

Supporting Information

Bicyclic (alkyl)(amino)carbene (BICAAC) as a metal-free catalyst for reduction of nitriles to amines

Nimisha Gautam, Ratan Logdi, Sreejyothi P, N. M. Rajendran, Ashwani K. Tiwari*
and Swadhin K. Mandal*

Department of Chemical Sciences, Indian Institute of Science Education and Research
Kolkata, Mohanpur 741246, India

*Correspondence to: swadhin.mandal@iiserkol.ac.in

Table of Contents:	Page
1) General Information	S3
2) Experimental Details	
2.1) Experimental procedure for optimisation study of hydroboration of nitriles	S3
2.2) General experimental procedures for BICAAC catalyzed hydroboration of nitriles	S5
2.3) Experimental procedure for gram-scale reaction	S6
2.4) Conversion vs time plot	S7
2.5) Control reactions	S7
2.6) Isotope experiment using DBpin	S13
2.7) Procedure for testing longevity of the catalyst	S15
2.8) Procedure for isolation of N,N-diborylamine	S16
2.9) Procedure for synthesis of amides from N,N-diborylamines	S19
3) Characterization	
3.1) ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Data of Isolated Products	S19
3.2) ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Isolated Products	S34

3.3) ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Data of N-substituted amide products	S78
3.4) ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of N-substituted amide products	S79
4) DFT studies	S82
5) References	S171

1) General Information

All catalytic and control reactions were carried out under argon or nitrogen atmosphere using standard Schlenk techniques or inside a glovebox. All solvents were dried over sodium/benzophenone mixture or CaH₂ and distilled prior to use. All chemicals were purchased from Sigma-Aldrich or Alfa Aesar or TCI-India and used as received. Analytical thin layer chromatography (TLC) was performed on a Merck 60 F254 silica gel plate (0.25 mm thickness). Column chromatography was performed on Merck 60 silica gel (100-200 mesh). The ¹H, ¹³C{¹H}, ¹⁹F{¹H} and ¹¹B{¹H} NMR spectra were recorded on JEOL ECS 400 MHz spectrometer and on a Bruker Avance III 500 MHz spectrometer in D₂O or DMSO-d₆ or CD₃OD with residual undeuterated solvent (eg. DMSO-d₆, 2.50/39.52) as an internal standard. Chemical shifts (δ) are given in ppm, and J values are given in Hz. Evaporation of solvents was performed under reduced pressure using a rotary evaporator. All the glassware were kept in an oven at 120 °C for overnight before use. High-resolution mass spectrometry (HRMS) was obtained on a Bruker maXis impact.

Pinacolborane was obtained from Sigma Aldrich and stored under inert atmosphere in the glovebox. BICAAC was synthesized^{S1} and stored under inert atmosphere in the MBraun glovebox maintained below 0.1 ppm of O₂ and H₂O level. The reactions were performed with a standard 15 mL reaction tube equipped with a stir bar and a screw cap. DBpin was prepared by following literature procedure.^{S2} The substrates (**2x-2z**, **2ad**) were synthesised according to the literature procedure.^{S3,S4,S5}

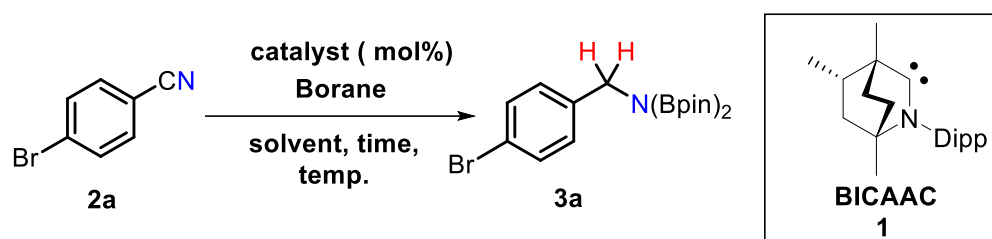
2) Experimental Details

2.1) Experimental procedure for optimisation study of hydroboration of nitriles

Inside a nitrogen-filled glovebox, an oven-dried 15 mL reaction tube was charged with 0.2 mmol of 4-bromo benzonitrile and a magnetic stirring bar, followed by addition of catalyst (5 mol%) and borane (0.5 mmol). The reaction mixture was stirred vigorously at room

temperature for 1-2 min. After that, the tube was sealed tightly with a screw cap and removed from the glovebox. The reaction tube was placed in a preheated oil bath at 60 °C and stirred for 16 h. After 16 h, the reaction mixture was cooled to room temperature and it was diluted with ~ 0.5-0.6 mL of CDCl₃ and ¹H NMR spectra was recorded to calculate the yield. NMR yields are based on unreacted substrate 2a.

Table S1. Optimisation of hydroboration of nitriles to diborylated amines

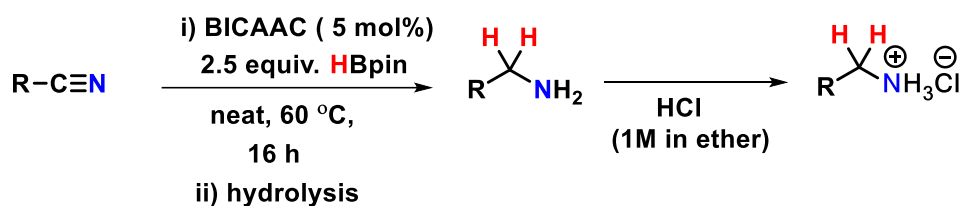


SI No.	Catalyst (mol%)	Borane (equiv.)	Solvent	Temp (°C)	Time (h)	NMR yield (%)
1	BICAAC (5)	HBpin (2.5)	THF	60	16	NR
2	BICAAC (5)	HBpin (2.5)	Toluene	60	16	NR
3	BICAAC (5)	HBpin (2.5)	ACN	60	16	NR
4	BICAAC (5)	HBpin (2.5)	Ether	60	16	NR
5	BICAAC (5)	HBpin (2.5)	DCM	60	16	NR
6	BICAAC (5)	HBpin (2.5)	Hexane	60	16	NR
7	BICAAC (5)	HBpin (2.5)	neat	60	16	91
8	-	HBpin (2.5)	neat	60	16	NR
9	BICAAC (5)	HBpin (2.0)	neat	60	16	73
10	BICAAC (5)	HBpin (2.5)	neat	RT	16	43
11	BICAAC (5)	HBpin (2.5)	neat	60	24	92
12	BICAAC(10)	HBpin (2.5)	neat	60	16	90
13	BICAAC (5)	HBpin (2.5)	neat	80	16	92
14	PPh ₃ (5)	HBpin (2.5)	neat	60	16	NR

15	Et ₃ N (5)	HBpin (2.5)	neat	60	16	NR
16	DBU (5)	HBpin (2.5)	neat	60	16	NR
17	Pyridine (5)	HBpin (2.5)	neat	60	16	NR
18	BICAAC (5)	9-BBN (2.5)	neat	60	16	NR
19	BICAAC (5)	NH ₃ BH ₃ (2.5)	neat	60	16	NR

Reaction conditions: 2a (0.2 mmol), borane (0.5 mmol), dry solvent (0.5 mL), NMR yields were based on unreacted substrate 2a, NR: no reaction.

2.2) General experimental procedure for BICAAC catalyzed hydroboration of nitriles

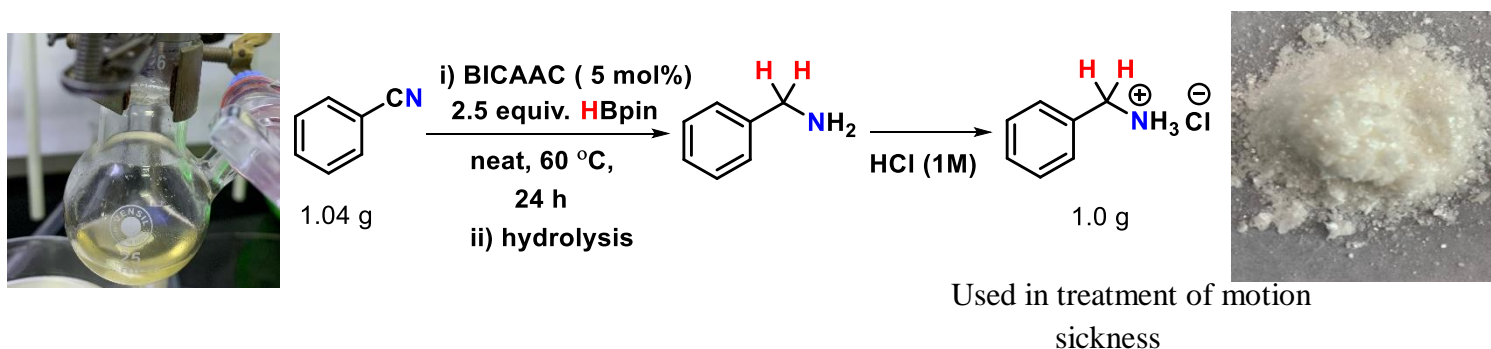


Scheme S1. General procedure for the hydroboration of nitriles to amine hydrochloride salts

Inside a nitrogen-filled glovebox, an oven-dried 15 mL reaction tube was charged with 0.2 mmol nitrile substrate and a magnetic stirring bar, followed by addition of BICAAC (5

mol%) and HBpin (0.5 mmol). Nitrile substrates were kept under high vacuum for 1 h prior to use. The reaction mixture was stirred vigorously at room temperature for 1-2 min. After that, the tube was sealed tightly with a screw cap and removed from the glovebox. The reaction tube was placed in a preheated oil bath at 60 °C and stirred for 16 h. After 16 h, the reaction mixture was cooled to room temperature and quenched by the addition of methanol (1 mL) and stirred overnight for hydrolysis. Subsequently, 0.5 mL HCl (1M in ether) was added dropwise into the reaction tube, and precipitation was observed. The precipitate was washed with n-hexane and diethyl ether and dried under the vacuum. The product was characterized by ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectroscopy using D_2O or DMSO-d_6 as the solvent.

2.3) Experimental procedure for gram-scale reaction



Scheme S2. Catalytic hydroboration of benzonitrile to benzylamine hydrochloride in gram-scale.

Inside a nitrogen-filled glovebox, BICAAC (5 mol%) and pinacolborane (2.5 equiv.) were added to an oven-dried 25 mL Schlenk flask. The solution was stirred vigorously at room temperature for 5 min. While continuously stirring, 1.04 g of benzonitrile substrate was added to the solution using a micropipette. After that, the flask was closed and removed from the glovebox. The reaction flask was placed in a preheated oil bath at 60 °C and stirred for 24 h. After 24 h, the reaction mixture was cooled to room temperature and quenched by the addition of methanol and stirred overnight for hydrolysis. Next, HCl (1M in ether) was added dropwise

into the reaction flask, and precipitation was observed. The precipitate was washed with n-hexane and diethyl ether and dried under the vacuum. The product was characterized by ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectroscopy using DMSO-d_6 as the solvent. Yield of the product is 70%.

2.4) Conversion vs time plot

We monitored the progress of the hydroboration reaction by looking at the conversion vs. time graph for 4-bromobenzonitrile substrate with catalyst BICAAC as shown in Fig. S1. The reaction was carried out at 60 °C for 16 h with 4-bromobenzonitrile and pinacolborane in presence of 5 mol% catalyst loading. The yield of the product was 30% after 2 h, and within 6 h, it furnishes a satisfactory yield of 84%. Finally, within 8 h, the reaction reaches near completion resulting in 91% conversion (Fig. S1).

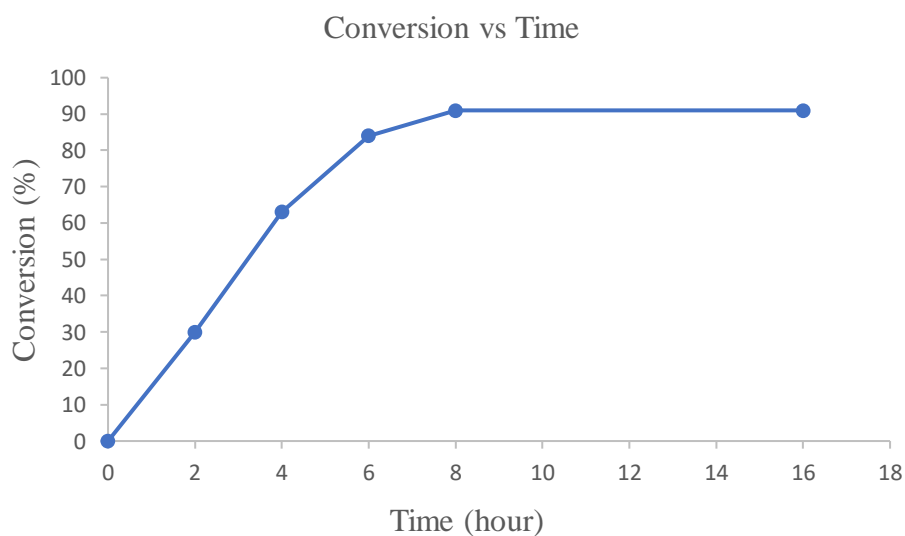
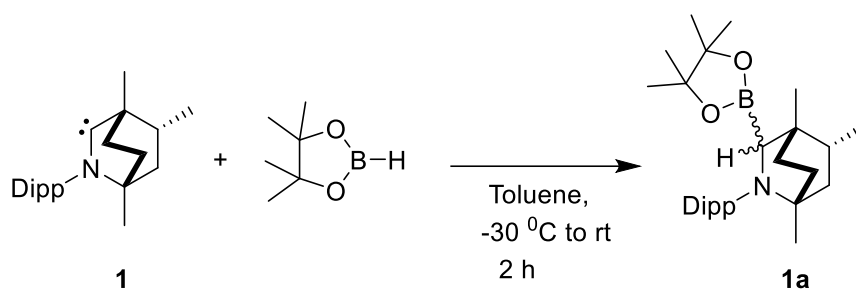


Fig. S1 Plot of conversion (%) versus time (hour) during the hydroboration of 4-bromobenzonitrile (0.2 mmol) and pinacolborane (0.5 mmol) catalyzed by BICAAC (5 mol %).

2.5) Control reactions

a) Preparation and Characterization of the BICAAC B-H insertion product



Scheme S3. Stoichiometric reaction of BICAAC (**1**) and HBpin resulting in the formation of BICAAC(H)·Bpin (**1a**)

Inside the glovebox, a 25 mL oven dried Schlenk flask was charged with BICAAC (0.16 mmol) and was dissolved in 1.5 mL of toluene and was cooled to -30 °C. To it, HBpin (1equiv.) was added and the reaction mixture was allowed to warm to RT and stirred for 2 h. Volatiles were then removed by evaporation under vacuum, affording a colourless and sticky compound. The diastereomeric mixture of the title compound (**1a**) was obtained in 81% yield. ^1H , $^{13}\text{C}\{^1\text{H}\}$ and ^{11}B NMR spectra were recorded in benzene- d_6 solvent.

^1H NMR (400 MHz, C_6D_6 , 25 °C), Diastereomeric Mixture: δ (ppm) = 7.07-7.01 (m, 4H), 6.98-6.93 (m, 2H), 4.11-4.00 (sept, $J = 6.8$ Hz, 1H), 3.97-3.86 (sept, $J = 6.8$ Hz, 1H), 3.65 (s, 1H, CHB), 3.54 (s, 1H, CHB), 3.52-3.44 (overlapping signal from diastereomers, 2H), 2.49-2.41 (m, 1H), 2.25-2.18 (m, 1H), 2.13-2.07 (m, 1H), 1.87-1.82 (m, 1H), 1.79-1.60 (m, 6H), 1.59-1.53 (m, 3H), 1.51-1.48 (m, 6H), 1.47 (s, 3H), 1.42 (broad d, 3H), 1.38 (broad d, 3H), 1.30-1.26 (m, 8H), 1.17-1.11 (m, 8H), 1.00 (broad d, 3H), 0.96 (s, 3H), 0.85 (s, 3H), 0.79 (s, 3H), 0.74-0.73 (m, 6H), 0.70 (s, 6H), 0.67 (s, 6H), 0.63 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6 , 25 °C): $\delta = 152.1, 152.0, 151.5, 150.2, 144.6, 144.3, 129.3, 128.6, 126.3, 126.1, 124.6, 124.3, 124.1, 82.9, 82.8, 52.9, 52.6, 47.9, 44.8, 41.1, 37.9, 37.5, 37.1, 36.5, 35.8, 35.3, 34.5, 29.7, 29.7, 28.0, 27.7, 26.1, 26.0, 25.8, 25.6, 25.3, 25.0, 24.7, 24.4, 24.3, 24.23, 24.17, 23.98,$

23.0, 20.0, 15.7; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6 , 25 °C): $\delta = 32.0$ (broad). HRMS: m/z calc. for $\text{C}_{28}\text{H}_{47}\text{BNO}_2$ $[\text{M}+\text{H}]^+$: 440.3694, found : 440.3679

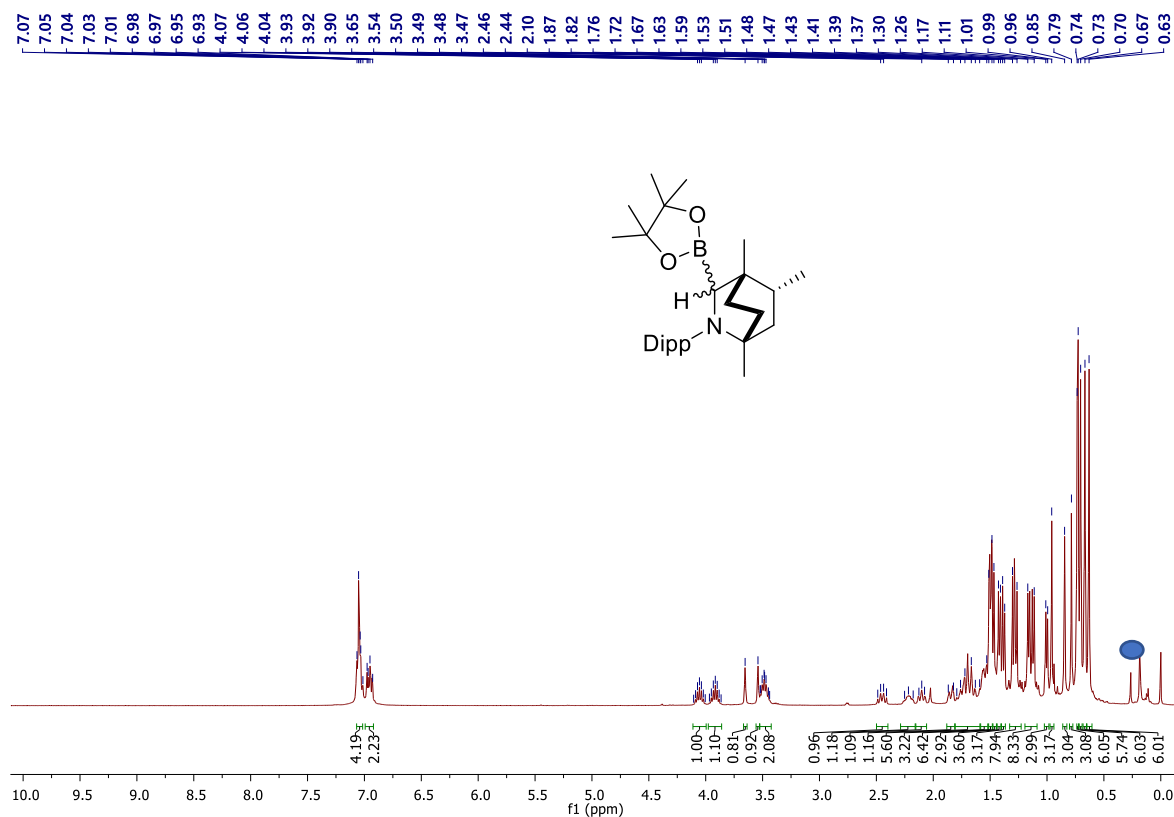


Fig. S2 ^1H NMR spectrum of diastereomeric mixture of BICAAC(H)·Bpin (**1a**) in C_6D_6 .

● denotes impurity peak.

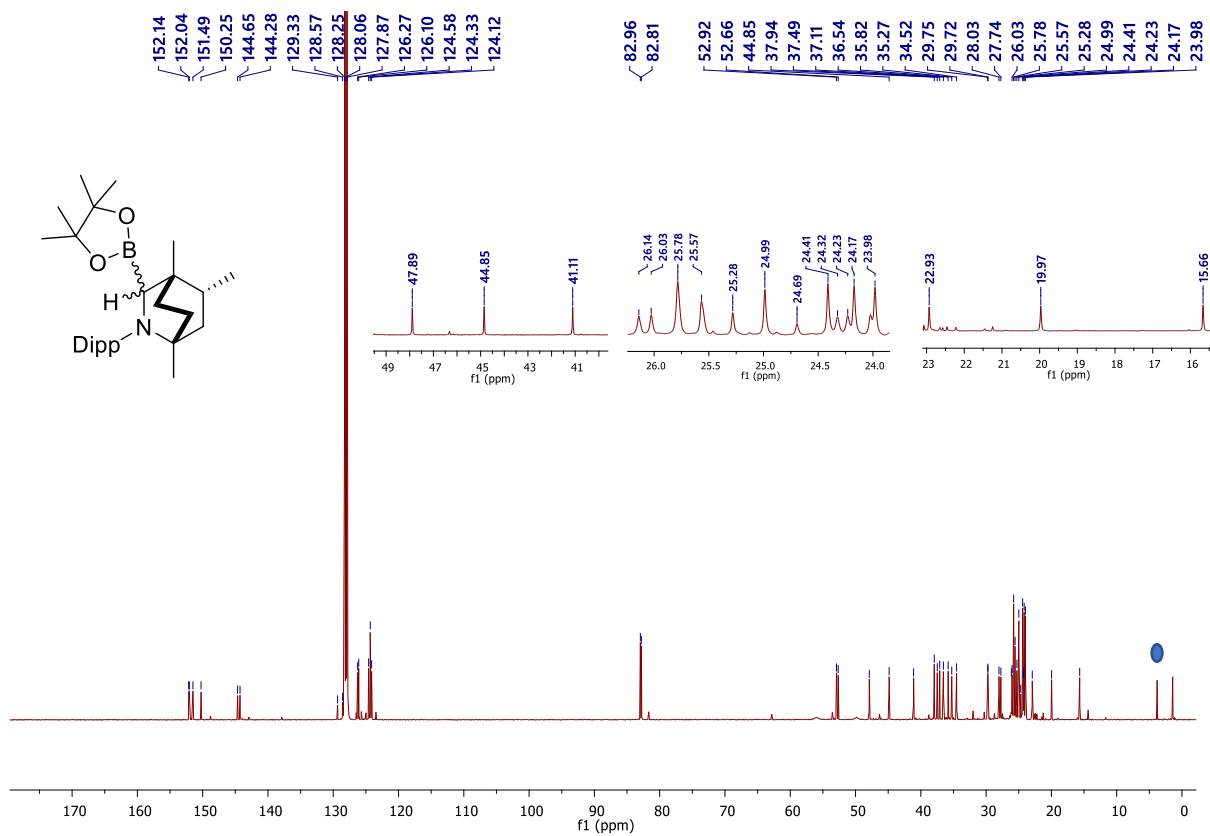


Fig. S3 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of BICAAC(H)·Bpin (**1a**) in C_6D_6 . ● denotes impurity peak.

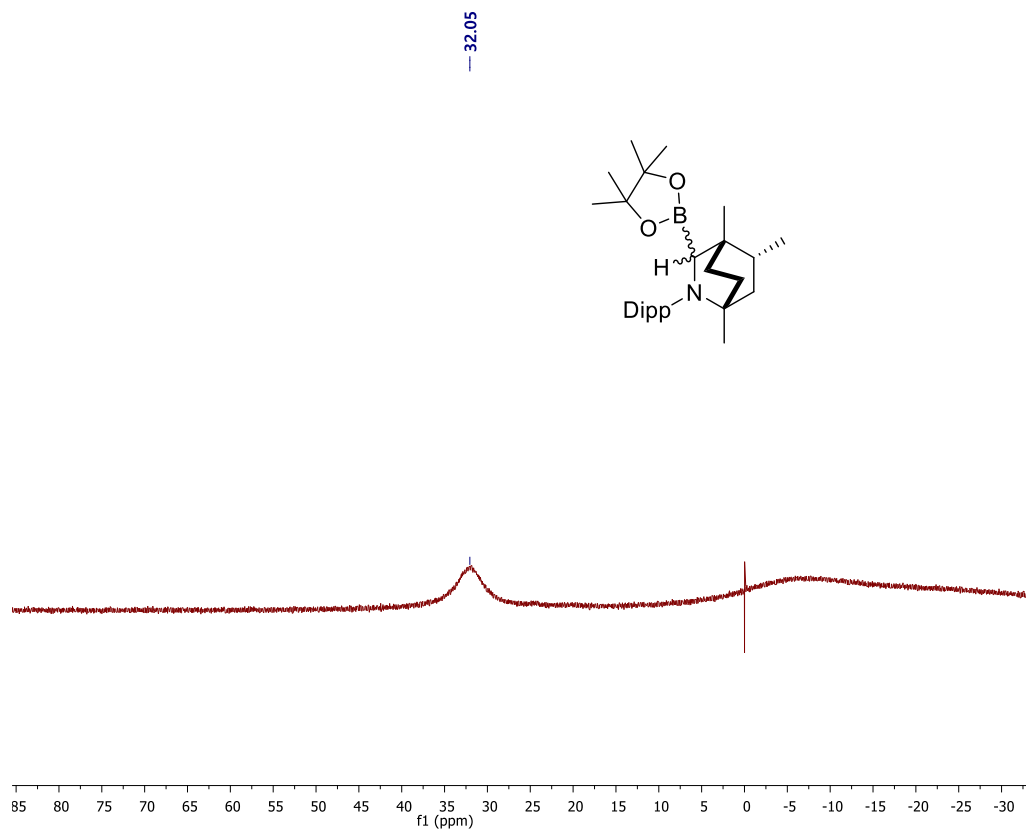


Fig. S4 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of BICAAC(H)·Bpin (**1a**) in C_6D_6

$C_{28}H_{47}BNO_2[M+H]^+$:calculated 440.3694, found 440.3679

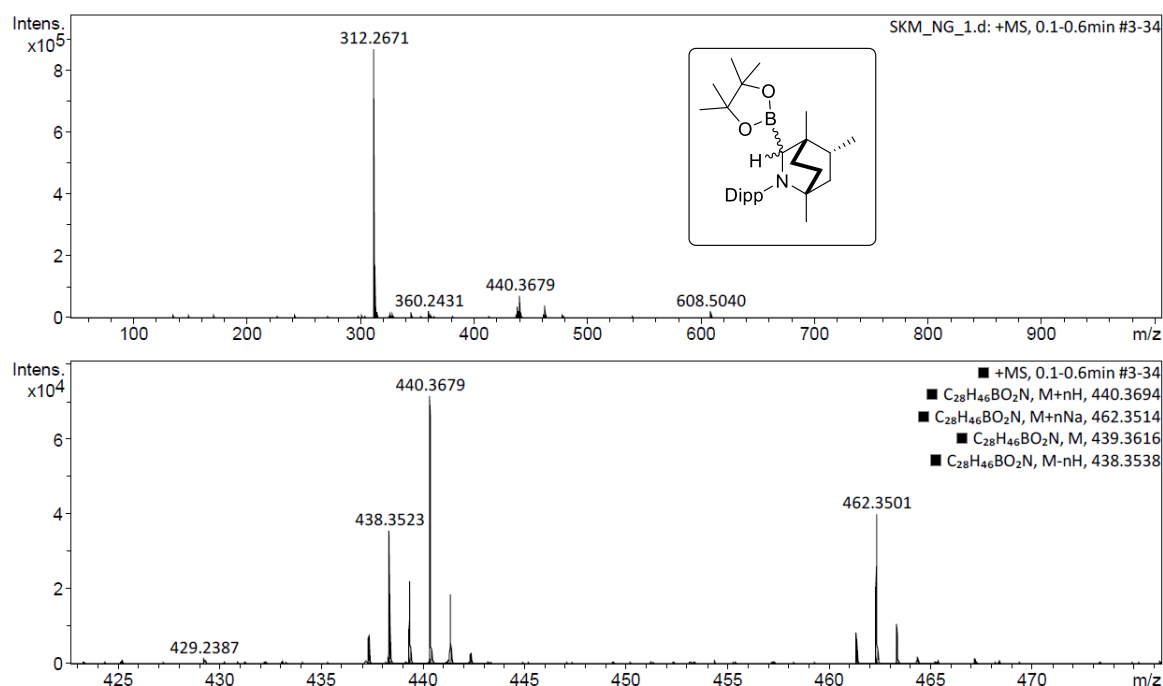
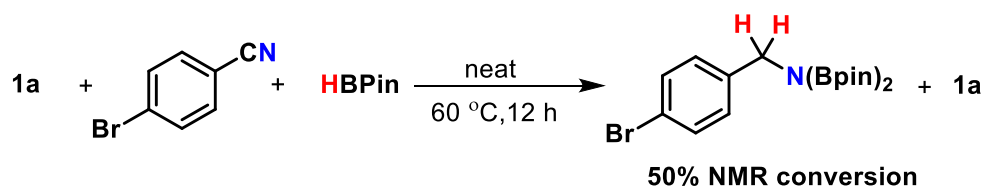


Fig. S5 HRMS spectrum of BICAAC(H)·Bpin (**1a**)

b) A control reaction between 1a, 4-bromo benzonitrile and HBpin



Scheme S4. Stoichiometric reaction of BICAAC(H)·Bpin (**1a**), 4-bromo benzonitrile and HBpin under neat condition

Inside an argon filled glovebox, a 25 mL Schlenk flask containing **1a** (0.16 mmol) was charged with 4-bromo benzonitrile (0.16 mmol) and HBpin (0.16 mmol). The Schlenk flask was next removed from the glovebox and was placed in a preheated oil bath at 60 °C and stirred for 12 h. After 12 h, the reaction mixture was cooled to room temperature and taken inside the glovebox. The reaction mixture was analysed by ¹H and ¹¹B{¹H} NMR spectroscopy using C₆D₆ solvent as a solvent.

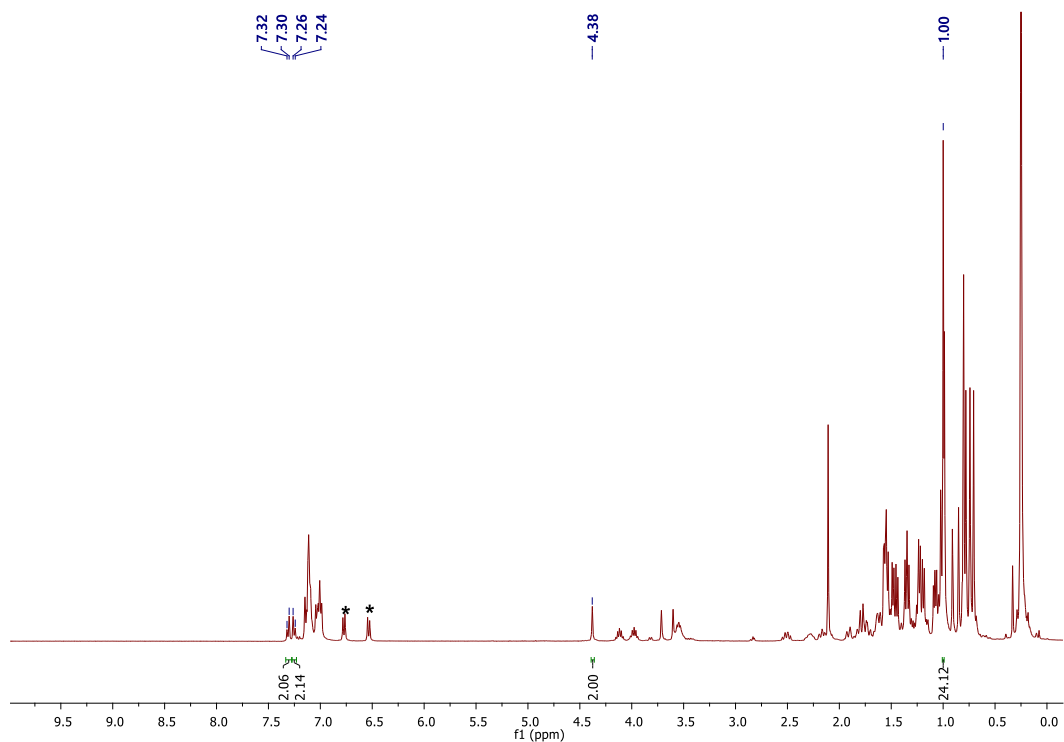


Fig. S6 ^1H NMR spectrum of reaction mixture in C_6D_6 . * indicates peak arising from unreacted 4-bromo benzonitrile.^{S6}

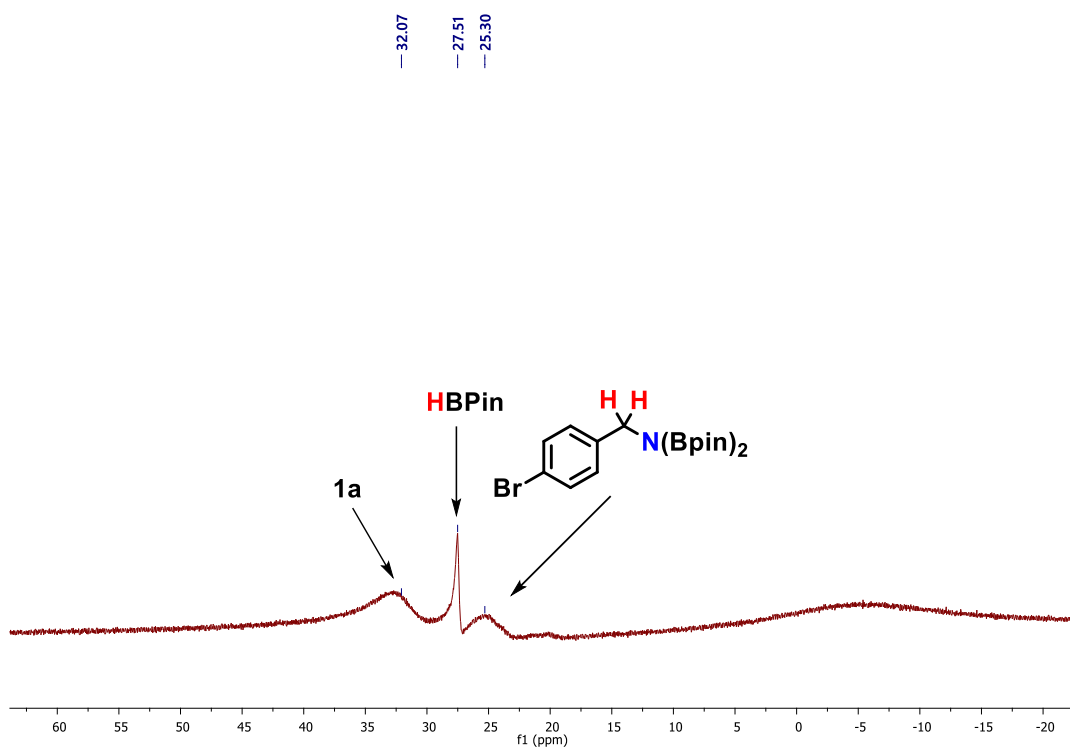
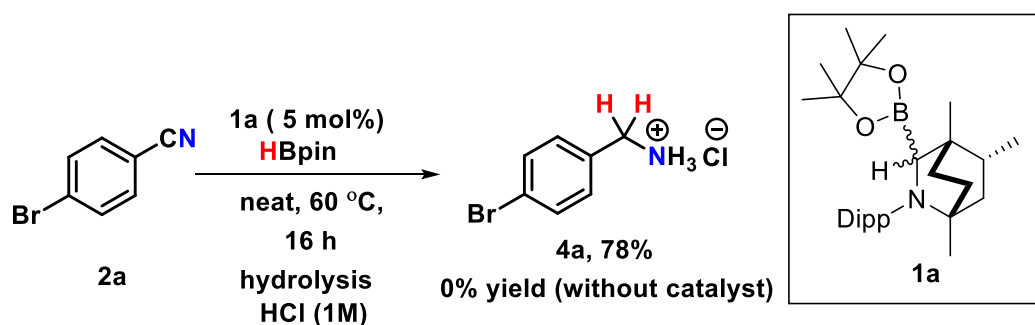


Fig. S7 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of reaction mixture in C_6D_6 .

c) BICAAC(H)·Bpin (**1a**) catalysed hydroboration of nitrile: As a proof to establish that **1a** is the catalytically active species

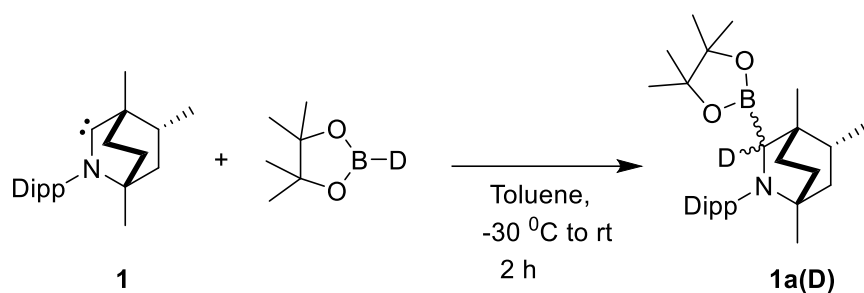


Scheme S5. Hydroboration of nitrile catalysed by BICAAC(H)·Bpin (**1a**)

4-bromo benzonitrile, **2a** was kept under vacuum for 1 h and then taken inside glove box. Inside an argon filled glovebox, an oven dried 15 mL reaction tube equipped with a magnetic bar was charged with 5 mol% of BICAAC(H)·Bpin (**1a**), 4-bromo benzonitrile (0.2 mmol) and HBpin (0.5 mmol). The tube was next sealed tightly with a screw cap and removed from the glovebox. The reaction tube was placed in a preheated oil bath at 60 °C and stirred for 16 h. After 16 h, the reaction mixture was cooled to room temperature and quenched by the addition of methanol (1 mL) and stirred overnight for hydrolysis. Next, 0.5 mL HCl (1M in ether) was added dropwise into the reaction tube, and precipitation was observed. The precipitate was washed with n-hexane and diethyl ether and dried under the vacuum. The corresponding product was then characterized by ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectroscopy using D_2O as the solvent. Yield of the product is 78%.

^1H NMR (400 MHz, D_2O , 25 °C)^{S7}: δ = 7.63 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 4.16 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, D_2O , 25 °C): δ = 132.2, 131.7, 130.7, 122.7, 42.5.

2.6) Isotope experiment using DBpin



Scheme S6. Stoichiometric reaction of BICAAC (**1**) and DBpin resulting in the formation of BICAAC(D)·Bpin [**1a(D)**]

Inside the glovebox, a 25 mL oven dried Schlenk flask was charged with BICAAC (0.16mmol) and was dissolved in 1.5 mL of toluene and was cooled to -30 °C. To it, DBpin (1equiv.) was added and the reaction mixture was allowed to warm to RT and stirred for 2 h. Volatiles were then removed by evaporation under vacuum, affording a colourless and sticky compound. The diastereomeric mixture of the title compound **1a(D)** was obtained. In the ^1H NMR spectrum, the two singlets characteristic signals of the addition product (-CH) at δ 3.65 and 3.54 ppm were missing. Further, a broad singlet at 32.9 ppm is obtained in $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (See Supporting Information, Fig. S8) confirms the formation of the addition product **1a(D)**. These findings suggest the incorporation of deuterium and confirms that the hydride present in the addition product **1a** originates from pinacolborane.

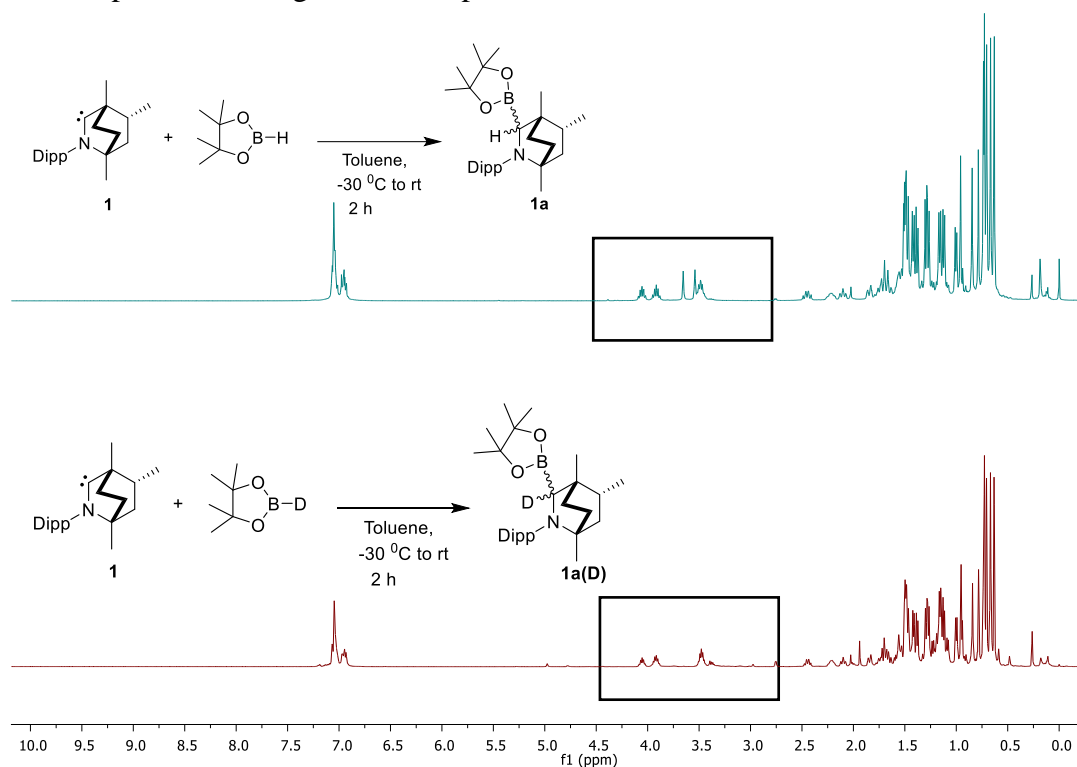


Fig. S8 Stack plots of ^1H NMR spectra (in C_6D_6) revealing incorporation of deuterated form

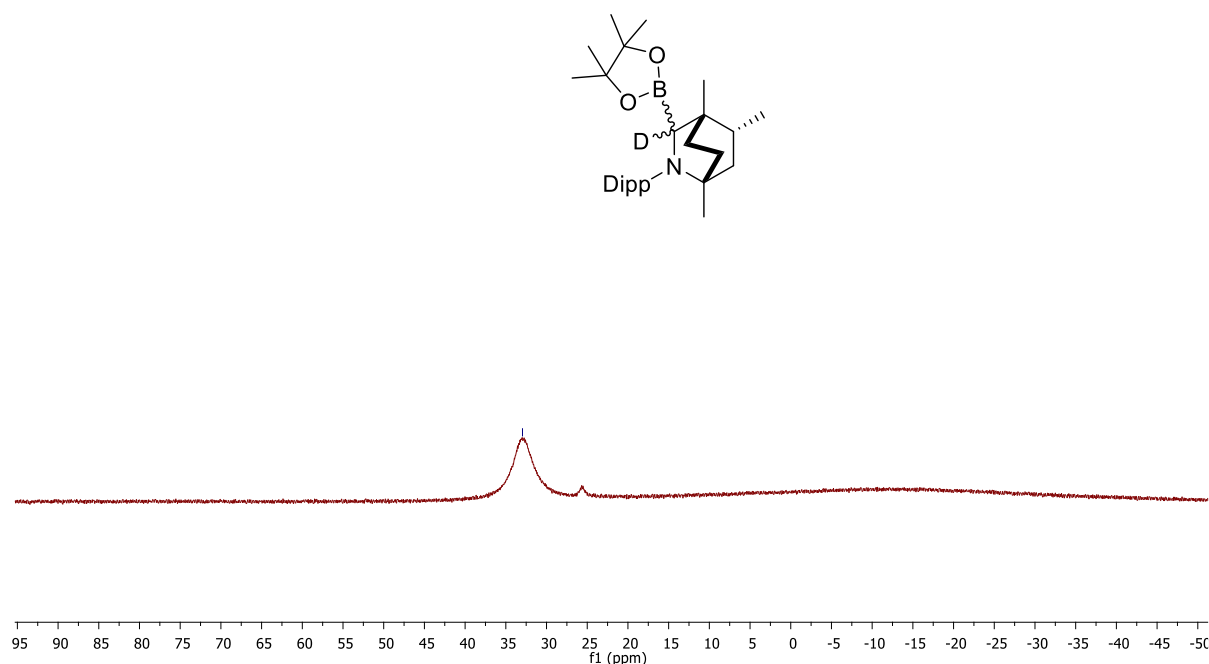


Fig. S9 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of BICAAC(D)-Bpin (**1b**) in C_6D_6

2.7) Procedure for testing longevity of the catalyst

Inside an argon filled glovebox, four oven dried 15 mL reaction tubes equipped with magnetic bar were taken and 0.2 mmol of benzonitrile, BICAAC catalyst (5 mol %), HBpin (0.5 mmol) were added in each of them. Next, the tubes were sealed tightly and removed from the glove box. Following this, it was placed in a preheated oil bath at 60 °C and stirred for 16 h.

After the first reaction time span (16 h), the first reaction tube was uncapped and its conversion was analysed by ^1H NMR spectroscopy. The rest 3 tubes were transferred to the glovebox and fresh 0.2 mmol of benzonitrile, HBpin (0.5 mmol) were added to all remaining three reaction tubes. No further addition of catalyst was made to any of these tubes. Next, these tubes were placed in a preheated oil bath at 60 °C and stirred for 16 h for the second cycle. After 16 h, the 2nd reaction tube was discontinued and analysed. This was continued till the fourth cycle and

its conversion was calculated similarly. It may be noted that the conversion is reported based on the average of two reactions.

In the first two runs, complete consumption of substrate to diborylated product was observed from the reaction mixture ^1H NMR spectrum. 77% and 72% of dihydroborylated product were obtained in the third and fourth cycle, respectively. This observation demonstrates the living nature of the catalyst.

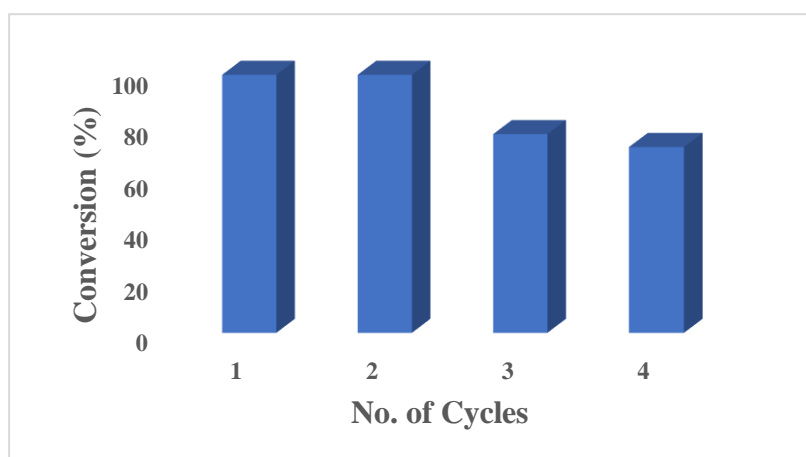
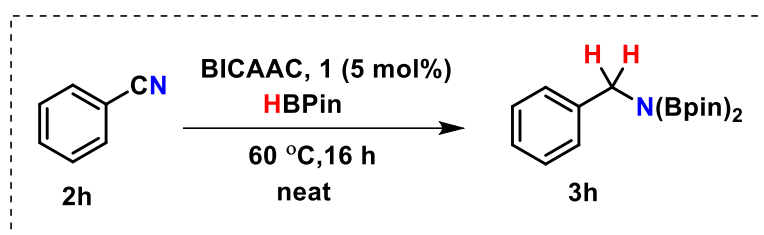
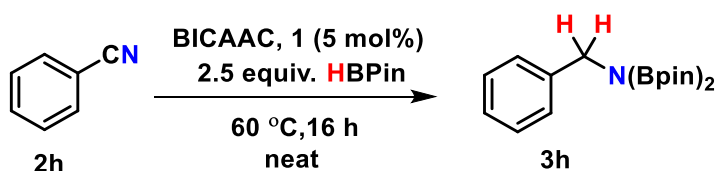


Fig. S10 Plot of conversion (%) versus no. of cycles in the diborylation of benzonitrile for the catalyst longevity test.

2.8) Procedure for isolation of N,N-diborylamine



Scheme S7. Synthesis of double hydroborated product (**3h**)

Inside a nitrogen-filled glovebox, BICAAC (5 mol%) and pinacolborane (1.25 mmol) were added to an oven-dried 25 mL Schlenk flask. The solution was stirred vigorously at room temperature for 2 min. To it, benzonitrile, **2h** (0.5 mmol) was added using a micropipette. After that, the flask was closed and removed from the glovebox. The reaction flask was placed in a preheated oil bath at 60 °C and stirred for 16 h. After 16 h, the reaction mixture was cooled to room temperature and taken inside the glovebox. White solid was observed in the flask, 0.5 mL of dry hexane was added to it and it was stored in the glovebox freezer at -30 °C for 30 minutes. Hexane was decanted from the solid after the Schlenk flask was retrieved from the freezer. The purified solid, **3h** was then kept under vacuum to remove any residual solvent. It was then characterised by ^1H , $^{13}\text{C}\{^1\text{H}\}$ and $^{11}\text{B}\{^1\text{H}\}$ NMR spectroscopy using CDCl_3 as solvent.

^1H NMR (400 MHz, CDCl_3 , 25 °C): δ = 7.28-7.26 (m, 2H), 7.20 (t, J = 7.6 Hz, 2H), 7.13-7.10 (m, 1H), 4.20 (s, 2H), 1.16 (s, 24H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 25 °C): δ = 143.1, 127.9, 127.6, 126.2, 82.4, 47.3, 24.6; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3 , 25 °C): δ = 25.2.

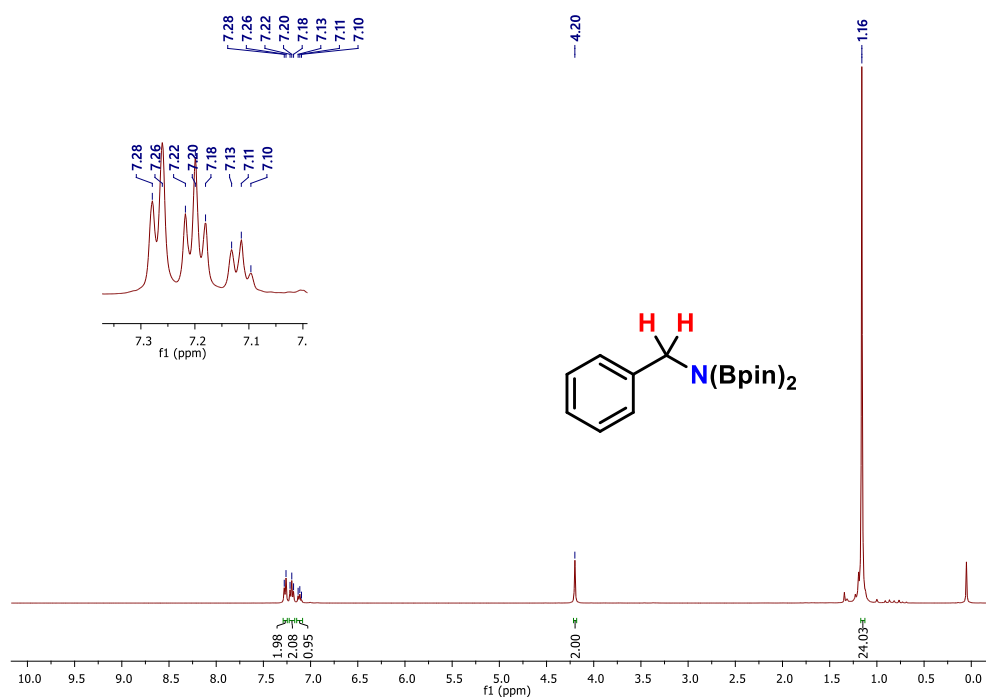


Fig. S11 ^1H NMR spectrum of **3h** in CDCl_3 .^{S7}

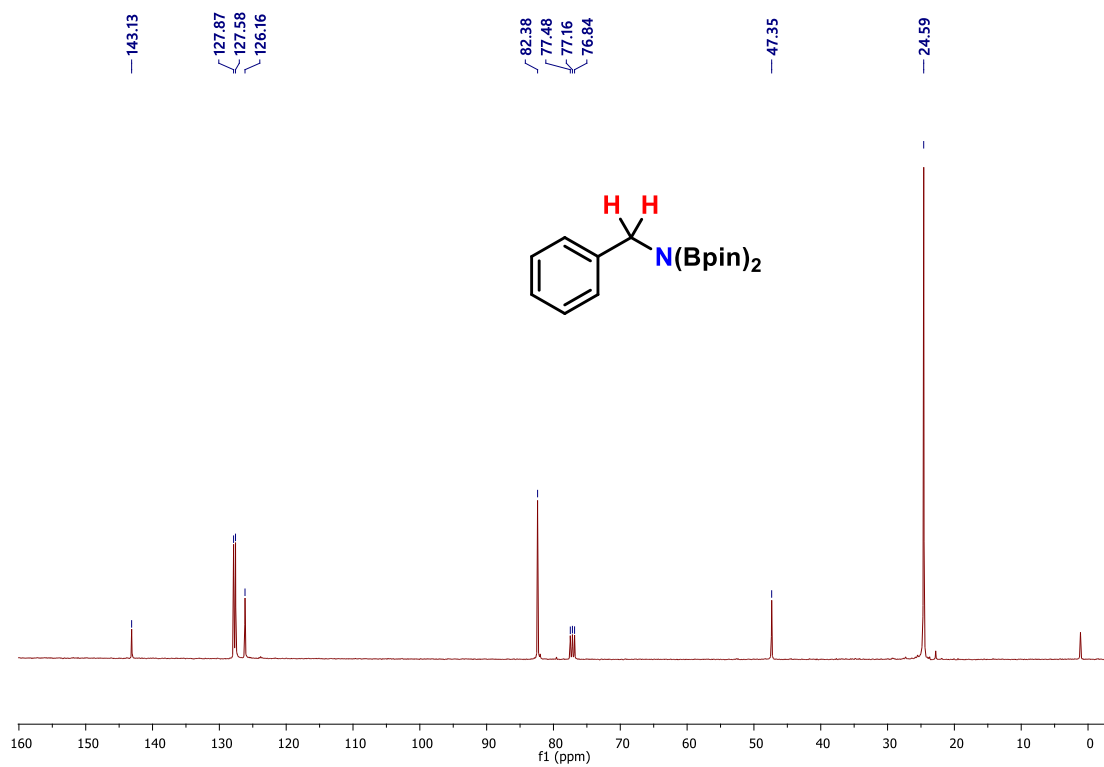


Fig. S12 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3h** in CDCl_3 .^{S7}

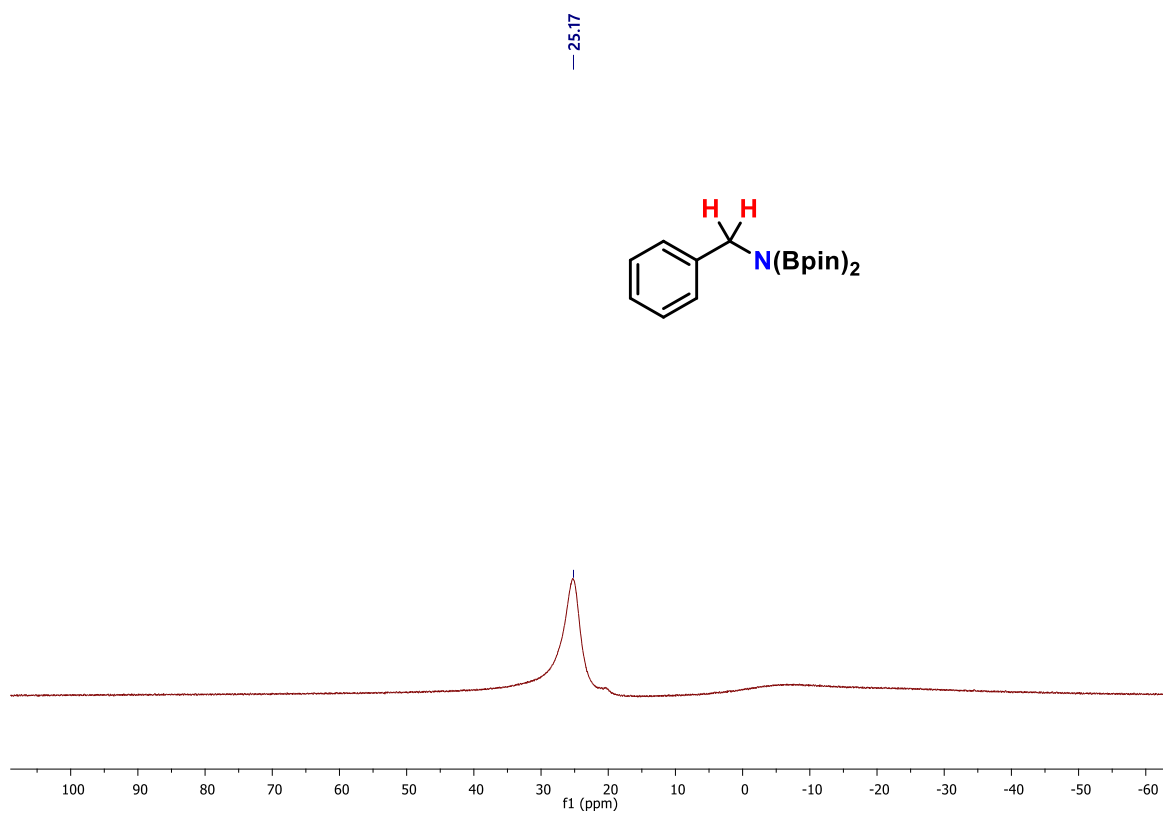
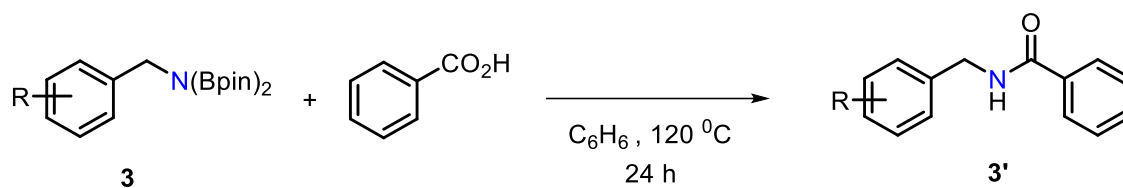


Fig. S13 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **3h** in CDCl_3 .^{S7}

2.9) Procedure for synthesis of amides from N,N-diborylamines

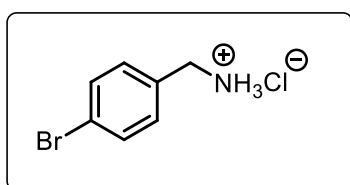


Scheme S8. Synthesis of N-substituted amides by direct C-N cross coupling.

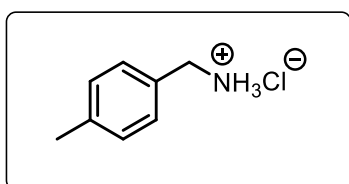
Inside a nitrogen-filled glovebox, 0.5 mmol of N,N-diborylamine, **3** obtained from our protocol in 0.3 mL benzene was taken in a sealed tube. To it, 0.5 mmol of benzoic acid in 0.2 mL benzene was added. Next the tube was sealed tightly with a screw cap and removed from the glovebox. The sealed tube was placed in a preheated oil bath at $120\text{ }^\circ\text{C}$ and stirred for 24 h. After 24 h, the reaction mixture was cooled to room temperature and solvent was removed under reduced pressure. The crude product was purified by column chromatography using hexane/ethyl acetate mixture to yield the desired products.

3) Characterization

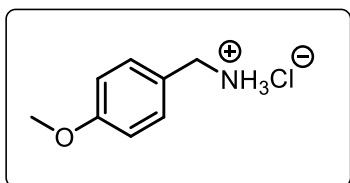
3.1) ^1H , $^{13}\text{C}\{^1\text{H}\}$ and ^{19}F NMR Data of Isolated Products



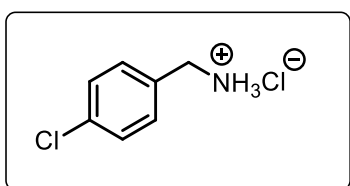
(4-bromophenyl)methan ammonium chloride (**4a**)^{S8}: ^1H NMR (400 MHz, D_2O , $25\text{ }^\circ\text{C}$): $\delta = 7.63$ (d, $J = 8.4$ Hz, 2H), 7.36 (d, $J = 8.4$ Hz, 2H), 4.16 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, D_2O , $25\text{ }^\circ\text{C}$): $\delta = 132.2$, 131.7 , 130.7 , 122.7 , 42.5 . Yield: 76%.



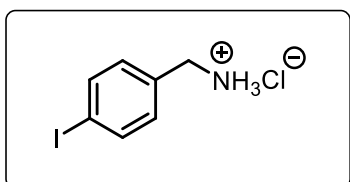
p-tolylmethan ammonium chloride (**4b**)^{S9}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.36-7.30 (m, 4H), 4.14 (s, 2H), 2.35 (s, 3H); **¹³C{¹H} NMR** (100 MHz, D₂O, 25 °C): δ = 139.6, 129.8, 129.6, 128.9, 42.9, 20.3. Yield: 86%.



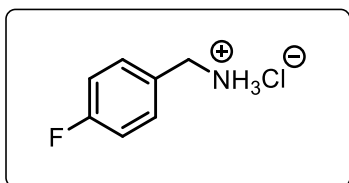
(4-methoxyphenyl)methan ammonium chloride (**4c**)^{S9}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.41 (d, *J* = 8.8 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 4.12 (s, 2H), 3.83 (s, 3H); **¹³C{¹H} NMR** (100 MHz, D₂O, 25 °C): δ = 159.4, 130.6, 125.2, 114.6, 55.4, 42.6. Yield: 86%.



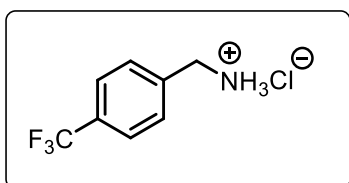
(4-chlorophenyl)methan ammonium chloride (**4d**)^{S10}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.48-7.41 (m, 4H), 4.17 (s, 2H); **¹³C{¹H} NMR** (100 MHz, D₂O, 25 °C): δ = 134.6, 131.2, 130.5, 129.2, 42.5. Yield: 86%.



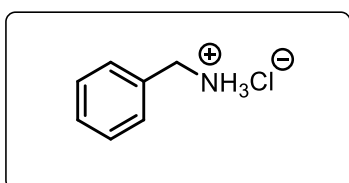
(4-iodophenyl)methan ammonium chloride (**4e**)^{S8}: $^1\text{H NMR}$ (400 MHz, D_2O , 25 °C): $\delta = 7.83$ (d, $J = 8.0$ Hz, 2H), 7.22 (d, $J = 8.4$ Hz, 2H), 4.14 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, D_2O , 25 °C): $\delta = 138.3, 132.3, 130.8, 94.7, 42.7$. Yield: 59%.



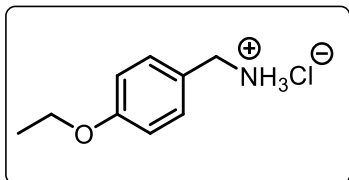
(4-fluorophenyl)methan ammonium chloride (**4f**)^{S11}: $^1\text{H NMR}$ (400 MHz, D_2O , 25 °C): $\delta = 7.47$ (dd, $J = 8.4, 5.2$ Hz, 2H), 7.20 (t, $J = 8.8$ Hz, 2H), 4.18 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, D_2O , 25 °C): $\delta = 162.9$ (d, $J = 243.9$ Hz), 131.1 (d, $J = 8.9$ Hz), 128.6 (d, $J = 2.5$ Hz), 116.0 (d, $J = 21.4$ Hz), 42.5; $^{19}\text{F}\{^1\text{H}\}$ NMR (470 MHz, D_2O , 25 °C): $\delta = -113.18$. Yield: 80%.



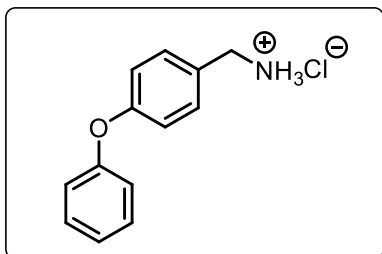
(4-(trifluoromethyl)phenyl)methan ammonium chloride (**4g**)^{S10}: $^1\text{H NMR}$ (400 MHz, D_2O , 25 °C): $\delta = 7.79$ (d, $J = 8.0$ Hz, 2H), 7.62 (d, $J = 8.0$ Hz, 2H), 4.28 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, D_2O , 25 °C): $\delta = 136.6, 130.4$ (q, $J = 32.0$ Hz), 129.3, 126.1 (q, $J = 3.8$ Hz), 125.1, 122.9, 120.7, 42.6; $^{19}\text{F}\{^1\text{H}\}$ NMR (470 MHz, D_2O , 25 °C, TMS): $\delta = -62.5$. Yield: 70%.



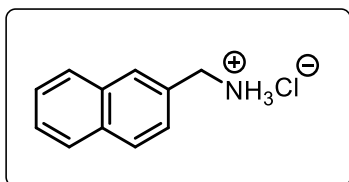
Phenylmethan ammonium chloride (**4h**)^{S10}: ¹H NMR (400 MHz, D₂O, 25 °C): δ = 7.51 (s, 5H), 4.21 (s, 2H); ¹³C{¹H} NMR (125 MHz, D₂O, 25 °C): δ = 132.6, 129.3, 128.9, 43.2. Yield: 84%.



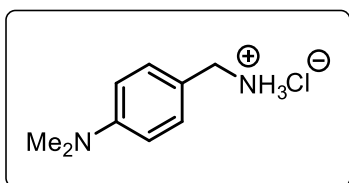
(4-ethoxyphenyl)methan ammonium chloride (**4i**)^{S12}: ¹H NMR (400 MHz, DMSO-d₆, 25 °C): δ = 8.50 (br s, 3H), 7.42 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 4.01 (q, *J* = 7.2 Hz, 2H), 3.90 (s, 2H), 1.31 (t, *J* = 7.2 Hz, 3H); ¹³C{¹H} NMR (100 MHz, DMSO-d₆, 25 °C): δ = 158.6, 130.5, 125.9, 114.3, 63.1, 41.6, 14.6. Yield: 67%.



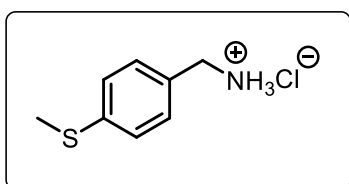
(4-phenoxyphenyl)methan ammonium chloride (**4j**)^{S13}: ¹H NMR (400 MHz, DMSO-d₆, 25 °C): δ = 8.64 (br s, 3H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.41-7.37 (m, 2H), 7.17-7.13 (m, 1H), 7.02-6.98 (m, 4H), 3.98 (s, 2H); ¹³C{¹H} NMR (100 MHz, DMSO-d₆, 25 °C): δ = 156.8, 156.4, 131.1, 130.1, 129.1, 123.7, 118.7, 118.5, 41.5. Yield: 81%.



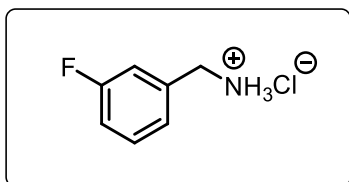
Naphthalen-2-ylmethan ammonium chloride (**4k**)^{S10}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.96-7.90 (m, 4H), 7.60-7.56 (m, 2H), 7.49 (dd, J = 8.4, 1.6 Hz, 1H), 4.29 (s, 2H); **¹³C{¹H}** NMR (125 MHz, D₂O, 25 °C): δ = 132.9 (d, J = 9.4 Hz), 130.1, 128.9, 128.2, 128.0, 127.7, 127.0 (d, J = 19.7 Hz), 125.9, 43.2. Yield: 71%.



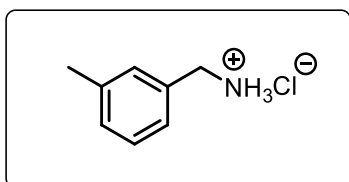
(4-(dimethylamino)phenyl)methan ammonium chloride (**4l**)^{S14}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.71 (br s, 3H), 7.66 (br s, 4H), 4.03-3.99 (m, 2H), 3.06 (s, 6H); **¹³C{¹H}** NMR (125 MHz, DMSO d₆, 25 °C): δ = 145.2, 130.6, 119.0, 44.2, 41.6. Yield: 78%.



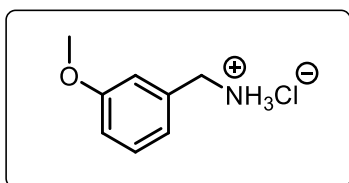
(4-(Methylthio)phenyl)methan ammonium chloride (**4m**)^{S15}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.43-7.37 (m, 4H), 4.17 (s, 2H), 2.52 (s, 3H); **¹³C{¹H}** NMR (125 MHz, D₂O, 25 °C): δ = 139.2, 129.6, 129.4, 126.6, 42.7, 14.4. Yield: 74%.



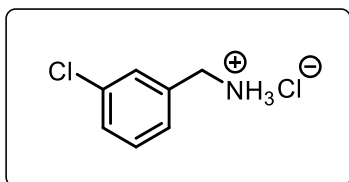
(3-fluorophenyl)methan ammonium chloride (**4n**)^{S9}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.50 (dd, J = 14.4, 8.0 Hz, 1H), 7.29 (d, J = 8.0 Hz, 1H), 7.26-7.20 (m, 2H), 4.22 (s, 2H); **¹³C{¹H} NMR** (125 MHz, D₂O, 25 °C): δ = 162.6 (d, J = 243.0 Hz), 134.8 (d, J = 7.9 Hz), 131.1 (d, J = 8.4 Hz), 124.7 (d, J = 2.7 Hz), 116.1 (d, J = 20.9 Hz), 115.7 (d, J = 22.4 Hz), 42.6; **¹⁹F{¹H} NMR** (470 MHz, D₂O, 25 °C): δ = -112.76. Yield: 70%.



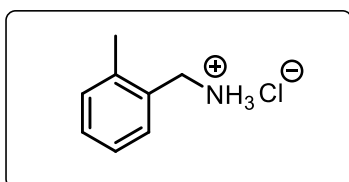
m-tolylmethan ammonium chloride (**4o**)^{S9}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.37 (t, J = 7.6 Hz, 1H), 7.27 (dd, J = 18.4, 8.0 Hz, 3H), 4.14 (s, 2H), 2.36 (s, 3H); **¹³C{¹H} NMR** (100 MHz, D₂O, 25 °C): δ = 139.5, 132.7, 129.8, 129.4, 129.2, 125.7, 43.1, 20.4. Yield: 62%.



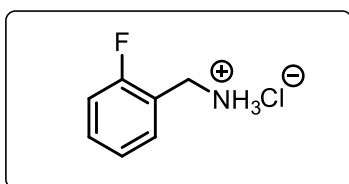
(3-methoxyphenyl)methan ammonium chloride (**4p**)^{S9}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.60 (br s, 3H), 7.30 (t, J = 7.6 Hz, 1H), 7.18 (s, 1H), 7.05 (d, J = 7.6 Hz, 1H), 6.94-6.91 (m, 1H), 3.96 (s, 2H), 3.76 (s, 3H); **¹³C{¹H} NMR** (100 MHz, DMSO d₆, 25 °C): δ = 159.3, 135.6, 129.6, 120.9, 114.5, 113.9, 55.2, 42.0. Yield: 66%.



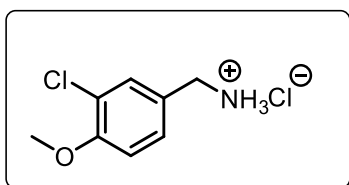
(3-chlorophenyl)methan ammonium chloride (**4q**)^{S10}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.51-7.40 (m, 4H), 4.20 (s, 2H) ppm; **¹³C{¹H} NMR** (125 MHz, D₂O, 25 °C): δ = 134.5, 134.2, 130.7, 129.2, 128.8, 127.2, 42.5. Yield: 79%.



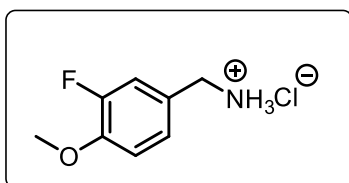
o-tolylmethan ammonium chloride (**4r**)^{S10}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.40-7.31 (m, 4H), 4.24 (s, 2H), 2.39 (s, 3H); **¹³C{¹H} NMR** (125 MHz, D₂O, 25 °C): δ = 137.2, 131.0, 130.9, 129.4, 129.1, 126.7, 40.5, 18.0. Yield: 41%.



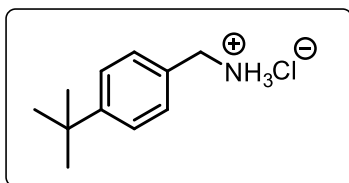
(2-fluorophenyl)methan ammonium chloride (**4s**)^{S16}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.54-7.48 (m, 2H), 7.32-7.24 (m, 2H), 4.28 (s, 2H); **¹³C{¹H} NMR** (125 MHz, D₂O, 25 °C): δ = 160.9 (d, J = 244.7 Hz), 131.7 (d, J = 8.5 Hz), 131.2 (d, J = 2.5 Hz), 125.0 (d, J = 3.1 Hz), 119.6 (d, J = 15.1 Hz), 115.8 (d, J = 21.0 Hz), 37.2 (d, J = 3.5 Hz); **¹⁹F{¹H} NMR** (470 MHz, D₂O, 25 °C): δ = -118.2. Yield: 30%.



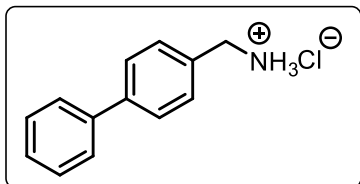
(3-chloro-4-methoxyphenyl)methan ammonium chloride (**4t**)^{S17}: **¹H NMR** (400 MHz, DMSO *d*₆, 25 °C): δ = 8.61 (br s, 3H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.46 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 1H), 3.93 (s, 2H), 3.85 (s, 3H); **¹³C{¹H} NMR** (100 MHz, DMSO *d*₆, 25 °C): δ = 154.5, 130.7, 129.4, 127.2, 120.7, 112.7, 56.2, 41.0. Yield: 79%.



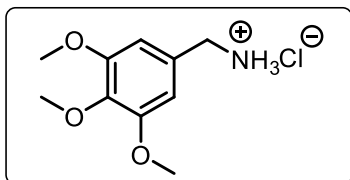
(3-fluoro-4-methoxyphenyl)methan ammonium chloride (**4u**)^{S17}: **¹H NMR** (400 MHz, DMSO *d*₆, 25 °C): δ = 8.62 (br s, 3H), 7.45 (dd, *J* = 12.4, 2.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.18 (t, *J* = 8.8 Hz, 1H), 3.93 (s, 2H), 3.83 (s, 3H); **¹³C{¹H} NMR** (125 MHz, DMSO *d*₆, 25 °C): δ = 151.0 (d, *J* = 242.5 Hz), 147.2 (d, *J* = 10.1 Hz), 126.8 (d, *J* = 6.7 Hz), 125.8, 116.8 (d, *J* = 18.7 Hz), 113.7, 56.1, 41.2; **¹⁹F{¹H} NMR** (470 MHz, D₂O, 25 °C): δ = -135.2. Yield: 92%.



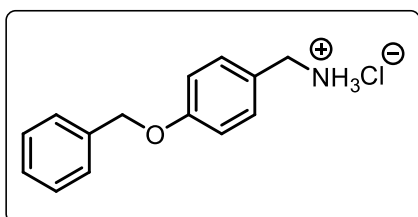
(4-(tert-butyl)phenyl)methan ammonium chloride (**4v**)^{S12}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.59 (br s, 3H), 7.45-7.39 (m, 4H), 3.94 (s, 2H), 1.27 (s, 9H); **¹³C{¹H} NMR** (125 MHz, DMSO d₆, 25 °C): δ = 150.9, 131.2, 128.8, 125.3, 41.8, 34.3, 31.1. Yield: 66%.



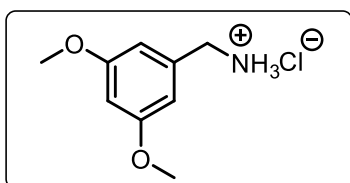
[1,1'-biphenyl]-4-ylmethan ammonium chloride (**4w**)^{S12}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.72 (br s, 3H), 7.68 (t, *J* = 8.4 Hz, 4H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 1H), 4.05 (s, 2H); **¹³C{¹H} NMR** (100 MHz, DMSO d₆, 25 °C): δ = 140.1, 139.5, 133.3, 129.6, 129.0, 127.7, 126.7, 41.8. Yield: 67%.



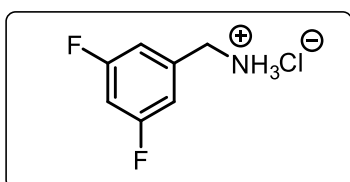
(3,4,5-trimethoxyphenyl)methan ammonium chloride (**4x**)^{S18}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.63 (br s, 3H), 6.95 (s, 2H), 3.93 (s, 2H), 3.78 (s, 6H), 3.64 (s, 3H); **¹³C{¹H} NMR** (100 MHz, DMSO d₆, 25 °C): δ = 152.8, 137.3, 129.7, 106.6, 60.0, 56.0, 42.4. Yield: 85%.



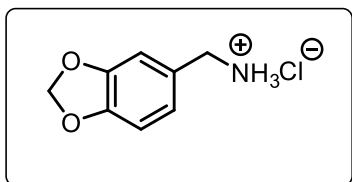
(4-(benzyloxy)phenyl)methan ammonium chloride (**4y**)^{S18}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.41 (br s, 3H), 7.45-7.30 (m, 7H), 7.03 (d, *J* = 8.4 Hz, 2H), 5.13 (s, 2H), 3.92 (s, 2H); **¹³C{¹H} NMR** (100 MHz, DMSO d₆, 25 °C): δ = 158.3, 136.9, 130.5, 128.4, 127.8, 127.6, 126.2, 114.8, 69.1, 41.6. Yield: 61%.



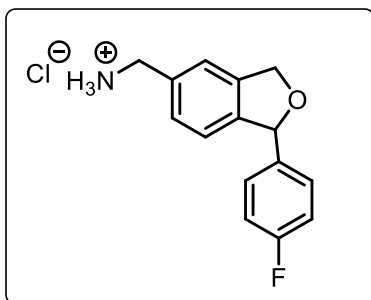
(3,5-dimethoxyphenyl)methan ammonium chloride (**4z**)^{S19}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.65 (br s, 3H), 6.75 (d, *J* = 2.0 Hz, 2H), 6.47 (t, *J* = 2.0 Hz, 1H), 3.92 (s, 2H), 3.74 (s, 6H); **¹³C{¹H} NMR** (100 MHz, DMSO d₆, 25 °C): δ = 160.5, 136.3, 106.9, 100.0, 55.3, 42.2. Yield: 88%.



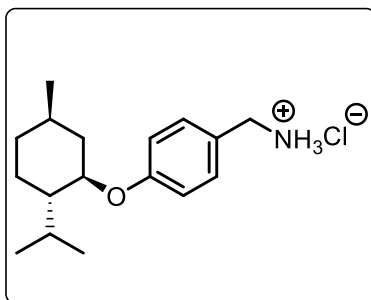
(3,5-difluorophenyl)methan ammonium chloride (**4aa**)^{S20}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 7.12-7.08 (m, 2H), 7.07-7.02 (m, 1H), 4.23 (s, 2H); **¹³C{¹H} NMR** (125 MHz, D₂O, 25 °C): δ = 163.9 (d, *J* = 13.4 Hz), 162.0 (d, *J* = 13.4 Hz), 136.1 (t, *J* = 10.0 Hz), 111.9 (q), 104.6 (t, *J* = 25.1 Hz), 42.3; **¹⁹F{¹H} NMR** (470 MHz, D₂O, 25 °C): δ = -109.2. Yield: 78%.



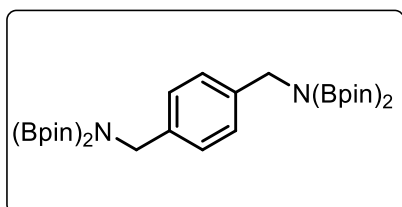
benzo[d][1,3]dioxol-5-ylmethan ammonium chloride (**4ab**)^{S14}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.56 (br s, 3H), 7.15 (s, 1H), 6.98-6.91 (m, 2H), 6.02 (s, 2H), 3.89 (s, 2H); **¹³C{¹H}** **NMR** (125 MHz, DMSO d₆, 25 °C): δ = 147.2, 127.7, 122.9, 109.5, 108.2, 101.2, 41.9. Yield: 88%.



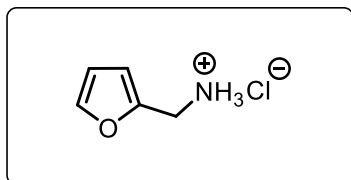
(1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-yl)methan ammonium chloride (**4ac**)^{S21}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.60 (br s, 3H), 7.52 (s, 1H), 7.41-7.35 (m, 3H), 7.20-7.16 (m, 2H), 7.09-7.07 (m, 1H), 6.19 (s, 1H), 5.31-5.27 (m, 1H), 5.14-5.11 (m, 1H), 4.01 (s, 2H); **¹³C{¹H}** **NMR** (125 MHz, DMSO d₆, 25 °C): δ = 161.7 (d, J = 242.5 Hz), 142.1, 139.1, 138.8 (d, J = 3.0 Hz), 133.8, 128.5 (t, J = 10.0 Hz), 122.1 (d, J = 23.4 Hz), 115.2 (d, J = 21.4 Hz), 84.0, 72.4, 41.9; **¹⁹F{¹H}** **NMR** (470 MHz, DMSO d₆, 25 °C): δ = -114.7. Yield: 84%.



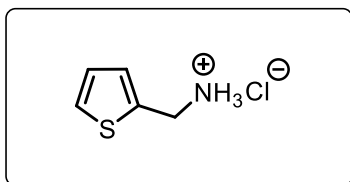
4-((1R,2S,5R)-2-Isopropyl-5-methylcyclohexoxy)phenylmethan ammonium chloride (**4ad**): $^1\text{H NMR}$ (400 MHz, CD_3OD , 25 °C): δ = 8.94 (d, J = 8.8 Hz, 2H), 8.53 (d, J = 8.8 Hz, 2H), 5.71 (dt, J = 10.4, 4.0 Hz, 1H), 5.60 (s, 2H), 3.72-3.66 (m, 2H), 3.33-3.26 (m, 2H), 3.14-3.02 (m, 2H), 2.78-2.68 (m, 2H), 2.55-2.51(m, 1H), 2.48 (d, J = 6.4 Hz, 6H), 2.32 (d, J = 6.8 Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CD_3OD , 25 °C): δ = 160.5, 131.7, 126.0, 117.0, 78.5, 49.5, 43.9, 41.4, 35.6, 32.4, 27.5, 24.9, 22.5, 21.0, 17.1; **HRMS**: m/z calc. for $[\text{C}_{17}\text{H}_{25}\text{O}-\text{Cl}-\text{NH}_3]^+$: 245.189, found: 245.189. Yield: 68%.



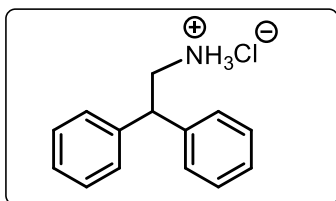
$\text{N,N}'$ -(1,4-phenylenebis(methylene))bis(4,4,5,5-tetramethyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine) (**3ae**)^{S7}: $^1\text{H NMR}$ (400 MHz, CDCl_3 , 25 °C): δ = 7.09 (s, 4H), 4.11 (s, 4H), 1.11 (s, 48H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C): δ = 140.7, 126.9, 82.3, 47.0, 24.6; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3 , 25 °C): δ = 26.02. Yield: 88%.



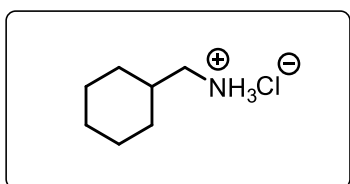
Furan-2-ylmethan ammonium chloride (**4af**)^{S22}: $^1\text{H NMR}$ (400 MHz, $\text{DMSO}-d_6$, 25 °C): δ = 8.64 (br s, 3H), 7.72 (s, 1H), 6.56-6.55 (m, 1H), 6.49-6.48 (m, 1H), 4.03 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, $\text{DMSO}-d_6$, 25 °C): δ = 147.7, 143.5, 110.9, 110.3, 34.9. Yield: 67%.



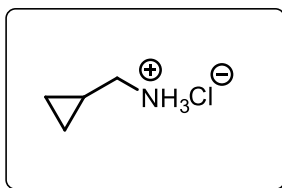
Thiophen-2-ylmethan ammonium chloride (**4ag**)^{S23}: $^1\text{H NMR}$ (400 MHz, DMSO d_6 , 25 °C): δ = 8.64 (br s, 3H), 7.57-7.55 (m, 1H), 7.29 (d, J = 2.8 Hz, 1H), 7.06 (dd, J = 4.8, 4.0 Hz, 1H), 4.20 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO d_6 , 25 °C): δ = 135.3, 129.1, 127.2, 36.6. Yield: 45%.



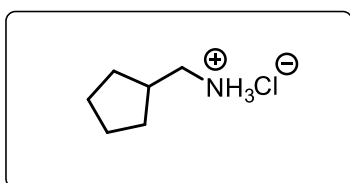
2,2-Diphenylethyl ammonium chloride (**4ah**)^{S24}: $^1\text{H NMR}$ (400 MHz, D_2O , 25 °C): δ = 7.38 (d, J = 4.4 Hz, 8H), 7.35-7.30 (m, 2H), 4.35 (t, J = 8.4 Hz, 1H), 3.72 (d, J = 8.4 Hz, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, D_2O , 25 °C): δ = 140.0, 129.3, 127.7, 48.6, 43.1. Yield: 67%.



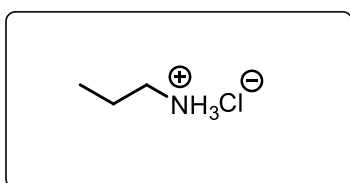
Cyclohexylmethan ammonium chloride (**4ai**)^{S25}: $^1\text{H NMR}$ (400 MHz, DMSO d_6 , 25 °C): δ = 8.12 (br s, 3H), 2.59 (d, J = 6.8 Hz, 2H), 1.75 -1.54 (m, 6H), 1.22-1.06 (m, 3H), 0.94-0.85 (m, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO d_6 , 25 °C): δ = 44.3, 35.4, 29.8, 25.6, 25.0. Yield: 59%.



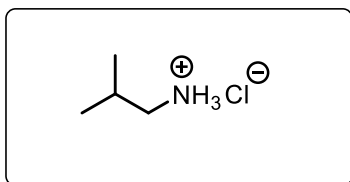
Cyclopropylmethan ammonium chloride (**4aj**)^{S12}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.17 (br s, 3H), 2.63 (d, *J* = 7.6 Hz, 2H), 1.06 -0.99 (m, 1H), 0.53-0.48 (m, 2H), 0.33-0.30 (m, 2H); **¹³C{¹H} NMR** (125 MHz, DMSO d₆, 25 °C): δ = 43.4, 8.5, 3.8. Yield: 65%.



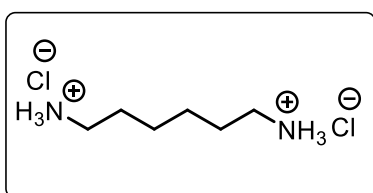
Cyclopentylmethan ammonium chloride (**4ak**)^{S25}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.16 (br s, 3H), 2.69 (d, *J* = 7.2 Hz, 2H), 2.14 -2.06 (m, 1H), 1.76-1.69 (m, 2H), 1.61-1.46 (m, 4H), 1.25-1.17 (m, 2H); **¹³C{¹H} NMR** (125 MHz, DMSO d₆, 25 °C): δ = 43.3, 37.5, 29.8, 24.6. Yield: 74%.



propyl ammonium chloride (**4al**)^{S26}: **¹H NMR** (400 MHz, D₂O, 25 °C): δ = 2.98 (t, *J* = 7.2 Hz, 2H), 1.74-1.64 (m, 2H), 0.99 (t, *J* = 7.6 Hz, 3H); **¹³C{¹H} NMR** (100 MHz, D₂O, 25 °C): δ = 41.2, 20.3, 10.1. Yield: 68%.



2-methylpropan-1- ammonium chloride (**4am**)^{S12}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.15 (br s, 3H), 2.59-2.57 (m, 2H), 1.89 (sept, *J* = 6.8 Hz, 1H), 0.91 (d, *J* = 6.8 Hz, 6H); **¹³C{¹H} NMR** (125 MHz, DMSO d₆, 25 °C): δ = 45.6, 30.7, 26.3, 19.9. Yield: 86%.



hexane-1,6-diammonium chloride (**4an**)^{S17}: **¹H NMR** (400 MHz, DMSO d₆, 25 °C): δ = 8.05 (br s, 6H), 2.74 (t, *J* = 7.2 Hz, 4H), 1.57-1.54 (m, 4H), 1.33-1.29 (m, 4H); **¹³C{¹H} NMR** (125 MHz, DMSO d₆, 25 °C): δ = 38.5, 26.7, 25.3. Yield: 50%.

3.2) ^1H and ^{13}C NMR Spectra of Products

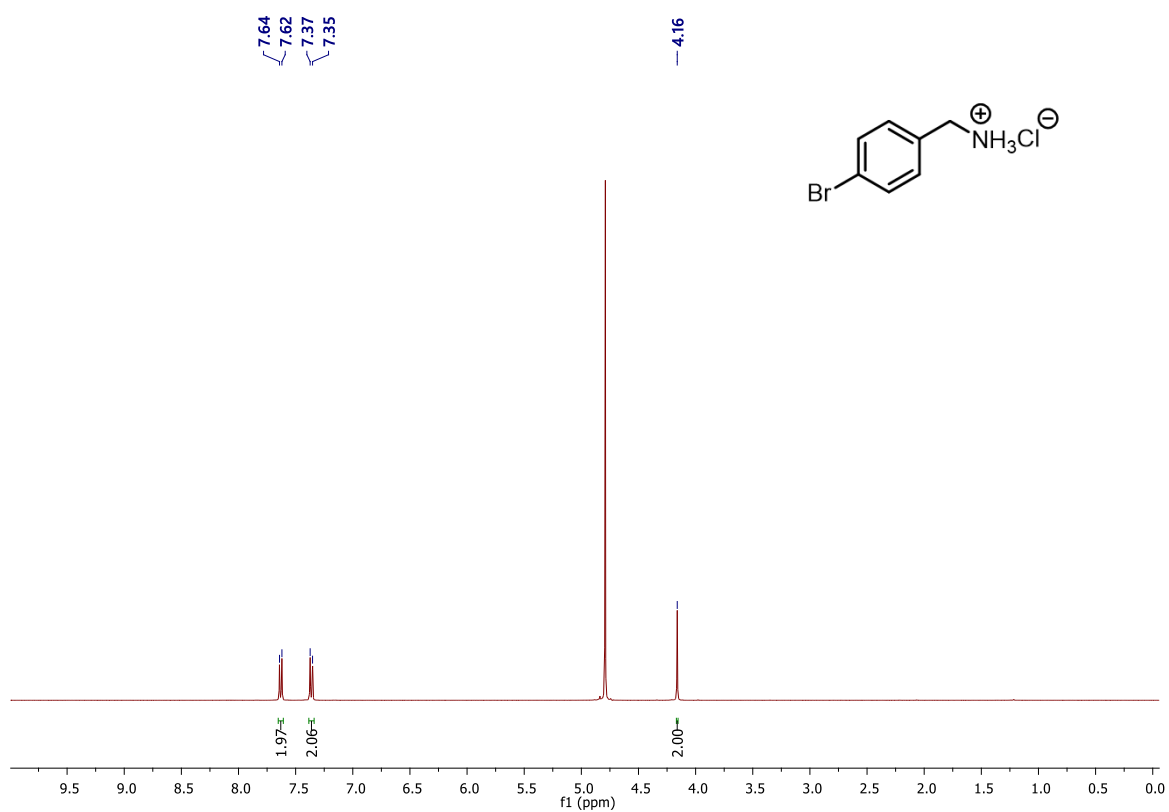


Fig. S14 ^1H NMR spectrum of **4a** in D_2O . ^{S8}

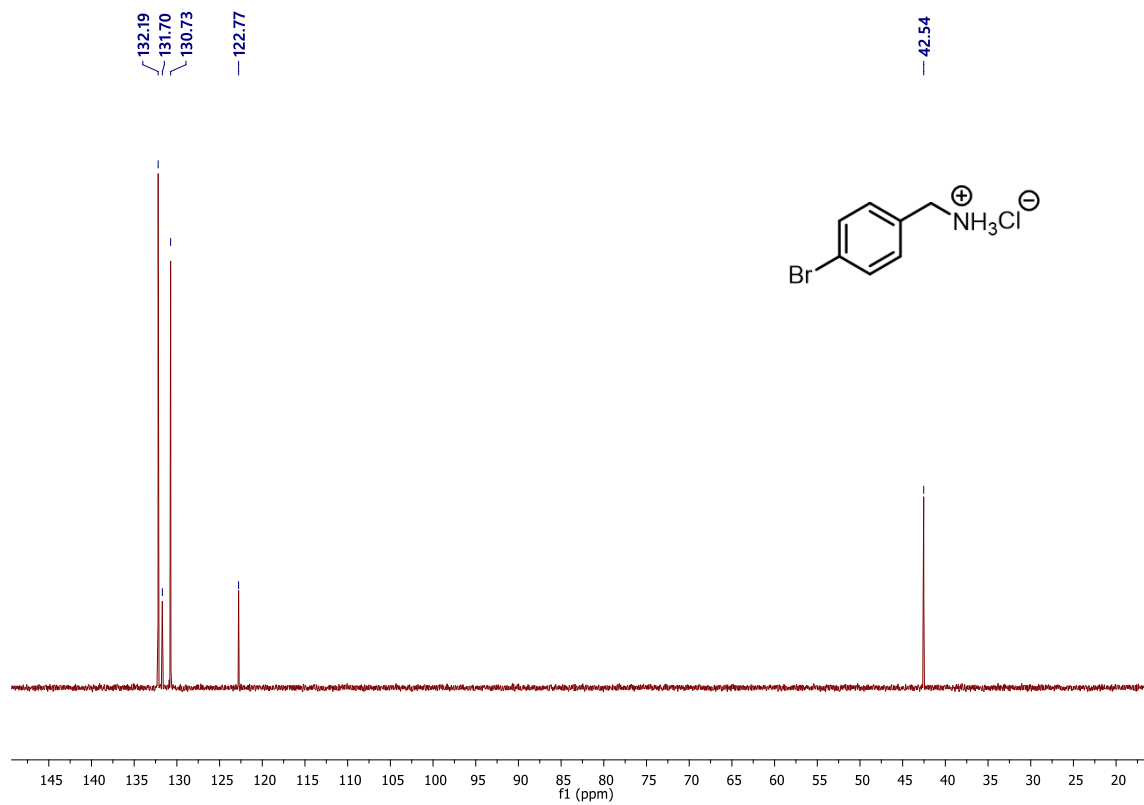


Fig. S15 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4a** in D_2O . ^{S8}

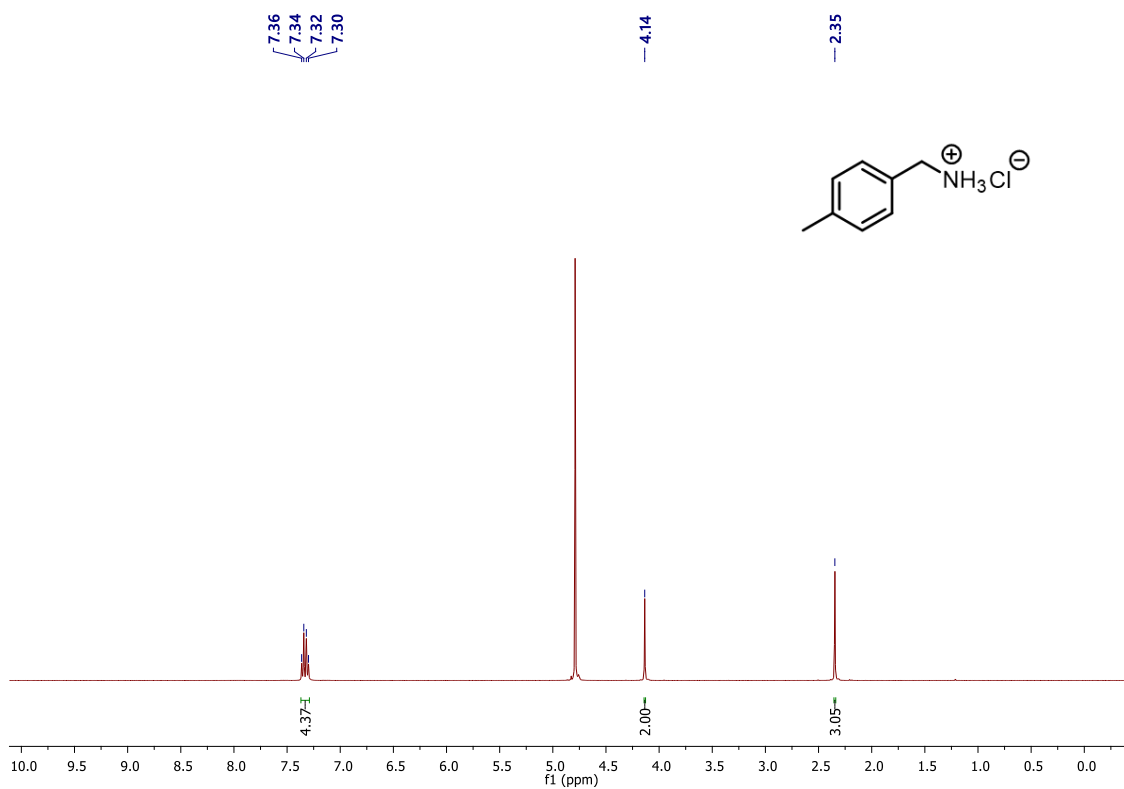


Fig. S16 ¹H NMR spectrum of **4b** in D₂O. ^{S9}

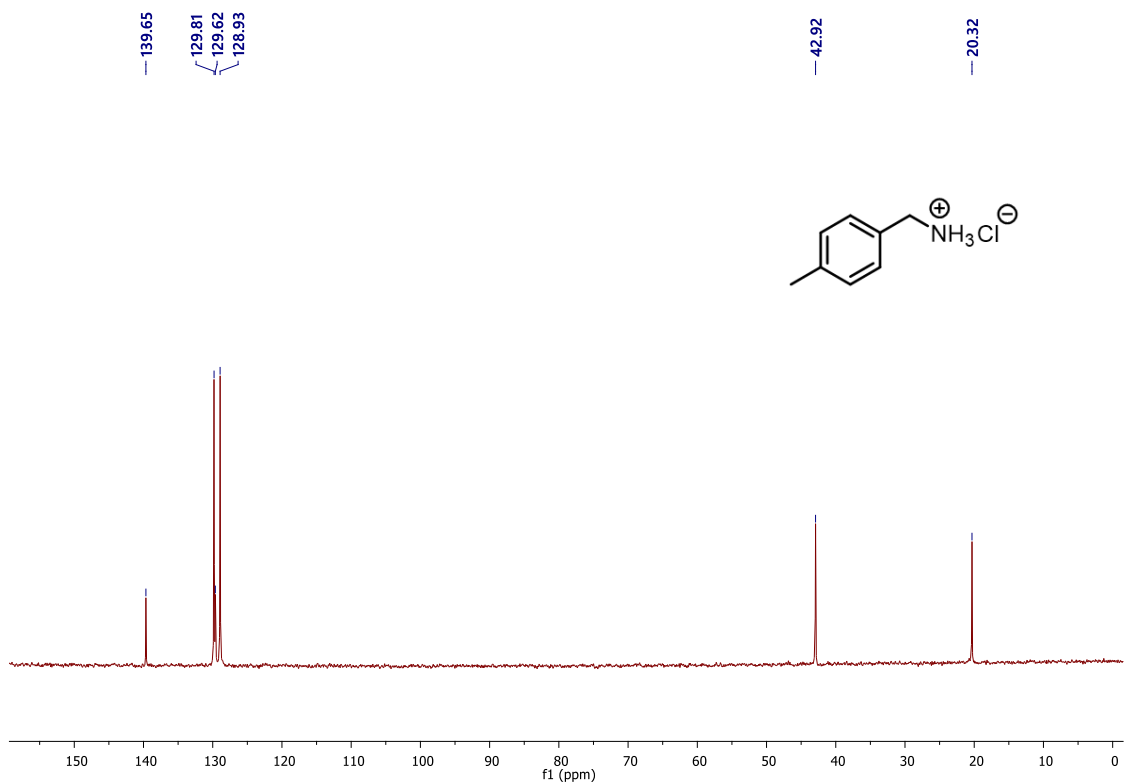


Fig. S17 ¹³C{¹H} NMR spectrum of **4b** in D₂O. ^{S9}

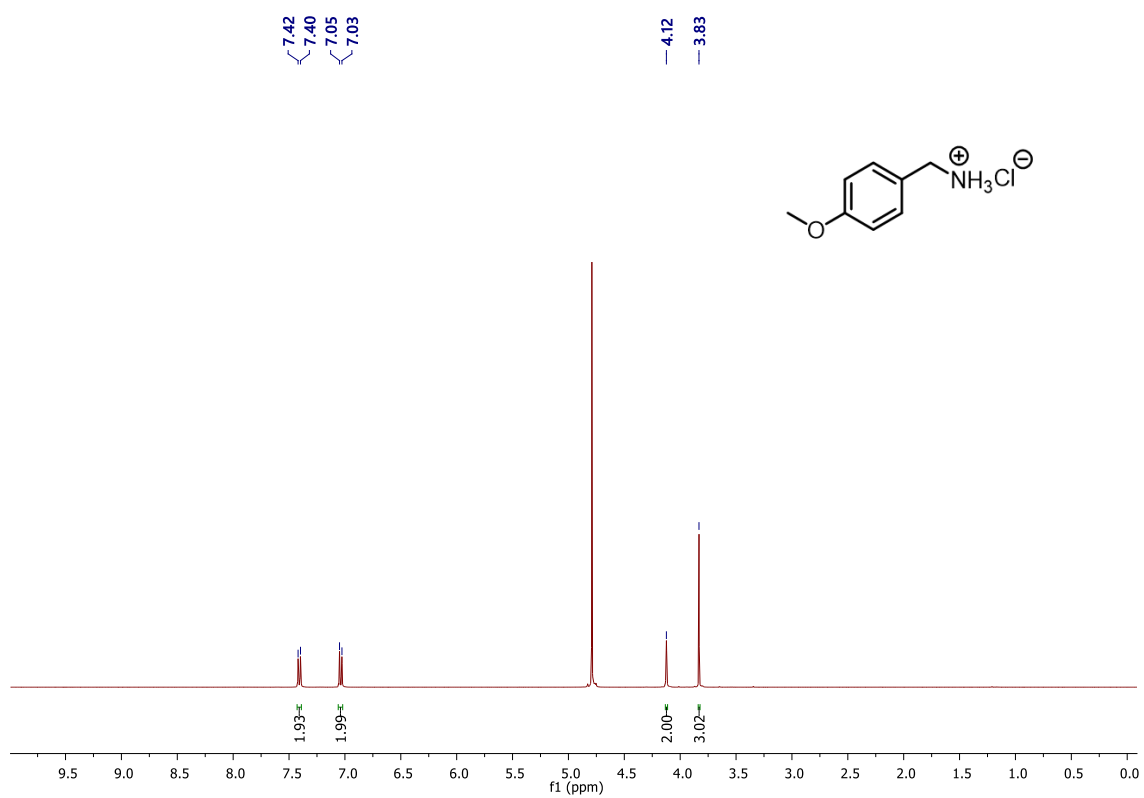


Fig. S18 ^1H NMR spectrum of **4c** in D_2O .^{S9}

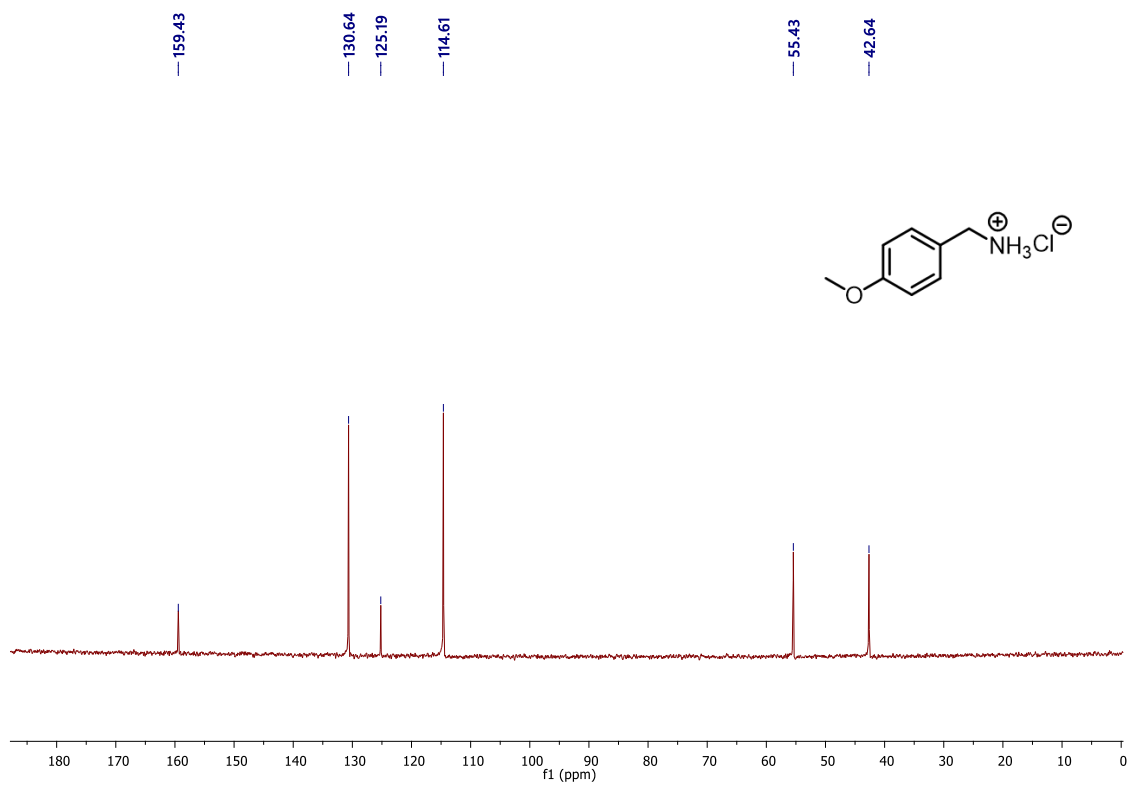


Fig. S19 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4c** in D_2O .^{S9}

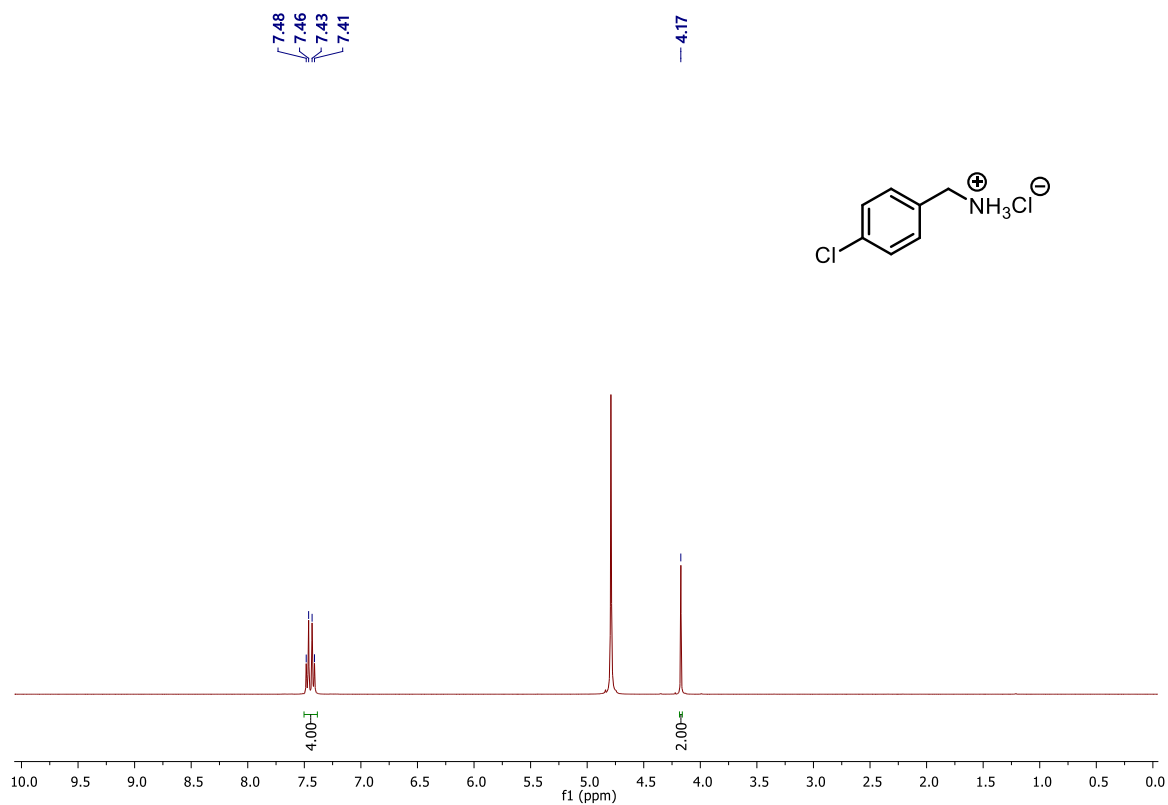


Fig. S20 ^1H NMR spectrum of **4d** in D_2O .^{S10}

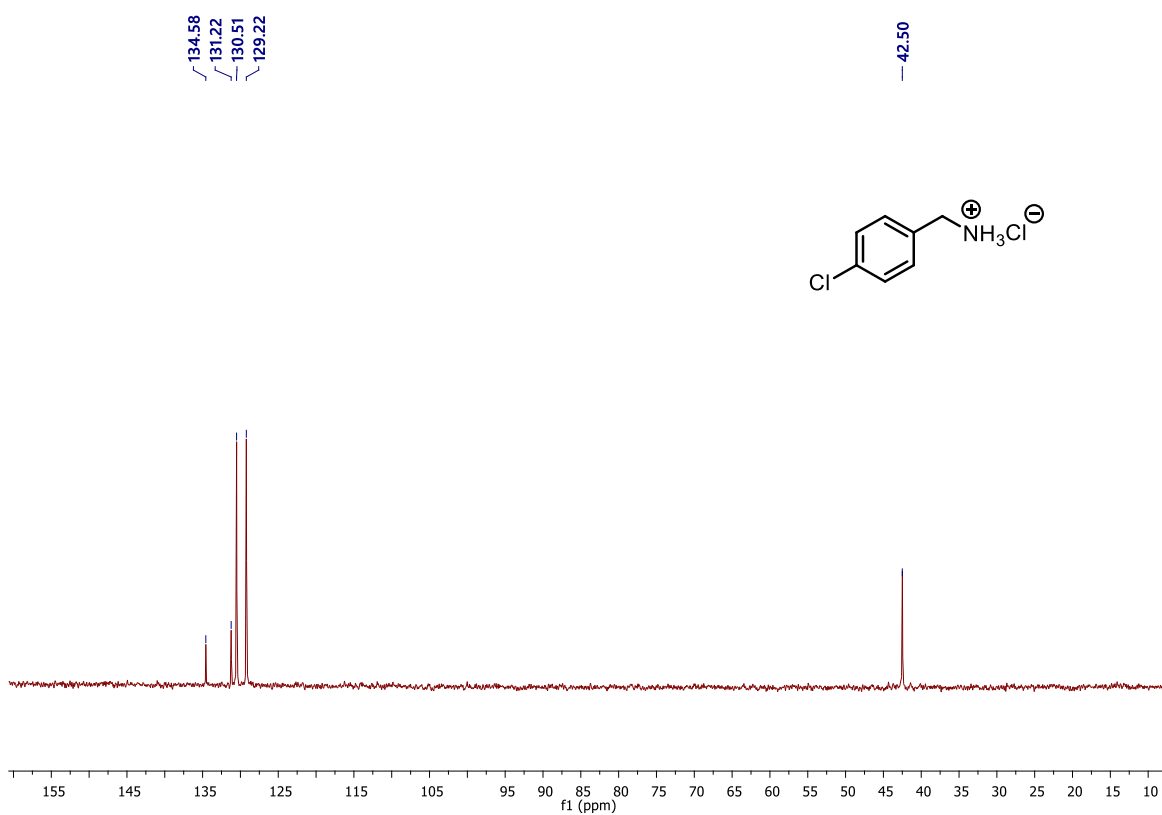


Fig. S21 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4d** in D_2O .^{S10}

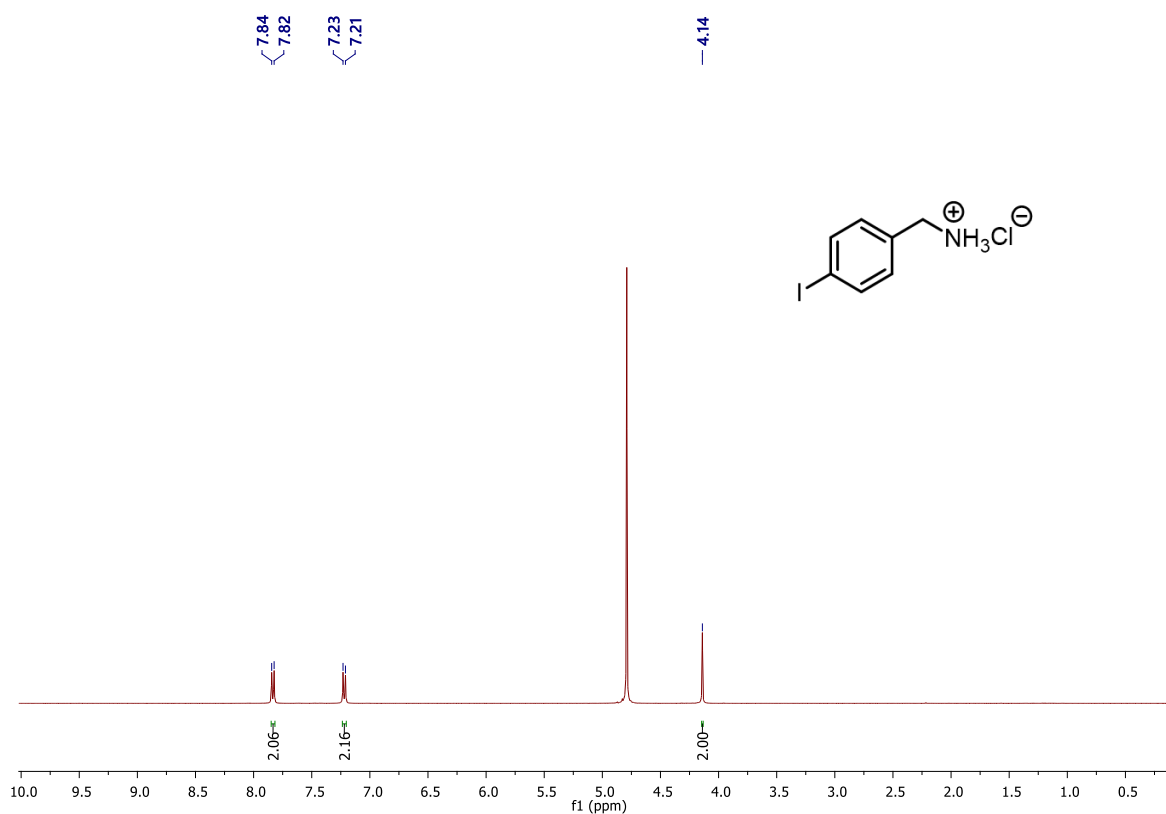


Fig. S22 ¹H NMR spectrum of **4e** in D₂O. ^{S8}

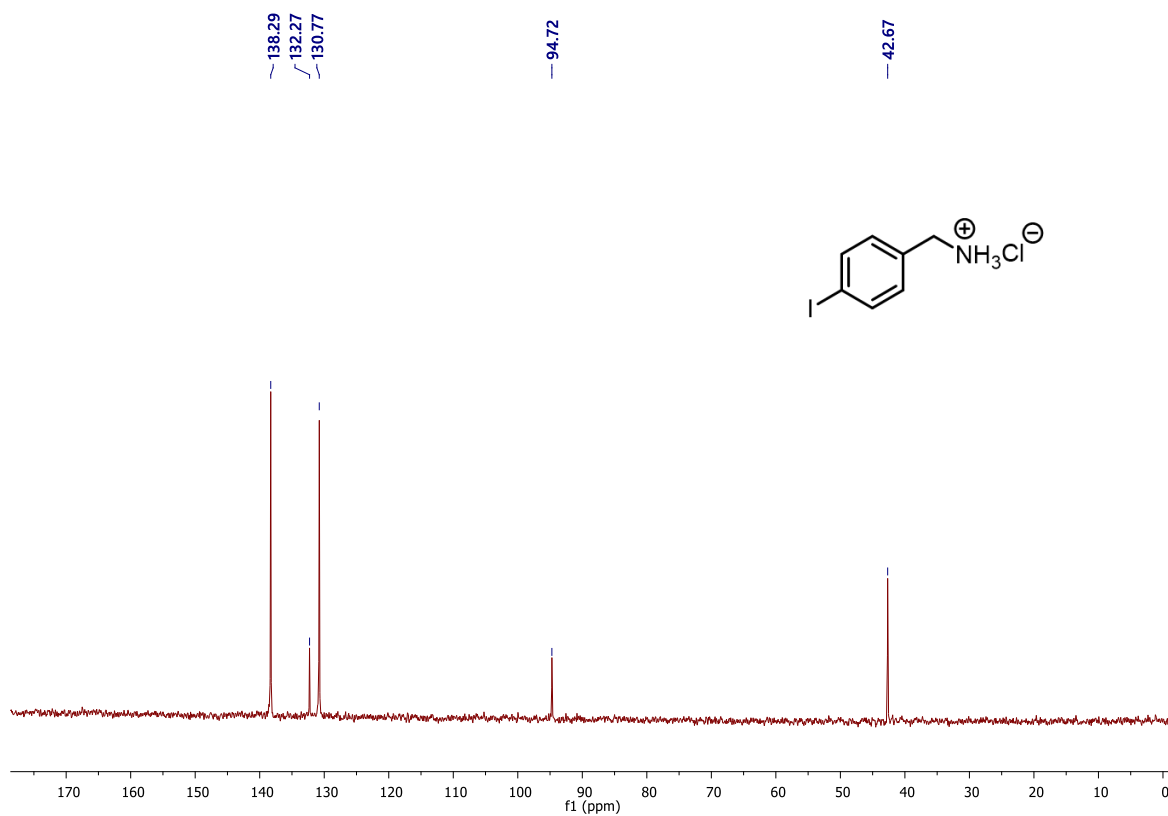


Fig. S23 ¹³C{¹H} NMR spectrum of **4e** in D₂O. ^{S8}

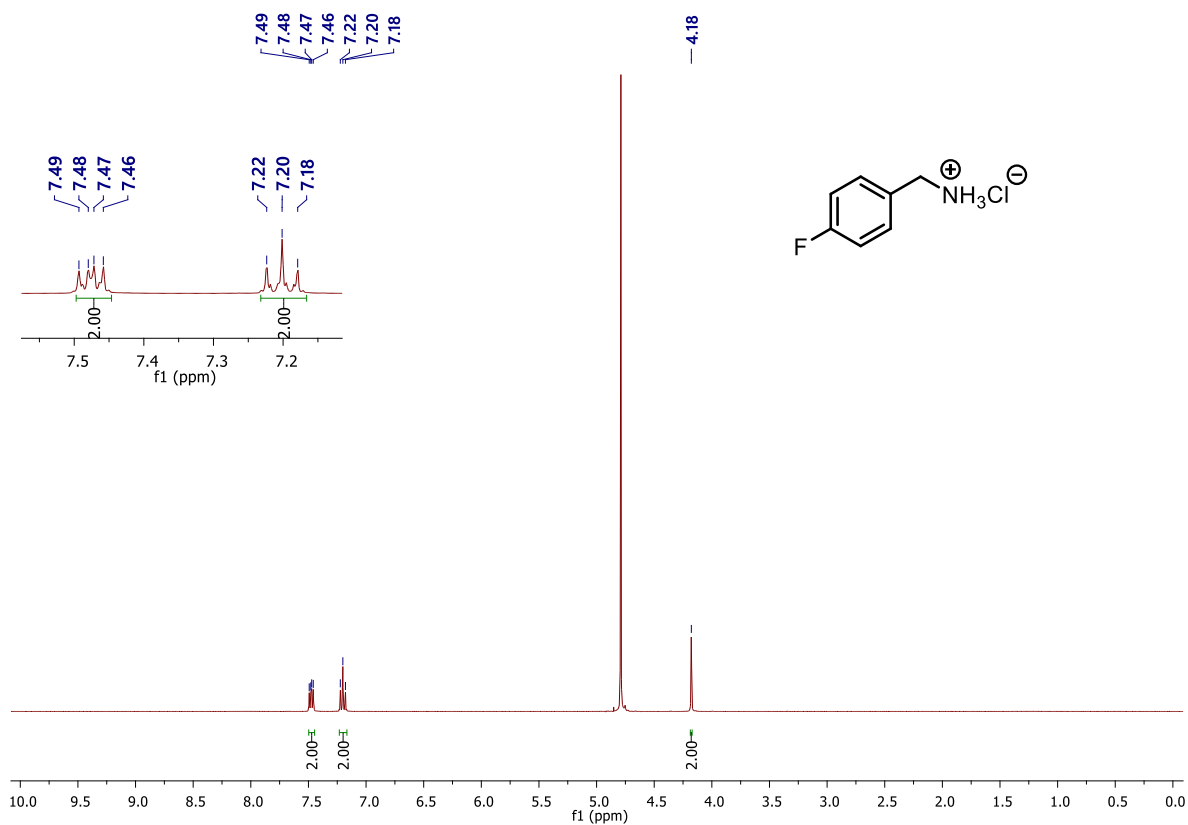


Fig. S24 ¹H NMR spectrum of **4f** in D₂O. ^{S11}

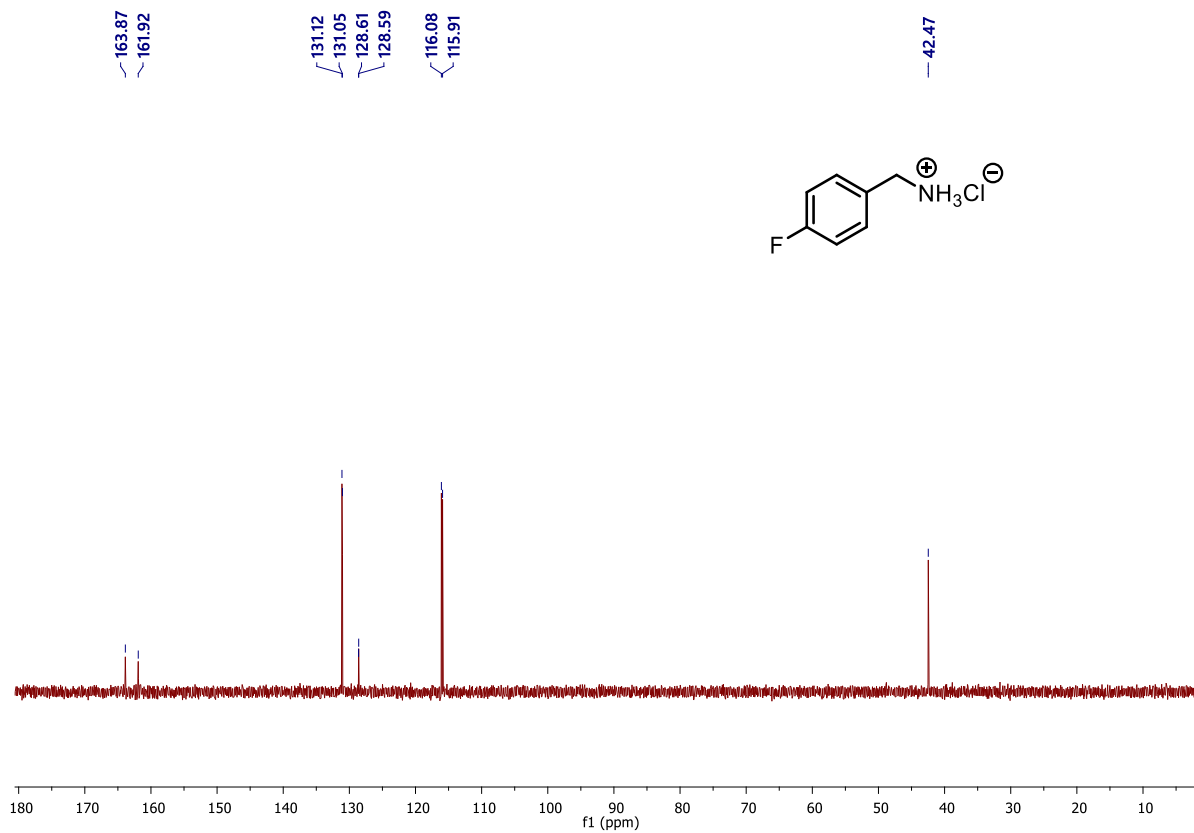


Fig. S25 ¹³C{¹H} NMR spectrum of **4f** in D₂O. ^{S11}

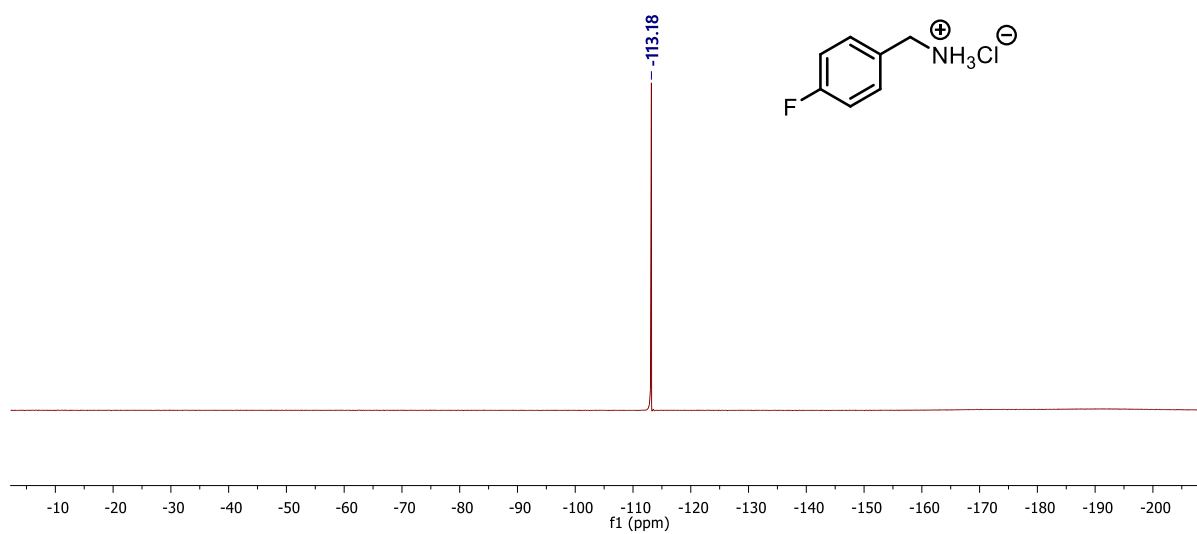


Fig. S26 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4f** in D_2O .^{S11}

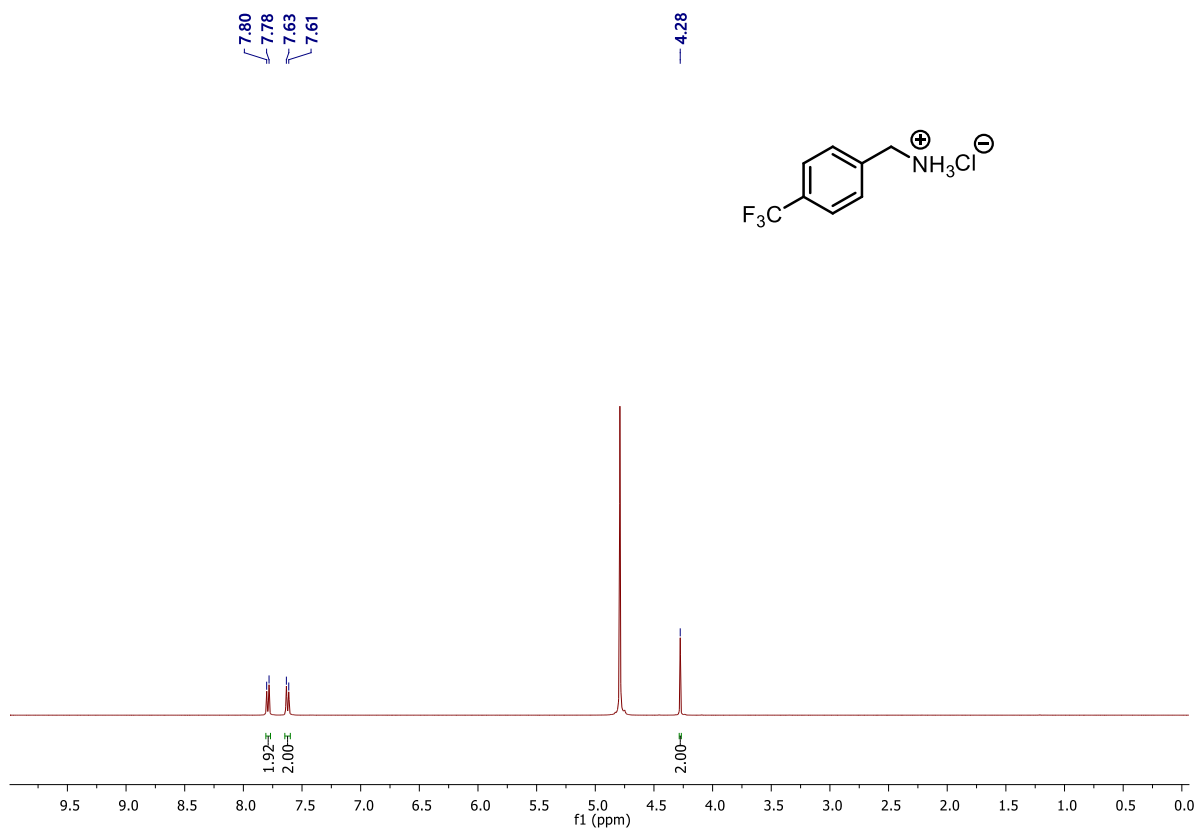


Fig. S27 ^1H NMR spectrum of **4g** in D_2O .^{S10}

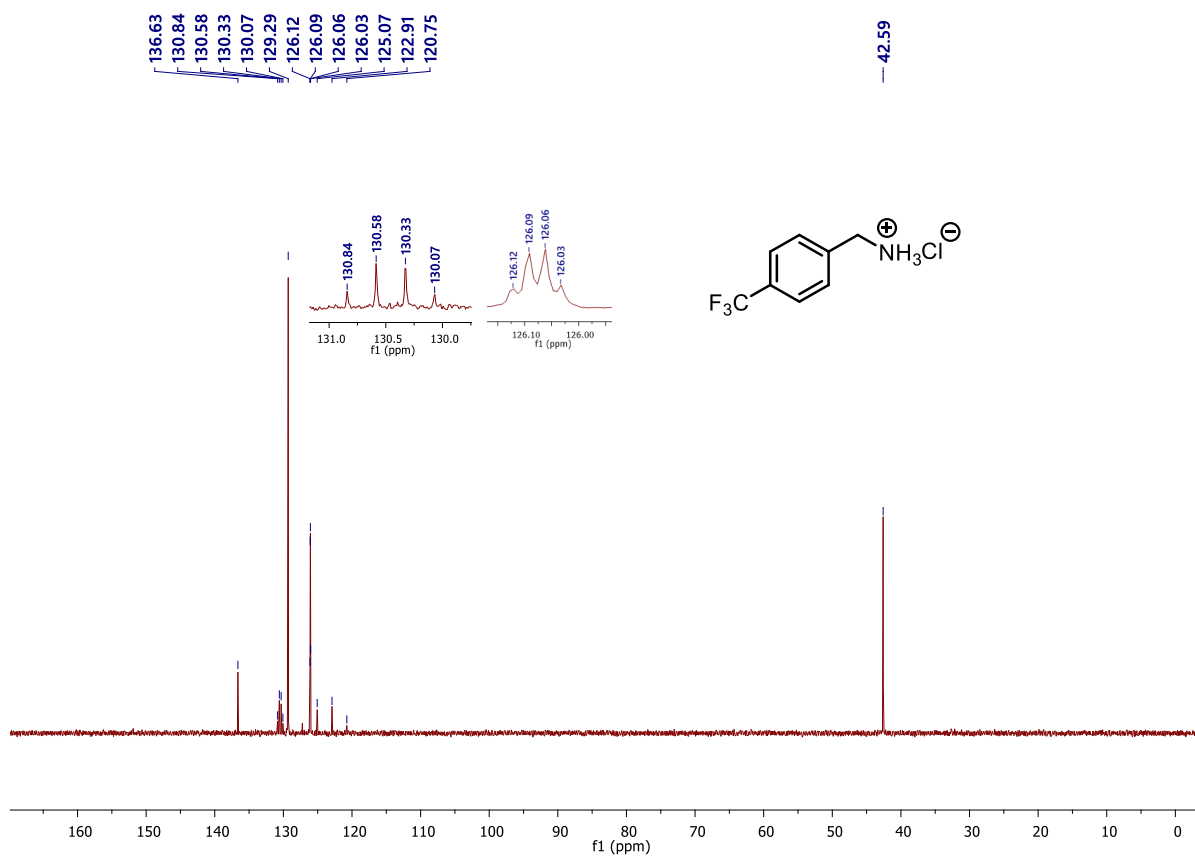


Fig. S28 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4g** in D_2O . ^{S10}

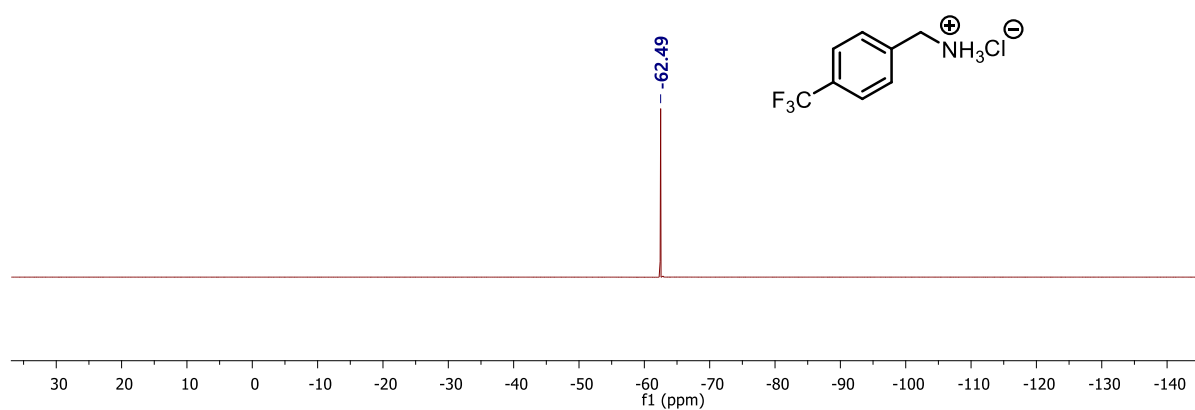


Fig. S29 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4g** in D_2O . ^{S26}

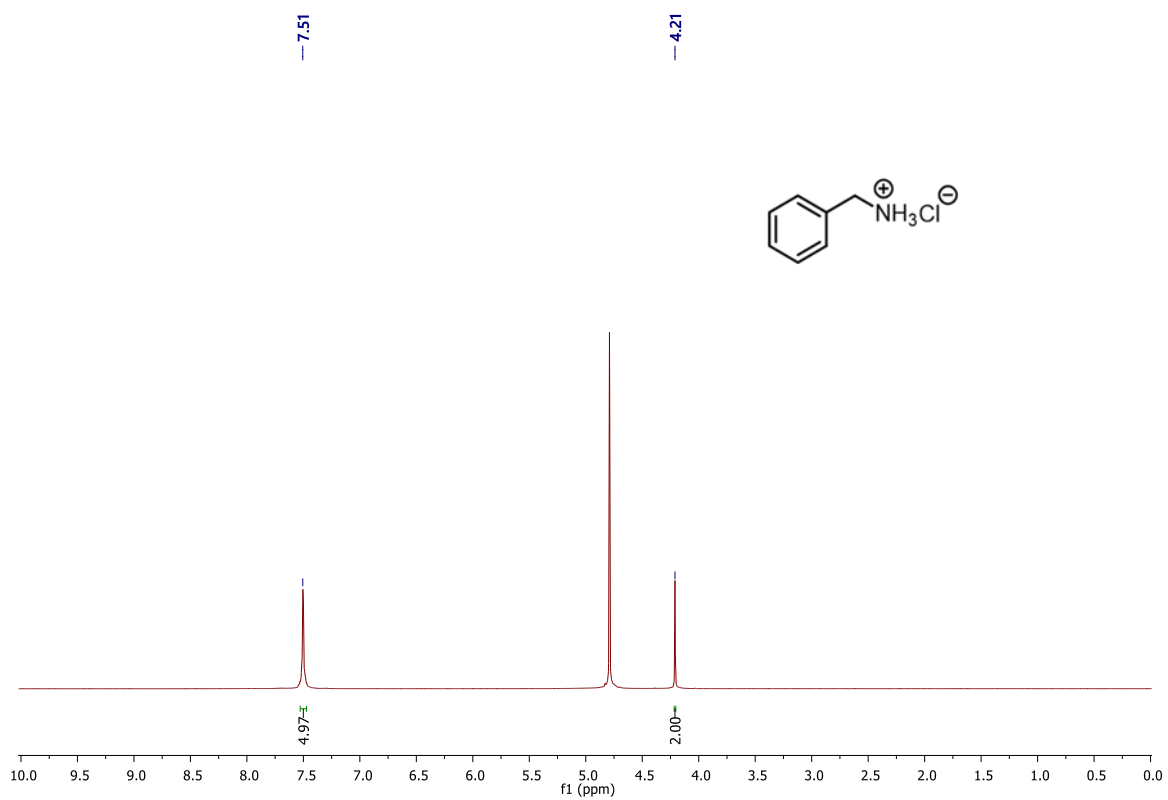


Fig. S30 ^1H NMR spectrum of **4h** in D_2O . ^{S10}

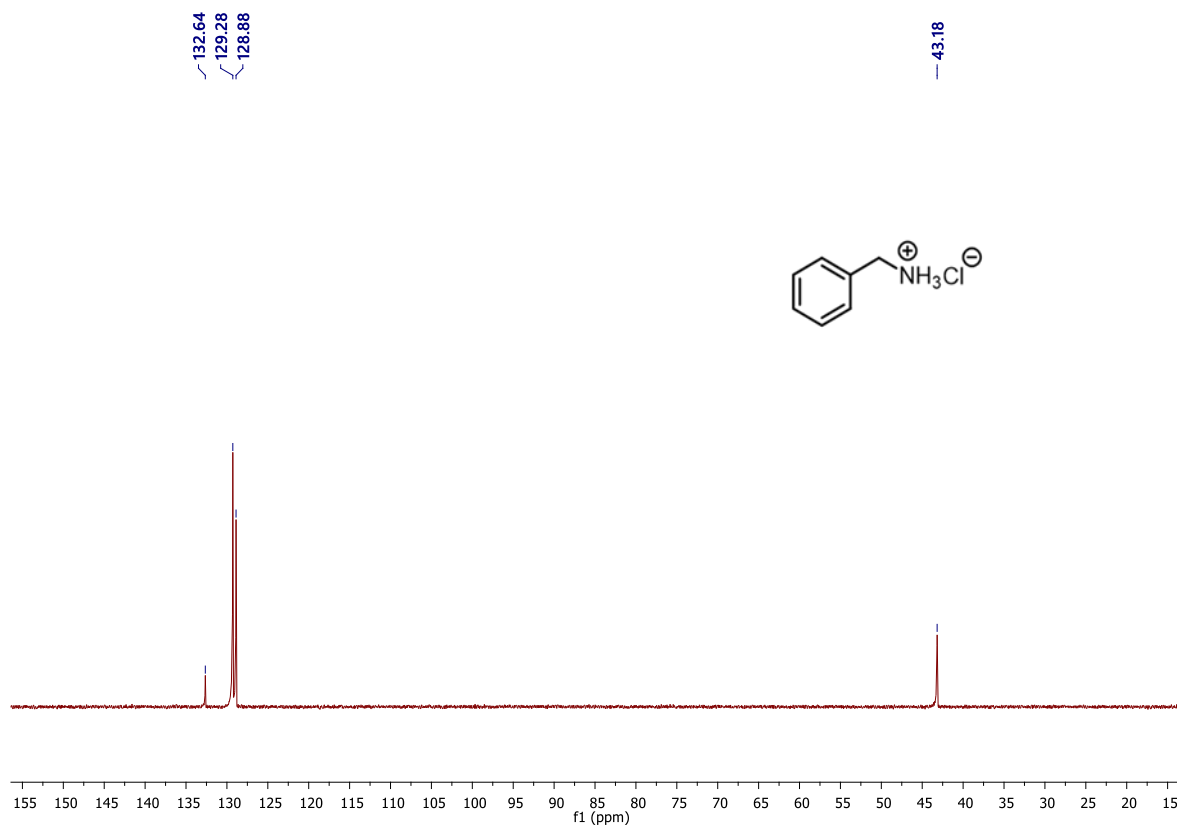


Fig. S31 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4h** in D_2O . ^{S10}

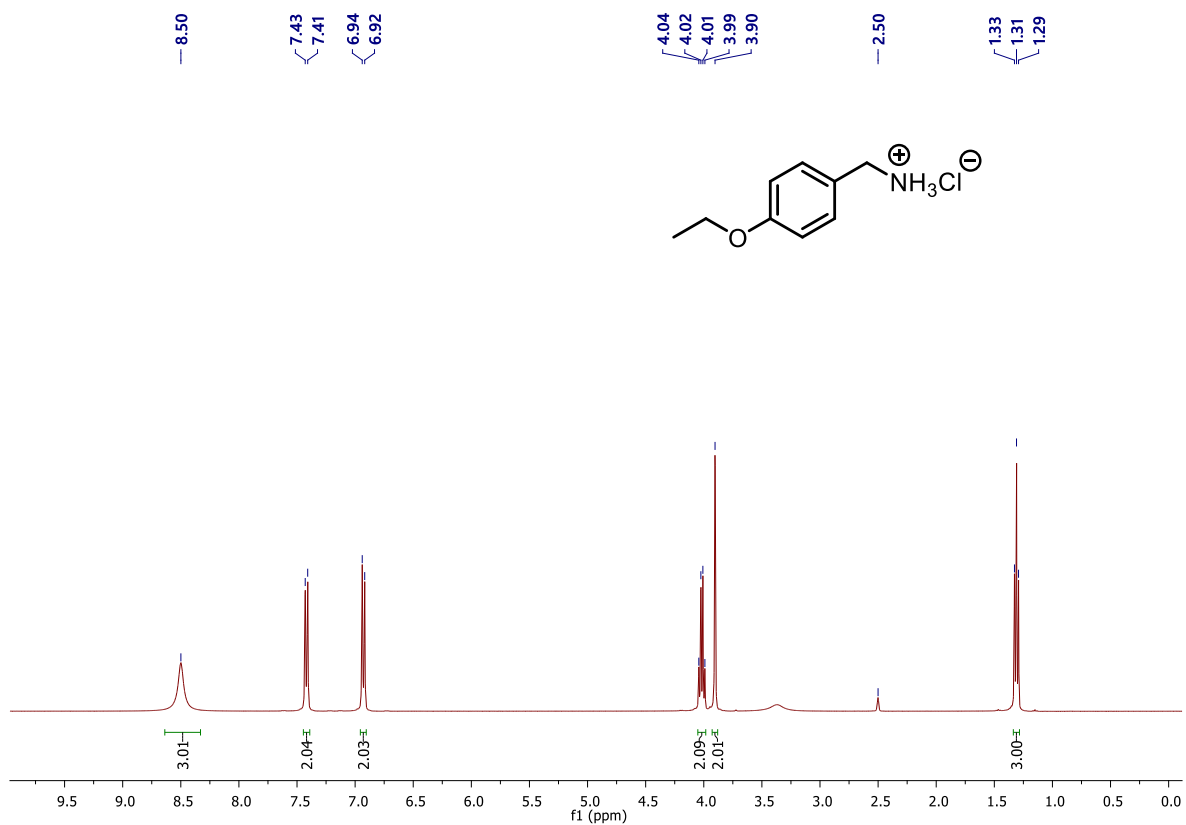


Fig. S32 ^1H NMR spectrum of **4i** in DMSO-d_6 .^{S12}

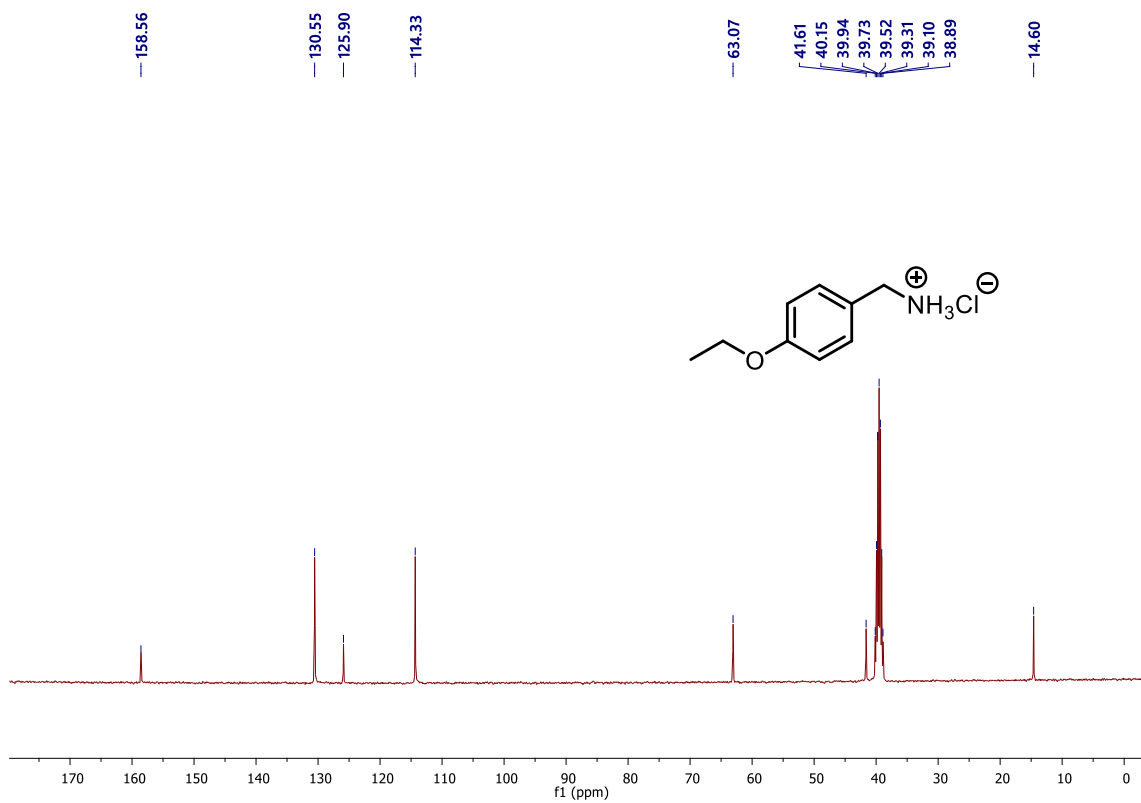


Fig. S33 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4i** in DMSO-d_6 .^{S12}

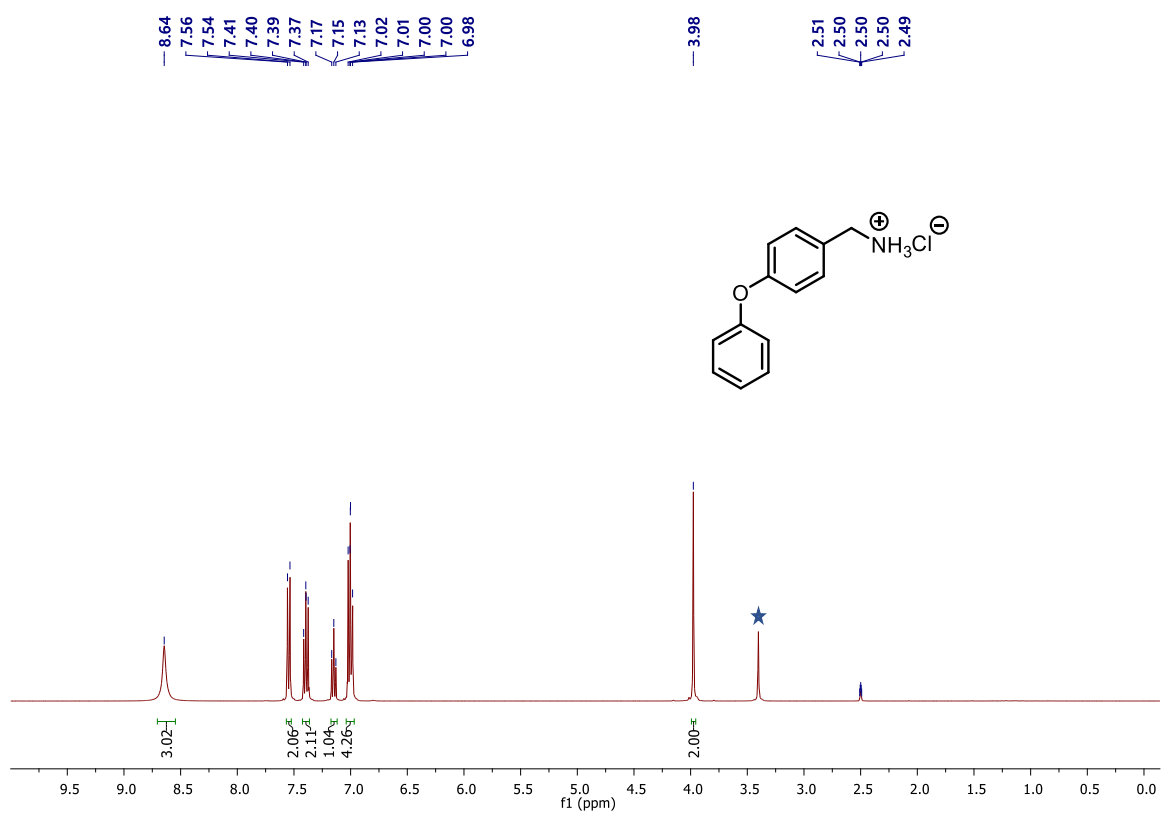


Fig. S34 ^1H NMR spectrum of **4j** in DMSO-d_6 . ★ denotes moisture peak in DMSO-d_6 . ^{S13}

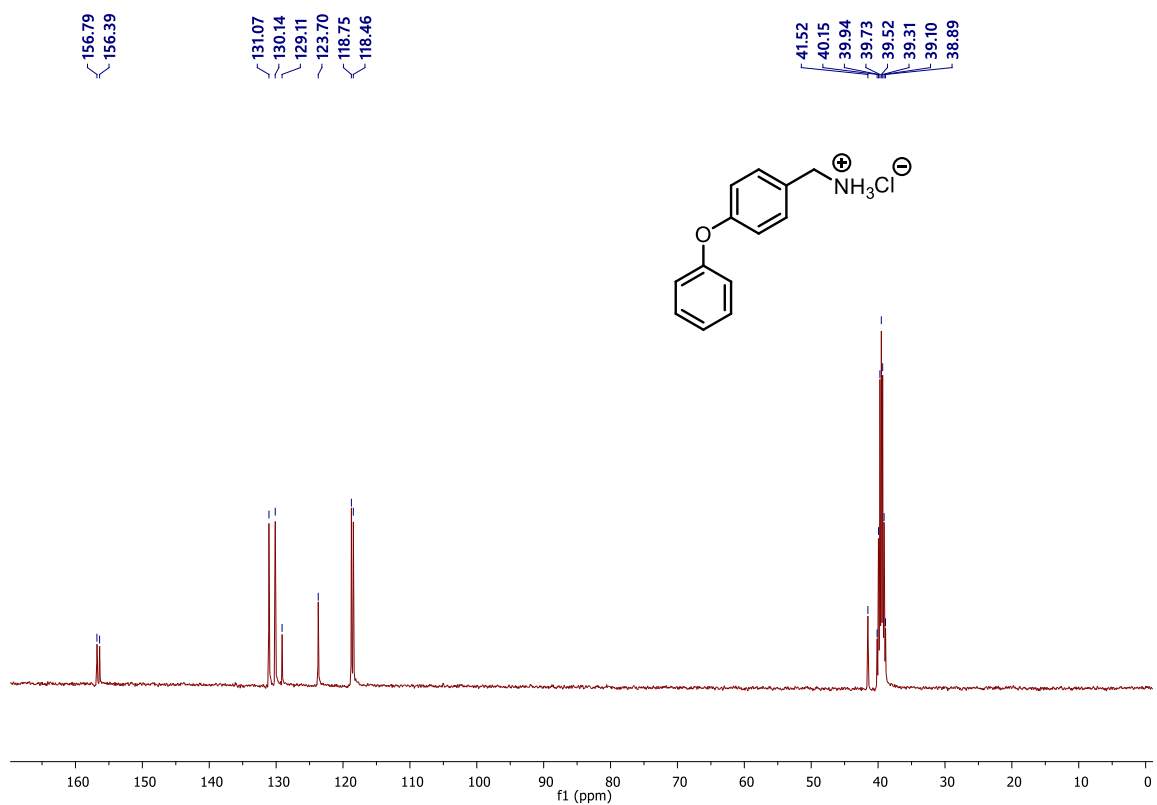


Fig. S35 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4j** in DMSO-d_6 . ^{S13}

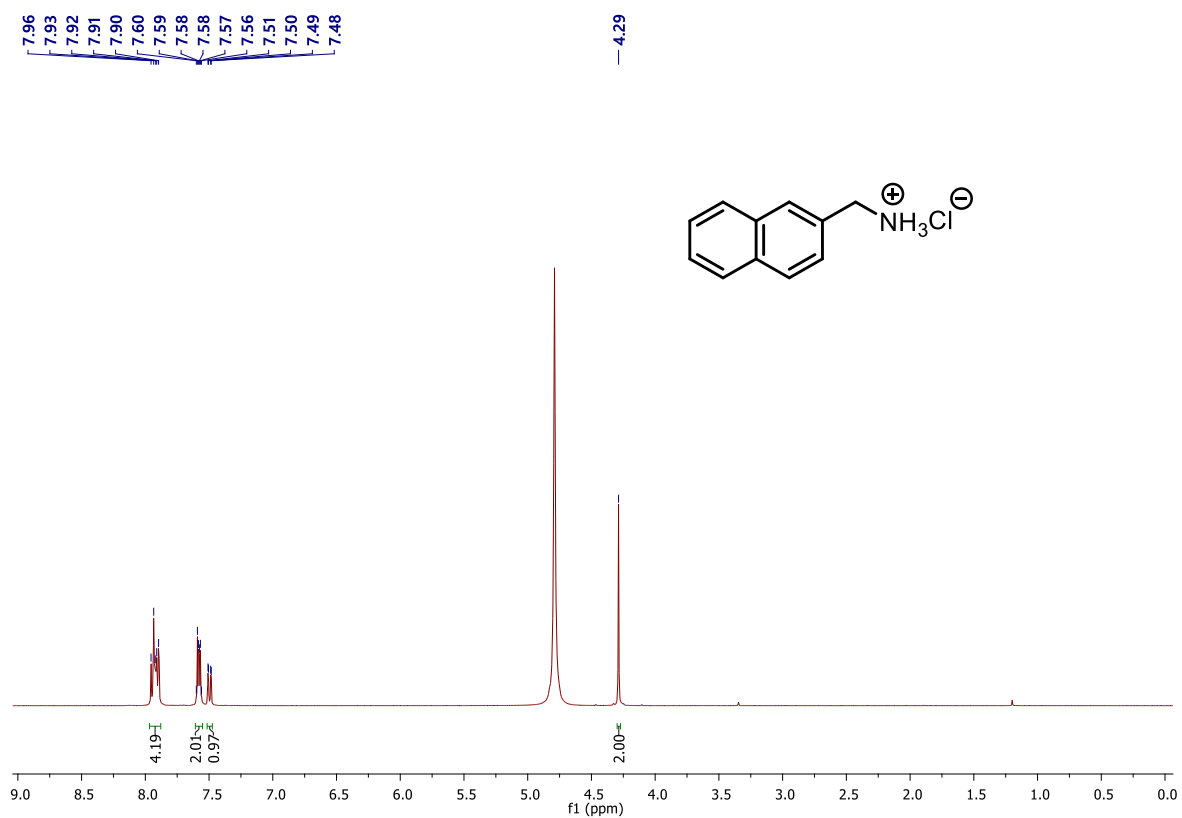


Fig. S36 ^1H NMR spectrum of **4k** in D_2O . ^{S10}

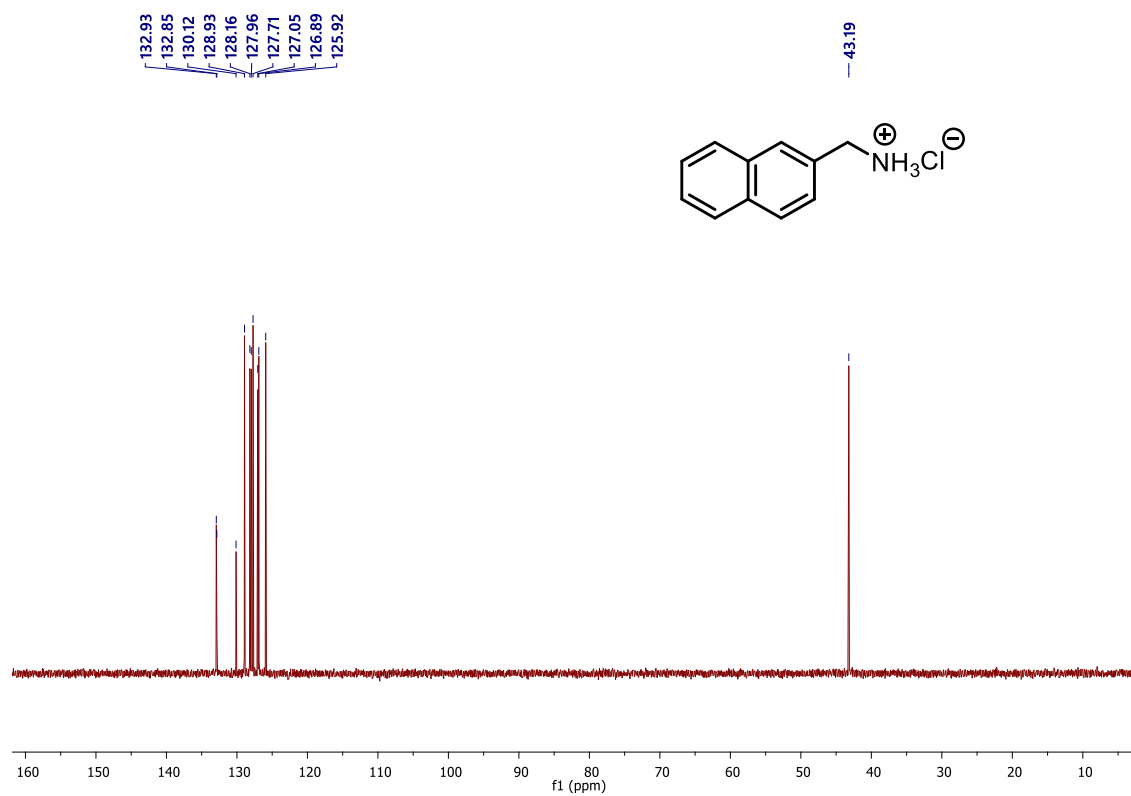


Fig. S37 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4k** in D_2O . ^{S10}

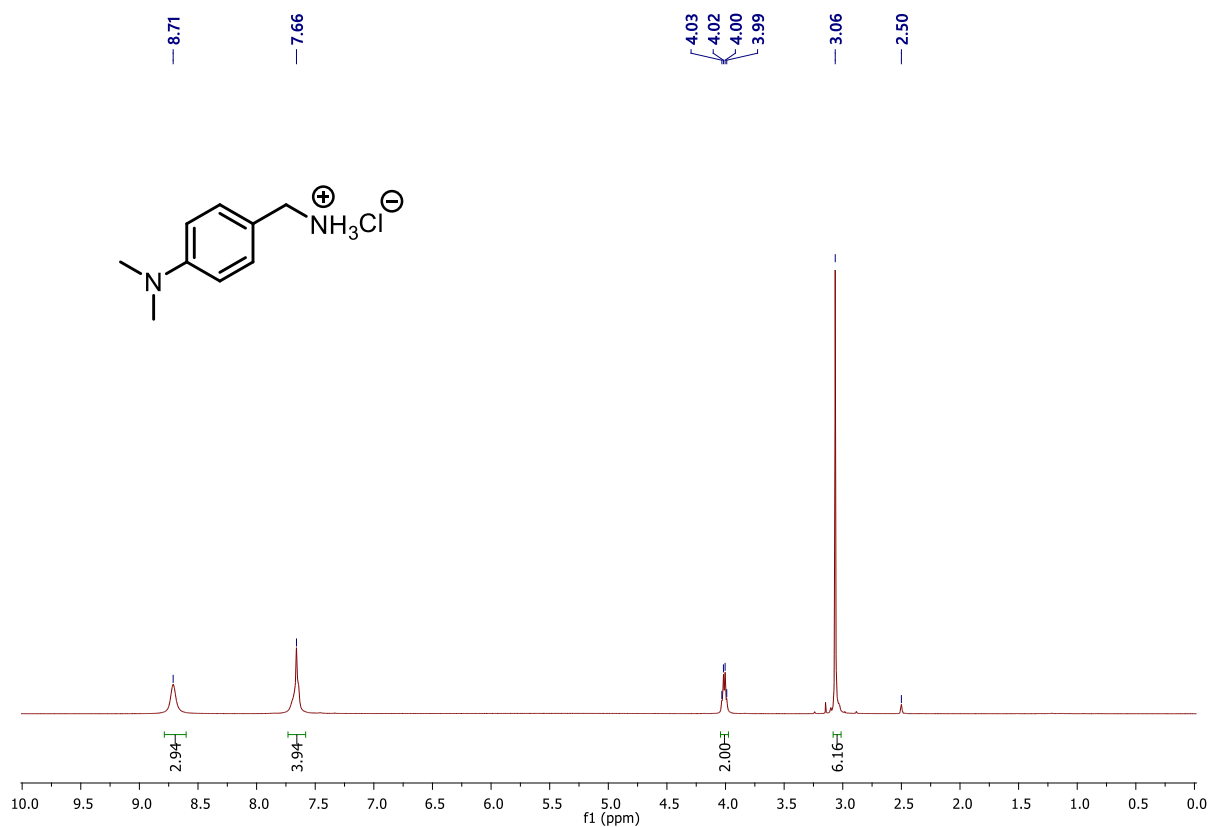


Fig. S38 ^1H NMR spectrum of **4I** in DMSO-d_6 .^{S14}

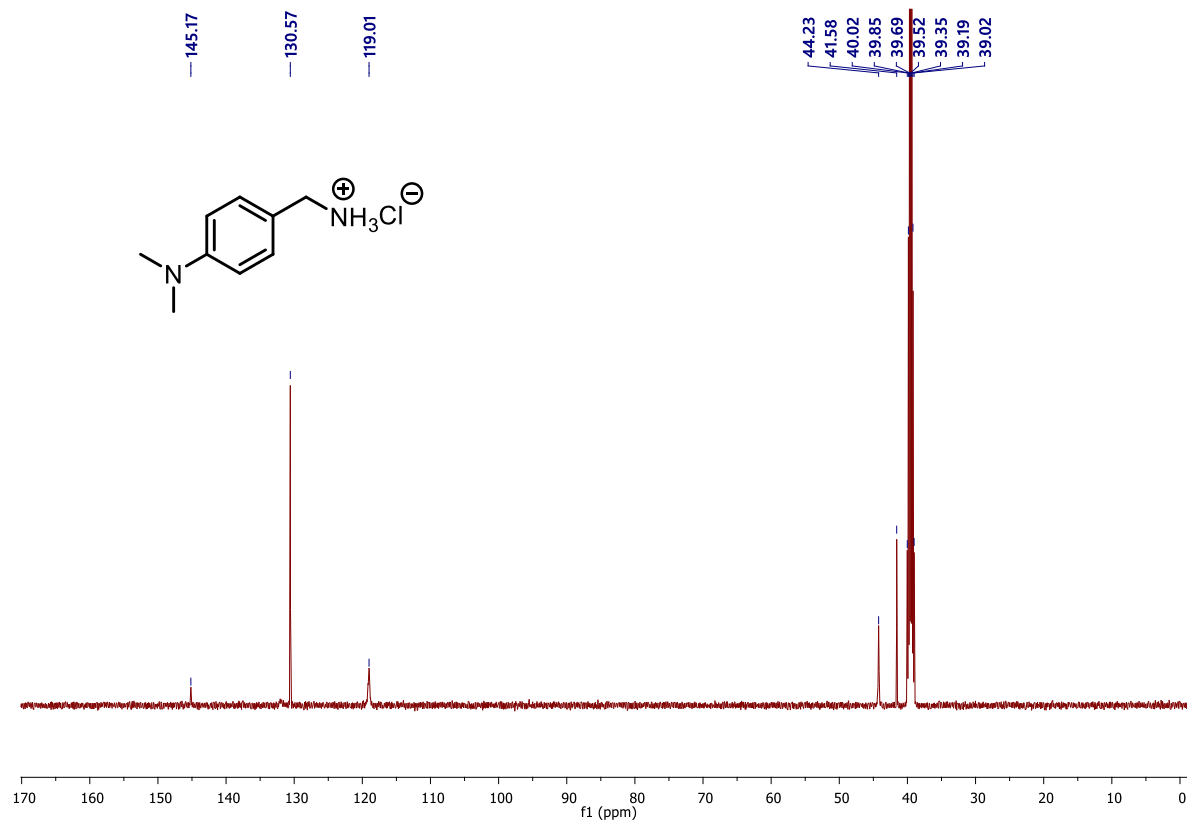


Fig. S39 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4I** in DMSO-d_6 .^{S14}

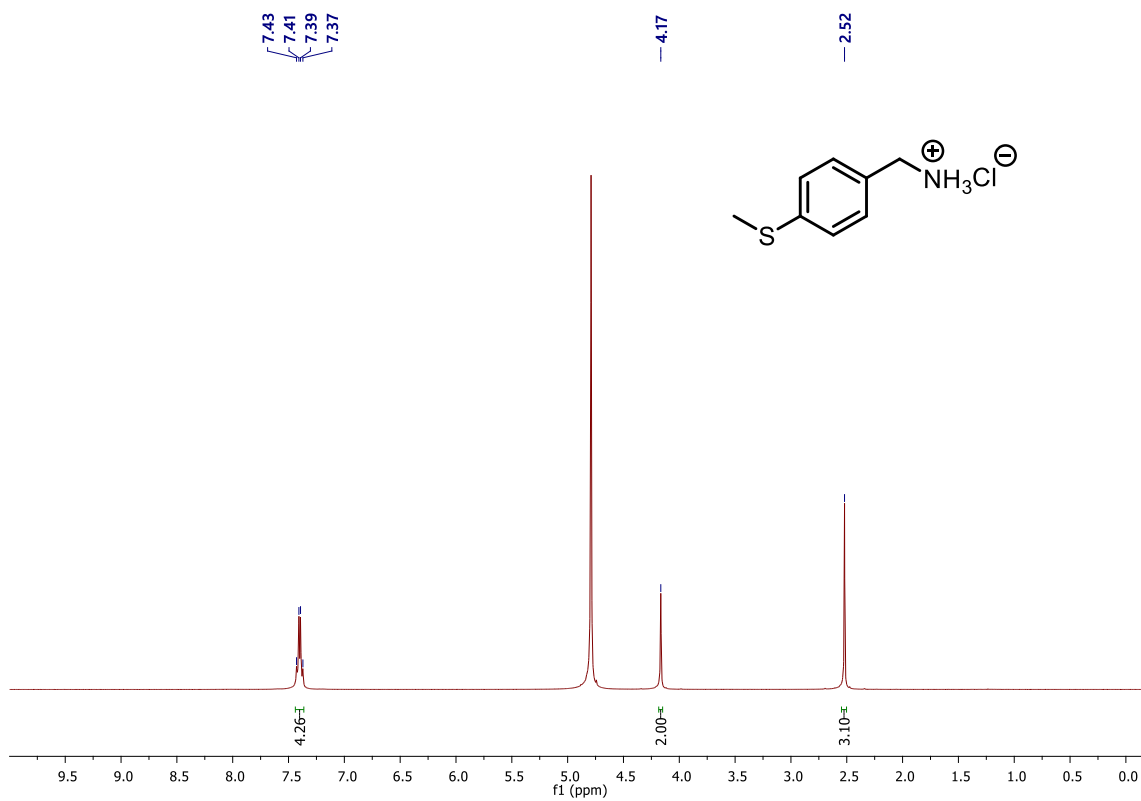


Fig. S40 ^1H NMR spectrum of **4m** in D_2O . ^{S15}

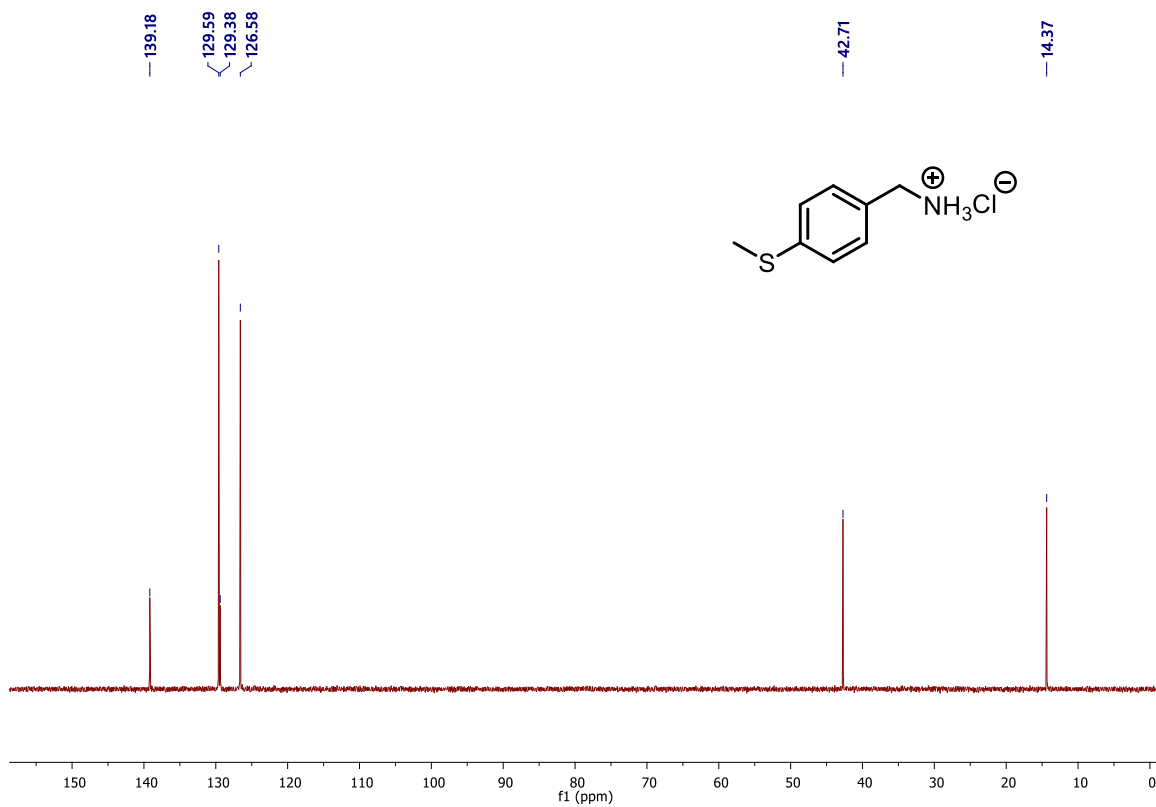


Fig. S41 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4m** in D_2O . ^{S15}

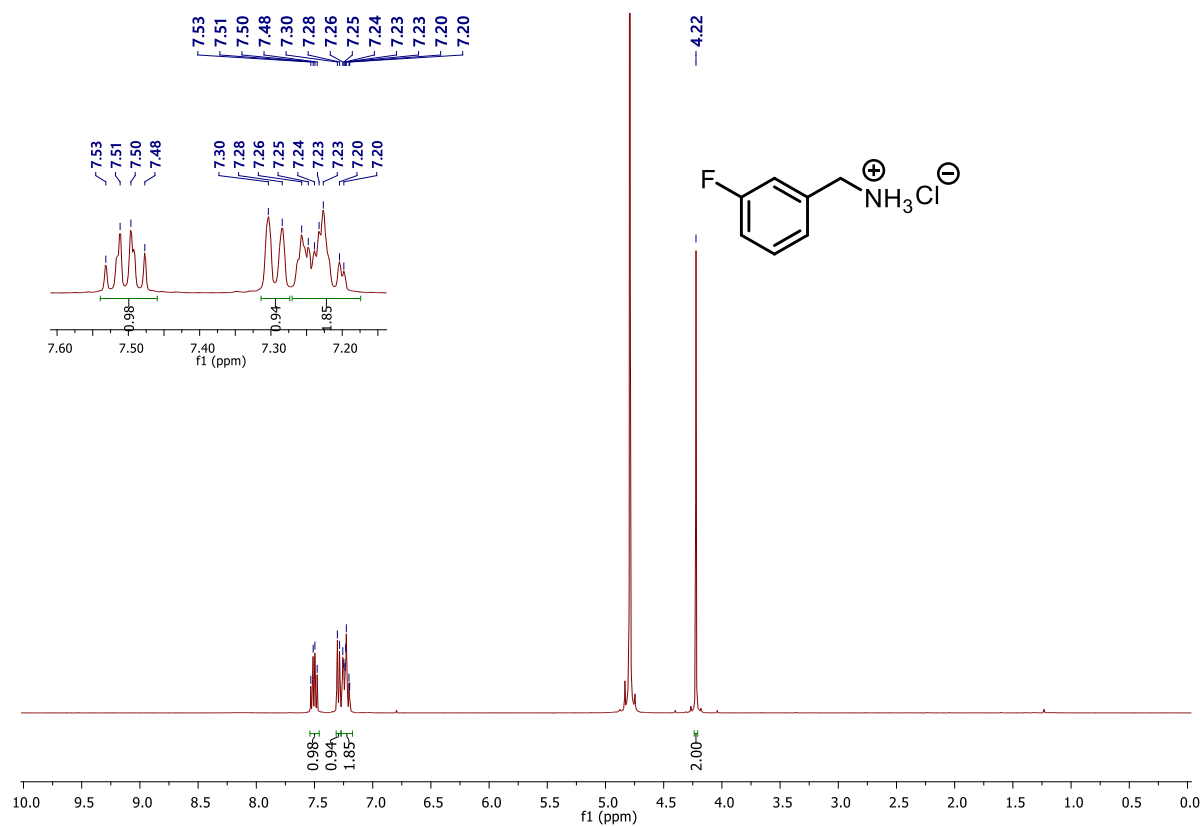


Fig. S42 ^1H NMR spectrum of **4n** in D_2O .^{S9}

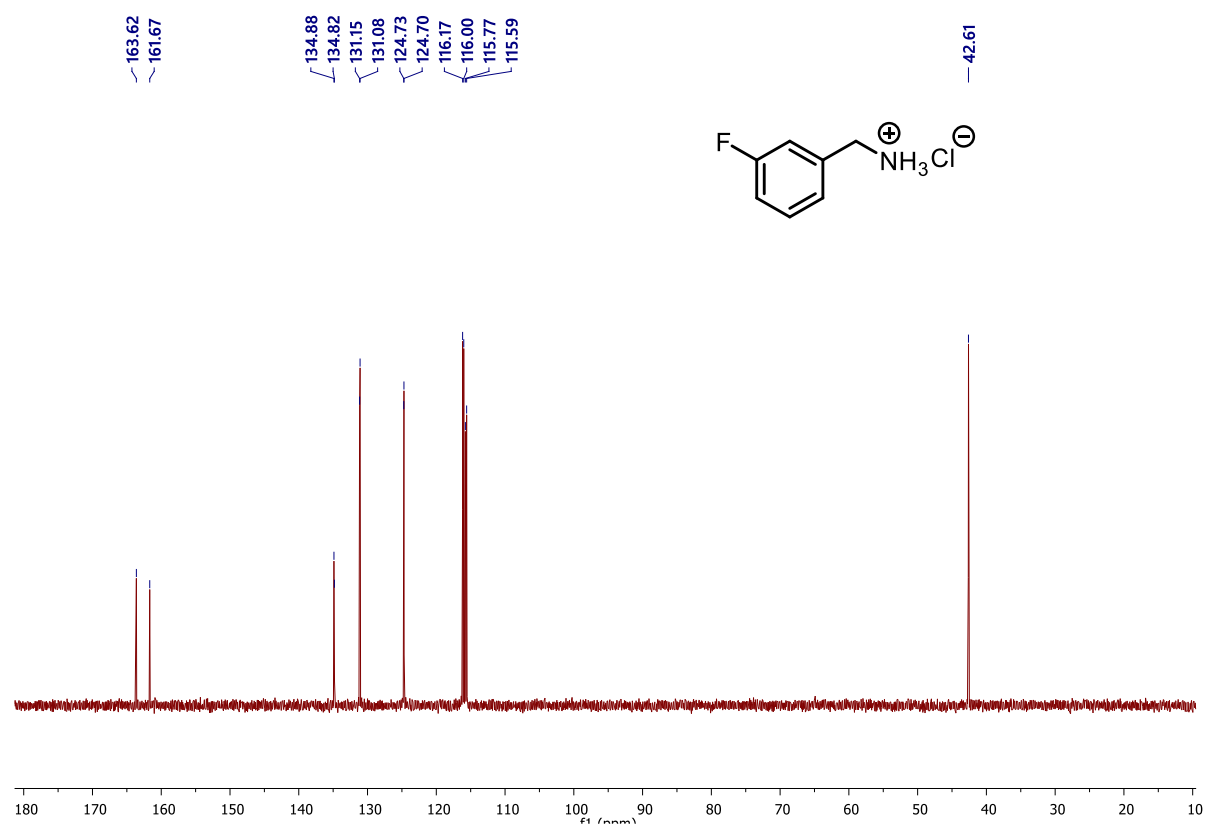


Fig. S43 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4n** in D_2O .^{S9}

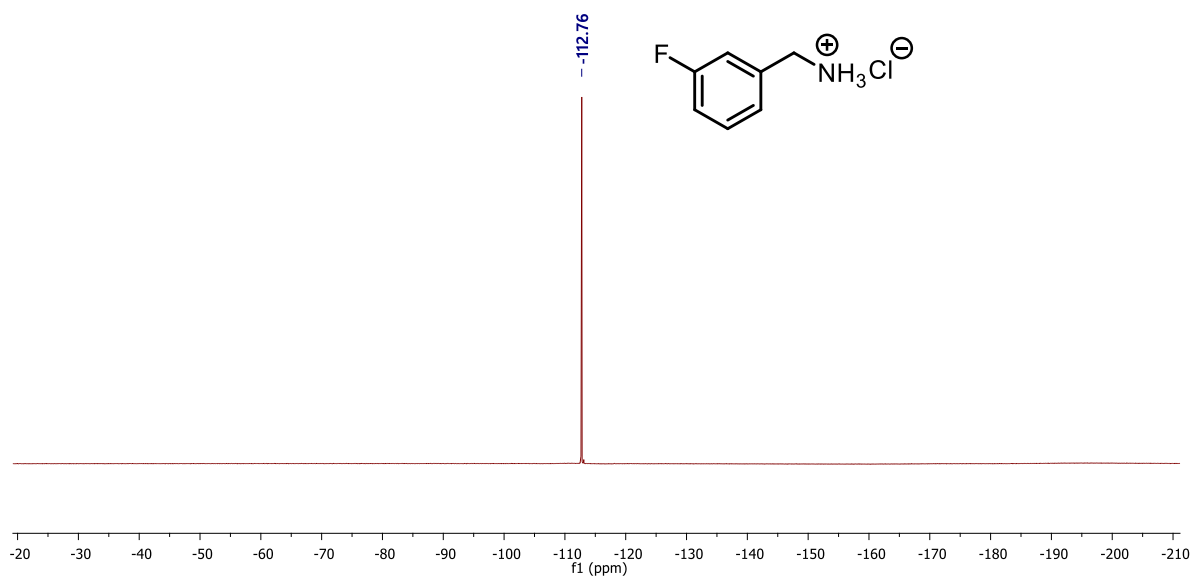


Fig. S44 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4n** in D_2O . ^{S28}

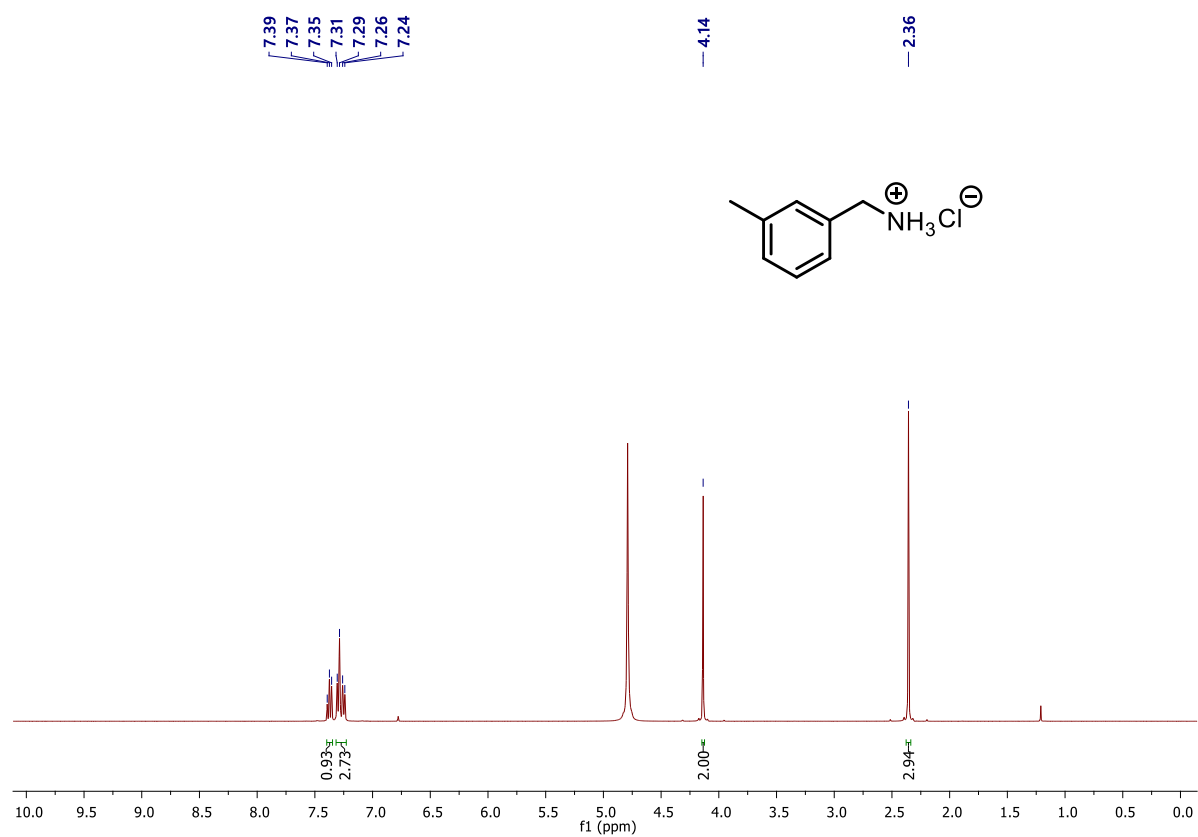


Fig. S45 ^1H NMR spectrum of **4o** in D_2O . ^{S9}

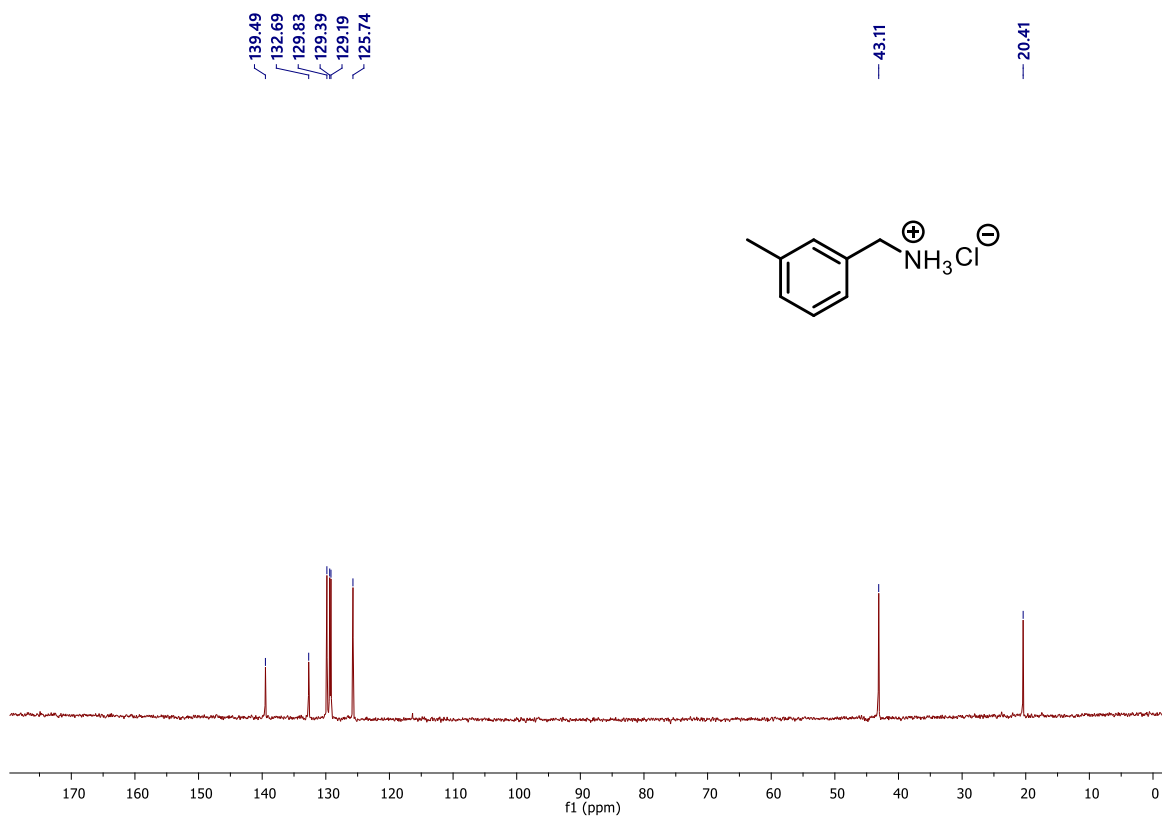


Fig. S46 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4o** in D_2O .^{S9}

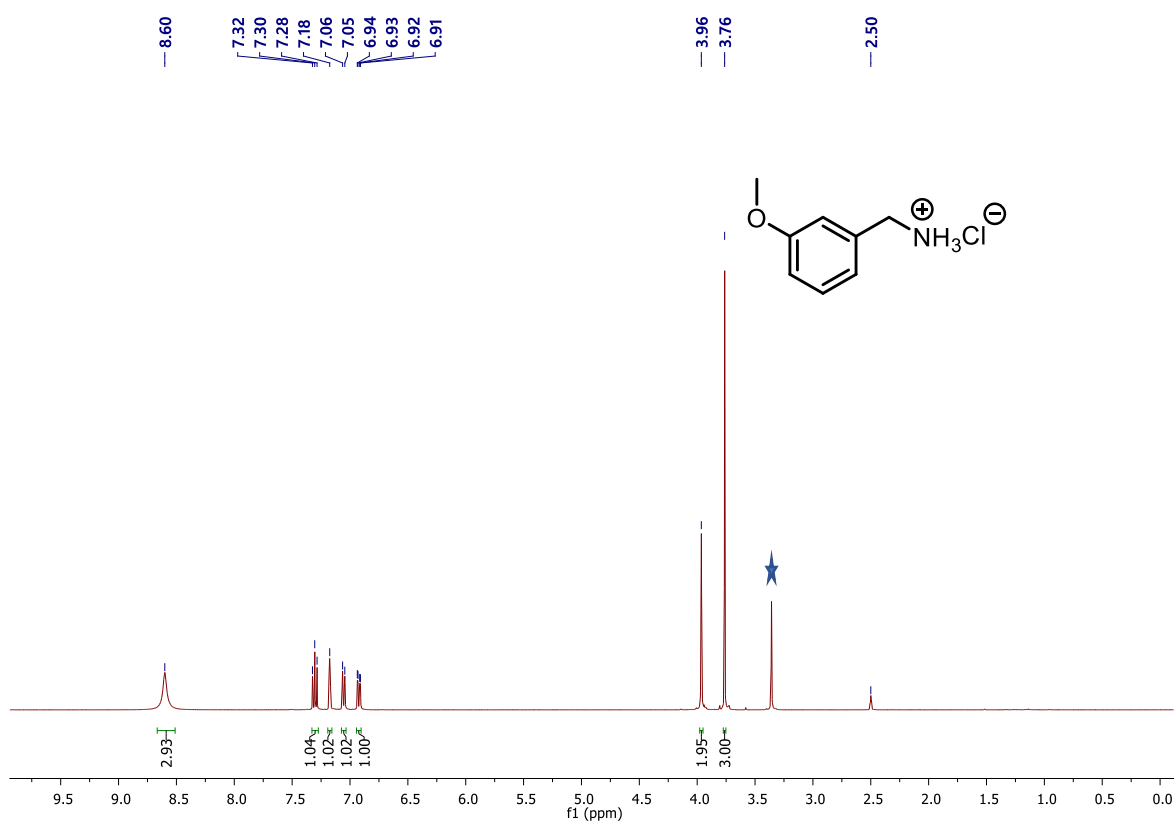


Fig. S47 ^1H NMR spectrum of **4p** in DMSO-d_6 .^{S9} ★ denotes moisture peak in DMSO-d_6 .

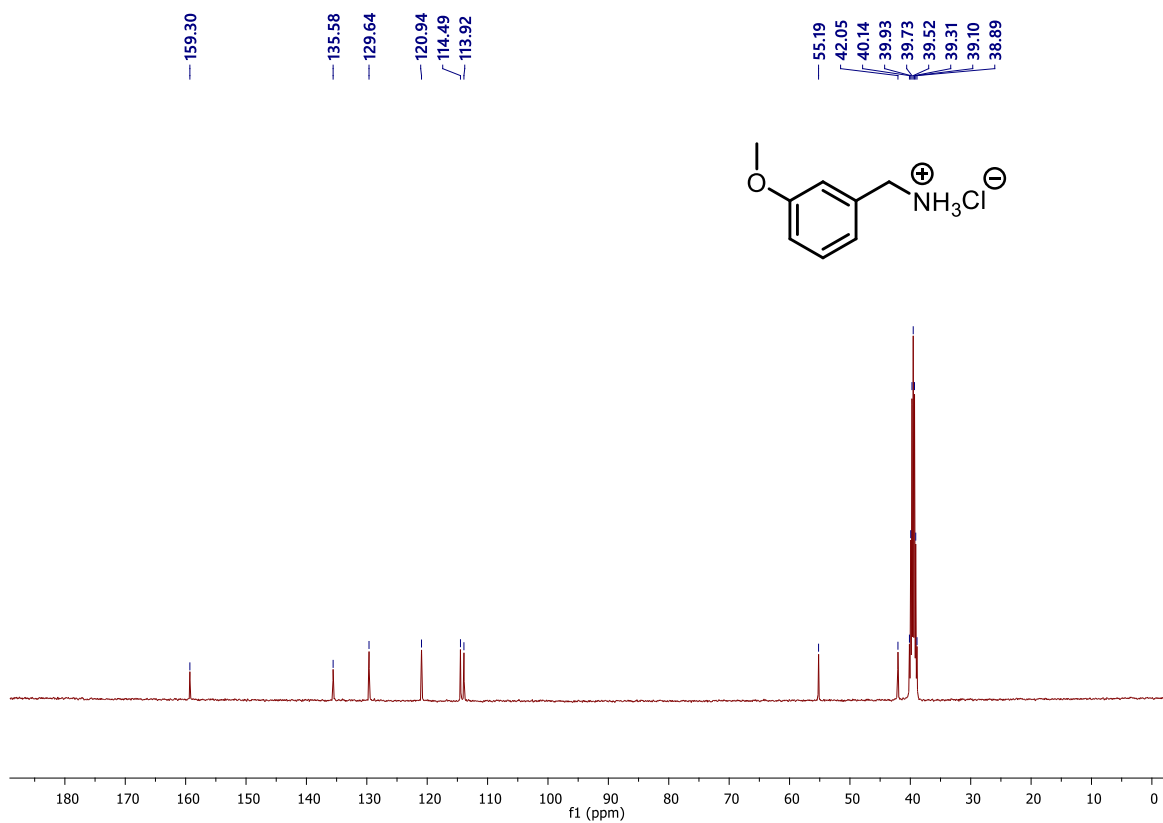


Fig. S48 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4p** in DMSO- d_6 . ^{S9}

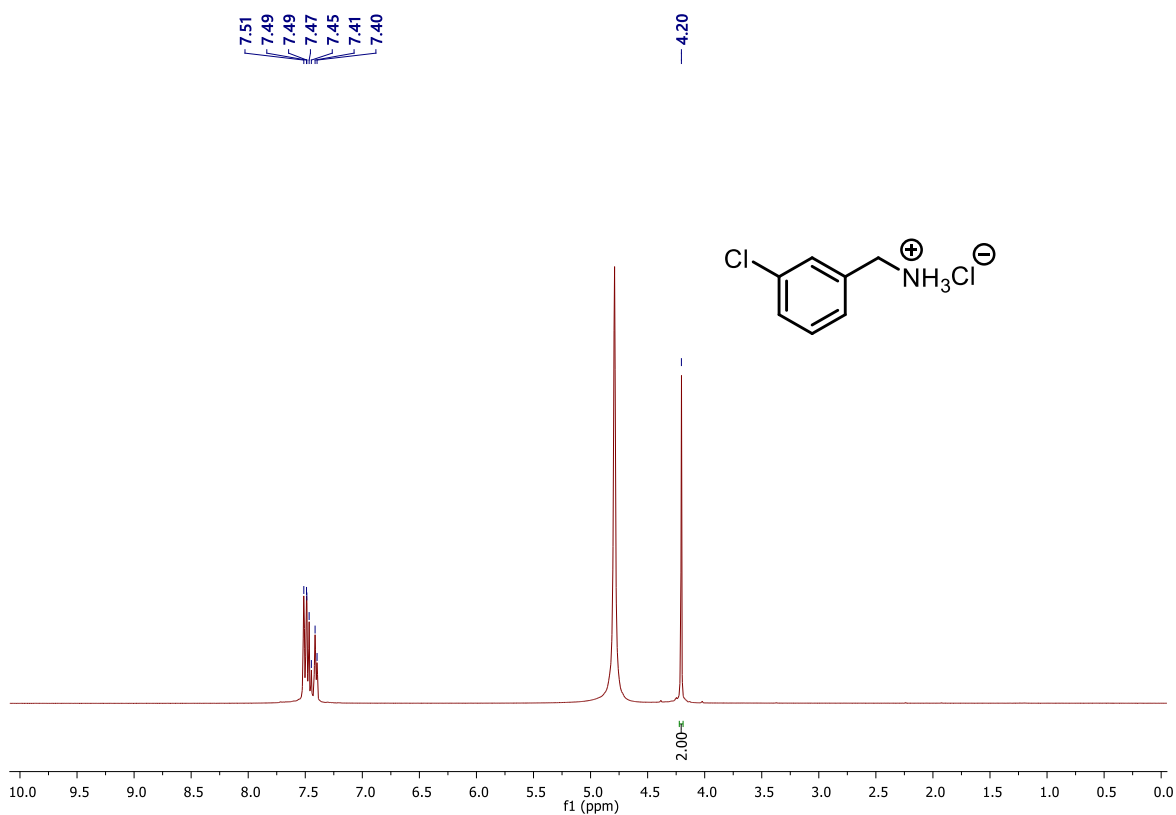


Fig. S49 ^1H NMR spectrum of **4q** in D_2O . ^{S10}

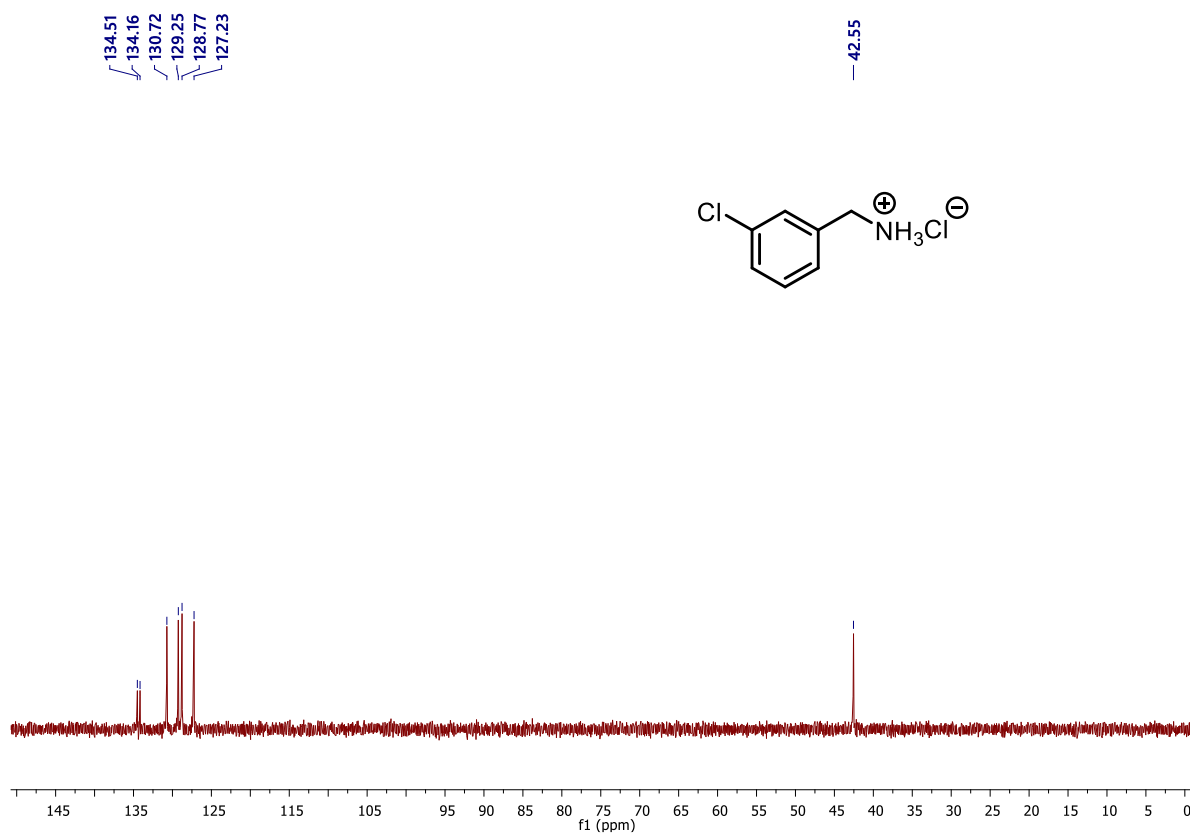


Fig. S50 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4q in D_2O . ^{S10}

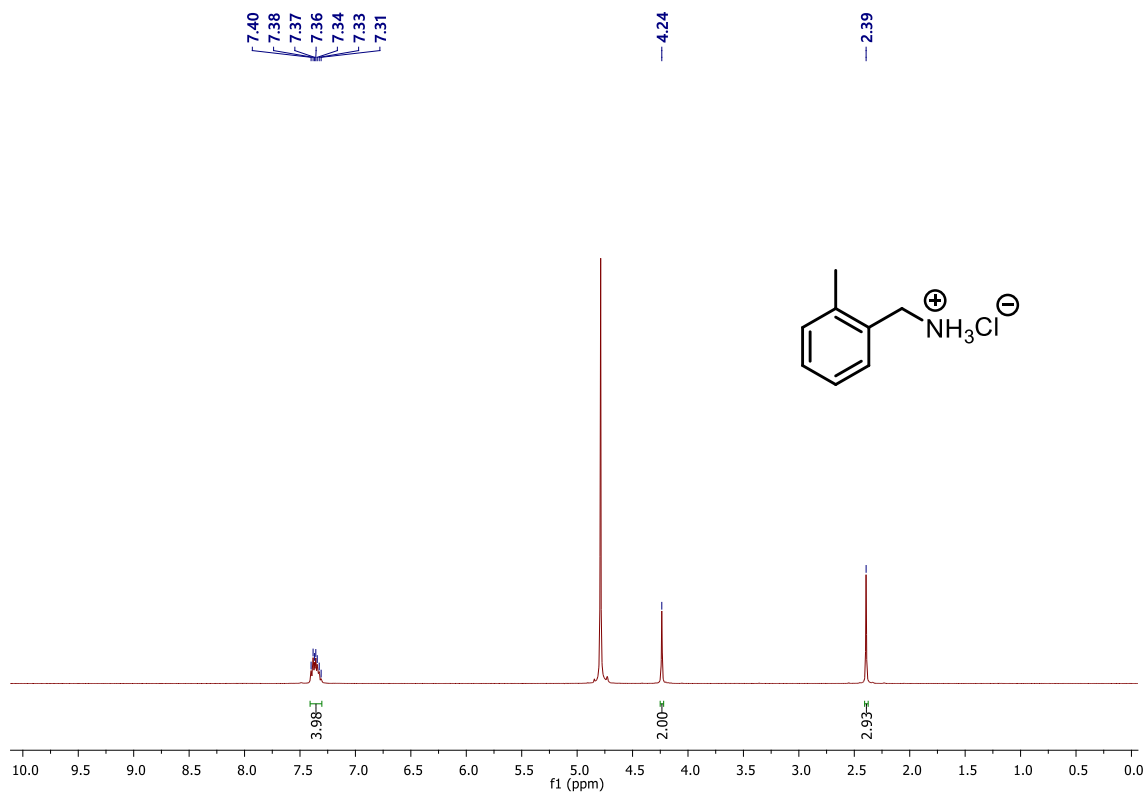


Fig. S51 ^1H NMR spectrum of 4r in D_2O . ^{S10}

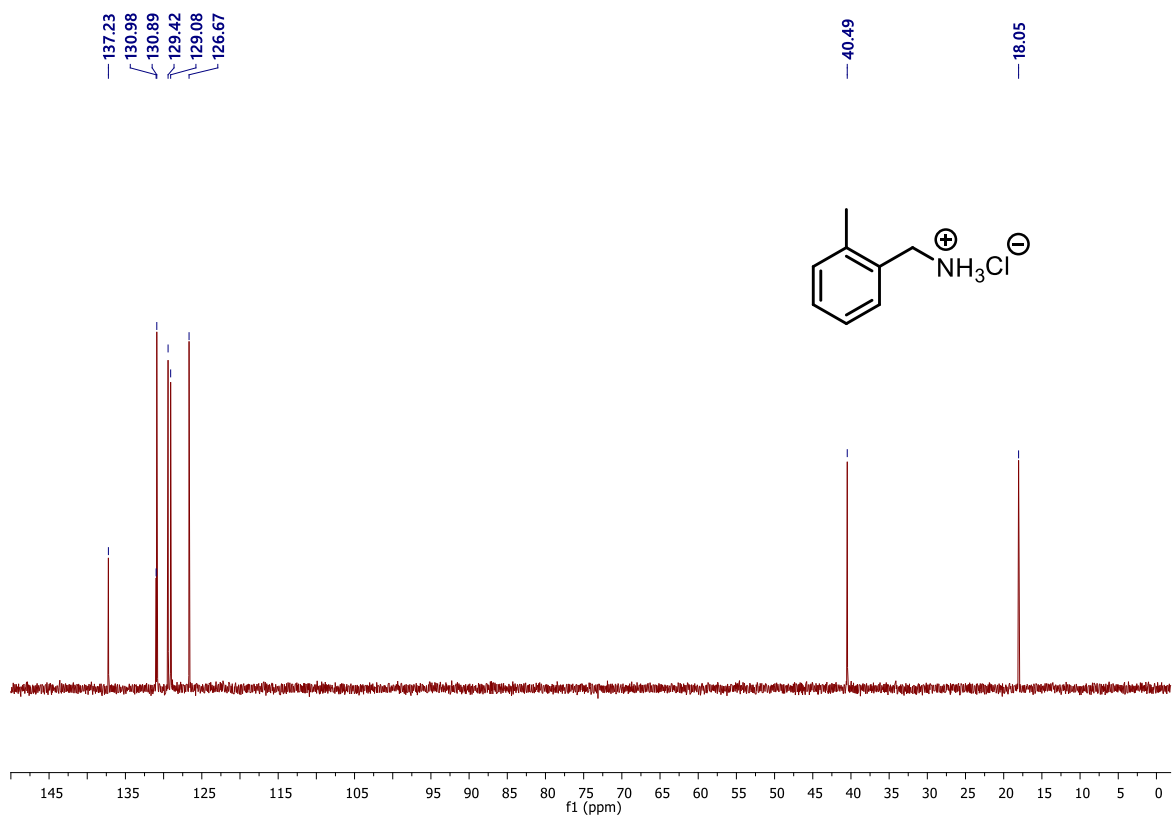


Fig. S52 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4r in D_2O . S10

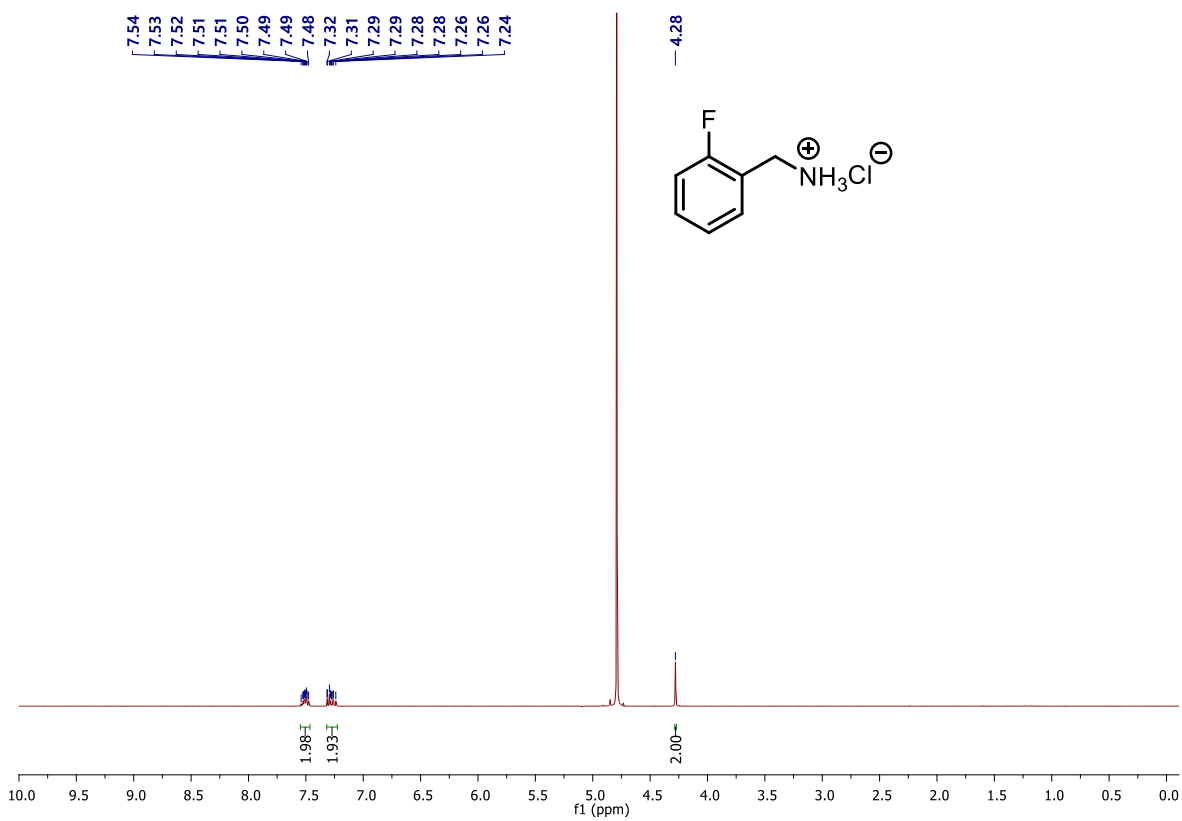


Fig. S53 ^1H NMR spectrum of 4s in D_2O . S16

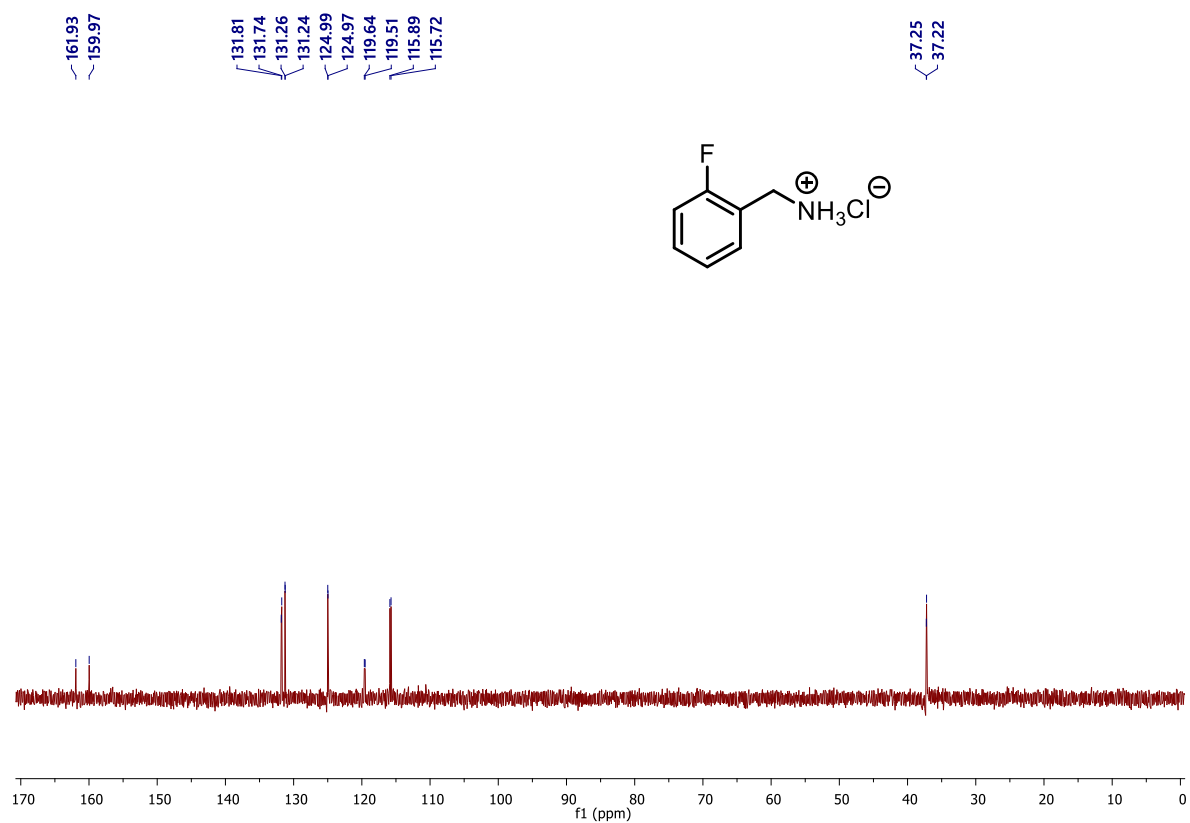


Fig. S54 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4s** in D_2O . ^{S16}

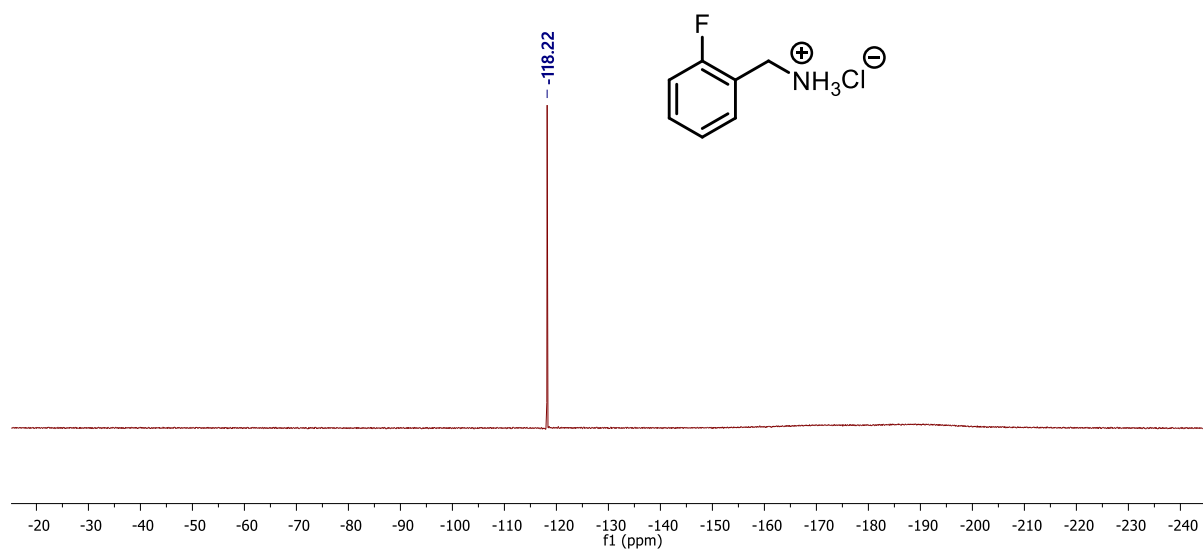


Fig. S55 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4s** in D_2O . ^{S28}

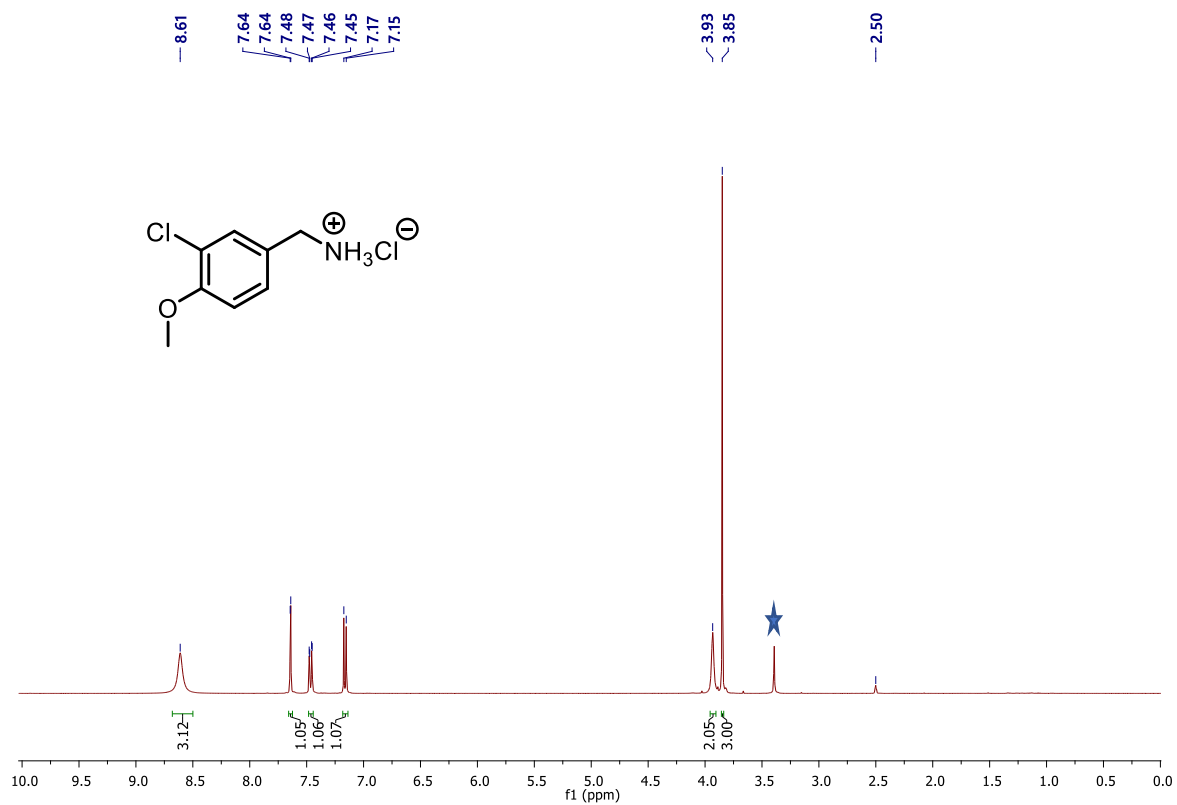


Fig. S56 ^1H NMR spectrum of 4t in DMSO- d_6 .^{S17} ★ denotes moisture peak in DMSO- d_6 .

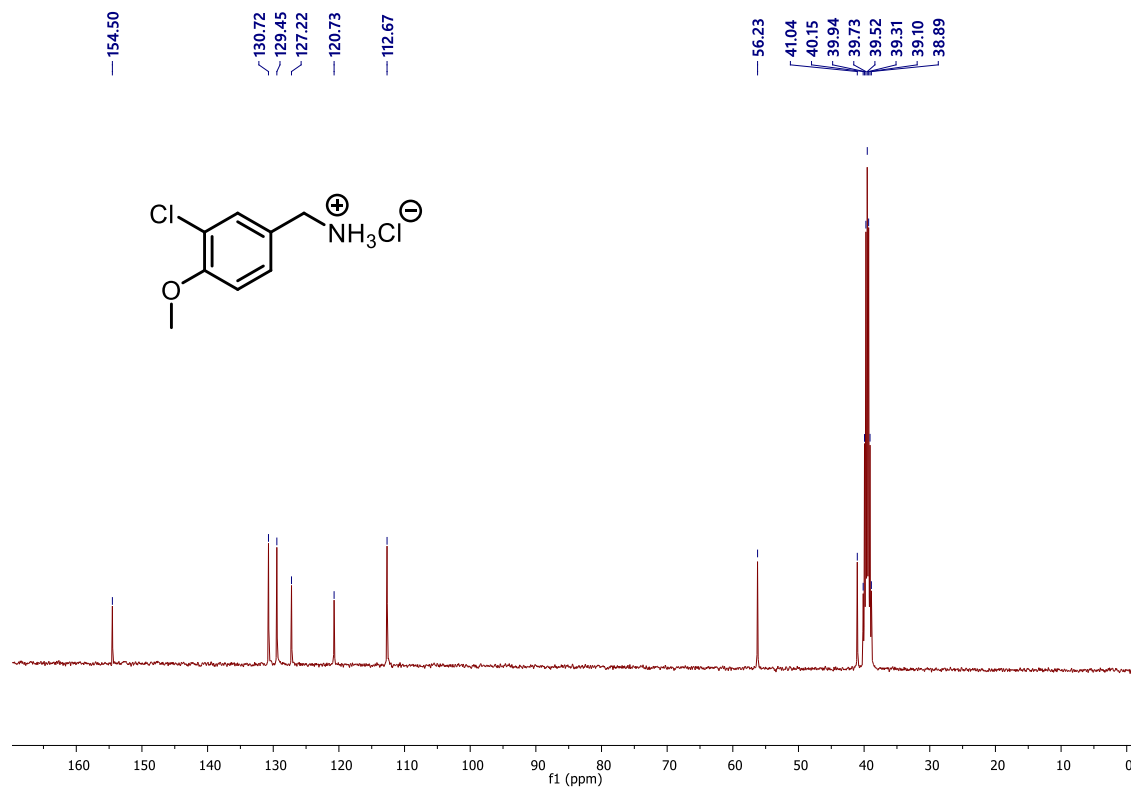


Fig. S57 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4t in DMSO- d_6 .^{S17}

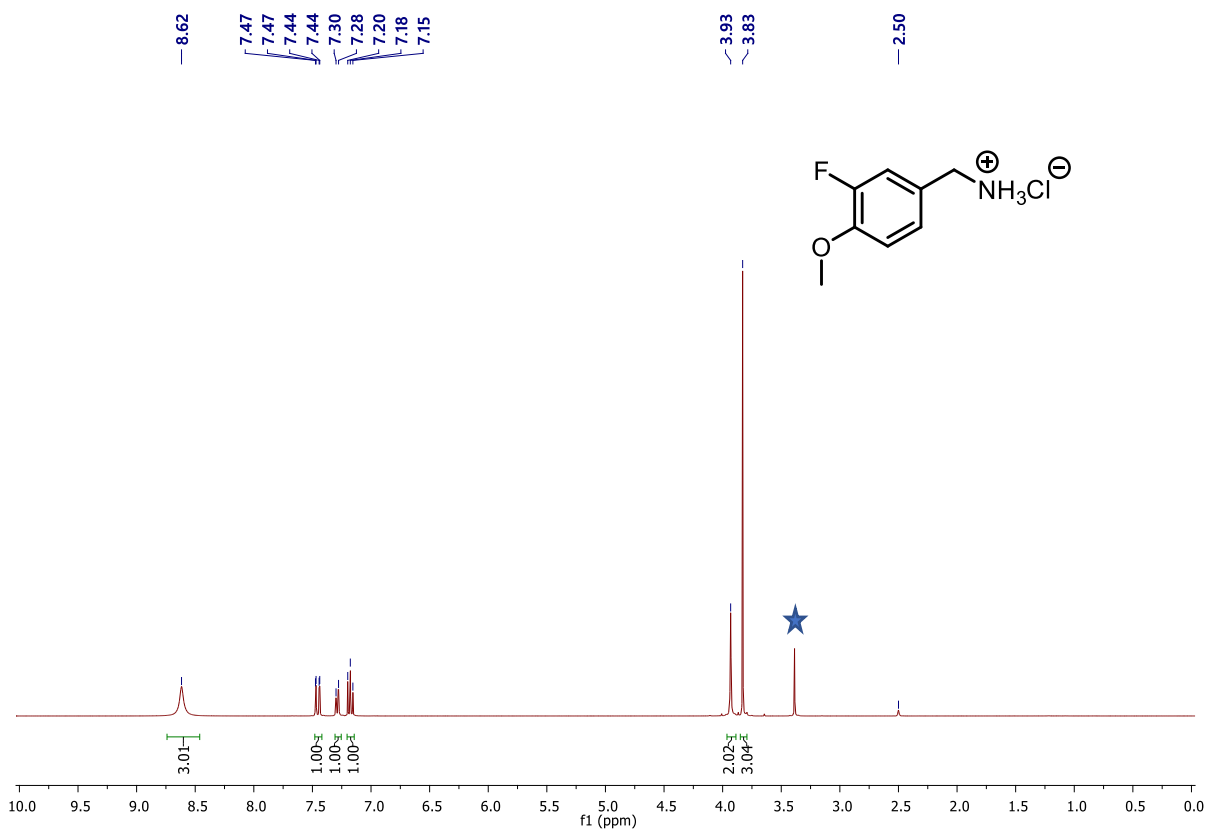


Fig. S58 $^1\text{H NMR}$ spectrum of **4u** in DMSO-d_6 .^{S17} ★ denotes moisture peak in DMSO-d_6 .

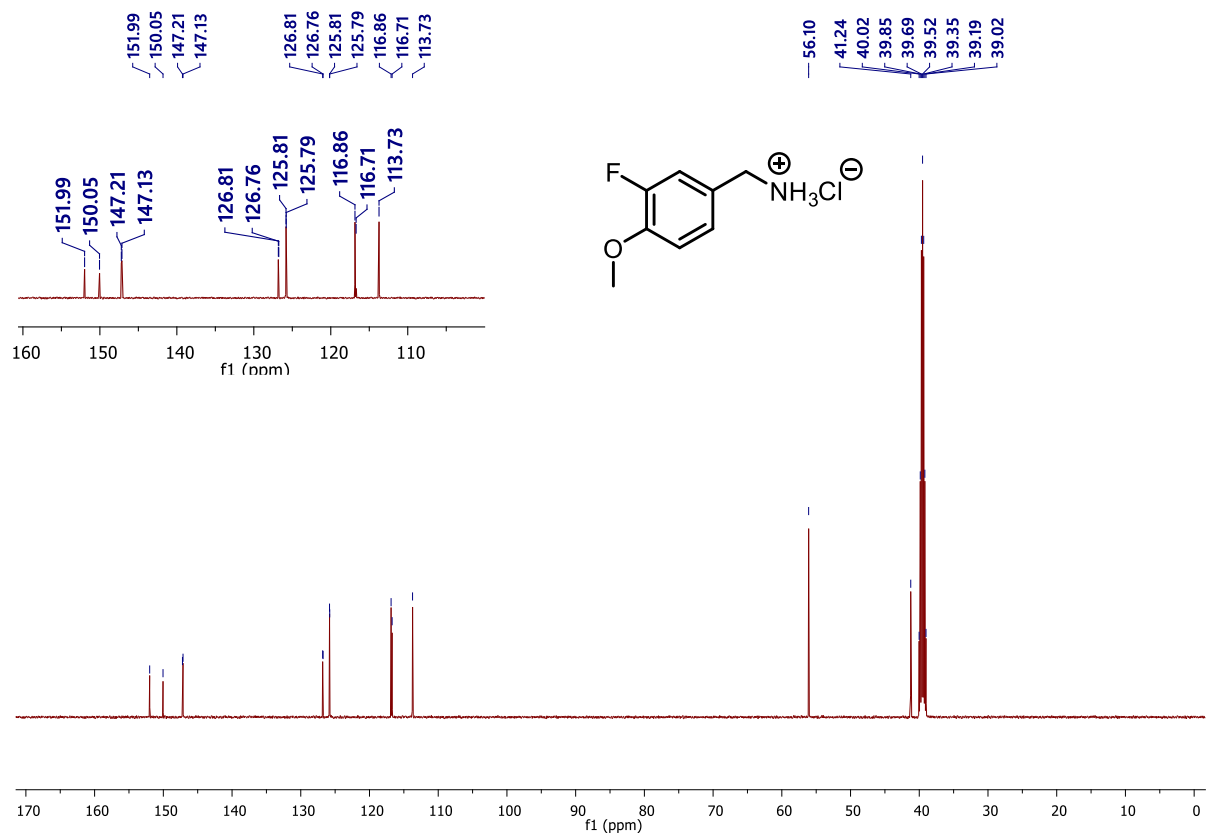


Fig. S59 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4u** in DMSO-d_6 .^{S17}

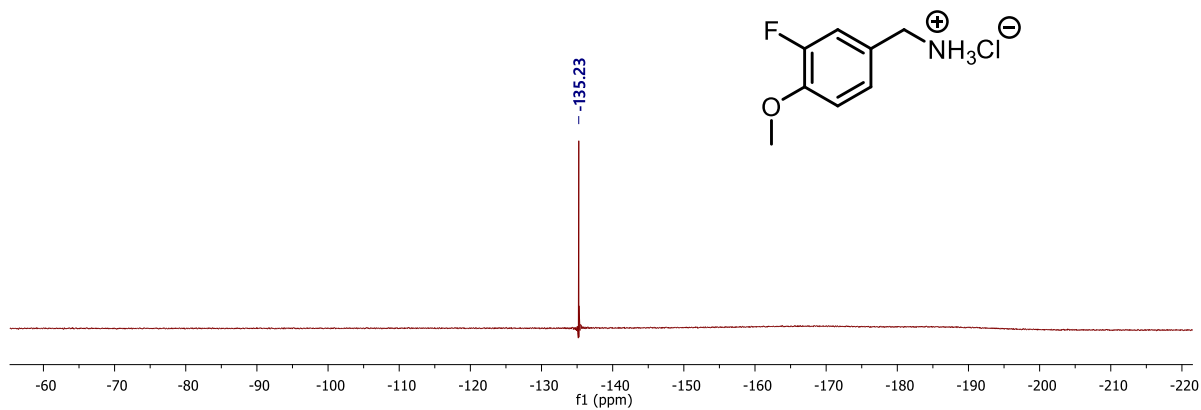


Fig. S60 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4u** in DMSO-d_6 .

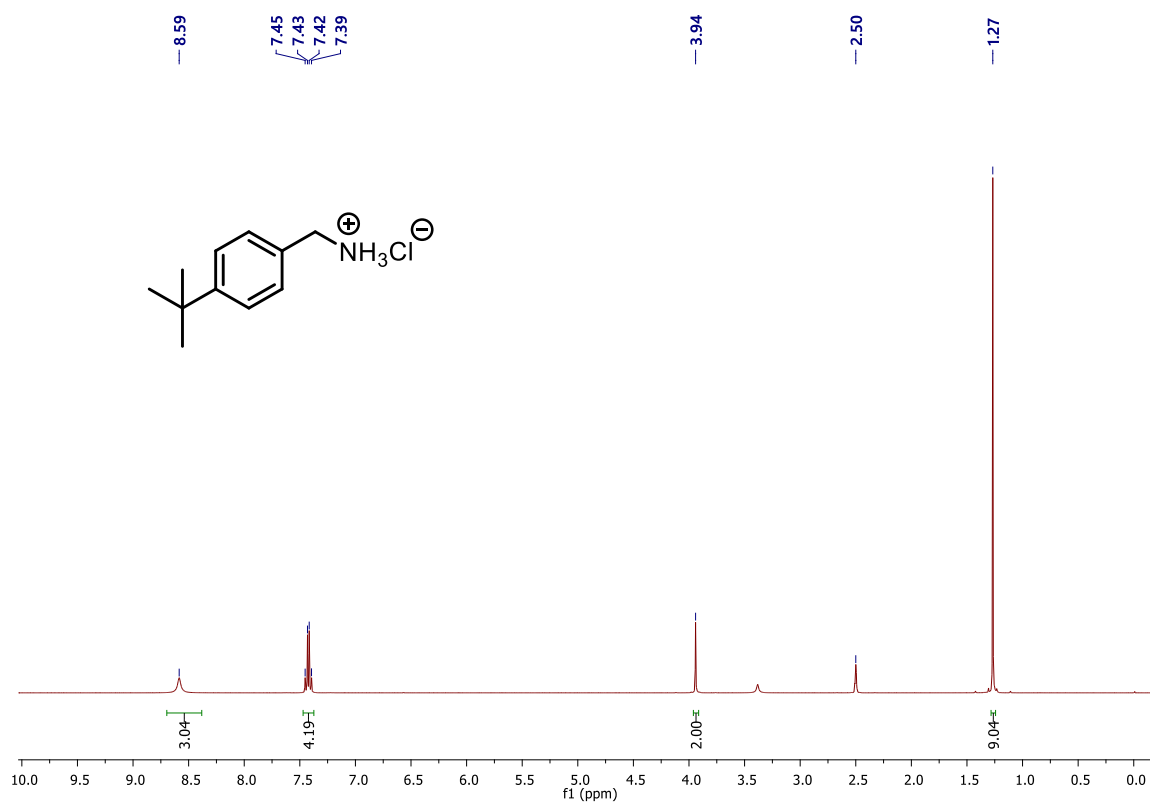


Fig. S61 ^1H NMR spectrum of **4v** in DMSO-d_6 .^{S12}

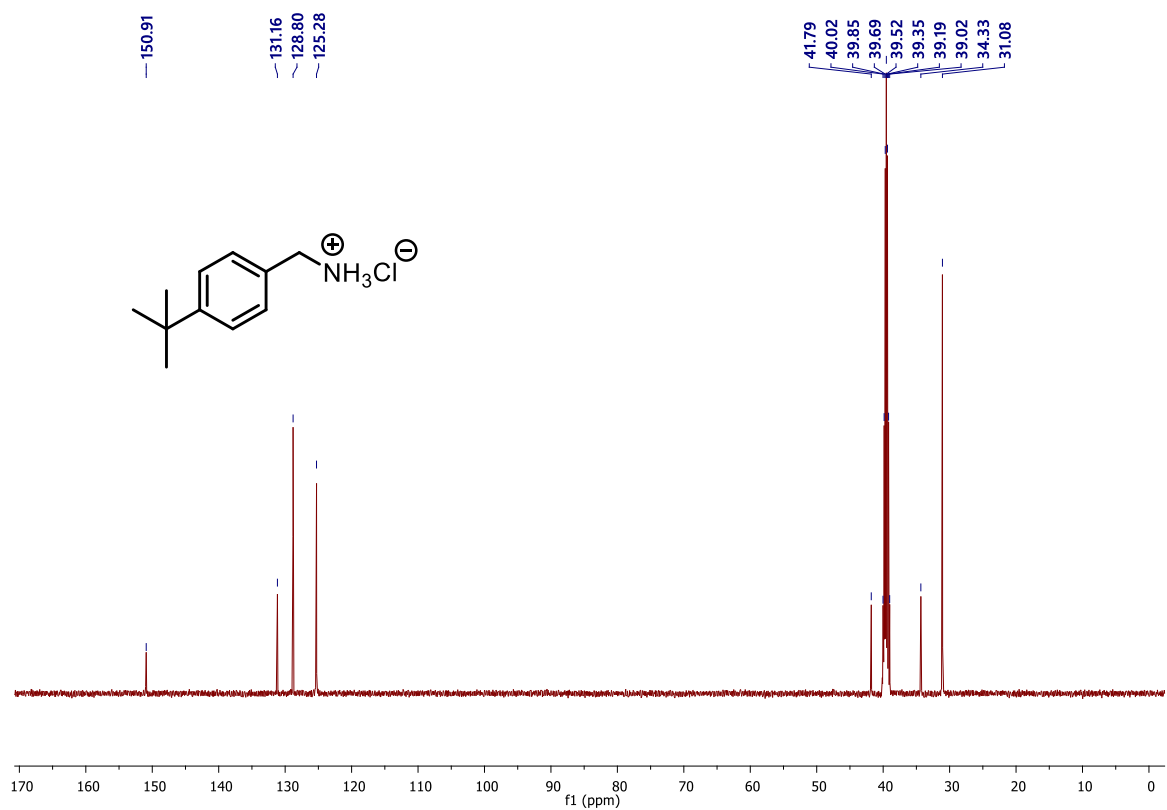


Fig. S62 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4v in DMSO- d_6 .^{S12}

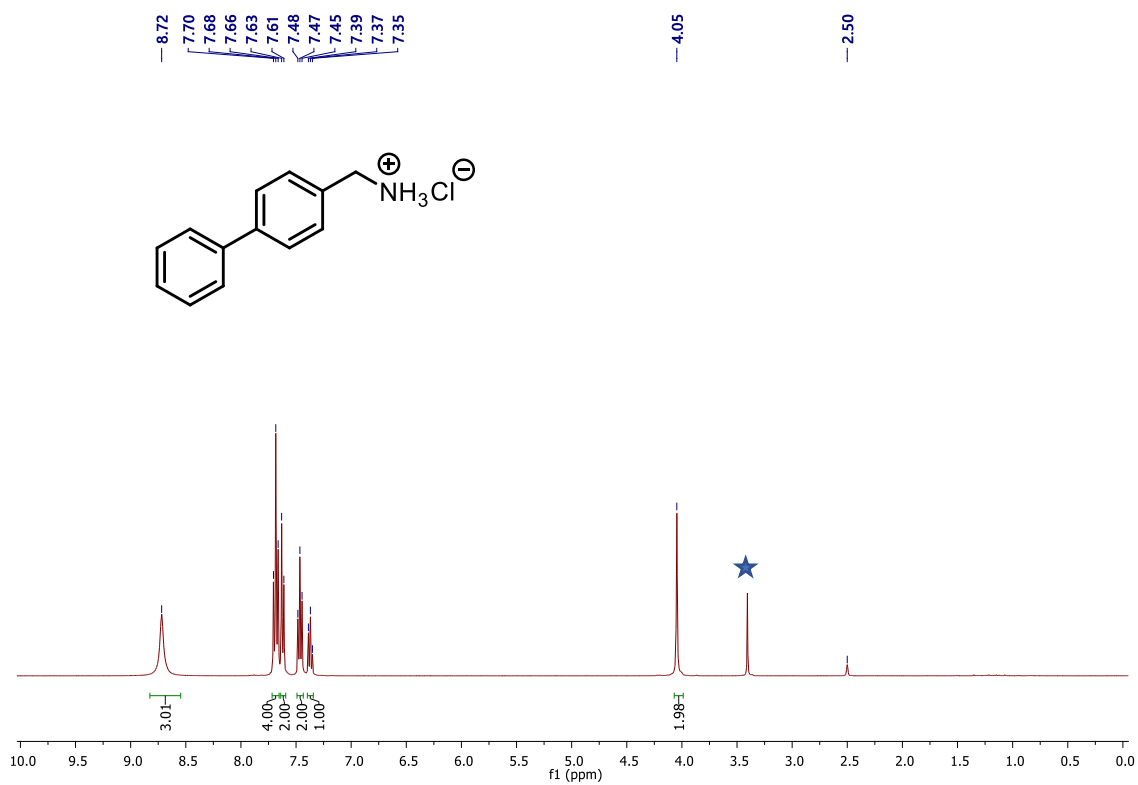


Fig. S63 ^1H NMR spectrum of 4w in DMSO- d_6 .^{S12} ★ denotes moisture peak in DMSO- d_6 .

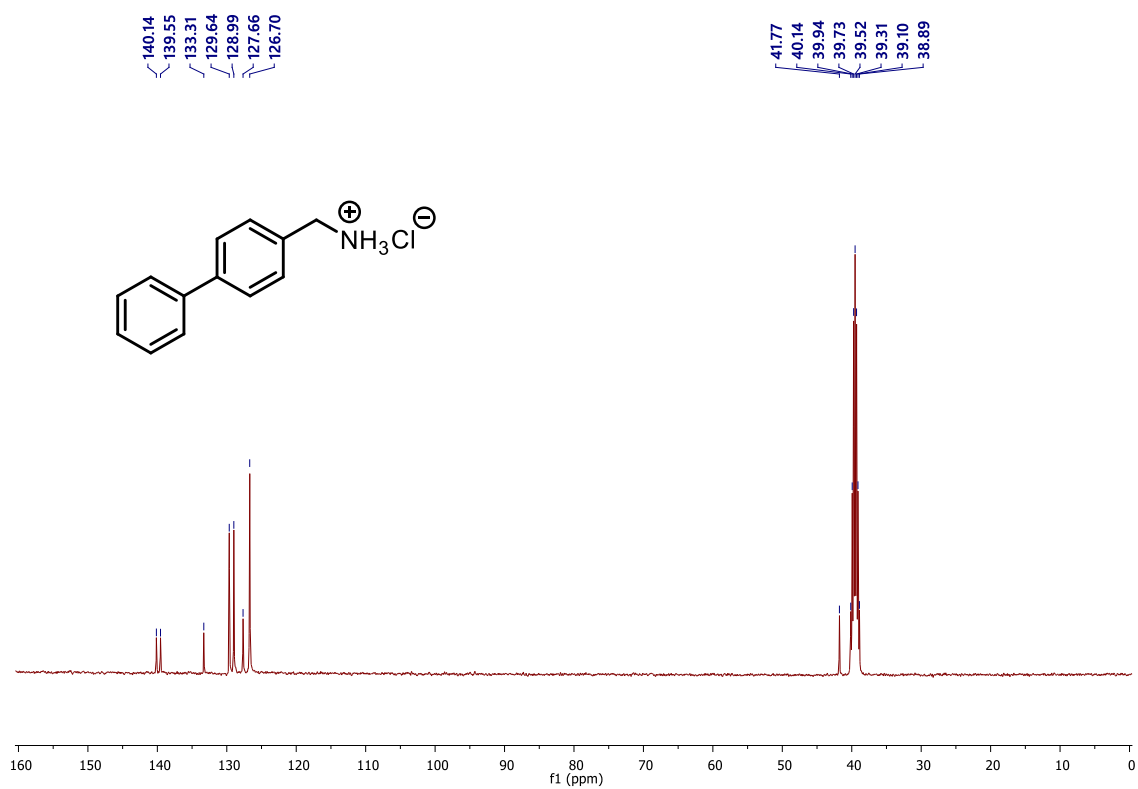


Fig. S64 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4w** in DMSO-d_6 .^{S12}

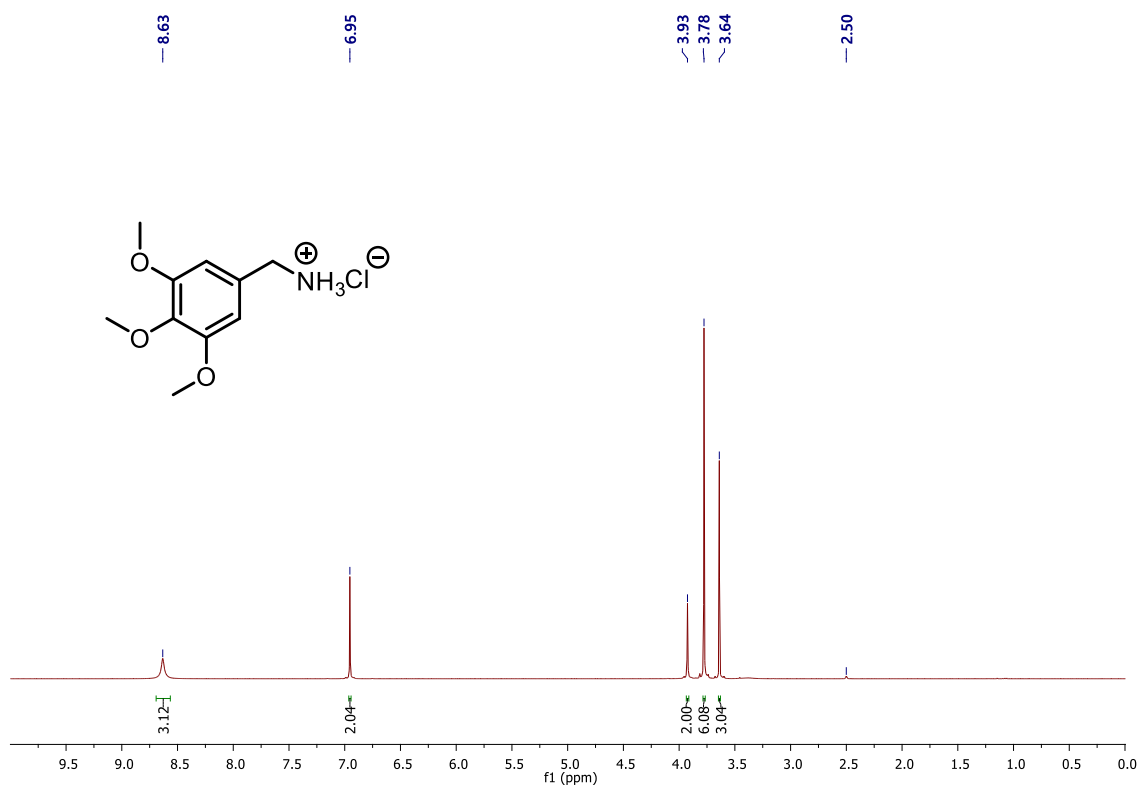


Fig. S65 ^1H NMR spectrum of **4x** in DMSO-d_6 .^{S18}

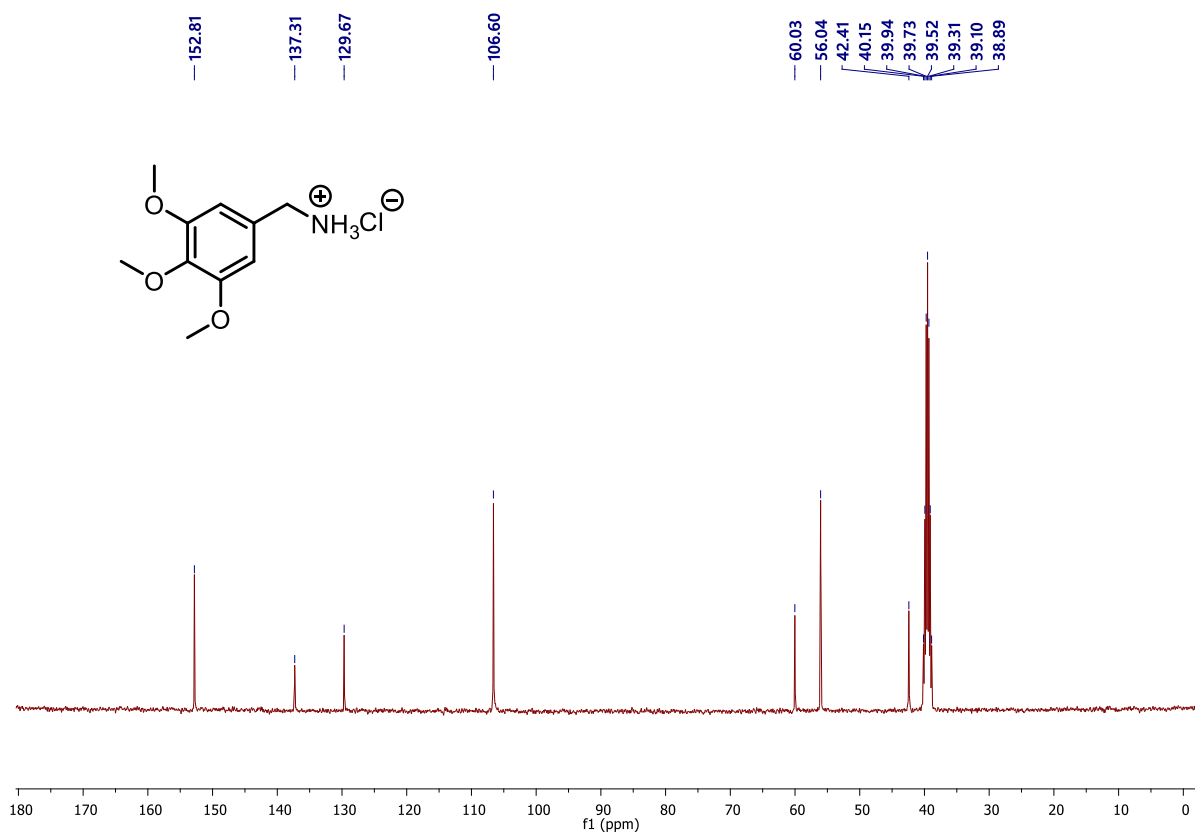


Fig. S66 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4x** in DMSO-d_6 . ^{S18}

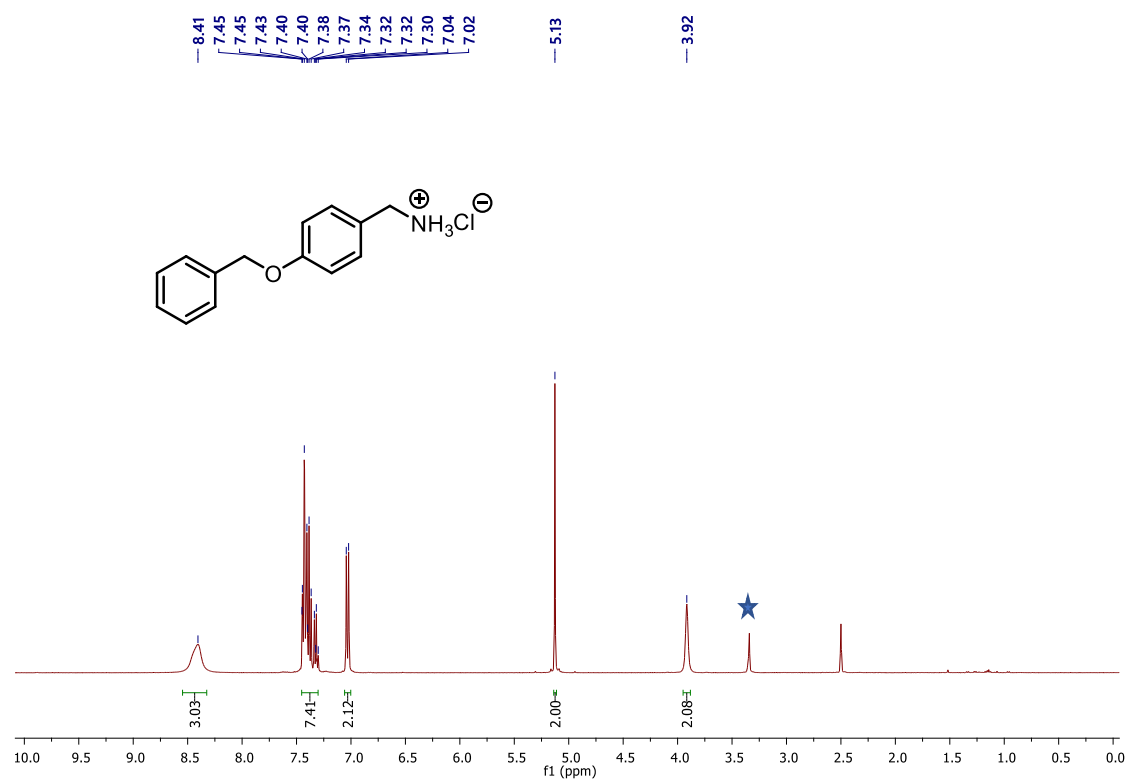


Fig. S67 ^1H NMR spectrum of **4y** in DMSO-d_6 . ^{S18} ★ denotes moisture peak in DMSO-d_6 .

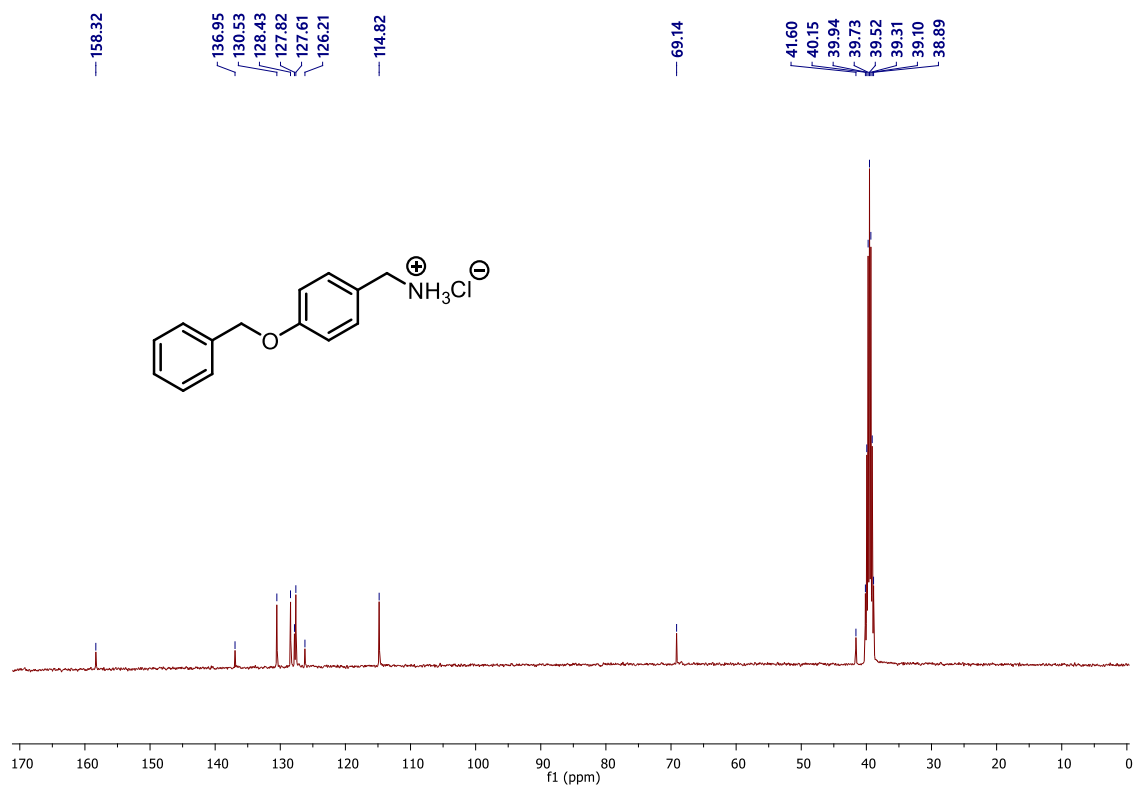


Fig. S68 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4y** in DMSO-d_6 .^{S18}

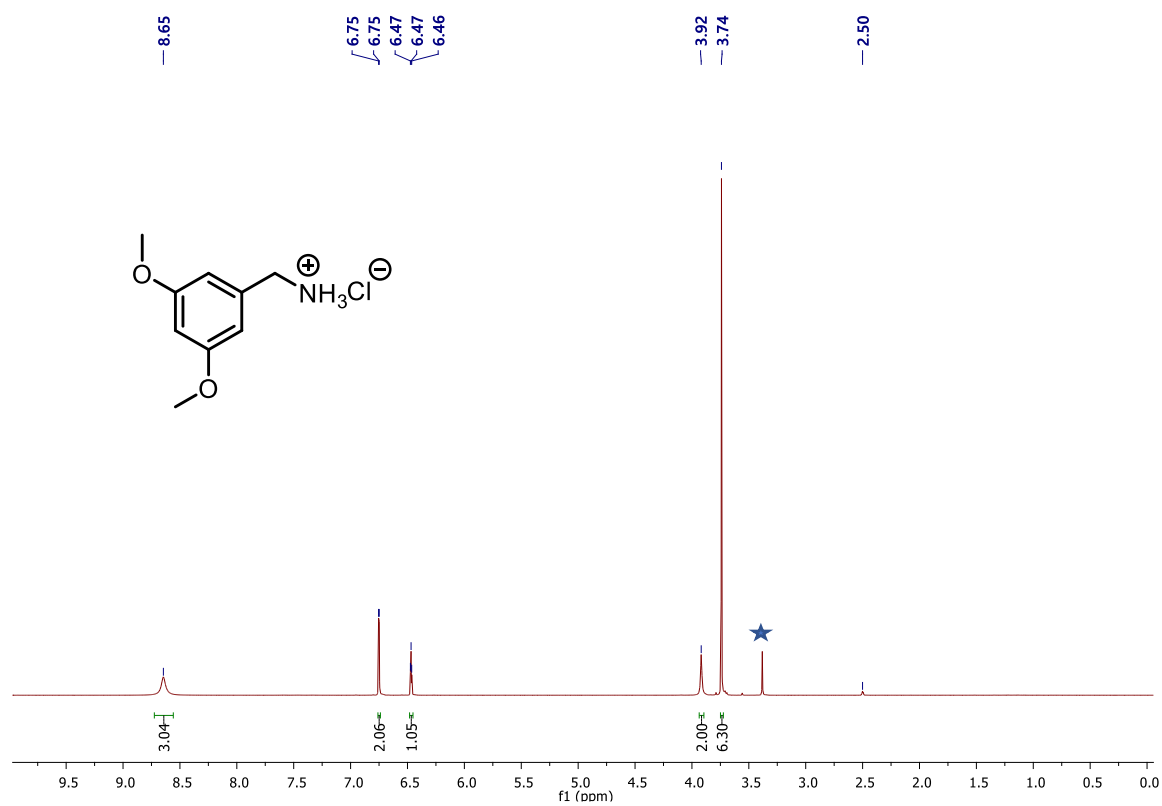


Fig. S69 ^1H NMR spectrum of **4z** in DMSO-d_6 .^{S19} ★ denotes moisture peak in DMSO-d_6 .

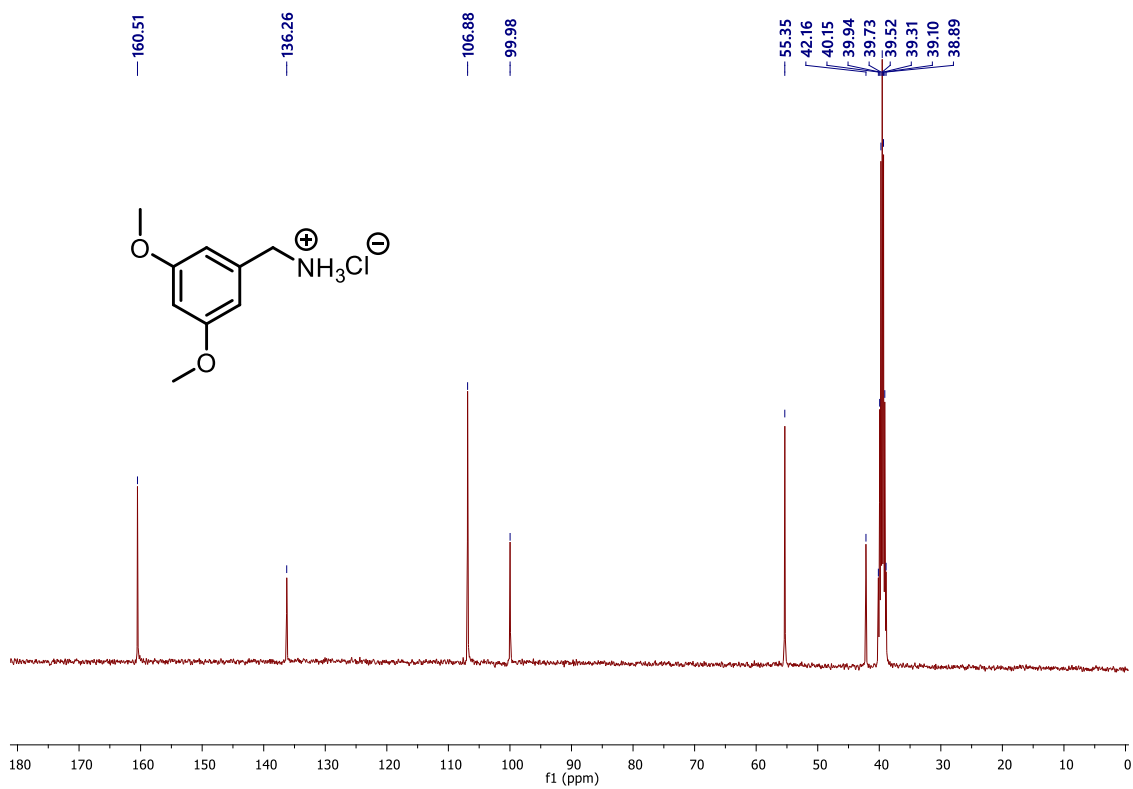


Fig. S70 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4z** in DMSO-d_6 .^{S19}

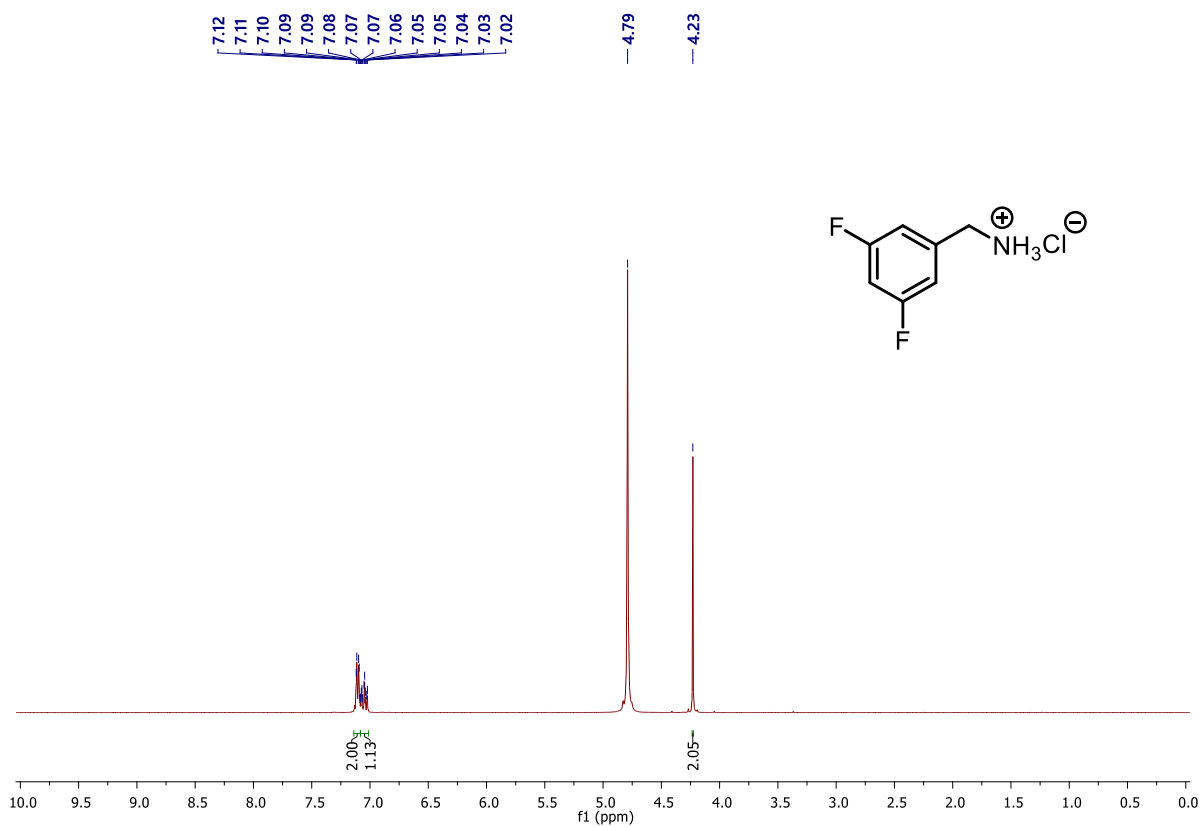


Fig. S71 ^1H NMR spectrum of **4aa** in D_2O .^{S20}

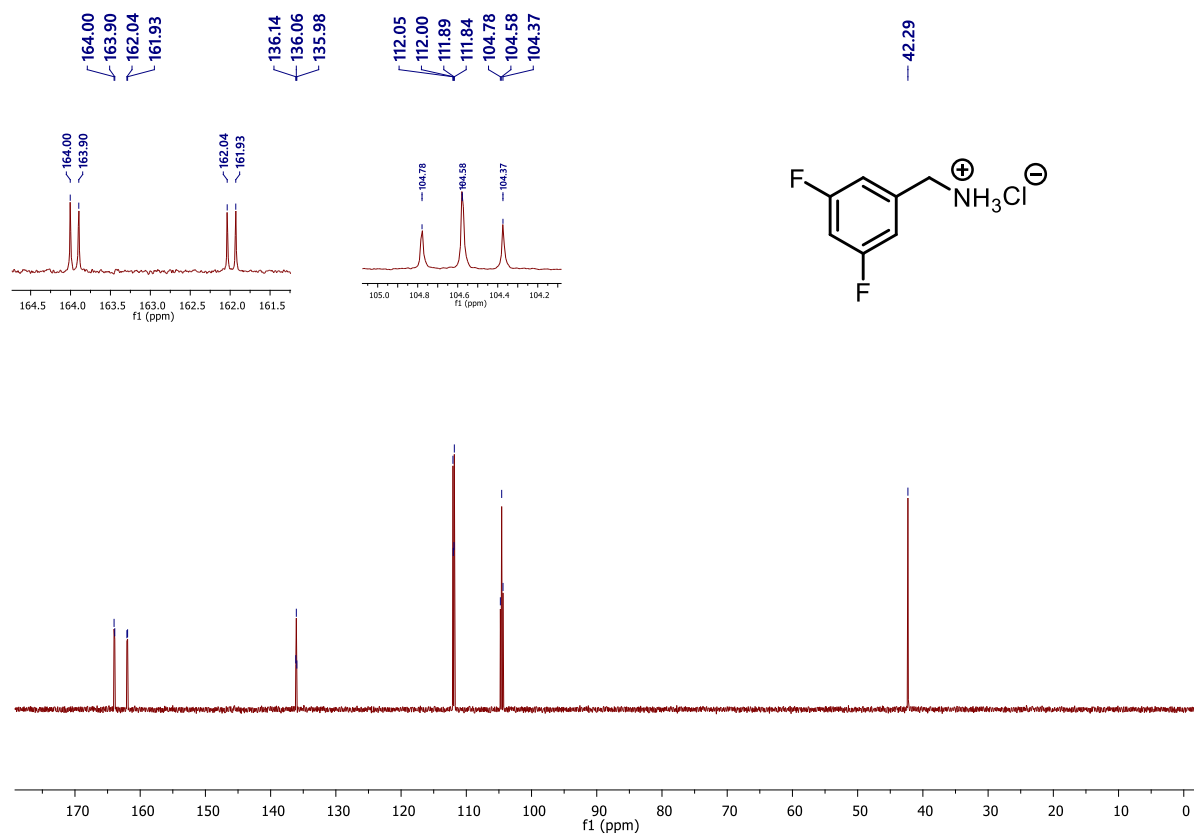


Fig. S72 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4aa in D_2O .^{S20}

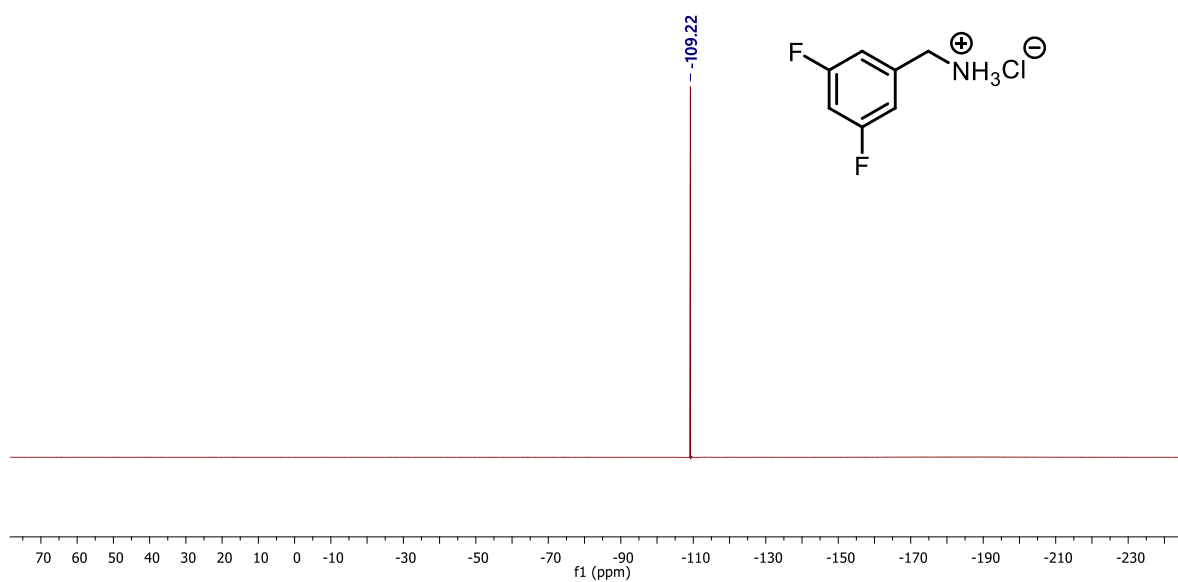


Fig. S73 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of 4aa in D_2O .

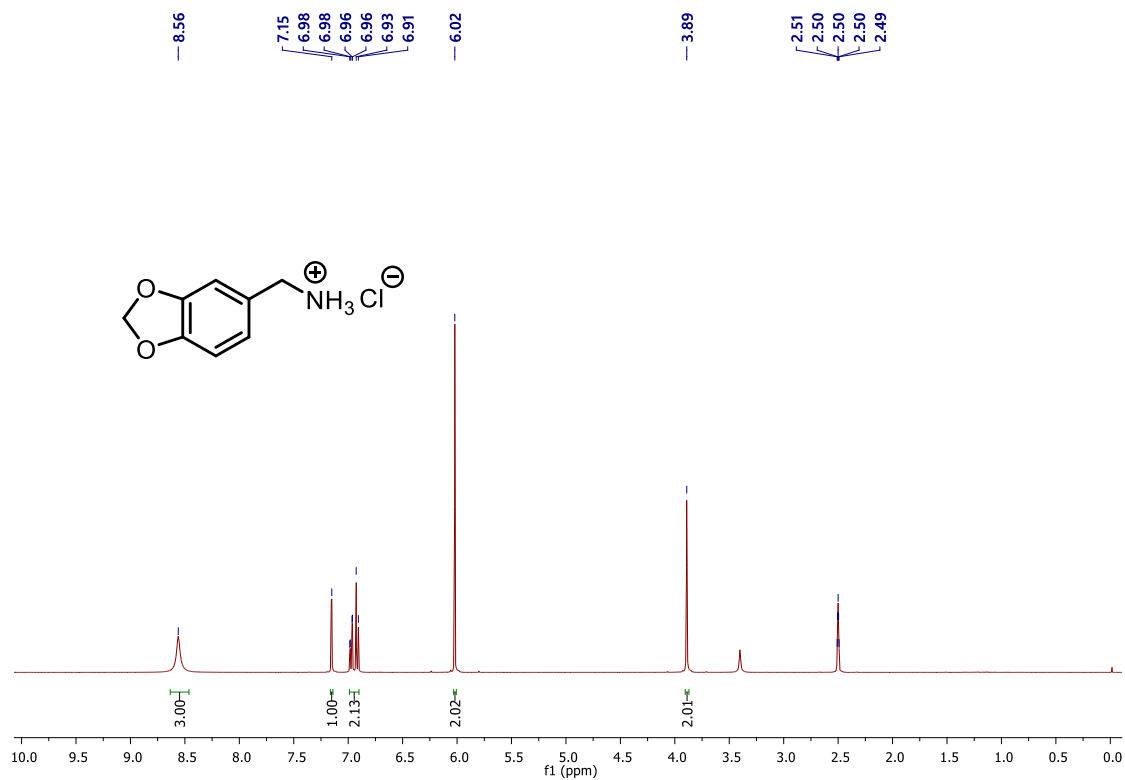


Fig. S74 ¹H NMR spectrum of **4ab** in DMSO-d₆.^{S14}

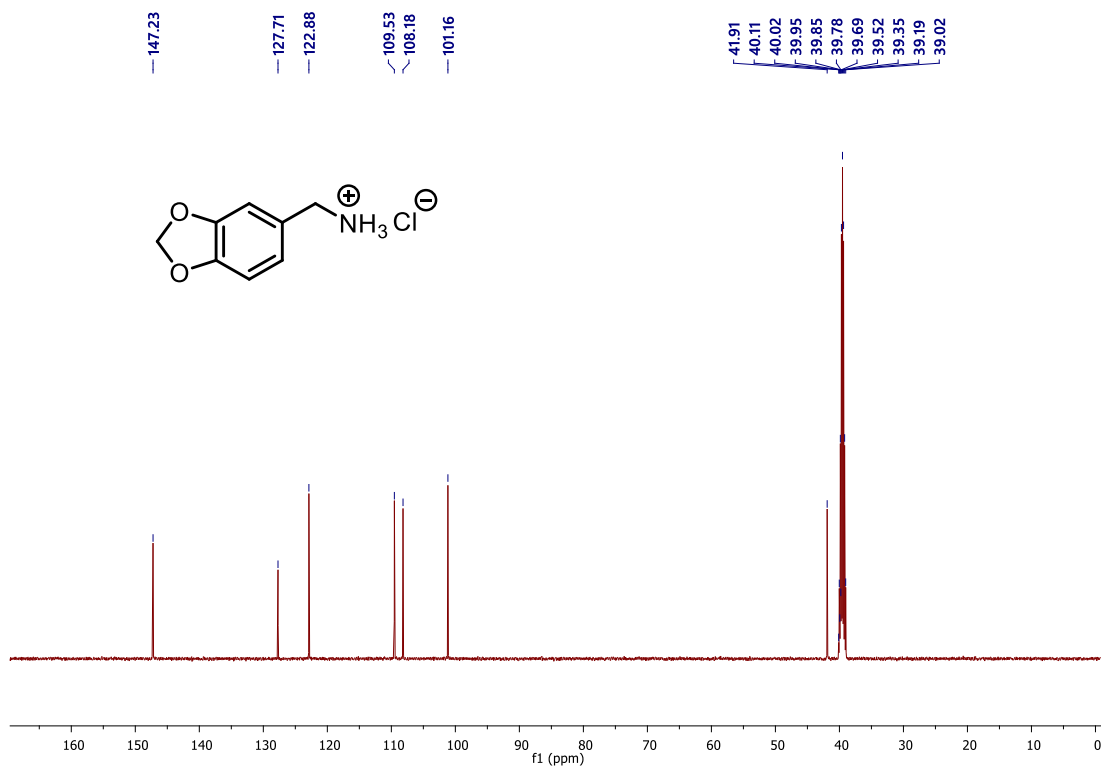


Fig. S75 ¹³C{¹H} NMR spectrum of **4ab** in DMSO-d₆.^{S14}

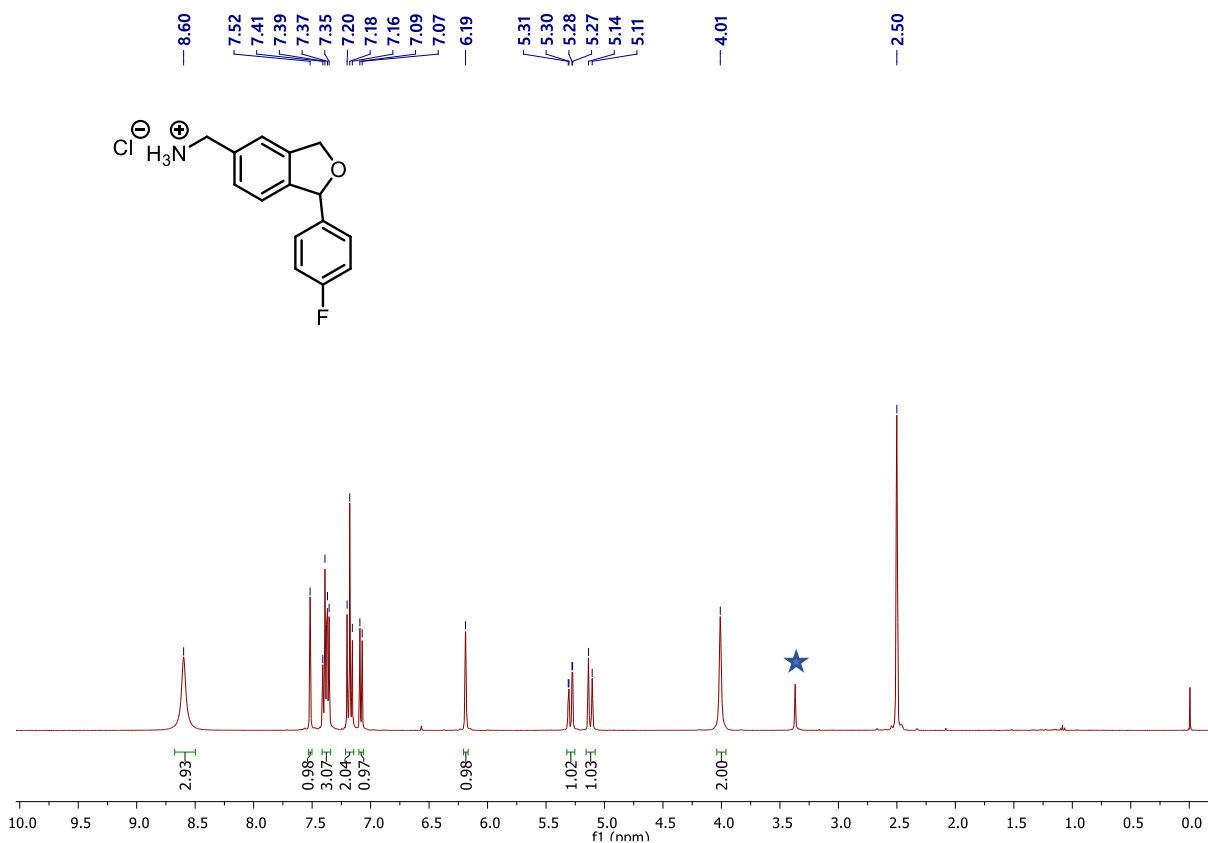


Fig. S76 ^1H NMR spectrum of **4ac** in DMSO-d_6 . \star denotes moisture peak in DMSO-d_6 .

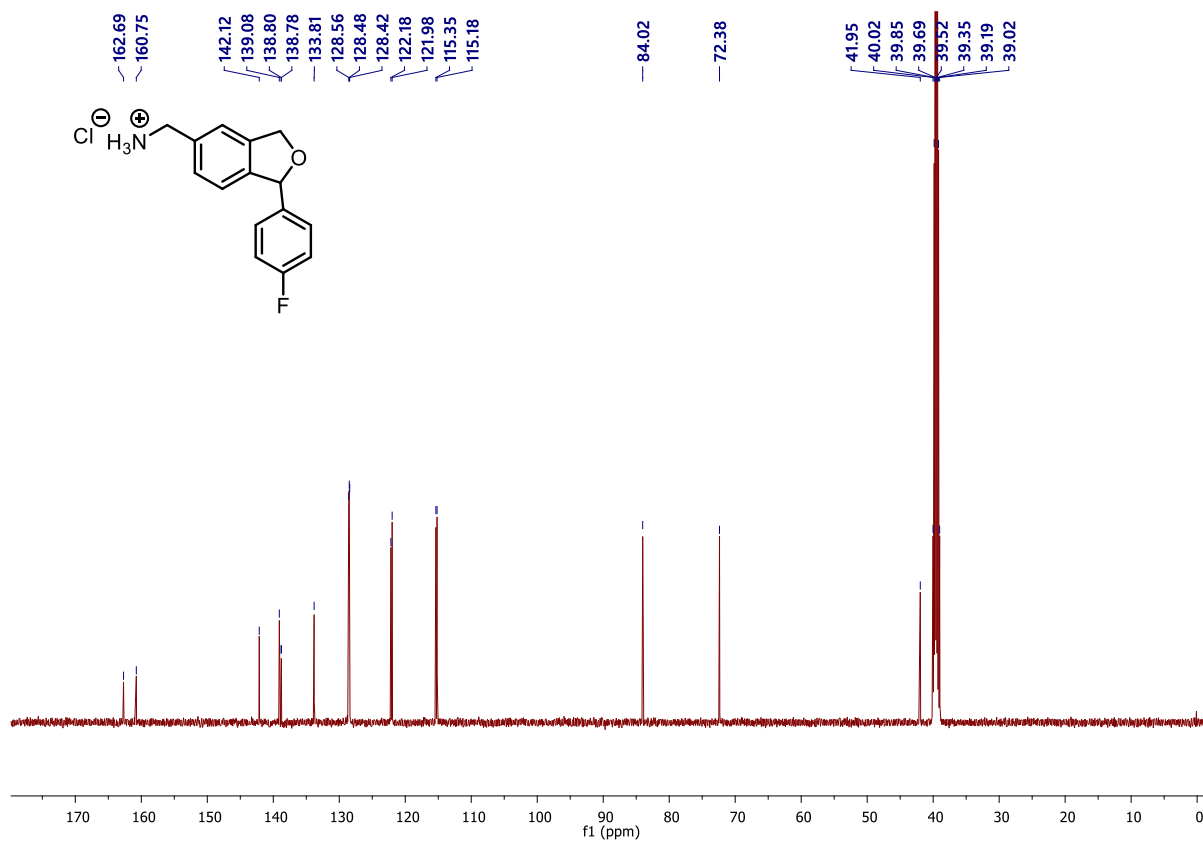


Fig. S77 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4ac** in DMSO-d_6 .

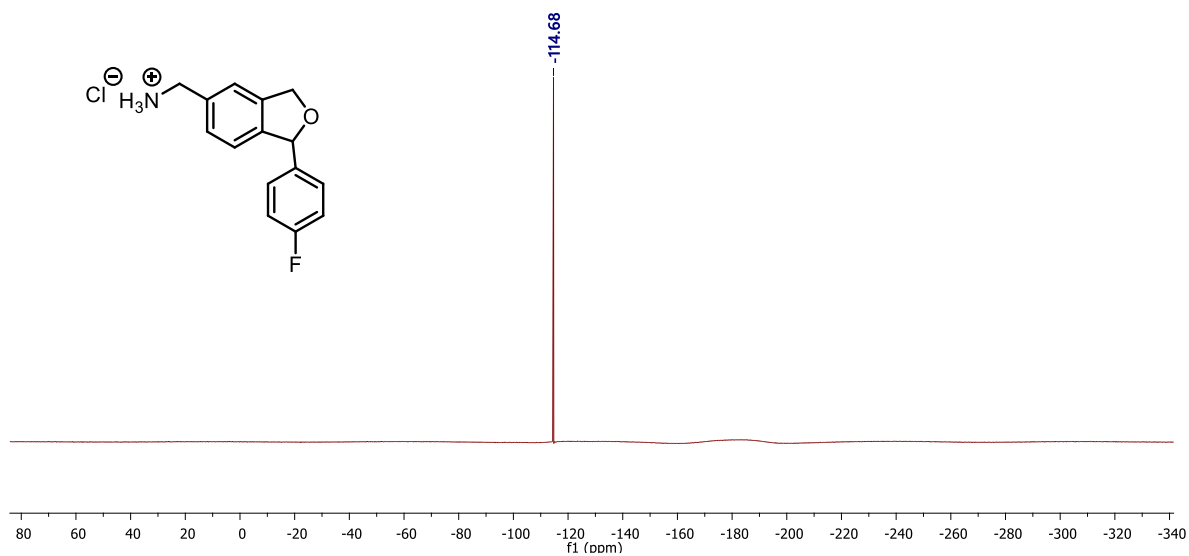


Fig. S78 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4ac** in DMSO-d_6 .

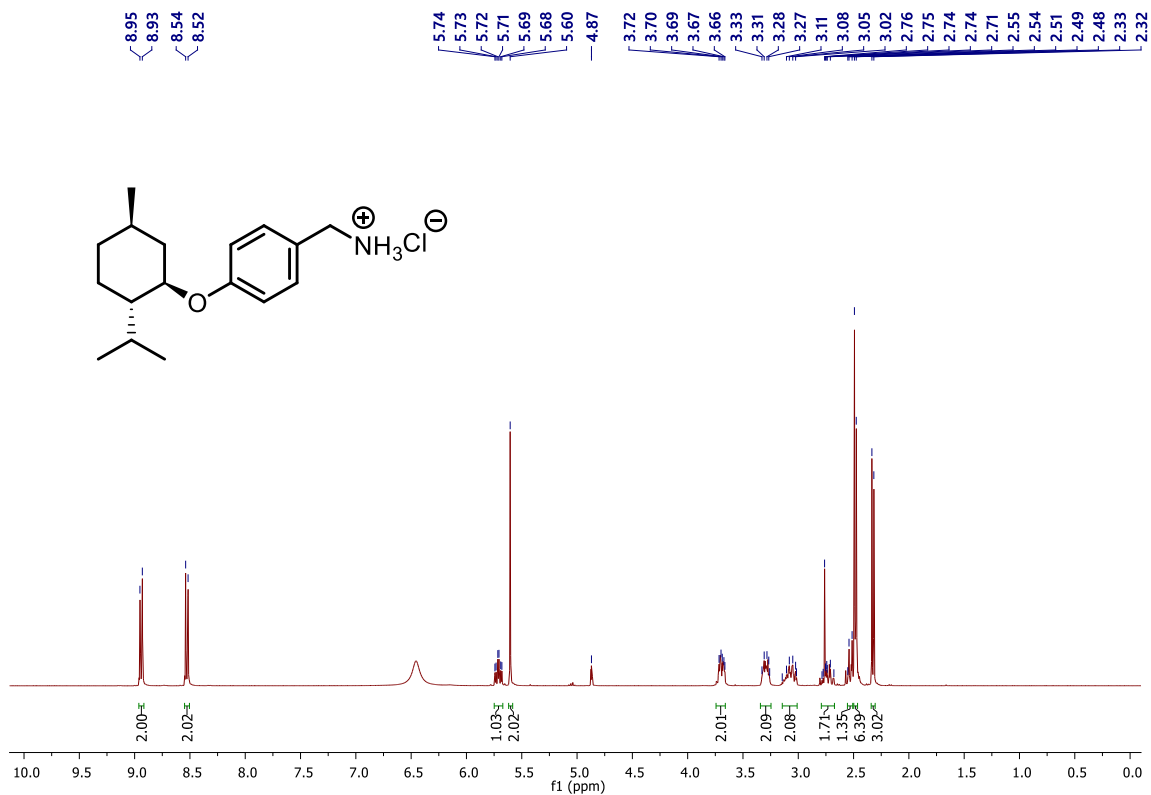


Fig. S79 ^1H NMR spectrum of **4ad** in CD_3OD .

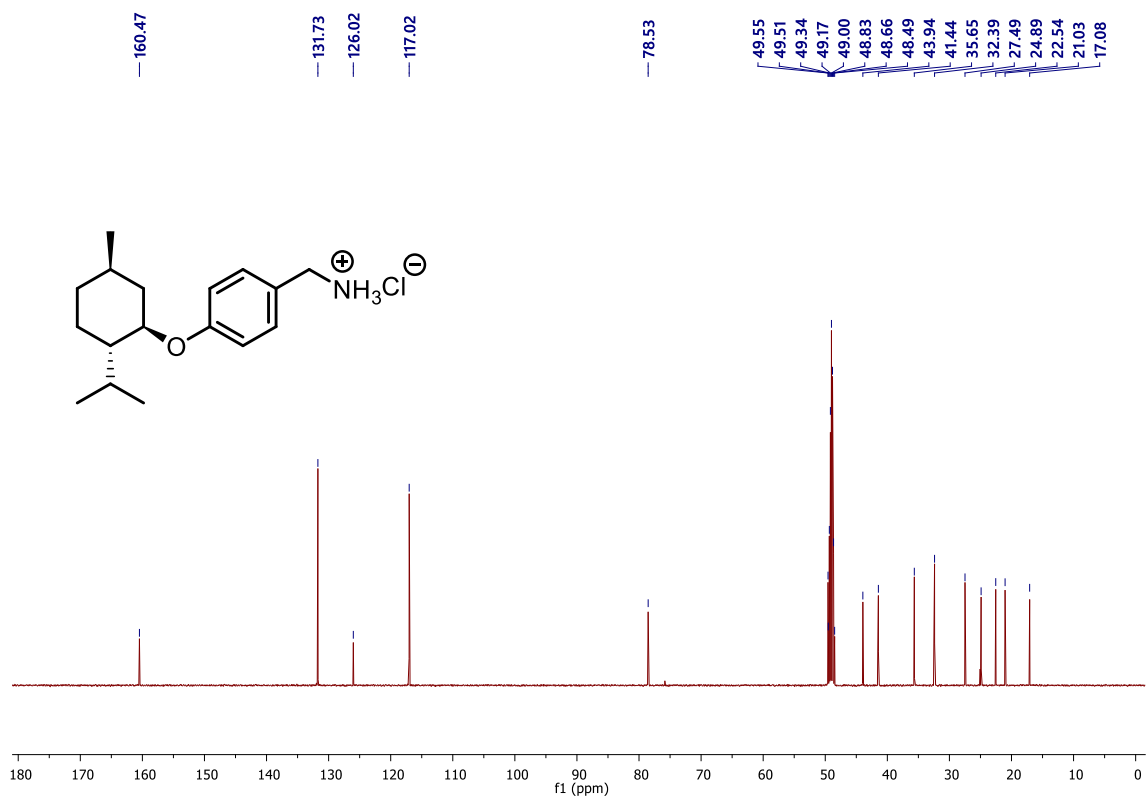


Fig. S80 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4ad** in CD_3OD .

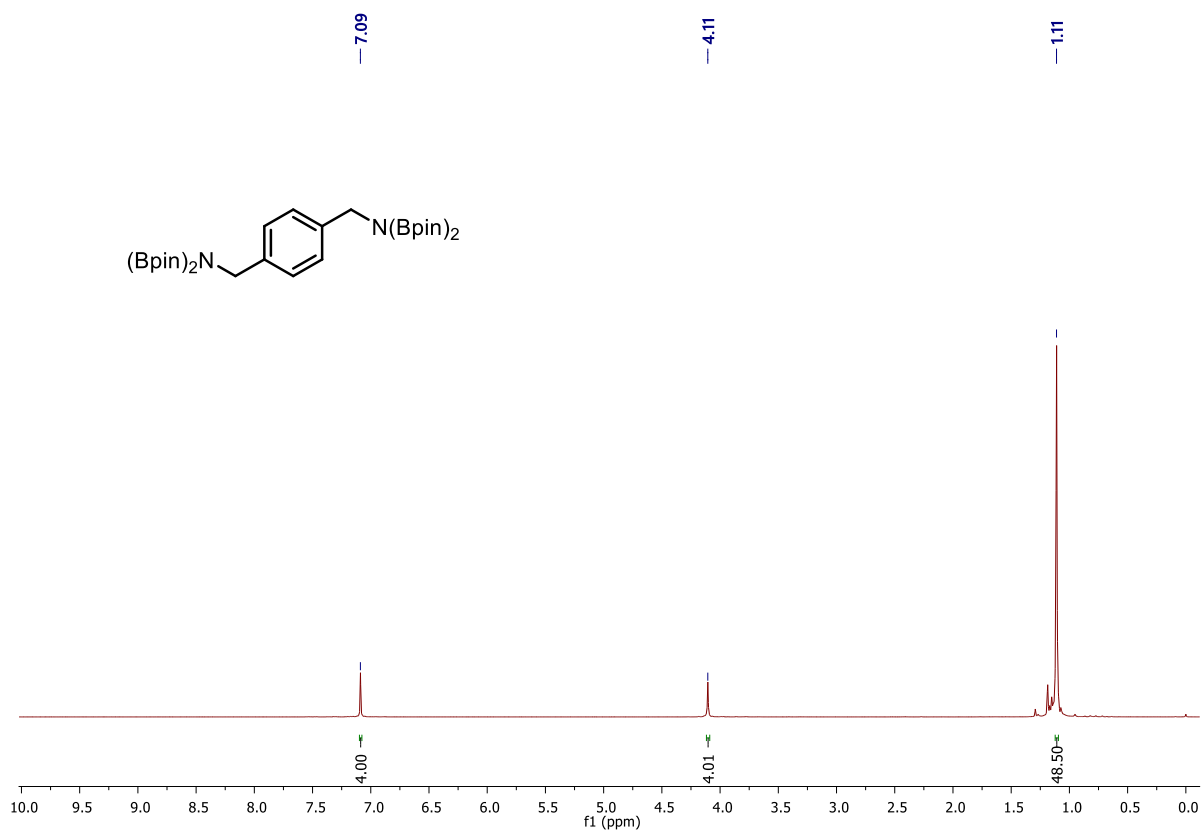


Fig. S81 ^1H NMR spectrum of **3ae** in CDCl_3 . ^{S7}

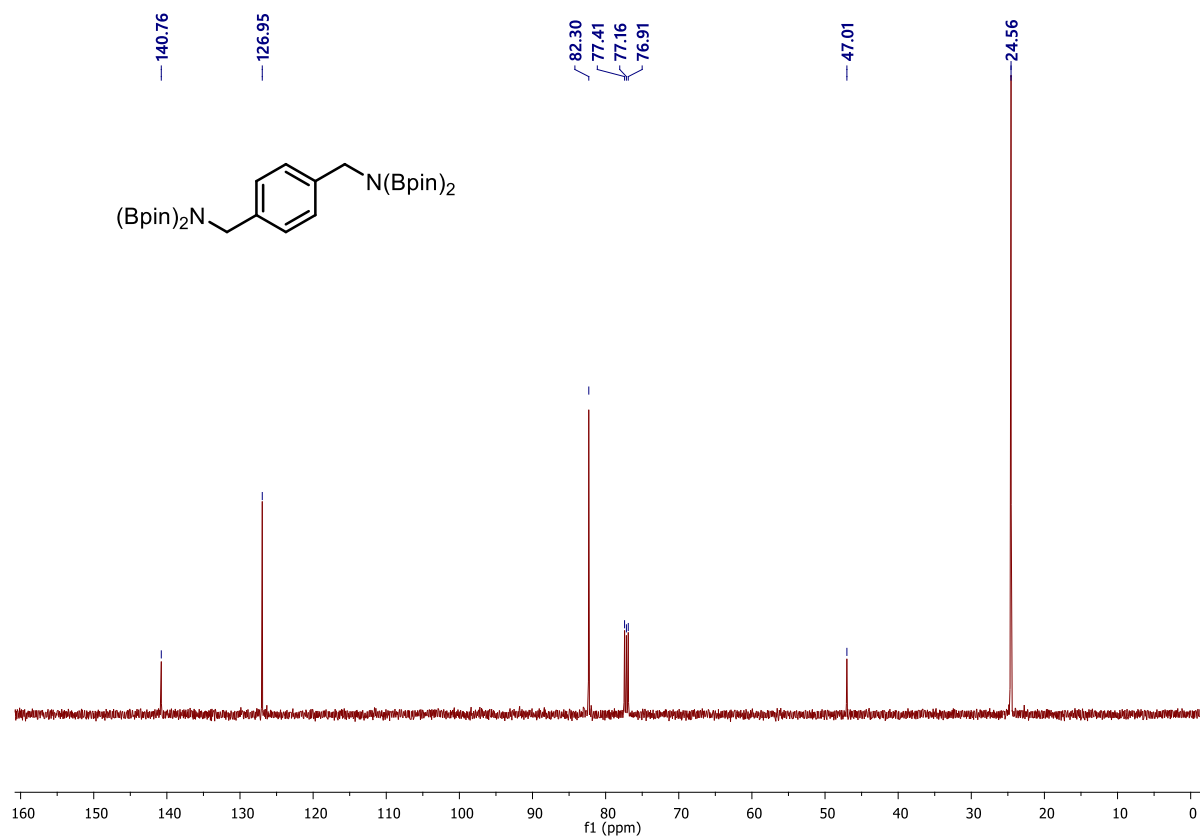


Fig. S82 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3ae** in CDCl_3 . ^{S7}

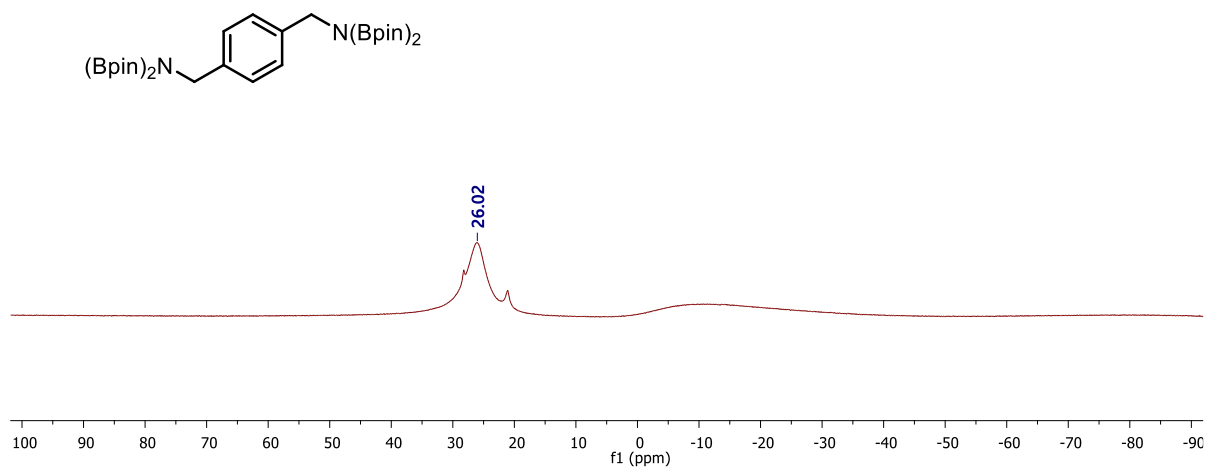


Fig. S83 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **3ae** in CDCl_3 . ^{S7}

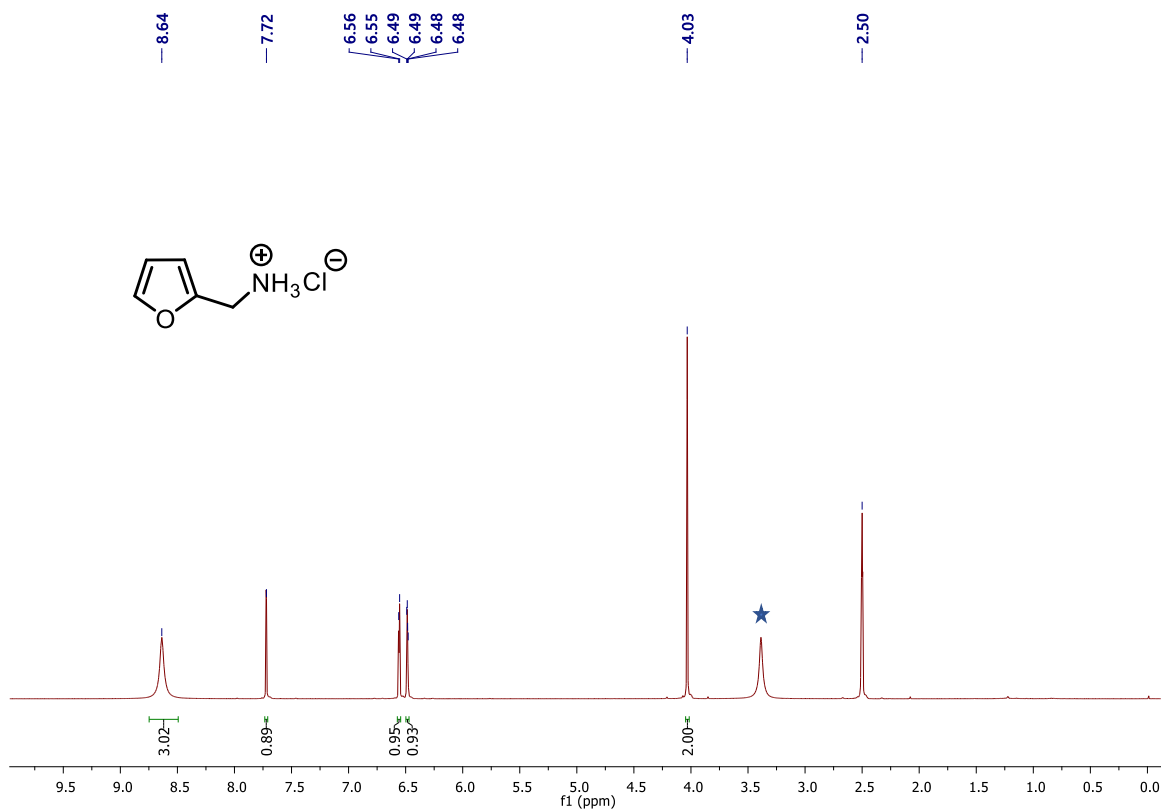


Fig. S84 ^1H NMR spectrum of **4af** in DMSO-d_6 . ^{S22} ★ denotes moisture peak in DMSO-d_6 .

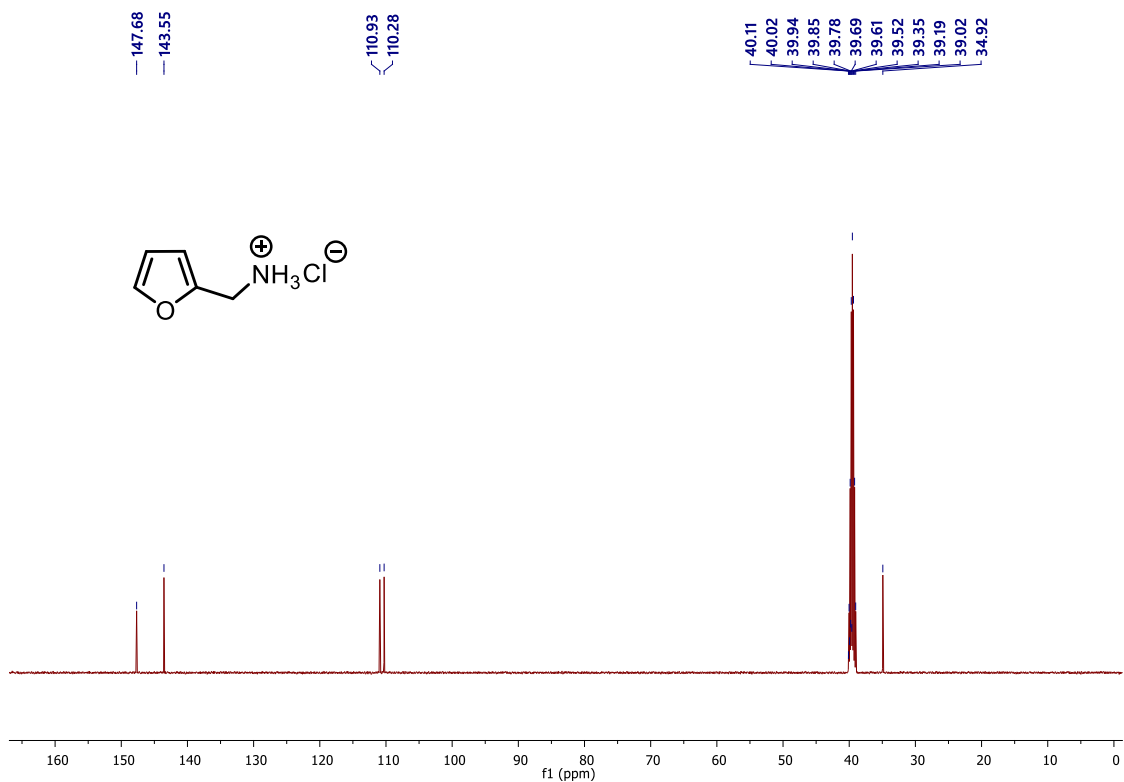


Fig. S85 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4af** in DMSO-d_6 . ^{S22}

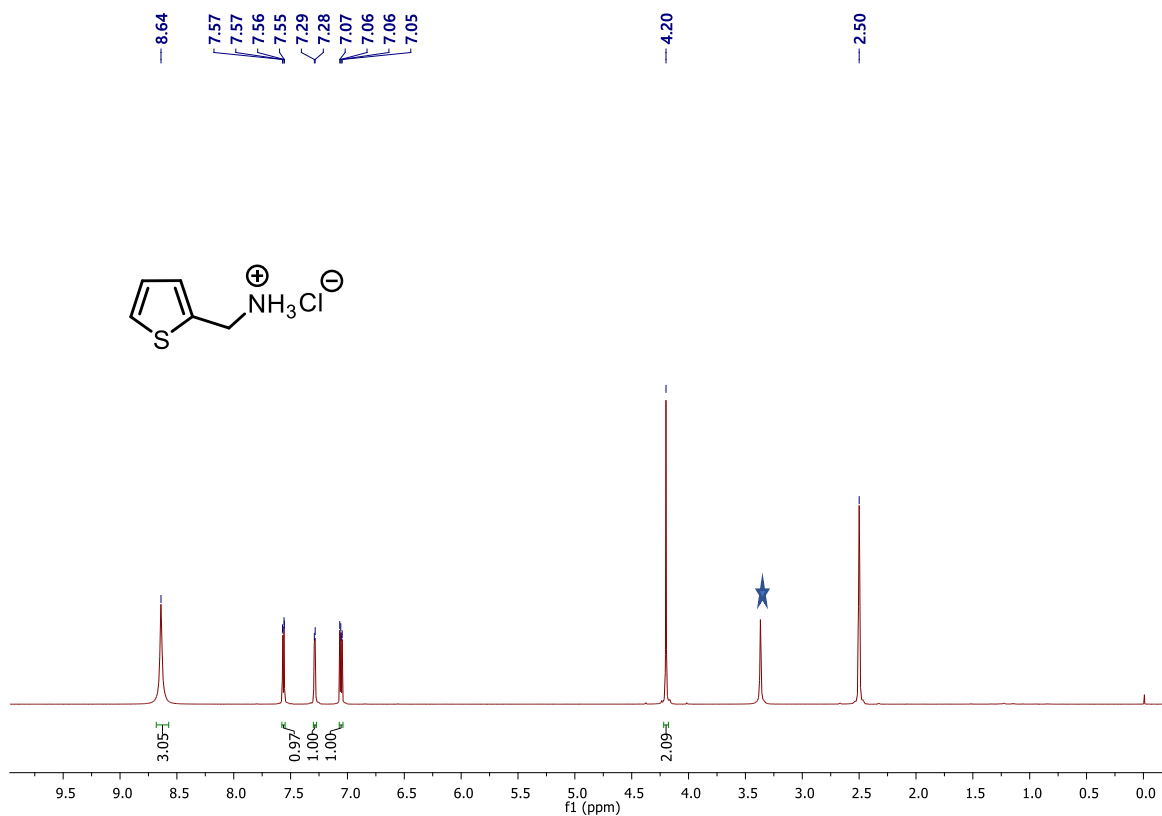


Fig. S86 ^1H NMR spectrum of **4ag** in DMSO-d_6 . $^{\text{S23}}$ ★ denotes moisture peak in DMSO-d_6 .

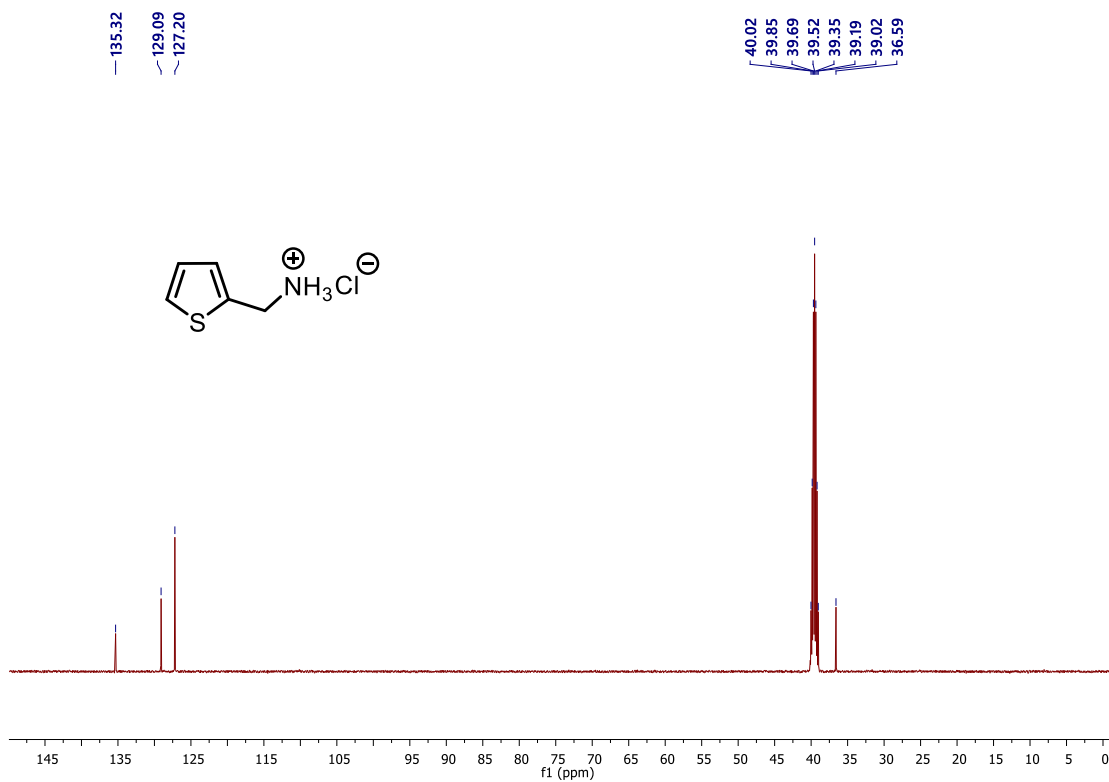


Fig. S87 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4ag** in DMSO-d_6 . $^{\text{S23}}$

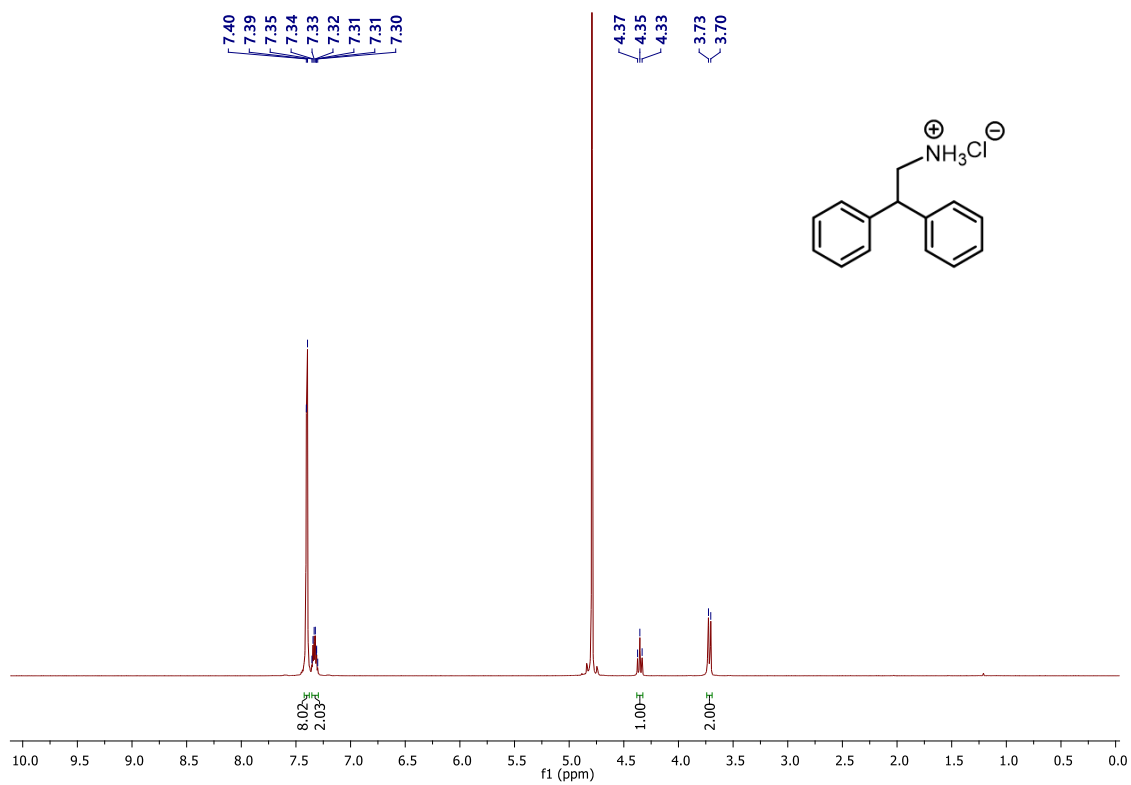


Fig. S88 ^1H NMR spectrum of **4ah** in D_2O . ^{S24}

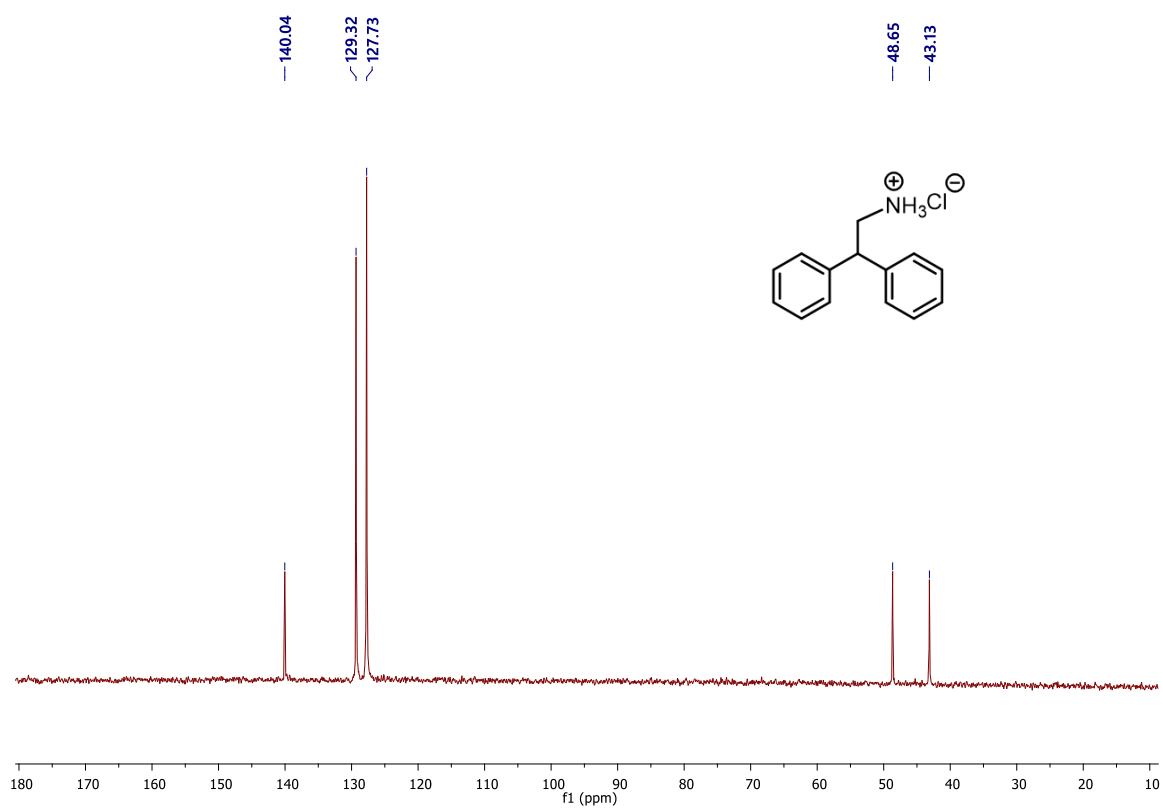


Fig. S89 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4ah** in D_2O . ^{S24}

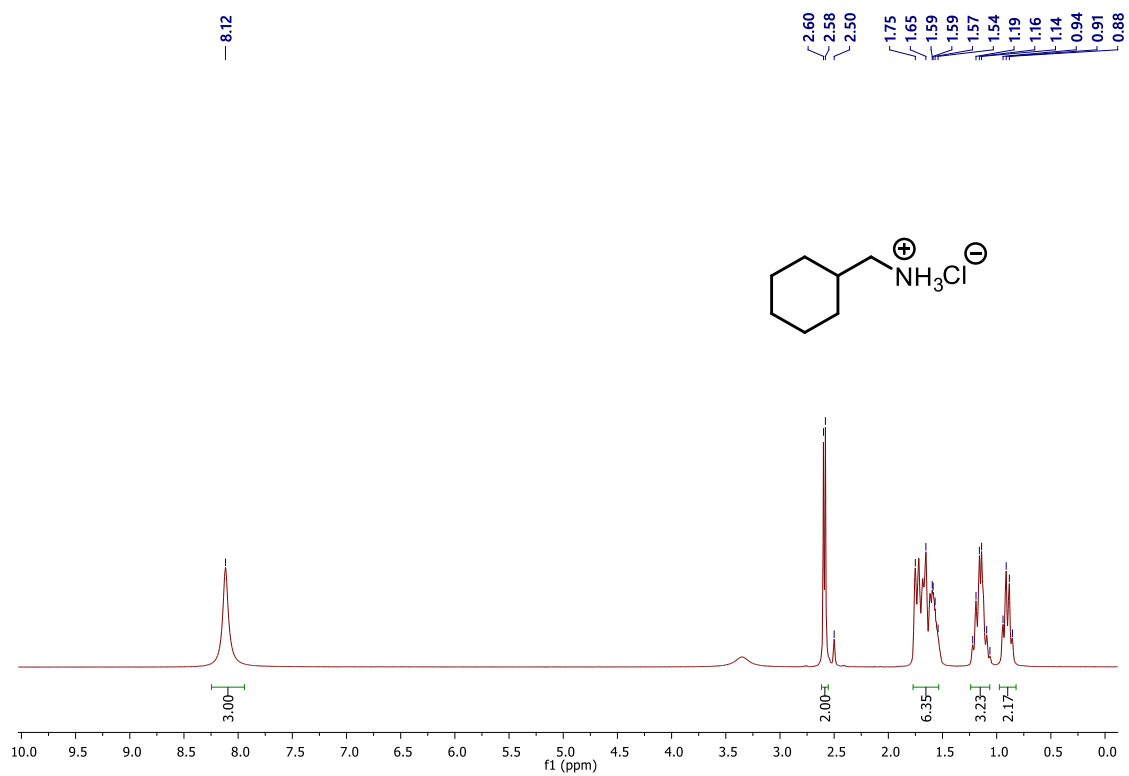


Fig. S90 ^1H NMR spectrum of **4ai** in DMSO-d_6 .^{S25}

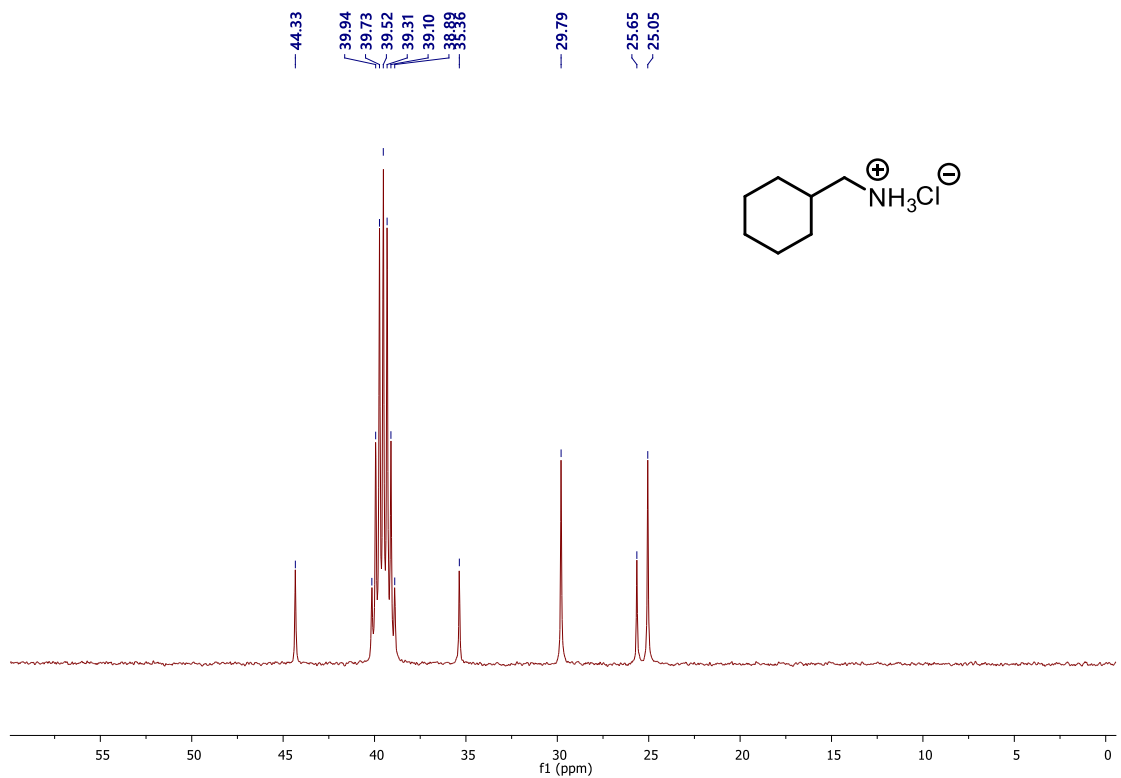


Fig. S91 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4ai** in DMSO-d_6 .^{S25}

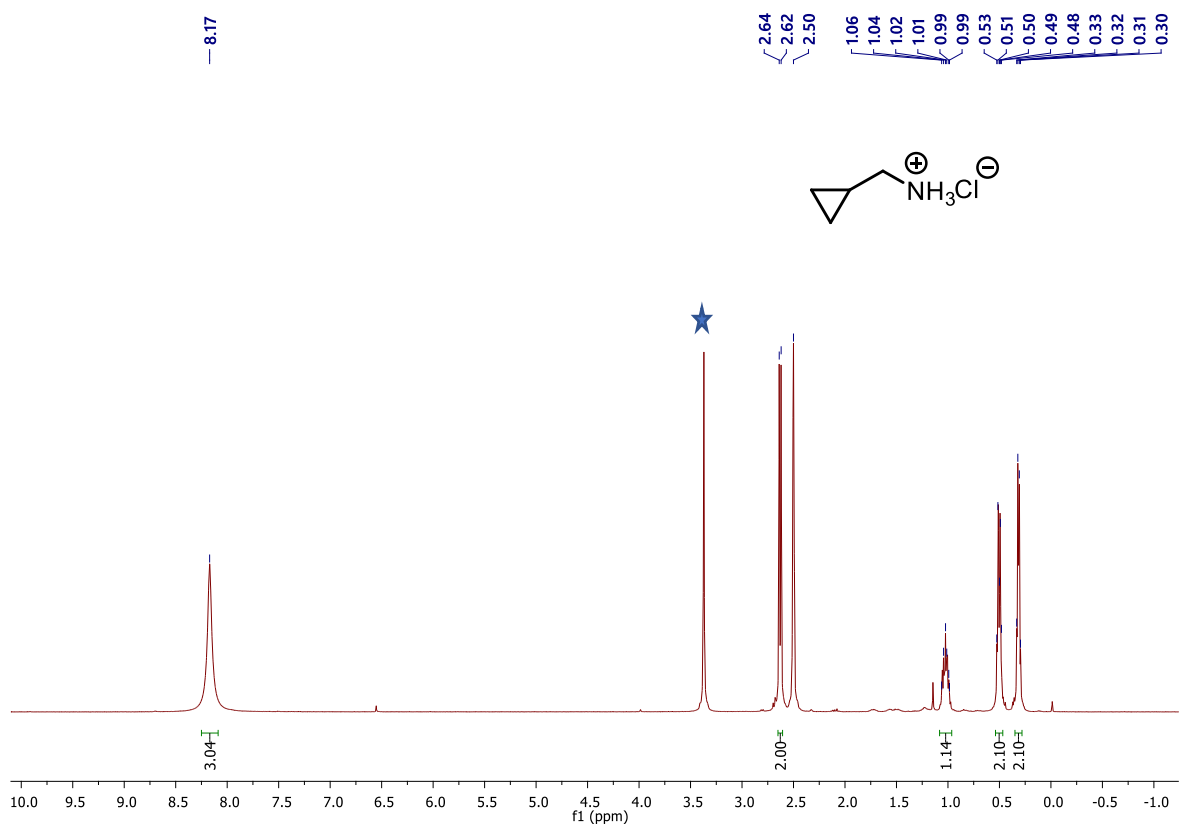


Fig. S92 ^1H NMR spectrum of **4aj** in DMSO-d_6 . ^{S12} ★ denotes moisture peak in DMSO-d_6 .

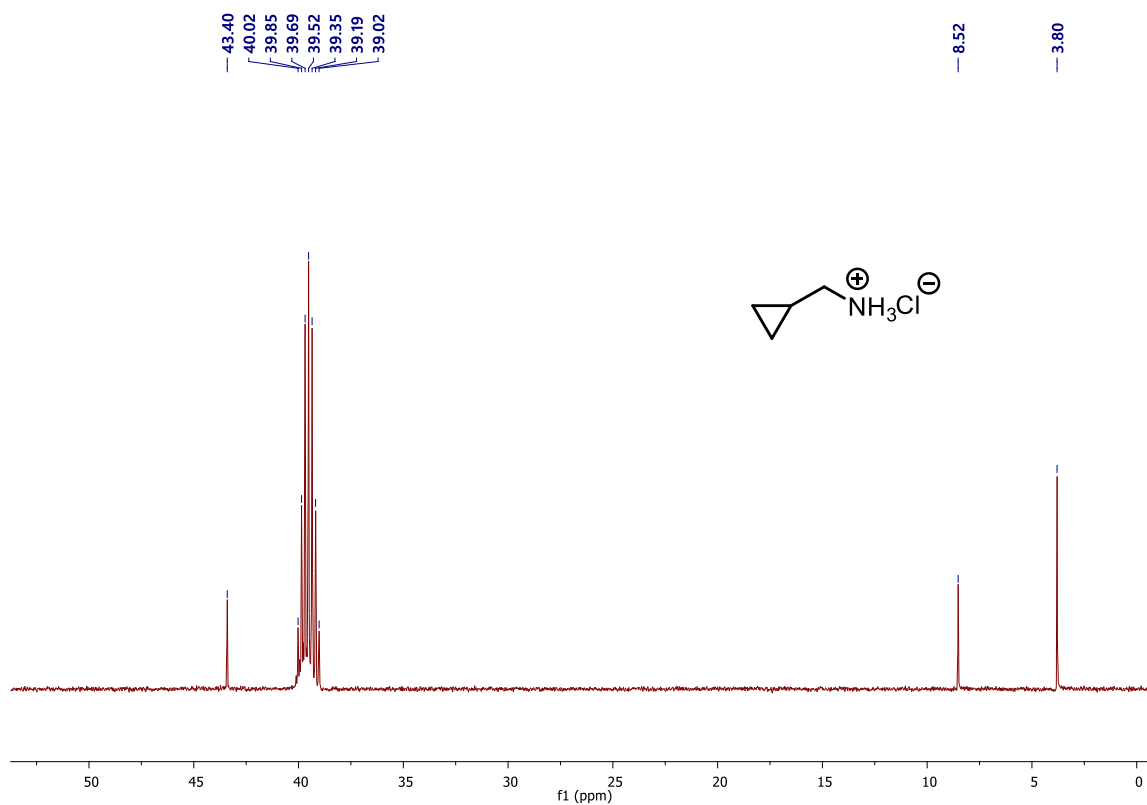


Fig. S93 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4aj** in DMSO-d_6 . ^{S12}

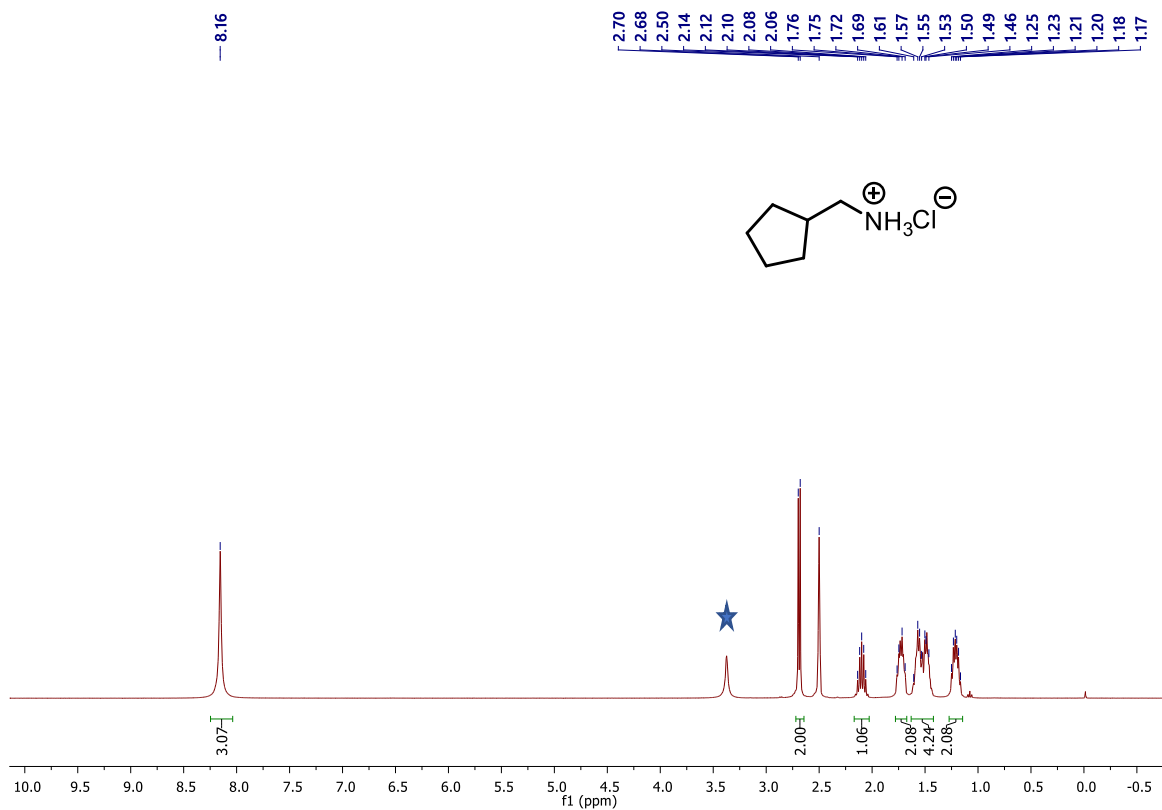


Fig. S94 ^1H NMR spectrum of **4ak** in DMSO-d_6 . ^{S25} ★ denotes moisture peak in DMSO-d_6 .

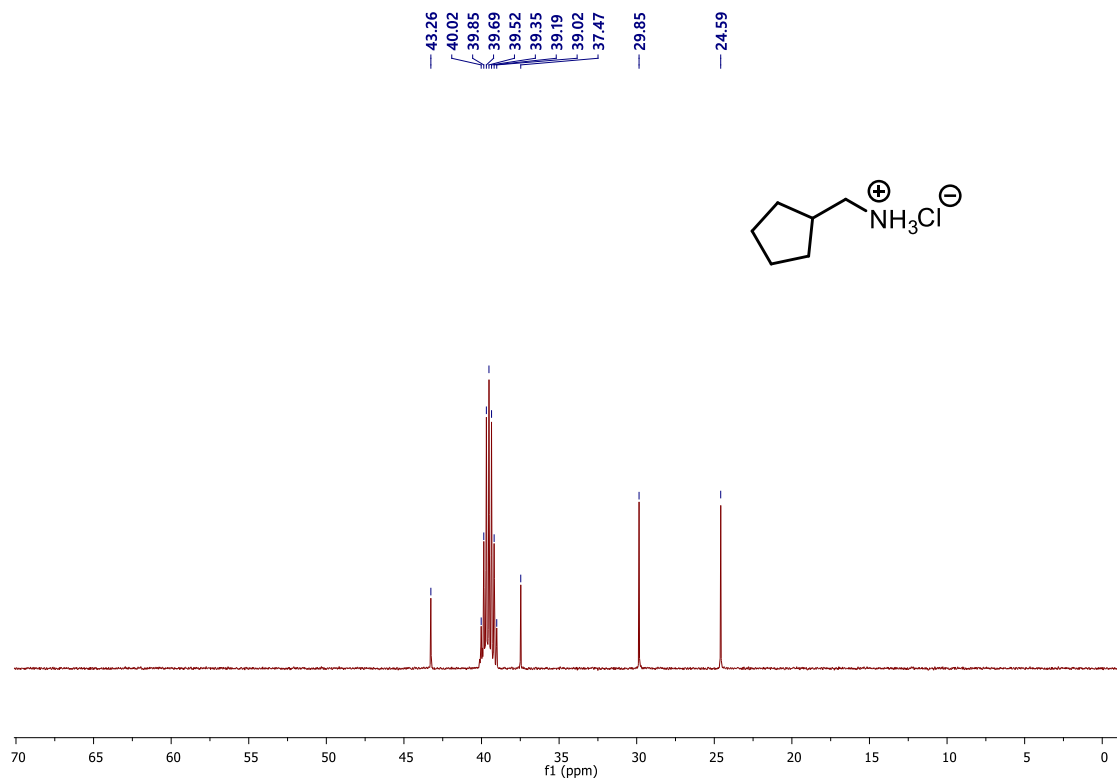


Fig. S95 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4ak** in DMSO-d_6 . ^{S25}

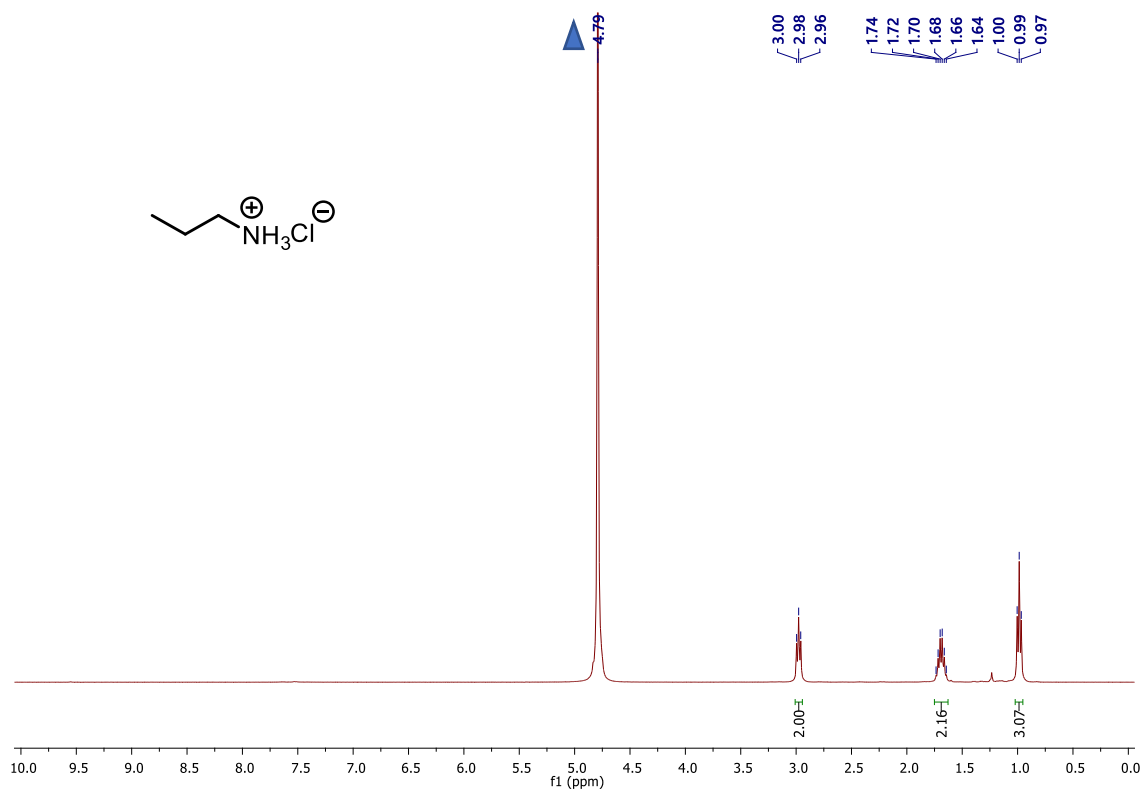


Fig. S96 ^1H NMR spectrum of **4al** in D_2O . ^{S26} ▲ denotes residual peak of D_2O .

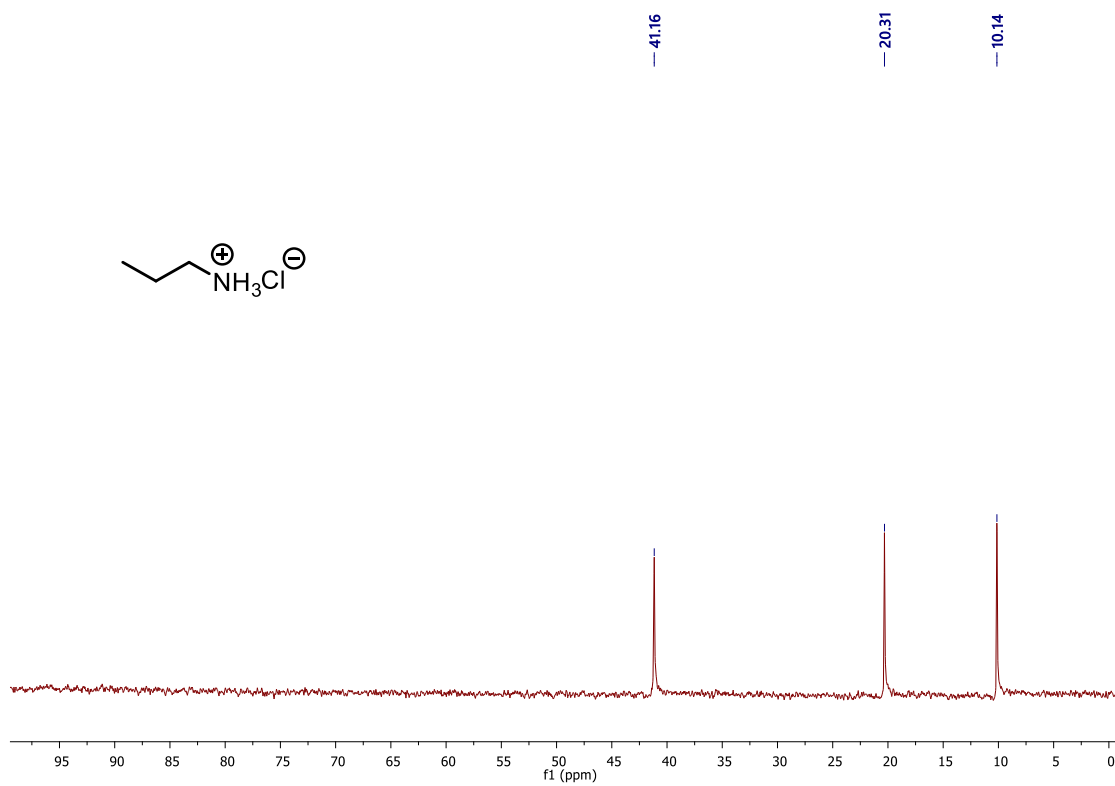


Fig. S97 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4al** in D_2O . ^{S26}

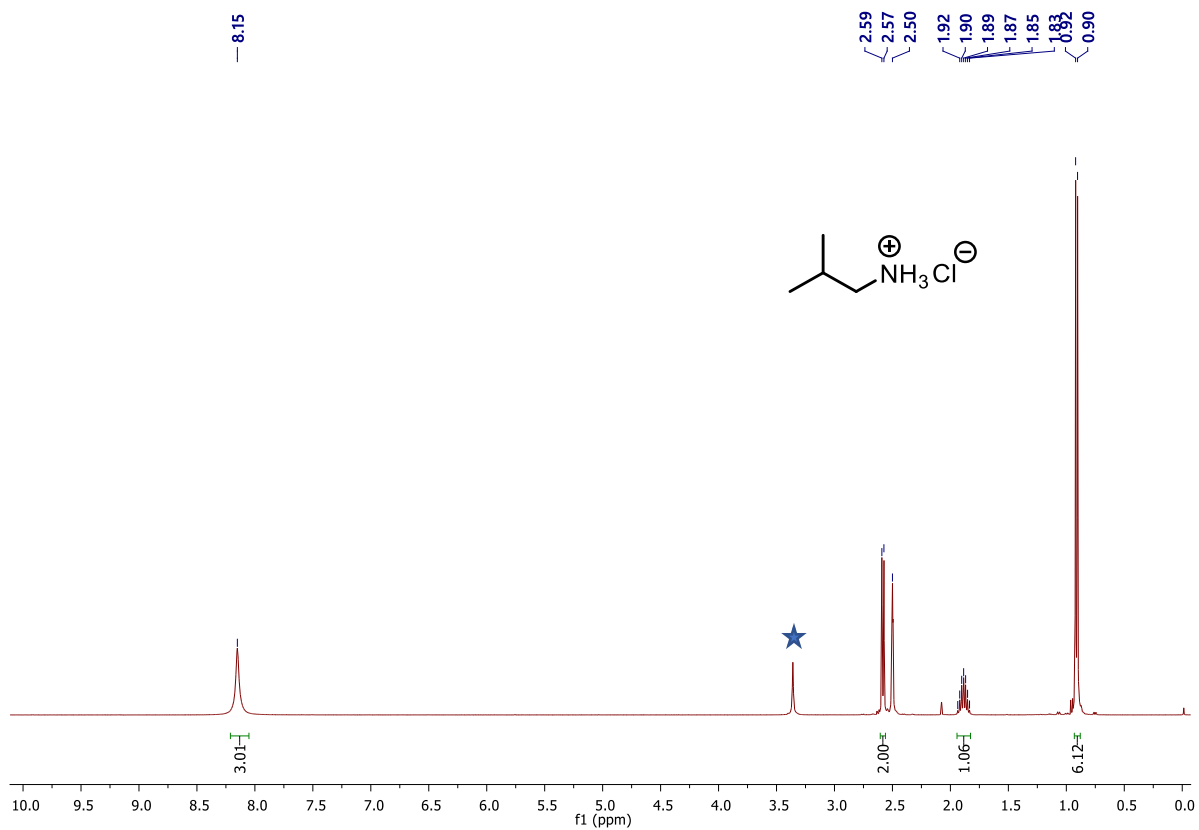


Fig. S98 ^1H NMR spectrum of **4am** in DMSO-d_6 . ^{S12} ★ denotes moisture peak in DMSO-d_6 .

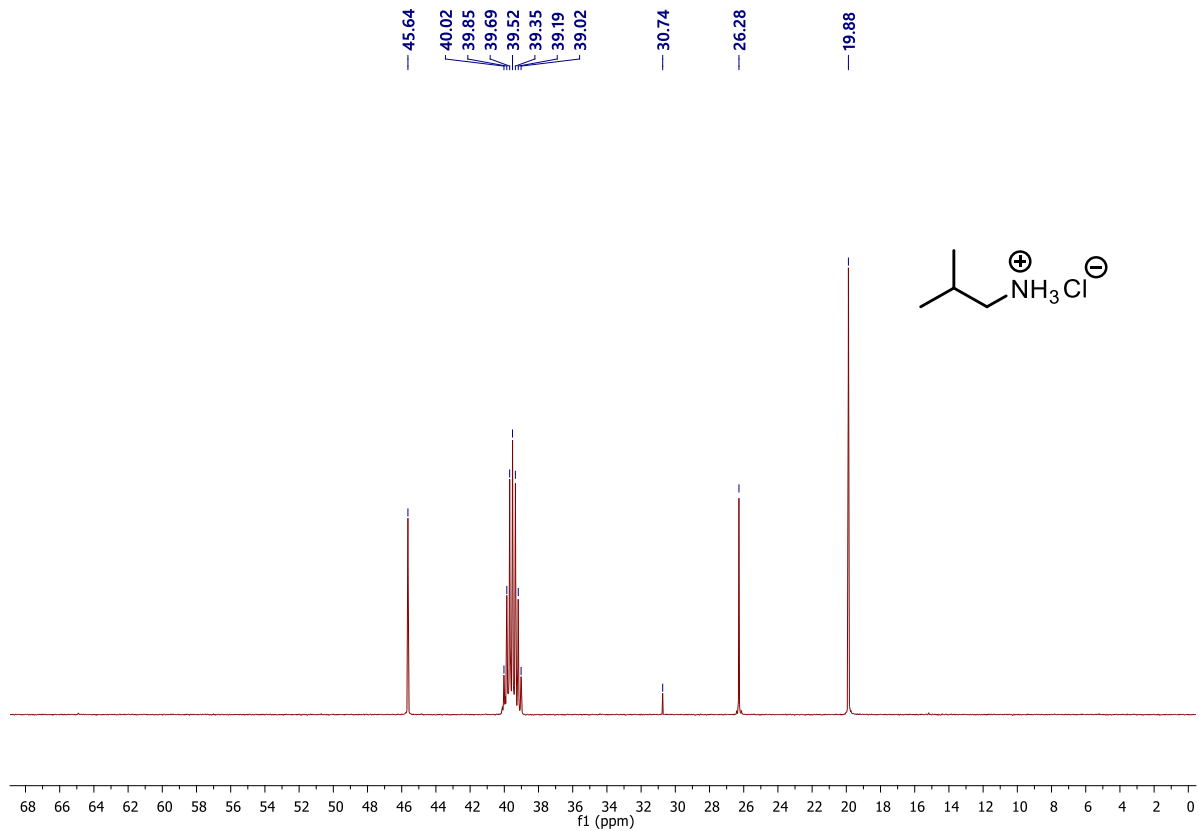


Fig. S99 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4am** in DMSO-d_6 . ^{S12}

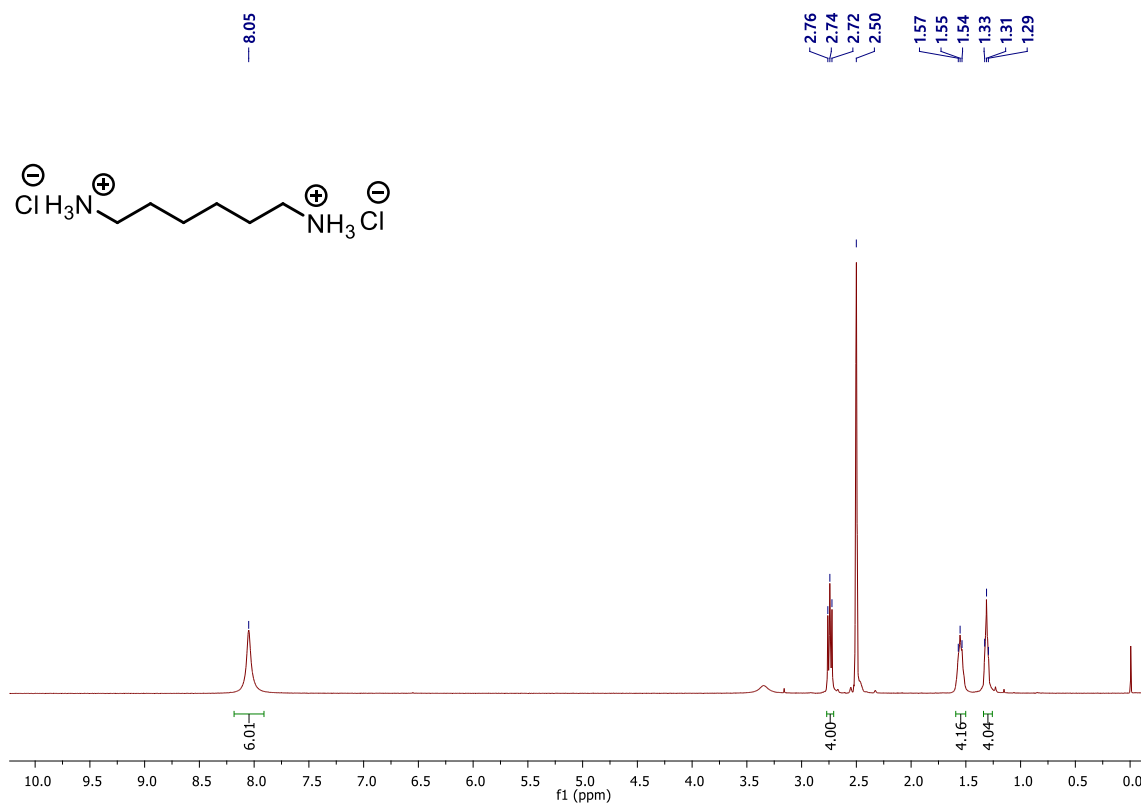


Fig. S100 ¹H NMR spectrum of **4an** in DMSO-d₆.^{S17}

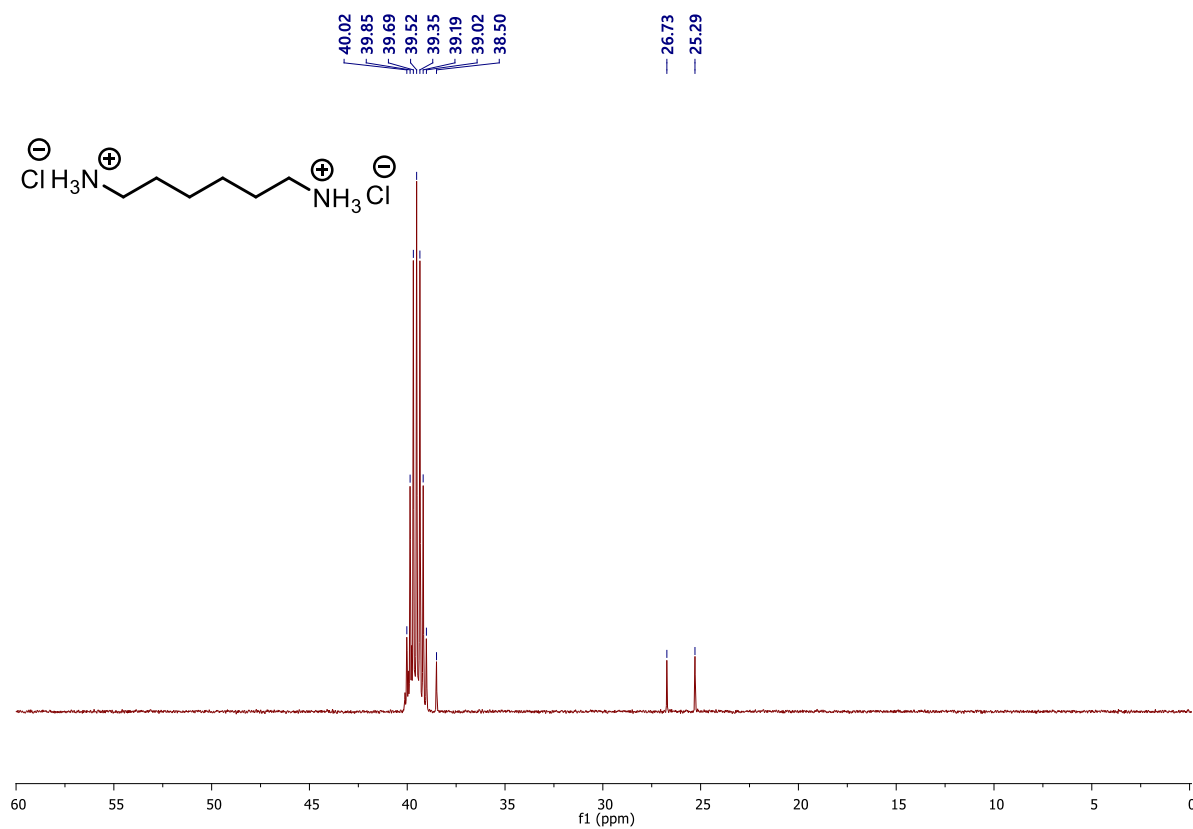
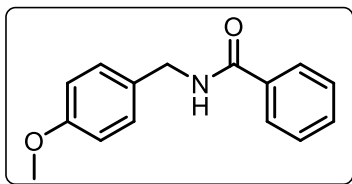
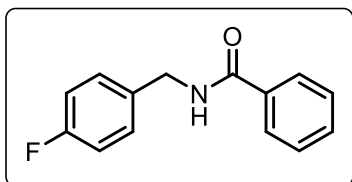


Fig. S101 ¹³C{¹H} NMR spectrum of **4an** in DMSO-d₆.^{S17}

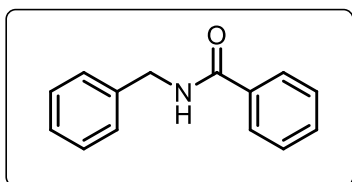
3.3) ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Data of N-substituted amide products



N-(4-methoxybenzyl)benzamide ($3c'$)^{S27}: ^1H NMR (500 MHz, CDCl_3 , 25 °C): δ = 7.80 (d, J = 7.5 Hz, 2H), 7.52-7.49 (m, 1H), 7.44-7.41 (m, 2H), 7.29 (d, J = 8.0 Hz, 2H), 6.89 (d, J = 8.0 Hz, 2H), 6.54 (br s, 1H), 4.58 (d, J = 5.5 Hz, 2H), 3.81 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C): δ = 167.4, 159.2, 134.6, 131.6, 130.4, 129.4, 128.7, 127.1, 114.3, 55.5, 43.7.



N-(4-fluorobenzyl)benzamide ($3f'$)^{S27}: ^1H NMR (400 MHz, CDCl_3 , 25 °C): δ = 7.79 (d, J = 7.2 Hz, 2H), 7.53-7.49 (m, 1H), 7.45-7.41 (m, 2H), 7.34-7.31 (m, 2H), 7.05-7.01 (m, 2H), 6.43 (br s, 1H), 4.60 (d, J = 5.6 Hz, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C): δ = 167.5, 162.4 (d, J = 244.2 Hz), 134.4, 134.2 (d, J = 3.4 Hz), 131.8, 129.7 (d, J = 7.9 Hz), 128.8, 127.1, 115.8 (d, J = 21.6 Hz), 43.5.



N-benzylbenzamide ($3h'$)^{S29}: ^1H NMR (400 MHz, CDCl_3 , 25 °C): δ = 7.71 (d, J = 7.2 Hz, 2H), 7.42 (t, J = 7.2 Hz, 1H), 7.33 (t, J = 7.2 Hz, 2H), 7.27-7.24 (m, 4H), 7.23-7.19 (m, 1H), 6.68 (br s, 1H), 4.54 (d, J = 6.0 Hz, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 25 °C): δ = 167.5, 138.3, 134.4, 131.6, 128.8, 128.6, 127.9, 127.6, 127.1, 44.1.

3.4) ^1H and ^{13}C NMR Spectra of N-substituted amide products

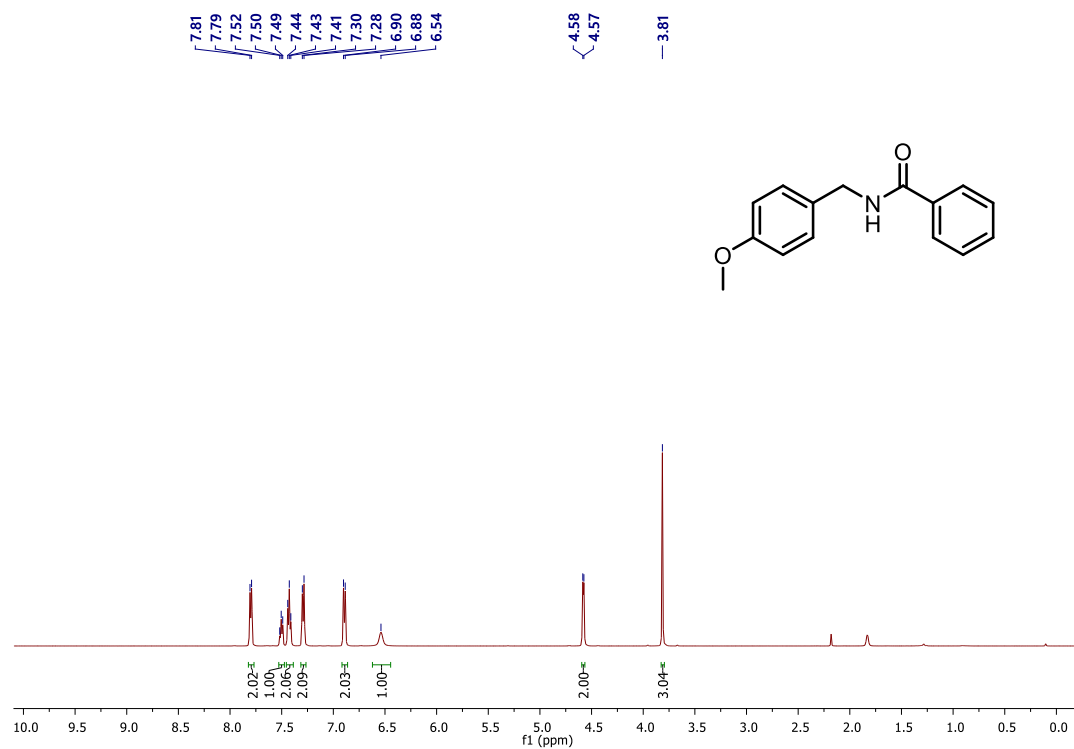


Fig. S102 ^1H NMR spectrum of **3c'** in CDCl_3 .^{S27}

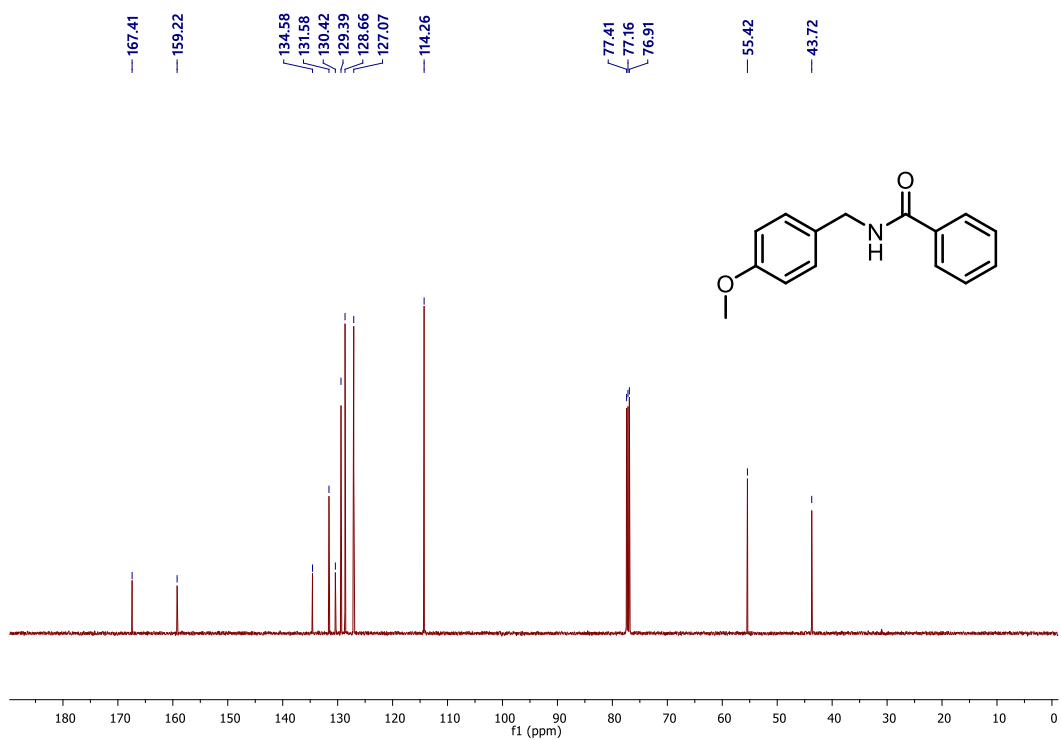


Fig. S103 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3c'** in CDCl_3 .^{S27}

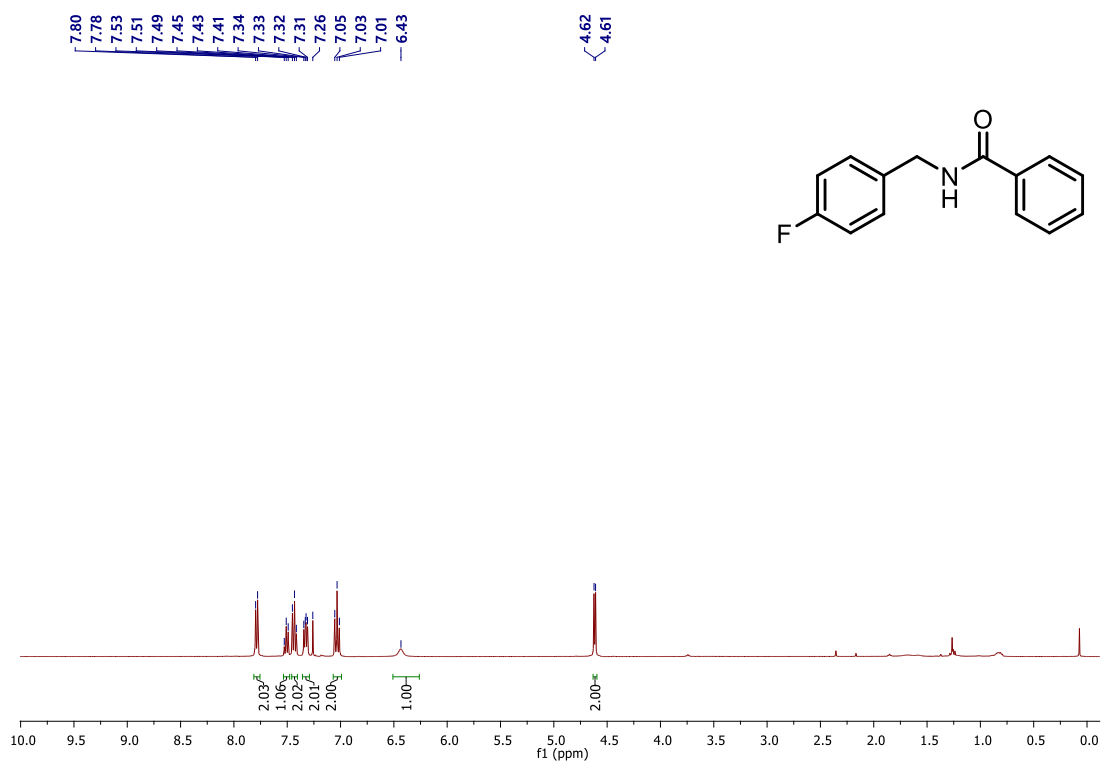


Fig. S104 $^1\text{H NMR}$ spectrum of **3f** in CDCl_3 .^{S27}

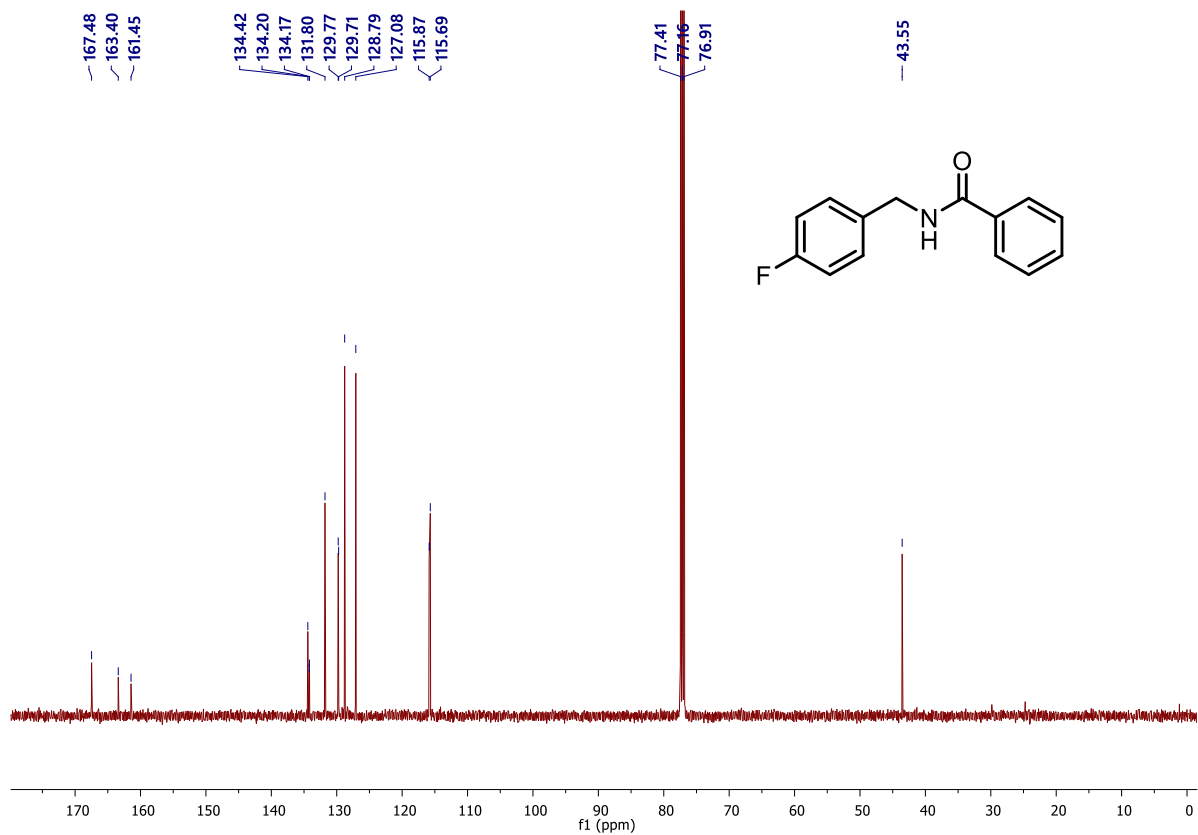


Fig. S105 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3f** in CDCl_3 .^{S27}

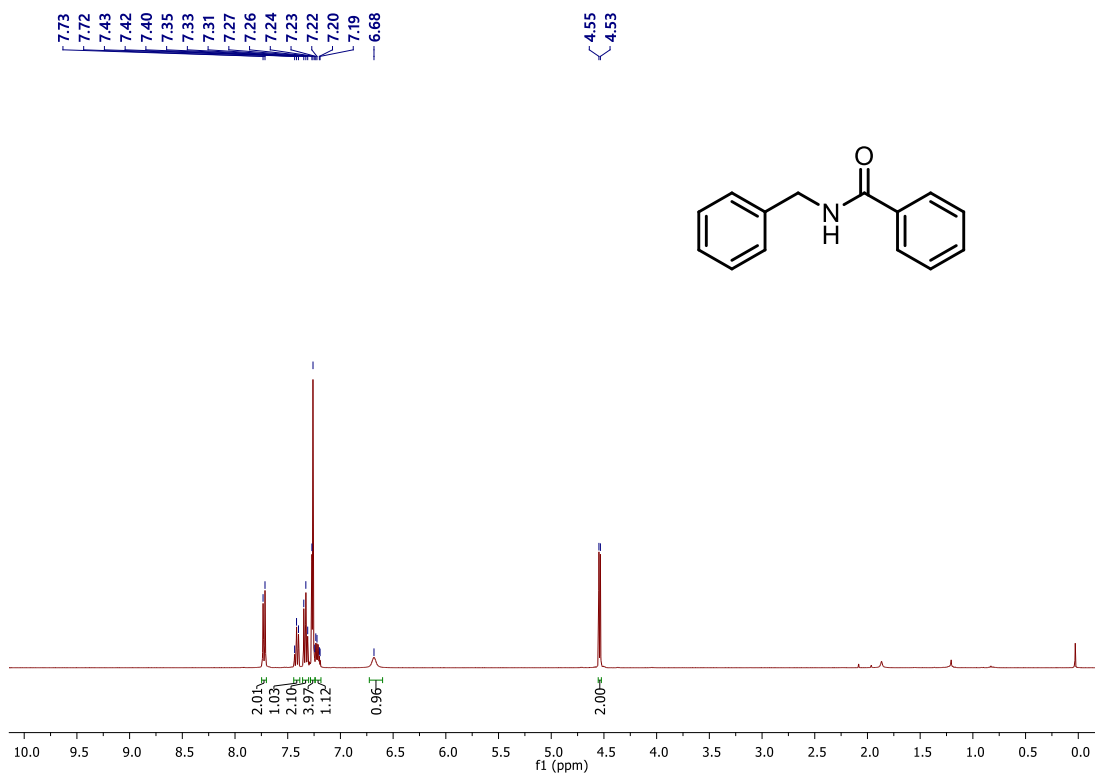


Fig. S106 ^1H NMR spectrum of **3h'** in CDCl_3 .^{S29}

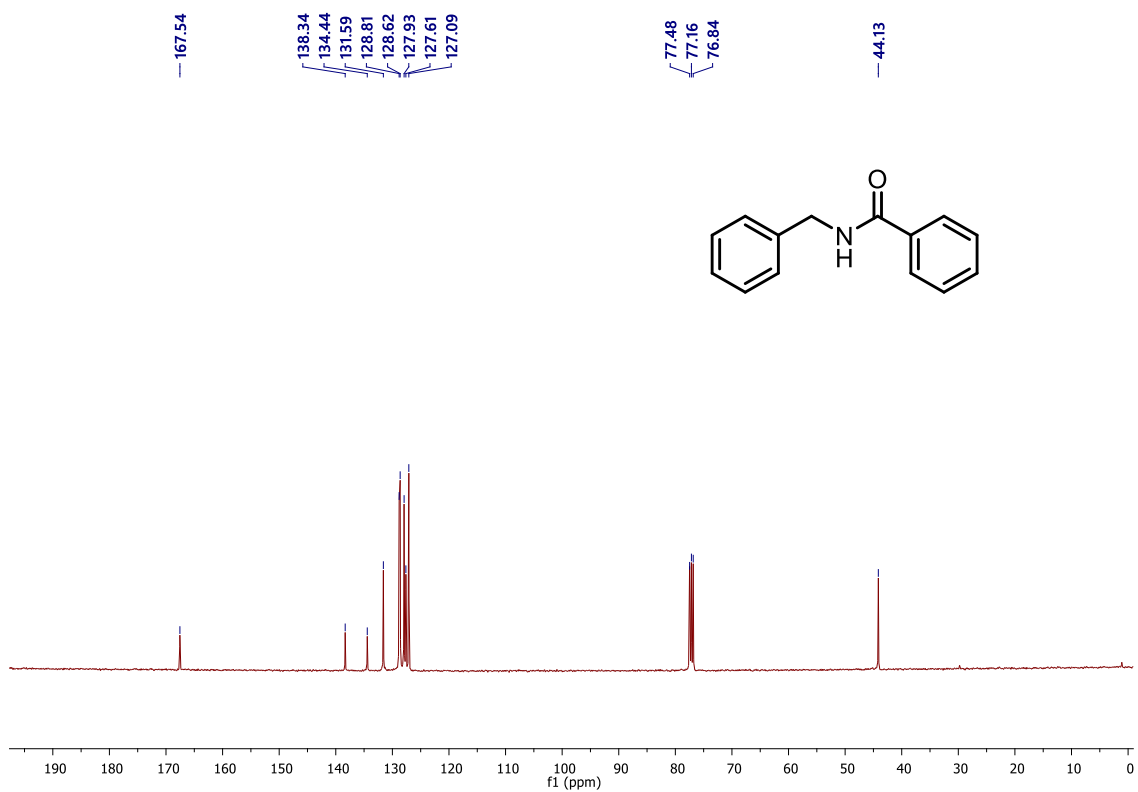


Fig. S107 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3h'** in CDCl_3 .^{S29}

4) DFT studies

For a better understanding of this reaction, particularly to know the role of the catalyst used here, a density functional theory (DFT) computation was carried out. Gaussian16 program package was employed for this calculation.^{S30, S31} M06-2X functional with 6-31G* basis was chosen for these calculations as this level of theory is proven as excellent for the main group elements.^{S32, S33} Geometries of all reactants, products, intermediates and transition states are optimized without any symmetry restriction. All optimized geometries are checked following frequency calculations. Transition states are verified by intrinsic reaction coordinate (IRC) calculations. The mechanistic investigation for the trans isomer is depicted in Fig. S108.

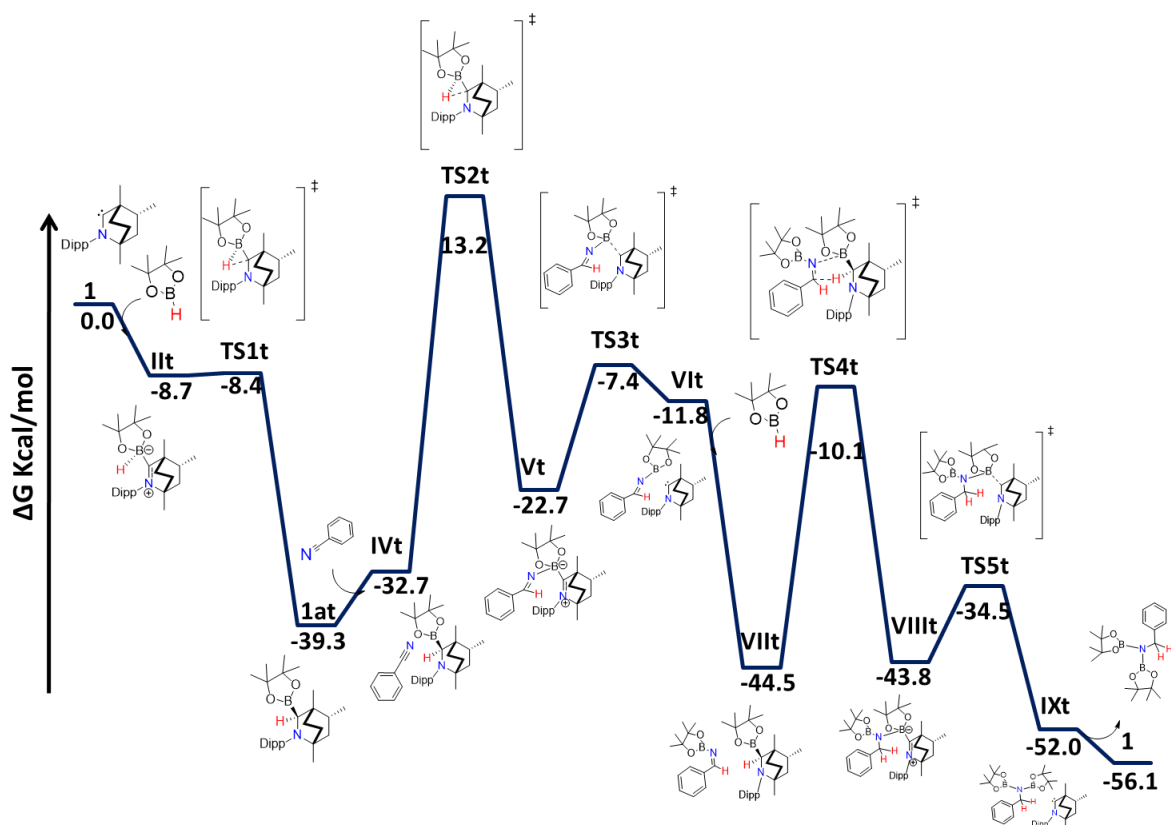


Fig. S108 Energy profile diagram of the reaction pathway for the trans isomer.

Z coordinates of the different complexes:

1

C	-3.10064500	0.32652800	0.20606200
C	-2.41543600	-0.79252800	-0.62808900
C	-0.96331900	-0.24208700	1.43914000

C	-2.20538100	0.66475900	1.42079500
H	-4.05454100	-0.08651500	0.56363000
H	-1.90101300	1.71636300	1.39700000
H	-2.74292700	0.51949700	2.36475700
C	-1.00054700	-0.37955400	-1.01635100
C	-1.49478100	-1.68443200	1.56237100
H	-0.67251700	-2.37898700	1.76152000
H	-2.15222700	-1.71892100	2.43829500
C	-2.25865800	-2.04445000	0.27513300
H	-1.72100000	-2.81190900	-0.29508900
H	-3.25100000	-2.45342900	0.49874700
N	-0.31710500	-0.12455900	0.08269500
C	-3.21802400	-1.14837900	-1.87572000
H	-3.19547000	-0.33119900	-2.60117400
H	-2.77969200	-2.02512300	-2.36301900
H	-4.26296100	-1.37440200	-1.62875300
C	-0.01460200	0.11656500	2.56976300
H	0.86387600	-0.53591300	2.57785400
H	0.33092000	1.15269100	2.49215800
H	-0.53992900	0.00029100	3.52335700
C	1.10074000	0.16938100	-0.02923400
C	1.52618700	1.50672100	-0.06815200
C	2.00959900	-0.89609900	-0.12086100
C	2.89573900	1.76202400	-0.14680800
C	3.37116600	-0.59312200	-0.20251700
C	3.81526300	0.72175500	-0.19972700
H	3.24791900	2.78833600	-0.17563200
H	4.09284000	-1.40103200	-0.27746700
H	4.87786400	0.93755700	-0.25692400
C	1.54895800	-2.33815000	-0.23859600

C	2.41700200	-3.31958300	0.55236300
C	1.47065700	-2.72495600	-1.72186400
H	0.53520500	-2.40293400	0.15940800
H	2.52190600	-3.01094600	1.59782200
H	1.96490100	-4.31624600	0.53141700
H	3.42052600	-3.41187700	0.12443500
H	0.78235700	-2.05318900	-2.24377600
H	2.45890400	-2.64954600	-2.18964900
H	1.11692600	-3.75627800	-1.83179200
C	0.52370500	2.64262400	-0.15102300
C	0.15119500	2.86605200	-1.62412600
C	1.00215400	3.94119400	0.49998000
H	-0.38365800	2.32784600	0.37081600
H	-0.22520900	1.93766500	-2.06722800
H	-0.61292500	3.64624800	-1.71671400
H	1.03488000	3.18253600	-2.18979300
H	1.34942100	3.77560000	1.52516800
H	1.81952500	4.39981800	-0.06614200
H	0.18294200	4.66625400	0.52678000
C	-3.40328700	1.58185000	-0.61449000
H	-4.11624000	1.38289500	-1.41895700
H	-3.83022500	2.36079500	0.02638500
H	-2.48574900	1.97928900	-1.06460800
IIC			
C	1.31219400	-3.13768400	0.24972000
C	0.57057200	-2.47635800	-0.95007800
C	2.52966900	-0.96324700	-0.16977000
C	2.44874800	-2.20574600	0.72825800
H	1.75207100	-4.06070400	-0.15074500

H	2.27995200	-1.89058000	1.76357200
H	3.41897600	-2.71396100	0.70392100
C	0.14486800	-1.07332800	-0.55321900
C	2.78188700	-1.43350400	-1.61629900
H	2.93724400	-0.56203800	-2.25955400
H	3.71943100	-2.00001200	-1.61516800
C	1.60287500	-2.29126600	-2.09397300
H	1.09169600	-1.82878400	-2.94448900
H	1.93307900	-3.28604000	-2.41387700
N	1.15738100	-0.34313000	-0.13886100
C	-0.57046800	-3.36063300	-1.44627300
H	-1.37355500	-3.44594300	-0.71581900
H	-1.01599500	-2.94468000	-2.35350100
H	-0.17059100	-4.35647400	-1.67341700
C	3.62507000	-0.00141500	0.26342500
H	3.68662800	0.86027900	-0.40588400
H	3.48047400	0.37526000	1.27629500
H	4.57922600	-0.53594400	0.22483600
H	-0.98125600	-0.48027000	-2.27153800
C	-3.03873400	0.83302200	-0.26344800
C	-3.30565700	-0.66159000	0.08939000
B	-1.31042100	-0.47704200	-1.06128900
O	-1.64188500	0.83170400	-0.51743700
O	-2.46248400	-1.33873100	-0.82576200
C	-3.33513600	1.82666100	0.85114300
H	-3.13626700	2.84350600	0.49864700
H	-4.38340300	1.76871200	1.16597500
H	-2.69365100	1.64485600	1.71587600
C	-3.77602300	1.24857300	-1.54070500
H	-4.85621600	1.33577100	-1.38166500

H	-3.39642900	2.22292900	-1.86389300
H	-3.59301800	0.52220700	-2.33869300
C	-2.83987700	-1.00290400	1.50801500
H	-3.46392000	-0.54600200	2.28420700
H	-2.86541600	-2.09041000	1.63499000
H	-1.80698700	-0.66216100	1.64456500
C	-4.74159600	-1.12228400	-0.12079300
H	-4.83779100	-2.17456700	0.16461200
H	-5.43750400	-0.53607900	0.49049600
H	-5.02675400	-1.02973600	-1.17086100
C	1.03345800	1.04806300	0.27211600
C	0.90354200	1.35665300	1.63643800
C	1.11749800	2.04212800	-0.71463600
C	0.90901700	2.70611700	1.99705100
C	1.11446800	3.37392400	-0.29907900
C	1.02390600	3.70884600	1.04455700
H	0.81343300	2.97301900	3.04580900
H	1.17486300	4.16043500	-1.04632900
H	1.02776600	4.75094800	1.34888100
C	1.16900600	1.74128500	-2.20467700
C	2.47623400	2.23247300	-2.83985600
C	-0.03960000	2.35673600	-2.92240800
H	1.10132600	0.65867100	-2.34609300
H	3.36068100	1.78713800	-2.37206000
H	2.49453400	1.98388900	-3.90612200
H	2.56818900	3.32033200	-2.75047000
H	-0.96451100	2.03036400	-2.44210600
H	0.00714100	3.45156700	-2.89763100
H	-0.04836400	2.04584300	-3.97222400
C	0.73001400	0.31452200	2.73424600

C	-0.46265100	0.64520900	3.64445700
C	1.97761500	0.17159600	3.61937000
H	0.52606600	-0.65010300	2.25803400
H	-1.35258700	0.90581000	3.07039300
H	-0.69987600	-0.21731200	4.27586400
H	-0.22892500	1.48438600	4.30820600
H	2.85404500	-0.18647800	3.07472700
H	2.23492300	1.13762200	4.06772500
H	1.78020900	-0.53432100	4.43324100
C	0.37200200	-3.51736800	1.39499400
H	-0.32413300	-4.30690900	1.10178100
H	0.94628800	-3.87641800	2.25542000
H	-0.22312900	-2.65517000	1.72032700

TS1c

C	-1.14628500	3.18915300	0.34460900
C	-0.41358100	2.51257500	-0.85223400
C	-2.52471200	1.13948300	-0.22034800
C	-2.39911400	2.35755200	0.71126200
H	-1.46964300	4.17040400	-0.02755400
H	-2.34558100	2.00698700	1.74865000
H	-3.31088000	2.95998600	0.62757000
C	-0.09894300	1.07806600	-0.42528600
C	-2.67793000	1.66578400	-1.65599100
H	-2.86116600	0.83103900	-2.33942600
H	-3.56905800	2.30265300	-1.68934000
C	-1.41048700	2.45157400	-2.03559600
H	-0.89675300	1.98764500	-2.88467000
H	-1.65690100	3.47907900	-2.32817400
N	-1.22801300	0.40154500	-0.11421600

C	0.79995800	3.33199200	-1.28078400
H	1.56552500	3.37866800	-0.50767000
H	1.26967300	2.89595200	-2.16658100
H	0.46719800	4.34815500	-1.52425400
C	-3.70863700	0.27321200	0.17928200
H	-3.81136000	-0.59983000	-0.47005500
H	-3.61951000	-0.08220400	1.20946100
H	-4.61935400	0.87449800	0.09843900
H	0.63906400	0.46802700	-1.78681900
C	3.03425500	-1.01358900	-0.18730900
C	3.55286200	0.45579600	-0.07920600
B	1.30883500	0.43722800	-0.58252600
O	1.61868400	-0.85150300	-0.06469300
O	2.50956600	1.20087900	-0.69879400
C	3.51706400	-1.94591000	0.91458600
H	3.06100800	-2.93145400	0.78179200
H	4.60628400	-2.06030300	0.87651100
H	3.23997000	-1.57511700	1.90376600
C	3.33483600	-1.62853800	-1.55556000
H	4.40529600	-1.80994000	-1.69441200
H	2.80965200	-2.58493300	-1.63467600
H	2.98319500	-0.97192500	-2.35888500
C	3.67580400	0.93628000	1.36888500
H	4.50605200	0.45439000	1.89546700
H	3.84854800	2.01669100	1.36169000
H	2.75098800	0.74486100	1.92175100
C	4.85573800	0.72474800	-0.82169300
H	5.14559400	1.77078900	-0.68458300
H	5.66366500	0.09217200	-0.43682000
H	4.74173600	0.54261800	-1.89211400

C	-1.21991400	-0.98980400	0.26920100
C	-1.11300300	-1.34429100	1.62229700
C	-1.35625500	-1.96392100	-0.73329100
C	-1.19279400	-2.69562400	1.96197100
C	-1.43034200	-3.30351900	-0.34860900
C	-1.36164200	-3.67107400	0.98856400
H	-1.11019900	-2.98620600	3.00624100
H	-1.53616300	-4.06999600	-1.11214200
H	-1.42534100	-4.71775300	1.27049900
C	-1.37790700	-1.61849800	-2.21304600
C	-2.68412500	-2.04605100	-2.89183600
C	-0.17045600	-2.24356500	-2.92093500
H	-1.27653700	-0.53383600	-2.31075800
H	-3.56016800	-1.58131800	-2.42790400
H	-2.67106200	-1.76468800	-3.95020600
H	-2.81693300	-3.13204800	-2.83812200
H	0.75237700	-1.94460000	-2.41901900
H	-0.23086100	-3.33789200	-2.91272100
H	-0.12831600	-1.91600400	-3.96511300
C	-0.83878000	-0.32293900	2.70877400
C	0.54514800	-0.58018800	3.31548800
C	-1.92169800	-0.29965900	3.79159100
H	-0.80863800	0.66175700	2.23789400
H	1.28161600	-0.67225600	2.51312200
H	0.83525100	0.23713500	3.98517600
H	0.55436500	-1.51122800	3.89377900
H	-2.90871400	-0.07144900	3.37588100
H	-1.99061300	-1.26626700	4.30223000
H	-1.68694900	0.45897500	4.54582100
C	-0.23333900	3.41981000	1.55095000

H	0.53495800	4.16759000	1.33877400
H	-0.81657600	3.77186500	2.40820900
H	0.27683600	2.49421900	1.84491800

1ac

C	-1.00136400	2.87495300	1.17374700
C	-0.46301800	2.71950700	-0.26960500
C	-2.52132600	1.16675600	0.08688200
C	-2.37045700	2.14594700	1.26873000
H	-1.16488300	3.95158600	1.32410300
H	-2.45345100	1.61222000	2.22211000
H	-3.19982800	2.86450500	1.23866000
C	-0.15649500	1.22668500	-0.58507100
C	-2.73012000	2.05716900	-1.15906900
H	-2.75058100	1.43576000	-2.06006400
H	-3.71494700	2.53258800	-1.08906000
C	-1.61100800	3.11932100	-1.22079100
H	-1.22026300	3.21593500	-2.24076700
H	-1.98975400	4.10748500	-0.92908400
N	-1.24499200	0.41773000	-0.02499000
C	0.75553700	3.59778000	-0.53751400
H	1.57352100	3.39848500	0.16277700
H	1.14212500	3.42094000	-1.54744900
H	0.48830400	4.65741200	-0.45229100
C	-3.70603200	0.23337900	0.26639200
H	-3.82527800	-0.42134600	-0.60376800
H	-3.58992300	-0.39487500	1.15191800
H	-4.61999800	0.82382700	0.38488300
H	-0.13639800	1.19822400	-1.69341800
C	2.91185300	-0.63425900	0.62798200

C	3.50679800	0.31288100	-0.46089200
B	1.28253000	0.69095400	-0.20971900
O	1.65054100	0.00757800	0.91898400
O	2.31682600	0.81082300	-1.10856300
C	3.72970600	-0.73180900	1.90525100
H	3.24697800	-1.42611500	2.59904000
H	4.73409900	-1.11103900	1.68732900
H	3.81789000	0.23898600	2.39736600
C	2.57427300	-2.02524800	0.09492500
H	3.47755600	-2.61199000	-0.09962900
H	1.96394500	-2.54671700	0.83826100
H	1.98445200	-1.96095400	-0.82661300
C	4.22681300	1.52043700	0.13577400
H	5.18558300	1.23764700	0.58074500
H	4.40983900	2.24951500	-0.65829500
H	3.61114400	1.99764800	0.90553900
C	4.37788600	-0.37663800	-1.49767700
H	4.74482700	0.35996400	-2.21786600
H	5.24219900	-0.85048700	-1.01984400
H	3.81442500	-1.13740400	-2.04206400
C	-1.15472200	-1.00864300	-0.13288800
C	-1.12644500	-1.79770400	1.04687200
C	-1.01309400	-1.65245200	-1.38536700
C	-0.91632500	-3.17371000	0.94797100
C	-0.76928600	-3.02946600	-1.43252200
C	-0.71525700	-3.79350000	-0.27816100
H	-0.89073900	-3.76953600	1.85726200
H	-0.64096300	-3.51022400	-2.39935500
H	-0.53325300	-4.86272100	-0.33234200
C	-1.15128900	-0.93010600	-2.71682400

C	-2.28278800	-1.53118700	-3.56064400
C	0.16926000	-0.92749800	-3.49759400
H	-1.42917400	0.10311900	-2.51452600
H	-3.22744500	-1.53448200	-3.00748800
H	-2.42198900	-0.94751700	-4.47688300
H	-2.06320900	-2.56296200	-3.85407200
H	0.97516900	-0.46019400	-2.92119000
H	0.47595700	-1.95145500	-3.74088600
H	0.05945700	-0.37997100	-4.43996300
C	-1.31352800	-1.21882300	2.44027800
C	-0.04899900	-1.36743700	3.29675400
C	-2.49678800	-1.86956400	3.17307000
H	-1.51504100	-0.15262100	2.32759000
H	0.80009100	-0.86983000	2.82585400
H	-0.21100400	-0.92944400	4.28821900
H	0.20129100	-2.42610000	3.43797000
H	-3.41444700	-1.86129700	2.57812300
H	-2.27676400	-2.91426900	3.41931800
H	-2.69220400	-1.34511100	4.11444300
C	-0.03857100	2.39250600	2.25842800
H	0.13851400	1.31715300	2.17728100
H	0.92999400	2.90213300	2.20920100
H	-0.46373900	2.59177600	3.24846500
IVc			
C	1.05545400	-0.83795100	3.20163800
C	0.07382000	0.17633000	2.56632200
C	-0.19669700	-2.15501700	1.43912500
C	0.68077100	-2.26106600	2.70290400
H	0.88504000	-0.78935100	4.28658400

H	1.58480700	-2.84462100	2.49542000
H	0.12284300	-2.81166100	3.47181700
C	0.25586000	0.22730300	1.02188400
C	-1.56575700	-1.63204500	1.92604300
H	-2.19617600	-1.42235200	1.05453200
H	-2.06914000	-2.42432300	2.49343100
C	-1.34902600	-0.37769500	2.80023700
H	-2.07810900	0.40669200	2.56460300
H	-1.46886300	-0.61696400	3.86505300
N	0.43286900	-1.15199000	0.54643400
C	0.18707700	1.57087300	3.17508300
H	1.20117800	1.97645400	3.09061500
H	-0.49155800	2.26503100	2.66749700
H	-0.07685300	1.54337800	4.23894000
C	-0.36858700	-3.49798400	0.75019200
H	-1.03546900	-3.41348800	-0.11484000
H	0.58713300	-3.89693200	0.40499100
H	-0.80160700	-4.21458700	1.45542500
H	-0.69015500	0.68326200	0.66975300
C	3.07881300	2.00617200	-0.76658900
C	2.20463900	3.19731100	-0.26299400
B	1.34061600	1.22494700	0.45089800
O	2.62974300	0.93082100	0.08672100
O	1.00314700	2.52640600	0.16823200
C	4.57668200	2.19338400	-0.58929700
H	5.10622500	1.32141600	-0.98410900
H	4.91842400	3.07742900	-1.13872100
H	4.84158700	2.30818600	0.46384300
C	2.75308200	1.58501900	-2.19852800
H	3.12276800	2.31423400	-2.92641800

H	3.2225400	0.61594900	-2.39421800
H	1.67298900	1.46015500	-2.33596100
C	2.79533300	3.88558700	0.96589300
H	3.67230600	4.48712400	0.70785200
H	2.03506100	4.53946100	1.40150100
H	3.08679800	3.14743700	1.72059100
C	1.84099600	4.21711600	-1.32929000
H	1.22431400	5.00461000	-0.88749300
H	2.74377400	4.67756600	-1.74531200
H	1.27497600	3.75349200	-2.14000700
C	0.67701000	-1.36988100	-0.84744400
C	1.87388200	-2.02172700	-1.24876400
C	-0.20502600	-0.89203700	-1.84599500
C	2.16923400	-2.14515600	-2.60645000
C	0.15192700	-1.01036400	-3.19470400
C	1.32855600	-1.62851400	-3.58319100
H	3.09050800	-2.64113900	-2.90268100
H	-0.52263500	-0.62360000	-3.95456400
H	1.58361700	-1.71791400	-4.63500200
C	-1.56509800	-0.26811300	-1.55725900
C	-2.69412500	-1.06536300	-2.22350500
C	-1.59813300	1.20346900	-1.99081500
H	-1.75052800	-0.30965600	-0.48352900
H	-2.67341200	-2.11360000	-1.90682000
H	-3.66764000	-0.64264100	-1.95098000
H	-2.61455000	-1.04403400	-3.31555600
H	-0.87910700	1.80456400	-1.42318600
H	-1.36074800	1.29753700	-3.05682900
H	-2.59477000	1.63040600	-1.83596200
C	2.87964000	-2.59761900	-0.26392900

C	4.21780700	-1.84804200	-0.31340800
C	3.13289100	-4.09287400	-0.51050200
H	2.46688900	-2.47266300	0.73792900
H	4.07813400	-0.78999300	-0.08746000
H	4.91771300	-2.27634700	0.41317900
H	4.67411100	-1.93605300	-1.30714000
H	2.20716400	-4.67244200	-0.56825400
H	3.67416800	-4.24797700	-1.45041300
H	3.74911100	-4.50823100	0.29402500
C	-3.51414000	1.99130500	0.76477100
C	-4.51613000	1.10951600	0.22410500
C	-5.25679000	1.50475500	-0.89531800
C	-4.73045400	-0.14043400	0.81446800
C	-6.20688400	0.64044800	-1.42618400
H	-5.07834600	2.47880600	-1.33897900
C	-5.67882600	-0.99902200	0.27042500
H	-4.15614700	-0.42579200	1.68998400
C	-6.41483700	-0.61056800	-0.84737500
H	-6.78234200	0.94170400	-2.29519100
H	-5.84327300	-1.97223300	0.72087800
H	-7.15341700	-1.28484200	-1.26902700
N	-2.70127900	2.69509400	1.19462800
C	2.53007300	-0.52902500	2.94582200
H	2.76696100	-0.59685300	1.88114700
H	2.80826900	0.47185300	3.29353500
H	3.16017600	-1.24929600	3.47975800

TS2c

C	-0.72355400	-1.35715000	-2.97492500
C	0.57809000	-0.82760000	-2.30353900

C	-0.53611200	-2.64691300	-0.83256700
C	-1.16087600	-2.64279300	-2.24069200
H	-0.44188000	-1.62431900	-4.00189800
H	-2.25056500	-2.72980700	-2.21014600
H	-0.79941000	-3.53584600	-2.76594700
C	0.24036800	-0.33272200	-0.85994100
C	0.95961300	-2.97017300	-1.04978200
H	1.48884300	-2.84193000	-0.09793000
H	1.05670800	-4.02541900	-1.32579100
C	1.51278000	-2.04967400	-2.14933800
H	2.52722700	-1.71023100	-1.91224100
H	1.57018300	-2.57483900	-3.11110800
N	-0.61450500	-1.26262200	-0.26342600
C	1.23553500	0.21870800	-3.20740500
H	0.68856400	1.16447900	-3.20675300
H	2.26657100	0.42582700	-2.91067800
H	1.26464800	-0.17143100	-4.23162900
C	-1.15331000	-3.68654600	0.08539600
H	-0.67194100	-3.68123200	1.06837200
H	-2.22178000	-3.53095100	0.22550800
H	-1.01384300	-4.67526200	-0.36264200
H	1.43099300	-0.34596500	-0.34101100
C	-1.43040300	3.09404200	-0.83796700
C	-0.82847500	3.07907900	0.60871600
B	0.08478300	1.36044700	-0.59241800
O	-0.63576200	2.13054200	-1.54041500
O	-0.32848500	1.74588500	0.71022000
C	-1.33369500	4.43285900	-1.55704100
H	-1.78404200	4.34582800	-2.55057800
H	-1.87130200	5.21173300	-1.00435100

H	-0.29338400	4.74060300	-1.68046100
C	-2.86789300	2.59031400	-0.84787000
H	-3.56532400	3.31583100	-0.41567700
H	-3.16718600	2.38698400	-1.88150700
H	-2.92752100	1.66164900	-0.27397200
C	0.32735300	4.07028200	0.78255800
H	-0.03914600	5.10200000	0.80773900
H	0.82659400	3.85724200	1.73320800
H	1.06468800	3.97535700	-0.01701900
C	-1.84118000	3.28899000	1.72823600
H	-1.32096100	3.26344900	2.69096300
H	-2.33877000	4.26070100	1.63087000
H	-2.59251700	2.49631000	1.73470900
C	-1.30447400	-0.96947400	0.97937100
C	-2.71796700	-0.85438900	1.01631600
C	-0.56169200	-0.75095400	2.15817200
C	-3.31827800	-0.37499400	2.18377100
C	-1.21206200	-0.29149900	3.30398900
C	-2.57852900	-0.06630400	3.31545300
H	-4.39955800	-0.26454900	2.20766600
H	-0.62926600	-0.10494900	4.20188100
H	-3.06895300	0.31296500	4.20691600
C	0.92816700	-1.02816200	2.26909300
C	1.19133700	-2.22951400	3.18731800
C	1.71187200	0.19618200	2.75935800
H	1.29624200	-1.29613700	1.27881100
H	0.67365500	-3.12868900	2.83805700
H	2.26529200	-2.44499700	3.22968500
H	0.84997900	-2.02409100	4.20771900
H	1.46736000	1.07810900	2.16170900

H	1.46964400	0.41709600	3.80500100
H	2.78950700	0.00486300	2.70748900
C	-3.66949300	-1.36697200	-0.06321000
C	-4.62934100	-0.32802100	-0.65968600
C	-4.52959700	-2.50968100	0.51640600
H	-3.07045900	-1.76216600	-0.88126000
H	-4.13094300	0.35836000	-1.34235000
H	-5.41581700	-0.84336300	-1.22191100
H	-5.11536100	0.26336800	0.12418700
H	-3.95282200	-3.21111000	1.12433900
H	-5.31745000	-2.10079400	1.15829900
H	-5.01806600	-3.06480700	-0.29161500
C	2.42299000	0.78185300	-0.37151400
C	3.77732600	0.32358300	-0.07744000
C	4.80894400	1.26719500	-0.16441700
C	4.05889600	-0.99262300	0.29039200
C	6.11474200	0.88453600	0.11355000
H	4.56676300	2.28617300	-0.44789900
C	5.36870100	-1.36655700	0.57193600
H	3.25003100	-1.71395500	0.35862100
C	6.39601500	-0.43057100	0.48229600
H	6.91515700	1.61416300	0.04439400
H	5.58607600	-2.38969800	0.86059100
H	7.41766200	-0.72499500	0.70074800
N	1.75505300	1.73410800	-0.65733600
C	-1.84040000	-0.31741200	-3.05015600
H	-2.72330400	-0.74944700	-3.53621200
H	-2.12649500	0.02488500	-2.05249100
H	-1.53044800	0.56739600	-3.61243600

Vc

C	-0.94064600	-1.90749100	-2.79744800
C	0.31807500	-1.32115100	-2.08446200
C	-1.09834300	-2.68694000	-0.39682400
C	-1.66263700	-2.86164000	-1.82072300
H	-0.55365500	-2.50688500	-3.63011700
H	-2.74805200	-2.72932900	-1.83460400
H	-1.48151700	-3.90578000	-2.10022400
C	-0.19032700	-0.51326000	-0.89248200
C	0.34718400	-3.22907300	-0.42852000
H	0.81604900	-3.06630100	0.54709300
H	0.29566800	-4.31192800	-0.58139100
C	1.12807900	-2.53267800	-1.55244700
H	2.11332300	-2.20313500	-1.21322200
H	1.29246400	-3.20877100	-2.39982500
N	-0.98255100	-1.20970500	-0.10813500
C	1.14468700	-0.51342800	-3.08895400
H	0.67870700	0.45002600	-3.30711300
H	2.14730900	-0.30950900	-2.71105200
H	1.23128800	-1.09192400	-4.01659200
C	-1.92620900	-3.40773500	0.64914200
H	-1.45896900	-3.34885200	1.63506000
H	-2.93556100	-3.00143700	0.72275200
H	-1.99833500	-4.46197900	0.36551400
H	2.01049800	-0.77334500	0.74416400
C	-0.43650000	3.17130100	-1.02311900
C	0.03129100	3.01827500	0.46678600
B	0.41245600	1.02801200	-0.60839400
O	-0.01012800	1.96105600	-1.64337800
O	-0.00849800	1.60905600	0.65039500

C	0.18444800	4.35153600	-1.76343500
H	-0.21130000	4.38953000	-2.78331800
H	-0.05458800	5.29976600	-1.26765400
H	1.26931000	4.24576900	-1.82453000
C	-1.95770500	3.24608500	-1.11867900
H	-2.34921200	4.20718300	-0.76752900
H	-2.25301300	3.11088600	-2.16456400
H	-2.40215600	2.44815600	-0.51708500
C	1.45925000	3.53363200	0.68949700
H	1.49783600	4.62755600	0.64571600
H	1.79505200	3.21729200	1.68276000
H	2.15138600	3.12070000	-0.04845300
C	-0.89240400	3.65019500	1.50334200
H	-0.47148700	3.48959900	2.50162500
H	-0.99144100	4.72978300	1.34229000
H	-1.88314300	3.19007800	1.48109100
C	-1.75848400	-0.58793300	0.97719400
C	-3.06010500	-0.12748600	0.69221900
C	-1.20258000	-0.45596200	2.26131800
C	-3.73828500	0.57846700	1.68890100
C	-1.93169700	0.24460200	3.22275100
C	-3.17591700	0.78637500	2.93912100
H	-4.73637300	0.95337800	1.47888400
H	-1.50217900	0.37634000	4.21171900
H	-3.71618300	1.34538100	3.69688700
C	0.13648200	-1.03647700	2.68011700
C	-0.03668900	-2.08569700	3.78898000
C	1.11778500	0.04750200	3.14644100
H	0.57238500	-1.53769000	1.81272000
H	-0.73171900	-2.88344500	3.51112200

H	0.93025700	-2.54038900	4.02811700
H	-0.41940400	-1.62141000	4.70392200
H	1.19755900	0.84007100	2.40067200
H	0.77882900	0.48824800	4.09104000
H	2.10676000	-0.39131700	3.32203100
C	-3.83368800	-0.46501300	-0.57635800
C	-4.35729800	0.74458300	-1.35732200
C	-5.02414300	-1.38068500	-0.24099700
H	-3.16687800	-1.00480800	-1.24356500
H	-3.55039700	1.31689900	-1.81244100
H	-5.02159700	0.40053300	-2.15749700
H	-4.93173100	1.42116100	-0.71539700
H	-4.74146100	-2.23993600	0.37235100
H	-5.78986500	-0.82451300	0.31045900
H	-5.48341300	-1.75292800	-1.16299100
C	2.54145200	-0.05747300	0.08662000
C	4.01546500	-0.23615500	0.11646600
C	4.84985600	0.57669600	-0.65736500
C	4.57731300	-1.23557800	0.91233100
C	6.22549000	0.39047500	-0.62765100
H	4.38765300	1.34546200	-1.26988600
C	5.95678300	-1.42423500	0.94242100
H	3.92310300	-1.86620400	1.51303500
C	6.78216800	-0.61005500	0.17193200
H	6.87135300	1.02440900	-1.22800800
H	6.38674400	-2.20296800	1.56519000
H	7.85844500	-0.75280700	0.19288600
N	1.95583500	0.79863100	-0.63028300
C	-1.81713200	-0.79678400	-3.39280500
H	-2.81654200	-1.17102400	-3.64130200

H	-1.92160600	0.05543100	-2.71173000
H	-1.36657500	-0.40923600	-4.31018400

TS3c

C	-1.42613000	-1.74204300	-2.87629400
C	-0.07091400	-1.22081300	-2.29955400
C	-1.23396700	-2.71877000	-0.54777100
C	-1.99336300	-2.78541400	-1.88783300
H	-1.17281700	-2.24654700	-3.81812800
H	-3.06863100	-2.64849200	-1.73471600
H	-1.86750300	-3.80358700	-2.27464400
C	-0.34876900	-0.48983000	-0.98486700
C	0.18921200	-3.25107100	-0.82209500
H	0.80511500	-3.09599600	0.07094000
H	0.13251600	-4.33083400	-0.99613300
C	0.76023000	-2.51113200	-2.03894300
H	1.81977200	-2.27756600	-1.91303400
H	0.69247000	-3.13135300	-2.94126300
N	-1.04311300	-1.26786600	-0.17389600
C	0.64162700	-0.30593200	-3.29081200
H	0.10218900	0.63548600	-3.41995100
H	1.63949000	-0.04284500	-2.92737800
H	0.74783600	-0.79949300	-4.26466400
C	-1.92036600	-3.52862200	0.53648600
H	-1.37827900	-3.48137200	1.48435600
H	-2.94037900	-3.18655600	0.71107900
H	-1.96385300	-4.57369500	0.21393500
H	2.15579400	-0.83902000	-0.67886100
C	-0.62758300	3.28161500	-1.16972600
C	-0.52433800	3.27108400	0.39360100

B	0.81047800	1.65965500	-0.48639900
O	0.49183900	2.48192400	-1.56447100
O	0.08869100	2.00476300	0.65879300
C	-0.49816500	4.65764700	-1.80670900
H	-0.58473500	4.56626300	-2.89340100
H	-1.29283800	5.32437500	-1.45325900
H	0.46981700	5.10854600	-1.57969300
C	-1.88167700	2.57820500	-1.67123400
H	-2.79153200	3.14653100	-1.45079600
H	-1.80549100	2.44166200	-2.75481500
H	-1.94021100	1.59163000	-1.20291400
C	0.42195100	4.35114800	0.92046800
H	0.00131100	5.35536900	0.80605900
H	0.60389400	4.16657200	1.98297200
H	1.38245800	4.30603800	0.39736100
C	-1.85638800	3.32565500	1.12698200
H	-1.67696400	3.31515200	2.20637200
H	-2.40805900	4.23862500	0.87497200
H	-2.47017500	2.45393600	0.88627000
C	-1.50858300	-0.77432500	1.12474700
C	-2.87292400	-0.46296500	1.30331900
C	-0.59115500	-0.62267200	2.18269200
C	-3.28287400	0.04663100	2.53803300
C	-1.05886500	-0.12188800	3.39917400
C	-2.38860000	0.22396800	3.58154300
H	-4.32944500	0.30258500	2.67959900
H	-0.35731900	0.00251700	4.21824800
H	-2.72753900	0.62038800	4.53378700
C	0.87479400	-1.00995800	2.09585500
C	1.13187800	-2.34554800	2.80872800

C	1.80384800	0.06706600	2.67062600
H	1.12493500	-1.13469400	1.04238400
H	0.53725500	-3.16390900	2.39051500
H	2.19009900	-2.61778400	2.72683300
H	0.88448500	-2.26568800	3.87327200
H	1.56265700	1.05105600	2.26291400
H	1.73237000	0.10621800	3.76336300
H	2.84367300	-0.17060000	2.42116500
C	-3.95488800	-0.66924600	0.25153400
C	-4.59510900	0.65050300	-0.19745400
C	-5.07628500	-1.59405000	0.75558500
H	-3.49636500	-1.12888800	-0.62452200
H	-3.86492800	1.33549500	-0.62740000
H	-5.36673200	0.45595700	-0.95035300
H	-5.07310300	1.15584500	0.64908000
H	-4.70323200	-2.51896300	1.20164400
H	-5.67856000	-1.08726200	1.51689400
H	-5.74568100	-1.85548200	-0.07063100
C	2.72716900	0.06960700	-0.43650600
C	4.16386600	-0.17798000	-0.17603700
C	5.03790800	0.87937100	0.09416000
C	4.64313300	-1.48879000	-0.17217800
C	6.37683600	0.62257600	0.35566800
H	4.63775300	1.88870500	0.09294000
C	5.98535100	-1.74726800	0.09328200
H	3.95530400	-2.30869400	-0.37349500
C	6.85269800	-0.69040300	0.35516600
H	7.05609600	1.44399300	0.56257600
H	6.35345200	-2.76858100	0.09615900
H	7.90049300	-0.88750800	0.56090600

N	2.18814200	1.20114600	-0.35904300
C	-2.43772900	-0.64470000	-3.20642300
H	-3.34696300	-1.08907700	-3.62635000
H	-2.72432400	-0.07256500	-2.31970700
H	-2.03837700	0.05944900	-3.94177500

VIc

C	-1.07545700	-1.67268400	-3.06783700
C	0.07709600	-1.10525300	-2.19058600
C	-1.33361200	-2.76157700	-0.79121400
C	-1.85381300	-2.71989600	-2.24025600
H	-0.60023400	-2.17194600	-3.92329100
H	-2.92909000	-2.51142400	-2.25210100
H	-1.73227500	-3.72577200	-2.65849200
C	-0.51340700	-0.45393700	-0.94522100
C	0.11729400	-3.27478900	-0.86063400
H	0.52455500	-3.36143700	0.15237800
H	0.10215600	-4.28454400	-1.28510000
C	0.94475100	-2.30630000	-1.72776600
H	1.81316700	-1.92720700	-1.17887100
H	1.34021200	-2.80809800	-2.61914300
N	-1.23917700	-1.34340600	-0.29561000
C	0.93661500	-0.11444100	-2.97136000
H	0.38927100	0.80711700	-3.18616700
H	1.82283500	0.16775500	-2.39528300
H	1.27310800	-0.55074600	-3.92011200
C	-2.21210600	-3.63344300	0.08952700
H	-1.84594700	-3.67124900	1.11924500
H	-3.24473900	-3.27086100	0.10974600
H	-2.21600100	-4.65124500	-0.31371800

H	1.92669400	0.04856400	0.22095400
C	-0.07673500	3.84041300	-0.81301800
C	-0.18784800	3.46035100	0.71342500
B	1.68333700	2.55162900	-0.20558900
O	1.26909400	3.44884500	-1.15240400
O	0.84423600	2.47171500	0.87593500
C	-0.23479700	5.32541700	-1.10879800
H	-0.12474300	5.49186100	-2.18394800
H	-1.22870700	5.67336400	-0.80743400
H	0.51990200	5.92199400	-0.59279800
C	-1.01301000	3.02881300	-1.70512100
H	-2.05705400	3.32276100	-1.55313400
H	-0.74899600	3.22032800	-2.75013100
H	-0.90262500	1.95710800	-1.50234900
C	0.16212300	4.61562800	1.64879000
H	-0.59760600	5.40260900	1.61880800
H	0.22719600	4.23153100	2.67038200
H	1.13121100	5.05137900	1.38720800
C	-1.50669600	2.81514100	1.11563800
H	-1.49880600	2.60425400	2.18997900
H	-2.35538800	3.47349200	0.89801000
H	-1.63226200	1.86479200	0.59067300
C	-1.85487400	-0.96124900	0.96429100
C	-3.20595400	-0.57507500	0.97244600
C	-1.08445400	-0.95345100	2.13938100
C	-3.77600500	-0.17344400	2.18108100
C	-1.70571400	-0.56263800	3.32900600
C	-3.03702100	-0.17318800	3.35664700
H	-4.81420100	0.14543800	2.19978800
H	-1.12718000	-0.55650600	4.24848400

H	-3.49664900	0.13452100	4.29090800
C	0.38286400	-1.34513200	2.18413900
C	0.57871600	-2.68852800	2.89909400
C	1.23597000	-0.25912500	2.85161100
H	0.73096700	-1.45149600	1.15210400
H	0.00960900	-3.49550100	2.42622100
H	1.63799700	-2.97045300	2.89842200
H	0.25271500	-2.61962400	3.94288500
H	1.06187600	0.71772900	2.39216200
H	1.01422100	-0.18762700	3.92215200
H	2.30018500	-0.50562300	2.75693200
C	-4.03710700	-0.51508600	-0.29652400
C	-4.12946600	0.92988300	-0.79939400
C	-5.43179400	-1.12538100	-0.12622300
H	-3.51809000	-1.08978700	-1.06548000
H	-3.13179800	1.33092900	-1.00093900
H	-4.71920700	0.98200000	-1.72139200
H	-4.60596300	1.57008200	-0.04775800
H	-5.38290800	-2.13674900	0.29018400
H	-6.05922700	-0.52057100	0.53650300
H	-5.93784000	-1.17624600	-1.09551400
C	2.87849700	0.56460100	0.01196000
C	4.08327200	-0.28899100	0.08471500
C	5.33673800	0.20990700	-0.28366300
C	3.97131800	-1.60407700	0.54334300
C	6.45987100	-0.60113300	-0.19505400
H	5.39809100	1.23510700	-0.63562600
C	5.09806200	-2.41643900	0.63613900
H	2.99364400	-1.98658800	0.83490300
C	6.34230400	-1.91446500	0.26493000

H	7.43229100	-0.21449300	-0.48423800
H	5.00598800	-3.43626400	0.99654400
H	7.22326700	-2.54556800	0.33295700
N	2.91885000	1.80081900	-0.27667600
C	-1.99946900	-0.58072500	-3.61336200
H	-2.82400100	-1.02685600	-4.18003500
H	-2.43069000	0.01442300	-2.80029000
H	-1.46685400	0.10259400	-4.28027400

VIIc

C	0.55743100	-2.13592000	-2.04906700
C	0.26638400	-0.62222800	-1.90734200
C	2.77578000	-1.00000000	-2.49465800
C	1.97743600	-2.31029600	-2.65587200
H	-0.18317100	-2.52315700	-2.76389300
H	2.50048400	-3.14171000	-2.16987400
H	1.92043700	-2.55713100	-3.72400600
C	1.23389300	0.02330800	-0.87371800
C	2.13552400	-0.00642700	-3.49009500
H	2.58777800	0.98315400	-3.36812200
H	2.37193100	-0.33055800	-4.50994700
C	0.60828400	0.02947000	-3.26423500
H	0.23585200	1.06054000	-3.27373900
H	0.07946700	-0.50777000	-4.06214100
N	2.57357600	-0.53098000	-1.10141800
C	-1.18733100	-0.33061000	-1.55045400
H	-1.48925200	-0.79018700	-0.60214200
H	-1.35220400	0.74763400	-1.44142300
H	-1.86747200	-0.69856800	-2.32742100
C	4.24881000	-1.18546500	-2.81600100

H	4.78954200	-0.23563500	-2.74080400
H	4.72032300	-1.90042400	-2.13852000
H	4.35335200	-1.56447000	-3.83751400
H	1.17600600	1.10490600	-1.11108100
C	0.82838000	-0.31499600	2.88207100
C	-0.36043200	0.61991900	2.49848600
B	0.78391300	-0.01604400	0.64024200
O	1.15569000	-0.91208200	1.60663100
O	-0.01457800	0.98629600	1.14308500
C	0.48126000	-1.41357700	3.87266000
H	1.37324400	-2.00765100	4.09186200
H	0.12018500	-0.97988400	4.81155800
H	-0.28669800	-2.07950600	3.47396400
C	2.07395700	0.44666300	3.33117800
H	1.94125900	0.88474300	4.32545500
H	2.91921800	-0.24778700	3.35687900
H	2.32495700	1.24245400	2.62059800
C	-1.69805100	-0.11462600	2.43638100
H	-2.07041100	-0.35567100	3.43687000
H	-2.43377300	0.51285100	1.92515500
H	-1.59926500	-1.04777700	1.86877700
C	-0.47491000	1.88792500	3.32766000
H	-1.32496000	2.48042000	2.97578200
H	-0.63898000	1.64449700	4.38295100
H	0.42817800	2.49699000	3.24217700
C	3.62932100	-0.12502800	-0.22212400
C	4.30504800	-1.09995500	0.55753300
C	3.96312300	1.23887700	-0.04245100
C	5.24018900	-0.69121800	1.50943000
C	4.88156700	1.60317900	0.94808100

C	5.51802000	0.65147400	1.72815900
H	5.74785500	-1.44501500	2.10655800
H	5.11352600	2.65579000	1.09194400
H	6.23397500	0.94993800	2.48819000
C	3.39777800	2.35680300	-0.90486300
C	4.51344800	3.12670700	-1.62290400
C	2.51768700	3.30955100	-0.08530800
H	2.78062000	1.90718900	-1.68109900
H	5.14039800	2.45045900	-2.21271900
H	4.08294700	3.87405200	-2.29798400
H	5.16232000	3.65237100	-0.91472800
H	1.70515800	2.76908300	0.41356300
H	3.11030300	3.81741500	0.68470700
H	2.07575500	4.07743600	-0.73028000
C	4.06147500	-2.59392400	0.41592800
C	3.44174400	-3.19478400	1.68451700
C	5.35442500	-3.35182500	0.07812600
H	3.35089500	-2.73422400	-0.39993000
H	2.49519500	-2.70723800	1.92250600
H	3.26371700	-4.26736100	1.54643600
H	4.11901100	-3.07730900	2.53939300
H	5.88282300	-2.91837300	-0.77577700
H	6.04555200	-3.34386200	0.92826400
H	5.12933700	-4.39880200	-0.15134900
C	0.41377500	-2.92625500	-0.74884300
H	1.17716100	-2.63187900	-0.02461200
H	-0.56700800	-2.78145300	-0.28301800
H	0.53042500	-3.99762300	-0.94786400
C	-4.78343000	-2.36767400	-0.76378700
C	-5.52982000	-2.05225700	0.57352900

B	-4.42609300	-0.22191500	-0.15723400
O	-4.47296100	-1.04834800	-1.25752100
O	-4.90982000	-0.81881900	0.98628800
C	-5.61339800	-3.10109100	-1.80466200
H	-5.00728400	-3.27637900	-2.69777800
H	-5.94429700	-4.07119000	-1.41836400
H	-6.48989200	-2.51896100	-2.09565600
C	-3.45502200	-3.08503100	-0.53451600
H	-3.60456500	-4.12726300	-0.23631300
H	-2.87247500	-3.06301900	-1.46049300
H	-2.87413000	-2.57902700	0.24411700
C	-7.01492500	-1.76185000	0.36267600
H	-7.57102700	-2.67064100	0.11362600
H	-7.42550900	-1.34143700	1.28444000
H	-7.15849700	-1.03290500	-0.44134000
C	-5.34194200	-3.08816600	1.67046900
H	-5.90270200	-2.78540600	2.55910800
H	-5.71452300	-4.06560600	1.34545000
H	-4.29033000	-3.18451400	1.94777100
C	-3.83445900	4.64517400	-0.86455200
C	-3.34083000	3.40530500	-0.45556900
C	-2.04095700	3.30550900	0.05276800
C	-1.25088300	4.44264900	0.15722600
C	-1.74908800	5.68229700	-0.24888300
C	-3.03999700	5.78362900	-0.76188600
H	-4.84496600	4.71605800	-1.26098300
H	-1.65964000	2.33444300	0.35659900
H	-0.24407400	4.36028500	0.55622900
H	-1.12919800	6.57009800	-0.16611200
H	-3.42659000	6.74693700	-1.07953800

C	-4.19674800	2.20490100	-0.55317200
N	-3.82458900	1.06791400	-0.15163700
H	-5.19004400	2.38170800	-0.99738800

TS4c

C	0.98657200	-2.20936800	-2.58762900
C	0.08930400	-0.96662100	-2.31897200
C	2.59132600	-0.30201200	-2.40493100
C	2.38719100	-1.71324400	-2.98822600
H	0.55143200	-2.70675600	-3.46451600
H	3.17465400	-2.40868000	-2.68593500
H	2.46471100	-1.63390400	-4.08035000
C	0.57120300	-0.21236300	-1.01350400
C	1.74565100	0.64021500	-3.29496900
H	1.67697600	1.61954000	-2.80479200
H	2.25294800	0.78849800	-4.25416500
C	0.35385400	0.01209800	-3.48845000
H	-0.42345200	0.78451800	-3.51786600
H	0.29376300	-0.53477500	-4.43823000
N	2.00118100	-0.24208900	-1.02852200
C	-1.36438500	-1.44864600	-2.34439200
H	-1.61544800	-2.00881100	-1.43760500
H	-2.08714500	-0.64020800	-2.47642600
H	-1.49665400	-2.11831500	-3.20347600
C	4.05584900	0.10111500	-2.44967300
H	4.21875800	1.11227000	-2.07170100
H	4.67733000	-0.57757500	-1.86821800
H	4.39365000	0.05912900	-3.49016500
H	0.12536600	0.88307600	-1.21864200
C	-0.35390200	-1.60414400	2.39928100

C	-0.13621500	-0.08421200	2.74338000
B	-0.28296300	-0.32517200	0.46243200
O	-0.58528900	-1.60490600	0.98780300
O	0.27465300	0.47696000	1.49878700
C	-1.54318100	-2.25394500	3.10063200
H	-1.62018300	-3.29641800	2.77626900
H	-1.40713300	-2.24134300	4.18834700
H	-2.47792500	-1.75540400	2.84218900
C	0.89622600	-2.43638100	2.65639000
H	1.11158300	-2.53569300	3.72560400
H	0.73861000	-3.43621500	2.24032600
H	1.75998700	-1.98154900	2.16463400
C	-1.42662500	0.60069800	3.20747400
H	-1.74786100	0.22452200	4.18426300
H	-1.23811600	1.67528300	3.30119100
H	-2.23973000	0.44407300	2.49165600
C	0.96368900	0.18175100	3.76599500
H	1.04744000	1.26031200	3.93607500
H	0.73548700	-0.29930000	4.72413800
H	1.93149000	-0.17383300	3.40454000
C	2.86214900	0.02354300	0.10965400
C	3.70033800	-0.99762800	0.63429900
C	2.93589600	1.31984000	0.67422600
C	4.49297100	-0.72225400	1.75438900
C	3.77379800	1.54858100	1.76656100
C	4.53476300	0.53538600	2.32848300
H	5.11371500	-1.51675600	2.16062000
H	3.82818200	2.54496500	2.19186100
H	5.16652200	0.73075100	3.18987500
C	2.16890900	2.51373800	0.12951100

C	3.04495300	3.39097300	-0.77650800
C	1.58454800	3.38700600	1.24227800
H	1.33416700	2.14274200	-0.46586500
H	3.39664200	2.85873700	-1.66372900
H	2.47196300	4.26275000	-1.11404200
H	3.92316800	3.75298500	-0.22951300
H	0.97105100	2.78627200	1.91764700
H	2.36980400	3.88940400	1.81706000
H	0.96559300	4.17061700	0.80033500
C	3.92383000	-2.37190400	0.00834300
C	3.52459900	-3.56263500	0.89058800
C	5.40636000	-2.56570800	-0.37164700
H	3.32377900	-2.42599700	-0.89322700
H	2.44547000	-3.66764500	0.98132500
H	3.91485600	-4.48717700	0.45015000
H	3.94470500	-3.47051700	1.89865800
H	5.85451100	-1.68513000	-0.83715300
H	6.00187400	-2.79670100	0.51837400
H	5.50869000	-3.41148000	-1.06046100
C	0.95699900	-3.21316800	-1.43383100
H	1.15067400	-2.73048600	-0.47288900
H	-0.02675300	-3.68632200	-1.35792300
H	1.69917200	-4.00531900	-1.58950000
C	-5.07586900	-0.78135400	-0.92535100
C	-4.80894400	-1.42390000	0.47401100
B	-2.98155600	-0.29020800	-0.20336400
O	-3.99502400	0.16732900	-1.02784600
O	-3.37474100	-1.34793000	0.57928500
C	-6.39612800	-0.03702300	-1.04542500
H	-6.49567800	0.37253100	-2.05458500

H	-7.23721300	-0.71552500	-0.86642500
H	-6.45151000	0.78974600	-0.33469300
C	-4.92228900	-1.78070100	-2.07032800
H	-5.76201300	-2.48171000	-2.10222700
H	-4.88982500	-1.23139900	-3.01561700
H	-3.99365500	-2.35109400	-1.97237400
C	-5.38402600	-0.59261100	1.62057100
H	-6.47645400	-0.64661000	1.65153200
H	-4.98861500	-0.97546600	2.56581400
H	-5.08750800	0.45753800	1.52576300
C	-5.23256700	-2.87749500	0.60609900
H	-4.99470600	-3.23491600	1.61202400
H	-6.31167000	-2.98131300	0.44897600
H	-4.70633400	-3.50954700	-0.11155800
C	-0.76474100	3.73376000	-1.46580600
C	-1.22686400	2.79494000	-0.53182400
C	-1.65744400	3.22844300	0.72537300
C	-1.65038300	4.58537800	1.03592900
C	-1.19105800	5.51270300	0.10501600
C	-0.73221400	5.08298800	-1.14358900
H	-0.43716900	3.39330700	-2.44662000
H	-2.03408400	2.49028400	1.42382200
H	-2.00683700	4.91821000	2.00577100
H	-1.18774400	6.57097100	0.34720800
H	-0.36867700	5.80508000	-1.86803100
C	-1.50956400	1.41016900	-0.94394000
N	-1.72680300	0.39782900	-0.10538900
H	-1.93096600	1.35082700	-1.95663200

VIIIc

C	1.75310300	-2.22591400	-2.58795100
C	0.58988400	-1.22146500	-2.29764900
C	2.86092200	0.01882100	-2.31341400
C	3.02533400	-1.40828100	-2.87335400
H	1.47039500	-2.74766100	-3.51001100
H	3.92695700	-1.89483800	-2.49342300
H	3.17570900	-1.29926900	-3.95375700
C	0.93759300	-0.53556300	-0.96750700
C	1.85314800	0.73793200	-3.23802400
H	1.56122700	1.68654100	-2.77168700
H	2.35179800	0.97469900	-4.18317700
C	0.64503200	-0.17863800	-3.44867300
H	-0.28701900	0.38488600	-3.50338200
H	0.73253200	-0.73738100	-4.38839100
N	2.16419200	-0.04994100	-0.96579700
C	-0.74169200	-1.98412500	-2.32115600
H	-0.93173900	-2.50213800	-1.37725900
H	-1.58439300	-1.31932600	-2.52172900
H	-0.70199900	-2.72323200	-3.13065400
C	4.17704400	0.77191000	-2.26544300
H	4.05700100	1.78599400	-1.87834300
H	4.91812900	0.25929300	-1.65640800
H	4.56380900	0.83401000	-3.28721600
H	-0.47275900	1.32309500	-1.64938000
C	-0.13129000	-1.82528500	2.21084000
C	-0.13957800	-0.30683000	2.60447400
B	-0.23758000	-0.47743100	0.29648300
O	-0.41832900	-1.81855000	0.81725400
O	0.24619200	0.33079500	1.39642600
C	-1.17182800	-2.67653000	2.93109000

H	-1.07254900	-3.71796600	2.60829700
H	-1.02413100	-2.63842700	4.01699400
H	-2.18050700	-2.34308000	2.68335200
C	1.25282700	-2.43615600	2.38780100
H	1.53436600	-2.56125300	3.43919900
H	1.26410800	-3.41836500	1.90286200
H	1.99229000	-1.79128400	1.90462700
C	-1.53198200	0.17709400	3.02488900
H	-1.80887200	-0.21162200	4.01132000
H	-1.52418600	1.27131900	3.07218400
H	-2.28993300	-0.13939100	2.30380300
C	0.86876300	0.07626600	3.68436900
H	0.78029800	1.14667700	3.89974900
H	0.68283700	-0.47545300	4.61335600
H	1.89328900	-0.11315500	3.35287400
C	2.86739500	0.48129800	0.22031000
C	3.89458100	-0.29518100	0.80577400
C	2.56254500	1.76868600	0.71193800
C	4.54266900	0.21286800	1.93664500
C	3.28403900	2.23702200	1.81103400
C	4.24977700	1.46714000	2.44006000
H	5.31783200	-0.38683400	2.40533400
H	3.06552100	3.22654700	2.19604200
H	4.77678800	1.84899700	3.30895300
C	1.51282600	2.69935800	0.12107100
C	2.14873900	3.75232000	-0.79797400
C	0.68943700	3.41048300	1.20208000
H	0.81623900	2.09959900	-0.46540100
H	2.68324300	3.31248900	-1.64561100
H	1.36855100	4.41129700	-1.19489000

H	2.86172700	4.36896000	-0.23867100
H	0.24293900	2.67702600	1.87588600
H	1.30132900	4.11398900	1.77680500
H	-0.11020700	3.98937400	0.73294100
C	4.46873800	-1.60110400	0.25545400
C	4.33260500	-2.81909500	1.18354200
C	5.97363100	-1.44271800	-0.05207000
H	3.94819000	-1.84221400	-0.66748100
H	3.32303100	-3.22336100	1.20456900
H	5.00289800	-3.61242900	0.83549000
H	4.61843000	-2.56691600	2.21043000
H	6.22999600	-0.48905200	-0.51790300
H	6.55657000	-1.51355900	0.87229500
H	6.30786100	-2.25240200	-0.70945200
C	1.89457200	-3.27679500	-1.48297200
H	1.94563000	-2.82590200	-0.48702600
H	1.02920700	-3.94534100	-1.48011500
H	2.79400200	-3.88400100	-1.63596800
C	-4.91348200	-1.13113200	-0.92068700
C	-4.59839600	-1.71710500	0.49028400
B	-2.79067800	-0.58940600	-0.29219300
O	-3.86324700	-0.17051800	-1.08515600
O	-3.16773800	-1.63727300	0.53971400
C	-6.25609700	-0.42635100	-1.03765800
H	-6.38983200	-0.05882900	-2.05919700
H	-7.07693600	-1.11562700	-0.81048100
H	-6.31182600	0.42785600	-0.35999200
C	-4.75881900	-2.17303500	-2.02919800
H	-5.57371100	-2.90372200	-2.01653800
H	-4.76375200	-1.66027400	-2.99533600

H	-3.80754900	-2.70576800	-1.92589000
C	-5.14513300	-0.84096400	1.61839500
H	-6.23558100	-0.90337100	1.69005600
H	-4.71284600	-1.17631800	2.56612600
H	-4.86384200	0.20679700	1.46457200
C	-5.01779000	-3.16464800	0.69414700
H	-4.75472100	-3.48193600	1.70760000
H	-6.10043700	-3.27696400	0.56853200
H	-4.50802300	-3.82492500	-0.01018200
C	-1.69059900	3.67799000	-1.43852900
C	-1.93663200	2.51580200	-0.70135400
C	-2.59205800	2.62348300	0.52107400
C	-2.98542900	3.86994900	1.00578800
C	-2.73148800	5.02369100	0.26981100
C	-2.08260600	4.92431400	-0.96108800
H	-1.17793300	3.60136000	-2.39722800
H	-2.76633000	1.72507100	1.10317500
H	-3.48773100	3.93893600	1.96652500
H	-3.03490200	5.99433200	0.65017800
H	-1.87913800	5.81800600	-1.54418000
C	-1.49336200	1.18034600	-1.27335800
N	-1.53306000	0.03951500	-0.37997400
H	-2.11465500	0.98881900	-2.16158200

TS5c

C	1.61607000	-2.86595800	-2.14549700
C	0.53110100	-1.76524800	-1.93724600
C	2.82788900	-0.65030600	-2.35167600
C	2.94686500	-2.17699900	-2.52298600
H	1.28026700	-3.45455400	-3.00922300

H	3.77801700	-2.56572100	-1.93031200
H	3.19809300	-2.36752400	-3.57323300
C	0.98651600	-0.88136900	-0.76280300
C	1.79910400	-0.13709200	-3.37879600
H	1.61265700	0.92433600	-3.17929600
H	2.23736600	-0.20887400	-4.38006000
C	0.50932400	-0.95513700	-3.25870500
H	-0.37399200	-0.31486900	-3.29968800
H	0.41378000	-1.67043600	-4.08537300
N	2.19801200	-0.40334800	-1.00012000
C	-0.82949500	-2.42829700	-1.69791500
H	-0.95667100	-2.70814300	-0.64680500
H	-1.65147900	-1.76089600	-1.96987600
H	-0.92068900	-3.32916000	-2.31833100
C	4.15542100	0.06623800	-2.55731500
H	4.02848300	1.15123900	-2.55413900
H	4.89747800	-0.17594200	-1.79812200
H	4.55223000	-0.22730100	-3.53473800
H	-0.51248600	0.92428000	-1.56798900
C	0.07656000	0.53544800	2.82654200
C	-0.14975600	-1.01588500	2.86955600
B	-0.75894200	-0.18706600	0.84407500
O	0.00756700	0.82884000	1.42402600
O	-0.94573000	-1.25187400	1.70983500
C	1.42102900	0.99556300	3.37108800
H	1.49829900	2.08496400	3.29480200
H	1.52348700	0.71864300	4.42693100
H	2.24988200	0.56016800	2.80643800
C	-1.06322200	1.30511800	3.49846400
H	-1.04470900	1.19803200	4.58778700

H	-0.96521800	2.36633800	3.24773200
H	-2.03287500	0.95234600	3.12881000
C	1.14514400	-1.79892400	2.70486600
H	1.77001000	-1.72260700	3.60034000
H	0.90381700	-2.85322300	2.53481500
H	1.69936100	-1.42481600	1.83798300
C	-0.91102300	-1.51237100	4.09189400
H	-1.00283500	-2.60129600	4.04412200
H	-0.38121900	-1.25130800	5.01500400
H	-1.91758300	-1.09090000	4.12475000
C	2.98445100	0.35838200	-0.02438100
C	4.01113800	-0.30721900	0.68864700
C	2.80841000	1.75292600	0.10758300
C	4.85383100	0.44692600	1.50925400
C	3.69570800	2.45329500	0.93112200
C	4.71388300	1.82014700	1.62438700
H	5.64022600	-0.06124400	2.06038300
H	3.57979400	3.52744000	1.02883700
H	5.38758500	2.39177300	2.25530100
C	1.73201500	2.56839600	-0.59694300
C	2.29447300	3.34609800	-1.79582800
C	1.05114800	3.56657500	0.35070400
H	0.96539000	1.87773500	-0.95034700
H	2.72755000	2.69910400	-2.56309200
H	1.49365100	3.93214800	-2.26039700
H	3.07515800	4.04205600	-1.46738500
H	0.63848400	3.05389800	1.22038600
H	1.74850000	4.34432400	0.68037100
H	0.23304400	4.06913800	-0.17249600
C	4.28601200	-1.80699300	0.63768600

C	4.39301100	-2.42516000	2.04333700
C	5.59240600	-2.15435300	-0.09737200
H	3.45179600	-2.28598200	0.12530200
H	3.63521400	-2.04173800	2.72435900
H	4.28385800	-3.51280900	1.97804900
H	5.37501800	-2.22342700	2.48494100
H	5.59772500	-1.87354900	-1.15132100
H	6.43843400	-1.65244700	0.38514600
H	5.76941800	-3.23422300	-0.04069700
C	1.70965700	-3.82906500	-0.95558600
H	1.74769500	-3.30046900	0.00210500
H	0.83321100	-4.48261400	-0.92263600
H	2.59882700	-4.46465900	-1.03631300
C	-4.96113400	-1.52366000	0.62314100
C	-5.03822900	-1.34563300	-0.92559900
B	-3.05524700	-0.58006900	-0.13234200
O	-3.55587100	-1.37444100	0.87915300
O	-3.96289500	-0.42492500	-1.17268800
C	-5.41582700	-2.88101000	1.13519900
H	-5.32539800	-2.90879200	2.22471100
H	-6.46360100	-3.06281400	0.87167400
H	-4.80153600	-3.68391200	0.72322100
C	-5.67712100	-0.40143800	1.37553200
H	-6.76506100	-0.48557400	1.29192400
H	-5.40115000	-0.45892400	2.43208100
H	-5.37001400	0.57781100	0.99305900
C	-4.71297000	-2.63603500	-1.67737000
H	-5.52676400	-3.36384600	-1.60072600
H	-4.55490300	-2.39755400	-2.73303800
H	-3.79659700	-3.09016000	-1.28611500

C	-6.33631900	-0.74242700	-1.43825400
H	-6.29806700	-0.66094300	-2.52833200
H	-7.18839300	-1.37720800	-1.17142800
H	-6.49664000	0.25641900	-1.02778200
H	-2.16007500	0.68164900	-2.11994300
C	-1.67757800	3.38869000	-1.96778600
C	-1.87492900	2.44246100	-0.95738700
C	-2.34134100	2.86879500	0.28259200
C	-2.59795500	4.21973000	0.51376300
C	-2.39403600	5.15743100	-0.49391400
C	-1.93392100	4.73665900	-1.74214800
H	-1.31475100	3.06015900	-2.94100000
H	-2.48207700	2.13666900	1.07100500
H	-2.95401900	4.53967400	1.48893600
H	-2.59210500	6.20926200	-0.31158900
H	-1.77502800	5.45989200	-2.53683500
C	-1.56013200	0.98884800	-1.25431800
N	-1.78494900	0.05519900	-0.16804200

IXc

C	2.03657100	-3.31647400	-1.40753700
C	1.06857200	-2.10400200	-1.31229300
C	3.36335400	-1.30737700	-2.19832800
C	3.39463400	-2.82652300	-1.95564500
H	1.58899400	-4.01831300	-2.12504000
H	4.20775100	-3.08007500	-1.26696100
H	3.63694300	-3.30891100	-2.90947400
C	1.67820300	-1.01838600	-0.43095400
C	2.29633500	-1.05866800	-3.28053200
H	2.29983600	-0.00442600	-3.57320600

H	2.57593300	-1.63695200	-4.16811200
C	0.92389000	-1.49213400	-2.73136200
H	0.24082200	-0.63689700	-2.67026500
H	0.44451100	-2.23051600	-3.38515000
N	2.84276500	-0.66227300	-0.94085600
C	-0.30373600	-2.52626100	-0.79371300
H	-0.27280300	-2.75816600	0.27533400
H	-1.02724800	-1.71589100	-0.92627600
H	-0.67303000	-3.40680500	-1.33553000
C	4.73276800	-0.78678400	-2.60212500
H	4.72460300	0.29256300	-2.77589000
H	5.48461800	-1.00088500	-1.83520300
H	5.03903900	-1.28348400	-3.52851500
H	-0.79254000	1.16461200	-0.96416400
C	0.11864600	1.42817400	2.71521600
C	-0.46298100	0.12581700	3.36638200
B	-1.46985800	0.49197100	1.38834700
O	-0.39758500	1.35829100	1.37332700
O	-1.66991700	-0.09673400	2.61207200
C	1.63779100	1.47425800	2.64130400
H	1.96275100	2.43114600	2.21915400
H	2.08123500	1.37168600	3.63853600
H	2.00806900	0.67835000	1.98974300
C	-0.44029400	2.70596500	3.33737500
H	-0.05410400	2.86432500	4.34902400
H	-0.14368300	3.55682900	2.71624700
H	-1.53391100	2.67371300	3.37785200
C	0.42980700	-1.09171400	3.13528300
H	1.34114900	-1.04018000	3.74029200
H	-0.12833300	-1.98894400	3.41905700

H	0.70908300	-1.16550600	2.07659200
C	-0.82172800	0.25617000	4.83800800
H	-1.21797100	-0.69646900	5.20031500
H	0.06602700	0.50674300	5.42896400
H	-1.58143400	1.02421100	4.99677200
C	3.56556000	0.44606700	-0.34233800
C	4.57523700	0.17334000	0.59668000
C	3.23165300	1.76256300	-0.69954200
C	5.25383900	1.24712400	1.17293100
C	3.95628700	2.80462100	-0.11225500
C	4.95717900	2.55657500	0.81503100
H	6.02780600	1.05641200	1.90999100
H	3.72028200	3.82987100	-0.38378100
H	5.50243900	3.38139300	1.26366000
C	2.12410800	2.11319400	-1.67915500
C	2.69664800	2.68365300	-2.98320200
C	1.12592800	3.10007800	-1.06219300
H	1.56979200	1.19839400	-1.90761800
H	3.40400500	1.99757000	-3.46007600
H	1.89053500	2.89300000	-3.69433100
H	3.22662800	3.62326200	-2.79069100
H	0.73129200	2.70900400	-0.12013000
H	1.59146700	4.07407700	-0.87424500
H	0.28578400	3.26579200	-1.74629800
C	4.87318000	-1.24344200	1.05275300
C	4.02079300	-1.57410600	2.28333300
C	6.35768400	-1.49779200	1.32452900
H	4.56507200	-1.92342000	0.25486000
H	2.95776000	-1.47214500	2.04500100
H	4.20987400	-2.59782000	2.62575800

H	4.25330400	-0.88578300	3.10479600
H	6.98151400	-1.18656800	0.48022800
H	6.70396800	-0.96463500	2.21591900
H	6.52486400	-2.56471200	1.50190900
C	2.20579800	-4.04578100	-0.07313800
H	2.57750700	-3.36252700	0.69944000
H	1.26258100	-4.47116900	0.27990600
H	2.92621100	-4.86458600	-0.17506700
C	-5.15439800	-1.87360200	0.72877900
C	-4.88137700	-2.00772400	-0.80354700
B	-3.36714700	-0.62877600	0.15264400
O	-3.92108900	-1.30966600	1.21065600
O	-3.99946300	-0.89664200	-1.04946500
C	-5.41136800	-3.18736600	1.44910400
H	-5.59257700	-2.99207900	2.50958800
H	-6.29371700	-3.68771500	1.03516200
H	-4.55318400	-3.85718300	1.36851500
C	-6.26219800	-0.86746100	1.03871200
H	-7.24815200	-1.25706100	0.76699900
H	-6.25157700	-0.65536100	2.11093700
H	-6.09464300	0.07194800	0.50199600
C	-4.10795000	-3.27952900	-1.14947500
H	-4.73753500	-4.17047600	-1.06312300
H	-3.74719100	-3.20308000	-2.17916200
H	-3.24129700	-3.39570100	-0.49032700
C	-6.10953100	-1.86994600	-1.68844700
H	-5.82051800	-1.98286100	-2.73741300
H	-6.84521700	-2.64583800	-1.45038100
H	-6.57597400	-0.89046200	-1.56583800
H	-2.02072100	0.25768500	-1.86471900

C	-3.68919800	2.23683600	-2.19304000
C	-2.66182300	2.20438400	-1.25015400
C	-2.40874700	3.34512400	-0.48147500
C	-3.16132100	4.50029200	-0.66515200
C	-4.17986200	4.52816000	-1.61701200
C	-4.44436600	3.39364300	-2.37825400
H	-3.90375900	1.34150800	-2.77092000
H	-1.61841600	3.31175100	0.26517000
H	-2.95408800	5.38193700	-0.06569100
H	-4.76629800	5.43065500	-1.76120900
H	-5.24113400	3.40714100	-3.11621400
C	-1.86292200	0.93973400	-1.02270700
N	-2.25240900	0.25453900	0.21865000

It

C	-2.28759500	2.66605100	0.56038200
C	-1.20900400	2.38116500	-0.54030600
C	-2.75075700	0.31472300	-0.21668500
C	-3.03795000	1.35396900	0.88140300
H	-2.98987900	3.37212600	0.09463400
H	-2.71459400	0.95432300	1.84903200
H	-4.11896600	1.52082700	0.94193800
C	-0.46775000	1.10683600	-0.18698600
C	-3.06648000	1.01703200	-1.55718400
H	-3.18419400	0.29810000	-2.37173400
H	-4.04233500	1.49929800	-1.43000800
C	-1.97766800	2.05273800	-1.84776400
H	-1.26354500	1.67929000	-2.59095700
H	-2.40443900	2.97927300	-2.24579200
N	-1.26514000	0.06822200	-0.11327100

C	-0.29410700	3.57807100	-0.78321700
H	0.33646900	3.79500600	0.07978100
H	0.37088600	3.38178800	-1.62736100
H	-0.90859300	4.45845000	-1.00596900
C	-3.55789800	-0.96310700	-0.06660900
H	-3.33296500	-1.67221100	-0.86934600
H	-3.37447900	-1.46315400	0.88629800
H	-4.61971100	-0.70521500	-0.12645700
C	3.01941800	-0.16560300	0.31276500
C	3.26301200	1.16868000	-0.48292100
B	1.10717000	1.18926300	0.29263900
O	1.73277300	0.01855000	0.88147200
O	1.95019300	1.58400200	-0.82950100
C	4.02657800	-0.40933800	1.43572100
H	3.79944200	-1.36161800	1.92675000
H	5.04981200	-0.46451500	1.04566600
H	3.97814300	0.38137800	2.18784100
C	2.97109600	-1.40636700	-0.57939000
H	3.95864700	-1.67370900	-0.97200900
H	2.58840300	-2.24199500	0.01599300
H	2.28833800	-1.25351300	-1.41554400
C	3.89811700	2.26088700	0.38587700
H	4.93705300	2.03217200	0.64462100
H	3.87578000	3.20125600	-0.17310500
H	3.32895700	2.40202900	1.30964400
C	4.07232200	0.99542300	-1.76189900
H	4.19432100	1.96617200	-2.25210800
H	5.06815200	0.59159000	-1.54632500
H	3.56340800	0.32395800	-2.45812000
C	-0.75400700	-1.27954500	0.09796200

C	-0.48586600	-1.73277400	1.39804100
C	-0.56526300	-2.08161300	-1.03908000
C	-0.04836600	-3.05181100	1.53584200
C	-0.10745500	-3.38544300	-0.84656200
C	0.13962100	-3.87159700	0.43127700
H	0.16237900	-3.43672700	2.52907600
H	0.05125500	-4.03030900	-1.70467000
H	0.48697100	-4.89157700	0.56549500
C	-0.84557900	-1.55212700	-2.43823200
C	-1.33811500	-2.63540800	-3.40167300
C	0.35764900	-0.81282600	-3.04066400
H	-1.65104500	-0.82217300	-2.34820500
H	-2.16627500	-3.21103800	-2.97544900
H	-1.68098700	-2.17424000	-4.33302400
H	-0.53770100	-3.33464200	-3.66427900
H	0.74109100	-0.02138800	-2.38474900
H	1.17537000	-1.51638900	-3.23348300
H	0.07333300	-0.36308300	-3.99899100
C	-0.63666100	-0.86509200	2.63930600
C	0.57776500	-0.96616500	3.57040300
C	-1.90832900	-1.22599600	3.42098500
H	-0.69909900	0.18037000	2.31787900
H	1.49219400	-0.75775500	3.01428000
H	0.47682600	-0.23382600	4.37816700
H	0.64489100	-1.95553400	4.03628000
H	-2.82155700	-1.09481600	2.83348100
H	-1.86941900	-2.27219600	3.74477800
H	-1.99225600	-0.60017000	4.31580200
H	0.92292600	2.04866500	1.18337200
C	-1.73990700	3.31195800	1.83025300

H	-1.31860500	4.30091600	1.63276200
H	-2.54496900	3.42938400	2.56347500
H	-0.95395600	2.69480800	2.27829100

TS1t

C	-1.57188100	3.11291600	0.33517100
C	-0.70744400	2.45295200	-0.78907400
C	-2.65463100	0.88298700	-0.08351100
C	-2.57767400	2.07523700	0.88049400
H	-2.13239800	3.91083100	-0.17364800
H	-2.27571600	1.72378700	1.87339500
H	-3.57514600	2.51659200	0.98839600
C	-0.24965400	1.05706000	-0.38131600
C	-2.93372300	1.48236400	-1.48131000
H	-3.27650000	0.71466800	-2.18037400
H	-3.76147100	2.19264300	-1.37142000
C	-1.66513700	2.18940200	-1.98113300
H	-1.14173100	1.57922000	-2.72703600
H	-1.90436600	3.14668600	-2.45693500
N	-1.29519700	0.25406300	-0.10173500
C	0.42136100	3.37728900	-1.22940300
H	1.17757500	3.49710700	-0.45184600
H	0.92894600	2.97990800	-2.11118700
H	0.00020500	4.36024700	-1.47279000
C	-3.73084200	-0.11589900	0.30493900
H	-3.75977200	-0.96016200	-0.39116300
H	-3.57601900	-0.51263800	1.31099700
H	-4.70161900	0.38827900	0.27454800
C	3.04474200	-0.75891600	-0.08960500
C	3.50253600	0.72114200	-0.28987100

B	1.24278500	0.68472700	-0.11676400
O	1.67278000	-0.61603800	0.28152000
O	2.31594000	1.33613900	-0.79096700
C	3.77636600	-1.51311400	1.01377500
H	3.35326800	-2.51849000	1.10418500
H	4.84357100	-1.60637400	0.78253900
H	3.67059100	-1.01344000	1.97924500
C	3.10338900	-1.56513200	-1.38764900
H	4.13138500	-1.83459700	-1.65257700
H	2.52080300	-2.48180100	-1.25135000
H	2.66615700	-0.99911000	-2.21445700
C	3.87578100	1.39722000	1.03260700
H	4.82254800	1.01853800	1.43060400
H	3.97530100	2.47277000	0.85819700
H	3.09440000	1.24500000	1.78510400
C	4.62026600	0.91243900	-1.30468100
H	4.87811900	1.97368200	-1.37073500
H	5.51730000	0.35953500	-1.00436800
H	4.31268800	0.57494800	-2.29644800
C	-1.10747800	-1.14413700	0.22188400
C	-0.84133300	-1.51426800	1.54891900
C	-1.17302000	-2.09518600	-0.81021600
C	-0.65668000	-2.86983800	1.82834900
C	-0.96564200	-3.43586300	-0.48679500
C	-0.71330400	-3.82433500	0.82381000
H	-0.44921100	-3.17640900	2.85021000
H	-1.00575200	-4.18833900	-1.26819500
H	-0.55940000	-4.87319500	1.05917500
C	-1.41487200	-1.67898600	-2.25068700
C	-2.20850800	-2.71070200	-3.05614400

C	-0.08925700	-1.35380100	-2.94893900
H	-2.00407200	-0.75959600	-2.23066100
H	-3.12207000	-3.01368900	-2.53443100
H	-2.48876900	-2.28880000	-4.02633800
H	-1.61665900	-3.61020100	-3.25495900
H	0.45383600	-0.56343500	-2.42162900
H	0.55353300	-2.24064300	-2.97518400
H	-0.26817500	-1.02794100	-3.97996600
C	-0.70138700	-0.50649200	2.67855200
C	0.66850700	-0.61729200	3.35973400
C	-1.82143000	-0.65174200	3.71622900
H	-0.75683300	0.49501300	2.24500400
H	1.46251100	-0.55268700	2.61285600
H	0.78877200	0.19050100	4.08976500
H	0.76974900	-1.56763600	3.89620800
H	-2.81401500	-0.50392900	3.27986900
H	-1.80264600	-1.64894600	4.16971600
H	-1.69224400	0.08276300	4.51830600
H	0.75803100	1.38748200	0.94362600
C	-0.77885500	3.76027500	1.46706700
H	-0.16514600	4.59256500	1.11284800
H	-1.46838600	4.15020000	2.22335200
H	-0.11964600	3.03272500	1.95392000

1at

C	-2.49059600	2.71621900	-0.02384600
C	-1.08324700	2.38834900	-0.59057500
C	-2.61130300	0.28921800	-0.76452600
C	-3.24956900	1.37642000	0.12948300
H	-3.00001700	3.33033700	-0.78154100

H	-3.23548600	1.04670200	1.17585100
H	-4.30416400	1.49805900	-0.14589700
C	-0.53732400	1.17523100	0.21238700
C	-2.45256000	0.94850400	-2.15208900
H	-2.28112900	0.19911300	-2.93175800
H	-3.38626700	1.46325100	-2.41333600
C	-1.27834000	1.94710000	-2.05641200
H	-0.34693200	1.48720100	-2.40869600
H	-1.46441600	2.82902100	-2.68181000
N	-1.25302200	-0.01216800	-0.26338300
C	-0.12861800	3.57538600	-0.50765900
H	0.17159200	3.77989500	0.52744000
H	0.77637500	3.37454300	-1.09260500
H	-0.59437800	4.48259600	-0.91035100
C	-3.48313200	-0.95326600	-0.79326800
H	-3.02118200	-1.75133800	-1.37886800
H	-3.65300800	-1.33253500	0.22055000
H	-4.45225000	-0.71347600	-1.24207300
C	3.07962400	0.47735300	0.97783000
C	3.19123800	0.86704000	-0.52738500
B	1.03212200	0.97571100	0.15805600
O	1.77229000	0.98519300	1.31511300
O	1.80930800	0.79171300	-0.95970200
C	4.11419800	1.11974900	1.88611000
H	3.95162700	0.78817600	2.91543200
H	5.12508300	0.82302000	1.58643900
H	4.04398800	2.20909900	1.86250900
C	3.02566400	-1.03480200	1.19169000
H	4.00639800	-1.49707000	1.04152900
H	2.69644300	-1.23369800	2.21580400

H	2.30388300	-1.50170200	0.51095800
C	3.63880900	2.31314800	-0.73117200
H	4.70008800	2.43999000	-0.49707600
H	3.47697400	2.58849900	-1.77719600
H	3.05727000	2.99384900	-0.10120100
C	4.04570100	-0.07355200	-1.36064900
H	4.03831300	0.24755000	-2.40652700
H	5.08127200	-0.05251300	-1.00360600
H	3.68041100	-1.10087500	-1.31321400
C	-0.76187600	-1.30290800	0.09600900
C	-0.74623800	-1.72189900	1.44736100
C	-0.20624900	-2.15051800	-0.89688400
C	-0.13814900	-2.93334700	1.78657200
C	0.36353800	-3.36747600	-0.51472500
C	0.41618000	-3.75666800	0.81735600
H	-0.11596200	-3.24192900	2.82911400
H	0.78370600	-4.01745500	-1.27865200
H	0.87750000	-4.69958600	1.09588200
C	-0.21667100	-1.80070700	-2.37588600
C	-1.06771900	-2.79195100	-3.18257200
C	1.19433100	-1.73884200	-2.97089100
H	-0.64900700	-0.80371200	-2.46600800
H	-2.08422800	-2.88753300	-2.79155200
H	-1.13351200	-2.47131700	-4.22786800
H	-0.61506900	-3.79009200	-3.16971100
H	1.77510700	-0.95467900	-2.48495400
H	1.72034300	-2.69420600	-2.85872900
H	1.13976900	-1.51560700	-4.04227900
C	-1.40813900	-0.92091900	2.55596800
C	-0.38763200	-0.42744800	3.58858100

C	-2.51760500	-1.73245300	3.23728200
H	-1.87960500	-0.04972600	2.09867500
H	0.40026300	0.16468000	3.11430000
H	-0.88073600	0.18638000	4.35045700
H	0.08402000	-1.27504800	4.10029000
H	-3.25307900	-2.09165700	2.51059300
H	-2.10950500	-2.60537400	3.75805600
H	-3.03752800	-1.11607900	3.97836900
H	-0.75116900	1.38362500	1.28015200
C	-2.49728200	3.50576100	1.28354200
H	-2.06127200	4.50196300	1.16390400
H	-3.52527600	3.63177300	1.63977100
H	-1.93967600	2.98291000	2.06976800

IVt

C	-0.87215200	-1.66068800	-2.75809500
C	0.13052900	-0.49549200	-2.53152100
C	0.85689300	-2.58093100	-1.14970200
C	-0.58896100	-2.72786900	-1.67614000
H	-0.63908300	-2.09054200	-3.74369200
H	-1.28860900	-2.61882000	-0.83512100
H	-0.73589800	-3.73670300	-2.08103000
C	0.18213900	-0.22129000	-1.00109100
C	1.74577400	-2.43303300	-2.40502800
H	2.80039900	-2.60355400	-2.16398300
H	1.46557600	-3.20420600	-3.13456600
C	1.50985900	-1.01874700	-2.98036400
H	2.27887300	-0.31488700	-2.63964800
H	1.55193400	-1.03392500	-4.07648000
N	0.93641900	-1.32041400	-0.38556600

C	-0.25462900	0.75603200	-3.31533600
H	-1.14292300	1.23937300	-2.89144600
H	0.56467200	1.48112200	-3.30084600
H	-0.46916900	0.50344700	-4.36095300
C	1.24090200	-3.77954900	-0.29912400
H	2.23376000	-3.65799600	0.14169200
H	0.52551700	-3.92155500	0.51812700
H	1.24580600	-4.68250200	-0.91800100
C	0.97958100	2.98278100	0.82720700
C	1.66750600	3.25244600	-0.54848300
B	0.74436300	1.18758000	-0.54075200
O	0.18216700	1.82092500	0.53445800
O	1.76118900	1.91770200	-1.11040200
C	0.05752400	4.09319900	1.30563600
H	-0.36414700	3.82034300	2.27752900
H	0.60995900	5.03199500	1.42315900
H	-0.76680100	4.24407700	0.60567000
C	1.96088500	2.57706700	1.92465100
H	2.55357700	3.43028300	2.26995900
H	1.39294300	2.17534200	2.76909600
H	2.63716900	1.78816600	1.57803100
C	0.78301900	4.05890300	-1.49846100
H	0.70149400	5.10200200	-1.17765200
H	1.22816800	4.03686600	-2.49753200
H	-0.22221700	3.62746200	-1.55535500
C	3.05387600	3.86718700	-0.45996700
H	3.47870300	3.95889500	-1.46365500
H	2.99250300	4.86885500	-0.02059900
H	3.73052400	3.26348000	0.14741500
C	1.48571200	-1.19077100	0.92407500

C	0.64574600	-1.16616500	2.06213000
C	2.88457000	-1.04203300	1.09821600
C	1.20755200	-1.00057100	3.32987100
C	3.40580600	-0.90461300	2.38749500
C	2.57930400	-0.87809300	3.50134600
H	0.55660400	-0.98253300	4.20075500
H	4.48099800	-0.80338900	2.51573200
H	3.00030200	-0.76285400	4.49580900
C	3.85758600	-1.01311900	-0.06805600
C	4.83236800	-2.19663400	-0.02870600
C	4.63211300	0.30833500	-0.13041600
H	3.26626000	-1.07784200	-0.97982100
H	4.31028100	-3.15788500	-0.00752000
H	5.48240000	-2.18288700	-0.91034700
H	5.47373900	-2.14718400	0.85860400
H	3.94339500	1.14061000	-0.29203800
H	5.20057500	0.48951000	0.78910900
H	5.34238500	0.29051900	-0.96442000
C	-0.86156600	-1.33977900	1.97055300
C	-1.59988200	-0.10635900	2.50871400
C	-1.32525000	-2.60228300	2.70876500
H	-1.11094700	-1.46659600	0.91331100
H	-1.36674500	0.77990500	1.91200300
H	-2.68299000	-0.26992400	2.50385400
H	-1.30717400	0.09359000	3.54586500
H	-0.80441100	-3.49520600	2.34998700
H	-1.14292300	-2.51899100	3.78574300
H	-2.40240100	-2.75000600	2.56649900
H	-0.87212000	-0.20718900	-0.64601100
C	-4.20192200	-0.60284300	0.33757300

C	-4.44163200	0.73692300	0.01224100
C	-5.72233800	1.28251200	0.15057300
C	-6.75999400	0.48440100	0.61698200
C	-6.52367300	-0.84971900	0.94242400
C	-5.24733100	-1.39141500	0.80274600
H	-3.20126700	-1.01132700	0.23117900
H	-5.89198200	2.32251300	-0.10698100
H	-7.75433100	0.90447400	0.72616800
H	-7.33699700	-1.46953300	1.30636000
H	-5.06343000	-2.43028000	1.05657600
C	-3.36996800	1.56651200	-0.47665200
N	-2.52494100	2.24539800	-0.88416100
C	-2.34070500	-1.24648300	-2.77998200
H	-2.58133600	-0.64867900	-3.66369800
H	-2.99044300	-2.12888000	-2.78124800
H	-2.59460900	-0.64567200	-1.90062000

TS2t

C	-1.18645500	-2.23653800	-2.34487300
C	-0.35629400	-0.91494500	-2.35297300
C	0.77782100	-2.70337900	-0.85797400
C	-0.68857800	-3.08163100	-1.15971900
H	-0.91531600	-2.75816800	-3.27354400
H	-1.30008000	-2.90098100	-0.26442300
H	-0.75604100	-4.15192800	-1.38789500
C	-0.09867100	-0.42367800	-0.89283300
C	1.47119700	-2.63597000	-2.24113700
H	2.55640200	-2.74088800	-2.17447900
H	1.12652600	-3.49567900	-2.82761900
C	1.04195700	-1.31629400	-2.89954100

H	1.75197500	-0.50830600	-2.68661000
H	0.98248200	-1.42526100	-3.98817500
N	0.74034100	-1.33011700	-0.26142000
C	-0.97708300	0.13110400	-3.27626100
H	-1.97737500	0.43357800	-2.96054000
H	-0.35095900	1.02558100	-3.32336100
H	-1.06141900	-0.29519500	-4.28336900
C	1.42904900	-3.71193700	0.07226400
H	2.46625600	-3.44949900	0.29666900
H	0.88548900	-3.78818300	1.01934500
H	1.42148100	-4.69248500	-0.41377400
C	1.07438100	2.95554700	0.57773000
C	1.22282000	3.22215800	-0.98519600
B	0.12320400	1.24670000	-0.64583500
O	0.49051400	1.65600400	0.66007800
O	0.93747900	1.94496800	-1.57596900
C	0.14425800	3.94257300	1.28444800
H	0.05937700	3.65275900	2.33629600
H	0.53476800	4.96519800	1.24059800
H	-0.85605700	3.92478600	0.84536900
C	2.39806500	2.89060900	1.33629800
H	2.90999100	3.85880500	1.34801300
H	2.18966900	2.58738300	2.36702600
H	3.05943500	2.13782100	0.90468000
C	0.21180300	4.23034900	-1.54766900
H	0.36815000	5.22976700	-1.12949400
H	0.35309100	4.28663300	-2.63147300
H	-0.81614400	3.92088900	-1.35666000
C	2.61423900	3.67789200	-1.41808200
H	2.65504300	3.69851300	-2.51118700

H	2.81253100	4.69030800	-1.04941500
H	3.40733300	3.02288800	-1.05808600
C	1.42702400	-1.03624000	0.97993200
C	0.71533900	-0.95403800	2.18929700
C	2.82485400	-0.83823800	0.96923700
C	1.40509200	-0.63333500	3.36075500
C	3.47125500	-0.51403100	2.16188700
C	2.77150700	-0.40282500	3.35526200
H	0.85366700	-0.56274900	4.29464900
H	4.54422900	-0.34226000	2.15131400
H	3.29004900	-0.14792900	4.27466000
C	3.66047900	-0.96431200	-0.29143800
C	4.91216400	-1.82549900	-0.08871900
C	4.02559800	0.40003300	-0.87757900
H	3.04254600	-1.45253200	-1.03561500
H	4.67606700	-2.78671800	0.37949200
H	5.39026800	-2.02170200	-1.05430200
H	5.65126900	-1.32068900	0.54211500
H	3.11766600	0.96134200	-1.11597700
H	4.63178100	0.98334900	-0.17323300
H	4.60679100	0.27550600	-1.79869800
C	-0.78081200	-1.18546400	2.29007000
C	-1.48848400	0.06555700	2.82773900
C	-1.10959300	-2.40802600	3.15540500
H	-1.15257600	-1.38880100	1.28380800
H	-1.24523200	0.93884200	2.21489500
H	-2.57379400	-0.07830900	2.84686600
H	-1.16675300	0.27466300	3.85410800
H	-0.63219800	-3.31530800	2.77128000
H	-0.77174300	-2.26360500	4.18723400

H	-2.19292700	-2.57414800	3.18094400
H	-1.31952700	-0.39128000	-0.38371600
C	-3.95526000	-0.72108500	0.62625200
C	-3.59822000	0.50982200	0.07329500
C	-4.55069300	1.52977200	-0.04179500
C	-5.85219400	1.30935500	0.39150700
C	-6.20710800	0.08030700	0.94496700
C	-5.25797300	-0.93247200	1.06345600
H	-3.20892200	-1.50588900	0.71390500
H	-4.25171000	2.48221000	-0.46705100
H	-6.59028600	2.09966800	0.29972200
H	-7.22411900	-0.08767500	1.28502000
H	-5.53120800	-1.88911800	1.49663800
C	-2.23873400	0.81451400	-0.37223000
N	-1.52529200	1.70924500	-0.72958200
C	-2.70304800	-2.08995500	-2.37064400
H	-3.04770600	-1.66777200	-3.31855700
H	-3.17455300	-3.07203400	-2.25192400
H	-3.07121000	-1.44879600	-1.56898200

Vt

C	-0.46964400	-3.03884100	-1.28535900
C	0.11812400	-1.74820100	-1.95291900
C	1.72187800	-2.63925100	-0.11287700
C	0.36845500	-3.37022400	-0.03399100
H	-0.31908000	-3.83224100	-2.03168700
H	-0.16031100	-3.05348600	0.87222500
H	0.54780400	-4.44774200	0.04949100
C	0.44206000	-0.72825700	-0.86916400
C	2.28828200	-2.95693300	-1.51393200

H	3.36440000	-2.77721100	-1.57265800
H	2.14998800	-4.03344900	-1.66525900
C	1.49913100	-2.15432400	-2.54565000
H	2.03635600	-1.24515400	-2.84021500
H	1.32626500	-2.73778600	-3.45550200
N	1.34476400	-1.17248500	-0.02925700
C	-0.74931400	-1.22433300	-3.09568800
H	-1.71022500	-0.86027800	-2.73849400
H	-0.24619600	-0.39295900	-3.59638600
H	-0.90076900	-2.03565200	-3.81803200
C	2.69017800	-3.05422400	0.98176700
H	3.64767100	-2.53249800	0.89183800
H	2.29550700	-2.86797900	1.98271400
H	2.87620900	-4.12736200	0.87522100
C	0.15077100	2.93272600	-0.07217200
C	-0.11375000	2.88913800	-1.63205900
B	-0.37792400	0.74995600	-0.78235100
O	-0.07432500	1.59704900	0.35682400
O	0.01201300	1.51190000	-1.96087700
C	-0.79549300	3.86771900	0.68334200
H	-0.56823100	3.82151200	1.75373000
H	-0.66982900	4.90611600	0.35556400
H	-1.84129800	3.58471200	0.54314600
C	1.58511900	3.29938800	0.30964500
H	1.82264400	4.34297300	0.07610900
H	1.70359500	3.14223500	1.38701500
H	2.30072600	2.65141000	-0.19549500
C	-1.52377000	3.35023100	-2.02588400
H	-1.67188000	4.41971200	-1.84275200
H	-1.65781300	3.15829600	-3.09448600

H	-2.29311100	2.78943700	-1.49075800
C	0.90044400	3.67929600	-2.45407600
H	0.67093300	3.56252400	-3.51747100
H	0.85744700	4.74656700	-2.20890800
H	1.91930800	3.32354000	-2.28467800
C	1.95560800	-0.34511100	1.00649900
C	1.29650800	-0.13473900	2.22532200
C	3.23774500	0.16736500	0.74301200
C	1.97867300	0.59069700	3.20520100
C	3.86512800	0.90239100	1.74894000
C	3.24677900	1.10535100	2.97583500
H	1.49665700	0.76553600	4.16224900
H	4.85342400	1.31404300	1.57325200
H	3.75286100	1.67058100	3.75252500
C	3.93215000	-0.06532500	-0.59122800
C	5.45690500	-0.13685200	-0.47241900
C	3.52896400	0.96224200	-1.65733800
H	3.60155900	-1.03653600	-0.95643700
H	5.77124900	-0.82896600	0.31574400
H	5.88507400	-0.47603400	-1.42070100
H	5.89101200	0.84467800	-0.25625000
H	2.44120400	1.03900900	-1.77646100
H	3.91427900	1.95434700	-1.39517300
H	3.96445400	0.68261100	-2.62359200
C	-0.10815300	-0.63521900	2.52353700
C	-0.96384700	0.45169500	3.18713100
C	-0.08399300	-1.87901900	3.42375600
H	-0.59353900	-0.89121400	1.57486300
H	-0.87458900	1.39033700	2.63621700
H	-2.01356700	0.13855300	3.19321900

H	-0.66572000	0.61346300	4.22897900
H	0.44826500	-2.72046400	2.97125700
H	0.40794000	-1.64768300	4.37530900
H	-1.10573100	-2.20673200	3.64237600
H	-2.30287000	1.29493600	0.96504600
C	-4.79383200	0.52053200	1.38827900
C	-4.04203100	0.17072600	0.26456900
C	-4.63607800	-0.59849400	-0.74166700
C	-5.95421200	-1.01741900	-0.61745700
C	-6.69602400	-0.67171200	0.51365100
C	-6.11500100	0.09963700	1.51639200
H	-4.33401700	1.12943100	2.16428000
H	-4.04088500	-0.84501800	-1.61598900
H	-6.41135900	-1.61133600	-1.40348200
H	-7.72685500	-0.99976800	0.60867100
H	-6.69098900	0.37485600	2.39479300
C	-2.62876400	0.61460700	0.16102800
N	-1.85060000	0.24948900	-0.76836700
C	-1.95723600	-2.98530500	-0.95301100
H	-2.56336700	-2.83697300	-1.85050900
H	-2.26459900	-3.92974100	-0.49028100
H	-2.18158700	-2.16730900	-0.26272300

TS3t

C	-0.53051000	-2.79285900	-1.70014700
C	0.19601100	-1.48710000	-2.16153900
C	1.63959700	-2.76789800	-0.42991200
C	0.23390800	-3.38824300	-0.50150500
H	-0.45183400	-3.48791000	-2.54946200
H	-0.30032500	-3.17689000	0.43146600

H	0.32222200	-4.47746600	-0.58806100
C	0.57649200	-0.61868400	-0.96314300
C	2.24024500	-2.92943500	-1.84430700
H	3.32654200	-2.80696300	-1.84690800
H	2.04932100	-3.96482100	-2.14991800
C	1.54313500	-1.94327700	-2.78710300
H	2.16911400	-1.06117900	-2.96484700
H	1.34603300	-2.39920300	-3.76390200
N	1.38188900	-1.30129900	-0.17004300
C	-0.60337000	-0.71033300	-3.20206100
H	-1.52088800	-0.30410400	-2.77416600
H	-0.01377800	0.13409600	-3.57209500
H	-0.85370500	-1.36177100	-4.04933200
C	2.50428500	-3.42191300	0.63583800
H	3.50895600	-2.99070200	0.67408900
H	2.06288300	-3.33547900	1.63192300
H	2.60190300	-4.48517400	0.39387900
C	0.38973100	3.26106100	0.15134300
C	0.08934000	3.45768100	-1.37805500
B	-0.85520700	1.52272900	-0.65829500
O	-0.49607000	2.19020100	0.50499000
O	-0.39351100	2.17171200	-1.79140800
C	0.06502500	4.46788500	1.02122500
H	0.29041500	4.23086800	2.06516300
H	0.67348600	5.33035500	0.72742200
H	-0.98986100	4.74176600	0.95282400
C	1.80385200	2.77658000	0.43298000
H	2.55588600	3.53997100	0.20623200
H	1.88108600	2.50287500	1.48977800
H	2.00309500	1.88217300	-0.15628200

C	-1.04336200	4.45329300	-1.63514400
H	-0.74989900	5.47955500	-1.39314700
H	-1.31653100	4.40529000	-2.69261500
H	-1.92833200	4.19190100	-1.04574800
C	1.30635300	3.82136800	-2.21600000
H	1.01025600	3.91909100	-3.26440700
H	1.73263000	4.77586800	-1.88776000
H	2.07628900	3.04935200	-2.14756300
C	1.93951100	-0.65998100	1.00783800
C	1.13307800	-0.44848100	2.13813200
C	3.28682800	-0.25018700	0.97015500
C	1.71974600	0.16974900	3.24823800
C	3.81952900	0.37021800	2.09935100
C	3.04572700	0.57444200	3.23605300
H	1.11962000	0.33558600	4.13769700
H	4.85443000	0.69616300	2.09390100
H	3.47789400	1.05282600	4.10984600
C	4.14565000	-0.44636400	-0.27186300
C	5.63354400	-0.62080100	0.04450200
C	3.95192400	0.67697600	-1.29926300
H	3.81447000	-1.36708100	-0.75138500
H	5.79595200	-1.37182400	0.82446500
H	6.16775200	-0.93789800	-0.85633900
H	6.08930700	0.31806900	0.37595600
H	2.90732400	0.74669200	-1.62040900
H	4.24674200	1.64375100	-0.87567800
H	4.57197500	0.48603000	-2.18228600
C	-0.31757900	-0.89742000	2.23050700
C	-1.21197900	0.14372700	2.91399900
C	-0.42524600	-2.22721800	2.99145700

H	-0.69822400	-1.03391900	1.21283900
H	-1.06205100	1.13326000	2.47657800
H	-2.26209200	-0.14538200	2.79131800
H	-1.01632500	0.19469500	3.99110100
H	0.16872000	-3.02318800	2.53425500
H	-0.07226200	-2.10068100	4.02147300
H	-1.46797700	-2.56066100	3.02798200
H	-2.80111100	1.69535900	0.96010100
C	-5.00098900	0.30049300	1.43928300
C	-4.22296700	0.18485900	0.28489600
C	-4.67923300	-0.60378200	-0.77617100
C	-5.88537100	-1.28421100	-0.67119100
C	-6.64782400	-1.18133000	0.49347800
C	-6.20650800	-0.38686100	1.54855100
H	-4.65162700	0.93007300	2.25502800
H	-4.07420500	-0.65501900	-1.67575800
H	-6.23889900	-1.89199400	-1.49859200
H	-7.59055500	-1.71421300	0.57347400
H	-6.80251900	-0.29964900	2.45170800
C	-2.93623300	0.91006500	0.19877900
N	-2.04817900	0.65761400	-0.67544100
C	-2.00925400	-2.62218100	-1.37207600
H	-2.15580000	-1.85231700	-0.60792500
H	-2.58214000	-2.32594200	-2.25513900
H	-2.42513100	-3.56640000	-1.00230600

VIt

C	-0.43636400	-2.57050600	-1.96370600
C	0.35978300	-1.26851000	-2.29453000
C	1.72758200	-2.77852400	-0.69384700

C	0.30908700	-3.34939700	-0.85768400
H	-0.42618500	-3.17230200	-2.88456400
H	-0.22273100	-3.26804200	0.09732200
H	0.37574100	-4.41651600	-1.09986200
C	0.76325500	-0.54237400	-1.01725400
C	2.36057600	-2.79076000	-2.10243000
H	3.44583900	-2.66254000	-2.05533300
H	2.18604200	-3.78928900	-2.52028100
C	1.68880500	-1.70968700	-2.96062100
H	2.33926900	-0.83246000	-3.06181900
H	1.48289600	-2.07480600	-3.97344700
N	1.51027700	-1.34559900	-0.28237900
C	-0.41237700	-0.33503900	-3.21957300
H	-1.29570200	0.07004600	-2.71928600
H	0.21687400	0.51648600	-3.49829000
H	-0.72032300	-0.85844400	-4.13435000
C	2.55568400	-3.56293000	0.30987900
H	3.56063000	-3.14418200	0.42395900
H	2.08490000	-3.58451200	1.29672800
H	2.65505400	-4.59307200	-0.04739200
C	0.21000900	3.44611500	0.39629200
C	0.05474100	3.73090100	-1.13969400
B	-1.30696700	2.03512400	-0.52770700
O	-0.93761200	2.61526000	0.66682800
O	-0.67932700	2.58586700	-1.61025700
C	0.14186400	4.68114700	1.28130700
H	0.24252600	4.38167600	2.32827900
H	0.96119000	5.36796000	1.04240800
H	-0.80633500	5.21026200	1.16562500
C	1.44239300	2.61150100	0.72770400

H	2.36686800	3.17452700	0.56182500
H	1.40115200	2.31247900	1.78081200
H	1.44541000	1.70172100	0.11955100
C	-0.81053800	4.95605900	-1.43298200
H	-0.30142500	5.88521400	-1.15930200
H	-1.03330500	4.97981500	-2.50299600
H	-1.75871800	4.90186900	-0.88879900
C	1.36767100	3.81375300	-1.90163700
H	1.16424800	4.00746100	-2.95877600
H	1.98966700	4.62843800	-1.51465100
H	1.92132700	2.87594600	-1.82339000
C	2.02538400	-0.85307500	0.98117500
C	1.18002700	-0.79020900	2.09952600
C	3.35820200	-0.40545000	1.03621400
C	1.71668700	-0.30727700	3.29800300
C	3.84004700	0.08978700	2.24730500
C	3.03047800	0.12862000	3.37726800
H	1.08475400	-0.26477100	4.18055000
H	4.86336600	0.44514100	2.31231400
H	3.42447300	0.50575400	4.31619900
C	4.23678600	-0.40011300	-0.20461600
C	5.72816600	-0.55178900	0.10247700
C	3.98311300	0.85925500	-1.04317300
H	3.94498900	-1.25624300	-0.81703700
H	5.92029700	-1.40280900	0.76405200
H	6.28350700	-0.70589100	-0.82770300
H	6.13630200	0.34704900	0.57648200
H	2.93307900	0.91517800	-1.34712400
H	4.22148500	1.75851500	-0.46350400
H	4.60965700	0.85256400	-1.94217200

C	-0.27895600	-1.21387300	2.06689200
C	-1.19298300	-0.15008100	2.68460600
C	-0.48102600	-2.55826300	2.77729700
H	-0.57722900	-1.31507100	1.02015300
H	-1.02248300	0.82775300	2.22472900
H	-2.24016500	-0.43550000	2.52997700
H	-1.03612800	-0.06164400	3.76551000
H	0.13610200	-3.35165800	2.34416800
H	-0.21586400	-2.47377200	3.83755800
H	-1.52933300	-2.86932300	2.71360500
H	-3.14674400	1.67040800	1.18392700
C	-5.10015200	-0.08559100	1.50372400
C	-4.36260000	0.07415300	0.32821100
C	-4.71599900	-0.65096600	-0.81449100
C	-5.78211500	-1.53922800	-0.77194800
C	-6.50513900	-1.70778900	0.41054500
C	-6.16573100	-0.97995700	1.54826200
H	-4.82893500	0.49115600	2.38549300
H	-4.14155700	-0.49097200	-1.72132500
H	-6.05699900	-2.09973900	-1.66023500
H	-7.33872500	-2.40297100	0.44133600
H	-6.73190700	-1.10661900	2.46569400
C	-3.21881800	1.00778600	0.30566400
N	-2.37191500	1.04625500	-0.64377700
C	-1.89371600	-2.31841800	-1.58433600
H	-1.97379000	-1.57698100	-0.78106600
H	-2.46287000	-1.93588200	-2.43594600
H	-2.37132500	-3.24626300	-1.24953800

VIII

C	0.54947300	1.44156900	2.92256500
C	0.73629200	0.01031800	2.34807200
C	2.94179800	1.37125500	2.10849300
C	1.77859300	2.28707100	2.53100000
H	0.53008700	1.32589500	4.01706400
H	1.53574600	2.95946200	1.69751200
H	2.09496300	2.92439800	3.36599100
C	1.17820700	0.13946100	0.85798600
C	3.09744100	0.31545200	3.21974500
H	4.04440700	-0.22300800	3.10741900
H	3.12929400	0.81829000	4.19536000
C	1.89348100	-0.64326400	3.13008200
H	2.17054600	-1.57658100	2.62164100
H	1.54002400	-0.92303700	4.13011300
N	2.56491900	0.65032900	0.86832800
C	-0.53637800	-0.80723800	2.55047700
H	-1.32404500	-0.52624900	1.84757800
H	-0.34420500	-1.87494500	2.42588500
H	-0.91599400	-0.64012900	3.56719700
C	4.20482500	2.20339300	1.93668000
H	5.04918200	1.60699000	1.58462500
H	4.04808700	3.01350000	1.21670600
H	4.47162400	2.64550100	2.90207400
C	0.88184300	-2.24631600	-2.05985900
C	0.25404000	-3.11758000	-0.93262500
B	0.96674100	-1.12670700	-0.08555400
O	1.59752500	-1.24573900	-1.30314200
O	0.06955400	-2.15205000	0.12652500
C	-0.17233000	-1.50807100	-2.88473000
H	0.33393700	-0.78011800	-3.52545600

H	-0.73741400	-2.19598600	-3.52100500
H	-0.87435700	-0.97344900	-2.23461400
C	1.84937500	-2.97599200	-2.97711800
H	1.31750300	-3.73509000	-3.56124700
H	2.29920100	-2.25936500	-3.66987300
H	2.65243000	-3.46500400	-2.42339400
C	-1.08589400	-3.73649900	-1.29395300
H	-0.98553800	-4.36286600	-2.18773600
H	-1.42685000	-4.37697000	-0.47340700
H	-1.84212800	-2.96951300	-1.47741800
C	1.20076600	-4.18749200	-0.39284600
H	0.76649200	-4.61002000	0.51763700
H	1.34738100	-4.99524000	-1.11657900
H	2.17536900	-3.76031500	-0.13902900
C	3.37964300	0.75097100	-0.29879300
C	3.14623500	1.73009700	-1.28583200
C	4.48043100	-0.12512200	-0.44668900
C	4.02367300	1.84143300	-2.36745400
C	5.34953900	0.03586300	-1.52623100
C	5.13177400	1.01593700	-2.48471500
H	3.84021800	2.59965100	-3.12527500
H	6.20460200	-0.62895800	-1.62504000
H	5.81529200	1.12919600	-3.32107600
C	4.72447300	-1.28329700	0.50542600
C	6.02277100	-1.13361700	1.30758200
C	4.74765300	-2.60962200	-0.26396800
H	3.88039000	-1.31008200	1.20067500
H	6.03138500	-0.22714000	1.91883400
H	6.16066900	-1.99204300	1.97457600
H	6.88762700	-1.09061900	0.63551900

H	3.87795700	-2.67434000	-0.92123900
H	5.64620100	-2.69526900	-0.88526600
H	4.74008200	-3.45975900	0.42762300
C	1.95307400	2.66946900	-1.23947800
C	1.00776400	2.36309400	-2.40806400
C	2.37102400	4.14418100	-1.24911200
H	1.41377400	2.48726400	-0.30625300
H	0.61297600	1.34409900	-2.32801200
H	0.16910700	3.06895200	-2.43283300
H	1.53353000	2.44569900	-3.36551700
H	3.05278200	4.36981200	-0.42327400
H	2.87727400	4.41077600	-2.18303500
H	1.49139700	4.79003700	-1.15157500
H	0.47813600	0.87420800	0.39648700
C	-0.74306300	2.14649200	2.51394500
H	-1.63927900	1.57816700	2.78066800
H	-0.80235600	3.12593200	3.00119400
H	-0.76577600	2.32025900	1.43258000
C	-4.70960100	-2.08322100	-0.30061400
C	-4.34687600	-1.85267600	1.20181500
B	-3.15685700	-0.45237100	-0.11357800
O	-3.62904900	-1.41043500	-0.98302400
O	-3.68404700	-0.57105900	1.15570200
C	-6.00106300	-1.37939800	-0.71470100
H	-6.08318300	-1.40974200	-1.80430700
H	-6.88064700	-1.86602400	-0.28291100
H	-5.99298400	-0.32899200	-0.40498100
C	-4.74322600	-3.54065100	-0.72990000
H	-5.52170900	-4.08071100	-0.18005400
H	-4.97152300	-3.60282500	-1.79769500

H	-3.78480300	-4.03147400	-0.55409000
C	-5.54122800	-1.75431600	2.13640900
H	-6.11585000	-2.68673700	2.12382400
H	-5.19247900	-1.58017500	3.15784800
H	-6.20066000	-0.93056800	1.85459000
C	-3.32605900	-2.85839700	1.72955000
H	-2.99308900	-2.53276400	2.71918300
H	-3.75645500	-3.86092600	1.81657600
H	-2.44500800	-2.89630900	1.07887100
C	-2.14079700	1.72649000	-0.71686800
N	-2.14739000	0.48851600	-0.47093000
C	-3.28475500	2.67081500	-0.72581500
C	-3.14277400	3.87064000	-1.42812400
C	-4.48129000	2.40637700	-0.04950700
C	-4.19271900	4.78063500	-1.49105200
H	-2.20415700	4.08184500	-1.93545100
C	-5.52525900	3.32229400	-0.10312800
H	-4.57559600	1.50523400	0.54945400
C	-5.38675100	4.50465700	-0.82977600
H	-4.07863900	5.70441600	-2.04928200
H	-6.44789900	3.12003200	0.43204700
H	-6.20610200	5.21578800	-0.86985800
H	-1.17967600	2.19450500	-0.96842000

TS4t

C	0.50655700	2.37036000	2.50830100
C	0.29121100	0.85893600	2.20030800
C	2.73921400	1.54734400	1.69103400
C	1.82216700	2.77531200	1.84366600
H	0.62645400	2.43094800	3.60028600

H	1.63302300	3.19168200	0.84346200
H	2.33929300	3.54877000	2.42381000
C	0.73557200	0.50000900	0.74706800
C	2.67260800	0.78280700	3.03134500
H	3.47366900	0.05234500	3.13169200
H	2.80443500	1.50903200	3.84308800
C	1.29436900	0.10622900	3.11114500
H	1.33710400	-0.93977300	2.78547000
H	0.91581800	0.11480500	4.13978200
N	2.12276200	0.66518600	0.64383400
C	-1.12622500	0.42135200	2.56695800
H	-1.88180600	0.95437800	1.98759500
H	-1.26736700	-0.65173900	2.41173300
H	-1.29836900	0.65625500	3.62556000
C	4.12684800	2.06310200	1.31993400
H	4.82951400	1.29249600	1.01190200
H	4.05396700	2.78391600	0.49896500
H	4.54034600	2.58287700	2.19070000
C	0.34680900	-2.48788100	-1.53229300
C	0.07067800	-3.11349800	-0.10624900
B	-0.07218300	-0.79260100	-0.02904100
O	0.62250700	-1.12294100	-1.24715500
O	-0.27641400	-1.99751400	0.70617200
C	-0.86825100	-2.55694200	-2.46578800
H	-0.64674500	-1.97710900	-3.36735500
H	-1.09860400	-3.58592200	-2.76153100
H	-1.75718600	-2.12137400	-2.00117900
C	1.56093600	-3.06457400	-2.25405700
H	1.45309800	-4.14170500	-2.42487000
H	1.67080400	-2.57011500	-3.22460600

H	2.47483700	-2.87675200	-1.68422600
C	-1.06124300	-4.13706900	-0.08152800
H	-0.80682200	-5.01284700	-0.69031400
H	-1.22221600	-4.46578300	0.94971000
H	-1.99757500	-3.70737900	-0.44108000
C	1.31776500	-3.70968700	0.52956800
H	1.08298900	-4.00804800	1.55638300
H	1.71222300	-4.57679400	-0.01072300
H	2.07653900	-2.92990200	0.56816400
C	3.00379000	0.20410400	-0.41756200
C	3.00027600	0.86468000	-1.66495700
C	3.99718700	-0.78193700	-0.16622500
C	3.95732600	0.53810600	-2.62795200
C	4.93575800	-1.06203400	-1.16513500
C	4.93016100	-0.41571100	-2.38899300
H	3.94424600	1.05825800	-3.58146800
H	5.69653700	-1.81168300	-0.96805900
H	5.67524100	-0.65103100	-3.14263700
C	4.18356200	-1.58177400	1.12460500
C	5.37904600	-1.09374400	1.96817600
C	4.47395200	-3.07541300	0.84248700
H	3.26279800	-1.50645600	1.71254100
H	5.27863800	-0.08221000	2.35813500
H	5.52357300	-1.76695000	2.82068400
H	6.29060900	-1.12606500	1.36048600
H	3.94972500	-3.45582600	-0.03492800
H	5.54546800	-3.23398600	0.68069400
H	4.18357400	-3.68216400	1.70598600
C	1.99941900	1.93935500	-2.05621700
C	1.24795100	1.50157800	-3.32388100

C	2.67016900	3.30161400	-2.27346000
H	1.28468700	2.06370400	-1.24056500
H	0.82829000	0.49973400	-3.18988600
H	0.44264600	2.20101000	-3.57497000
H	1.92406300	1.47553200	-4.18453200
H	3.18247600	3.64623400	-1.36991400
H	3.40829400	3.25682800	-3.08127100
H	1.92137600	4.05425500	-2.54569100
H	0.03481200	1.35678700	0.04042000
C	-0.60468700	3.34482800	2.13276200
H	-1.56211600	3.08962000	2.59554300
H	-0.32871300	4.34964000	2.47277000
H	-0.74867000	3.39636500	1.05090400
C	-4.96260500	-1.12573600	-0.45010200
C	-4.45334700	-1.79409700	0.86684200
B	-2.77468300	-0.62436600	-0.09896700
O	-3.92247700	-0.17209900	-0.72729000
O	-3.02692900	-1.69591000	0.73049800
C	-6.28578600	-0.38679800	-0.32406000
H	-6.55789800	0.04467700	-1.29132200
H	-7.08319500	-1.07156100	-0.01561500
H	-6.21702900	0.42543300	0.40306600
C	-5.00586000	-2.10095300	-1.62529400
H	-5.82809200	-2.81608000	-1.52464000
H	-5.14507000	-1.53254500	-2.54868100
H	-4.06622200	-2.65796700	-1.70559500
C	-4.83365000	-1.00344700	2.11903900
H	-5.90355400	-1.07657900	2.33671400
H	-4.27181700	-1.40224400	2.96794300
H	-4.57180800	0.05494600	2.00931500

C	-4.83581700	-3.25639400	1.03423900
H	-4.41409500	-3.63745700	1.96848700
H	-5.92488600	-3.36786200	1.07551800
H	-4.44943400	-3.86598100	0.21507600
C	-1.19265500	1.14485500	-0.85340300
N	-1.48200700	-0.06745600	-0.33479600
C	-2.03691900	2.35530800	-0.80763500
C	-1.65846300	3.42923300	-1.62483400
C	-3.12687400	2.52452200	0.05612900
C	-2.34854600	4.63487800	-1.59073100
H	-0.80094700	3.31445200	-2.28270300
C	-3.82078500	3.72669800	0.08714400
H	-3.43595400	1.71507700	0.70556200
C	-3.43514000	4.78601400	-0.73312200
H	-2.03804000	5.45471600	-2.23064600
H	-4.66433400	3.84131900	0.76076000
H	-3.97775800	5.72567500	-0.70043700
H	-0.49816500	1.13536600	-1.69410900

VIII

C	0.62788700	2.06029200	2.68092500
C	0.57565000	0.52547000	2.41639400
C	2.92900500	1.44725700	1.83990500
C	1.94876100	2.59754500	2.11906800
H	0.62522000	2.17014000	3.77459000
H	1.77463700	3.13803900	1.17999100
H	2.42373900	3.30116800	2.81136000
C	1.01476000	0.23621100	0.98306100
C	3.00955200	0.58860300	3.11541900
H	3.83878700	-0.11735800	3.07164500

H	3.21499100	1.27132000	3.94790200
C	1.66985200	-0.13030900	3.30290500
H	1.73968600	-1.18943300	3.02902400
H	1.33915300	-0.08720200	4.34548700
N	2.26396400	0.60636100	0.76290000
C	-0.77442300	-0.06947300	2.81038400
H	-1.59792800	0.38213900	2.26232100
H	-0.80757100	-1.14248300	2.60892700
H	-0.92641700	0.10457500	3.88277000
C	4.26657900	2.04318200	1.41808600
H	4.98980700	1.31285000	1.06341500
H	4.13291400	2.78436700	0.62624700
H	4.68803900	2.55197300	2.29104800
C	0.36137700	-2.06255000	-1.82317300
C	0.21748800	-2.89868100	-0.49173100
B	-0.03295000	-0.60917100	-0.06428800
O	0.62081800	-0.74714200	-1.35511200
O	-0.15297400	-1.94484700	0.49041900
C	-0.91572800	-2.05640900	-2.67466300
H	-0.77754400	-1.34813300	-3.49842600
H	-1.12250200	-3.04346800	-3.10256200
H	-1.79203900	-1.73508900	-2.10432000
C	1.53520100	-2.47915500	-2.70695000
H	1.44417800	-3.52258700	-3.02997500
H	1.55655800	-1.84380700	-3.59838400
H	2.48651800	-2.34528900	-2.18398200
C	-0.84203700	-3.99452400	-0.54584900
H	-0.61000100	-4.73422700	-1.32107700
H	-0.88253100	-4.50367300	0.42191500
H	-1.82898000	-3.56953700	-0.73590100

C	1.54457400	-3.48226400	-0.02890700
H	1.41607500	-3.90425100	0.97322800
H	1.93688400	-4.25919200	-0.69400700
H	2.26248400	-2.66456200	0.03318100
C	3.07446600	0.35693000	-0.43592100
C	2.92719300	1.20776900	-1.54682300
C	4.11476300	-0.60003600	-0.38565000
C	3.82269100	1.07707100	-2.60937900
C	4.97587900	-0.68489000	-1.48475500
C	4.84367100	0.14164800	-2.58792000
H	3.71340000	1.72975100	-3.47018600
H	5.77464200	-1.42030900	-1.46414800
H	5.53188500	0.05740500	-3.42303100
C	4.41965700	-1.56080400	0.76622200
C	5.67023600	-1.15864100	1.57331100
C	4.70419500	-2.99188400	0.25236200
H	3.55129700	-1.59547100	1.43440600
H	5.57596700	-0.22429400	2.12531600
H	5.90456000	-1.94802500	2.29564100
H	6.52764300	-1.06052900	0.89817600
H	4.11376400	-3.25447800	-0.62555000
H	5.76126900	-3.09828500	-0.01343600
H	4.49169300	-3.72065400	1.04044400
C	1.85199200	2.27295700	-1.67555900
C	1.04853900	2.07619300	-2.96913500
C	2.44196300	3.68970600	-1.64357100
H	1.16538300	2.17546500	-0.82947900
H	0.67290100	1.05155600	-3.02823500
H	0.20198000	2.77116600	-2.99413800
H	1.66760100	2.28362600	-3.84820200

H	2.97145000	3.90201400	-0.71000800
H	3.14928100	3.83452100	-2.46740300
H	1.64256600	4.42984100	-1.75234600
H	-0.61320100	1.61460900	-1.25202800
C	-0.55416000	2.83457100	2.10966000
H	-1.49258100	2.58289500	2.60791300
H	-0.39205700	3.91169600	2.22491800
H	-0.67849100	2.62444100	1.04072400
C	-4.76257500	-1.41564300	-0.29703200
C	-4.25260700	-1.87079500	1.11136100
B	-2.61530600	-0.70139700	0.05661300
O	-3.76676100	-0.46755200	-0.69171900
O	-2.83571100	-1.68244600	1.01491200
C	-6.11985900	-0.72467000	-0.28992800
H	-6.39438700	-0.45219200	-1.31291100
H	-6.89424900	-1.38921900	0.10939900
H	-6.09174200	0.19074000	0.30485000
C	-4.75889000	-2.54251800	-1.32955400
H	-5.54719100	-3.27591300	-1.13202700
H	-4.92364300	-2.10767300	-2.31937600
H	-3.79523700	-3.06050200	-1.34404900
C	-4.74993100	-0.96350900	2.23852400
H	-5.81843700	-1.09988600	2.43272300
H	-4.19262800	-1.20233700	3.14898100
H	-4.57350300	0.08957900	1.99442700
C	-4.53255700	-3.32723600	1.45142300
H	-4.13692100	-3.55169900	2.44617200
H	-5.61012100	-3.52565900	1.45590200
H	-4.05159900	-3.99808800	0.73627800
C	-1.57450600	1.10460600	-1.16476000

N	-1.43493800	0.05851600	-0.16199400
C	-2.61733700	2.18139700	-0.90535900
C	-2.89925900	3.08903900	-1.92969900
C	-3.28296000	2.33675200	0.30987000
C	-3.80933100	4.12546500	-1.74583100
H	-2.40376400	2.97031700	-2.89187200
C	-4.19730800	3.36933200	0.50188300
H	-3.07773800	1.63753300	1.11501200
C	-4.46409600	4.27068800	-0.52503600
H	-4.01283700	4.81646300	-2.55885300
H	-4.70549100	3.46684400	1.45746000
H	-5.17879100	5.07472400	-0.37802400
H	-1.77190100	0.68618700	-2.16530400

TS5t

C	0.74041300	2.27493600	2.47540100
C	0.83042900	0.72141400	2.42423500
C	3.08134900	1.75938700	1.68494400
C	2.01228200	2.85357100	1.83291100
H	0.71972800	2.54540600	3.54132500
H	1.78609300	3.25511600	0.83729100
H	2.42379200	3.67698100	2.42796500
C	1.26200400	0.25050200	1.03659000
C	3.24841000	1.09407500	3.06417200
H	4.13698700	0.45977500	3.09114900
H	3.40956100	1.89649100	3.79365100
C	1.97451600	0.30080000	3.38312700
H	2.14193800	-0.77764700	3.27152900
H	1.64934400	0.46599800	4.41631500
N	2.46181900	0.73619800	0.75730900

C	-0.46476500	0.05259300	2.86671100
H	-1.29740700	0.30880400	2.21338300
H	-0.36339500	-1.03686500	2.83353200
H	-0.71570600	0.35210200	3.89245700
C	4.37693800	2.36341400	1.16274100
H	5.14255700	1.61906000	0.94700900
H	4.21241000	2.93738400	0.24784700
H	4.76475500	3.04556000	1.92653400
C	0.43842500	-2.35107800	-1.77596500
C	0.20356800	-3.03831200	-0.38480000
B	-0.50625400	-0.87370800	-0.33327700
O	0.29981400	-0.95674300	-1.47404600
O	-0.66795400	-2.11926700	0.27615900
C	-0.66132900	-2.69116000	-2.78523000
H	-0.54656900	-2.03996300	-3.65698100
H	-0.60935500	-3.73261000	-3.11837600
H	-1.65170400	-2.50599700	-2.35221800
C	1.81297800	-2.58934500	-2.38185500
H	1.98206100	-3.65793800	-2.55871300
H	1.88690800	-2.06603900	-3.34063600
H	2.60164700	-2.20310800	-1.73102000
C	-0.48388000	-4.39548500	-0.46310900
H	0.13211200	-5.10944200	-1.02135200
H	-0.63092100	-4.78593500	0.54836600
H	-1.45997500	-4.32363500	-0.94715100
C	1.47195200	-3.15634800	0.45052900
H	1.18818500	-3.40168600	1.47914000
H	2.12391000	-3.94825400	0.07086200
H	2.01060900	-2.20462400	0.45983800
C	3.22011400	0.35583900	-0.42672600

C	2.95709900	0.98274100	-1.66069700
C	4.28326600	-0.56498000	-0.29321000
C	3.79419200	0.69211300	-2.74128900
C	5.08884600	-0.81384300	-1.40808700
C	4.85877000	-0.18783000	-2.62283900
H	3.60984400	1.17577300	-3.69543700
H	5.90963600	-1.51982500	-1.31678400
H	5.50023500	-0.39058000	-3.47494100
C	4.61025700	-1.34529300	0.97717600
C	5.91217800	-0.88099300	1.65247900
C	4.77655000	-2.84780500	0.67558400
H	3.77731800	-1.22595900	1.67818400
H	5.87917500	0.14509100	2.02018700
H	6.13923600	-1.53294500	2.50309700
H	6.74523800	-0.95462400	0.94445900
H	4.06296300	-3.19886400	-0.06965200
H	5.78324400	-3.05699300	0.29782500
H	4.64286000	-3.43418100	1.59012400
C	1.83429500	1.98490500	-1.88213100
C	1.04381700	1.67671900	-3.16203800
C	2.36909700	3.42228000	-1.96455700
H	1.14905400	1.91291100	-1.03074200
H	0.67210800	0.64950500	-3.14988600
H	0.19229400	2.36138500	-3.24539400
H	1.65992700	1.82820800	-4.05433000
H	2.88813300	3.73307000	-1.05456000
H	3.07228300	3.52003000	-2.79952500
H	1.54334700	4.12127500	-2.13441600
H	-0.76694900	1.48952000	-1.48178900
C	-0.51086500	2.84155500	1.81286300

H	-1.41679200	2.57094400	2.36030900
H	-0.46093800	3.93502000	1.76684700
H	-0.61451000	2.46145900	0.78949400
C	-4.83375300	-1.63331000	-0.07132400
C	-4.52161700	-1.40829000	1.44268200
B	-2.85638600	-0.56399800	0.15848300
O	-3.92074600	-0.72172800	-0.70861500
O	-3.12859700	-1.04970200	1.41698700
C	-6.25391400	-1.29409800	-0.49260700
H	-6.37476700	-1.49001500	-1.56174100
H	-6.97612800	-1.91083200	0.05356900
H	-6.47735200	-0.24067400	-0.31255700
C	-4.44783800	-3.03706300	-0.53695000
H	-5.12817400	-3.79852700	-0.14328200
H	-4.48252400	-3.06705600	-1.62984900
H	-3.42702200	-3.27120300	-0.21481200
C	-5.28569600	-0.22099100	2.02763500
H	-6.34592100	-0.45528700	2.16569100
H	-4.85284800	0.02797600	3.00086000
H	-5.20278200	0.65506600	1.37635900
C	-4.69653400	-2.63694000	2.32176100
H	-4.46767300	-2.37826400	3.35949100
H	-5.72913100	-3.00043700	2.27757500
H	-4.02253100	-3.43899500	2.01501600
C	-1.74163000	1.01534500	-1.34310200
N	-1.62113700	0.06602600	-0.24043500
C	-2.76696700	2.11185800	-1.12988300
C	-3.12950200	2.90812200	-2.21977300
C	-3.34689800	2.38211400	0.10955900
C	-4.03923600	3.94987000	-2.07653900

H	-2.69583400	2.69900800	-3.19585700
C	-4.26494700	3.42072800	0.25734500
H	-3.07623400	1.77797500	0.97144100
C	-4.61341800	4.21037400	-0.83352700
H	-4.30746000	4.55472500	-2.93776100
H	-4.70619900	3.61092600	1.23185100
H	-5.32847700	5.01926000	-0.71931700
H	-1.96967300	0.50711500	-2.29277800

IXt

C	-2.59257600	-2.31245800	2.49867700
C	-2.76332600	-0.77854400	2.68770600
C	-4.52678000	-1.64468300	1.00482800
C	-3.63819800	-2.80953900	1.47295800
H	-2.79633800	-2.77367400	3.47551600
H	-3.14266600	-3.27402700	0.61452700
H	-4.29015700	-3.57554300	1.90802600
C	-2.68156600	-0.06102100	1.34724600
C	-5.24322000	-1.12260800	2.26739800
H	-6.01912300	-0.40078200	1.99237300
H	-5.75660200	-1.97283700	2.72993400
C	-4.19738700	-0.51446000	3.21974200
H	-4.33574700	0.56976700	3.31138000
H	-4.28543400	-0.93053300	4.23018000
N	-3.60566100	-0.54722400	0.54217100
C	-1.73601100	-0.20144700	3.65648500
H	-0.72749000	-0.25213600	3.23750200
H	-1.95443400	0.85491400	3.84548800
H	-1.74648100	-0.73551200	4.61496800
C	-5.51240900	-2.06914100	-0.07035200

H	-6.13816400	-1.23042600	-0.39066400
H	-5.00335500	-2.47165100	-0.95189400
H	-6.16388500	-2.85001700	0.33529100
C	0.39324500	2.61880100	-1.01066400
C	0.99280100	2.90238600	0.40315400
B	2.27294500	1.40801700	-0.68653800
O	1.08462800	1.40564000	-1.38548400
O	2.33300200	2.37992700	0.28014100
C	0.78374400	3.68155900	-2.03754000
H	0.51825100	3.32071500	-3.03502300
H	0.25844500	4.62414500	-1.85722400
H	1.86191600	3.87152800	-2.01400500
C	-1.10680200	2.38207000	-1.03167700
H	-1.63210000	3.30894400	-0.77193600
H	-1.42232500	2.08815400	-2.03876200
H	-1.41799500	1.60304800	-0.32931000
C	1.07273900	4.37231700	0.78019800
H	0.07294200	4.81993200	0.78658900
H	1.49969700	4.46991100	1.78227800
H	1.70581500	4.92651700	0.08413900
C	0.29616600	2.09885600	1.49921600
H	0.89937200	2.15293500	2.41051800
H	-0.70763200	2.47930000	1.71101300
H	0.18631200	1.04841900	1.20824100
C	-3.79798100	0.09361000	-0.74781800
C	-3.21467800	-0.47234000	-1.89345900
C	-4.52037400	1.29533300	-0.80306200
C	-3.39752500	0.17753900	-3.11458600
C	-4.66305200	1.91935000	-2.04566900
C	-4.11911100	1.36301200	-3.19478500

H	-2.95708000	-0.24213800	-4.01340600
H	-5.20829100	2.85669500	-2.11040500
H	-4.24710100	1.85832700	-4.15260900
C	-5.08963900	1.96326400	0.43705100
C	-6.53172800	2.44054100	0.24182300
C	-4.17550400	3.10776900	0.88992800
H	-5.09555500	1.22904600	1.24341200
H	-7.17533000	1.63015700	-0.11620100
H	-6.93578700	2.80765200	1.19077300
H	-6.59447700	3.26304100	-0.47805700
H	-3.18102500	2.71491300	1.12431900
H	-4.07809900	3.86232500	0.10050200
H	-4.58432600	3.59602100	1.78165000
C	-2.31352400	-1.68771100	-1.79163800
C	-0.88336300	-1.24365800	-1.46204700
C	-2.32500600	-2.57830400	-3.03504800
H	-2.66763800	-2.29487900	-0.95462000
H	-0.85709300	-0.63231000	-0.55333300
H	-0.24126400	-2.11860600	-1.31856700
H	-0.46725900	-0.63472600	-2.27304500
H	-3.34206100	-2.86311200	-3.32539900
H	-1.85142100	-2.08285600	-3.88905100
H	-1.75087900	-3.48867500	-2.83573000
H	2.36750500	-0.11699500	-2.73887000
C	-1.17790600	-2.70655900	2.06960900
H	-0.43575900	-2.45829800	2.83415900
H	-1.12146300	-3.78578200	1.88677000
H	-0.89106100	-2.19856400	1.14109600
C	6.67548200	-0.23709400	0.18386300
C	6.08471300	0.58658300	1.37341500

B	4.55141400	0.39232300	-0.26375700
O	5.49308300	-0.57149600	-0.56628200
O	4.93284700	1.20848300	0.77458400
C	7.38643000	-1.51970100	0.58450600
H	7.76808400	-2.02164600	-0.30901300
H	8.23356900	-1.30020500	1.24346700
H	6.70764900	-2.20488500	1.09572800
C	7.56613400	0.60518300	-0.72826400
H	8.52134200	0.84281600	-0.25026400
H	7.76426200	0.04153800	-1.64391000
H	7.06826200	1.54103500	-1.00092400
C	5.57430800	-0.30570100	2.50448900
H	6.39788900	-0.76137900	3.06268600
H	4.97948700	0.30415000	3.18946200
H	4.93556400	-1.10335200	2.11031800
C	7.00146200	1.66837700	1.92053300
H	6.50299000	2.18690000	2.74410400
H	7.93060200	1.23016300	2.30095900
H	7.24545300	2.40512200	1.15285200
C	3.07584200	-0.52603600	-2.01145900
N	3.32134700	0.47894600	-0.98091700
C	2.52247000	-1.83822700	-1.48202700
C	2.21851600	-2.85465300	-2.39291300
C	2.29325400	-2.06492700	-0.12662300
C	1.68907900	-4.06558400	-1.96259200
H	2.39191800	-2.68658600	-3.45399500
C	1.77057300	-3.28224400	0.31065700
H	2.51136600	-1.28136200	0.59338900
C	1.46068100	-4.28383800	-0.60332100
H	1.45367500	-4.84082300	-2.68608500

H	1.59924400	-3.44298900	1.37130800
H	1.04848800	-5.22871800	-0.26205300
H	4.01290500	-0.73272300	-2.53916600

HBpin

C	0.77976800	-0.18565100	-0.05472600
C	-0.77971300	-0.18578100	0.05465200
B	-0.00012700	1.93368800	0.00004300
O	1.06297300	1.18422000	-0.41935900
O	-1.06322600	1.18398700	0.41940100
C	1.34703600	-1.10824700	-1.12147000
H	2.43794800	-1.03453300	-1.12535700
H	1.07386700	-2.14838100	-0.91347500
H	0.98346600	-0.83974300	-2.11501500
C	1.46935000	-0.43486700	1.28538700
H	1.35822000	-1.47496500	1.60611200
H	2.53438200	-0.21289900	1.17943200
H	1.05960000	0.21758900	2.06263200
C	-1.46944400	-0.43494000	-1.28537100
H	-1.35801500	-1.47495600	-1.60623400
H	-2.53451500	-0.21338500	-1.17900500
H	-1.06017200	0.21766100	-2.06273200
C	-1.34668900	-1.10849300	1.12139200
H	-2.43759700	-1.03489500	1.12539900
H	-1.07341500	-2.14860200	0.91328900
H	-0.98299100	-0.84005900	2.11492300
H	0.00002600	3.12095600	0.00028700

PhCN

C	0.09084700	-1.21463400	-0.00000100
---	------------	-------------	-------------

C	1.48043600	-1.20837800	-0.00000300
C	2.17420000	0.00002100	0.00000300
C	1.48036300	1.20842100	0.00000000
C	0.09081000	1.21461900	-0.00000400
C	-0.60294700	-0.00004300	0.00000300
H	-0.46257900	-2.14749800	0.00000200
H	2.02258200	-2.14820200	-0.00000500
H	3.25959800	0.00007400	0.00000600
H	2.02251800	2.14824100	0.00000000
H	-0.46270800	2.14742800	0.00000100
C	-2.04316800	-0.00003100	0.00000100
N	-3.20037900	0.00001500	0.00000000

5) References

- S1. E. Tomás-Mendivil, M. M. Hansmann, C. M. Weinstein, R. Jazzar, M. Melaimi and G. Bertrand, *J. Am. Chem. Soc.*, 2017, **139**, 7753-7756.
- S2. H.-C. Yu, S. M. Islam and N. P. Mankad, *ACS Catal.*, 2020, **10**, 3670-3675.
- S3. B. V. Rokade and K. R. Prabhu, *J. Org. Chem.*, 2012, **77**, 5364-5370.
- S4. T. Yabuta, M. Hayashi and R. Matsubara, *J. Org. Chem.*, 2021, **86**, 2545-2555.
- S5. S. Ando, M. Tsuzaki and T. Ishizuka, *J. Org. Chem.*, 2020, **85**, 11181-11189.
- S6. X. Wang and X. Xu, *RSC Adv.*, 2021, **11**, 1128-1133.
- S7. D. Bedi, A. Brar and M. Findlater, *Green Chem.*, 2020, **22**, 1125-1128.
- S8. H. Dai and H. Guan, *ACS Catal.*, 2018, **8**, 9125-9130.
- S9. K. Sarkar, K. Das, A. Kundu, D. Adhikari and B. Maji, *ACS Catal.*, 2021, 2786-2794.
- S10. S.-F. Hou, J.-Y. Chen, M. Xue, M. Jia, X. Zhai, R.-Z. Liao, C.-H. Tung and W. Wang, *ACS Catal.*, 2020, **10**, 380-390.

- S11. L. Zhao, C. Hu, X. Cong, G. Deng, L. L. Liu, M. Luo and X. Zeng, *J. Am. Chem. Soc.*, 2021, **143**, 1618-1629.
- S12. M. Bhunia, S. R. Sahoo, A. Das, J. Ahmed, P. Sreejyothi and S. K. Mandal, *Chem. Sci.*, 2020, **11**, 1848-1854.
- S13. N. Gandhamsetty, J. Jeong, J. Park, S. Park and S. Chang, *J. Org. Chem.*, 2015, **80**, 7281-7287.
- S14. G. Hahn, P. Kunas, N. de Jonge and R. Kempe, *Nat. Catal.*, 2019, **2**, 71-77.
- S15. K. Ganguli, A. Mandal, B. Sarkar and S. Kundu, *Tetrahedron*, 2020, **76**, 131439.
- S16. Q. Guan, M. Jiang, J. Wu, Y. Zhai, Y. Wu, K. Bao and W. Zhang, *Green Chem.*, 2016, **18**, 5794-5799.
- S17. S. Das, H. S. Das, B. Singh, R. K. Haridasan, A. Das and S. K. Mandal, *Inorg. Chem.*, 2019, **58**, 11274-11278.
- S18. K. Murugesan, Z. Wei, V. G. Chandrashekar, H. Jiao, M. Beller and R. V. Jagadeesh, *Chem. Sci.*, 2020, **11**, 4332-4339.
- S19. M. K. Bisai, K. Gour, T. Das, K. Vanka and S. S. Sen, *Dalton Trans.*, 2021, **50**, 2354-2358.
- S20. A. D. Ibrahim, S. W. Entsminger and A. R. Fout, *ACS Catal.*, 2017, **7**, 3730-3734.
- S21. C. Bornschein, S. Werkmeister, B. Wendt, H. Jiao, E. Alberico, W. Baumann, H. Junge, K. Junge and M. Beller, *Nat. Commun.*, 2014, **5**, 4111.
- S22. M. Sheng, S. Fujita, J. Yamasaki, K. Nakajima, S. Yamazoe, T. Mizugaki and T. Mitsudome, *JACS Au*, 2021, **1**, 501-507.
- S23. H. S. Das, S. Das, K. Dey, B. Singh, R. K. Haridasan, A. Das, J. Ahmed and S. K. Mandal, *Chem. Commun.*, 2019, **55**, 11868-11871.
- S24. J. Pecak, W. Eder, B. Stöger, S. Realista, P. N. Martinho, M. J. Calhorda, W. Linert and K. Kirchner, *Organometallics*, 2020, **39**, 2594-2601.

- S25. J. Neumann, C. Bornschein, H. Jiao, K. Junge and M. Beller, *Eur. J. Org. Chem.*, 2015, 5944-5948.
- S26. W. Yao, J. Wang, Y. Lou, H. Wu, X. Qi, J. Yang and A. Zhong, *Org. Chem. Front.*, 2021, **8**, 4554-4559.
- S27. W. Q. Wang, Y. Yuan, Y. Miao, B. Y. Yu, H. J. Wang, Z. Q. Wang, W. Sang, C. Chen and F. Verpoort, *Appl. Organomet. Chem.*, 2020, **34**, e5323.
- S28. C. Li, S. Song, Y. Li, C. Xu, Q. Luo, Y. Guo and X. Wang, *Nat. Commun.*, 2021, **12**, 3813.
- S29. V. Adebomi, M. Sriram, X. Streeby and M. Raj, *Org. Lett.*, 2021, **23**, 6189-6193.
- S30. P. Hohenberg and W. Kohn, *Phys. Rev.*, 1964, **136**, B864-B871.
- S31. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, et al. Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT, 2016.
- S32. R. Logdi, A. Bag and A. K. Tiwari, *J. Phys. Chem. A* 2021, **125**, 5718-5725.
- S33. R. Logdi, A. Bag and A. K. Tiwari, *J. Mol. Graphics Modell.*, 2019, **93**, 107437.