

Supporting Information

Silver(I)-N-heterocyclic carbene complexes derived from clotrimazole: antiproliferative activity and interaction with an artificial membrane-based biosensor

Heba A. Mohamed,^a Samantha Shepherd,^b Nicola William,^a Helen A. Blundell,^a Madhurima Das,^a Christopher M. Pask,^a Benjamin R. M. Lake,^a Roger M. Phillips,^{b} Andrew Nelson,^{a*} and Charlotte E. Willans^{a*}*

^a School of Chemistry, University of Leeds, Woodhouse Lane, Leeds, LS2 9JT, UK.

^b School of Applied Sciences, Department of Pharmacy, University of Huddersfield, Queensgate, Huddersfield, HD1 3DH, UK.

1. ¹H and ¹³C{¹H} NMR spectra of imidazolium salts	Page S2
2. ¹H and ¹³C{¹H} NMR spectra of silver complexes	Page S15
3. Molecular Structures of Imidazolium Salts	Page S28
4. X-Ray Crystallographic Information for Imidazolium Salts	Page S32
5. X-Ray Crystallographic Information for Silver Complexes	Page S40
6. Expanded RCVs	Page S45

1. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of imidazolium salts

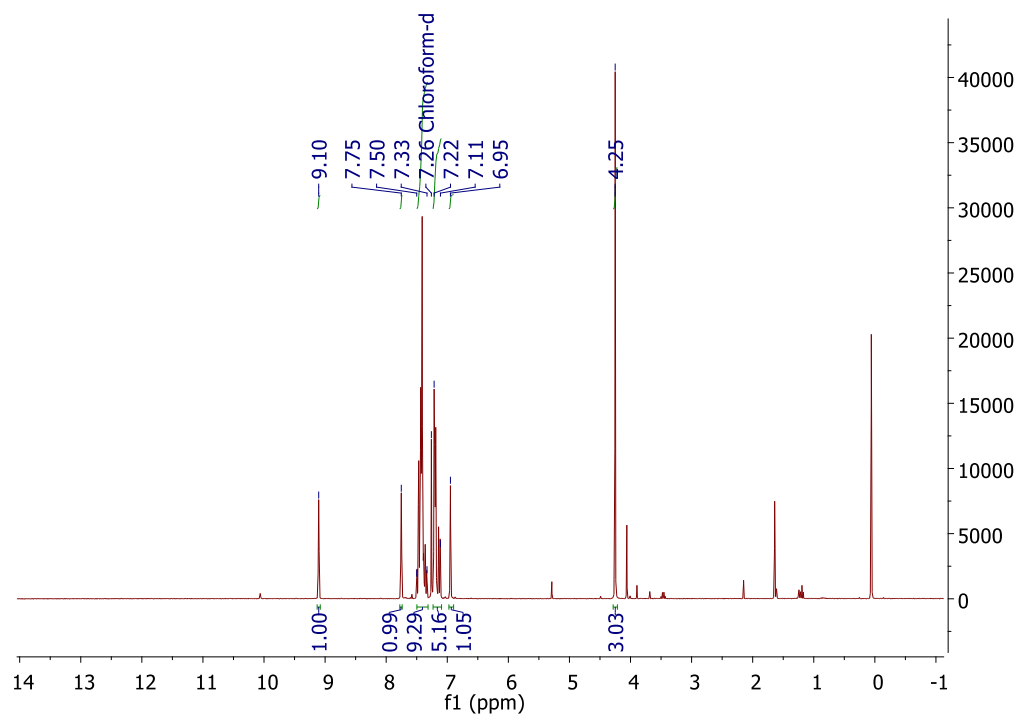


Figure S1a. ^1H NMR spectrum of imidazolium salt **1a** (300 MHz, CDCl_3)

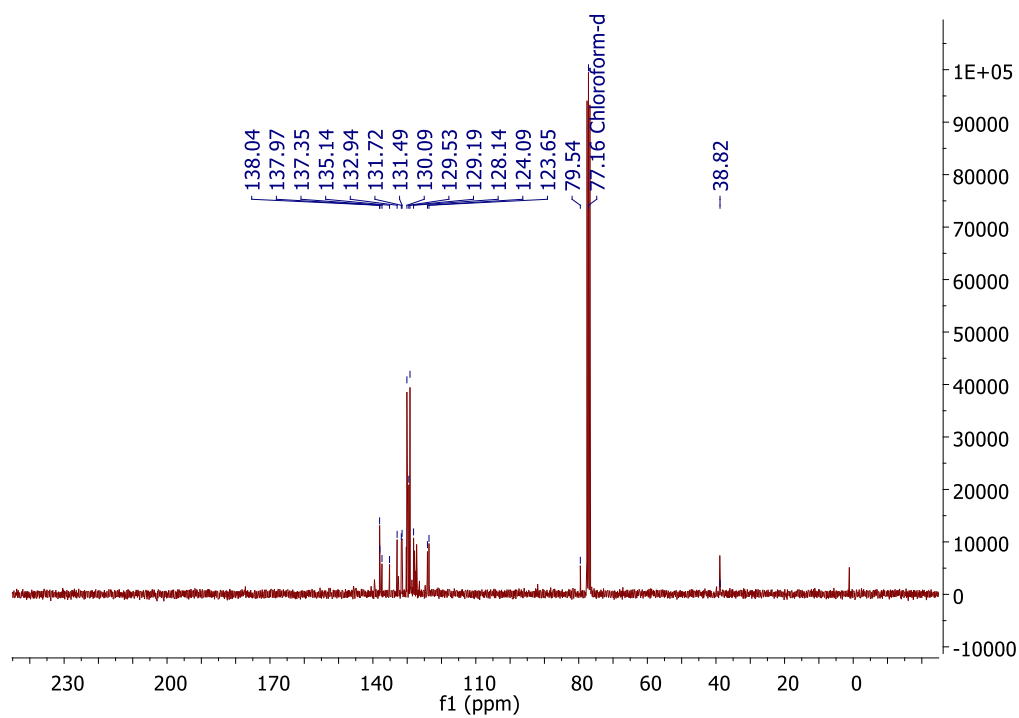


Figure S1b. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of imidazolium salt **1a** (75 MHz, CDCl_3)

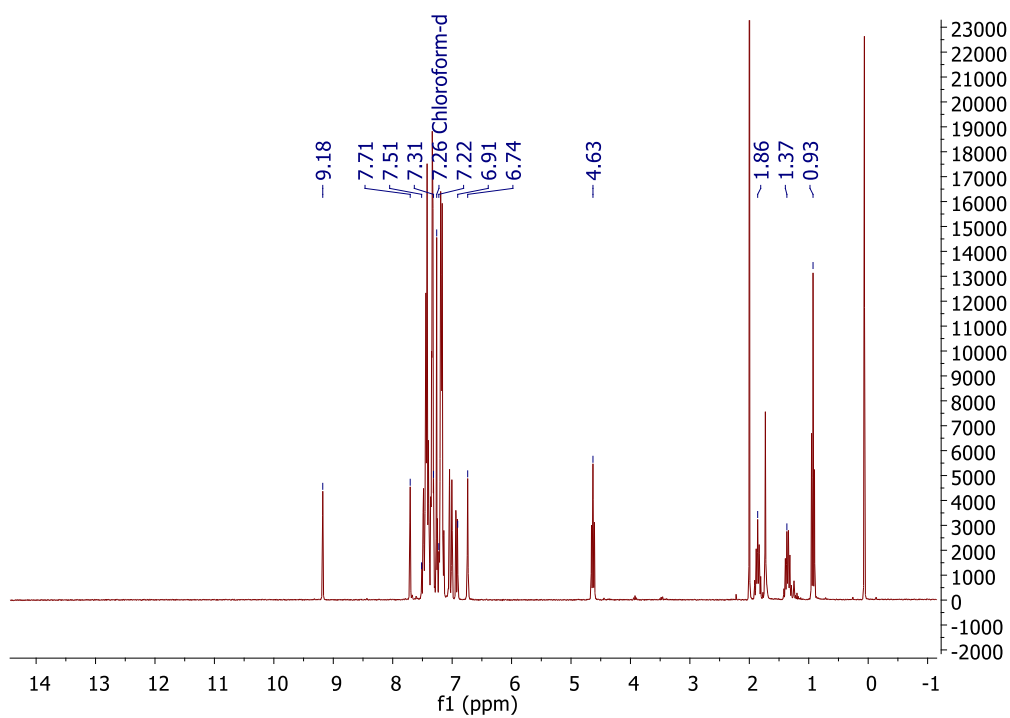


Figure S2a. ^1H NMR spectrum of imidazolium salt **1c** (300 MHz, CDCl_3)

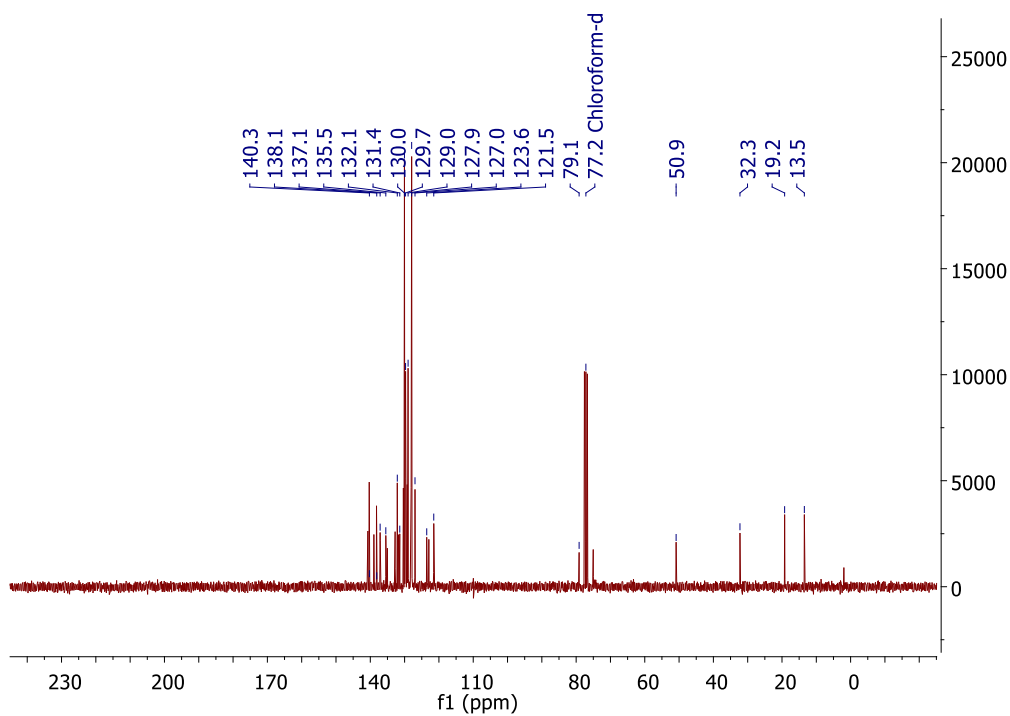


Figure S2b. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of imidazolium salt **1c** (75 MHz, CDCl_3)

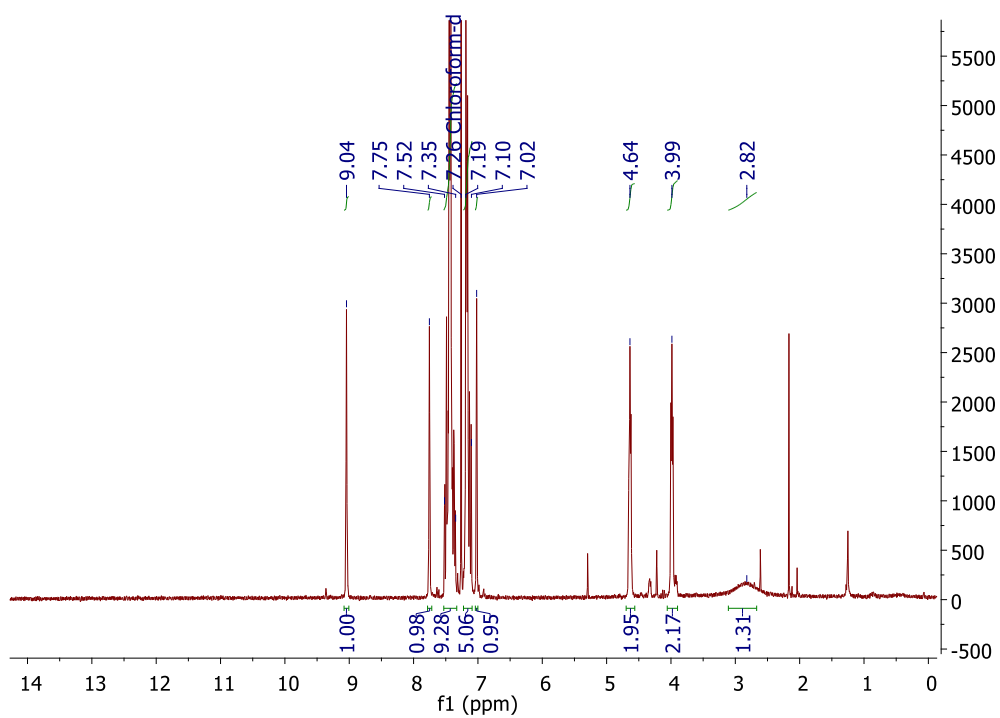


Figure S3a. ¹H NMR spectrum of imidazolium salt **1e** (300 MHz, CDCl₃)

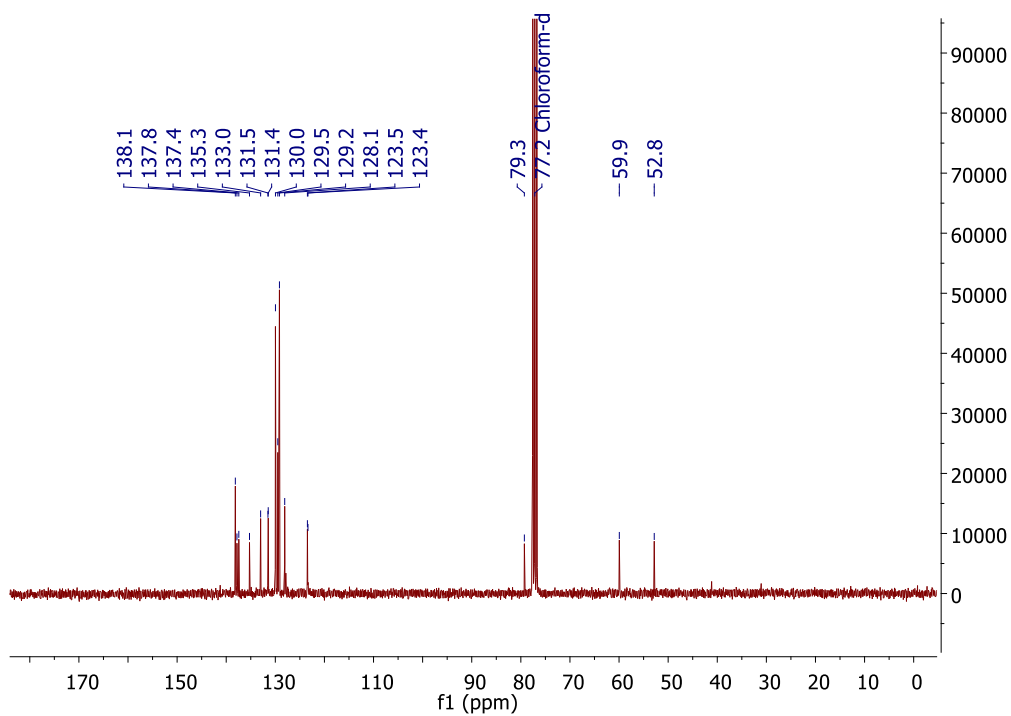


Figure S3b. ¹³C{¹H} NMR spectrum of imidazolium salt **1e** (75 MHz, CDCl₃)

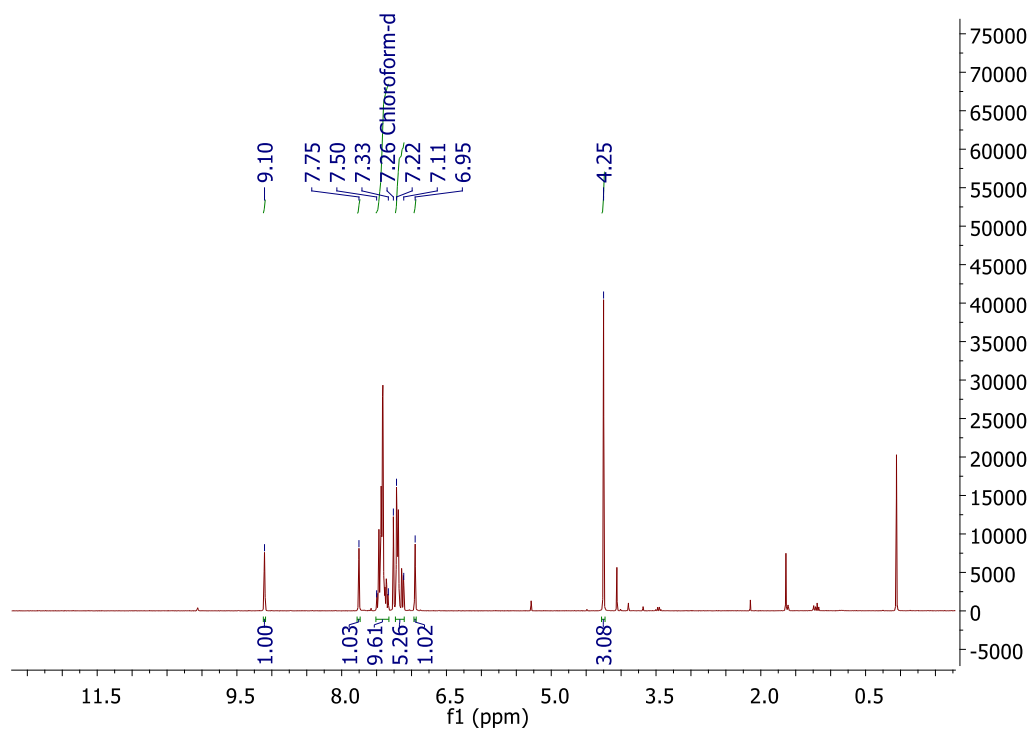


Figure S4a. ¹H NMR spectrum of imidazolium salt **2a** (300 MHz, CDCl₃)

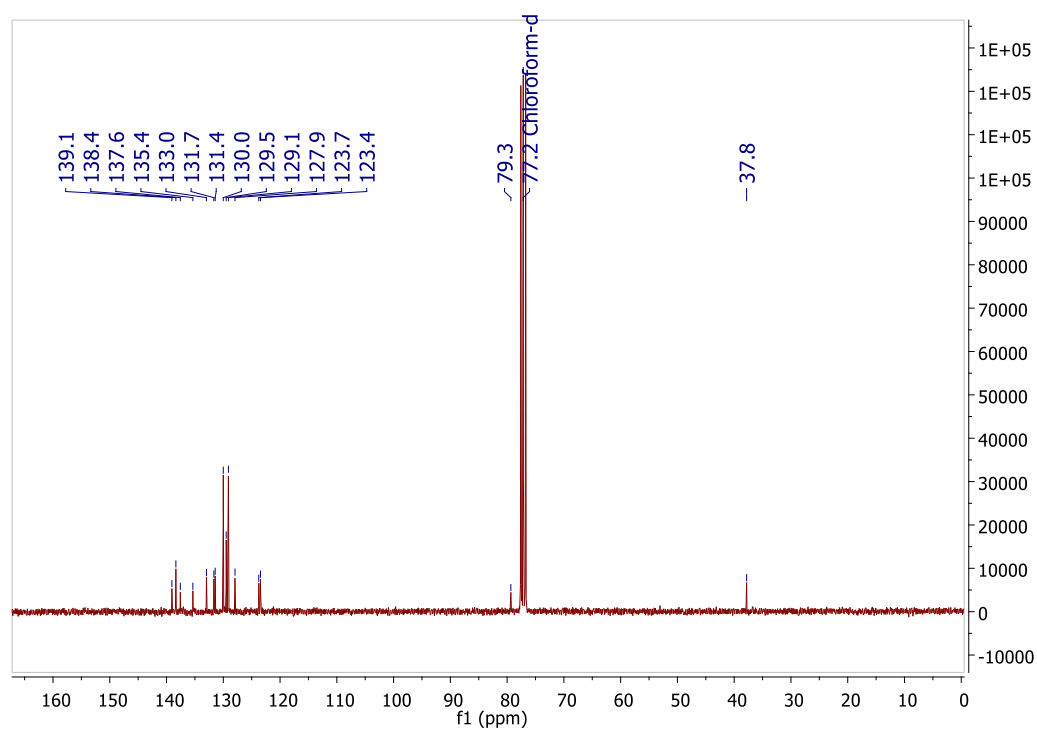


Figure S4b. ¹³C{¹H} NMR spectrum of imidazolium salt **2a** (75 MHz, CDCl₃)

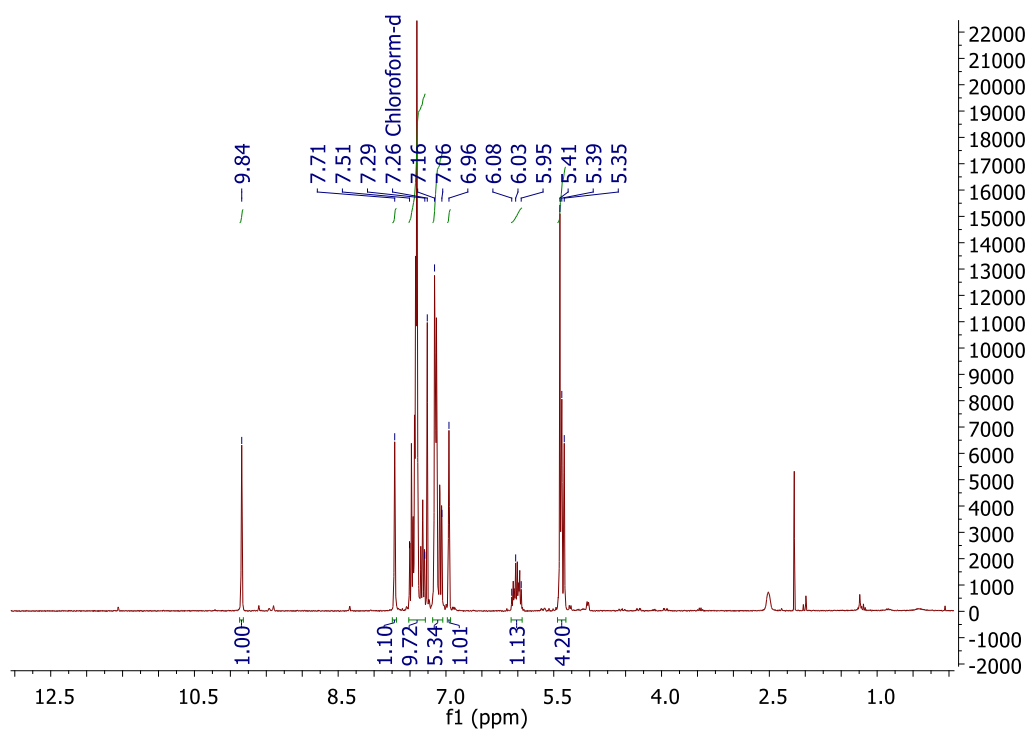


Figure S5a. ¹H NMR spectrum of imidazolium salt **2b** (300 MHz, CDCl₃)

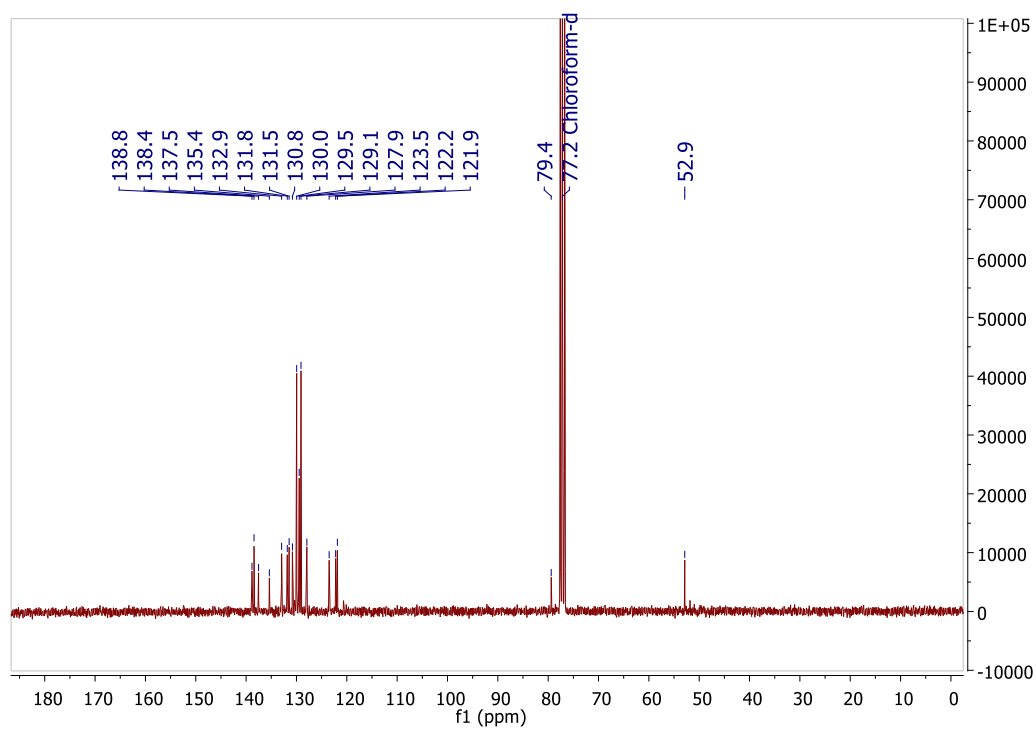


Figure S5b. ¹³C{¹H} NMR spectrum of imidazolium salt **2b** (75 MHz, CDCl₃)

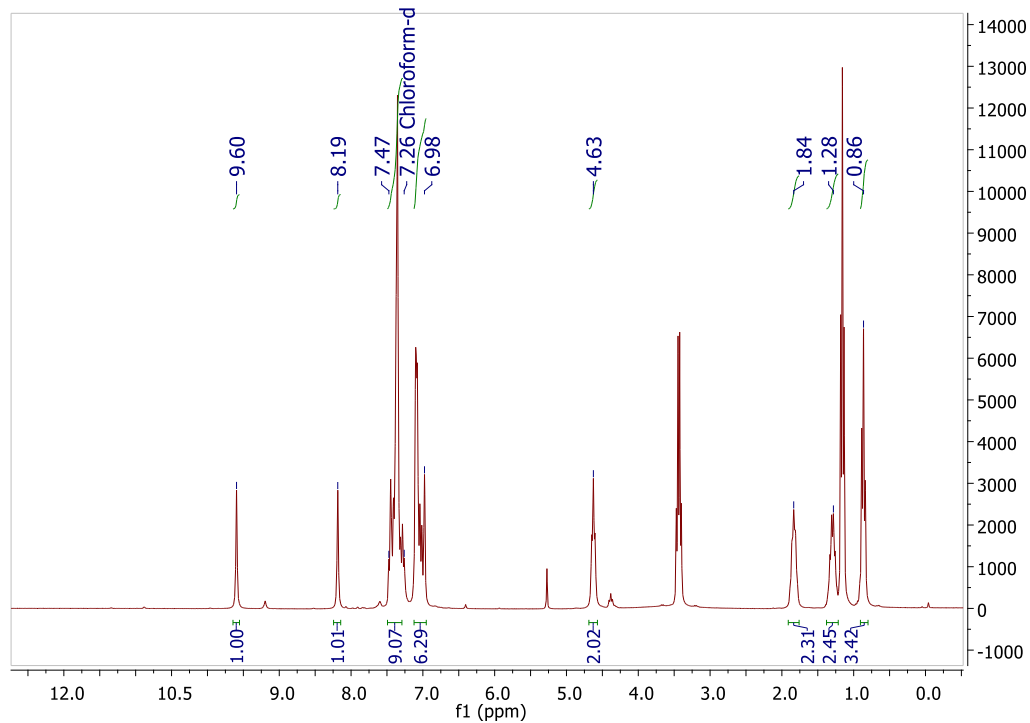


Figure S6a. ¹H NMR spectrum of imidazolium salt **2c** (300 MHz, CDCl₃)

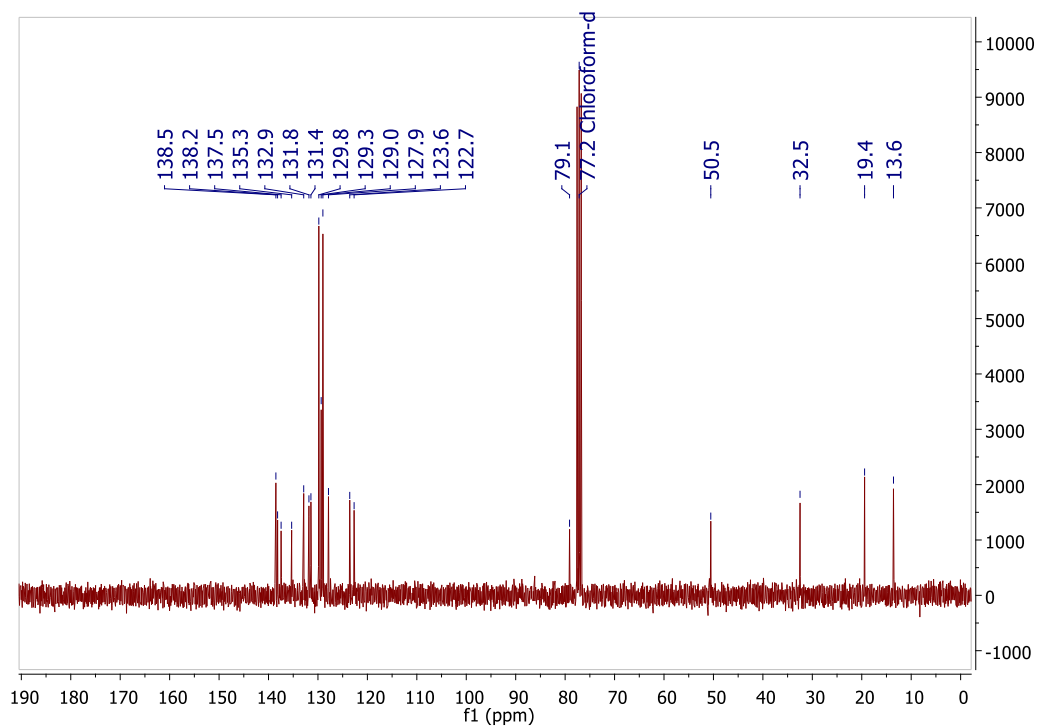


Figure S6b. ¹³C{¹H} NMR spectrum of imidazolium salt **2c** (75 MHz, CDCl₃)

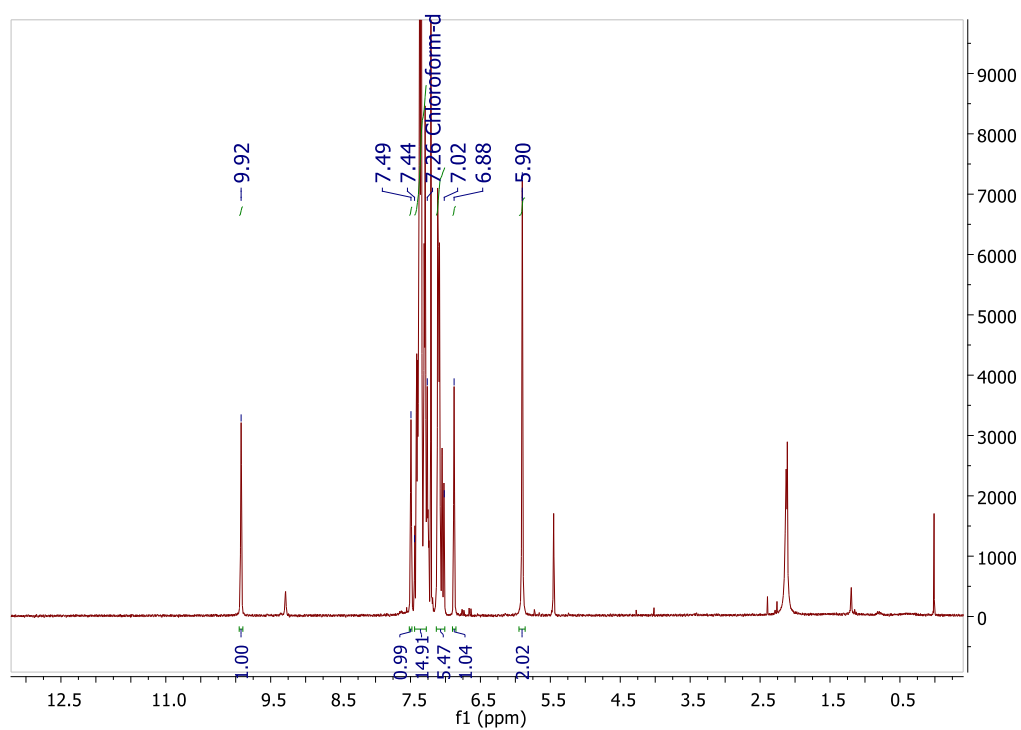


Figure S7a. ¹H NMR spectrum of imidazolium salt **2d** (300 MHz, CDCl₃)

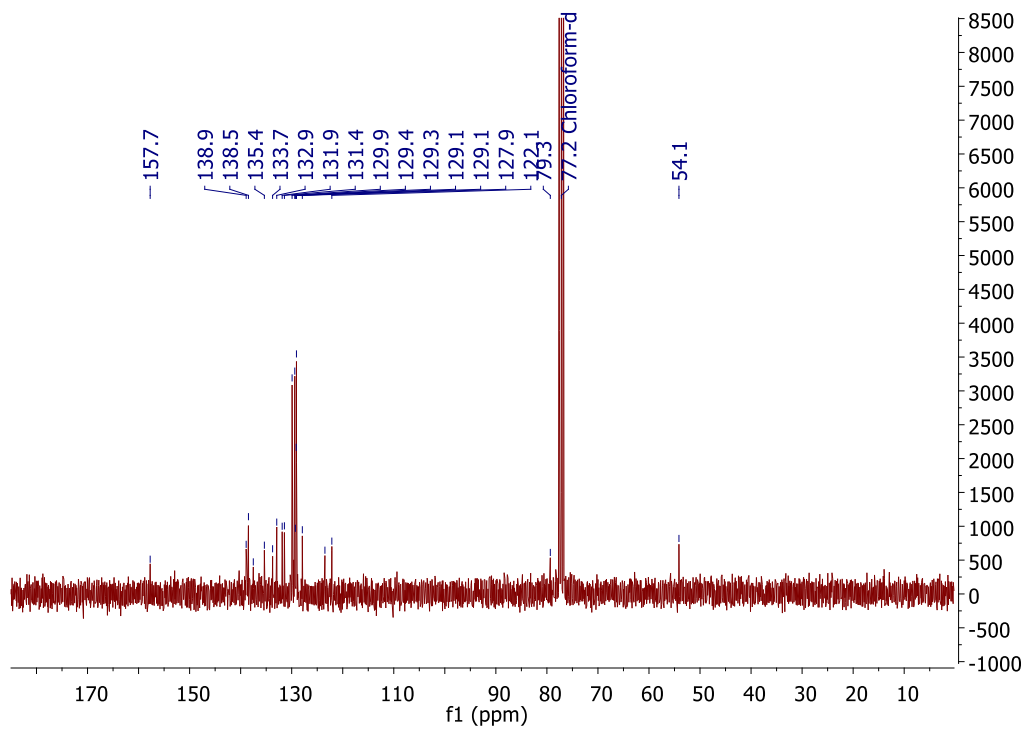


Figure S7b. ¹³C{¹H} NMR spectrum of imidazolium salt **2d** (75 MHz, CDCl₃)

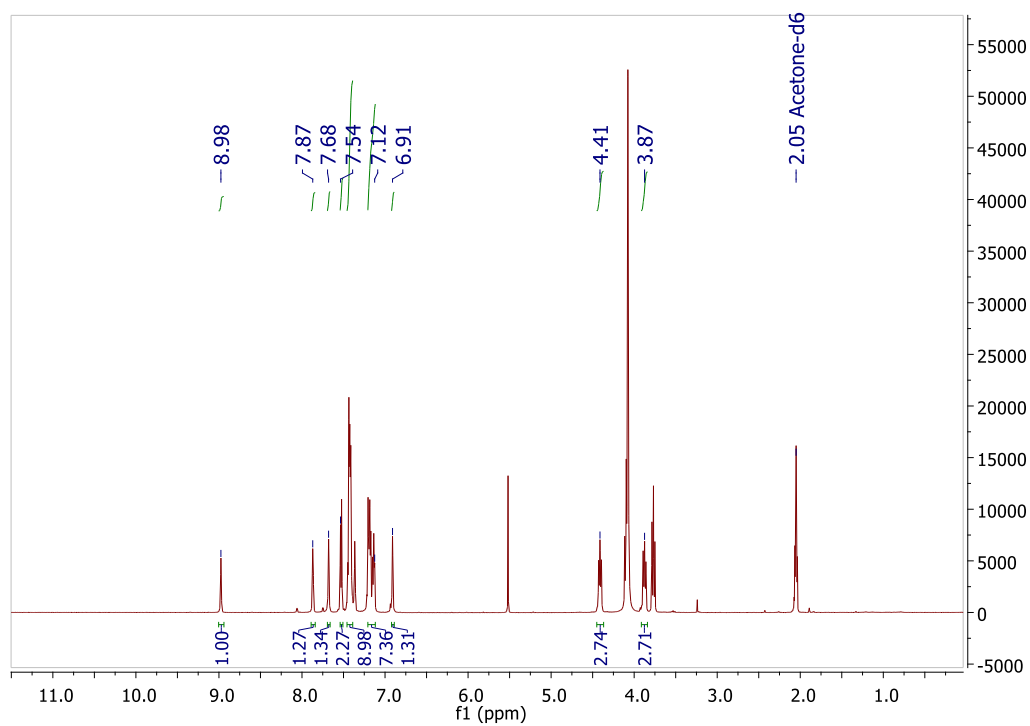


Figure S8a. ^1H NMR spectrum of imidazolium salt **2e** (300 MHz, Acetone- d_6)

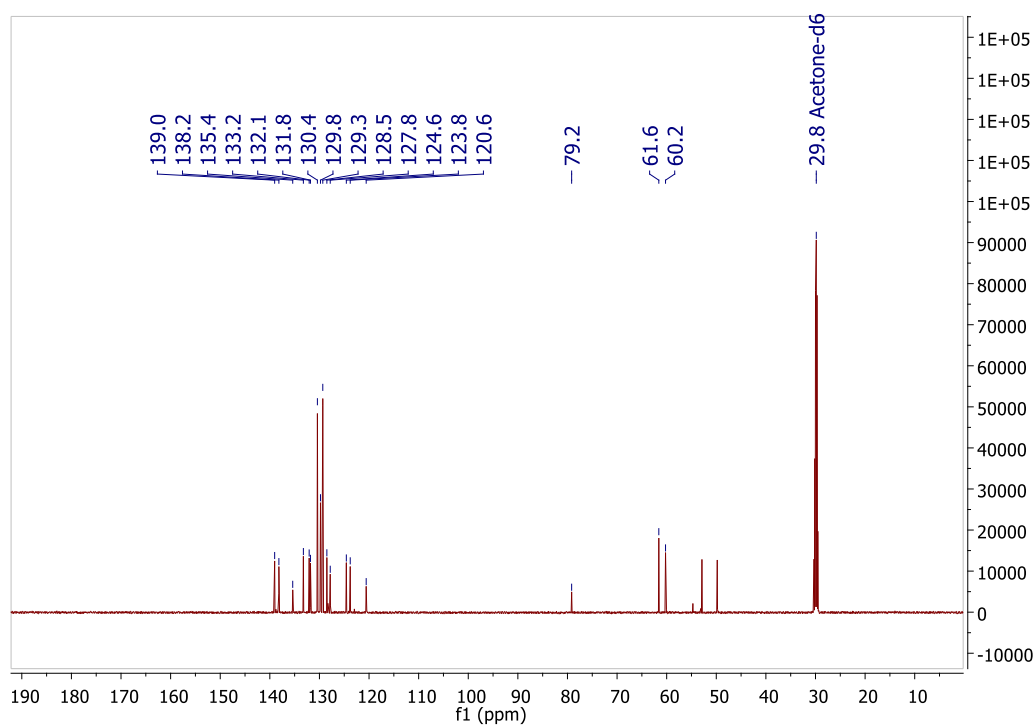


Figure S8b. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of imidazolium salt **2e** (75 MHz, Acetone- d_6)

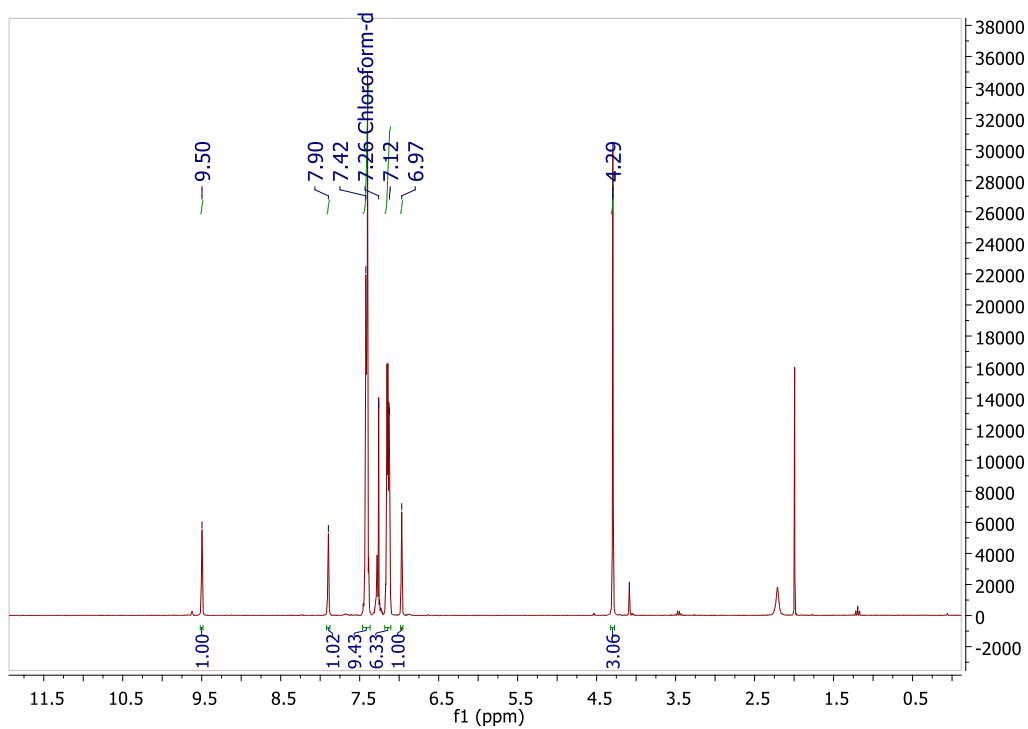


Figure S9a. ¹H NMR spectrum of imidazolium salt **3a** (300 MHz, CDCl₃)

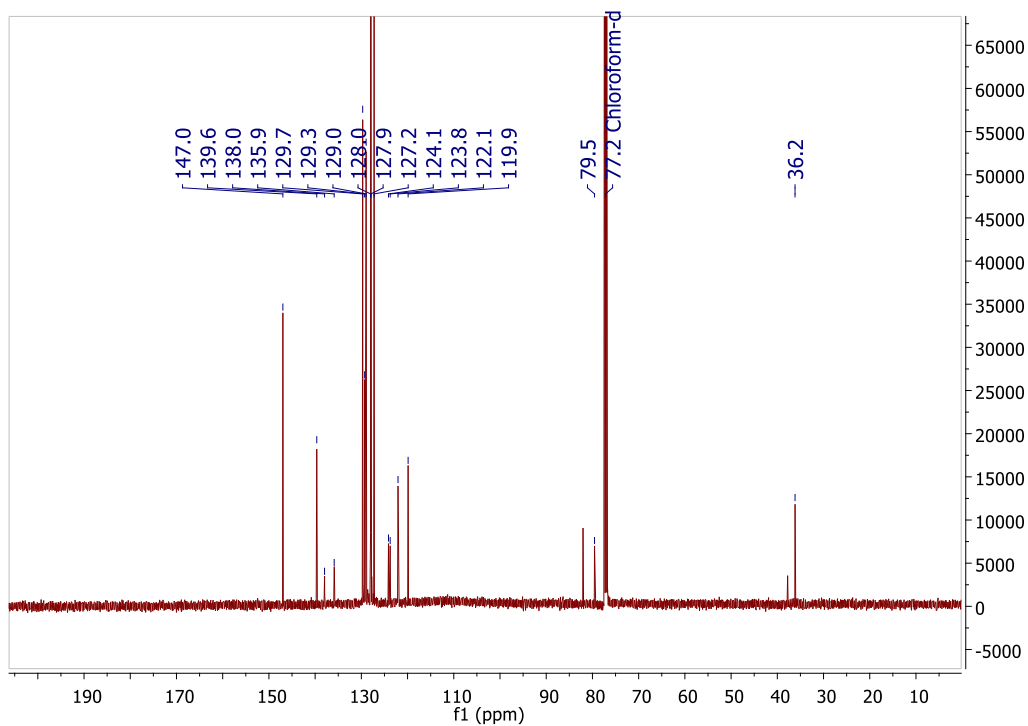


Figure S9b. ¹³C{¹H} NMR spectrum of imidazolium salt **3a** (75 MHz, CDCl₃)

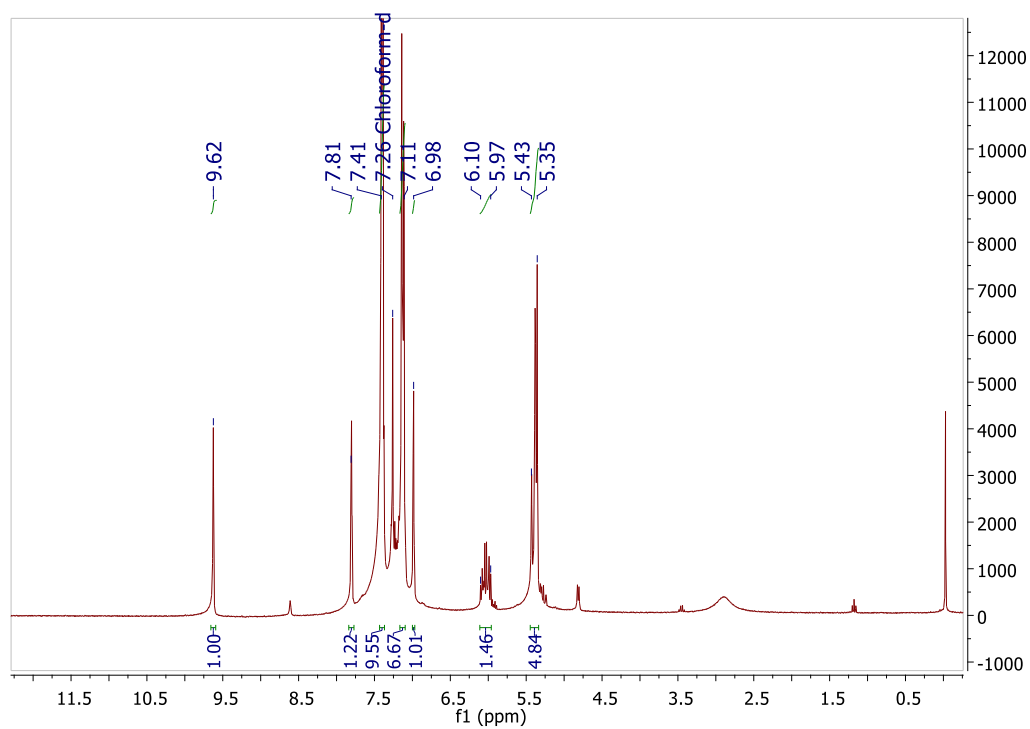


Figure S10a. ¹H NMR spectrum of imidazolium salt **3b** (300 MHz, CDCl₃)

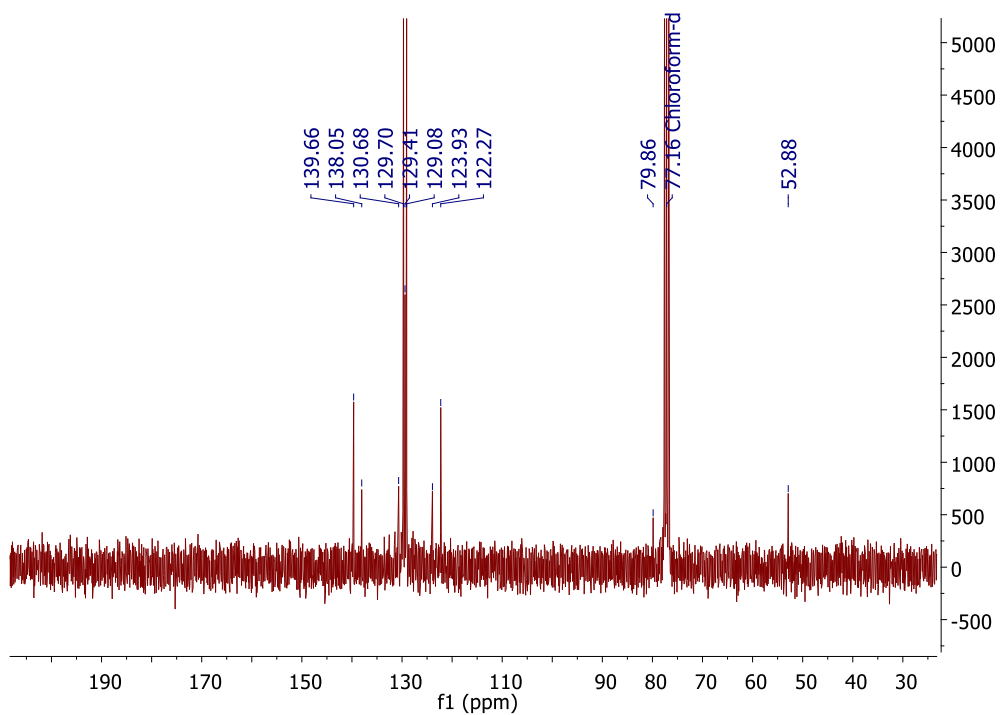


Figure S10b. ¹³C{¹H} NMR spectrum of imidazolium salt **3b** (75 MHz, CDCl₃)

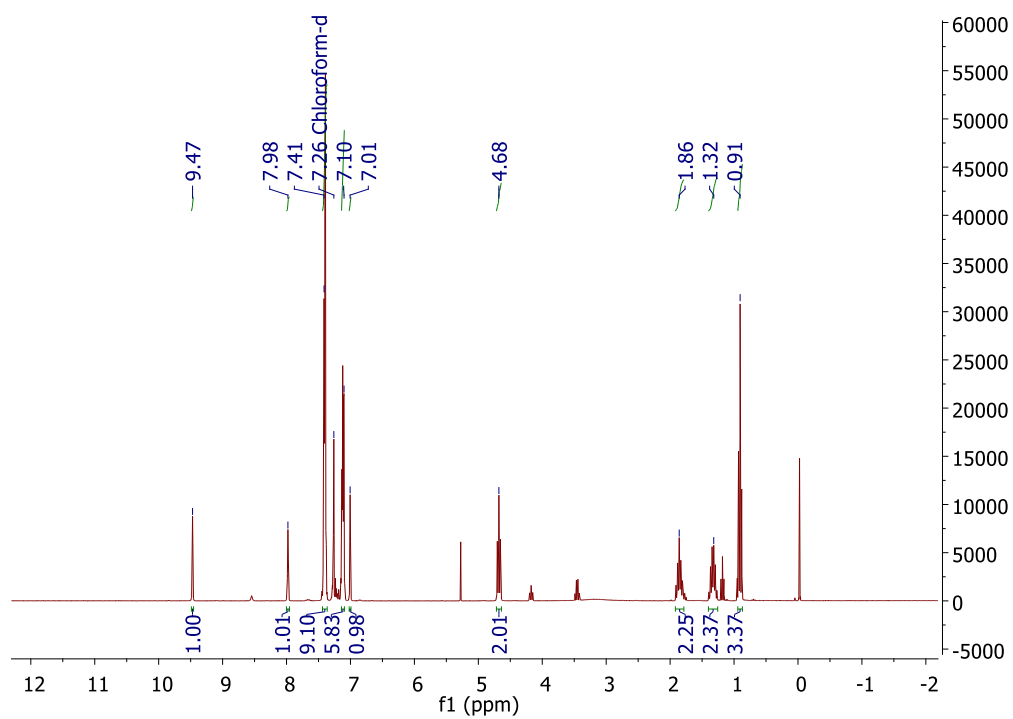


Figure S11a. ¹H NMR spectrum of imidazolium salt **3c** (300 MHz, CDCl₃)

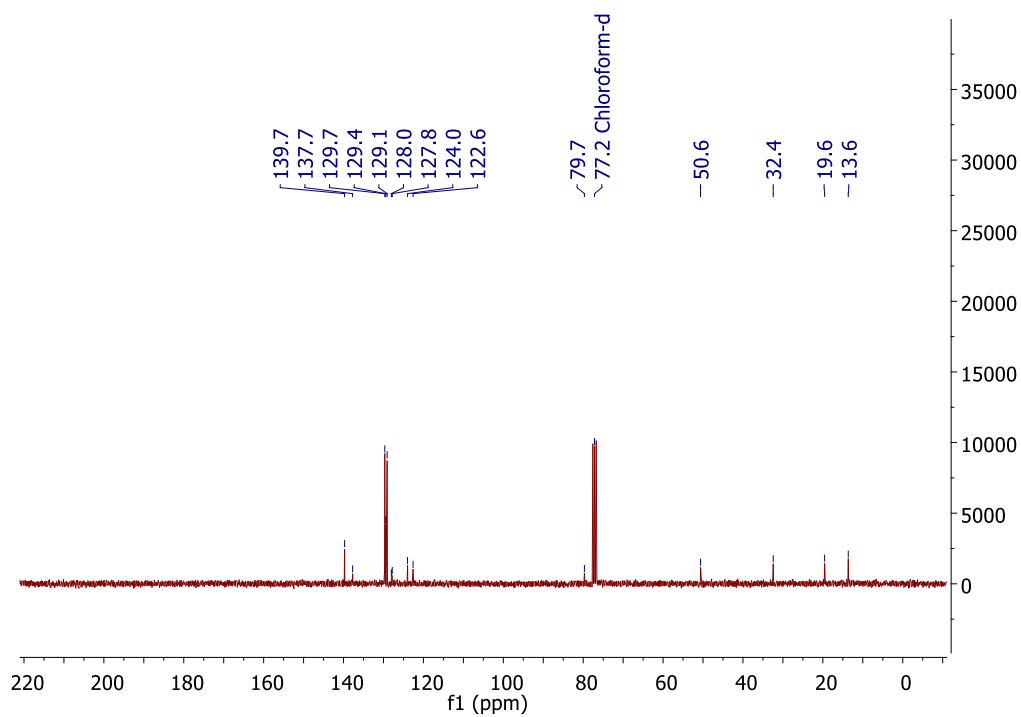


Figure S11b. ¹³C{¹H} NMR spectrum of imidazolium salt **3c** (75 MHz, CDCl₃)

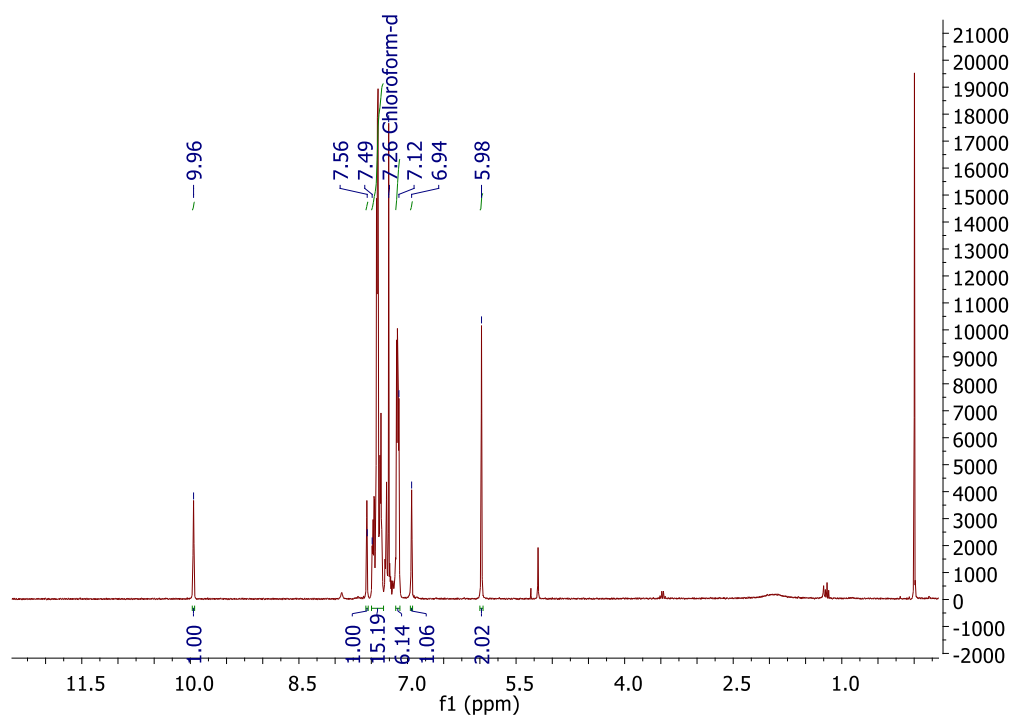


Figure S12a. ¹H NMR spectrum of imidazolium salt **3d** (300 MHz, CDCl₃)

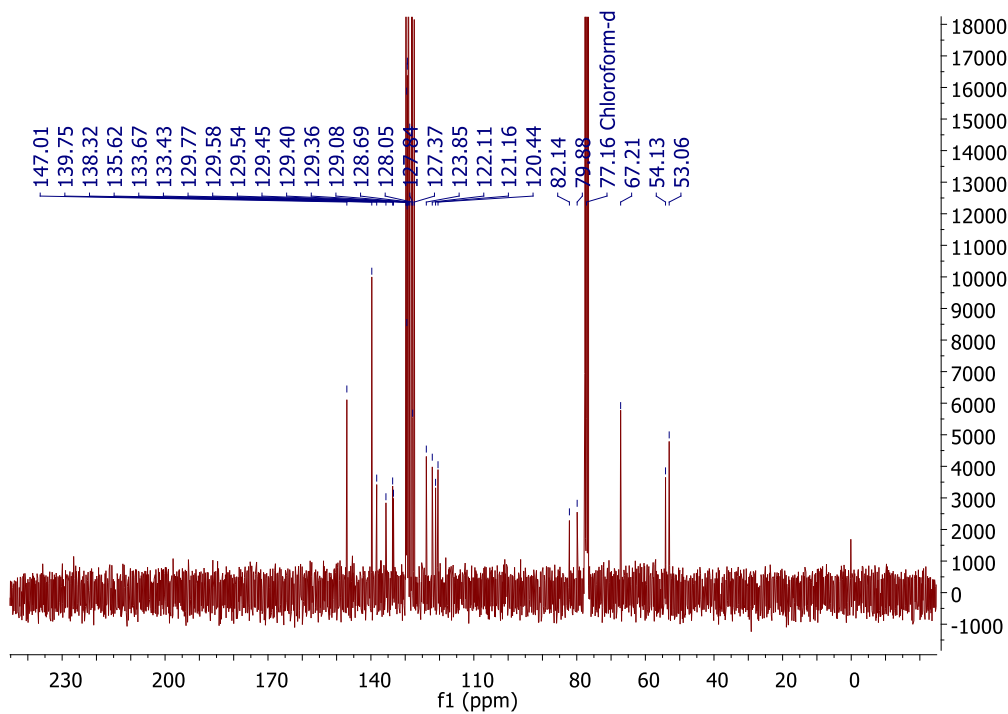


Figure S12b. ¹³C{¹H} NMR spectrum of imidazolium salt **3d** (75 MHz, CDCl₃)

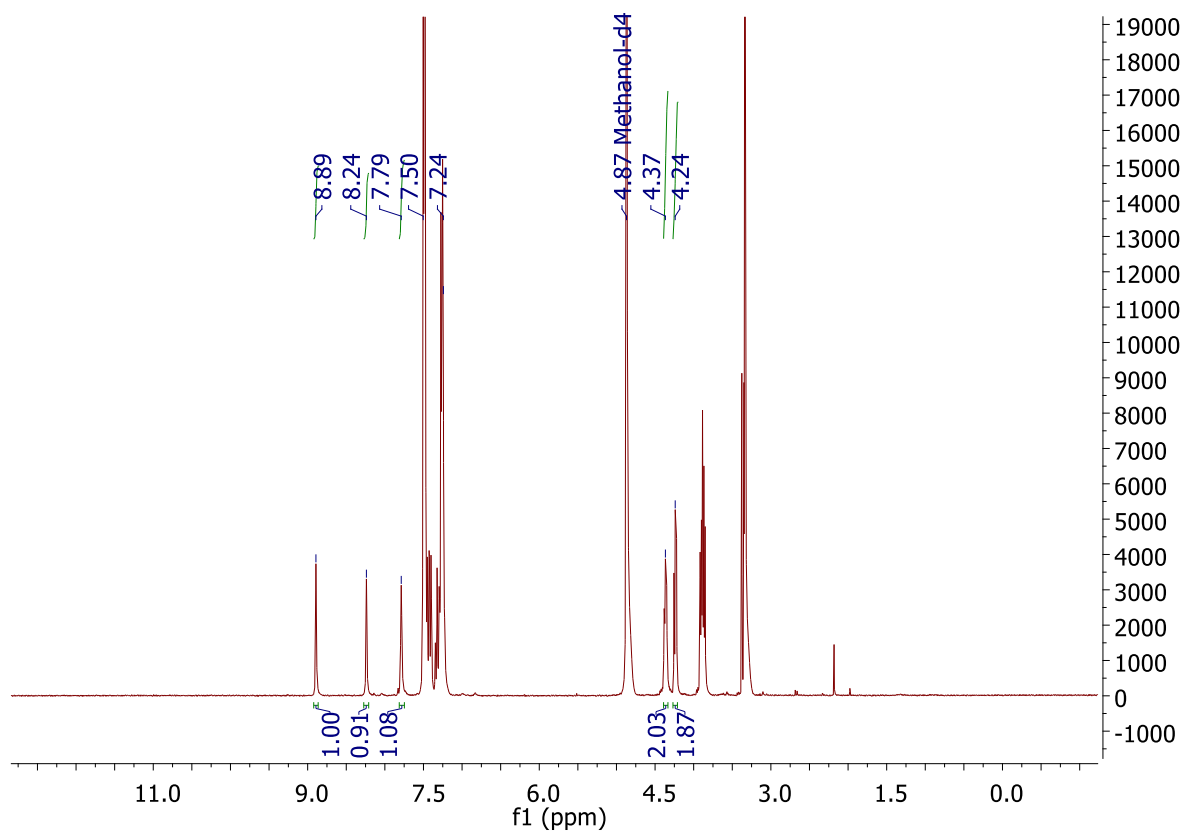


Figure S13a. ¹H NMR spectrum of imidazolium salt **3e** (300 MHz, Methanol-d₄)

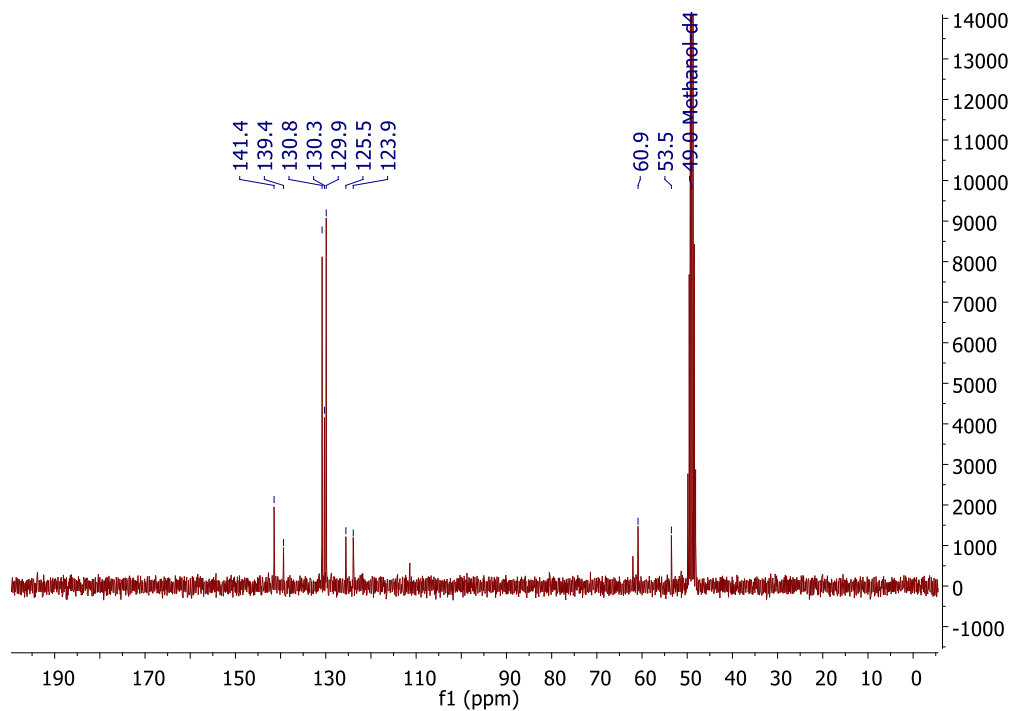


Figure S13b. ¹³C {¹H} NMR spectrum of imidazolium salt **3e** (300 MHz, Methanol-d₄)

2. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of silver complexes

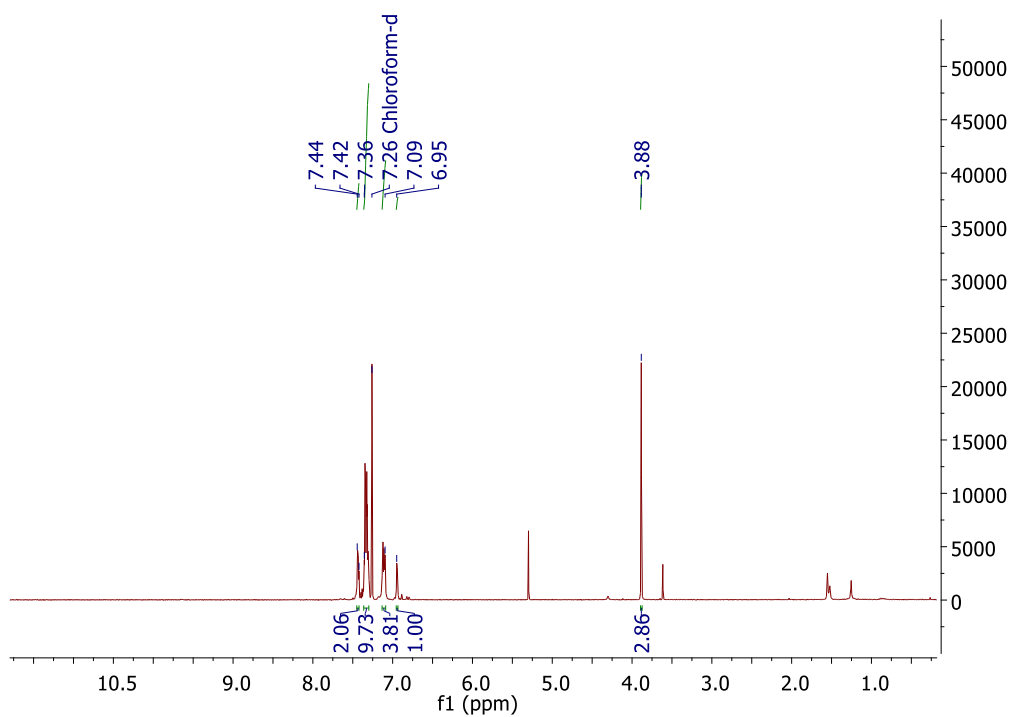


Figure S14a. ^1H NMR spectrum of complex **4a** (300 MHz, CDCl_3)

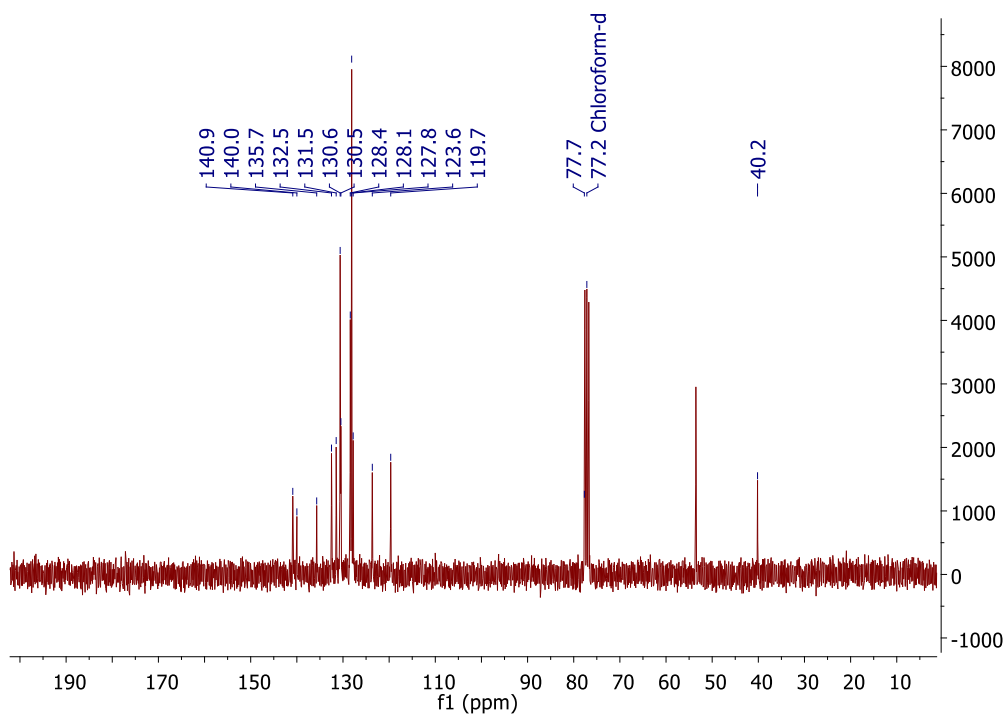


Figure S14b. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **4a** (75 MHz, CDCl_3)

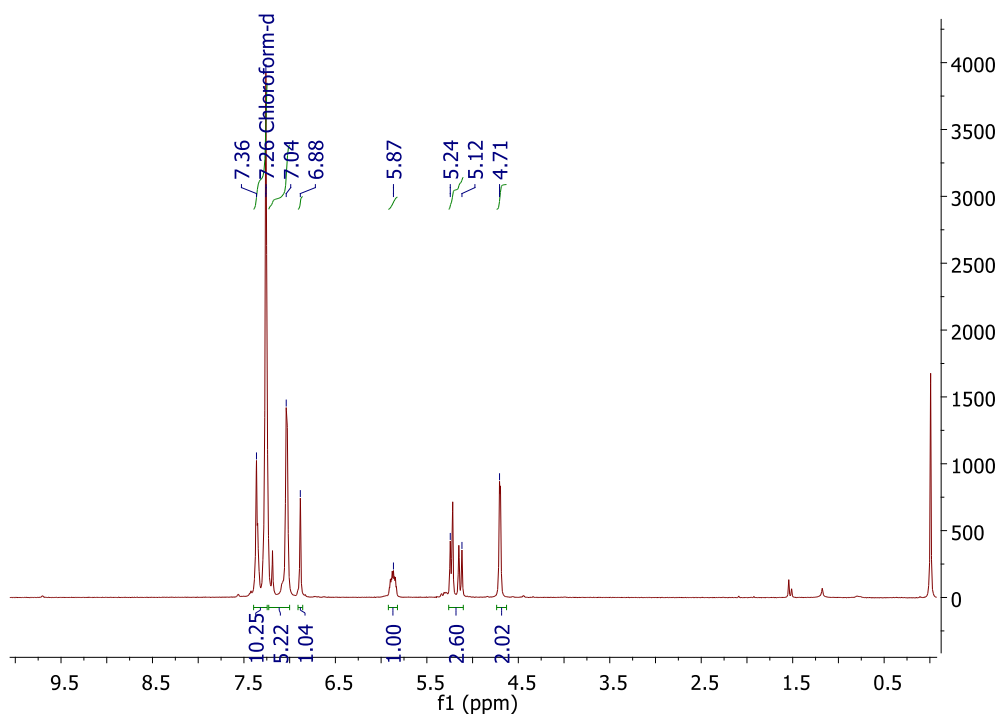


Figure S15a. ¹H NMR spectrum of complex **4b** (300 MHz, CDCl₃)

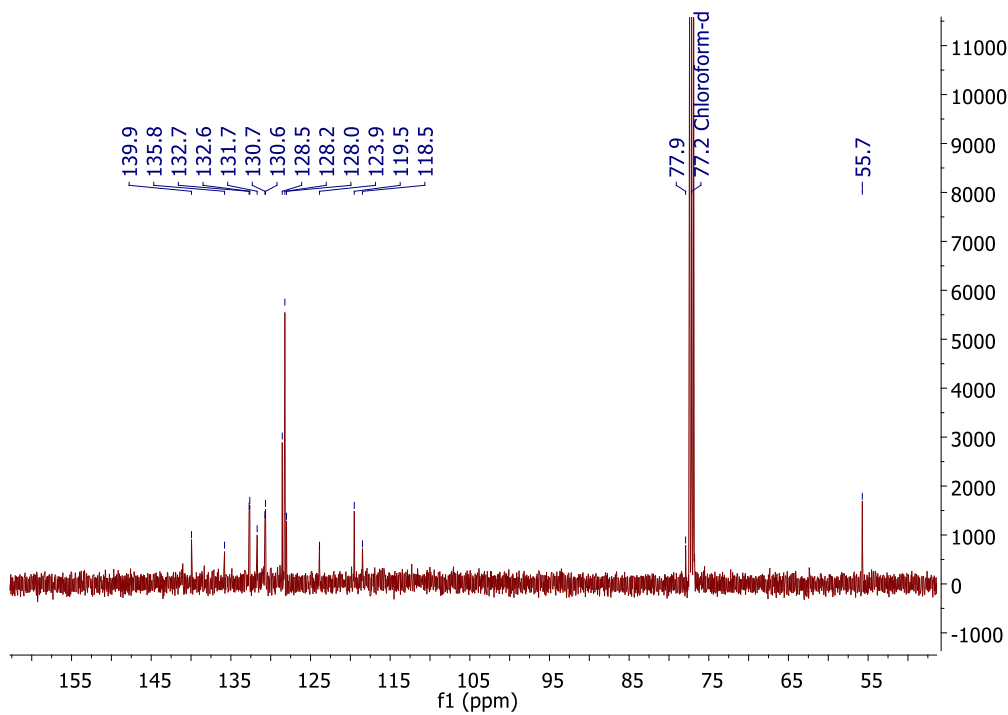


Figure S15b. ¹³C{¹H} NMR spectrum of complex **4b** (75 MHz, CDCl₃)

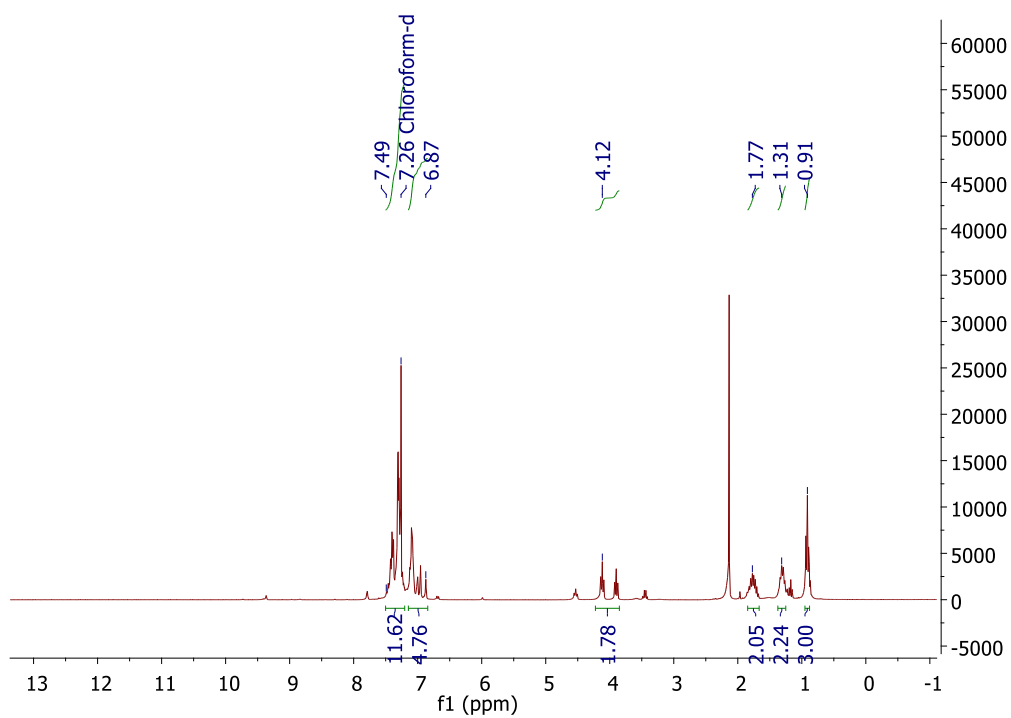


Figure S16a. ¹H NMR spectrum of complex **4c** (300 MHz, CDCl₃)

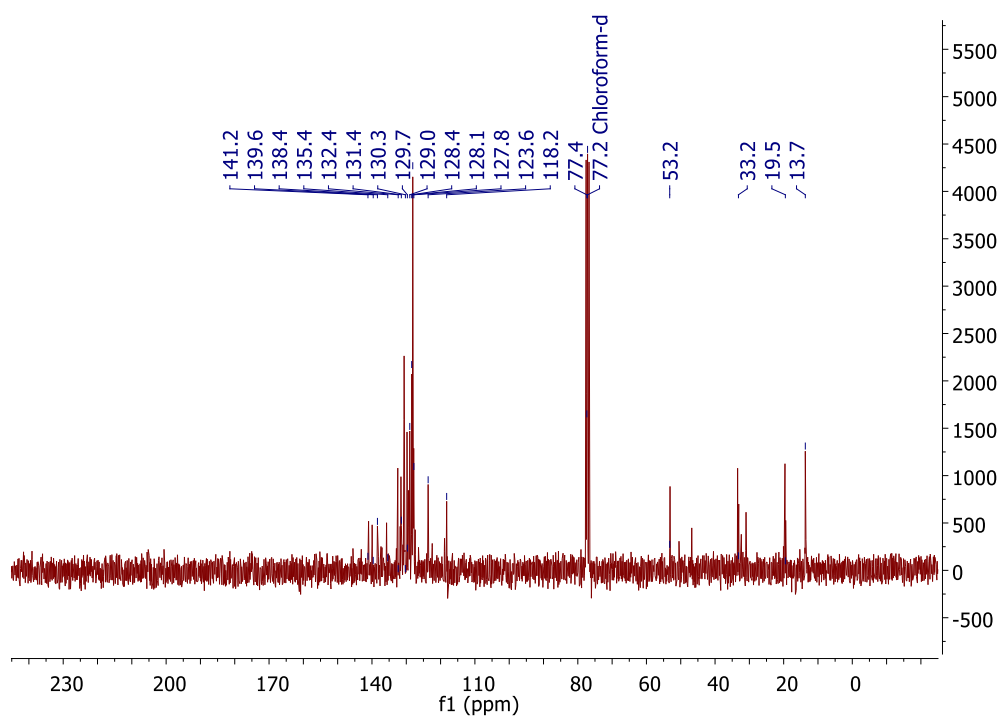


Figure S16b. ¹³C{¹H} NMR spectrum of complex **4c** (75 MHz, CDCl₃)

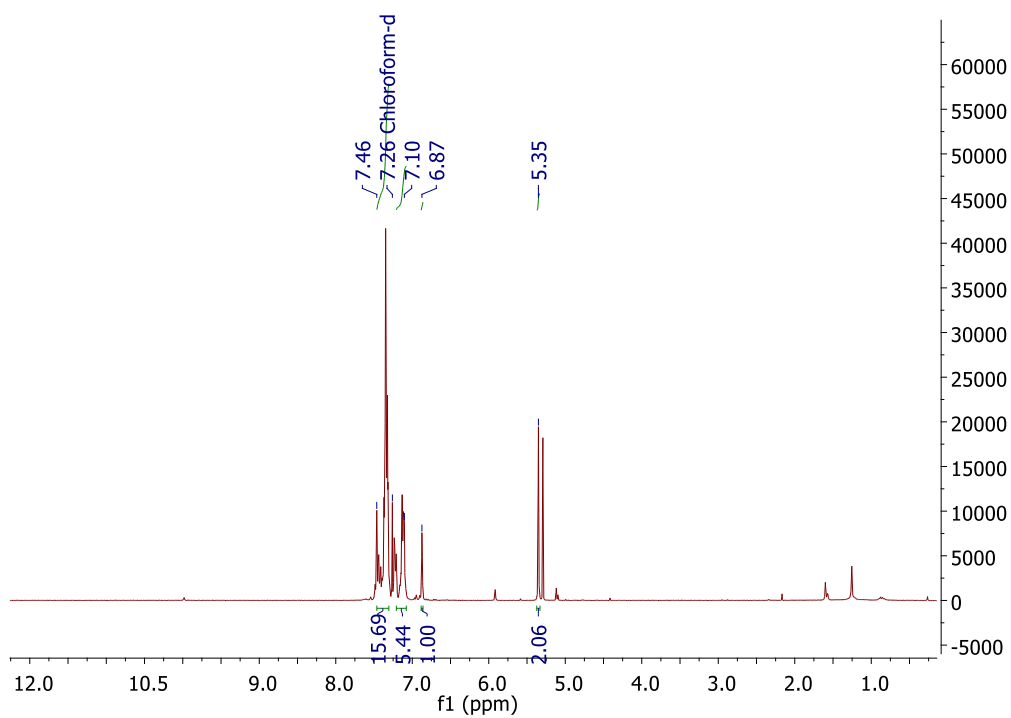


Figure S17a. ¹H NMR spectrum of complex **4d** (300 MHz, CDCl₃)

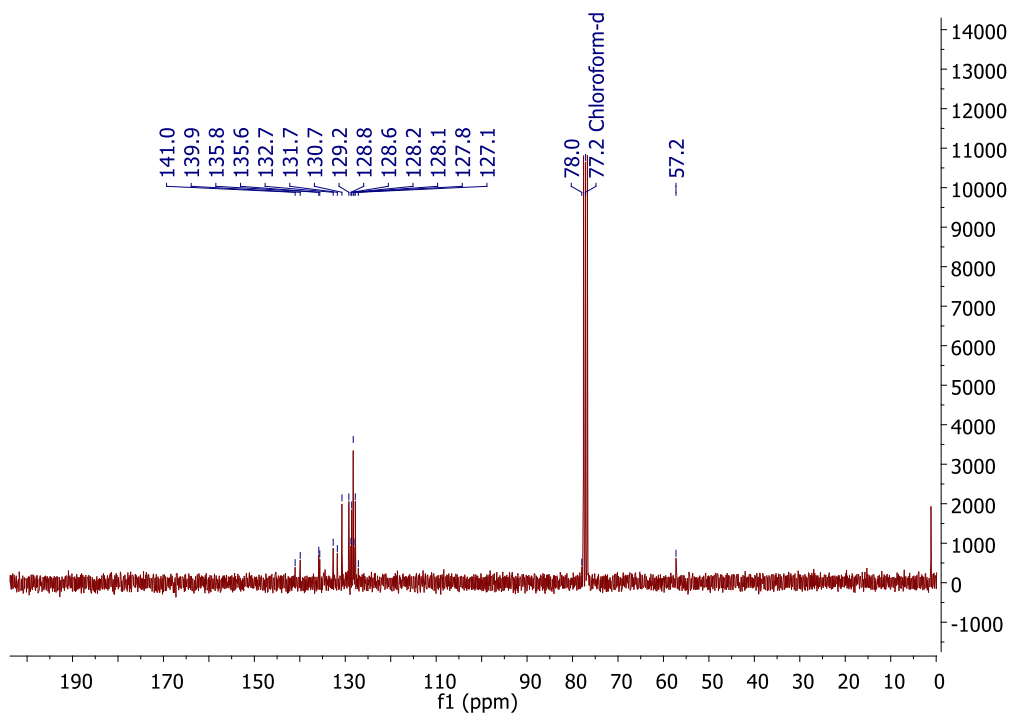


Figure S17b. ¹³C{¹H} NMR spectrum of complex **4d** (75 MHz, CDCl₃)

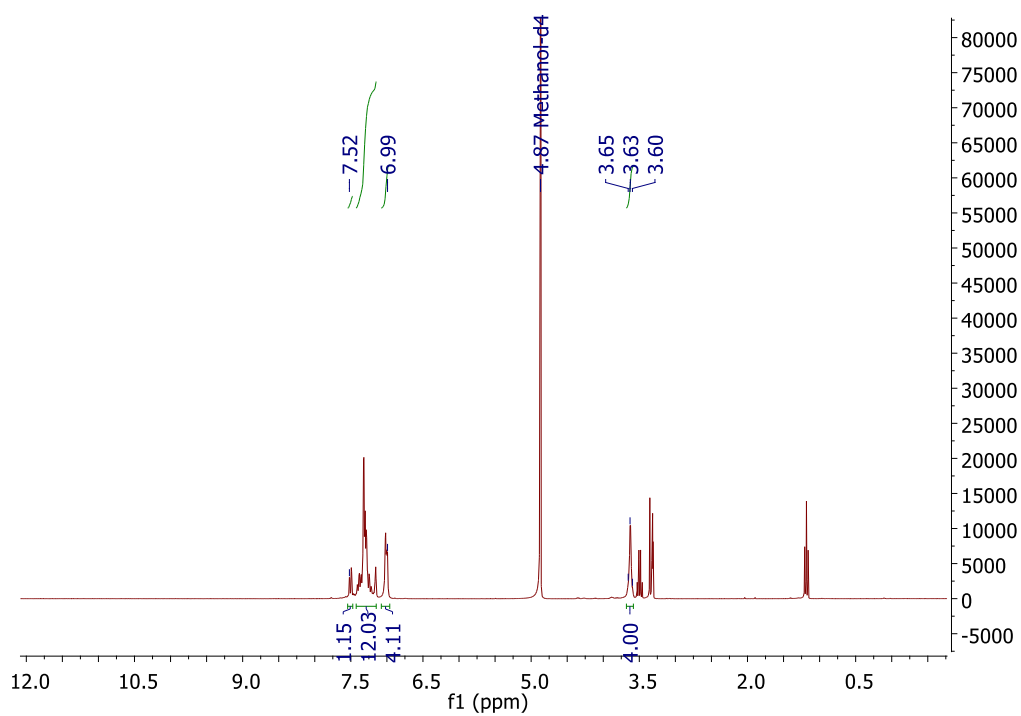


Figure S18a. ¹H NMR spectrum of complex **4e** (300 MHz, Methanol-d₄)

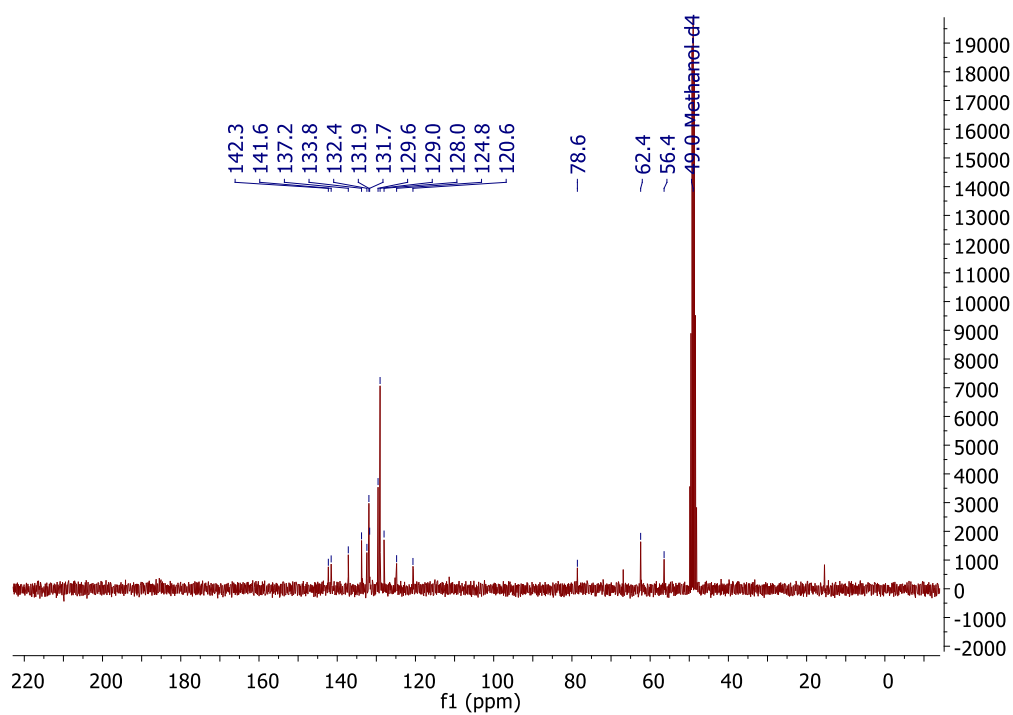


Figure S18b. ¹³C{¹H} NMR spectrum of complex **4e** (75 MHz, Methanol-d₄)

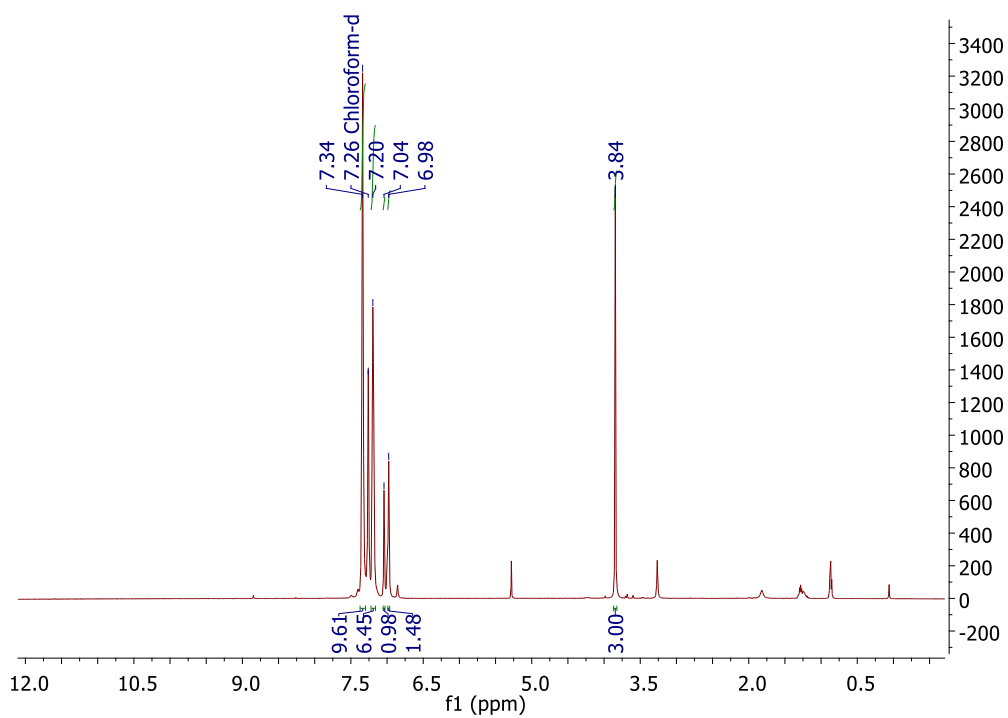


Figure S19a. ¹H NMR spectrum of complex **5a** (300 MHz, CDCl₃)

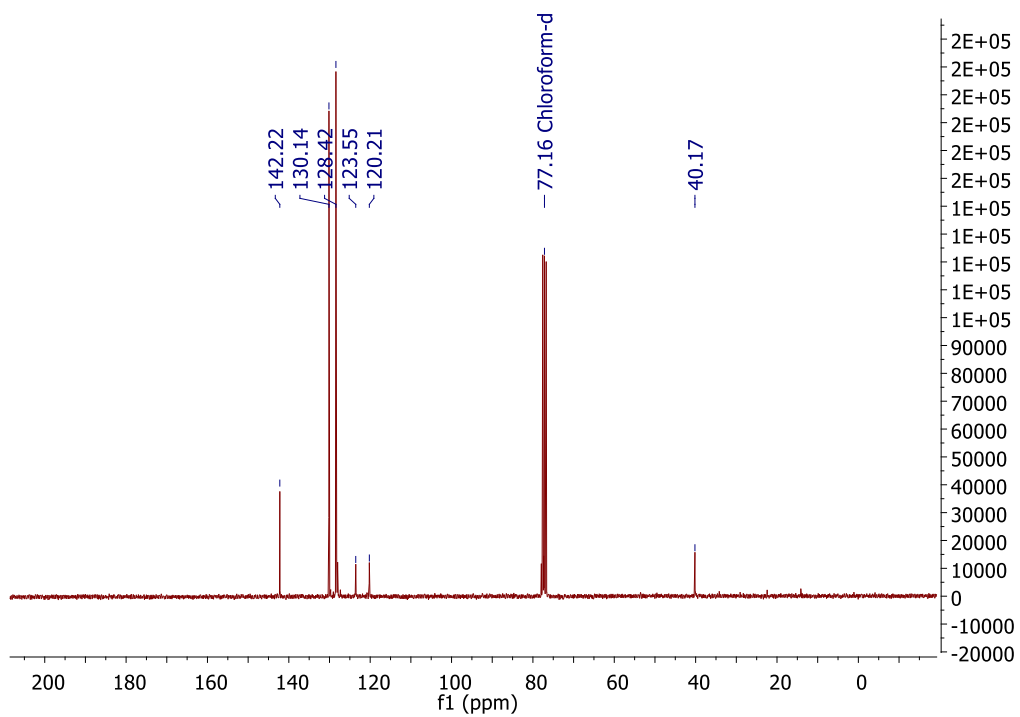


Figure S19b. ¹³C{¹H} NMR spectrum of complex **5a** (75 MHz, CDCl₃)

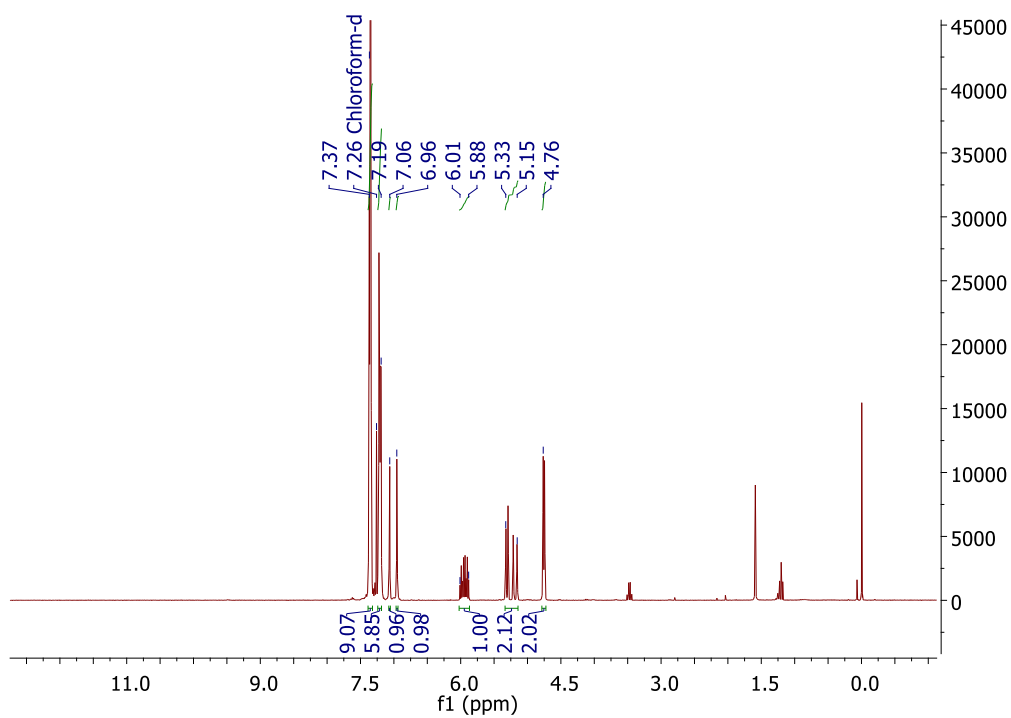


Figure S20a. ¹H NMR spectrum of complex **5b** (300 MHz, CDCl₃)

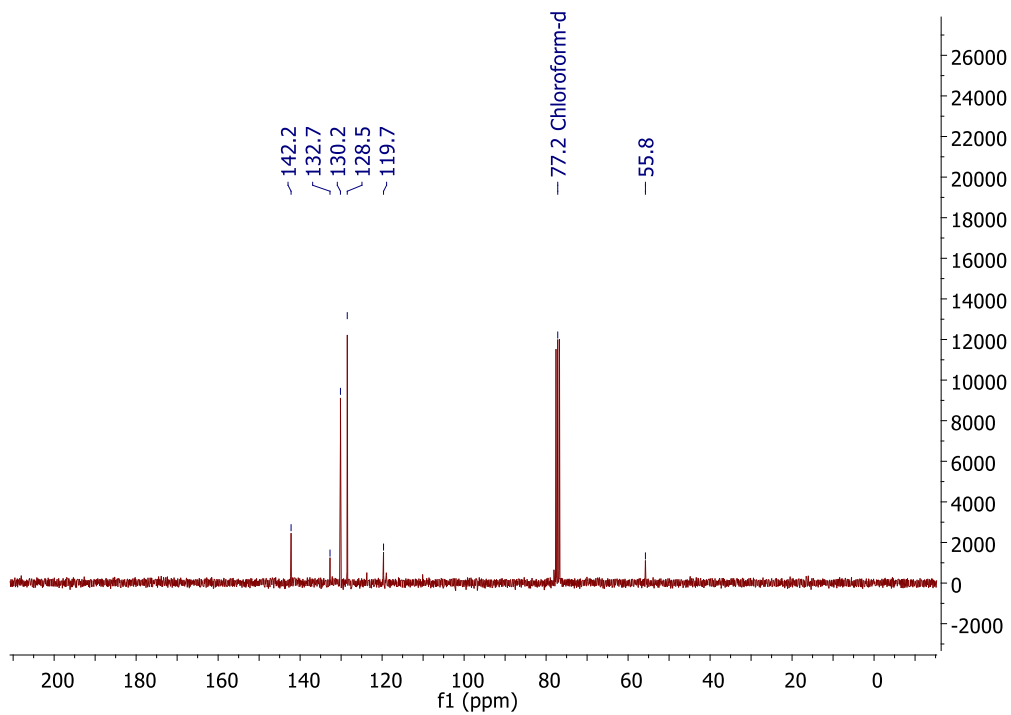


Figure S20b. ¹³C{¹H} NMR spectrum of complex **5b** (75 MHz, CDCl₃)

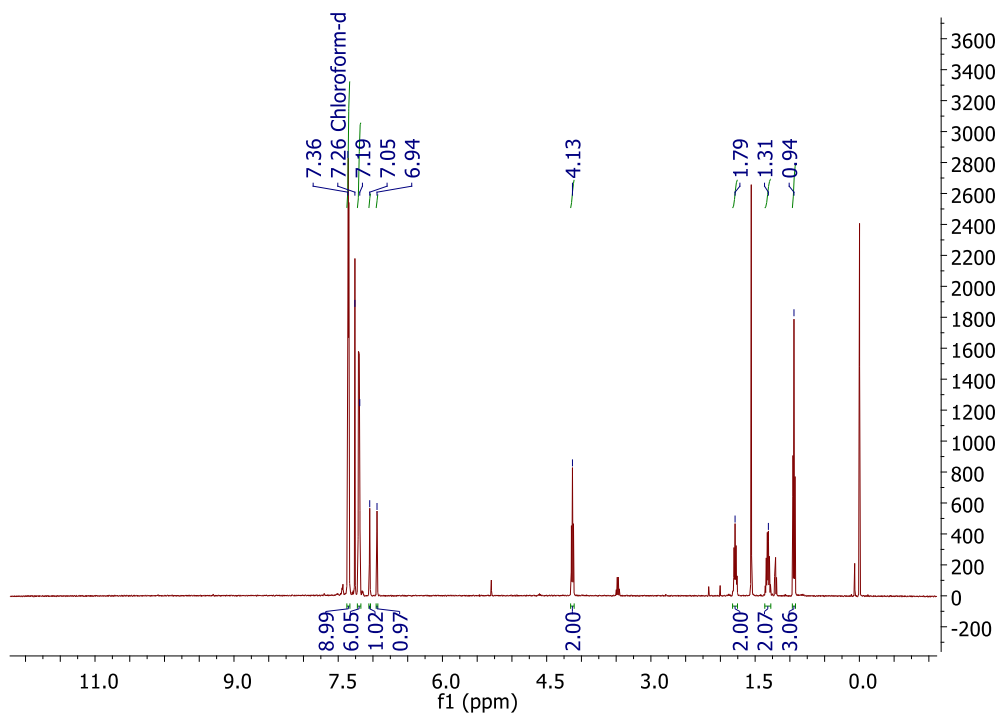


Figure S21a. ¹H NMR spectrum of complex **5c** (300 MHz, CDCl₃)

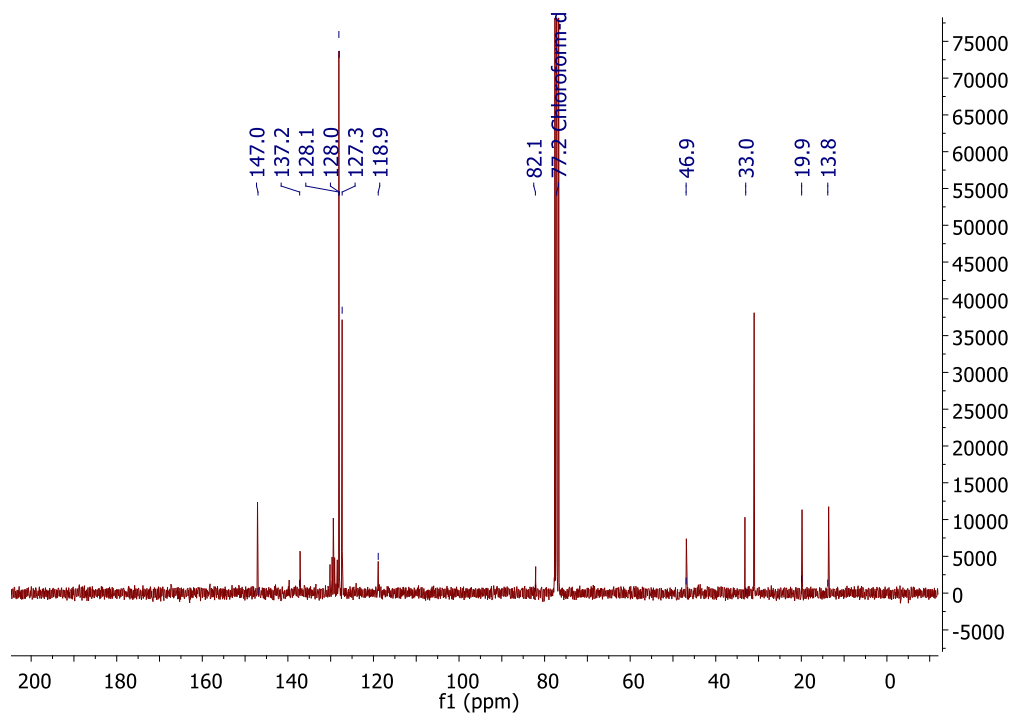


Figure S21b. ¹³C{¹H} NMR spectrum of complex **5c** (75 MHz, CDCl₃)

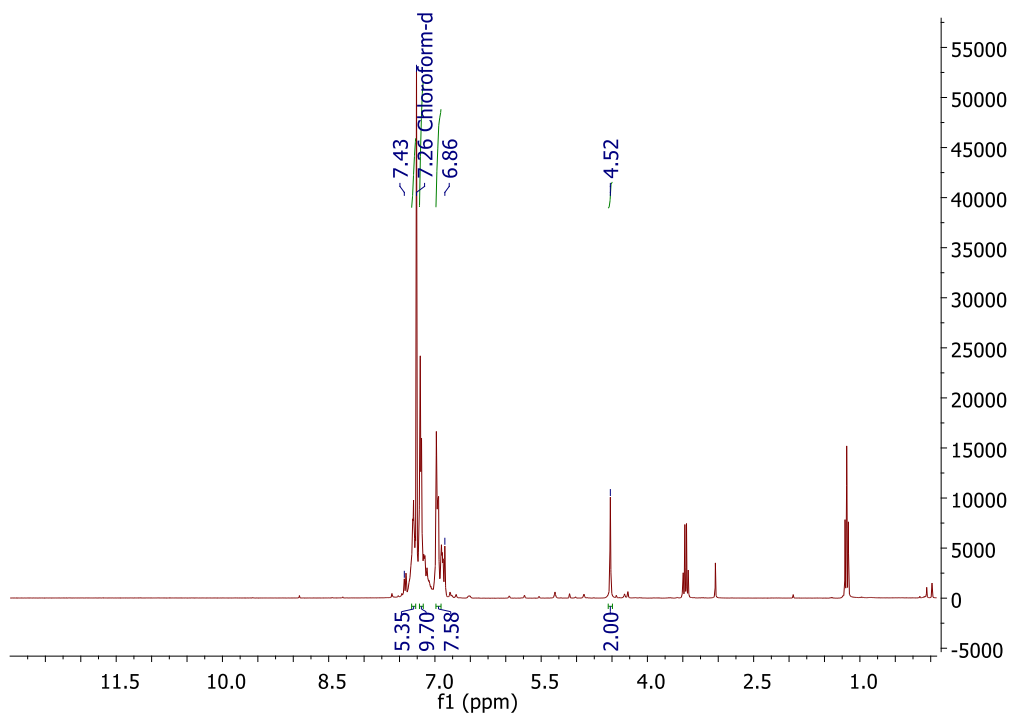


Figure S22a. ¹H NMR spectrum of complex **5d** (300 MHz, CDCl₃)

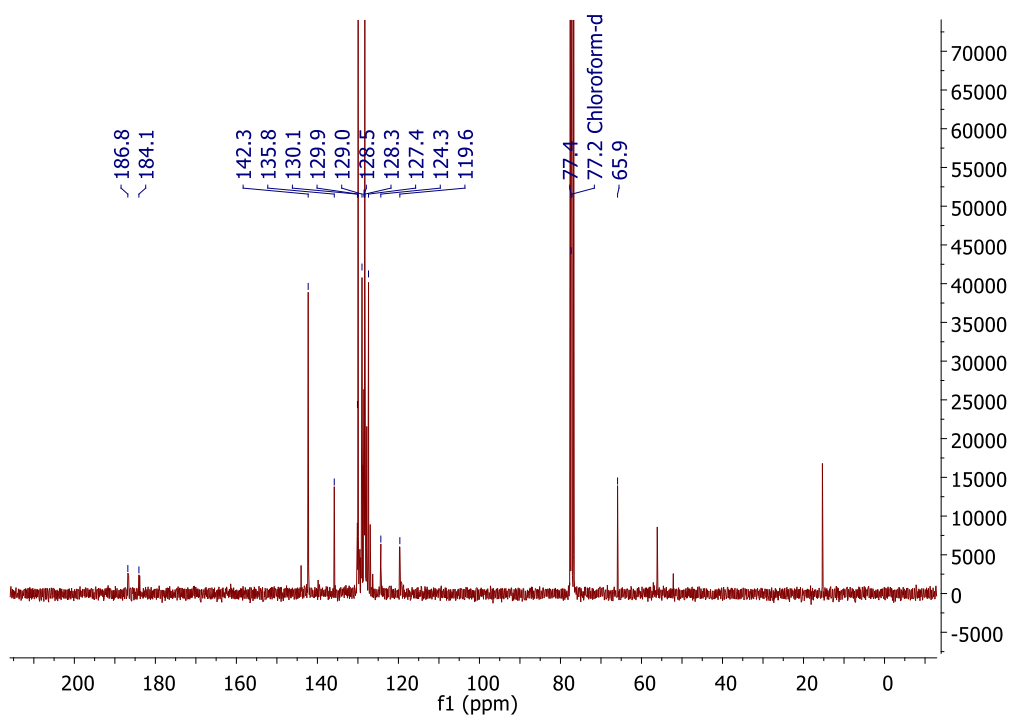


Figure S22b. ¹³C{¹H} NMR spectrum of complex **5d** (75 MHz, CDCl₃)

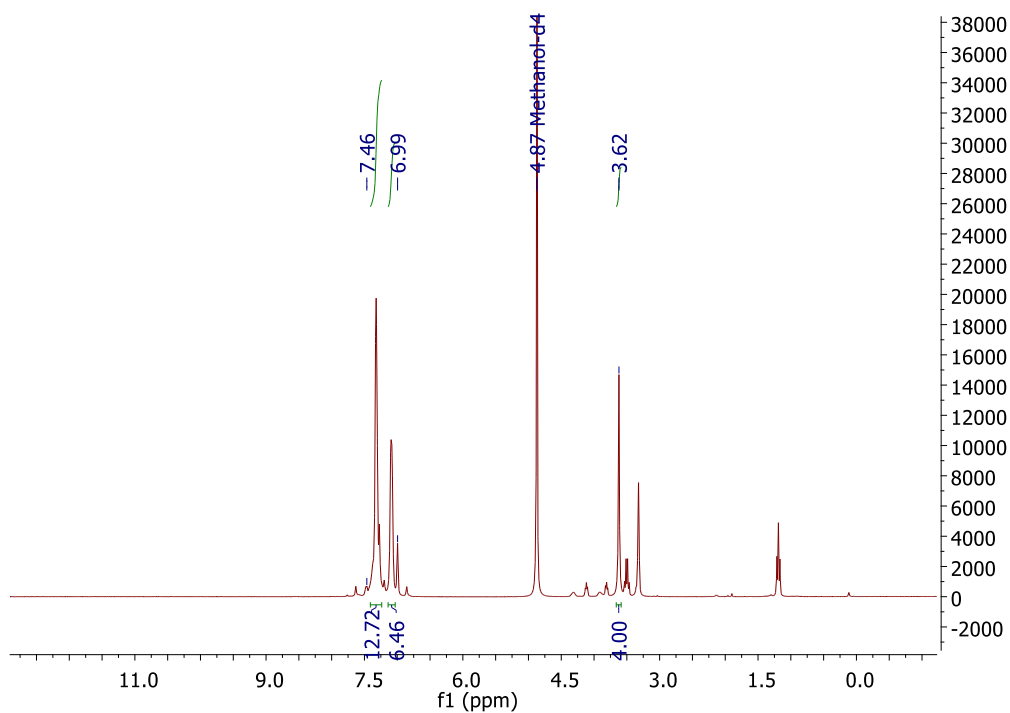


Figure S23a. ¹H NMR spectrum of complex **5e** (300 MHz, Methanol-d₄)

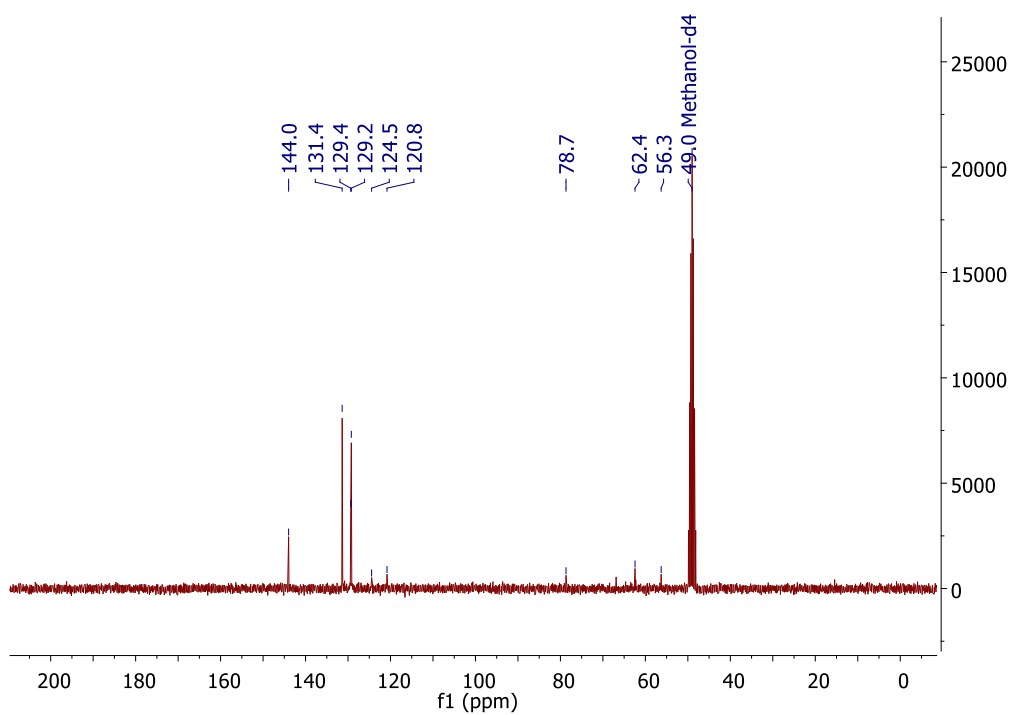


Figure S23b. ¹³C{¹H} NMR spectrum of complex **5e** (300 MHz, Methanol-d₄)

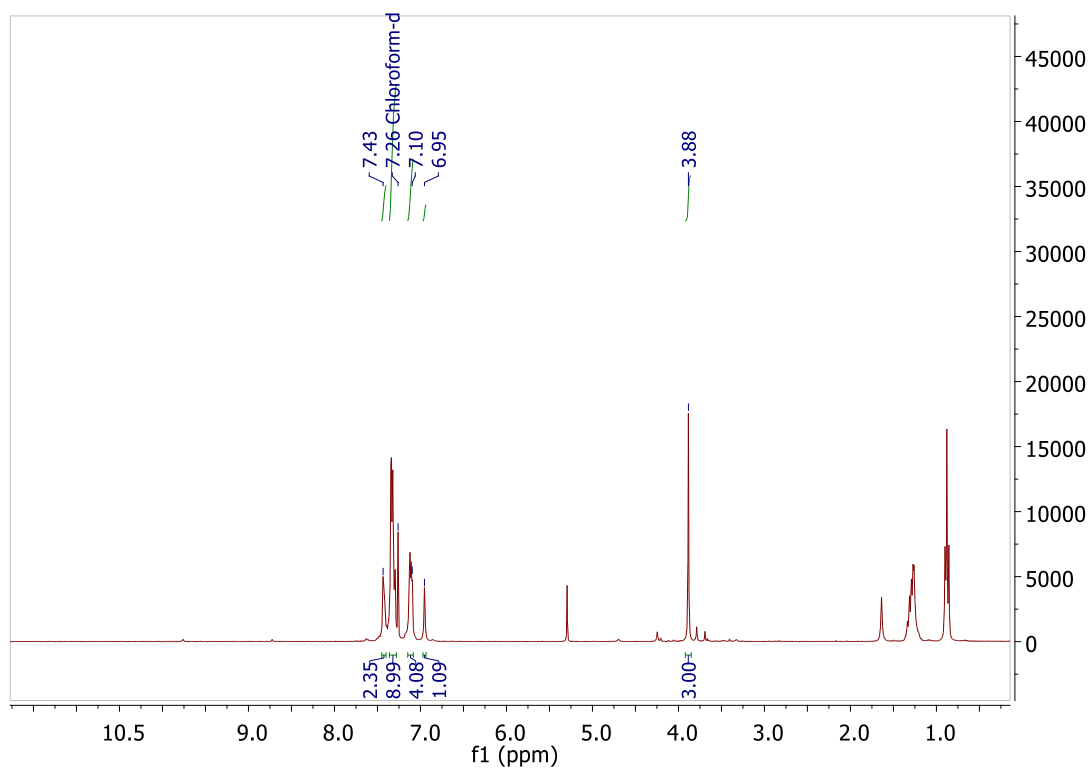


Figure S24a. ¹H NMR spectrum of complex **6a** (300 MHz, CDCl₃)

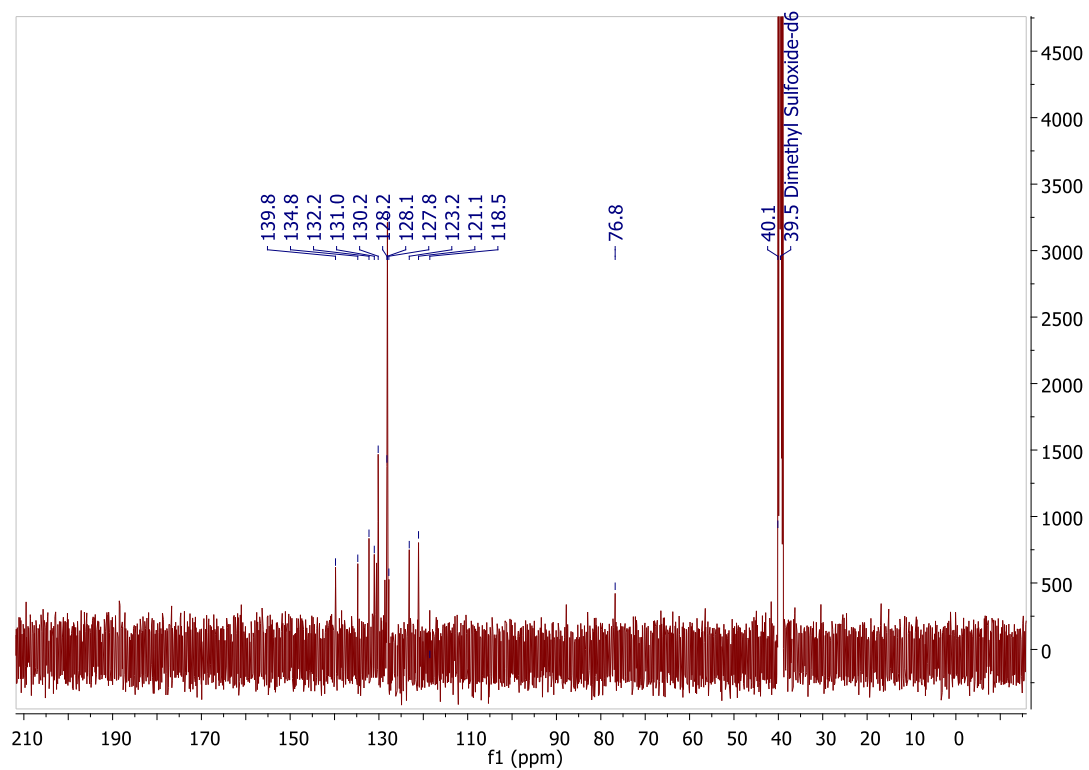


Figure S24b. ¹³C{¹H} NMR spectrum of complex **6a** (75 MHz, DMSO-d₆)

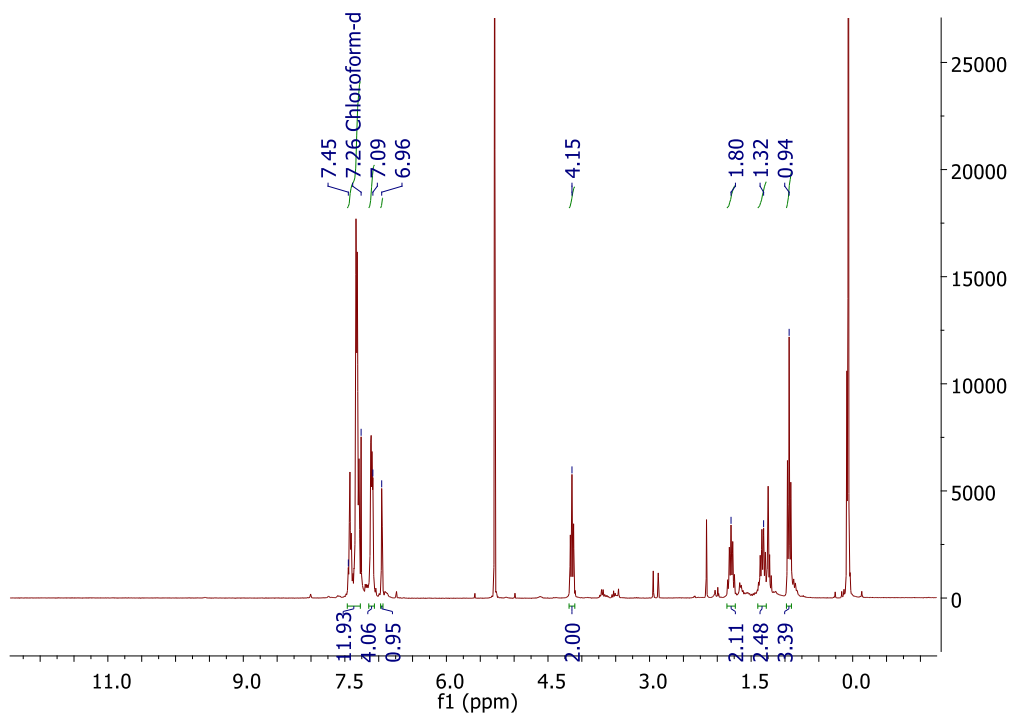


Figure S25a. ^1H NMR spectrum of complex **6c** (300 MHz, CDCl_3)

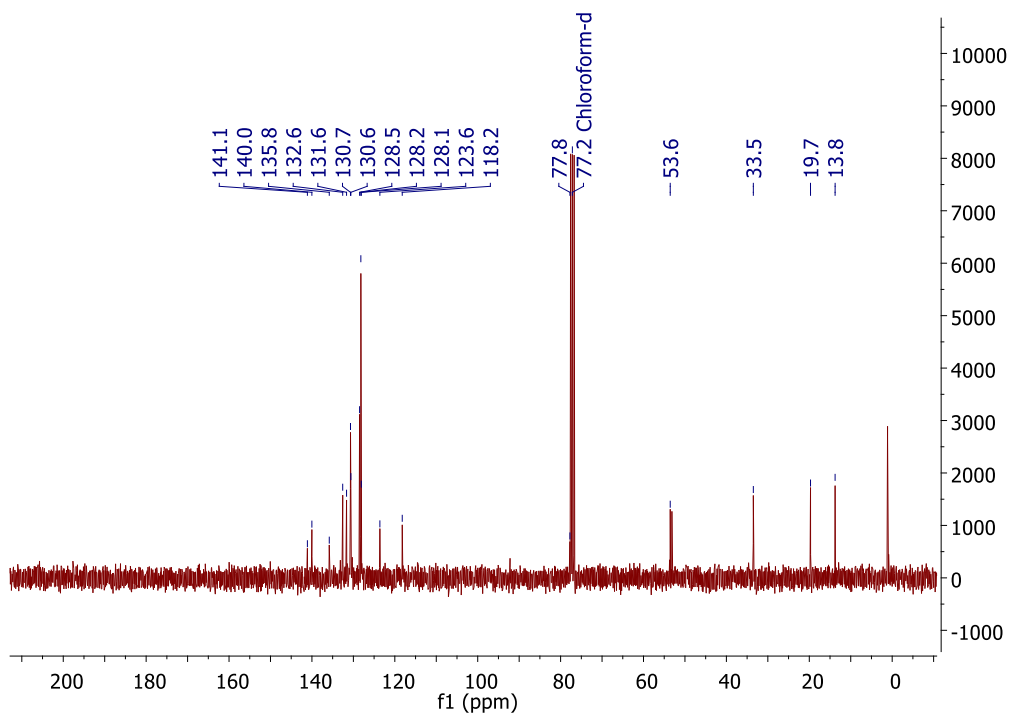


Figure S25b. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **6c** (75 MHz, CDCl_3)

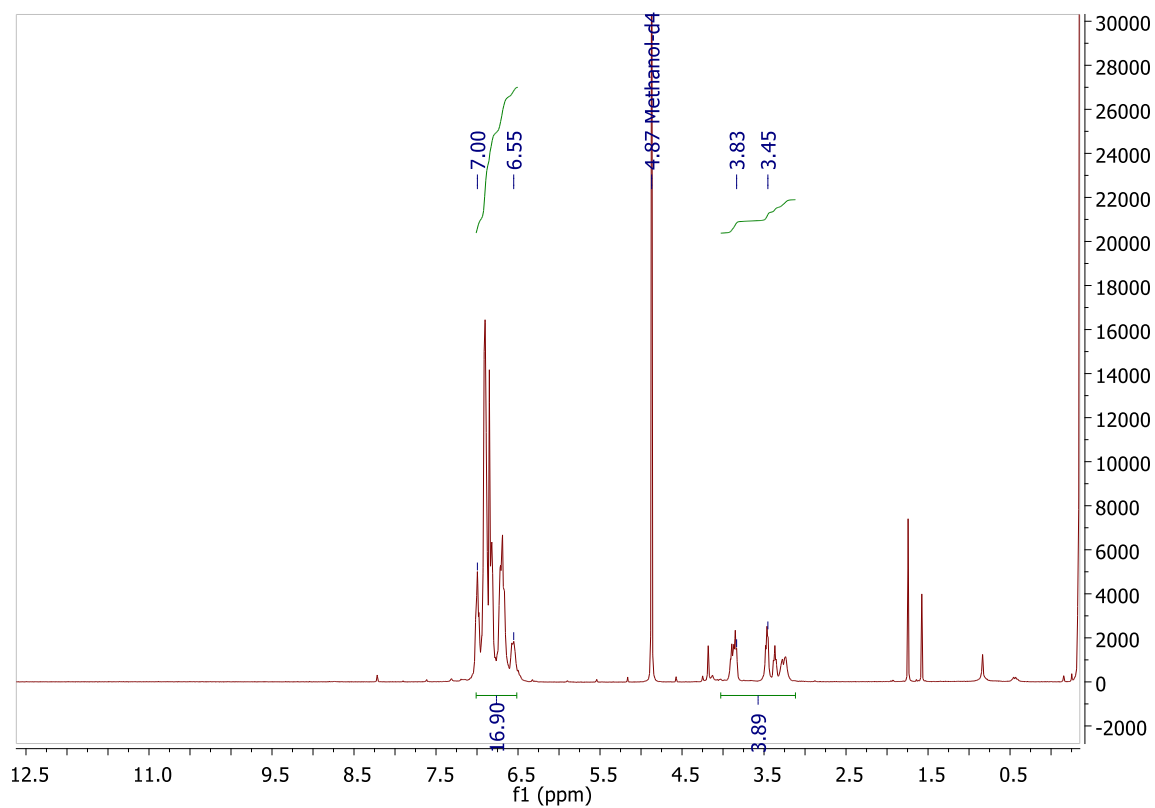


Figure S26a. ^1H NMR spectrum of complex **6e** (300 MHz, MeOD- d_4)

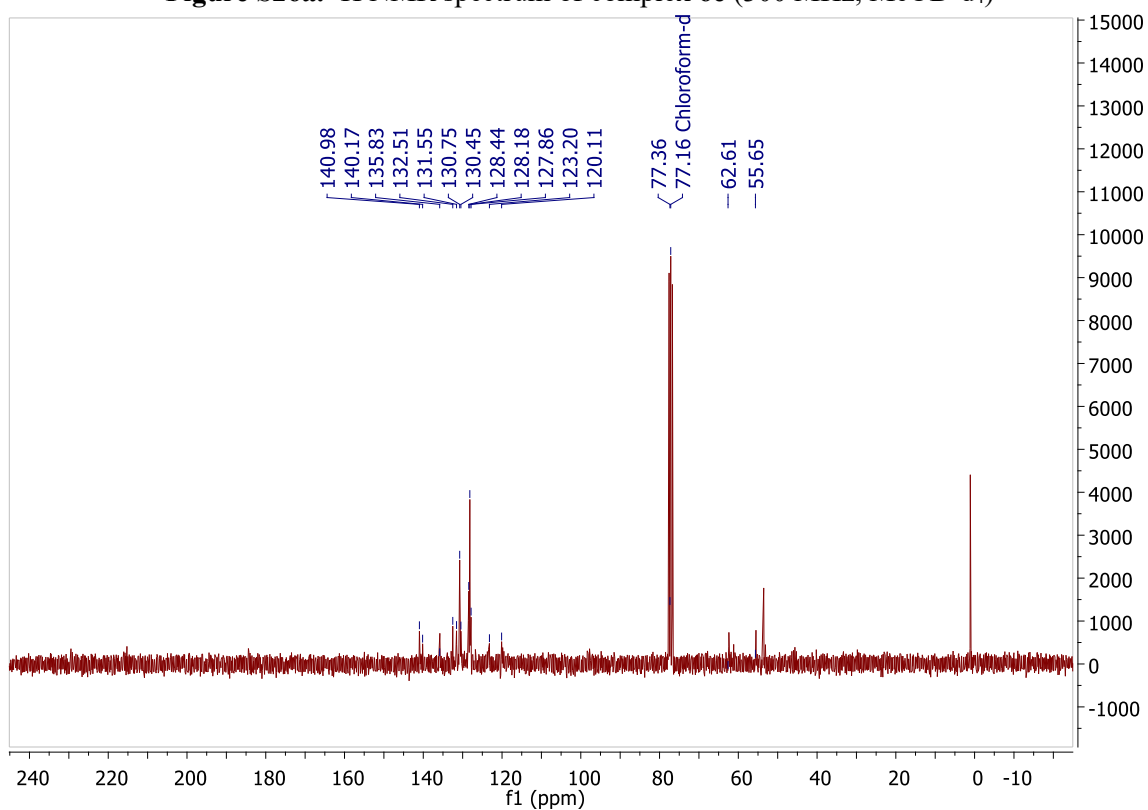


Figure S26b. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex **6e** (75 MHz, CDCl_3)

3. Molecular Structures of Imidazolium Salts

Ellipsoids are drawn at 50% probability level and H atoms are omitted for clarity. Where observed, anion- π interactions are shown.

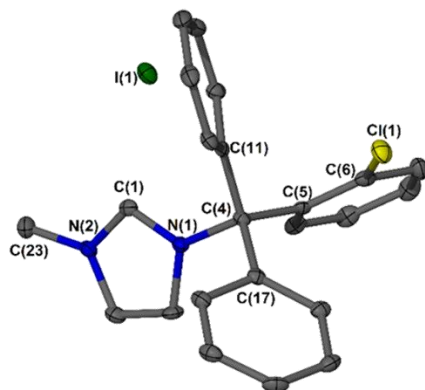


Figure S27. Molecular structure of imidazolium salt 1a.

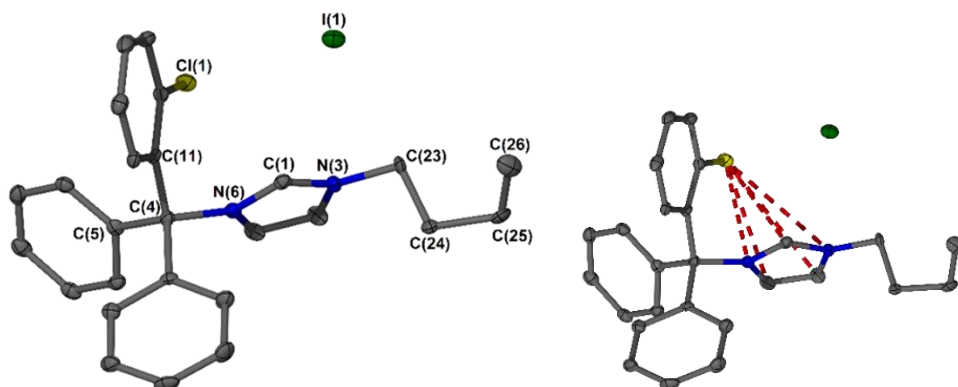


Figure S28. Molecular structure of imidazolium salt 1c.

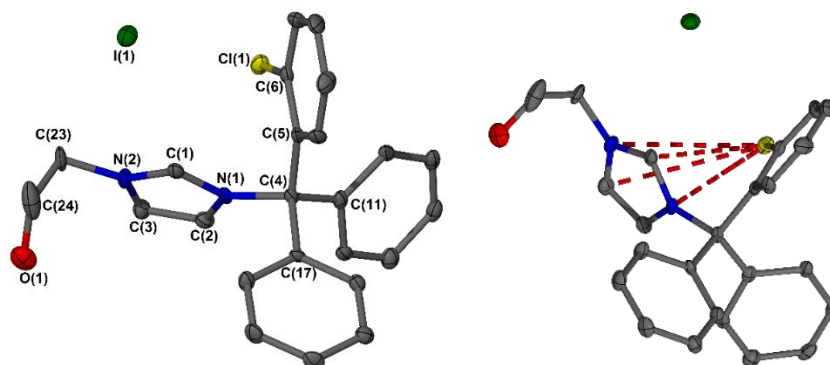


Figure S29. Molecular structure of imidazolium salt 1e.

Table S1. Selected bond lengths and angles for imidazolium salts 1			
Bond Lengths (Å) and angles (°)	1a	1c	1e
N1-C1-N2	108.9(2)	109.2(2)	109.0(4)
N1-C4-C5	107.1(3)	106.31(19)	106.0(3)
N1-C4-C17	108.3(3)	110.4(2)	108.0(3)
N1-C4-C11	104.4(3)	107.8(2)	110.6(3)
C5-C4-C11	112.8(3)	113.2(2)	111.9(3)
C17-C4-C11	114.0(3)	109.6(2)	109.1(3)
C17-C4-C5	109.8(3)	113.2(2)	111.1(3)
C6-Cl1	1.741(4)	1.745(3)	1.747(5)
N1-C4	1.508(4)	1.513(3)	1.519(5)
N2-C23	1.465(4)	1.478(3)	1.469(5)
Cl1.....C1	5.511	3.188	3.201
I1.....C1	3.729	3.815	3.630
Cl1.....I1	6.864	4.771	4.443

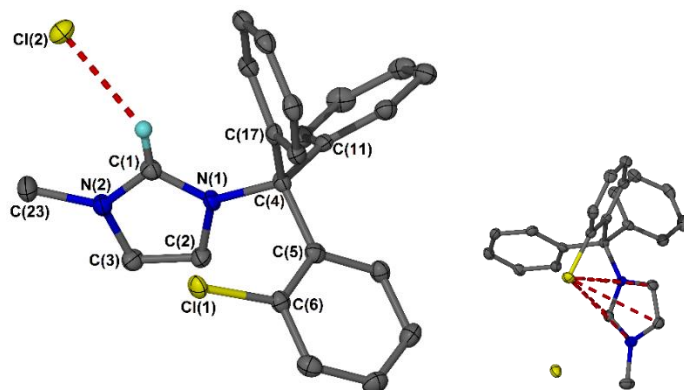


Figure S30. Molecular structure of imidazolium salt **2a**.

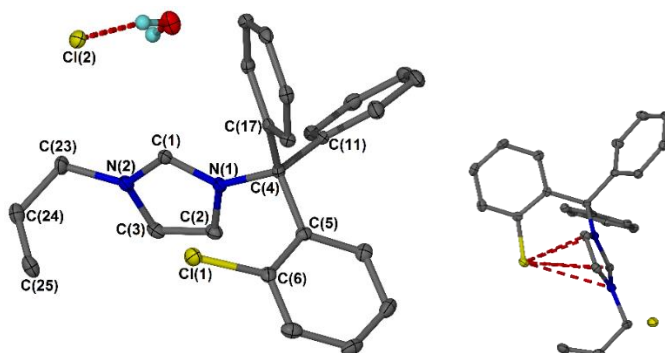


Figure S31. Molecular structure of imidazolium salt **2b**.

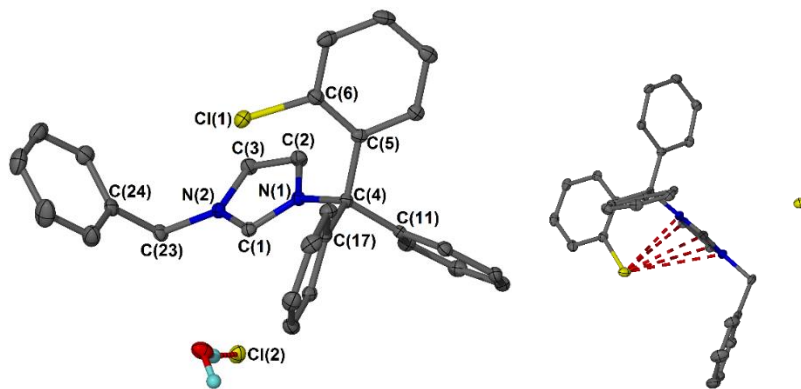


Figure S32. Molecular structure of imidazolium salt **2d**.

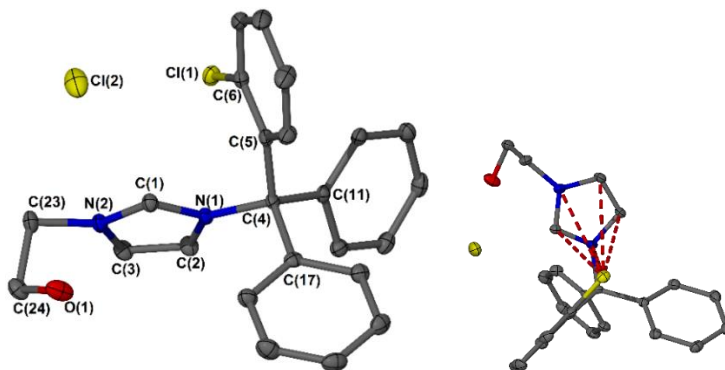


Figure S33. Molecular structure of imidazolium salt **2e**.

Table S2. Selected bond lengths and angles for imidazolium salts 2				
Bond Lengths (Å) and angles (°)	2a	2b	2d	2e
N(1)-C(1)-N(2)	108.1 (3)	108.53 (17)	108.21 (16)	108.99 (14)
N(1)-C(4)	1.514 (4)	1.503 (2)	1.516 (2)	1.509 (2)
N(2)-C(23)	1.478 (4)	1.467 (2)	1.485 (2)	1.470 (2)
Cl(1)-C(6)	1.755 (3)	1.745 (2)	1.752 (2)	1.7471 (17)
Cl(1)····C(1)	3.271	3.255	3.256	3.230
Cl(2)····C(1)	3.323	3.432	3.782	3.371
Cl(1)····Cl(2)	5.661	5.415	7.026	4.247

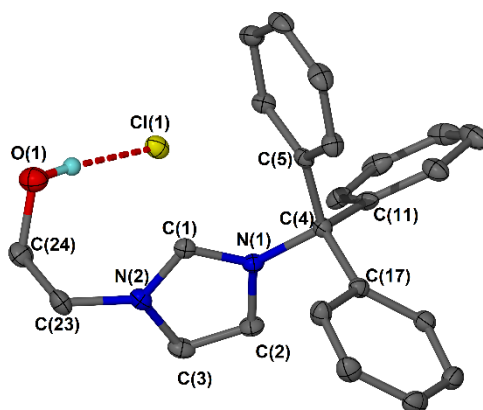


Figure S34. Molecular structure of imidazolium salt **3e**.

Table S3. Selected bond lengths and angles for imidazolium salt 3	
Bond Lengths (Å) and angles (°)	3e
N(1)-C(1)-N(2)	108.62 (13)
N(1)-C(4)	1.5086 (18)
N(2)-C(23)	1.4723 (19)
Cl(1)····C(1)	3.608

4. X-Ray Crystallographic Information for Imidazolium Salts

Table S4. Crystal data and structure refinement for **1a**

Empirical formula	C ₂₃ H ₂₀ ClIN ₂
Formula weight	486.76
Temperature/K	99.98(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	11.1938(5)
b/Å	14.6954(5)
c/Å	25.1005(10)
$\alpha/^\circ$	90.00
$\beta/^\circ$	90.00
$\gamma/^\circ$	90.00
Volume/Å ³	4129.0(3)
Z	8
$\rho_{\text{calc}}/\text{mg}/\text{mm}^3$	1.566
m/mm ⁻¹	1.690
F(000)	1936.0
Crystal size/mm ³	0.21 × 0.11 × 0.07
2 Θ range for data collection	6.5 to 56.56°
Index ranges	-14 ≤ h ≤ 9, -19 ≤ k ≤ 18, -33 ≤ l ≤ 27
Reflections collected	13104
Independent reflections	5081[R(int) = 0.0410]
Data/restraints/parameters	5081/0/245
Goodness-of-fit on F ²	1.032
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0414, wR ₂ = 0.0820
Final R indexes [all data]	R ₁ = 0.0662, wR ₂ = 0.0924
Largest diff. peak/hole / e Å ⁻³	2.02/-1.09

Table S5. Crystal data and structure refinement for **1c**

Empirical formula	C ₂₆ H ₂₆ N ₂ ClI
Formula weight	528.84
Temperature/K	99.8(6)
Crystal system	triclinic
Space group	P-1
a/Å	9.0800(4)
b/Å	10.6879(6)
c/Å	12.7305(6)
$\alpha/^\circ$	79.385(4)
$\beta/^\circ$	70.251(4)
$\gamma/^\circ$	79.962(4)
Volume/Å ³	1134.47(10)
Z	2
ρ_{calc} mg/mm ³	1.548
m/mm ⁻¹	1.545
F(000)	532.0
Crystal size/mm ³	0.28 × 0.16 × 0.11
2 Θ range for data collection	5.62 to 56.56°
Index ranges	-12 ≤ h ≤ 10, -9 ≤ k ≤ 14, -14 ≤ l ≤ 16
Reflections collected	8893
Independent reflections	5543[R(int) = 0.0353]
Data/restraints/parameters	5543/0/300
Goodness-of-fit on F ²	1.049
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0362, wR ₂ = 0.0723
Final R indexes [all data]	R ₁ = 0.0450, wR ₂ = 0.0780
Largest diff. peak/hole / e Å ⁻³	0.73/-0.49

Table S6. Crystal data and structure refinement for **1e**

Empirical formula	C ₂₄ H ₂₂ N ₂ OCl _{1.26} I _{0.74}
Formula weight	493.01
Temperature/K	100.0(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.7680(5)
b/Å	10.5147(6)
c/Å	12.2516(7)
α /°	77.789(5)
β /°	72.958(5)
γ /°	79.794(4)
Volume/Å ³	1047.43(10)
Z	2
ρ_{calc} /mg/mm ³	1.563
m/mm ⁻¹	1.324
F(000)	497.3
Crystal size/mm ³	0.26 × 0.14 × 0.1
2 Θ range for data collection	5.92 to 56.56°
Index ranges	-11 ≤ h ≤ 10, -13 ≤ k ≤ 14, -16 ≤ l ≤ 12
Reflections collected	8180
Independent reflections	5163[R(int) = 0.0315]
Data/restraints/parameters	5163/2/270
Goodness-of-fit on F ²	1.240
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0585, wR ₂ = 0.1120
Final R indexes [all data]	R ₁ = 0.0679, wR ₂ = 0.1165
Largest diff. peak/hole / e Å ⁻³	1.14/-0.84

Table S7. Crystal data and structure refinement for **2a**

Empirical formula	C ₂₃ H ₂₀ N ₂ Cl ₂
Formula weight	395.31
Temperature/K	100.0(3)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	8.2285(3)
b/Å	14.0099(5)
c/Å	8.8801(3)
α /°	90.00
β /°	105.303(4)
γ /°	90.00
Volume/Å ³	987.41(6)
Z	2
ρ_{calc} mg/mm ³	1.330
m/mm ⁻¹	3.019
F(000)	412.0
Crystal size/mm ³	0.09 × 0.05 × 0.04
2 Θ range for data collection	10.32 to 133.04°
Index ranges	-9 ≤ h ≤ 6, -16 ≤ k ≤ 14, -10 ≤ l ≤ 9
Reflections collected	3657
Independent reflections	2561[R(int) = 0.0318]
Data/restraints/parameters	2561/1/254
Goodness-of-fit on F ²	1.116
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0363, wR ₂ = 0.0864
Final R indexes [all data]	R ₁ = 0.0392, wR ₂ = 0.0875
Largest diff. peak/hole / e Å ⁻³	0.32/-0.19
Flack parameter	-0.001(16)

Table S8. Crystal data and structure refinement for **2b**

Empirical formula	C ₂₅ H ₂₄ N ₂ OCl ₂
Formula weight	439.36
Temperature/K	99.9(4)
Crystal system	orthorhombic
Space group	Pbca
a/Å	8.7356(5)
b/Å	19.9479(8)
c/Å	24.8334(12)
$\alpha/^\circ$	90.00
$\beta/^\circ$	90.00
$\gamma/^\circ$	90.00
Volume/Å ³	4327.4(4)
Z	8
ρ_{calc} mg/mm ³	1.349
m/mm ⁻¹	0.320
F(000)	1840.0
Crystal size/mm ³	0.31 × 0.2 × 0.15
2 Θ range for data collection	6.4 to 56.56°
Index ranges	-9 ≤ h ≤ 11, -14 ≤ k ≤ 26, -26 ≤ l ≤ 32
Reflections collected	15101
Independent reflections	5342[R(int) = 0.0497]
Data/restraints/parameters	5342/3/277
Goodness-of-fit on F ²	1.029
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0479, wR ₂ = 0.0909
Final R indexes [all data]	R ₁ = 0.0727, wR ₂ = 0.1023
Largest diff. peak/hole / e Å ⁻³	0.37/-0.39

Table S9. Crystal data and structure refinement for **2d**

Empirical formula	C ₂₉ H ₂₆ N ₂ OCl ₂
Formula weight	489.42
Temperature/K	99.9(4)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	10.7546(7)
b/Å	25.2780(12)
c/Å	10.1699(7)
α /°	90.00
β /°	115.850(8)
γ /°	90.00
Volume/Å ³	2488.1(3)
Z	4
ρ_{calc} mg/mm ³	1.307
m/mm ⁻¹	0.286
F(000)	1024.0
Crystal size/mm ³	0.33 × 0.15 × 0.12
2 Θ range for data collection	6.58 to 56.56°
Index ranges	-14 ≤ h ≤ 14, -27 ≤ k ≤ 33, -10 ≤ l ≤ 13
Reflections collected	11440
Independent reflections	6126[R(int) = 0.0397]
Data/restraints/parameters	6126/3/307
Goodness-of-fit on F ²	1.042
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0493, wR ₂ = 0.1045
Final R indexes [all data]	R ₁ = 0.0679, wR ₂ = 0.1174
Largest diff. peak/hole / e Å ⁻³	0.81/-0.43

Table S10. Crystal data and structure refinement for **2e**

Empirical formula	C ₂₄ H ₂₂ Cl ₂ N ₂ O
Formula weight	425.33
Temperature/K	120.0(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.6119(7)
b/Å	10.5213(8)
c/Å	11.8588(7)
α /°	79.723(6)
β /°	73.537(6)
γ /°	80.616(6)
Volume/Å ³	1006.70(13)
Z	2
ρ_{calc} /mg/mm ³	1.403
m/mm ⁻¹	0.341
F(000)	444.0
Crystal size/mm ³	0.11 × 0.06 × 0.03
2 Θ range for data collection	5.946 to 56.564°
Index ranges	-10 ≤ h ≤ 11, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	15179
Independent reflections	4984[R(int) = 0.0403]
Data/restraints/parameters	4984/0/282
Goodness-of-fit on F ²	1.039
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0439, wR ₂ = 0.0871
Final R indexes [all data]	R ₁ = 0.0616, wR ₂ = 0.0947
Largest diff. peak/hole / e Å ⁻³	0.39/-0.52

Table S11. Crystal data and structure refinement for **3e**

Empirical formula	C ₂₄ H ₂₃ N ₂ OCl
Formula weight	390.89
Temperature/K	120.15
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	12.6173(5)
b/Å	13.0098(5)
c/Å	12.7200(5)
α /°	90
β /°	107.183(5)
γ /°	90
Volume/Å ³	1994.76(15)
Z	4
ρ_{calc} mg/mm ³	1.302
m/mm ⁻¹	0.209
F(000)	824.0
Crystal size/mm ³	0.46 × 0.35 × 0.19
2 Θ range for data collection	6.558 to 56.564°
Index ranges	-16 ≤ h ≤ 12, -17 ≤ k ≤ 11, -16 ≤ l ≤ 15
Reflections collected	9414
Independent reflections	4908[R(int) = 0.0382]
Data/restraints/parameters	4908/1/257
Goodness-of-fit on F ²	1.071
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0446, wR ₂ = 0.0972
Final R indexes [all data]	R ₁ = 0.0583, wR ₂ = 0.1096
Largest diff. peak/hole / e Å ⁻³	0.26/-0.27

5. X-Ray Crystallographic Information for Silver Complexes

Table S12. Crystal data and structure refinement for **4e**

Empirical formula	C ₄₈ H ₄₀ AgCl ₃ N ₄ O ₂
Formula weight	919.06
Temperature/K	119.98(18)
Crystal system	monoclinic
Space group	C2/c
a/Å	21.311(2)
b/Å	15.0537(13)
c/Å	14.0953(13)
α /°	90.00
β /°	90.886(10)
γ /°	90.00
Volume/Å ³	4521.3(7)
Z	4
ρ_{calc} /mg/mm ³	1.350
m/mm ⁻¹	0.665
F(000)	1880.0
Crystal size/mm ³	0.12 × 0.08 × 0.06
2 θ range for data collection	6.14 to 50.06°
Index ranges	-24 ≤ h ≤ 25, -17 ≤ k ≤ 17, -16 ≤ l ≤ 16
Reflections collected	13428
Independent reflections	3919[R(int) = 0.0858]
Data/restraints/parameters	3919/1/275
Goodness-of-fit on F ²	1.042
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.1018, wR ₂ = 0.2844
Final R indexes [all data]	R ₁ = 0.1554, wR ₂ = 0.3228
Largest diff. peak/hole / e Å ⁻³	1.49/-0.64

Table S13. Crystal data and structure refinement for **5a**

Empirical formula	C ₂₃ H ₂₀ N ₂ ClAg
Formula weight	467.73
Temperature/K	110.01(10)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	13.5174(5)
b/Å	9.9426(3)
c/Å	15.6082(6)
$\alpha/^\circ$	90.00
$\beta/^\circ$	106.551(4)
$\gamma/^\circ$	90.00
Volume/Å ³	2010.80(12)
Z	4
ρ_{calc} mg/mm ³	1.545
m/mm ⁻¹	1.145
F(000)	944.0
Crystal size/mm ³	0.41 × 0.16 × 0.14
2 Θ range for data collection	6.24 to 56.56°
Index ranges	-18 ≤ h ≤ 17, -9 ≤ k ≤ 13, -20 ≤ l ≤ 20
Reflections collected	15088
Independent reflections	4992[R(int) = 0.0523]
Data/restraints/parameters	4992/0/245
Goodness-of-fit on F ²	1.253
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0757, wR ₂ = 0.1738
Final R indexes [all data]	R ₁ = 0.0850, wR ₂ = 0.1784
Largest diff. peak/hole / e Å ⁻³	4.70/-0.82

Table S14. Crystal data and structure refinement for **5b**

Empirical formula	C ₂₅ H ₂₂ N ₂ ClAg
Formula weight	493.77
Temperature/K	120.01(10)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	7.2098(3)
b/Å	10.3663(5)
c/Å	13.7678(6)
α /°	90.00
β /°	92.764(4)
γ /°	90.00
Volume/Å ³	1027.79(8)
Z	2
ρ_{calc} /mg/mm ³	1.595
m/mm ⁻¹	1.124
F(000)	500.0
Crystal size/mm ³	0.5 × 0.39 × 0.29
2 Θ range for data collection	5.92 to 61°
Index ranges	-8 ≤ h ≤ 10, -12 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected	10205
Independent reflections	5255[R(int) = 0.0591]
Data/restraints/parameters	5255/1/262
Goodness-of-fit on F ²	1.081
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0377, wR ₂ = 0.0926
Final R indexes [all data]	R ₁ = 0.0387, wR ₂ = 0.0939
Largest diff. peak/hole / e Å ⁻³	0.55/-0.69
Flack parameter	0.00(3)

Table S15. Crystal data and structure refinement for **5d**

Empirical formula	C _{58.75} H _{49.5} AgCl _{2.5} N ₄ O _{0.25}
Formula weight	1012.02
Temperature/K	120.0(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	13.3752(3)
b/Å	18.7972(4)
c/Å	19.9989(6)
α /°	90.00
β /°	103.388(3)
γ /°	90.00
Volume/Å ³	4891.4(2)
Z	4
ρ_{calc} mg/mm ³	1.374
m/mm ⁻¹	0.593
F(000)	2086.0
Crystal size/mm ³	0.2166 × 0.1046 × 0.0771
2 Θ range for data collection	6.02 to 56.56°
Index ranges	-17 ≤ h ≤ 17, -23 ≤ k ≤ 25, -26 ≤ l ≤ 26
Reflections collected	55175
Independent reflections	12129[R(int) = 0.0473]
Data/restraints/parameters	12129/2/620
Goodness-of-fit on F ²	1.051
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0564, wR ₂ = 0.1381
Final R indexes [all data]	R ₁ = 0.0728, wR ₂ = 0.1493
Largest diff. peak/hole / e Å ⁻³	1.21/-1.70

Table S16. Crystal data and structure refinement for **6c**

Empirical formula	C _{106.5} H ₁₀₆ N ₈ Cl ₆ Ag ₄ I ₂
Formula weight	2395.97
Temperature/K	99.93(16)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	19.1036(18)
b/Å	23.4773(18)
c/Å	24.0473(14)
α /°	90.00
β /°	102.591(7)
γ /°	90.00
Volume/Å ³	10525.9(14)
Z	4
ρ_{calc} /mg/mm ³	1.512
m/mm ⁻¹	12.262
F(000)	4788.0
Crystal size/mm ³	0.14 × 0.06 × 0.04
2 Θ range for data collection	6.56 to 113.84°
Index ranges	-20 ≤ h ≤ 19, -18 ≤ k ≤ 25, -26 ≤ l ≤ 21
Reflections collected	27795
Independent reflections	14093[R(int) = 0.1021]
Data/restraints/parameters	14093/8/1160
Goodness-of-fit on F ²	0.976
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.1000, wR ₂ = 0.2512
Final R indexes [all data]	R ₁ = 0.1859, wR ₂ = 0.3281
Largest diff. peak/hole / e Å ⁻³	1.92/-2.21

6. Expanded RCVs

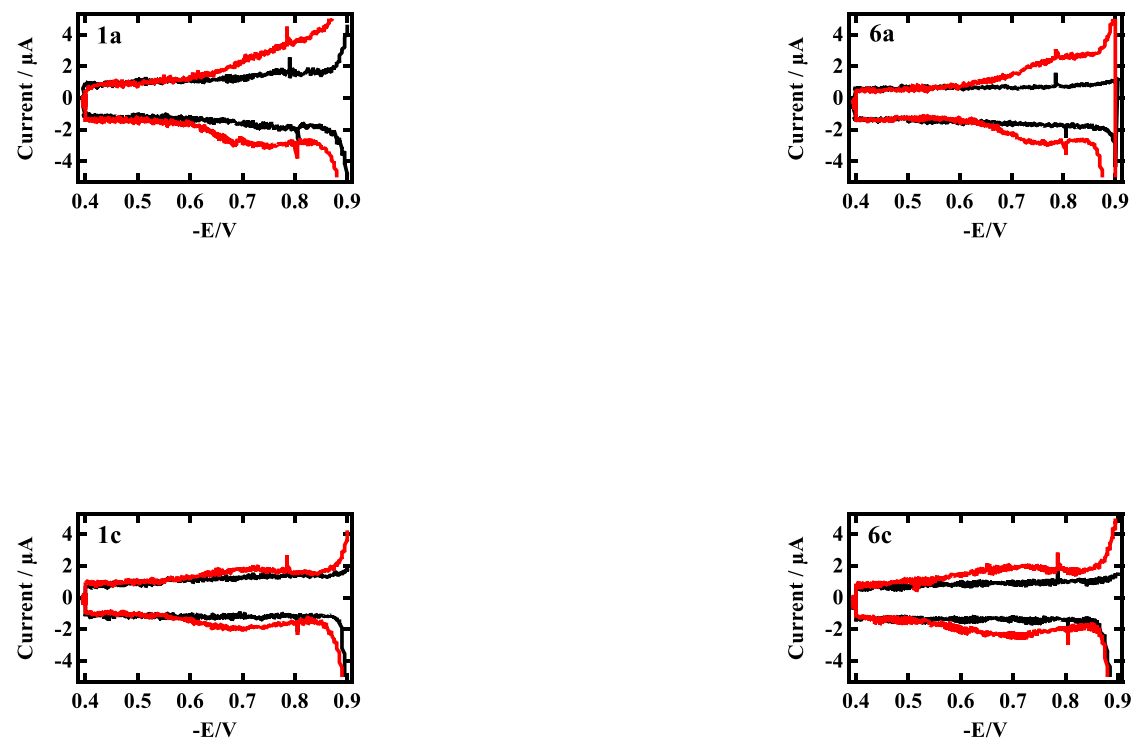


Figure S35. Expanded RCVs for imidazolium salts **1a** and **1c** and silver complexes **6a** and **6c**.