Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Synthesis of Hydroxyl- and Amine-functionalized N-Heterocyclic Carbene Gold(I) Complexes and Peptide Conjugates

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1. Additional Figures (X-ray packing)

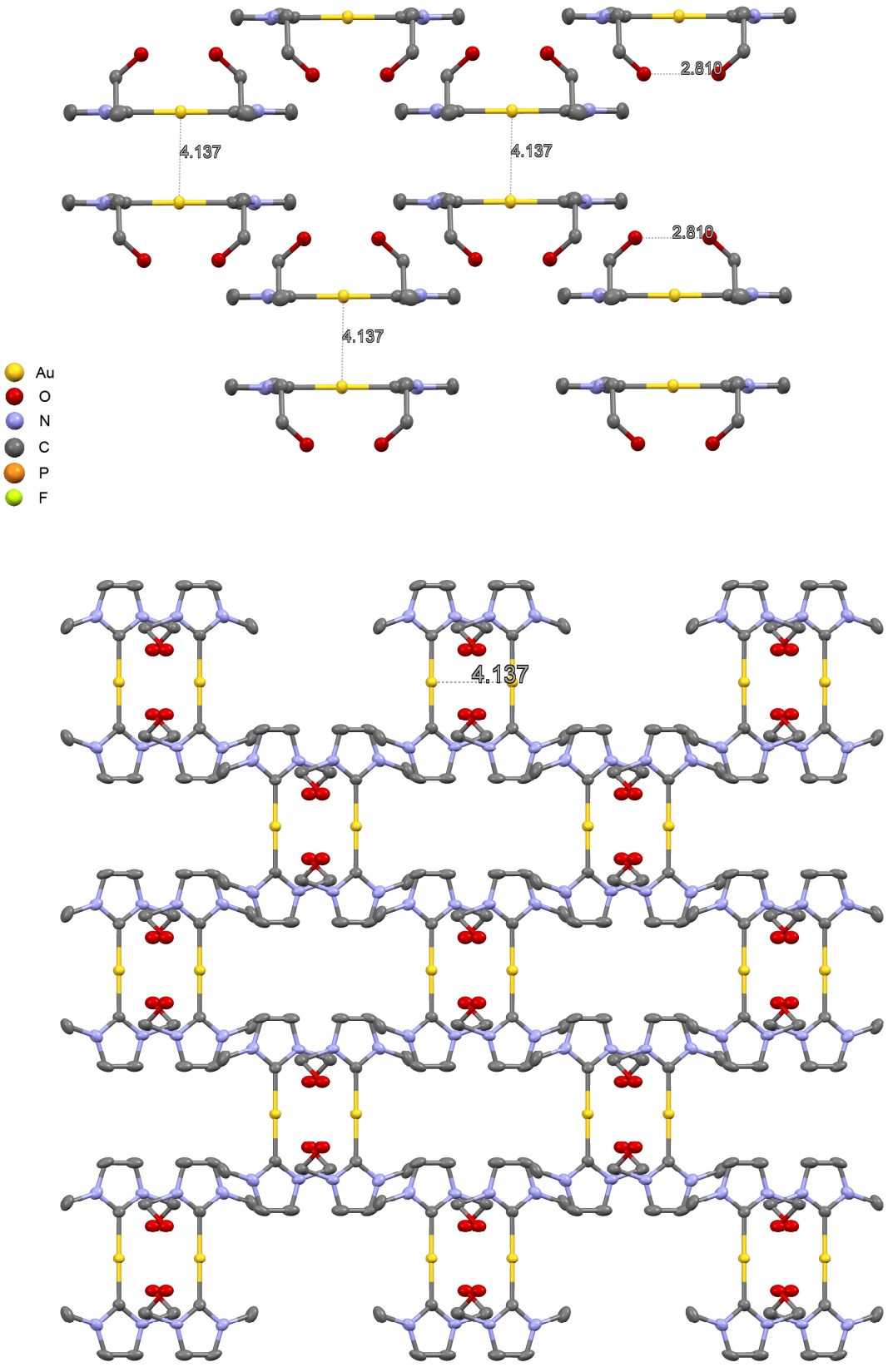


Figure S1: Additional views of the crystal packing of complex **5b** (50 % probability level; PF_6^- anions and hydrogen atoms are omitted for clarity). Selected distances are given in Å.

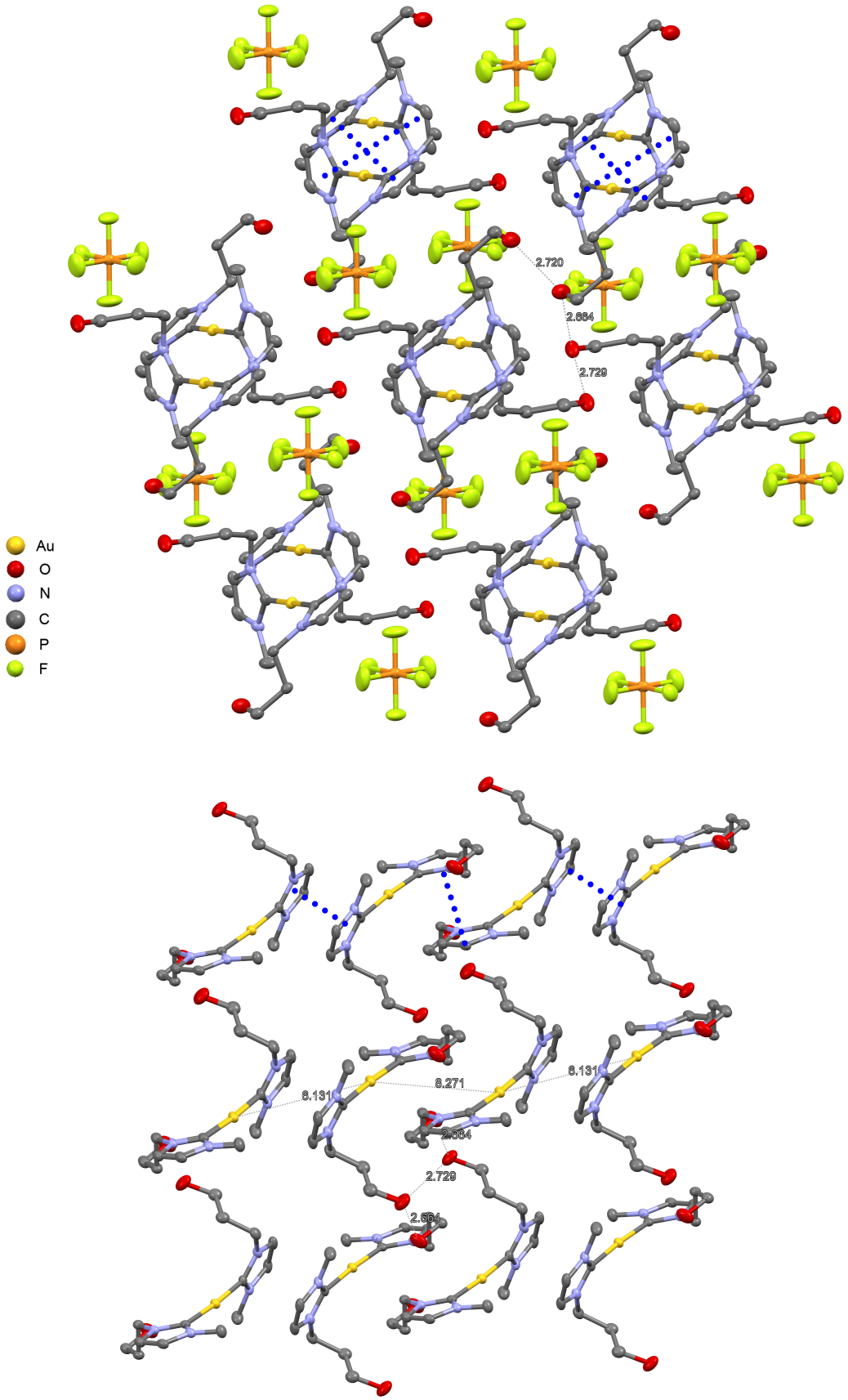


Figure S2: Additional views of the crystal packing of complex **7b** (50 % probability level; hydrogen atoms and in the lower view PF_6^- anions are omitted for clarity). Head-to-tail π–π interactions are indicated by dotted blue lines. Selected distances are given in Å.

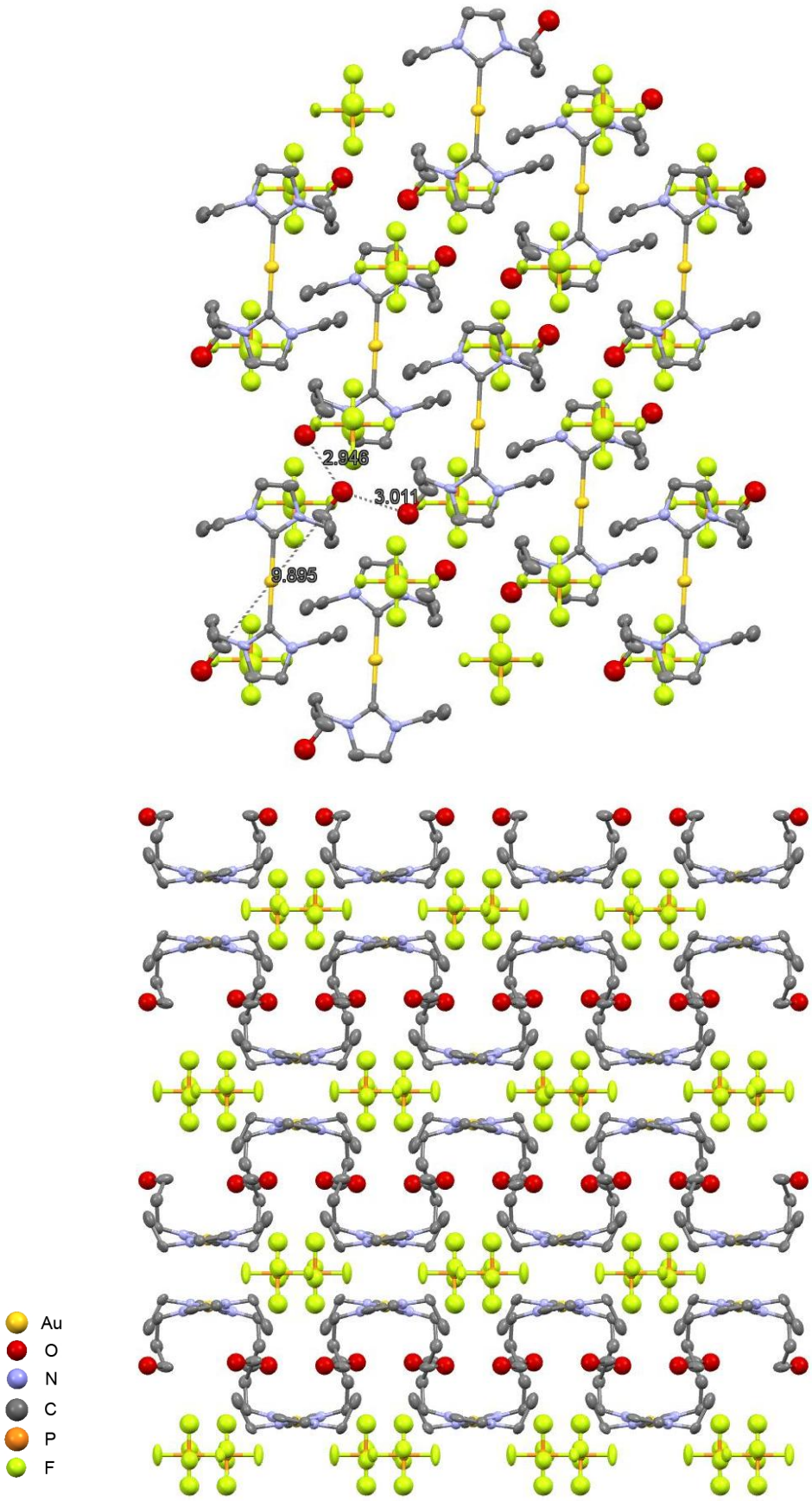


Figure S3: Additional views of the crystal packing of complex **8b** (50 % probability level; hydrogen atoms are omitted for clarity). Selected distances are given in Å.

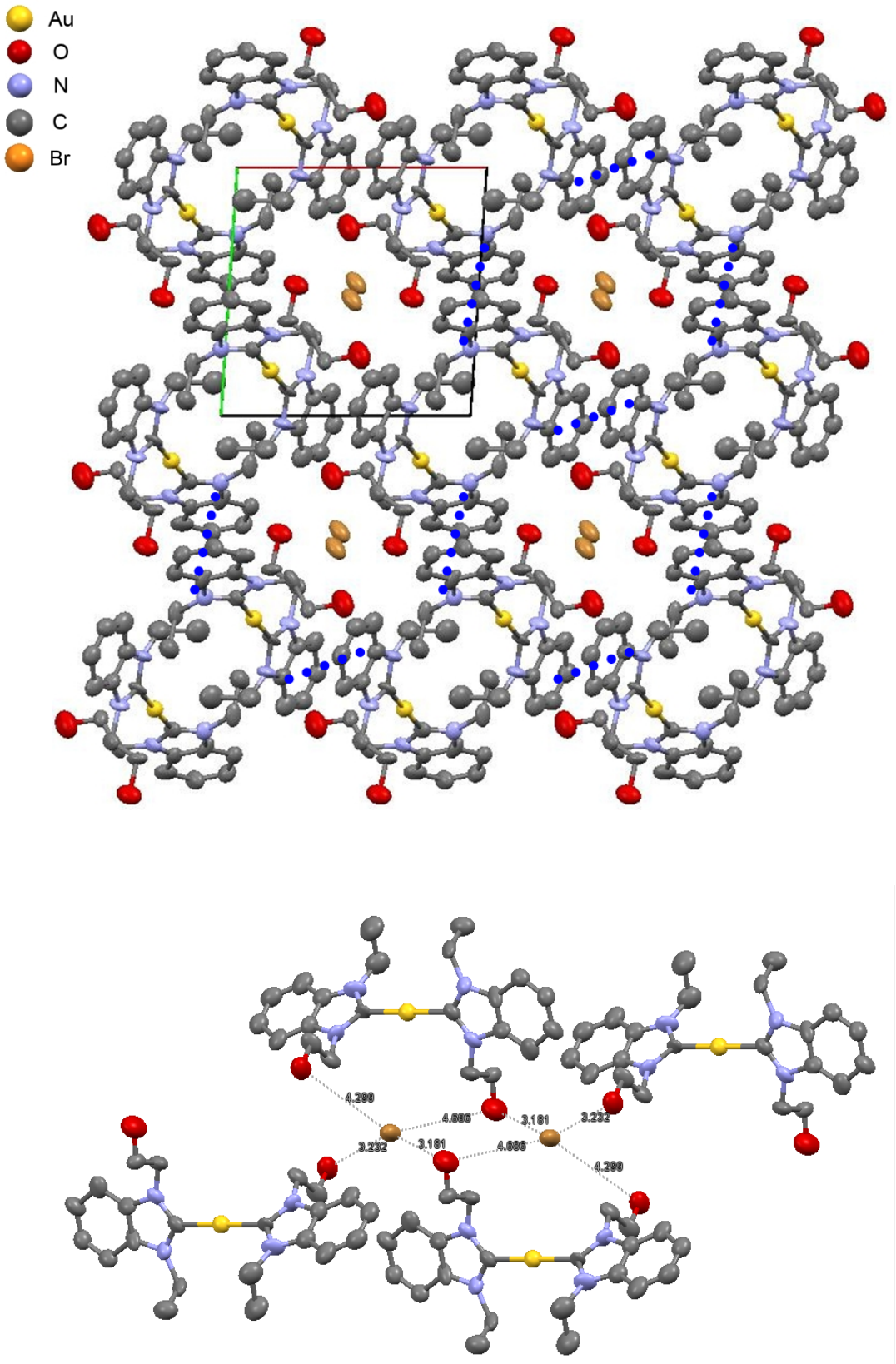


Figure S4: Additional views of the crystal packing of complex **9a** (50 % probability level; hydrogen atoms are omitted for clarity). Head-to-tail π–π interactions are indicated by dotted blue lines. Selected distances are given in Å.

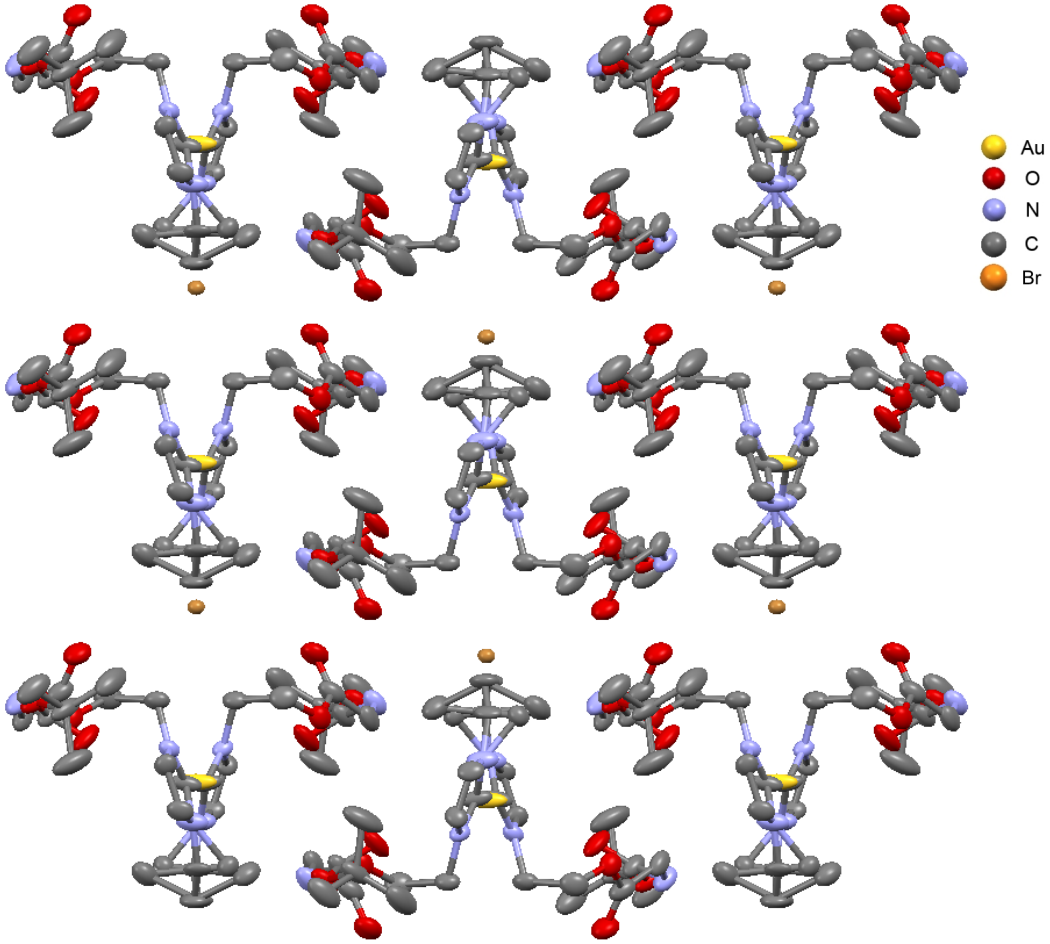


Figure S5: View of the crystal packing of complex **11'** (50 % probability level; hydrogen atoms are omitted for clarity).

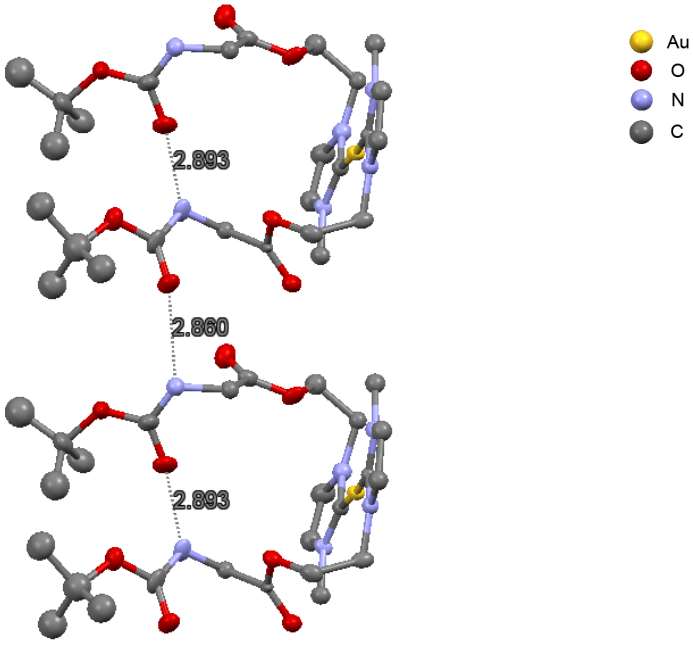
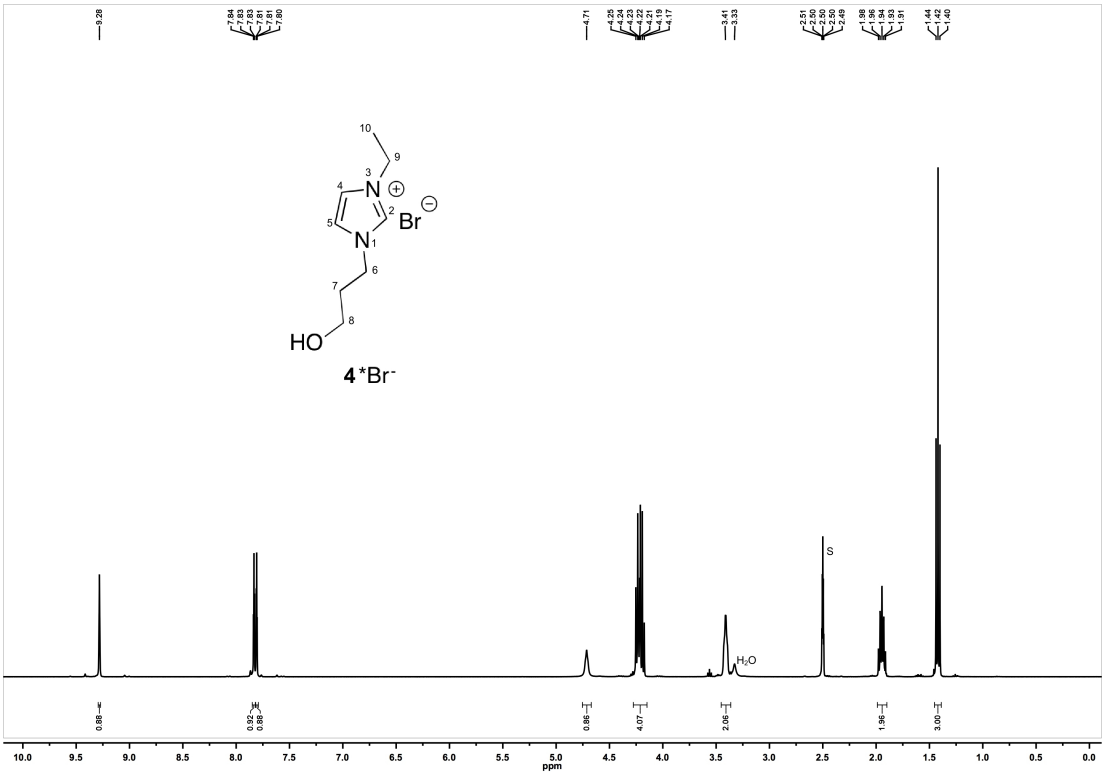


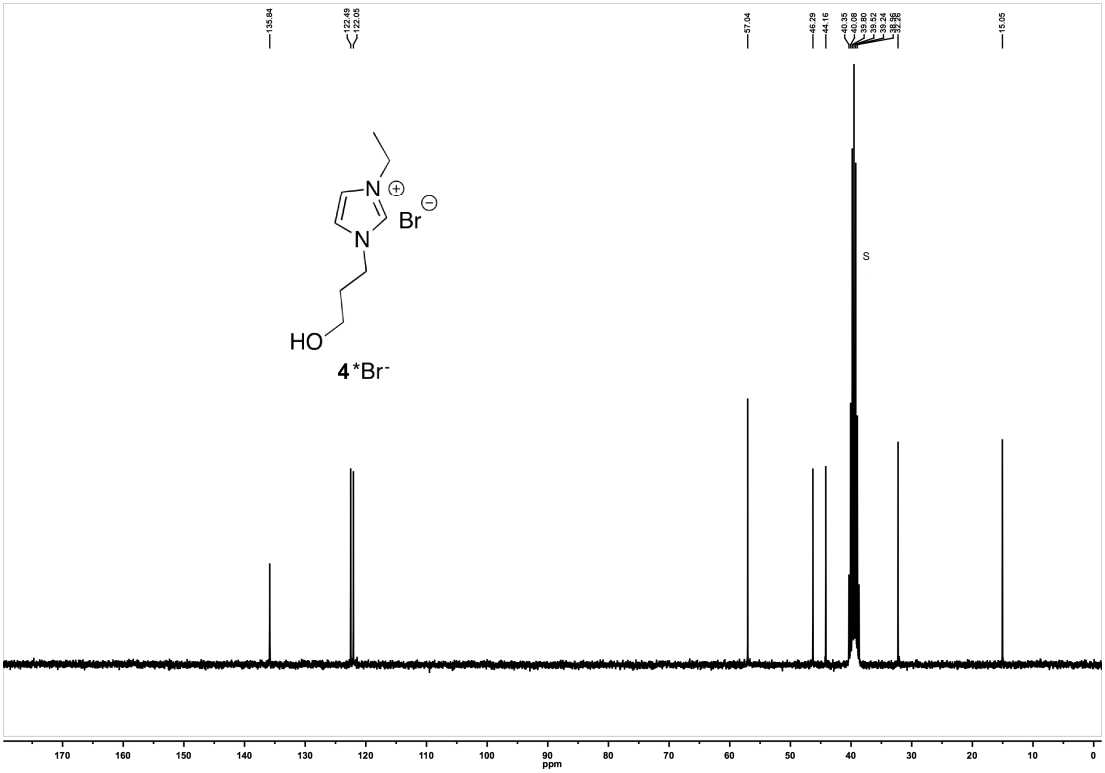
Figure S6: Additional view of the crystal packing of complex **10** (50 % probability level; hydrogen atoms are omitted for clarity). Selected distances of the hydrogen bonding pattern and are given in Å.

2. Substance Characterization: NMR spectra

Legend: ^{1}H-NMR above, ^{13}C{^{1}H}-NMR below, S: solvent

1-Ethyl-3-(3-hydroxypropyl)imidazoliumbromide 4*Br (DMSO-*d6*)





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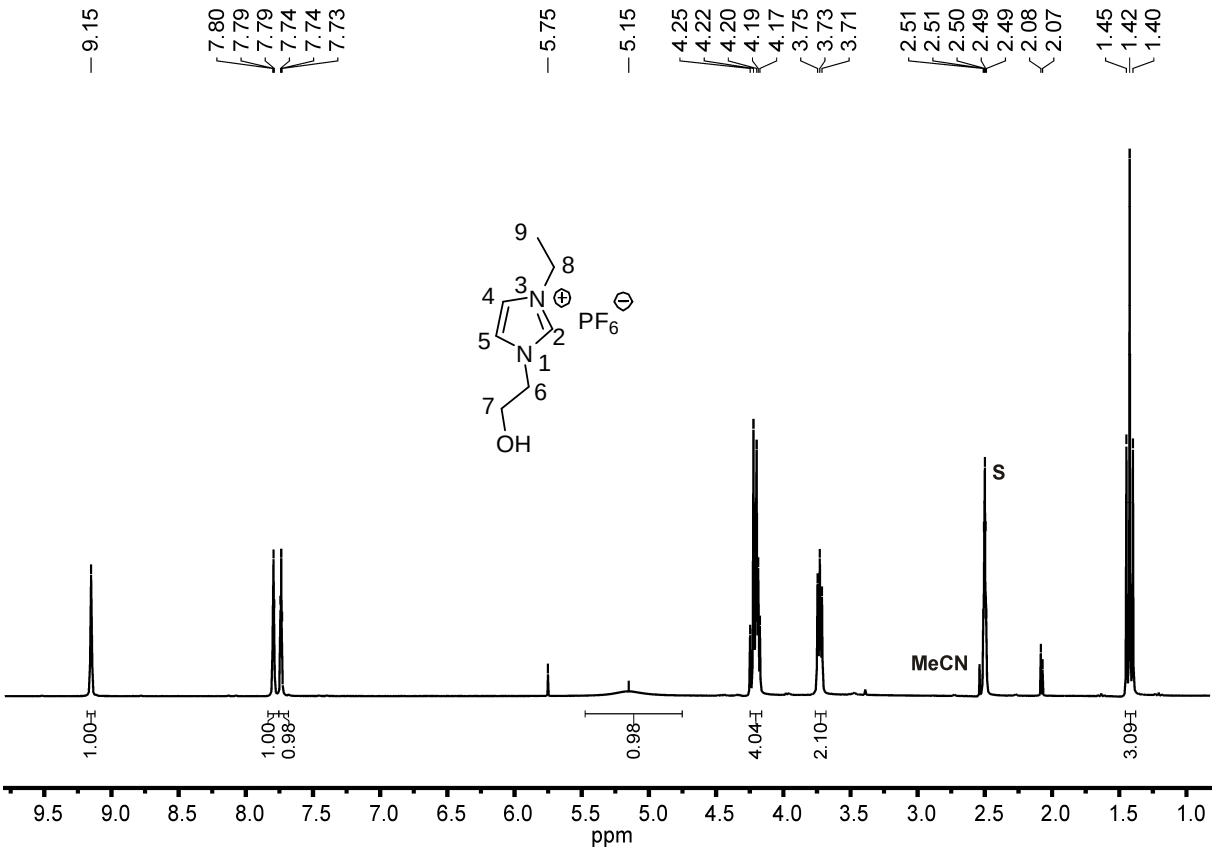

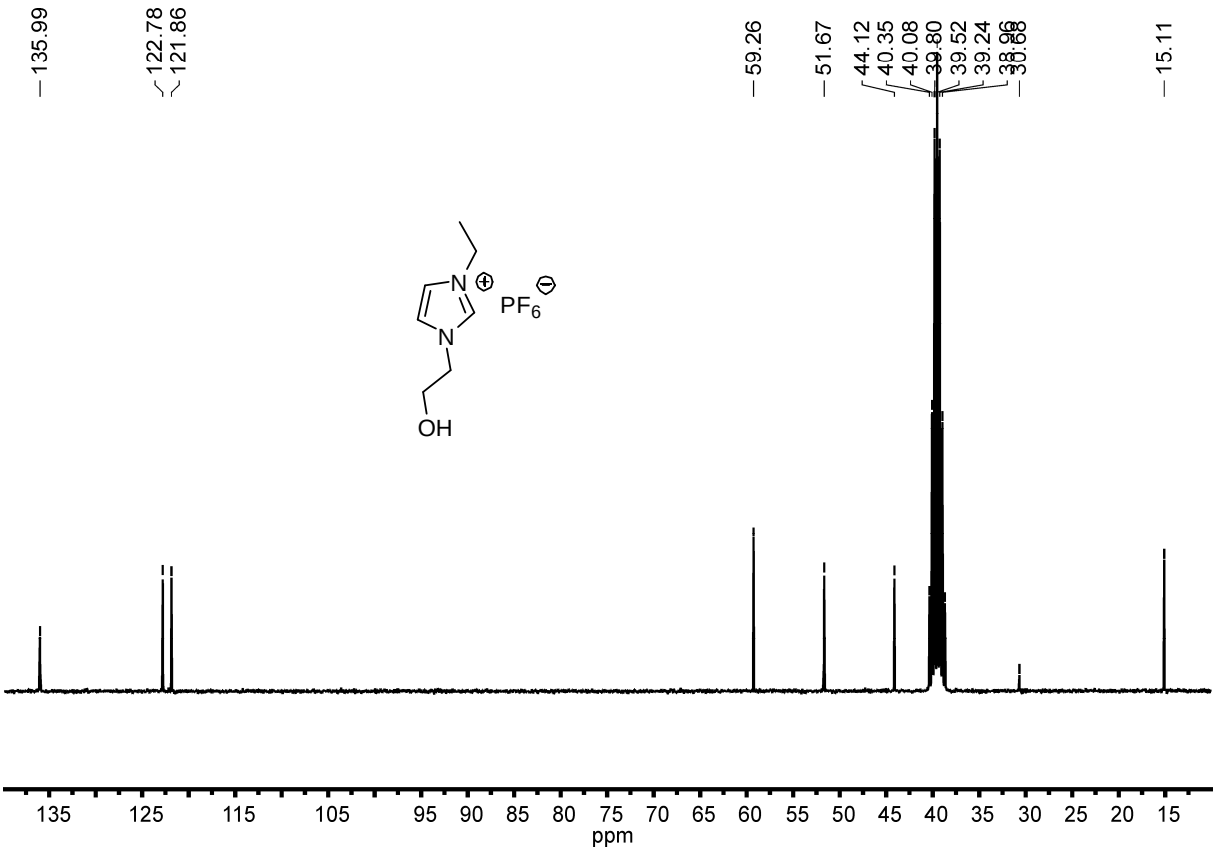

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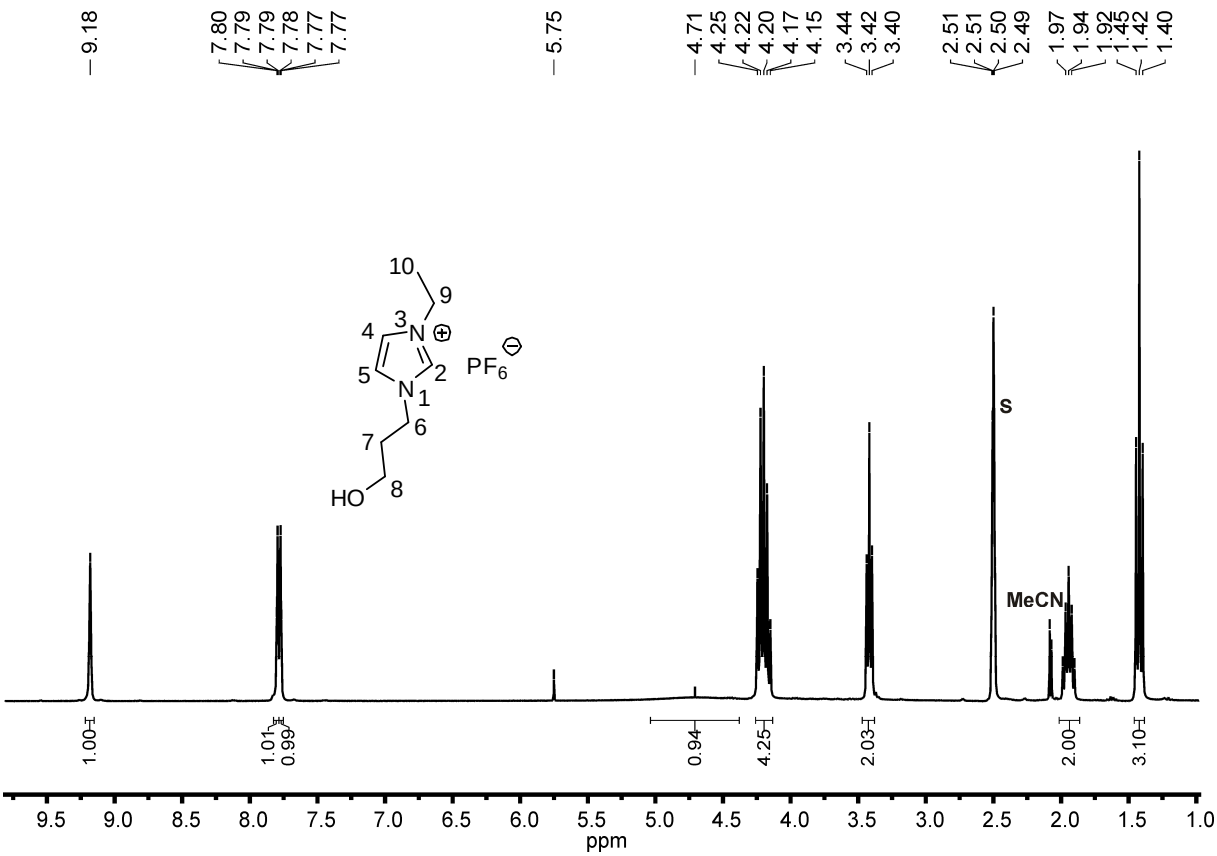
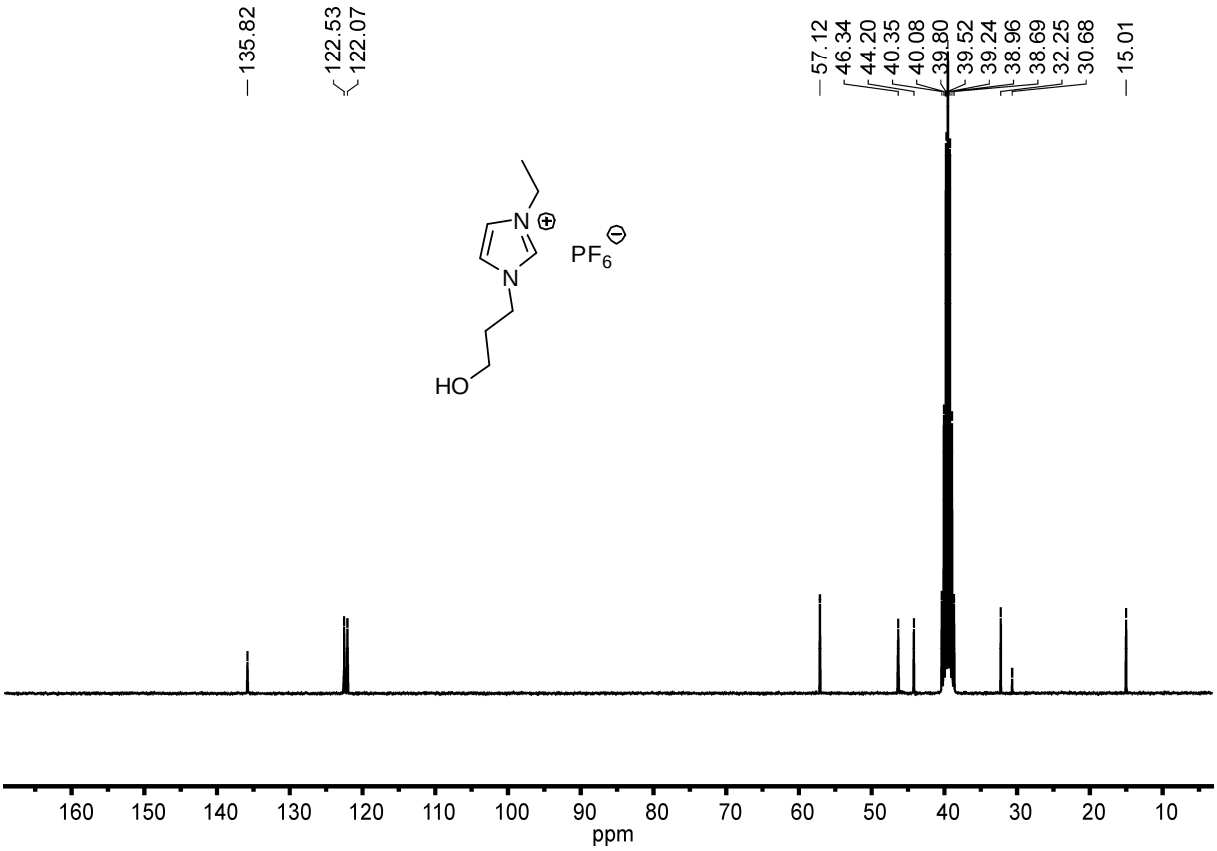
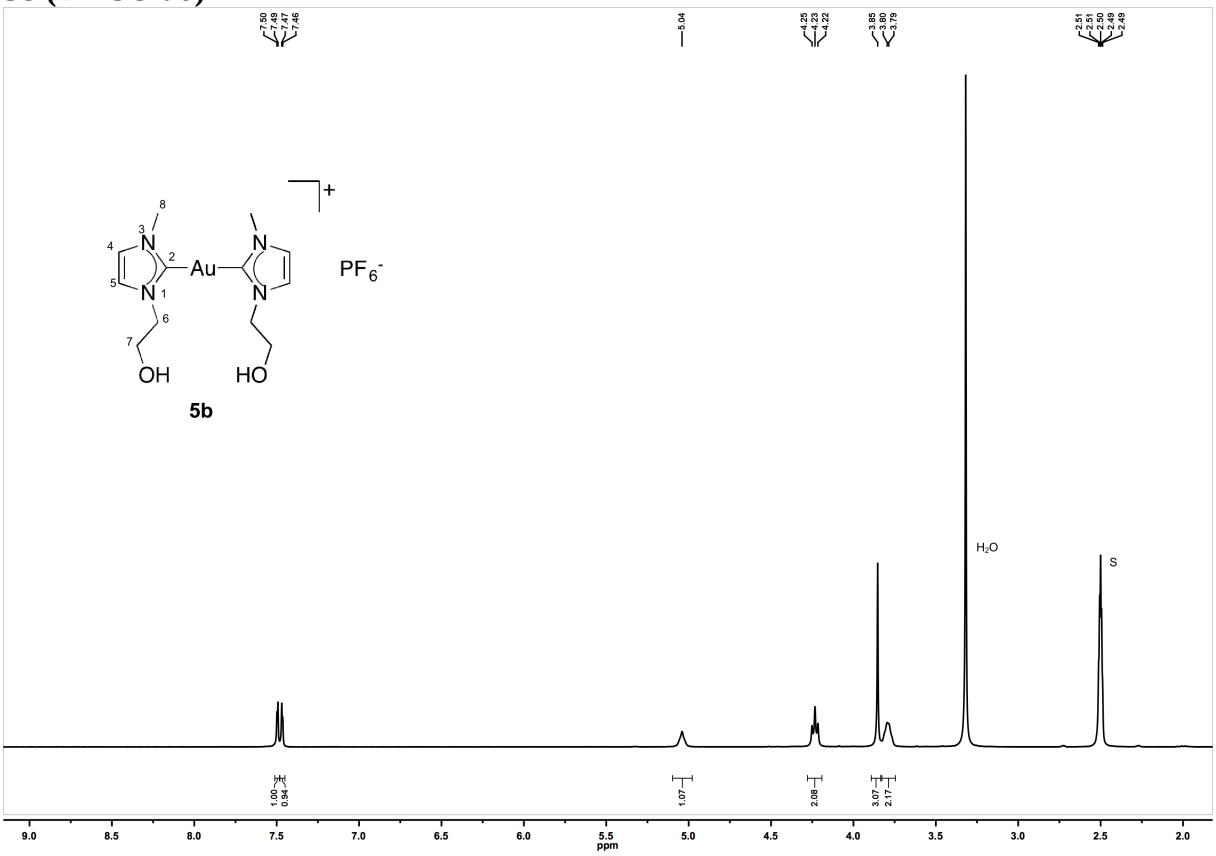


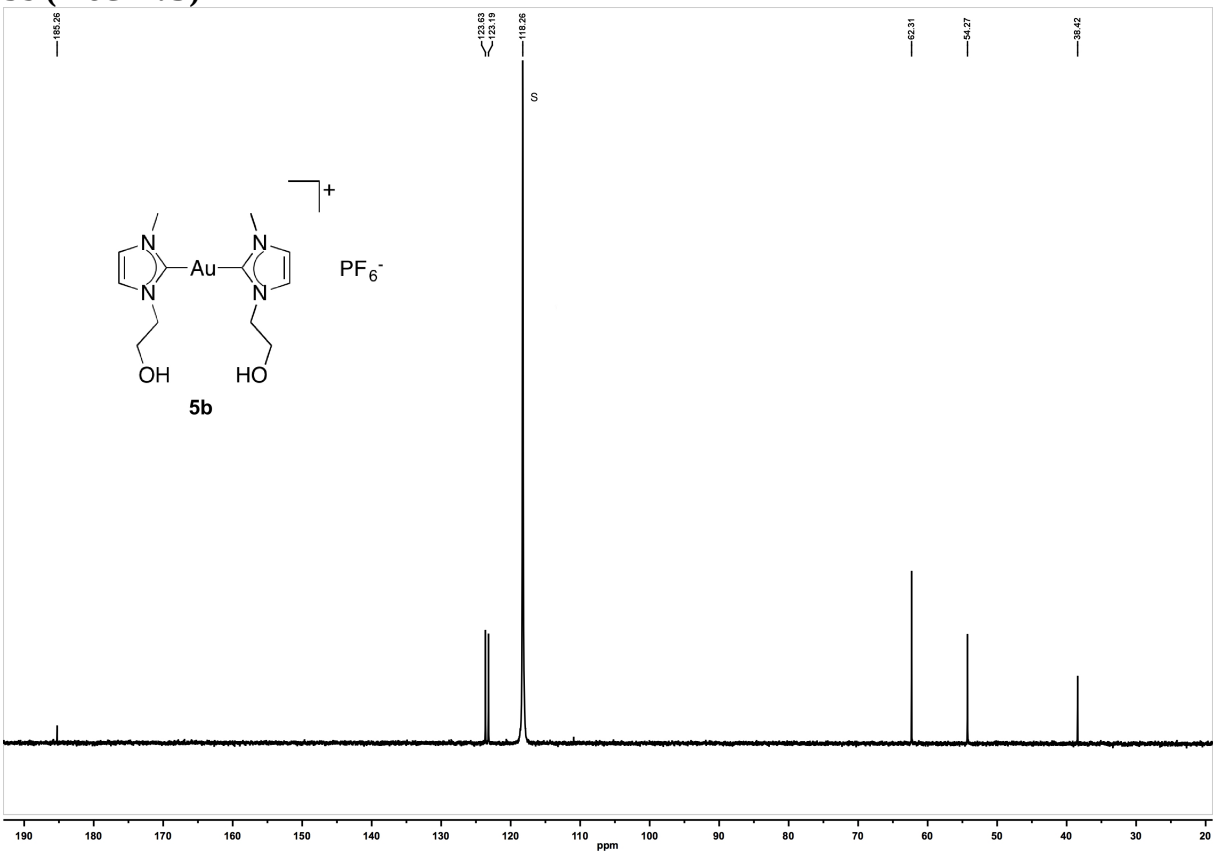


5b (DMSO-*d6*)



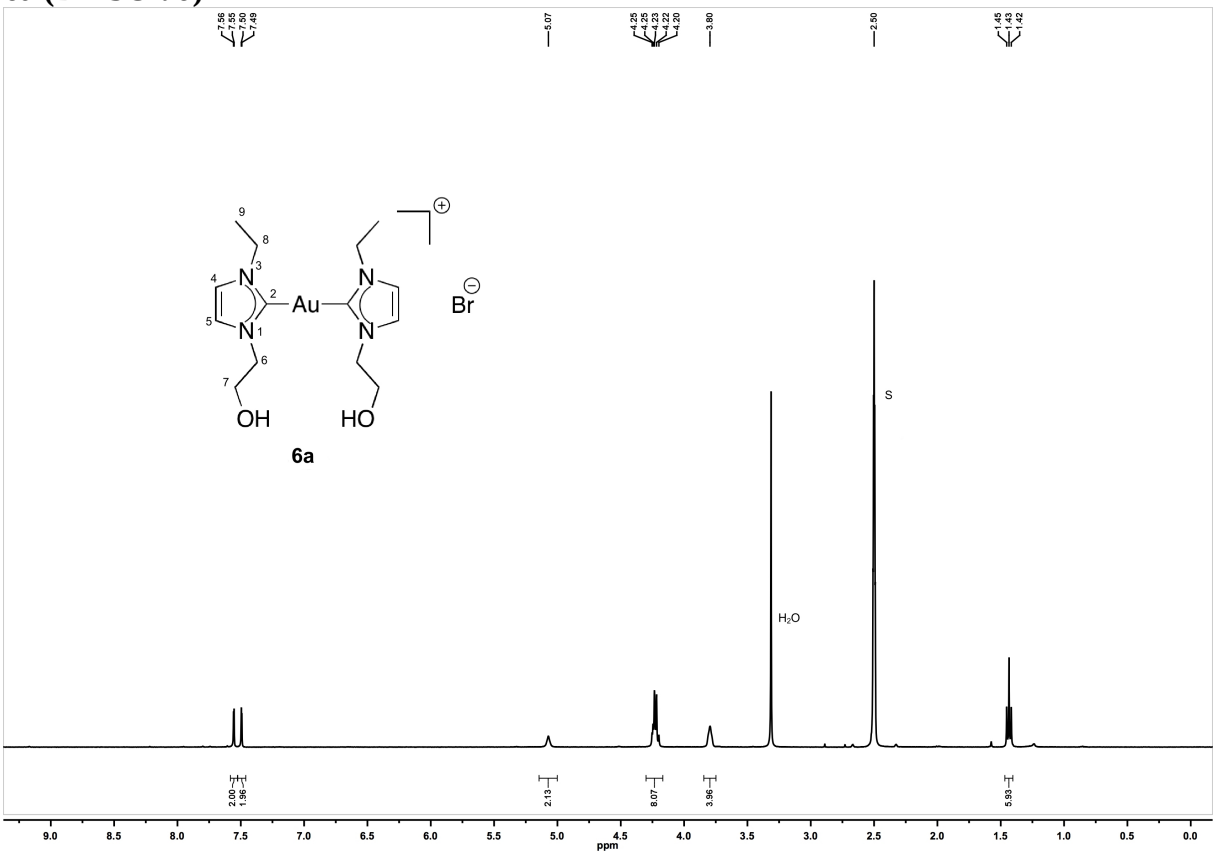
5b

5b (MeCN-*d3*)

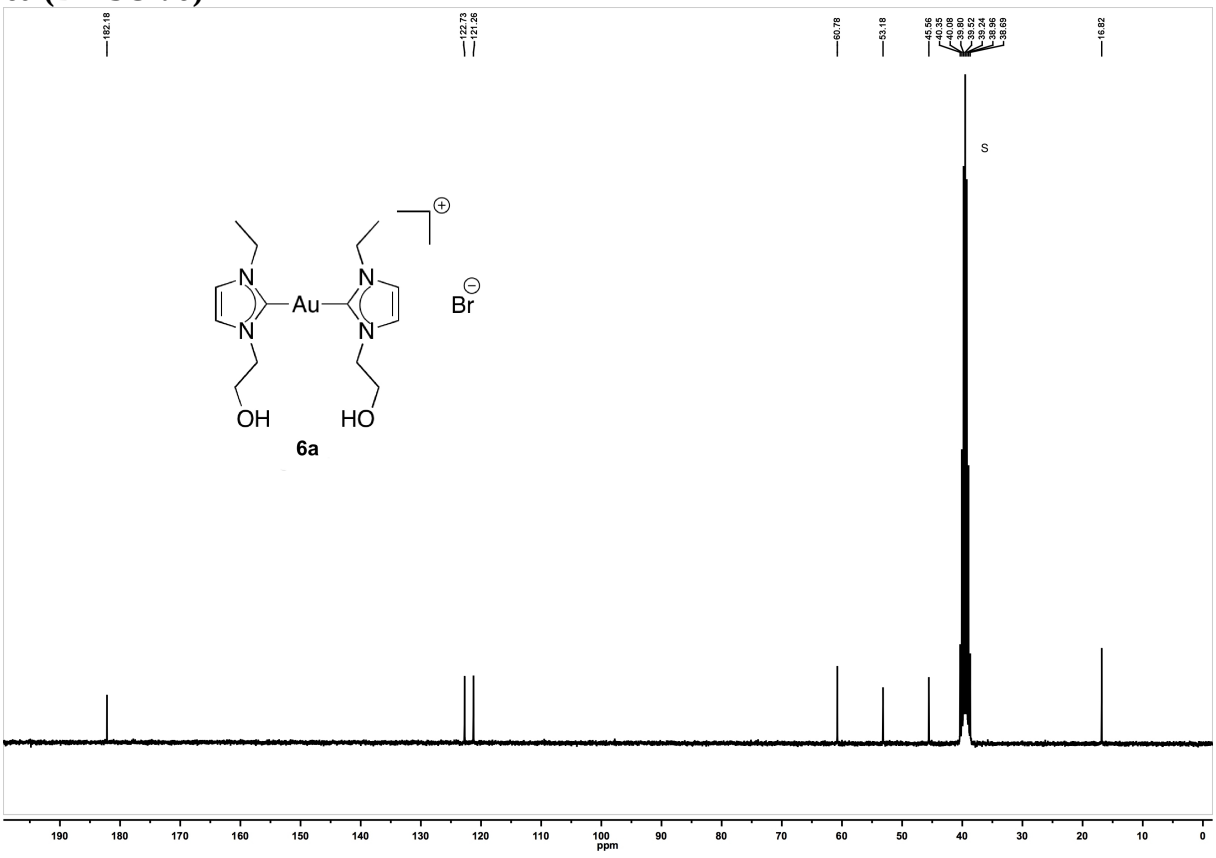


5b

6a (DMSO-*d6*)



6a (DMSO-*d6*)



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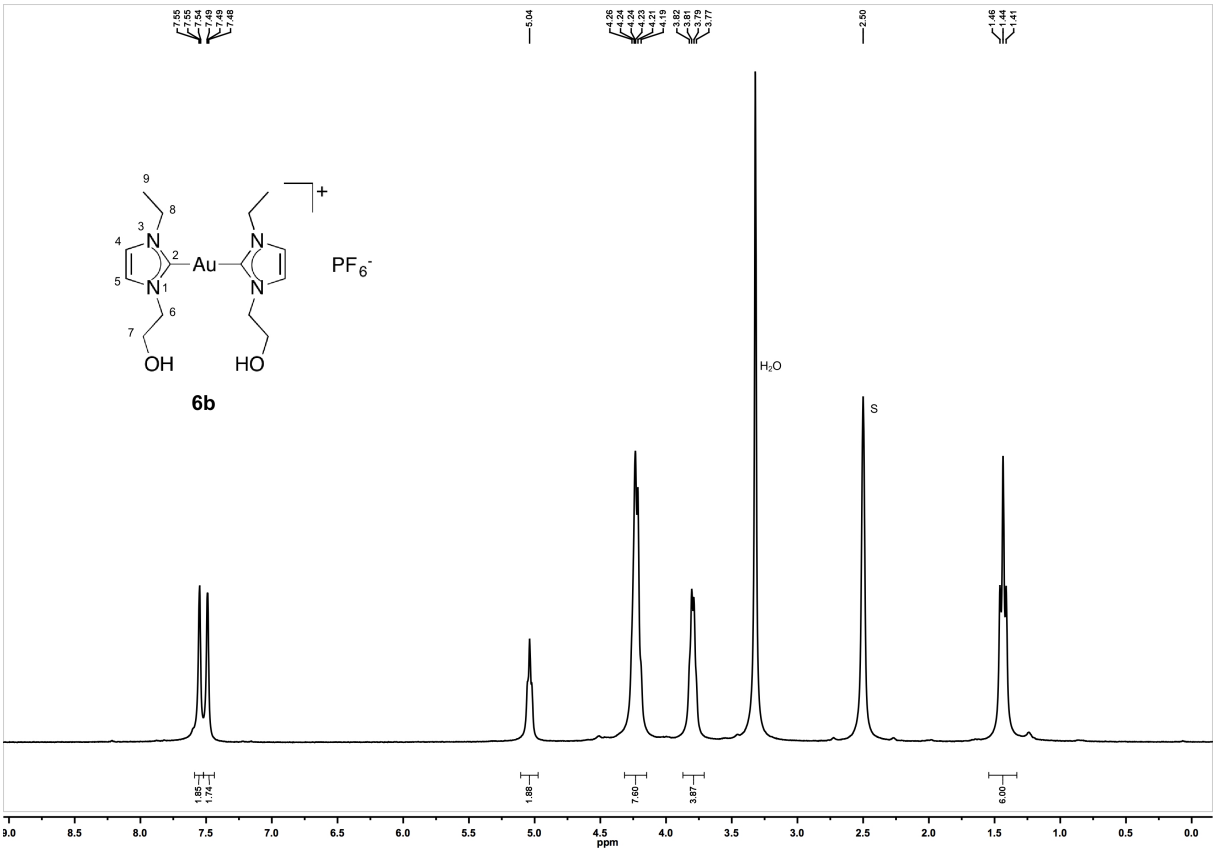
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1.44
1.41
9
8
3
4
N
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Au
N
5
N
1
N
6
7
OH
HO
PF6-
6b
H2O
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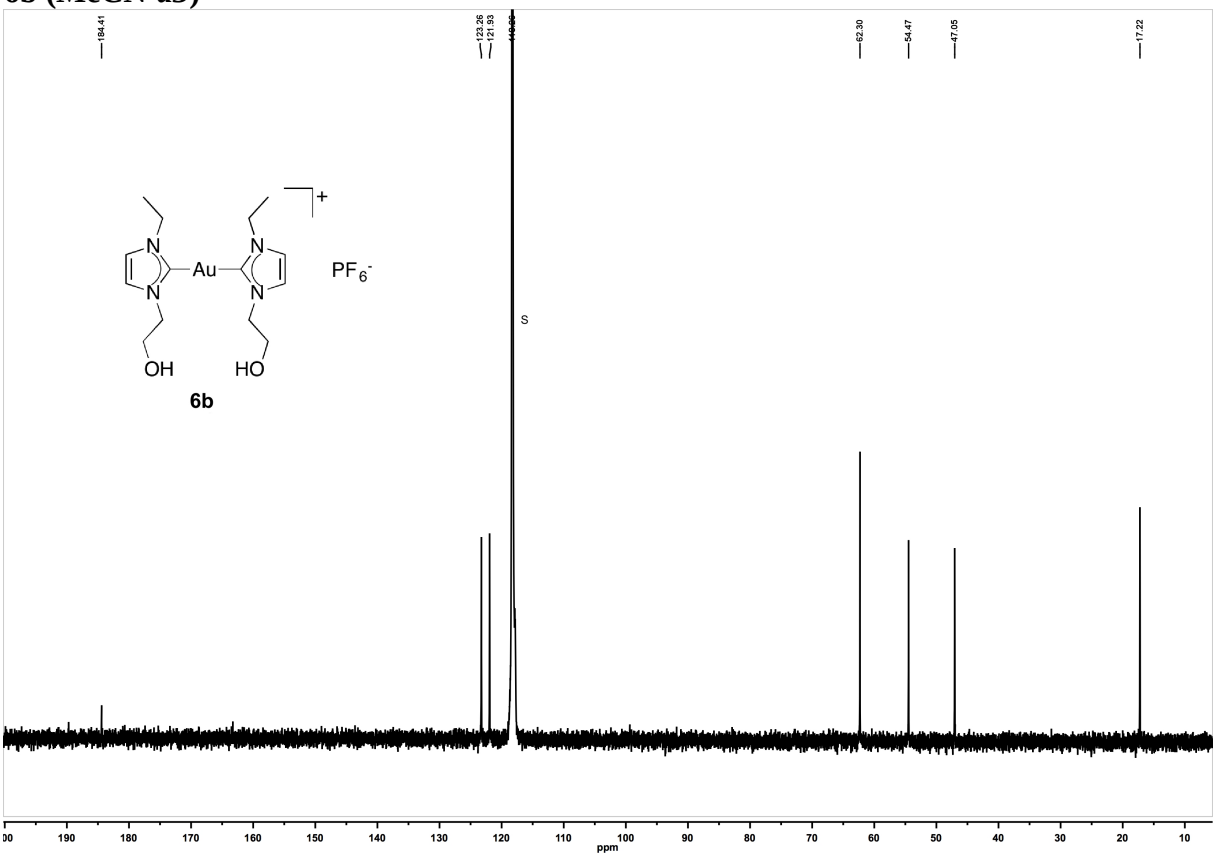
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17.22
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Au
N
N
PF6-
OH
HO
6b
S
190
180
170
160
150
140
130
120
110
100
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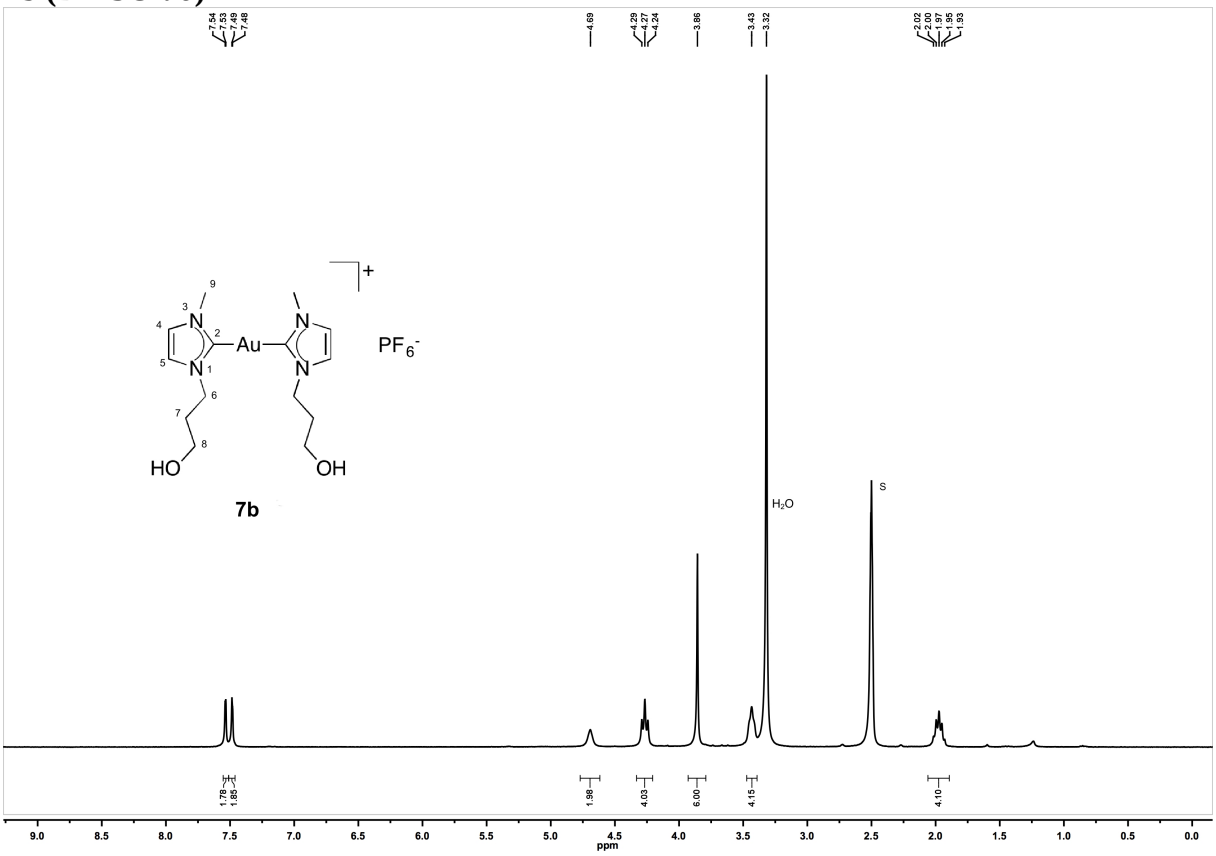
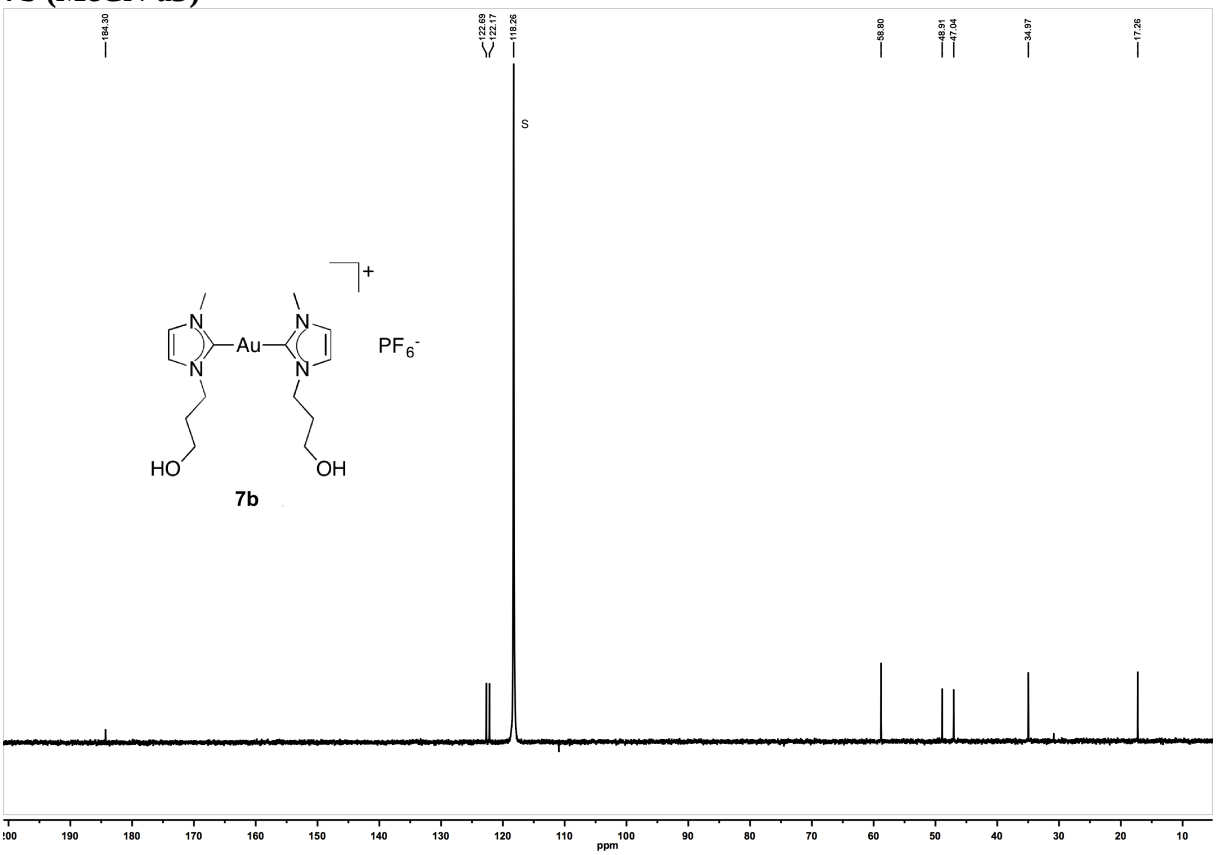
70
60
50
40
30
20
10
ppm

7b (DMSO-*d6*)



7b

7b (MeCN-*d3*)



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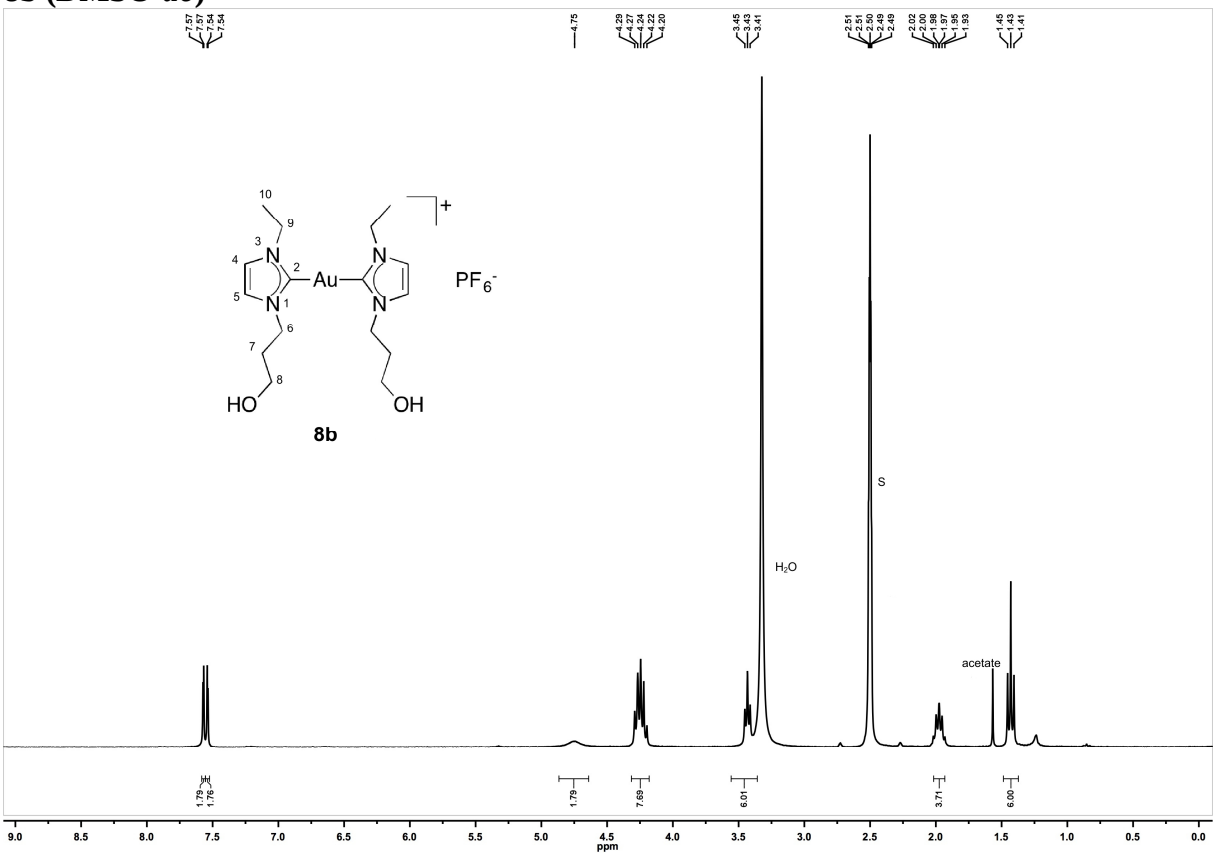
8b (DMSO-*d6*)



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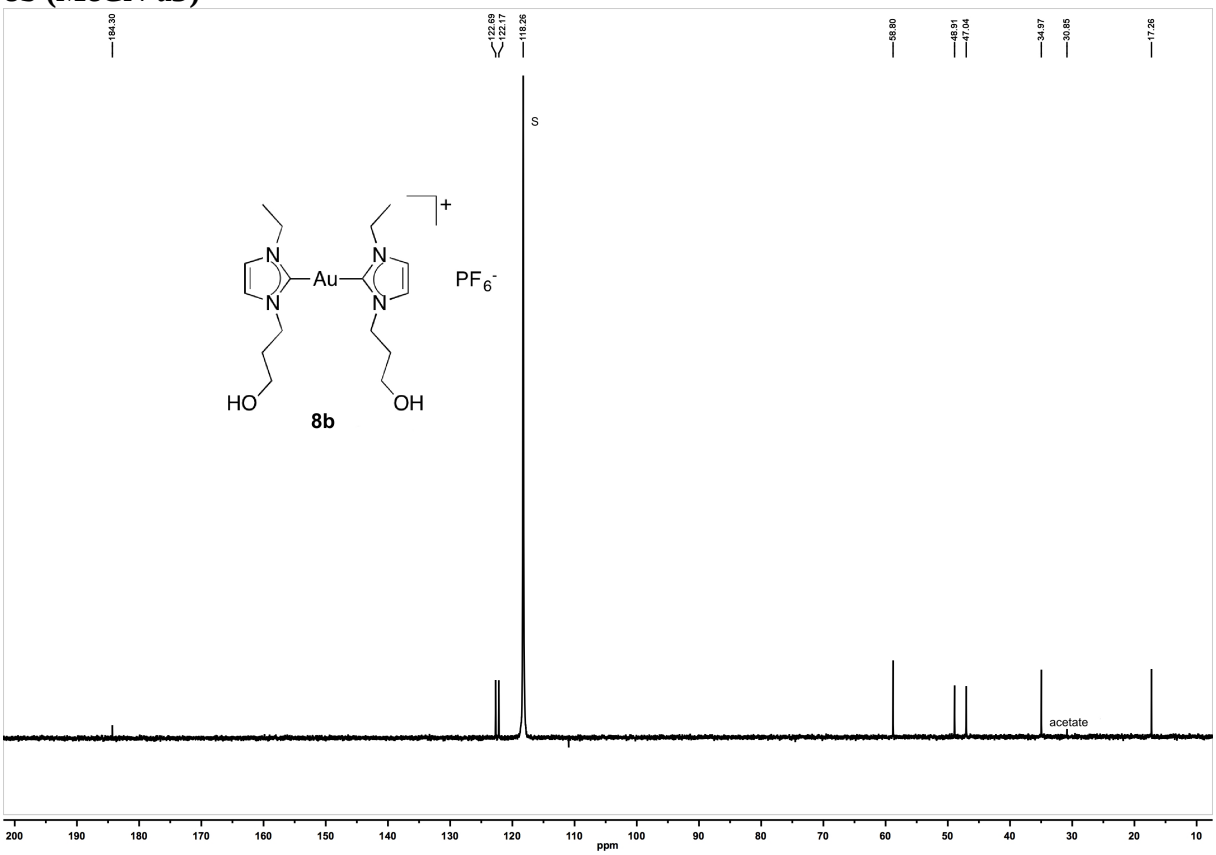

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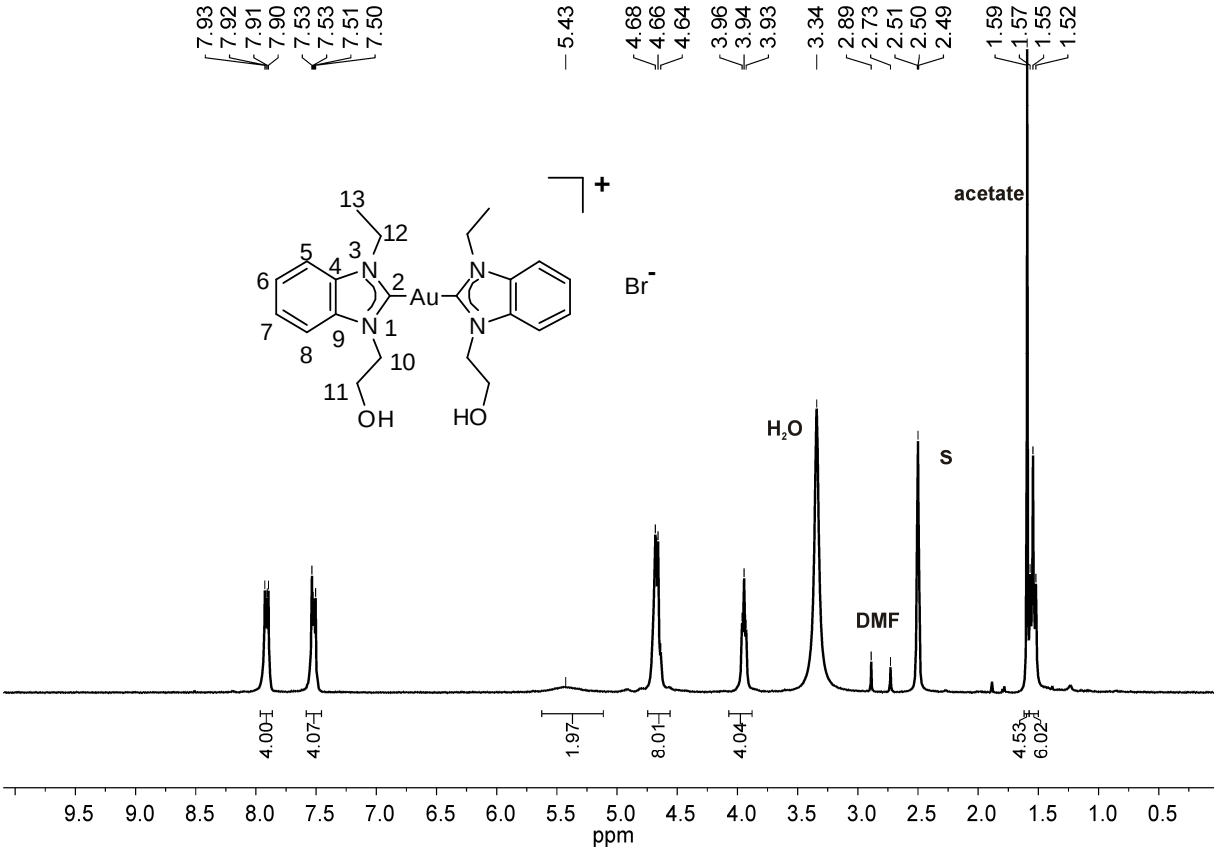

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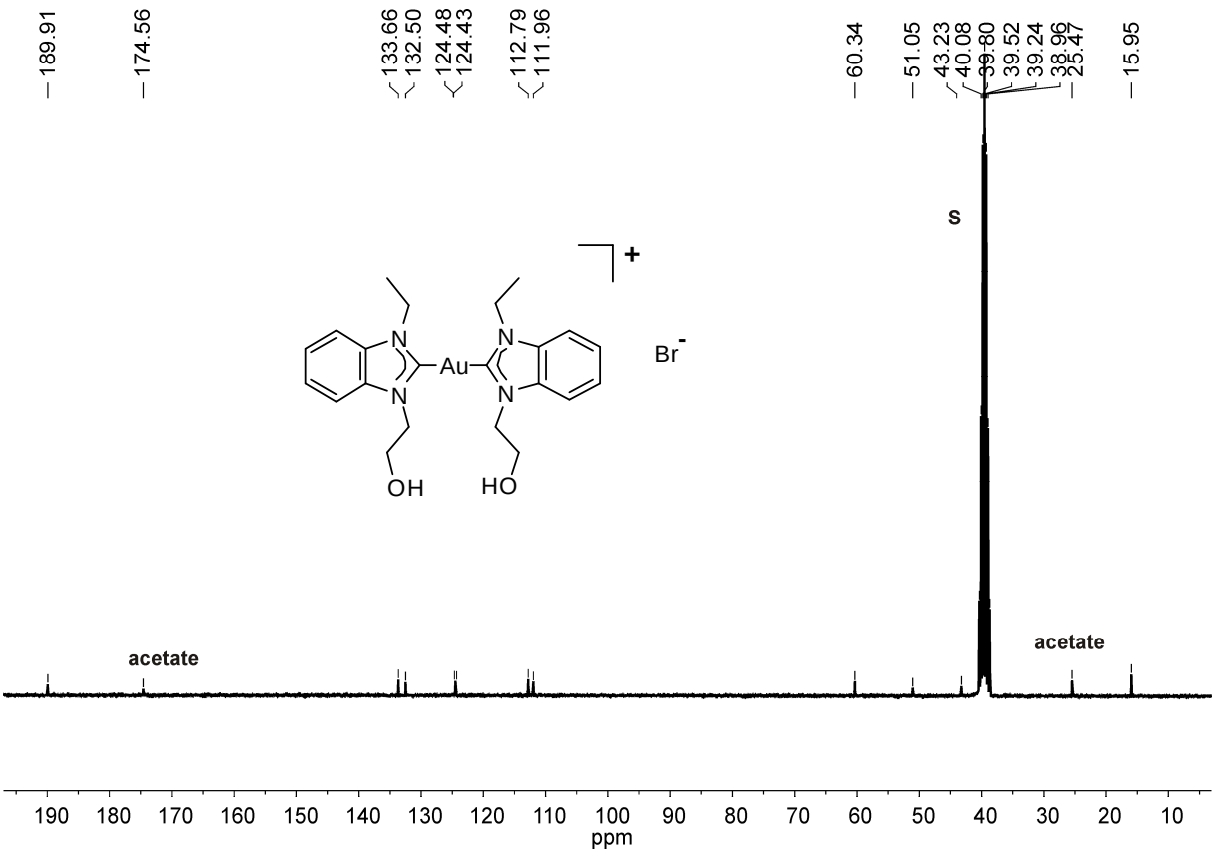

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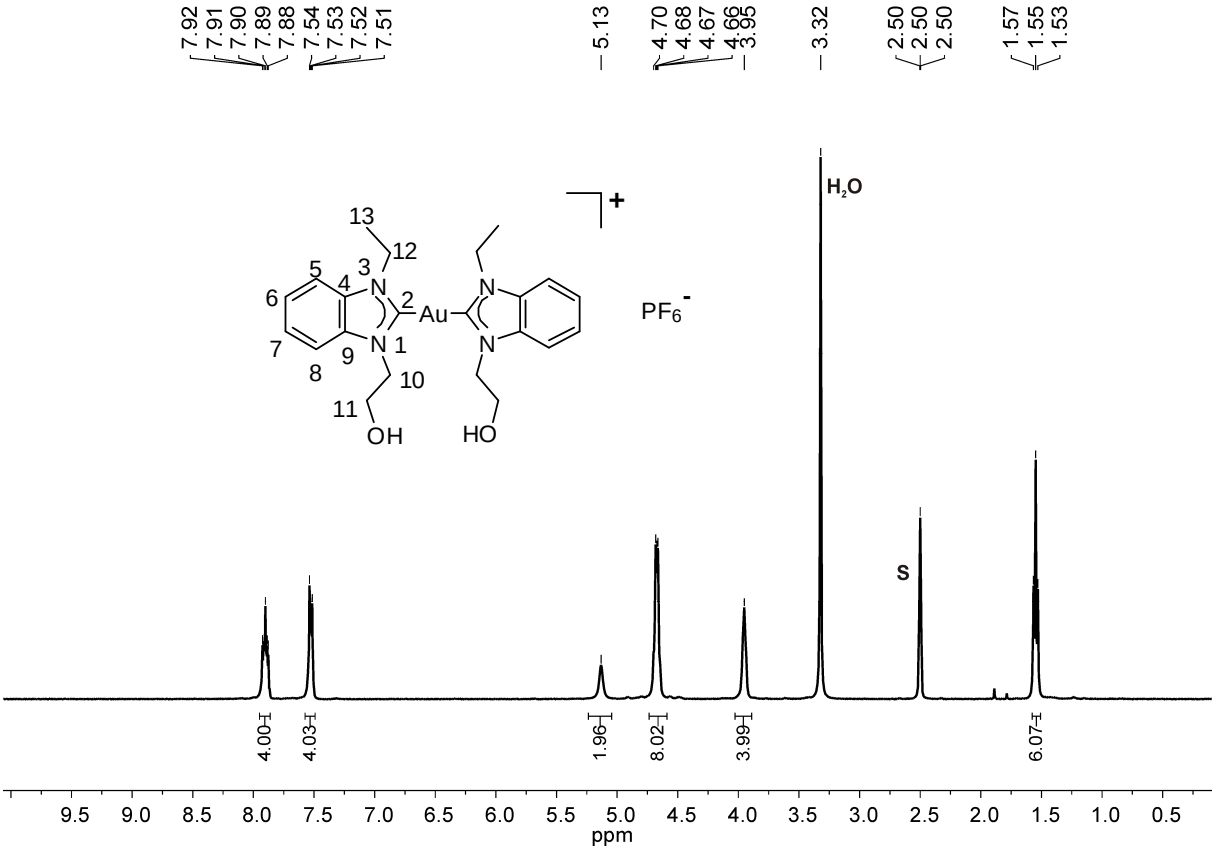

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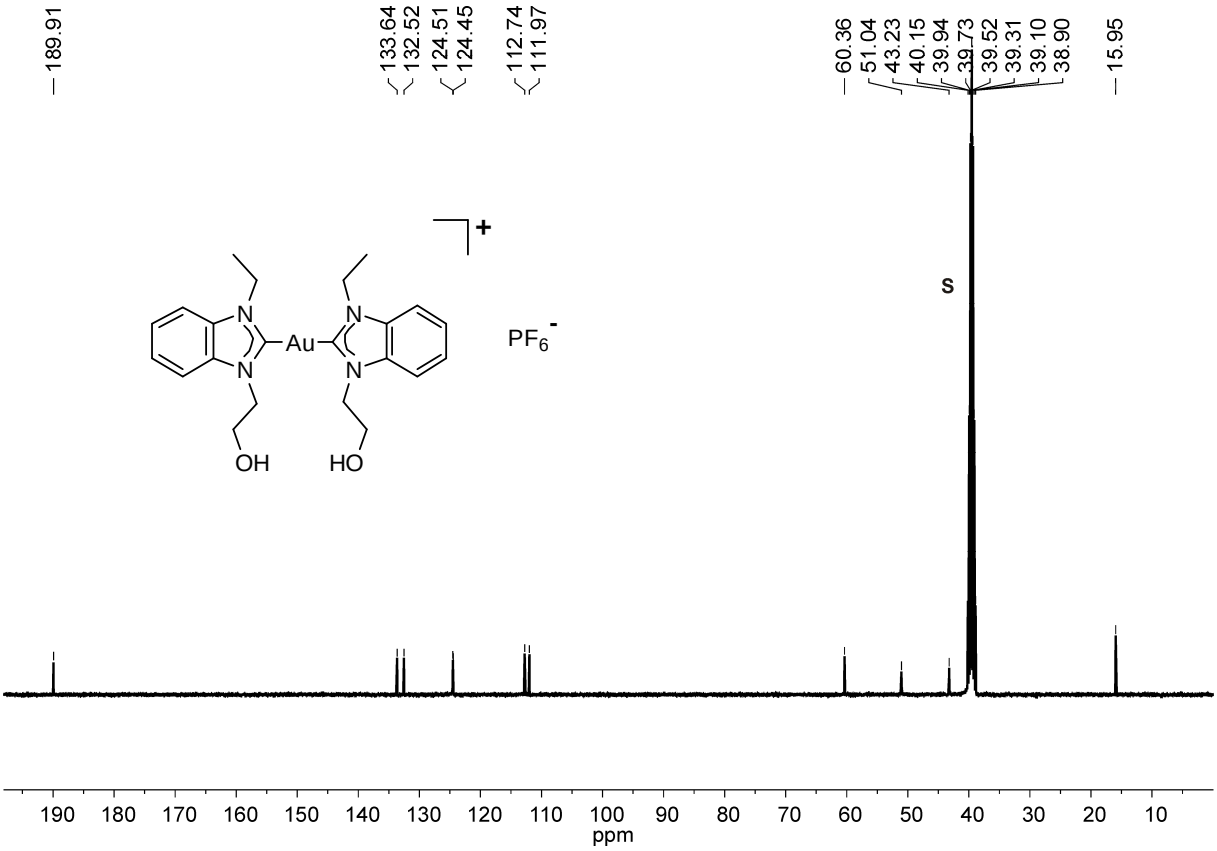

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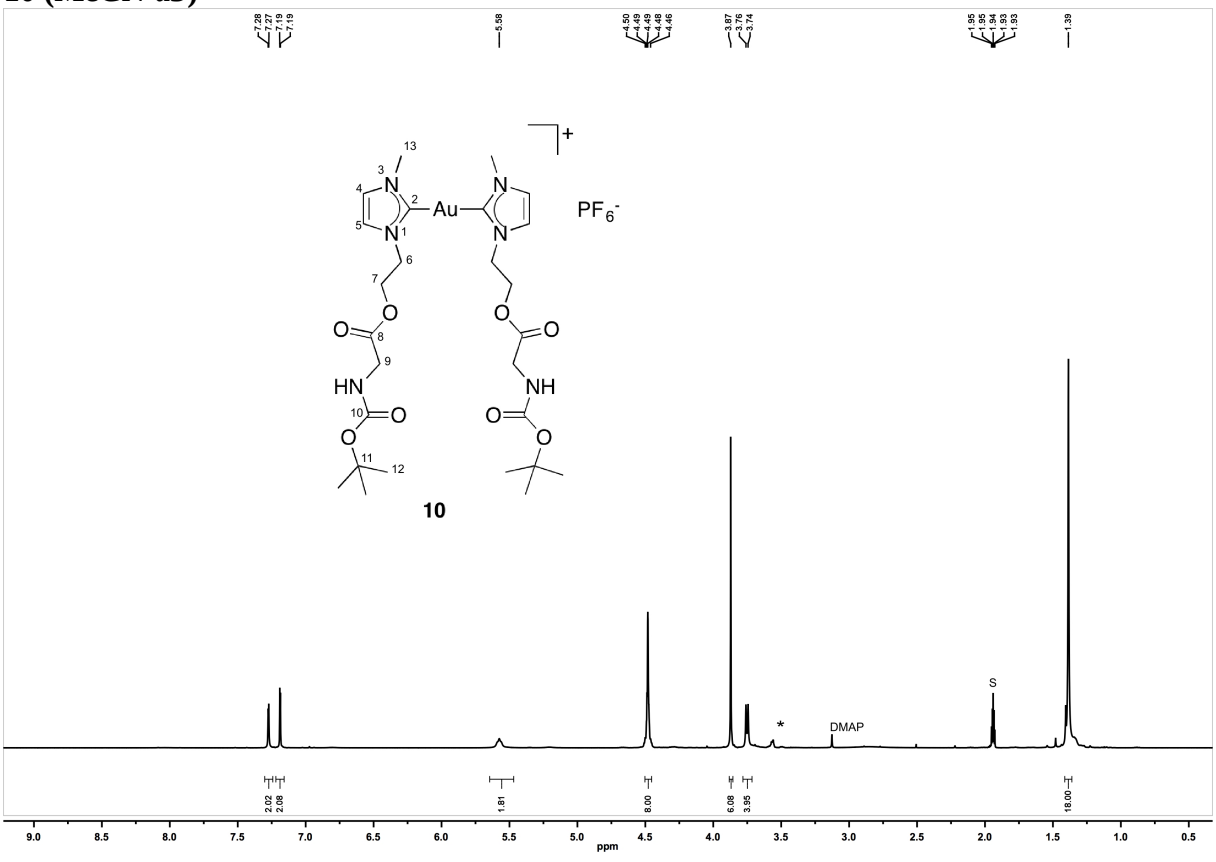

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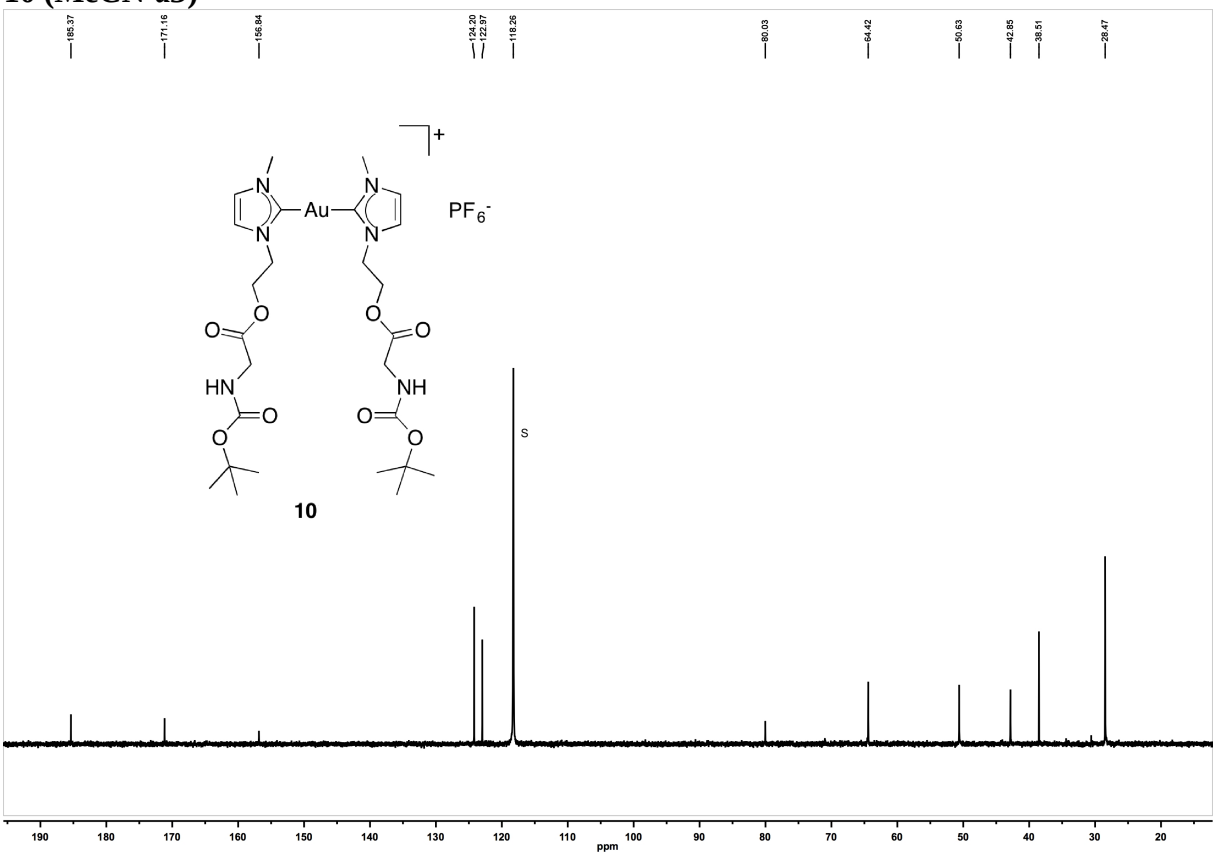

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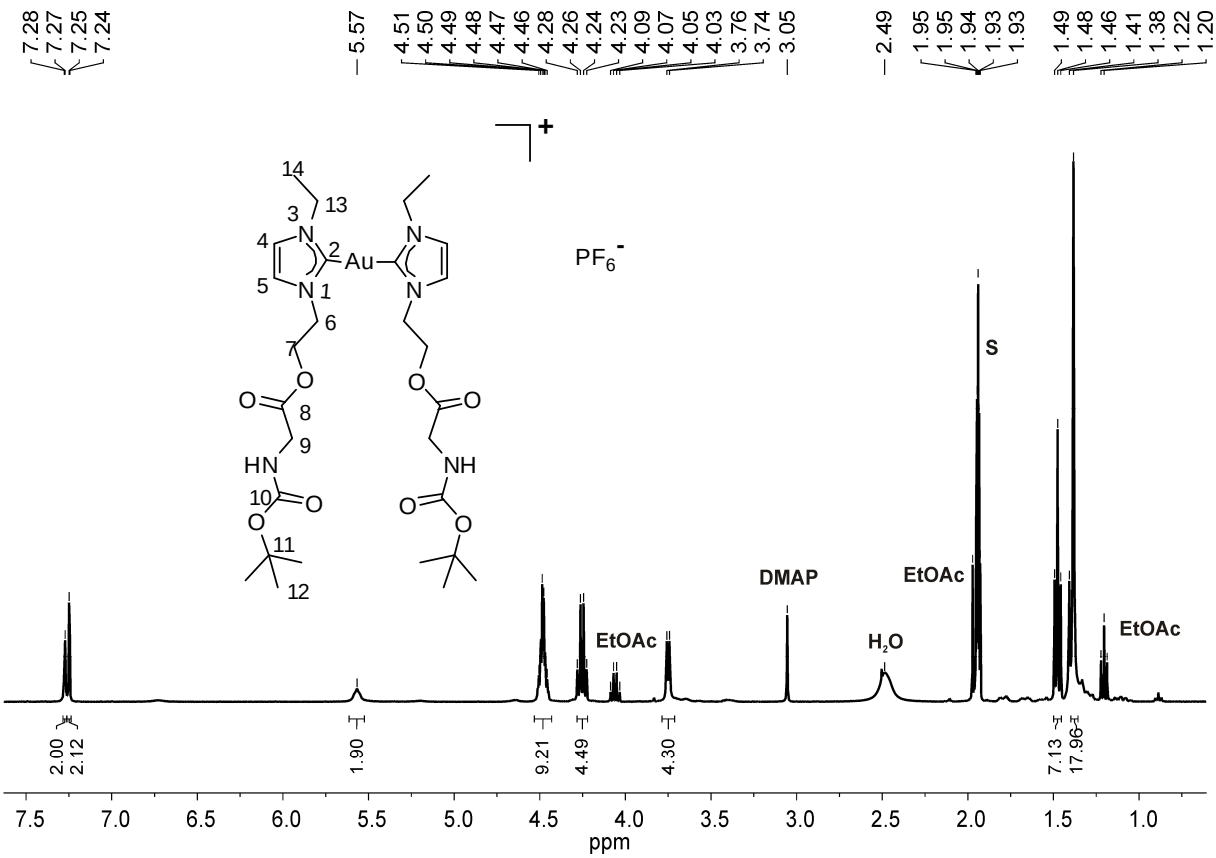
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3.05
2.49
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1.93
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1.41
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DMAP
EtOAc
H2O
EtOAc
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ppm

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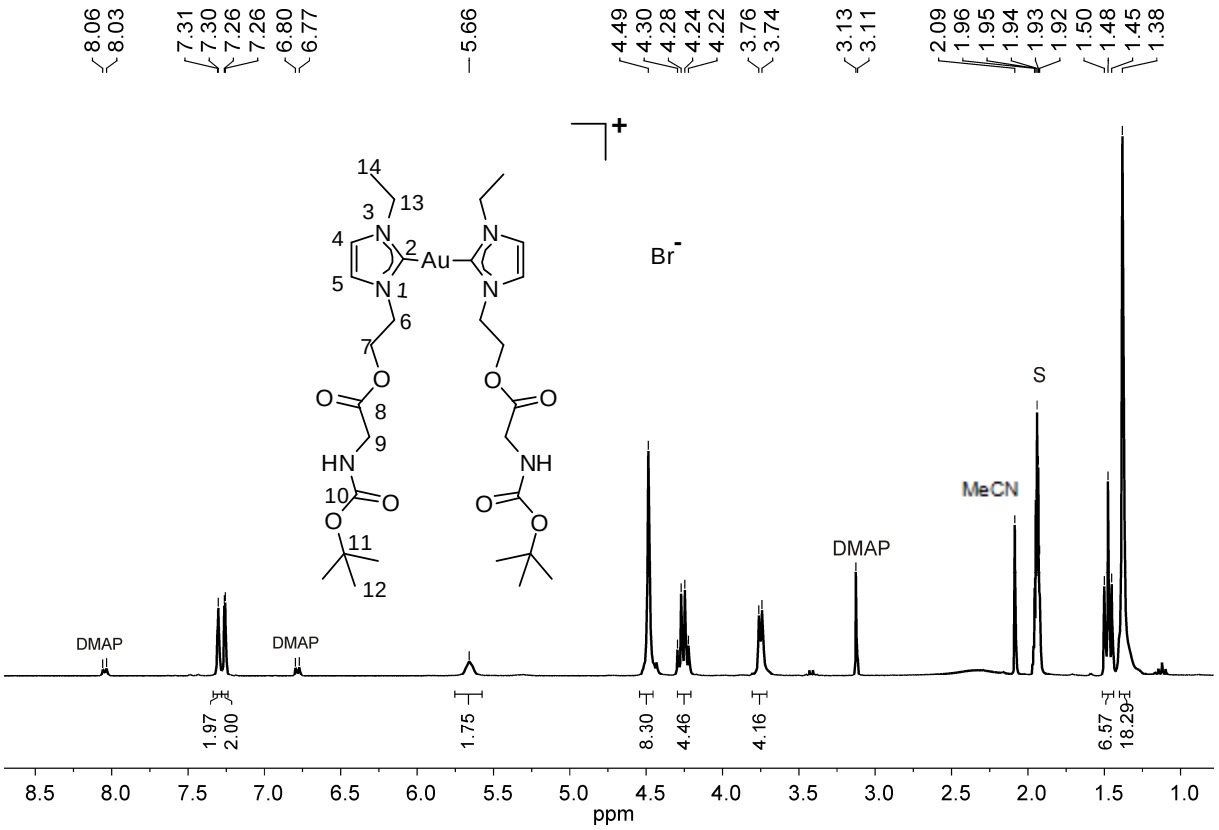

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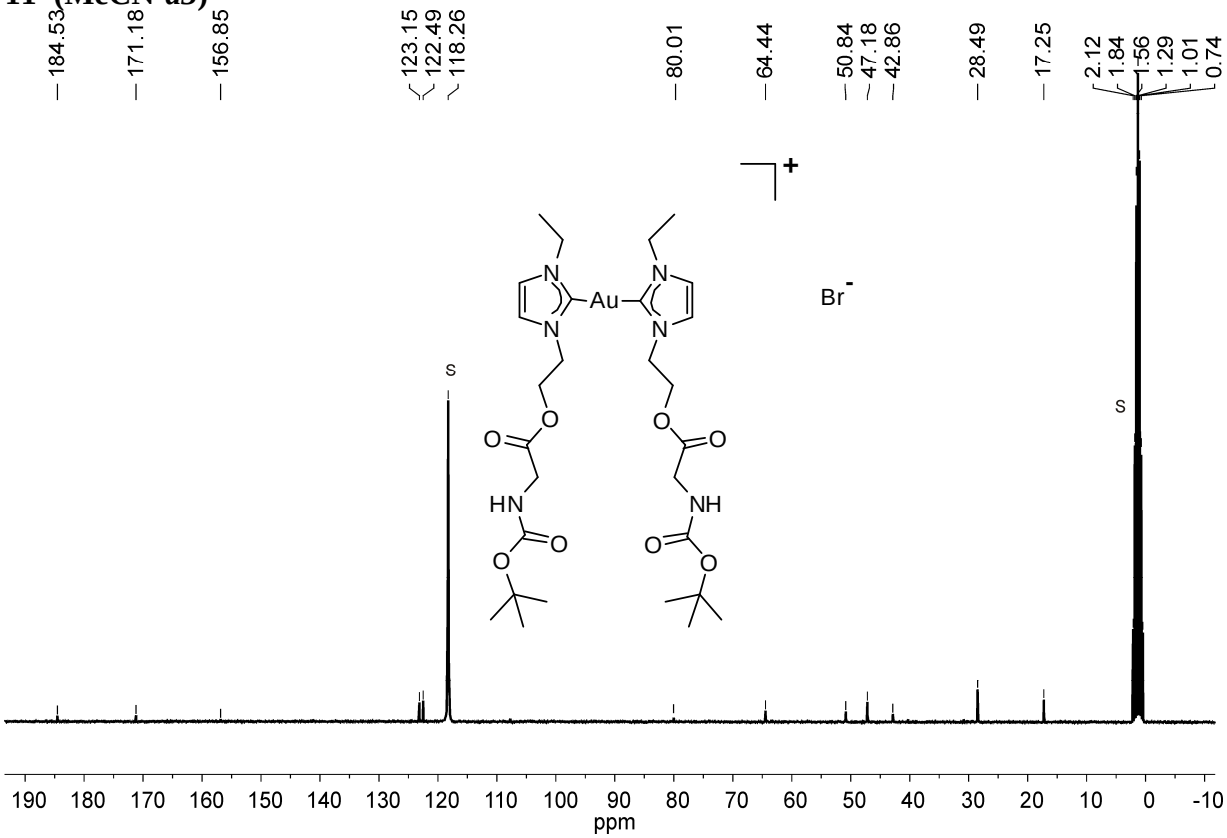

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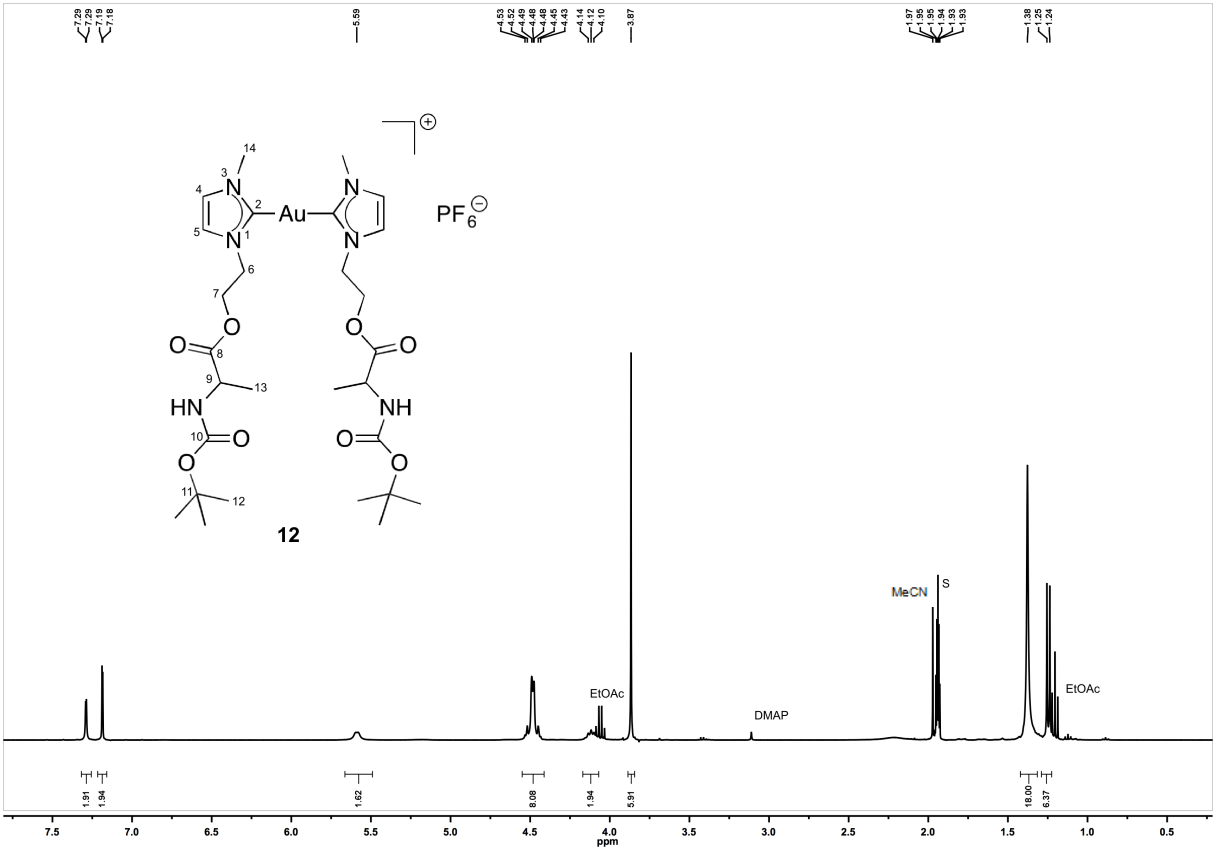

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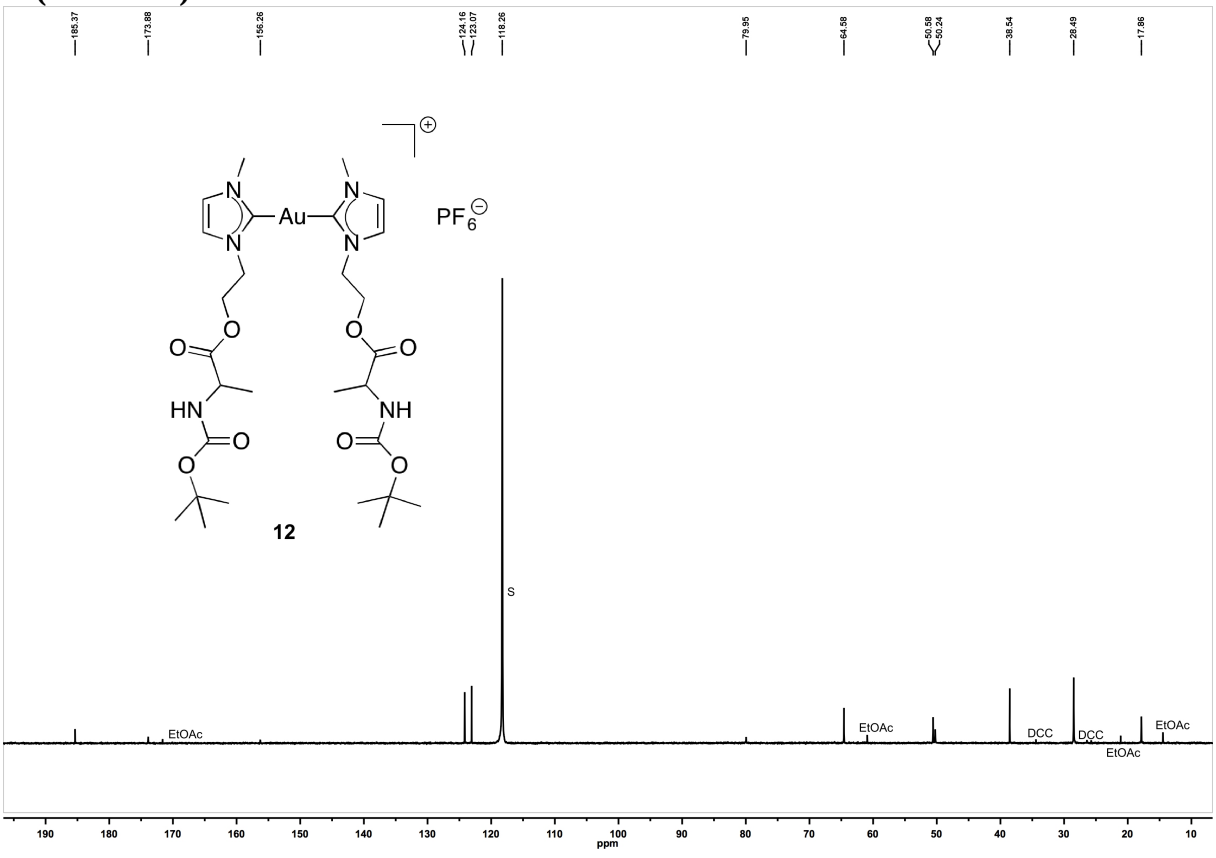

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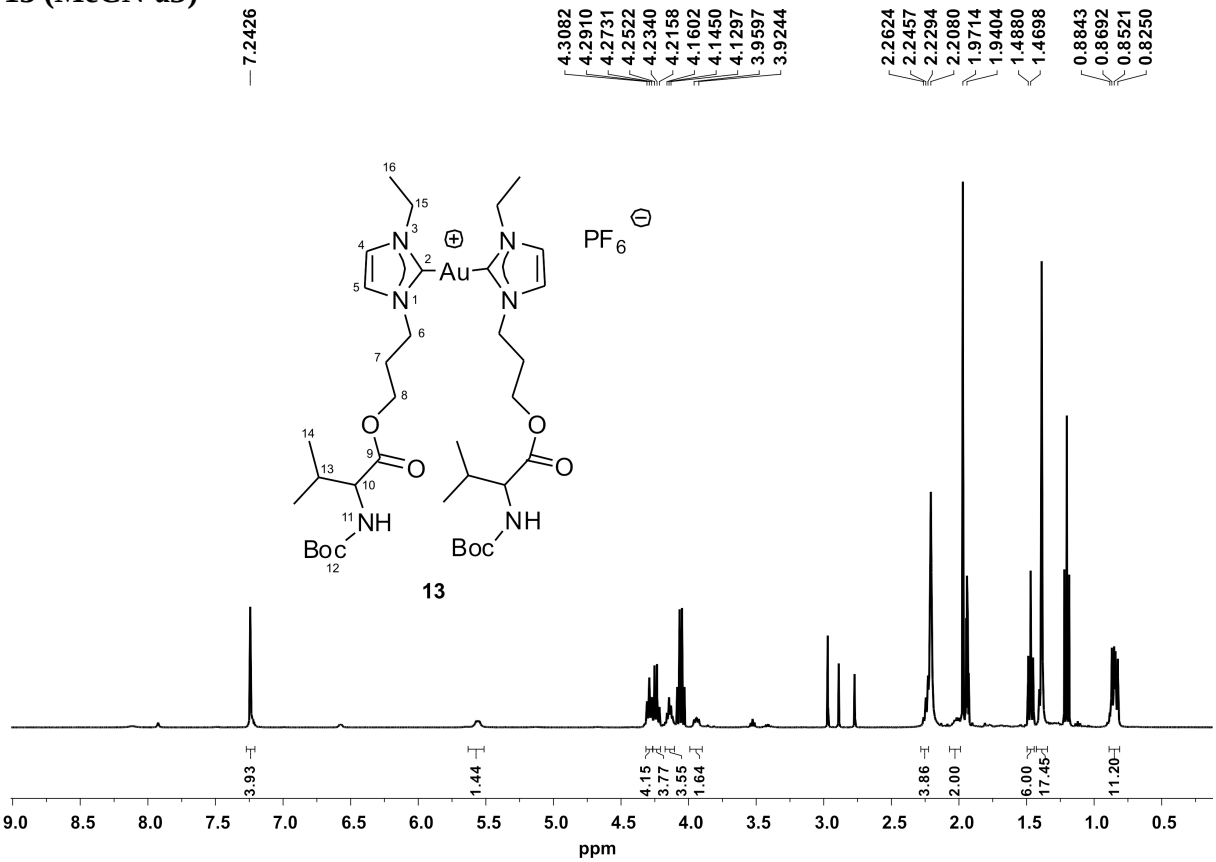

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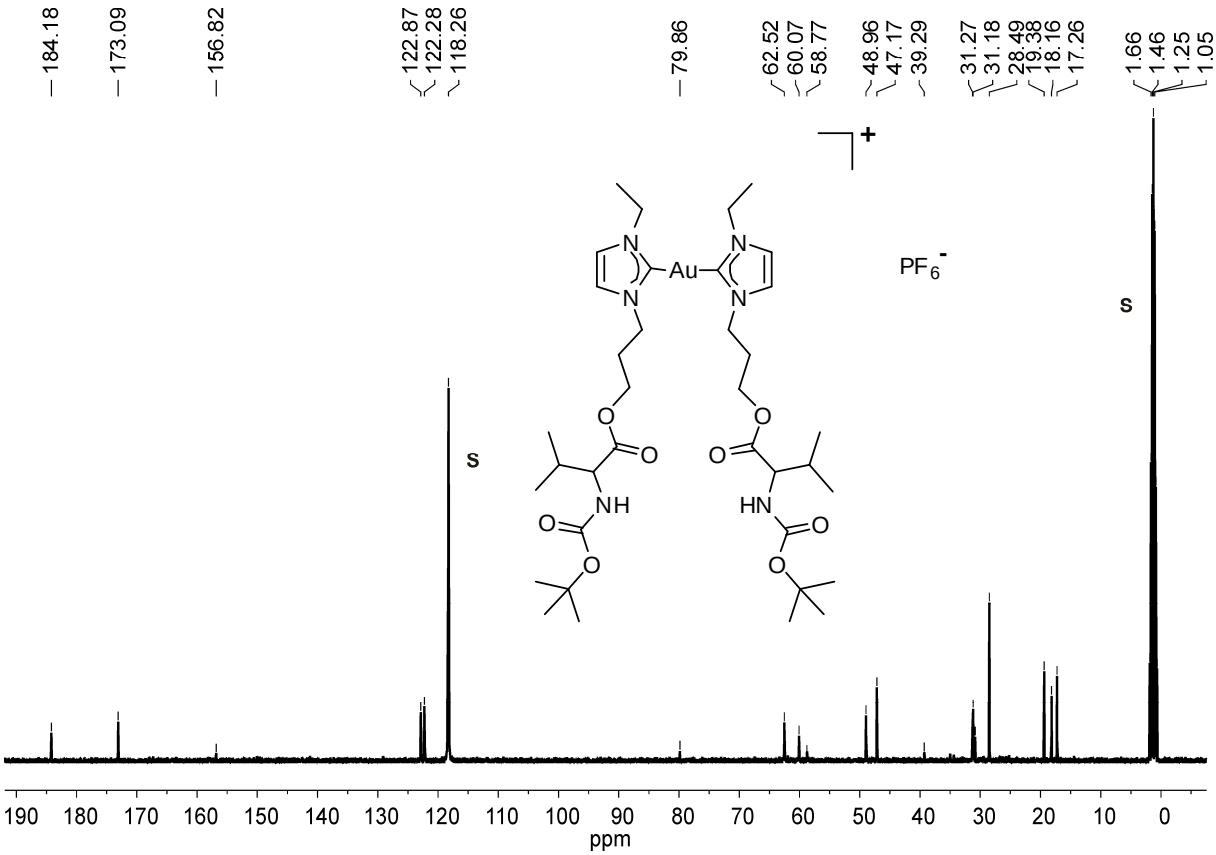

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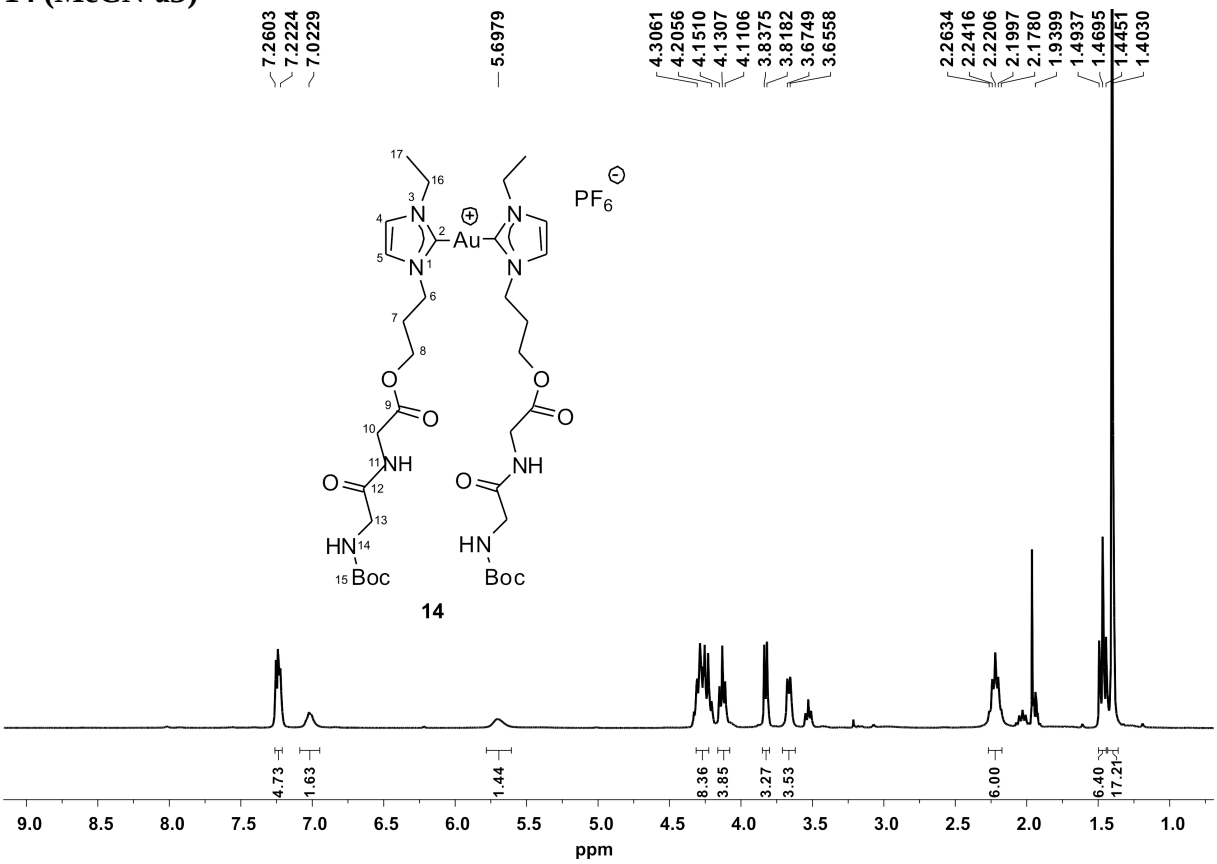

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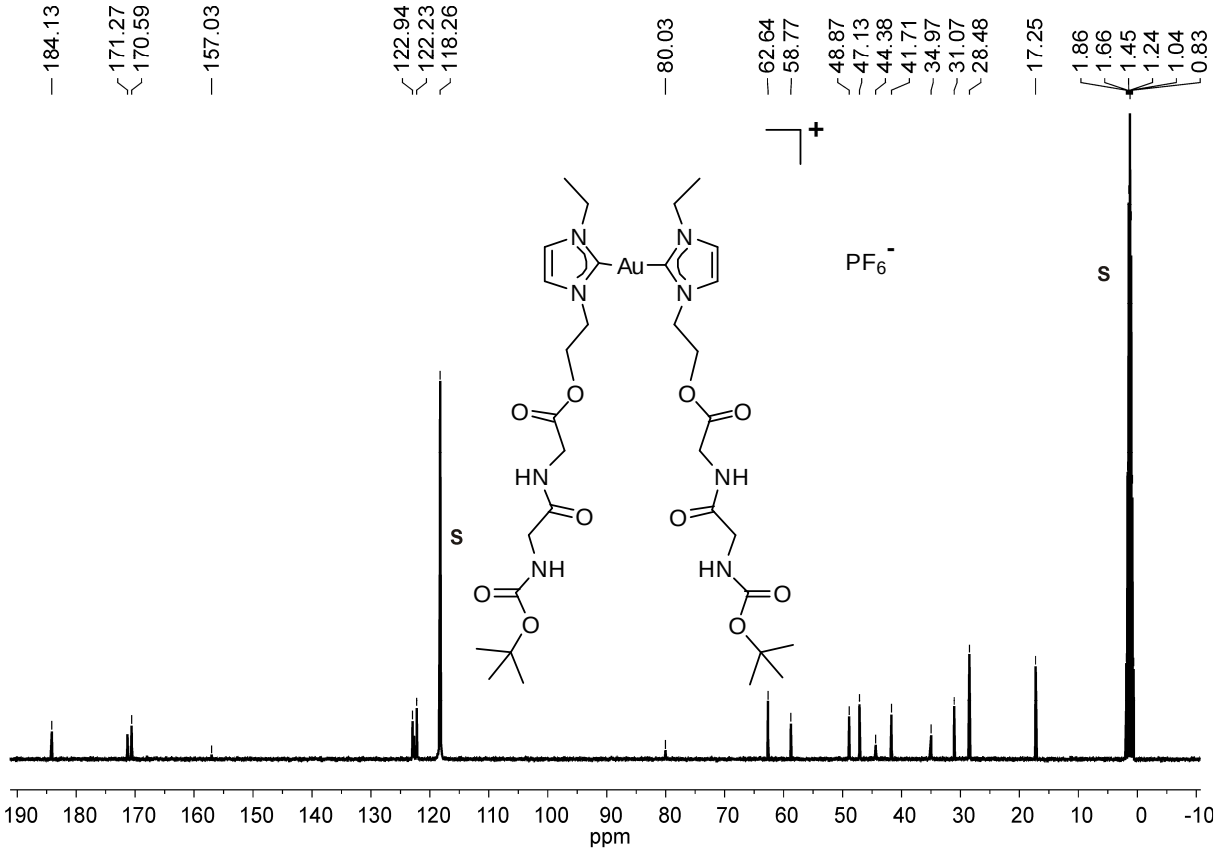

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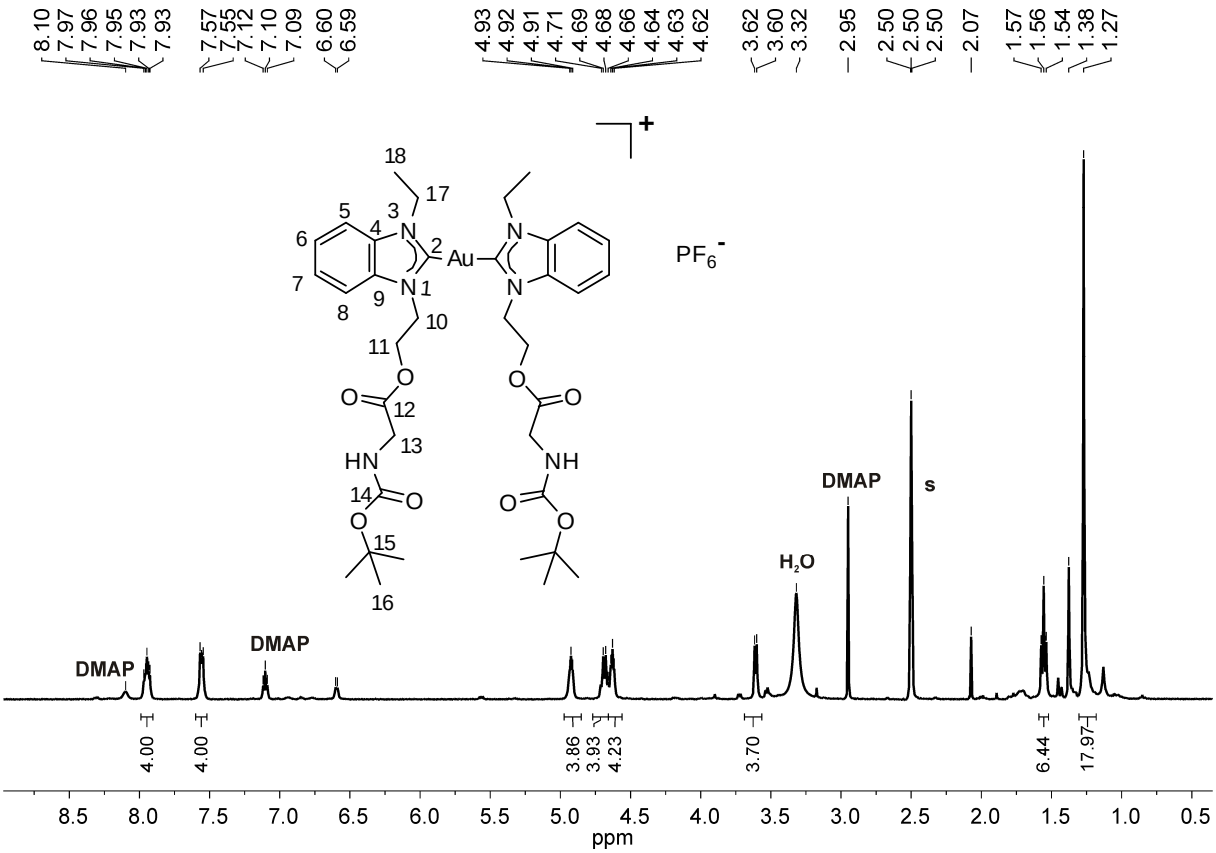

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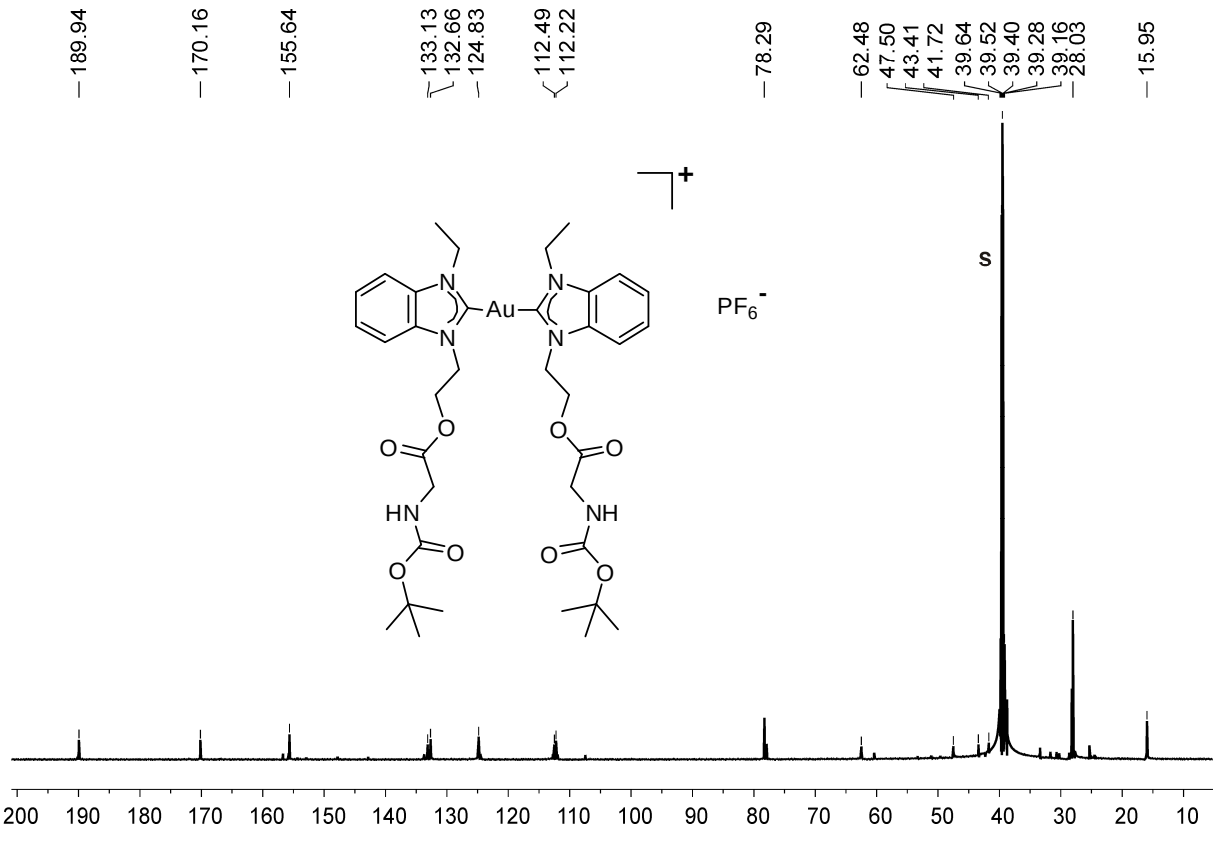

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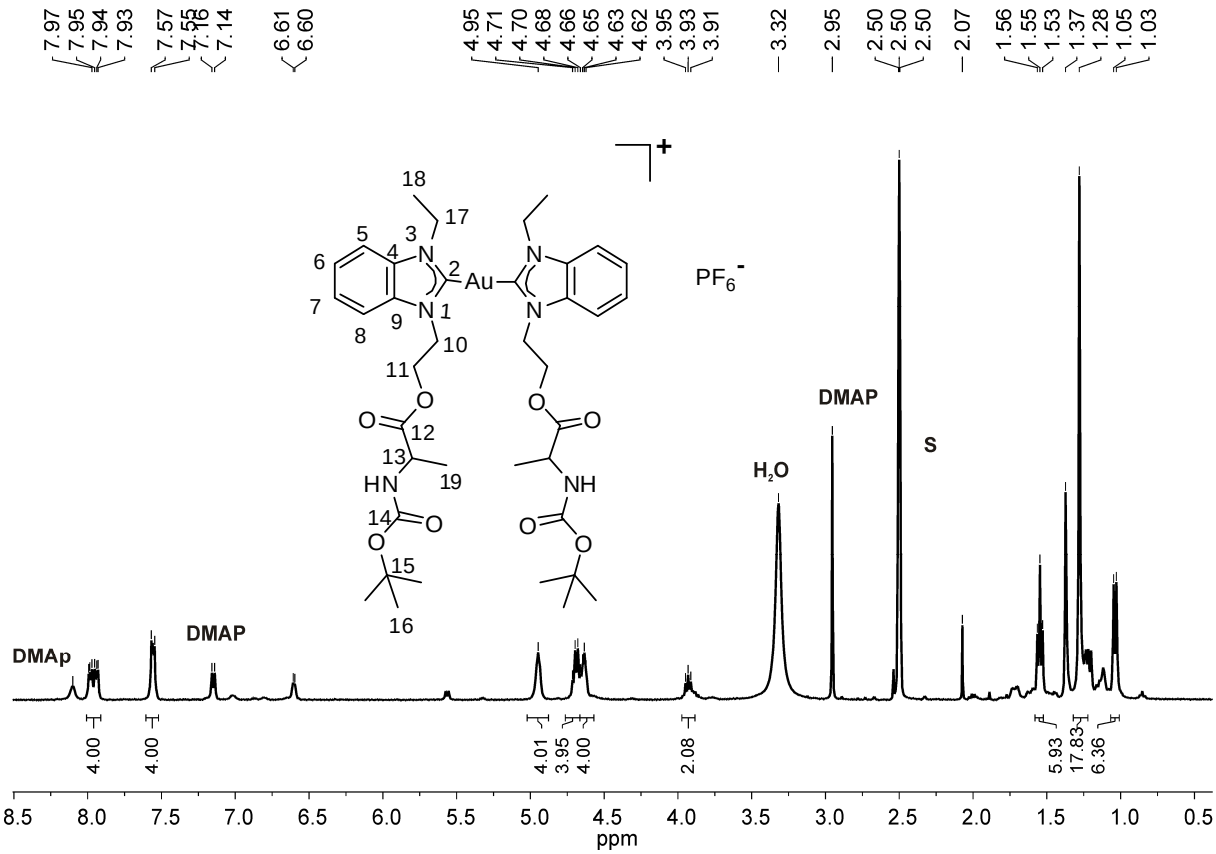

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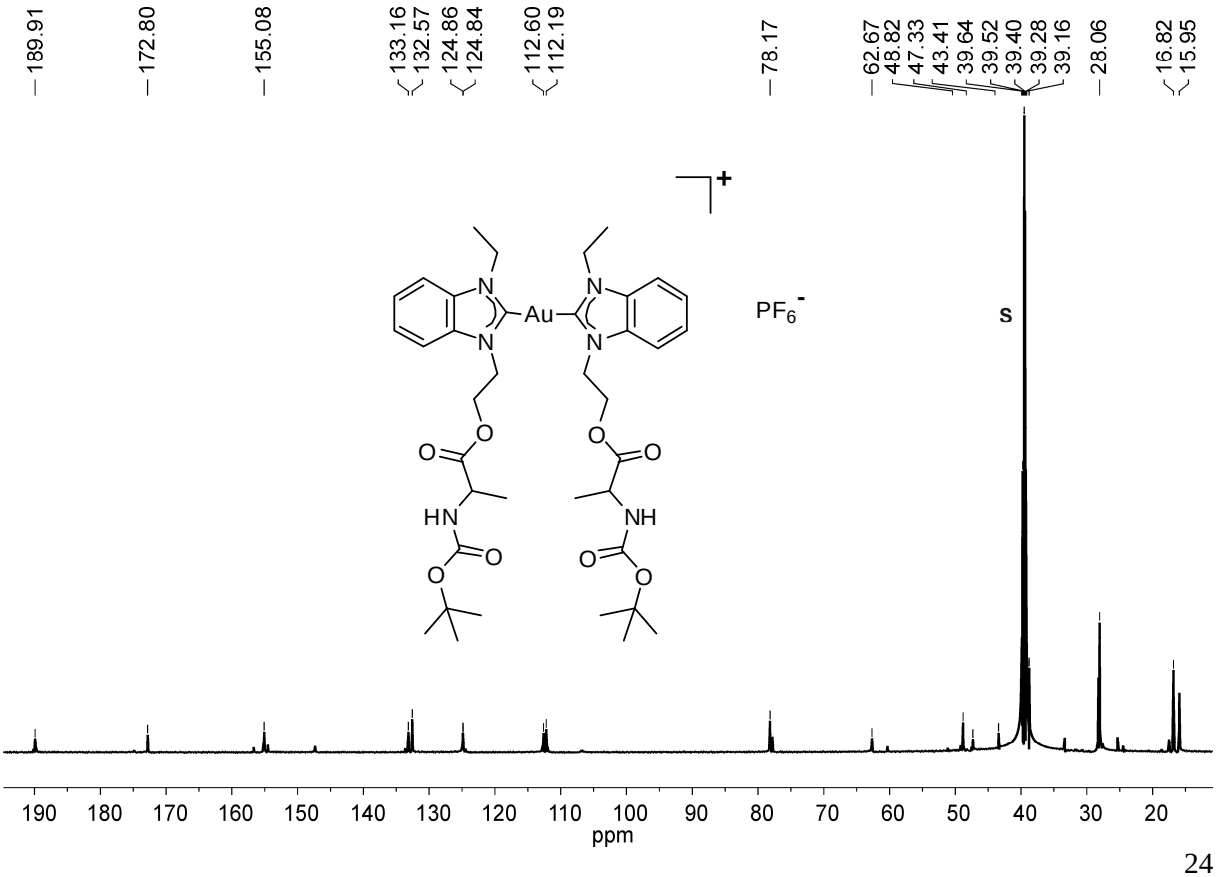

3. Bacterial cell growth assay

Microbiological cell growth experiments were performed to verify putative cytotoxic effects of the heterocyclic Gold(I) compounds. Therefore, *Streptococcus mutans* (Gram-positive) and *Aggregatibacter actinomycetemcomitans* (Gram-negative) (DSMZ, Braunschweig, Germany) were grown in brain heart infusion broth (BHI; BD Difco, Le Pont de Claix, France) according to the manufacturer´s protocol at 37°C. Bacterial growth of liquid cell cultures was quantified photometrically by reading the optical density at 600 nm hourly over a period of 24 hours. The non-peptide heterocyclic substances were added to the cell culture at final concentrations of 10/30/100 µM at the beginning of the experiments. All experiments were carried out in triplicates (n=3).

All compounds being tested failed to affect cell growth of both bacteria strains at all concentrations up to 0.1 mM.