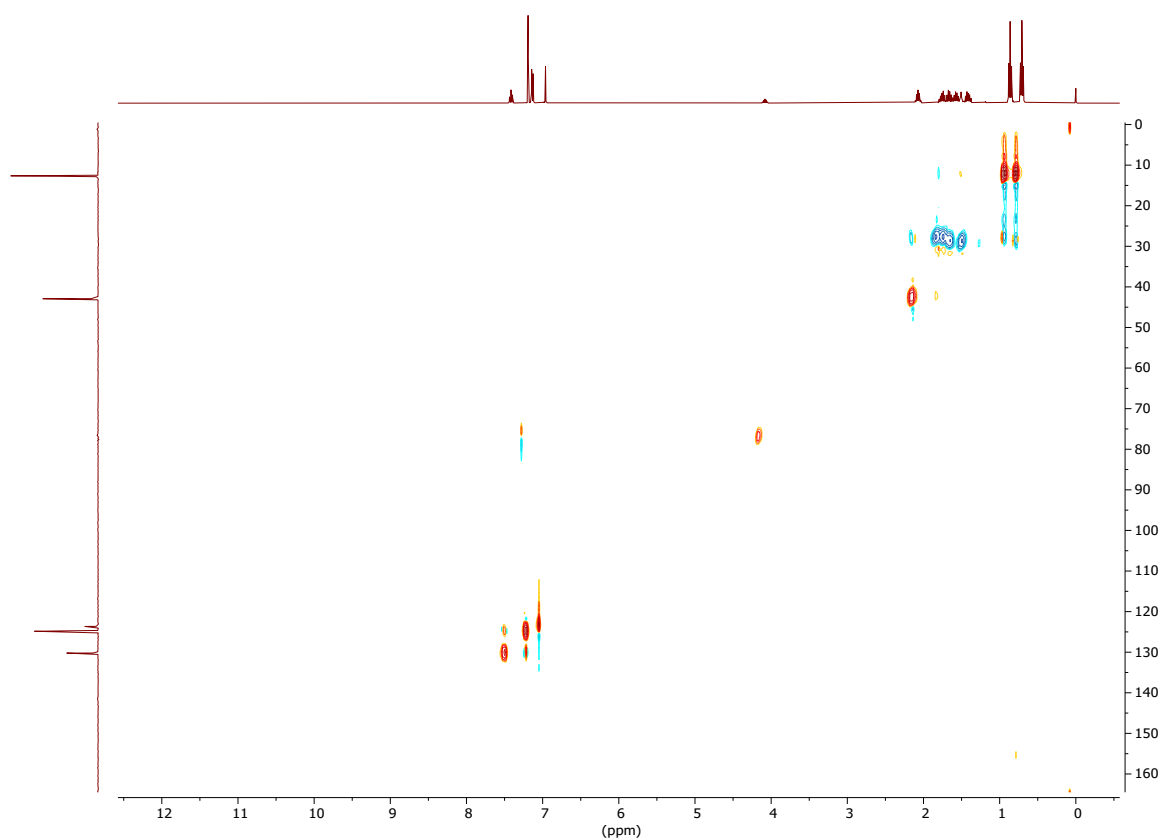
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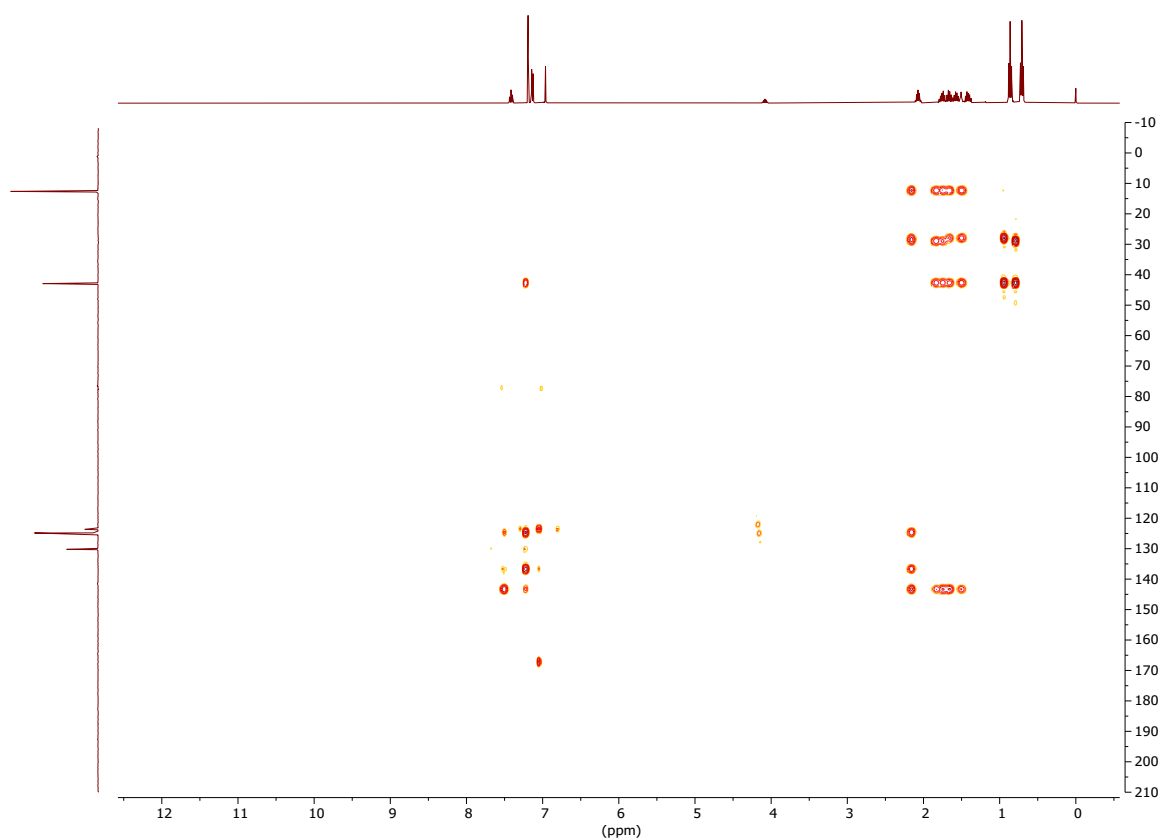
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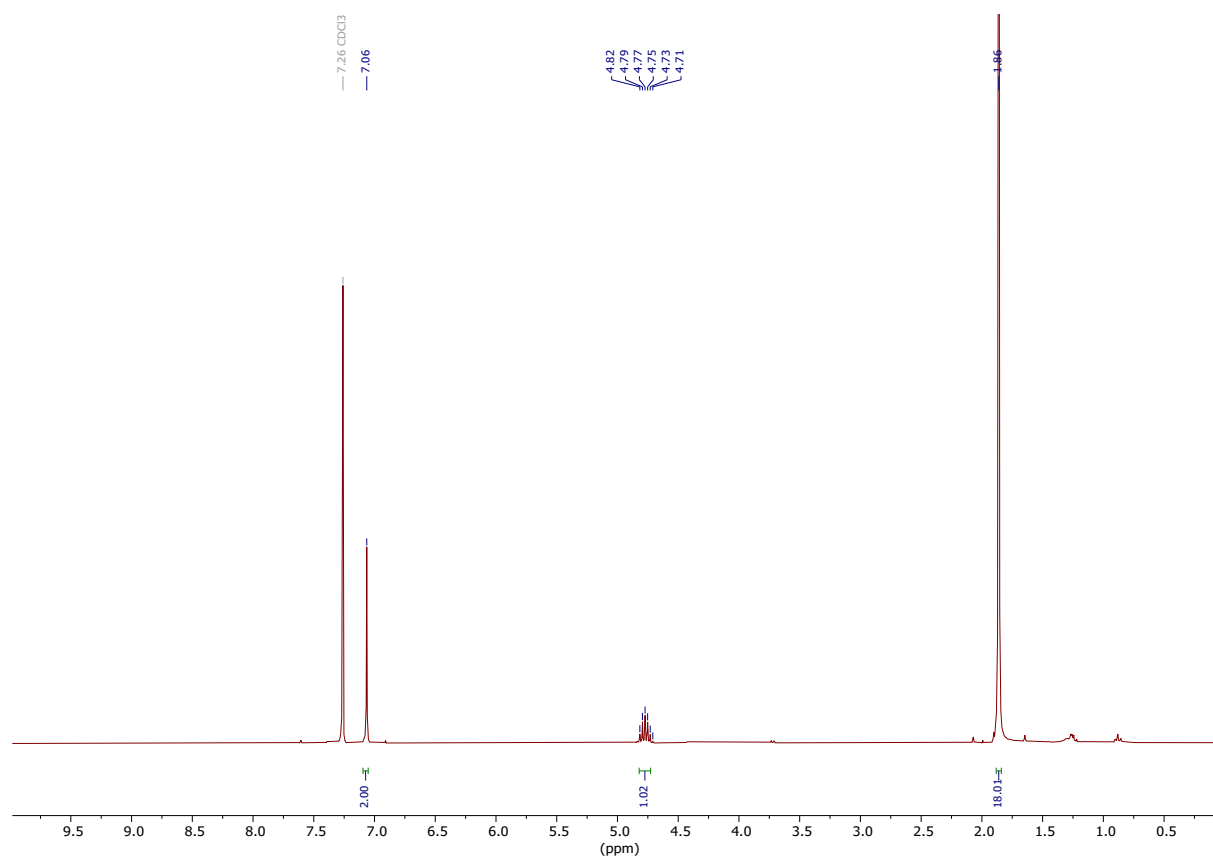
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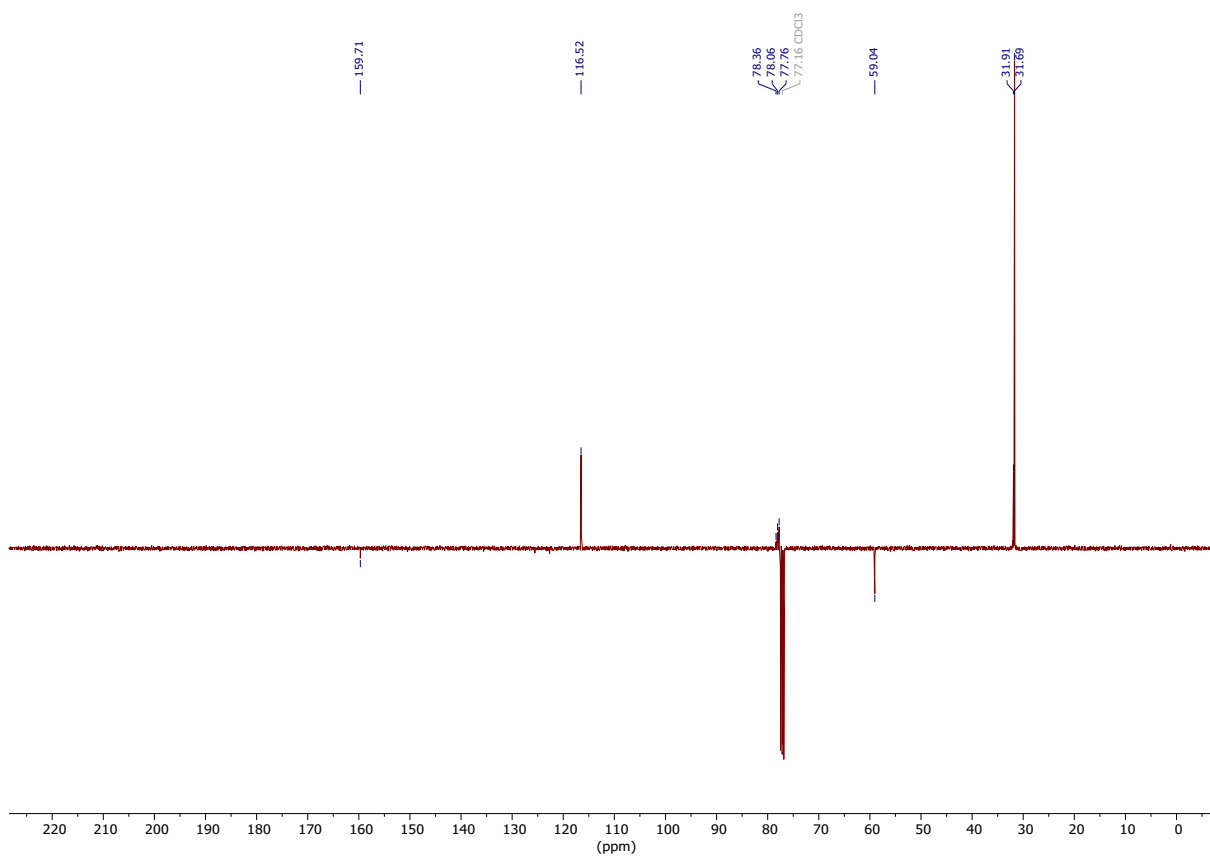
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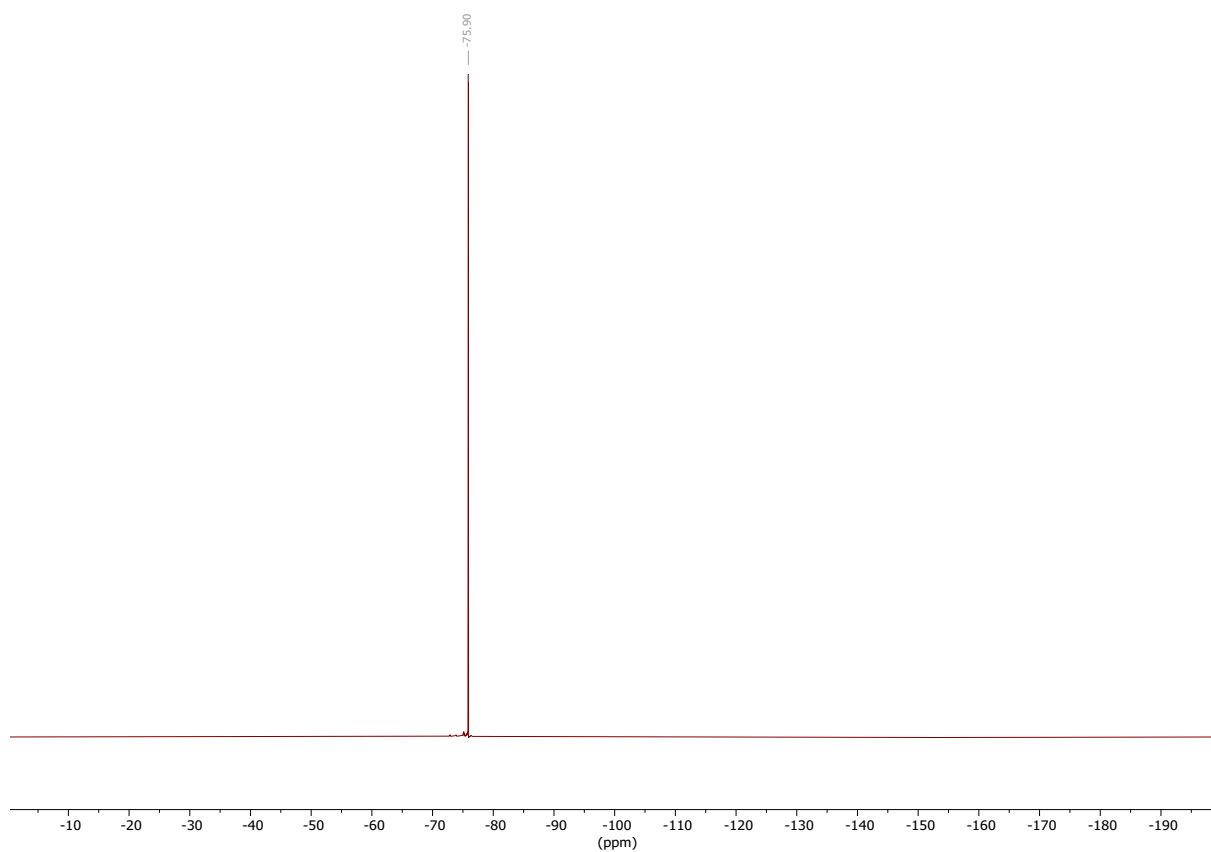
^1H NMR of $[\text{Au}(\text{t}^{\text{Bu}})(\text{OCH}(\text{CF}_3)_2)]$ (1h)



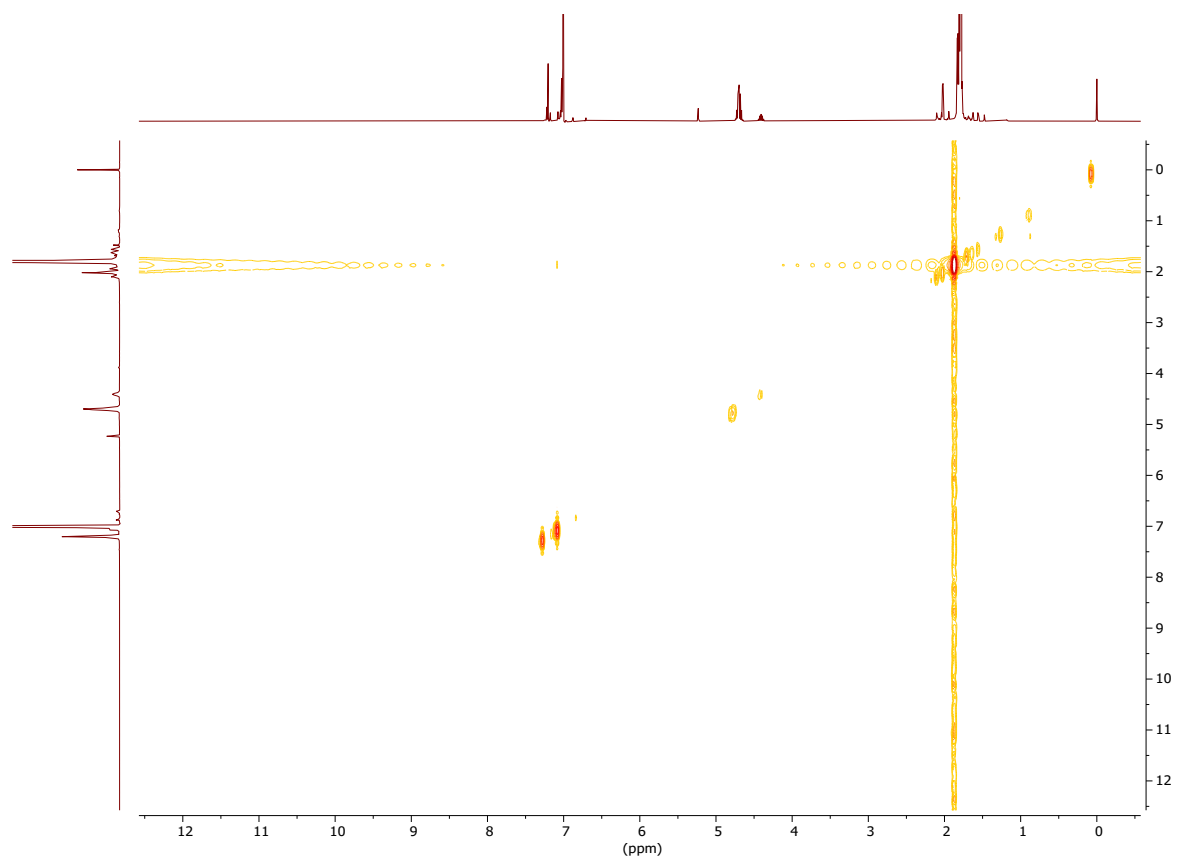
¹³C NMR of 1h



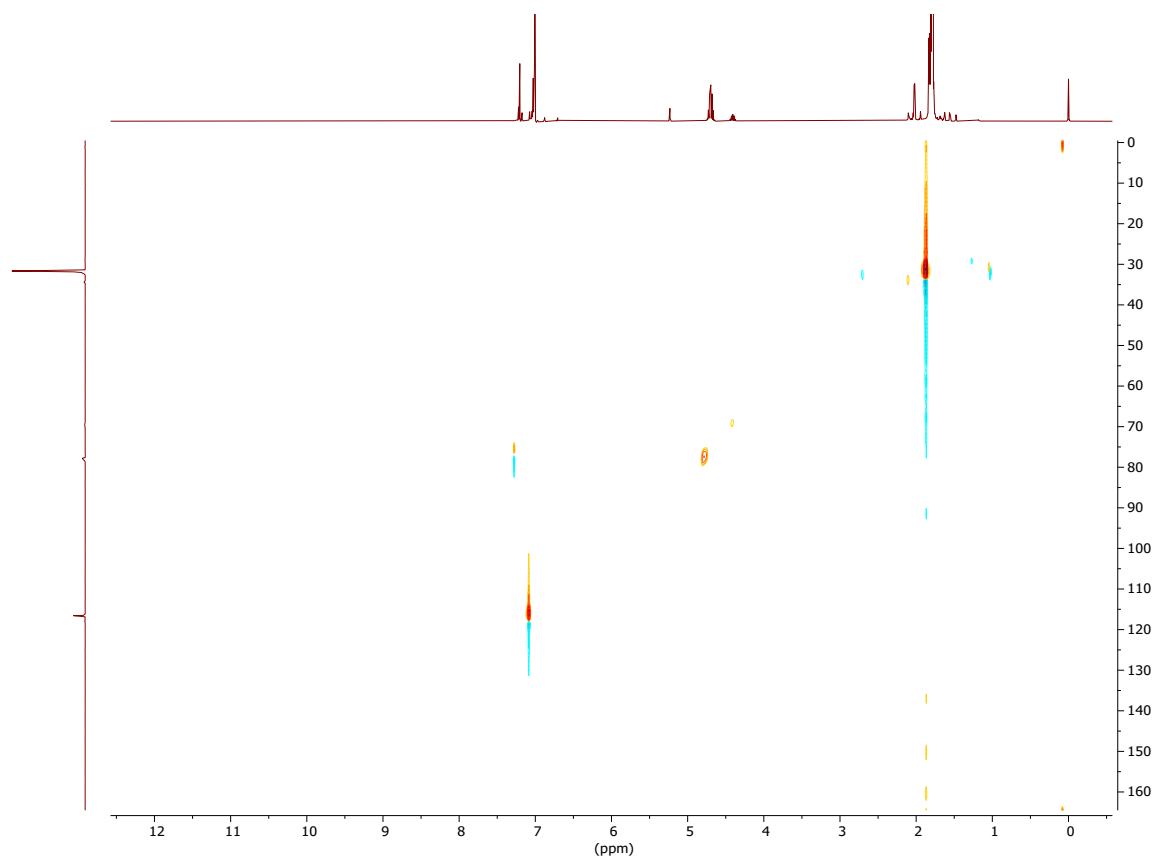
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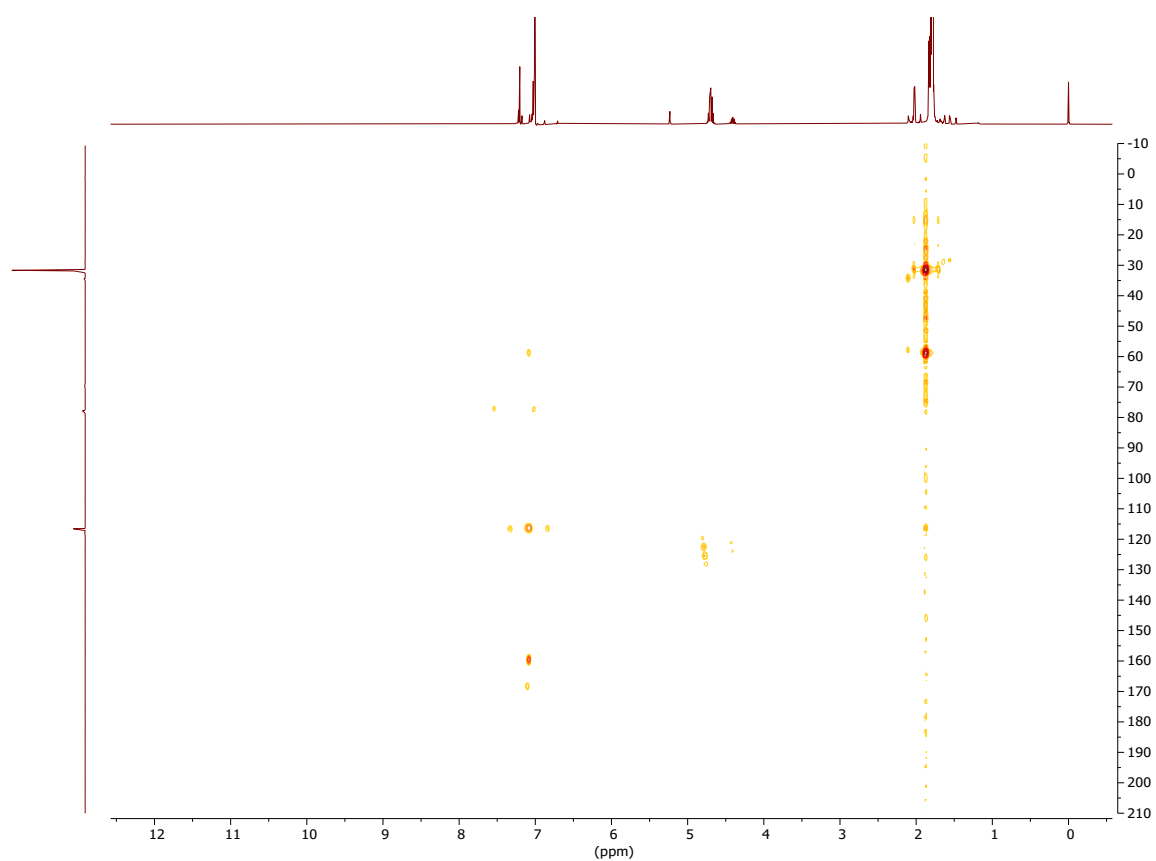
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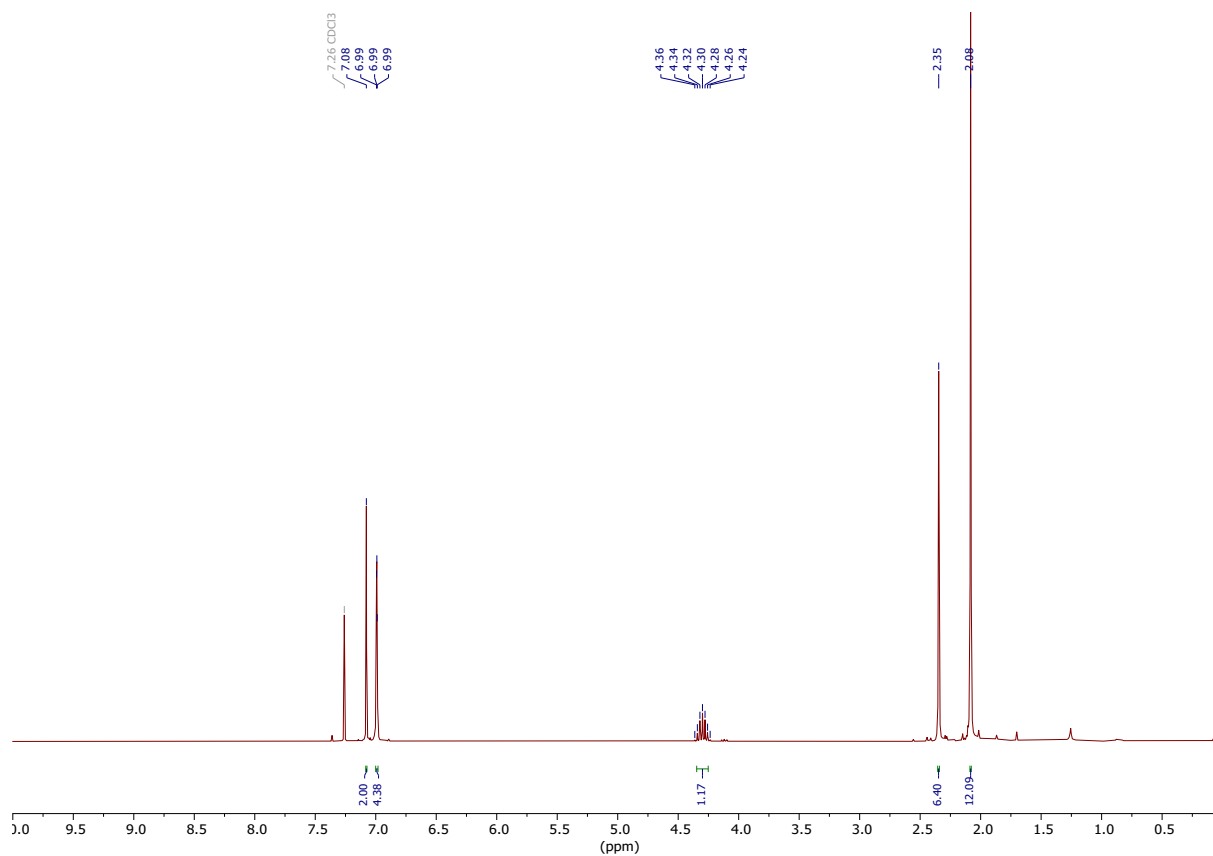
HSQC NMR of 1h



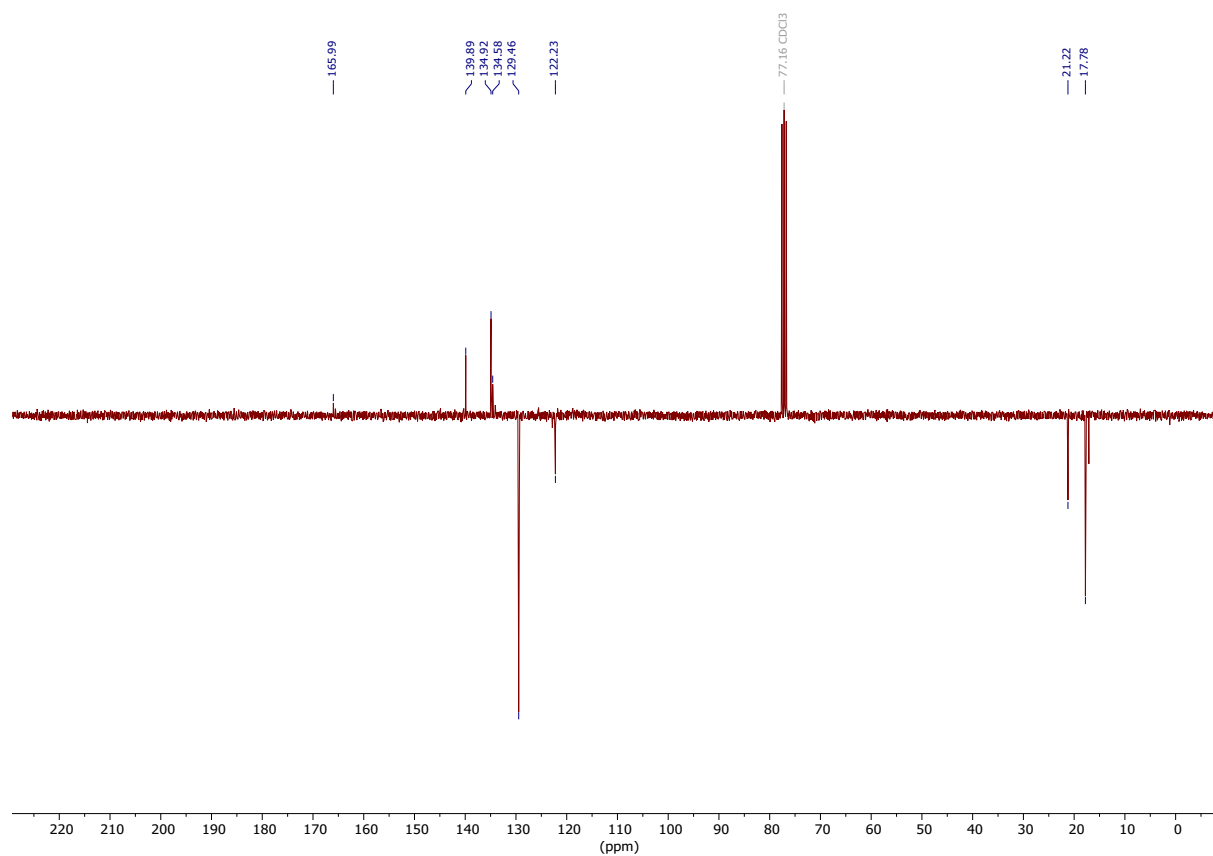
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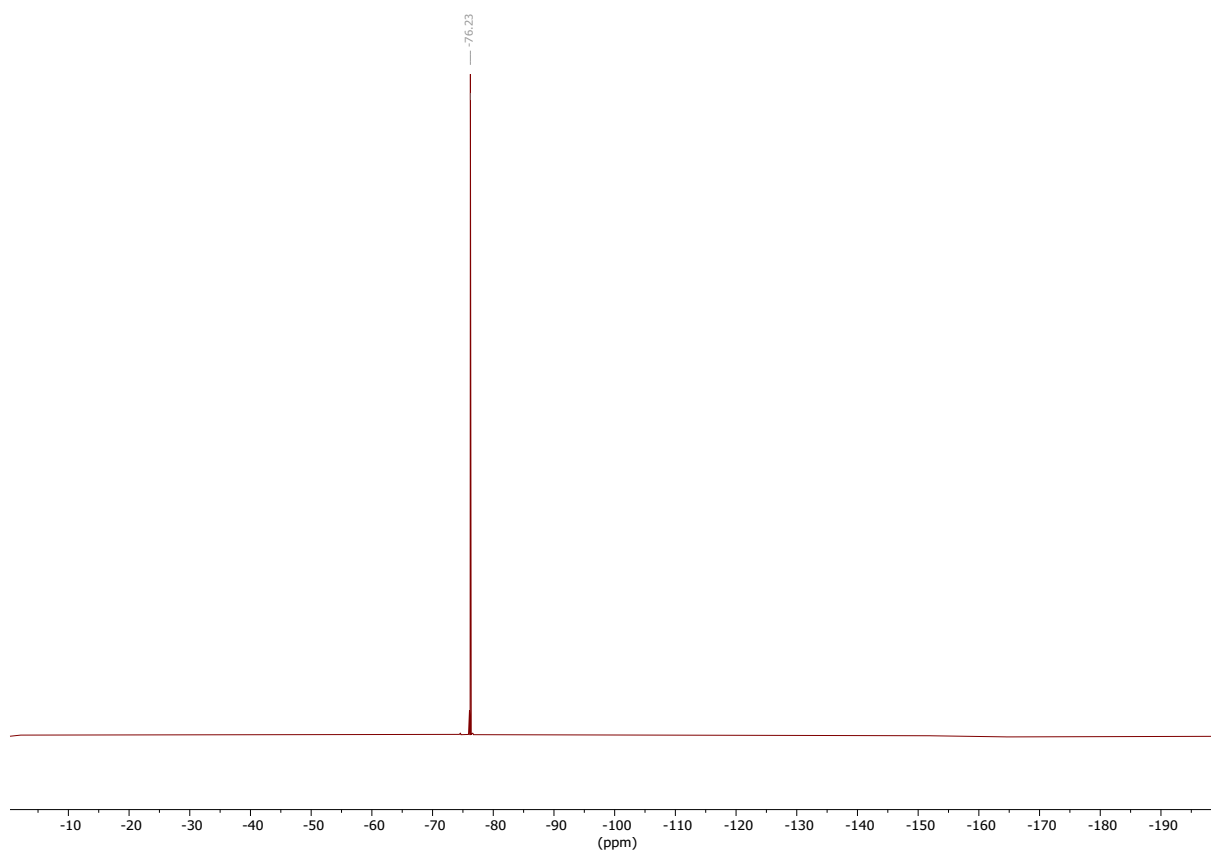
^1H NMR of $[\text{Au}(\text{IMes})(\text{OCH}(\text{CF}_3)_2)]$ (1i)



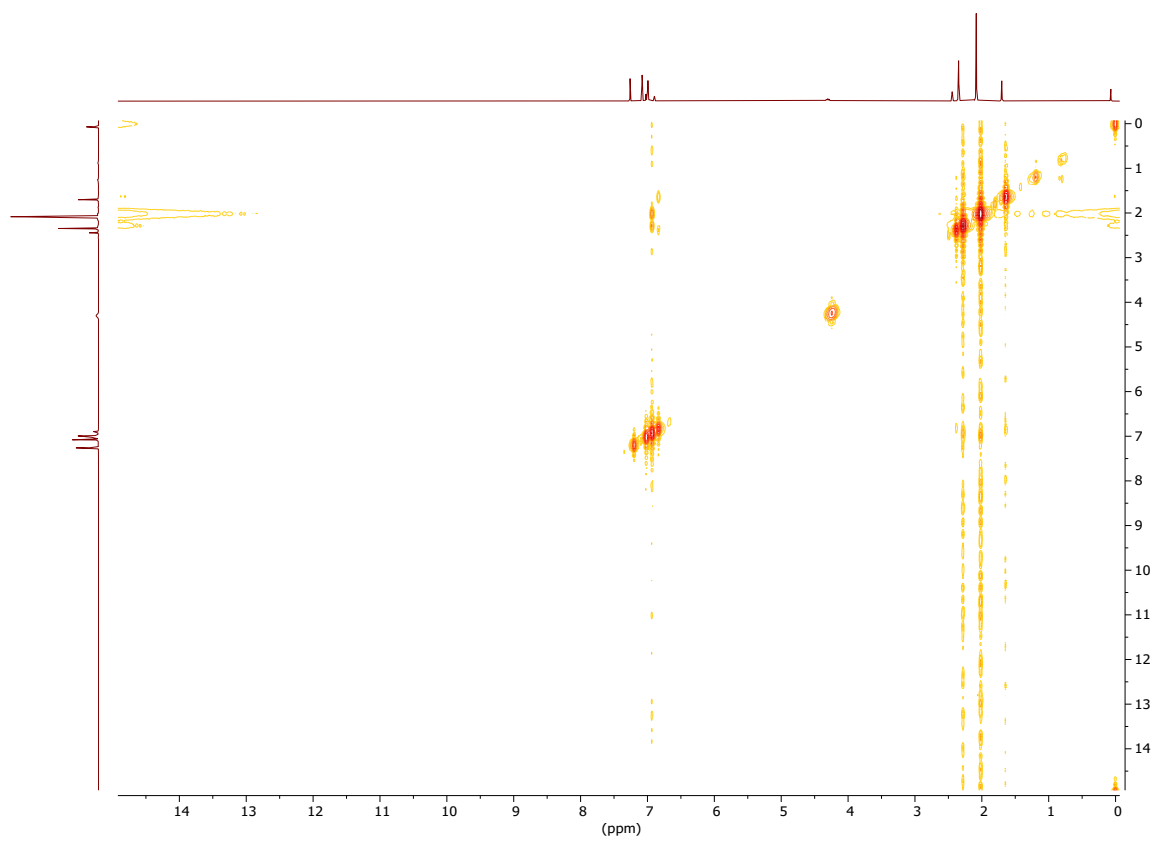
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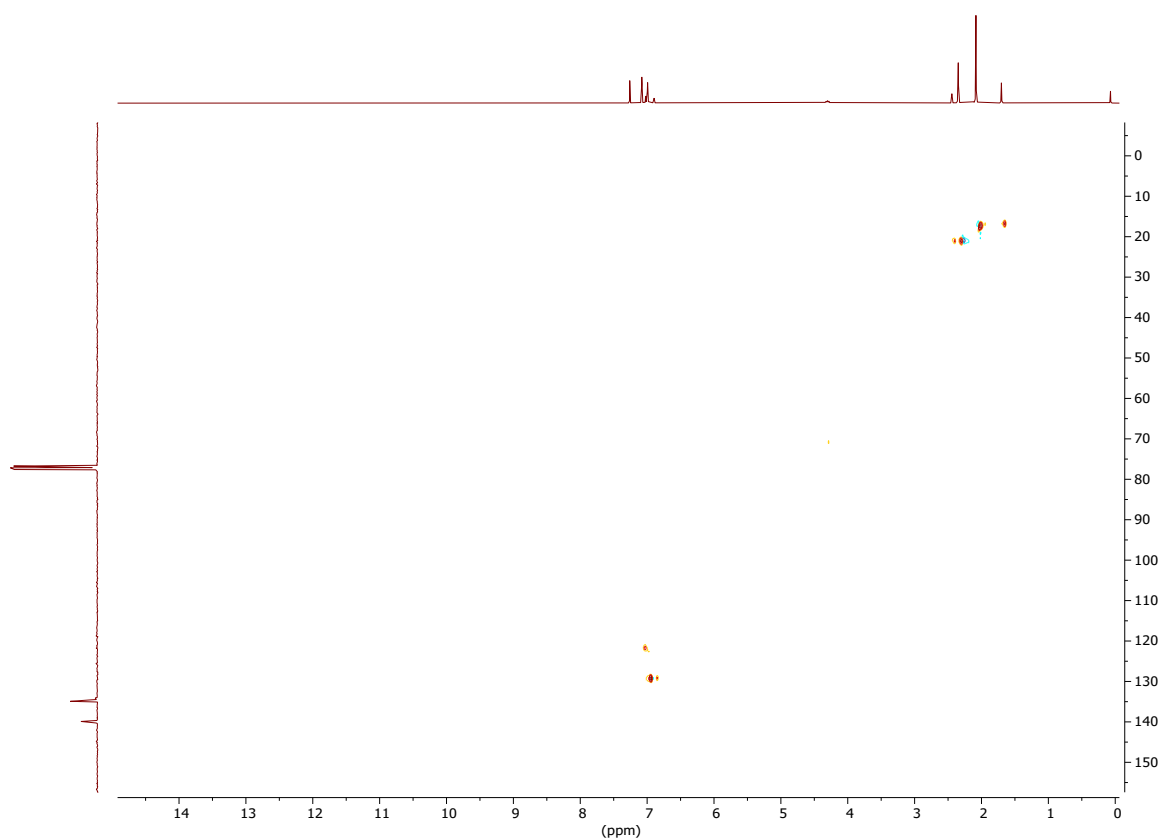
^{19}F NMR of **1i**



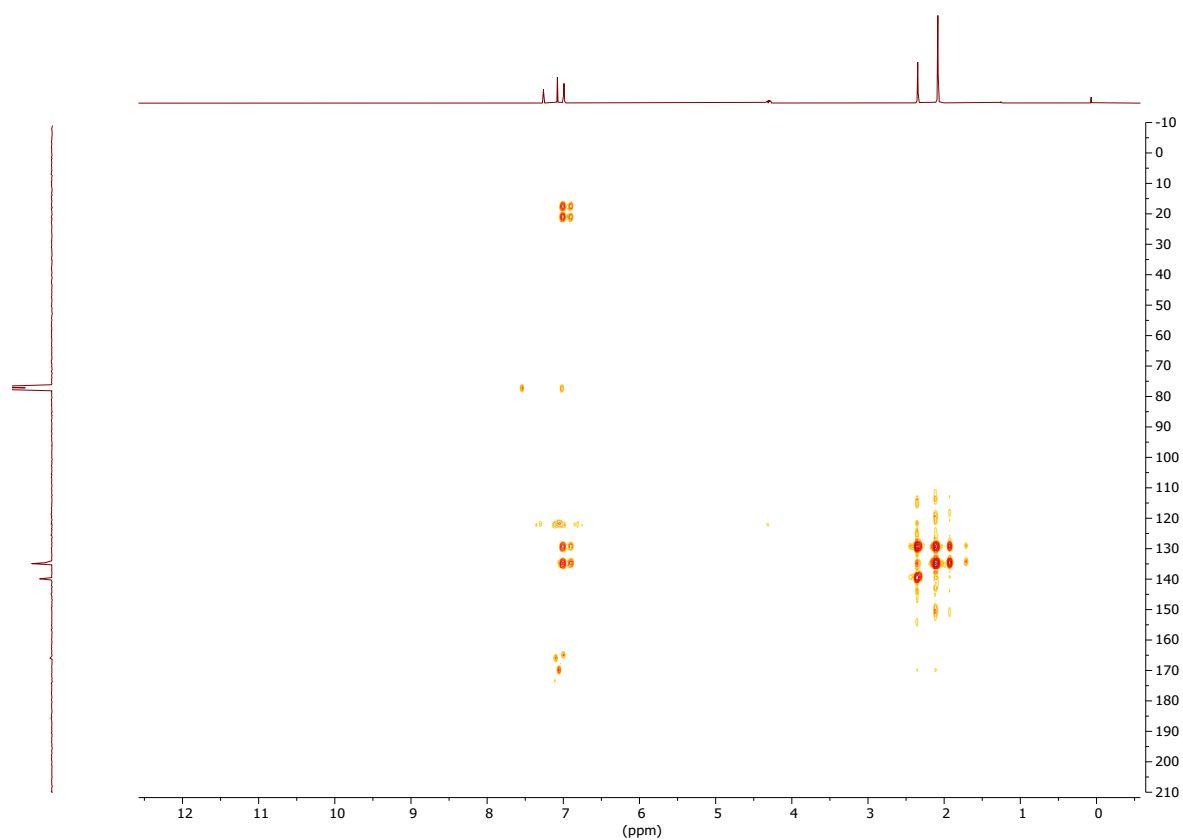
COSY NMR of 1i



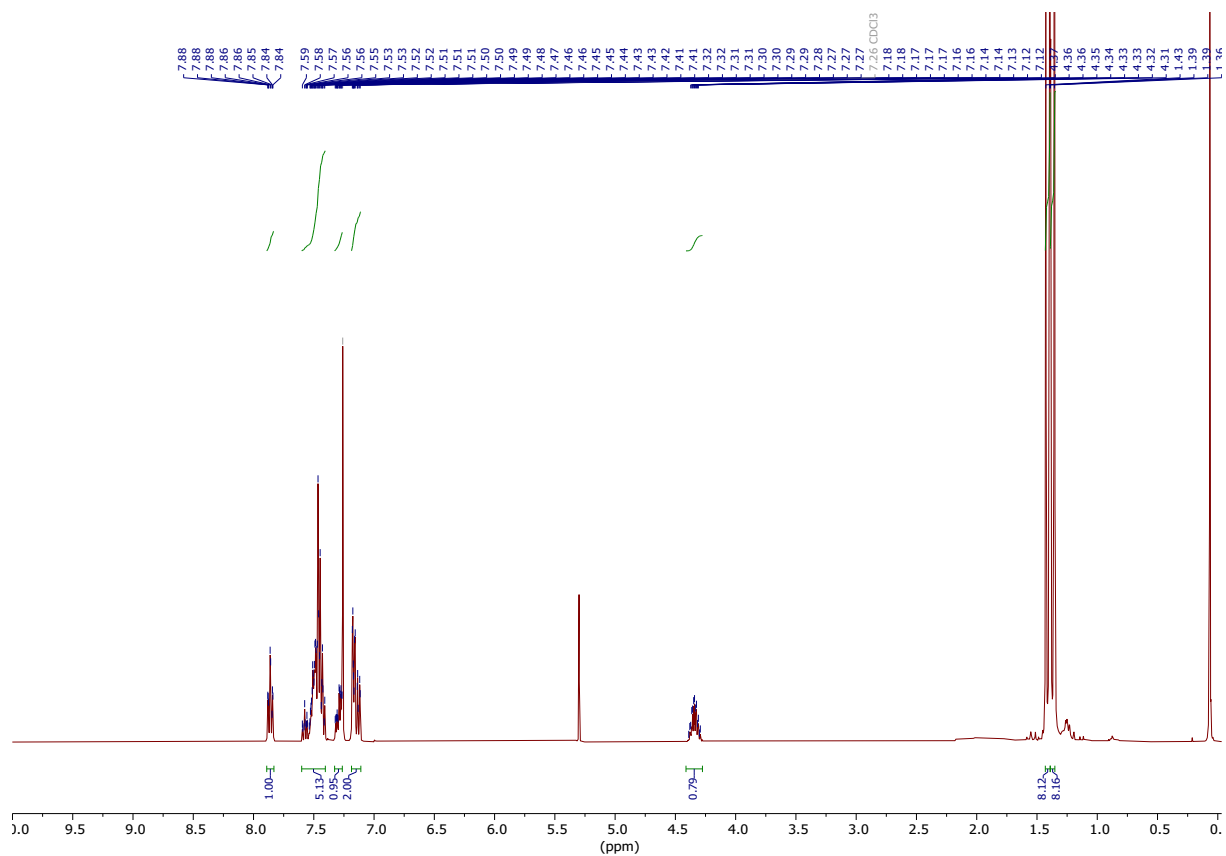
HSQC NMR of 1i



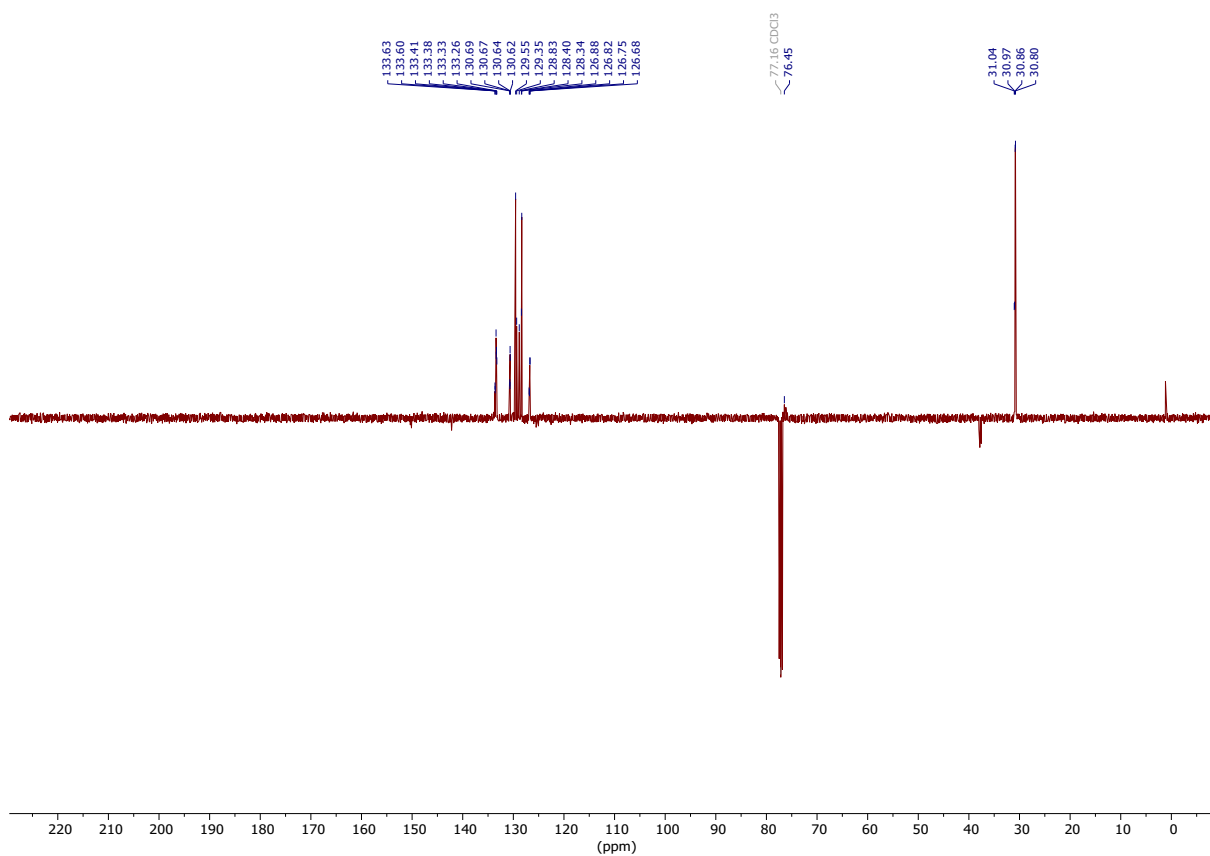
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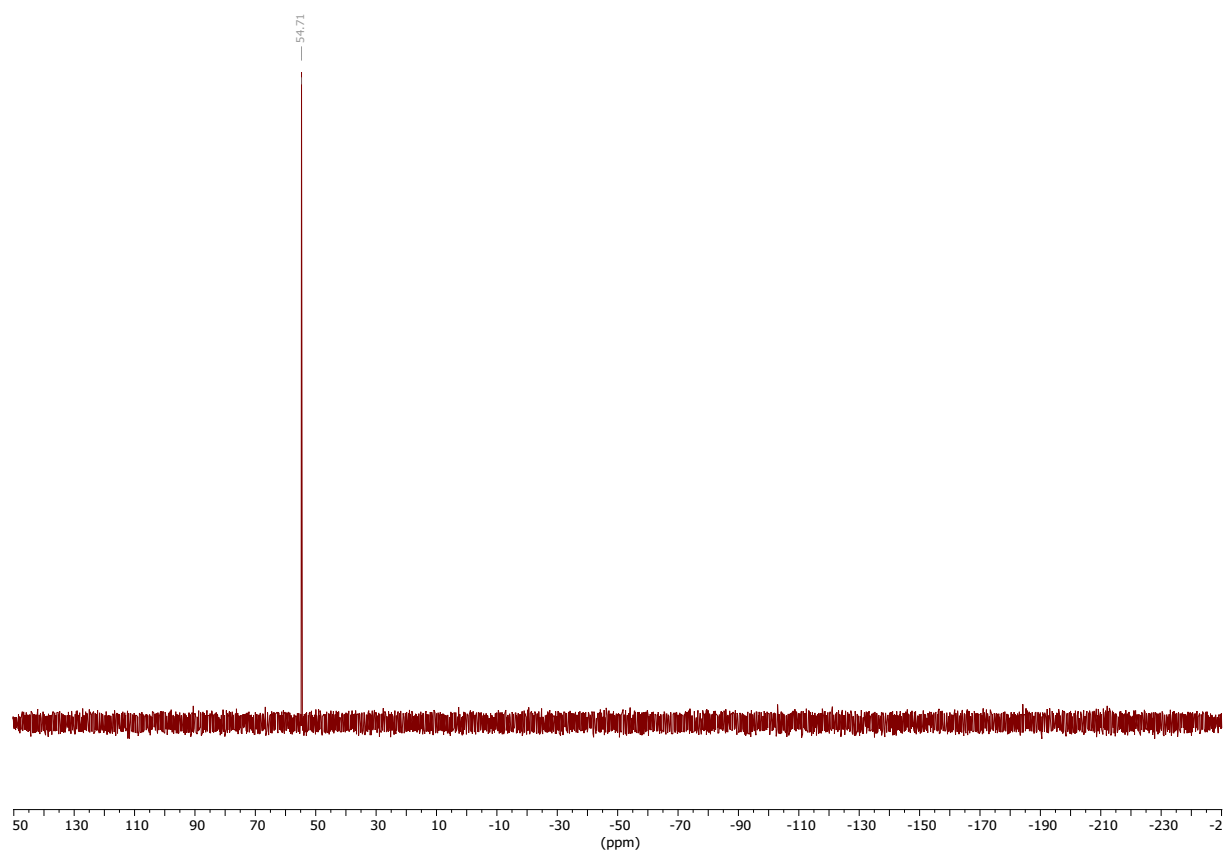
¹H NMR of [Au(JohnPhos)(OCH(CF₃)₂)] (1j)



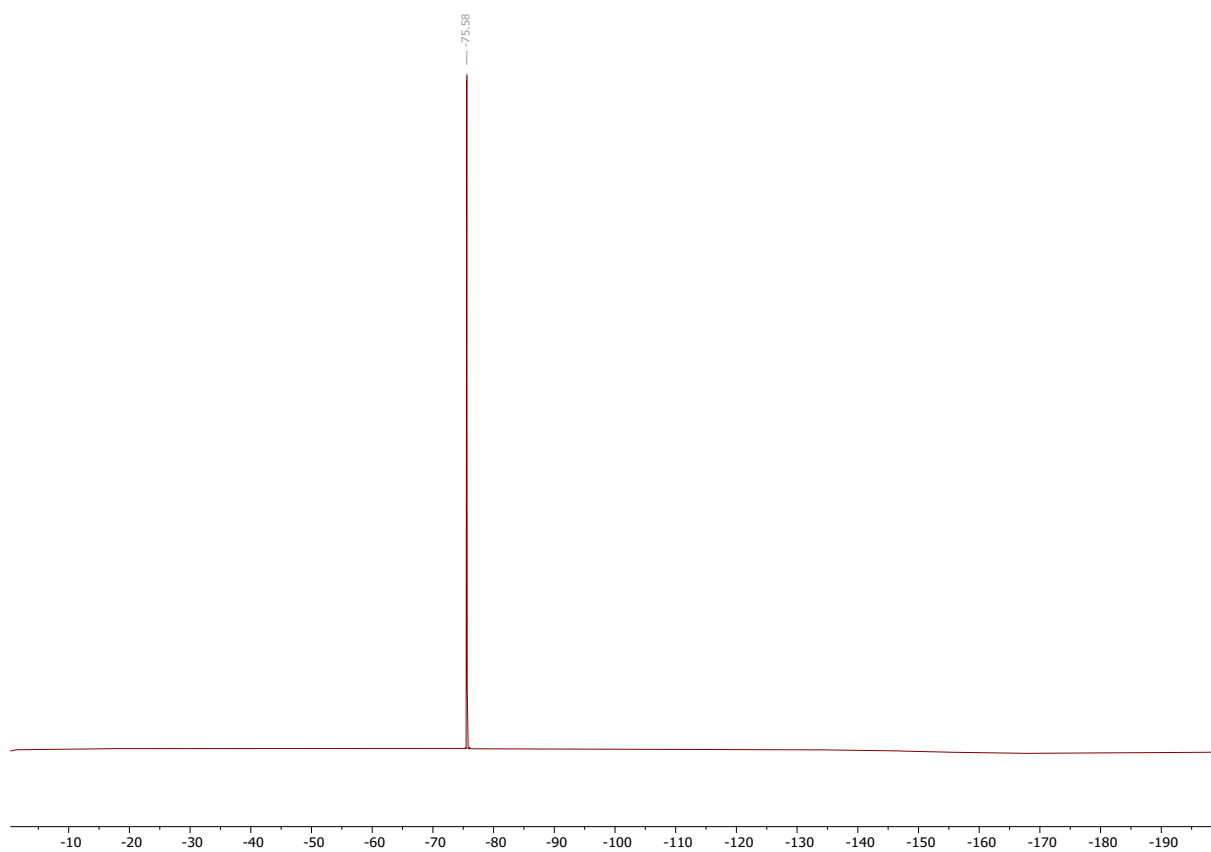
¹³C NMR of 1j



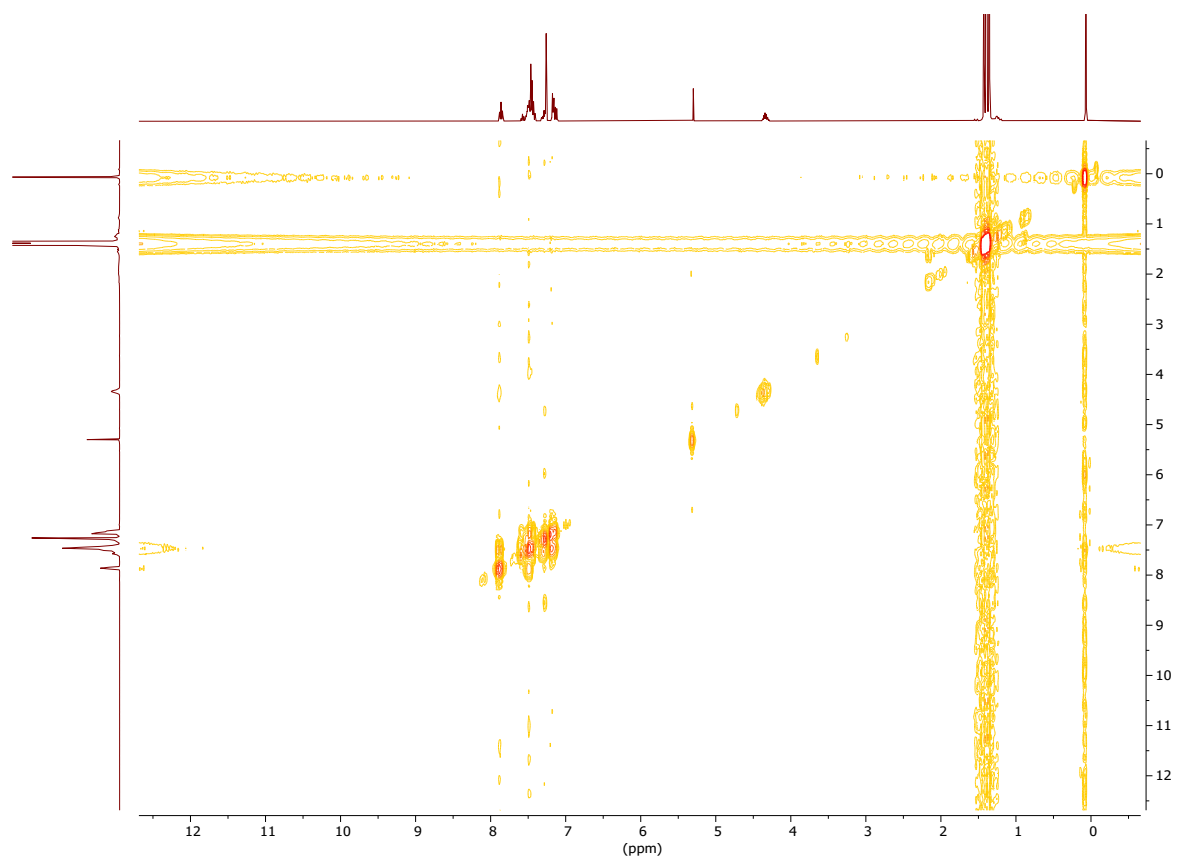
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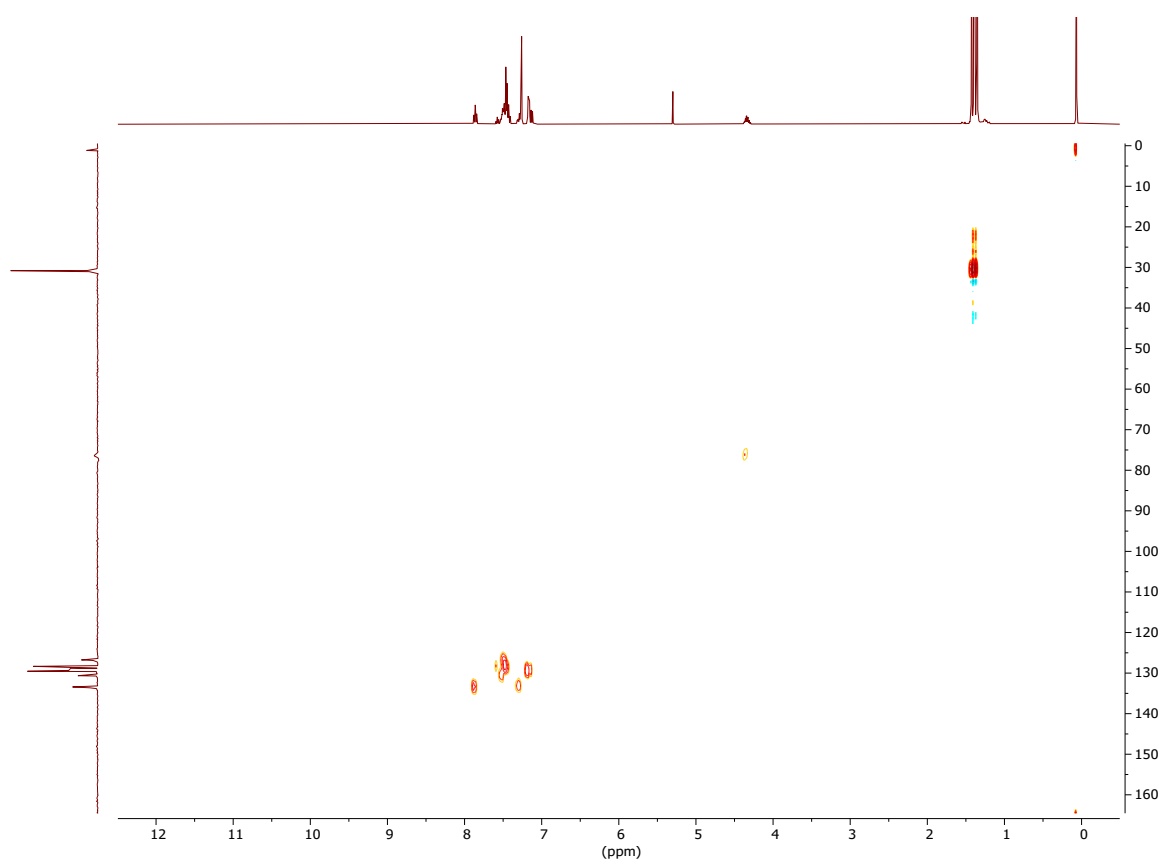
^{19}F NMR of 1j



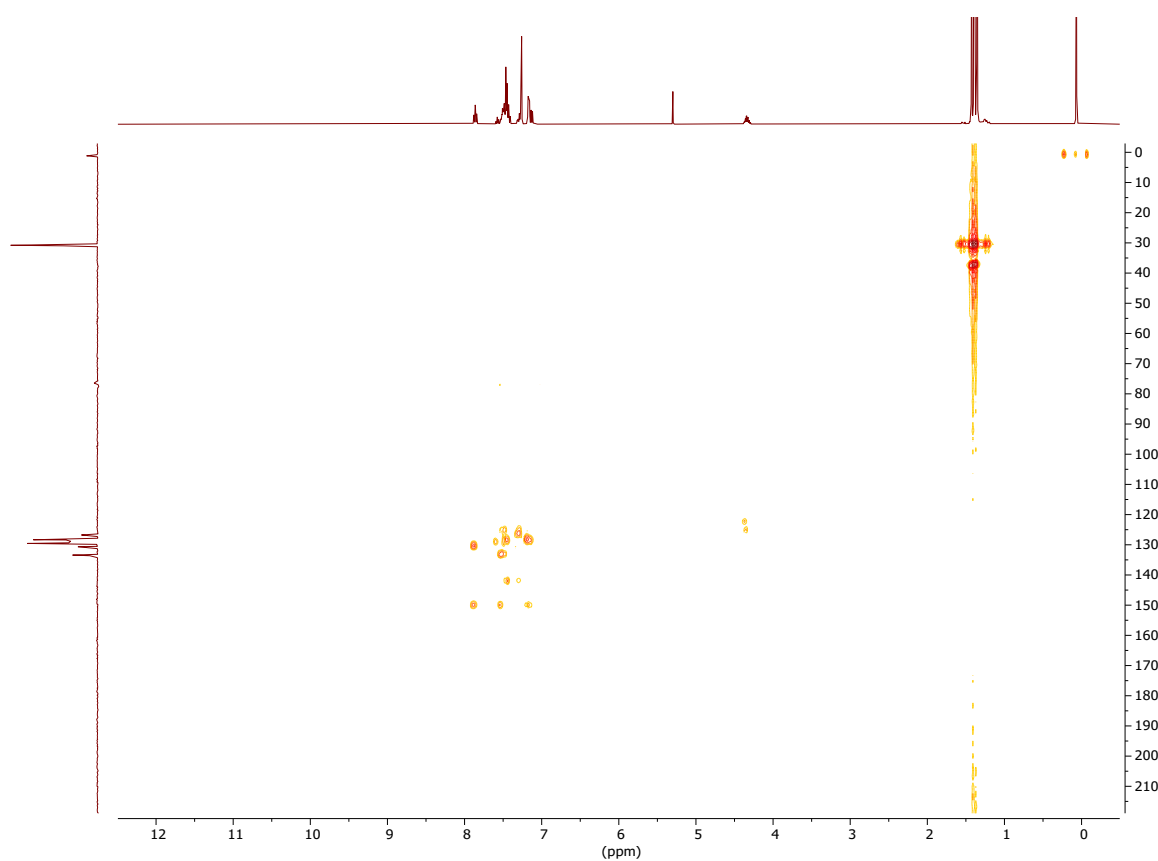
COSY NMR of 1j



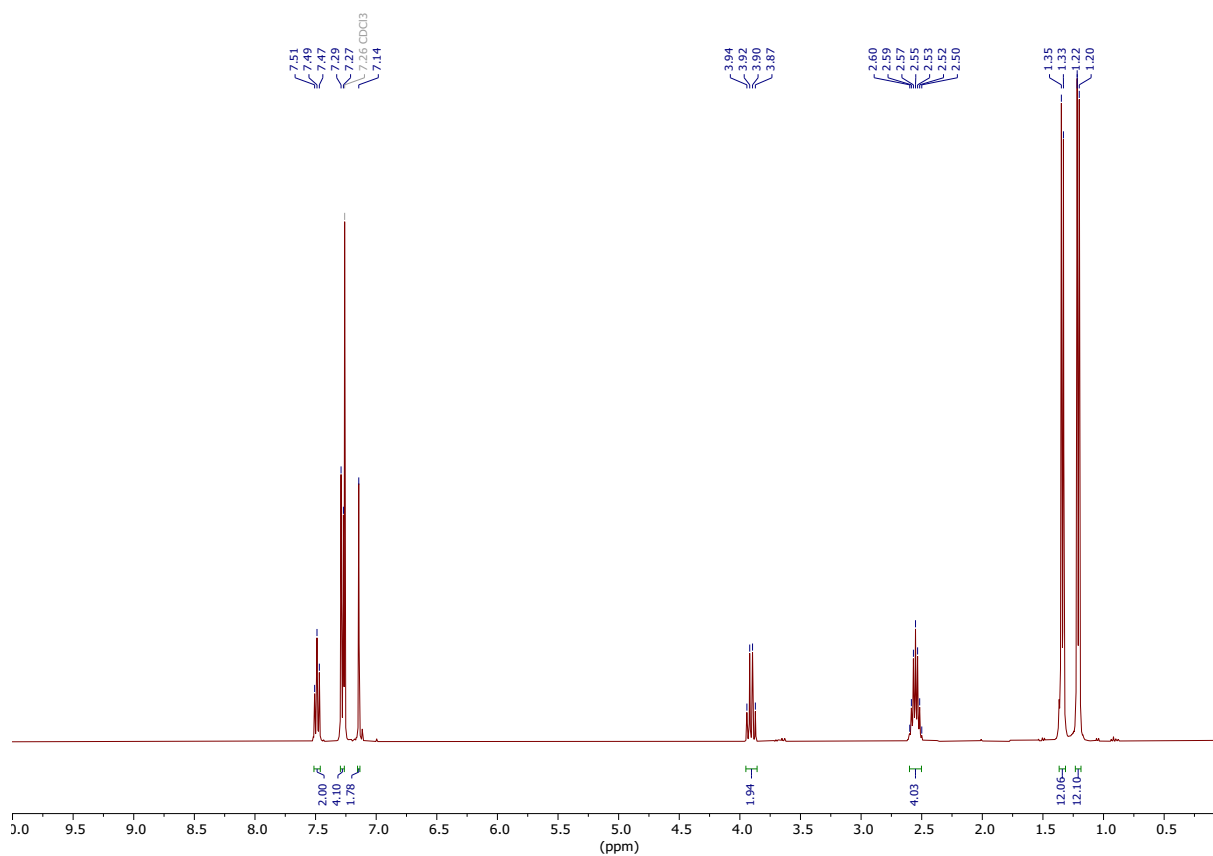
HSQC NMR of 1j



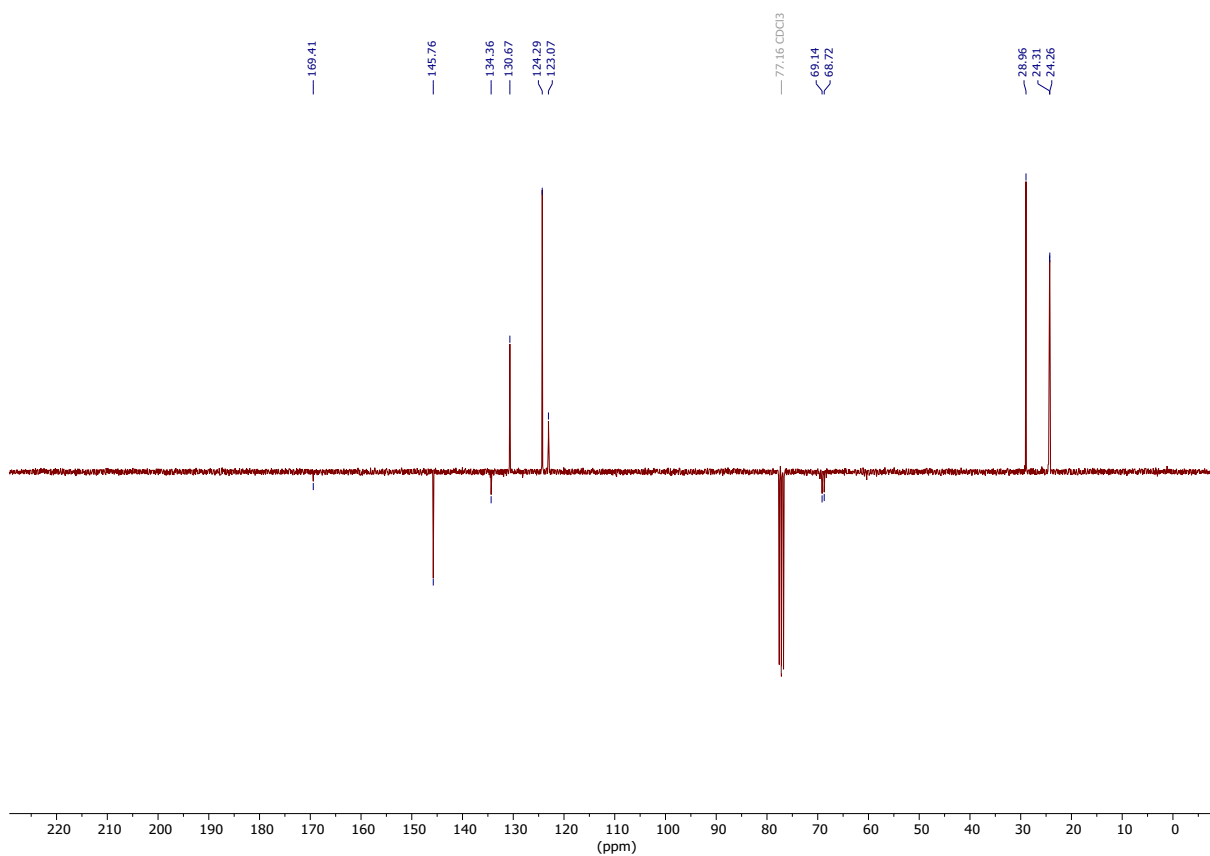
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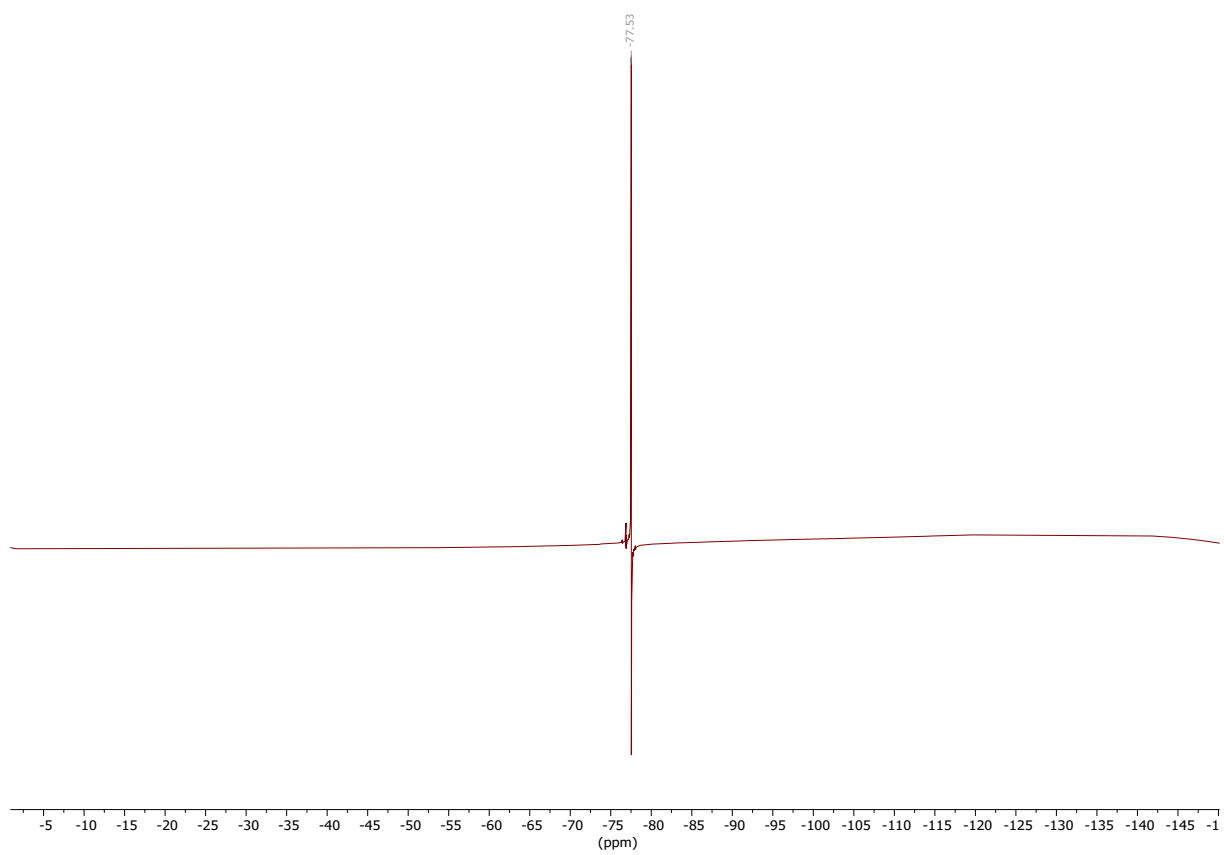
^1H NMR of $[\text{Au}(\text{IPr})(\text{OCH}_2\text{CF}_3)]$ (**2a**)



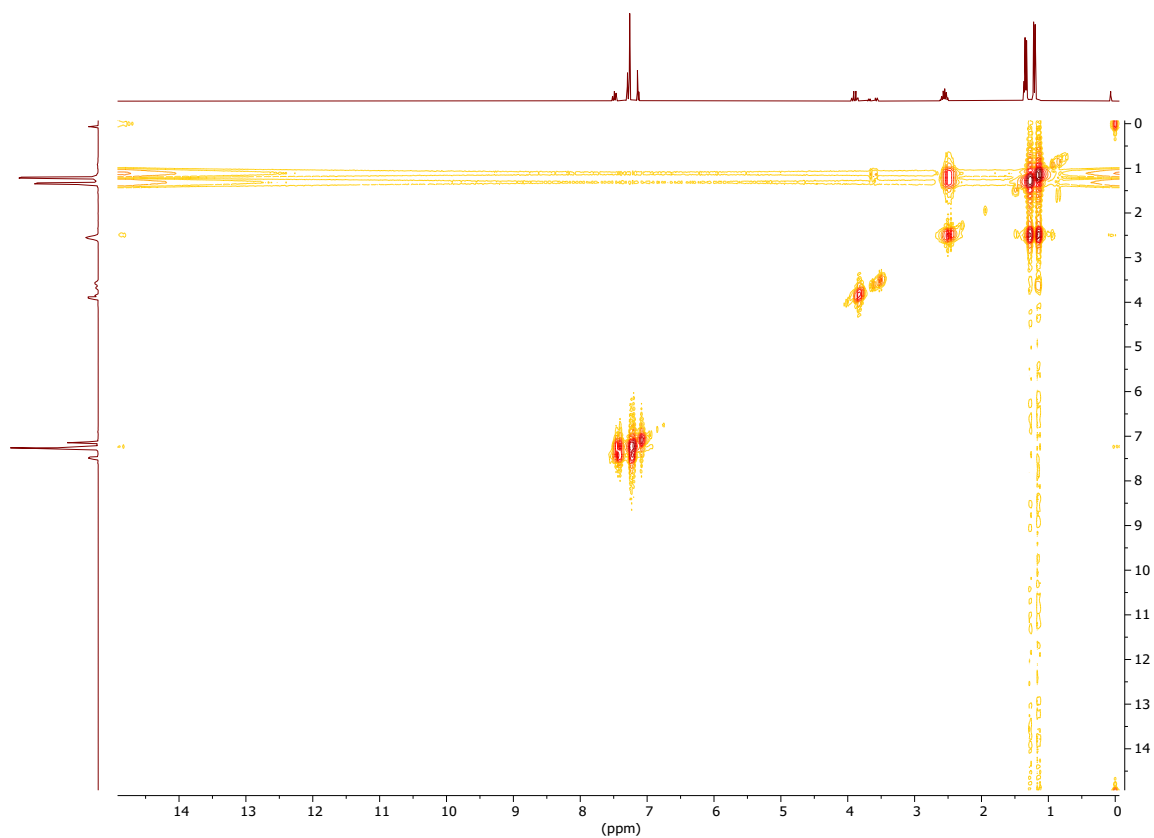
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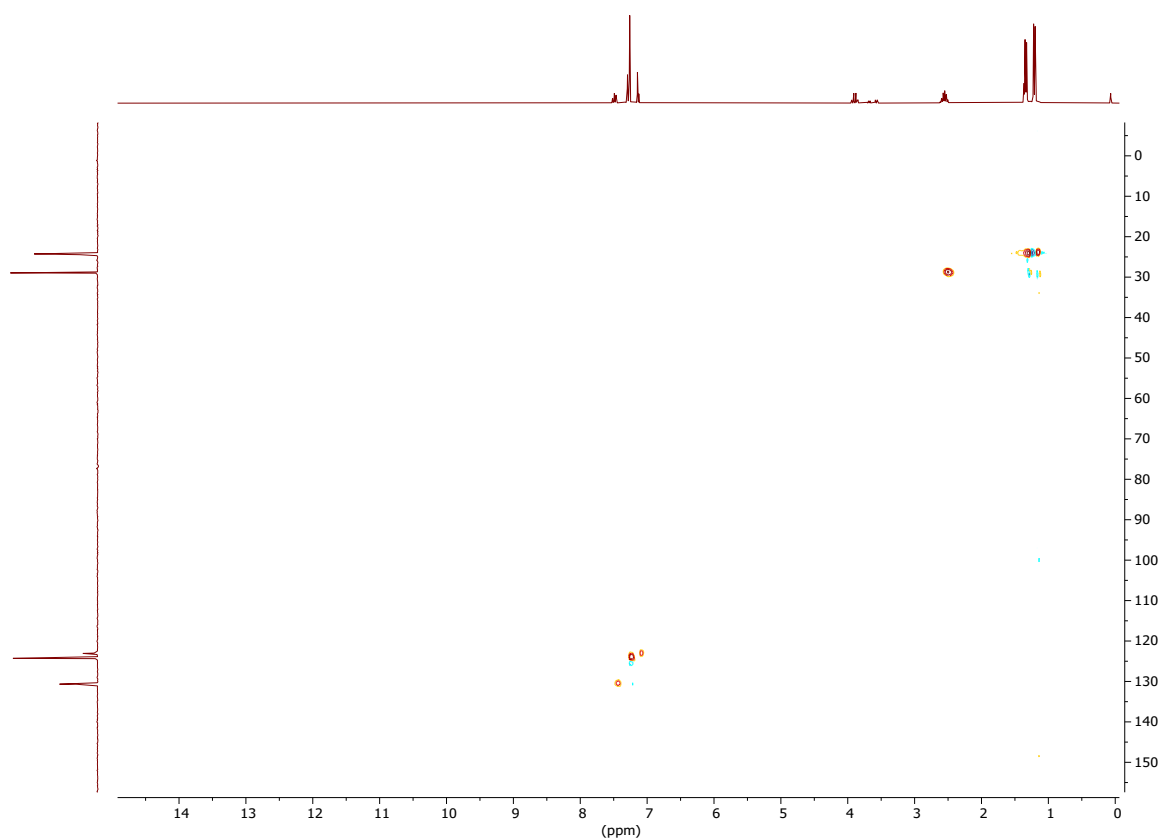
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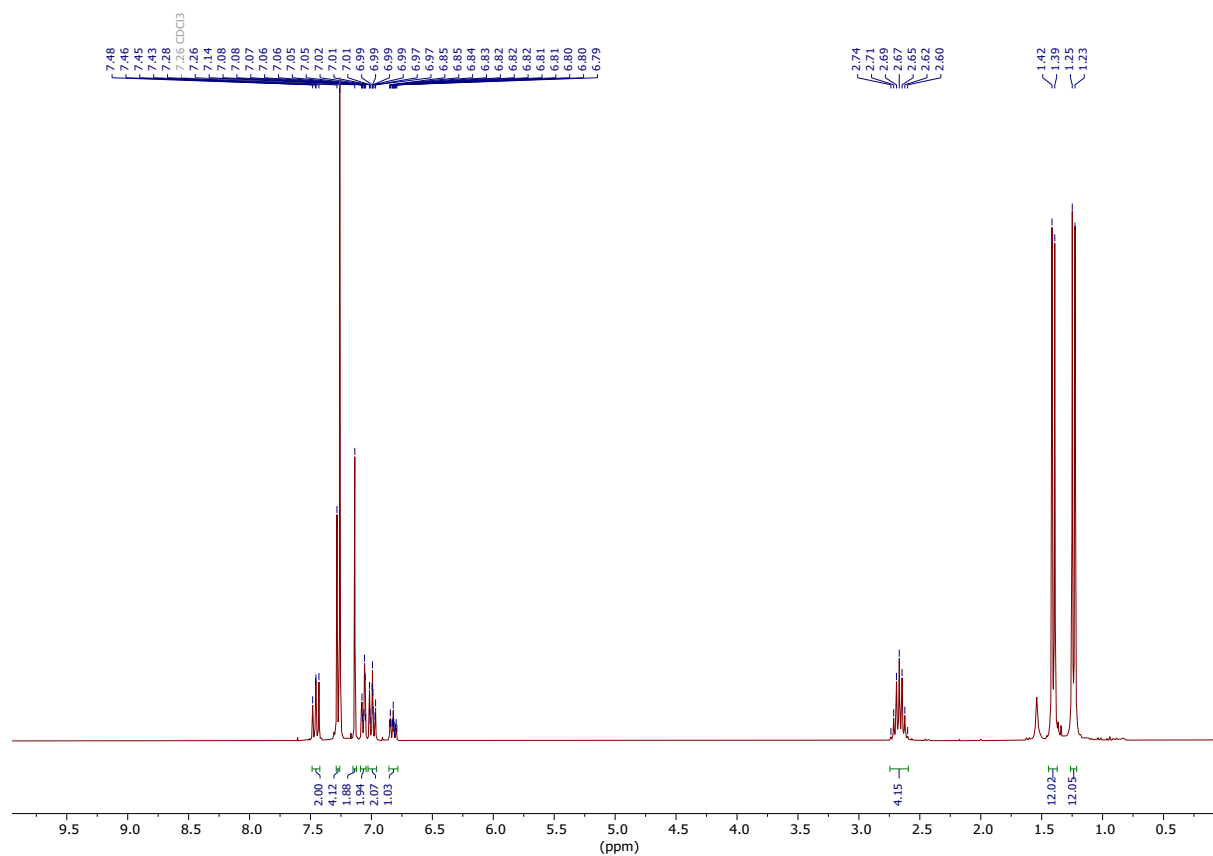
COSY NMR of 2a



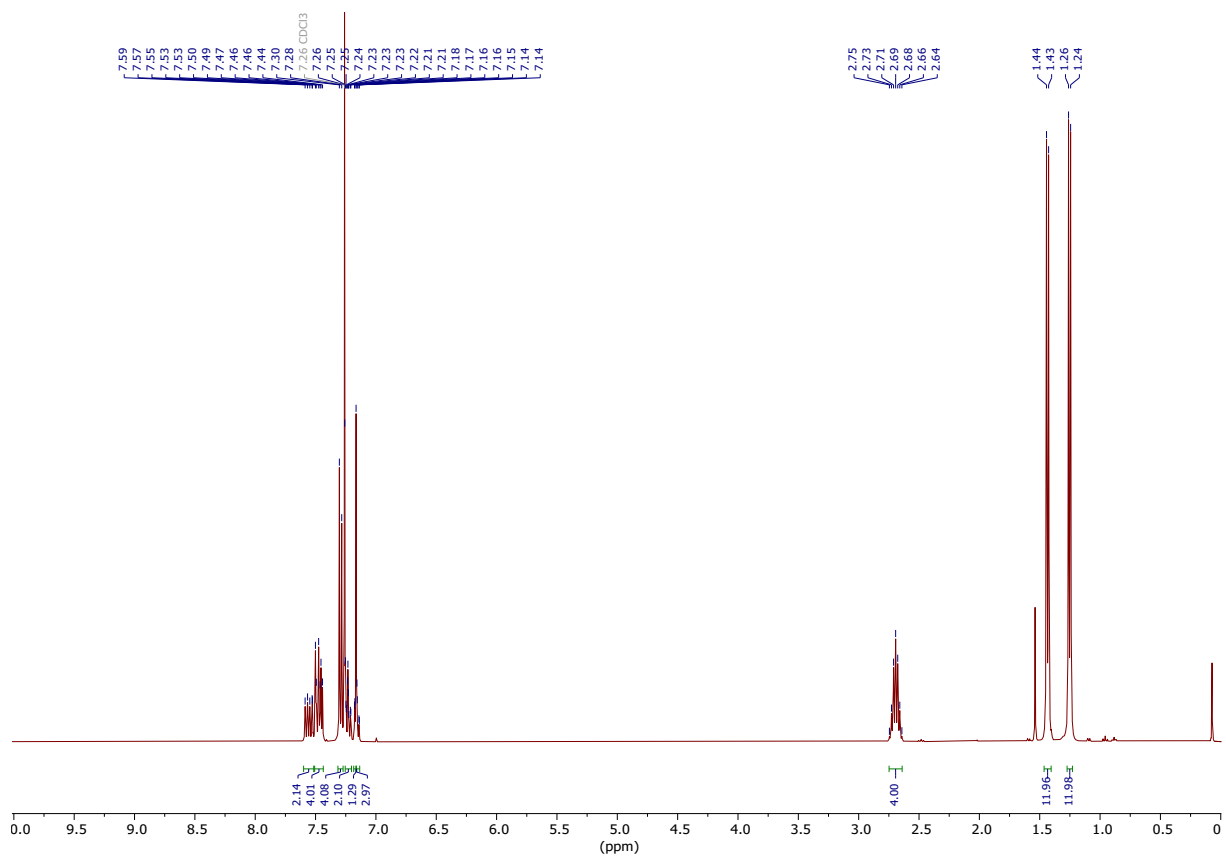
HSQC NMR of 2a



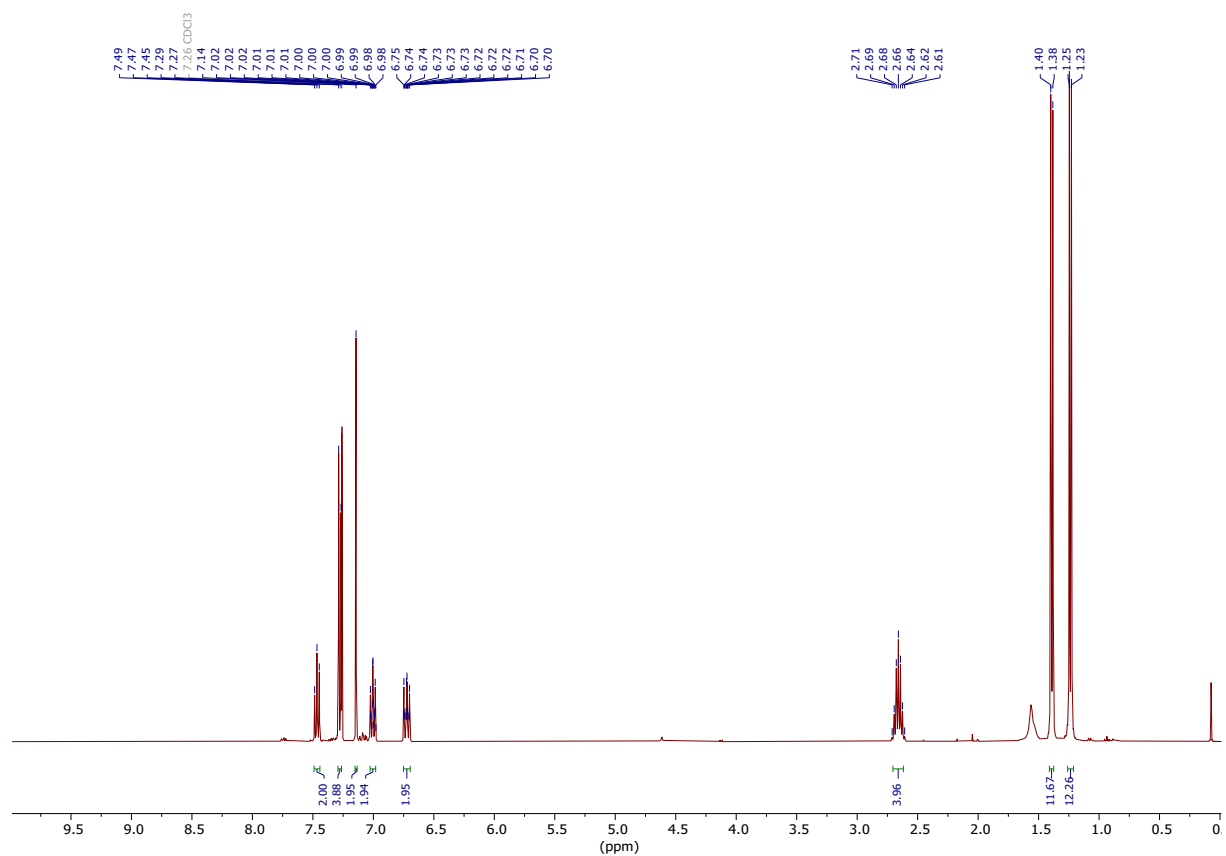
^1H NMR of $[\text{Au}(\text{IPr})\text{Ph}]$ (3a)



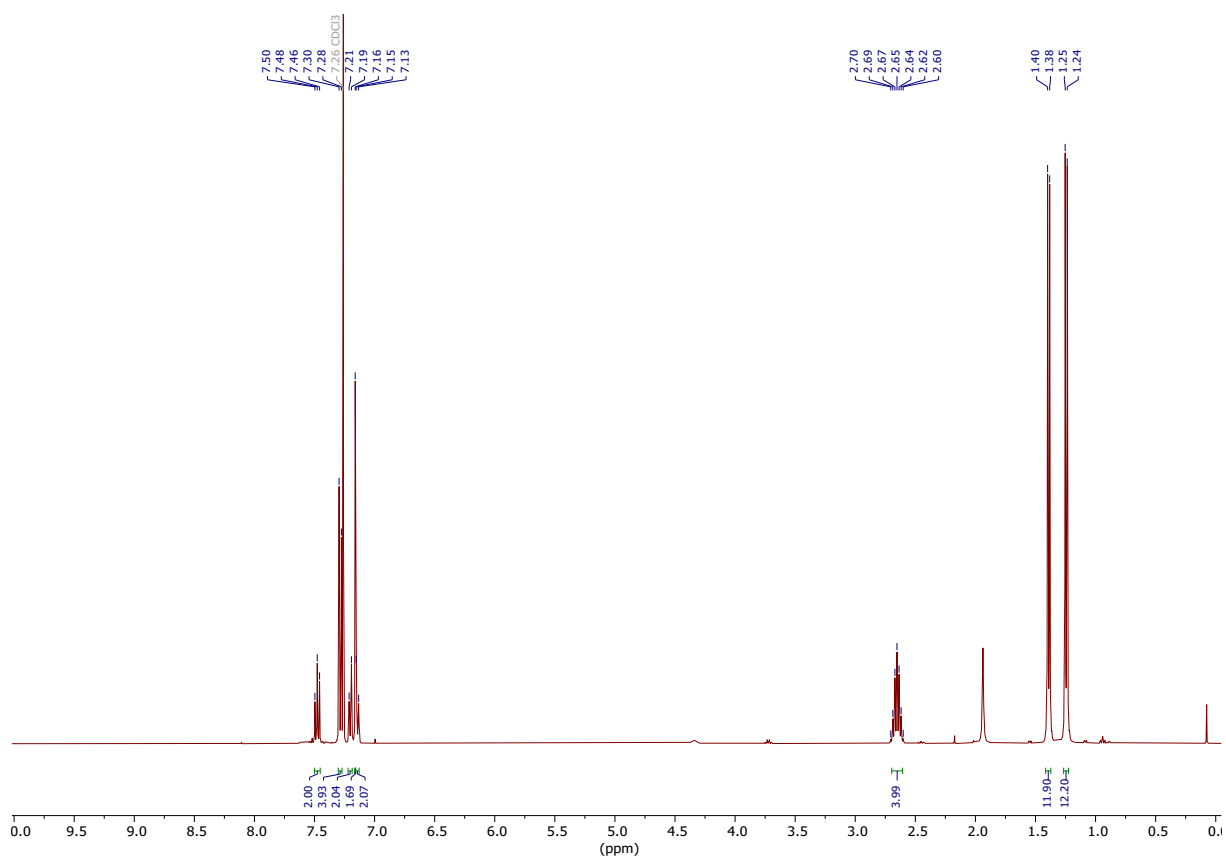
^1H NMR of $[\text{Au}(\text{IPr})_2\text{-Naphthyl}]$ (3b)



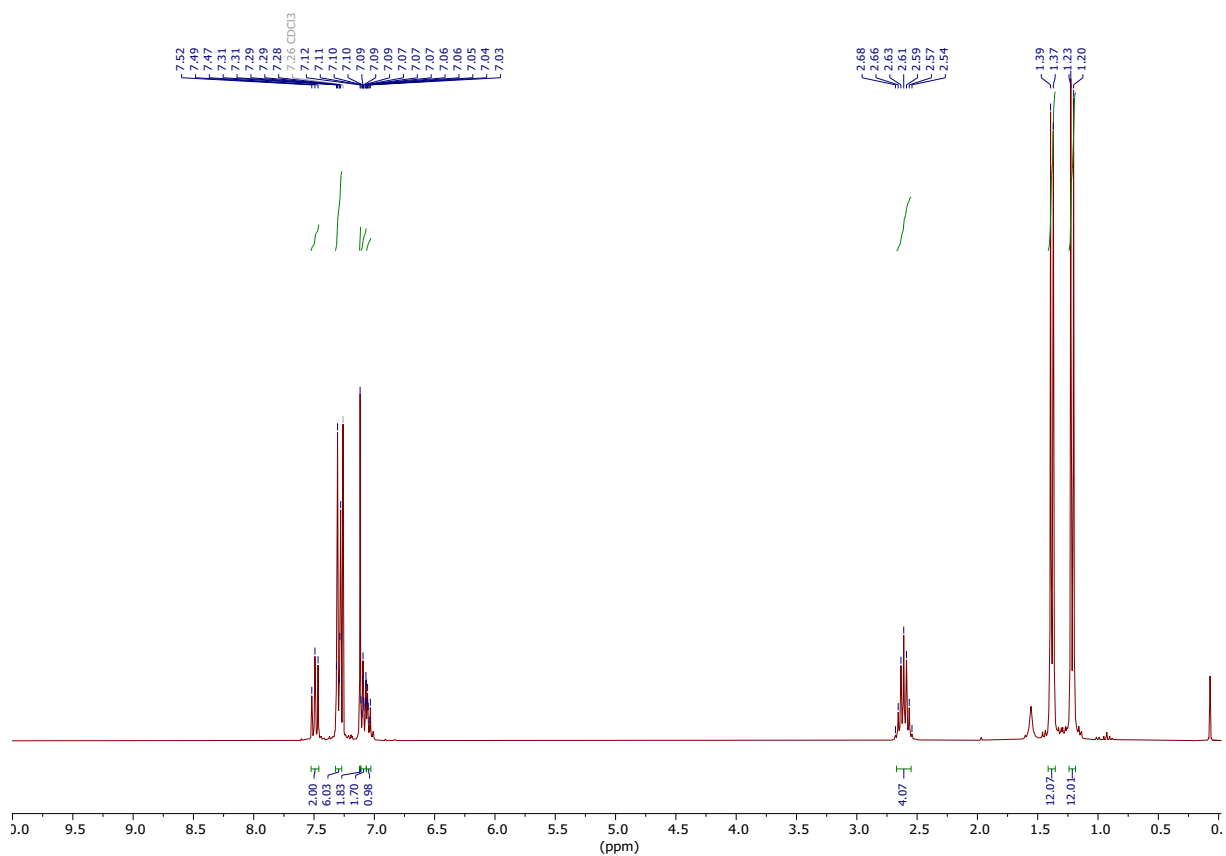
^1H NMR of $[\text{Au}(\text{IPr})\text{PhF}]$ (3c)



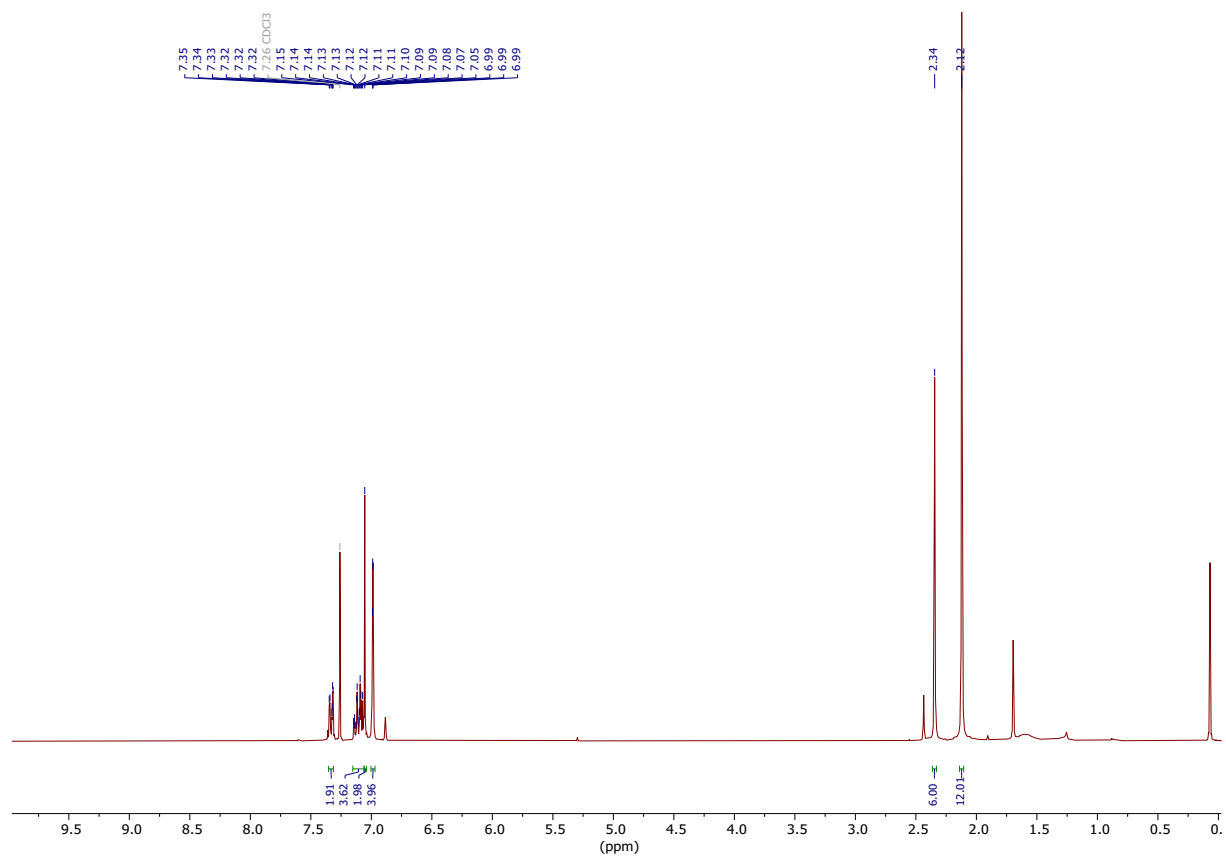
^1H NMR of $[\text{Au}(\text{IPr})\text{PhCF}_3]$ (3d)



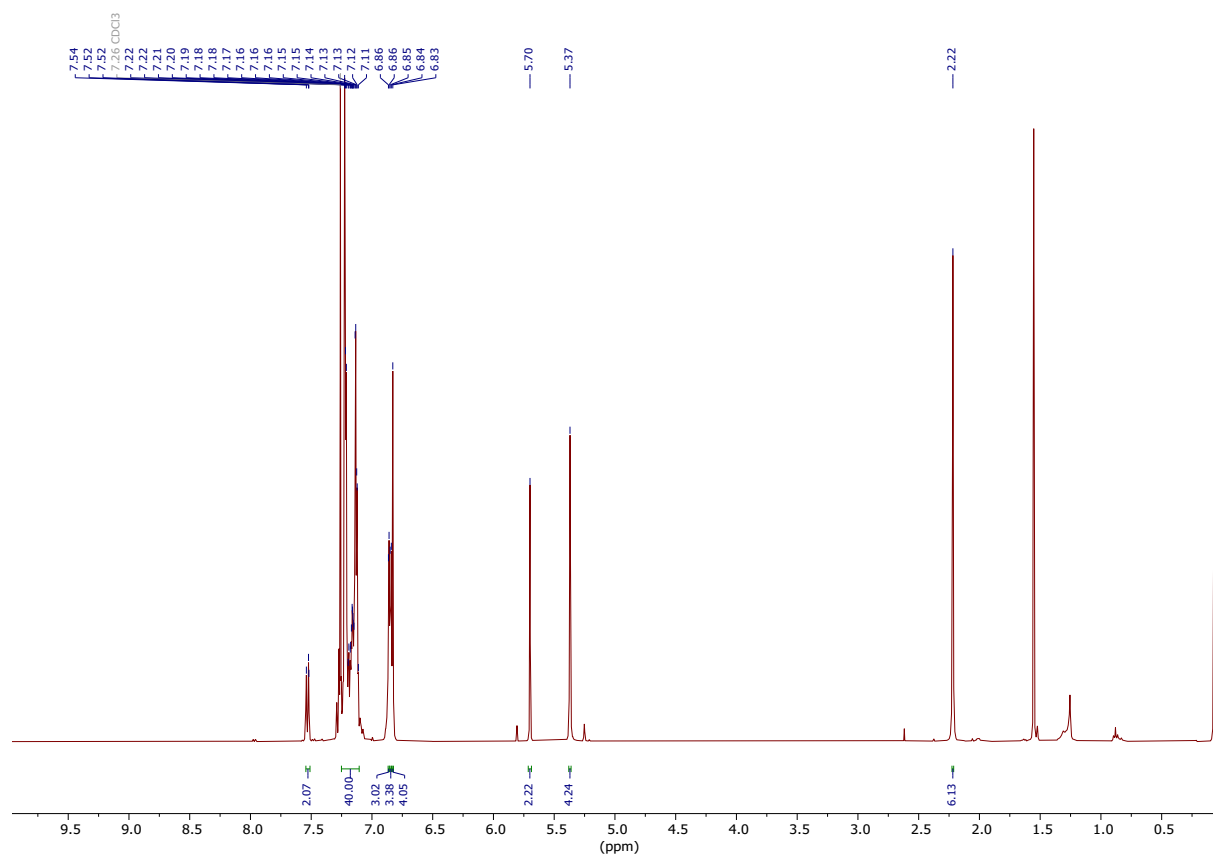
¹H NMR of [Au(IPr)Phenylacetylene] (4a)



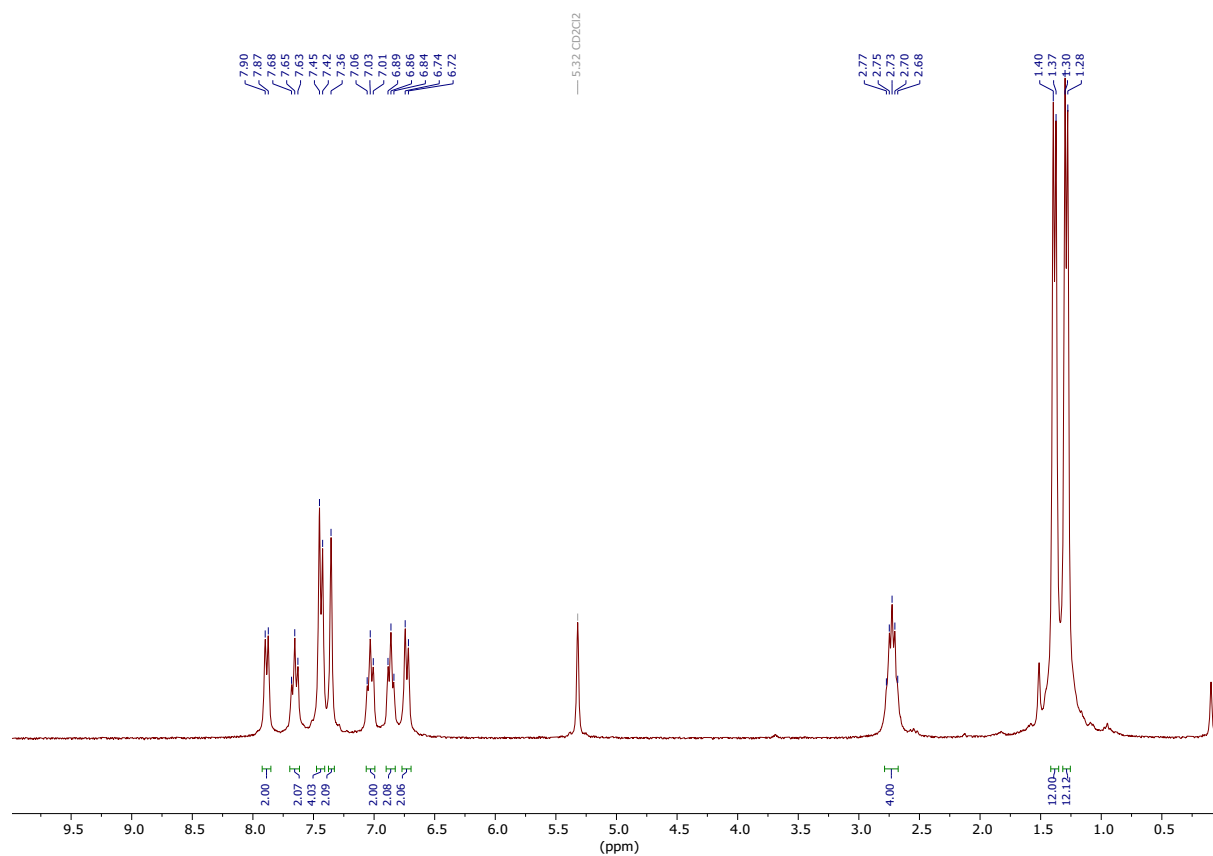
^1H NMR of $[\text{Au}(\text{IMes})\text{Phenylacetylene}]$ (**4b**)



^1H NMR of $[\text{Au}(\text{IPr}^*)\text{Phenylacetylene}]$ (4c)

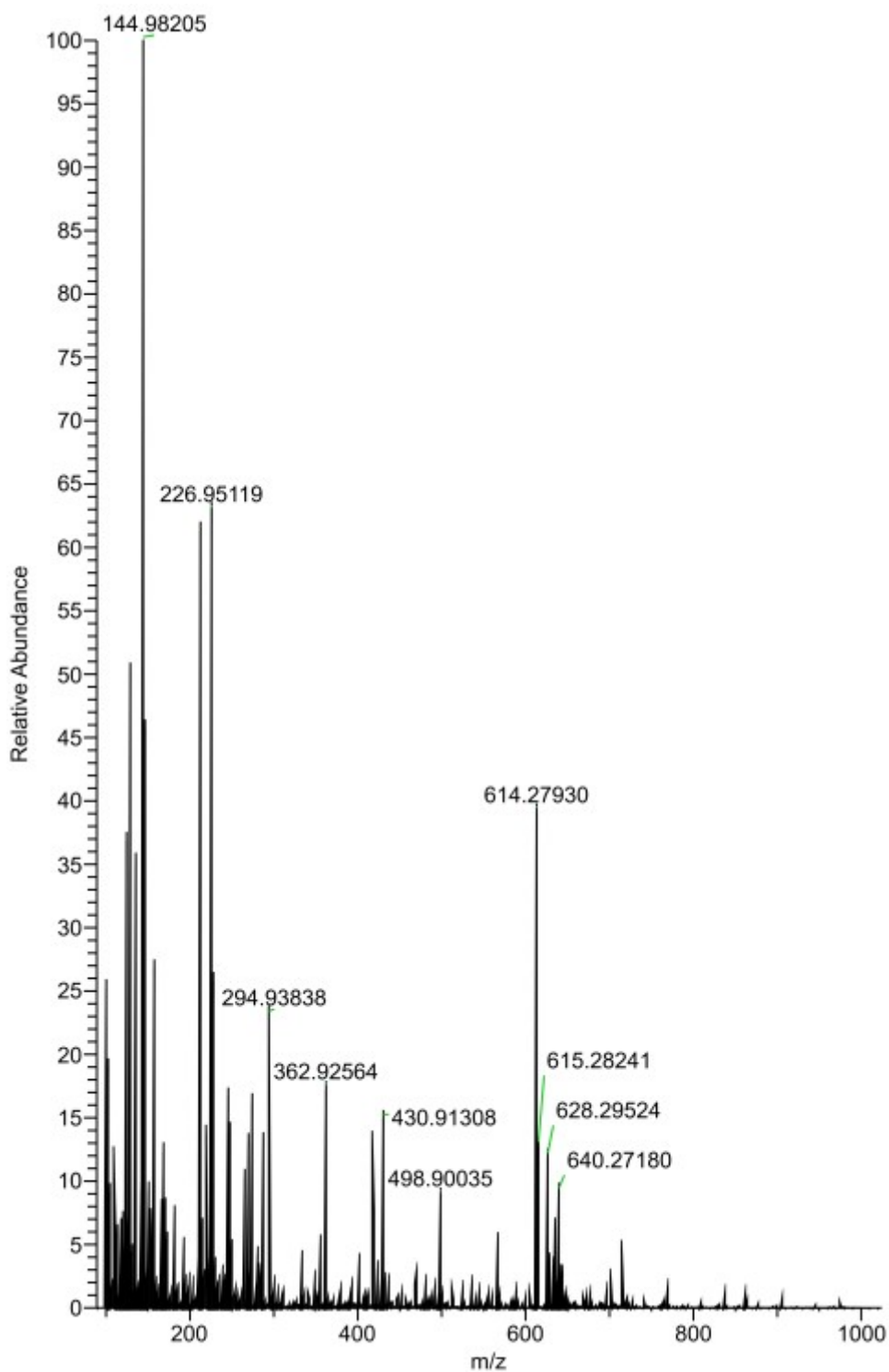


^1H NMR of $[\text{Au}(\text{IPr})\text{Cbz}]$ (5)

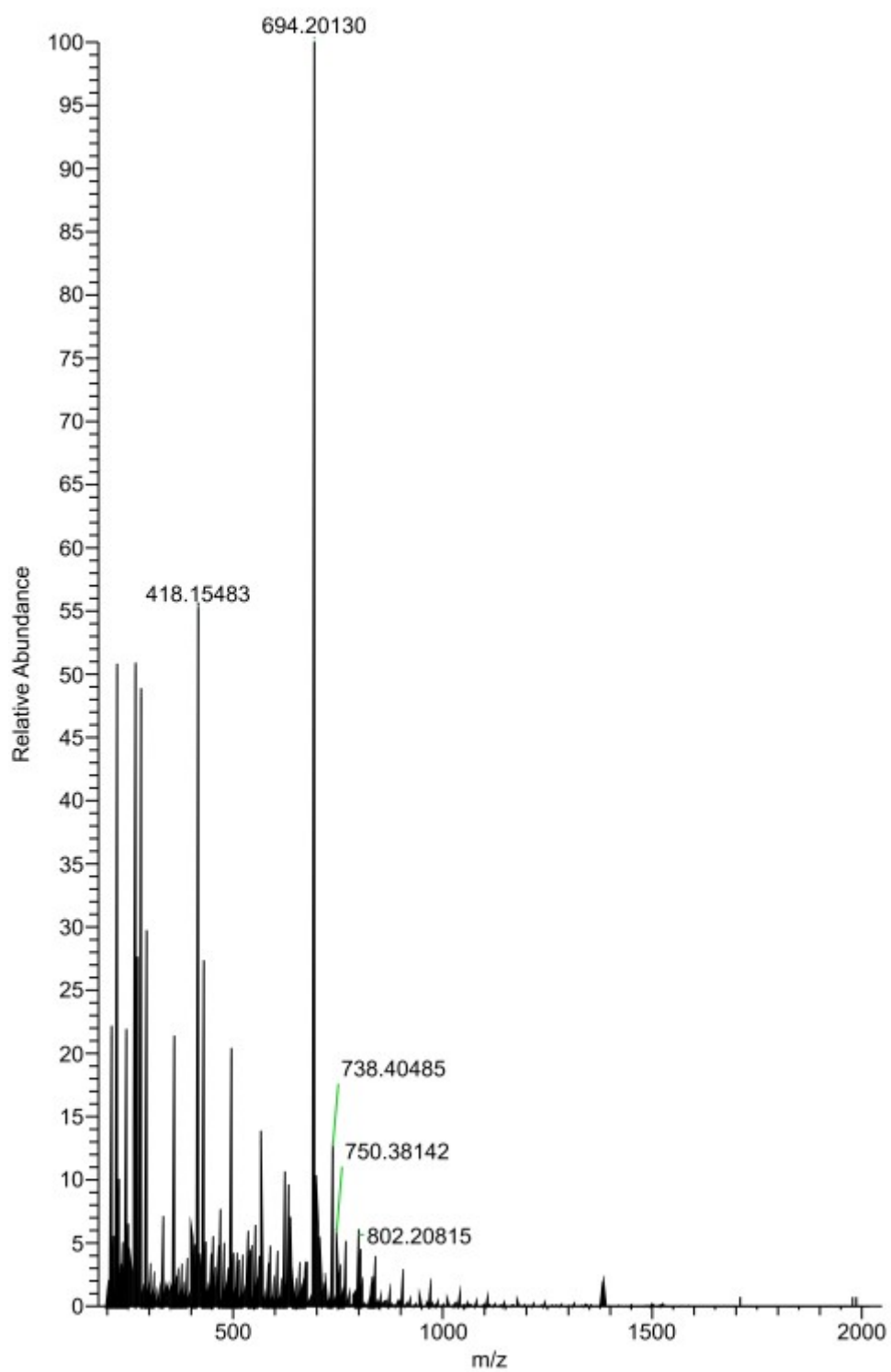


HRMS Data

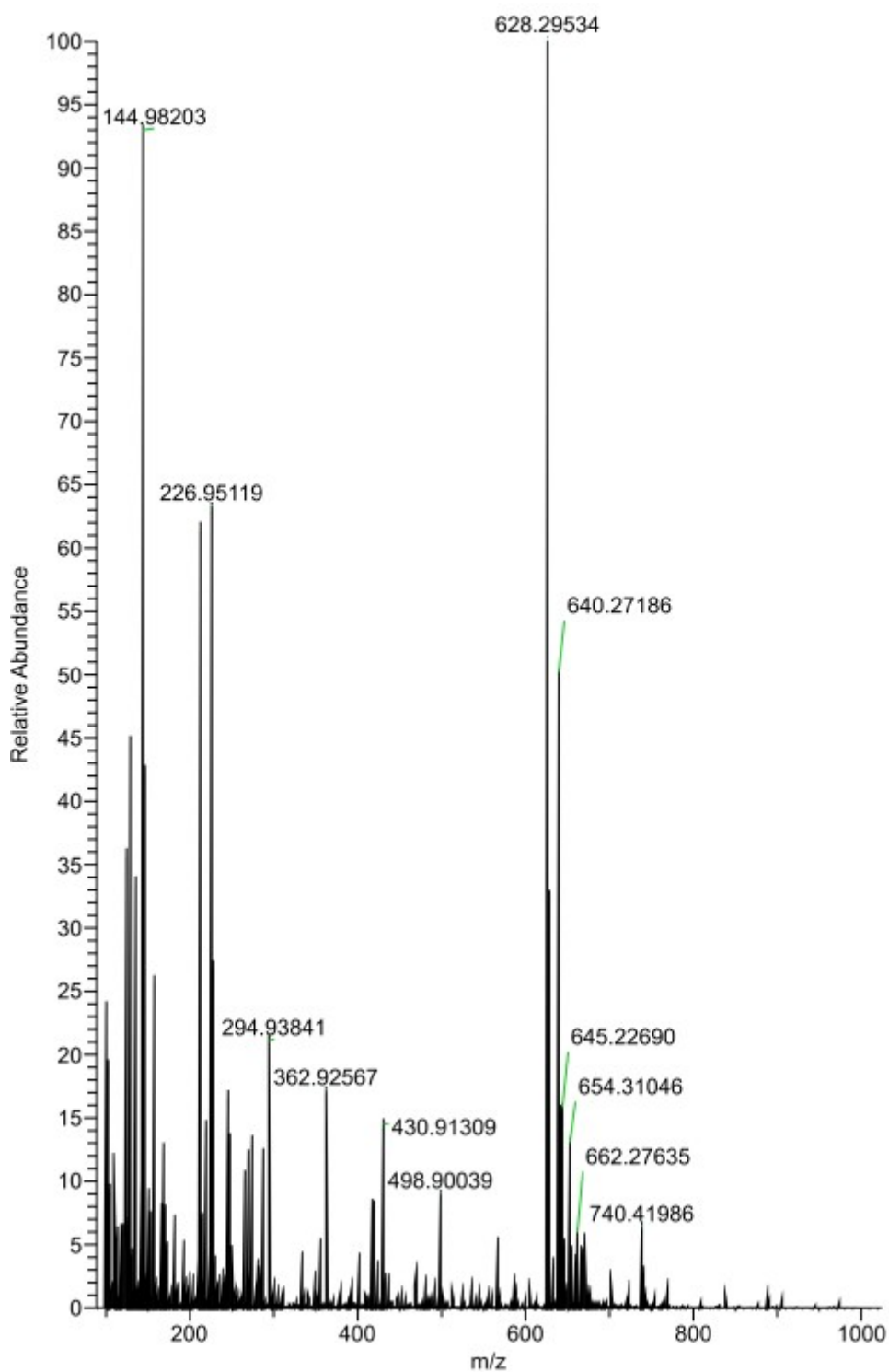
HRMS of $[\text{Au}(\text{SIPr})(\text{OCH}(\text{CF}_3)_2)]$ (1b)



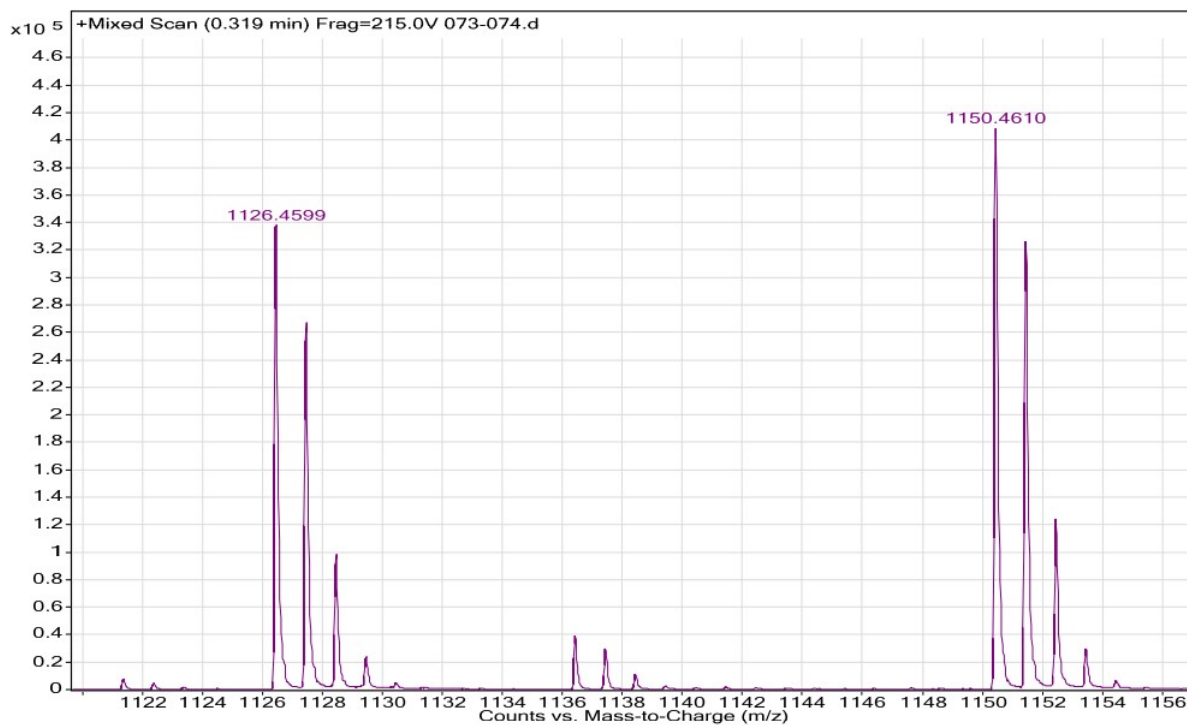
HRMS of $[\text{Au}(\text{IPr}^{\text{Cl}})(\text{OCH}(\text{CF}_3)_2)]$ (1c)



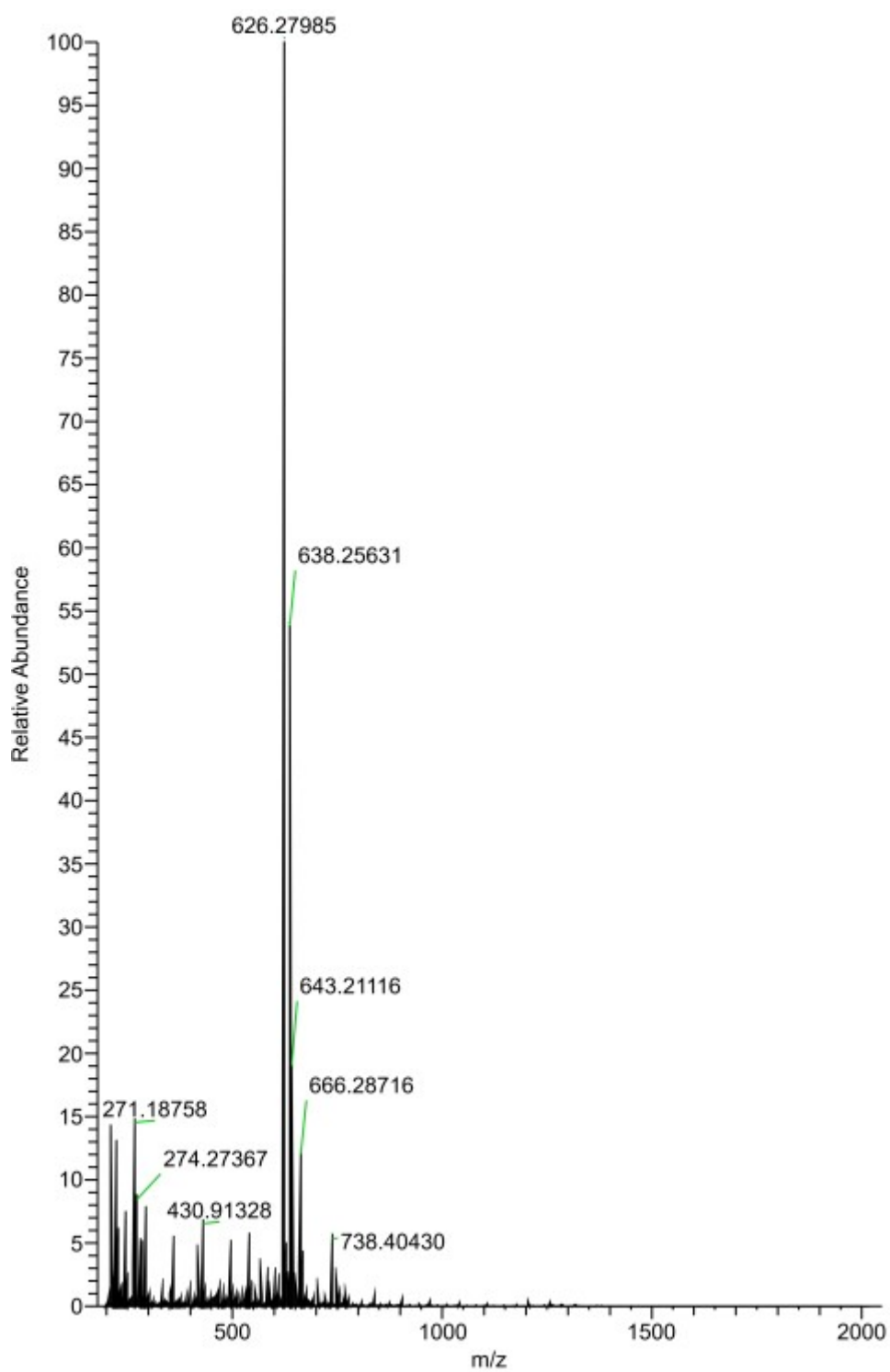
HRMS of $[\text{Au}(\text{IPr}^{\text{Me}})(\text{OCH}(\text{CF}_3)_2)]$ (1d)



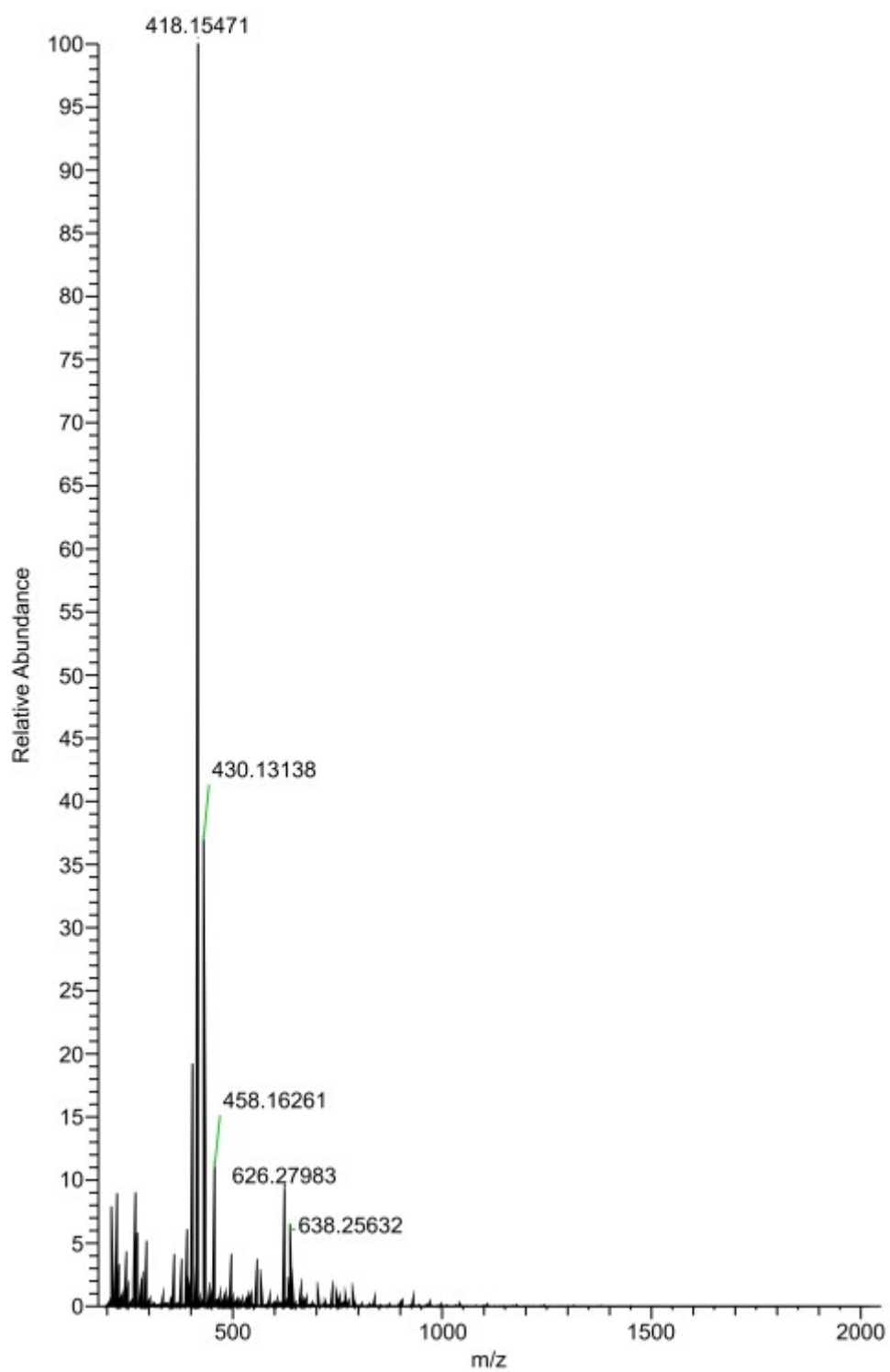
HRMS of [Au(IPr*)(OCH(CF₃)₂)] (1f)



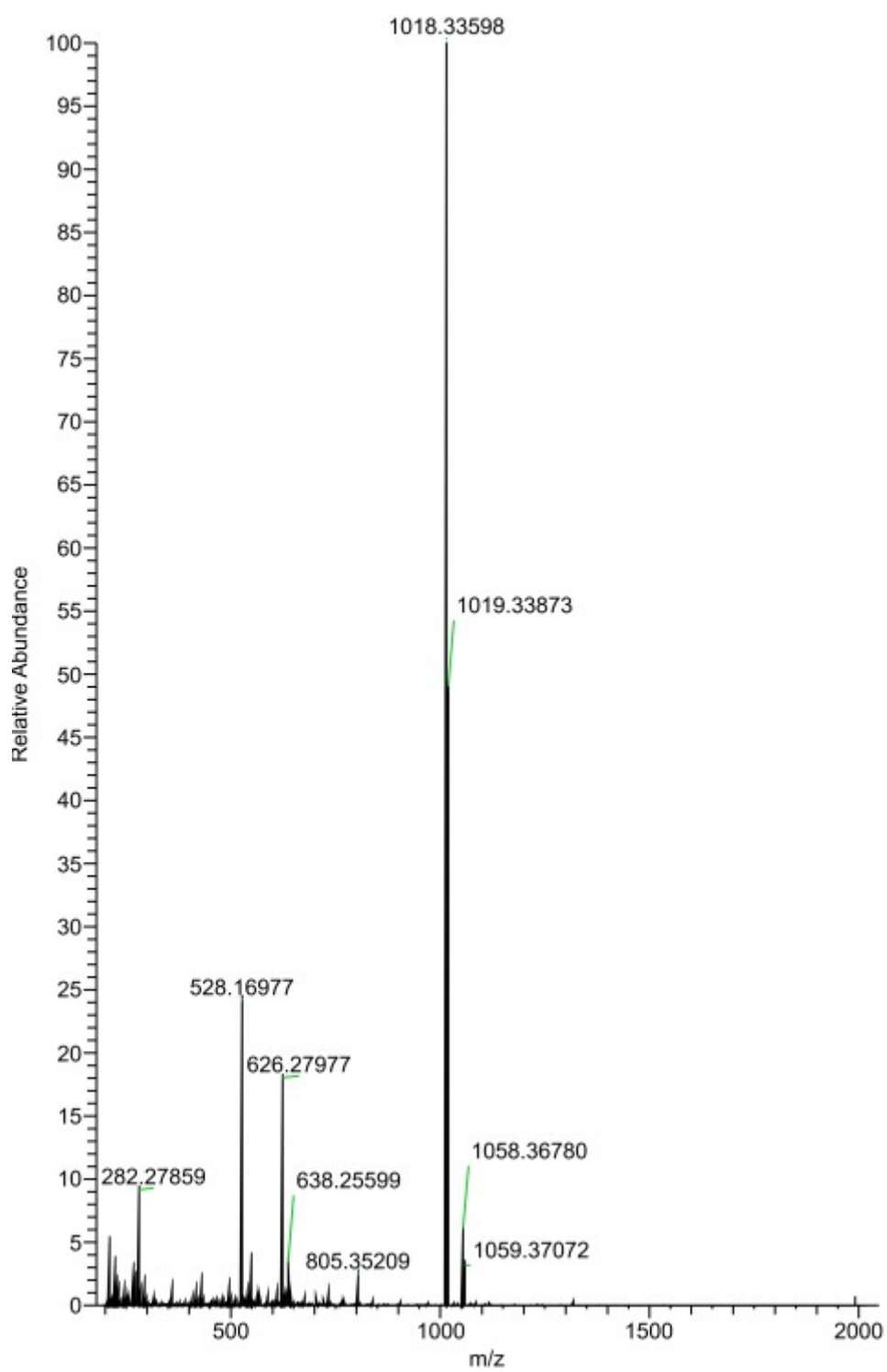
HRMS of [Au(IPent)(OCH(CF₃)₂)] (1g)



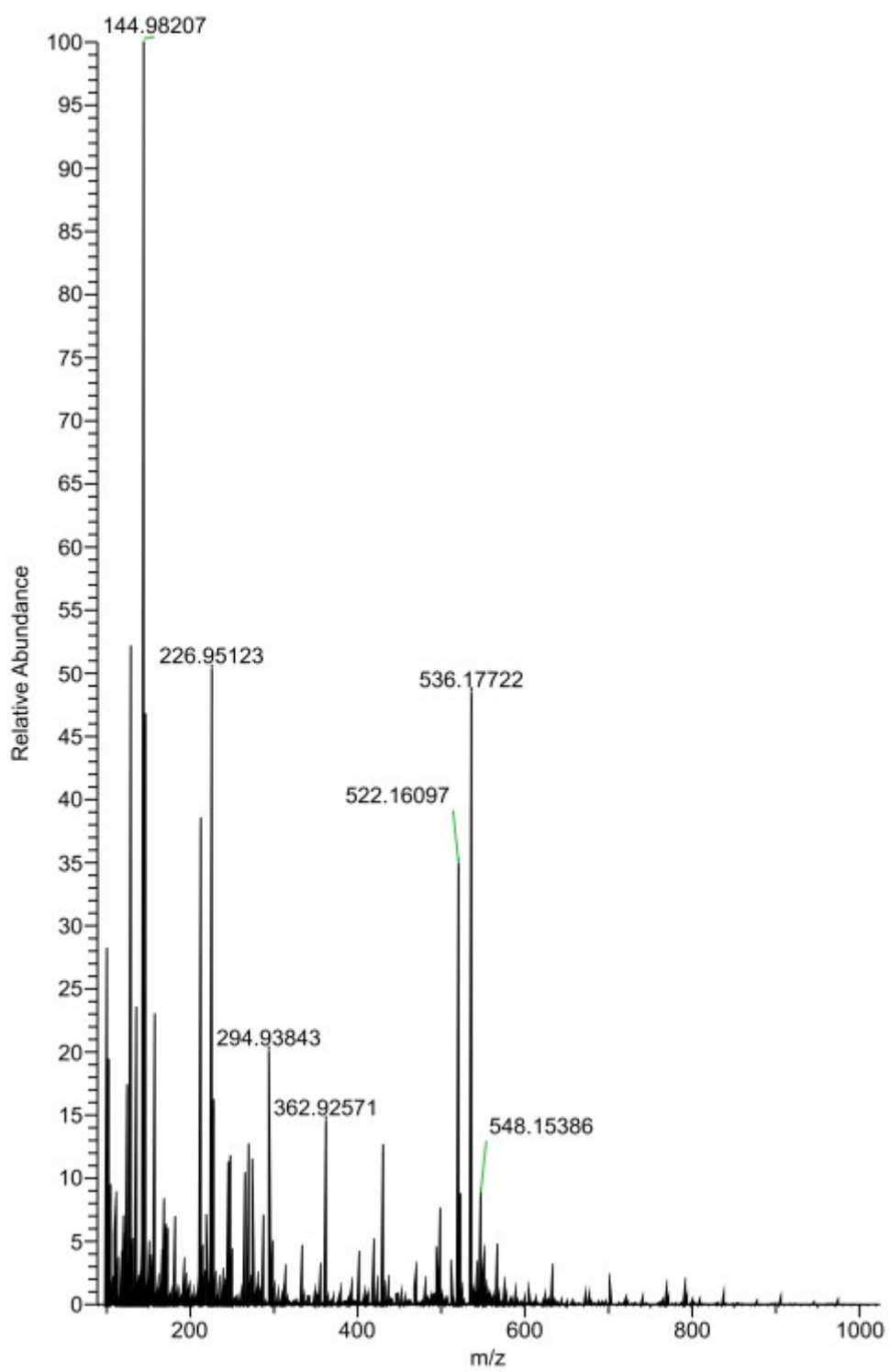
HRMS of $[\text{Au}(\text{I}^t\text{Bu})(\text{OCH}(\text{CF}_3)_2)]$ (1h)



HRMS of [Au(IMes)(OCH(CF₃)₂)] (1i)



HRMS of [Au(JohnPhos)(OCH(CF₃)₂)] (1j)



HRMS of [Au(IPr)(OCH₂CF₃)] (2a)

