Supporting Information

Studies on gold(I) and gold(III) alcohol functionalised NHC complexes

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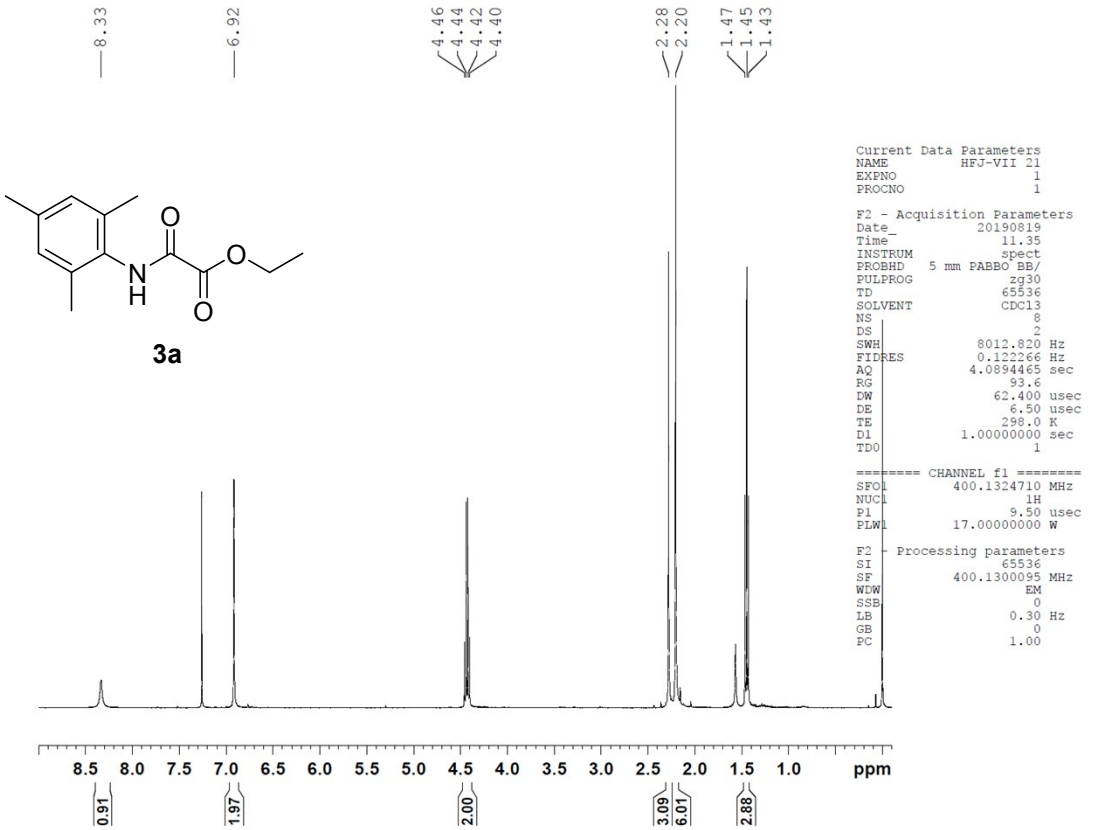
^{1}H and ^{13}C NMR spectra of:

^{1}H and ^{13}C NMR Spectra

^{1}H NMR data for compound **3a**



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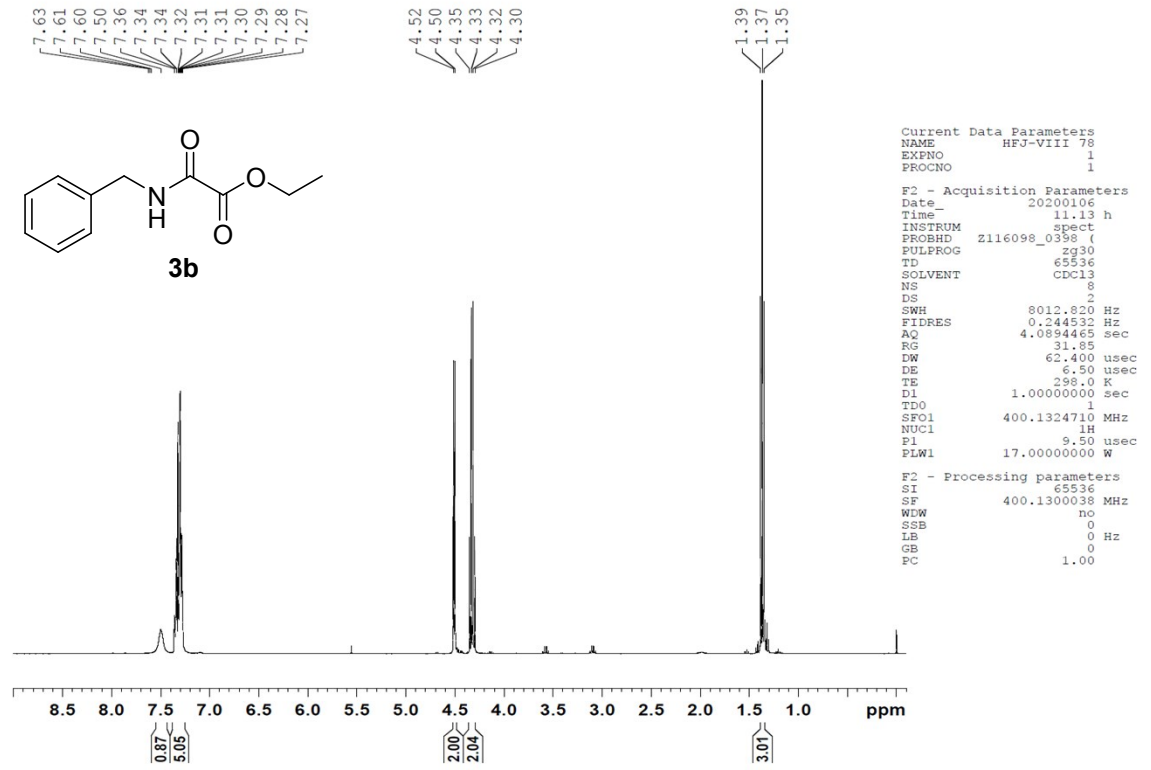

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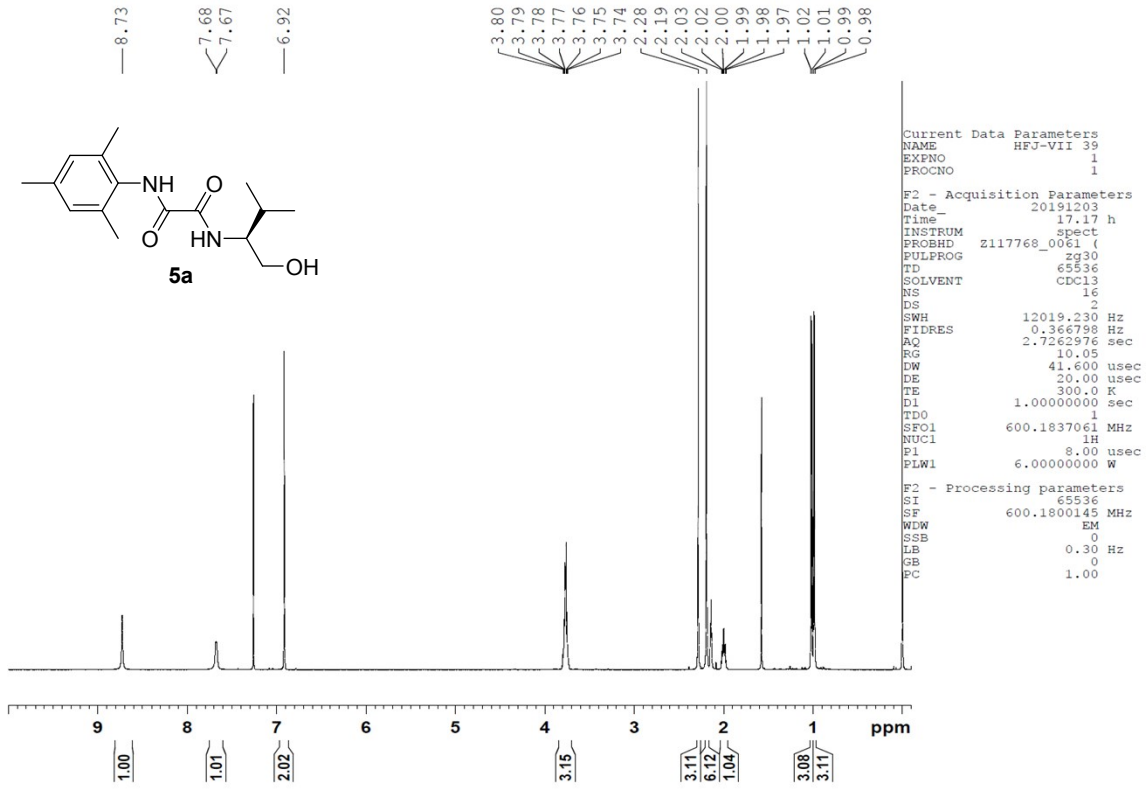

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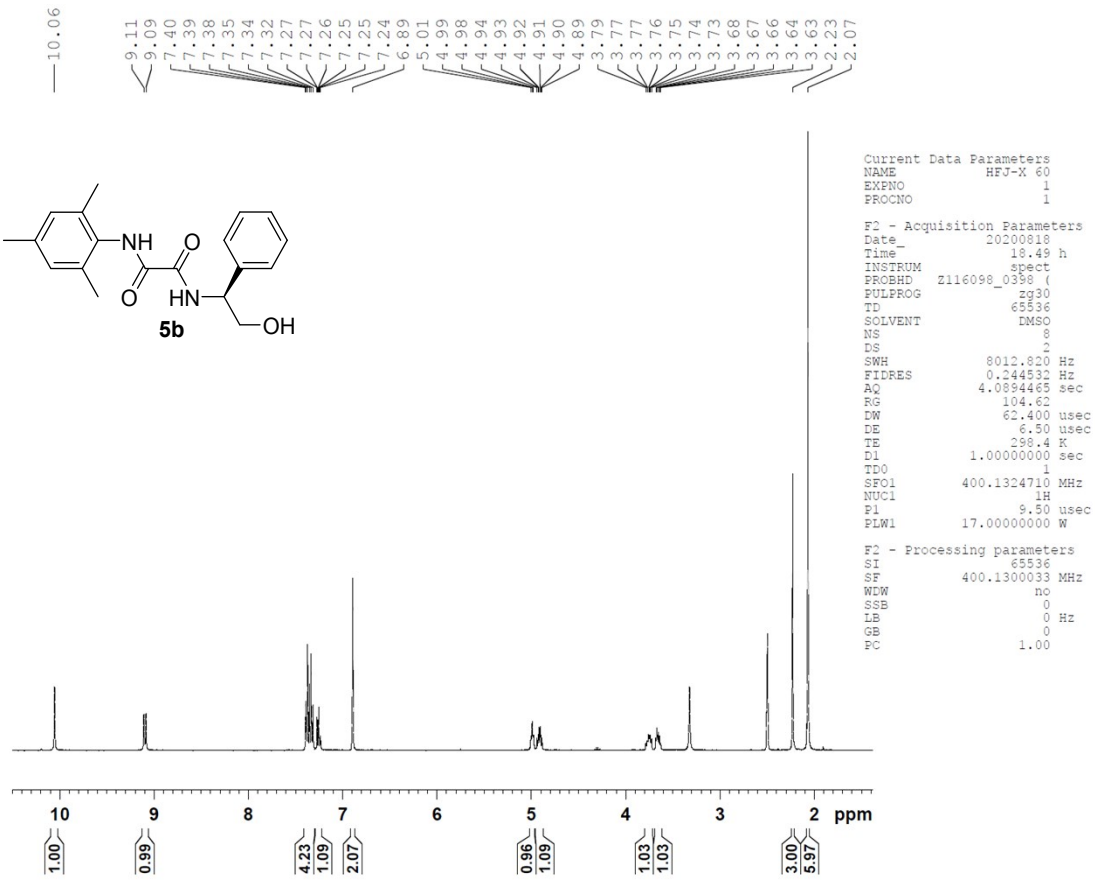

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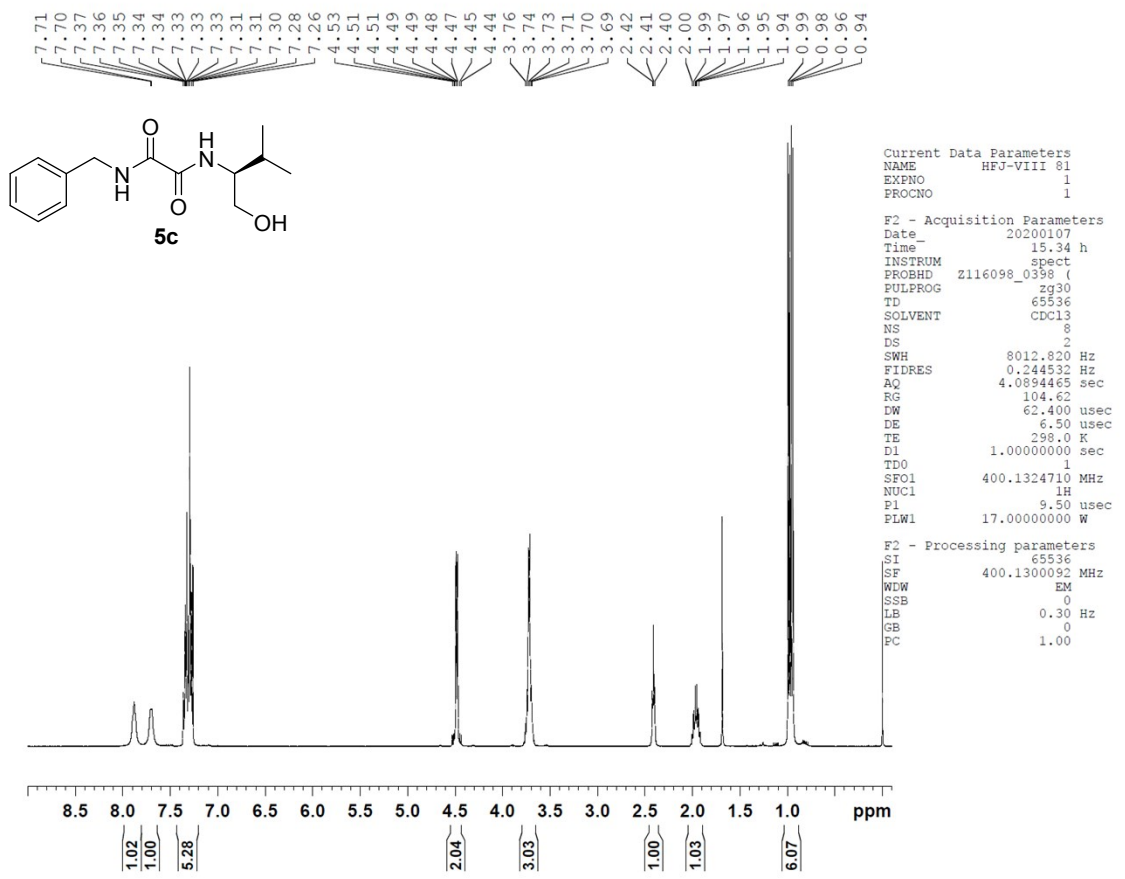

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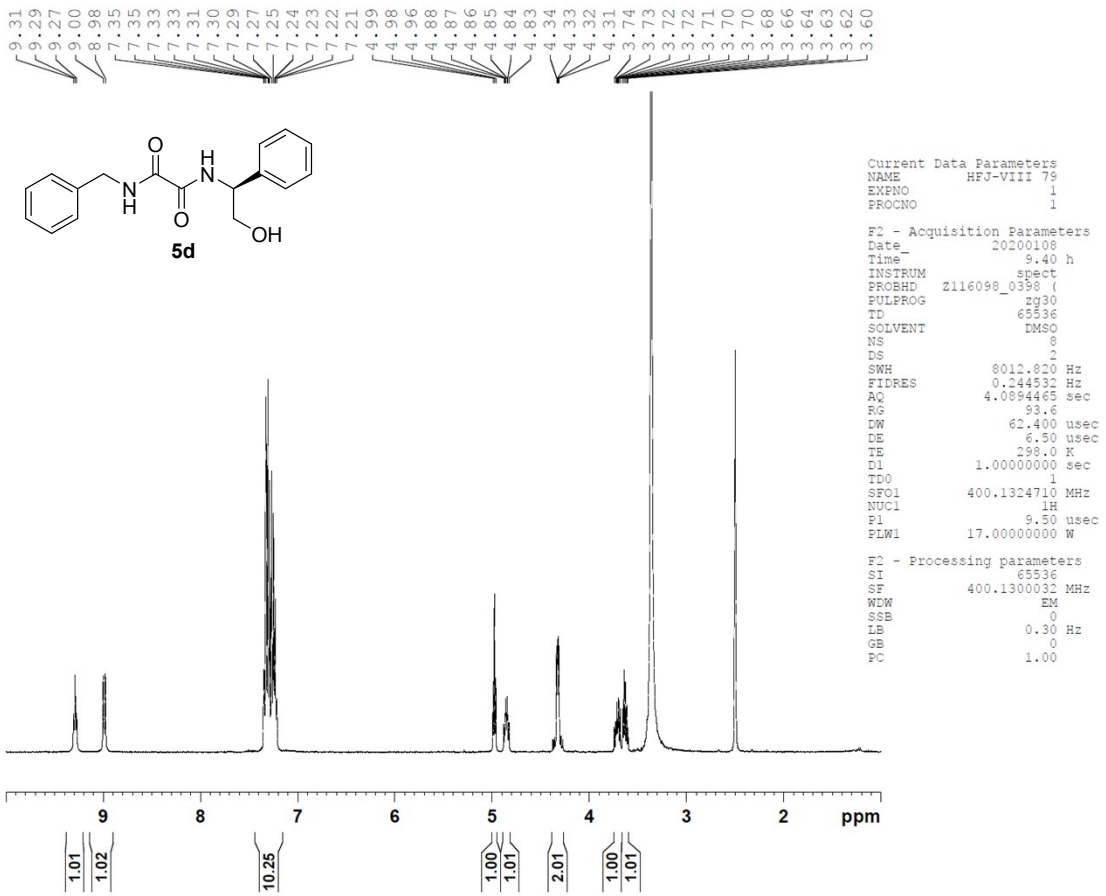

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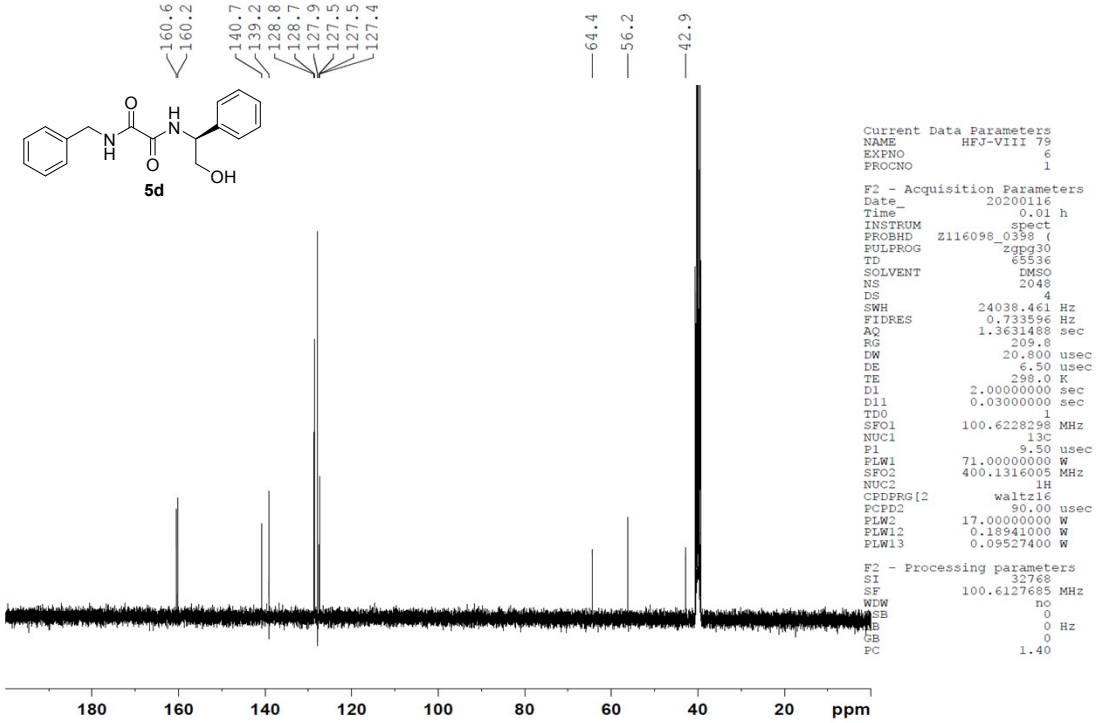

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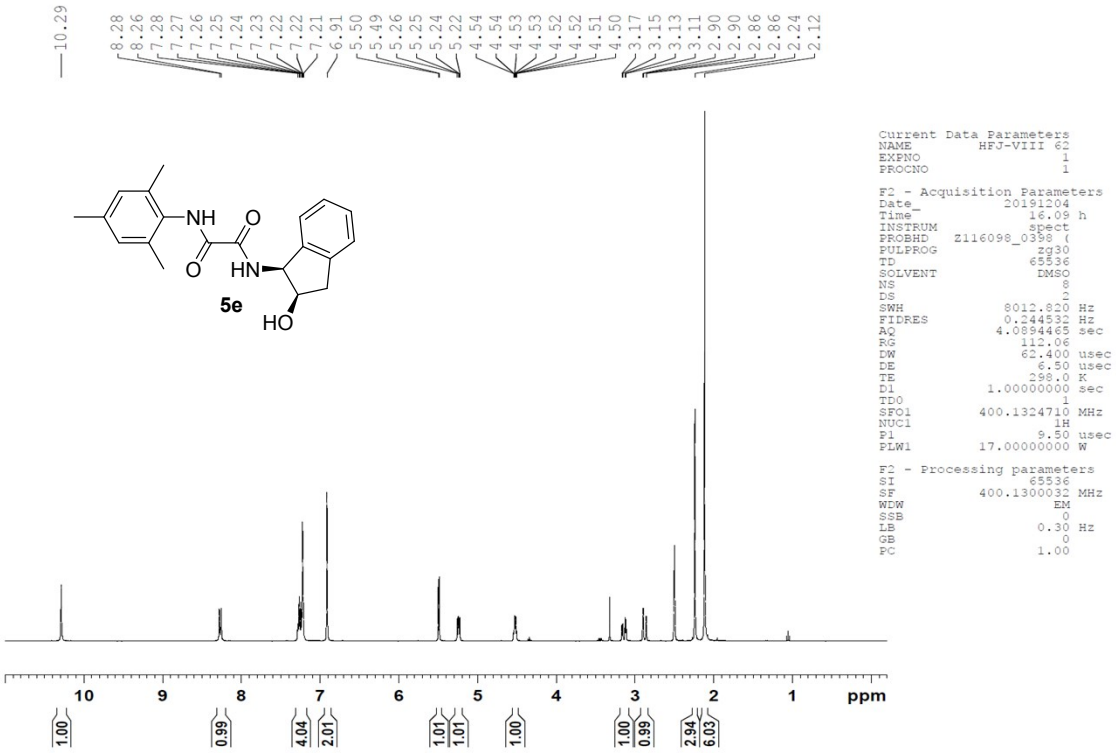

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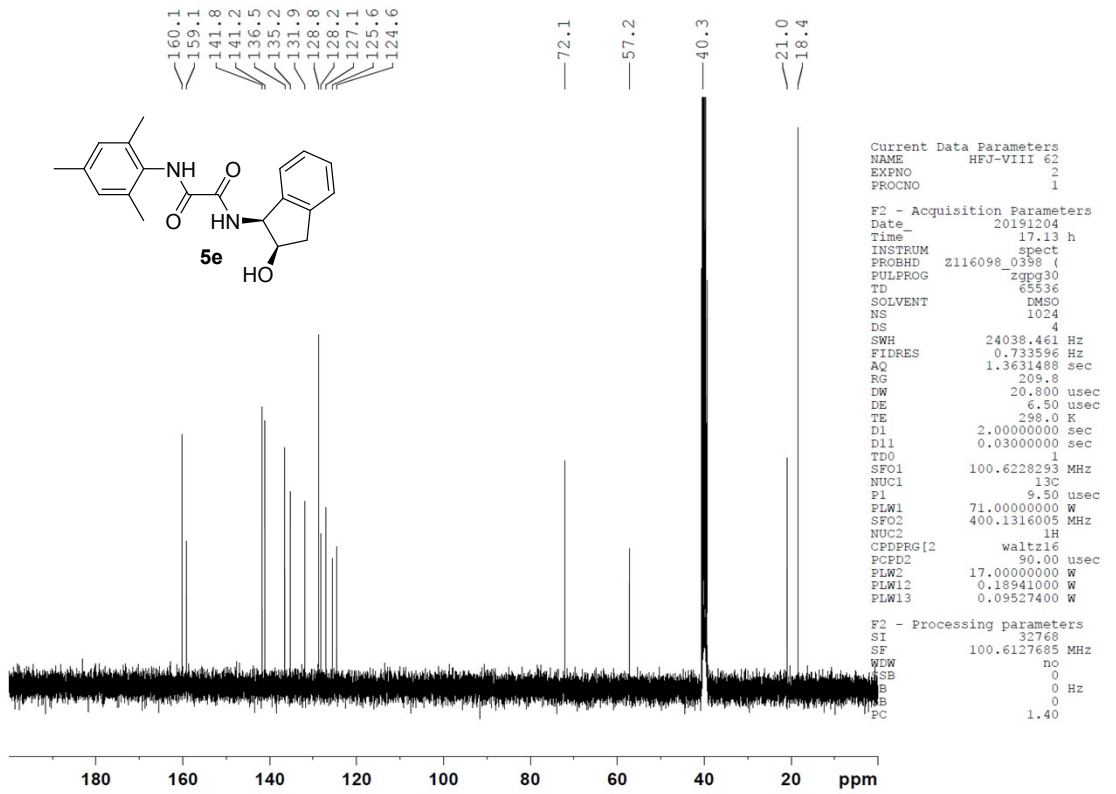

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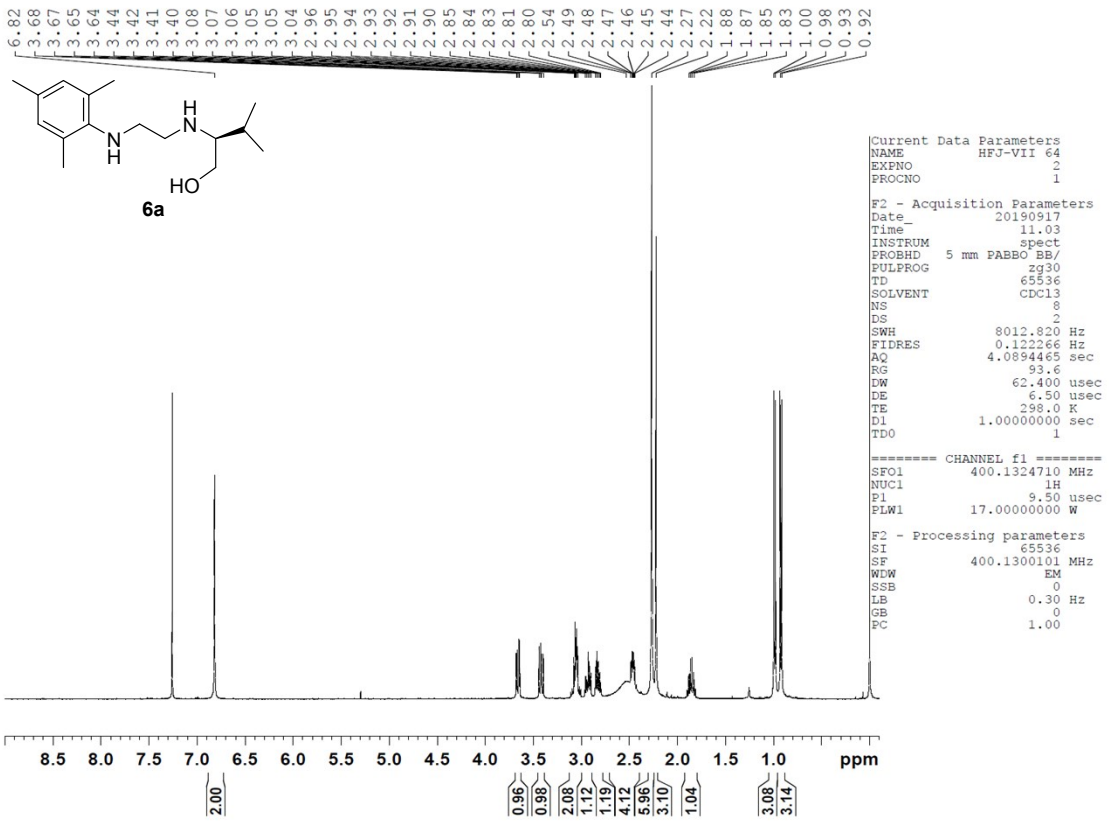

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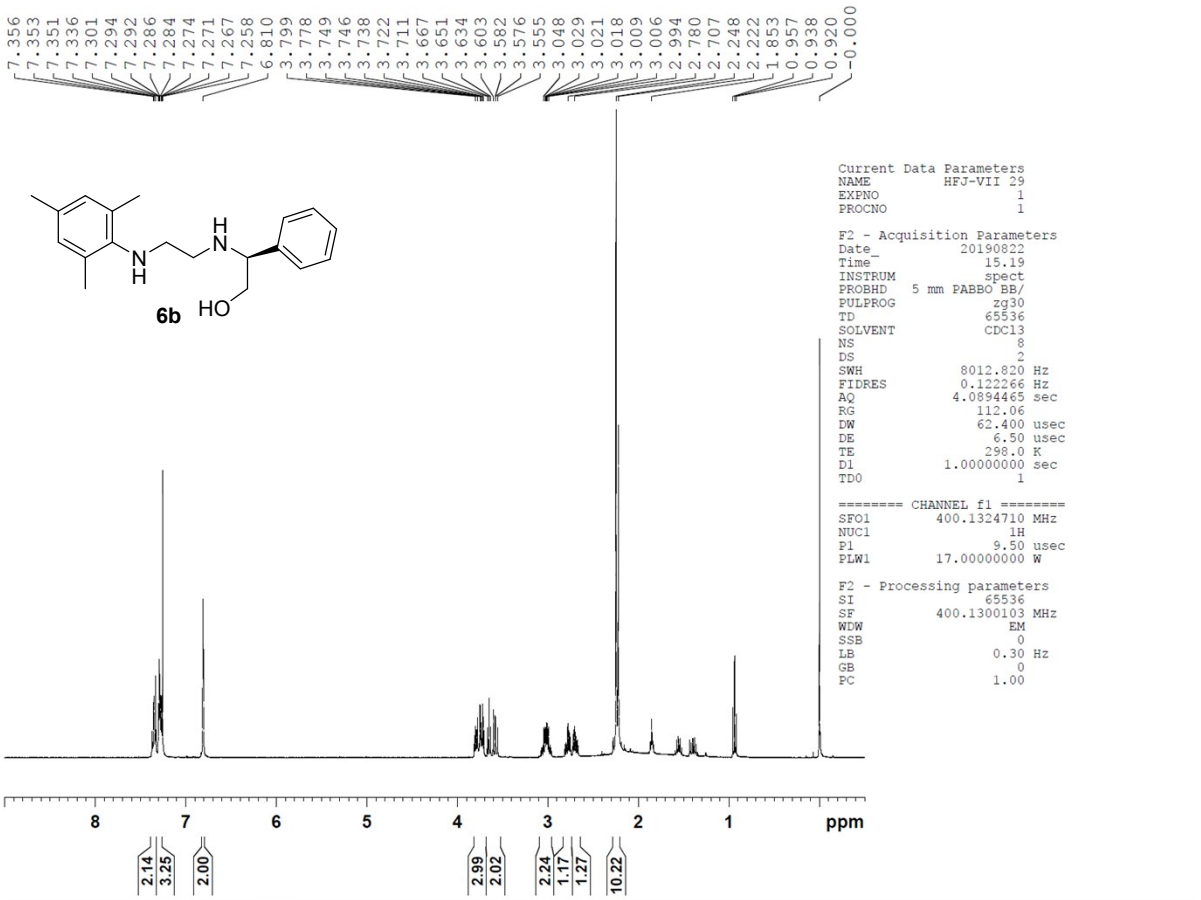

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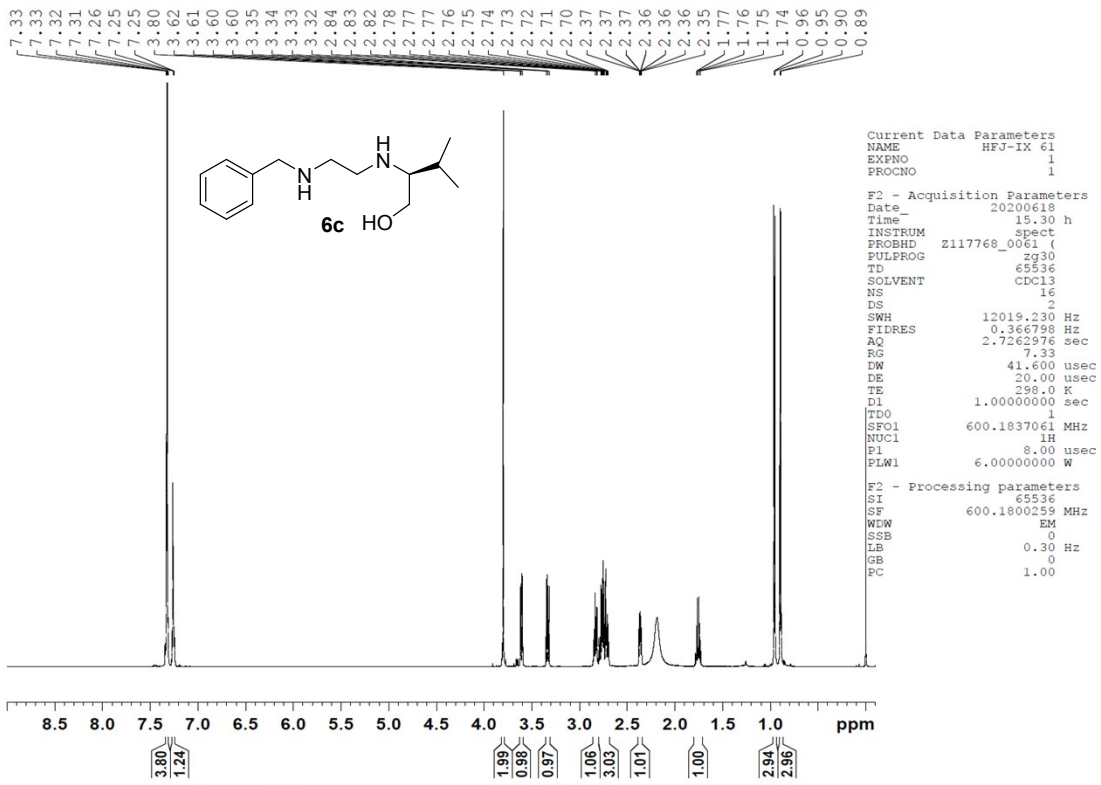

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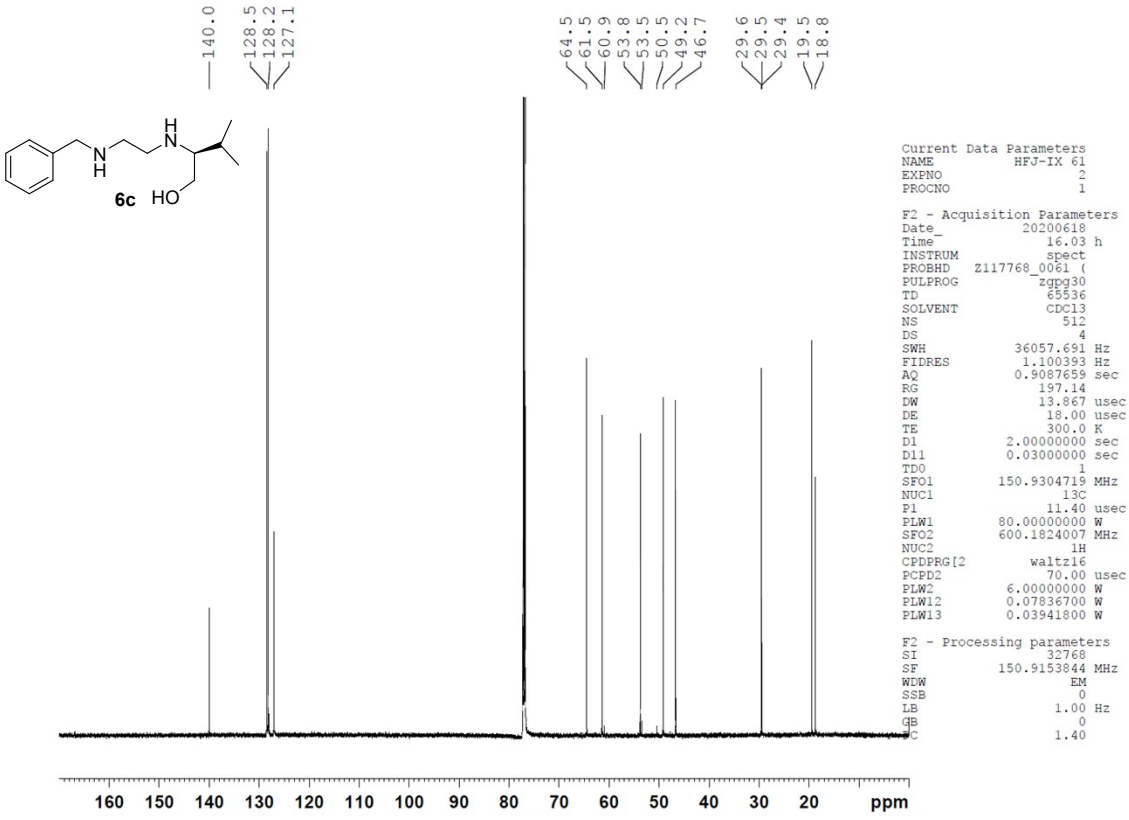

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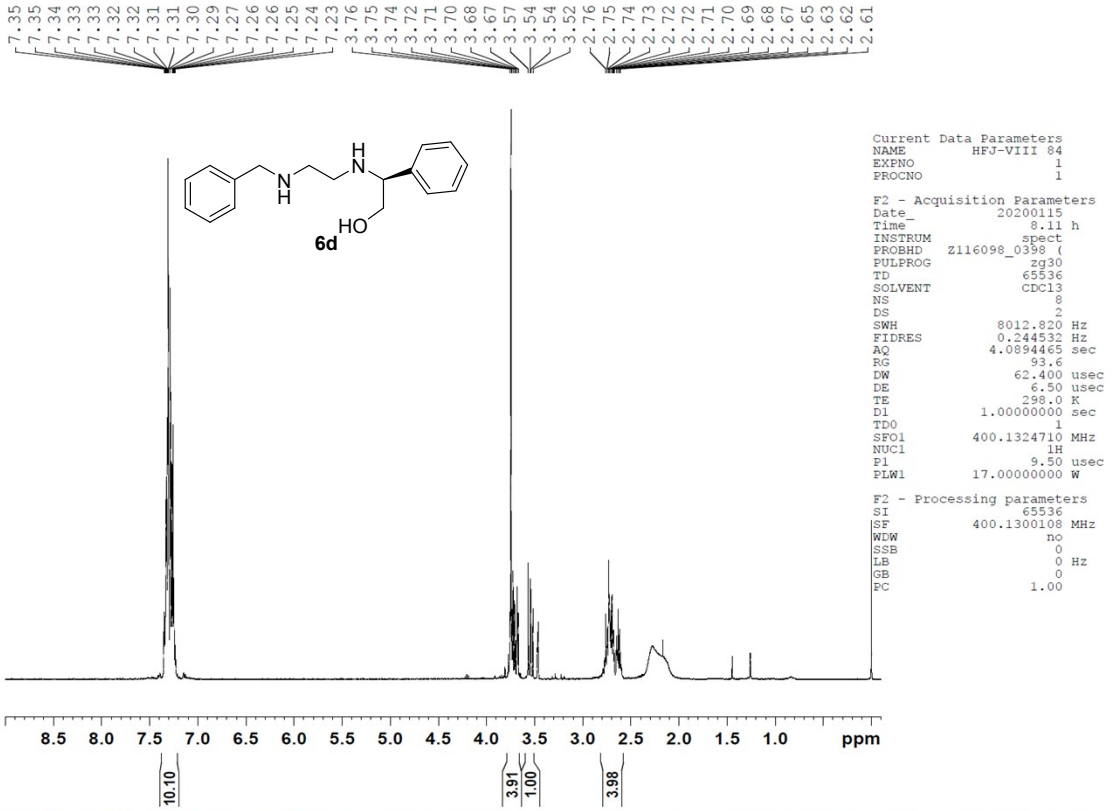

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DW 62.400 usec
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TE 298.0 K
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P1 9.50 usec
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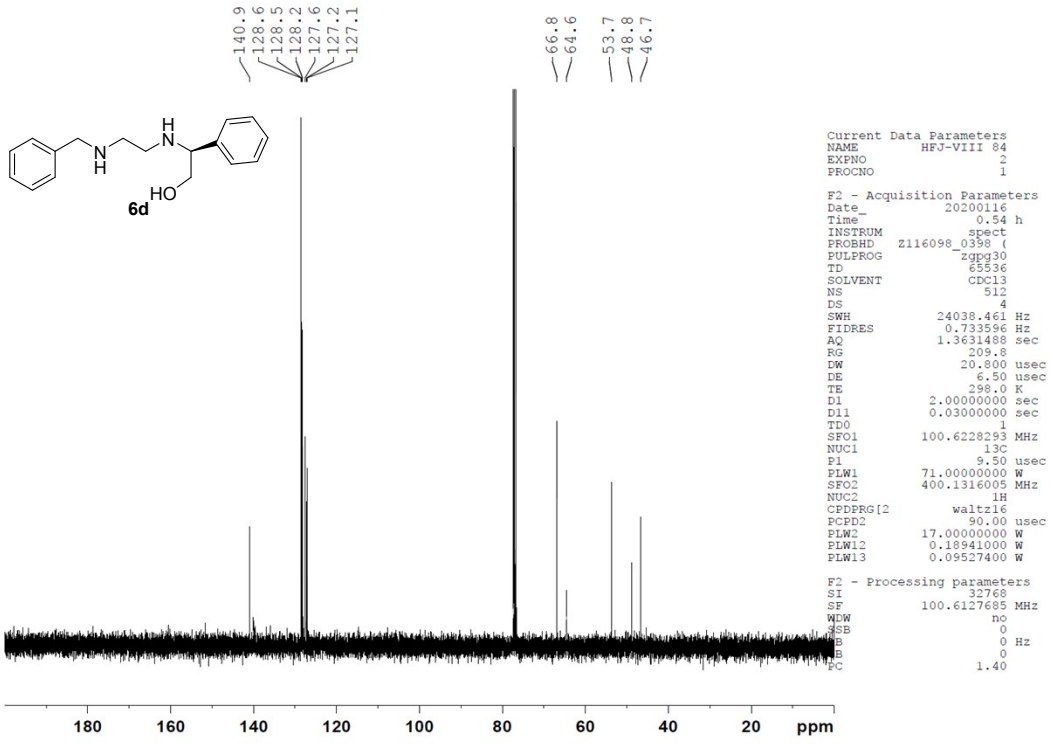

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FIDRES 0.733596 Hz
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DW 20.800 usec
DE 6.50 usec
TE 298.0 K
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D11 0.03000000 sec
TD0 1
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NUC1 13C
P1 9.50 usec
PLW1 71.00000000 W
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NUC2 1H
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PLW13 0.09527400 W

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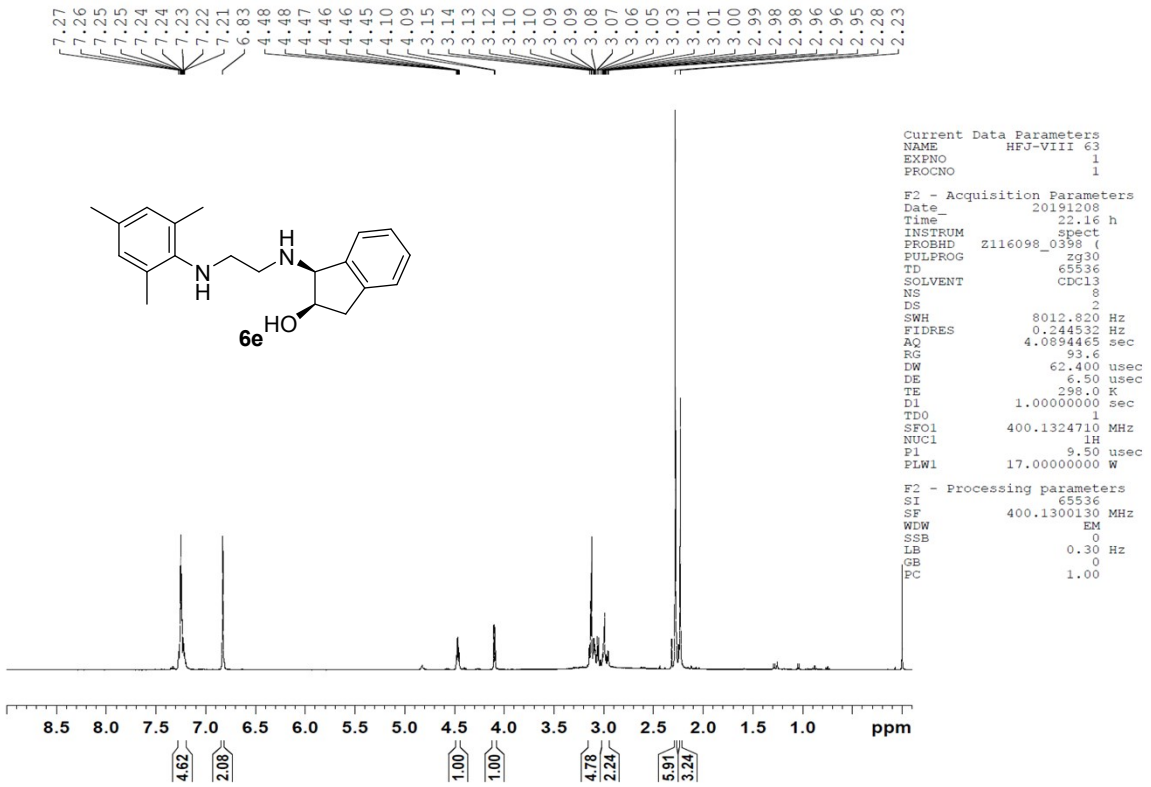

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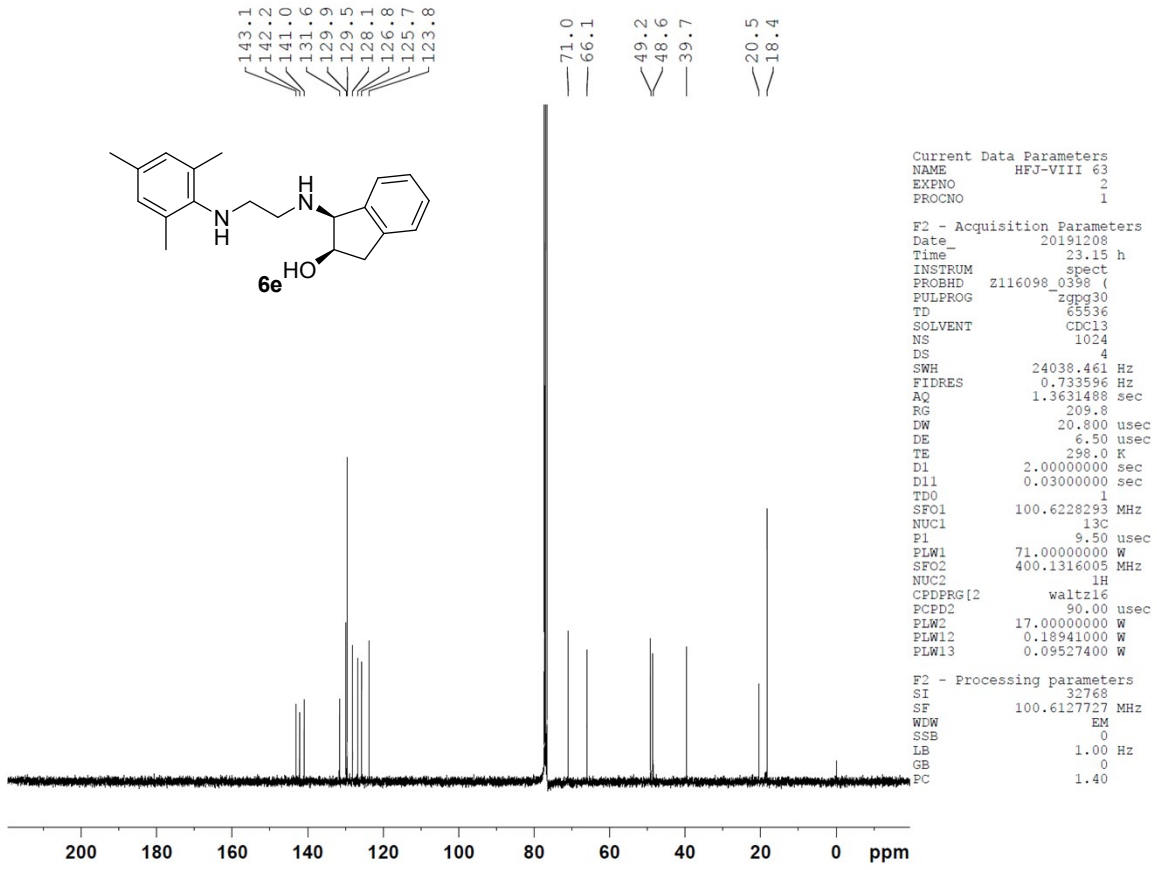

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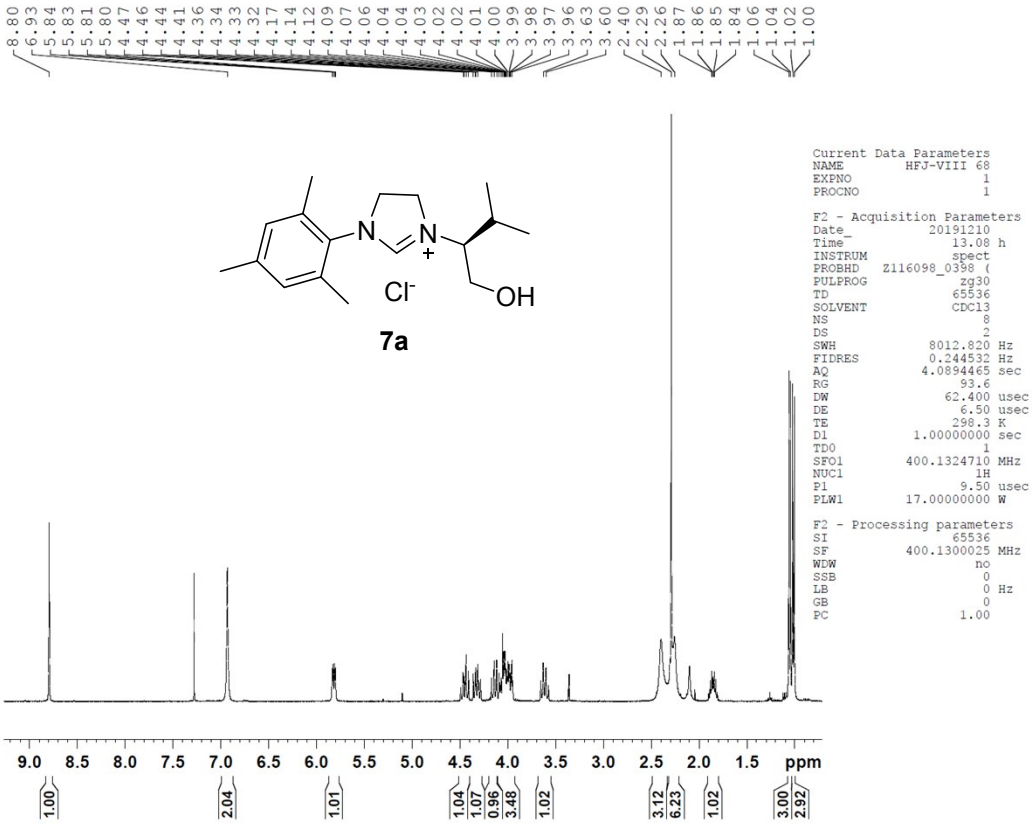

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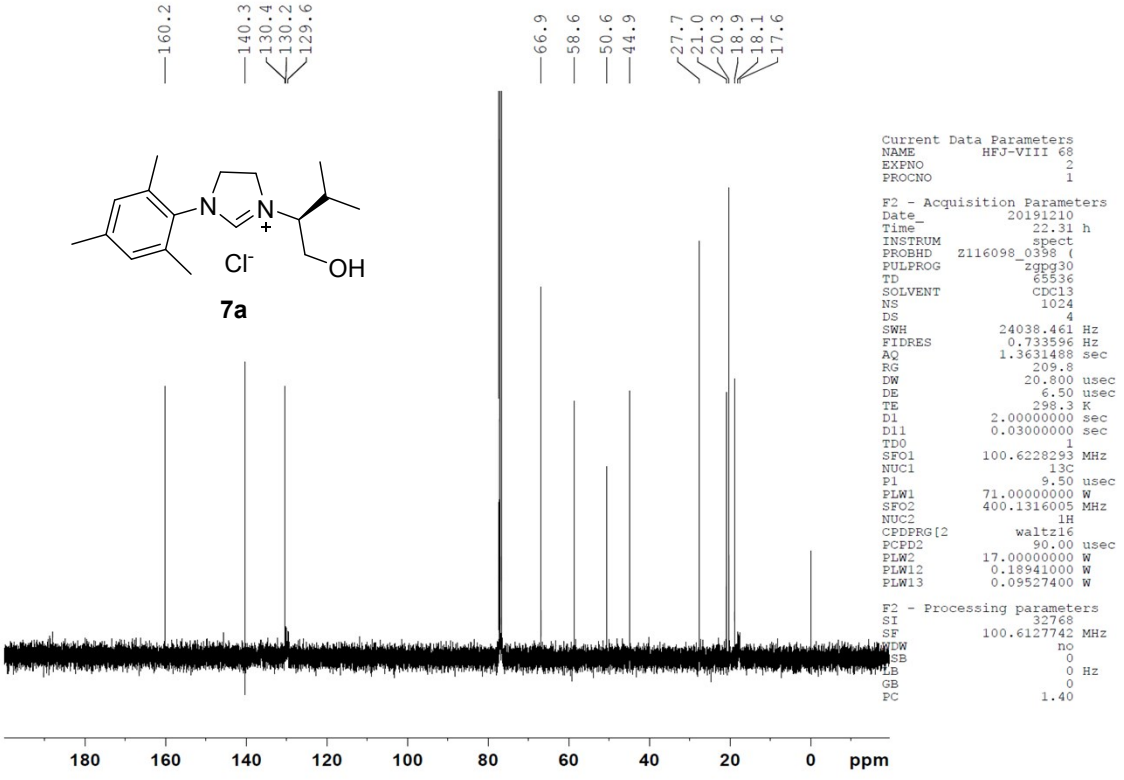

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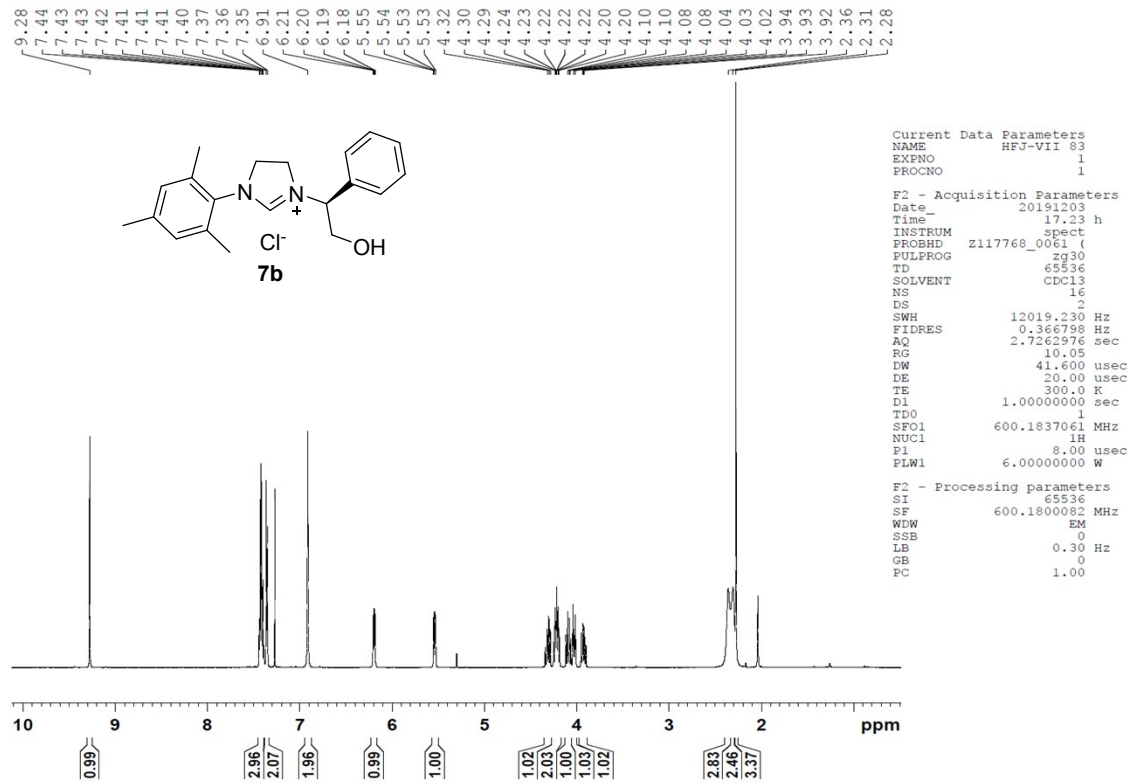

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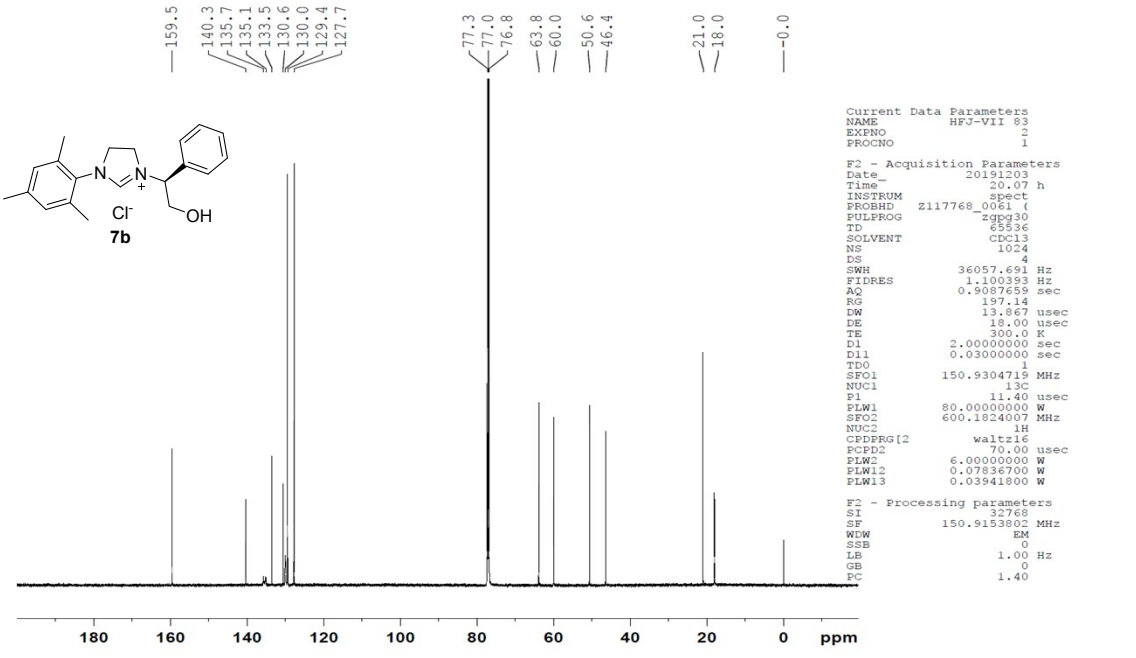

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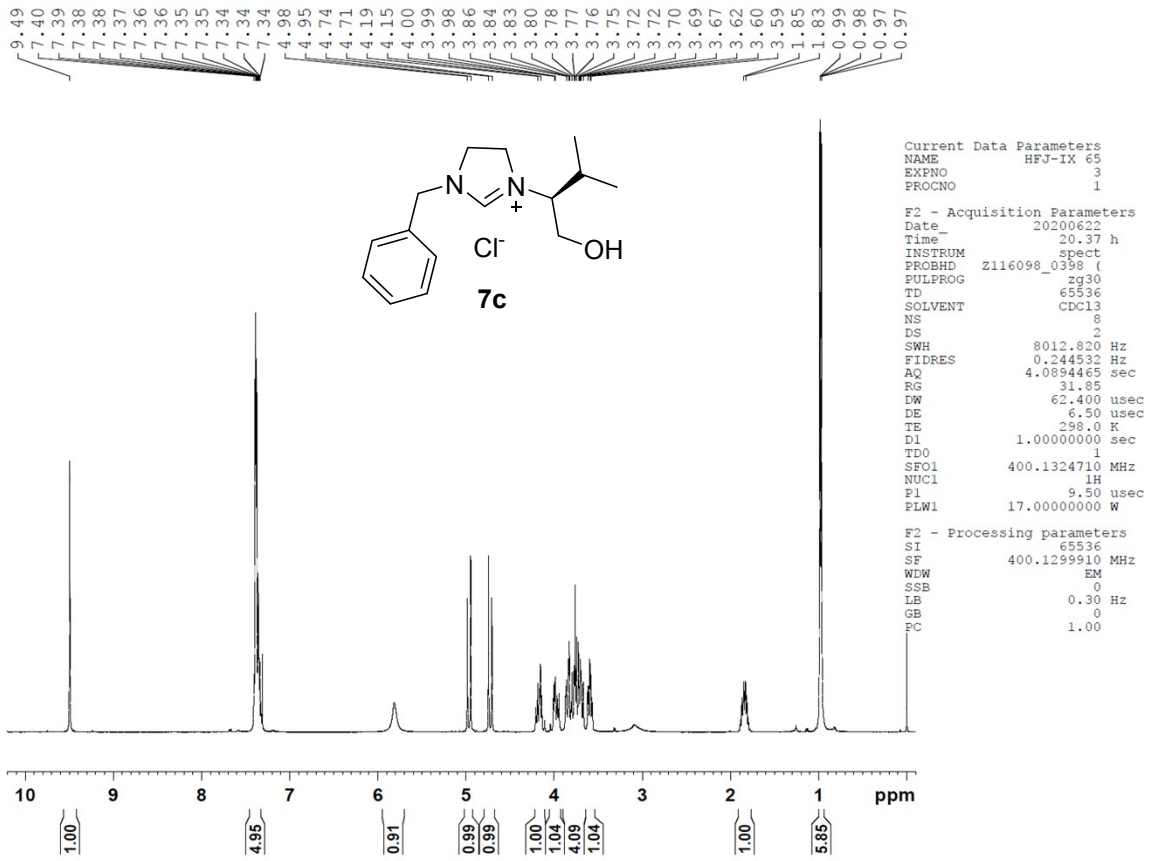

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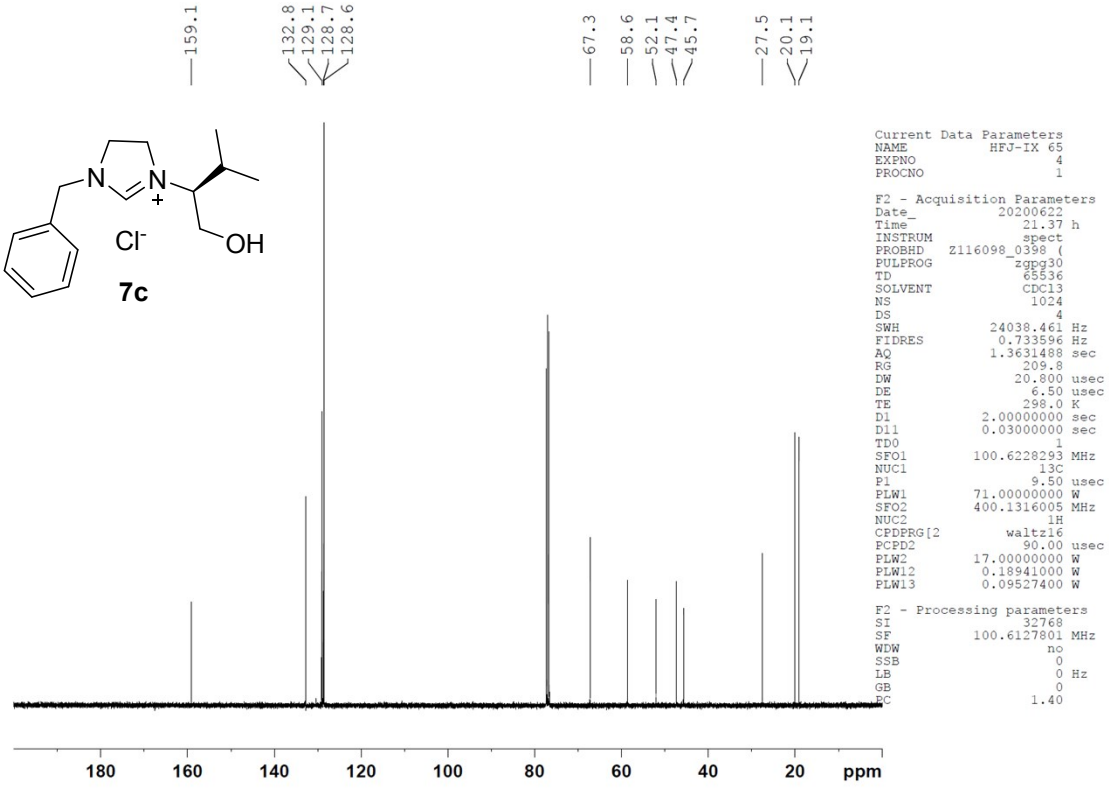

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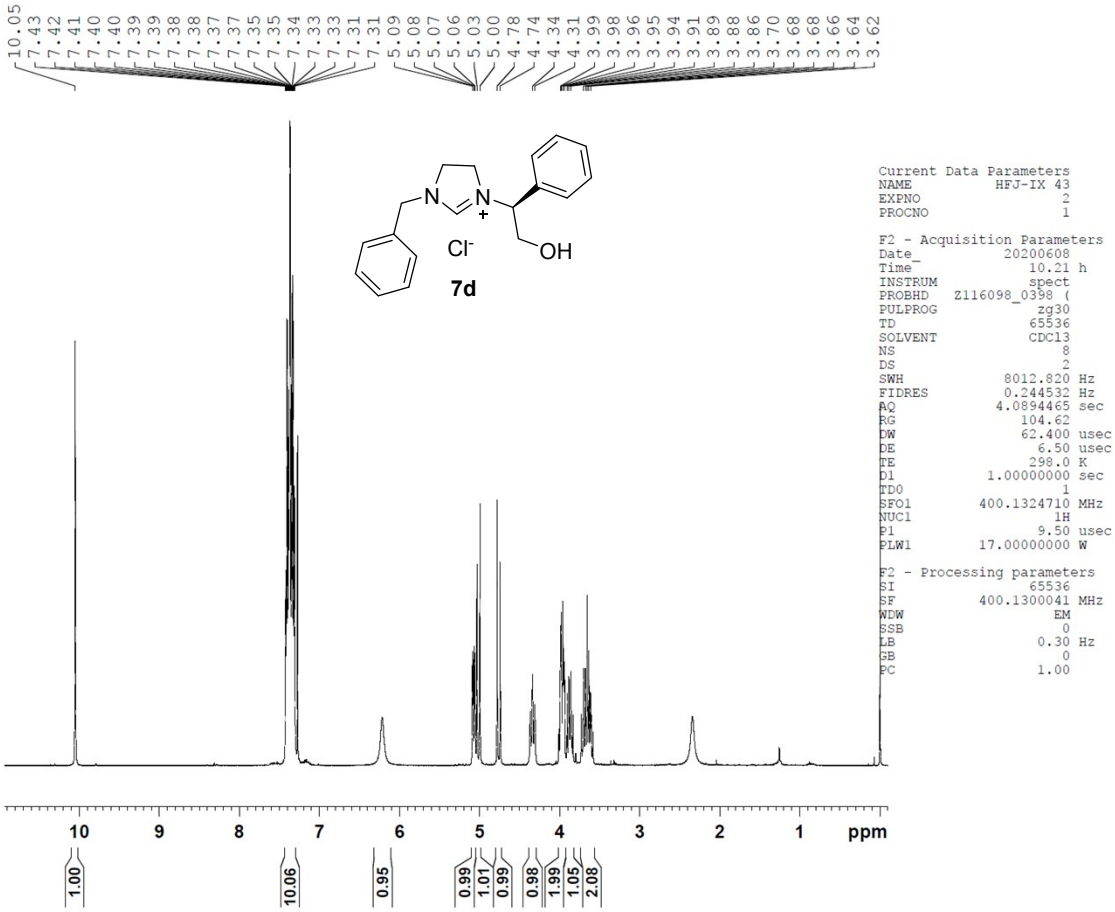


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DW                 62.400 usec
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TE                 298.0 K
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F2 - Processing parameters
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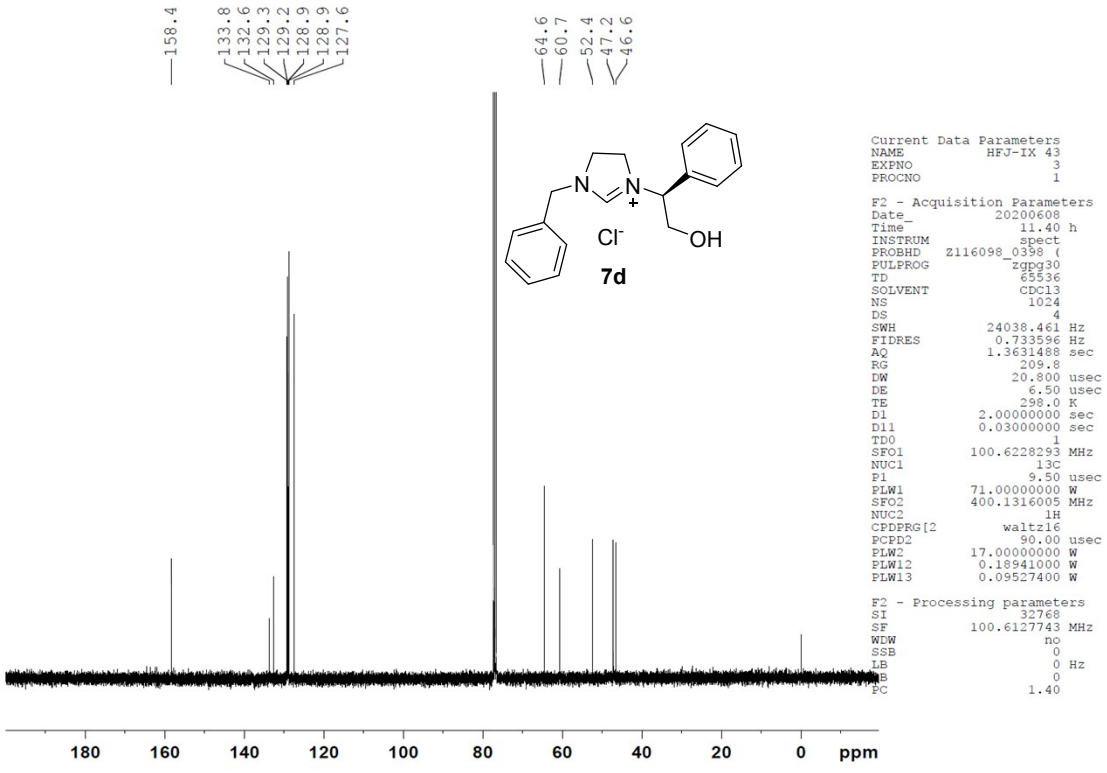


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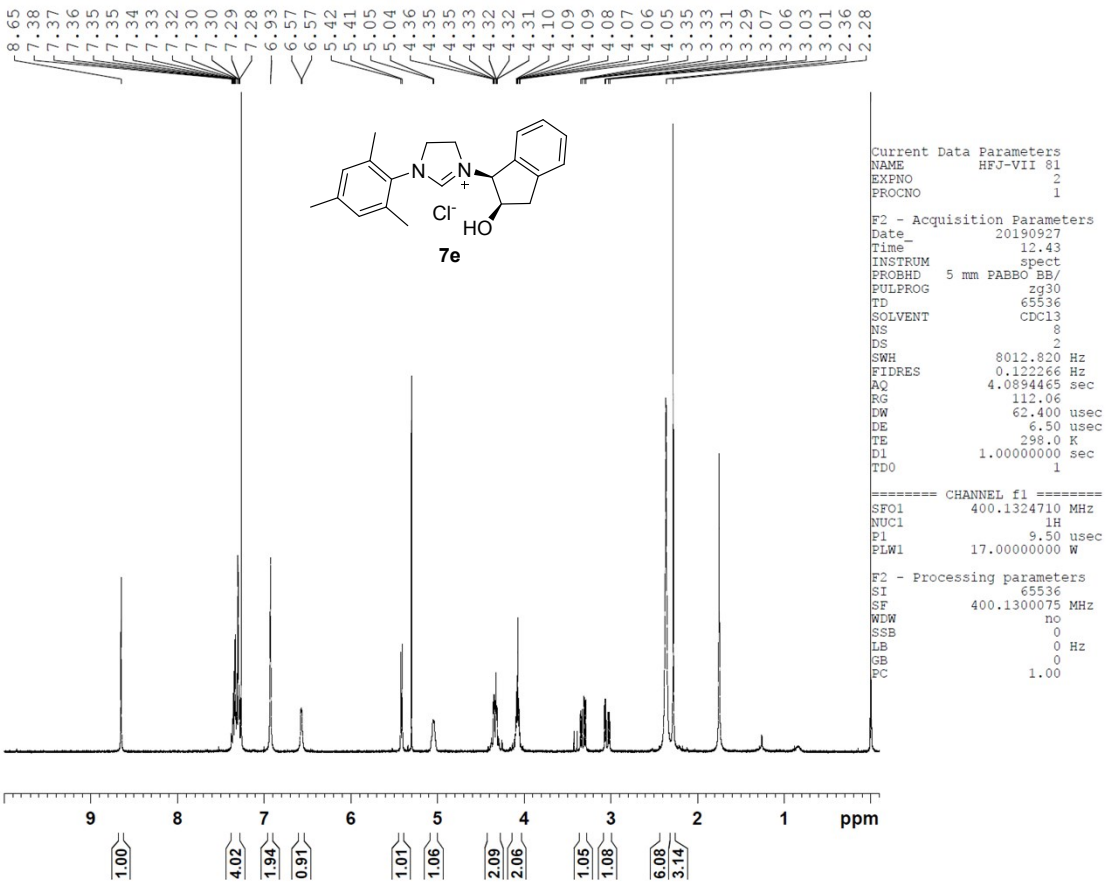

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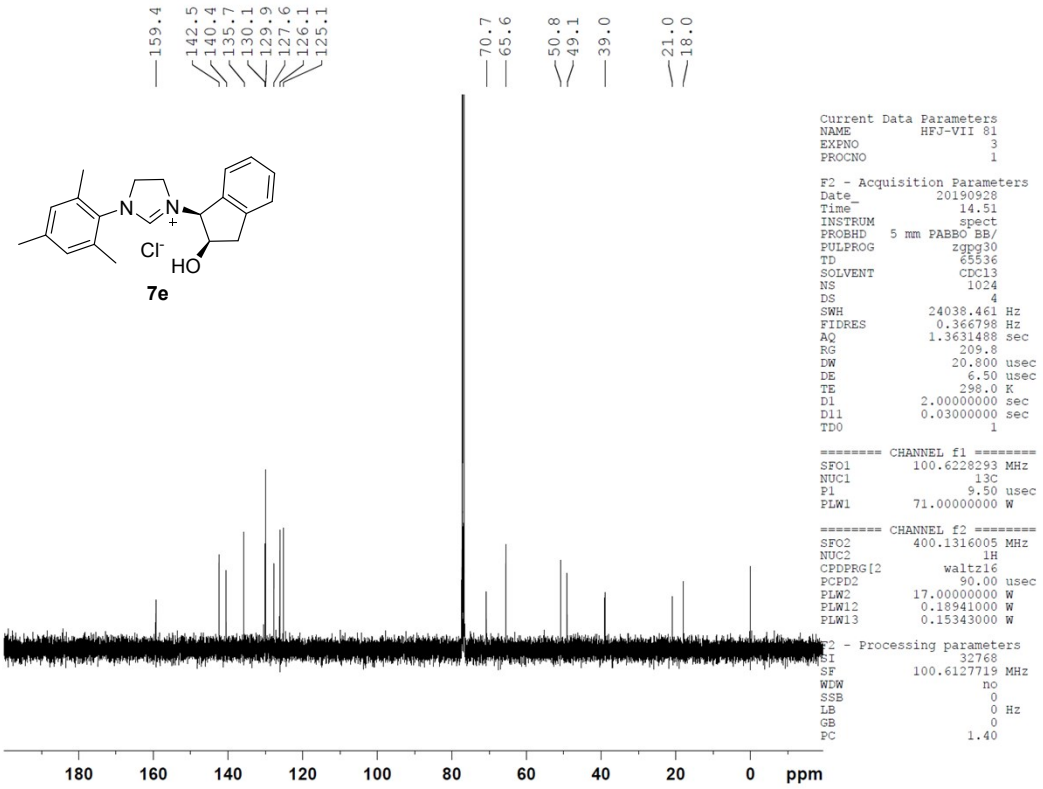

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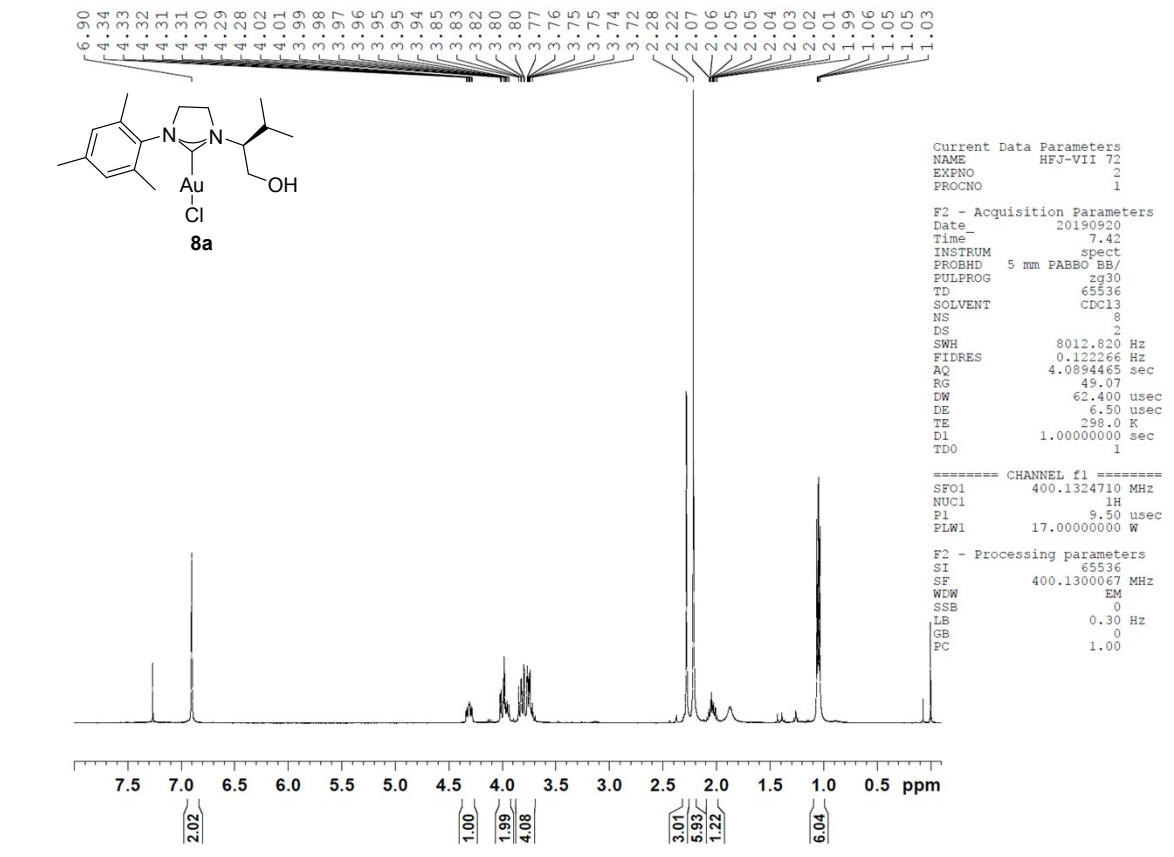

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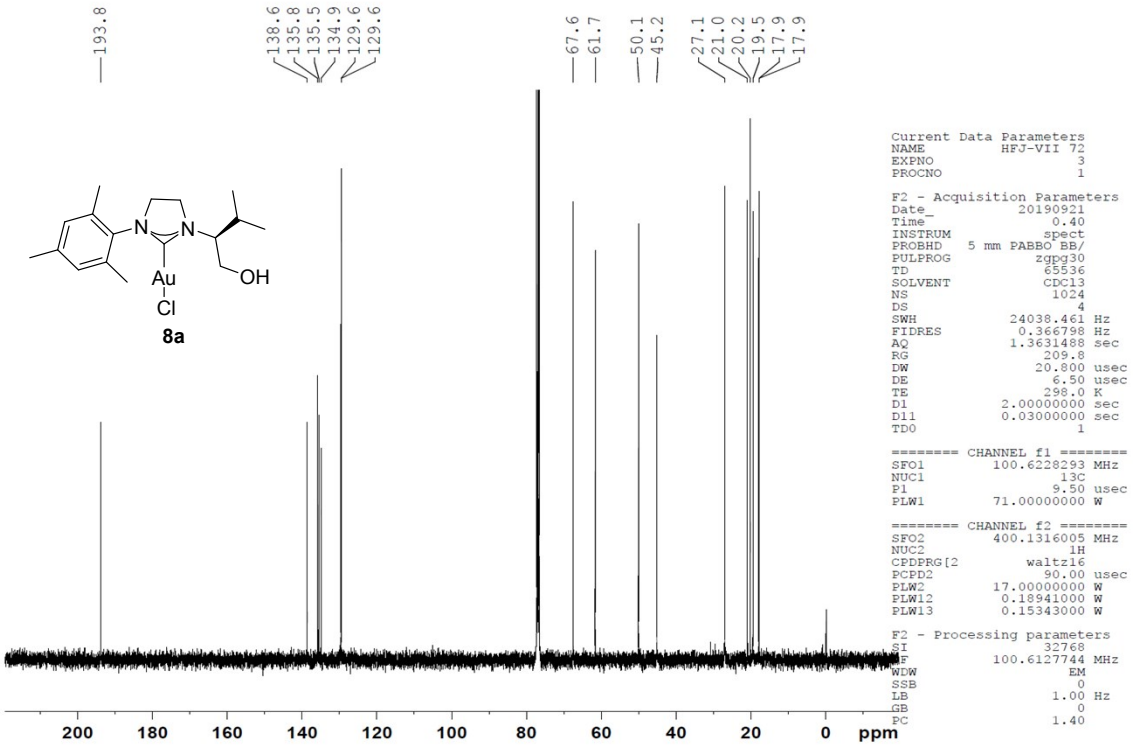

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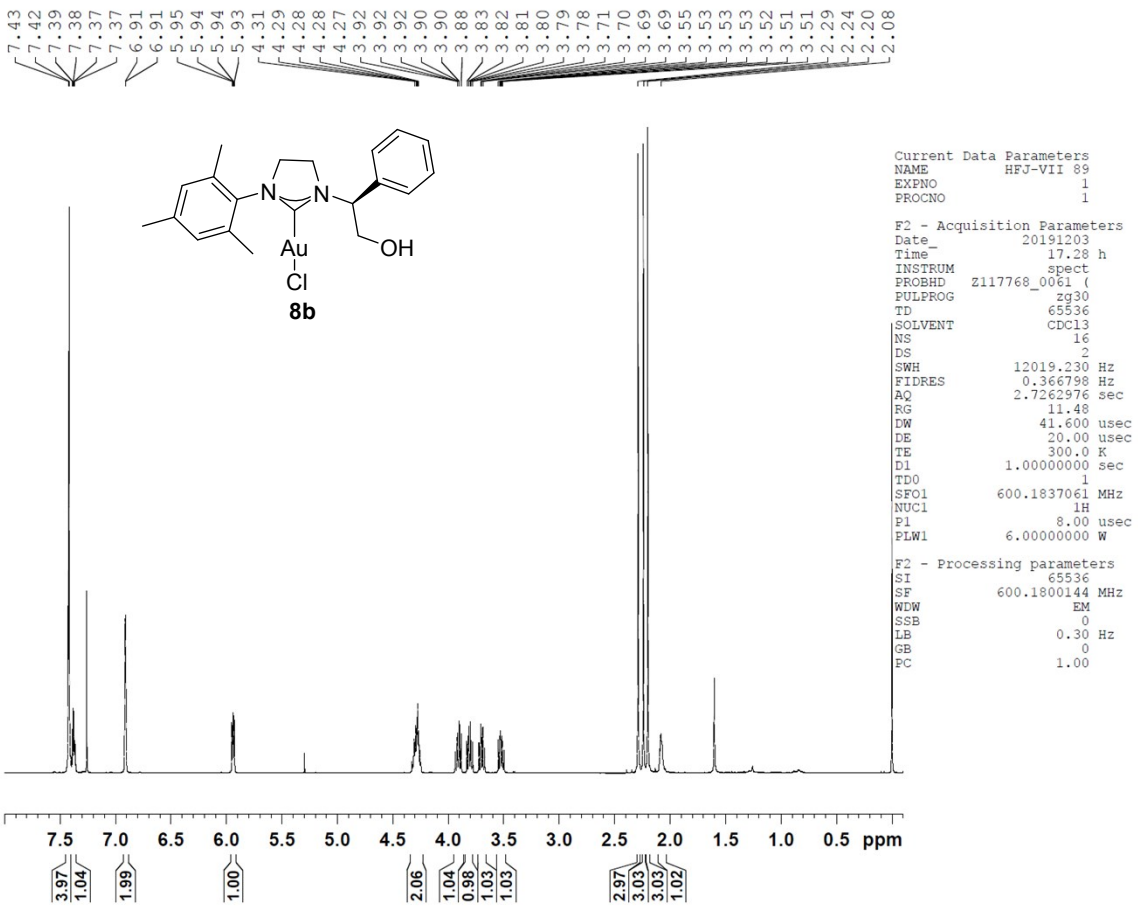

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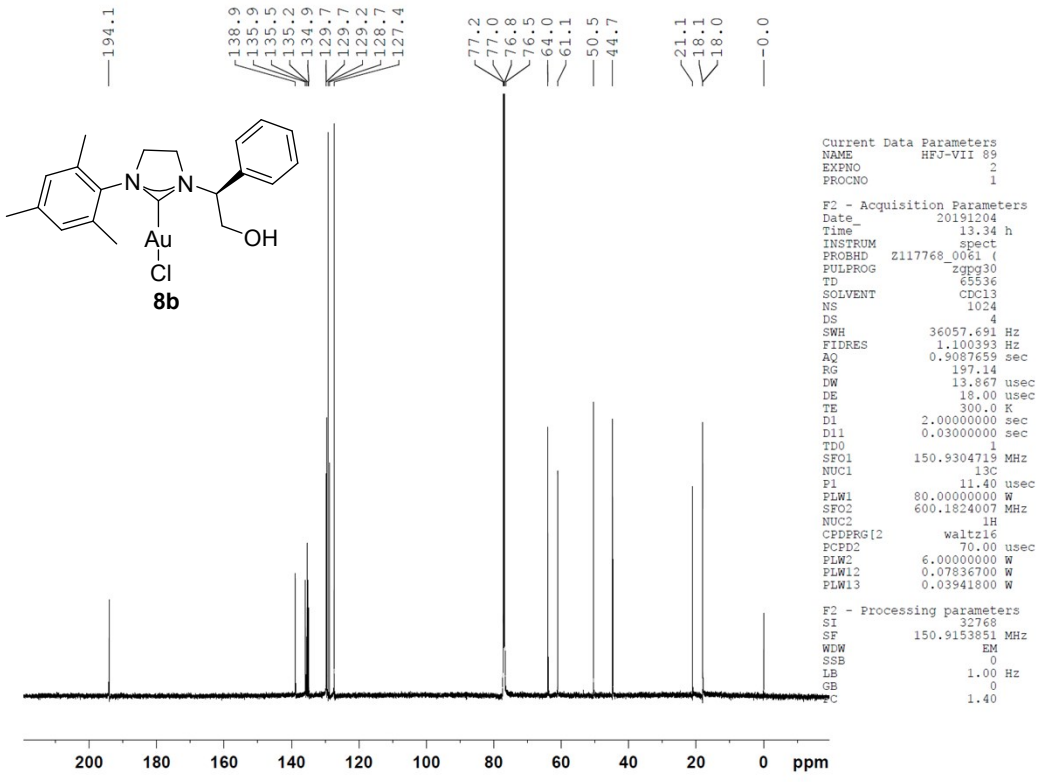

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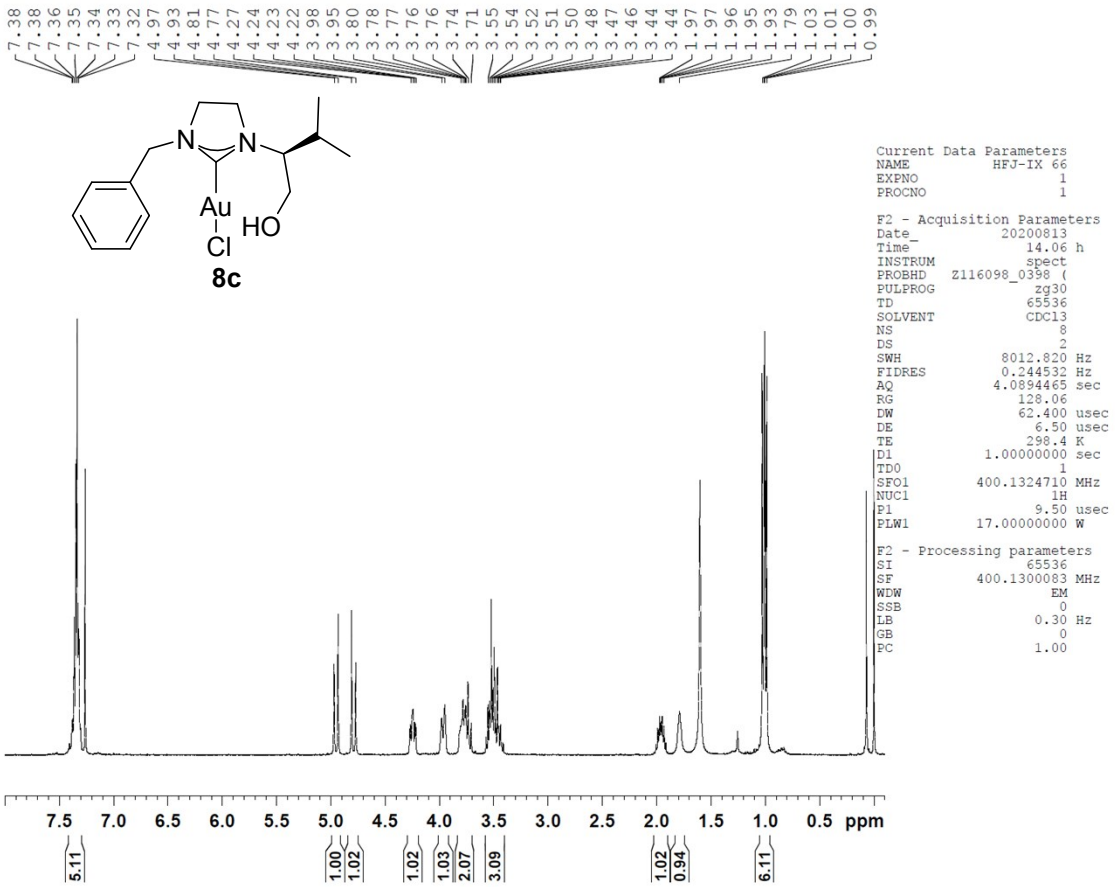

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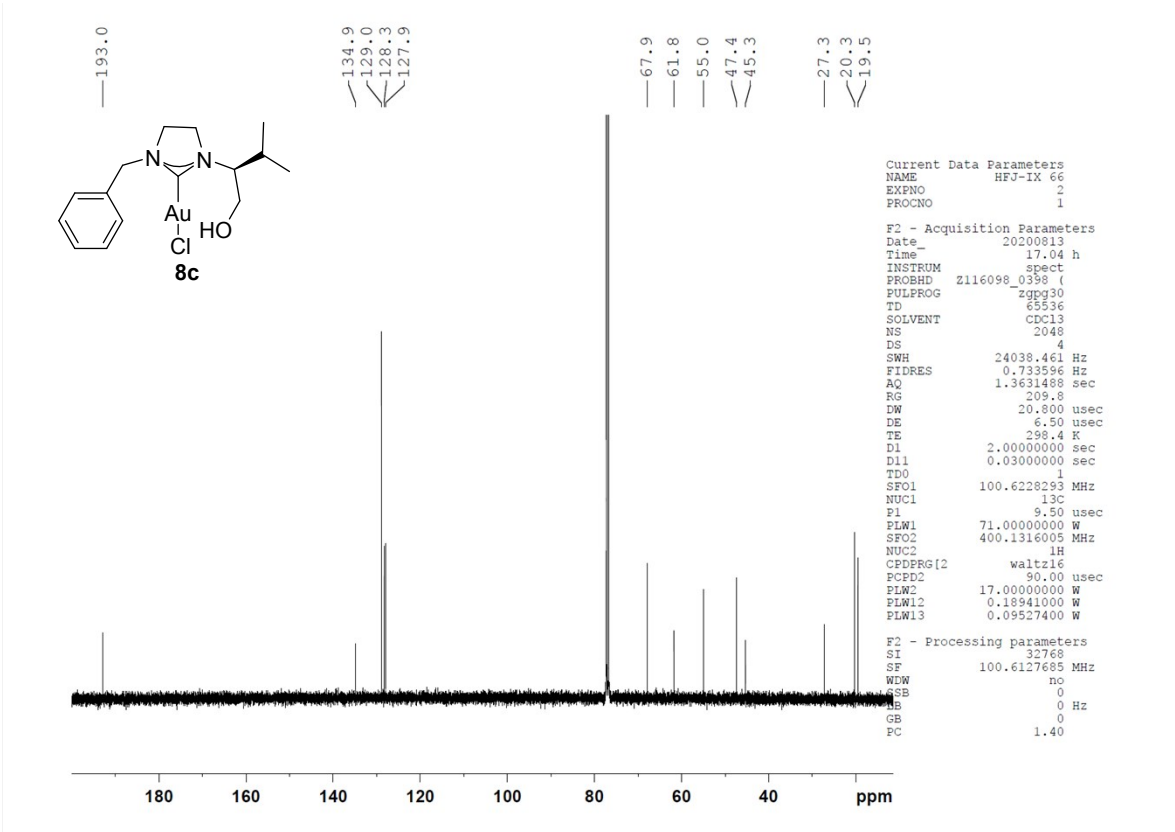

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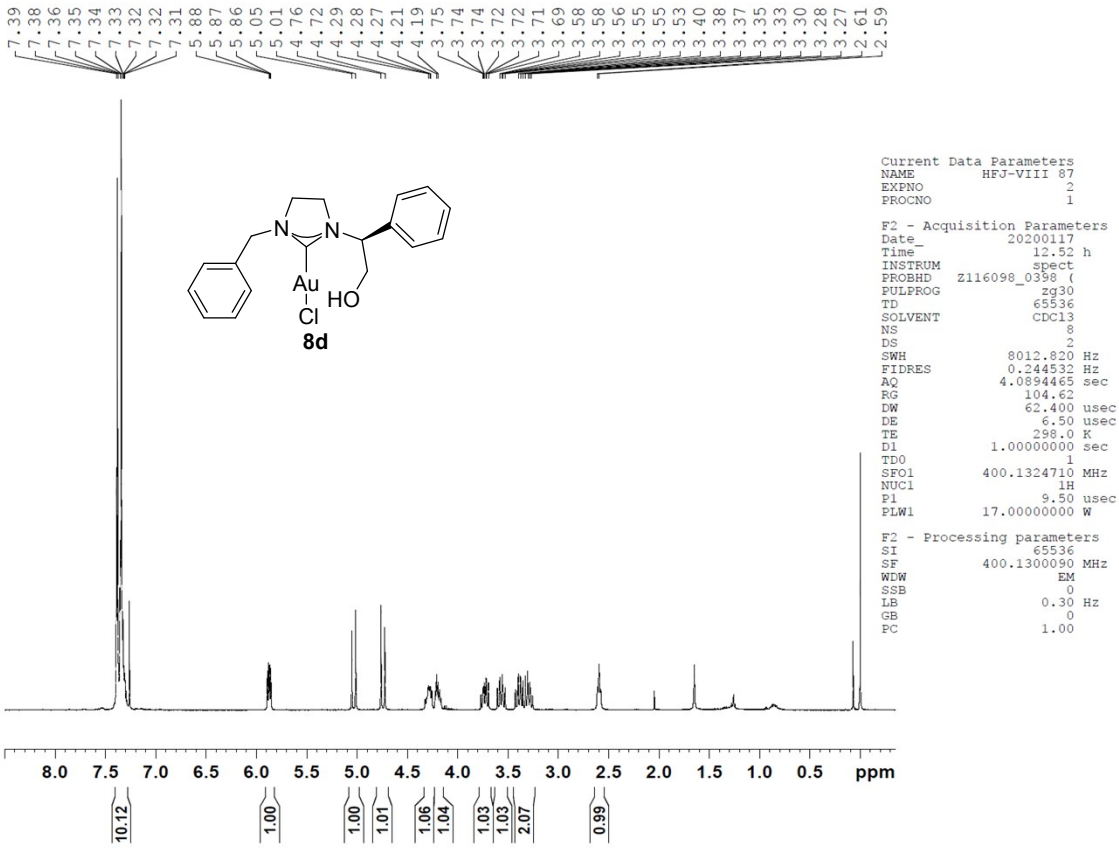

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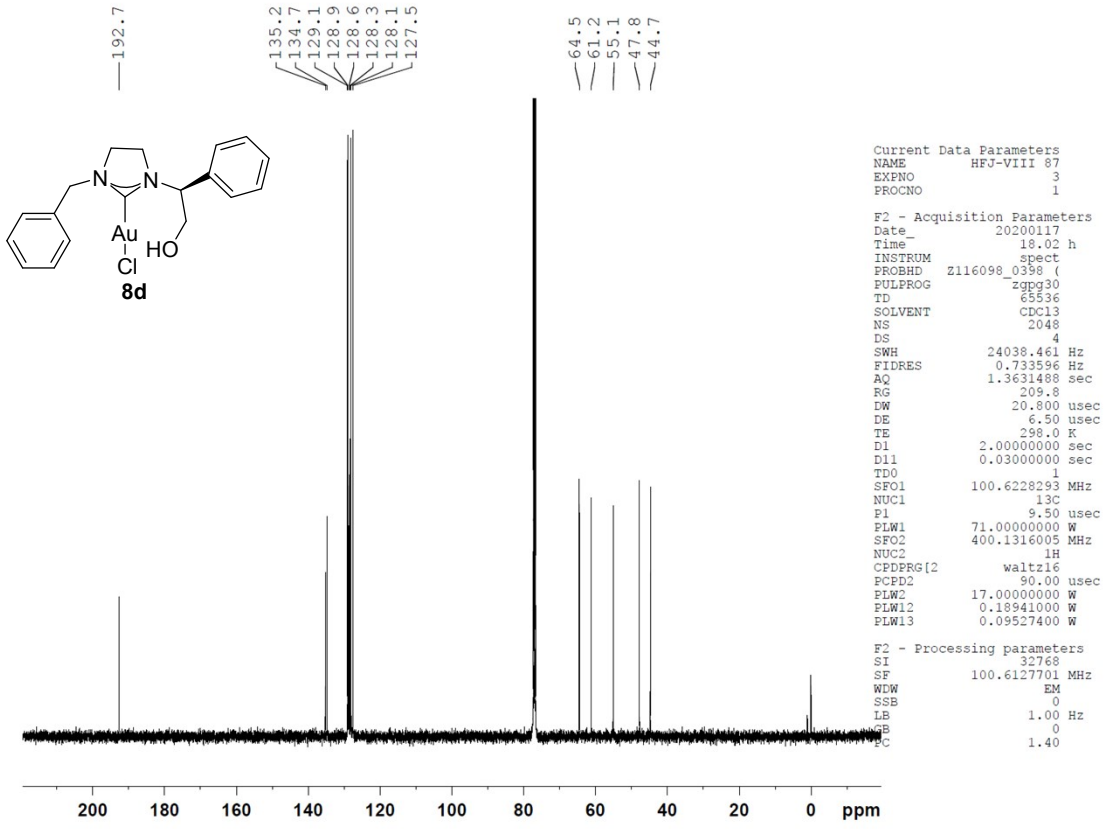

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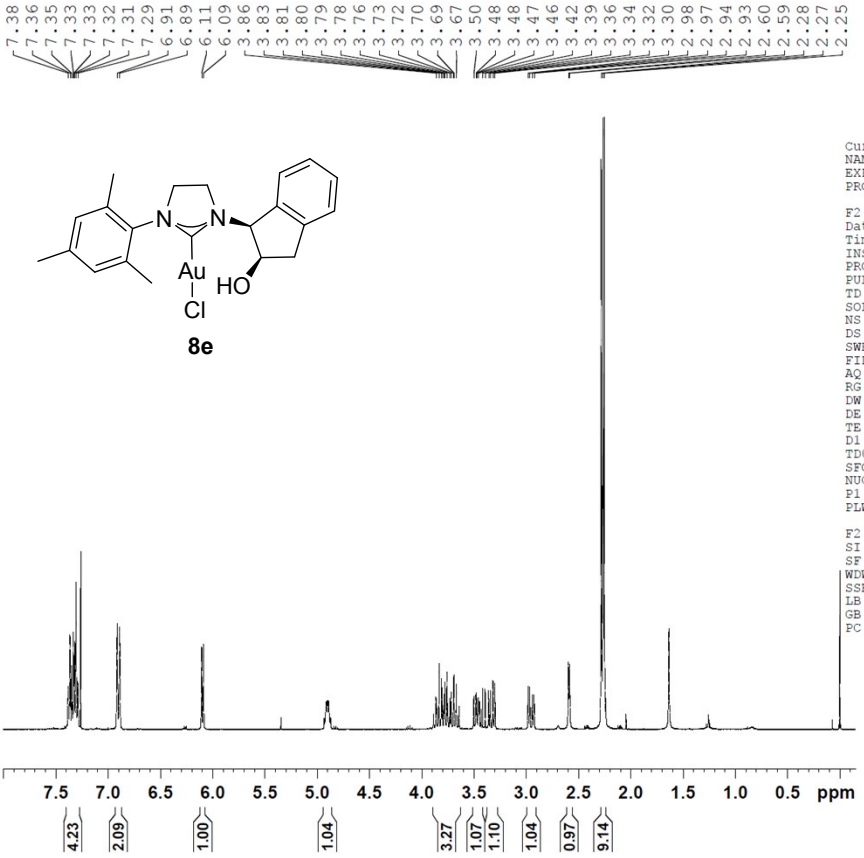

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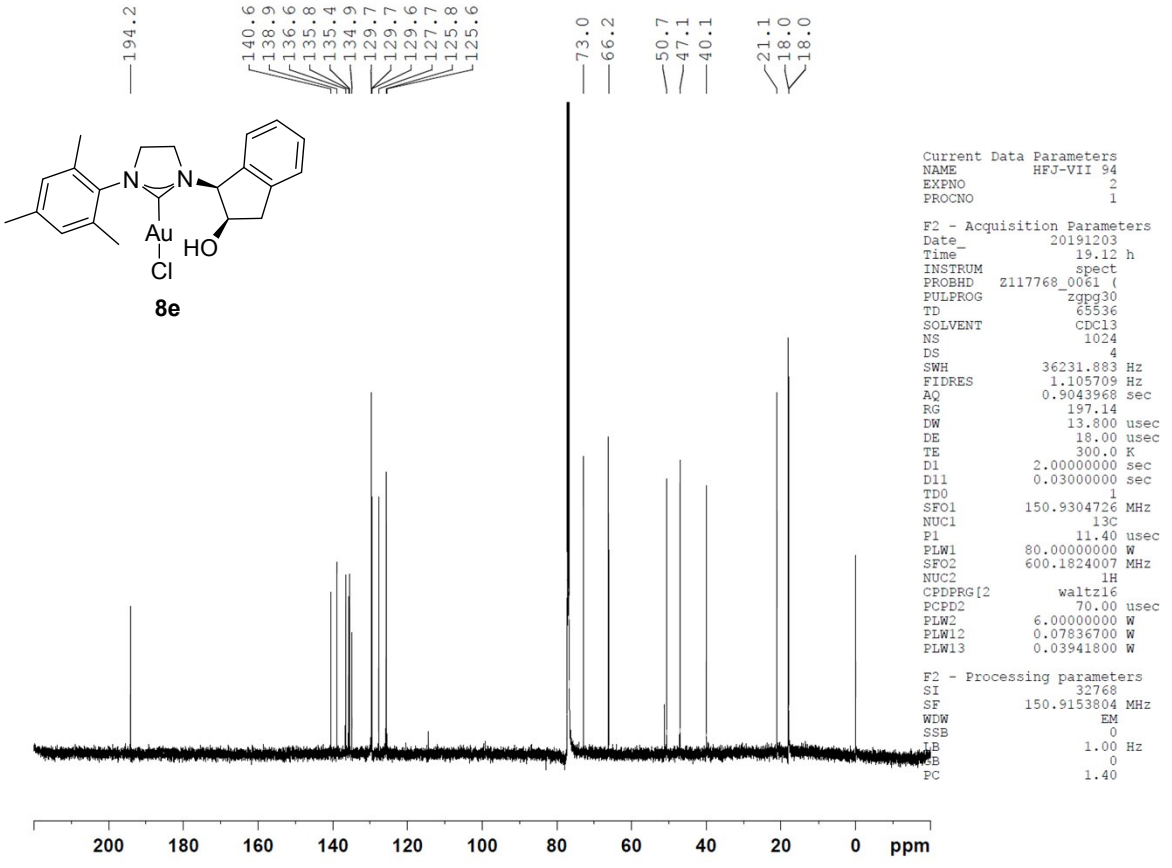

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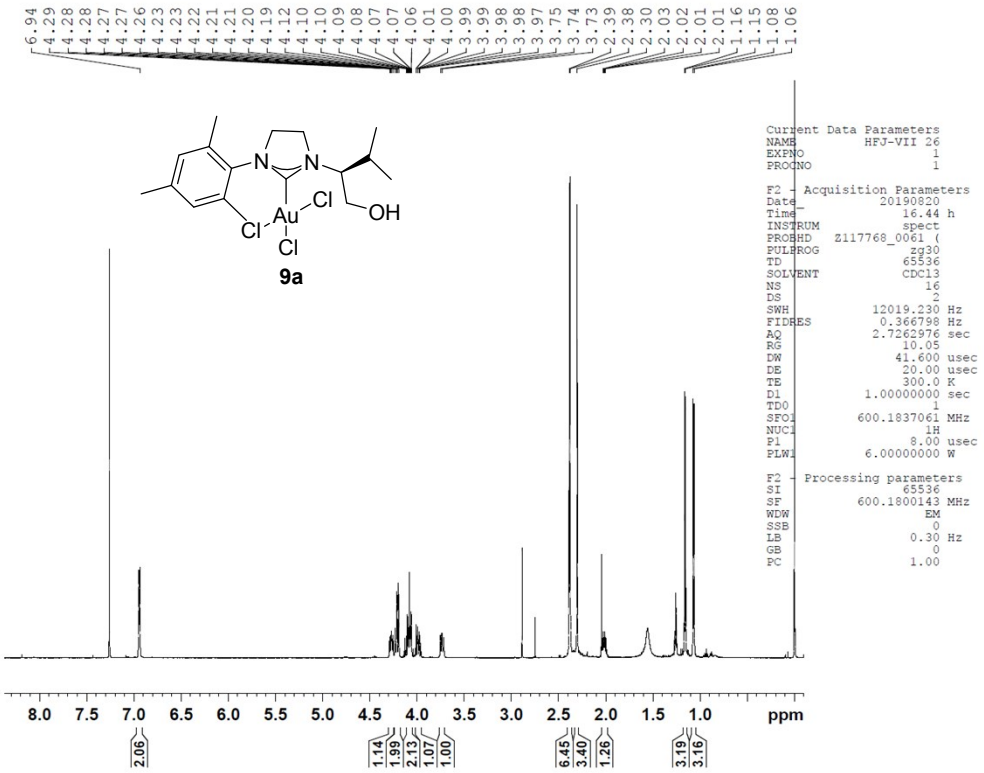

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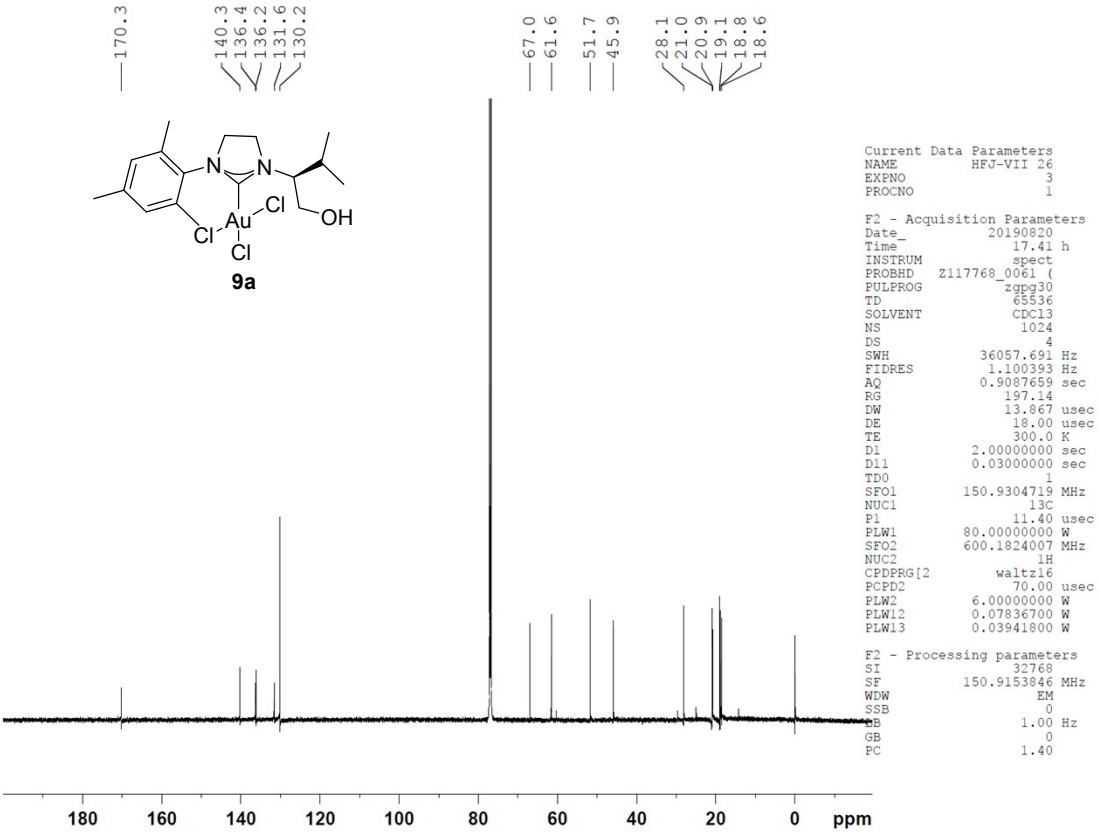

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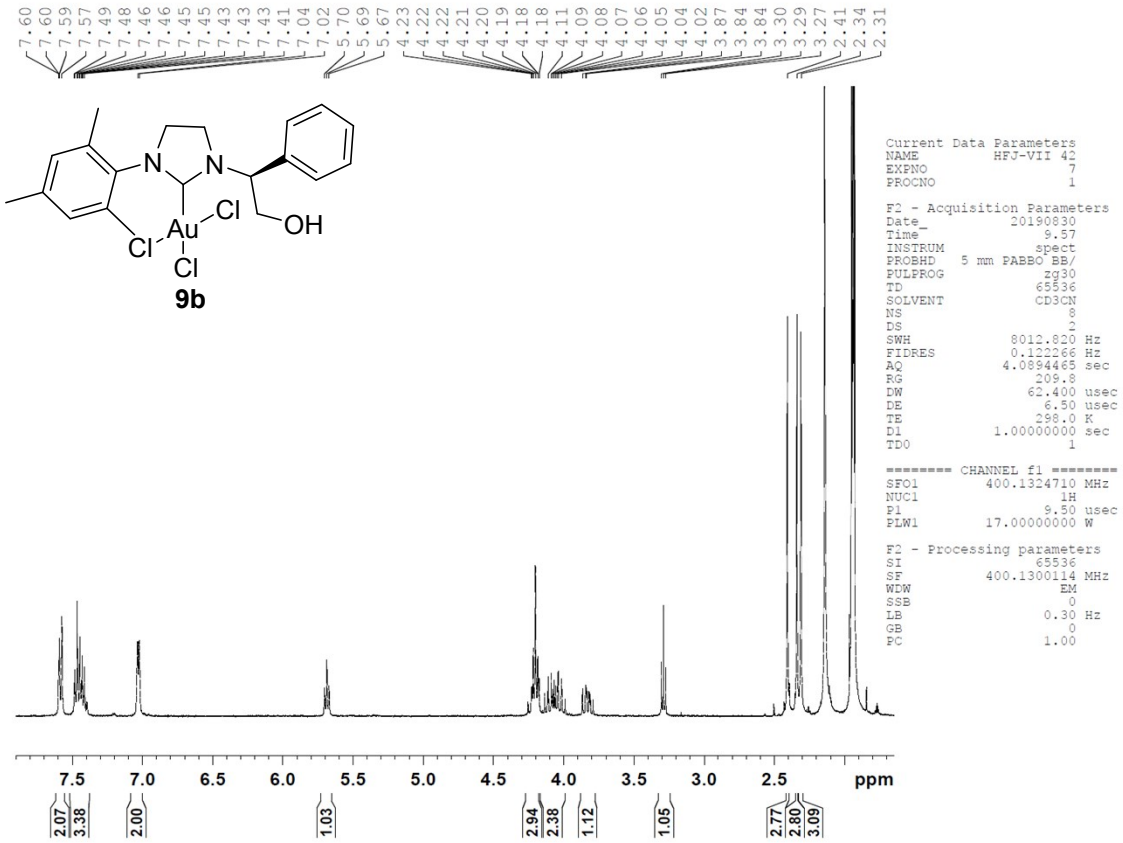

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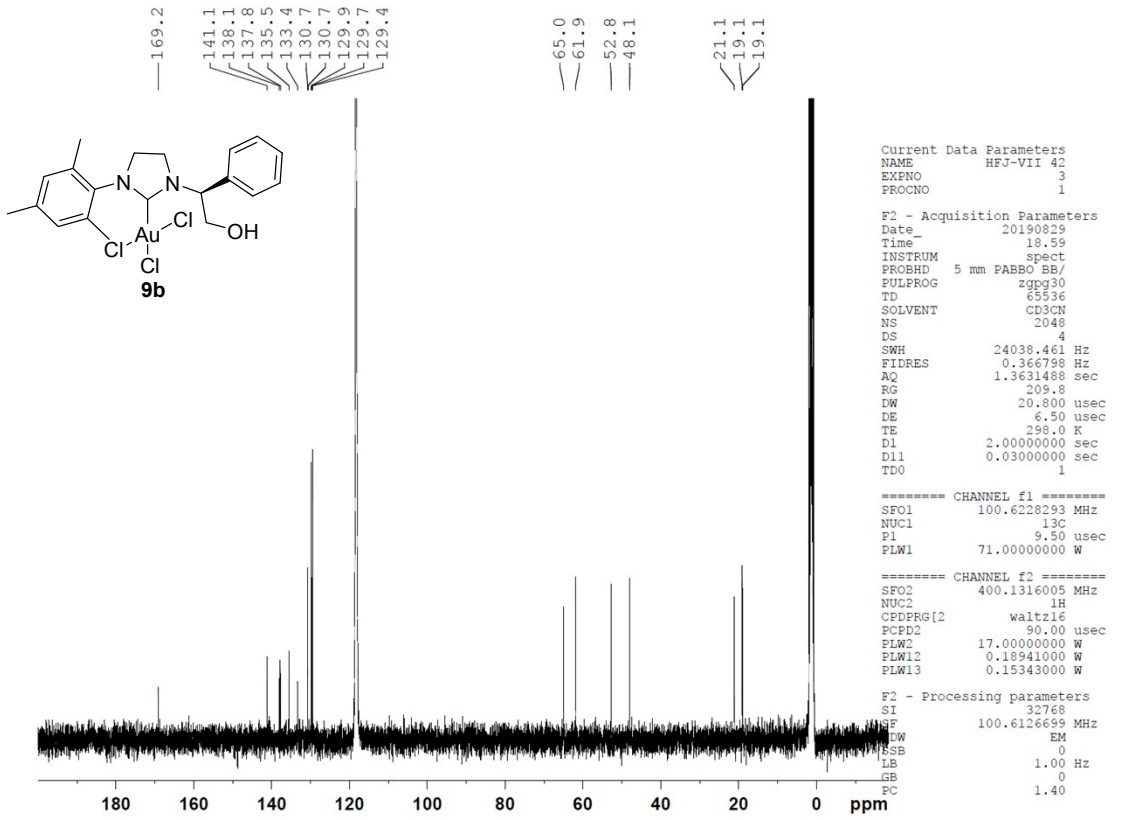

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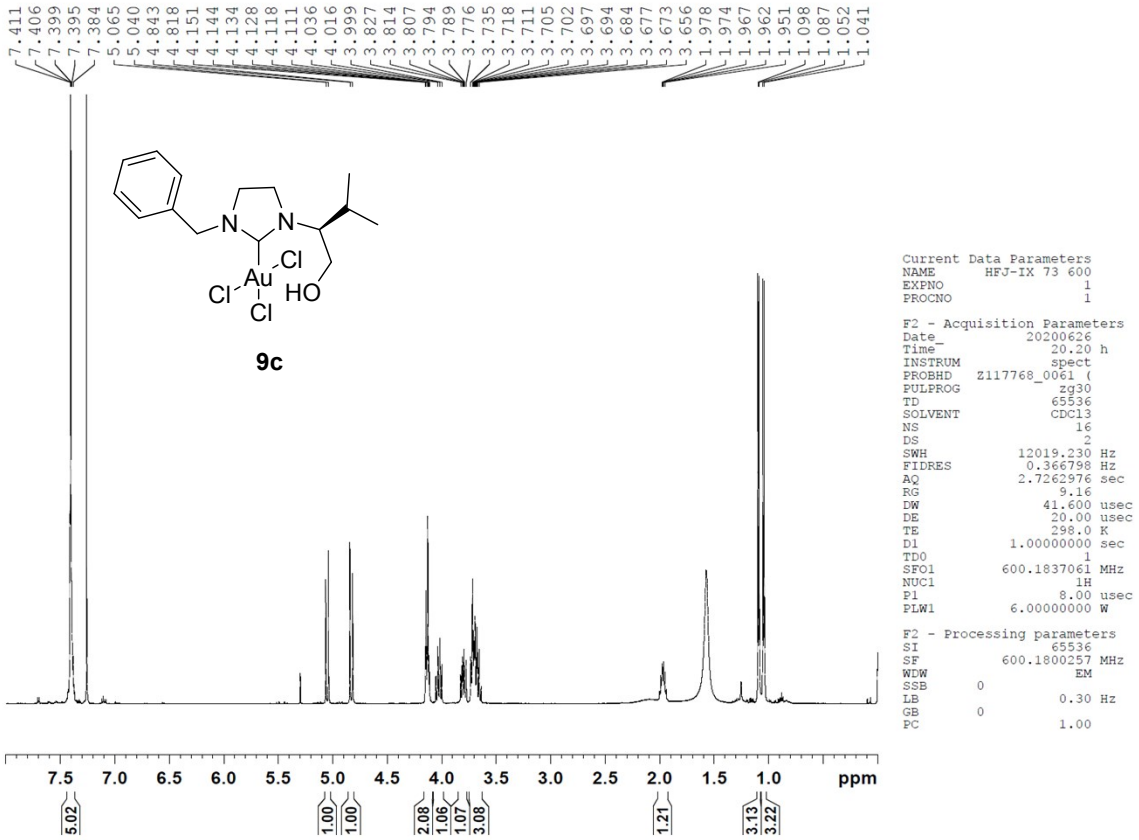

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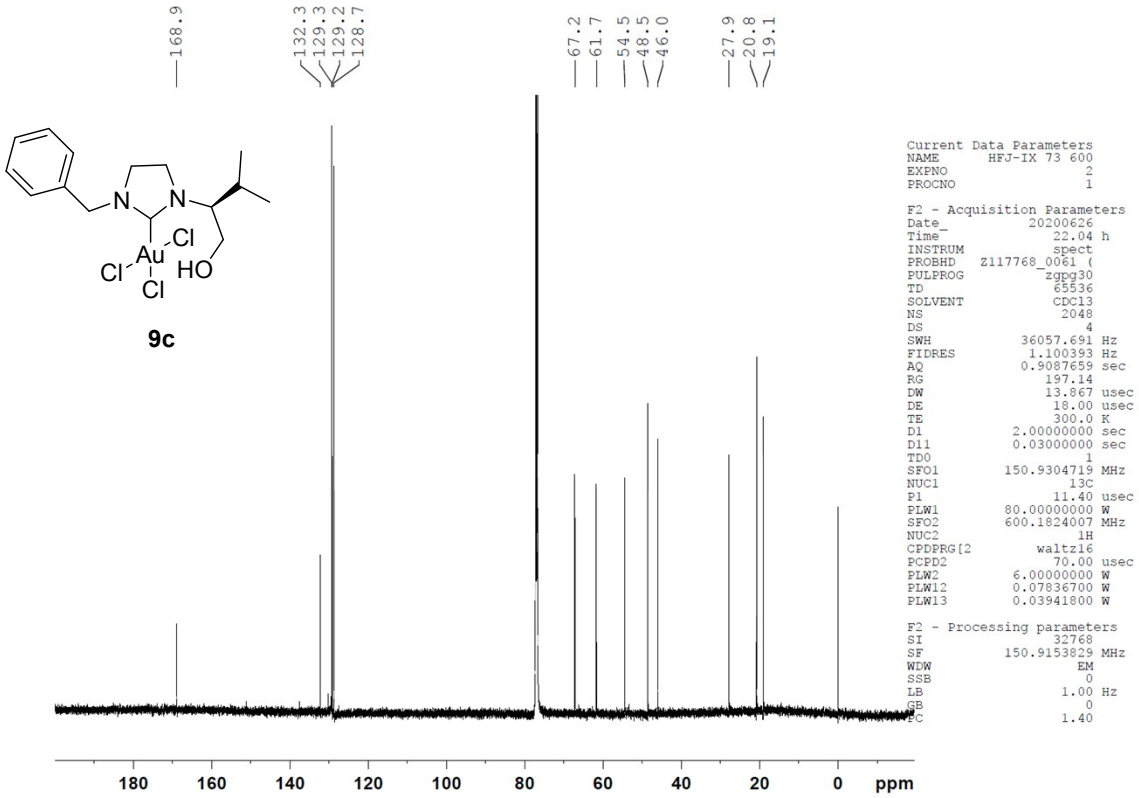

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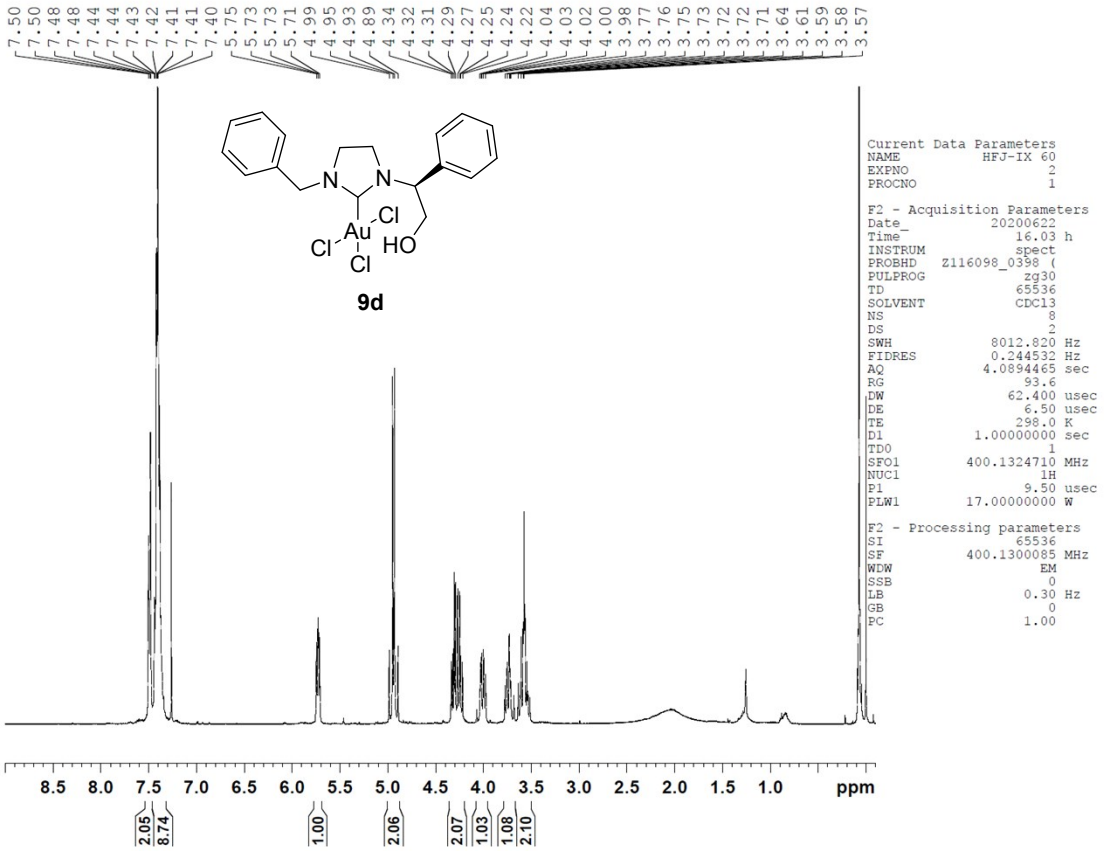

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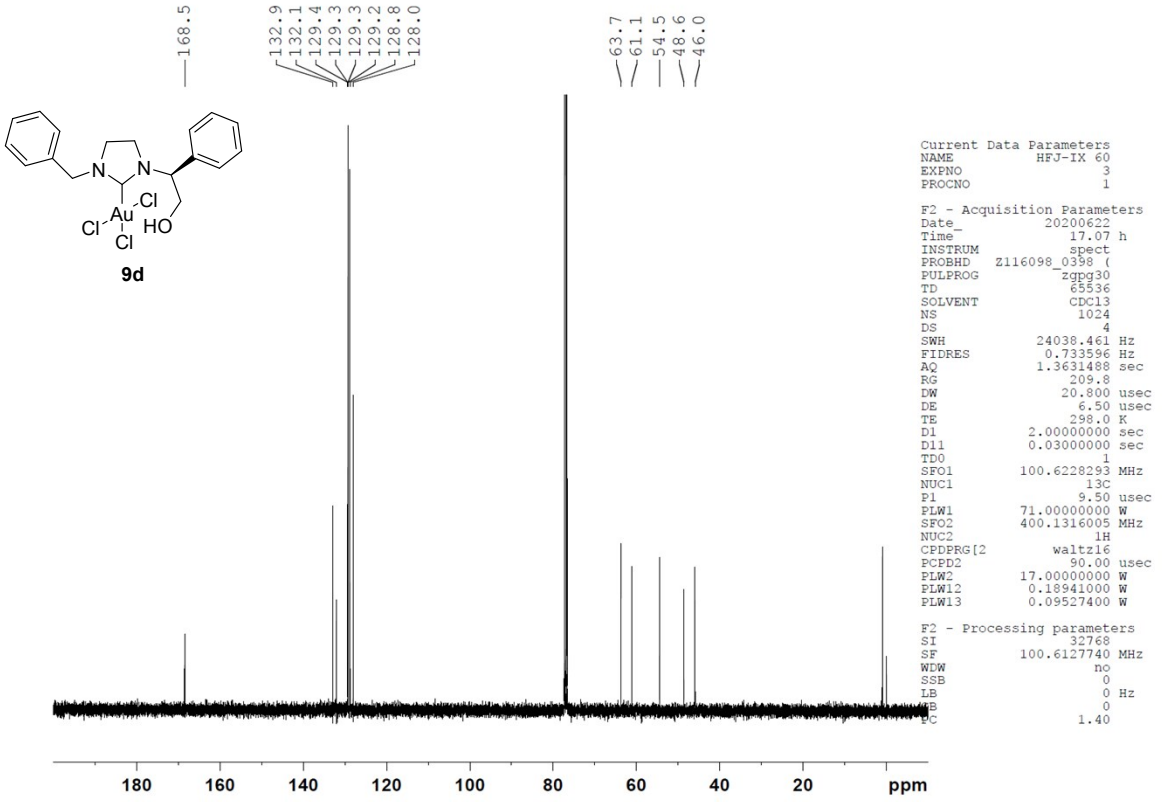

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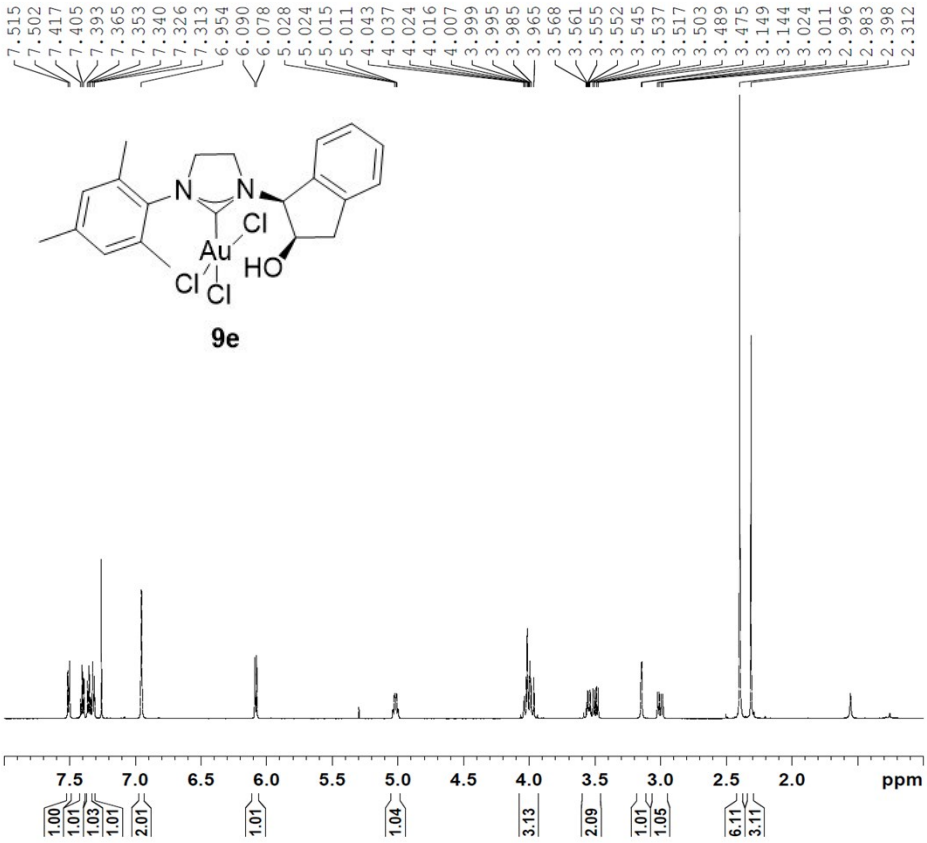


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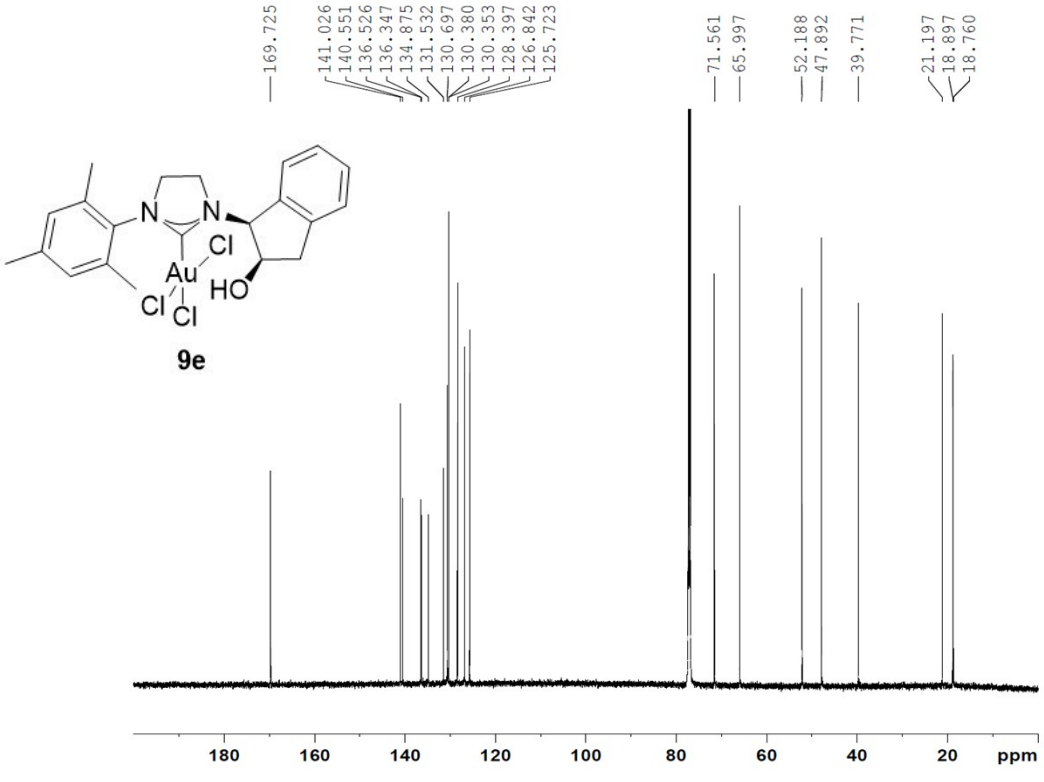
^{13}C NMR data for compound **9e**

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PROCNO                 1

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SOLVENT            CDCl3
NS                  2048
DS                     4
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FIDRES         1.100393 Hz
AQ             0.9087659 sec
RG                197.14
DW                13.867 usec
DE                18.00 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.9304719 MHz
NUC1                 13C
P1                11.40 usec
PLW1         80.00000000 W
SFO2         600.1824007 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             70.00 usec
PLW2          6.00000000 W
PLW12         0.07836700 W
PLW13         0.03941800 W

F2 - Processing parameters
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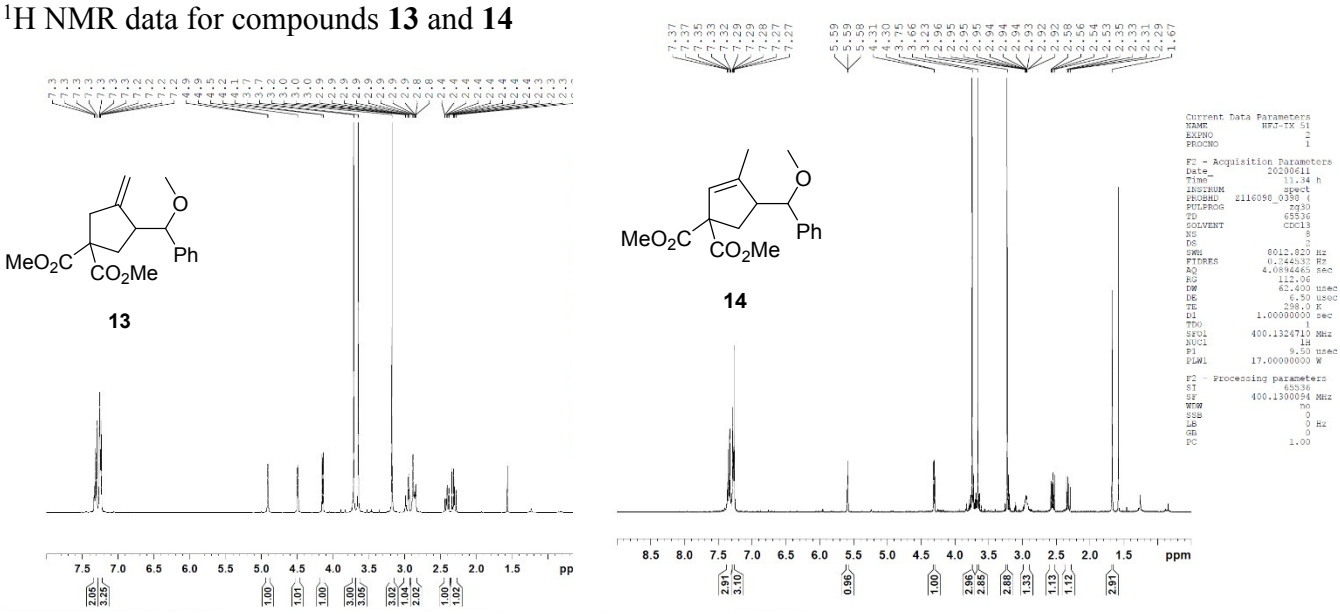
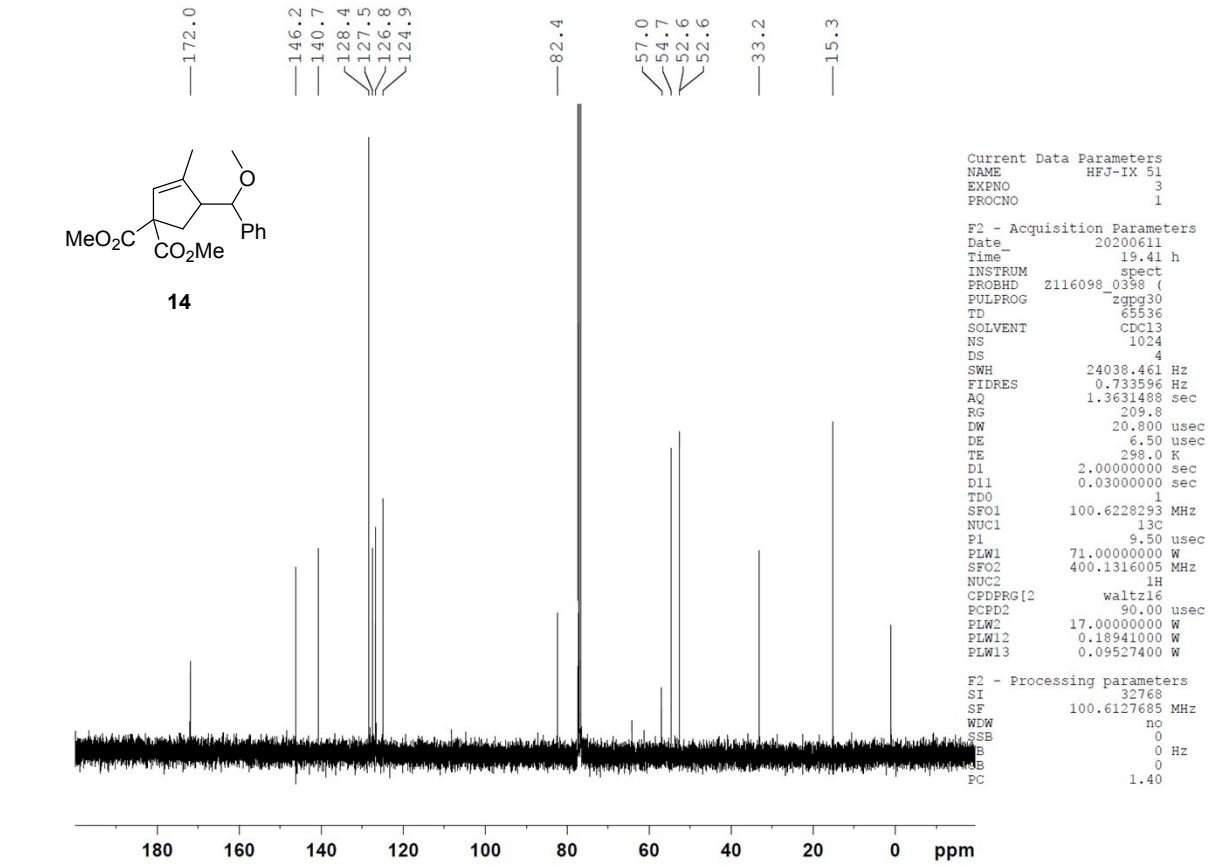
^{1}H NMR data for compounds **13** and **14**



^{13}C NMR data for compound **14**

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RG                 209.8
DW                20.800 usec
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TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
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NUC1                  13C
P1                  9.50 usec
PLW1          71.00000000 W
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          17.00000000 W
PLW12          0.18941000 W
PLW13          0.09527400 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   no
SSB                    0
LB                 0 Hz
GB                     0
PC                  1.40
```

Crystallographic data

Single crystals of complexes **8b,d,e** and **9a,b,e** were crystallized by slow diffusion of diethyl ether into a dichloromethane solution of the complexes. Suitable crystals were selected and were collected on a Bruker D8 APEX-II diffractometer equipped with a CCD camera using Mo Kα radiation (λ = 0.71073 Å). Crystals were mounted on a fiber loop using Fomblin oil. Data reduction was performed with SAINT,5 absorption corrections for the area detector were performed using SADABS,6 or with CrysAlisPro. Structures were solved by direct methods and refined by least squares methods on F2 using the SHELX7-8 and the OLEX2 software suits.9-11 The data were collected at 170 K for all complexes. The X-ray structures (cif) of data have been deposited with the Cambridge Crystallographic Data Centre.

Table S1 Crystal data and structure refinement for 8b.

Identification code	2056825
Empirical formula	$C_{20}H_{24}AuClN_2O$
Formula weight	540.83
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	8.4305(2)
b/Å	14.1308(4)
c/Å	9.2329(2)
α/°	90
β/°	115.9010(10)
γ/°	90
Volume/Å^3	989.43(4)
Z	2
ρ_{calc}g/cm^3	1.815
μ/mm^{-1}	7.579
F(000)	524.0
Crystal size/mm^3	0.22 × 0.16 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.904 to 61.354
Index ranges	-12 ≤ h ≤ 12, -20 ≤ k ≤ 20, -13 ≤ l ≤ 13
Reflections collected	26060
Independent reflections	6119 [R_{int} = 0.0527, R_{sigma} = 0.0488]
Data/restraints/parameters	6119/1/230
Goodness-of-fit on F^2	0.933
Final R indexes [I>=2σ (I)]	R_1 = 0.0233, wR_2 = 0.0469
Final R indexes [all data]	R_1 = 0.0267, wR_2 = 0.0480
Largest diff. peak/hole / e Å^{-3}	0.66/-0.79
Flack parameter	0.017(6)

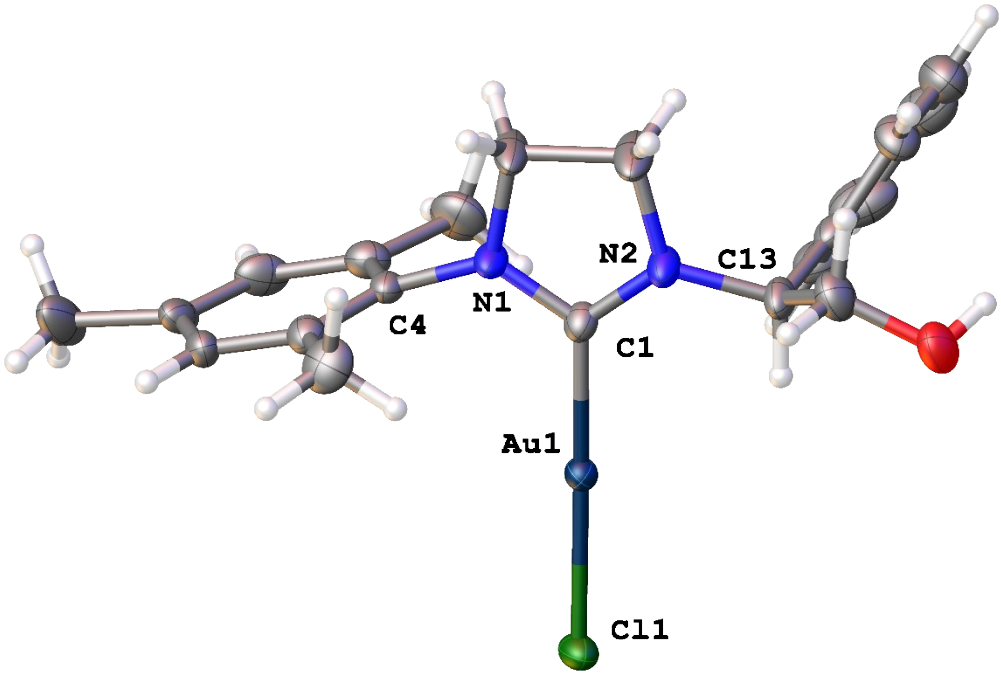

Figure S1. ORTEP plot (50% probability ellipsoids) of complex **8b**. Selected bond lengths (Å) and angles (°): Au1 Cl1 2.2870(13), Au1 C1 1.980(5), C1 N2 1.325(6), C1 N1 1.329(6), C1 Au1 Cl1 177.61(16),C1 N2 C13 124.7(4), C1 N1 C4 126.2(4)

Table S2 Crystal data and structure refinement for 8d.

Identification code	2056945
Empirical formula	$C_{18}H_{20}AuClN_2O$
Formula weight	512.78
Temperature/K	170
Crystal system	triclinic
Space group	P1
a/Å	8.2937(11)
b/Å	9.0157(12)
c/Å	13.7482(18)
α/°	73.077(2)
β/°	75.363(2)
γ/°	64.382(2)
Volume/Å3	877.2(2)
Z	2
ρcalcg/cm3	1.941
μ/mm-1	8.543
F(000)	492.0
Crystal size/mm3	0.12 × 0.09 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.124 to 53.45
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -17 ≤ l ≤ 17
Reflections collected	21897
Independent reflections	7470 [Rint = 0.0816, Rsigma = 0.0938]
Data/restraints/parameters	7470/9/417
Goodness-of-fit on F2	0.965
Final R indexes [I>=2σ (I)]	R1 = 0.0382, wR2 = 0.0895
Final R indexes [all data]	R1 = 0.0445, wR2 = 0.0929
Largest diff. peak/hole / e Å-3	1.50/-1.65
Flack parameter	0.076(16)

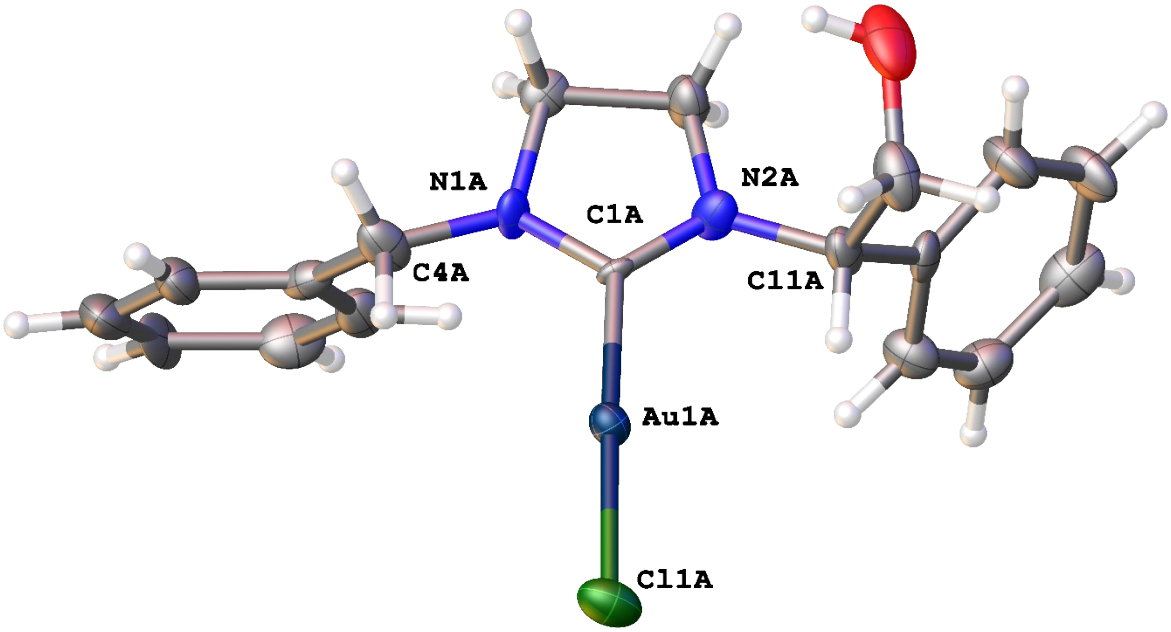

Figure S2. ORTEP plot (50% probability ellipsoids) of complex **8d**. Selected bond lengths (Å) and angles (°): Au1A-Cl1A 2.279(6), Au1B Cl1B 2.279(6) , Au1B C1B 1.97(3), Au1A C1A 2.009(17), C1B Au1B Cl1B 178.5(7), C1A Au1A Cl1A 178.1(6), C1B N2B C11B 123.4(19), C1A N2A C11A 127.2(17), C1B N1B C4B 126.3(19), C1A N1A C4A 125.0(18)

Table S3 Crystal data and structure refinement for 8e

Identification code	2056827
Empirical formula	$C_{21}H_{24}AuClN_2O$
Formula weight	552.84
Temperature/K	150(2)
Crystal system	monoclinic
Space group	C2
a/Å	20.526(12)
b/Å	8.886(5)
c/Å	11.161(7)
α/°	90
β/°	94.890(9)
γ/°	90
Volume/Å^3	2028(2)
Z	4
ρ_{calc}g/cm^3	1.810
μ/mm^{-1}	7.397
F(000)	1072.0
Crystal size/mm^3	0.38 × 0.12 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.662 to 56.724
Index ranges	$-27 \leq h \leq 27$, $-11 \leq k \leq 11$, $-14 \leq l \leq 14$
Reflections collected	22187
Independent reflections	4995 [R_{int} = 0.1393, R_{sigma} = 0.1163]
Data/restraints/parameters	4995/1/239
Goodness-of-fit on F^2	0.858
Final R indexes [I>=2σ (I)]	R_1 = 0.0436, wR_2 = 0.0828
Final R indexes [all data]	R_1 = 0.0625, wR_2 = 0.0886
Largest diff. peak/hole / e Å^{-3}	1.55/-2.48
Flack parameter	0.066(14)

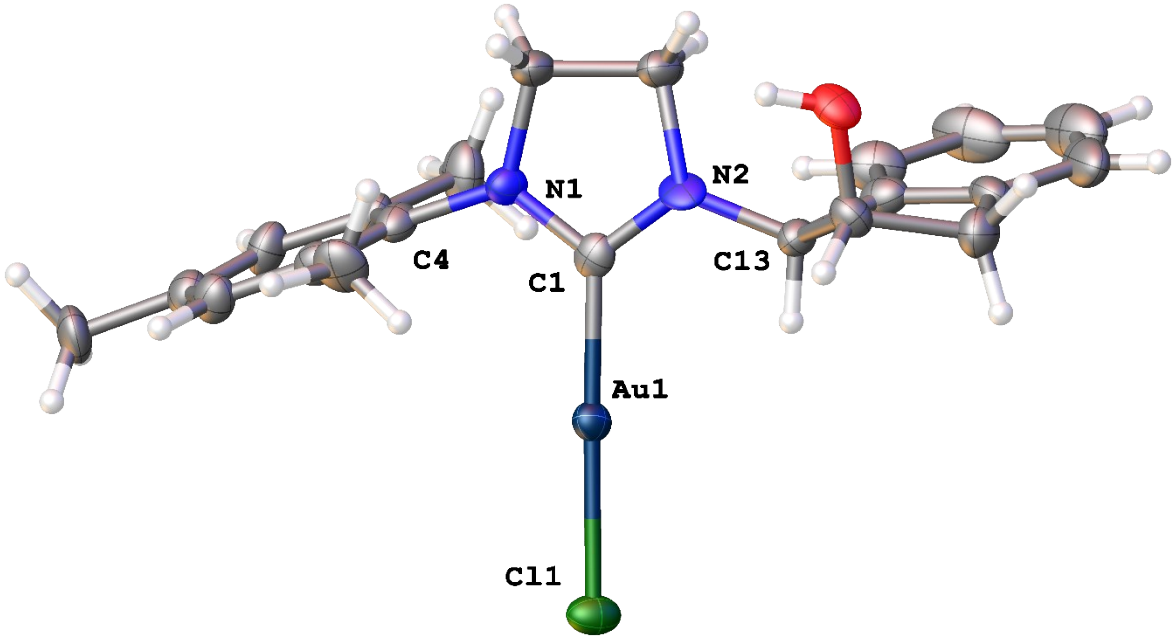

Figure S3. ORTEP plot (50% probability ellipsoids) of complex **8e**. Selected bond lengths (Å) and angles (°): Au1 Cl1 2.295(3), Au1 C1 1.972(12), C1 Au1 Cl1 178.3(3), C1 N1 C4 124.2(9), C1 N2 C13 122.1(10)

Table S4 Crystal data and structure refinement for 9a.

Identification code	2056823
Empirical formula	$C_{17}H_{26}AuCl_3N_2O$
Formula weight	577.71
Temperature/K	150(2)
Crystal system	hexagonal
Space group	$P6_5$
a/Å	15.7328(14)
b/Å	15.7328(14)
c/Å	15.4038(14)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	3301.9(7)
Z	6
ρ_{calc}g/cm^3	1.743
μ/mm^{-1}	7.054
F(000)	1680.0
Crystal size/mm^3	0.36 × 0.28 × 0.16
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.99 to 61.41
Index ranges	$-18 \leq h \leq 22$, $-22 \leq k \leq 19$, $-22 \leq l \leq 21$
Reflections collected	29813
Independent reflections	6763 [R_{int} = 0.0668, R_{sigma} = 0.0664]
Data/restraints/parameters	6763/1/223
Goodness-of-fit on F^2	0.980
Final R indexes [I>=2σ (I)]	R_1 = 0.0318, wR_2 = 0.0621
Final R indexes [all data]	R_1 = 0.0396, wR_2 = 0.0644
Largest diff. peak/hole / e Å^{-3}	1.63/-0.97
Flack parameter	0.006(6)

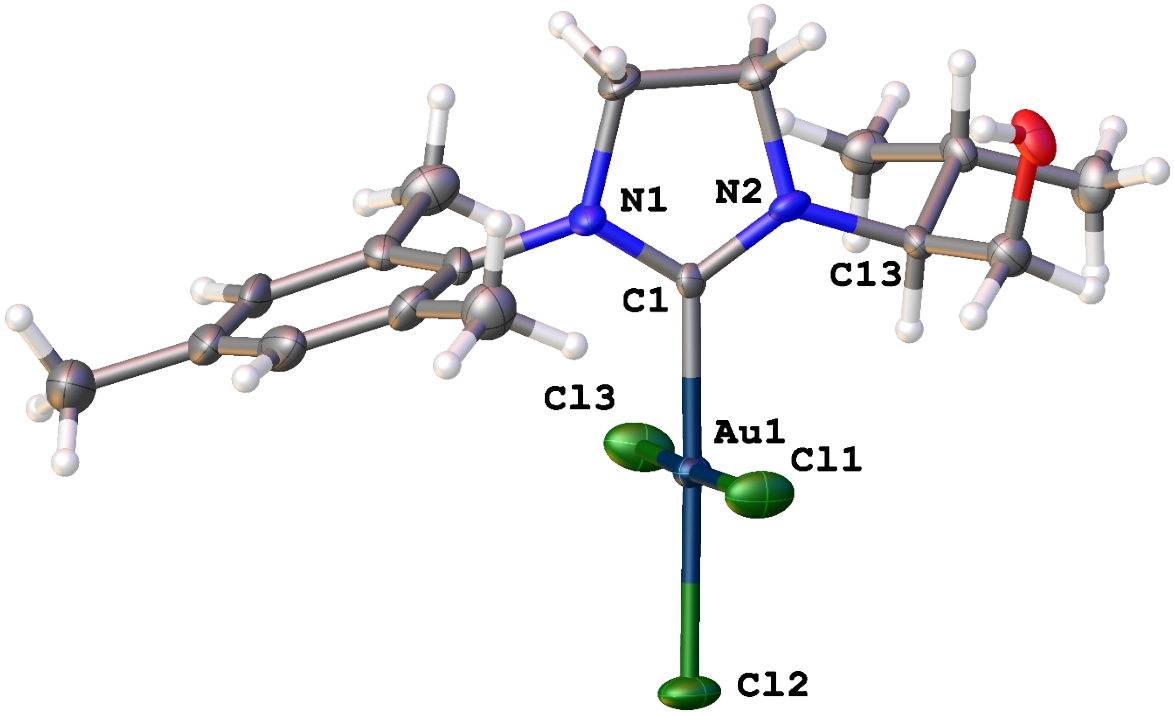

Figure S4. ORTEP plot (50% probability ellipsoids) of complex **9a**. Selected bond lengths (Å) and angles (°): Au1 Cl1 2.2747(19) Au1 Cl2 2.3269(17) Au1 Cl3 2.265(2) Au1 C1 2.016(6) N2 C13 1.469(8) N1 C4 1.440(8) C1 N2 C13 127.3(5)C1 N1 C4 127.4(5) Cl1 Au1 Cl2 90.50(7) Cl3 Au1 Cl1 176.05(9) Cl3 Au1 Cl2 89.82(7) C1 Au1 Cl1 88.39(19) C1 Au1 Cl2 178.1(2) C1 Au1 Cl3 91.39(19).
Planes :
A: C1 Cl3 Cl1 Au1 Cl2 Au1 (-0.020), C1 (-0.052), Cl1 (0.058), Cl2 (-0.045), Cl3 (0.058), RMSD/A: 0.049
B: C2 C3 N2 C1 N1 C2 (0.037), N1 (-0.027), C1 (0.003), N2 (0.023), C3 (-0.036), RMSD/A: 0.028
Angle between A-B: 89.8(2)

Table S5 Crystal data and structure refinement for 9b.

Identification code	2056946
Empirical formula	$C_{40}H_{48}Au_2Cl_6N_4O_2$
Formula weight	1223.45
Temperature/K	180
Crystal system	monoclinic
Space group	P21
a/Å	8.3792(5)
b/Å	15.8615(10)
c/Å	8.5517(5)
α/°	90
β/°	109.7410(10)
γ/°	90
Volume/Å3	1069.78(11)
Z	1
ρ_{calc} g/cm3	1.899
μ/mm^{-1}	7.263
F(000)	592.0
Crystal size/mm3	0.15 × 0.09 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.06 to 57.618
Index ranges	-11 ≤ h ≤ 11, -21 ≤ k ≤ 21, -11 ≤ l ≤ 11
Reflections collected	30817
Independent reflections	5567 [Rint = 0.0673, Rsigma = 0.0502]
Data/restraints/parameters	5567/1/248
Goodness-of-fit on F2	1.049
Final R indexes [I>=2σ (I)]	R1 = 0.0320, wR2 = 0.0771
Final R indexes [all data]	R1 = 0.0382, wR2 = 0.0798
Largest diff. peak/hole / e Å-3	3.08/-0.73
Flack parameter	0.027(6)

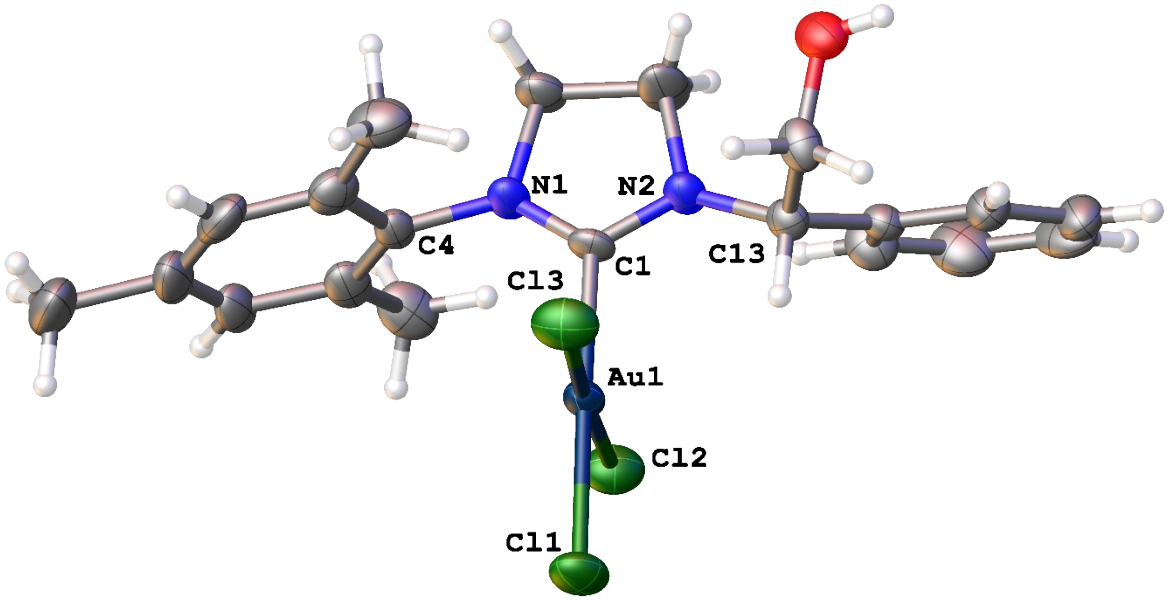

Figure S5. ORTEP plot (50% probability ellipsoids) of complex **9b**. Selected bond lengths (Å) and angles (°): Au1 C1 2.055(7), Au1 Cl1 2.324(2), Au1 Cl2 2.270(2), Au1 Cl3 2.278(2), Cl2 Au1 Cl3 176.68(11), C1 Au1 Cl1 178.7(2), C1 Au1 Cl2 88.6(2), C1 Au1 Cl3 90.3(2), C1 N1 C4 129.2(7), C1 N2 C13 127.3(7), Cl2 Au1 Cl3 176.68(11)
Planes
A: C1, C2, N1, N2, C3: C2 -0.009, N1 0.002, C1 0.008, N2 -0.014, C3 0.013
B: Cl1, Cl2, Cl3 Au1: Cl3 -0.030, Au1 0.032, C1 0.015, Cl2 -0.030, Cl1 0.013.
A/B: 85.5(3)

Table S6 Crystal data and structure refinement for 9e.

Identification code	2056822
Empirical formula	$C_{21}H_{24}AuCl_3N_2O$
Formula weight	623.74
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	8.3572(9)
b/Å	13.6260(15)
c/Å	9.7363(10)
α/°	90
β/°	100.369(2)
γ/°	90
Volume/Å^3	1090.6(2)
Z	2
ρ_{calc}g/cm^3	1.899
μ/mm^{-1}	7.127
F(000)	604.0
Crystal size/mm^3	0.3 × 0.26 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.252 to 60.996
Index ranges	$-11 \le h \le 11$, $-19 \le k \le 19$, $-13 \le l \le 13$
Reflections collected	16650
Independent reflections	6551 [R_{int} = 0.0366, R_{sigma} = 0.0585]
Data/restraints/parameters	6551/1/257
Goodness-of-fit on F^2	0.774
Final R indexes [I>=2σ (I)]	R_1 = 0.0222, wR_2 = 0.0457
Final R indexes [all data]	R_1 = 0.0238, wR_2 = 0.0463
Largest diff. peak/hole / e Å^{-3}	1.48/-0.88
Flack parameter	0.014(5)

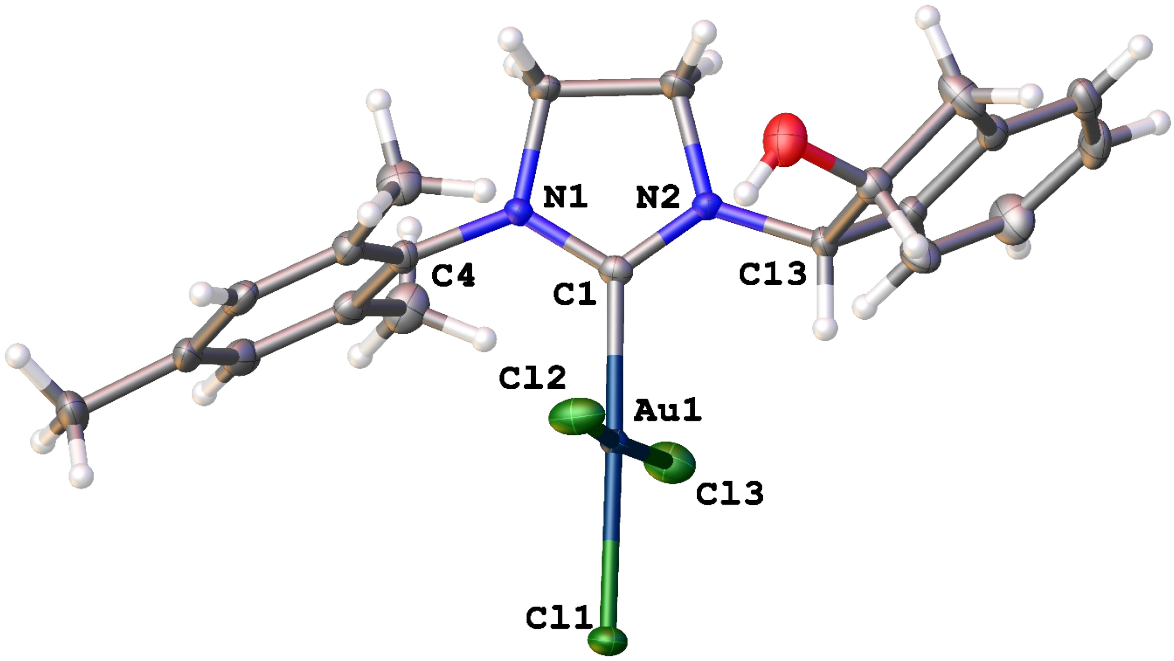

Figure S6. ORTEP plot (50% probability ellipsoids) of complex **9e**. Selected bond lengths (Å) and angles (°): Au1 Cl3 2.2876(13), Au1 Cl1 2.3290(12), Au1 Cl2 2.2845(12), Au1 C1 2.009(5), Cl3 Au1 Cl1 90.44(5), Cl2 Au1 Cl3 174.61(6), Cl2 Au1 Cl1 90.91(5), C1 Au1 Cl3 87.72(13) , C1 Au1 Cl1 177.26(13), C1 Au1 Cl2 91.10(13), C1 N2 C13 125.4(4), C1 N1 C4 125.8(4).
Planes :
A: C1 Au1 Cl3 Cl2 Cl1: Cl2 (0.076), Cl1 (-0.058), Cl3 (0.078), C1 (-0.069), Au1 (-0.027), RMSD/A: 0.064
B: C2 N1 C1 N2 C3: C3 (0.011), N2 (-0.007), C1 (-0.002),N1 (0.009), C2 (-0.011), RMSD/A: 0.009
A-B: 100.42(14)