Electronic Supporting Information For:

Antibacterial silver and gold complexes of imidazole and 1,2,4-triazole derived *N*-heterocyclic carbenes

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NMR Stability Studies

Time course ^{1}H-NMR studies

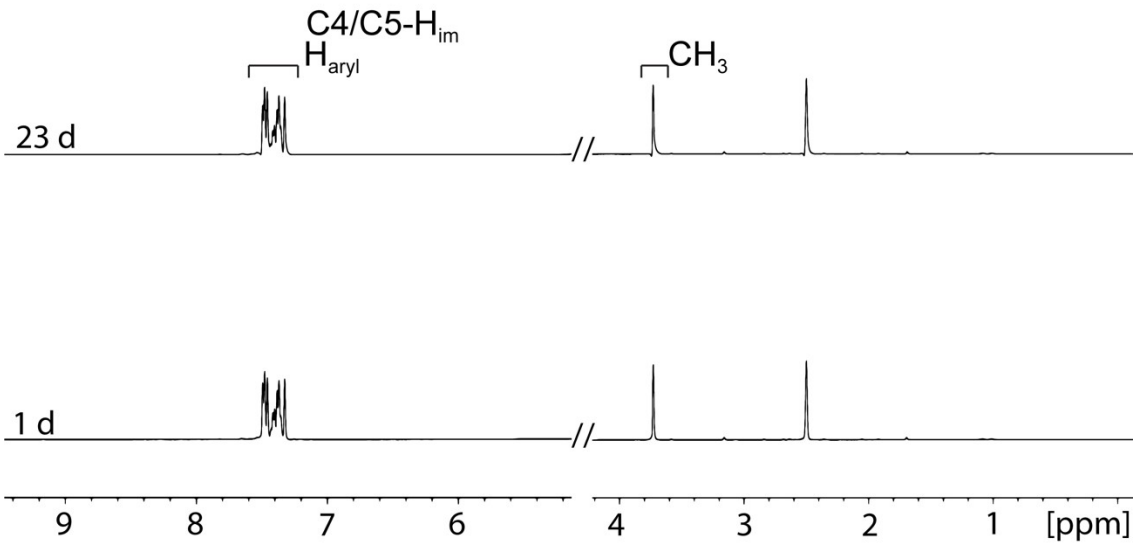


Figure S1. Selected ^{1}H NMR spectra recorded for a solution of the gold(I) complex **4a** in a mixture of 300 µL DMSO-d_6 and 300 µL H_2O over a period of 23d at 25.0 ± 0.1 °C.

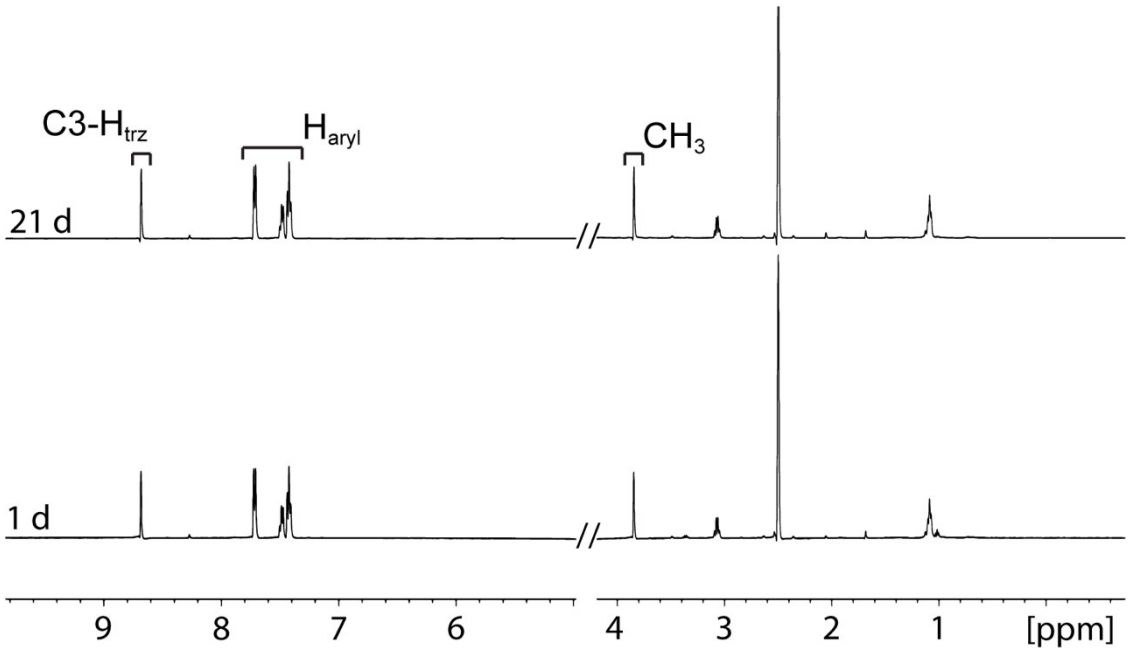


Figure S2. Selected ^{1}H NMR spectra recorded for a solution of the gold(I) complex **4c** in a mixture of 300 μL DMSO-d_6 and 300 μL H_2O over a period of 21d at 25.0 ± 0.1 °C.

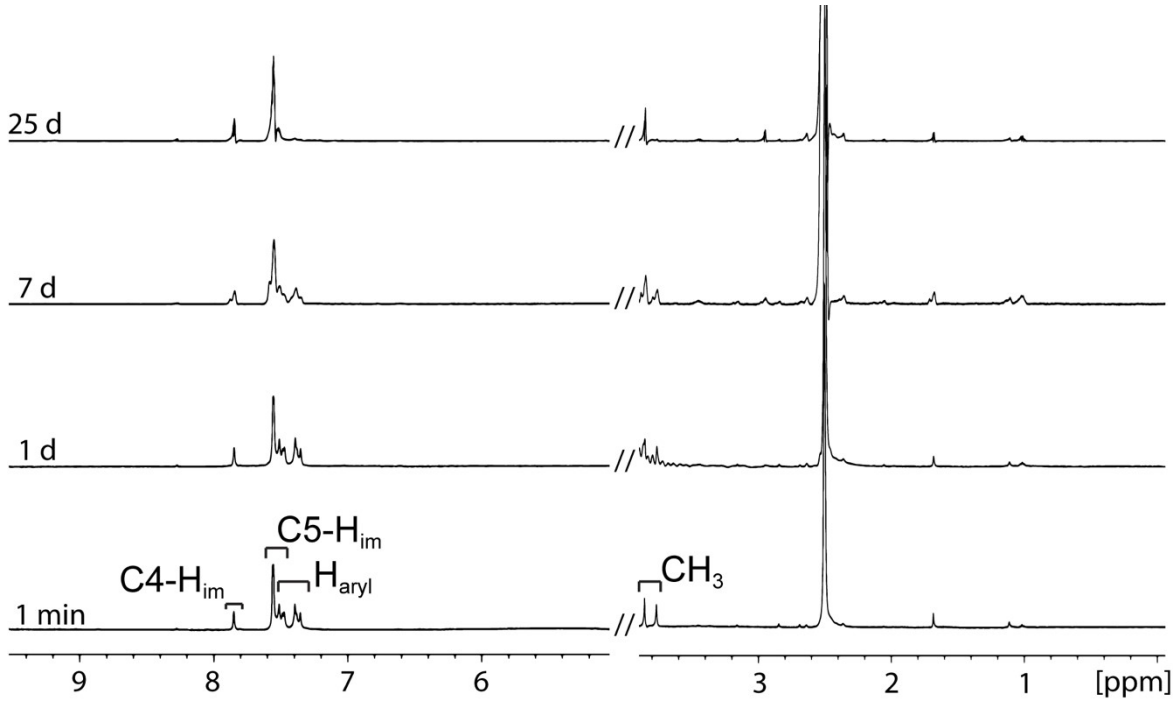


Figure S3. Selected ^{1}H NMR spectra recorded for a solution of the silver(I) complex **3a** in a mixture of 300 μL DMSO-d_6 and 300 μL H_2O over a period of 25 d at 25.0 ± 0.1 °C.

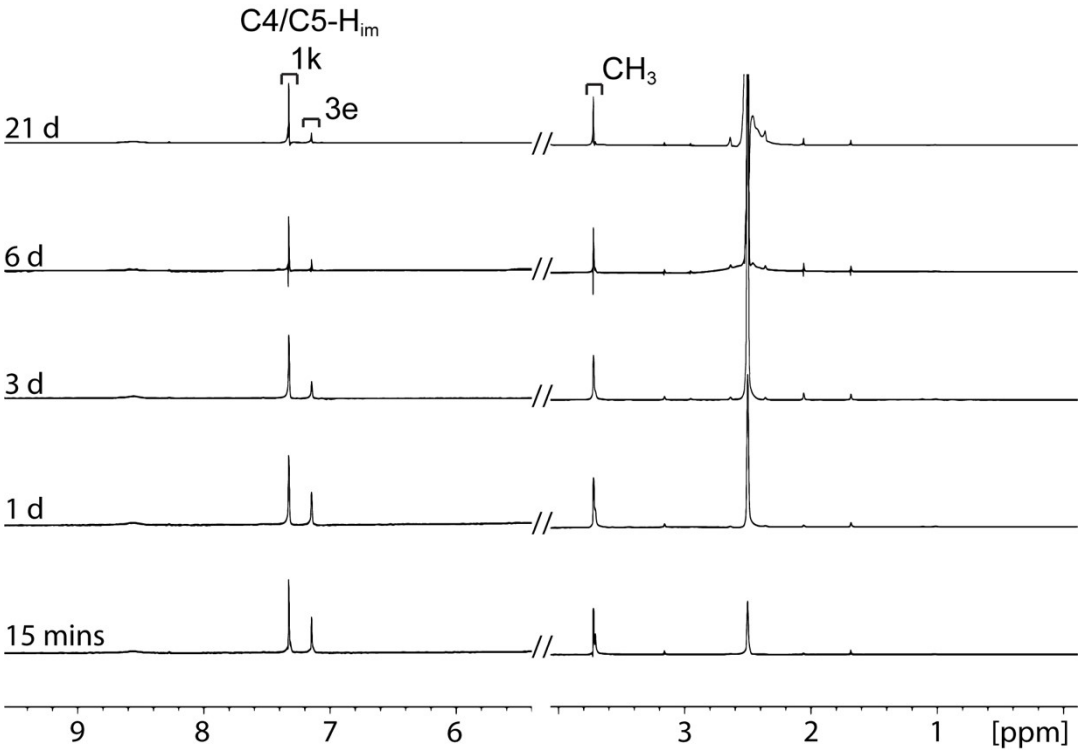


Figure S4. Selected ^{1}H NMR spectra recorded for a solution of the silver(I) complex **3e** in a mixture of 300 μL DMSO-d_6 and 300 μL H_2O over a period of 21d at 25.0 ± 0.1 °C.

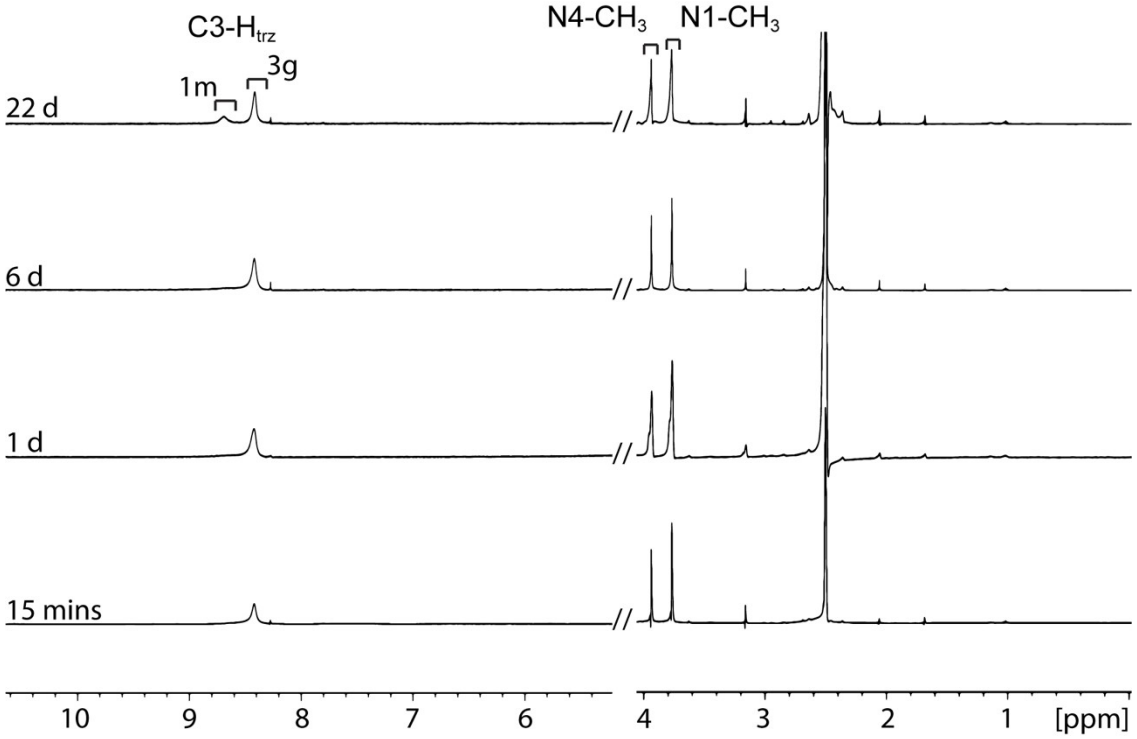


Figure S5. Selected ^{1}H NMR spectra recorded for a solution of the silver(I) complex **3g** in a mixture of 300 μL DMSO-d_6 and 300 μL H_2O over a period of 22 d at 25.0 ± 0.1 °C.

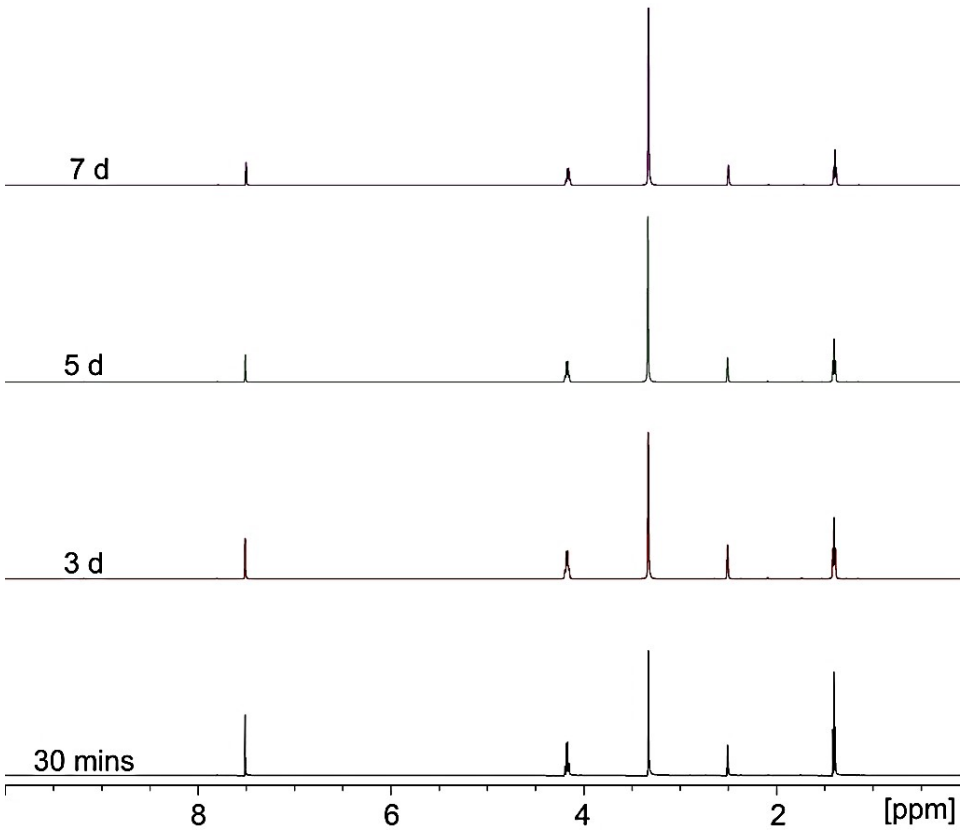


Figure S6. Stacked ^{1}H-NMR spectrums of compound **3f** in DMSO-d_6 over a period 7 days.

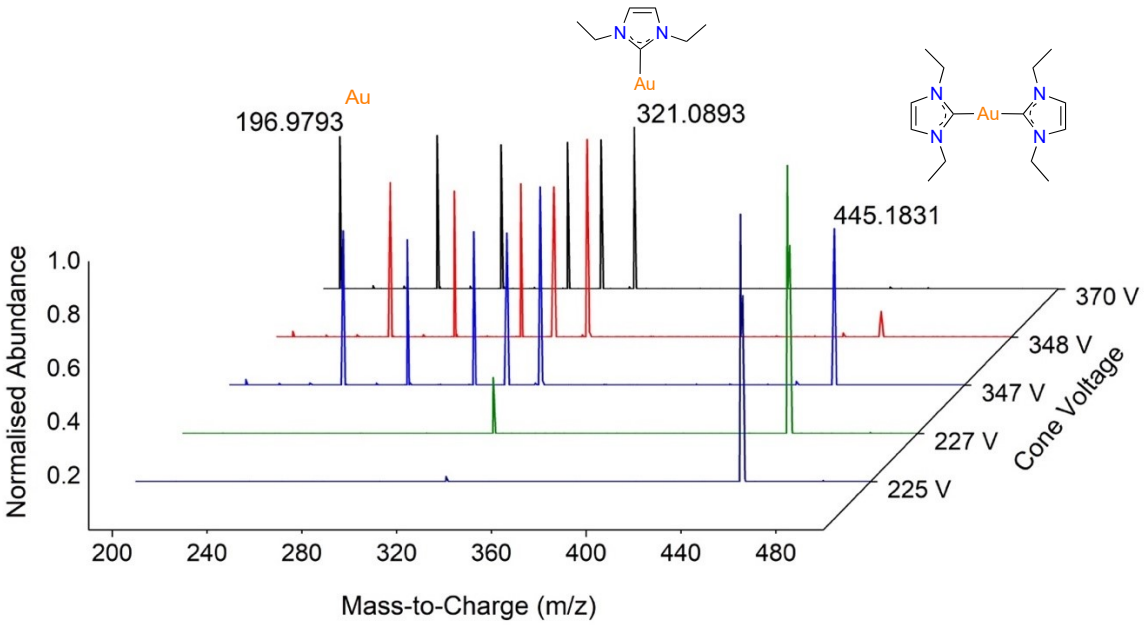


Figure S7. Normalised ESI-HR-MS plots at selected cone voltages for gold(I) complex **4f**.

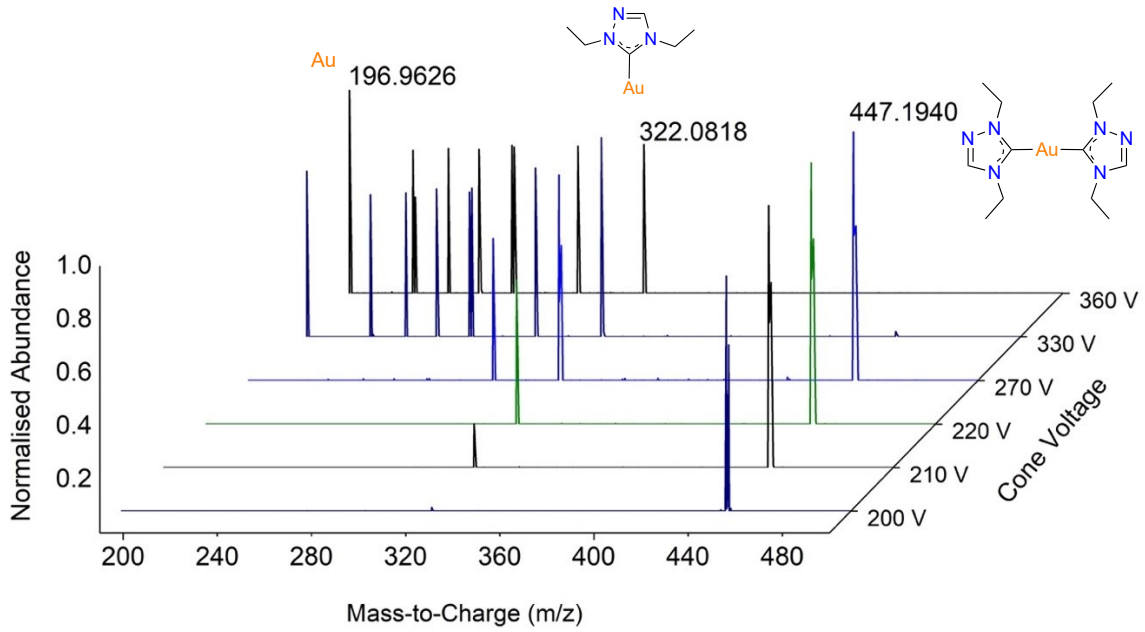


Figure S8. Normalised ESI-HR-MS plots at selected cone voltages for gold(I) complex **4h**.

Further crystallographic Information

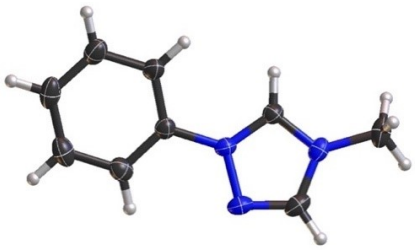


Figure S9. Representation of X-ray crystal structure of **1e**, the iodide anion has been omitted for clarity.

Table S1. Crystallographic data for **1e**, **3a**, **3c**

Identification code	**1e**	**3a**	**3c**
Empirical formula	$C_9H_{10}IN_3$	$C_{20}H_{20}Ag_2Cl_2N_4$	$C_9H_9Ag_2I_2N_3$
Formula weight	287.10	603.04	628.73
Temperature/K	150(2)	150(15)	150(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1$	P2/n
a/Å	7.83570(10)	11.2662(2)	12.9749(2)
b/Å	12.72860(10)	7.39800(10)	7.37600(10)
c/Å	14.2408(2)	12.5768(2)	32.9550(5)
α/°	90	90	90
β/°	131.433(2)	96.300(2)	120.190(2)
γ/°	90	90	90
Volume/Å^3	1064.87(3)	1041.91(3)	2726.10(8)
Z	4	2	8
ρ_{calc}g/cm^3	1.791	1.922	3.064
μ/mm^{-1}	23.302	2.149	58.438
F(000)	552.0	592.0	2272.0
Crystal size/mm^3	0.04 × 0.03 × 0.02	0.08 0.04 × 0.04	0.03 × 0.02 × 0.02
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.816 to 142.474	6.4 to 49.406	6.866 to 142.48
Index ranges	-9 ≤ h ≤ 9, -15 ≤ k ≤ 15, -13 ≤ l ≤ 17	13 ≤ h ≤ 13, -8 ≤ k ≤ 8, -14 ≤ l ≤ 14	-15 ≤ h ≤ 11, -9 ≤ k ≤ 8, -38 ≤ l ≤ 40
Reflections collected	21563	21372	27986
Independent reflections	2066 [R_{int} = 0.0585, R_{sigma} = 0.0182]	3544 [R_{int} = 0.0731, R_{sigma} = 0.0449]	5280 [R_{int} = 0.0609, R_{sigma} = 0.0336]
Data/restraints/parameters	2066/0/119	3544/1/255	5280/0/296
Goodness-of-fit on F^2	1.083	1.045	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0273, wR_2 = 0.0754	R_1 = 0.0275, wR_2 = 0.0579	R_1 = 0.0364, wR_2 = 0.1048
Final R indexes [all data]	R_1 = 0.0275, wR_2 = 0.0757	R_1 = 0.0300, wR_2 = 0.0596	R_1 = 0.0404, wR_2 = 0.1082
Largest diff. peak/hole / e Å^{-3}	1.33/-1.01	0.37/-0.34	2.25/-1.54

Table S2. Crystallographic data for **4b** and **5b**

Identification code	**Complex 4b**	**Complex 5b**
Empirical formula	$C_{22}H_{24}AuIN_4$	$C_{20}H_{34}Au_2Br_2N_{12}O$
Formula weight	668.32	1012.34
Temperature/K	150(2)	150(2)
Crystal system	monoclinic	triclinic

Space group	$P2_1/n$	P-1
a/Å	9.89520(10)	9.54745(7)
b/Å	17.19070(10)	9.97551(6)
c/Å	13.18180(10)	17.05412(8)
α/°	90	99.8735(4)
β/°	90.2300(10)	90.4278(5)
γ/°	90	112.6243(6)
Volume/Å^3	2242.28(3)	1472.226(16)
Z	4	2
ρ_{calc}g/cm^3	1.980	2.284
μ/mm^{-1}	23.242	21.953
F(000)	1264.0	948.0
Crystal size/mm^3	0.05 × 0.04 × 0.04	0.06 × 0.02 × 0.02
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.452 to 129.486	9.782 to 130.164
Index ranges	-11 ≤ h ≤ 11, -19 ≤ k ≤ 20, -15 ≤ l ≤ 15	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -19 ≤ l ≤ 20
Reflections collected	16824	26139
Independent reflections	3783 [R_{int} = 0.0278, R_{sigma} = 0.0197]	5012 [R_{int} = 0.0522, R_{sigma} = 0.0227]
Data/restraints/parameters	3783/0/255	5012/2/347
Goodness-of-fit on F^2	1.079	1.188
Final R indexes [I>=2σ (I)]	R_1 = 0.0182, wR_2 = 0.0455	R_1 = 0.0334, wR_2 = 0.0876
Final R indexes [all data]	R_1 = 0.0191, wR_2 = 0.0460	R_1 = 0.0335, wR_2 = 0.0876
Largest diff. peak/hole / e Å^{-3}	0.62/-0.93	2.68/-2.26

Antibacterial Activity of the imidazolium and triazolium salts.

Table S3. Minimum Inhibitory Concentration (MIC μg·mL^{-1}) values of the imidazolium and 1,2,4-triazolium precursor pro-ligand salts.

Compound	Gram-positive		Gram-negative	
	E. faecium[a]	*S. aureus*[b]	*A. baumannii*[c]	*E. coli*[d]
1c$_{Im,}$ (R_1 = Ph, R_2 = Me)	>128	>128	>128	>128
1d$_{Im,}$ (R_1 = Ph, R_2 = Et)	>128	>128	>128	>128
1e$_{trz,}$ (R_1 = Ph, R_2 = Me)	>128	>128	128	>128

1f$_{trz,}$ (R_1 = Ph, R_2 = Et)	>128	>128	>128	>128
1k$_{Im,}$ (R_1 = R_2 = Me)	>128	>128	>128	>128
1l$_{Im,}$ (R_1 = R_2 = Et)	>128	>128	>128	>128
1m$_{trz,}$ (R_1 = R_2 = Me)	>128	>128	>128	>128
1n$_{trz,}$ (R_1 = R_2 = Et)	>128	>128	>128	>128
2a$_{Bis\text{-}im,}$ (R_1 = Et, n = 2)	>128	>128	>128	>128
2b$_{Bis\text{-}trz,}$ (R_1 = Et, n = 2)	>128	>128	>128	>128

[a]*E. faecium* ATCC® BAA-2127, [b]*S. aureus* ATCC® 9144™, [c]*A. baumannii* ATCC® 17978™, and [d]*E. coli* ATCC® BAA-2340™

Synthesis

General Details

All reagents were purchased from Sigma-Aldrich, Alfa Aesar or Chem Supply and were of analytical grade or higher and were used without further purification unless otherwise stated. 400 and 500 MHz NMR spectrometers were employed to record ^{1}H and ^{13}C-NMR spectra. Chemical shifts (δ) are displayed in parts per million (ppm) referenced to residual solvent signals $CDCl_3$ (δ_H = 7.26 and δc = 77.16 ppm) and DMSO-d_6 (δ_H = 2.50 and δ_C = 39.52 ppm). ^{1}H-NMR spectroscopic data are reported in the order of multiplicity, which is characterized as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad), coupling constant (J) in hertz (Hz) and number of protons.

1a. Compound **1a** was synthesised following a modified literature procedure.[1] To a solution of imidazole (3.00 g, 44.06 mmol) and bromobenzene (5.07 mL, 48.00 mmol) in degassed DMSO (30 mL), potassium carbonate (12.00 g, 88.12 mmol), CuI (0.84 g, 4.41 mmol) and proline (0.50 g, 4.41 mmol) were added under nitrogen atmosphere and this mixture was stirred at 120 °C for 48 h. The resultant mixture was then cooled to RT and diluted with water followed by extraction with ethyl acetate (3 × 50 mL). The combined organic layers were washed with brine (30 mL) followed by drying over anhydrous $MgSO_4$. The crude product was purified via column chromatography to obtain a yellow liquid. Yield: 2.93 g, 46%. ^{1}H-NMR (500.14 MHz, $CDCl_3$) δ 7.79 (s, 1H, C2-H_{im}), 7.43 – 7.40 (m, 2H, H_{aryl}), 7.32 – 7.29 (m, 3H, H_{aryl}), 7.22 (s, 1H, C5-H_{im}), 7.15 (s, 1H, C4-H_{im}) ^{13}C-NMR (125.77 MHz, $CDCl_3$) δ 136.3 (C_q), 134.5 ($C2_{im}$), 129.4 ($C4_{im}$), 128.8 (C_{aryl}), 126.4 (C_{aryl}), 120.4 (C_{aryl}), 117.2 ($C5_{im}$) HRESI-MS: [$C_9H_8N_2^+$] *m/z* = 145.0705 calcd. = 145.0760.

1b. This compound was prepared using the same method for **1a** from 1,2,4-triazole (1.00 g, 43.50 mmol) bromobenzene (5.0 mL, 47.80 mmol) potassium carbonate (12.00 g, 86.88 mmol), CuI(0.83 g, 4.34 mmol), and proline (0.50 g, 4.34 mmol). Volatiles were removed under reduced pressure producing a yellow crystalline solid. Yield: 3.48 g, 55%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 9.31 (s, 1H, C5-H_{trz}), 8.25 (s, 1H, C3-H_{trz}), 7.88 – 7.86 (m, 2H, H_{aryl}), 7.59 – 7.55 (m, 2H, H_{aryl}), 7.44 – 7.40 (m, 1H, H_{aryl}).^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 152.9 ($C5_{trz}$), 142.8 ($C3_{trz}$) 137.2 (C_q), 130.2 (C_{aryl}), 128.3 (C_{aryl}), 119.9 (C_{aryl}). HRESI-MS: [$C_8H_7N_3^+$] *m/z* = 146.0704 calcd. = 146.0704.

1c. To a solution of 1-phenyl-1*H*-imidazole (**1a**) (0.20 g, 1.38 mmol) in acetonitrile was added iodomethane (0.12 mL, 1.94 mmol). The resulting mixture was heated under reflux for 24 h and then cooled to RT and volatiles were removed under reduced pressure producing a yellow oil. The crude product was recrystallised with acetonitrile and ether producing a crystalline white powder. Yield: 0.26 g, 65%. ^{1}H-NMR (400.13 MHz, $CDCl_3$) δ 10.15 (s, 1H, C2-H_{im}), 7.79 (s, 1H, C4-H_{im}), 7.75 (s, 1H, C5-H_{im}), 7.71 – 7.69 (m, 2H, H_{aryl}), 7.50 – 7.42 (m, 3H, H_{aryl}), 4.17 (s, 3H, CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 136.4 ($C2_{im}$), 135.2 (C_q) 130.7 (C_{aryl}) 130.2 (C_{aryl}), 124.9 (C_{im}), 122.3 (C_{aryl}), 121.5 (C_{im}) 36.7 (CH_3) HRESI-MS: [$C_{10}H_{11}N_2^+$] *m/z* = 159.0926 calcd. = 159.0917.

1d. This compound was prepared using the same method as **1c** from **1a** (0.60 g, 4.16 mmol), and iodoethane (0.40 mL, 5.00 mmol) yielding a light brown powder. Yield: 0.95 g, 76%. ^{1}H-NMR (400.13 MHz, $CDCl_3$) δ 10.29 (s, 1H, C2-H_{im}), 7.84 (s 1H, C4-H_{im}), 7.77 (s, 1H, C5-H_{im}), 7.71-7.69 (m, 2H, H_{aryl}), 7.44-7.37 (m, 3H, H_{aryl}) 4.52 (q, J = 8.0 Hz, 2H, CH_2CH_3), 1.55 (t, J = 8.0 Hz, 3H, CH_2CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 135.6 ($C2_{im}$), 135.3 (C_q), 130.6 (C_{aryl}), 130.2 (C_{aryl}), 123.5 (C_{im}), 122.4 (C_{aryl}), 121.6 (C_{im}). 45.3 (CH_2CH_3), 15.3 (CH_2CH_3). HRESI-MS: [$C_{11}H_{13}N_2^+$] *m/z* = 173.1089 calcd. = 173.1073.

1e was prepared using the same method as **1c** from **1b** (0.60 g, 4.13 mmol) and iodomethane (0.36 mL, 5.79 mmol) yielding a white powder. Yield: 0.95 g, 80%. ^{1}H-NMR (400.13 MHz, $CDCl_3$) δ 11.57 (s, 1H, C5-H_{trz}), 9.17 (s, 1H, C3-H_{trz}), 7.96 – 7.92 (m, 2H, H_{aryl}), 7.55 – 7.47 (m, 3H, H_{aryl}), 4.33 (s, 3H, CH_3). ^{13}C-NMR (125.77 MHz, $CDCl_3$) δ 145.2 ($C5_{trz}$), 140.8 ($C3_{trz}$), 134.7 (C_q), 130.9 (C_{aryl}), 130.3 (C_{aryl}), 120.8 (C_{aryl}), 36.1 (CH_3). HRESI-MS: [$C_9H_{10}N_3^+$] *m/z* = 160.0868, calcd. = 160.0869.

1f was prepared using the same methods as **1c** from **1b** (0.60 g, 4.13 mmol) and iodoethane (0.47 mL, 5.79 mmol) to give **1f** as a crystalline white powder. Yield: 1.05 g, 84%. ^{1}H-NMR (400.13 MHz,

$CDCl_3$) δ 11.84 (s, 1H, C5-H_{trz}), 9.13 (s, 1H, C3-H_{trz}), 8.06 – 8.02 (m, 2H, H_{aryl}), 7.58 – 7.50 (m, 3H, H_{aryl}), 4.78 (q, J = 7.4 Hz, 2H, CH_2CH_3), 1.74 (t, J = 7.4 Hz, 3H, CH_2CH_3). ^{13}C-NMR (125.77 MHz, $CDCl_3$) δ 143.9 ($C5_{trz}$), 140.2 ($C3_{trz}$), 134.8 (C_q), 131.0 (C_{aryl}), 130.3 (C_{aryl}), 120.7 (C_{aryl}), 45.0 (CH_2CH_3), 15.7 (CH_2CH_3). HRESI-MS: $[C_{10}H_{12}N_3^+]$ m/z = 174.1024 calcd. = 174.1026.

1g and **1k.** A mixture of imidazole (2.00 g, 29.37 mmol), iodomethane (3.65 mL, 58.74 mmol) and potassium carbonate (4.06 g, 29.37 mmol) in acetone (30 mL) was stirred at RT for 24 h. The reaction mixture was filtered and volatiles were removed under reduced pressure producing an off-white powder. The crude product was redissolved in acetone (10 mL) followed by the addition of ethyl acetate (15 mL) to obtain a white powder **1k** that was collected and washed with ethyl acetate. The solvent of the filtrate was removed under reduced pressure to yield mono-alkylated product **1g** as a yellow oil. **1g**: Yield: 0.86 g, 36%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 7.58 (s, 1H, C2-H_{im}), 7.10 (s, 1H, C5-H_{im}), 6.92 (s, 1H, C4-H_{im}) 3.64 (s, 3H, N3-CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 138.3 ($C2_{im}$), 128.9 ($C5_{im}$), 120.9 ($C4_{im}$) 33.1 (CH_3). **1k**: (Yield: 1.84 g, 27%). ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 9.06 (s, 1H, C2-H_{im}), 7.69 (m, 2H, H_{im}), 3.85 (s, 6H, N1-CH_3, N3-CH_3). ^{13}C-NMR (100.62 MHz, DMSO-d_6) δ 137.5 ($C2_{im}$), 123.9 ($C4_{im}$, $C5_{im}$), 36.2 (CH_3). HRESI-MS: $[C_5H_9N_2^+]$ m/z = 97.0760 calcd. = 97.0741.

1h and **1l**. These compounds were prepared using the same methods as **1g** and **1k** from imidazole (2 g, 29.37 mmol), iodoethane (4.72 mL, 58.74 mmol), and potassium carbonate (4.06 g, 29.37 mmol), yielding **1h** as a yellow oil, and **1l** as a white crystalline powder. **1h**: Yield: 0.59 g, 21%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 7.64 (s, 1H, C2- H_{im}), 7.17 (s, 1H, C4-H_{im}), 6.90 (s, C5-H_{im}), 3.97 (q, J = 7.3, 2, CH_2CH_3), 1.32 (t, J = 7.3, 3H, CH_2CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 137.2 ($C2_{im}$), 128.7 ($C5_{im}$), 119.3 ($C4_{im}$) 41.4 (CH_2CH_3) 16.7 (CH_2CH_3). **1l**: Yield: 1.42 g, 19%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 9.25 (s, 1H, C2-H_{im}), 7.82 (s, 2H H_{im}), 4.20 (q, J = 7.3, 4H, CH_2CH_3), 1.45 – 1.40 (m, 6H, CH_2CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 135.9 ($C2_{im}$), 122.5 ($C4_{im}$, $C5_{im}$), 44.7 (CH_2CH_3), 15.5 (CH_2CH_3). HRESI-MS: $[C_7H_{13}N_2^+]$ m/z = 126.1077 calcd. = 126.3031.

1i and **1m**. These compounds were prepared using the same methods as **1g** and **1k** from 1,2,4-triazole (2.00 g, 28.96 mmol), iodomethane (3.61 mL, 57.92 mmol), and potassium carbonate (4 g, 28.98 mmol) yielding **1i** as a yellow oil, and **1m** as a white crystalline powder. **1i**: Yield: 0.87 g, 36%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 8.45 (s, 1H, C5-H_{trz}), 7.94 (s, 1H, C3-H_{trz}), 3.87 (s, 3H, N1-CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 151.8 ($C5_{trz}$), 144.9 ($C3_{trz}$), 36.1 (N1-CH_3). **1m:** Yield: 1.7 g, 26%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 9.99 (s, 1H, C5-H_{trz}), 9.12 (s, 1H, C3-H_{trz}), 4.07 (s, 3H,

N4-CH_3), 3.90 (s, 3H, N1-CH_3). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 145.8 (C5$_{trz}$), 143.8 (C3$_{trz}$), 39.1 (N4-CH_3), 34.5 (N1-CH_3). HRESI-MS: [$C_4H_8N_3^+$] *m/z* = 98.0712 calcd. = 98.0713.

1j and **1n**. These compounds were prepared using the same methods as **1g** and **1k** from 1,2,4-triazole (2 g, 29.00 mmol), iodoethane (4.66 mL, 57.91 mmol), and potassium carbonate (7.38 g, 29.00 mmol) yielding **1j** as a yellow oil, and **1n** as a white crystalline powder. **1j**: Yield: 2.15 g, 76%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 8.50 (s, 1H, C5-H_{trz}), 7.94 (s, 1H, C3-H_{trz}), 4.20 (q, J = 7.3 Hz, 2H, N1-CH_2CH$_3$), 1.36 (t, J = 7.3 Hz, 3H, N1-CH$_2$$CH_3$). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 151.6 (C5$_{trz}$), 143.7 (C3$_{trz}$), 44.3 (N1-CH_2CH$_3$), 15.4 (N1-CH$_2$$CH_3$). **1n**: Yield: 1.61 g, 22%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 10.16 (s, 1H, C5-H_{trz}), 9.24 (s, 1H, C3-H_{trz}), 4.39 (q, J = 7.3 Hz, 2H, N4-CH_2CH$_3$), 4.28 (q, J = 7.3 Hz, 2H, N1-CH_2CH$_3$), 1.47 (t, J = 7.3 Hz, 6H, CH$_2$$CH_3$). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 144.8 (C5$_{trz}$), 142.4 (C3$_{trz}$), 47.6 (N4-CH_2CH$_3$), 43.5(N1-CH_2CH$_3$), 14.9 (N4-CH$_2$$CH_3$) 14.1 (N1-CH$_2$$CH_3$). HRESI-MS: [$C_6H_{12}N_3^+$] *m/z* = 126.1023 calcd. = 126.1026.

Compounds **2a – 2c** were prepared using slightly modified procedures from Zhao and co-workers.[2] **2a.** A mixture of 1-ethyl-imidazole **1h** (200 mg, 2.08 mmol) and dibromoethane (0.18 mL, 4.81 mmol) in acetonitrile (10 mL) was heated at reflux for 24 h. The off-white precipitate was collected followed by washing with acetonitrile and dried under vacuum to obtain the pure product as a white solid. Yield: 264 mg, 67%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 9.32 (s, 2H, C2-H$_{im}$), 7.86 (s, 4H, C4-H$_{im}$), 7.71 (s, 4H, C5-H$_{im}$), 4.75 (s, 4H, CH_2CH_2), 4.21 (q, J = 7.3 Hz, 4H, N1-CH_2CH$_3$), 1.41 (t, J = 7.3 Hz, N3-CH$_2$$CH_3$). ^{13}C-NMR (100.62 MHz, DMSO-d_6) δ 136.9 (C2$_{im}$), 123.0 (C4$_{im}$), 122.9 (C5$_{im}$), 48.9 (C$_{ethylene}$), 44.9 (CH_2CH$_3$), 15.4 (CH$_2$$CH_3$). HRESI-MS: [$C_{12}H_{20}N_4^{2+}$] *m/z* = 110.0702 calcd. = 110.0839.

2b. In a sealed tube, a mixture of 1-ethyl-1,2,4-triazole **1j** (500 mg, 5.15 mmol) and dibromoethane (0.89 mL, 10.30 mmol) was stirred at 120 °C for 4 h. The resultant solid was collected followed by washing with acetonitrile (10 mL) to obtain the pure product as a white solid. Yield: 226 mg, 23%. ^{1}H-NMR (400.13 MHz, DMSO-d_6) δ 10.21 (s, 2H, C5-H_{trz}), 9.19 (s, 2H, C3-H_{trz}), 4.85 (s, 4H, N4-CH_2CH_2), 4.43 (q, J = 7.2 Hz, 4H, N1-CH_2CH$_3$), 1.57 – 1.42 (m, 6H, N1-CH$_2$$CH_3$). ^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 145.1 (C5$_{trz}$), 143.0 (C3$_{trz}$), 47.8 (C$_{ethylene}$). 47.0 (CH_2CH$_3$), 14.0 (CH$_2$$CH_3$). HRESI-MS: [$C_{10}H_{18}N_6^{2+}$] *m/z* = 111.0746 calcd. = 111.0791.

2c. This compound was prepared using the same methods as **2b** from **1i** (400 mg, 4.81 mmol), and dibromoethane (0.42 mL, 4.82 mmol), producing a white powder. Yield: 203 mg, 24%. ^{1}H-NMR

(400.13 MHz, DMSO-d_6) δ 10.13 (s, 5H C5-H_{trz}), 9.17 (s, 2H C3-H_{trz}), 4.85 (s, 4H, N4-CH_2CH_2), 4.10 (s, 6H, CH_3).^{13}C-NMR (125.77 MHz, DMSO-d_6) δ 145.1 (C5$_{trz}$), 143.8 (C3$_{trz}$), 47.1 (C$_{ethylene}$) 19.0 (C-CH_3). HRESI-MS: [$C_8H_{14}N_6^{2+}$] *m/z* = 97.0756 calcd. = 97.0635.

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

Figure S10. ^{1}H-NMR spectrum of compound **1a** ($CDCl_3$).

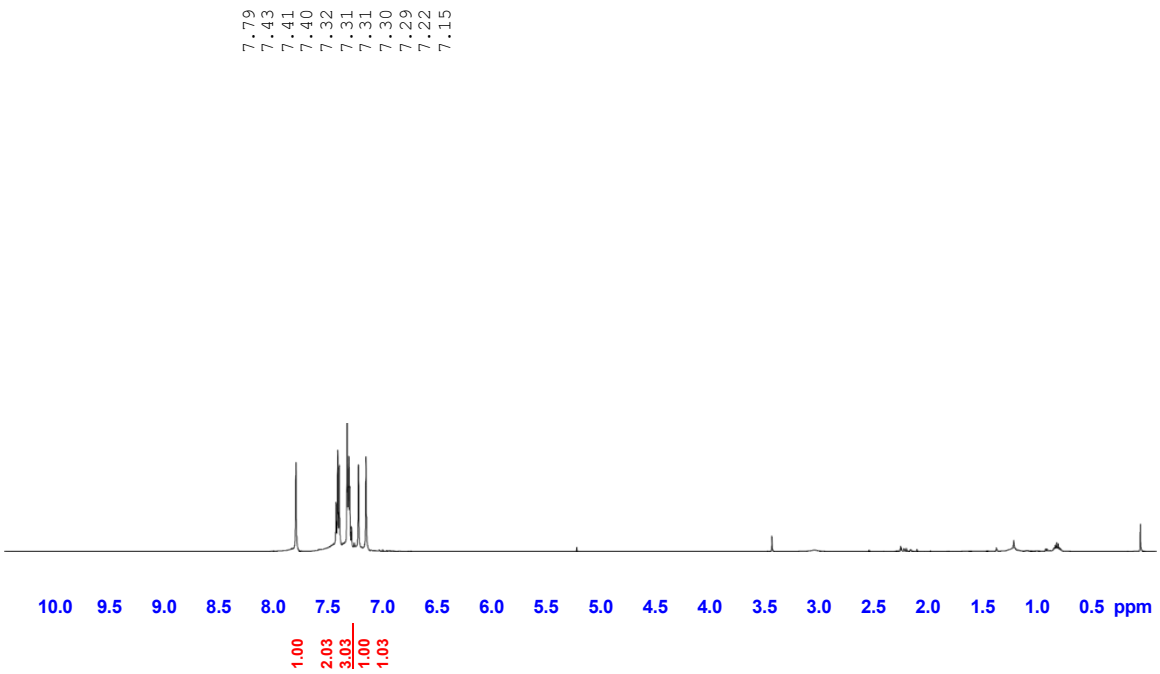

7.79
7.43
7.41
7.40
7.32
7.31
7.31
7.30
7.29
7.22
7.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.03
3.03
1.00
1.03

Figure S11. ^{13}C-NMR spectrum of compound **1a** ($CDCl_3$).

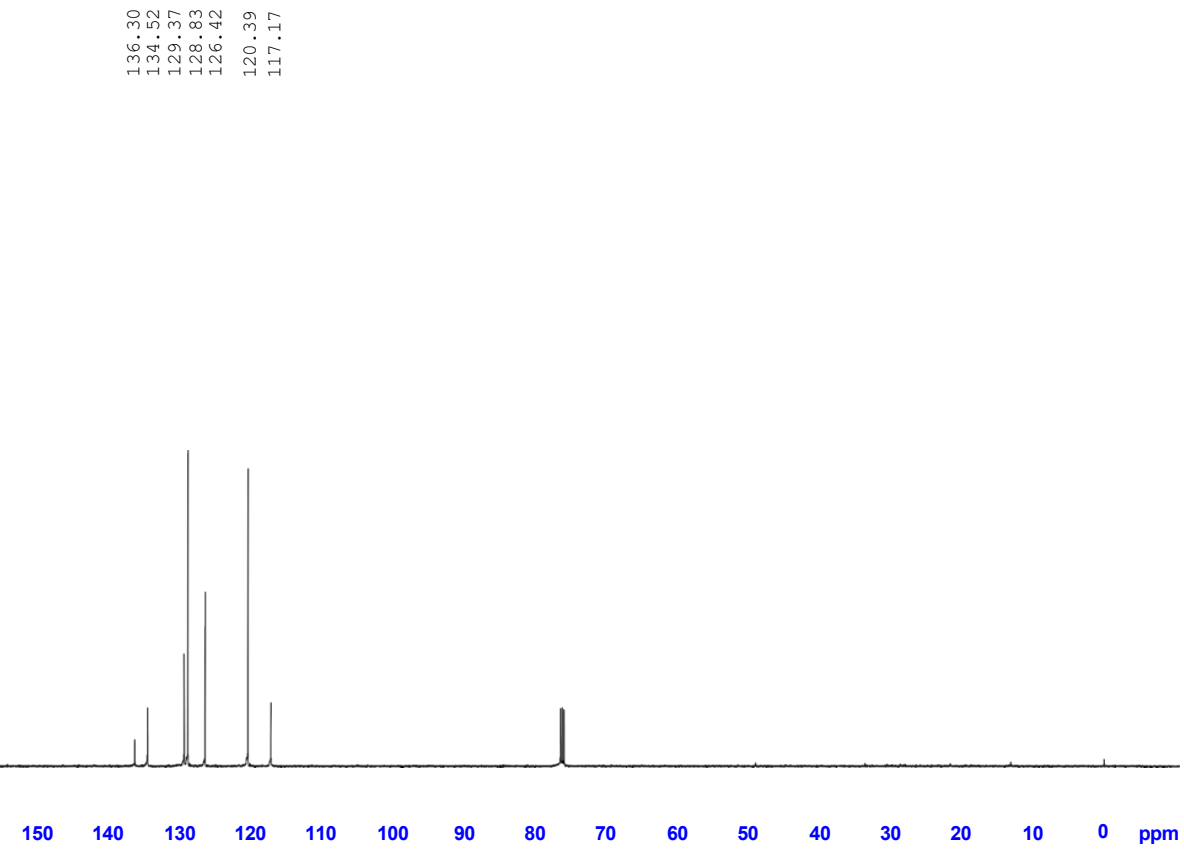


Figure S12. ^{1}H-NMR spectrum of compound **1b** (DMSO-d_6).

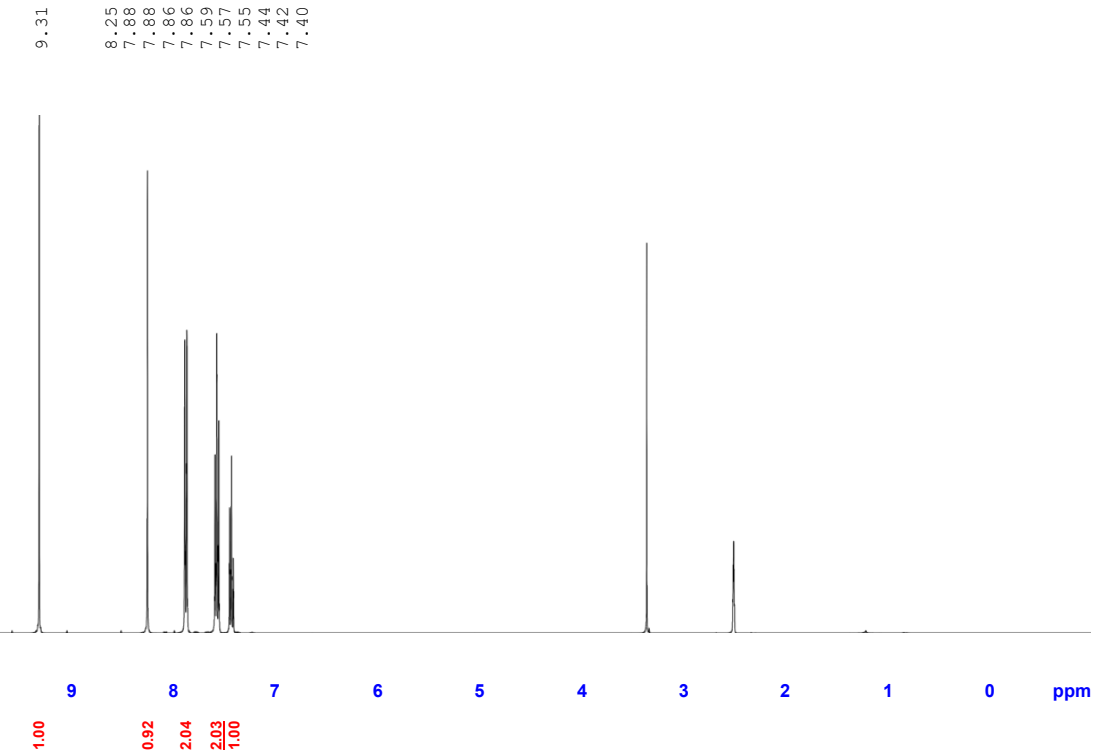


Figure S13. ^{13}C-NMR spectrum of compound **1b** (DMSO-d_6).

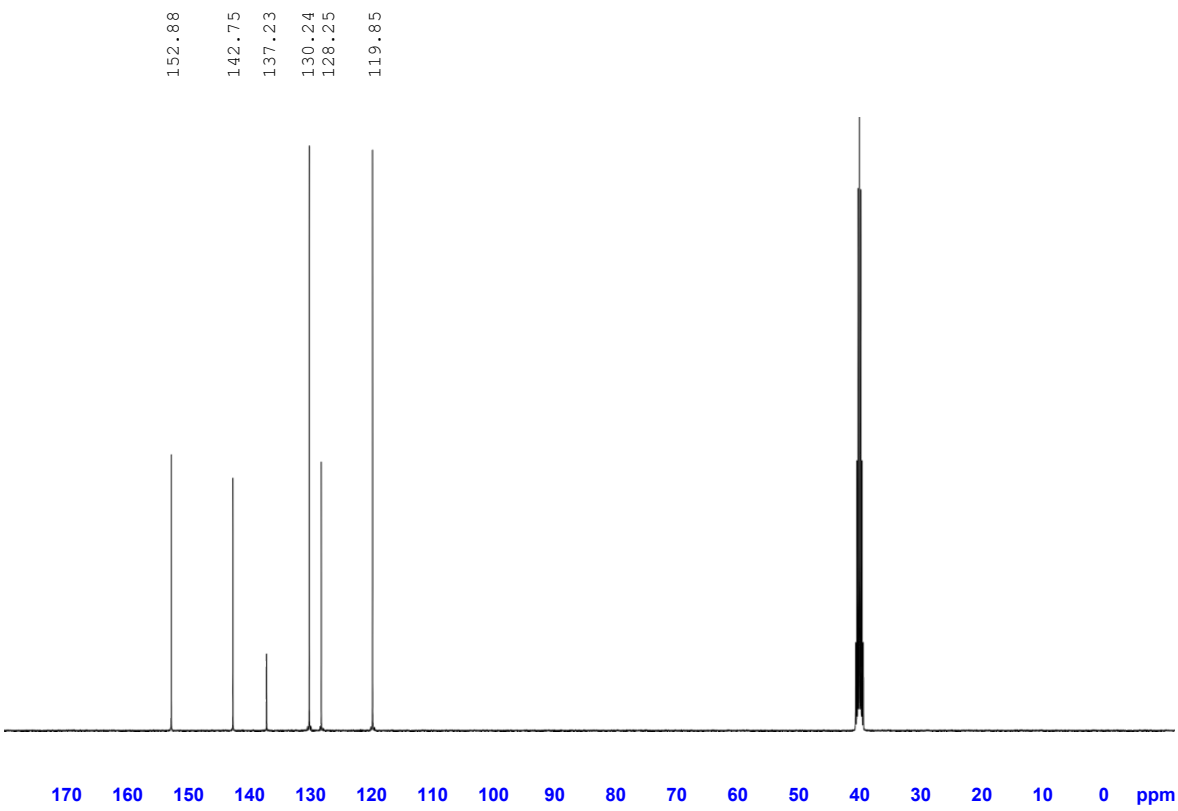

152.88
142.75
137.23
130.24
128.25
119.85
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Figure S14. ^{1}H-NMR spectrum of compound **1c** ($CDCl_3$).

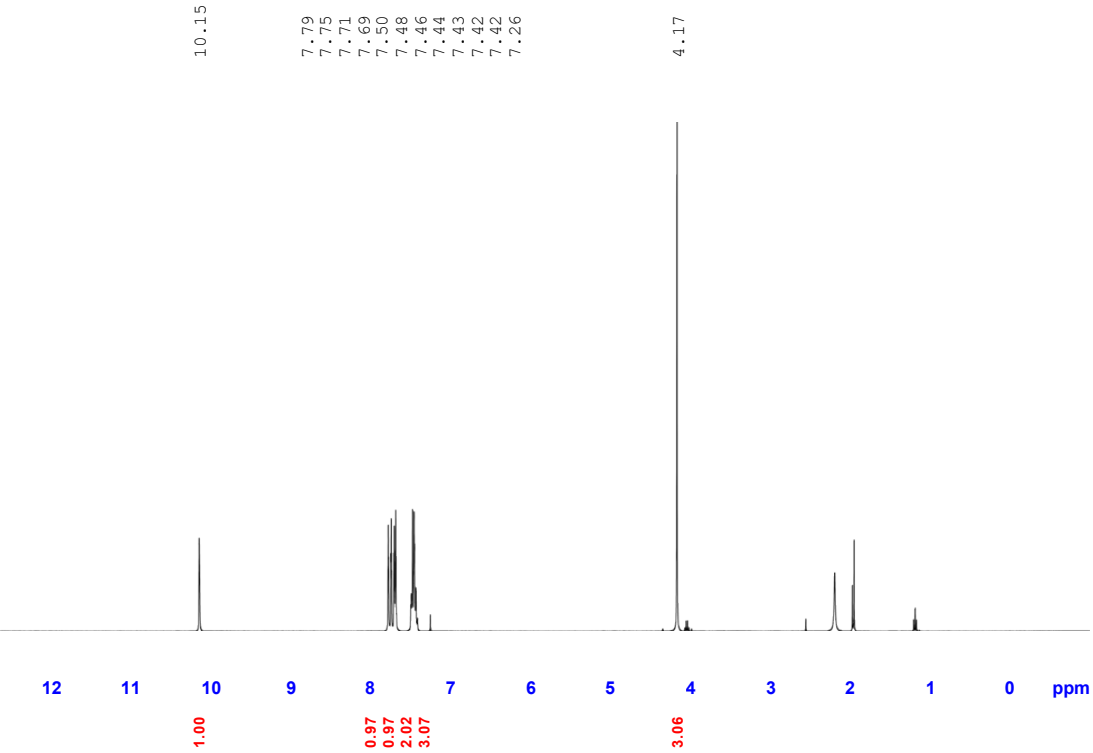


Figure S15. ^{13}C-NMR spectrum of compound **1c** (DMSO-d_6).

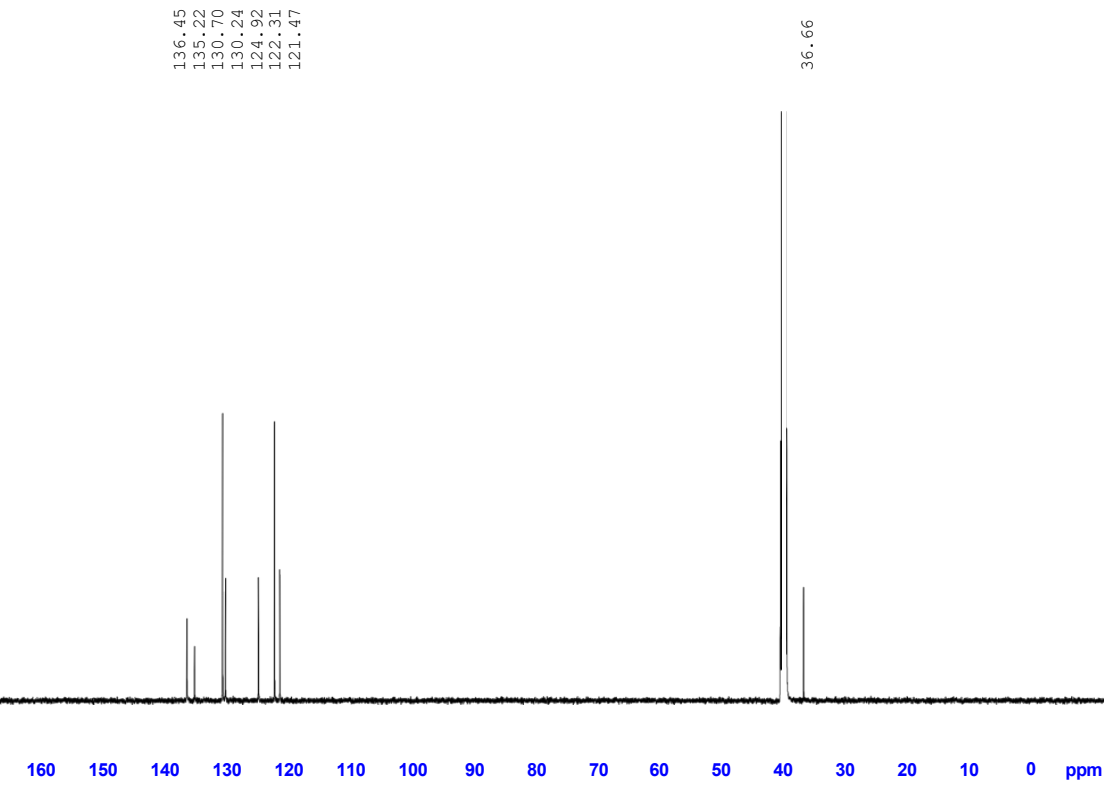


Figure S16. ^{1}H-NMR spectrum of compound **1d** ($CDCl_3$).

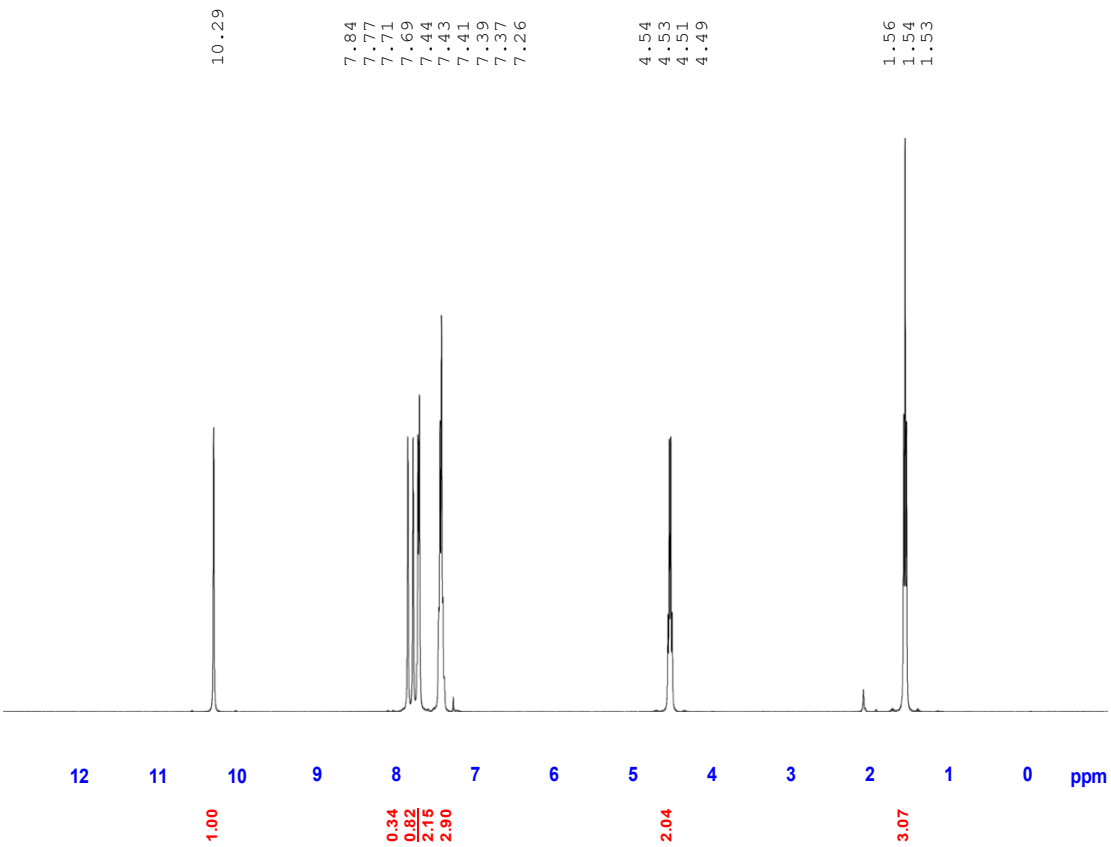


Figure S17. ^{13}C-NMR spectrum of compound **1d** (DMSO-d_6).

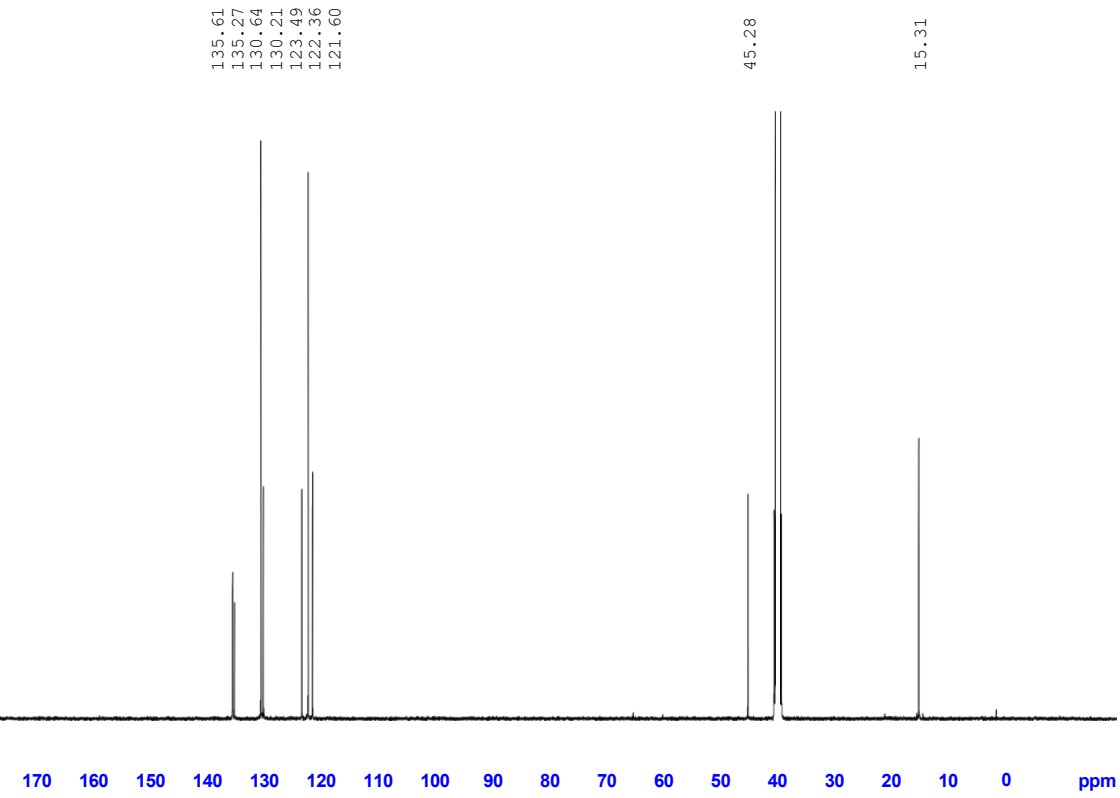

135.61
135.27
130.64
130.21
123.49
122.36
121.60
45.28
15.31
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

Figure S18. ^{1}H-NMR spectrum of compound **1e** ($CDCl_3$).

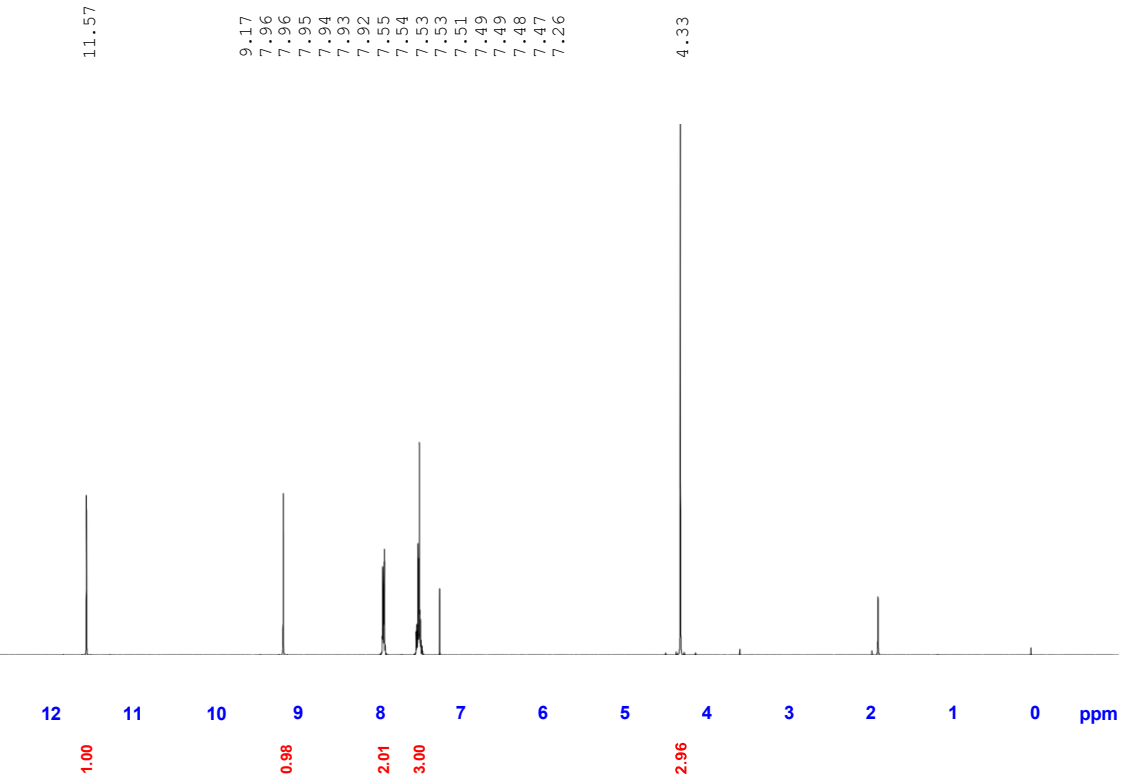


Figure S19. ^{13}C-NMR spectrum of compound **1e** ($CDCl_3$).

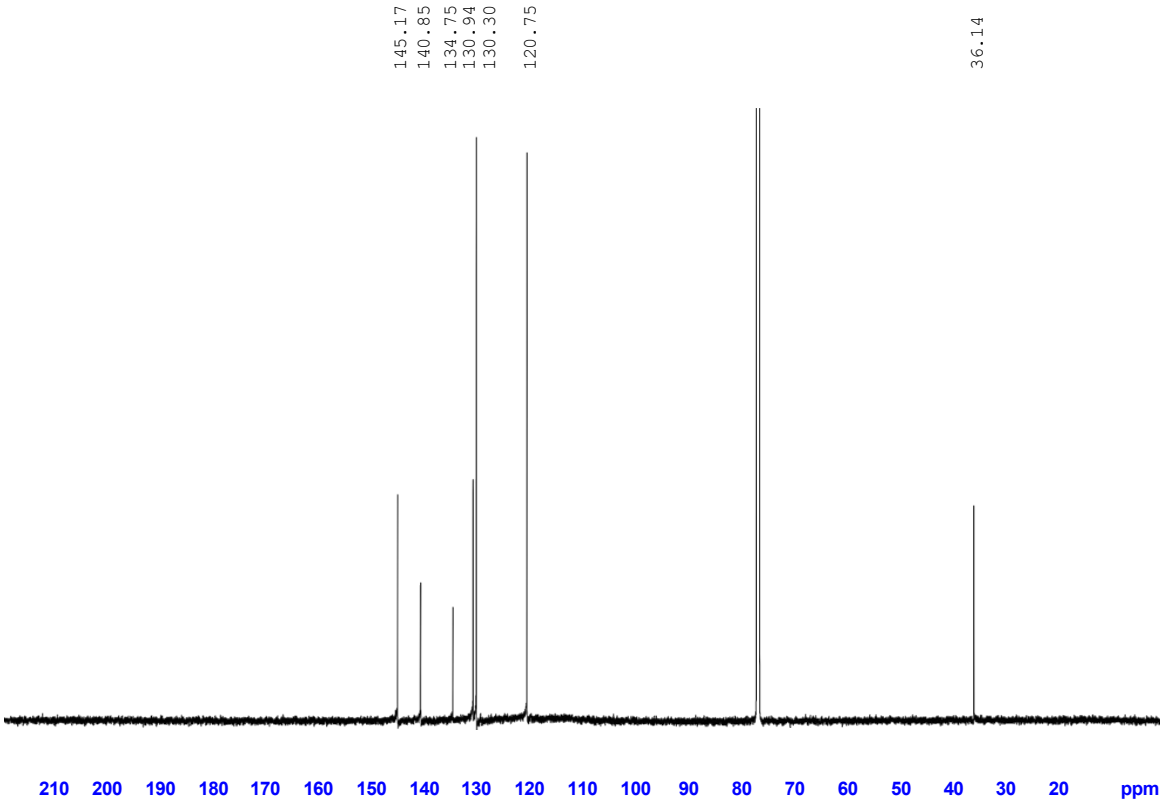


Figure S20. ^{1}H-NMR spectrum of compound **1f** ($CDCl_3$).

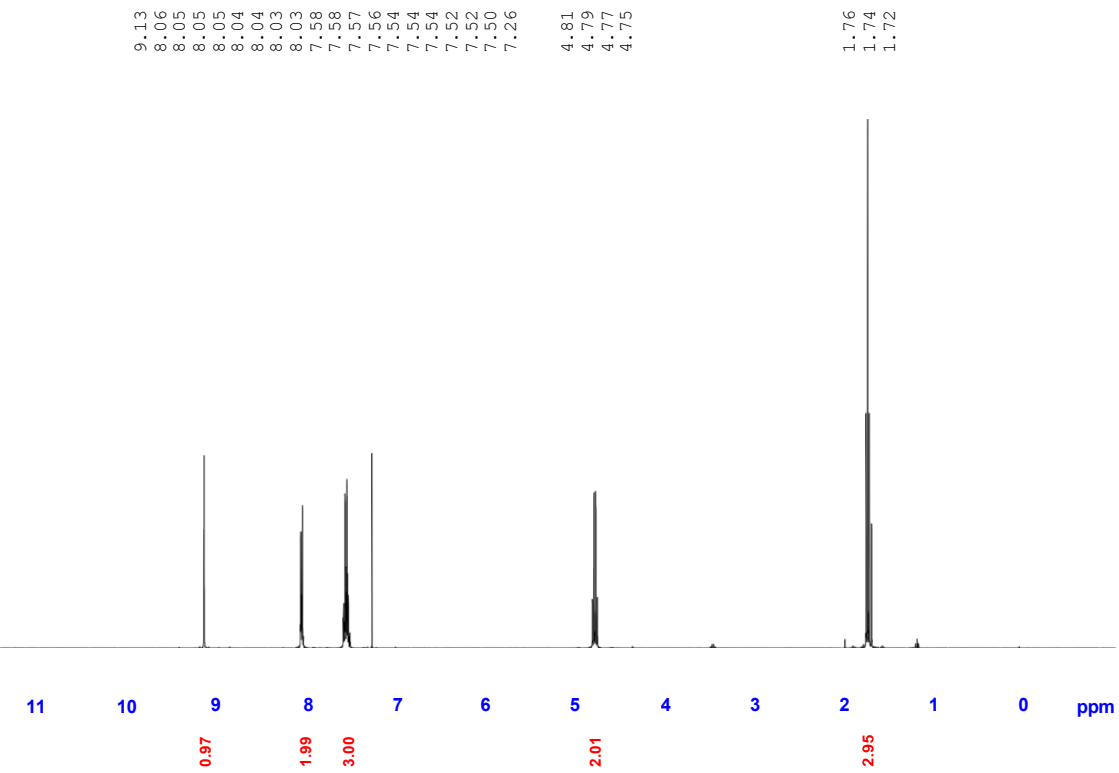


Figure S21. ^{13}C-NMR spectrum of compound **1f** ($CDCl_3$).

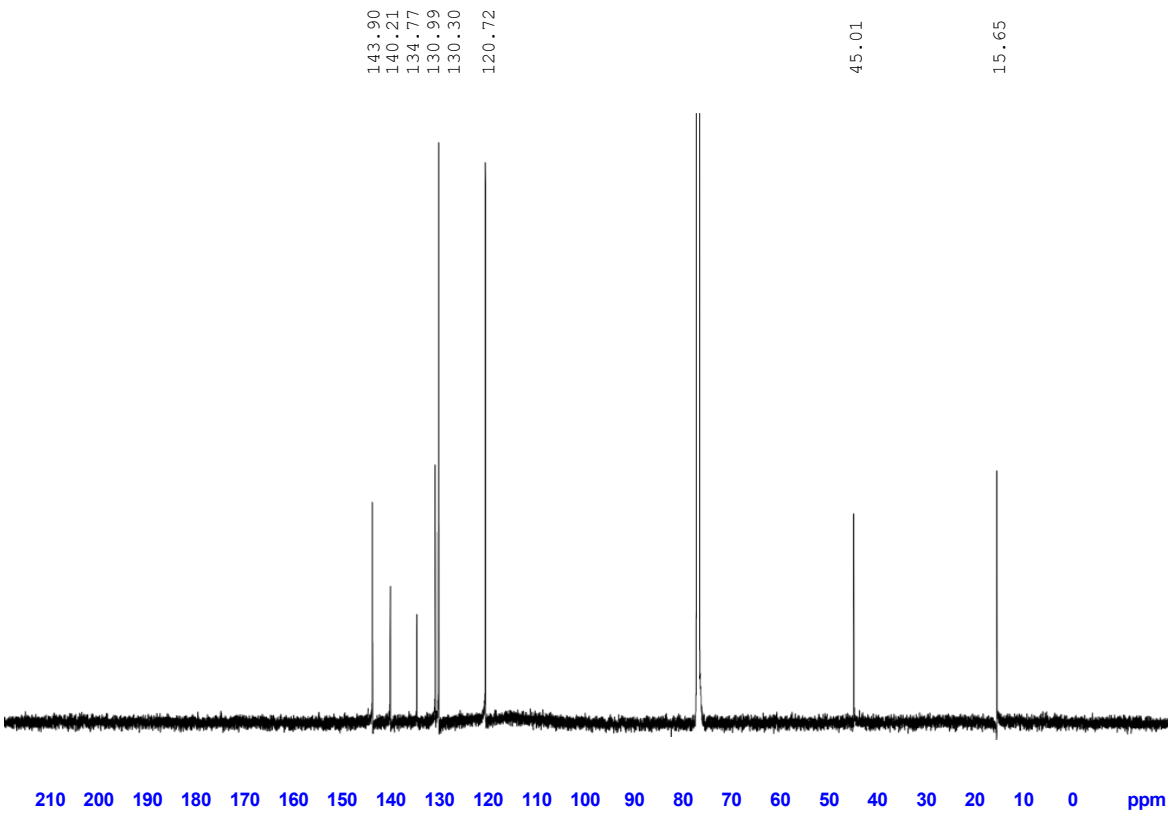

143.90
140.21
134.77
130.99
130.30
120.72
45.01
15.65
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Figure S22. ^{1}H-NMR spectrum of compound **1g** (DMSO-d_6).

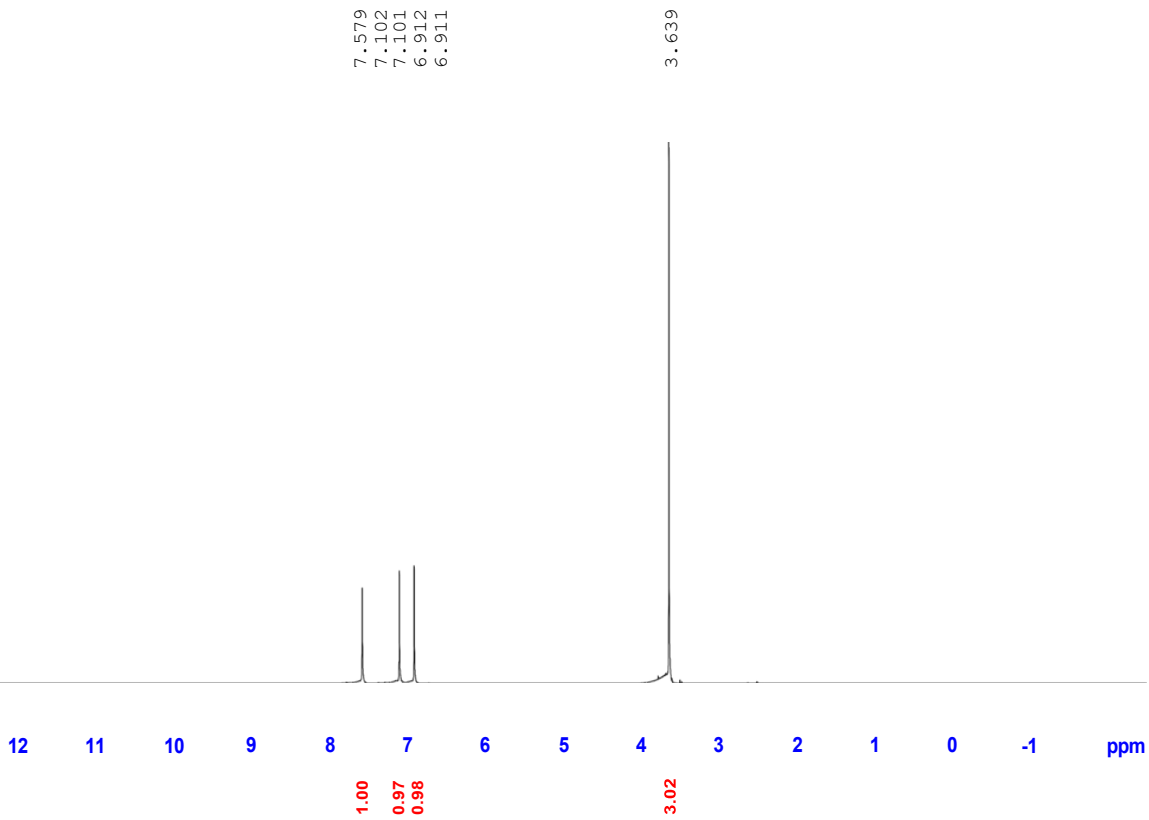


Figure S23. ^{13}C-NMR spectrum of compound **1g** (DMSO-d_6).

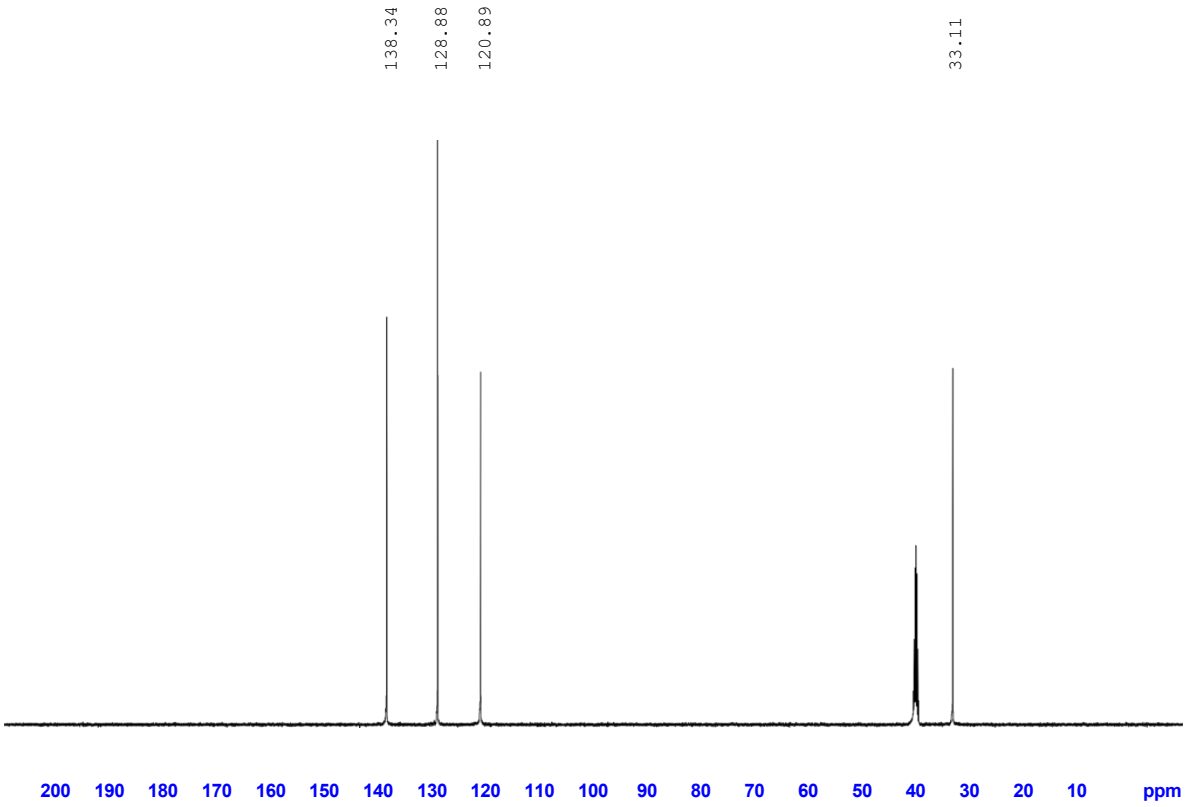


Figure S24. ^{1}H-NMR spectrum of compound **1h (**DMSO-d_6).

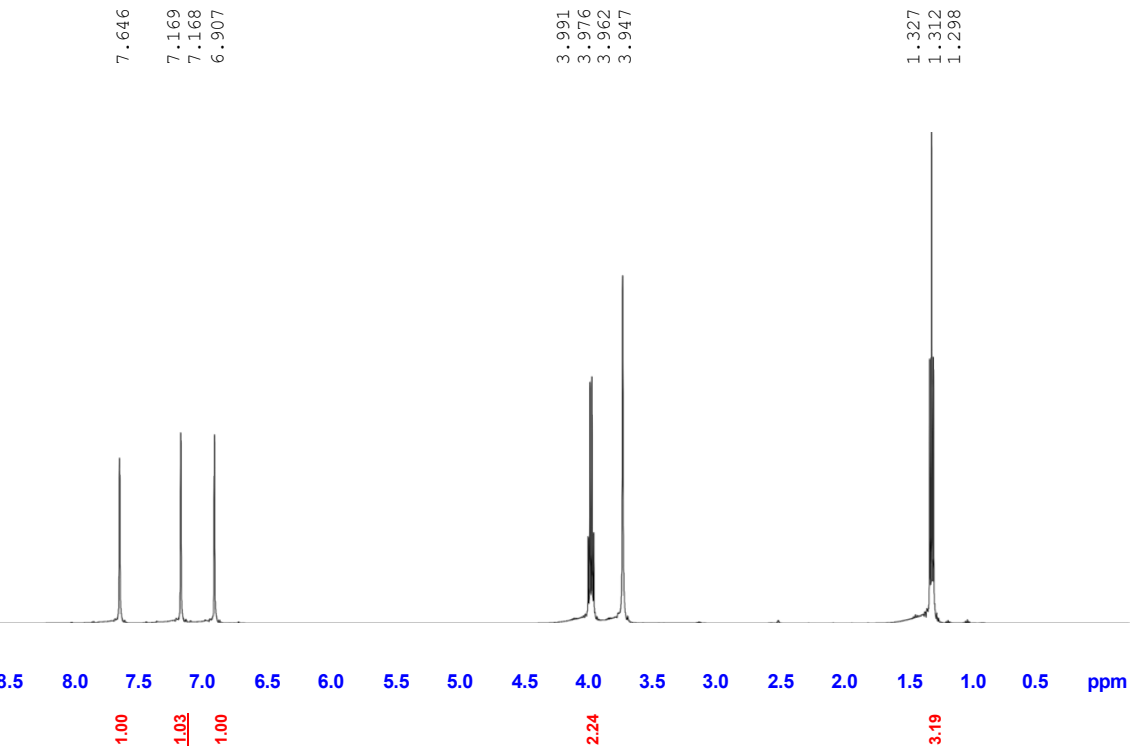


Figure S25.[13]C-NMR spectrum of compound **1h (**DMSO-d_6).

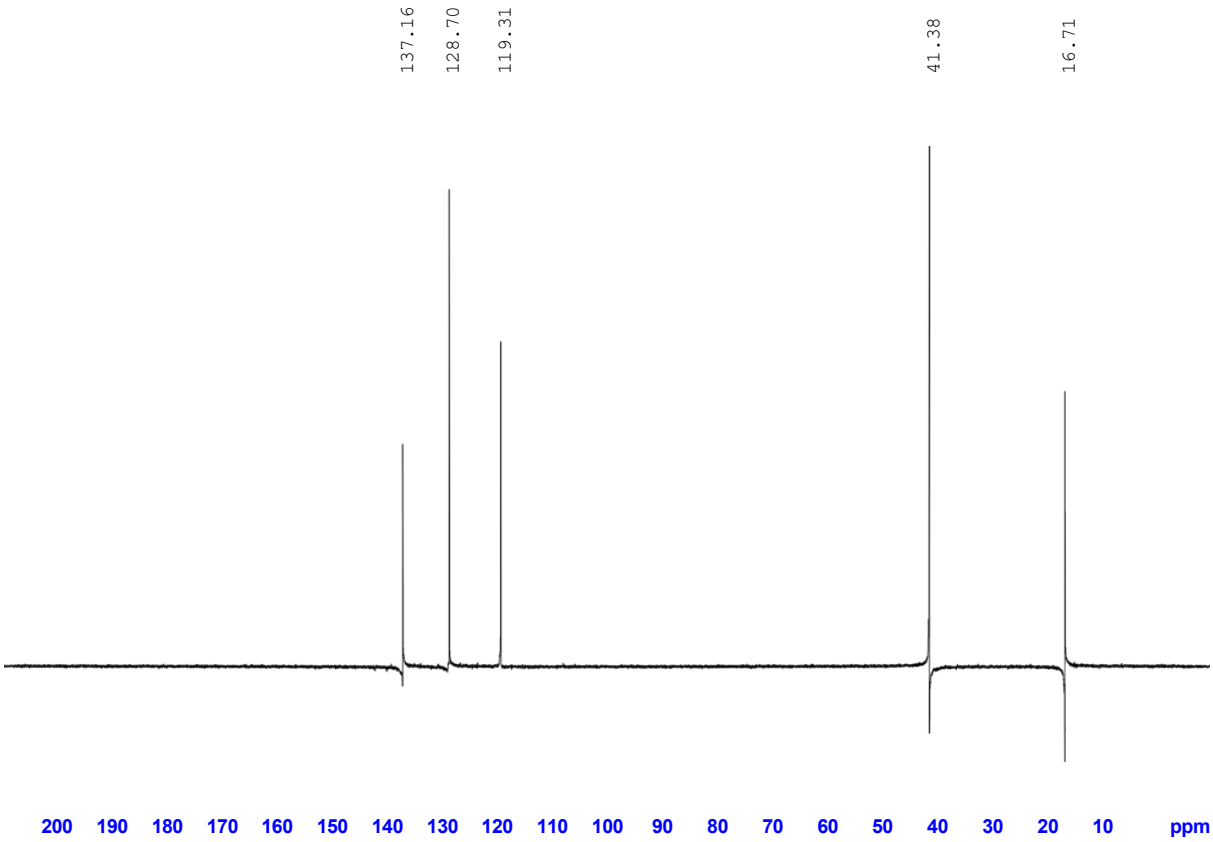


Figure S26. ^{1}H-NMR spectrum of compound **1i (**DMSO-d_6).

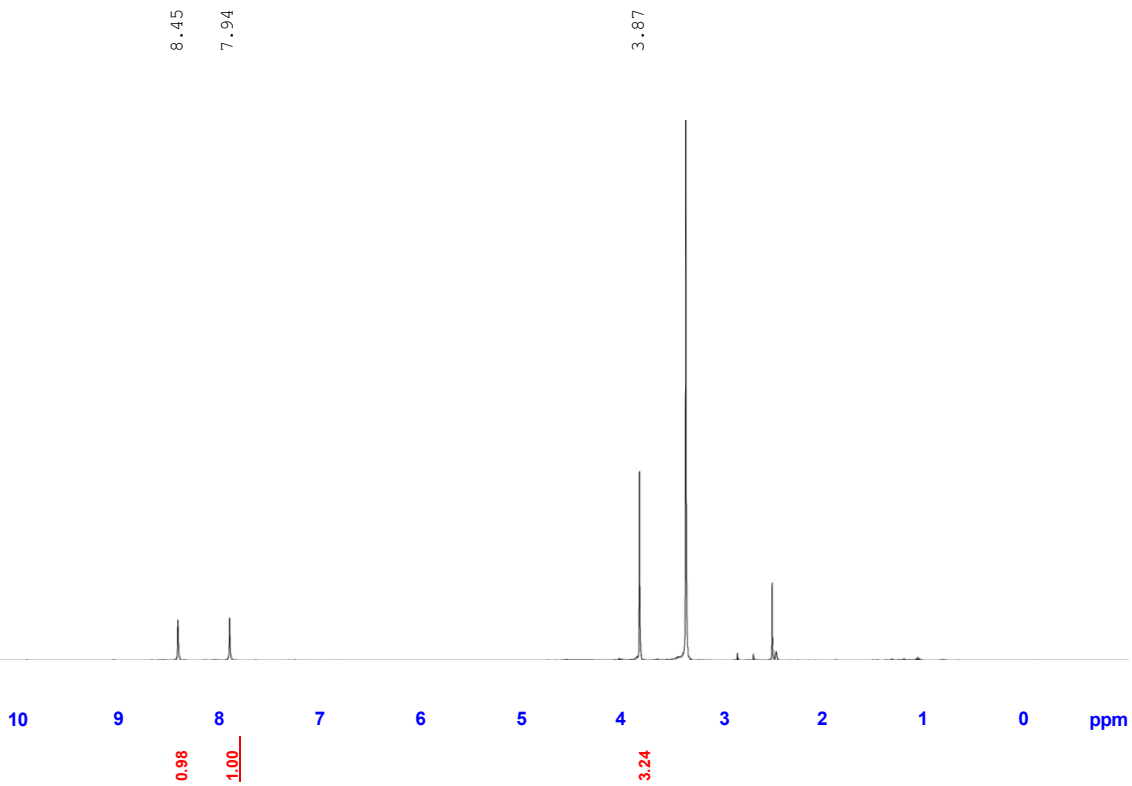


Figure S27. ^{13}C-NMR spectrum of compound **1i (**DMSO-d_6).

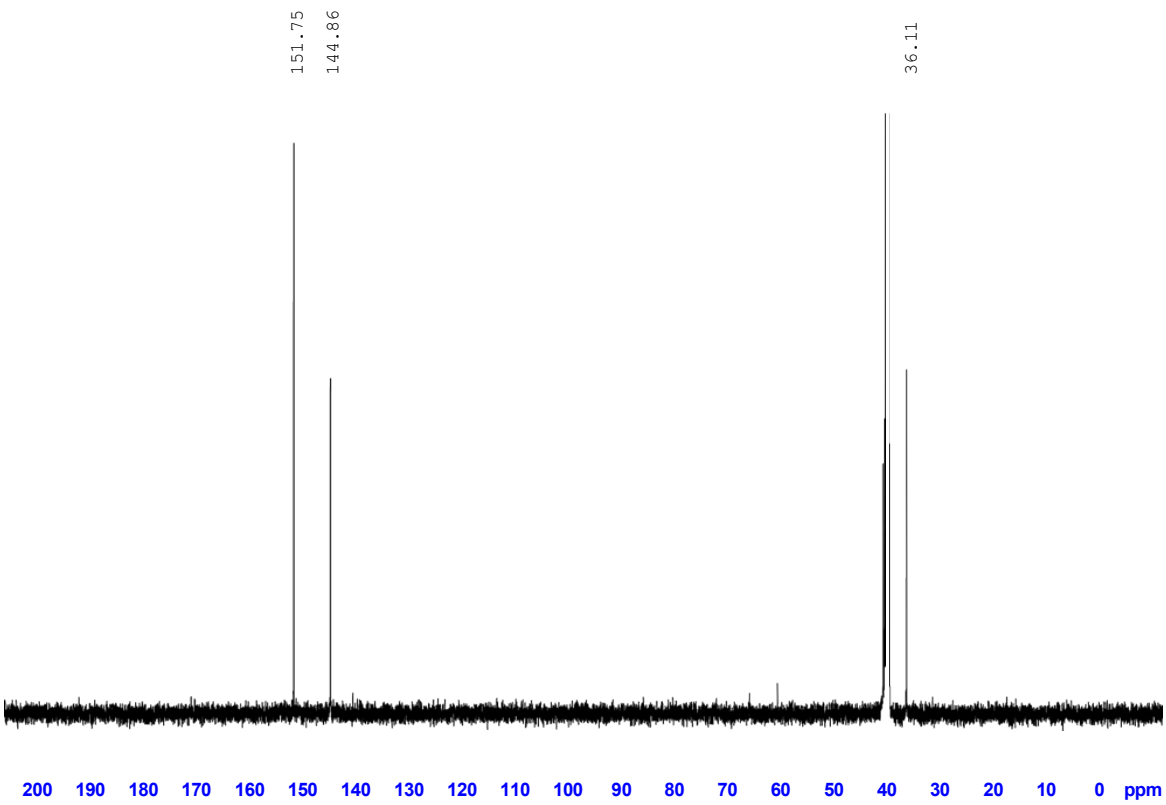

151.75
144.86
36.11
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Figure S28. ^{1}H-NMR spectrum of compound **1j** (DMSO-d_6).

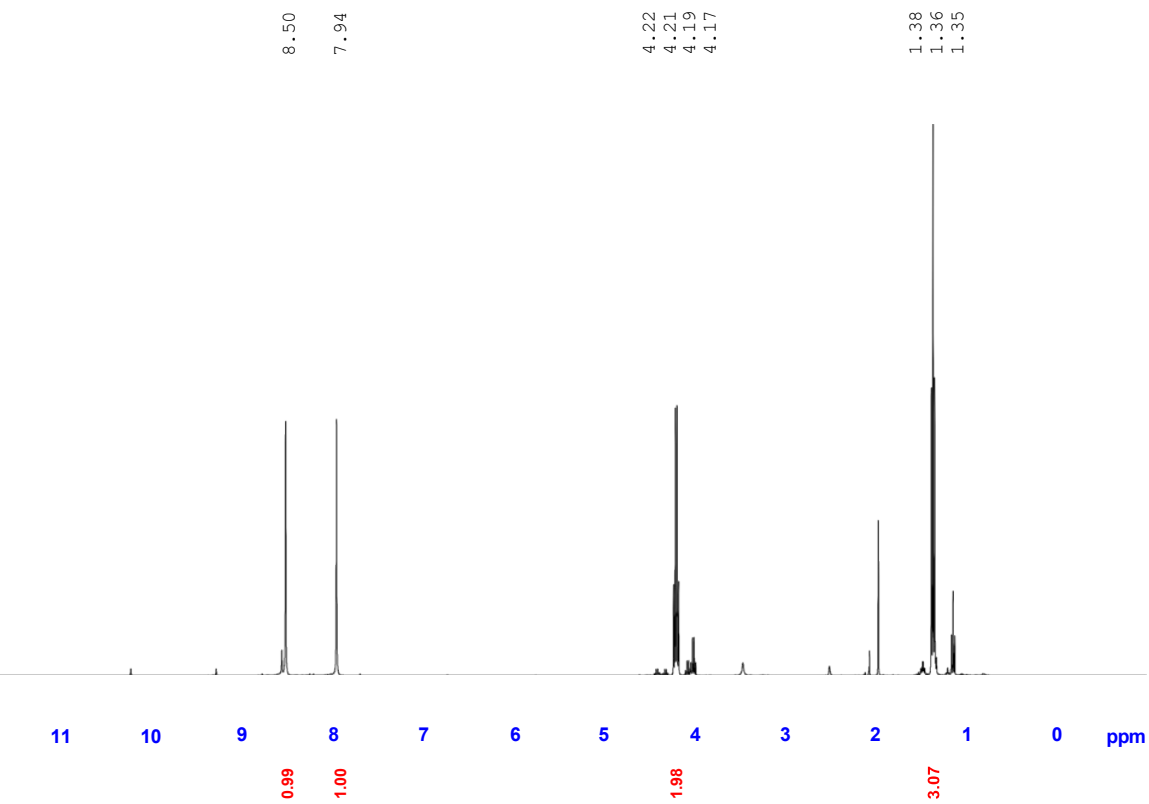


Figure S29. ^{13}C-NMR spectrum of compound **1j** (DMSO-d_6).

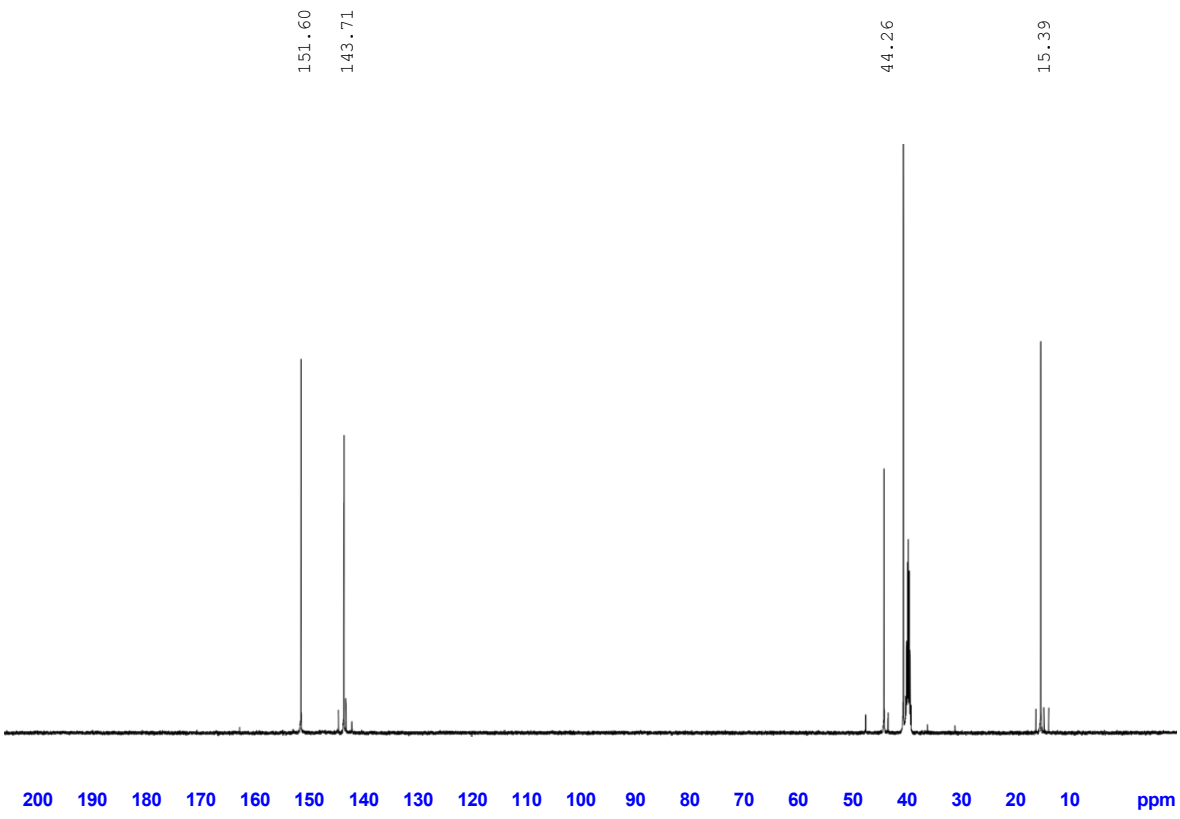

151.60
143.71
44.26
15.39
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Figure S30. ^{1}H-NMR spectrum of compound **1k (**DMSO-d_6).

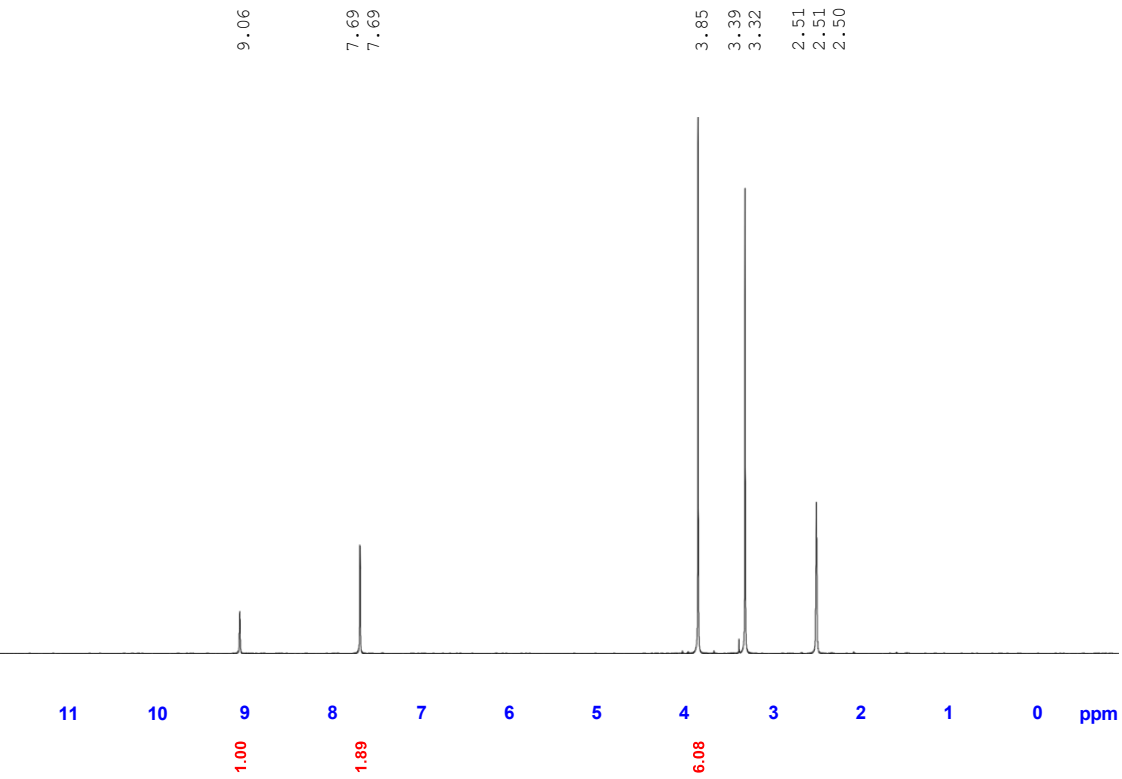


Figure S31. ^{13}C-NMR spectrum of compound **1k (**DMSO-d_6).

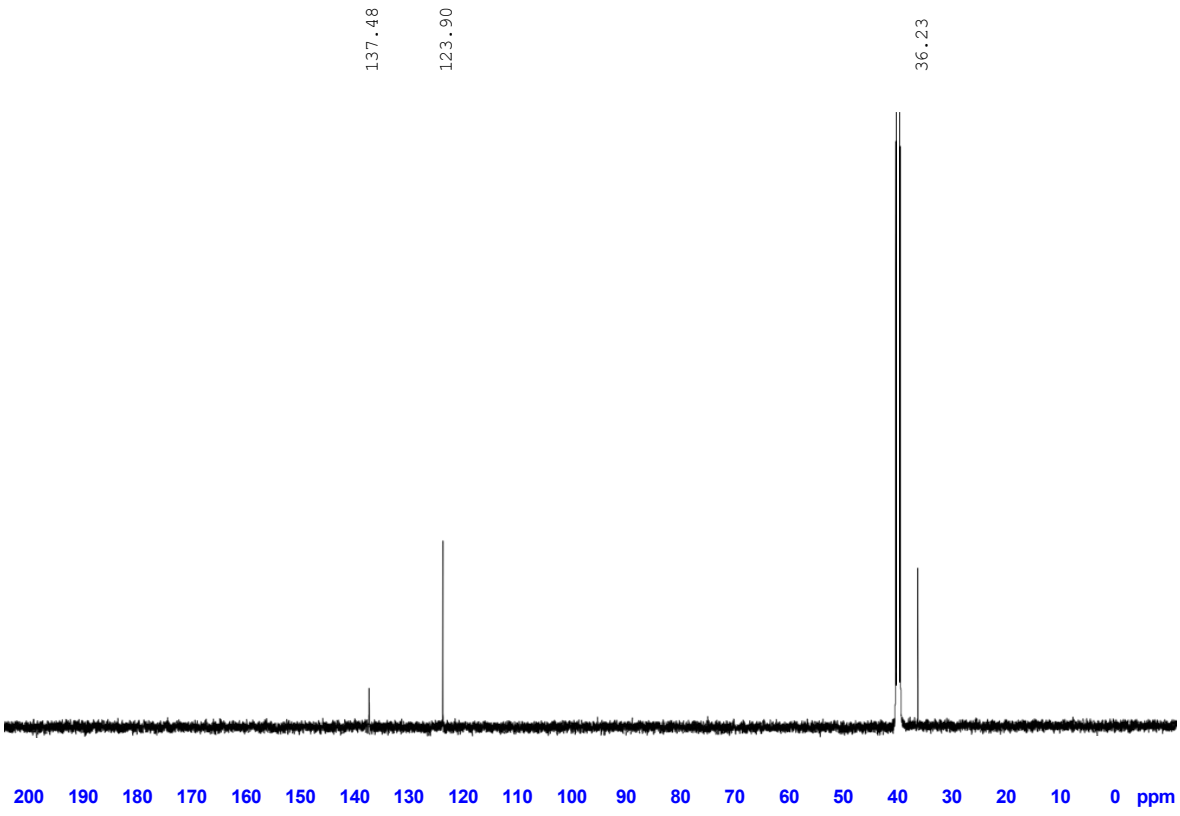


Figure S32. ^{1}H-NMR spectrum of compound **1l (**DMSO-d_6).

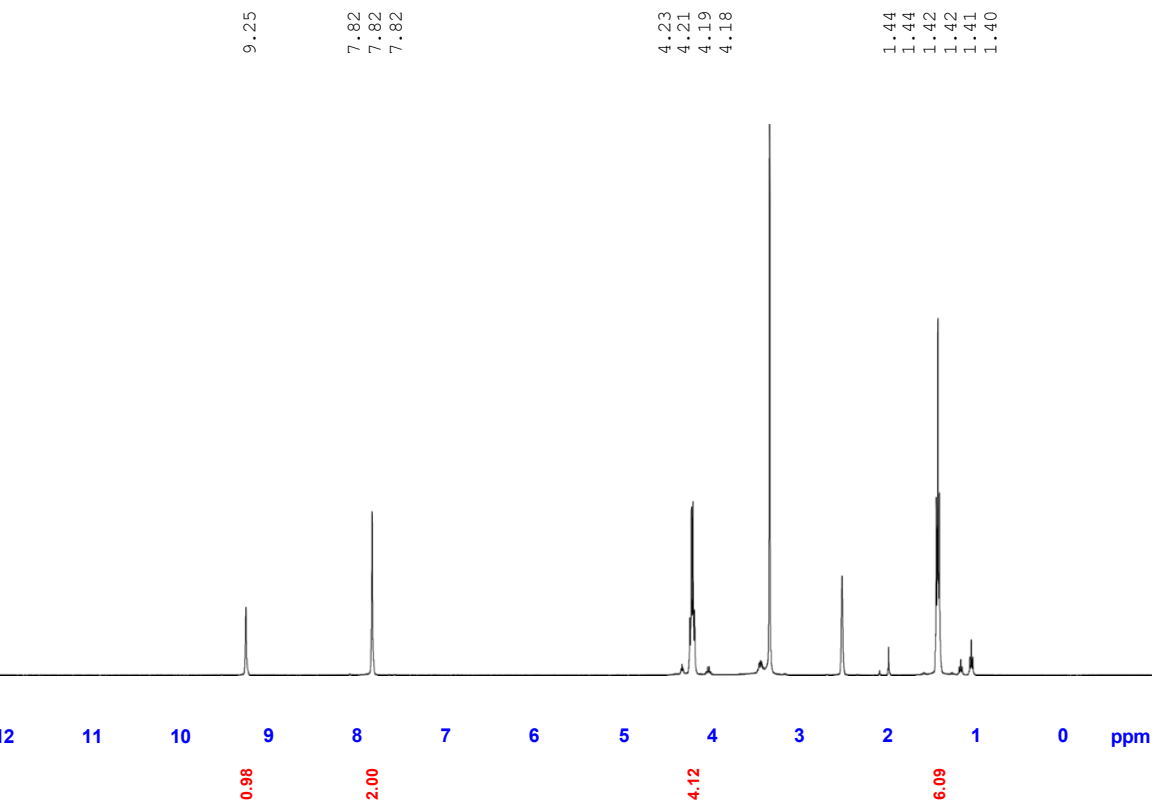


Figure S33. ^{13}C-NMR spectrum of compound **1l** (DMSO-d_6).

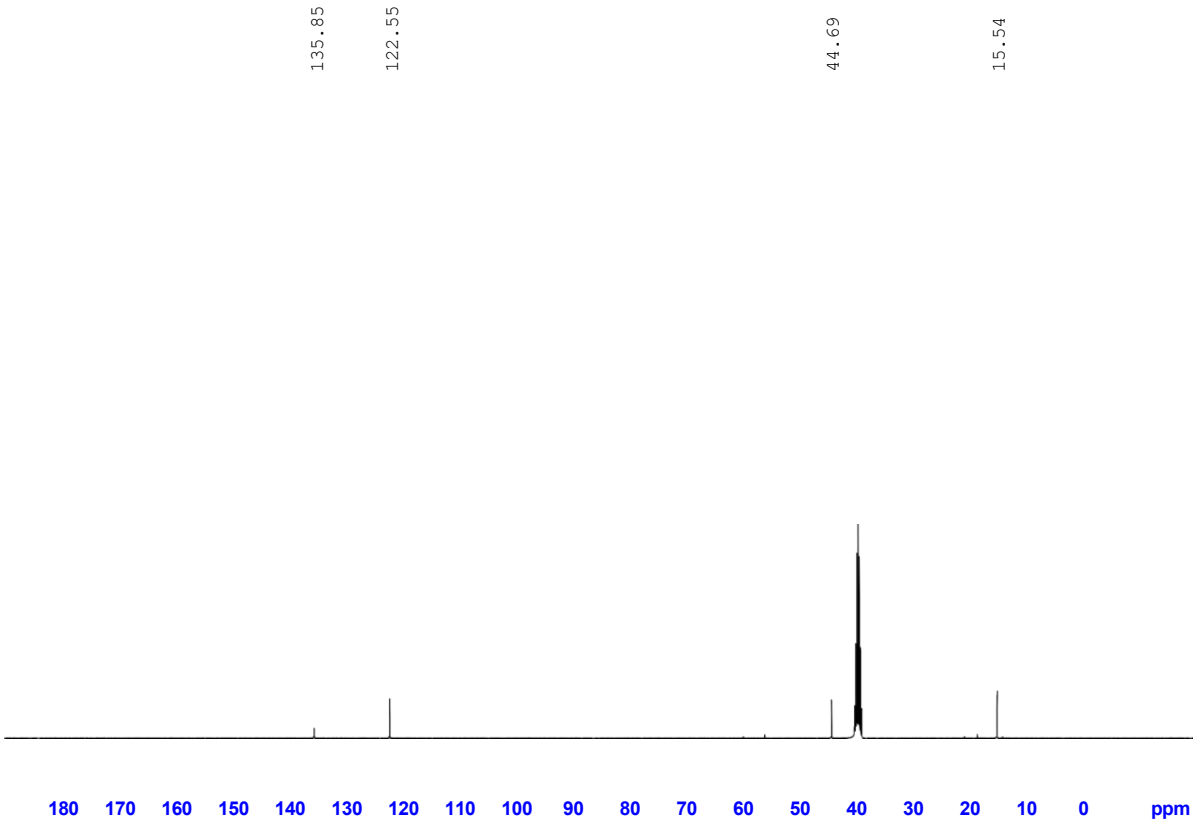


Figure S34. ^{1}H-NMR spectrum of compound **1m (**DMSO-d_6).

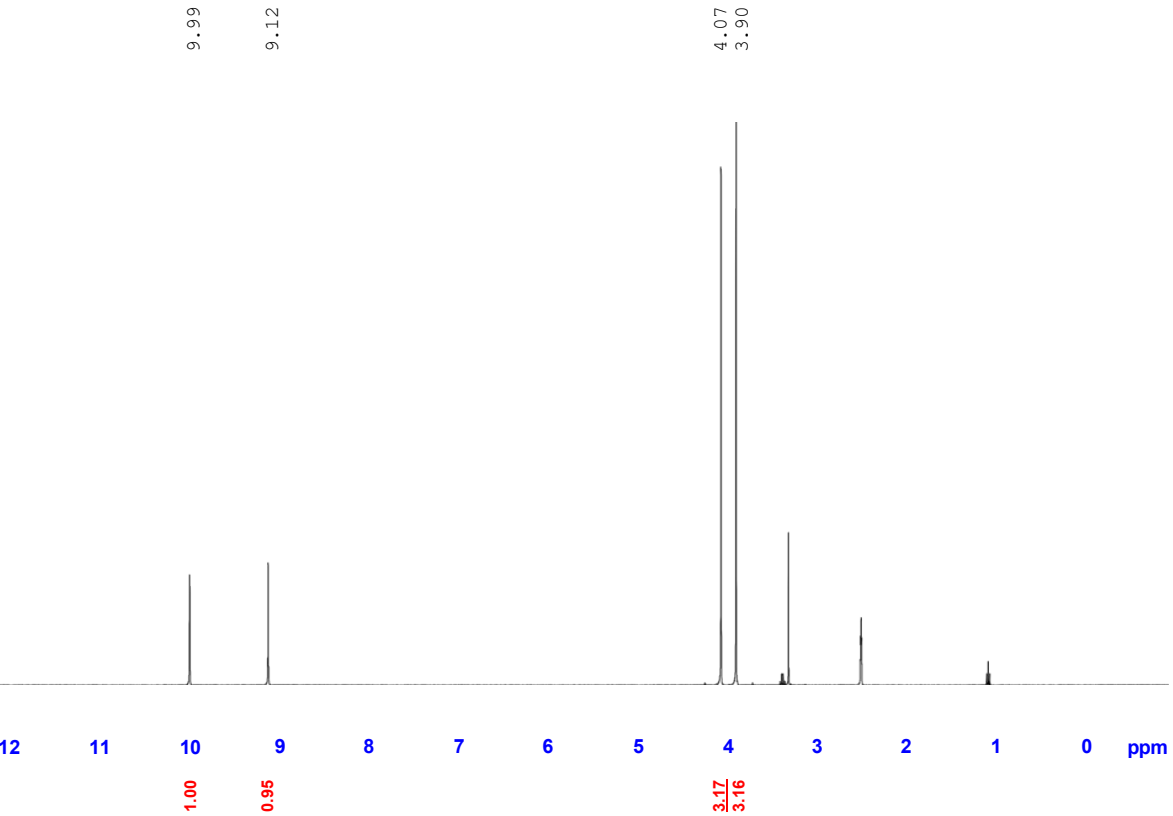


Figure S35. ^{13}C-NMR spectrum of compound **1m (**DMSO-d_6).

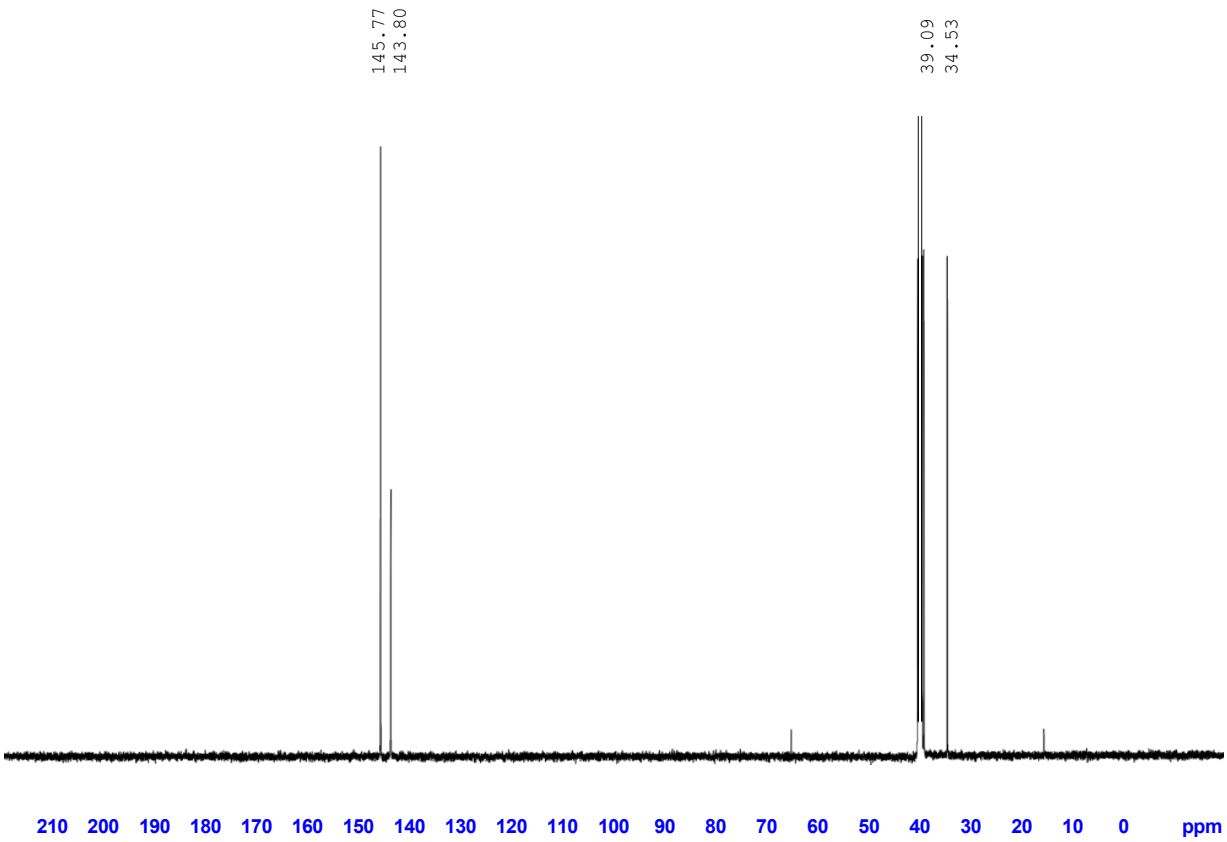

145.77
143.80
39.09
34.53
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Figure S36. ^{1}H-NMR spectrum of compound **1n (**DMSO-d_6).

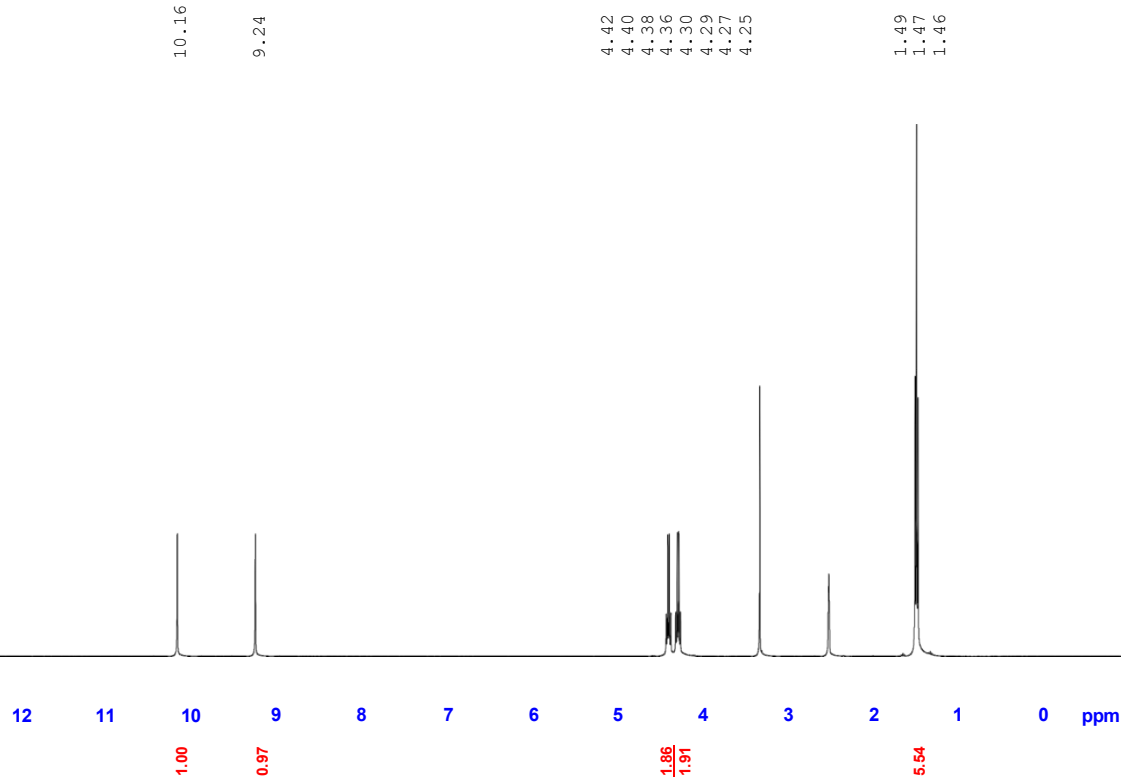


Figure S37. ^{13}C-NMR spectrum of compound **1n (**DMSO-d_6).

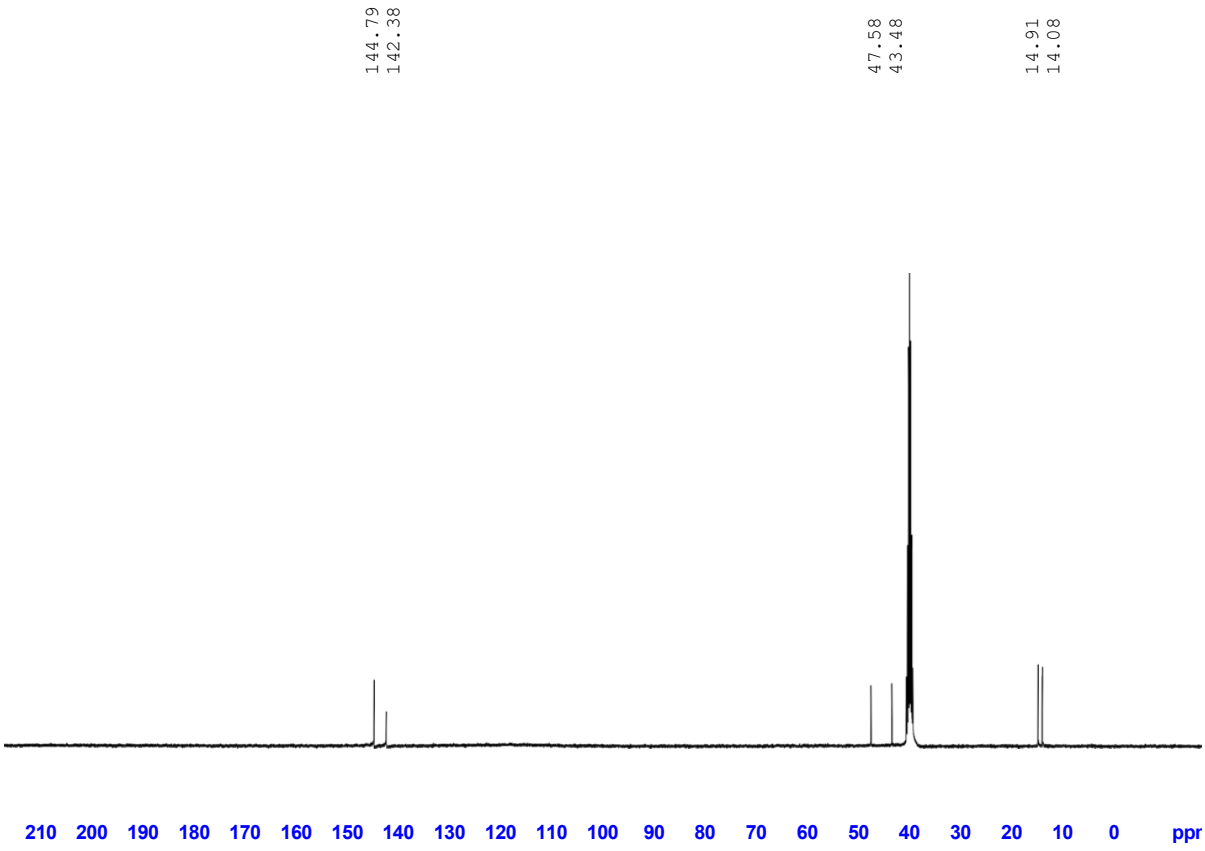


Figure S38. ^{1}H-NMR spectrum of compound **3a (**DMSO-d_6).

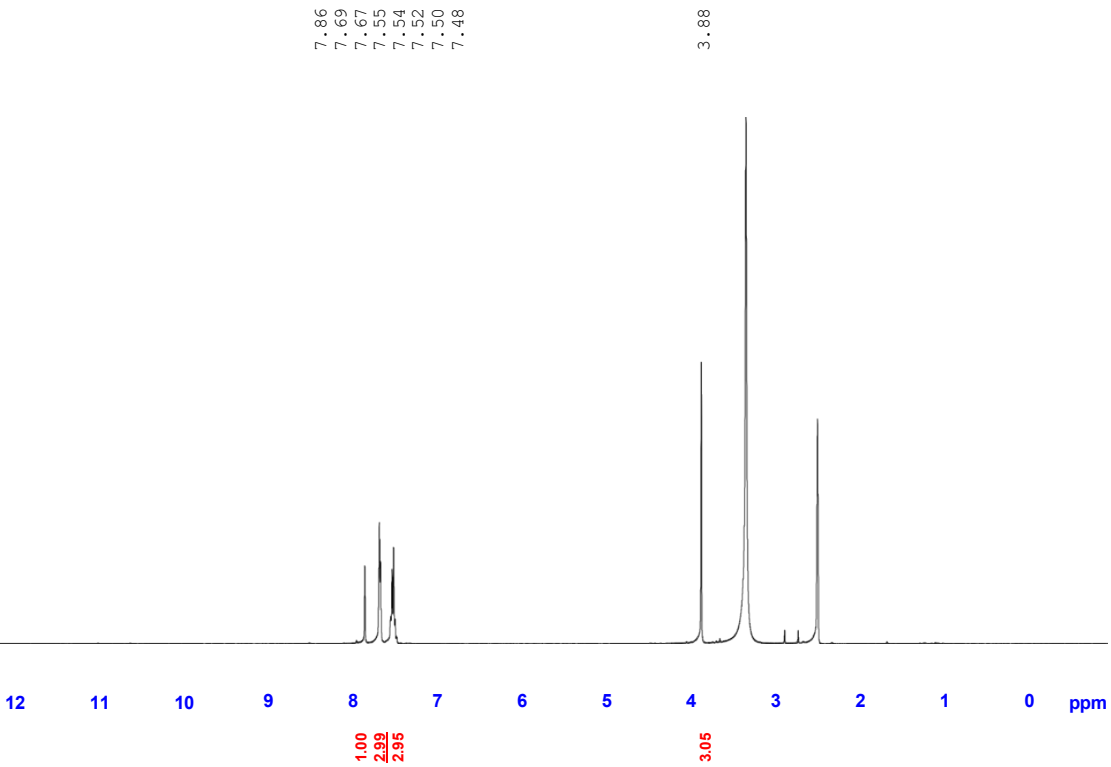

7.86
7.69
7.67
7.55
7.54
7.52
7.50
7.48
3.88
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.99
2.95
3.05

Figure S39. ^{13}C-NMR spectrum of compound **3a (**DMSO-d_6).

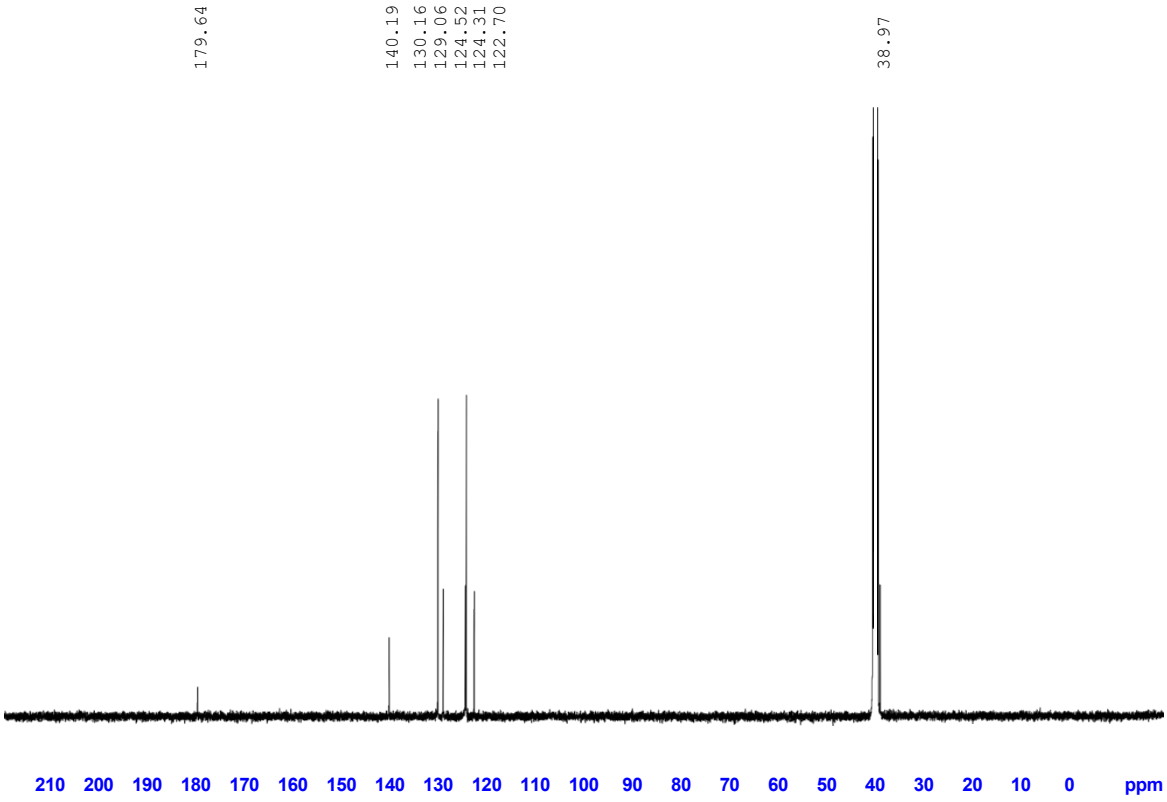


Figure S40. ^{1}H-NMR spectrum of compound **3b (**DMSO-d_6).

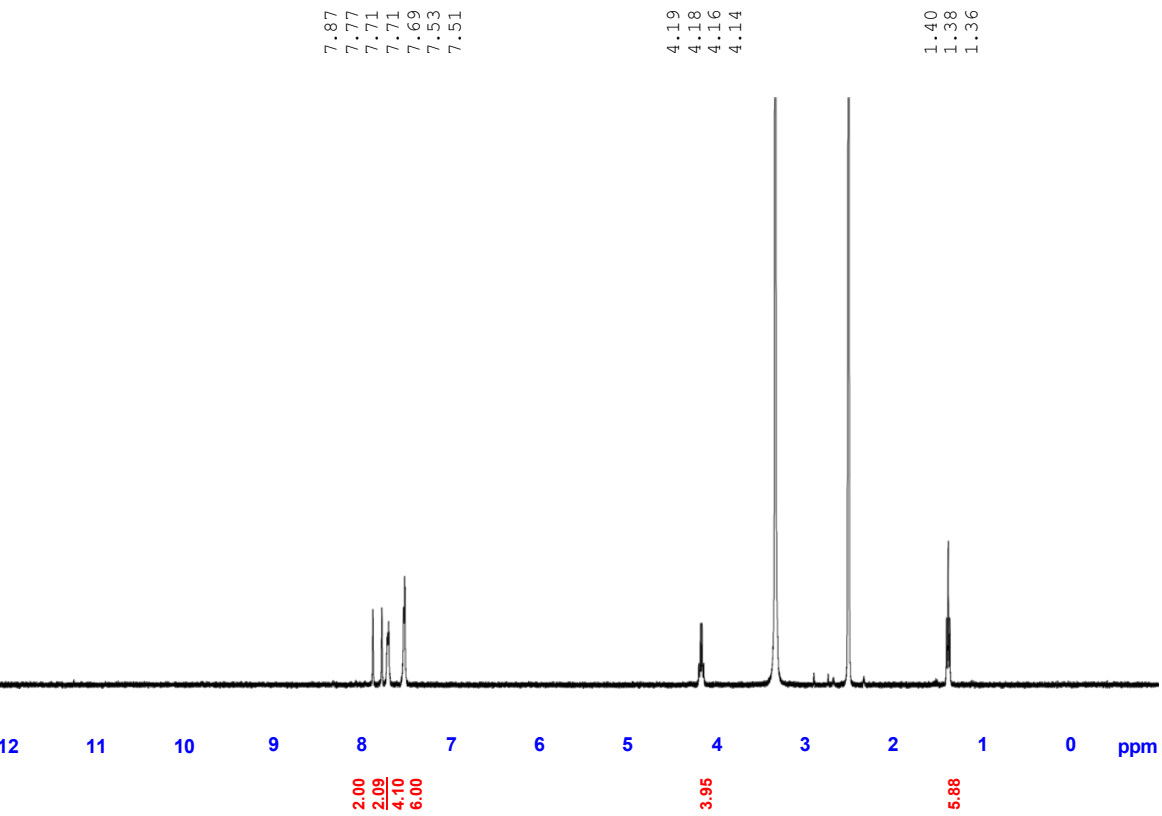


Figure S41. ^{13}C-NMR spectrum of compound **3b (**DMSO-d_6).

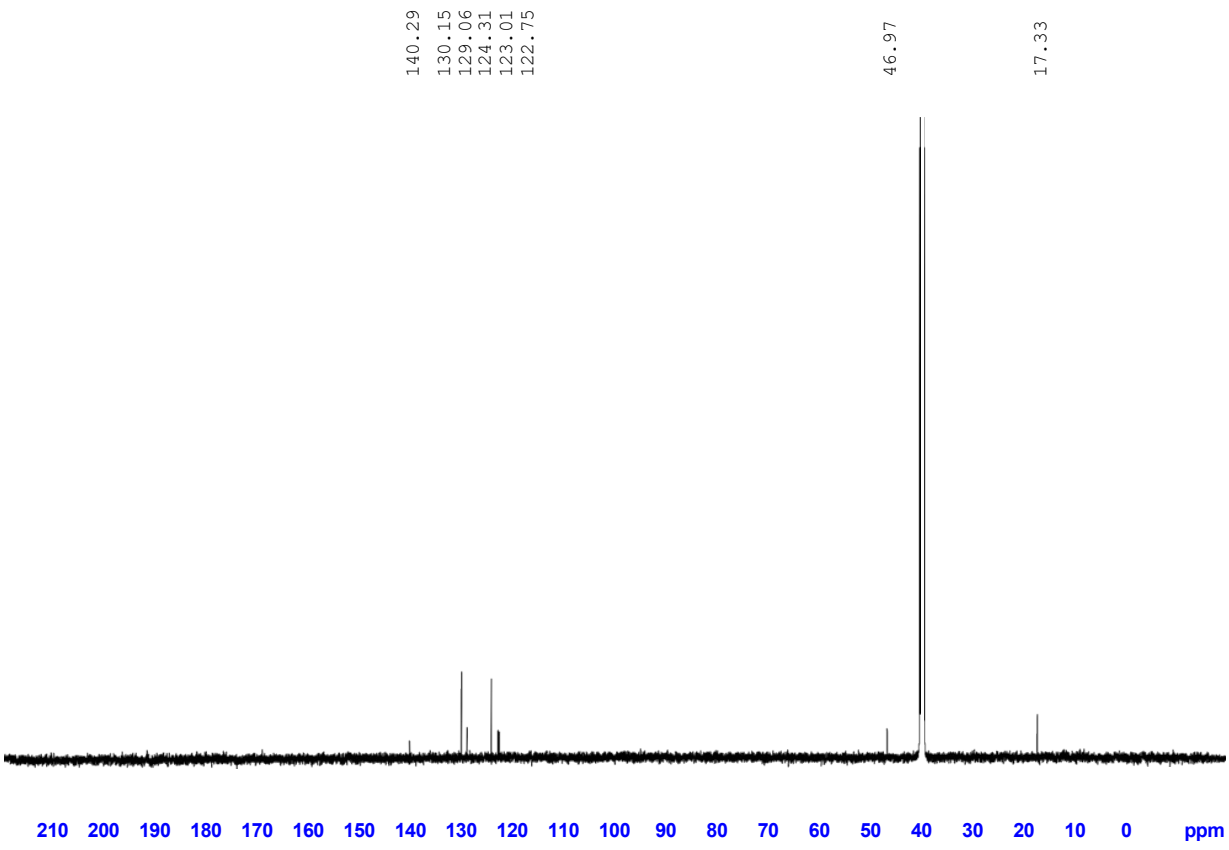


Figure S42. ^{1}H-NMR spectrum of compound **3c (**DMSO-d_6).

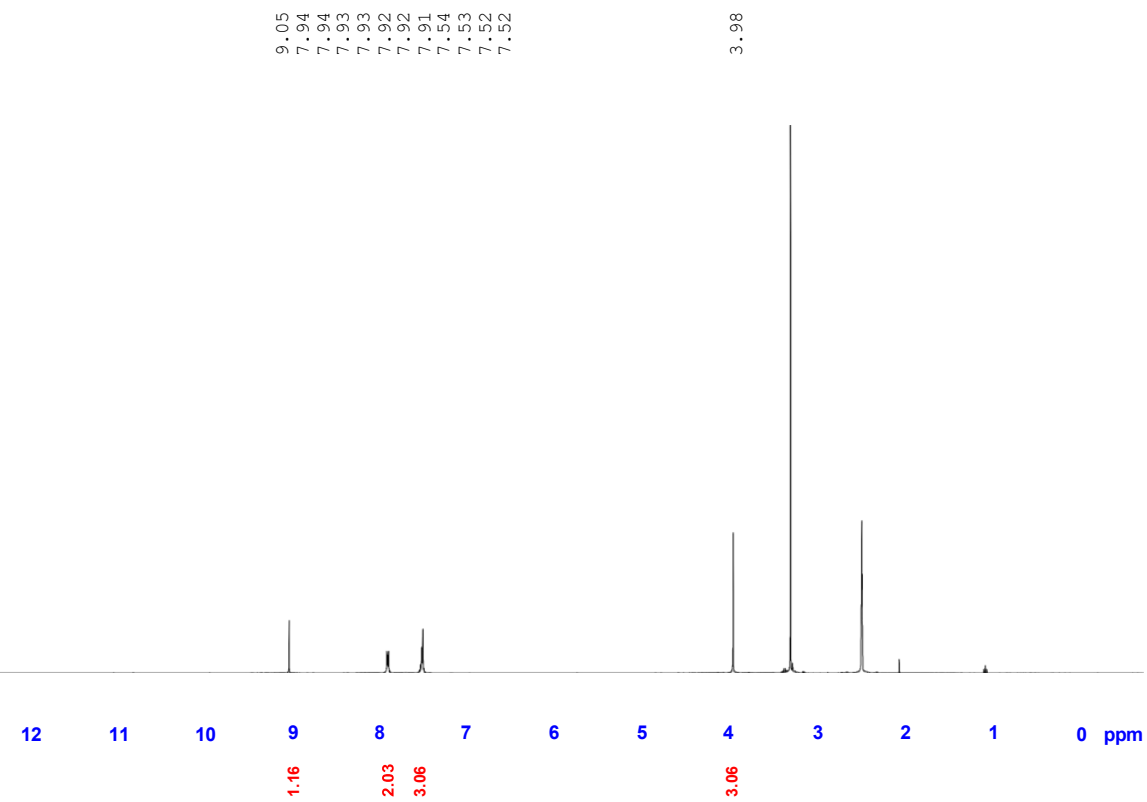


Figure S43. ^{13}C-NMR spectrum of compound **3c (**DMSO-d_6).

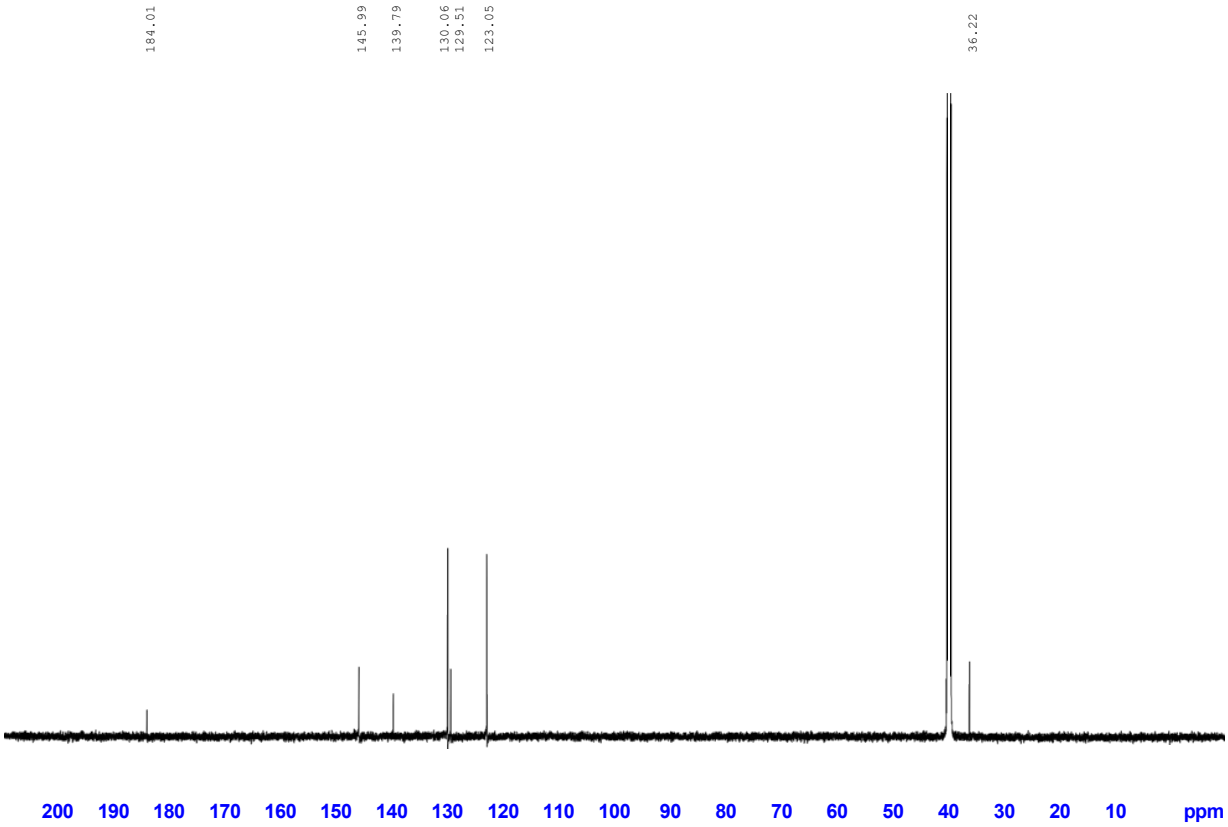


Figure S44. ^{1}H-NMR spectrum of compound **3d (**DMSO-d_6).

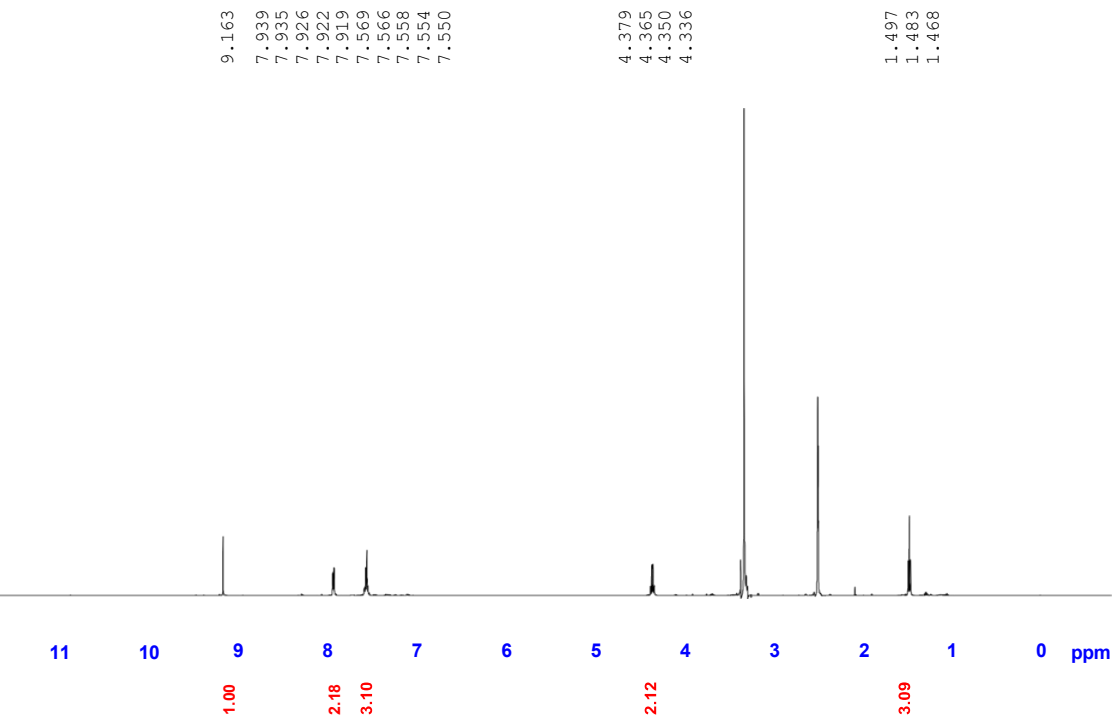


Figure S45. ^{13}C-NMR spectrum of compound **3d (**DMSO-d_6).

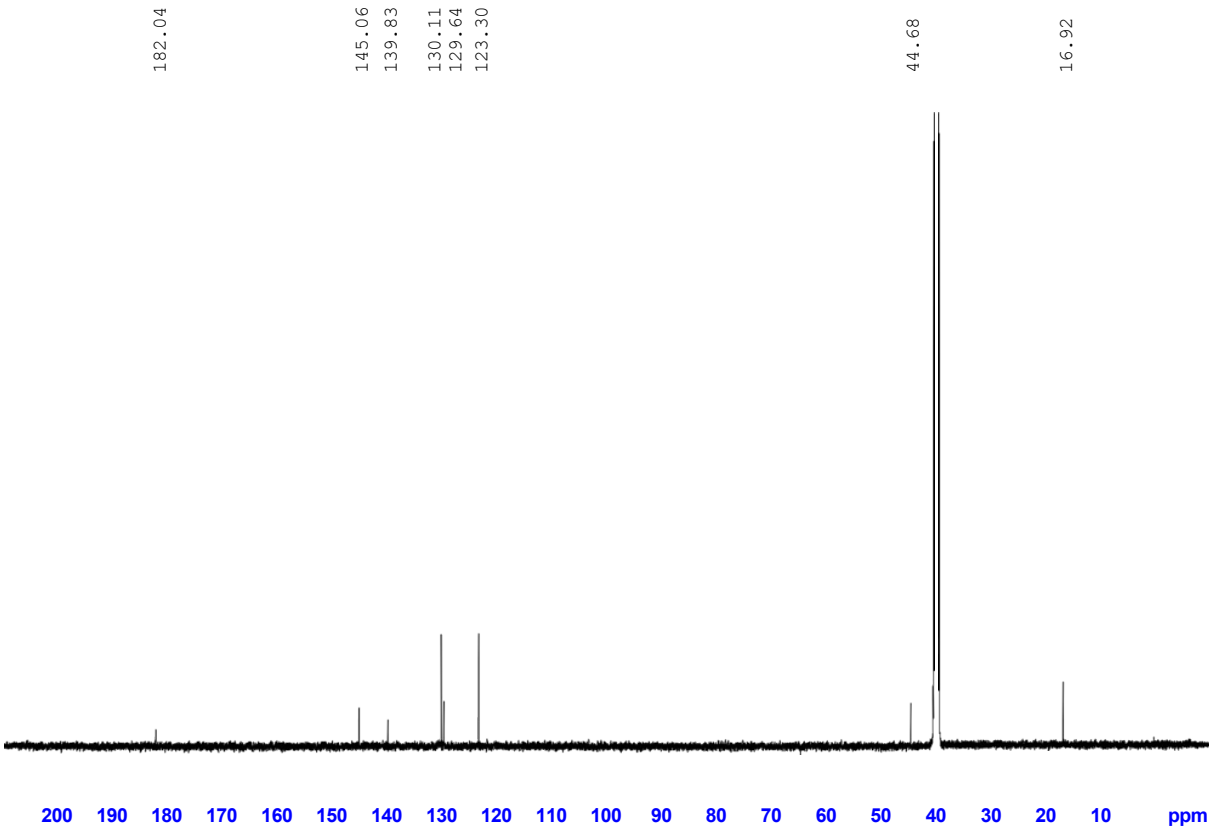


Figure S46. ^{1}H-NMR spectrum of compound **3e (**DMSO-d_6).

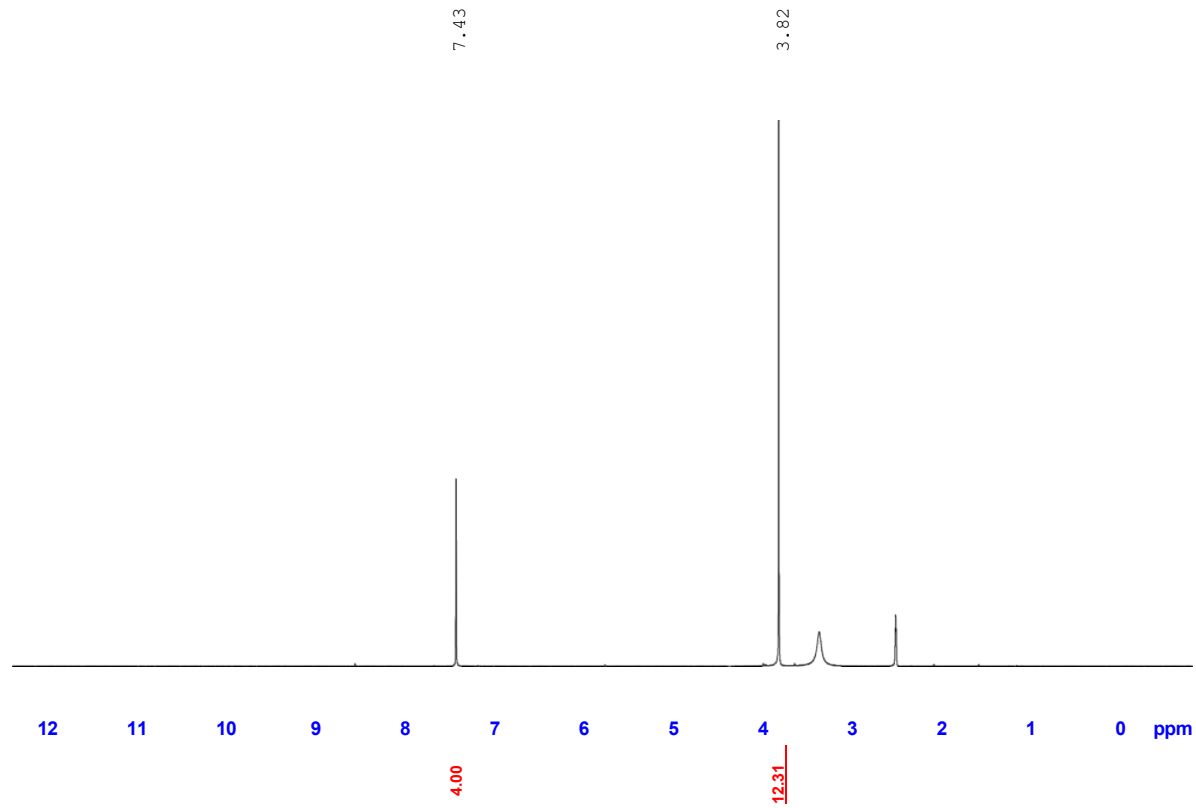


Figure S47. ^{13}C-NMR spectrum of compound **3e (**DMSO-d_6).

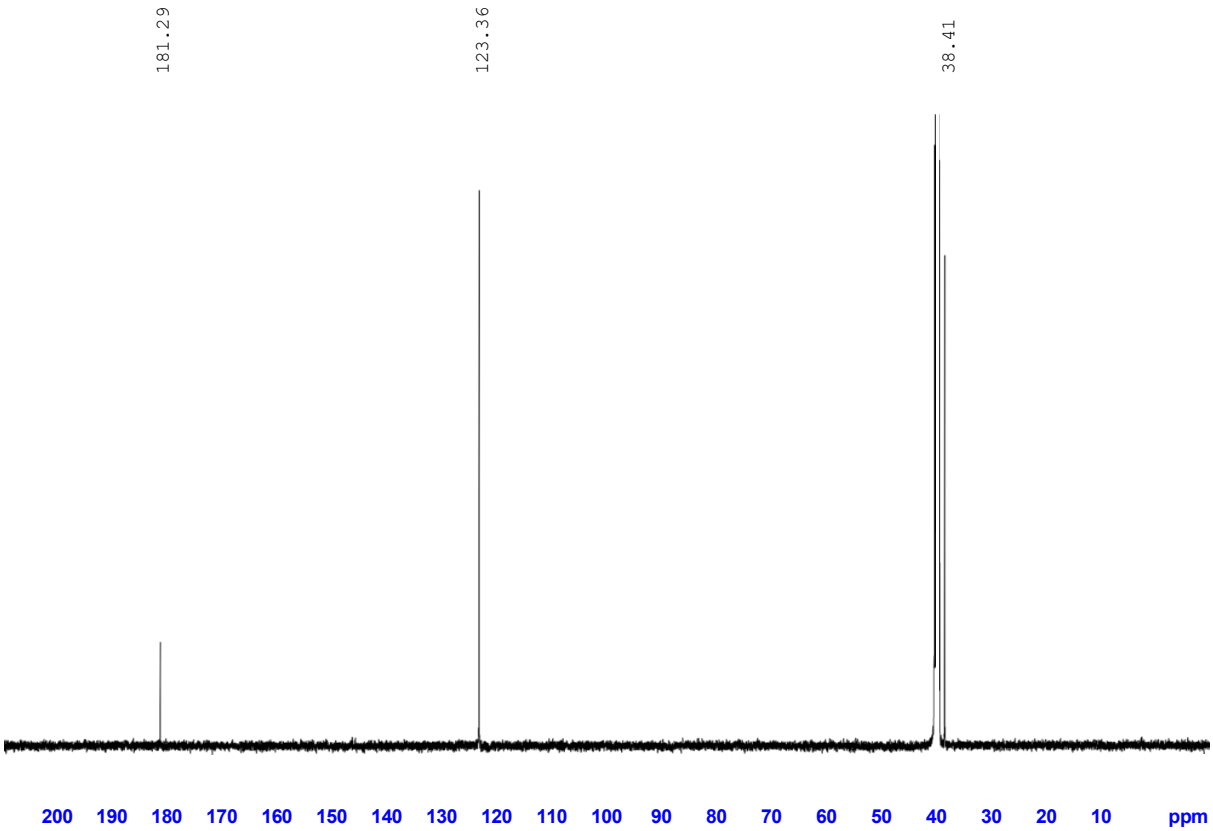


Figure S48. ^{1}H-NMR spectrum of compound **3f (**DMSO-d_6).

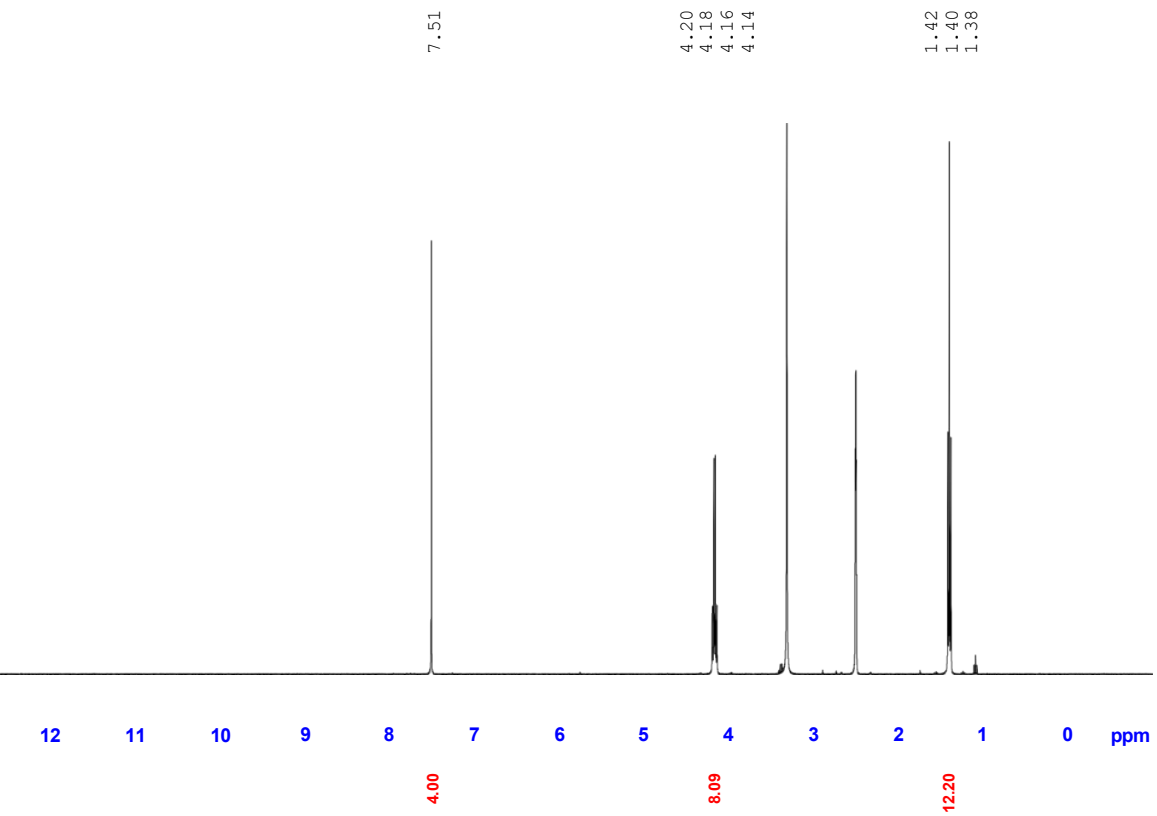

7.51
4.20
4.18
4.16
4.14
1.42
1.40
1.38
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
8.09
12.20

Figure S49. ^{13}C-NMR spectrum of compound **3f (**DMSO-d_6).

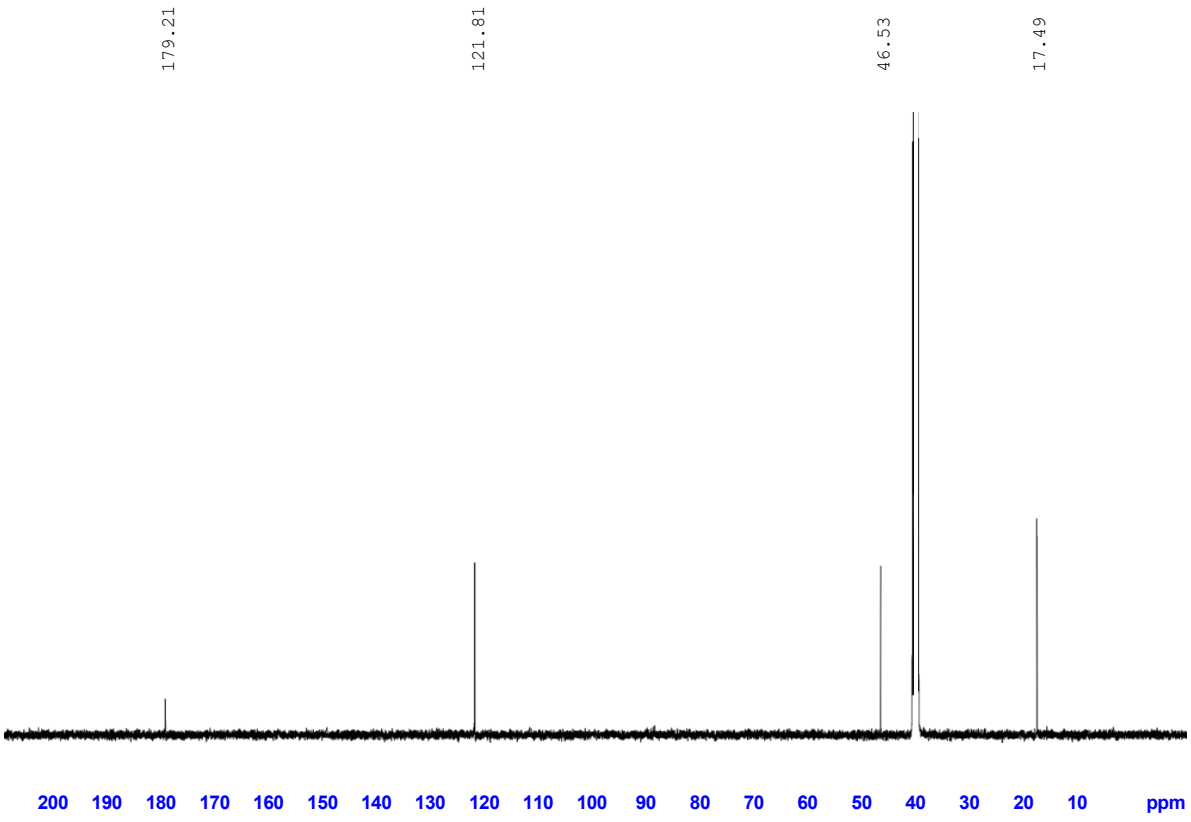


Figure S50. ^{1}H-NMR spectrum of compound **3g (**DMSO-d_6).

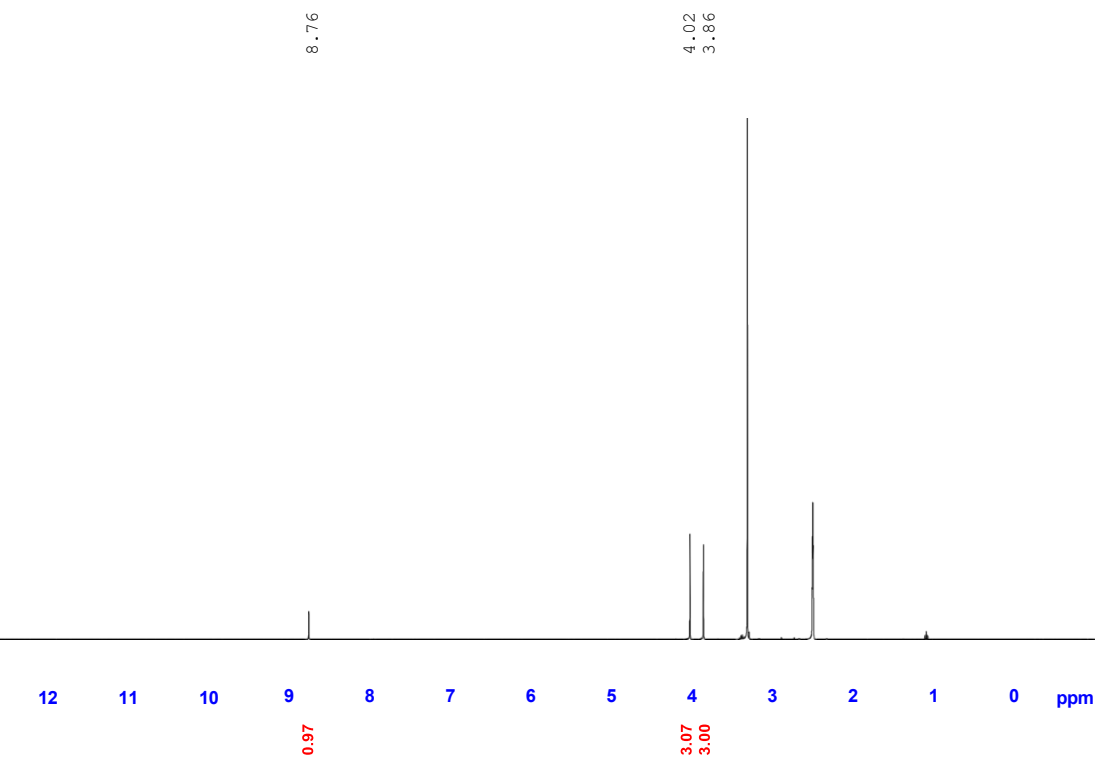

8.76
4.02
3.86
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
3.07
3.00

Figure S51. ^{13}C-NMR spectrum of compound **3g** (DMSO-d_6).

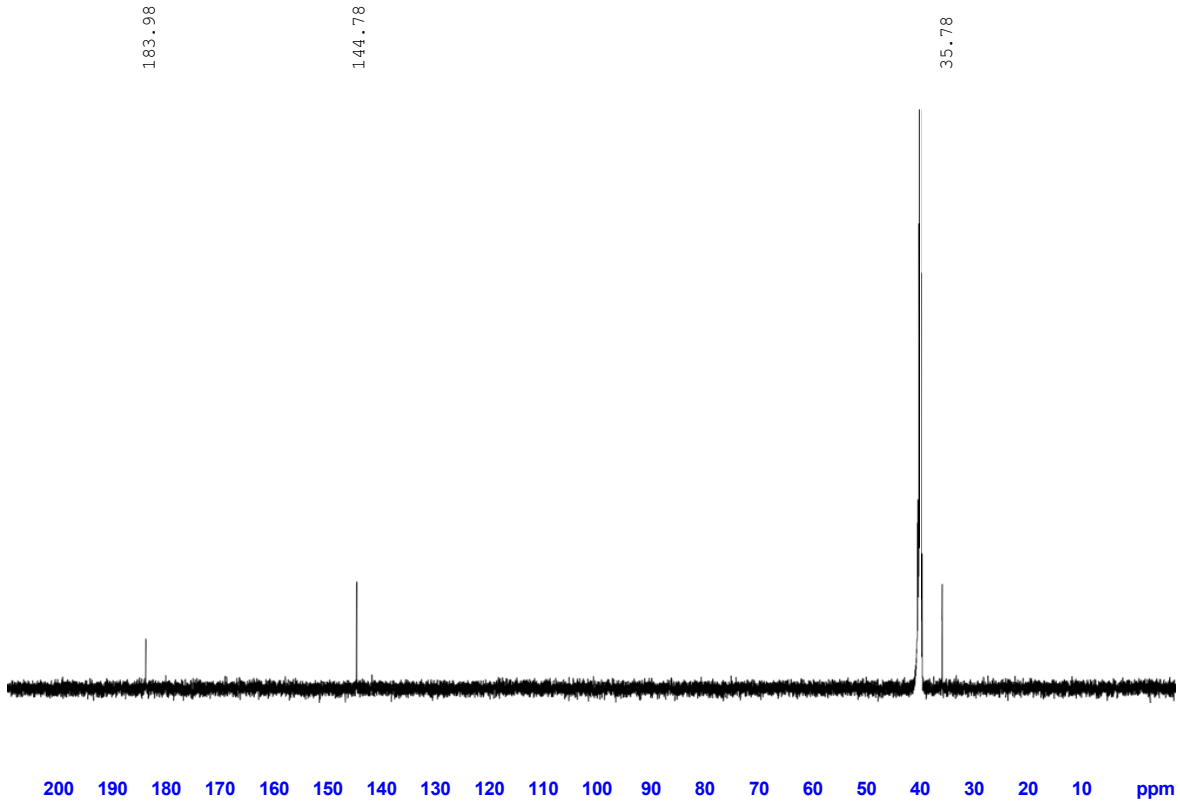


Figure S52. ^{1}H-NMR spectrum of compound **3h (**DMSO-d_6).

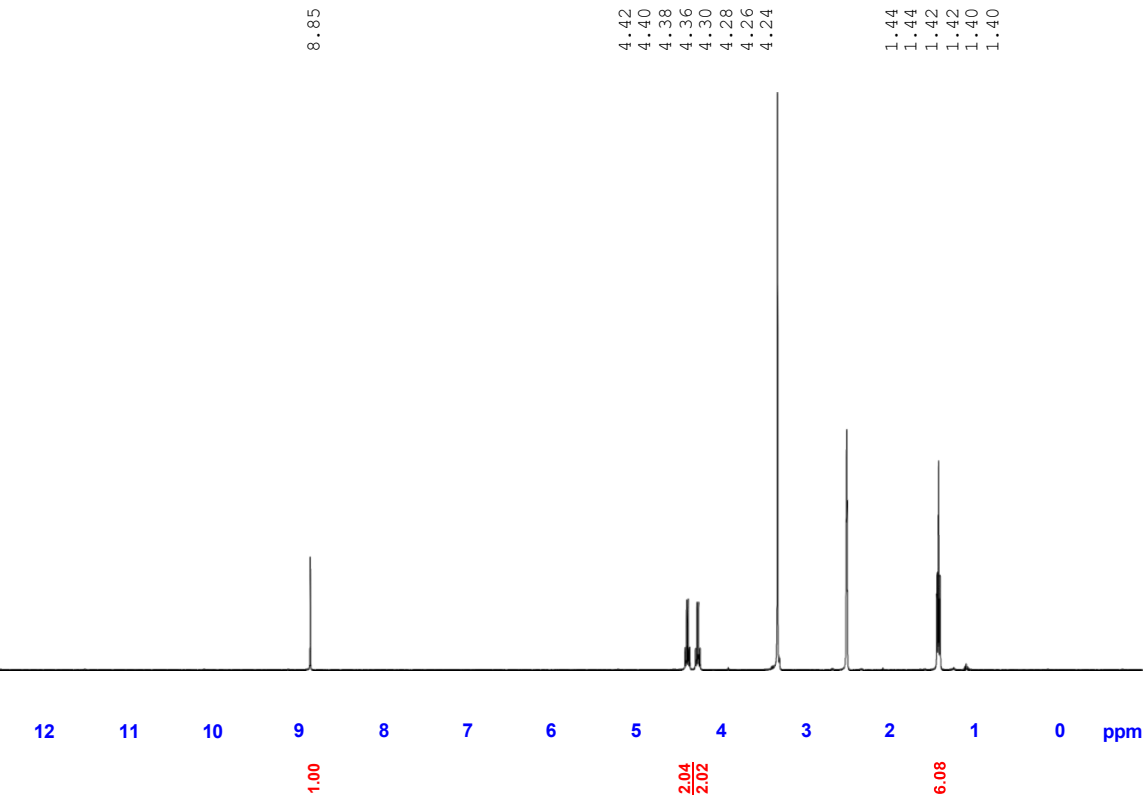


Figure S53. ^{13}C-NMR spectrum of compound **3h (**DMSO-d_6).

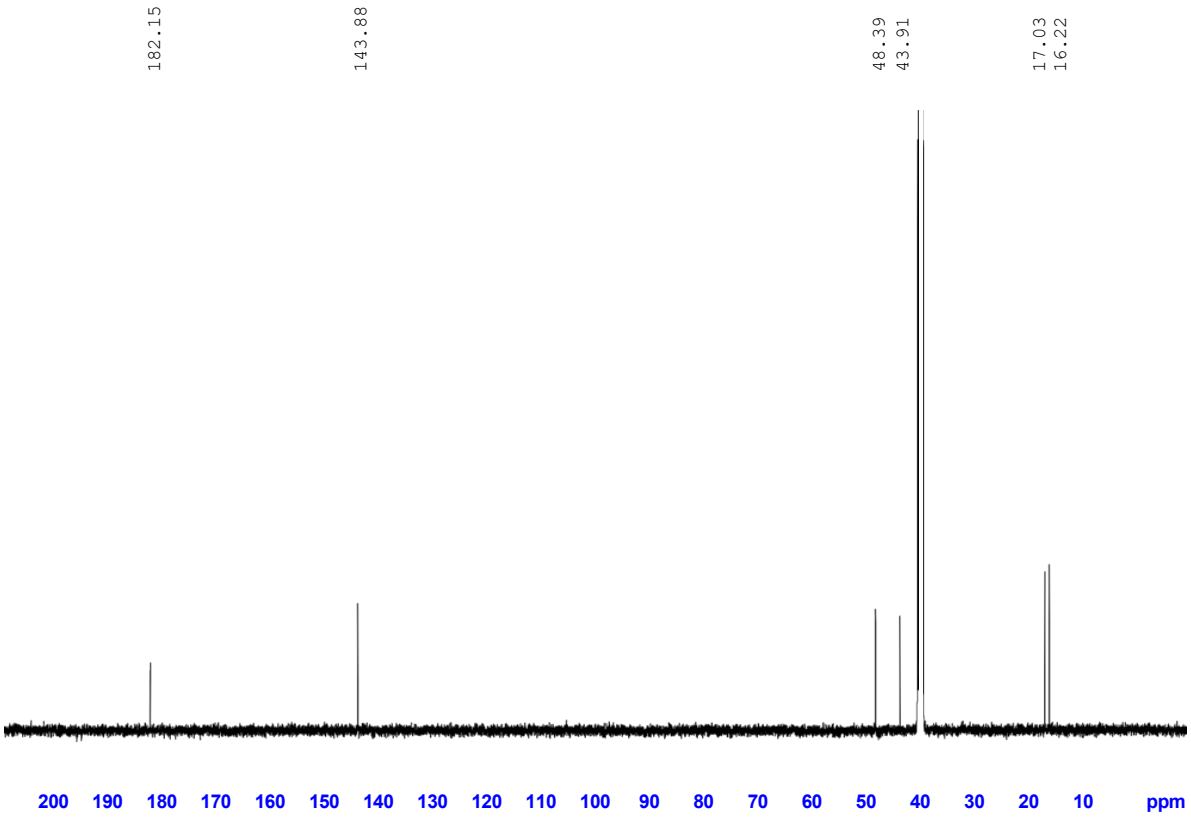


Figure S54. ^{1}H-NMR spectrum of compound **4a (**DMSO-d_6).

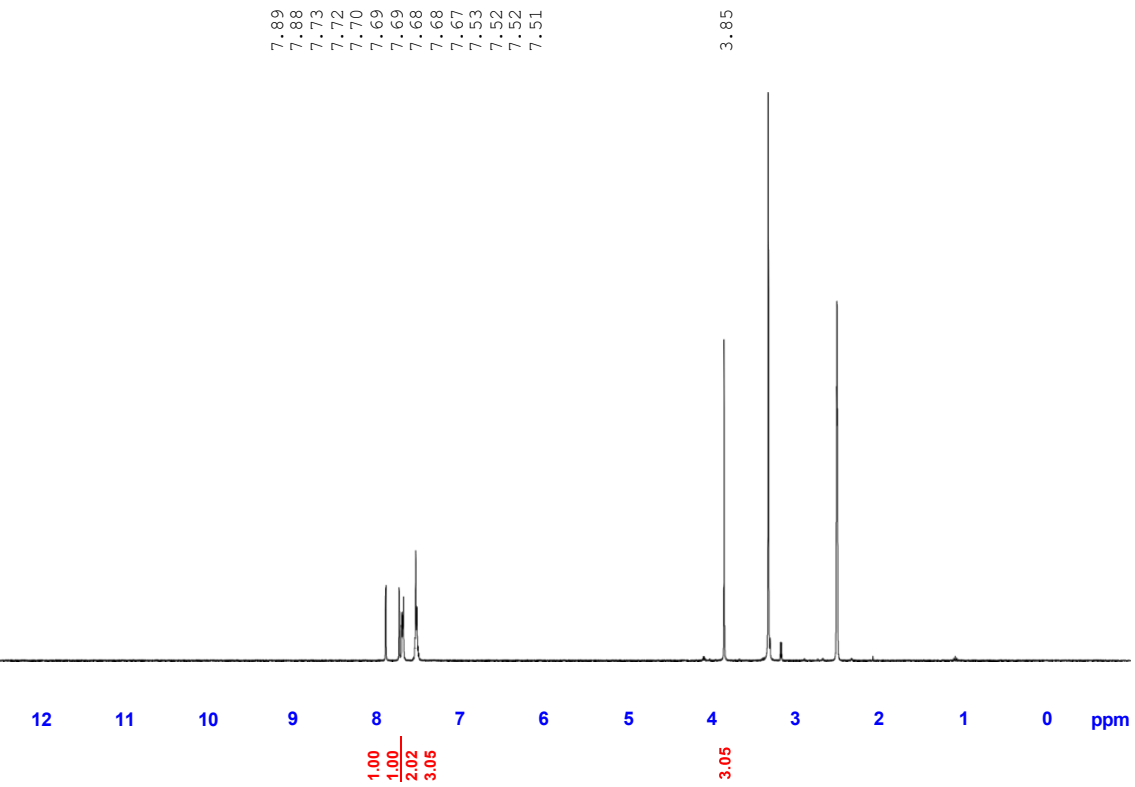


Figure S55. ^{13}C-NMR spectrum of compound **4a (**DMSO-d_6).

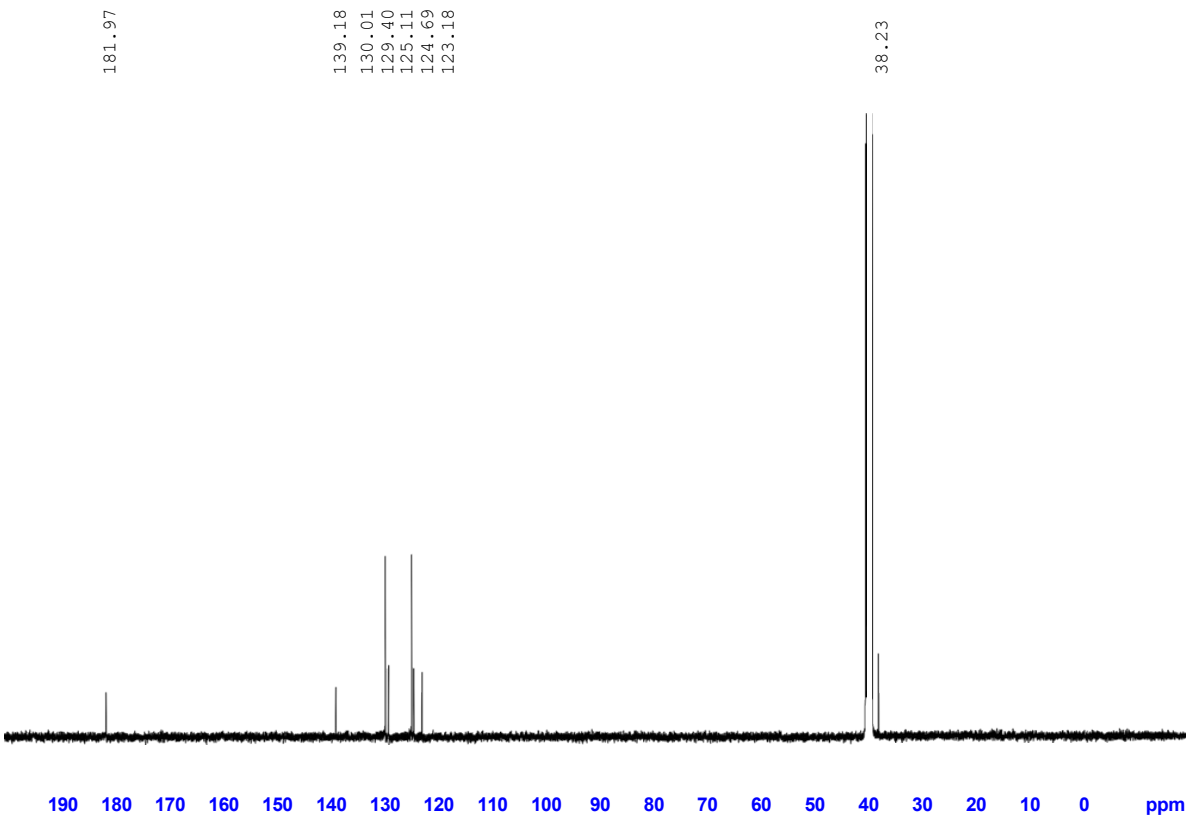


Figure S56. ^{1}H-NMR spectrum of compound **4b (**DMSO-d_6).

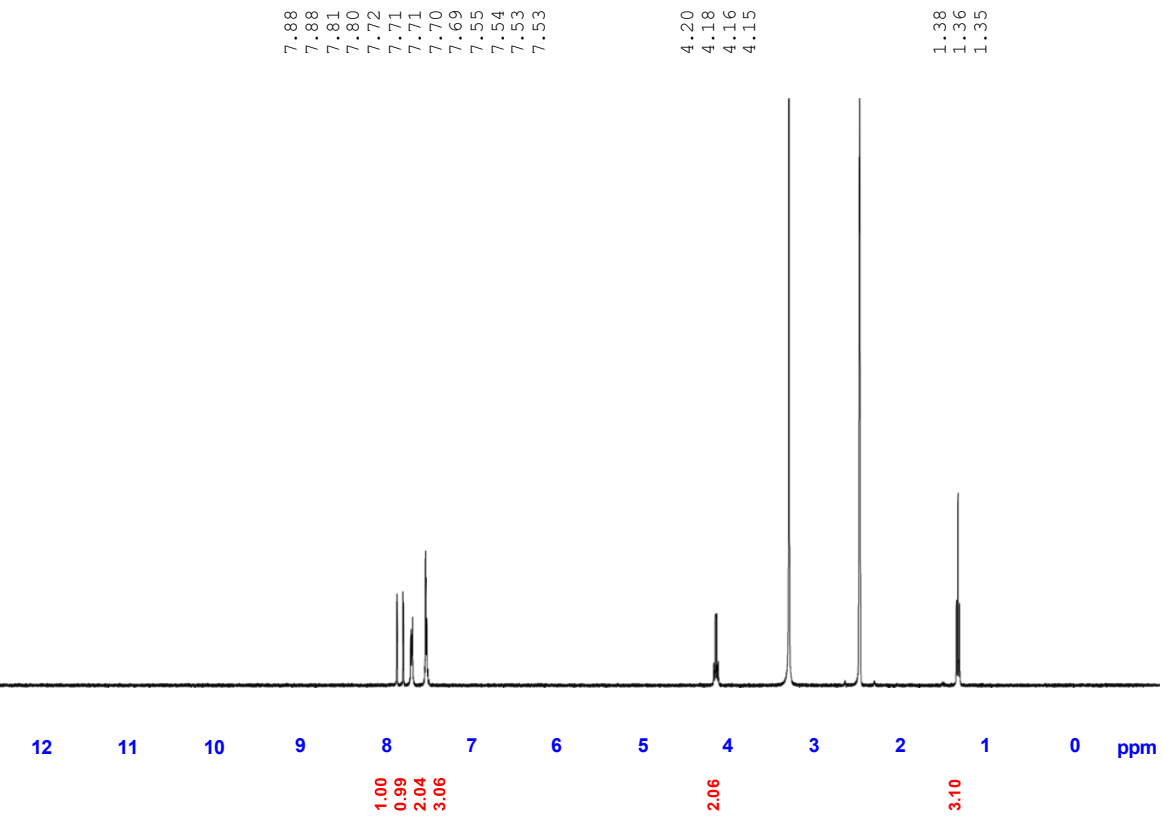


Figure S57. ^{13}C-NMR spectrum of compound **4b (**DMSO-d_6).

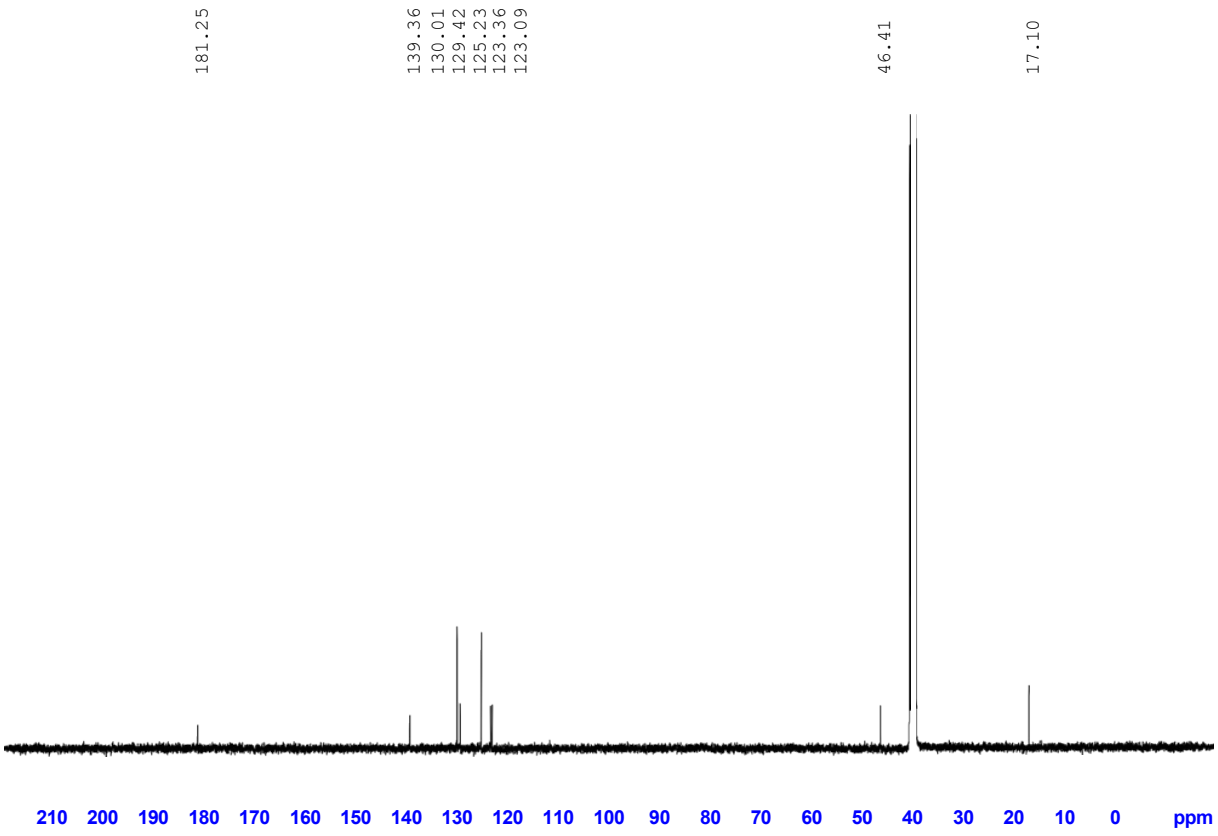

181.25
139.36
130.01
129.42
125.23
123.36
123.09
46.41
17.10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Figure S58. ^{1}H-NMR spectrum of compound **4c (**DMSO-d_6).

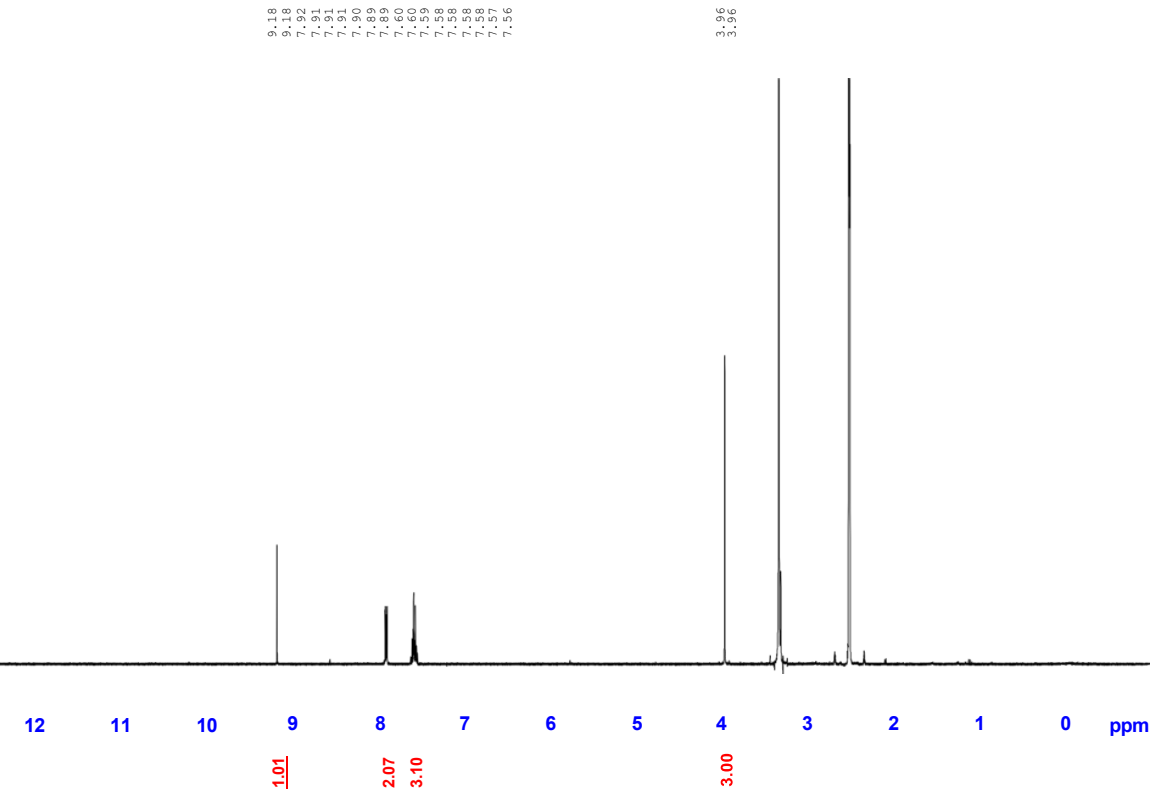


Figure S59. ^{13}C-NMR spectrum of compound **4c (**DMSO-d_6).

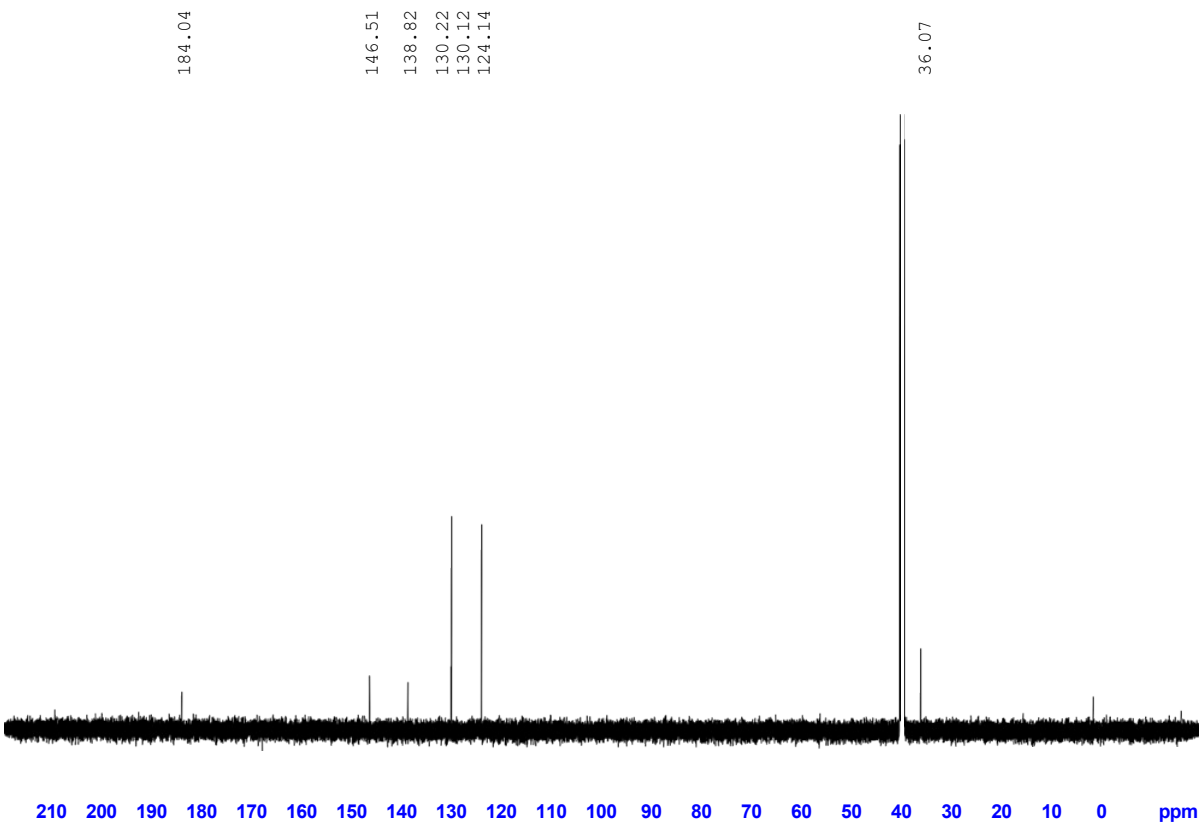


Figure S60. ^{1}H-NMR spectrum of compound **4d (**DMSO-d_6).

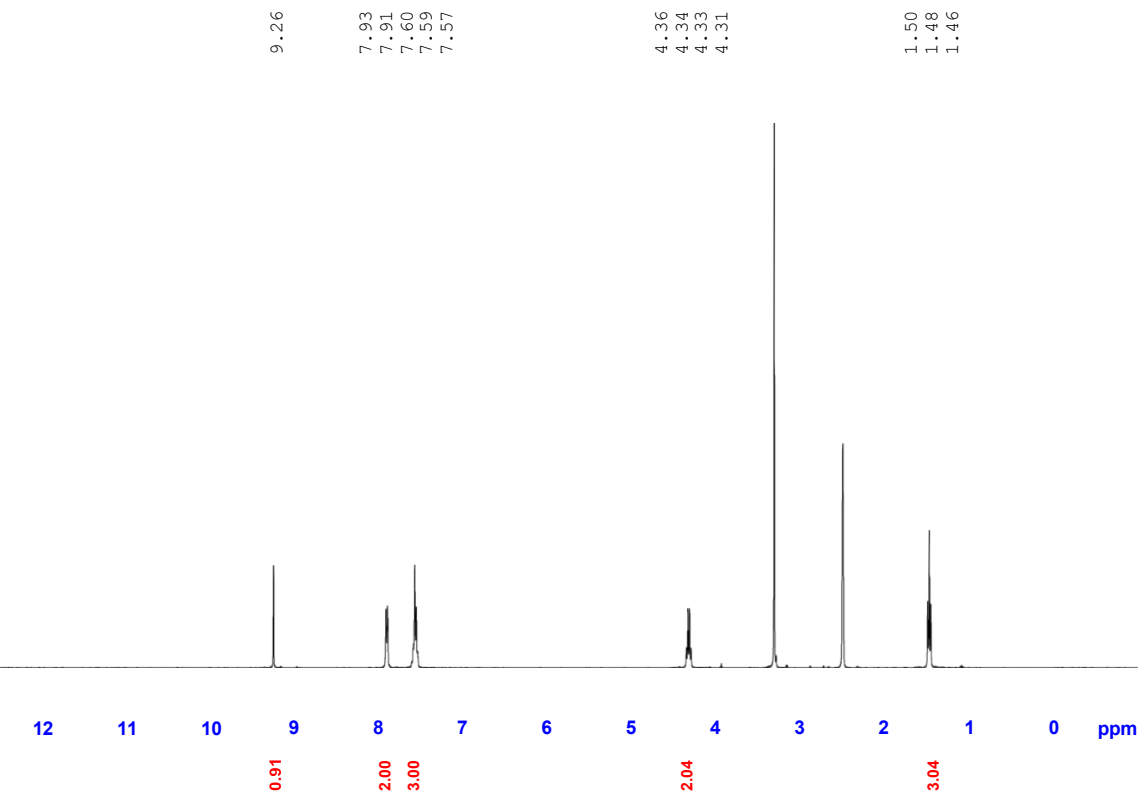


Figure S61. ^{13}C-NMR spectrum of compound **4d (**DMSO-d_6).

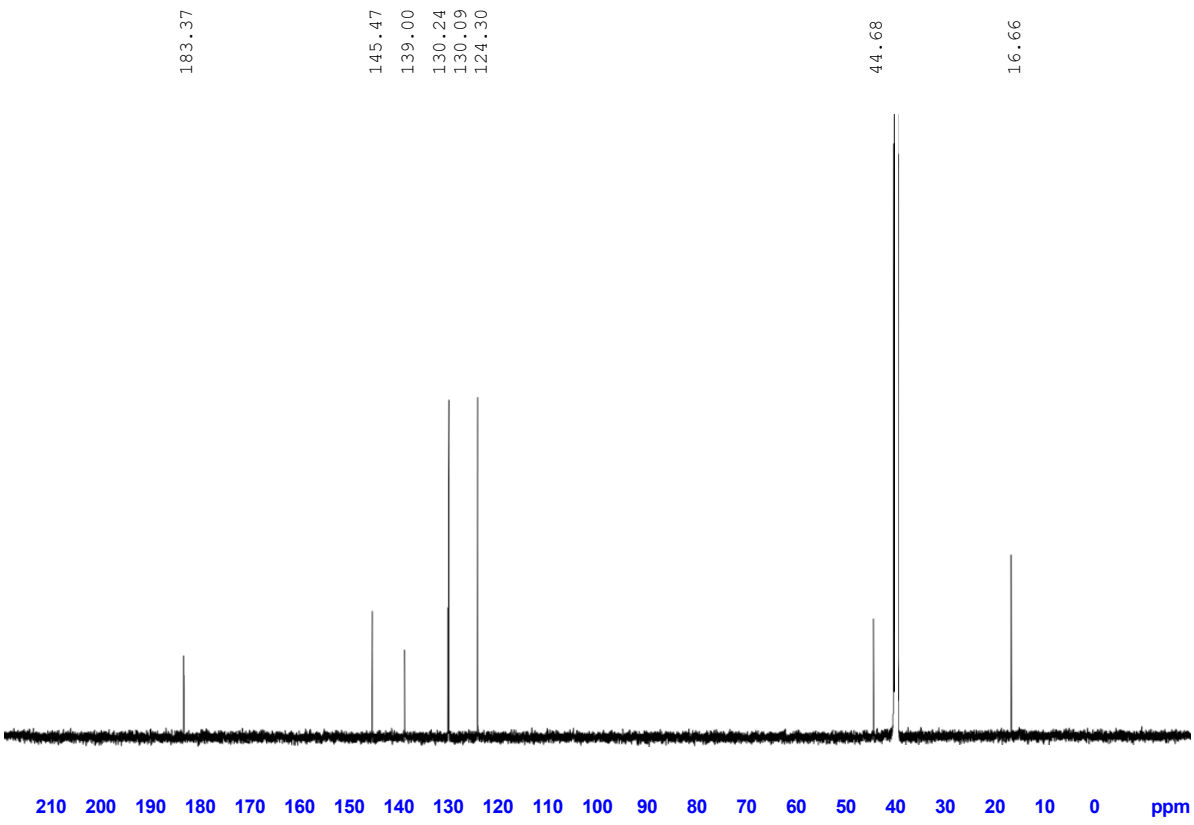


Figure S62. [1]H-NMR spectrum of compound **4e (**DMSO-d_6).

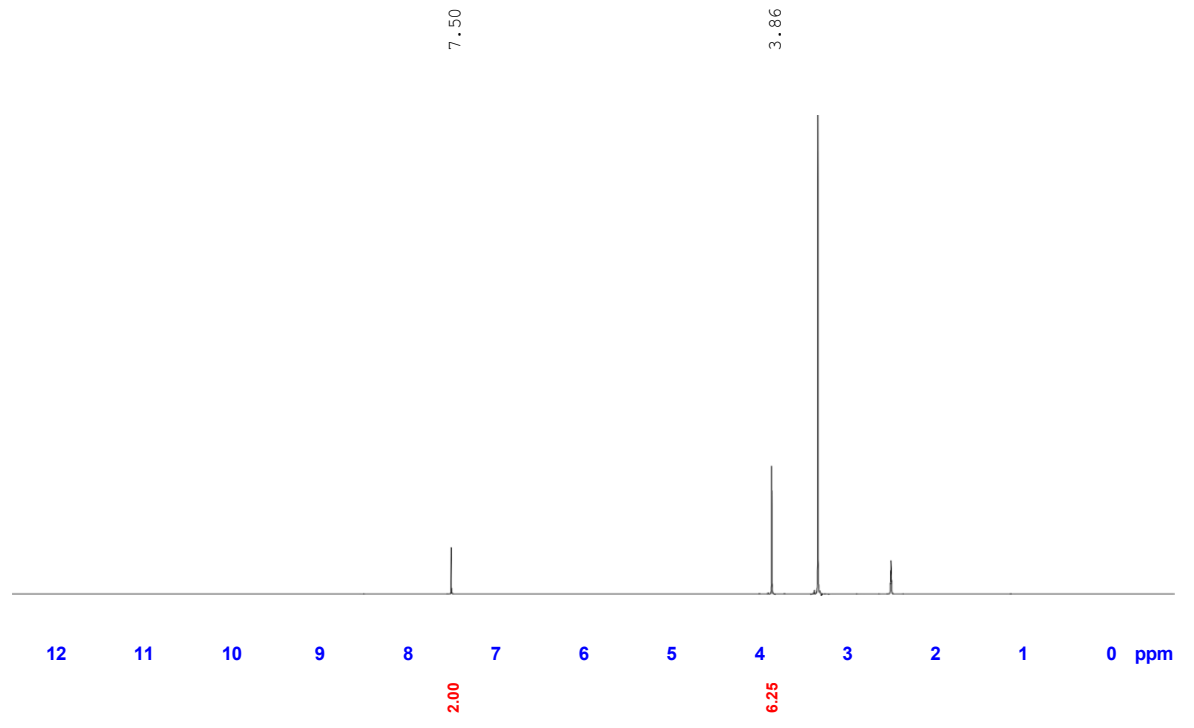


Figure S63. [13]C-NMR spectrum of compound **4e (**DMSO-d_6).

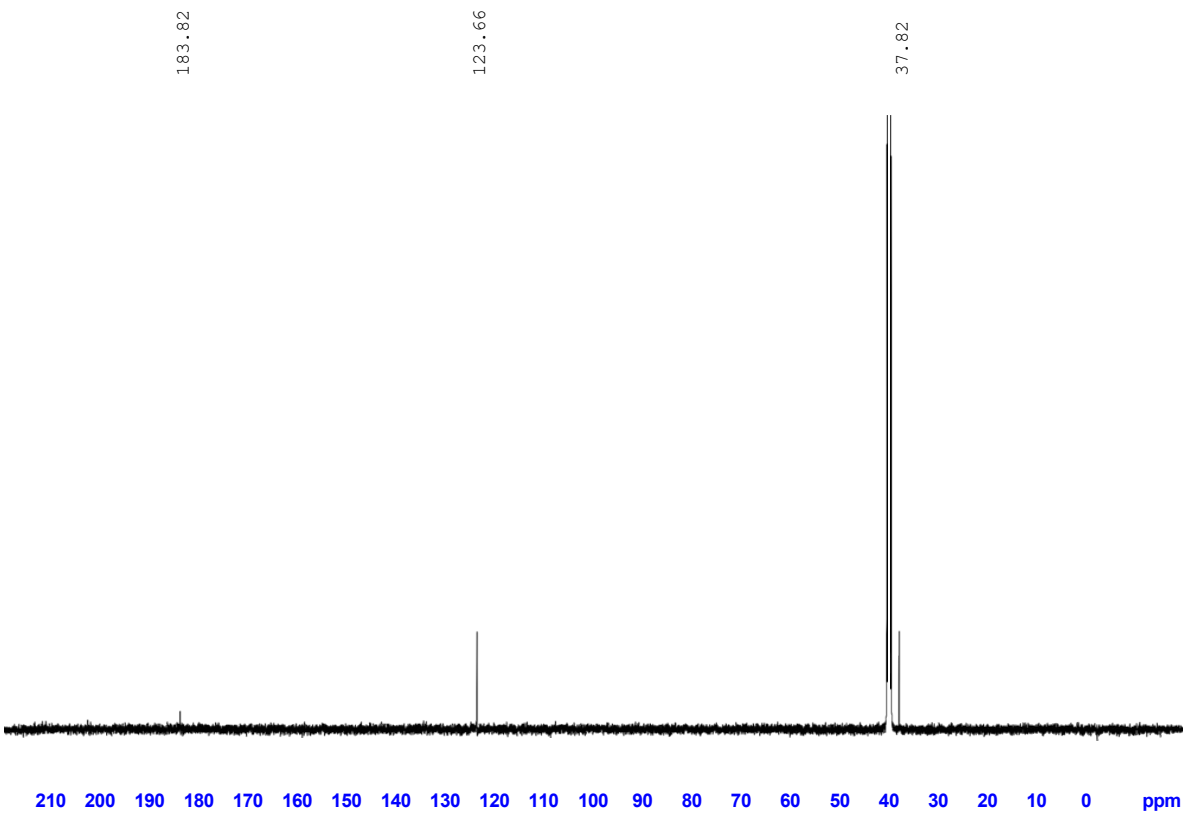

183.82
123.66
37.82
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Figure S64. ^{1}H-NMR spectrum of compound **4f (**DMSO-d_6).

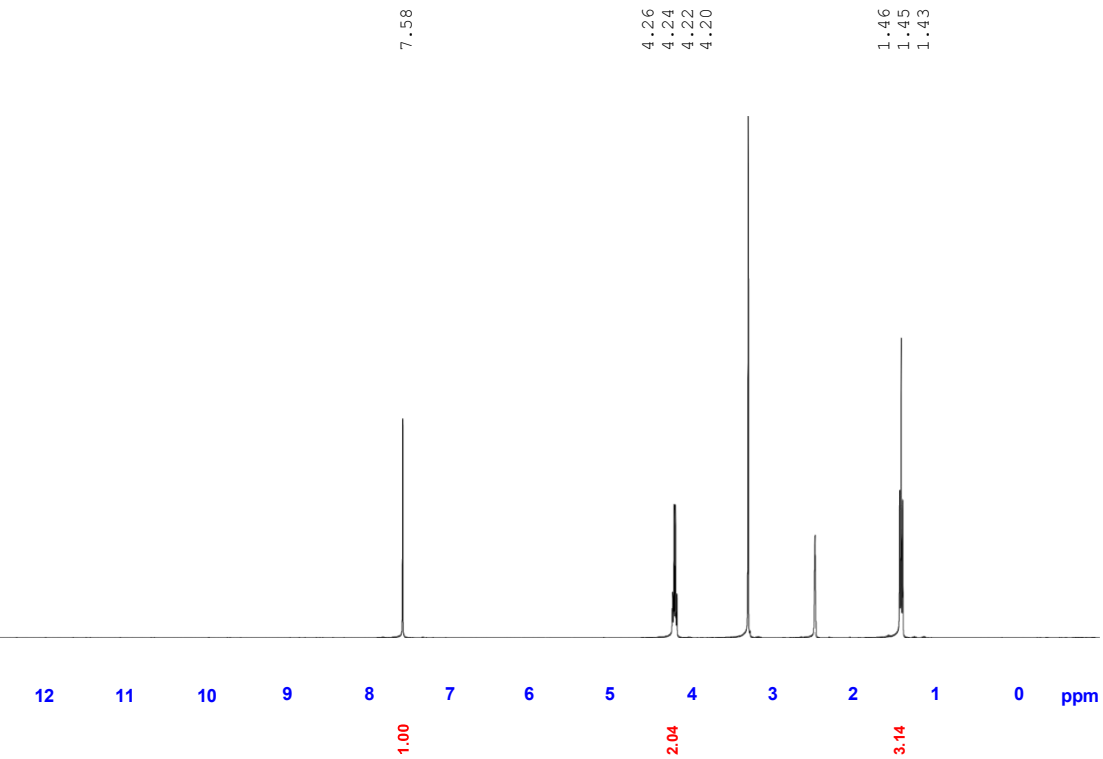


Figure S65. ^{13}C-NMR spectrum of compound **4f (**DMSO-d_6).

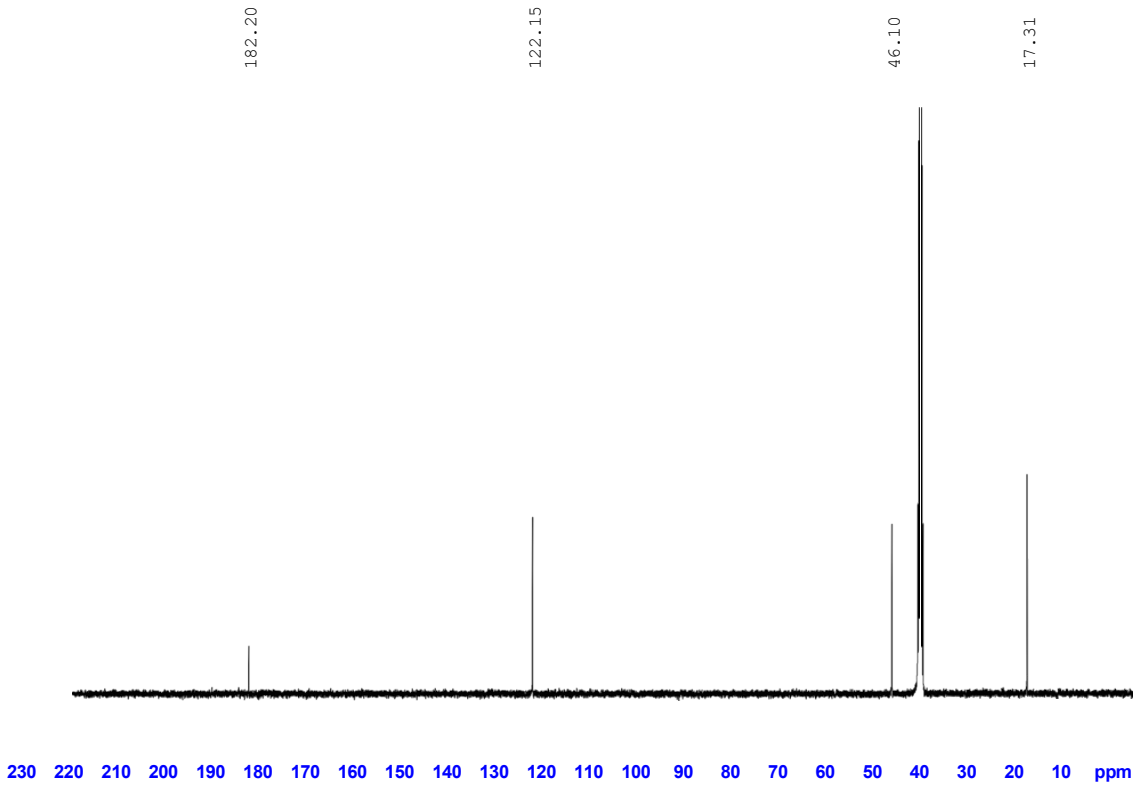


Figure S66. ^{1}H-NMR spectrum of compound **4g (**DMSO-d_6).

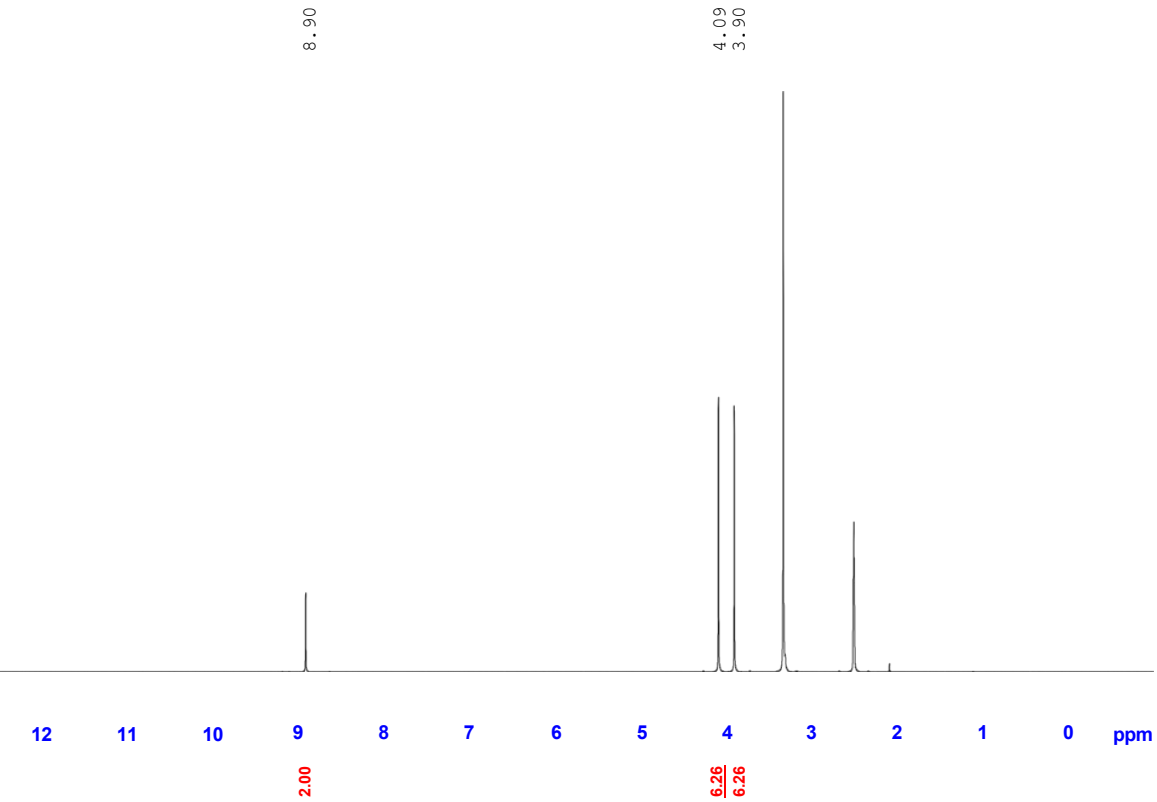


Figure S67. ^{13}C-NMR spectrum of compound **4g (**DMSO-d_6).

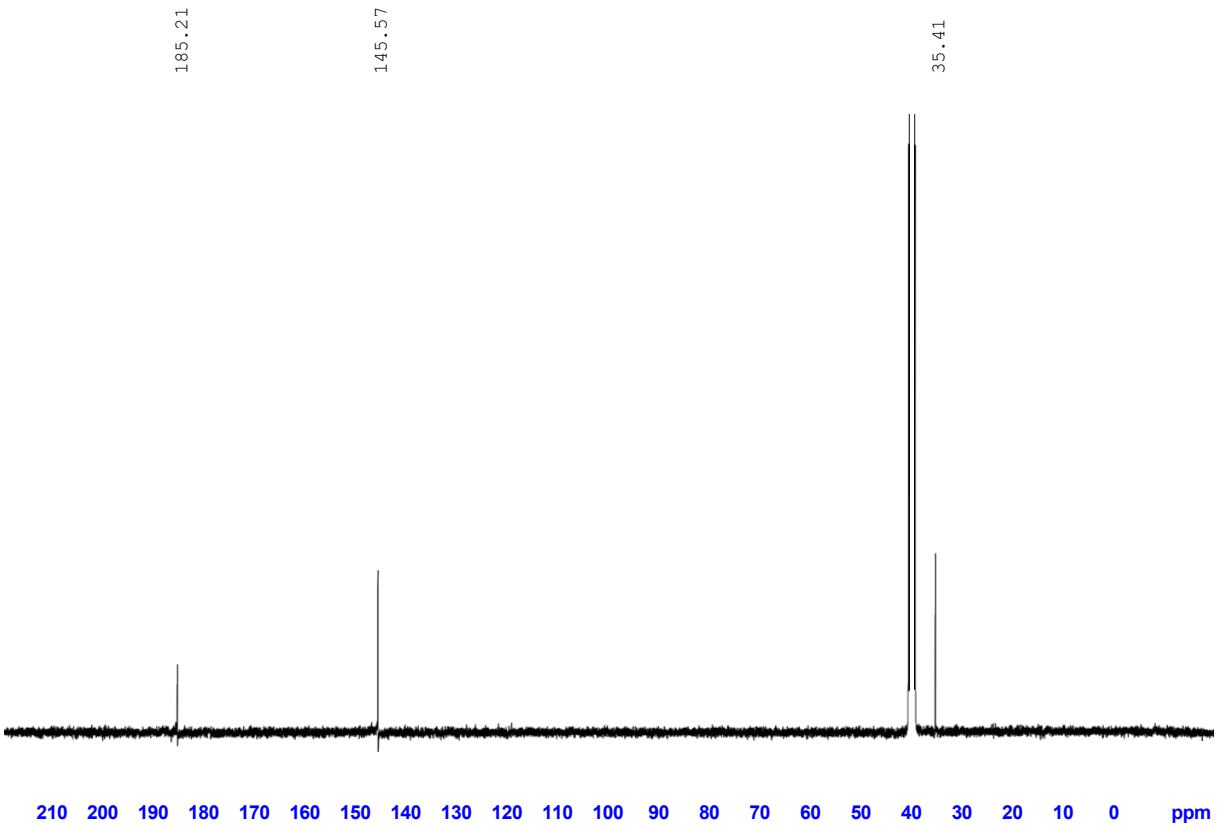


Figure S68. ^{1}H-NMR spectrum of compound **4h (**DMSO-d_6).

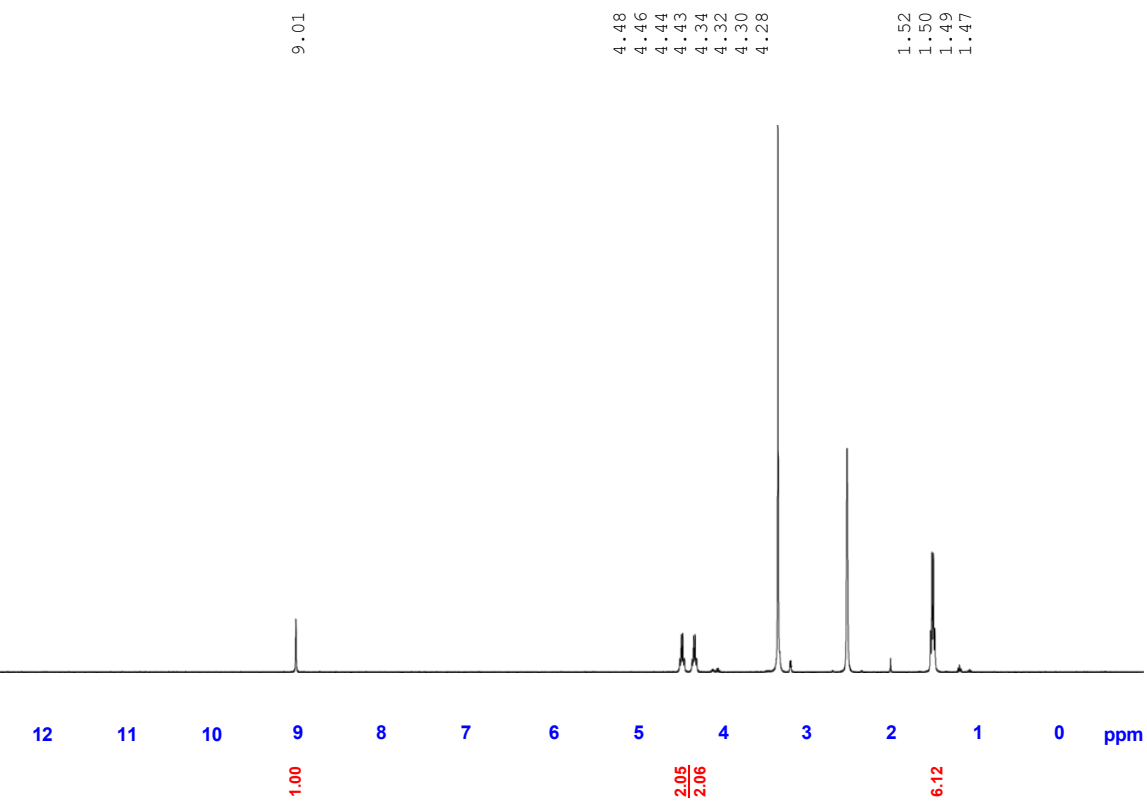

9.01
4.48
4.46
4.44
4.43
4.34
4.32
4.30
4.28
1.52
1.50
1.49
1.47
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.05
2.06
6.12

Figure S69. ^{13}C-NMR spectrum of compound **4h (**DMSO-d_6).

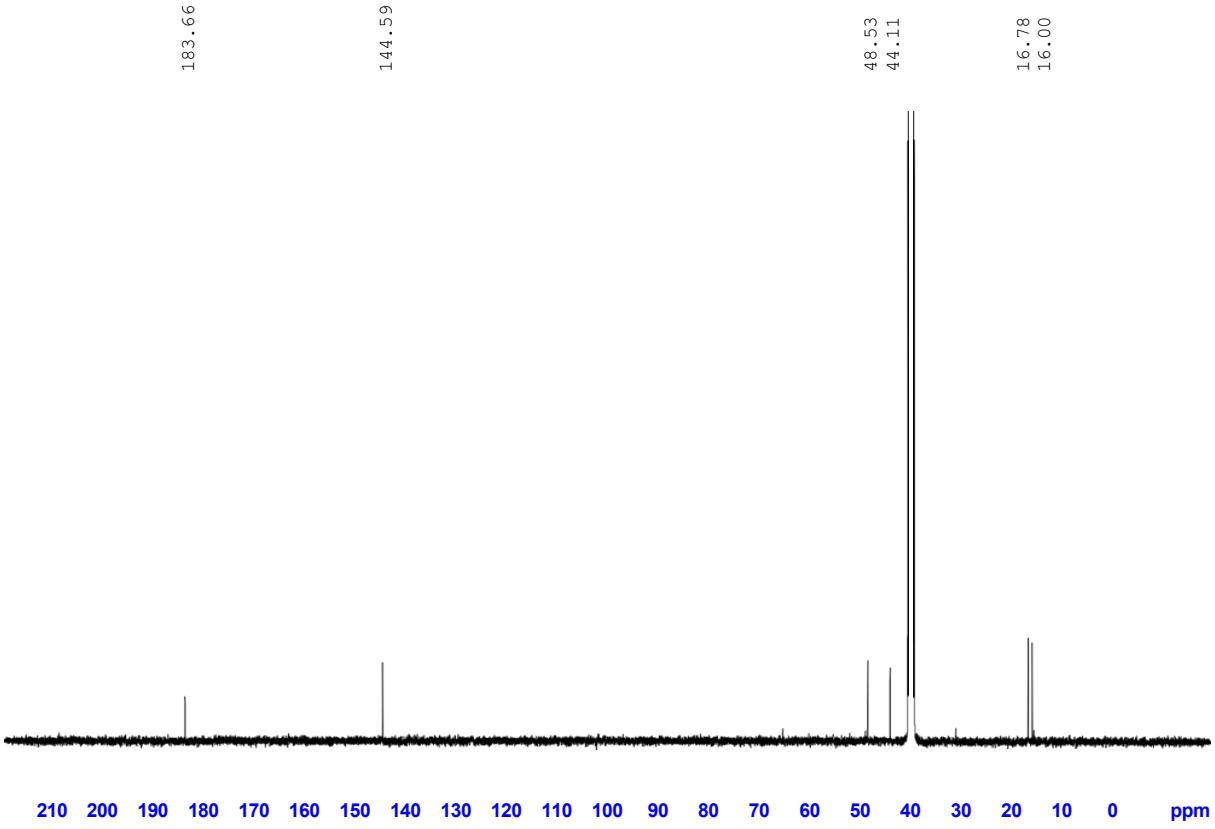


Figure S70. ^{1}H-NMR spectrum of compound **2a (**DMSO-d_6).

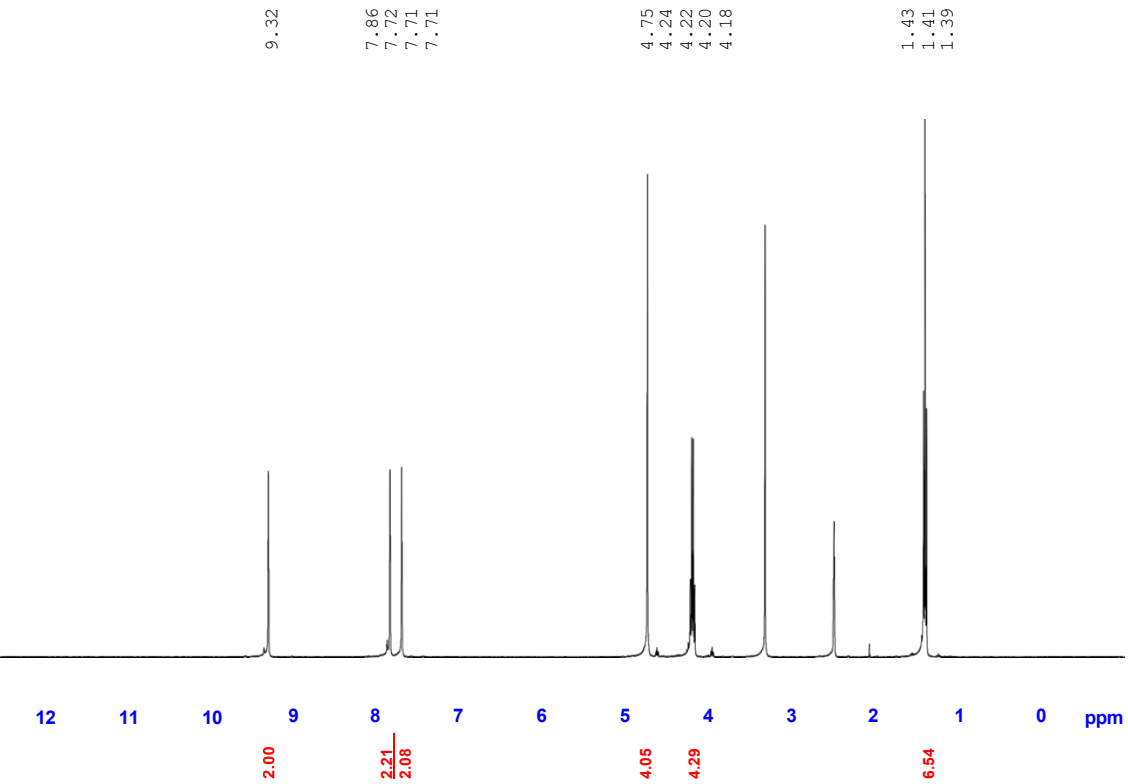


Figure S71. ^{13}C-NMR spectrum of compound **2a (**DMSO-d_6).

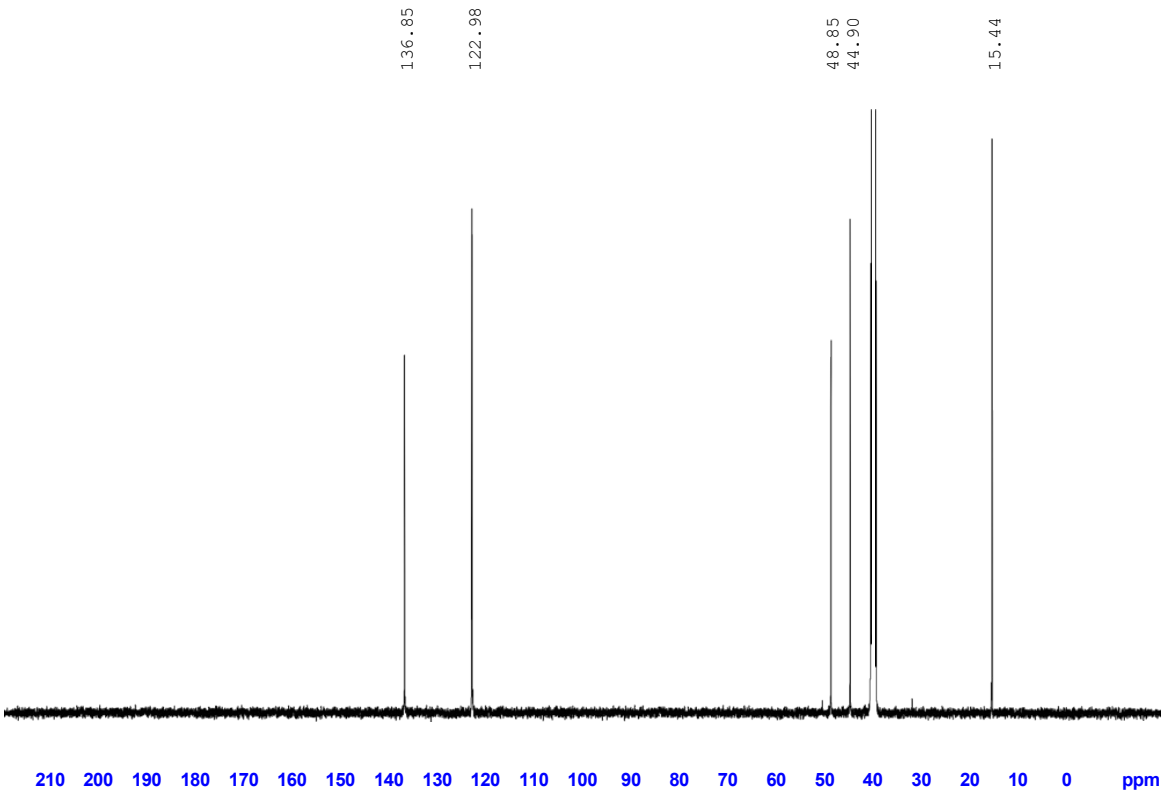


Figure S72. ^{1}H-NMR spectrum of compound **2b (**DMSO-d_6).

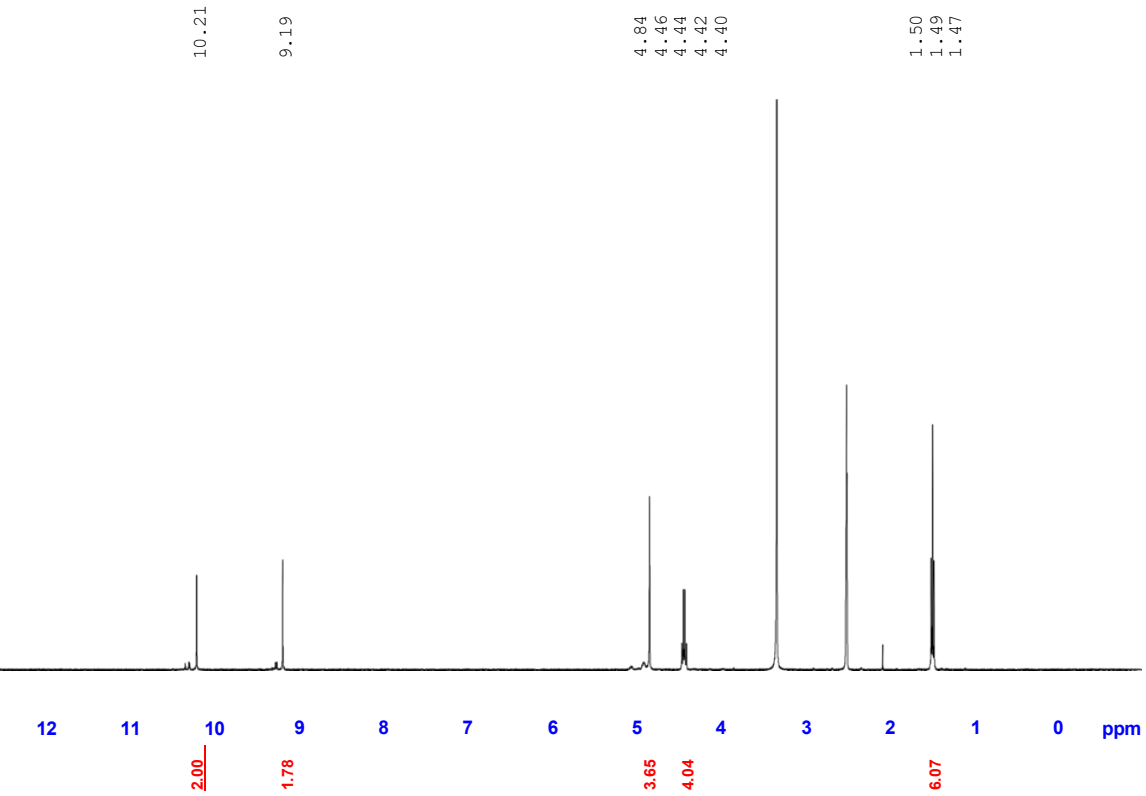


Figure S73. ^{13}C-NMR spectrum of compound **2b (**DMSO-d_6).

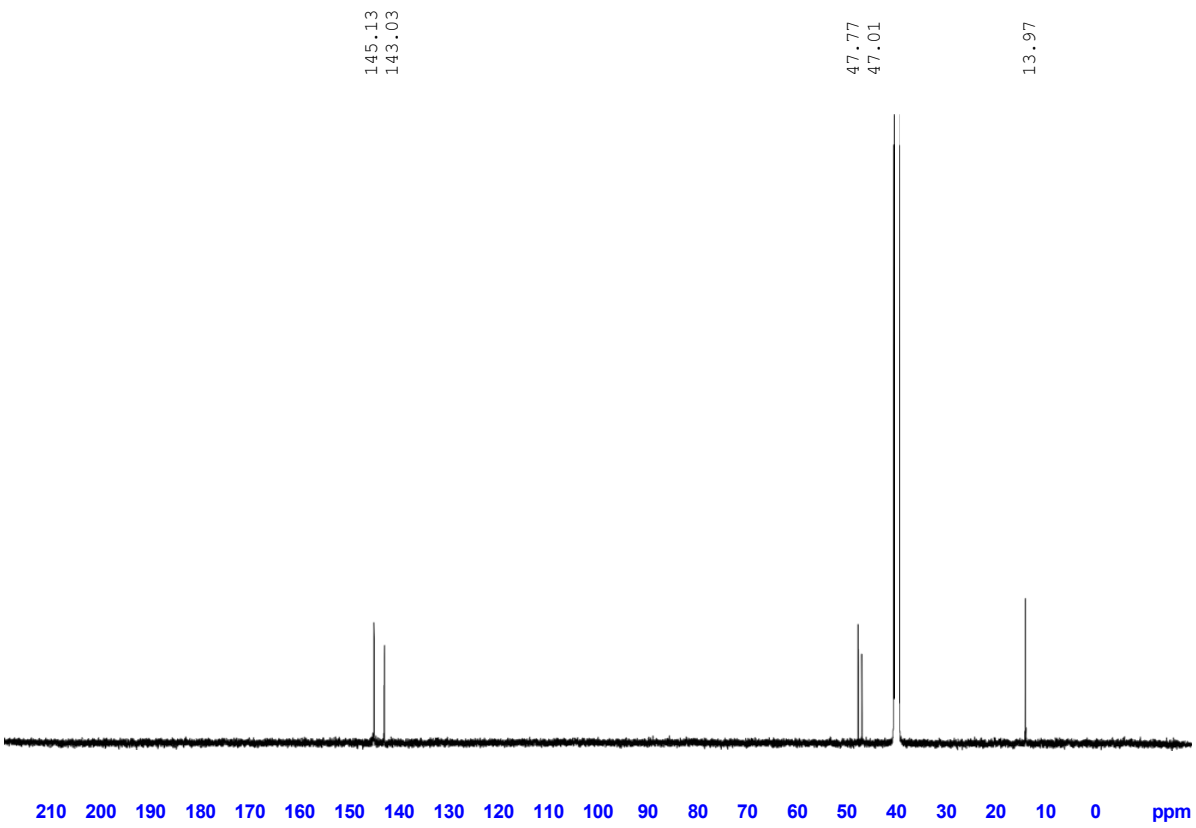


Figure S74. ^{1}H-NMR spectrum of compound **2c (**DMSO-d_6).

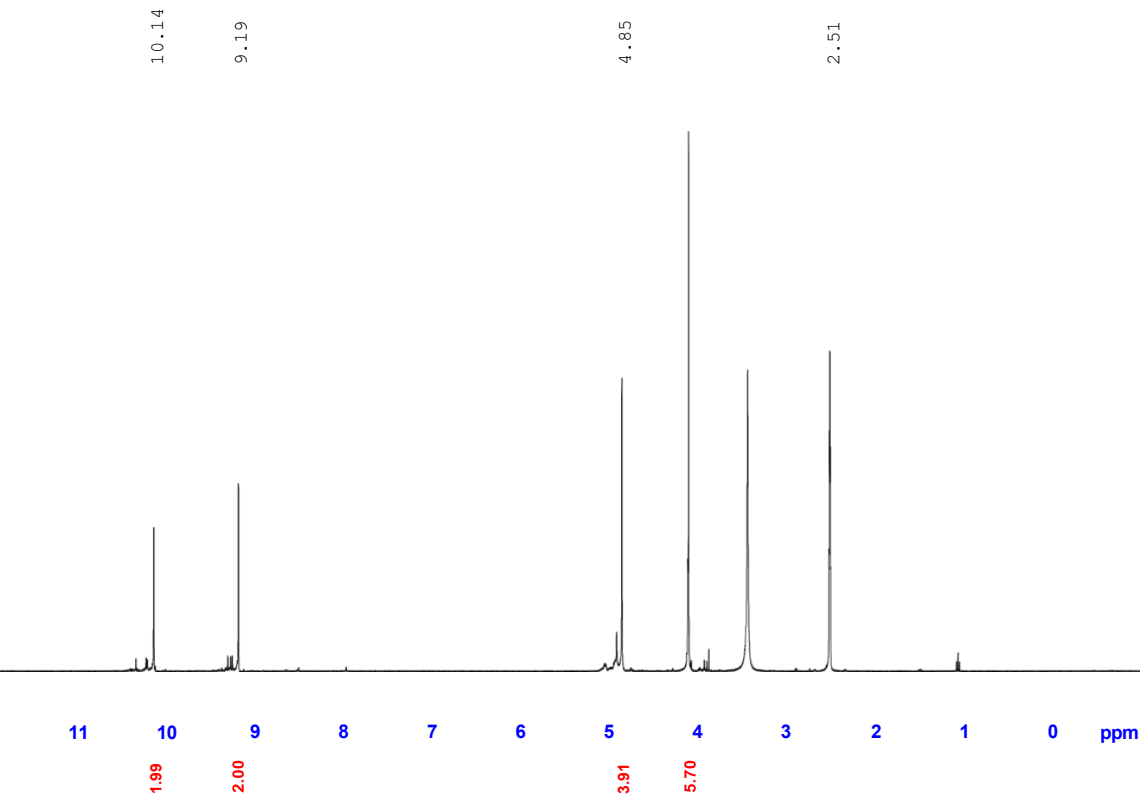


Figure S75. ^{13}C-NMR spectrum of compound **2c (**DMSO-d_6).

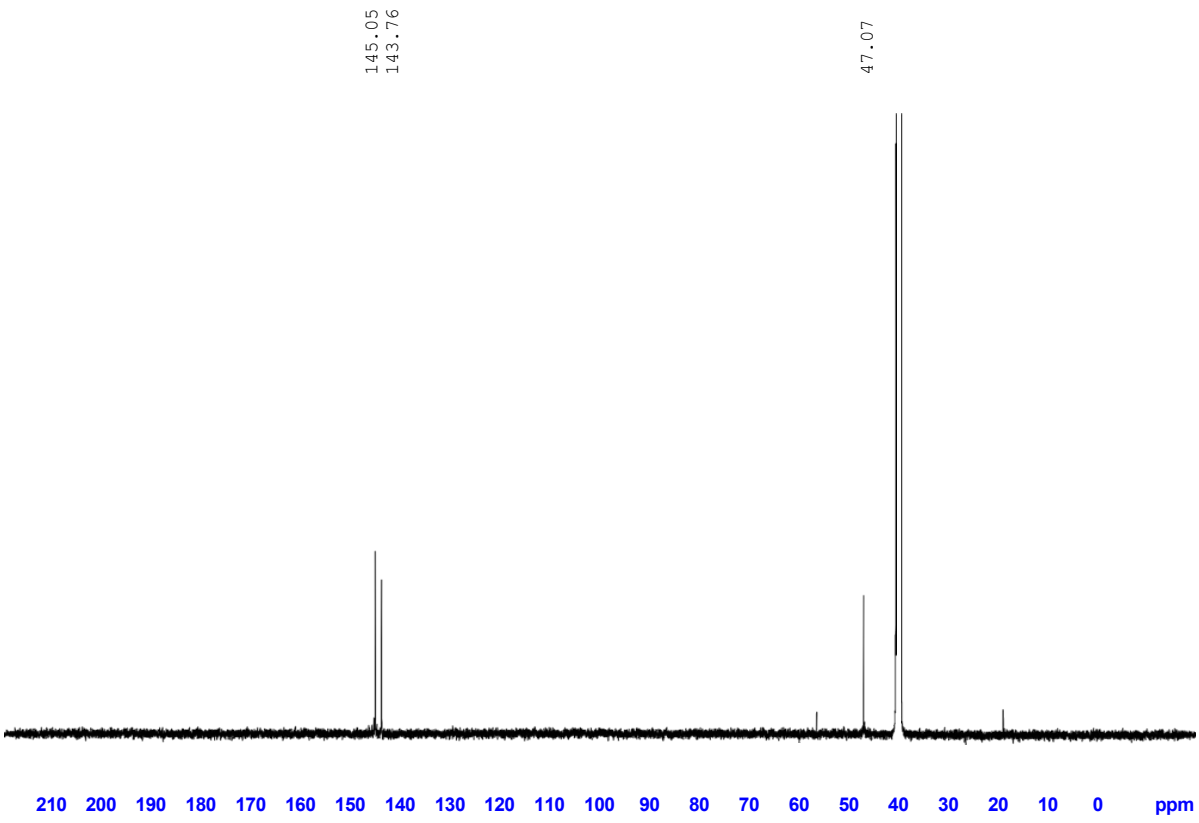


Figure S76. ^{1}H-NMR spectrum of compound **5a (**DMSO-d_6).

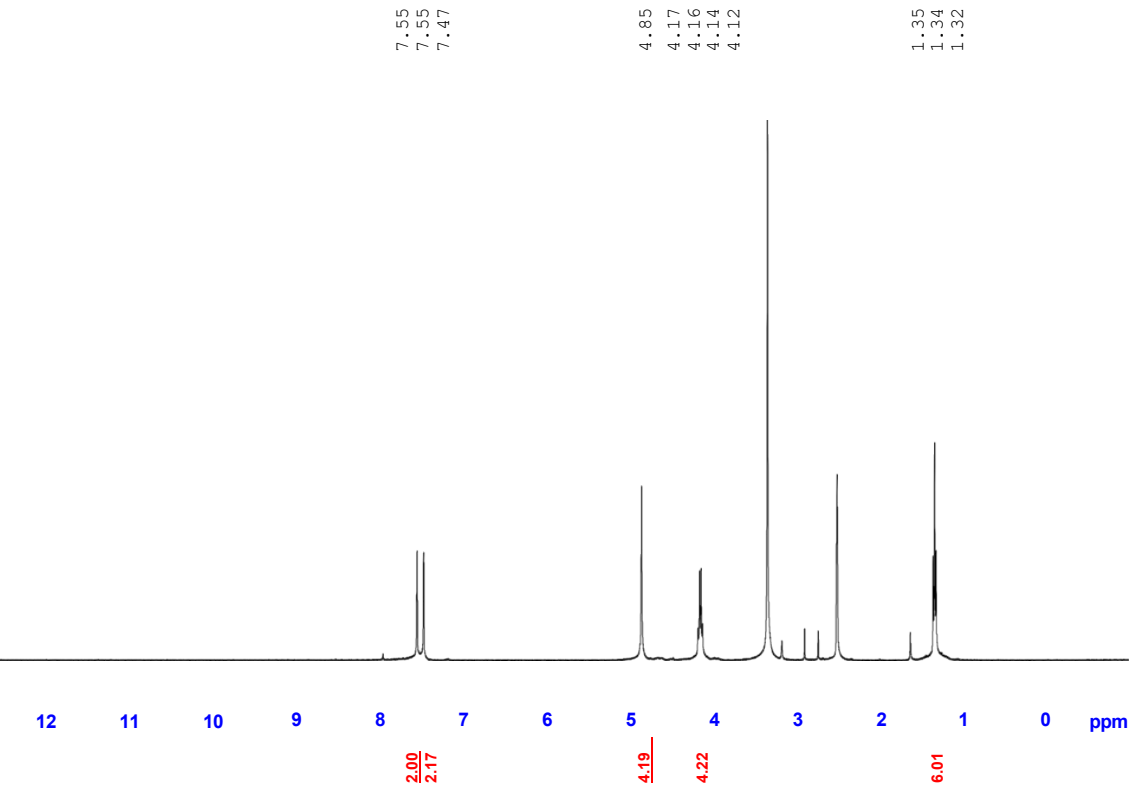


Figure S77. ^{13}C-NMR spectrum of compound **5a (**DMSO-d_6).

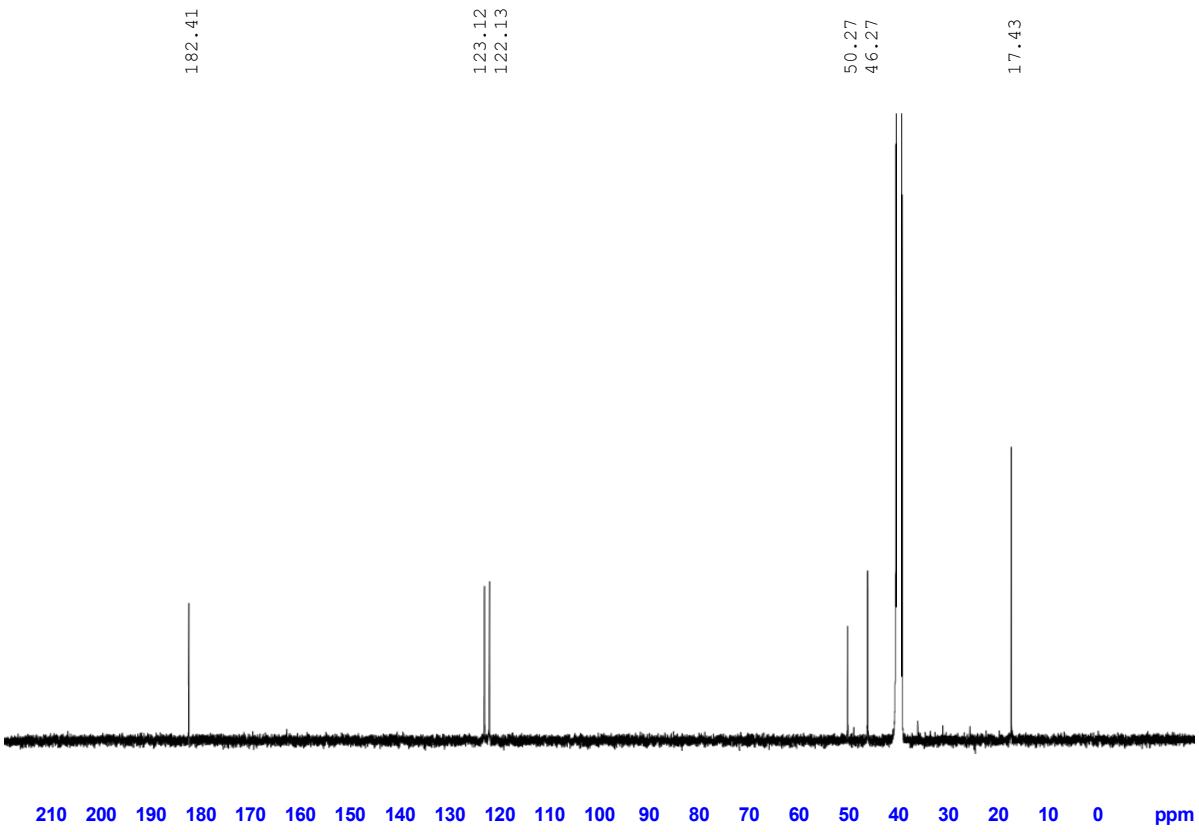


Figure S78. ^{1}H-NMR spectrum of compound **5b (**DMSO-d_6).

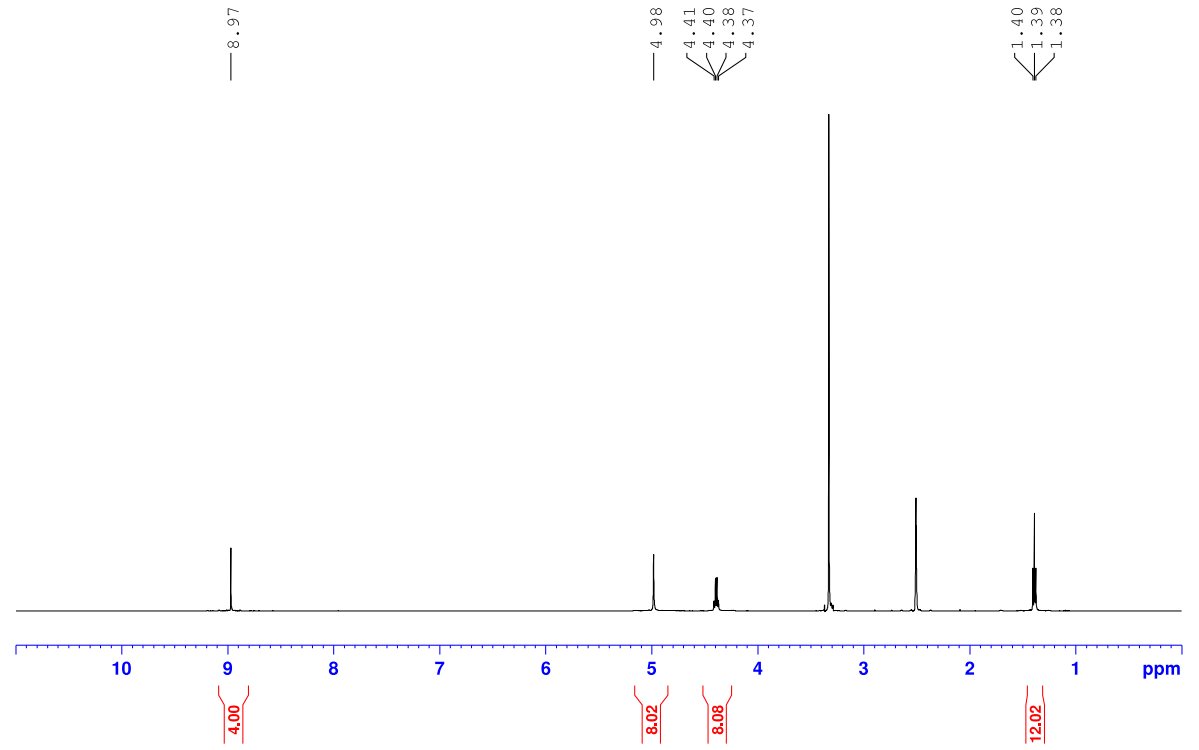


Figure S79. ^{13}C-NMR spectrum of compound **5b (**DMSO-d_6).

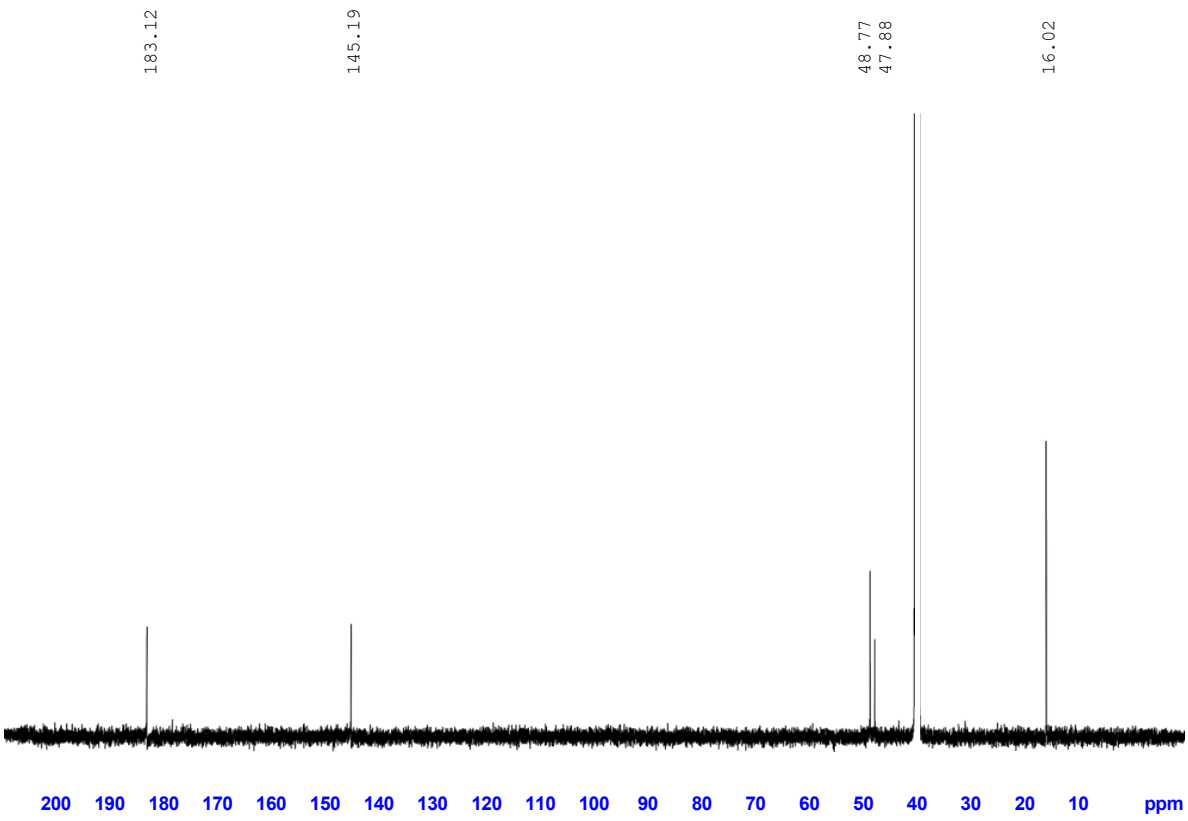

183.12
145.19
48.77
47.88
16.02
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Figure S80. ^{1}H-NMR spectrum of compound **5c (**DMSO-d_6).

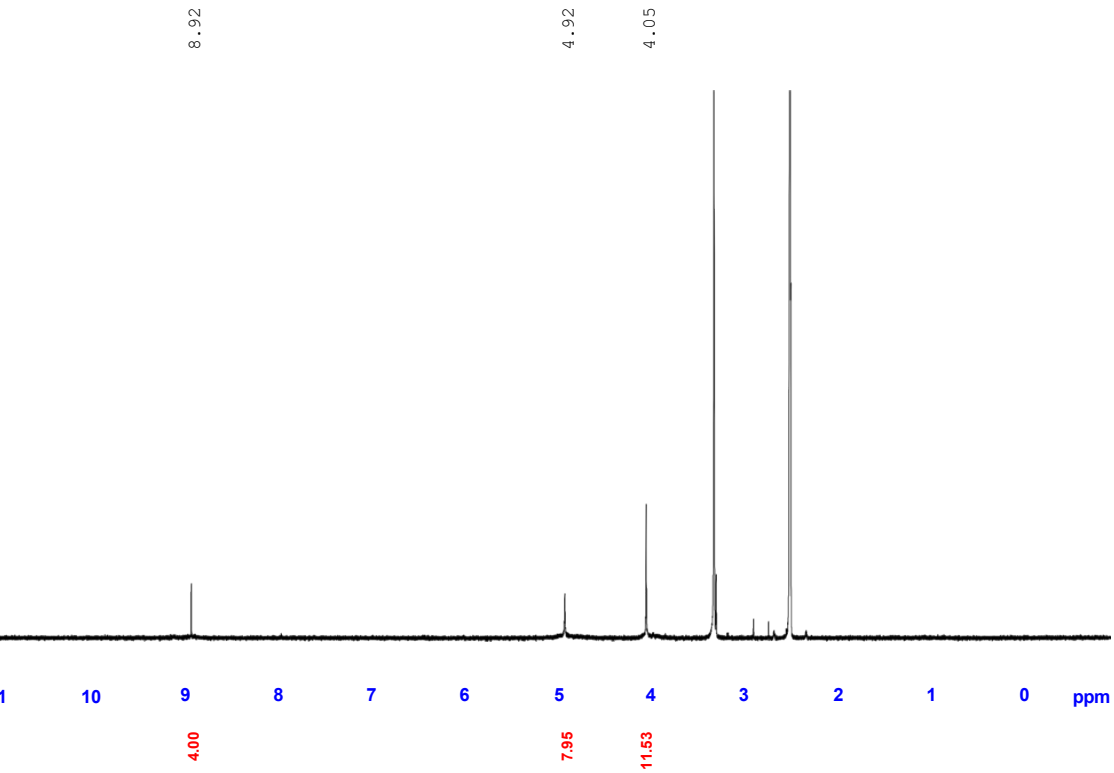
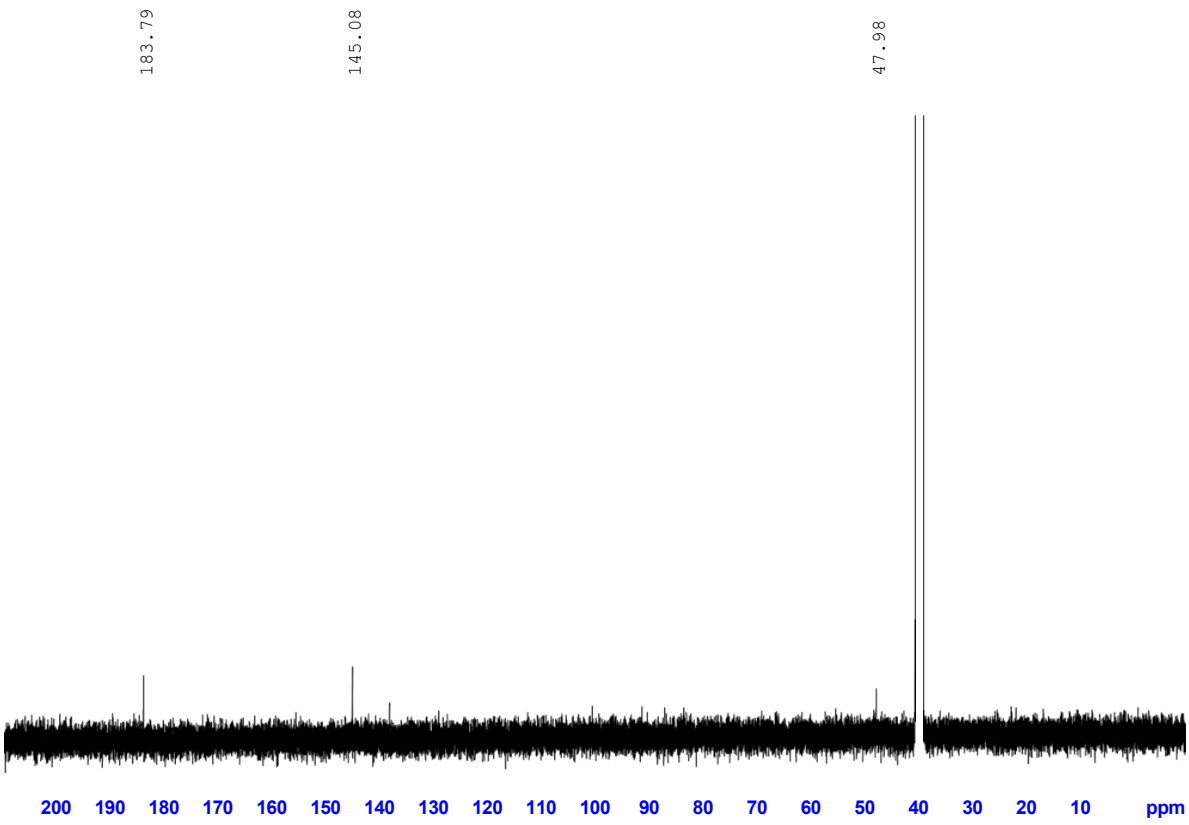


Figure S81. ^{13}C-NMR spectrum of compound **5c (**DMSO-d_6).



High Resolution Mass Spectra and Mass Spectra

Figure S82. HRMS spectra of compound **4a**.

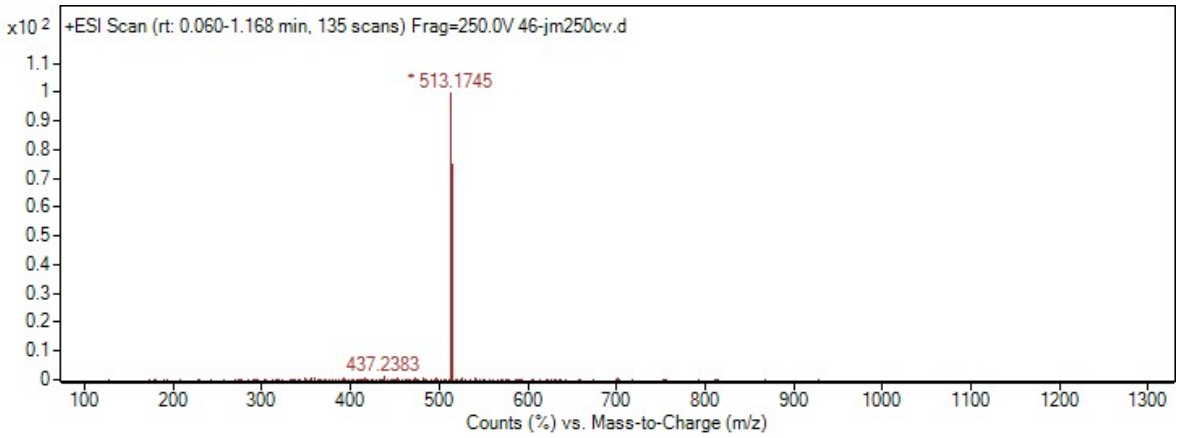


Figure S83. HRMS spectra of compound **4b**.

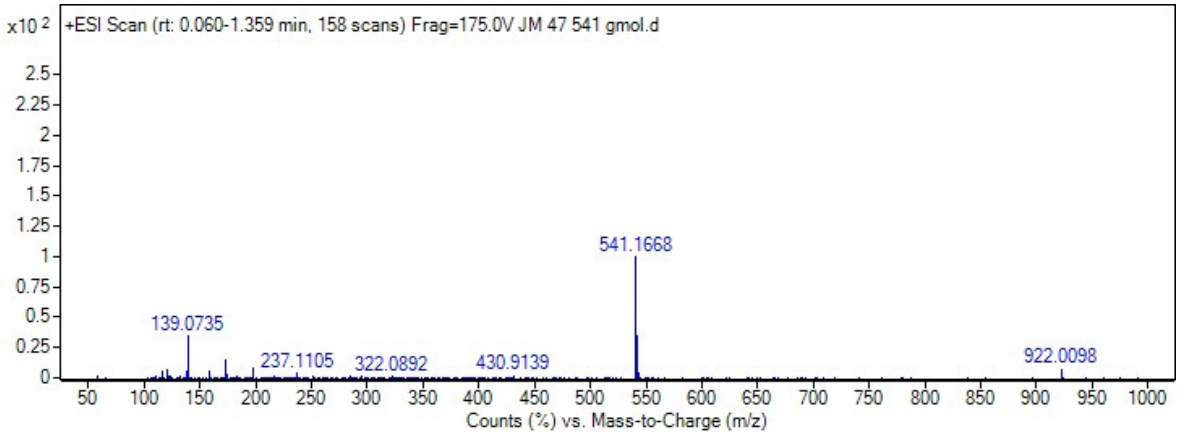


Figure S84. HRMS spectra of compound **4c**.

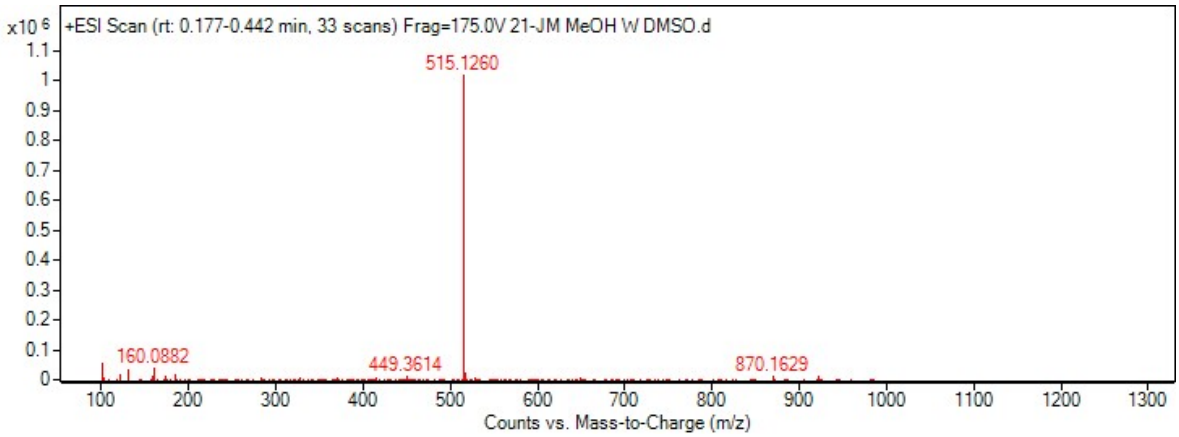


Figure S85. HRMS spectra of compound **4d**.

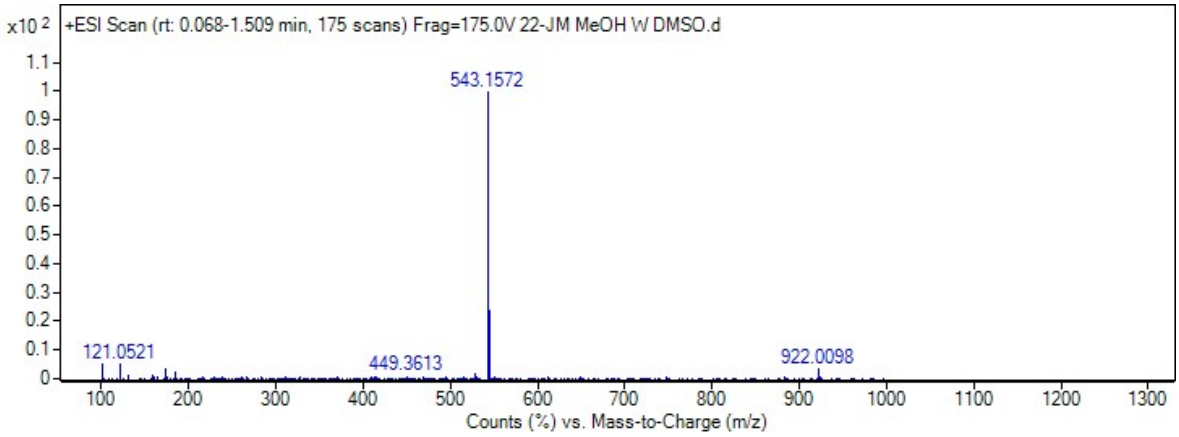


Figure S86. HRMS spectra of compound **4e**.

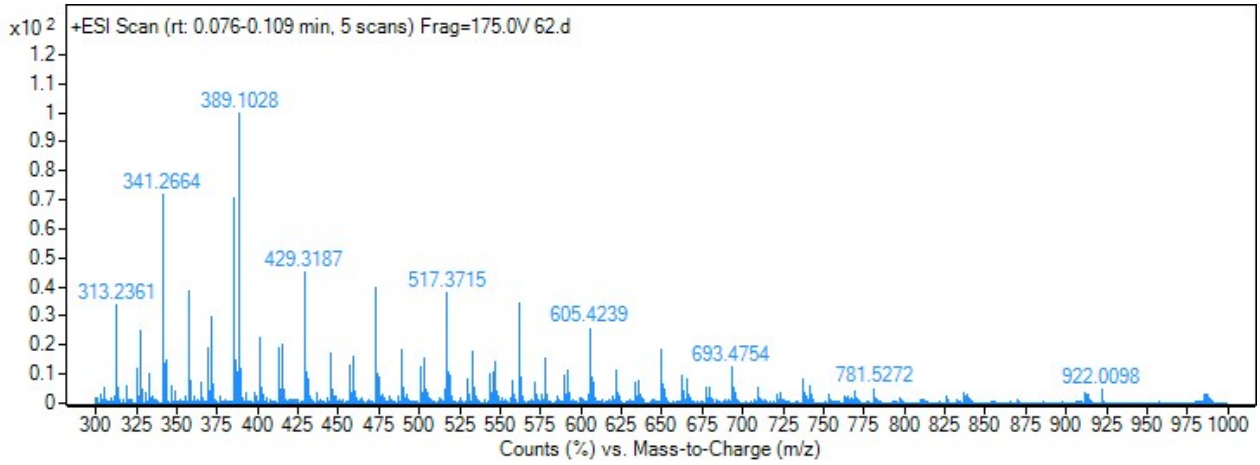


Figure S87. HRMS spectra of compound **4f**.

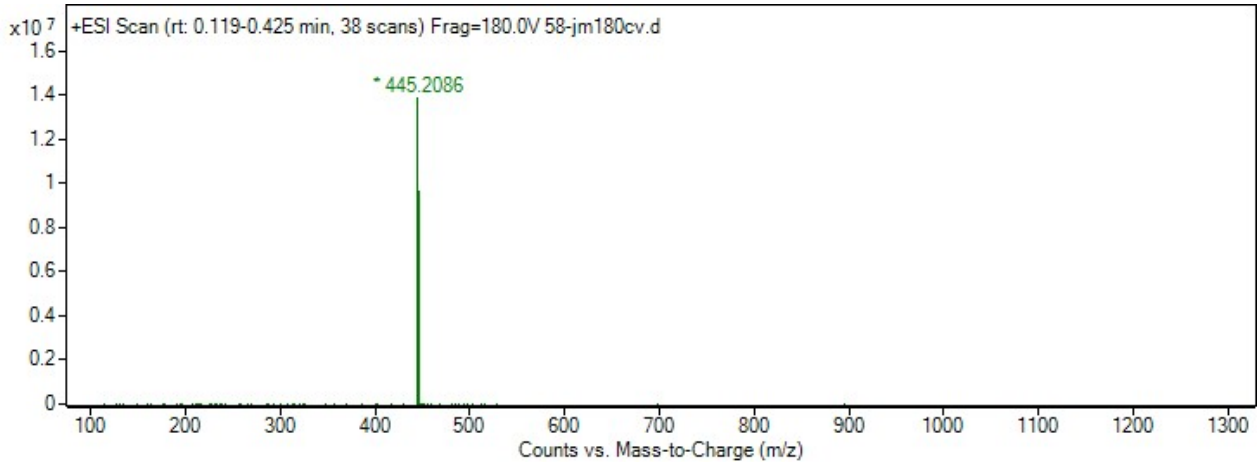


Figure S88. HRMS spectra of compound **4g**.

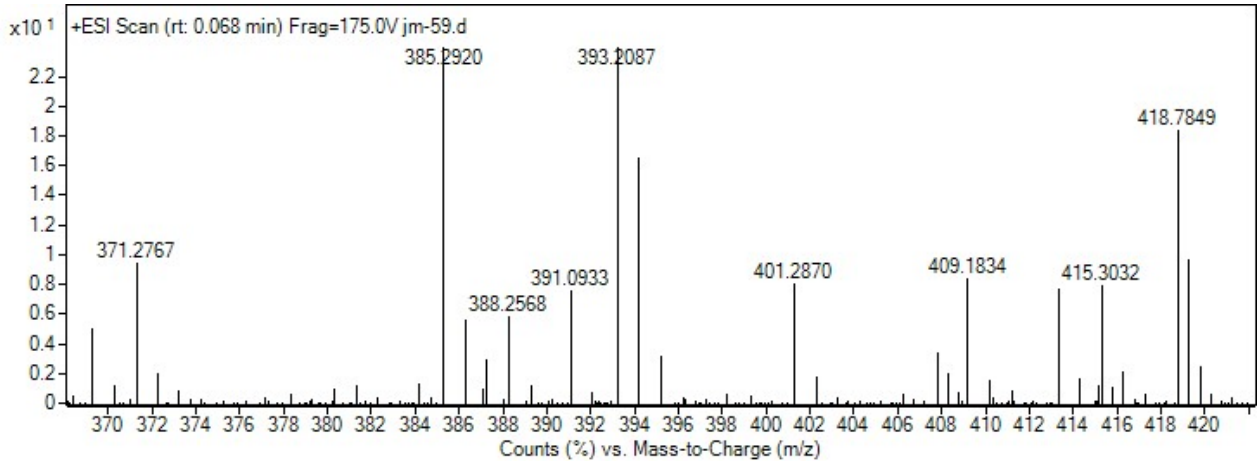


Figure S89. HRMS spectra of compound **4h**.

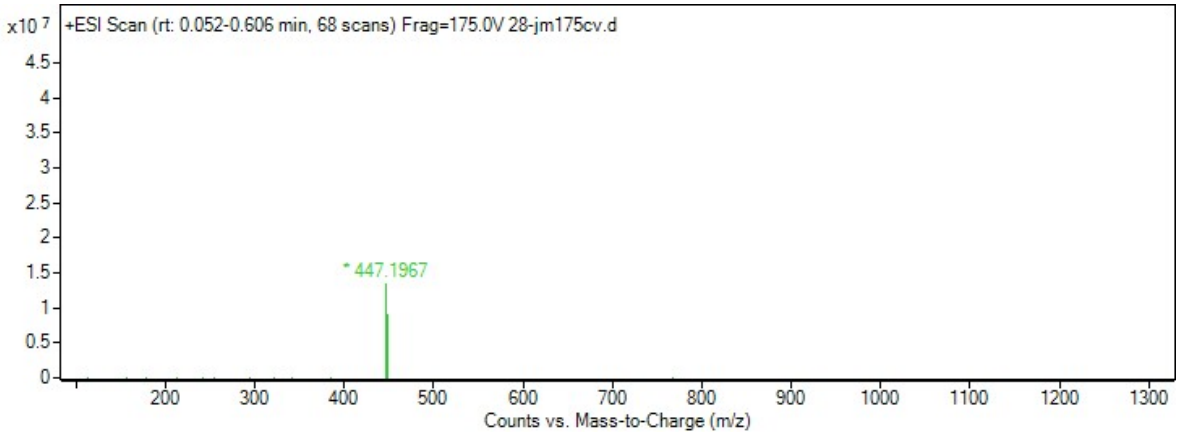


Figure S90. LRMS spectra of compound **5a**.

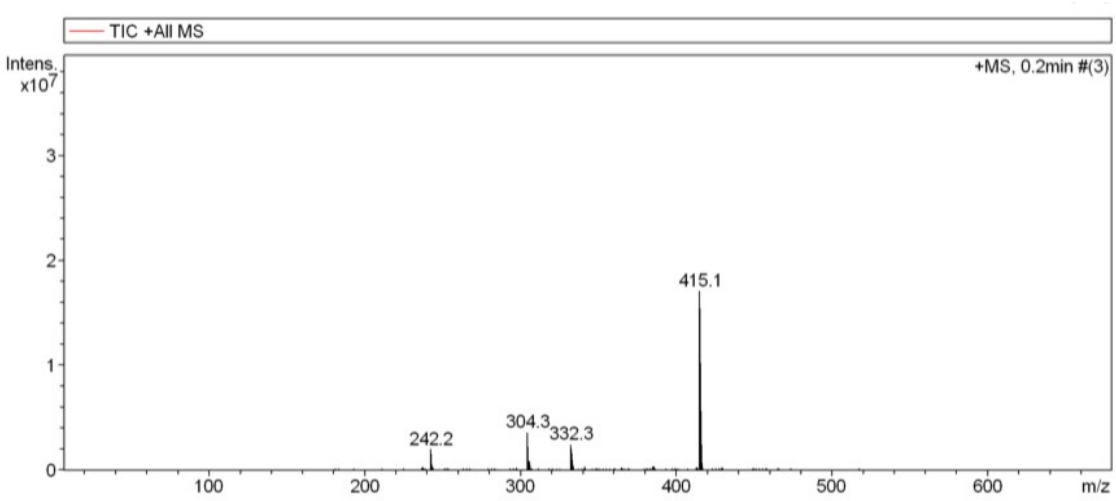
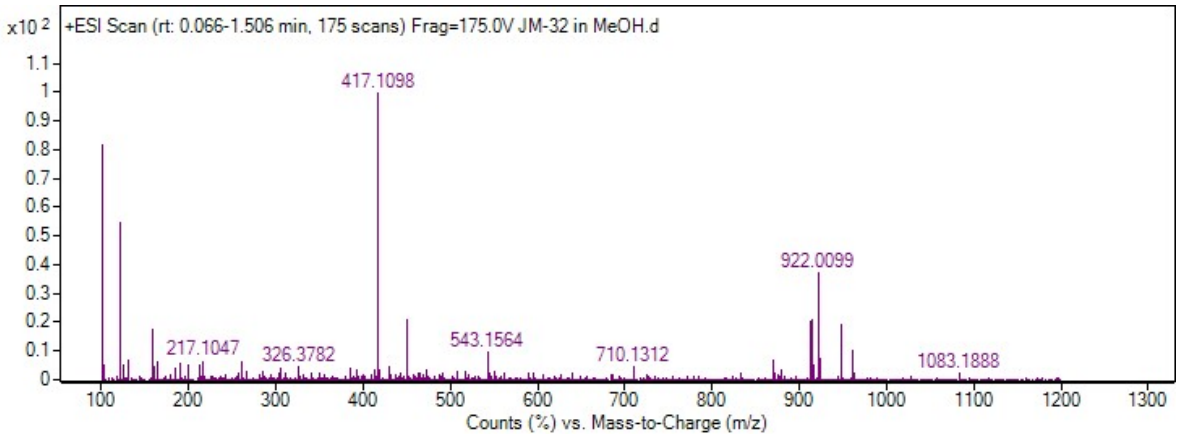


Figure S91. HRMS spectra of compound **5b**.



Computational ESI

The following tables are total energies (Eh) for all species presented in the work. Level of theory for each step shown in table. The solvated free energy is calculated using the following equation:

$$Solvated\ free\ energy = Solv\ Energy + (Free\ energy - Energy)$$

Table S4. Free carbene ligand energies

	PBE-D3BJ/def2-tzvp		PWPB95-D3BJ/def2-tzvpp	
ligands	**Energy**	**Free energy**	**Solv Energy (DCE)**	**Solv free energy (DCE)**
a	-496.111815	-495.973036	-496.361275	-496.222497
c	-512.151355	-512.024047	-512.401736	-512.2744288
e	-304.534703	-304.442796	-304.692637	-304.6007294
g	-320.57445	-320.493747	-320.734439	-320.6537365

Table S5. Bis and mono ligated carbene complexes

	PBE-D3BJ/def2-tzvp		PWPB95-D3BJ/def2-tzvpp	
Complexes	**Energy**	**Free energy**	**Solv Energy (DCE)**	**Solv free energy (DCE)**
3a bis carbene	-1139.1855	-1138.88367	-1139.60546	-1139.303632
3a mono carbene	-642.955803	-642.818132	-643.157185	-643.0195147
3c bis carbene	-1171.24366	-1170.96553	-1171.67295	-1171.394816
3c mono carbene	-658.981388	-658.854644	-659.189313	-659.0625693
3e bis carbene	-756.028806	-755.823043	-756.268047	-756.0622838
3e mono	-451.375937	-451.285833	-451.489583	-451.3994792

carbene				
3g bis carbene	-788.089142	-787.907634	-788.339294	-788.157786
3g mono carbene	-467.402888	-467.324369	-467.523639	-467.4451197
4a bis carbene	-1127.92252	-1127.62079	-1128.33604	-1128.034316
4a mono carbene	-631.697786	-631.560513	-631.856576	-631.7193035
4c bis carbene	-1159.98283	-1159.70389	-1160.40164	-1160.122705
4c mono carbene	-647.723021	-647.596527	-647.886437	-647.7599435
4e bis carbene	-744.794961	-744.588753	-745.00008	-744.7938748
4e mono carbene	-440.131797	-440.042073	-440.190428	-440.1007042
4g bis carbene	-776.856924	-776.674778	-777.06941	-776.8872606
4g mono carbene	-456.158117	-456.078953	-456.22184	-456.1426719

Table S6. Intermediates and Transition states for the decomposition mechanisms for 3e.

	PBE-D3BJ/def2-tzvp		**PWPB95-D3BJ/def2-tzvpp**	
	Energy	**Free energy**	**Solv Energy (DMSO)**	**Solv free energy (DMSO)**
H_2O	-76.3773	-76.3749	-76.4265	-76.4242
AgI_2	-742.6193	-742.6488	-742.3500	-742.3795
3e	-756.0288	-755.8230	-756.2731	-756.0673
3e-AgI_2	-1,498.7743	-1,498.5767	-1,498.6415	-1,498.4439
$TS1_{3c}$	-1,498.7476	-1,498.5516	-1,498.6243	-1,498.4283
$[3e\text{-}I]_2$	-1,498.7704	-1,498.5724	-1,498.6411	-1,498.4432
[3e-I]	-749.3696	-749.2832	-749.3113	-749.2249

[3e-I]$_{H2O}$	-825.7639	-825.6582	-825.7404	-825.6346
TS2$_{3c}$	-825.7311	-825.6243	-825.7075	-825.6008
[Ag-OH].L-H	-825.7391	-825.6310	-825.7191	-825.6109
[I-Ag-OH]	-520.6268	-520.6450	-520.5183	-520.5365
LH	-304.9620	-304.8565	-305.2038	-305.0984
3e.H_2O	-832.4175	-832.1928	-832.7009	-832.4762
TS3$_{3e}$	-832.3863	-832.1605	-832.6698	-832.4440
[LAgOH].LH	-832.4055	-832.1804	-832.6836	-832.4586
[LAgOH]	-527.3887	-527.2894	-527.4837	-527.3844
[LAgH_2O]	-527.8007	-527.6898	-527.9552	-527.8442

Table S7. Intermediates and Transition states for the decomposition mechanisms for 3c.

	PBE-D3BJ/def2-tzvp		**PWPB95-D3BJ/def2-tzvpp**	
	Energy	**Free energy**	**Solv Energy (DMSO)**	**Solv free energy (DMSO)**
3c	-1,171.2437	-1,170.9655	-1,171.6789	-1,171.4007
3c-AgI2	-1,913.9926	-1,913.7236	-1,914.0498	-1,913.7808
TS1 3c	-1,913.9751	-1,913.7052	-1,914.0423	-1,913.7724
[3c-I]2	-1,913.9938	-1,913.7238	-1,914.0526	-1,913.7826
[3c-I]	-956.9783	-956.8551	-957.0130	-956.8898
3c-I + H2O	-1,033.3722	-1,033.2309	-1,033.4430	-1,033.3018
TS2 3c	-1,033.3421	-1,033.1992	-1,033.4125	-1,033.2696
[LAgH2O].L	-1,033.3452	-1,033.2036	-1,033.4121	-1,033.2705
[LAgH2O]	-521.1536	-521.1605	-520.9931	-521.0000
TS3 3c	-1,033.3445	-1,033.2047	-1,033.4091	-1,033.2693
[LAgOH].LH	-1,033.3452	-1,033.2036	-1,033.4121	-1,033.2705
[LAgOH]	-520.6268	-520.6450	-520.5183	-520.5365
LH	-512.5623	-512.4223	-512.8853	-512.7453

Coordinates for calculated structures

Free carbene

a

C	-2.24022097510778	1.64735111619209	-0.10726786016784
N	-1.02078735402482	2.29610454781694	-0.10880984384869
C	0.05845182716848	1.41221334896967	-0.07463825803467
C	-0.47942237215058	0.16444655151147	-0.04883853138972
N	-1.86027416724611	0.33840489738282	-0.07112600199661
H	1.09332431791449	1.72891518693042	-0.03306395642677
H	0.00018126338848	-0.80757457565880	-0.00796592534005
C	-2.81604596934260	-0.75443293017166	-0.06905342071048
H	-3.81762292354632	-0.31287249436351	-0.06669767824932
H	-2.68772916334322	-1.38031864751338	0.82594486107173
H	-2.69387037152429	-1.38064168954803	-0.96473912869491
H	-0.61311699018178	7.59074861942290	-0.23143837818412
C	-0.69419852173700	6.50324539314674	-0.20920996160135
C	-1.85834155380010	5.89121097046887	0.26459630118636
H	-2.69150145639477	6.50134847917517	0.61726494034354
C	-1.96649235683511	4.50301370418321	0.30139222938812
H	-2.86414987707605	4.00253556846828	0.66261573418094
C	-0.90247544047234	3.71275954202238	-0.14910050239026
C	0.26114779913482	4.31836945033494	-0.63603636284564
H	1.07829561665361	3.70895097329379	-1.02261603076477
C	0.36218644540381	5.71032322652069	-0.65880126373554
H	1.27194380661920	6.17449352761497	-1.04275376688993

c

C	-2.19383852661069	1.68517912707436	0.02084834259893
N	-1.02263236681364	2.34807443827517	-0.18865596943466
N	0.08035334400748	1.54750206848540	-0.45683763830474
C	-0.42649859363749	0.34587541144394	-0.41240380837713
N	-1.77542805642577	0.38882965126536	-0.13036161018660
H	0.14439749433114	-0.56339207319891	-0.57581289414163

C	-2.65114031100171	-0.76557111568495	-0.01212003566627
H	-3.64327573232527	-0.39582398585548	0.26423295379244
H	-2.28525377944125	-1.45026892755603	0.76533762717678
H	-2.71540760858242	-1.30409171078994	-0.96788764385860
H	-0.42503757921083	7.61837396474308	-0.04343726485716
C	-0.54563649879525	6.53465477799329	-0.07371955719236
C	-1.79867026695060	5.95863756629247	0.15368253608070
H	-2.66241310771590	6.59181413400062	0.36259695982066
C	-1.96138574859704	4.57550282356760	0.11675221689110
H	-2.92780240416454	4.10418066901640	0.29077892179560
C	-0.85471618741227	3.76210069906547	-0.15120129381880
C	0.40418775786927	4.32478057871832	-0.38048942949354
H	1.25070739494070	3.67261292009265	-0.58700649624141
C	0.55001498826839	5.71185348257578	-0.33993446902975
H	1.53323737696770	6.14980407807538	-0.51899091585353

e

C	-5.72390485691747	3.19497309347027	-1.81574371401401
N	-5.95172675366701	4.07157534772028	-2.84523190889514
C	-7.29589053585254	4.37981810961843	-3.01388413393855
C	-7.96452719597403	3.67611961395203	-2.05800095390127
N	-6.99545001988785	2.97331237860612	-1.35287805461776
C	-4.88245145130648	4.61659981282155	-3.66073890128932
H	-7.66236184711166	5.05622085991221	-3.77871674406353
H	-3.94591408883197	4.16972762954287	-3.31155079175480
H	-4.82632374481124	5.71007648700995	-3.55502543309924
H	-5.03376397555543	4.36770880695927	-4.72127167463430
C	-7.28002438021749	2.08806449316356	-0.23898716961987
H	-6.32333684212180	1.68711350240584	0.11131433194992
H	-7.93040361052687	1.25862136465482	-0.55344086230189
H	-7.76937595072617	2.63453883576880	0.58056560686261
H	-9.02428133629196	3.62209494689397	-1.83262895148282

g

C	-2.18011165317003	1.62719896086524	-0.42851769024726
N	-1.33666302570011	2.07570520570196	0.52986535260950
N	-0.20776173526759	1.30732145310757	0.75997473554121
C	-0.35639335548292	0.33099016851888	-0.09776659377811
N	-1.51589346823150	0.48545271253841	-0.82265792675819
H	0.34488364673747	-0.48956338374022	-0.21854005171602
C	-1.99555661223159	-0.41568559200891	-1.85647885205197
H	-2.91795514225731	0.01309120230765	-2.26051813647501
H	-2.20895090608057	-1.41032404658342	-1.44027138963007
H	-1.25482683529255	-0.51318273965924	-2.66234714071798
C	-1.51955301553949	3.27736615687545	1.31821974456168
H	-2.45614936301406	3.74175103395088	0.99527968192959
H	-0.68129704714317	3.96809383394313	1.15587362577748
H	-1.57272524772658	3.02534986098261	2.38582028525514

3a bis carbene

C	-2.18987538247691	1.62506155120274	-0.32736418001034
N	-1.03822445711579	2.30930093058582	-0.05540091671794
C	-0.00794602889724	1.44338606765805	0.28212631138999
C	-0.52965547175398	0.18634350702815	0.23101751324585
N	-1.85770569112652	0.32100088420750	-0.14016230085030
H	0.97946190125143	1.79568168315469	0.55421076637740
H	-0.07525741705280	-0.77638056253943	0.43357188788253
C	-2.77053124157630	-0.79942708206363	-0.33128279991161
Ag	-3.97981056353038	2.44272861957070	-0.97867326204857
C	-5.75765252795295	3.24807553171360	-1.67637599930390
N	-6.02606928752741	4.51427590062125	-2.08938294436973
C	-7.32434839072803	4.62759796974894	-2.55974204724217
C	-7.89398493451127	3.39652237903644	-2.43755690746433
N	-6.92439931915705	2.56864770978395	-1.89007314689877
C	-5.06410235025547	5.60951365454475	-2.07290873933122
H	-7.73196295995292	5.56172756403375	-2.92796827212849
H	-8.89589104076323	3.04885410139119	-2.65761142716812
H	-3.76030629027829	-0.40277183238548	-0.58386777226652

H	-2.83940444992166	-1.38866421629270	0.59222744799354
H	-2.41656717260116	-1.44126414205538	-1.14839719841982
H	-4.14621061869887	5.25945285533295	-1.58744519051515
H	-5.47303861415348	6.45803085084966	-1.50955345550418
H	-4.83443618100876	5.92846885152032	-3.09790401165762
H	-0.59579428315093	7.58704440936269	-0.34402539831783
C	-0.68840276678055	6.50217382978002	-0.28522645201462
C	-1.72439976299633	5.92753521683459	0.45513506699392
H	-2.43496055028649	6.56126933900472	0.98733446409500
C	-1.83913565726312	4.53953063455700	0.54398907386720
H	-2.62029279709284	4.07744019892212	1.14840522181151
C	-0.91465228650185	3.73359854304164	-0.12612141606448
C	0.12680525916450	4.29725263723611	-0.86542034507716
H	0.83003267554450	3.65310836274963	-1.39506503015531
C	0.23794626629538	5.68634173436143	-0.93877774262951
H	1.04814718834188	6.13103307190082	-1.51724900627111
C	-7.11060493320181	1.17992353859748	-1.59714717661648
C	-7.62363609943000	0.33285361068954	-2.58113578743763
H	-7.86527055509251	0.72809849365098	-3.56874071028663
C	-7.79568726543714	-1.02182748654017	-2.29377747173897
H	-8.19354809824486	-1.68765314270844	-3.06005691755280
C	-7.45044834276744	-1.52426173060403	-1.03710009310195
H	-7.58894403249130	-2.58319884210621	-0.81698201198547
C	-6.94142308355921	-0.66699499549254	-0.05853863021895
H	-6.69388998952947	-1.05100191545184	0.93192577280040
C	-6.77492268740208	0.69146368996008	-0.33145544691053
H	-6.41336083472905	1.37855386100639	0.43414505263102

3a mono carbene

Ag	-4.04188195824773	2.35344892345727	-1.00514313386690
C	-5.76541805603049	3.24857755501466	-1.70757956920495
N	-6.01773065124926	4.52014586031543	-2.09762956964591
C	-7.32749486728363	4.64154175348155	-2.53184019899928
C	-7.90403085990135	3.41264633837297	-2.40425979838213

N	-6.93117984849109	2.56994547242965	-1.88976147010145
C	-5.05143068127722	5.61389351223837	-2.09613124622370
H	-7.73569626603858	5.58221155880863	-2.88295898824783
H	-8.91321802455797	3.07250025043492	-2.60282854542229
H	-4.11582468162074	5.25261810762219	-1.65661950838908
H	-5.43499268922069	6.44856987792064	-1.49663978590466
H	-4.86484359218026	5.95230938852100	-3.12299914673931
C	-7.11436515273433	1.17729666552403	-1.59636088317303
C	-7.59460566119850	0.32636212491105	-2.59248689738179
H	-7.81759632126673	0.71696123723730	-3.58630380664086
C	-7.75749482107664	-1.02906935603862	-2.30382949721600
H	-8.12857242780855	-1.70208489491675	-3.07705334508805
C	-7.43484912562378	-1.52403852096487	-1.03784835869267
H	-7.56279485202821	-2.58451429345412	-0.81978709366191
C	-6.95977636602056	-0.66138421525251	-0.04776823232885
H	-6.73153170124683	-1.04173764090439	0.94824863188691
C	-6.80401879609106	0.69927225714609	-0.31939290548350
H	-6.49429530900575	1.39437910709552	0.46291452490723

3c bis carbene

C	-2.16575903499210	1.67629356492085	-0.33686302544887
N	-1.02743252511724	2.35964621861372	-0.07395937513680
N	0.04806655074137	1.55651909458536	0.21313358113135
C	-0.44719105861714	0.34760828389475	0.14019003790817
N	-1.78283981828372	0.37561271643004	-0.18339483675228
H	0.11959355005213	-0.56126023595266	0.31686917229653
C	-2.63983135259874	-0.79245660309350	-0.36598579594525
Ag	-3.98721723101717	2.44859530975210	-0.95814069317462
C	-5.77714662963697	3.19998103377286	-1.68611638004967
N	-6.06638878027152	4.44814446184407	-2.15562498997243
C	-7.35390413089086	4.44731498373075	-2.63701939149653
N	-7.91204854747964	3.27239874566759	-2.49512113469275
N	-6.92906031983611	2.52215743074369	-1.89932616319343
C	-5.15029190333890	5.58504640003874	-2.17471832265552

H	-7.84341047553028	5.31234302257906	-3.07360978948862
H	-3.66205679126932	-0.44638575988254	-0.55370349236774
H	-2.62503410696375	-1.41092034400565	0.53988709644668
H	-2.29391953870861	-1.38489530358874	-1.22227442482632
H	-4.22375862681271	5.29198325181699	-1.66912540755276
H	-5.59987903169894	6.43536021225764	-1.64728945149006
H	-4.92453900741135	5.87100910377814	-3.20966348294214
H	-0.43017435318275	7.62153737800584	-0.19800968814910
C	-0.55505822358618	6.53868868539273	-0.17073358572020
C	-1.69729068601194	5.98152437879653	0.40887961769697
H	-2.45727927671020	6.62571853114060	0.85281746577573
C	-1.85424457179852	4.59592927631658	0.45923248658403
H	-2.71589507585036	4.14738650205078	0.95525801592840
C	-0.86290241584652	3.77996725938199	-0.09214329859530
C	0.29080234503060	4.32184171730281	-0.65959601524444
H	1.05671996077402	3.66023079861824	-1.06288184579164
C	0.43875311151929	5.70795336557893	-0.69459816185847
H	1.33673490023840	6.14008905321723	-1.13675339630455
C	-7.17946055688306	1.14887445639511	-1.58894214678063
C	-7.87773340180903	0.36323388266527	-2.50651966950673
H	-8.23791084360330	0.80708819198911	-3.43401881136503
C	-8.10234703786995	-0.98091983899975	-2.21120865023486
H	-8.64637098838648	-1.60240602082551	-2.92283309170823
C	-7.63285588861387	-1.53013159898749	-1.01534076785615
H	-7.81616801076715	-2.58098297675702	-0.78948279307904
C	-6.94955962795305	-0.72744799105820	-0.09888032622064
H	-6.61520614336795	-1.14343178958814	0.85235041926515
C	-6.72562338200025	0.62146943979285	-0.37712474555511
H	-6.23996824393995	1.27054255976810	0.35258835362296

3c mono carbene

Ag	-4.05260814015702	2.33343213430612	-0.98862572733022
C	-5.78455946868523	3.19795588774867	-1.71949826105707
N	-6.05946421373975	4.45539403738066	-2.15980186397438

C	-7.36208944684430	4.46968684749240	-2.59917291503738
N	-7.92823514711302	3.29759669659261	-2.45100852889566
N	-6.94166127498276	2.52698379768032	-1.89581575595909
C	-5.13596311655919	5.58789465983815	-2.19645914501964
H	-7.85532064261571	5.34456858173216	-3.01190986422696
H	-4.19486612008091	5.28560432857240	-1.72651959335427
H	-5.56276430097515	6.43211219271157	-1.64192475512549
H	-4.94636832986400	5.88357702351599	-3.23554319933822
C	-7.18854828538838	1.15084089712755	-1.58561668008227
C	-7.85826641805420	0.35797124816579	-2.51693601217680
H	-8.20410203892687	0.79376665517100	-3.45383156526008
C	-8.06878060487504	-0.98862112095826	-2.22197835361263
H	-8.58881270038534	-1.61991956243582	-2.94267893300312
C	-7.61237286609555	-1.52902877353893	-1.01671335604445
H	-7.78091489406620	-2.58299306017872	-0.79477636446762
C	-6.95948257323932	-0.71780913809018	-0.08627432584378
H	-6.63618561369220	-1.12926529274668	0.87016357565984
C	-6.75182258158698	0.63473971117111	-0.36156762713432
H	-6.31766003117282	1.29573451914207	0.39132181498362

3e bis carbene

C	-2.14060598705824	1.62315679959411	-0.46746850705626
N	-1.32689548351427	2.11623192774529	0.50707058872441
C	-0.21163133876129	1.31662817570336	0.68036169339168
C	-0.32618677782563	0.29139798136729	-0.20987265424153
N	-1.50776967216556	0.49701575548648	-0.89895585773141
H	0.32462571097489	-0.55264771650324	-0.40601195377982
C	-2.00337433083876	-0.38676384078126	-1.94661860400772
Ag	-3.94072848961592	2.41319171965136	-1.14357635415576
C	-5.74019206355699	3.20257344971627	-1.82151995058427
N	-5.93517520987610	4.07263321597680	-2.85100182229942
C	-7.27694112079803	4.36948244626295	-3.00845295287461
C	-7.94565978517579	3.66626197172324	-2.05186761846363
N	-6.99128379166009	2.96237132947015	-1.33987703317476

C	-4.87473063738293	4.63223943521836	-3.67961971789077
H	-7.63939823861834	5.04464089337707	-3.77475391094946
H	-2.94397100638179	0.02447027940968	-2.32926193976849
H	-2.18441224936383	-1.39066666585166	-1.54143108313417
H	-1.27460296077939	-0.44863593849582	-2.76489767598836
H	-3.92191154083444	4.19367218503037	-3.36346672634884
H	-4.83148043010267	5.72210765052075	-3.55614964788449
H	-5.05336636972868	4.39060043075050	-4.73509995196172
C	-1.58734927793141	3.32876904495794	1.27261927782586
C	-7.29692535349223	2.07839748103726	-0.22209310532088
H	-2.53692300476491	3.75416748615263	0.93003425810131
H	-0.78333796197002	4.05844623096174	1.11202559756757
H	-1.65948658579431	3.09318232773126	2.34215528475504
H	-6.35661414135676	1.66171799875032	0.15521114946639
H	-7.94966113997998	1.26047036335845	-0.55318986240298
H	-7.79275409771628	2.64023414782705	0.57983944657511
H	0.55855023178697	1.53897169472026	1.40961404675195
H	-9.00364266941713	3.60916228343097	-1.82417765073992

3e mono carbene

Ag	-3.96008622643690	2.42502435792149	-1.14841324385542
C	-5.74851677142449	3.20535838265984	-1.82533604081455
N	-5.92611028630003	4.07328078836841	-2.85268200410721
C	-7.26923164084685	4.36781116896428	-3.00463871666057
C	-7.93820366272607	3.66408687119837	-2.04788574016888
N	-6.98807719422861	2.95638110124769	-1.33359016815455
C	-4.86961032418851	4.63674667277526	-3.68753197335501
H	-7.63132049803351	5.04413819824332	-3.77029686539405
H	-3.91019243450776	4.20744233527822	-3.37873888019020
H	-4.83487777540200	5.72636496300118	-3.56446923090452
H	-5.05345155847710	4.38865415224365	-4.74003595911438
C	-7.30201994297555	2.07186467565561	-0.21568498572173
H	-6.36855405190411	1.64865590709916	0.17119377003972
H	-7.95501680049789	1.25781661302409	-0.55385705897072

H	-7.79904009283620	2.63847846488745	0.58133458569369
H	-8.99615581861439	3.60765234963194	-1.81916319732160

3g bis carbene

C	-2.16362802303153	1.62015756747009	-0.42315001488924
N	-1.34230204362095	2.09172502665786	0.53638085273483
N	-0.23383693101746	1.32095246618844	0.74866493099318
C	-0.37355792625362	0.33965445324286	-0.10676819932211
N	-1.52804708480988	0.48195557112958	-0.83644681800387
H	0.32834386266434	-0.47975598007952	-0.22667133849456
C	-1.99600819294944	-0.43567311452380	-1.87100468492287
Ag	-3.95478899010708	2.42799063710861	-1.10212050687113
C	-5.74809946676932	3.23296904382676	-1.77822847614436
N	-5.95624407675515	4.11596117458610	-2.80156453591842
C	-7.30318159861690	4.36702860945941	-2.89166698855631
N	-7.96847590091448	3.69481931716915	-1.98621868584843
N	-6.99467282463184	3.00853044225601	-1.31642374463336
C	-4.92386227940709	4.71043004598485	-3.64538005382486
H	-7.75317668988958	5.03450470666408	-3.61999531871337
H	-2.91728306109053	-0.02943077307049	-2.30128706955292
H	-2.20244550216340	-1.42161480612224	-1.43630451953259
H	-1.23865846786680	-0.53124267736214	-2.65868569212076
H	-3.97051746316495	4.22083028043858	-3.42111500320207
H	-4.83770750825313	5.78483290516737	-3.43975704648440
H	-5.17117577029463	4.55622186707467	-4.70261775394903
C	-1.51513627206743	3.29461371358014	1.33605946168514
C	-7.38883589639582	2.13803708453889	-0.21936533590804
H	-2.44939197818568	3.77791292236757	1.03224779327537
H	-0.66834455420113	3.97041322367486	1.16721244597761
H	-1.55865758579985	3.02389723357900	2.39768849643045
H	-6.48640024013856	1.67854694555156	0.19688924094969
H	-8.06854281119332	1.36340570554257	-0.59384797662347
H	-7.89961389247466	2.72946240739915	0.54974397886995

3g mono carbene

Ag	-3.94684297611960	2.69108182679747	-0.92867724068053
C	-5.75281416387603	3.29673917514705	-1.73129235450767
N	-5.95070330099001	4.10056296530781	-2.81478064125280
C	-7.30471579454447	4.23756520660535	-2.98976604036455
N	-7.96903859773567	3.56729286885557	-2.08028014414524
N	-6.99452624642004	2.99544463048991	-1.31550892677178
C	-4.90902249927996	4.71021245980303	-3.64060267799998
H	-7.75981373393742	4.82603675182326	-3.78058833742823
H	-4.27600805916464	3.93079772521044	-4.08091715071426
H	-4.30108914734851	5.39321917736354	-3.03541926471653
H	-5.38914553342758	5.27675364608809	-4.44531145190051
C	-7.39391333683891	2.16241491317103	-0.18900510850219
H	-6.49284440442747	1.79050302957628	0.30916703975270
H	-7.99482686118282	1.32279689612653	-0.55726166221963
H	-7.98999075380677	2.76214990053460	0.50857575475124

4a bis carbene

C	-2.16869446884915	1.66838851408239	-0.44934814082881
N	-1.03831785838481	2.36005901945012	-0.10817268207297
C	-0.00201334158199	1.49014384465155	0.19731881434668
C	-0.49555309570619	0.22964049017028	0.05398095076488
N	-1.81622135390914	0.35857513518915	-0.33815438975994
H	0.97192123802488	1.84261205692767	0.51451440085728
H	-0.02520036690092	-0.73495069763314	0.20553450685117
C	-2.69641456617857	-0.77076260808856	-0.61918186212845
Au	-3.94836124524844	2.42622184296723	-1.08308535305754
C	-5.71326642663719	3.16943472890688	-1.77335331170959
N	-5.95734235768018	4.41731889263389	-2.25857685355252
C	-7.26164124051659	4.53152296326942	-2.70621444976995
C	-7.85786142630127	3.32615595356169	-2.49503969996211
N	-6.90049869631347	2.50459408212679	-1.91848446710198
C	-4.97398802806600	5.49286570890859	-2.33202920052780
H	-7.65509759826800	5.45117973158787	-3.12341013391111

H	-8.87300231807818	2.99214954021047	-2.67201043379365
H	-3.69290622182979	-0.38384033754411	-0.85876145575477
H	-2.75977721936688	-1.42278379377903	0.26159788801505
H	-2.31291130272142	-1.34532845642069	-1.47248249256443
H	-4.05231866813585	5.15567520616160	-1.84535928004950
H	-5.35584662617341	6.38252679431921	-1.81489029379571
H	-4.76327278679620	5.74174186531141	-3.38041271317335
H	-0.53978533251397	7.64247015197028	0.06854918189031
C	-0.64956450315451	6.55816838928206	0.02591509482875
C	-1.67486166878332	5.93051126320619	0.73800963710164
H	-2.36076829582034	6.52137862372786	1.34664436120542
C	-1.81219942046726	4.54179777270332	0.69864327820076
H	-2.58832334832043	4.03851446915826	1.27594053941005
C	-0.91946199336014	3.78989167461972	-0.07008522924294
C	0.10984348622772	4.40703883526427	-0.78546475969374
H	0.79004037718723	3.80627034872562	-1.39131008543515
C	0.24245211566459	5.79542989097210	-0.73162339063447
H	1.04379676574572	6.28124097415421	-1.28950560587437
C	-7.14175909057432	1.14271082465580	-1.53496706229422
C	-7.66300468294197	0.25181998963887	-2.47664102053718
H	-7.84937157565464	0.58520682839429	-3.49878122024471
C	-7.92075778563032	-1.06724303050426	-2.10002683436513
H	-8.32653109772219	-1.76617507199637	-2.83231203813677
C	-7.65406118891160	-1.49100834972840	-0.79594658596598
H	-7.86084049613946	-2.52154141051523	-0.50470825466584
C	-7.13356536139970	-0.59137380450069	0.13786689039770
H	-6.94319459119721	-0.91393184354425	1.16244314761621
C	-6.87973107838422	0.73261138138816	-0.22485240240305
H	-6.50412638493083	1.45151745115748	0.50383138242180

4a mono carbene

Au	-4.03948931035729	2.38672220151081	-1.18836156773296
C	-5.72903742051179	3.16594688504320	-1.81733563645506
N	-5.94294818271672	4.42407383256629	-2.26830145705496

C	-7.26578628379151	4.55467773876297	-2.65495179075441
C	-7.87234569440743	3.35457945669849	-2.43224043167765
N	-6.91163078702725	2.50323479807735	-1.90881477426555
C	-4.94704131506743	5.49057539859016	-2.36792362076721
H	-7.66038010927633	5.48629623687260	-3.04425055835865
H	-8.89850783125500	3.03594959335255	-2.57210206764206
H	-4.00671002184909	5.13432725417458	-1.93473447772897
H	-5.29486900361089	6.37010929282391	-1.81256232222303
H	-4.78893456532394	5.75421853500807	-3.42112654064259
C	-7.14988838213436	1.13368645271072	-1.52634182156948
C	-7.61035038462318	0.23507168785827	-2.49061875522495
H	-7.75760713827384	0.56062669084888	-3.52156348308261
C	-7.85679364983078	-1.08678023539127	-2.11668252801205
H	-8.21241137501566	-1.79863833086706	-2.86216212007044
C	-7.63992561898163	-1.49716201484417	-0.79889758293714
H	-7.83415879218332	-2.53140379165264	-0.51289536043413
C	-7.18232729780848	-0.58524070915398	0.15518486762693
H	-7.02904998657361	-0.90125254894922	1.18754432999985
C	-6.93906770605039	0.74234225626598	-0.20170118123442
H	-6.62017989493001	1.47201959429349	0.54387869154157

4c bis carbene

C	-2.12557909886241	1.71470893330740	-0.51454273888775
N	-1.02099917134451	2.40811149358089	-0.14326299554201
N	0.06474944510186	1.60874186809475	0.10713205382170
C	-0.38666750856765	0.39899419998490	-0.10043798714211
N	-1.70791772841400	0.41408994127304	-0.47074747468043
H	0.20454812876500	-0.50489352285623	0.01113501122120
C	-2.51247935256699	-0.76205238578082	-0.79577960573321
Au	-3.93398526244202	2.41674267751934	-1.12574308404045
C	-5.71206284585890	3.10345367593506	-1.83603775809465
N	-5.96700939683509	4.31866931250136	-2.40728722622643
C	-7.26897776628372	4.32546525334777	-2.84068556982247
N	-7.86740276383920	3.19409238781020	-2.57198797690429

N	-6.89777377291829	2.45456749373907	-1.94469069823918
C	-5.01366289870189	5.41529018601515	-2.56461468966896
H	-7.74125440570085	5.16730836738209	-3.33792517006222
H	-3.54655366739517	-0.44077603712606	-0.95874490989230
H	-2.47868800226707	-1.47556628977077	0.03676985758248
H	-2.13084367142069	-1.23998129304674	-1.70697320170704
H	-4.08835918200450	5.14771602555683	-2.04371135657792
H	-5.42743216805479	6.33191143562137	-2.12641258420728
H	-4.79939741931917	5.57900787838695	-3.62838045012894
H	-0.46430829958330	7.65588304559356	0.36682627870325
C	-0.58491580704363	6.57736856374468	0.25837072680992
C	-1.73313057492615	5.95013340761959	0.74777888403242
H	-2.50367087438906	6.53351170316285	1.25354362844856
C	-1.88688108755097	4.56811994285884	0.62512347115096
H	-2.75788300572254	4.06390054540276	1.04505587636458
C	-0.88325067570566	3.82808495719981	-0.00563769617270
C	0.27608515333591	4.43967955677338	-0.48768916168829
H	1.05298776141220	3.83570091458926	-0.95582137532104
C	0.41868165056091	5.82014578253704	-0.35176769968843
H	1.32097003228042	6.30527892911440	-0.72555309304896
C	-7.21619622064520	1.13044370552214	-1.49800678231555
C	-7.97719417133158	0.30638491422726	-2.33004691051566
H	-8.31589054308808	0.67703549747856	-3.29721172940973
C	-8.29619825961513	-0.98061442057413	-1.89834997561099
H	-8.89007597237290	-1.63026152380408	-2.54212975425908
C	-7.85979453974786	-1.43583794353755	-0.65128061658265
H	-8.11791099223659	-2.44142709718664	-0.31710983002831
C	-7.11048368787967	-0.59575831831786	0.17585424565633
H	-6.79597110848118	-0.93641181604970	1.16322853860606
C	-6.78930148720039	0.69757838550062	-0.23974373426969
H	-6.24500600153944	1.37631051466957	0.41769835947131

4c mono carbene

Au	-4.02470806697366	2.36949158697243	-1.22332622079983

C	-5.72696686786483	3.09748699095767	-1.87628088259307
N	-5.95488124483850	4.32831479169069	-2.41091550380985
C	-7.27474384635843	4.35741688498781	-2.78532788481522
N	-7.88152291104036	3.23032694820559	-2.50543498000803
N	-6.91170465315767	2.45532135190654	-1.93114246908939
C	-4.98786177740648	5.41368507145865	-2.59148076671647
H	-7.75320634593713	5.21415737079521	-3.25091961044059
H	-4.04724119608611	5.12851743310316	-2.11011600051627
H	-5.37414274935116	6.32739600014948	-2.12447020016968
H	-4.81613256621513	5.58354701142362	-3.66147399789553
C	-7.22632418766976	1.12567359489437	-1.48600118634159
C	-7.94634222223853	0.29116207602923	-2.34248485493364
H	-8.25790374595016	0.65011661199335	-3.32329026818638
C	-8.25332999513252	-0.99992896917809	-1.91477301915182
H	-8.81207172749493	-1.66438937447245	-2.57436267542599
C	-7.84562092035343	-1.44126813772142	-0.65281765153841
H	-8.09088765243925	-2.45197813715921	-0.32500350531545
C	-7.13943894779469	-0.58685927830654	0.19706548242950
H	-6.84659345890863	-0.92101822807215	1.19279442989797
C	-6.82971210082562	0.71103400337660	-0.21187241278240
H	-6.33000368186295	1.40346098866545	0.46705942510218

4e bis carbene

C	-2.17254724968744	1.63769839575080	-0.47954709634677
N	-1.35897396455175	2.13621347193193	0.49349436326100
C	-0.24699023738864	1.33323147158069	0.66543838013785
C	-0.36455169627246	0.30527483979595	-0.22093101686021
N	-1.54515427544183	0.50751453655149	-0.91096979574990
H	0.28519855733194	-0.54042140243194	-0.41413694495413
C	-2.04082667840087	-0.38163805460273	-1.95625540726055
Au	-3.94037913058680	2.41362967950346	-1.14388940698118
C	-5.70811874744542	3.18818420428122	-1.80979915896535
N	-5.89867763087705	4.06270290229434	-2.83742190649781
C	-7.24058063633352	4.35617353686126	-2.99241749475783

C	-7.90958451752369	3.64869039000806	-2.03947908877031
N	-6.95862595306772	2.94202360419896	-1.32733544930718
C	-4.83930354250113	4.62831270866251	-3.66609138814327
H	-7.60392437050704	5.03382664231553	-3.75626625572976
H	-2.98228529269893	0.02595476850647	-2.33990024033478
H	-2.21820535898149	-1.38429180762562	-1.54610523893672
H	-1.31108913589741	-0.44498645195388	-2.77371921946263
H	-3.88414350143624	4.19640319211939	-3.34872107319194
H	-4.80475317454475	5.71867471420975	-3.54337715044392
H	-5.01707959506614	4.38471674208374	-4.72139997586672
C	-1.61316404153251	3.35273695010728	1.25786986640886
C	-7.26857849828886	2.05320725942261	-0.21253538408116
H	-2.56118506345308	3.78241298167283	0.91701982093416
H	-0.80480862325533	4.07706856090801	1.09412604320071
H	-1.68279077744844	3.11811325854391	2.32790091401714
H	-6.33035670304745	1.63424552927177	0.16667312366030
H	-7.92166280061288	1.23803578665572	-0.55005806617929
H	-7.76768999129937	2.61361492029235	0.58851127806422
H	0.52509088927223	1.55568129731532	1.39283050021382
H	-8.96809403235589	3.59047591616881	-1.81394076857661

4e mono carbene

Au	-4.02052495568785	2.45240796994239	-1.17162313916339
C	-5.72239150879603	3.19419094361022	-1.81539914277107
N	-5.88405955377089	4.06451609003632	-2.84135502071774
C	-7.22865496216440	4.35186866455001	-2.98778997537957
C	-7.89804246237042	3.64376491099125	-2.03444352783662
N	-6.95467614734198	2.93213202454159	-1.31639005079722
C	-4.82521789418417	4.63347764200958	-3.67534687478140
H	-7.59196403927740	5.03007446970445	-3.75152824539916
H	-3.86493028364124	4.20812404788338	-3.36581137271450
H	-4.79972979359695	5.72293361105689	-3.54910468210370
H	-5.01174490123727	4.38491103150191	-4.72722191002019
C	-7.27031813605027	2.04146468695044	-0.19948637296899

H	-6.33850080098273	1.61534394246712	0.18653828710793
H	-7.92538965870584	1.23258240873800	-0.54577250914299
H	-7.76866421554787	2.60939269953063	0.59571021374663
H	-8.95674351204465	3.58573258498579	-1.80852384285802

4g bis carbene

C	-2.19810331477489	1.63783099953692	-0.43690862000879
N	-1.37208370699711	2.11947210735800	0.51560501021719
N	-0.26821097322776	1.34528297816439	0.72667831726827
C	-0.41565673221957	0.35655570655169	-0.11855967730906
N	-1.57138009642138	0.49211136472942	-0.84545593281458
H	0.28381389220125	-0.46597722244471	-0.23304992766628
C	-2.04475277839975	-0.43671924514128	-1.86976661598786
Au	-3.95486352869948	2.42593722480267	-1.10438519530728
C	-5.71388836180707	3.21416235669855	-1.76540410007376
N	-5.91573947986400	4.10757565718180	-2.78194462314098
C	-7.26258739082239	4.35300016349941	-2.87205481466100
N	-7.93009701350379	3.67002362221805	-1.97661283933715
N	-6.96169316930216	2.97889894744994	-1.30804810340306
C	-4.88309734449336	4.71552857128142	-3.61857979929667
H	-7.71259994099940	5.02645275426482	-3.59516175687452
H	-2.96740002979250	-0.03480686775377	-2.30062318132151
H	-2.24870325493000	-1.41784109200960	-1.42285013631837
H	-1.28918564062082	-0.54062890706446	-2.65827934498028
H	-3.92724203099581	4.23092416274218	-3.39517220727797
H	-4.80611008491784	5.78902267972251	-3.40410739513406
H	-5.12798571898608	4.56791684539098	-4.67745600362876
C	-1.53449360210421	3.33117882477533	1.30692095832689
C	-7.36118363943240	2.09622884009956	-0.22070475598171
H	-2.46688380723539	3.81862825997064	1.00455247888748
H	-0.68297753578844	3.99875626698682	1.12841271328562
H	-1.57314165167847	3.06777325232269	2.37073885458640
H	-6.46121131645434	1.63389896063403	0.19724656580317
H	-8.03806180007580	1.32531418496455	-0.60821687787431

H	-7.87872911715695	2.68063460276740	0.54945444762298

4g mono carbene

Au	-4.02532416639317	2.47542165963934	-1.13048059402948
C	-5.72630520057466	3.22077911352721	-1.76770292967781
N	-5.90166581451585	4.10912928630027	-2.78533495636817
C	-7.25030668685407	4.34719075424366	-2.87012744410622
N	-7.91584284697455	3.66224651895528	-1.97241724016521
N	-6.95915120998420	2.96880182401937	-1.29552080600619
C	-4.86851594156023	4.71972920142864	-3.62659185346404
H	-7.70321524032045	5.01876244653397	-3.59370628177003
H	-3.91192795292623	4.22898227536853	-3.42177337962317
H	-4.78883229497754	5.78963037852351	-3.39816708876433
H	-5.13033448726731	4.57997319561944	-4.68191405962019
C	-7.36324435149810	2.08421398894268	-0.20711258101259
H	-6.46895025447094	1.61580503166204	0.21550779149792
H	-8.04132427646345	1.31947541981682	-0.60364282464348
H	-7.88014921281922	2.67537847911923	0.55783678915299

Structures for 3e mechanism

AgI_2

Ag	-0.0000000036026	0.0000000030595	0.00000000001444
I	0.00000000180131	-0.00000000152978	2.63879085661082
I	0.00000000180131	-0.00000000152978	-2.63879085662527

3e.AgI_2

C	-2.23158293952058	1.47279361334950	-1.06117155060219
N	-1.11436930070931	2.11375002082184	-0.61942089169539
C	-0.22554511742009	1.22831859260588	-0.03636586416826
C	-0.79591184629567	-0.00688475815678	-0.12103960136252
N	-2.01076957877651	0.16354638829549	-0.75827338463902
H	-0.44322860550193	-0.97547677890520	0.21202437492424
C	-2.99281812777848	-0.89091431553805	-0.95887607406631

Ag	-4.01653895394462	2.31125385650297	-1.72201780694210
C	-5.78440330854018	3.15199820165180	-2.42379879009095
N	-5.90400316911834	4.29954738149751	-3.14658480108779
C	-7.22649331251901	4.68331351813837	-3.26630811822912
C	-7.96420149271484	3.73913531027639	-2.61597566136124
N	-7.06658452703205	2.81621783626916	-2.11033409757304
C	-4.77321174828362	5.08420802169715	-3.61967409490179
H	-7.52657886119152	5.58618615748919	-3.78397698047378
H	-3.57357038649956	-0.66411265691030	-1.86071050840032
H	-3.67506921683459	-0.92775930813660	-0.09644681271157
H	-2.47655670002343	-1.85031409107734	-1.08402590269288
H	-3.96599842870455	4.40090599851725	-3.90802821422117
H	-4.41568142416935	5.74180756665698	-2.81224965075285
H	-5.08279754693926	5.67588782321861	-4.48937983329297
C	-0.90909485072903	3.55349967440817	-0.68380265925266
C	-7.44813609780612	1.62405564508562	-1.36561839127269
H	-1.68652372236048	3.99227277309389	-1.31748608901869
H	0.08335493875813	3.77165811391657	-1.09978212296790
H	-1.00491351514025	3.99908572159978	0.31505679787230
H	-6.65034945161795	1.36531353429743	-0.65624069971198
H	-7.62688439216726	0.78301456572824	-2.05009181091861
H	-8.36200630111685	1.83281251722824	-0.79707761072631
H	0.72248314180809	1.54596328463764	0.38105303363002
H	-9.03387926751755	3.64875414343703	-2.47129282533777
Ag	-4.52370349232268	3.49773600617213	0.94084051020173
I	-3.97580212603221	5.93519052193886	0.11105598721483
I	-5.03215855553806	1.04950821169241	1.78315906862887

$TS1_{3e}$

C	1.72633364322064	-0.55856657663988	0.84373726713943
N	2.66526445605366	-0.92275110860641	-0.07533305826015
C	3.14248363952333	-2.20181870904477	0.16676046396786
C	2.47960627191915	-2.65640133249771	1.26815703792289
N	1.62606335963470	-1.64245073087999	1.66583609264104

H	2.54753718164943	-3.60074394776934	1.79518764743372
C	0.69867053582707	-1.72322607727661	2.79249878680454
Ag	0.46915056308387	1.11033887871493	1.04019365627650
C	-1.53174813575407	1.11836812001359	-0.42032587920047
N	-1.82577423434645	2.19975796856652	-1.20836080335679
C	-2.18231333759538	1.81785119607410	-2.48749399629707
C	-2.11059874335701	0.45514806210763	-2.51886000754669
N	-1.71444025126220	0.05075580036178	-1.26030273556592
C	-1.80933456070337	3.58121071472194	-0.74625143985072
H	-2.46076222375852	2.53034052113221	-3.25520960311060
H	-0.31035157807521	-2.00794147345512	2.46047278860388
H	0.63385920977184	-0.73886595029650	3.27153475843179
H	1.07425733984730	-2.45929138865529	3.51263633132625
H	-1.16421626981686	4.18656377254517	-1.39712270783954
H	-1.41942826022979	3.60228487165006	0.27945044216729
H	-2.82721908334077	3.99401524040054	-0.75605681917219
C	3.11601616945006	-0.06182544614884	-1.15520228673787
C	-1.53871000086171	-1.33534097129310	-0.85046029636753
H	2.53407326488101	0.86544571948212	-1.10829841079105
H	2.95216210702918	-0.54762942897449	-2.12675536465884
H	4.18289975788139	0.17380407655100	-1.04110700986925
H	-2.15419645434148	-1.53643589481633	0.04127503545682
H	-0.48325264224817	-1.52099406516796	-0.60889115900641
H	-1.84962079501722	-1.99004882389911	-1.67232393896334
H	3.90576161899244	-2.66848268550339	-0.44454898117676
H	-2.31494113167834	-0.24511190246029	-3.32038054650902
Ag	-2.18593073143475	0.94801716105484	1.78657205919987
I	-0.37446657767971	2.99371600455906	2.89655870070873
I	-3.49683410726405	-1.20969159455036	2.63241397619956

[3e-I]$_2$

C	-3.66806144818878	1.30000734911505	-1.19154399451469
N	-3.50640447528425	1.25399744385572	0.15999762756508
C	-2.27454682271801	0.72684427540732	0.50132803991768

C	-1.63745091432296	0.44496116297910	-0.66916714777294
N	-2.49751214869441	0.81261231974592	-1.68599783970623
H	-0.66563339086933	0.00624915680263	-0.85862524469247
C	-2.26404163678940	0.53583146599164	-3.09320785001857
Ag	-5.28544500021997	2.02527794077548	-2.27556118317879
H	-2.47497508686532	-0.52473387253761	-3.29469496580152
H	-1.22370529952918	0.76920194489988	-3.35159162157266
H	-2.93951335389255	1.16181899990394	-3.68770363777172
C	-4.55047596044461	1.58317338704080	1.11320528713912
H	-5.29354432939823	2.20983885570635	0.60642210506318
H	-4.12534108496867	2.13369926448976	1.96191553271232
H	-5.03250095208469	0.66221060113130	1.47219790337762
H	-1.96425404906111	0.58646694639277	1.52940101651289
I	-7.07545237988862	3.31045658065709	-3.67871083340069
C	-7.89349784033403	-0.13407849373300	-2.27779817178877
N	-8.44682696202553	-0.15314792826836	-3.52098279504134
C	-9.66207240159676	0.50385149360529	-3.53983592053196
C	-9.89278035209745	0.93316395042049	-2.26791768761555
N	-8.80696343609223	0.52733304788594	-1.51411117987470
H	-10.71767436646182	1.49520643388925	-1.84770146584740
C	-8.59733969338919	0.88010114490094	-0.12179166424240
Ag	-6.10030530545669	-1.00076681734346	-1.68715568507634
H	-7.80516357473375	0.23730197763758	0.27946906268525
H	-9.52054834973001	0.72282432976545	0.45023993572496
H	-8.28811853989621	1.93270782770018	-0.04592350237511
C	-7.75810673396591	-0.63161935441988	-4.70772682060038
H	-7.29353626483889	0.21979864130634	-5.22645185433377
H	-8.46904359094050	-1.13675552104582	-5.37325714702702
H	-6.97993229314407	-1.33830358372951	-4.39695098038259
H	-10.24516105525183	0.62362390130657	-4.44451285852032
I	-4.07902925692430	-2.48012154403525	-0.94135414250998

[3e-I]

C	-2.31126210010713	1.34406416666384	-0.31991145973844

N	-1.87295510102232	1.37362885225984	0.97085634107981
C	-0.73136116317216	0.60720589264403	1.13514416415790
C	-0.44043308134566	0.07847041812940	-0.08648608656148
N	-1.41372925130853	0.53941428700116	-0.95696371025588
H	0.36404618791168	-0.57542125144978	-0.40185583418211
C	-1.47719842907454	0.20843387859504	-2.37285400802495
Ag	-3.96174555569553	2.30357623201805	-1.12473546056268
H	-1.58796960310476	-0.87600831301850	-2.50551701970723
H	-0.56756042133822	0.55018643443447	-2.88441380854248
H	-2.34804618004922	0.71837467051240	-2.80066760112007
C	-2.52582181326785	2.11916278771363	2.03690831611006
H	-1.83914939073860	2.86801079982711	2.45353829050147
H	-2.85310591146457	1.43730484075178	2.83299561518479
H	-3.39911839893661	2.62485236005024	1.60885928288621
H	-0.22947853975215	0.50263100235826	2.08981081967808
I	-6.01850811803381	3.50876040920901	-2.12101104720300

H_2O

O	-2.14457894072702	3.09418542284217	-2.61004134309271
H	-1.65204034978344	3.92534373702200	-2.51302025270523
H	-1.85014564798955	2.73946477463584	-3.46462723160205

[3e-I].H_2O

C	-2.18692800113969	0.99774276047968	-0.58722056592225
N	-1.93851163967537	0.96314403817275	0.75169032862246
C	-0.63814314946287	0.56601099226742	1.01051147084765
C	-0.05009284238505	0.33930385591448	-0.19791687874008
N	-1.01082845108897	0.60889156151578	-1.15755471761995
H	0.95122350990368	0.01014740532513	-0.44915169371816
C	-0.79886399965720	0.48720957475734	-2.59170421204354
Ag	-3.95212693706419	1.53668342421478	-1.52878873981994
H	-0.54832097464722	-0.54939819614988	-2.85416633014160
H	0.01227830751089	1.15345743501725	-2.91440894902194
H	-1.72822664747962	0.77531014562290	-3.09636421279760

C	-2.90304039468169	1.33640184466914	1.78108305402781
H	-2.65353760434800	2.32445847765830	2.19144339211978
H	-2.88000110288000	0.59263571692114	2.58796982382051
H	-3.91181103754644	1.36647184838196	1.34626765449566
H	-0.24615246036626	0.47712378156947	2.01678513793002
I	-6.19641191637171	2.24766184924894	-2.64244909263872
O	-6.13205890218455	1.43635367060200	0.90886111709906
H	-6.53082802557730	0.57046134121220	0.71809681740923
H	-6.26254450325841	1.91982137799919	0.06212966369159

$TS2_{3e}$

C	2.24695338955520	-0.39292715930829	0.51209588778970
N	1.79879636437996	-1.45873438456733	1.23977973679275
C	1.89533394175229	-2.64268070760120	0.53281078970270
C	2.44196483854581	-2.32868112537742	-0.67621036457954
N	2.65039243125624	-0.96105445160780	-0.66398768561329
H	2.69373044193335	-2.95597572337555	-1.52343439681484
C	3.18489140264840	-0.20124976691987	-1.78311532582807
Ag	0.25087686399669	1.25105159711179	0.29014072005894
H	2.50011889878856	-0.25456139512056	-2.64069600605838
H	4.16755691432093	-0.59400358302588	-2.07753636161889
H	3.28948684520441	0.84371009164754	-1.47266071858854
C	1.13520283990972	-1.33276077854430	2.52830360077373
H	1.47155969638255	-0.40652829946289	3.00578832830862
H	1.39626362206615	-2.18704418338053	3.16561276166243
H	0.04504231815726	-1.28520286210225	2.38340977491585
H	1.56834158751655	-3.59420807151623	0.93546821432060
O	2.29330456107463	2.34970591657505	0.58447235476177
H	2.51861997208190	1.36301799806718	0.77018863477973
H	2.37078595161399	2.83779420494311	1.42238437896122
I	-2.05410529378466	0.07627750546544	0.18699385437346

[AgIOH].LH

C	4.35856066010374	0.34381386473576	0.42685678890684

N	4.53776401965471	-0.60286710101598	1.36573092805612
C	5.00221396303862	-1.75555879031900	0.76019950948083
C	5.14049056457008	-1.48025678401031	-0.57106253208235
N	4.74167573680365	-0.17067113501695	-0.75541325649347
H	5.47104689572985	-2.10285761070539	-1.39288276712916
C	4.63150256946702	0.54882143841267	-2.02365576442070
Ag	1.45125435556851	0.53848402062177	0.12934563922271
H	4.19864914377692	-0.12414729152097	-2.77313770710886
H	5.62295381218068	0.88571219144931	-2.35403531310025
H	3.95155078899216	1.40069202430662	-1.85223285392606
C	4.04967032985499	-0.50661633548617	2.73649321941985
H	4.00910361758121	0.54839183249546	3.02612042415432
H	4.73112485030454	-1.04720339946622	3.40318883617426
H	3.03642012087293	-0.94018025280886	2.77533143737913
H	5.17150127282971	-2.66788001910514	1.31784338137041
O	2.56999799762163	2.21707744668578	-0.43146235312807
H	3.93237110828900	1.35537050120233	0.53225987178599
H	2.01948195979526	3.01421754260159	-0.48107986553449
I	0.73955573296463	-1.79954843055631	1.00697307777292

LH

C	3.86166028158448	0.02068470157162	0.57292484086737
N	3.80571668881322	-1.18827331484266	1.15315820655961
C	4.42135701345270	-2.10555149331479	0.32282290601759
C	4.85437943831218	-1.42232753701722	-0.77954619184714
N	4.49563350168962	-0.09928087354280	-0.60406684331750
H	5.38246839215324	-1.76309773489362	-1.66257046963629
C	4.76450927437442	0.99083807107470	-1.54548507614650
H	4.27852002366967	0.77433741213011	-2.50419076706743
H	5.84681909987767	1.09018474732690	-1.69009138549055
H	4.36426884586269	1.92378514114207	-1.13637815544336
C	3.19255677230219	-1.48703464905397	2.45002377068024
H	2.79005157235997	-0.56272194464188	2.87627680817029
H	3.95022067153807	-1.90093713509642	3.12587577322135

H	2.38003134545523	-2.21028088322069	2.31283767249744
H	4.50078230950866	-3.15492901328677	0.58209064764656
H	3.46194812184596	0.94013831876545	0.98597787138834

[AgIOH]

Ag	0.35383046419453	1.31640094725006	0.39101840650331
O	2.16138750510486	2.29281161757808	0.52185408830465
H	2.14959844452767	2.68749698800962	1.41089591710299
I	-1.93285253222706	0.04800139876224	0.13994354118905

3e.H_2O

C	-2.20029017085864	1.61585433934553	-0.35555818187010
N	-1.50167113109274	1.92811429855477	0.77170461216051
C	-0.33755656138769	1.18560556995784	0.86159548020735
C	-0.30260042524043	0.38551908540213	-0.24148052933806
N	-1.44726084694076	0.66088757208705	-0.96676206323878
H	0.42790788592813	-0.34843208864040	-0.56084338390107
C	-1.77392090408917	0.04057549632840	-2.24559222168636
Ag	-3.98919606212377	2.41921156717883	-1.04462503255020
C	-5.78258292730621	3.20105807507572	-1.74451294382756
N	-6.00400415814650	3.84677344837148	-2.92263858968713
C	-7.33021197300225	4.21943905095530	-3.04722786099887
C	-7.96222770707088	3.79601029703811	-1.91671821758037
N	-7.00163322854547	3.17782912425718	-1.13671163536795
C	-4.98446415397000	4.11722271503981	-3.92952395212263
H	-7.70936721242997	4.74468539879066	-3.91596480400779
H	-2.84133784508588	0.18814153540903	-2.44161206664020
H	-1.55520491109857	-1.03283544807764	-2.19844027446131
H	-1.20064217040183	0.51478283892902	-3.05165801436875
H	-4.03105514418067	3.68409782623775	-3.60351395116248
H	-4.86595631834582	5.20099798437983	-4.06037371557979
H	-5.27886897347185	3.66735381974268	-4.88673986025722
C	-1.93111089496415	2.89647382969974	1.77179916029226
C	-7.27036576835143	2.57994719072172	0.16430132268290

H	-2.85641475521456	3.36574692357893	1.42002737653515
H	-1.16161941841595	3.66723523024903	1.90763340774699
H	-2.11832377837168	2.39597225013391	2.73079997485984
H	-6.34195481275466	2.13180412571618	0.53507009517463
H	-8.03655418708436	1.79968816130760	0.07077400563627
H	-7.61365093010916	3.34624404071375	0.87147079991163
H	0.35304707698363	1.27989427860572	1.69135494438362
H	-8.99810247934671	3.88047006411766	-1.60983436643109
O	-1.68571104333054	3.08688971543191	-3.57536426756586
H	-1.16986080314125	3.65230447581797	-2.97603533626087
H	-1.29783397943798	3.24691168644266	-4.45292197558662

TS3$_{3e}$

C	2.10411962371552	-0.46006135090919	0.49173775425811
N	1.79761631339669	-1.54213652227760	1.26605403284152
C	2.04338721259055	-2.73404697170988	0.60660124848209
C	2.51836188755733	-2.39927520395727	-0.62811909901119
N	2.54601747726748	-1.01680015327335	-0.67405020289517
H	2.84115297030576	-3.02331727862494	-1.45390469590295
C	3.00179727977400	-0.24121869246920	-1.82173896943296
Ag	0.18650652211063	1.43501945984977	0.27104721578728
C	-1.76627494657786	1.06477922189961	-0.25447660260025
N	-2.30438677785723	-0.12683336881138	-0.63757903879840
C	-3.65218396949801	0.00359755335494	-0.92332132431602
C	-3.96910973650273	1.31186347769737	-0.71357715450014
N	-2.80615353232275	1.94151633652590	-0.30694478945929
C	-1.56540615890612	-1.37740682880124	-0.74451516131845
H	-4.26364237056685	-0.83012114671339	-1.24798393560266
H	2.34901771434935	-0.41775103894667	-2.68696322054163
H	4.03046769969361	-0.52136572276334	-2.08228026245365
H	2.97500750237558	0.82039967195789	-1.55513223935753
H	-0.52830848888853	-1.19033491918036	-0.44496124327279
H	-1.58573010354276	-1.74262909892868	-1.77953445886766
H	-2.00622001787858	-2.13491631102275	-0.08343166562505

C	1.30370629872569	-1.44863313130921	2.63296538529926
C	-2.71948912279351	3.35964503721458	0.01848855441235
H	1.10234033939102	-0.39554328303533	2.85453903813760
H	2.05189629630860	-1.83138009716949	3.33963050320907
H	0.37588905162205	-2.02510870100646	2.74294337003822
H	-1.68235172859848	3.58654386166597	0.28833273849997
H	-3.37714513519302	3.59422040039651	0.86524710167633
H	-3.00963938624067	3.96411123622088	-0.85024815142005
H	1.87726680549697	-3.70443728182101	1.06078090401206
H	-4.91069356801266	1.83786001926409	-0.81913928454144
O	2.21207248469822	2.25219992153519	0.77606161350923
H	2.44267017909139	1.25910942146817	0.88942508761449
H	2.38744138490932	2.73245148367986	1.60404695213969

[LAgOH].LH

C	-2.98854156100841	0.31163241330241	2.27072312518772
N	-2.29055535207476	0.79479783432390	3.31370951383009
C	-2.43194871467160	-0.05717698836299	4.39632243047455
C	-3.23810315367286	-1.08281701604098	3.98954851273962
N	-3.56848562903423	-0.83287547276452	2.67034902616580
H	-3.59613527438910	-1.95563386110392	4.52236712476997
C	-4.41062142639657	-1.65920563322584	1.80353568854469
Ag	-5.03955521617956	1.88213677162755	-1.27526900138033
C	-6.44462595339686	3.07510658942928	-2.14593367841598
N	-6.31919806527405	4.37972736119793	-2.52015844192274
C	-7.48159984799893	4.84763541823001	-3.10764047963711
C	-8.36423901983066	3.81029879882496	-3.10342111828246
N	-7.71360692775234	2.74041236523110	-2.51418733930796
C	-5.11683031090324	5.18133157848111	-2.34095621815982
H	-7.58239493262103	5.86198512253222	-3.47522123471316
H	-4.42715450999708	-1.18129819257587	0.81342872372990
H	-5.42423201750765	-1.71444996755294	2.21950543488746
H	-3.98561793113484	-2.66793472391374	1.73352295410061
H	-4.36858798980063	4.56298281646108	-1.83287788226100

H	-5.33887606053287	6.06512269118702	-1.72885836948508
H	-4.72419834637824	5.49995003589290	-3.31538803728127
C	-1.50622410101700	2.02674332329802	3.29352452729807
C	-8.31327176315952	1.42749220187606	-2.32158109111702
H	-1.58851529262793	2.47463455433016	2.29820244477466
H	-0.45397495153862	1.80239031909451	3.50726258993723
H	-1.89307463099795	2.72762823965345	4.04345386963633
H	-7.56662271319790	0.77803171380103	-1.85137143757491
H	-8.60841033142881	1.00075070120288	-3.28893521176111
H	-9.19424607798747	1.50399414709009	-1.67096950363618
H	-1.95391920906937	0.13384574609685	5.34974237743011
H	-9.38337343085649	3.74579989393659	-3.46590364797860
O	-3.65215250171961	0.67239603402238	-0.37517826899511
H	-3.10281722502032	0.70248064614926	1.21903995818939
H	-3.00059335702267	0.40774519346776	-1.04592639428639

[LAgOH]

Ag	-5.03713838380886	1.80096660274758	-1.41455750023749
C	-6.43400058134331	3.03574872943631	-2.21104981969617
N	-6.31041059614460	4.35495648911589	-2.54514132259802
C	-7.49122944590256	4.86182760558628	-3.06229235910509
C	-8.38873210448486	3.83742958593189	-3.05570318833649
N	-7.72746658019581	2.73699022632842	-2.53597776026690
C	-5.08685588551446	5.12250492023215	-2.38063167360510
H	-7.59312956914313	5.89056286323179	-3.38702839078413
H	-4.33924108329837	4.46334168706595	-1.92412845780741
H	-5.26308690642808	5.98550392280059	-1.72429824600479
H	-4.71923767705419	5.47168882147079	-3.35522665882096
C	-8.32983107171024	1.42658791102027	-2.34917998652993
H	-7.55565253999593	0.75206756197601	-1.96541679246822
H	-8.70770462029761	1.04168590505847	-3.30594268034180
H	-9.15404810790324	1.48315282279814	-1.62511589661443
H	-9.42448343418299	3.80144557926015	-3.37208054788922
O	-3.77097037520005	0.49599705635633	-0.59773216111106

H	-2.87916388349166	0.88044114398296	-0.56827391408275

[LAgH$_2$O]

Ag	-4.48163095558252	3.66608381311816	-1.91558387218590
C	-6.45567390039852	3.86374088815405	-2.39157936006979
N	-7.09522919766275	3.34857824733529	-3.47527410114423
C	-8.43536201252523	3.68904917249789	-3.46076087639289
C	-8.63799887412474	4.43637207909104	-2.33935555238611
N	-7.41607672069494	4.53190399231379	-1.69895423551489
C	-6.47286635166902	2.54392316410211	-4.52077706313654
H	-9.12298261600822	3.37635355738378	-4.23782868974648
H	-5.40686744313956	2.43765879169017	-4.29243028691682
H	-6.58684759851598	3.03884861438255	-5.49332453787133
H	-6.93636321726472	1.55004302893310	-4.55672748393040
C	-7.20713274718864	5.25711083907234	-0.45113903878106
H	-6.15123037080981	5.17283238682704	-0.17256808400772
H	-7.82757916380653	4.82493813988162	0.34397310342341
H	-7.46338110235769	6.31572445872545	-0.58376263609572
H	-9.53625450286603	4.90111271509486	-1.95003404205764
O	-2.36511483740282	3.40692491532514	-1.46915621217600
H	-2.08691018276415	2.85814109106157	-0.71519868298738
H	-1.75865457371803	4.16713401111004	-1.50574589672249

Structures for 3c mechanism

3c.AgI$_2$

C	-2.40619671494676	1.59119376386139	-0.57671836108628
N	-1.22137745746332	2.06970634245290	-0.12687242149666
N	-0.28196033497851	1.09398667597941	0.11878450864157
C	-0.91679608934406	-0.01233894455715	-0.17303961362377
N	-2.20073071745488	0.24065490322817	-0.58410772593320
H	-0.48758153695081	-1.00605173070144	-0.09767851660402
C	-3.18474346983598	-0.75120077051579	-1.00771411011208
Ag	-4.06897368175103	2.52587959097914	-1.42432521445521

C	-5.97354415131998	3.01964188342153	-2.11838315085740
N	-6.39201514561610	3.97100367431092	-3.00298051459014
C	-7.66343761870354	3.65966391782314	-3.41747277658674
N	-8.10167270094086	2.57003817686018	-2.84101269279569
N	-7.05299618545221	2.20317609491867	-2.03241776947263
C	-5.60914681098232	5.12090382059567	-3.43917790422669
H	-8.22817038024789	4.24642098142633	-4.13445135691951
H	-4.08547970051001	-0.66934599843870	-0.38673881525602
H	-2.74691832336313	-1.74945326970091	-0.89445424780585
H	-3.46476142770560	-0.58717758675373	-2.05954875744314
H	-5.73803757144549	5.95526621258027	-2.73714439997297
H	-5.94596664733473	5.42352382903364	-4.43723750013349
H	-4.54731795754742	4.83945371269446	-3.48627439159314
H	0.08413906685507	7.16963946091459	0.44397380960820
C	-0.18361090826305	6.11741818955765	0.34061205768296
C	-1.49483680175275	5.70206027511518	0.58000122177860
H	-2.25429519996715	6.42552377820580	0.87904189355429
C	-1.84288467896371	4.35929517500020	0.44620610149257
H	-2.86108079829699	4.02098547454464	0.64051831780449
C	-0.86892110442986	3.43847780652569	0.05671041501298
C	0.44775756645863	3.83742575635209	-0.17670378274793
H	1.18477271700928	3.09770757005243	-0.48445618479276
C	0.78450352220401	5.18159833558287	-0.03049870808872
H	1.80924013569113	5.50058800474209	-0.22412445352405
C	-7.14557256297784	1.00624496341965	-1.26192494392049
C	-7.67311690916623	-0.14248953625211	-1.85158937927316
H	-8.00317863202754	-0.10833618994363	-2.88822084903203
C	-7.73475124023071	-1.31826467875323	-1.10422276912169
H	-8.13498365382048	-2.22298852318467	-1.56288610876478
C	-7.26855256200802	-1.34484553729513	0.21232126659531
H	-7.31632570746135	-2.26909265526070	0.78989293717434
C	-6.74940482547550	-0.18434287081473	0.79249486134700
H	-6.40069917800352	-0.19411308772345	1.82614864254576
C	-6.69049415870332	1.00067245709722	0.05832426747214

H	-6.30181307316449	1.91779880971196	0.50008820472598
Ag	-3.33679810997265	1.88462849163172	-4.21159177466329
I	-1.82985643688262	3.97435826268797	-3.66236722531987
I	-4.93596798945500	-0.15830977561266	-4.57517884822256

$TS1_{3c}$

C	1.64950611716463	-0.56241436893735	1.04974324836994
N	2.31101123751576	-0.56944911613351	-0.13347925828994
N	3.12762045767135	-1.66576380112422	-0.31466482978276
C	2.96916737286127	-2.34314871033812	0.79273794953054
N	2.09447010827323	-1.71244813378262	1.64340806527333
H	3.47078904288304	-3.27947333418112	1.01593130370240
C	1.67422983629346	-2.19042394117981	2.95545246087659
Ag	0.15346119965371	0.69558367351325	1.79685768171603
C	-1.58178794095081	0.72936473019460	-0.20803958799311
N	-1.46330790198698	1.56724602416385	-1.27948191108760
N	-1.55109369899033	0.93049821293946	-2.50168081718095
C	-1.72749387575980	-0.32197242680643	-2.17660244037159
N	-1.74341292535229	-0.48943453064503	-0.81714721712423
H	2.55234144271783	-2.49235107939383	3.53942872370242
H	0.98830636537589	-3.04175710288104	2.85346019787344
H	1.15799291177210	-1.36859772930154	3.46576874523470
C	-2.01360960543155	-1.72758188118498	-0.10441536286855
H	-2.98766834214546	-1.64466340443389	0.40555493959028
H	-1.22707016033919	-1.89519144390685	0.64343683578427
H	-2.02683098354264	-2.55631595359277	-0.82182792861095
H	-1.84785141750159	-1.12976491131904	-2.89115844608542
Ag	-2.61638021727423	1.08386699790196	1.74194104538821
I	-0.94094951938702	2.09001423387017	3.84485847562666
I	-5.11365827007486	0.16366913642788	1.57116152470699
H	-0.61084697875213	5.53079136900629	0.87753863654782
C	-0.79216266076747	5.01999930622239	-0.06903442477734
C	-0.79368518629082	5.73161667355897	-1.27079421532641
H	-0.61204729662615	6.80704890038106	-1.27363818254774

C	-1.04350974198656	5.05537515671160	-2.46714103674341
H	-1.05958151355894	5.60061671474352	-3.41199642983997
C	-1.27847351583331	3.68135600637564	-2.47065966668196
H	-1.46513042709717	3.14330276780471	-3.39748543408914
C	-1.26196501144757	2.97784131353083	-1.26181604537356
C	-1.02724997988113	3.64634651251412	-0.05670218192392
H	-1.02553430172066	3.10815166464339	0.89157666045420
H	1.83581378792149	3.76561357218859	-1.56396990288541
C	1.97457500266020	2.71688970218255	-1.82783921854122
C	2.07739007356907	1.76410060768395	-0.81559146556376
H	2.04619088100177	2.05941537152879	0.23376187057863
C	2.22945501846546	0.41899473315162	-1.16029962795091
C	2.30380442070940	0.01846471626278	-2.49598070091216
H	2.43677907573041	-1.03604175253389	-2.73451250218631
C	2.20859470408721	0.98338100390799	-3.49739149811884
H	2.25702122071493	0.67735466237348	-4.54299622262695
C	2.03778799220244	2.32950076025773	-3.16732433670060
H	1.94846094417799	3.07896257797954	-3.95424781097054

[3c-I]$_2$

C	-3.13459305564108	1.52524129137756	-1.34614211725207
N	-2.06080154154158	2.26939599465155	-0.99059861222640
N	-0.97059103699725	1.53100806840398	-0.59547595226812
C	-1.39541130999328	0.29837806060171	-0.70238168916561
N	-2.70067599857855	0.25204636738920	-1.12358622657151
H	-0.79795340546200	-0.57934762501462	-0.48101378811636
C	-3.42596763833517	-0.94929001012092	-1.50729152146614
Ag	-4.94739507199666	2.17095225492340	-2.12042582298752
H	-4.50037980102519	-0.75247843417031	-1.42582528220319
H	-3.14835715947490	-1.77340742273041	-0.83968268122917
H	-3.16936531062516	-1.20154221835271	-2.54705185530582
H	-1.64540673331630	7.52833462889596	-1.41558556206240
C	-1.73310917984388	6.44469985784798	-1.32511012184206
C	-2.84136596289894	5.88498871558963	-0.68468465517784

H	-3.62039199789806	6.52647509149174	-0.27078729269180
C	-2.95474373826758	4.49986618542444	-0.55891483529223
H	-3.80892557873867	4.04884913121963	-0.05340342522057
C	-1.95047435708501	3.68687860952104	-1.08735340722540
C	-0.83635120825465	4.23073673215767	-1.72963939042675
H	-0.07967003715979	3.56321806934608	-2.14128162181552
C	-0.73278125549855	5.61694900665549	-1.84338455557045
H	0.13170249803103	6.05076948578612	-2.34736950278510
I	-7.29608190050974	3.02873154350424	-2.84365751592069
C	-4.60085946222065	3.45607608130605	-5.38789970880675
N	-5.54764153392313	3.27365103554863	-6.33970278324144
N	-6.30688361045062	4.39150618274837	-6.59444272049152
C	-5.82144250307746	5.27691745823006	-5.76327919643260
N	-4.78414720636886	4.75972128177095	-5.03021059034278
H	-6.19049437462249	6.29190150887079	-5.66146166167919
C	-4.10317676707084	5.42583759503192	-3.93160787314144
Ag	-3.13375006098141	2.12063288971891	-4.76500927240634
H	-4.68931922953920	5.29735709707853	-3.01126087889405
H	-3.98752950068880	6.49190276566893	-4.16002485816522
H	-3.11664600900960	4.96962338445013	-3.79567541440751
H	-6.53597648267776	-1.22371222121251	-8.94897508675111
C	-6.33954839535355	-0.29644676839519	-8.40923263584664
C	-6.03294918526398	-0.33215524057402	-7.04753912119142
H	-5.99990538173264	-1.28413939440384	-6.51669049320344
C	-5.78576143942885	0.84963802742754	-6.35016682946052
H	-5.59549685554622	0.84476749680221	-5.27663028498860
C	-5.82762053103112	2.06368051519831	-7.03867828500185
C	-6.14806378473866	2.11720566462802	-8.39606703642060
H	-6.19239031265347	3.08237899451533	-8.89940288829182
C	-6.40592627081687	0.92886321628039	-9.07762967363719
H	-6.65241693440115	0.96133396959777	-10.13960699715805
I	-1.13053462979043	0.48275258121334	-4.40418440411598

[3c-I]

C	-2.15812989524955	1.51386995917266	-0.95713202807968
N	-1.17479337939598	2.04667057400137	-0.18902955796812
N	-0.22855249535061	1.13240051176802	0.22166499378945
C	-0.64884685645233	0.00914686111651	-0.29840297296618
N	-1.80754617291590	0.19278785921801	-1.00929629680380
H	-0.15038002463745	-0.94758524312713	-0.17981735953403
C	-2.55205887460705	-0.83250149155098	-1.73076066506533
Ag	-3.78662537727387	2.36430925634375	-1.91192462555396
H	-3.57018555789948	-0.90487527327569	-1.33019017021695
H	-2.03867528317640	-1.79322002343015	-1.60971336336269
H	-2.60610687308407	-0.57332647205111	-2.79499731353961
H	-0.55203109705197	7.13204197752788	1.17435854634438
C	-0.68386386110565	6.08452356473703	0.90097198224891
C	-1.96599506712194	5.56967675339694	0.70006409594511
H	-2.84182533853676	6.20815753378730	0.81910492468039
C	-2.14304801400989	4.23075467140411	0.35411081391442
H	-3.14464482224954	3.82263832546958	0.21362402627079
C	-1.02027874366132	3.41549890926302	0.19246080283349
C	0.26819406682762	3.91540196395830	0.39723520627027
H	1.12550138161967	3.25523541165543	0.27538986345284
C	0.42883287896623	5.25291253664273	0.75504973284284
H	1.43331814470943	5.64777982570285	0.91191161079624
I	-5.80849128324318	3.35520246926953	-3.17047724749875

[3c-I].H_2O

C	-2.05601276602456	1.60015638871220	-1.05176879705560
N	-1.16906555142529	2.08103234417257	-0.14606897175560
N	-0.44221582974782	1.10357094757931	0.49584278070320
C	-0.90486846264574	-0.00581398349316	-0.01884172228197
N	-1.87998355778381	0.24695773375600	-0.95099424896485
H	-0.56450300835629	-0.99910362896581	0.25587635444167
C	-2.61603161617220	-0.75383132229189	-1.71276815078263
Ag	-3.34411399503324	2.59146387965306	-2.34239931065793
H	-3.30405796206922	-1.30301779482896	-1.05677152557031

H	-1.91649168978474	-1.45454820517492	-2.18537910829864
H	-3.19186275806188	-0.23295178905197	-2.48612039524619
H	-0.17217861364822	7.17101786375394	0.93890686918050
C	-0.38198888481872	6.12242707650575	0.72351580557316
C	-1.68177098738422	5.71761200535477	0.41443891307086
H	-2.50405222685618	6.43328904537937	0.38769022836971
C	-1.95878681733951	4.37795600502005	0.14207931375510
H	-2.98739700904792	4.08099050215589	-0.06945188011893
C	-0.91275325876604	3.45450634280111	0.16364745347467
C	0.39221240245622	3.84041899136208	0.47983803354160
H	1.18541408811191	3.09423901016690	0.50084773780400
C	0.64998937118262	5.18065440442396	0.76311769350265
H	1.66703326119275	5.49014182641406	1.00724555176527
I	-4.97477096395223	3.74903367035396	-4.00426290156264
O	-5.00998406233943	5.06778165593319	-0.62988083811506
H	-5.86103619768238	4.67873334846522	-0.36920438894648
H	-4.99469695500373	4.93780717614303	-1.60483761502549

$TS2_{3c}$

C	2.39428883000066	-0.26842485724568	0.79174786969530
N	1.71425122034147	-1.39778193555655	1.16678453066187
C	1.82727089499545	-2.34655516920336	0.18339824042344
N	2.56919534960865	-1.92057574292224	-0.80433883292634
N	2.91200748249223	-0.64503359309982	-0.40985948145907
Ag	0.67959715241110	1.64421973704943	0.72303022442287
C	0.84543699113007	-1.49414437910702	2.33082261952097
H	1.29902722662674	-0.94865118883940	3.16512172503884
H	0.72748340639417	-2.54833802784730	2.60817865482605
H	-0.13612753047667	-1.05562601990062	2.09218526282541
H	1.36485098243927	-3.32748734866661	0.22395228036168
O	2.60223195206842	2.28080846621026	1.90978359716256
H	2.73866220259614	1.28603545543722	1.73875859114506
H	2.43514664596589	2.39358905643541	2.86142874158286
I	-1.61759943152272	0.81758372851987	-0.13545592538034

H	4.32432733750994	1.54135020599469	0.25074128137522
C	4.37672556600230	1.27745118021820	-0.80357624079288
C	3.69906572449965	0.15572161502687	-1.28995653789844
C	3.76841854537712	-0.19049427484810	-2.64270760874106
H	3.22971751111226	-1.06707496186712	-2.99754776941706
C	4.52227376257968	0.59729516697067	-3.51097788062682
H	4.57277919379862	0.32902235843951	-4.56703434696589
C	5.19742049643008	1.72508774417843	-3.03998620436387
H	5.78151384337157	2.34116384495167	-3.72465910653238
C	5.11936442699016	2.05994471829324	-1.68667250015107
H	5.64483203115761	2.93683793827831	-1.30648386878688

[AgIH$_2$O].L

C	5.81086907778020	0.31494243563965	0.87989375177854
N	5.79480444521265	-0.98673513640077	1.28751287510887
C	7.06829223926591	-1.49721026043182	1.21566616948897
N	7.91555775112848	-0.59996806666975	0.78443776156928
N	7.11730714219913	0.50651665497266	0.57932434417794
Ag	2.23976818860455	0.32143070032295	0.01619277507250
C	4.60610157252346	-1.72861667829887	1.70038932511824
H	4.01483220564602	-1.11880008413488	2.39186419201022
H	4.92049206805761	-2.64914635083798	2.20565360831332
H	3.97809974395273	-1.97789189100293	0.83365184670755
H	7.33337150177898	-2.51553727072063	1.48154262855010
H	4.56719300217447	1.29973708728086	0.70302745258451
H	3.45562193178792	2.44074670161906	1.19166078899808
I	0.87651533128477	-1.82491276795793	-0.33821628399717
H	5.84061476946398	2.54479371996008	-0.59856861972473
C	6.91429106189601	2.69630730476395	-0.49124652345993
C	7.71395241142341	1.71235390268466	0.09803123656744
C	9.09433009634883	1.88676829788721	0.22445944164250
H	9.69397554533721	1.10002372822793	0.67882384835648
C	9.67637671530406	3.06544477848226	-0.24034814814350
H	10.75368126989644	3.20378468448131	-0.14212746548356

C	8.89035744348927	4.06220032398898	-0.82161095385653
H	9.35051329886586	4.98262718146990	-1.18285655542862
C	7.51224277407802	3.87177315019480	-0.94366552220871
H	6.89127241779987	4.64004430106159	-1.40603295098635
O	3.69299398779968	1.88470966931763	0.43012643194454

[AgIH$_2$O]

Ag	-3.08127219783262	1.78199618815039	-4.37566050119282
I	-4.71551038706295	0.22879327869423	-3.17611784675171
O	-1.61243563151368	3.12368336435388	-5.45498314507485
H	-0.68716887830595	2.91313864879257	-5.23903842953405
H	-1.68283891028481	3.05240863480891	-6.42298605334655

TS3$_{3e}$

C	5.78550965978304	0.34365746145471	0.98753329270369
N	5.74140339728412	-0.94934642631747	1.40056023563979
C	6.99900737253500	-1.48418416877109	1.27324613025720
N	7.84665664549712	-0.60451485891117	0.80425890990015
N	7.07446346385389	0.52012369719067	0.63049886108882
Ag	2.55409405942074	0.35660615724907	-0.29849268879741
C	4.54537317397279	-1.66215144140510	1.84661246281440
H	4.00385569551133	-1.04765843010094	2.57373271289157
H	4.85468253547948	-2.60091497114777	2.31956448832116
H	3.88245147389668	-1.87116482701031	0.99193261795349
H	7.25208224890853	-2.50807062987820	1.52816436751971
H	4.75785797217405	1.19231527638618	0.87067710676412
H	3.34478827522572	2.34686437560019	1.27449637152740
I	1.50664023092161	-1.87446019459207	-1.04432803714156
H	5.76261367800877	2.67315262888999	-0.29247094035298
C	6.85041756830865	2.75847091827595	-0.33088772133647
C	7.66865437461122	1.71504007485606	0.11314904979968
C	9.06137865084509	1.80993660108879	0.06080625479979
H	9.67093716763145	0.97784498391035	0.40826017937153
C	9.64197470723362	2.97285352150860	-0.44328770288773

H	10.72890812544179	3.05137236780016	-0.48701344155041
C	8.84219199869862	4.02805065312167	-0.88626189833968
H	9.30151167282872	4.93535566293520	-1.28038360158085
C	7.45137692651889	3.91488178000286	-0.82662377621245
H	6.81865721572952	4.73111355035069	-1.17725524638035
O	3.77593970267950	1.91021235331295	0.52109746792738

[AgIOH].LH

C	4.33722710399510	0.00722273293160	0.74222552285661
N	3.77847267195759	-1.20989725179788	0.91818442785045
C	4.37611478457000	-2.05589121570901	0.01995725199327
N	5.29975112944375	-1.44195178309544	-0.67866326696514
N	5.26376224001867	-0.15220922723786	-0.21609826362739
Ag	1.86675036272968	1.47675473130129	-0.07587435866421
C	2.61295892704885	-1.49475684803692	1.74957439438449
H	2.53177646895042	-0.71744498111592	2.51551648835364
H	2.73610480175180	-2.47656264047110	2.22073880180618
H	1.71587855746069	-1.46863721345579	1.10893550898901
H	4.10822579723703	-3.10028380337410	-0.09541636287034
H	4.05164318442809	0.96251517223611	1.26419898184214
H	2.79611790144277	3.06935768337906	1.80082531876528
I	0.65417301943493	-0.34238634863187	-1.46938037349016
H	4.93975562006492	2.50395399638168	0.01842450100605
C	5.82566328894878	2.19888201233339	-0.55409918144540
C	6.12285183237351	0.84934938712931	-0.76842861554681
C	7.23185514559281	0.44408800952044	-1.51436871490301
H	7.42269155158147	-0.61670982141491	-1.66746952218346
C	8.06837668788958	1.41871753691390	-2.05476653414042
H	8.93625601292839	1.11380809154062	-2.64052718918222
C	7.79899977963440	2.77352857006112	-1.84747651442769
H	8.45681851892990	3.53189363222105	-2.27400030604388
C	6.68265546630164	3.15454859726678	-1.09956134818803
H	6.46078121611083	4.21105375956460	-0.94436460970393
O	3.22594963557409	2.44690507715978	1.19379517393495

LH

C	2.28683991252285	-0.28814106648984	0.67658189870967
N	1.65772177646681	-1.38161989311569	1.15374968276432
C	1.90167865634774	-2.38406641591268	0.24823987326442
N	2.65306395942648	-1.96318102864084	-0.74293216927775
N	2.89058294055403	-0.64930945527391	-0.46013949387370
C	0.83306283635858	-1.46037693434602	2.36448045357033
H	1.26606778341966	-0.82148017702325	3.14131493393894
H	0.82603448990052	-2.49777053244034	2.71428336318085
H	-0.19123323516964	-1.13796564832614	2.14025112355249
H	1.52484956152171	-3.39708342062834	0.35141926704000
H	2.27839208528959	0.70122353275169	1.11940142960248
H	4.44166570266779	1.40710427344072	0.28883872543175
C	4.42654504455907	1.22053897203646	-0.78594130196682
C	3.69560970463914	0.15951144309779	-1.32642696614330
C	3.71757123470559	-0.14019918822961	-2.68955529877347
H	3.14124360081940	-0.97996089965039	-3.07529988282998
C	4.48694375931624	0.66020802144187	-3.53140573517547
H	4.51406816611561	0.44214397041833	-4.59896489933171
C	5.21295511607499	1.73645529285701	-3.01462464448872
H	5.81257344974153	2.35733831184279	-3.68051554429946
C	5.18372873184550	2.01384536005819	-1.64532353231960
H	5.76699658537675	2.84000675763219	-1.23897328477528

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