Supporting Information

Iodine-Mediated Decarboxylative Coupling to Synthesize β-Sulfonyl-ene-amines/2,3-Diarythio-pyrroles from α-Amino Acids and Sodium Sulfinates

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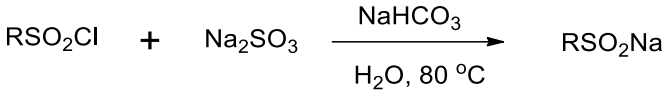
General remark

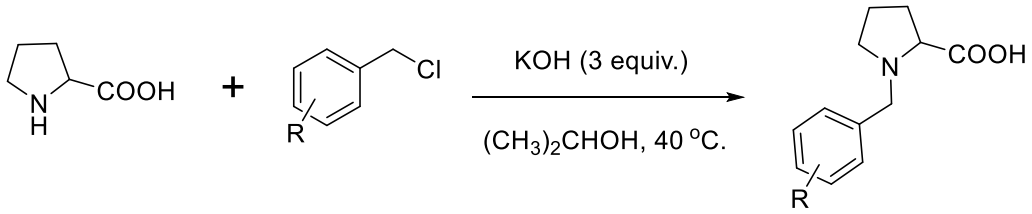
^{1}H NMR and ^{13}C NMR spectra were recorded on 400MHz and 100MHz in $CDCl_3$ (BRUKER 400M). All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. Unless otherwise noted, commercially available reagents and solvents were used without further purification.

Typical Experimental Procedure for the Preparation of Sodium Sulfinates[1]



Sodium sulfite (2.50 g, 0.02 mol, 2 eq.), sodium bicarbonate (1.68 g, 0.02 mol, 2 eq.) and the corresponding aryl sulfonyl chloride (0.01 mmol, 1 eq.) were dissolved in distilled water (9.60 mL). The reaction mixture was stirred for 4 h at 80 °C. After cooling to rt, the solvent was evaporated and the white residue was extracted with ethanol (25 mL) to obtain the desired aryl sulfinate as white crystalline powder.

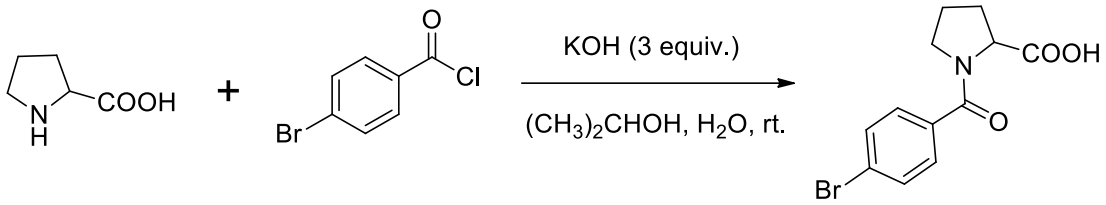
General procedure for synthesis of *a*-amino acids[2]



To a dry 25 mL flask, *L*-proline (1.15 g, 10 mmol) and potassium hydroxide (1.68 g, 30 mmol) were dissolved in isopropanol (7 mL) and heated to 40 °C. Benzylchloride (2 mL, 12 mmol) was added slowly over 0.5 h via a dropping funnel. The reaction mixture was stirred overnight at the same temperature and then was allowed to cool to room temperature. Concentrated HCl was added to adjust the PH of solution to 4-5. Chloroform (4 mL) was added and the reaction mixture was allowed to stir at room

temperature for 12 h. The reaction mixturewas filtered to remove the white precipitate and the precipitate was washed with chloroform (3×5 mL). The organic layers were combined and concentrated to yield a pale viscous liquid, which was treated with acetone (4 mL). A large amount of white solid appeared. The mixture was further cooled to 0 ºC, and then was filtered and the precipitatewas washed with cold acetone (3×5 mL). The solid was dried under vacuum to yield the benzylated acid as a white solid, which was used further without any purification. (**1a-1j, 1o**)

1k was prepared in the method[3]

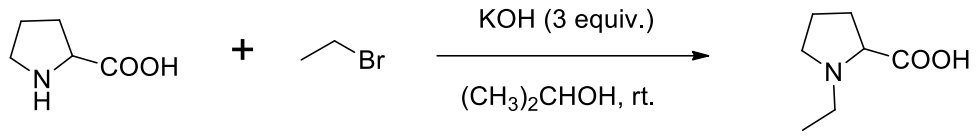


L-Proline (800 mg, 6.95 mmol) was dissolved in IPA (30 mL), followed by the addition of KOH pellets (1.17 g, 20.85 mmol) and H_2O (10 mL). Reaction was stirred at rt while an IPA solution of 4-bromobenzoyl chloride (1.65 g, 7.64 mmol) was added via syringe pump over 1 h. Reaction was allowed to stir an additional 1 h, after which time the reaction was cooled to 0 ºC. The solution was then acidified to pH 5, DCM was added, and the reaction stirred for 13 h at rt. After this time, the precipitate was filtered off and washed with DCM (2×5 mL), and the combined organic filtrate extracts were concentrated to provide an off-white solid without further purification.

1l was prepared in the method[4]

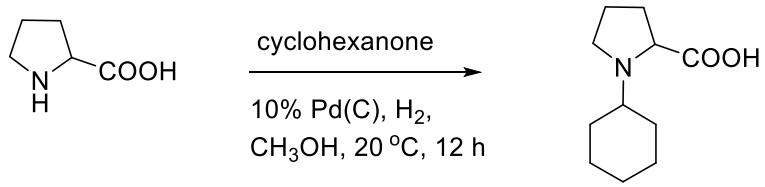
L-Proline (2.0 g, 17.4 mmol) was dissolved in methanol (20 mL) and to this solution was added 40% aqueous formaldehyde solution (1.4 mL, 19.1mmol). This was followed by the addition of 10% Pd/C catalyst (500 mg) and the resulting slurry was stirred in a hydrogen atmosphere overnight. The slurry was then filtered through a Celite pad to remove the catalyst. The pad was washed with methanol and the combined filtrates were concentrated under reduced pressure. The residue was taken up in ethanol-benzene (1:1, 100 mL) and concentrated a second time to provide a solid, which was recrystallized from methanol-diethyl ether. In this way *N*-methyl proline was isolated as fine needles.

1m was prepared in the method[5]



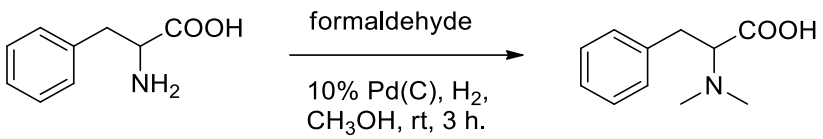
To a dry 25 mL flask, *L*-proline (1.15 g, 10 mmol) and potassium hydroxide (1.68 g, 30 mmol) were dissolved in isopropanol (7 mL) and the resulting mixture was stirred at rt. bromoethane (2 mL, 12 mmol) was added slowly over 0.5 h via a dropping funnel. The reaction mixture was stirred 6 h at the same temperature. Concentrated HCl was added to adjust the PH of solution to 5-6. Chloroform (4 mL) was added and the reaction mixture was allowed to stir at room temperature for 5 h. The reaction mixturewas filtered to remove the white precipitate and the precipitate was washed with chloroform (3×5 mL). The organic layers were combined and concentrated to yield a pale viscous liquid, which was treated with acetone (4 mL). A large amount of white solid appeared. The mixture was further cooled to 0 ºC, and then was filtered and the precipitatewas washed with cold acetone (3×5 mL). The solid was dried under vacuum to yield the *N*-Ethyl-*L*-proline as a white solid, which was used further without any purification.

1n was prepared in the method[6]



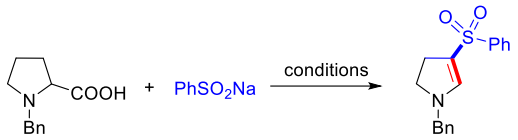
Palladium on carbon (10% by wt, dry, 0.12 g) was suspended in methanol (10 mL) in a dry 50 mL flask, which was flushed with N_2. *L*-proline (1.15 g, 10 mmol) and cyclohexanone (1.2 mL, 11 mmol) were added to this suspension. The flask was charged with H_2 and was kept under a balloon of H_2 for 12 h. At this time, the reaction was purged with N_2 and filtered through Celite. Removal of the methanol under reduced pressure led to the unpurified acid

1p was prepared in the method[7]



A suspension of 10% Pd/C (0.7 g) in methanol (2 mL) was added to a mixture of *L*-Phenylalanine (3.3 g, 20 mmol), formaldehyde (11mL of 37% wt. in water), 1N HCl (10 mL) and methanol (10 mL), and exposed to H_2 (60 psi) for 3 hours. The reaction mixture was filtered through diatomaceous earth (Celite), and the filtrate was concentrated in vacuo. The resulting crude material was recrystallized from isopropanol to provide the white needle product.

Table S1. Optimization reaction conditions. [a]

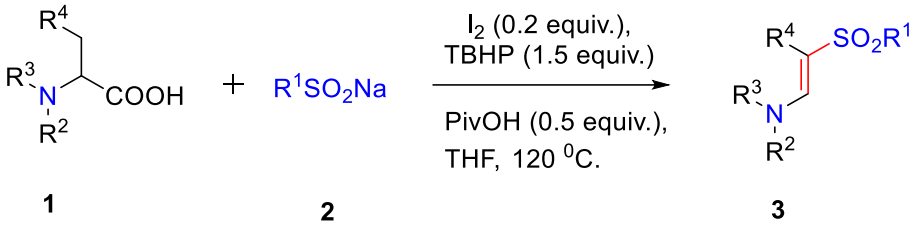


1a **2a** **3aa**

Entry	Solvents	Temperature (°C)	Reaction time (h)	Yields (%)[b]
1	THF	120	12	78
2	toluene	120	12	56
3	DMF	120	12	50
4	DMA	120	12	48
5	DMSO	120	12	64
6	EtOH	120	12	30
7	Acetonitrile	120	12	52
8	THF	60	12	-
9	THF	80	12	-
10	THF	100	12	45
11	THF	**130**	**12**	**75**
12	THF	120	6	32
13	THF	120	8	49
14	THF	120	10	68
15	THF	120	14	78
16	THF	120	16	78

[a] Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), I_2 (20 %) TBHP (1.5 equiv.), PivOH (20%), solvents (2 mL), Ar. [b] Yields of isolated products.

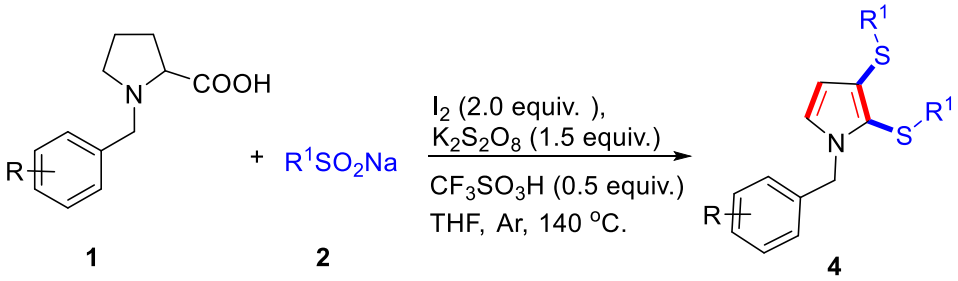
General procedure for synthesis of substituted sulfones from *α*-amino acids and sodium sulfonates:



1 **2** **3**

The *α*-amino acids (**1**, 0.3 mmol), sodium sulfonates (**2**, 0.6 mmol), iodine (0.2 equiv), TBHP (1.5 equiv), PivOH (0.5 equiv) were mixed in THF (2 mL) and this mixture was carried out under Ar at 120 ºC for 12 h. The reaction mixture was cooled to room temperature and then washed with saturated sodium thiosulfate (5 mL), extracted with ethyl acetate (15 mL×3). The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/EtOAc (4:1) to afford the desired products **3**.

General procedure for synthesis of substituted sulfones from *α*-amino acids and sodium sulfonates:

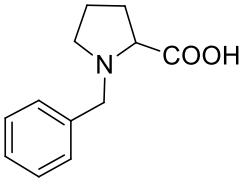


1 **2** **4**

The *α*-amino acids (**1**, 0.3 mmol), sodium sulfonates (**2**, 3+1.5 equiv.), iodine (2 equiv.), $K_2S_2O_8$ (1.5 equiv.), F_3CSO_3H (0.5 equiv.) were mixed in THF (2 mL) and this mixture was carried out under Ar at 140ºC for 24 h. And 3 equiv. of **2** was added at

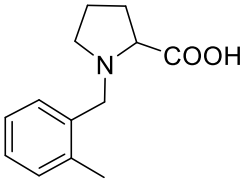
beginning and 1.5 equiv. was added 5 hours later. The reaction mixture was cooled to room temperature and then washed with saturated sodium thiosulfate (5 mL), extracted with ethyl acetate (15 ml×3). The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/EtOAc (8:1) to afford the desired products **4**.

The data of products:



1-benzylpyrrolidine-2-carboxylic acid (1a)

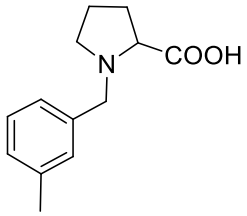
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 9.21 (s, 1 H), 7.46-7.44 (m, 2 H), 7.39-7.29 (m, 3 H), 4.38-4.35 (d, *J* = 12.8 Hz, 1 H), 4.20-4.16 (d, *J* = 13.2 Hz, 1 H), 3.83-3.80 (m, 1 H), 3.70-3.64 (m, 1 H), 2.90-2.83 (m, 1 H), 2.37-2.21 (m, 2 H), 2.07-1.87 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 171.2, 131.3, 130.5, 129.4, 129.1, 67.7, 57.9, 53.4, 29.0, 23.0. The NMR data same with reference *Angew. Chem. Int. Ed.*, 2009, **48**, 792.



1-(2-methylbenzyl)pyrrolidine-2-carboxylic acid (1b)

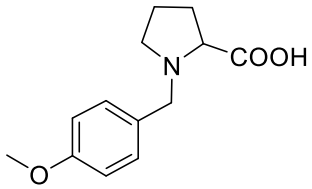
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.47-7.45 (d, *J* = 7.2 Hz, 1 H), 7.30-7.17 (m, 3 H), 6.88 (s, 1 H), 4.50-4.46 (d, *J* = 13.2 Hz, 1 H), 4.25-4.21 (d, *J* = 13.2 Hz, 1 H), 3.91-3.88 (m, 1 H), 3.65-3.60 (m, 1 H), 2.99-2.92 (m, 1 H), 2.44-2.38 (m, 4 H), 2.27-2.17 (m, 1 H), 2.04-1.94 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 171.4, 137.8, 131.2, 131.2, 129.7, 129.5, 126.6, 68.2, 55.3, 53.6, 28.8, 23.0, 19.5. The

NMR data same with reference *Angew. Chem. Int. Ed.*, 2009, **48**, 792.



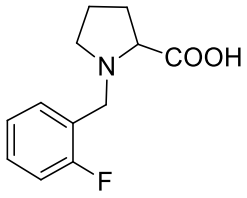
1-(3-methylbenzyl)pyrrolidine-2-carboxylic acid (1c)

White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 9.12 (s, 1 H), 7.30-7.24 (m, 3 H), 7.19-7.16 (m, 1 H), 4.36-4.33 (d, *J* = 12.8 Hz, 1 H), 4.17-4.14 (d, *J* = 12.8 Hz, 1 H), 3.86-3.82 (m, 1 H), 3.71-3.65 (m, 1 H), 2.92-2.85 (m, 1 H), 2.38-2.22 (m, 5 H), 2.08-1.86 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 170.9, 138.9, 131.2, 130.8, 130.2, 129.0, 127.5, 67.7, 57.8, 53.3, 28.9, 22.9, 21.3. The NMR data same with reference *Angew. Chem. Int. Ed.*, 2009, **48**, 792.



1-(4-methoxybenzyl)pyrrolidine-2-carboxylic acid (1d)

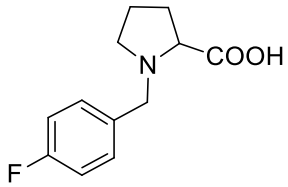
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.96 (s, 1 H), 7.38-7.36 (d, *J* = 8.8 Hz, 2 H), 6.89-6.87 (d, *J* = 8.8 Hz, 2 H), 4.31-4.28 (d, *J* = 12.8 Hz, 1 H), 4.23-4.19 (d, *J* = 13.2 Hz, 1 H), 3.84-3.82 (m, 1 H), 3.80 (s, 3 H), 3.78-3.68 (m, 1 H), 2.93-2.86 (m, 1 H), 2.34-2.22 (m, 2 H), 2.05-1.87 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 170.8, 160.5, 132.11, 122.4, 114.5, 67.4, 57.1, 55.3, 53.1, 28.9, 22.9. The NMR data same with reference *Chem. Sci.*, 2022, **13**, 9507.



1-(2-fluorobenzyl)pyrrolidine-2-carboxylic acid (1e)

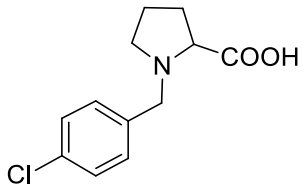
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 9.60 (s, 1 H), 7.54-7.50 (m, 1 H), 7.39-7.29 (m, 1 H), 7.17-7.08 (m, 2 H), 4.38-4.35 (d, *J* = 13.2 Hz, 1 H), 4.17-4.14 (d, *J* = 13.2 Hz, 1 H), 3.74-3.70 (m, 1 H), 3.59-3.54 (m, 1 H), 2.85-2.78 (m, 1 H), 2.37-2.17

(m, 2 H), 2.01-1.89 (m, 2 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, ppm): δ = 172.1, 162.6-160.2 (d, *J* = 247 Hz, 1 C), 132.7-132.6 (d, *J* = 3 Hz, 1 C), 131.3-131.2 (d, *J* = 9 Hz, 1 C), 124.8-124.7 (d, *J* = 4 Hz, 1 C), 119.9-119.8 (d, *J* = 14 Hz, 1 C), 115.9-115.8 (d, *J* = 22 Hz, 1 C), 67.3, 53.6, 51.1, 29.2, 23.2. The NMR data same with reference *Chem. Sci.*, 2022, **13**, 9507.



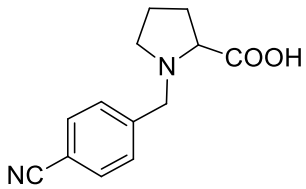
1-(4-fluorobenzyl)pyrrolidine-2-carboxylic acid (1f)

White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.45-7.41 (m, 2 H), 7.07-7.03 (m, 2 H), 4.30-4.26 (d, *J* = 13.2 Hz, 1 H), 4.12-4.09 (d, *J* = 12.8 Hz, 1 H), 3.77-73 (m, 1 H), 3.63-3.58 (m, 1 H), 2.84-2.77 (m, 1 H), 2.37-2.17 (m, 2 H), 2.02-1.88 (m, 2 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, ppm): δ = 171.6, 164.4-161.9 (d, *J* = 248 Hz, 1 C), 132.2-132.1 (d, *J* = 8 Hz, 2 C), 127.8, 116.2-116.0 (d, *J* = 21 Hz, 2 C), 67.5, 57.5, 53.6, 29.2, 23.2. The NMR data same with reference *Bioorgan. & Med. Chem.*, 2020, **28**, 115216.



1-(4-chlorobenzyl)pyrrolidine-2-carboxylic acid (1g)

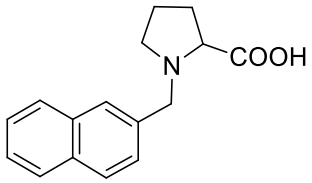
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.36-7.32 (m, 4 H), 4.19-4.16 (d, *J* = 12.8 Hz, 1 H), 4.98-3.95 (d, *J* = 12.8 Hz, 1 H), 3.68-3.64 (m, 1 H), 3.48-3.43 (m, 1 H), 2.76-2.69 (m, 1 H), 2.32-2.21 (m, 2 H), 2.19-1.90 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 172.3, 135.1, 131.2, 131.1, 129.3, 67.2, 58.1, 53.8, 29.5, 23.8. The NMR data same with reference *Bioorgan. Med. Chem.*, 2015, **23**, 1569.



1-(4-cyanobenzyl)pyrrolidine-2-carboxylic acid (1h)

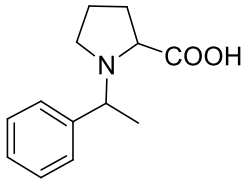
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.70-7.68 (d, *J* = 8.0 Hz, 2 H),

7.49-7.47 (d, *J* = 8.0 Hz, 2 H), 4.13-4.09 (d, *J* = 13.2 Hz, 1 H), 4.85-3.81 (d, *J* = 13.2 Hz, 1 H), 3.55-3.52 (m, 1 H), 3.25-3.20 (m, 1 H), 2.63-2.56 (m, 1 H), 2.35-2.25 (m, 1 H), 2.19-2.13 (m, 1 H), 1.98-1.82 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 175.3, 132.7, 129.7, 124.9, 118.1, 112.3, 66.5, 59.2, 54.2, 30.0, 24.4. The NMR data same with reference *J. Med. Chem.*, 1992, **35**, 4393.



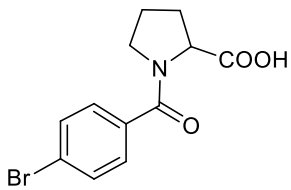
1-(naphthalen-2-ylmethyl)pyrrolidine-2-carboxylic acid (1i)

White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.25-8.23 (d, *J* = 8.4 Hz, 1 H), 7.87-7.85 (d, *J* = 8.4 Hz, 2 H), 7.58-7.54 (m, 2 H), 7.50-7.47 (m, 1 H), 7.44-7.40 (m, 1 H), 4.4.81-4.78 (d, *J* = 13.2 Hz, 1 H), 4.48-4.44 (d, *J* = 13.2 Hz, 1 H), 3.87-3.83 (m, 1 H), 3.49-3.44 (m, 1 H), 2.90-2.83 (m, 1 H), 2.35-2.29 (m, 1 H), 2.23-2.19 (m, 1 H), 1.91-1.86 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 172.3, 133.9, 131.9, 130.2, 129.6, 129.0, 128.5, 127.4, 126.3, 125.2, 123.1, 68.0, 55.5, 53.9, 30.9, 29.2, 23.4. The NMR data same with reference *Tetrahedron Lett.*, 2000, **41**, 1841.



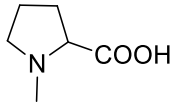
1-(1-phenylethyl)pyrrolidine-2-carboxylic acid (1j)

White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.17 (s, 1 H), 7.50-7.36 (m, 5 H), 4.63-4.62 (d, *J* = 5.6 Hz, 1 H), 3.89-3.85 (m, 1 H), 3.62-3.56 (m, 1 H), 3.06-2.86 (m, 1 H), 2.29-2.20 (m, 2 H), 2.04-1.92 (m, 1 H), 1.80-1.75 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 171.4, 129.5, 129.2, 129.1, 128.8, 66.7, 62.9, 50.9, 29.3, 23.0, 18.8. The NMR data same with reference *Tetrahedron Lett.*,1996, 37, 4819.



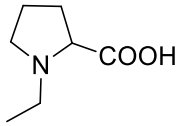
1-(4-bromobenzoyl)pyrrolidine-2-carboxylic acid (1k)

White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.35 (s, 1 H), 7.56-7.54 (d, *J* = 8.4 Hz, 2 H), 7.46-7.44 (d, *J* = 8.4 Hz, 2 H), 4.70-4.67 (m, 1 H), 3.62-3.48 (m, 2 H), 2.36-2.27 (m, 1 H), 2.17-2.13 (m, 1 H), 2.11-1.97 (m, 1 H), 1.92-1.87 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 174.9, 169.6, 134.4, 131.7, 129.0, 124.9, 59.5, 50.2, 29.1, 25.2. The NMR data same with reference *Bioorg. Med. Chem*. **2015**, 23, 1569.



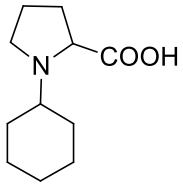
1-methylpyrrolidine-2-carboxylic acid (1l)

White solid, ^{1}H NMR (400 MHz, D_2O, ppm): δ = 4.08-4.04 (m, 1 H), 3.74-3.71 (m, 1 H), 3.22-3.25 (m, 1 H), 2.95 (s, 3 H), 2.56-2.49 (m, 1 H), 2.15-1.98 (m, 3 H); ^{13}C NMR (100 MHz, CD_2O, ppm): δ = 172.4, 69.4, 56.5, 40.8, 28.4, 22.5. The NMR data same with reference *J. Org. Chem.*, 2003, **68**, 2652.



1-ethylpyrrolidine-2-carboxylic acid (1m)

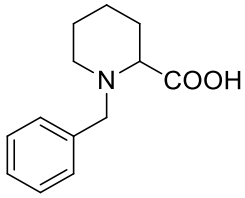
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.46 (s, 1 H), 4.05-3.99 (m, 1 H), 3.77-3.61 (m, 1 H), 3.34-3.28 (m, 1 H), 3.21-3.12 (m, 1 H), 2.88-2.81 (m, 1 H), 2.41-2.25 (m, 2 H), 2.06-1.98 (m, 2 H), 1.42-1.38 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 170.5, 69.3, 54.4, 50.4, 29.5, 23.5, 11.0. The NMR data same with reference *Chem. Com.*, 2010, **46**, 7834.



1-cyclohexylpyrrolidine-2-carboxylic acid (1n)

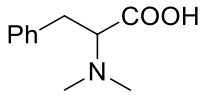
White solid, ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.31 (s, 1 H), 3.94-3.88 (m, 2 H), 3.22-3.17 (m, 1 H), 2.99-2.92 (m, 1 H), 2.43-2.21 (m, 2 H), 2.17-2.09 (m, 2 H), 1.97-1.88 (m, 4 H), 1.72-1.56 (m, 1 H), 1.53-1.32 (m, 2 H), 2.1.30-1.23 (m, 2 H), 1.20-1.12 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 170.6, 66.3, 63.3, 51.6, 30.0, 28.8, 28.2, 25.1, 24.8, 24.7, 24.1. The NMR data same with reference *Adv. Synth. Catal.*,

2008, **350**, 385.



1-benzylpiperidine-2-carboxylic acid (1o)

White solid, ^{1}H NMR (400 MHz, D_2O, ppm): δ = 7.35-7.30 (m, 5 H), 4.22-4.19 (d, *J* = 12.4 Hz, 1H), 3.86-3.83 (d, *J* = 12.4 Hz, 1 H), 3.27-3.17 (m, 2 H), 2.70-2.62 (m, 1 H), 2.00-1.96 (d, *J* = 13.2 Hz, 1 H), 1.61-1.23 (m, 5 H); ^{13}C NMR (100 MHz, D_2O, ppm): δ = 175.4, 131.5, 129.9, 129.7, 67.3, 59.5, 50.8, 28.3, 22.6, 21.5. The NMR data same with reference *Angew. Chem. Int. Ed.*, 2009, **48**, 792.

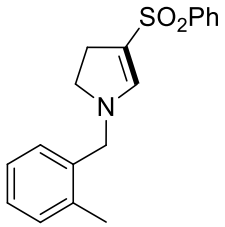


2-(dimethylamino)-3-phenylpropanoic acid (1p)

White solid, ^{1}H NMR (400 MHz, D_2O, ppm): δ = 7.44-7.33 (m, 5 H), 3.87-3.83 (m, 1 H), 3.36-3.31 (m, 1 H), 3.15-3.10 (m, 1 H), 2.97 (s, 3 H), 2.91 (s, 3 H); ^{13}C NMR (100 MHz, D_2O, ppm): δ = 172.2, 135.2, 129.2, 128.9, 127.4, 72.1, 42.8, 40.5, 33.9. The NMR data same with reference *Chem. Comm.*, 2010, **46**, 7834.

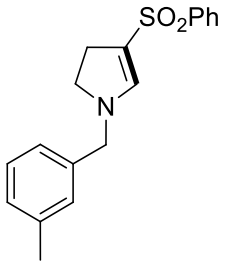
benzyl-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3aa)

White solid, mp 69-71 °C. (Isolated yield 78%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 2 H), 7.53-7.47 (m,3 H), 7.37-7.31 (m, 3 H), 7.23-7.20 (m, 2 H), 7.10 (s, 1 H), 4.19 (s, 2 H), 3.43-3.38 (m, 2 H), 2.72-2.67 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.9, 142.5, 135.8, 131.9, 128.9, 128.9, 128.1, 128.1, 126.7, 106.7, 54.6, 52.2, 27.7； HRMS (ESI) (m/z) calcd for $C_{17}H_{18}NO_2S$ $[M+H]^+$ 300.1053, found 300.1056.



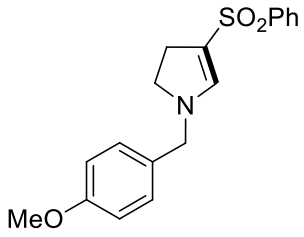
1-(2-methylbenzyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ba)

White solid, mp 72-74 °C. (Isolated yield 67%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84-7.82 (m, 2 H), 7.52-7.45 (m, 3 H), 7.24-7.14 (m, 4 H), 7.00 (s, 1 H), 4.17 (s, 2 H), 3.45-3.40 (m, 2 H), 2.73-2.67 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.7, 142.6, 136.7, 133.6, 131.9, 130.8, 129.1, 128.9, 128.3, 126.6, 126.3, 106.2, 52.7, 52.5, 27.7, 19.1； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.1209, found 314.1204.



1-(3-methylbenzyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ca)

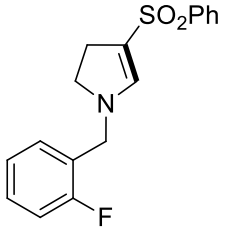
White solid, mp 79-81 °C. (Isolated yield 72%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 2 H), 7.54-7.46 (m, 3 H), 7.25-7.22 (m, 1 H), 7.13-7.09 (m, 2 H), 7.02-7.00 (m, 2 H), 4.15 (s, 2 H), 3.43-3.38 (m, 2 H), 2.72-2.67 (m, 2 H), 2.35 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.0, 142.6, 138.6, 135.7, 131.9, 128.9, 128.8, 128.8, 128.8, 126.7, 125.1, 106.4, 54.5, 52.2, 27.7, 21.4； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.1209, found 314.1213.



1-(4-methoxybenzyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3da)

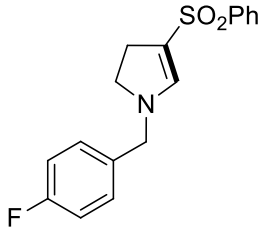
White solid, mp 89-91 °C. (Isolated yield 73%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.82 (m, 2 H), 7.52-7.45 (m, 3 H), 7.14-7.12 (m, 2 H), 7.07 (s, 1 H), 7.89-7.86 (m,

2 H), 4.12 (s, 2 H), 3.80 (s, 3 H), 3.41-3.36 (m, 2 H), 2.70-2.65(m 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.4, 150.9, 142.6, 131.9, 129.4, 128.9, 127.7, 126.6, 114.2, 106.4, 55.3, 53.9, 52.1, 27.7； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_3S$ $[M+H]^+$ 330.1159, found 330.1155.



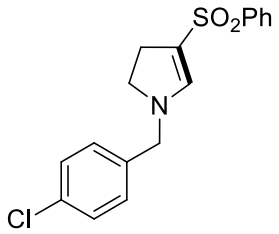
1-(2-fluorobenzyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ea)

White solid, mp 98-100 °C. (Isolated yield 82%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.82 (m, 2 H), 7.54-7.46 (m, 3 H), 7.34-7.28 (m, 1 H), 7.24-7.20 (m, 1 H), 7.15-7.12 (m, 1 H), 7.10-7.05(m, 2 H), 4.25 (s, 2 H), 3.47-3.42 (m, 2 H), 2.71-2.66 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 162.3-159.8 (d, *J* = 257 Hz, 1 C), 150.8, 142.5, 131.9, 130.4-130.4 (d, *J* = 4 Hz, 1 C), 130.2-130.1 (d, *J* = 8 Hz, 1 C), 128.9, 126.7, 124.5-124.4 (d, *J* = 4 Hz, 1 C), 122.9-122.8(d, *J* = 15 Hz, 1 C), 115.9-115.7 (d, *J* = 21 Hz, 1 C), 106.9, 52.2, 47.9-47.8 (d, *J* = 3 Hz, 1 C), 27.7； HRMS (ESI) (m/z) calcd for $C_{17}H_{17}FNO_2S$ $[M+H]^+$ 318.0959, found 318.0964.



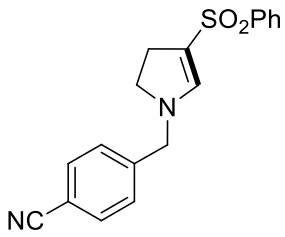
1-(4-fluorobenzyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3fa)

White solid, mp 65-67 °C. (Isolated yield 75%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.53-7.46 (m, 3 H), 7.21-7.17 (m, 2 H), 7.08 (s, 1 H), 7.06-7.01 (m, 2 H), 4.16(s, 2 H), 3.41-3.35 (m, 2 H), 2.72-2.66 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 163.7-161.2 (d, *J* = 256 Hz, 1 C), 150.8, 142.4, 132.0, 131.6-131.6 (d, *J* = 3 Hz, 1 C), 129.8- 129.7 (d, *J* = 8 Hz, 2 C), 128.9, 126.7, 115.9-115.7 (d, *J* = 22 Hz, 2 C), 107.2, 53.9, 52.2, 27.7； HRMS (ESI) (m/z) calcd for $C_{17}H_{17}FNO_2S$ $[M+H]^+$ 318.0959, found 318.0960.



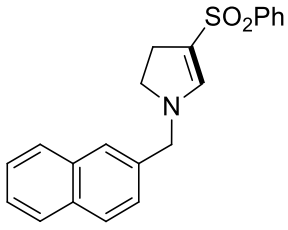
1-(4-chlorobenzyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ga)

White solid, mp 96-99 °C. (Isolated yield 70%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 2 H), 7.54-7.47 (m, 3 H), 7.33-7.31 (m, 2 H), 7.17-7.15 (m, 2 H), 7.08 (s, 1 H), 4.16 (s, 2 H), 3.40-3.35 (m, 2 H), 2.72-2.67 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.7, 142.3, 134.4, 133.9, 132.1, 129.4, 129.1, 128.9, 126.7, 107.4, 53.9, 52.2, 27.7；HRMS (ESI) (m/z) calcd for $C_{17}H_{17}ClNO_2S$ $[M+H]^+$ 334.0663, found 334.0669.



4-((4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrol-1-yl)methyl)benzonitrile(3ha)

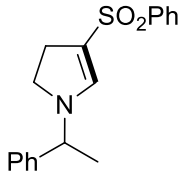
White solid, mp 83-85 °C. (Isolated yield 69%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.84 (m, 2 H), 7.66-7.64 (m, 2 H), 7.58-7.48 (m, 3 H), 7.37-7.35 (m, 2 H), 7.10 (s, 1 H), 4.26 (s, 2 H), 3.42-3.37 (m, 2 H), 2.75-2.70 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.6, 142.1, 141.5, 132.7, 132.2, 129.0, 128.5, 126.7, 118.4, 112.1, 108.6, 54.3, 52.5, 27.8；HRMS (ESI) (m/z) calcd for $C_{18}H_{17}N_2O_2S$ $[M+H]^+$ 325.1005, found 325.1007.



1-(naphthalen-2-ylmethyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ia)

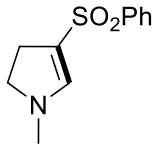
White solid, mp 108-110 °C. (Isolated yield 65%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.93-7.85 (m, 2 H), 7.83-7.80 (m, 3 H), 7.55-7.42 (m, 6 H), 7.38-7.37 (m, 1 H), 7.08 (s, 1 H), 4.60 (s, 2 H), 3.50-3.45 (m, 2 H), 2.72-2.67 (m, 2 H); ^{13}C NMR (100 MHz,

$CDCl_3$, ppm): δ = 150.6, 142.5, 133.9, 131.9, 131.4, 131.2, 129.2, 128.9, 128.9, 127.1, 126.7, 126.7, 126.1, 125.3, 123.1, 106.9, 52.9, 52.5, 27.7； HRMS (ESI) (m/z) calcd for $C_{21}H_{20}NO_2S$ $[M+H]^+$ 350.1209, found 350.1202.



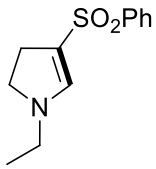
1-(1-phenylethyl)-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ja)

White solid, mp 84-86 °C. (Isolated yield 57%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 2 H), 7.53-7.46 (m, 3 H), 7.37-7.27 (m, 3 H), 7.23-7.19 (m, 3 H), 4.23-4.18 (m, 1 H), 3.39-3.34 (m, 2 H), 2.68-2.63 (m, 2 H), 1.55-1.53 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.7, 142.6, 141.2, 131.9, 128.9, 127.9, 126.63, 126.5, 106.2, 58.8, 51.2, 27.2, 20.9； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 315.1209, found 315.1215.



1-methyl-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3la)

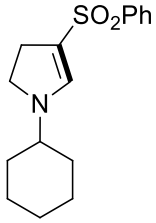
White solid, mp 72-74 °C. (Isolated yield 45%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.54-7.46 (m, 3 H), 6.94 (s, 1 H), 3.47-3.42 (m, 2 H), 2.81 (s, 3 H), 2.73-2.68 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.2, 142.7, 131.9, 128.9, 126.6, 106.0, 54.7, 37.1, 28.1；HRMS (ESI) (m/z) calcd for $C_{11}H_{14}NO_2S$ $[M+H]^+$ 224.0740, found 224.0743.



1-ethyl-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ma)

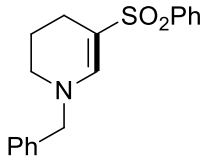
White solid, mp 76-78 °C. (Isolated yield 67%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.83 (m, 2 H), 7.52-7.46 (m, 3 H), 7.02 (s, 1 H), 3.51-3.46 (m, 2 H), 3.11-3.06 (s, 2 H), 2.72-2.67 (m, 2 H), 1.18-1.14 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ

= 150.7, 142.8, 131.8, 128.9, 126.6, 105.5, 52.1, 44.7, 27.6, 13.4；HRMS (ESI) (m/z) calcd for $C_{12}H_{16}NO_2S$ $[M+H]^+$ 238.0896, found 238.0899.



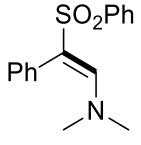
1-cyclohexyl-4-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3na)

White solid, mp 97-99 °C. (Isolated yield 66%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84-7.82 (m, 2 H), 7.51-7.46 (m, 3 H), 7.11 (s, 1 H), 3.56-3.51 (m, 2 H), 2.93-2.88 (m, 1 H), 2.69-2.64(m, 2 H), 1.88-1.79 (m, 4 H), 1.67-1.63 (m, 1 H), 1.33-1.21 (m, 4 H), 1.17-1.10 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 149.0, 142.9, 131.5, 128.8, 126.5, 104.3, 58.0, 50.1, 31.6, 26.9, 25.4, 25.1； HRMS (ESI) (m/z) calcd for $C_{16}H_{22}NO_2S$ $[M+H]^+$ 292.1366, found 292.1363.



1-benzyl-5-(phenylsulfonyl)-1,2,3,4-tetrahydropyridine(3oa)

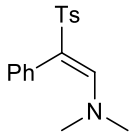
White solid, mp 95-97 °C. (Isolated yield 87%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 2 H), 7.52-7.46 (m, 4 H), 7.38-7.30 (m, 3 H), 7.21-7.19 (m, 2 H), 4.31 (s, 2 H), 2.97-2.94 (m, 2 H), 2.17-2.16 (m, 2 H), 1.79-1.73 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 144.5, 142.7, 136.4, 131.7, 128.9, 128.8, 128.0, 127.5, 126.8, 100.7, 59.7, 44.9, 20.9, 19.6； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.1209, found 314.1212.



***(E)*-*N*,*N*-dimethyl-2-phenyl-2-(phenylsulfonyl)ethenamine(3pa)**

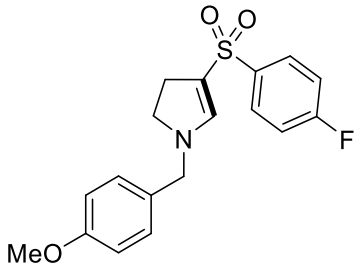
White solid, mp 153--155 °C. (Isolated yield 69%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.55-7.52 (m, 3 H), 7.43-7.40 (m, 1 H), 7.34-7.30 (m, 2 H), 7.24-7.15 (m, 3 H), 7.07-7.04 (m, 2 H), 2.67 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.3, 142.4,

133.6, 131.5, 131.5, 128.3, 127.9, 127.6, 127.3, 106.4, 42.7；HRMS (ESI) (m/z) calcd for $C_{16}H_{18}NO_2S$ $[M+H]^+$288.1053, found 288.1058.



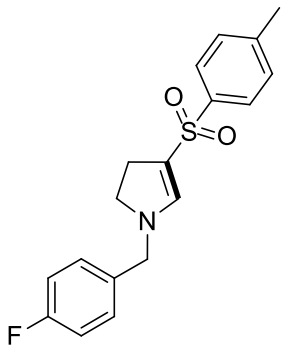
***(E)-N,N*-dimethyl-2-phenyl-2-tosylethenamine(3qa)**

White solid, mp 164-167 °C. (Isolated yield 64%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.50 (s, 1 H), 7.43-7.41 (m, 2 H), 7.23-7.16 (m, 3 H), 7.12-7.06 (m, 4 H), 2.66 (s, 6 H), 2.35 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.0, 142.0, 139.5, 133.6, 131.7, 128.9, 127.8, 127.5, 127.3, 106.7, 42.7, 21.5；HRMS (ESI) (m/z) calcd for $C_{17}H_{20}NO_2S$ $[M+H]^+$ 302.1209, found 302.1203.



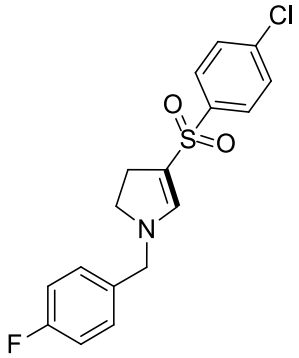
4-((4-fluorophenyl)sulfonyl)-1-(4-methoxybenzyl)-2,3-dihydro-1*H*-pyrrole(3df)

White solid, mp 133-135 °C. (Isolated yield 63%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.82 (m, 2 H), 7.17-7.12 (m, 4 H), 7.07 (s, 1 H), 6.89-6.87 (d, *J* = 8.4 Hz, 2 H), 4.13 (s, 2 H), 3.81 (s, 3 H), 3.43-3.38 (m, 2 H), 2.69-2.64 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 165.9-163.5 (d, *J* = 251 Hz, 1 C), 159.5, 150.9, 138.8-138.7 (d, *J* = 3 Hz, 1 C), 129.4-129.3 (d, *J* = 10 Hz, 2 C), 129.3, 127.6, 116.1-115.9 (d, *J* = 22 Hz, 2 C), 114.3, 106.1, 55.3, 53.9, 52.1, 27.6； HRMS (ESI) (m/z) calcd for $C_{18}H_{19}FNO_3S$ $[M+H]^+$ 348.1064, found 348.1063.



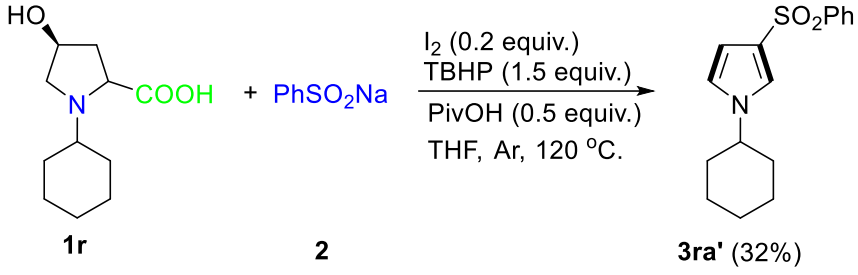
1-(4-fluorobenzyl)-4-tosyl-2,3-dihydro-1*H*-pyrrole((3fc))

White solid, mp 103-105 °C. (Isolated yield 72%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.73-7.71 (d, *J* = 8.4 Hz, 2 H), 7.29-7.27 (d, *J* = 8.0 Hz, 2 H), 7.21-7.17 (m, 2 H), 7.06-7.01 (m, 3 H), 4.15 (s, 2 H), 3.39-3.34 (m, 2 H), 2.70-2.65 (m, 2 H), 2.41 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 163.7-161.2 (d, *J* = 245 Hz, 1 C), 150.4, 142.7, 139.5, 131.7-131.7 (d, *J* = 3 Hz, 1 C), 129.8-129.7 (d, *J* = 8 Hz, 2 C), 129.6, 126.8, 115.9-115.7 (d, *J* = 21 Hz, 2 C), 107.8, 53.9, 52.2, 27.8, 21.5； HRMS (ESI) (m/z) calcd for $C_{18}H_{19}FNO_2S$ $[M+H]^+$ 332.1115, found 332.1118.



4-((4-chlorophenyl)sulfonyl)-1-(4-fluorobenzyl)-2,3-dihydro-1*H*-pyrrole((3fg))

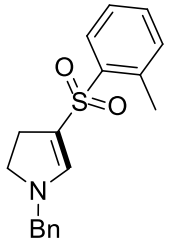
White solid, mp 117-119 °C. (Isolated yield 67%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.79-7.75 (m, 2 H), 7.47-7.44 (m, 2 H), 7.21-7.17 (m, 2 H), 7.08-7.02 (m, 3 H), 4.17 (s, 2 H), 3.43-3.38 (m, 2 H), 2.71-2.66 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 163.8-161.3 (d, *J* = 246 Hz, 1 C), 151.0, 141.0, 138.4, 131.4-131.4 (d, *J* = 4 Hz, 1 C), 129.8-129.7 (d, *J* = 8 Hz, 2 C), 129.2, 128.2, 115.9-115.7 (d, *J* = 21 Hz, 2 C), 106.5, 53.8, 52.2, 27.6; HRMS (ESI) (m/z) calcd for $C_{17}H_{16}ClFNO_2S$ $[M+H]^+$ 352.0569, found 352.0569.



1-cyclohexyl-3-(phenylsulfonyl)-1*H*-pyrrole(3ra')

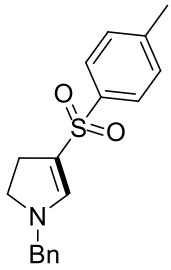
White solid, mp 58-60 °C. (Isolated yield 32%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.94-7.92 (d, *J* = 6.8 Hz, 2 H), 7.51-7.45 (m, 3 H), 7.33 (s, 1 H), 6.70-6.69 (m, 1 H), 6.43 (s, 1 H), 3.83-3.75 (m, 1 H), 2.09-2.06 (m, 2 H), 1.90-1.87 (m, 2 H), 1.75-1.72 (m,

1 H), 1.43-1.33 (m, 2 H), 1.26-1.19 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.9, 132.2, 128.9, 126.8, 123.5, 122.6, 121.1, 108.4, 59.6, 34.3, 25.4, 25.2； HRMS (ESI) (m/z) calcd for $C_{16}H_{20}NO_2S$ $[M+H]^+$ 290.1209, found 290.1205.



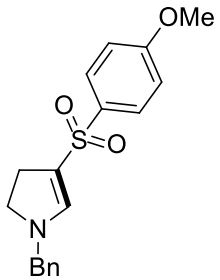
1-benzyl-4-(o-tolylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ab)

White solid, mp 150-152 °C. (Isolated yield 76%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.98-7.95 (m, 1 H), 7.43-7.21 (m, 8 H), 7.13 (s, 1 H), 4.21 (s, 2 H), 3.42-3.37 (m, 2 H), 2.65-2.60 (m, 5 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.3, 139.6, 137.2, 135.9, 132.4, 132.3, 129.1, 128.9, 128.1, 128.0, 126.2, 106.4, 54.6, 52.2, 27.8, 20.1； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.1209, found 314.1211.



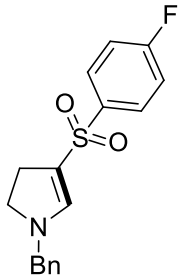
1-benzyl-4-tosyl-2,3-dihydro-1*H*-pyrrole(3ac)

White solid, mp 144-146 °C. (Isolated yield 61%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.73-7.71 (d, *J* = 8.4 Hz, 2 H), 7.37-7.30 (m, 3 H), 7.29-7.27 (d, *J* = 8.0 Hz, 2 H), 7.22-7.20 (m, 2 H), 7.07 (s, 1 H), 4.18 (s, 2 H), 3.41-3.36 (m, 2 H), 2.70-2.65 (m, 2 H), 2.41 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.6, 142.6, 139.6, 135.9, 129.5, 128.9, 128.1, 126.7, 107.3, 54.6, 52.2, 27.8, 21.5； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.1209, found 314.1215.



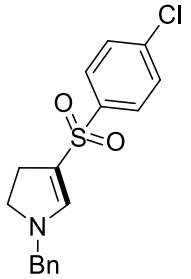
1-benzyl-4-((4-methoxyphenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole(3ad)

White solid, mp 107-109 °C. (Isolated yield 60%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.78-7.76 (d, *J* = 9.2 Hz, 2 H), 7.37-7.30 (m, 3 H), 7.23-7.21 (m, 2 H), 7.05 (s, 1 H), 6.96-6.94 (d, *J* = 9.2 Hz, 2 H), 4.17 (s, 2 H), 3.85 (s, 3 H), 3.41-3.36 (m, 2 H), 2.69-2.64 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.5, 150.2, 135.9, 134.3, 128.8, 128.8, 128.1, 128.0, 114.1, 107.8, 55.6, 54.7, 52.3, 27.8； HRMS (ESI) (m/z) calcd for $C_{18}H_{20}NO_3S$ $[M+H]^+$ 330.1159, found 330.1156.



1-benzyl-4-((4-fluorophenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole(3ae)

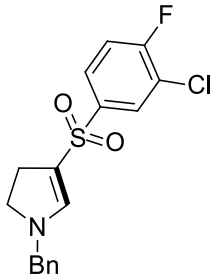
White solid, mp 108-110 °C. (Isolated yield 59%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 2 H), 7.38-7.31 (m, 3 H), 7.26-7.15 (m, 2 H), 7.14-7.13 (m, 2 H), 7.10 (s, 1 H), 4.20 (s, 2 H), 3.46-3.39 (m, 2 H), 2.71-2.66 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 166.0-163.5 (d, *J* = 252 Hz, 1 C), 151.0, 138.7-138.6 (d, *J* = 3 Hz, 1 C), 135.7, 129.4, 129.3, 128.9, 128.1-128.1 (d, *J* = 8 Hz, 2 C), 116.2-115.9 (d, *J* = 22 Hz, 2 C), 106.3, 54.5, 52.2, 27.6； HRMS (ESI) (m/z) calcd for $C_{17}H_{17}FNO_2S$ $[M+H]^+$ 318.0959, found 318.0962.



1-benzyl-4-((4-chlorophenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole(3af)

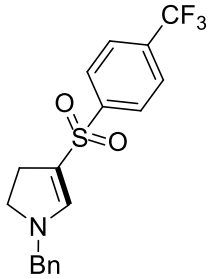
White solid, mp 141-143 °C. (Isolated yield 68%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.78-7.7.76 (m, 2 H), 7.46-7.44 (m, 2 H), 7.38-7.31 (m, 3 H), 7.22-7.20 (m, 2 H), 7.10 (s, 1 H), 4.20 (s, 2 H), 3.45-3.40 (m, 2 H), 2.71-2.66 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.3, 141.2, 138.3, 135.6, 129.2, 128.9, 128.2, 128.0, 105.9, 54.5,

52.2, 27.9；HRMS (ESI) (m/z) calcd for $C_{17}H_{17}ClNO_2S$ $[M+H]^+$ 334.0663, found 334.0668.



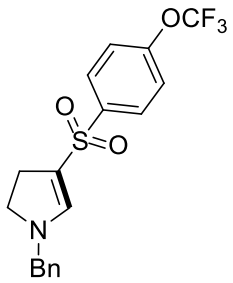
1-benzyl-4-((3-chloro-4-fluorophenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole(3ag)

White solid, mp 76-78 °C. (Isolated yield 45%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.92-7.89 (m, 1 H), 7.75-7.71 (m, 1 H), 7.39-7.32 (m, 3 H), 7.24-7.21 (m, 3 H), 7.12 (s, 1 H), 4.22 (s, 2 H), 3.48-3.43 (m, 2 H), 2.73-2.68 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 161.4-158.9 (d, *J* = 255 Hz, 1 C), 151.6, 139.9-139.8 (d, *J* = 3 Hz, 1 C), 135.5, 129.6, 128.9, 128.2, 128.0, 127.1-127.0 (d, *J* = 9 Hz, 2 C), 122.2-122.0 (d, *J* = 18 Hz, 1 C), 117.2-117.0 (d, *J* = 22 Hz, 1 C), 105.3, 54.5, 52.1, 27.5；HRMS (ESI) (m/z) calcd for $C_{17}H_{16}ClFNO_2S$ $[M+H]^+$ 352.0569, found 352.0563.



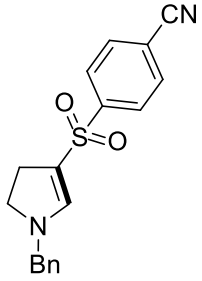
1-benzyl-4-((4-(trifluoromethyl)phenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole(3ah)

White solid, mp 93-95 °C. (Isolated yield 55%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.97-7.95 (d, *J* = 8.0 Hz, 2 H), 7.76-7.74 (d, *J* = 8.0 Hz, 2 H), 7.39-7.32 (m, 3 H), 7.22 (d, *J* = 1.2 Hz, 2 H), 7.20 (s, 1 H), 4.22 (s, 2 H), 3.48-3.43 (m, 2 H), 2.73-2.67 (m, 2 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm): δ = 151.9, 146.2, 135.4, 133.8-133.4 (d, *J* = 32 Hz, 1 C), 128.9, 128.2, 128.0, 127.1, 126.2-126.0 (m, 1 C), 124.8, 122.1, 105.0, 54.4, 52.2, 27.5；HRMS (ESI) (m/z) calcd for $C_{18}H_{17}F_3NO_2S$ $[M+H]^+$ 368.0927, found 368.0931.



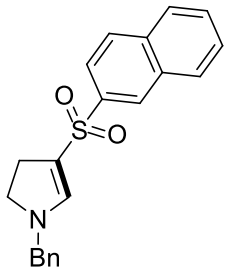
1-benzyl-4-((4-(trifluoromethoxy)phenyl)sulfonyl)-2,3-dihydro-1*H*-pyrrole(3ai)

White solid, mp 113-115 °C. (Isolated yield 61%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.89-7.87 (m, 2 H), 7.39-7.30 (m, 5 H), 7.23-7.21 (m, 2 H), 7.12 (s, 1 H), 4.21 (s, 2 H), 3.47-3.42 (m, 2 H), 2.73-2.68 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.6, 151.4, 141.1, 135.6, 128.9, 128.8, 128.2, 128.1, 120.9, 119.0, 105.7, 54.5, 52.2, 27.6； HRMS (ESI) (m/z) calcd for $C_{18}H_{17}F_3NO_3S$ $[M+H]^+$ 384.0876, found 384.0879.



4-((1-benzyl-4,5-dihydro-1*H*-pyrrol-3-yl)sulfonyl)benzonitrile(3aj)

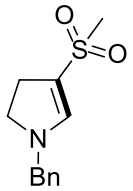
White solid, mp 102-105 °C. (Isolated yield 43%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.95-7.93 (d, *J* = 8.4 Hz, 2 H), 7.79-7.77 (d, *J* = 8.4 Hz, 2 H), 7.39-7.33 (m, 3 H), 7.22-7.20 (m, 2 H), 7.14 (s, 1 H), 4.24 (s, 2 H), 3.50-3.45 (m, 2 H), 2.74-2.69 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.3, 147.0, 135.3, 132.8, 129.0, 128.3, 128.02, 127.2, 117.7, 115.5, 104.3, 54.4, 52.1, 27.4； HRMS (ESI) (m/z) calcd for $C_{18}H_{17}N_2O_2S$ $[M+H]^+$ 325.1005, found 325.1009.



1- benzyl-4-(naphthalen-2-ylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3ak)

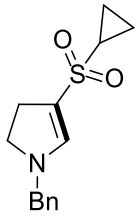
White solid, mp 131-133 °C. (Isolated yield 54%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.41 (s, 1 H), 7.96-7.88 (m, 3 H), 7.83-7.81 (m, 1 H), 7.63-7.56 (m, 2 H), 7.37-7.30 (m, 3 H), 7.26-7.20 (m, 2 H), 7.16 (s, 1 H), 4.20 (s, 2 H), 3.42-3.37 (m, 2 H), 2.74-2.69

(m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.1, 139.4, 135.8, 134.6, 132.4, 129.2, 129.2, 128.9, 128.4, 128.1, 128.0, 127.9, 127.6, 127.3, 122.5, 106.8, 54.6, 52.2, 27.7；HRMS (ESI) (m/z) calcd for $C_{21}H_{20}NO_2S$ $[M+H]^+$ 350.1209, found 350.1214.



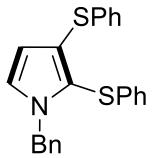
1-benzyl-4-(methylsulfonyl)-2,3-dihydro-1*H*-pyrrole (3am)

White solid, mp 68-69 °C. (Isolated yield 82%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.39-7.31 (m, 3 H), 7.24-7.22 (m, 2 H),7.00 (s, 1 H), 4.19 (s, 2 H), 3.51-3.46 (m, 2 H), 2.92-2.85 (m, 5 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.1, 135.8, 128.9, 128.5, 128.1, 106.4, 54.6, 52.4, 43.0, 28.1；HRMS (ESI) (m/z) calcd for $C_{12}H_{16}NO_2S$ $[M+H]^+$ 238.0896, found 238.0899.



1-benzyl-4-(cyclopropylsulfonyl)-2,3-dihydro-1*H*-pyrrole(3an)

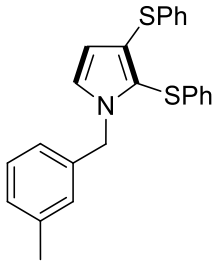
White solid, mp 77-79 °C. (Isolated yield 69%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.39-7.31 (m, 3 H), 7.25-7.23 (m, 2 H),7.00 (s, 1 H), 4.19 (s, 2 H), 3.49-3.43 (m, 2 H), 2.91-2.86 (m, 2 H), 2.40-2.34 (m, 1 H), 1.17-1.13 (m, 2 H), 0.95-0.90 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.9, 136.0, 128.9, 128.1, 128.0, 106.6, 54.7, 52.4, 31.6, 28.3, 4.6；HRMS (ESI) (m/z) calcd for $C_{14}H_{18}NO_2S$ $[M+H]^+$ 264.1053, found 264.1057.



1-benzyl-2,3-bis(phenylthio)-1*H*-pyrrole (4a)

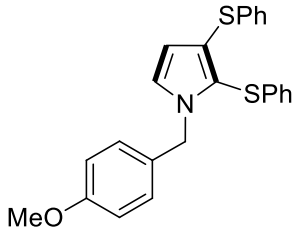
White solid, mp 150-152 °C. (Isolated yield 69%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.25-7.23 (m, 3 H), 7.18-7.17 (m, 4 H), 7.12-7.02 (m, 6 H), 6.95-6.93 (m, 3 H), 6.45-6.44 (m, 1 H), 5.18 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 138.8, 137.3, 137.1, 128.9, 128.7, 128.7, 127.7, 127.4, 127.3, 126.6, 125.7, 125.4, 125.2, 123.6, 120.4,

115.1, 51.7； HRMS (ESI) (m/z) calcd for $C_{23}H_{20}NS_2$ $[M+H]^+$ 374.1032, found 374.1038.



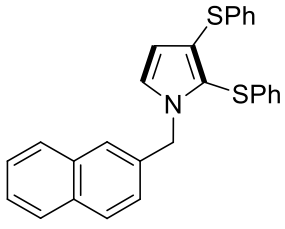
1-(3-methylbenzyl)-2,3-bis(phenylthio)-1*H*-pyrrole (4b)

White solid, mp 158-160 °C. (Isolated yield 46%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.18-7.16 (m, 4 H), 7.14-7.10 (m, 3 H), 7.07-7.02 (m, 3 H), 6.95-6.93 (m, 3 H), 6.86-6.84 (d, *J* = 7.6 Hz, 1 H), 6.76 (s, 1), 6.45-6.44 (d, *J* = 2.8 Hz, 1 H), 5.14 (s, 2 H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 138.9, 138.4, 137.4, 137.0, 128.9, 128.7, 128.6, 128.5, 128.2, 127.2, 126.6, 125.6, 125.5, 125.2, 124.5, 123.6, 120.3, 115.1, 51.7, 21.3；HRMS (ESI) (m/z) calcd for $C_{24}H_{22}NS_2$ $[M+H]^+$ 388.1188, found 388.1192.



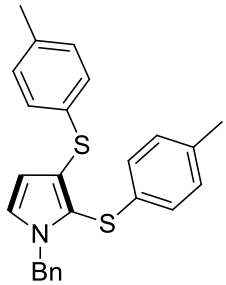
1-(4-methoxybenzyl)-2,3-bis(phenylthio)-1*H*-pyrrole (4c)

White solid, mp 156-158 °C. (Isolated yield 70%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.17-7.16 (d, *J* = 4.4 Hz, 4 H), 7.12-7.10 (m, 2 H), 7.07-7.03 (m, 2 H), 7.00-6.97 (d, *J* = 8.8 Hz, 2 H), 6.94-6.91 (m, 3 H), 6.78-6.76 (d, *J* = 8.8 Hz, 2 H), 6.43-6.42 (d, *J* = 3.2 Hz, 1 H), 5.10 (s, 2), 3.76 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.2, 138.9, 137.5, 129.0, 129.0, 128.9, 128.6, 127.2, 126.5, 125.6, 125.2, 125.2, 123.3, 120.3, 115.0, 114.1, 55.3, 51.2； HRMS (ESI) (m/z) calcd for $C_{24}H_{22}NOS_2$ $[M+H]^+$ 404.1138, found 404.1144.



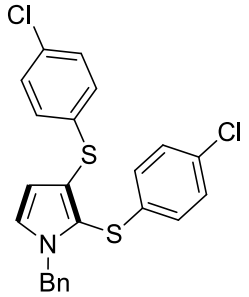
1-(naphthalen-2-ylmethyl)-2,3-bis(phenylthio)-1*H*-pyrrole (4d)

White solid, mp 163-165 °C. (Isolated yield 67%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.84 (d, *J* = 8.0 Hz, 1 H), 7.79-7.77 (d, *J* = 8.0 Hz, 1 H), 7.74-7.72 (d, *J* = 8.0 Hz, 1 H), 7.50-7.33 (m, 3 H), 7.20-7.19 (m, 3 H), 7.17-7.14 (m, 2 H), 7.11-7.07 (m, 2 H), 7.05-7.00 (m, 3 H), 6.77-6.76 (d, *J* = 3.2 Hz, 1 H), 6.41-6.40 (d, *J* = 3.2 Hz, 1 H), 5.60 (s, 2); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.0, 137.1, 133.7, 132.3, 131.0, 129.0, 128.8, 128.8, 128.7, 127.2, 127.0, 126.6, 126.4, 126.0, 125.9, 125.4, 125.2, 123.8, 122.9, 120.4, 115.1, 49.6； HRMS (ESI) (m/z) calcd for $C_{27}H_{22}NS_2$ $[M+H]^+$ 424.1188, found 424.1183.



1- benzyl-2,3-bis(*p*-tolylthio)-1*H*-pyrrole (4e)

White solid, mp 149-152 °C. (Isolated yield 52%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.25-7.23 (m, 3 H), 7.11-7.09 (m, 2 H), 7.03-6.98 (m, 4 H), 6.94-6.92 (d, *J* = 8.0 Hz, 2 H), 6.88-6.85 (m, 3 H), 6.39-6.38 (d, *J* = 8.0 Hz, 1 H), 5.16 (s, 2 H), 2.67 (s, 3 H), 2.44 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 137.3, 135.5, 135.2, 135.0, 133.7, 129.6, 129.4, 128.6, 128.0, 127.6, 127.3, 127.0, 125.1, 123.6, 121.1, 114.6, 51.6, 20.9, 20.9； HRMS (ESI) (m/z) calcd for $C_{25}H_{24}NS_2$ $[M+H]^+$ 402.1345, found 402.1340.



1-benzyl-2,3-bis((4-chlorophenyl)thio)-1*H*-pyrrole (4f)

White solid, mp 165-167 °C. (Isolated yield 59%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.25-7.23 (m, 3 H), 7.13-7.11 (m, 2 H), 7.06-6.7.00 (m, 6 H), 6.98-6.97 (d, *J* = 3.2 Hz, 2 H), 6.79-6.77 (m, 2 H), 6.45 (d, *J* = 2.8 Hz, 1 H), 5.17 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 137.2, 136.8, 135.6, 131.7, 131.2, 129.0, 128.8, 128.7, 128.6,

127.9, 127.8, 127.3, 125.8, 123.3, 120.3, 115.3, 51.9；HRMS (ESI) (m/z) calcd for $C_{23}H_{18}Cl_2NS_2$ $[M+H]^+$ 442.0252, found 442.0256.

Refrence:

[1] a)Liu, L. K.; Chi, Y.; Jen, K.-Y. *J. Org. Chem.* **1980**, *45*, 406; b) Zhou, X.-Y.; Luo, J.-Y.; Liu, J.; Peng, S.-M.; Deng, G.-J. *Org. Lett.*, **2011**, *13*, 1432; c) Natalie U.; Georg M. *Org. Lett.* **2013**, *15*, 188.

[2] a) Bi, H.-P.; Zhao, L.; Liang, Y.-M; Li, C.-J. *Angew. Chem. Int. Ed*. **2009**, *48*, 792; b) Tang, Y.-Q.; Lu, J.-M.; Wang, X.-R.; Shao, L.-X.; *Tetrahedron*. **2010**, *66*, 7970.

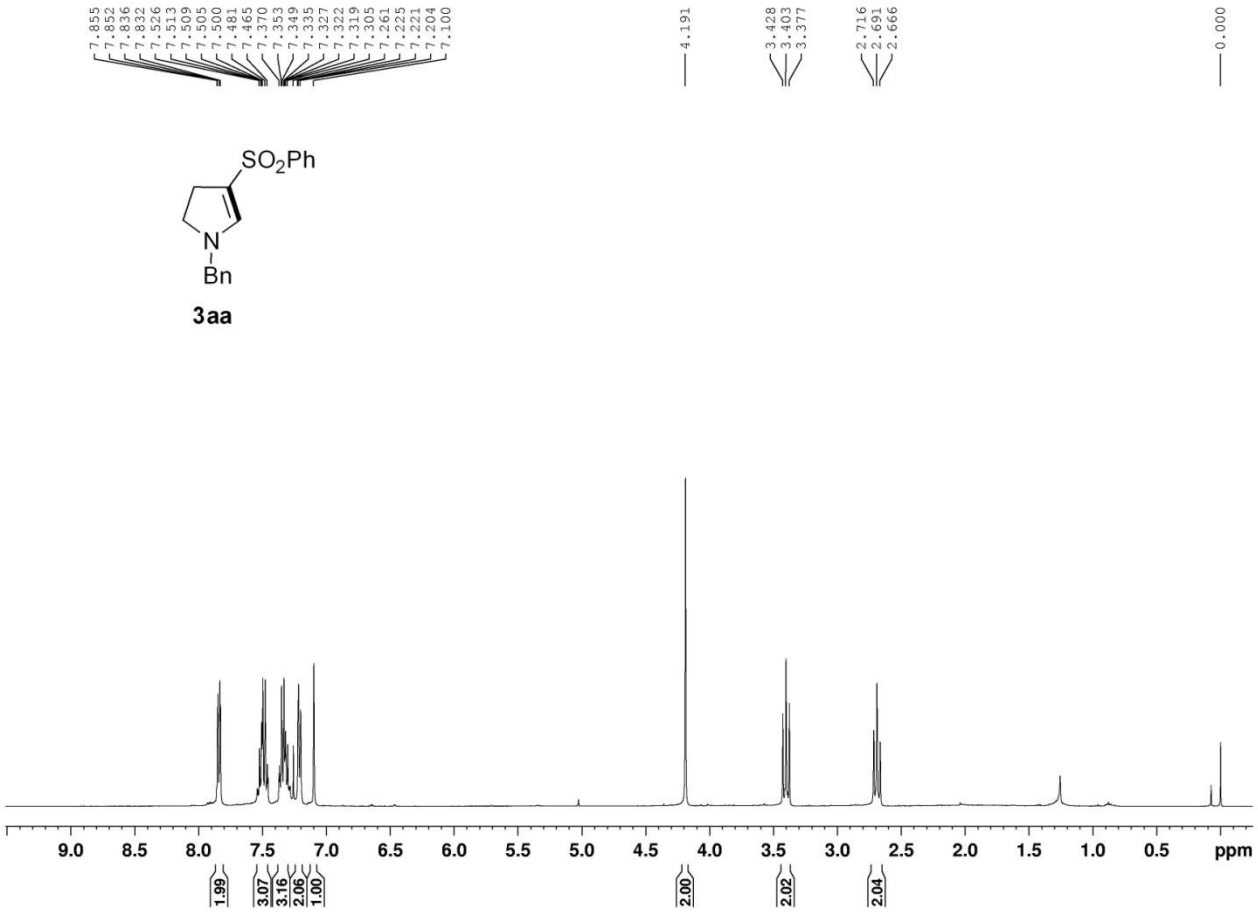
[3] Scott, J. B.; Philip, C. D.; Janice, A. S.; Craig, J. D.; Xiang, J. N.; Richard, F. K.; David, J. M.; Scott, D. L. *Bioorg. Med. Chem*. **2015**, 23, 1569.

[4] Luigi, A.; John, S. B.; Robert, T. C. B.; Andrew B. H.; Marianne, M. S. *J. Org. Chem.* **2003**, *68*, 2652.

[5] Ren, L.-Y.; Feng, W.-H. *From Huaxue Shiji*, **2010**,32, 928.

[6] Wen, Y. H.; Gao, B.; Fu, Y. Z.; Dong, S. X.; Liu, X. H.; Feng, X. M. *Chem. Eur. J.* **2008**, 14, 6789.

[7] Makonen, B.; Piyssena, H. from PCT Int. Appl., 2012039717, 29 Mar **2012**.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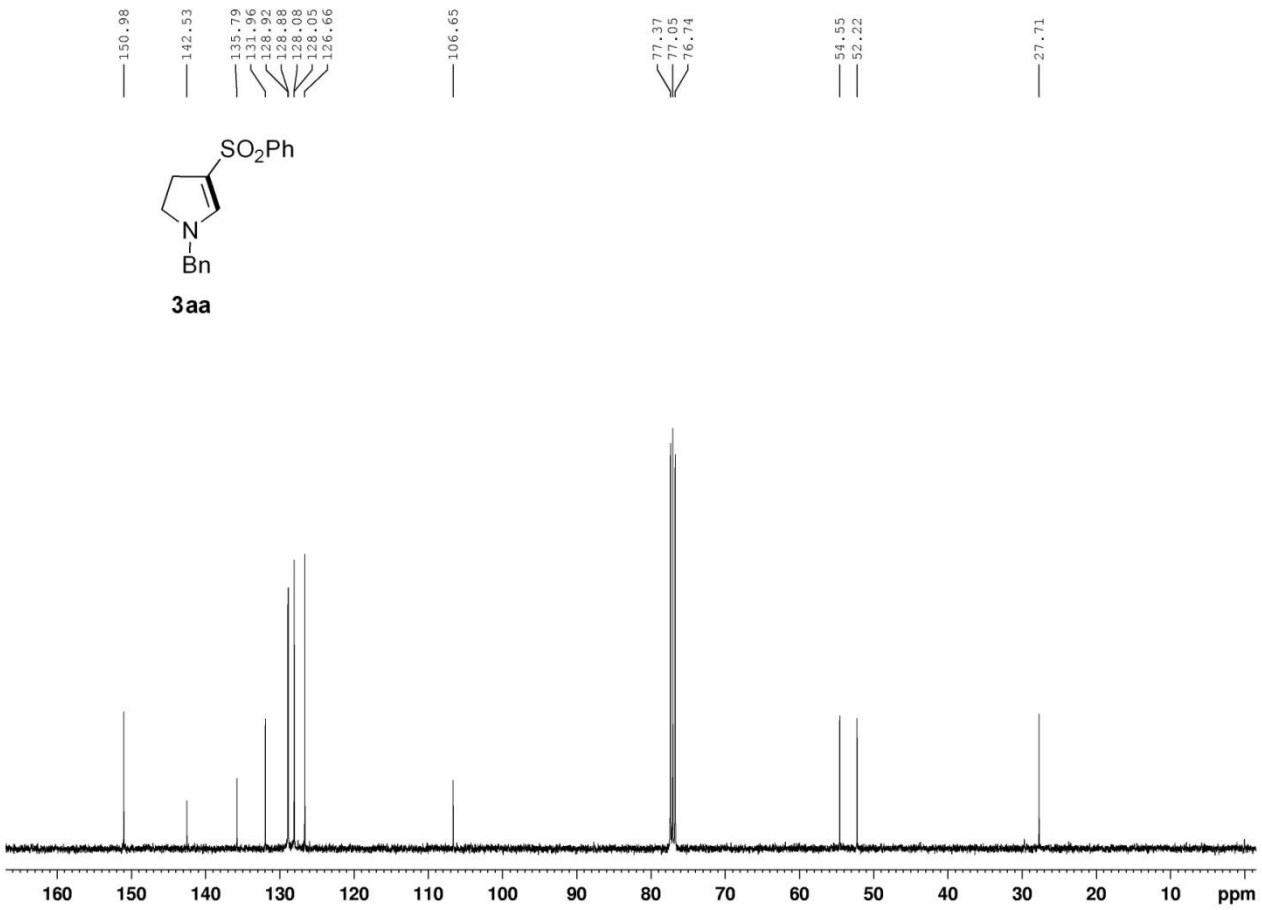
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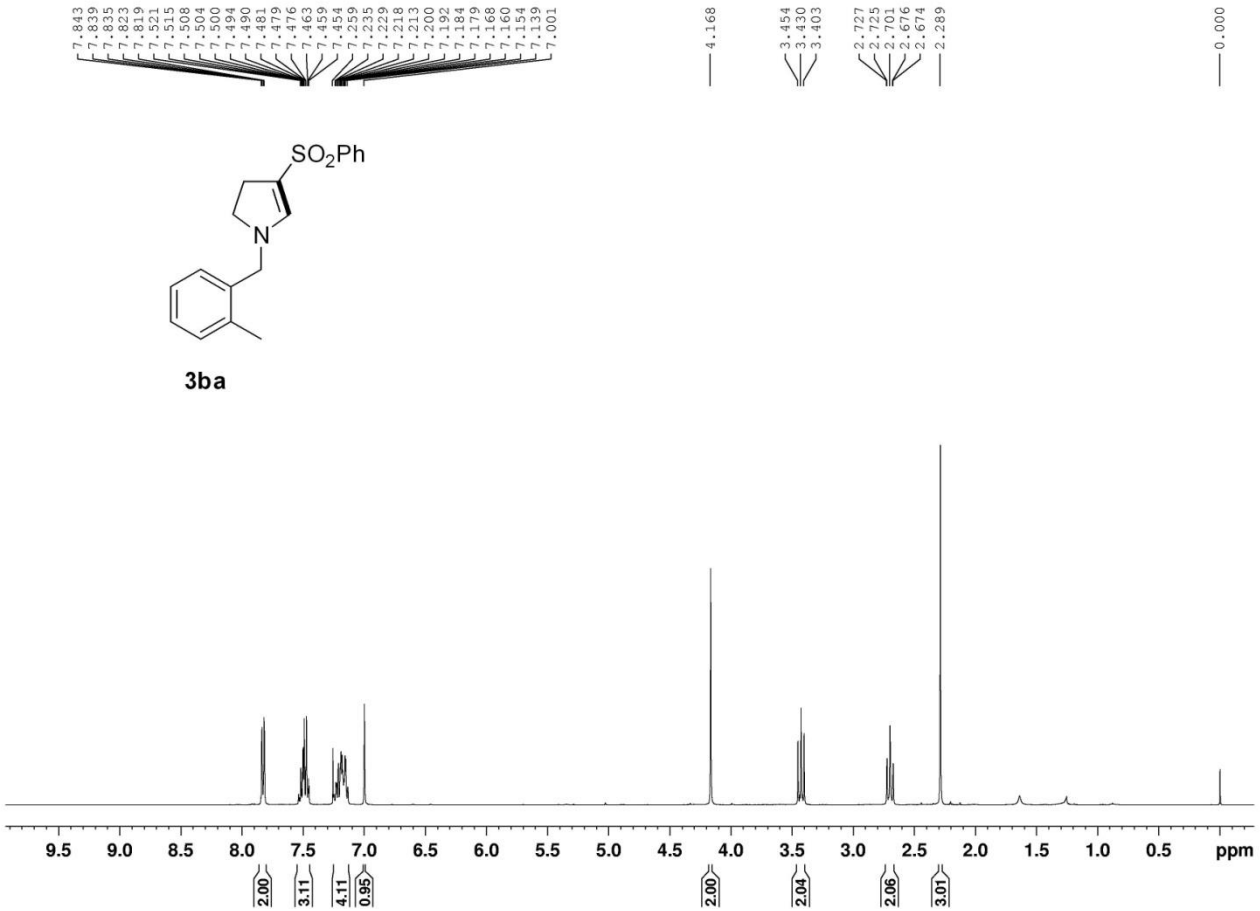
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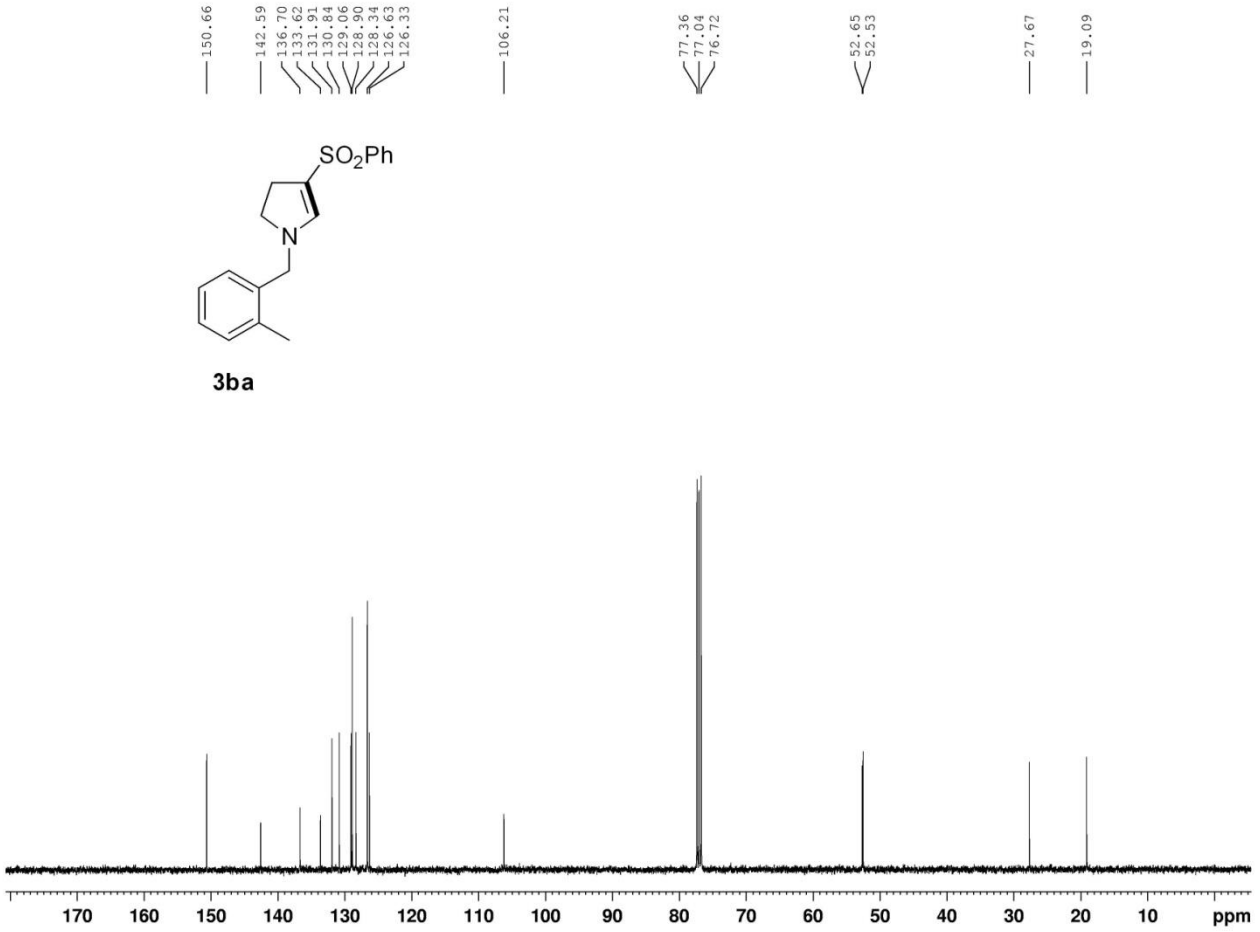
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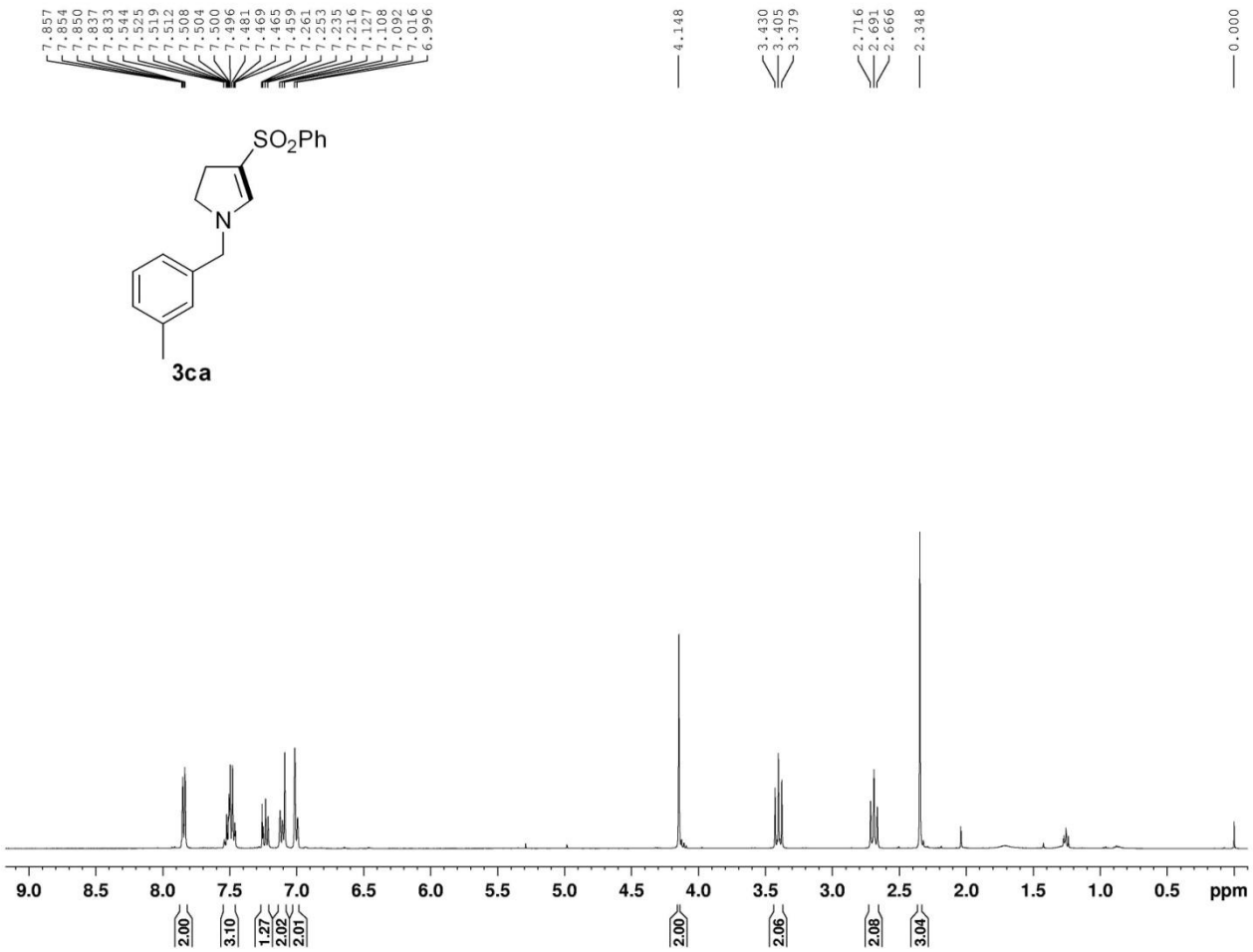
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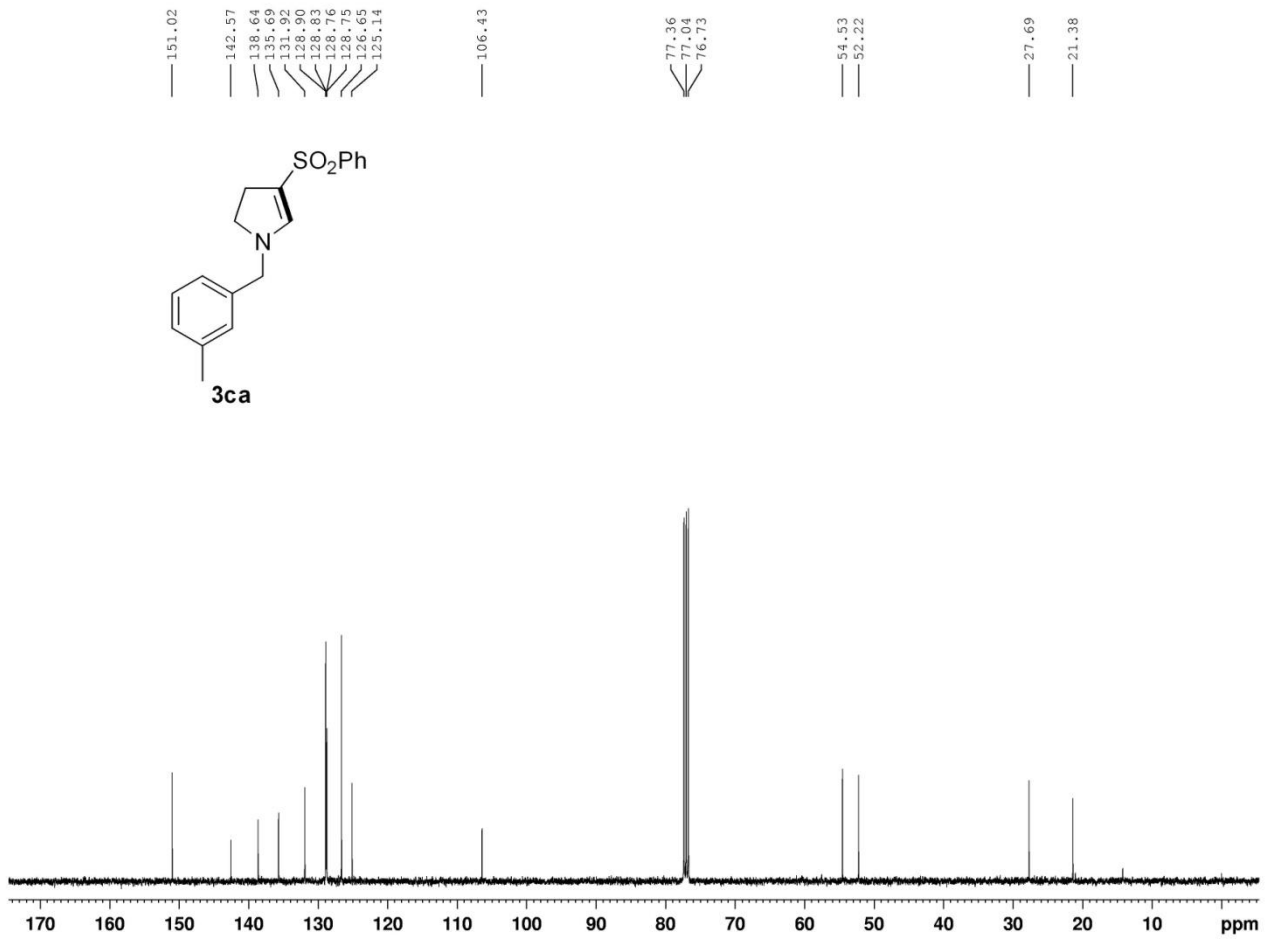
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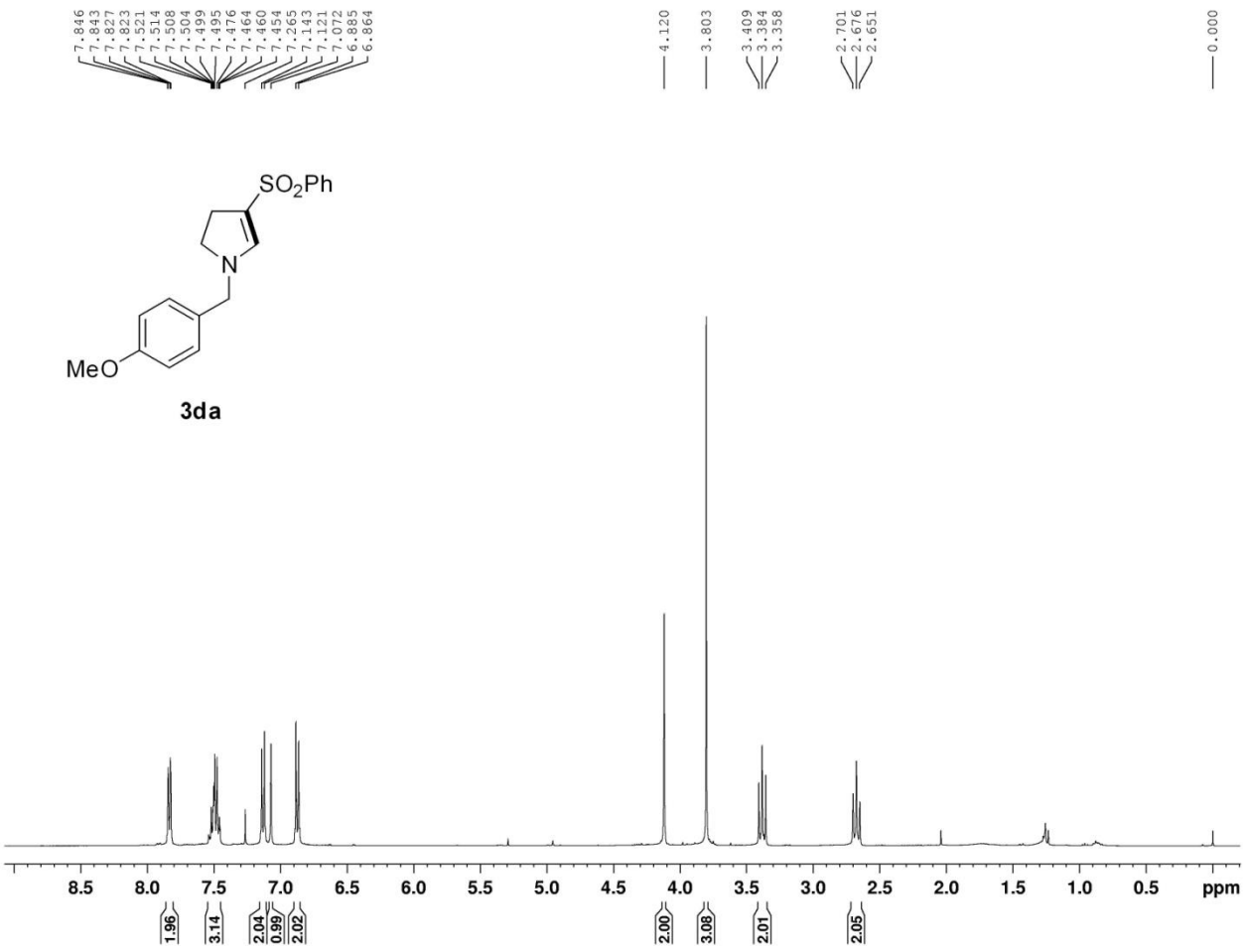
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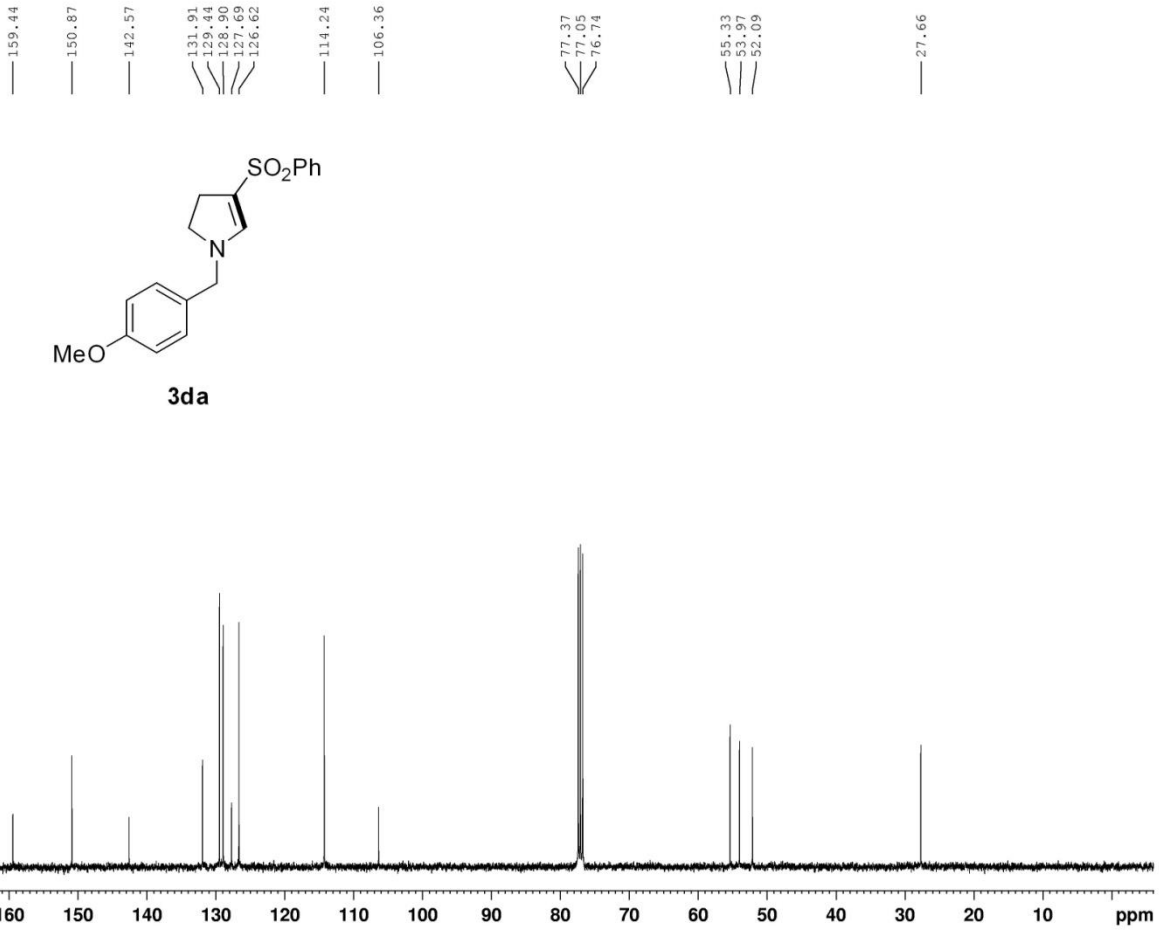
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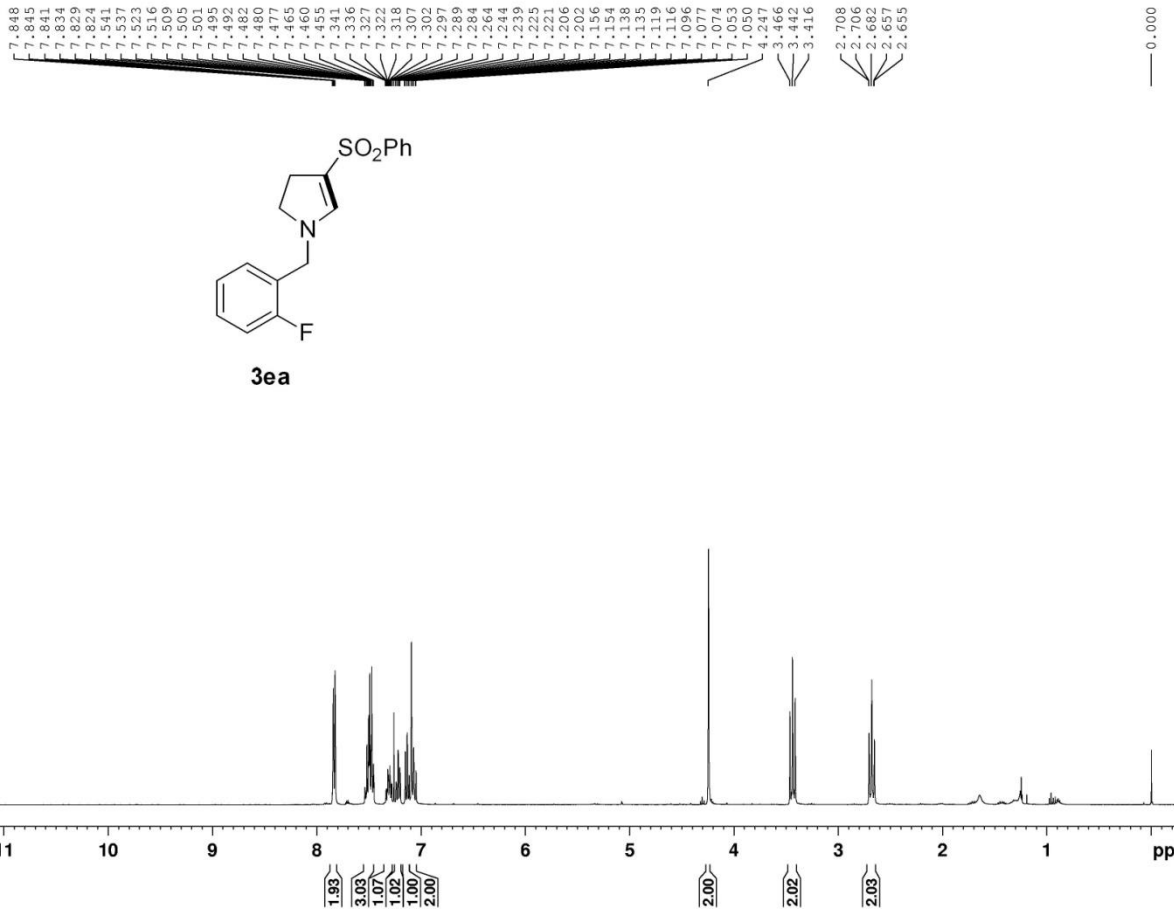
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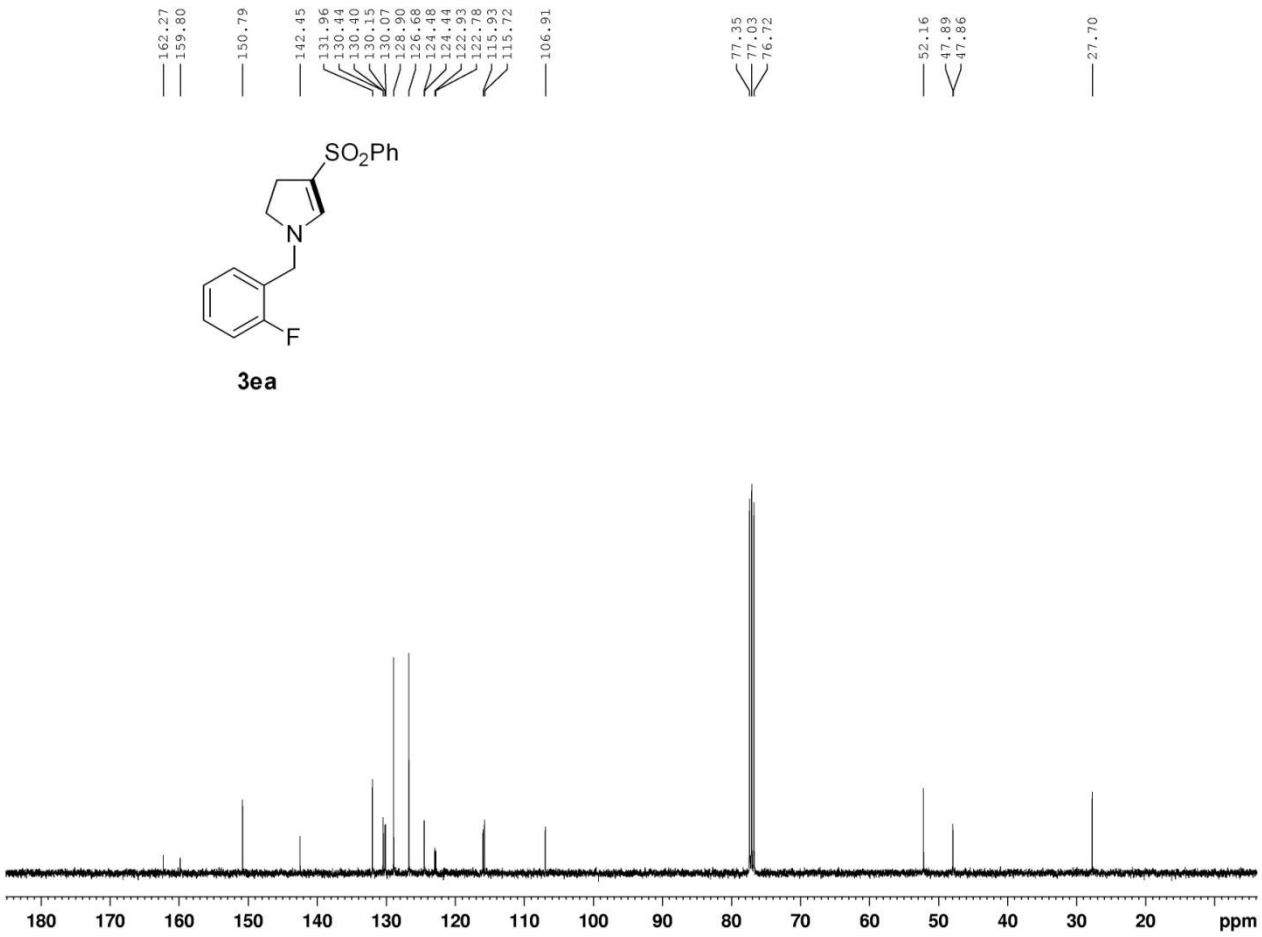
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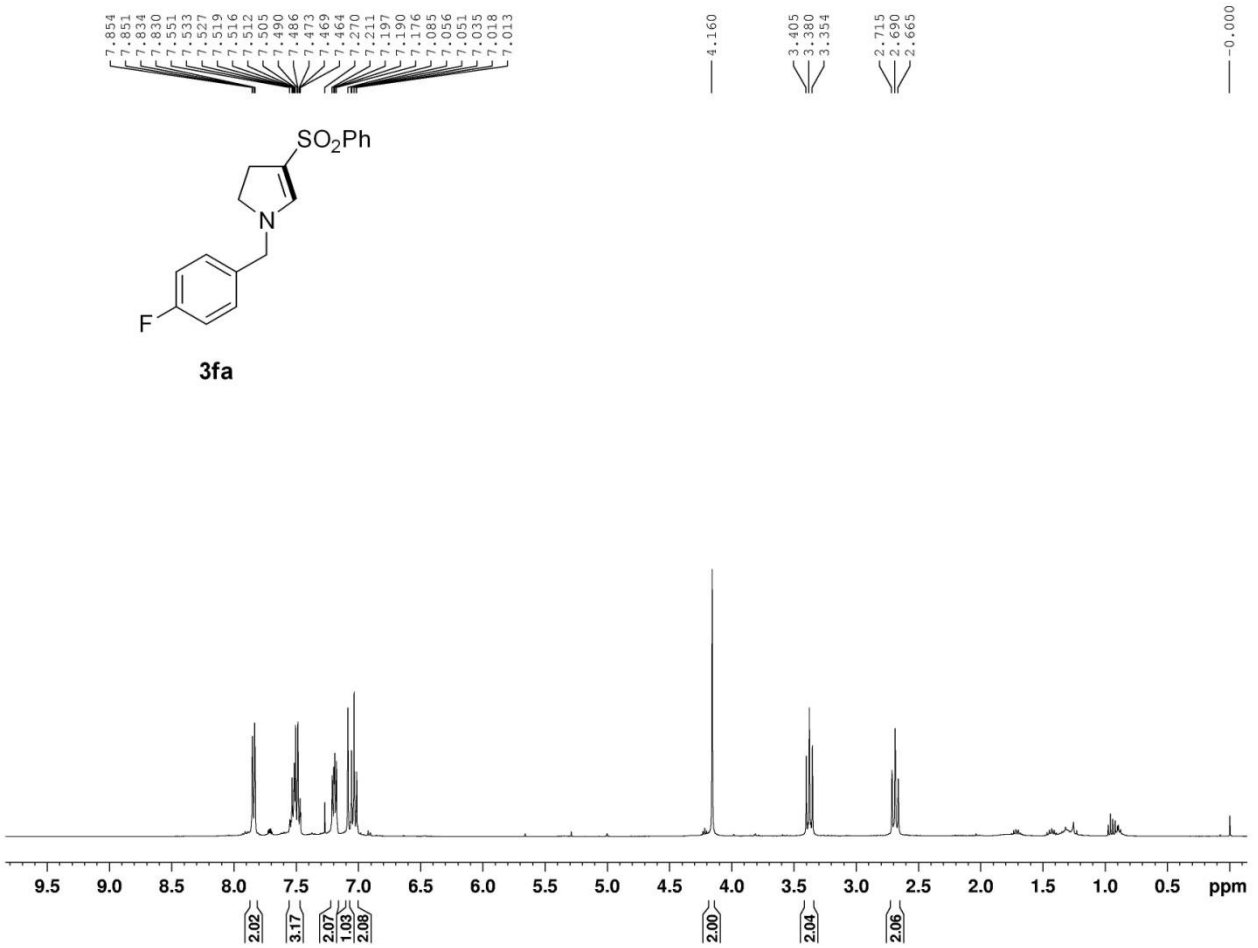
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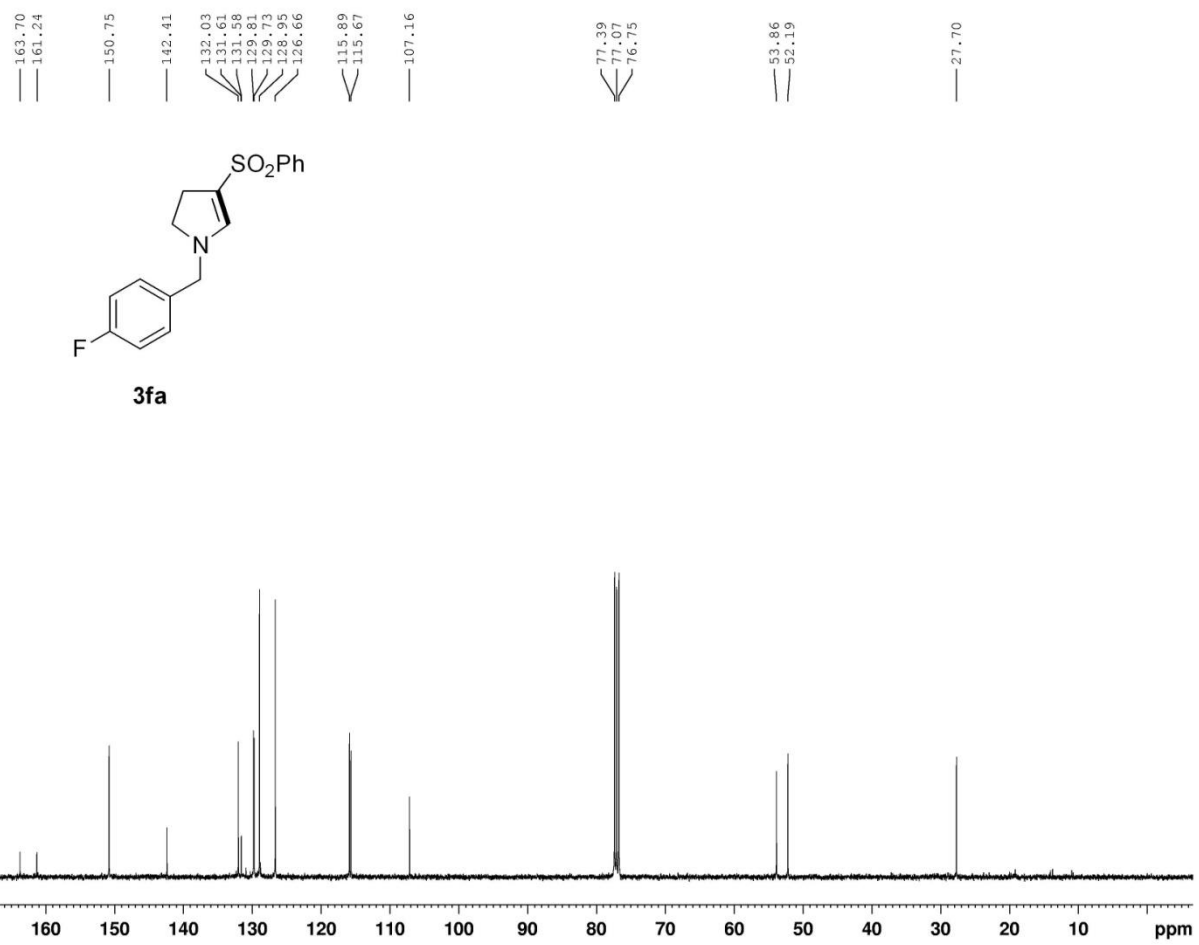
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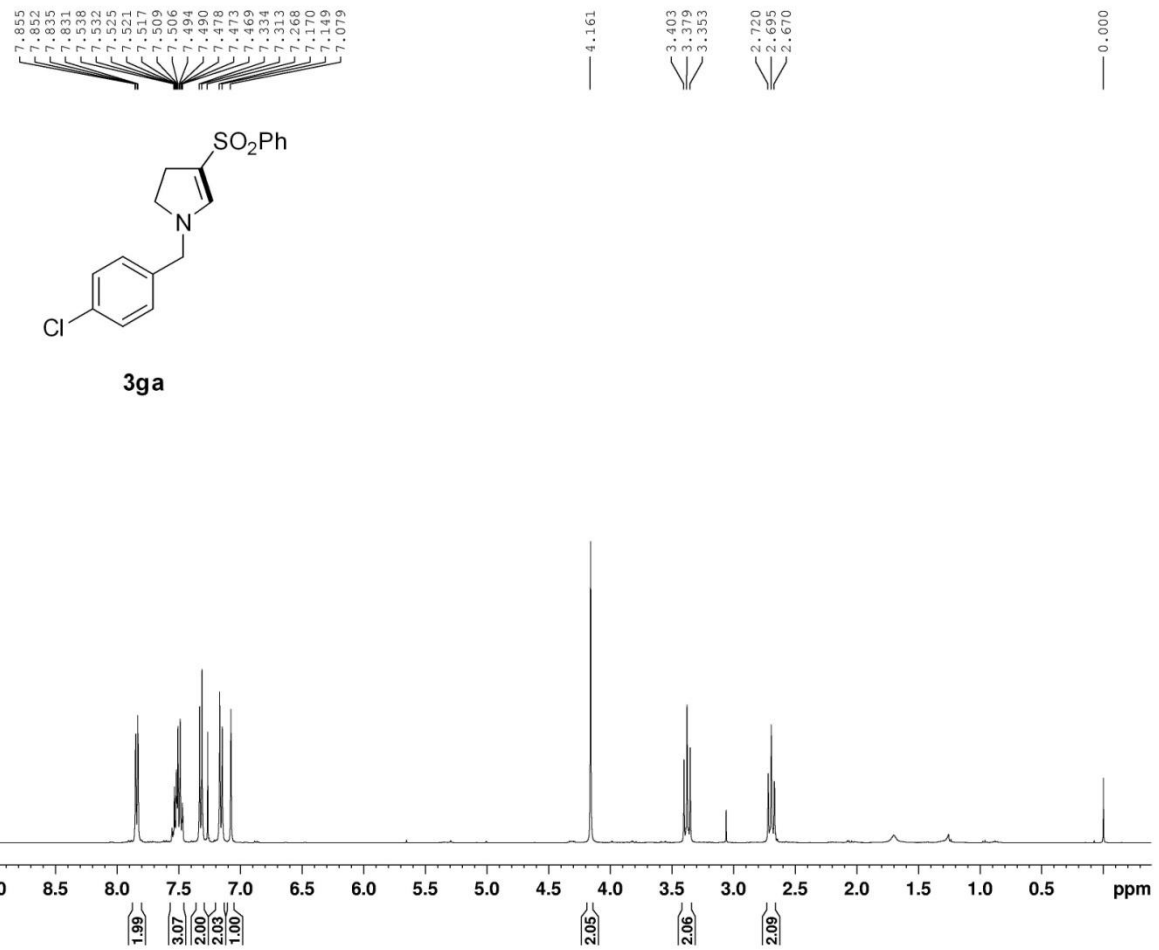
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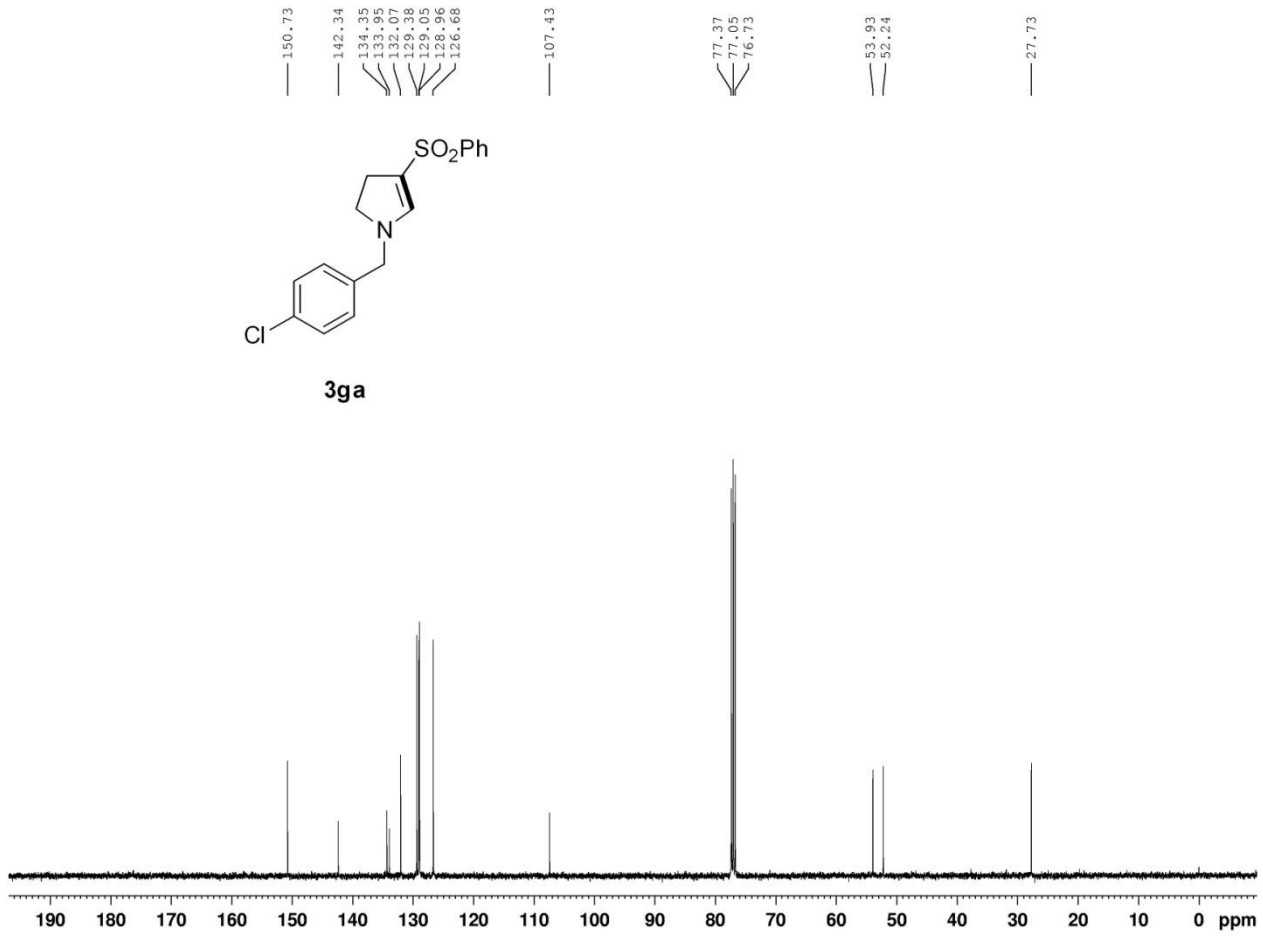
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Cl
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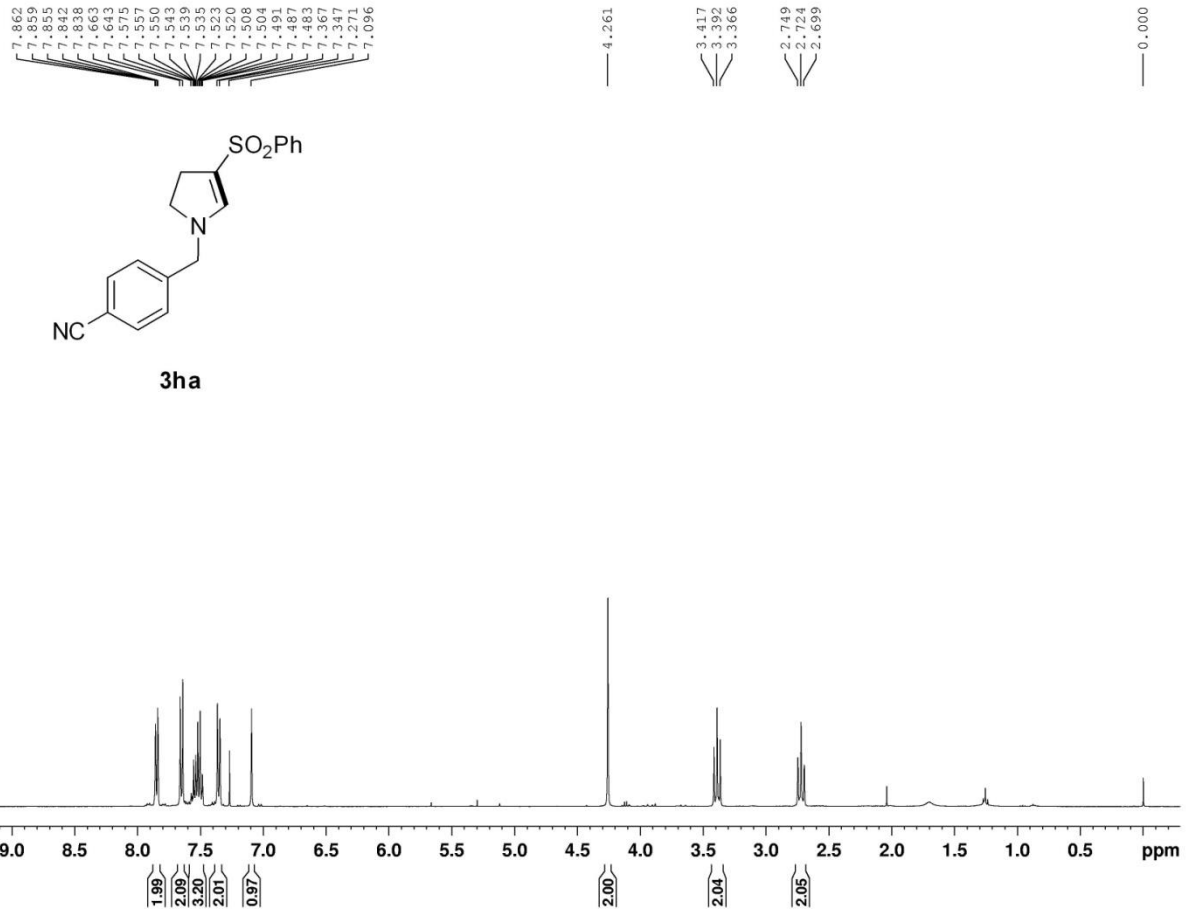
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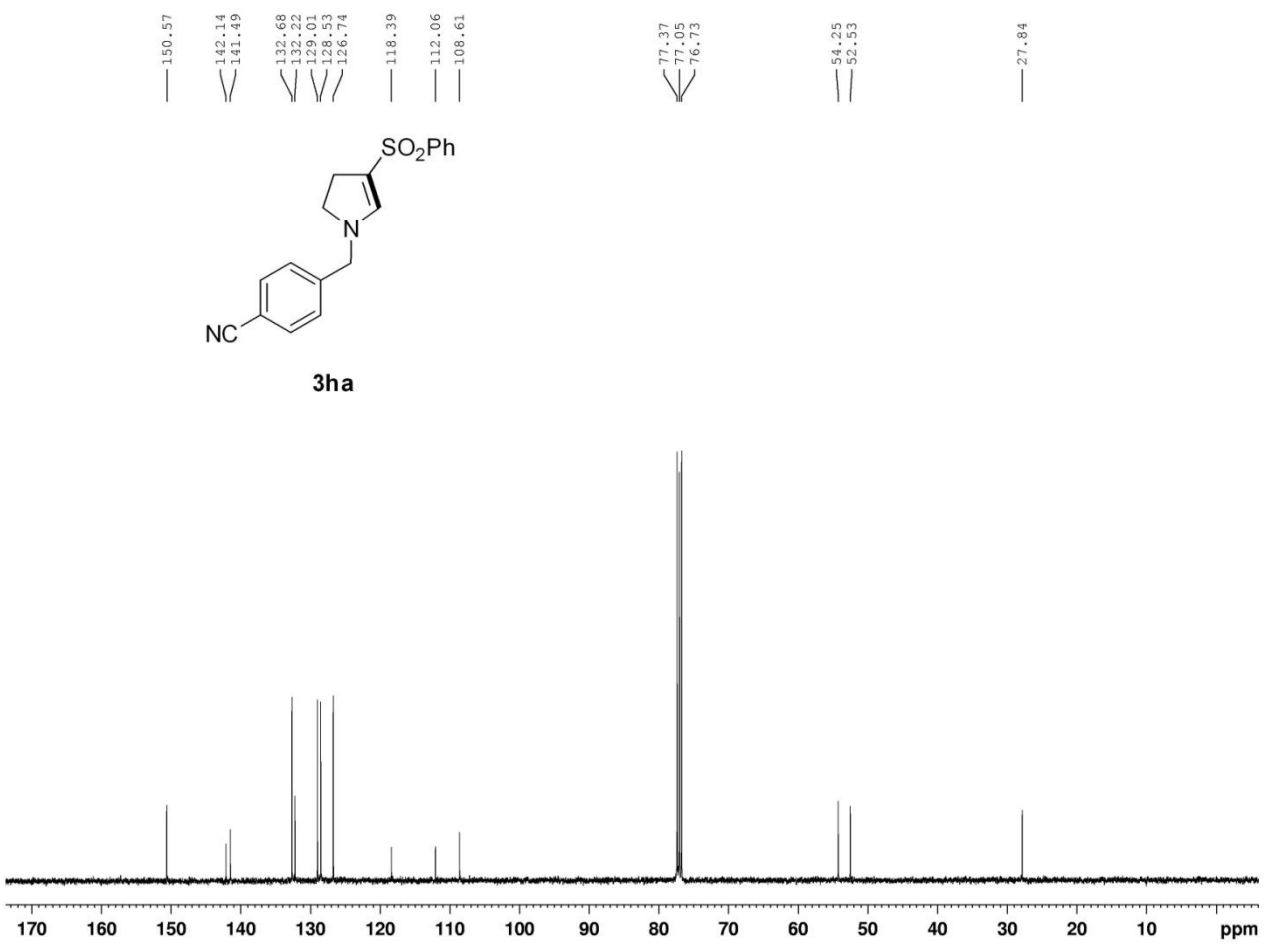
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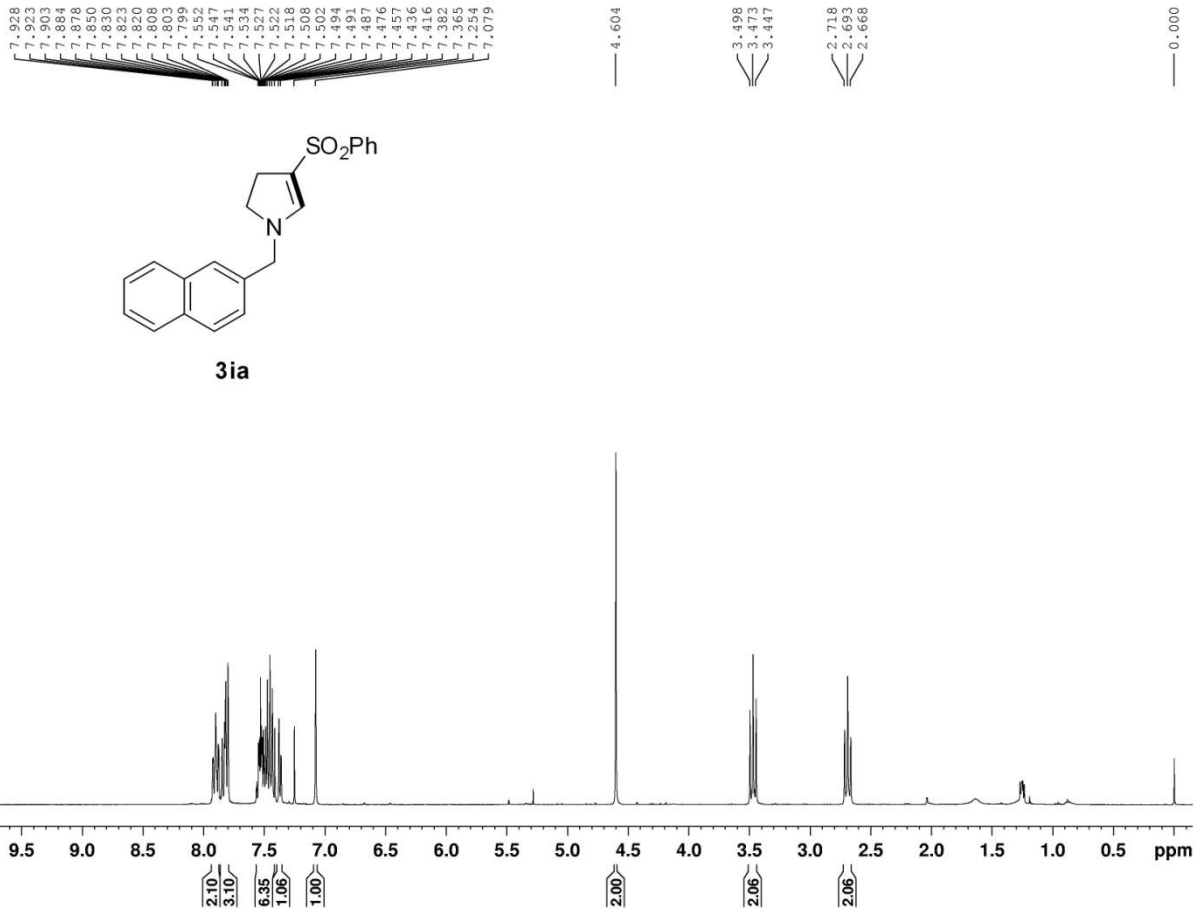
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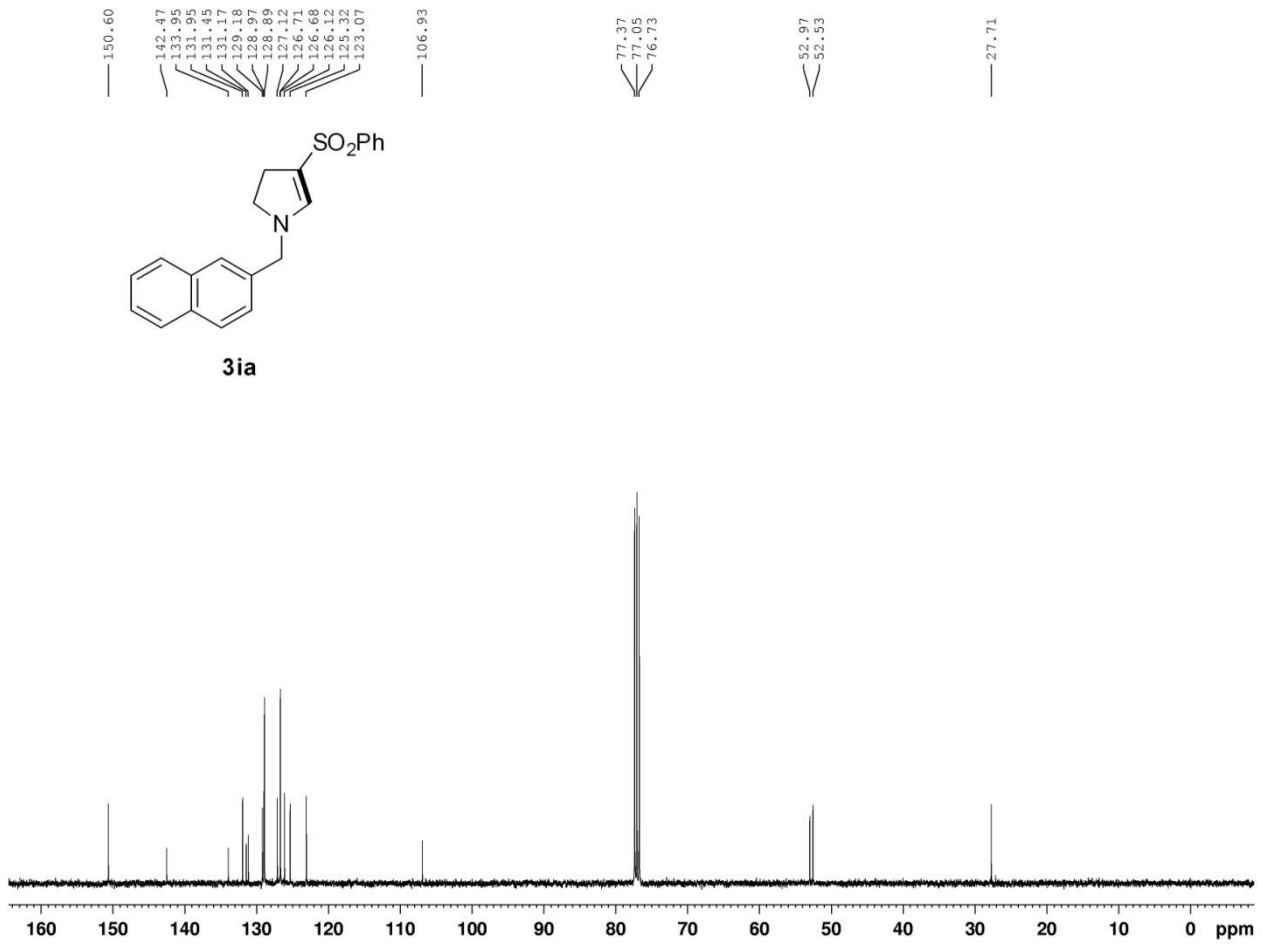
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126.12
125.32
123.07
106.93
77.37
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76.73
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52.53
27.71
SO2Ph
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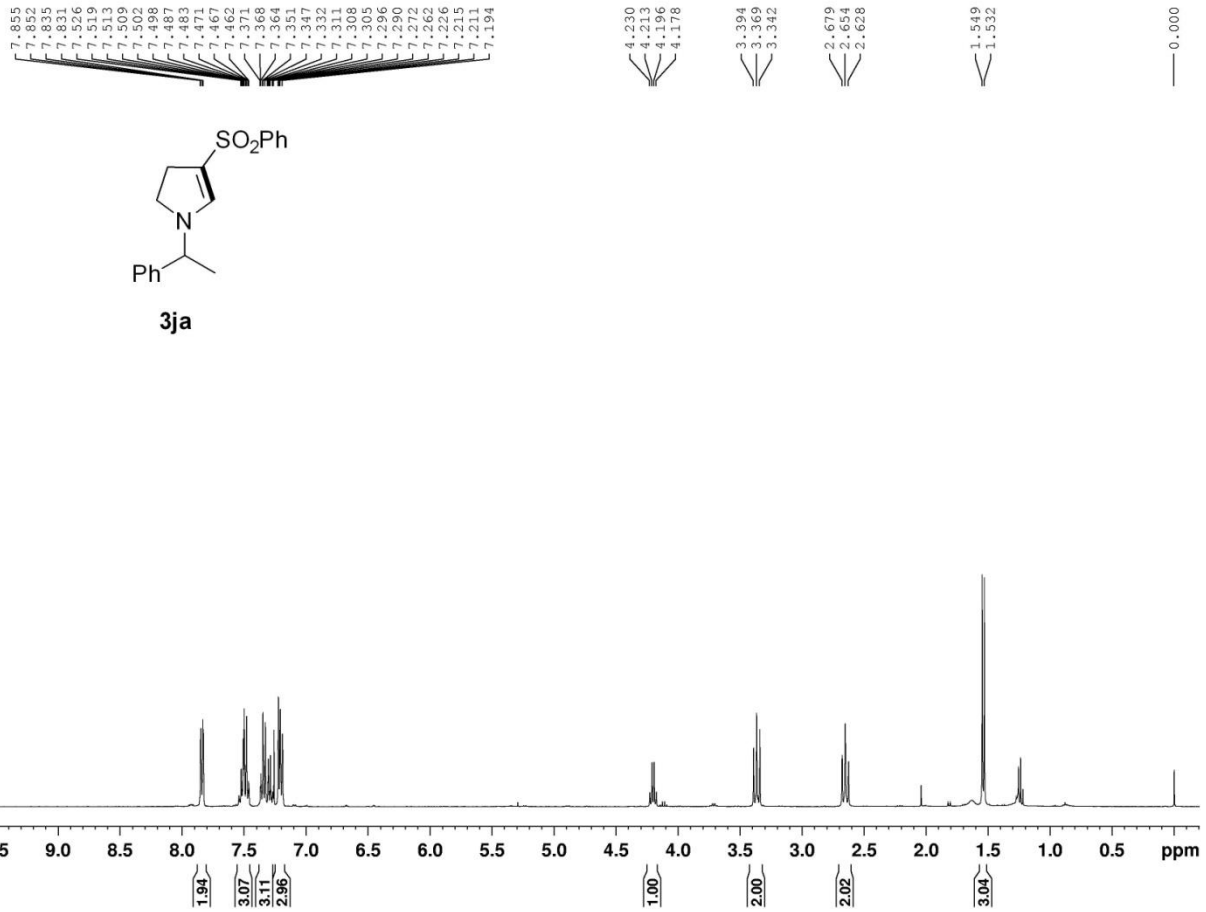
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Ph
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8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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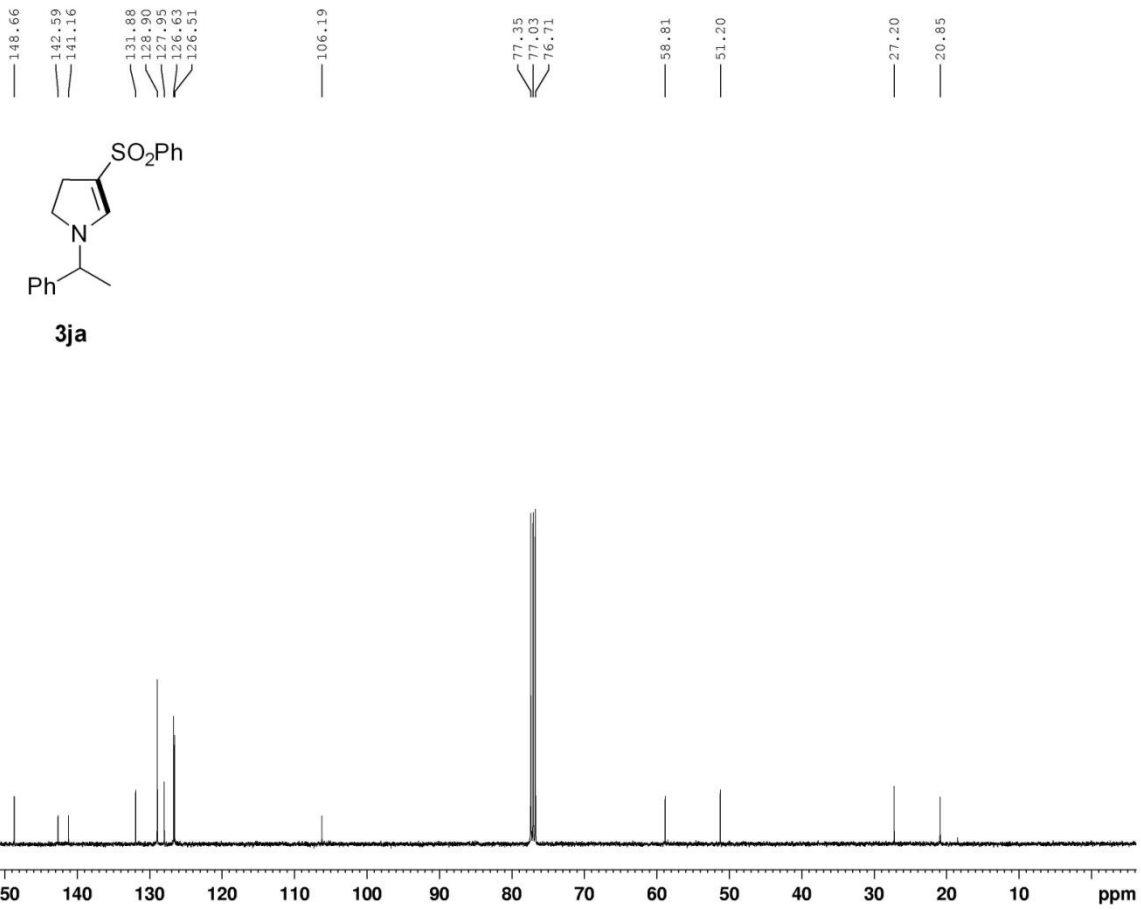
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51.20
27.20
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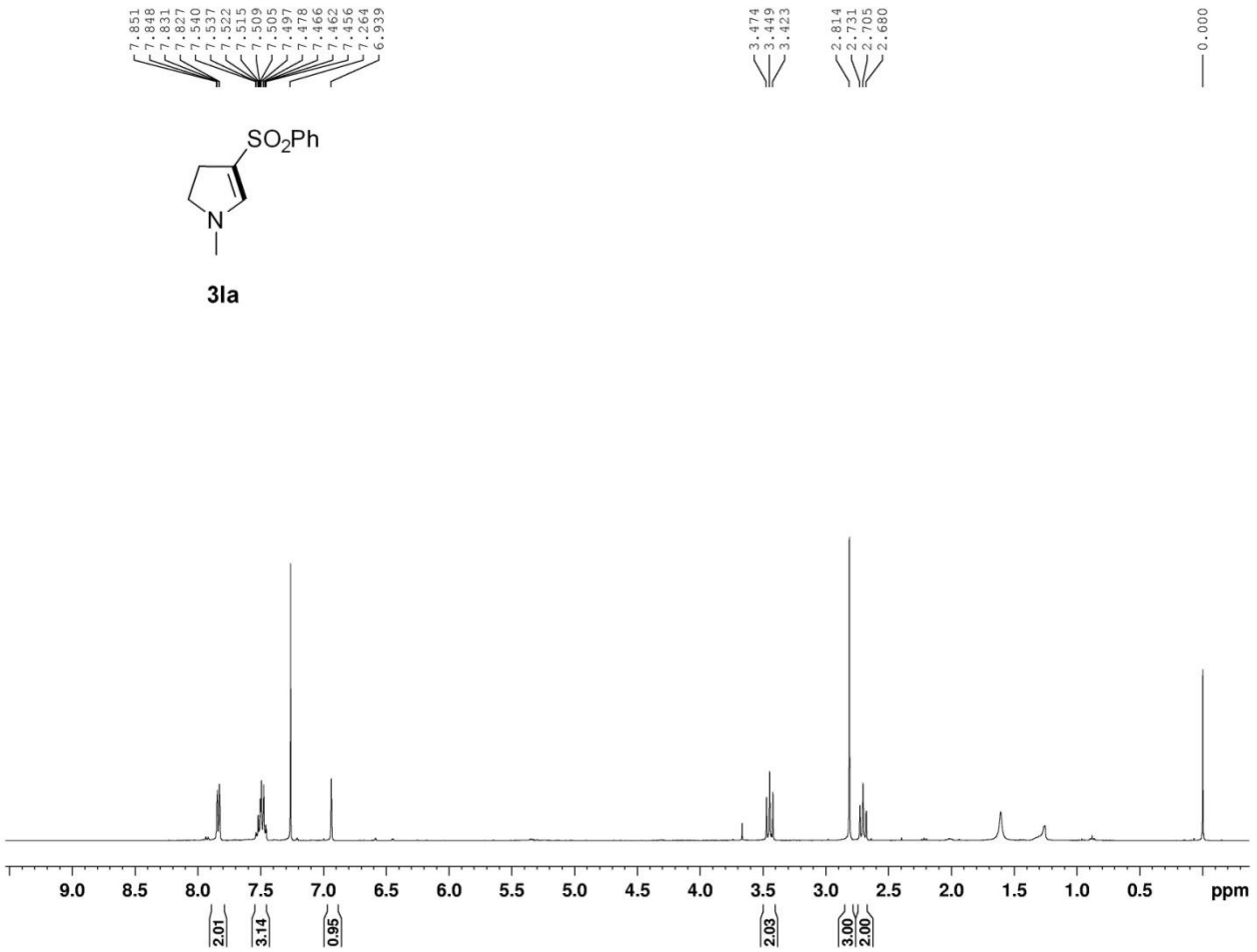
ppm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6.0
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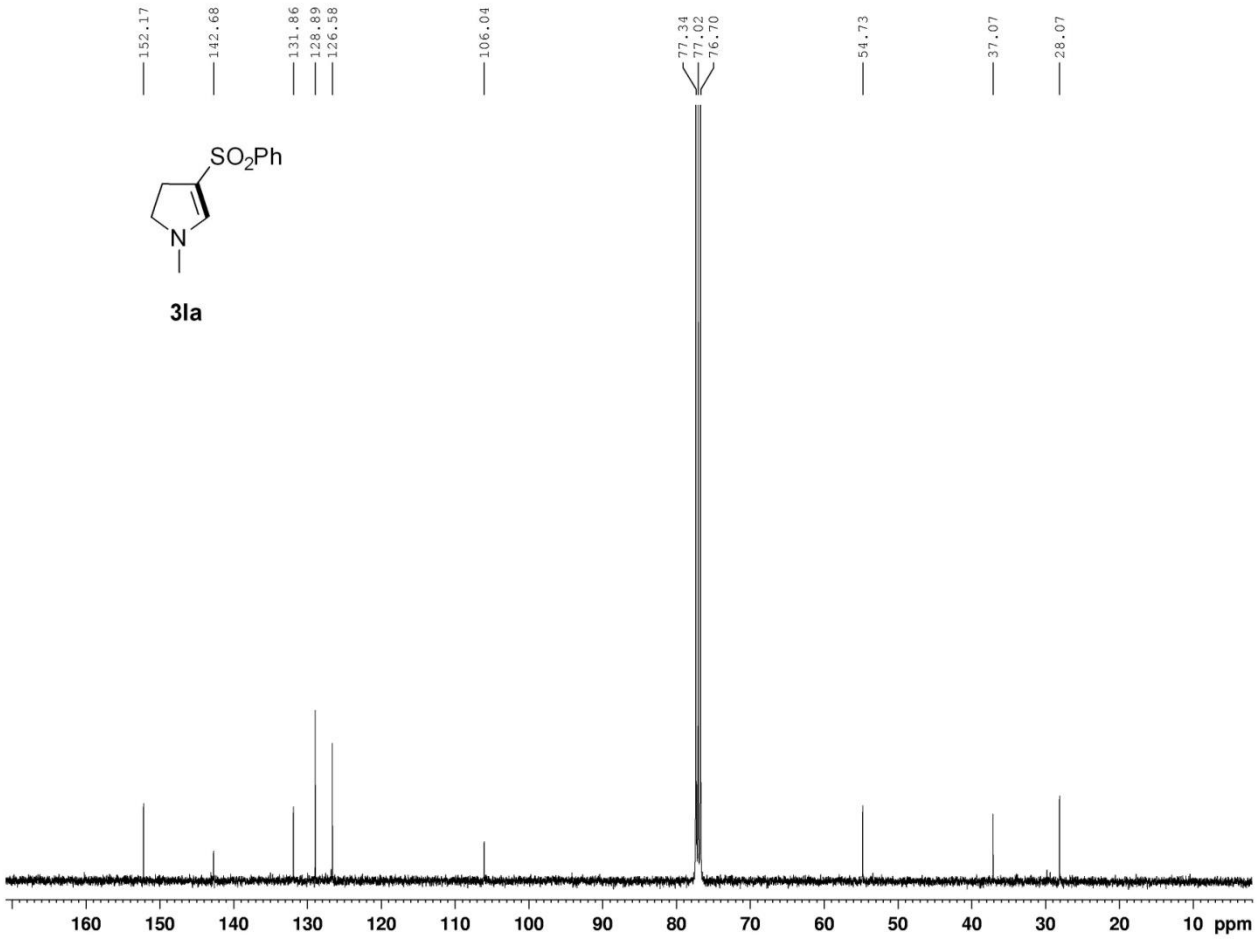
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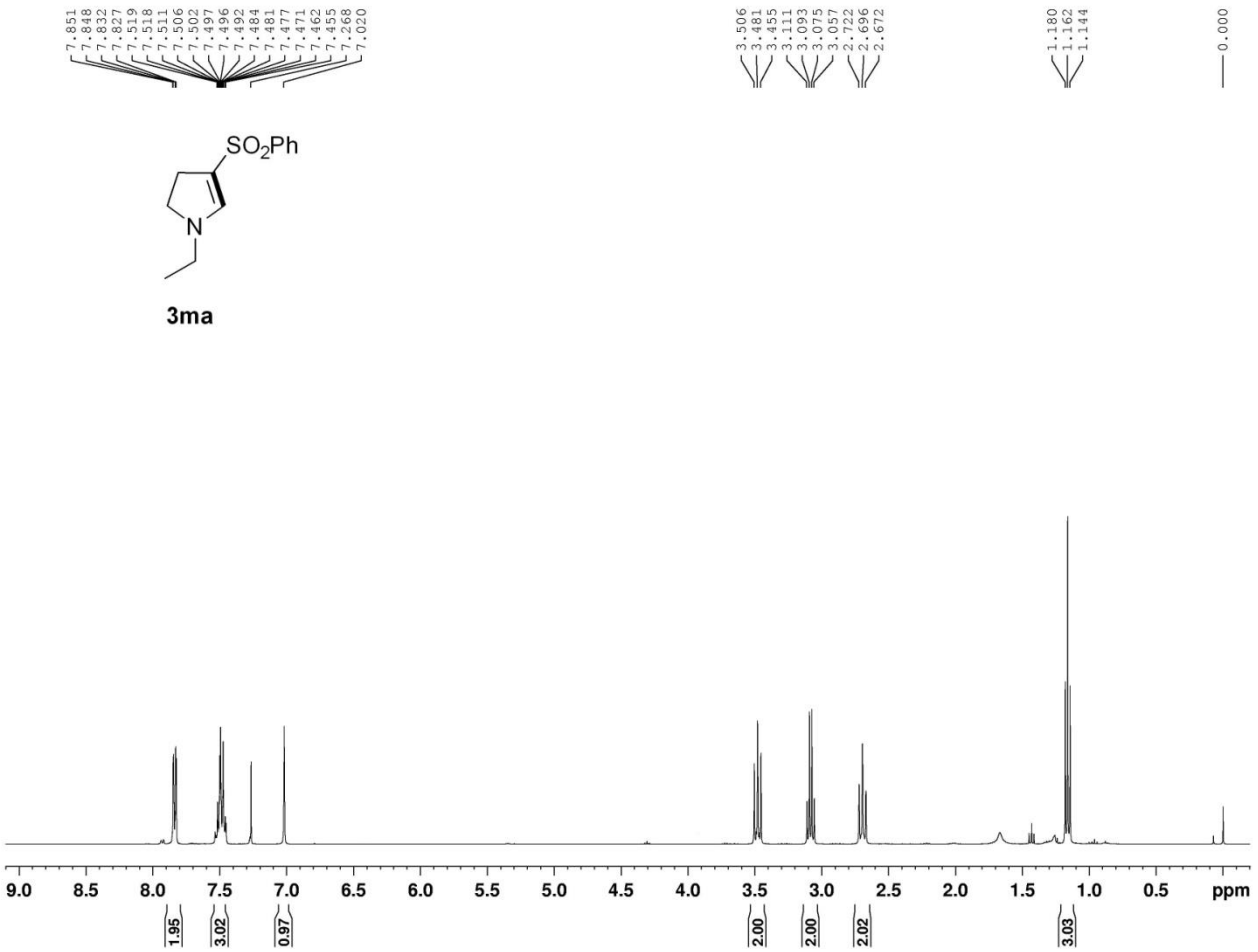
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3.455
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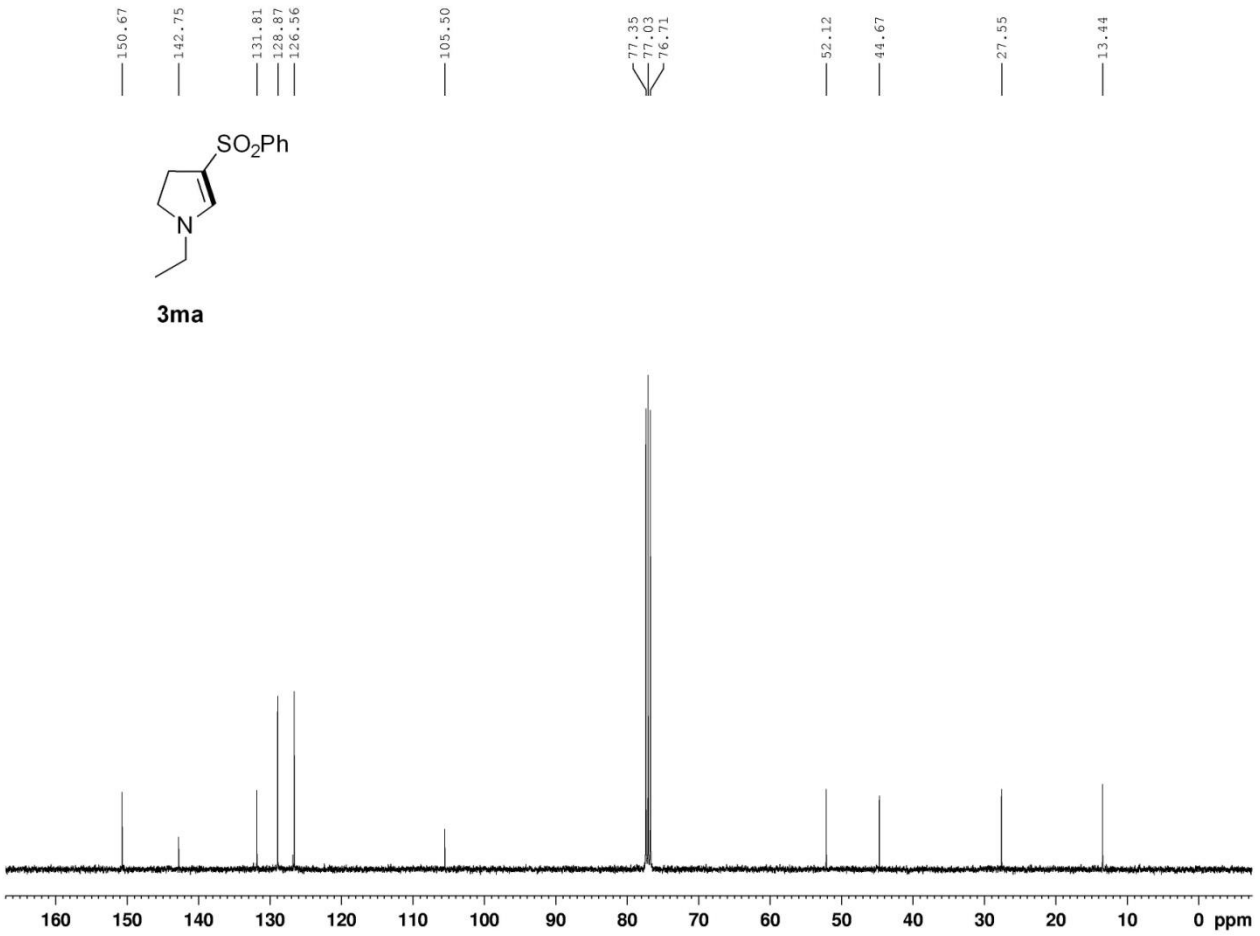
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SO2Ph
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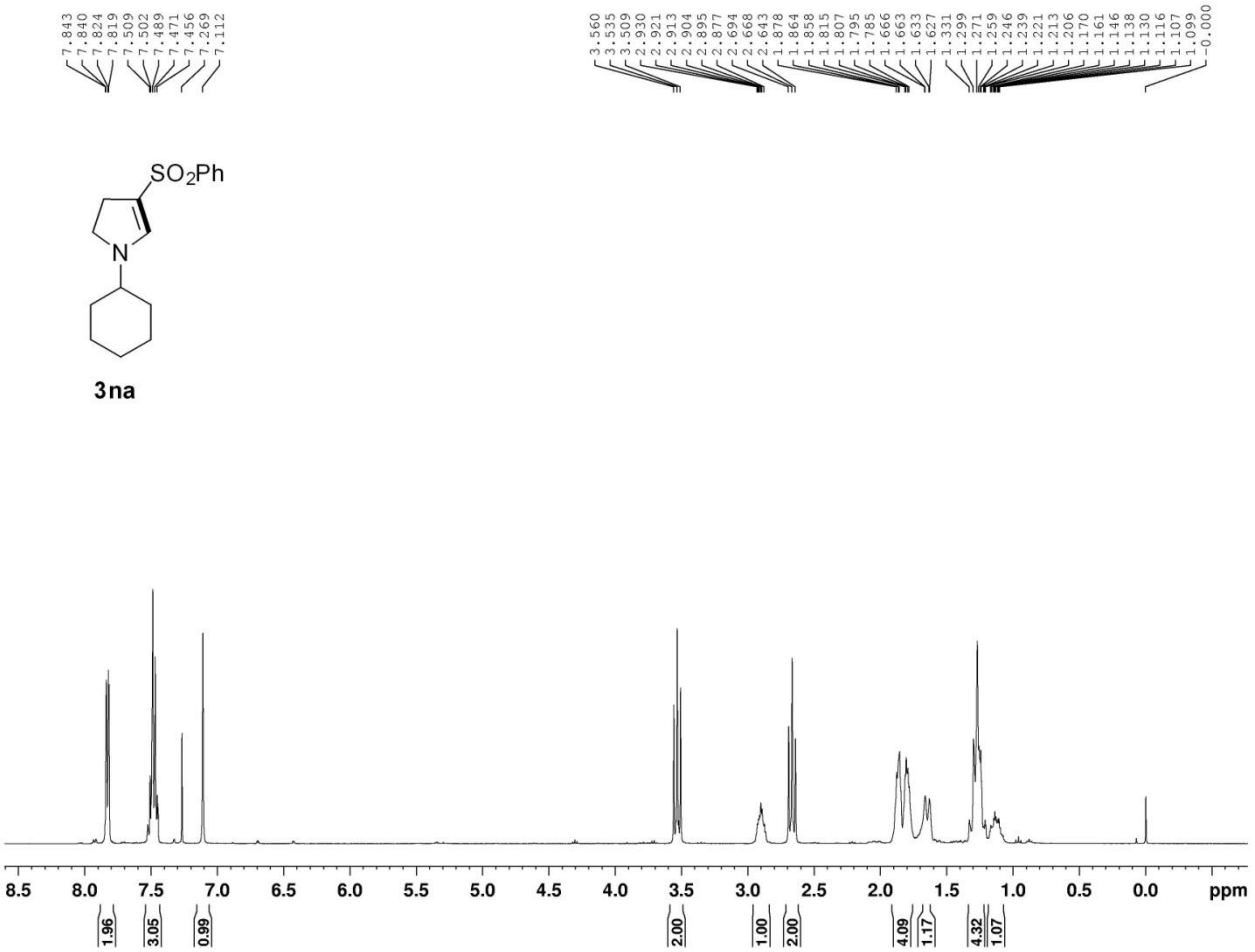
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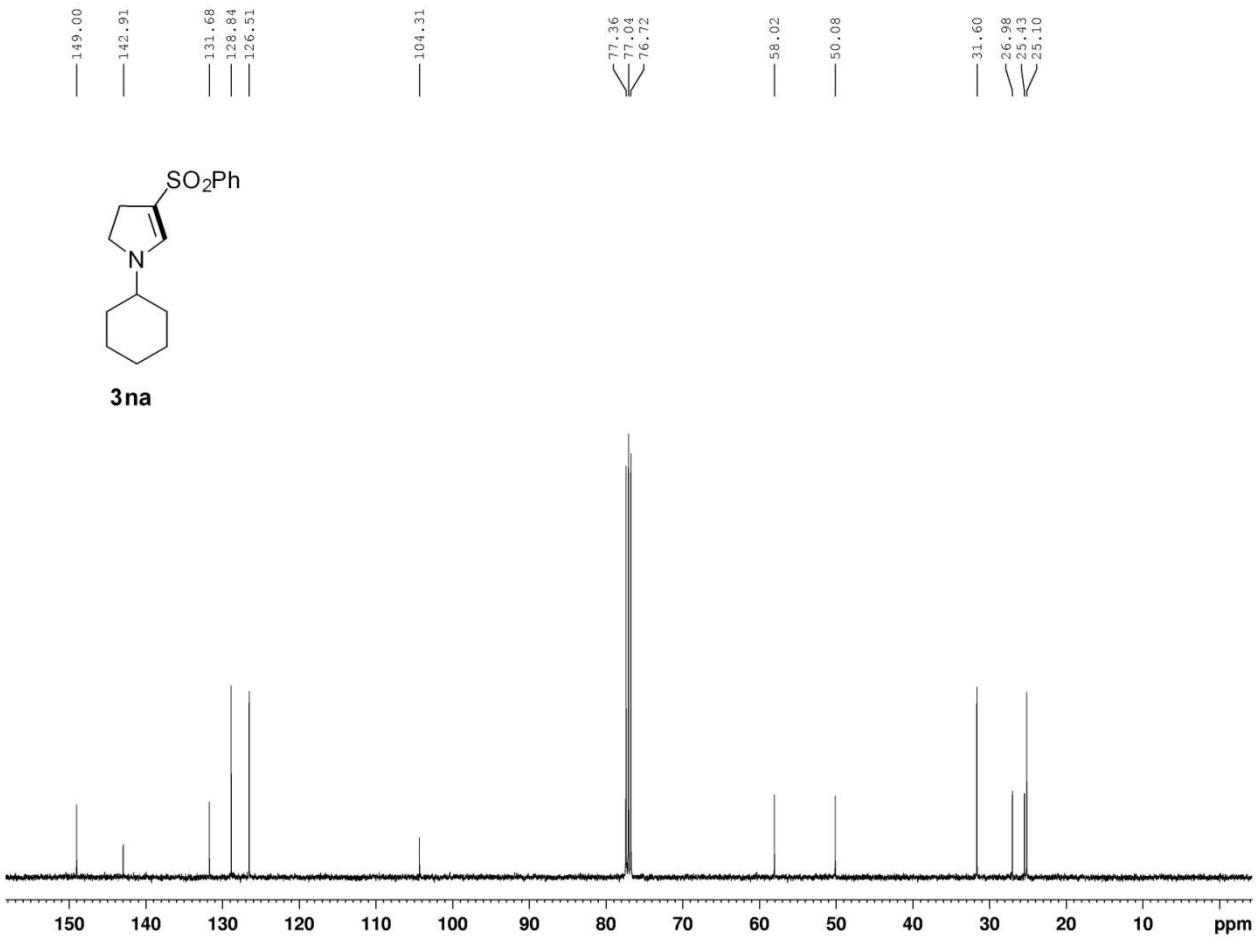
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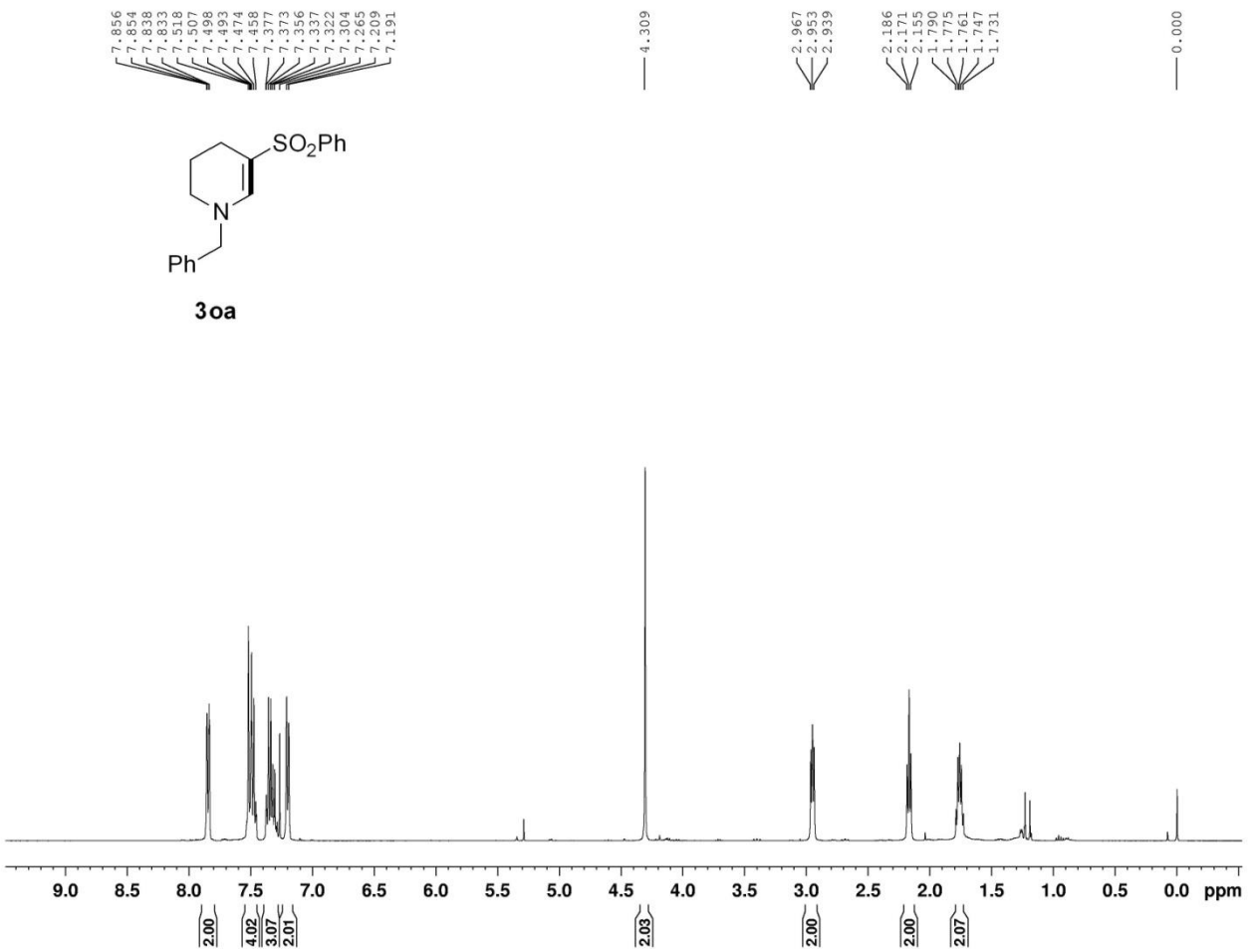
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N
Ph
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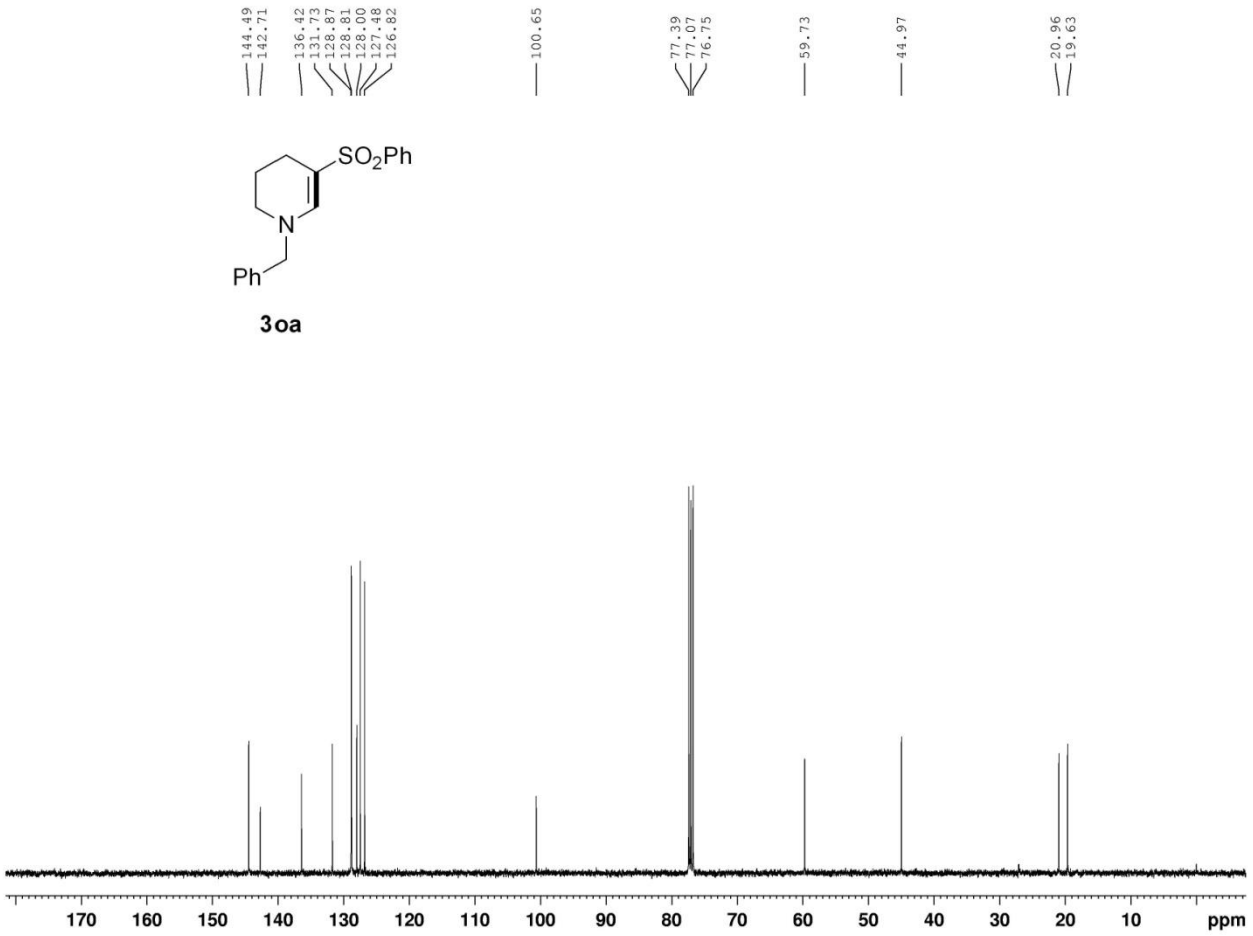
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N
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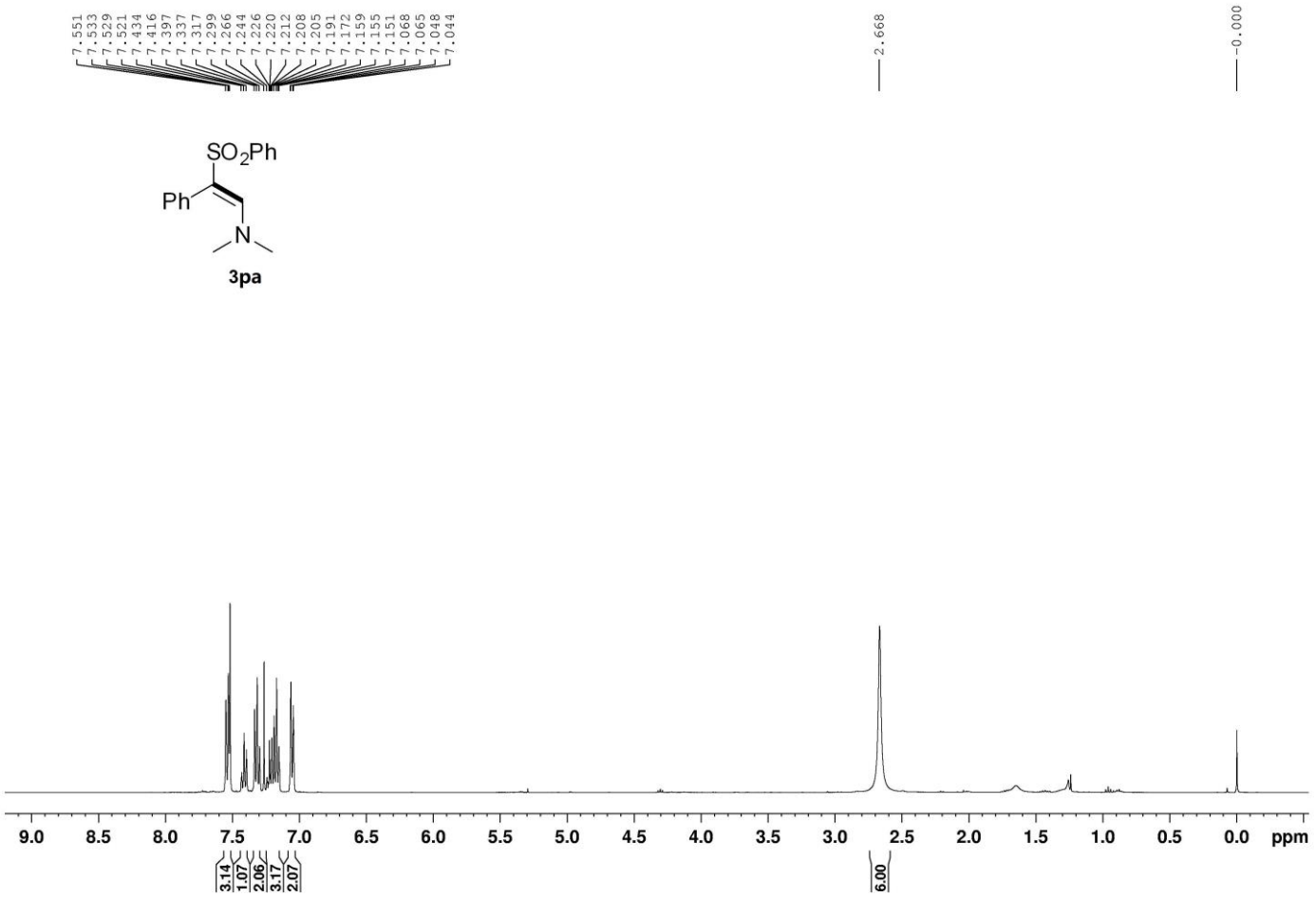
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7.155
7.151
7.068
7.065
7.048
7.044
2.668
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SO2Ph
Ph
N
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8.5
8.0
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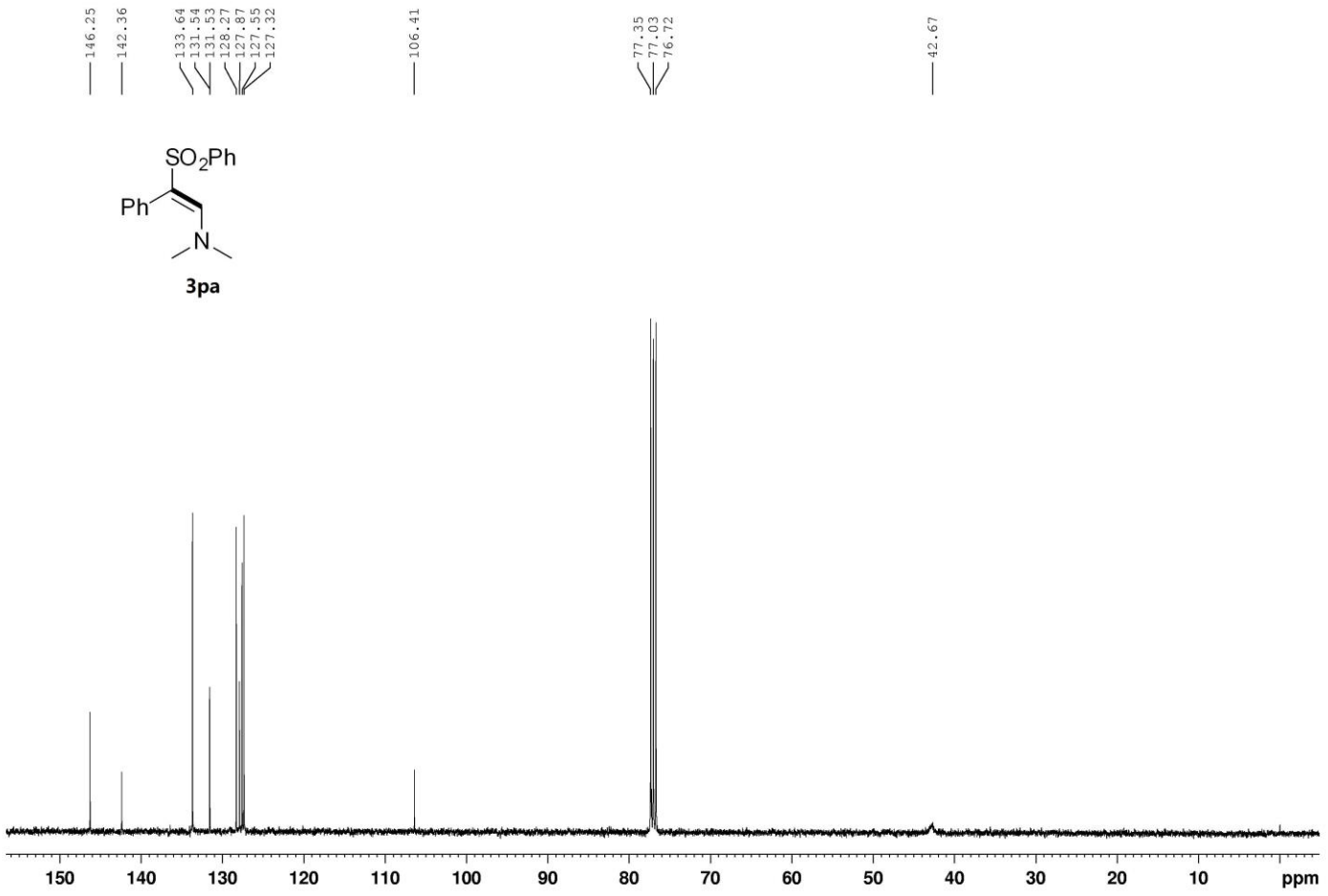
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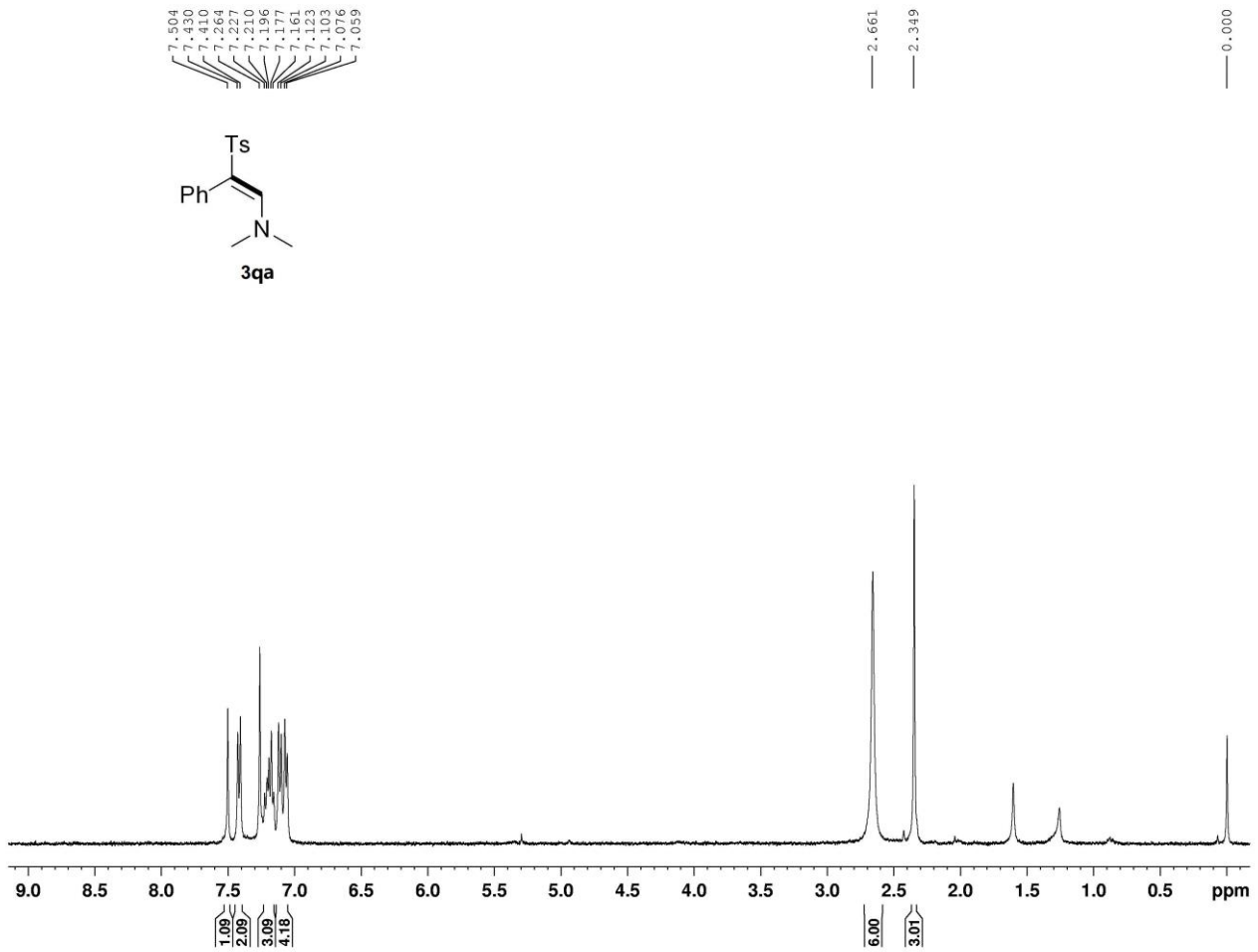
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Ph
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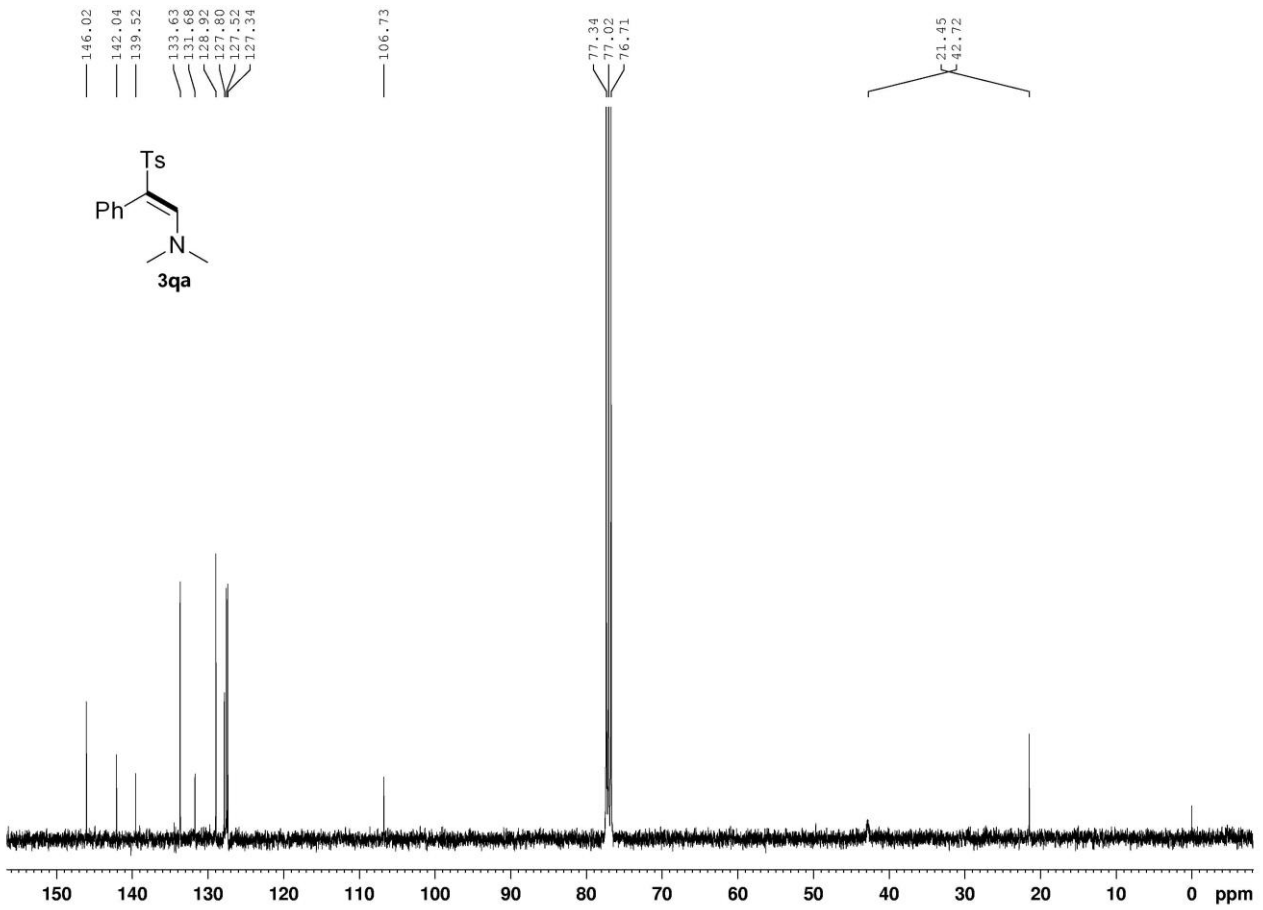
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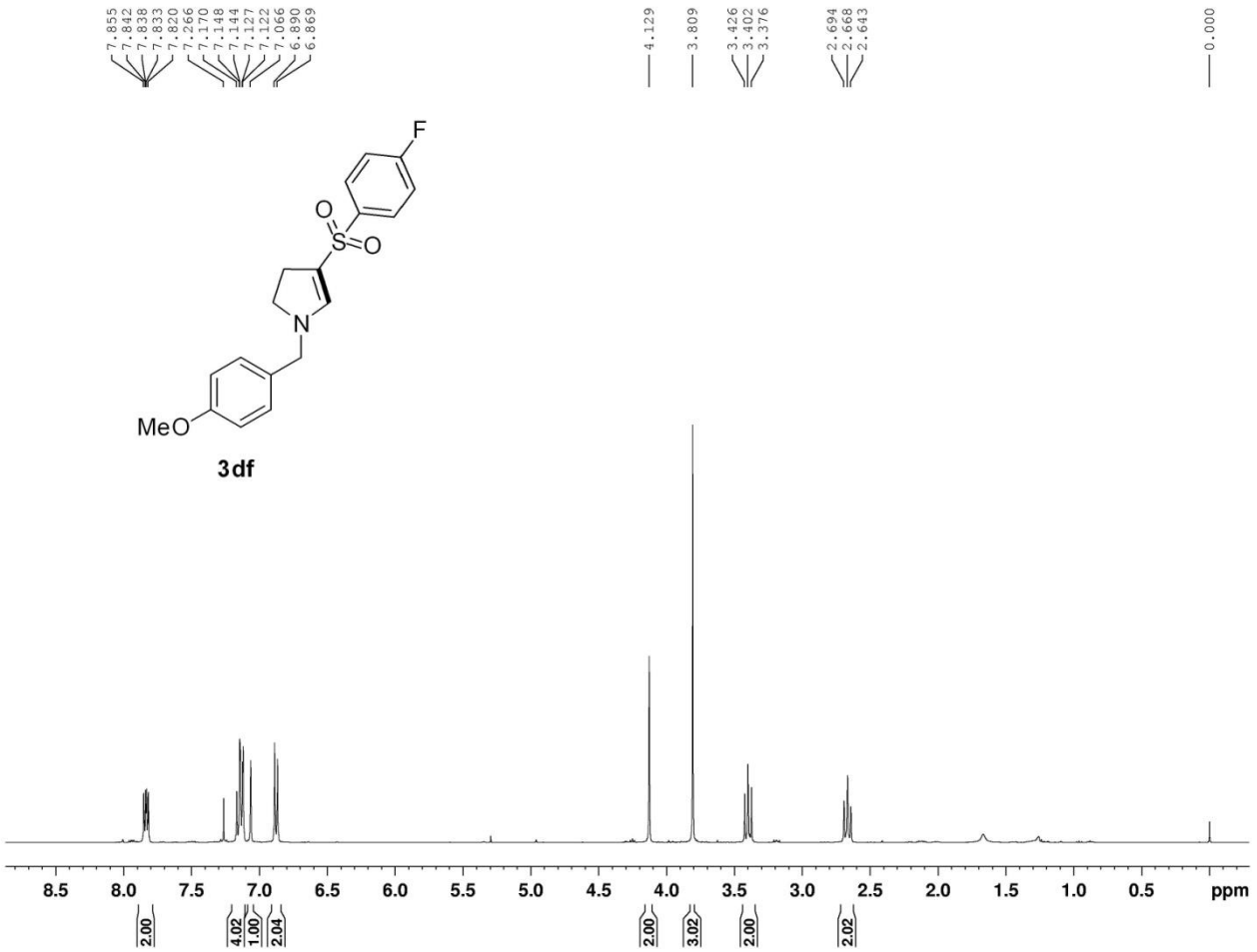
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S
O
N
MeO
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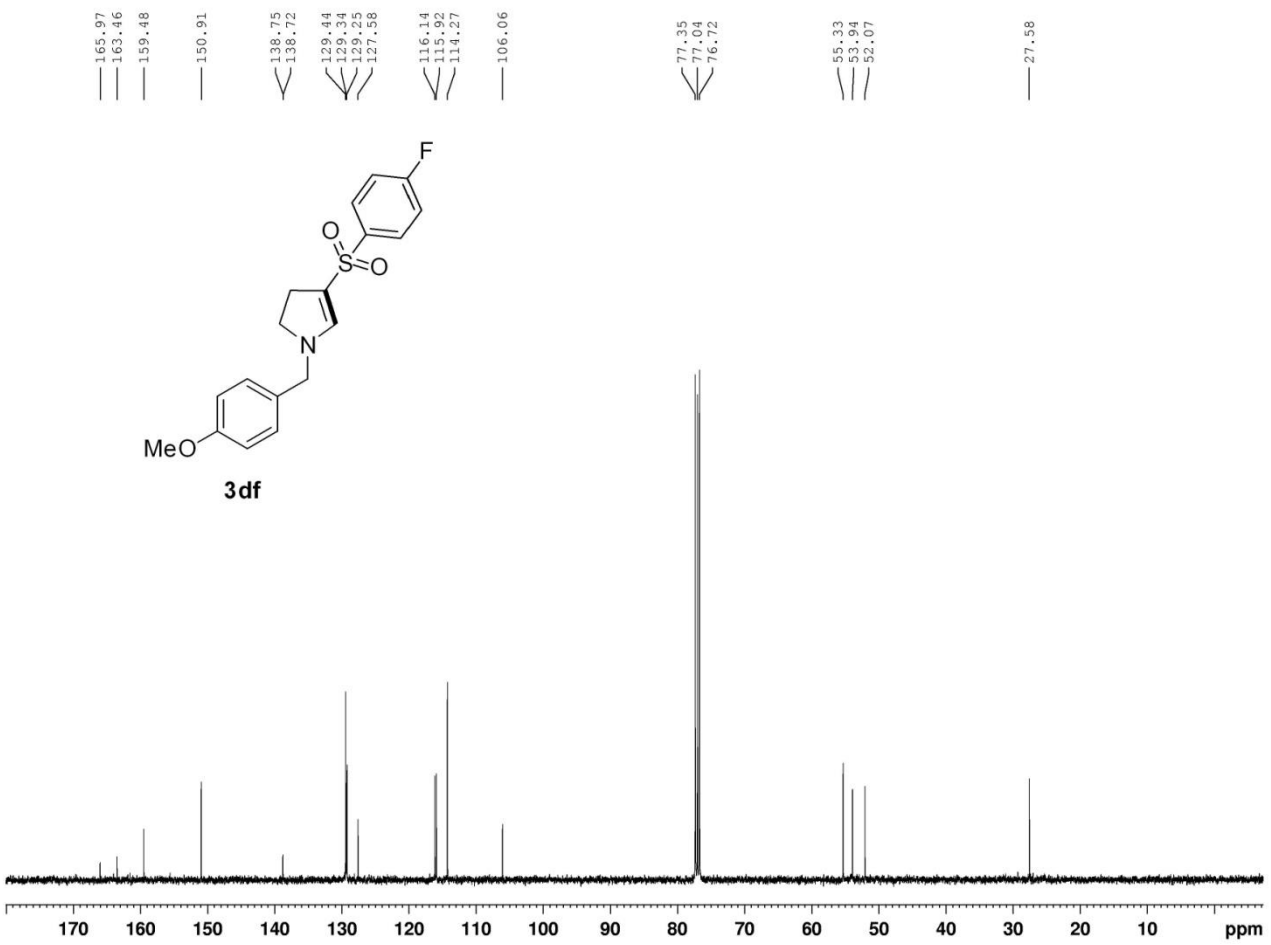
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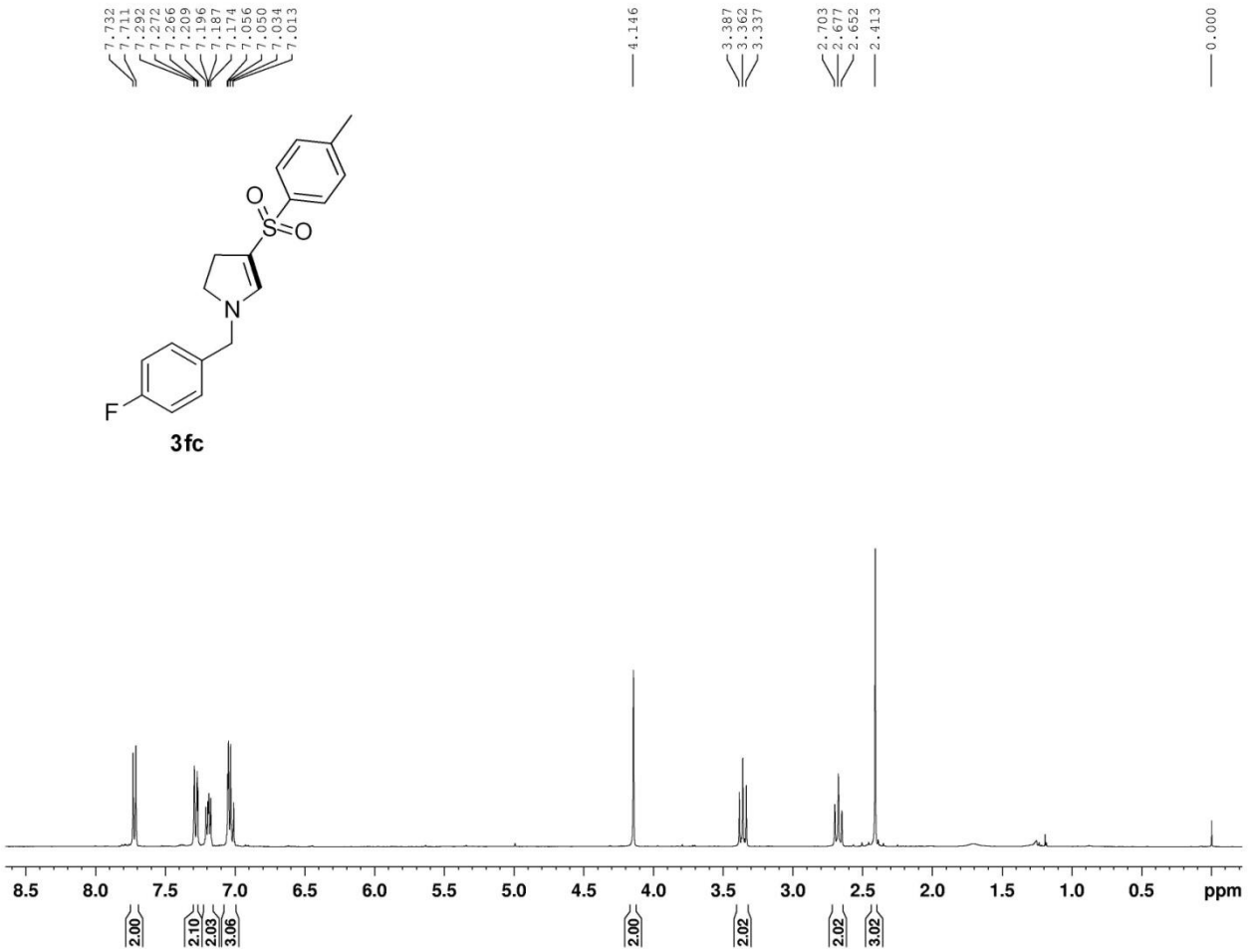
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S
O
N
F
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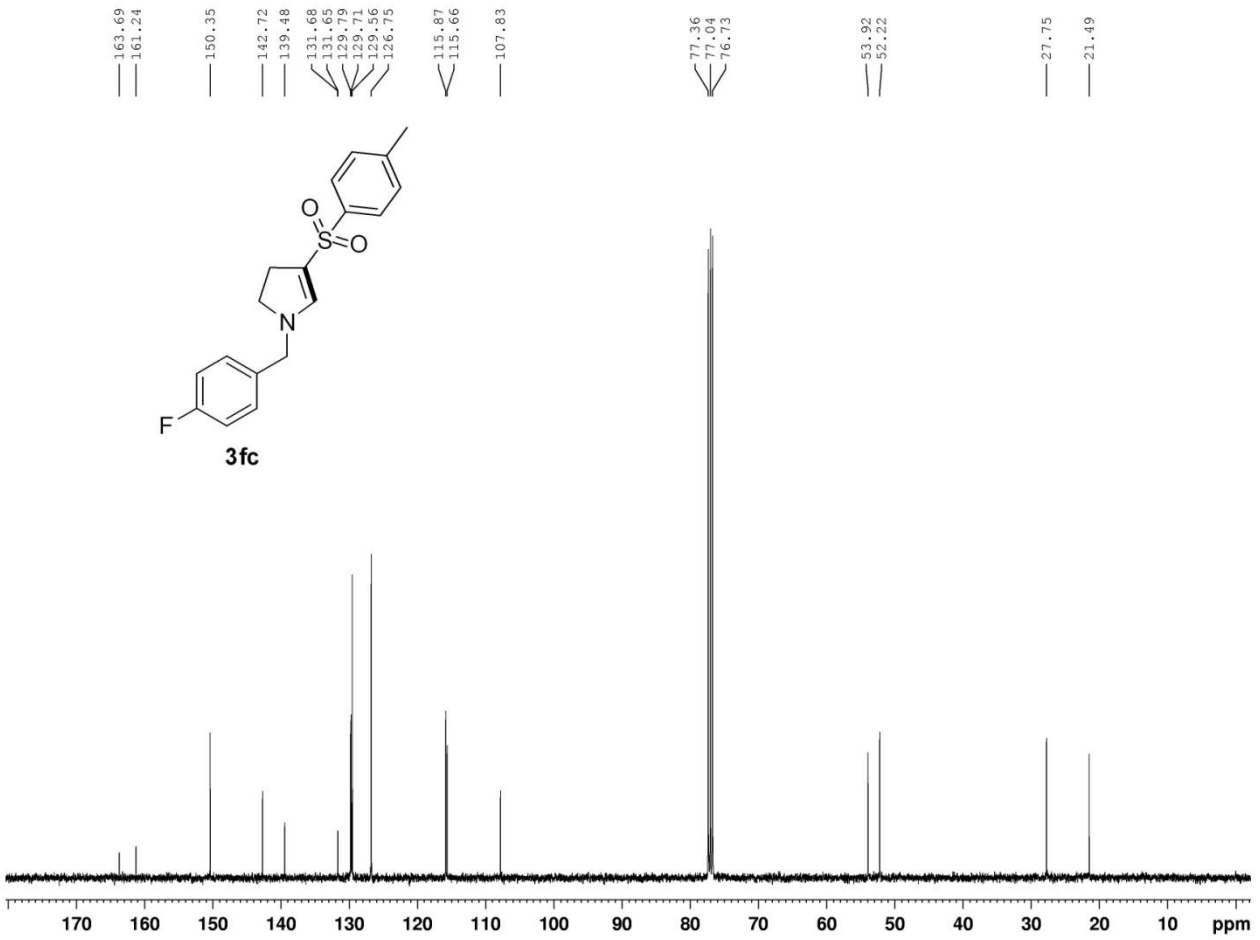
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77.04
76.73
53.92
52.22
27.75
21.49
O
S
O
N
F
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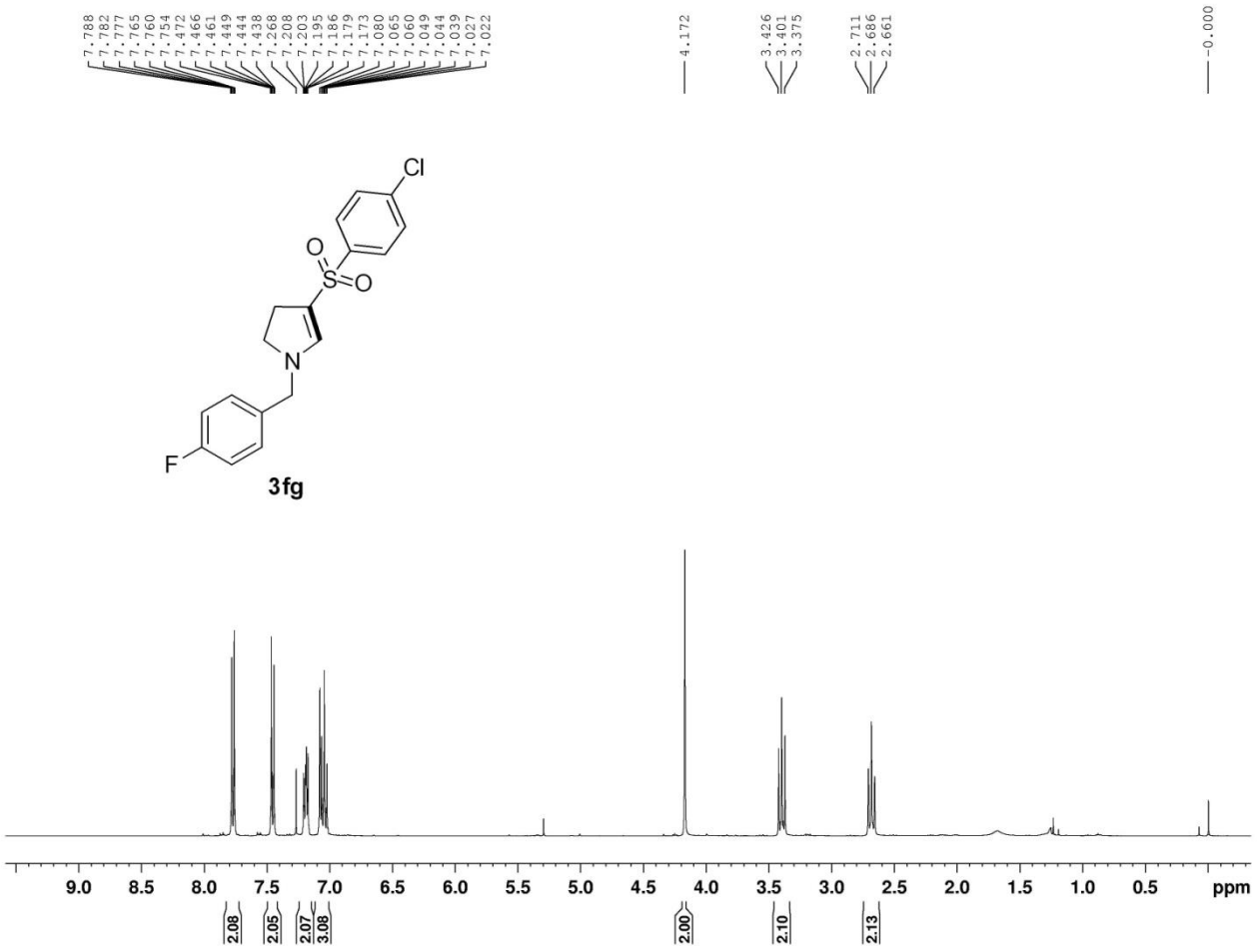
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S
O
N
F
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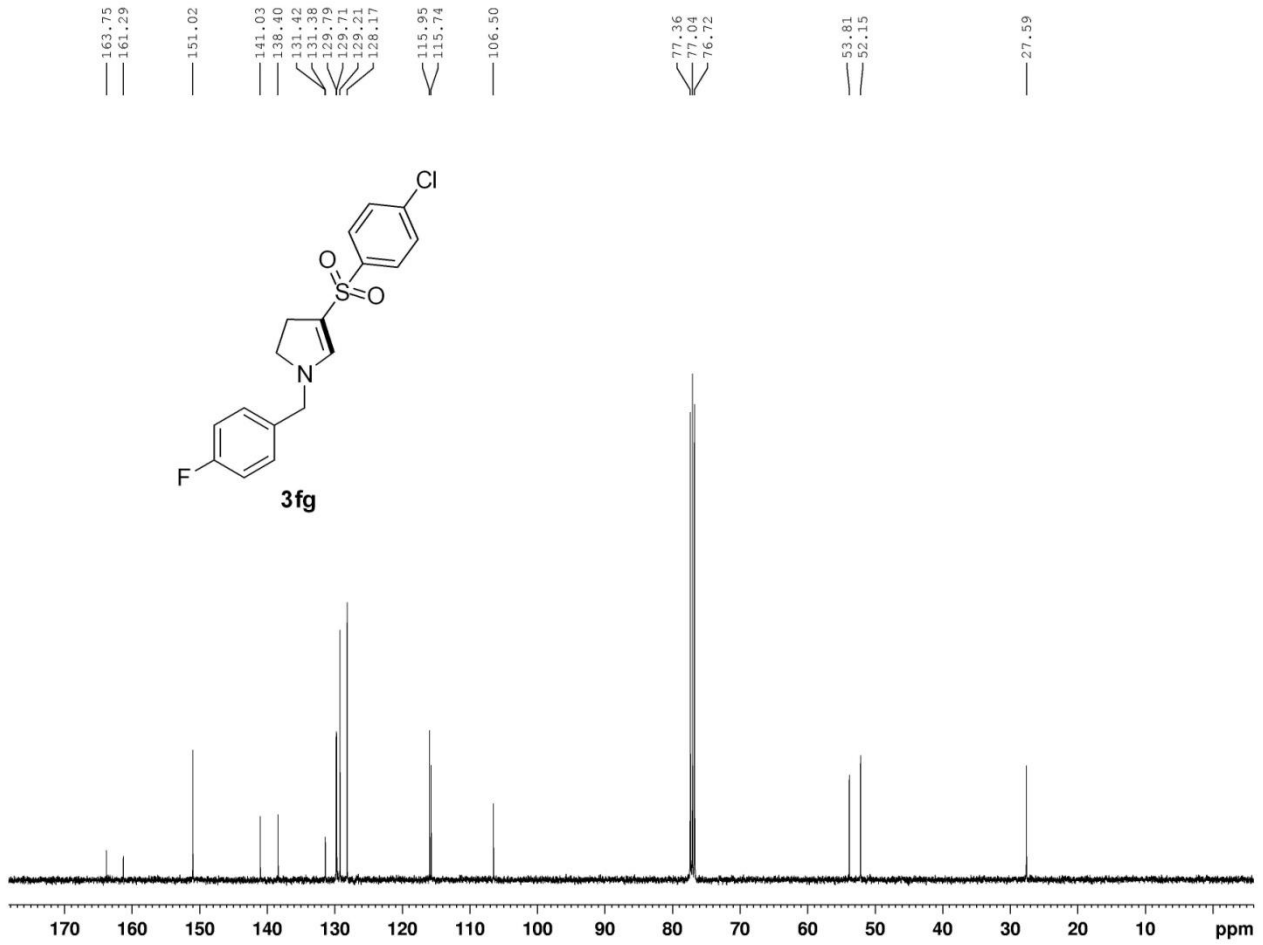
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S
O
N
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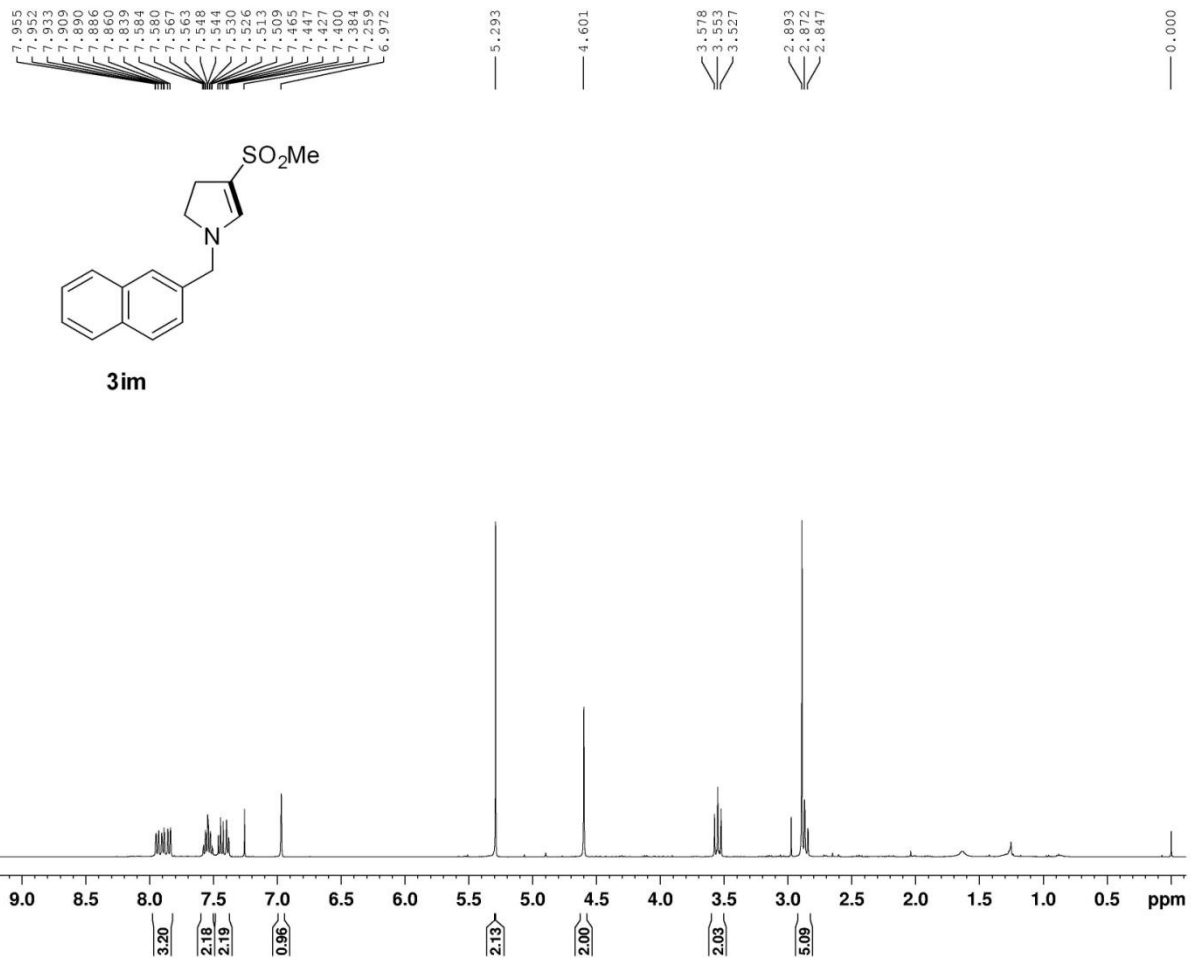
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7.530
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7.259
6.972
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N
3im
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7.0
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4.0
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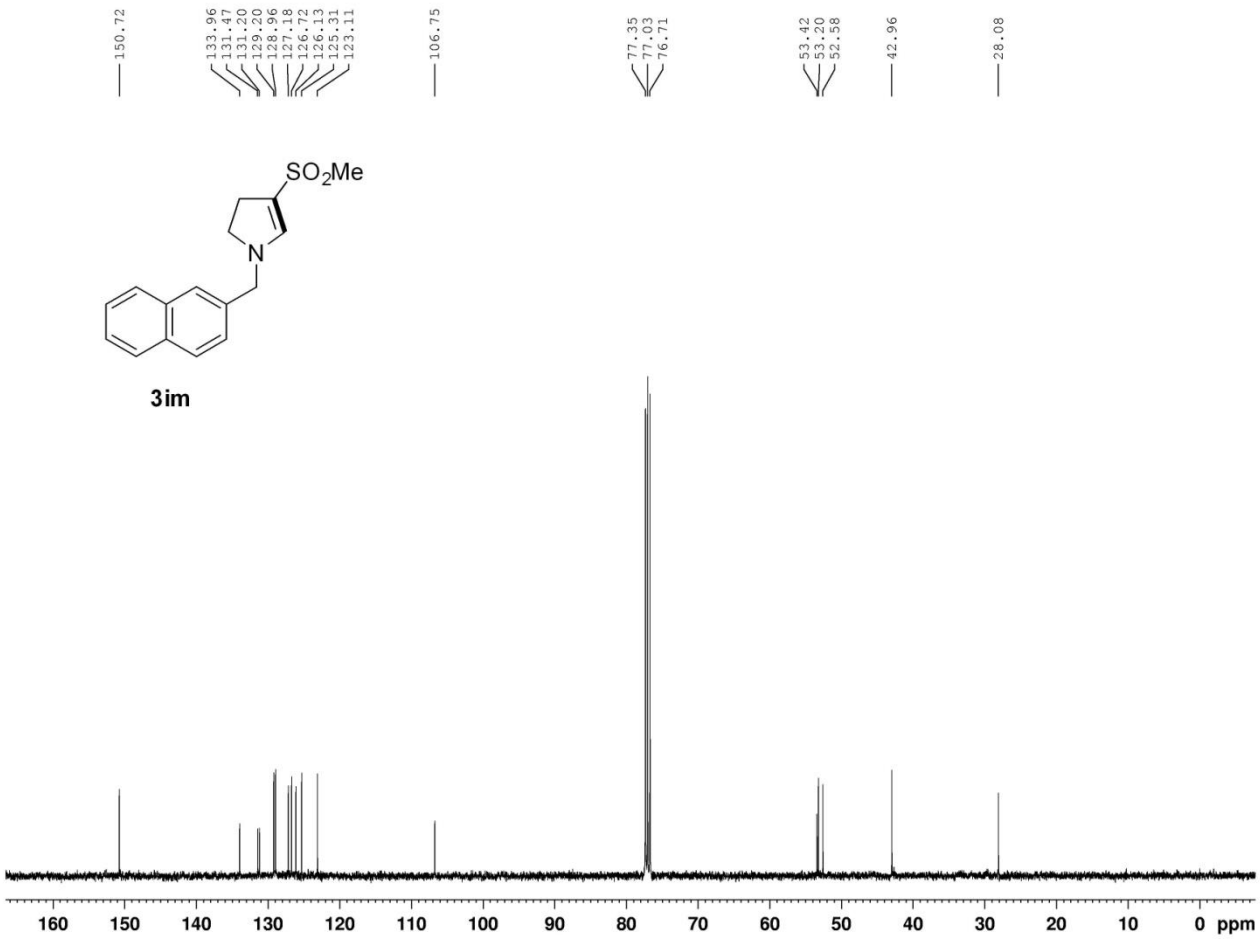
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77.03
76.71
53.42
53.20
52.58
42.96
28.08
SO2Me
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60
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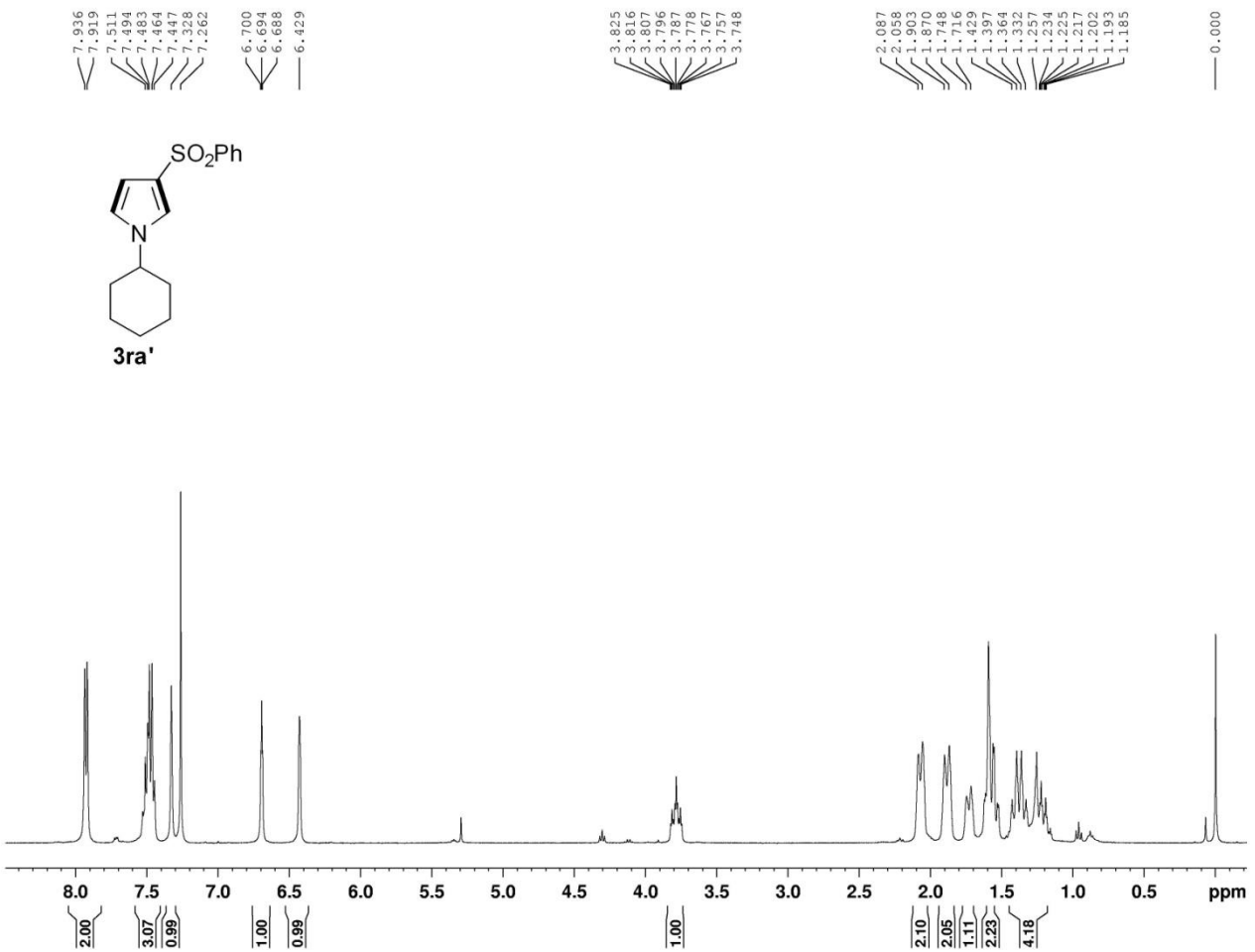
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3.807
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3.778
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3.757
3.748
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2.058
1.903
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1.429
1.397
1.364
1.332
1.257
1.234
1.225
1.217
1.202
1.193
1.185
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N
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7.0
6.5
6.0
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5.0
4.5
4.0
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3.0
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2.0
1.5
1.0
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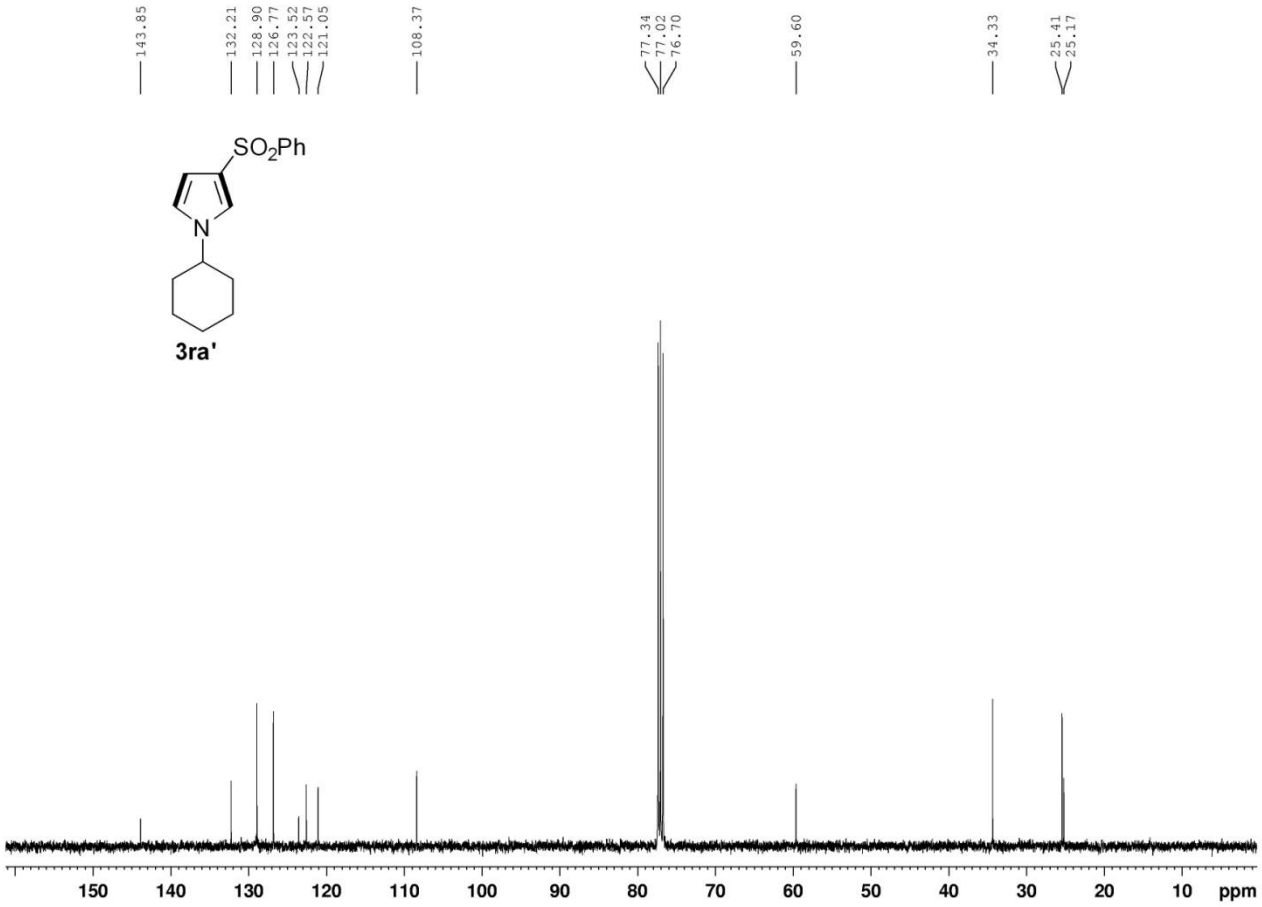
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25.41
25.17
SO2Ph
N
3ra'
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140
130
120
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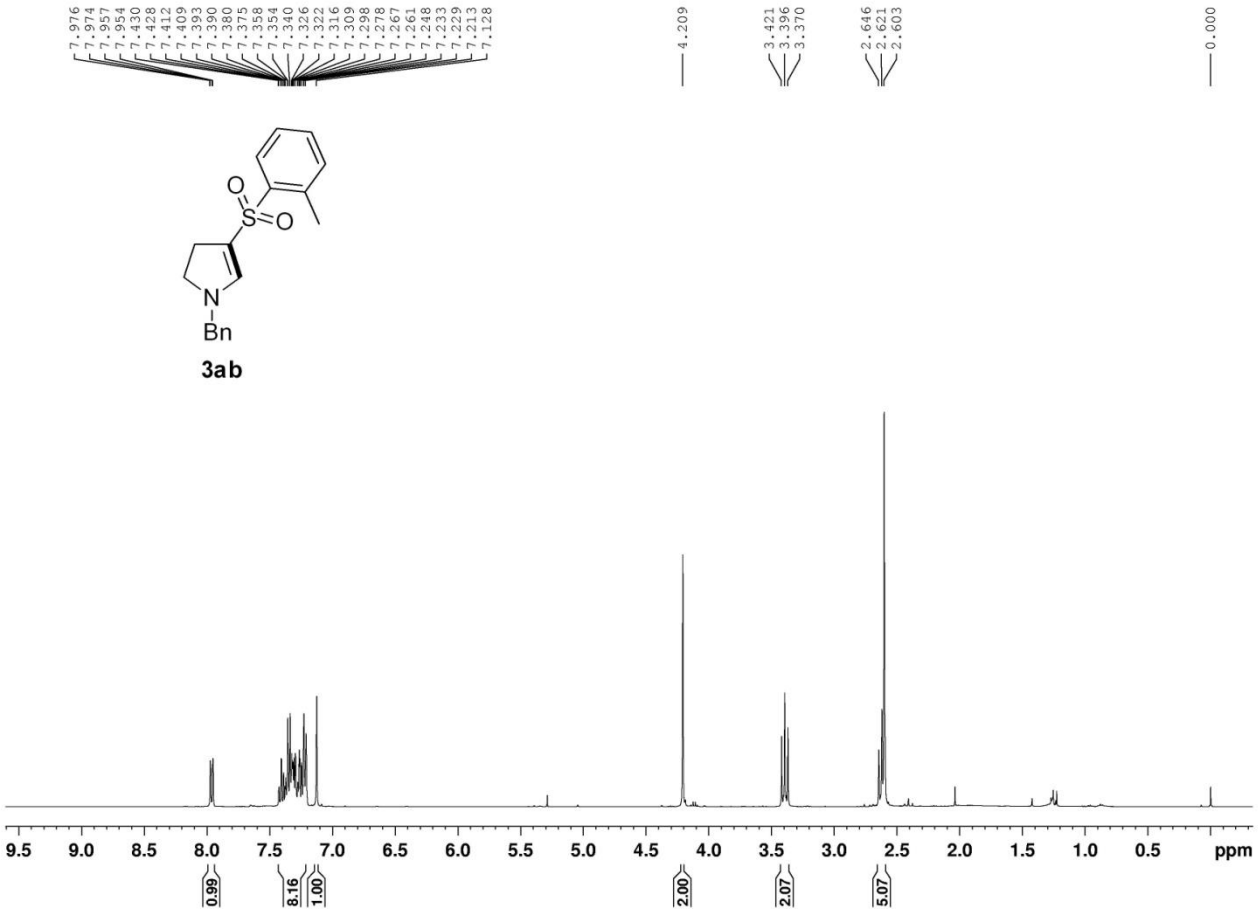
30
20
10
ppm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7.358
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7.229
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O
N
Bn
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7.5
7.0
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6.0
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4.0
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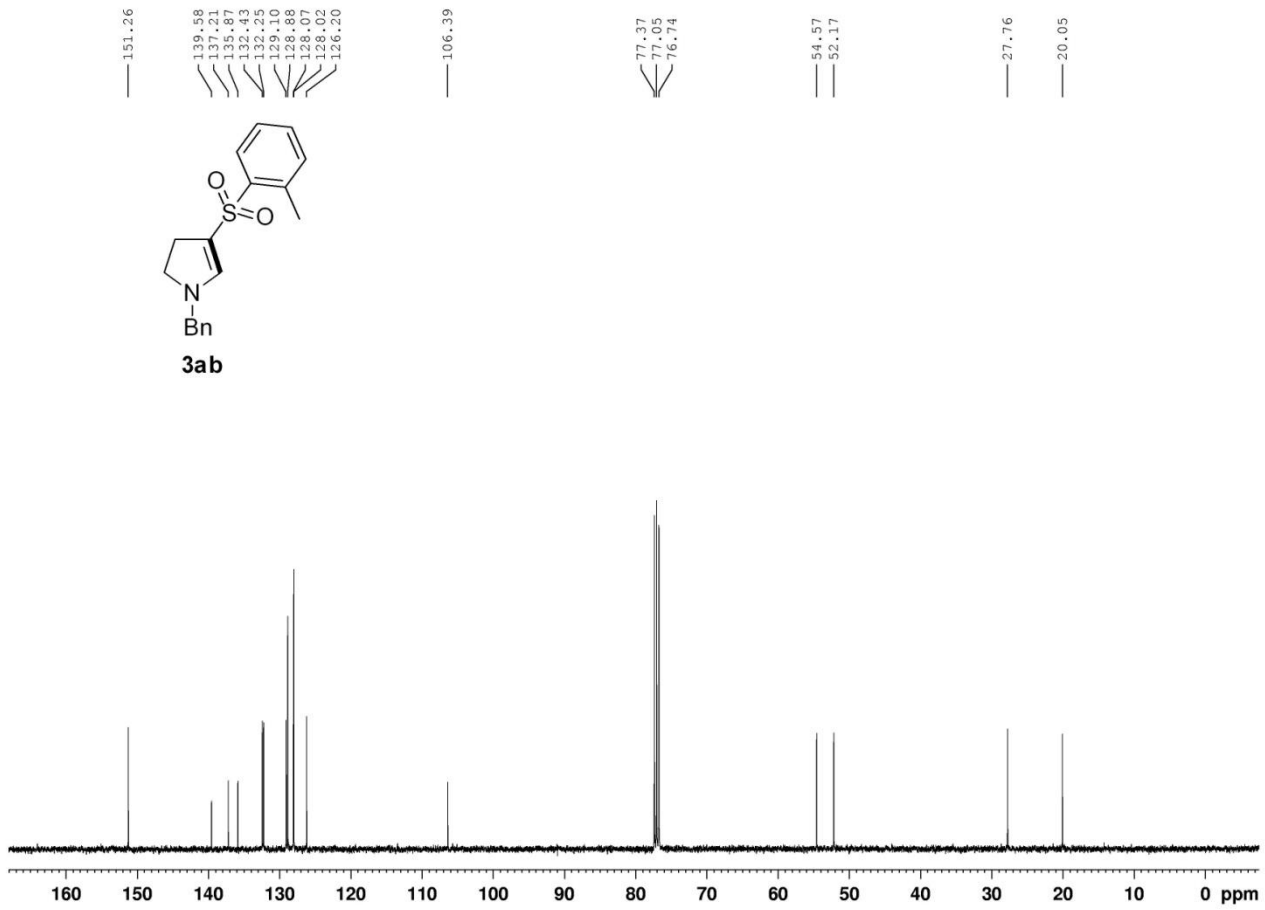
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77.05
76.74
54.57
52.17
27.76
20.05
O
S
O
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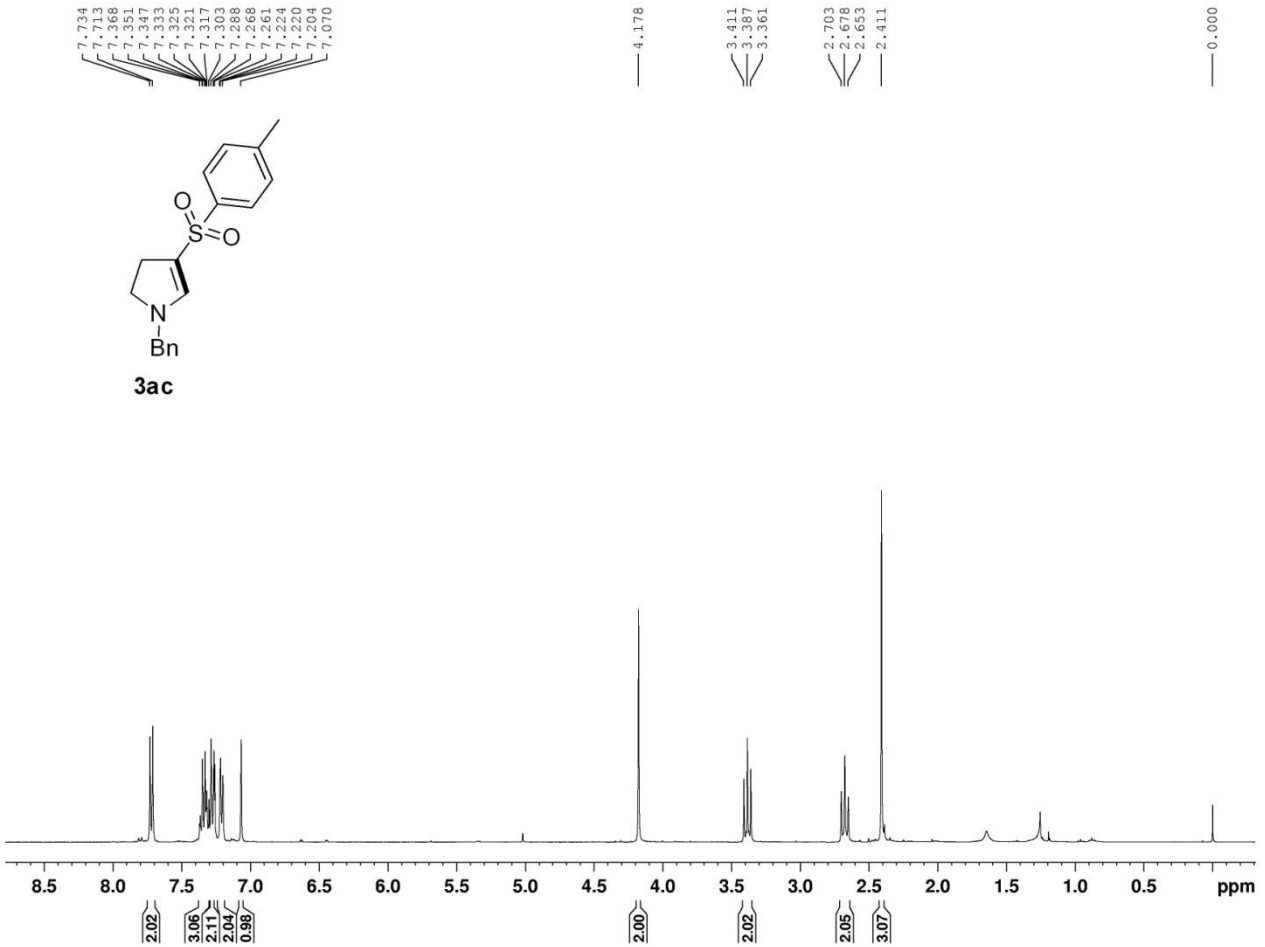
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7.220
7.204
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3.387
3.361
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2.678
2.653
2.411
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S
O
N
Bn
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6.0
5.5
5.0
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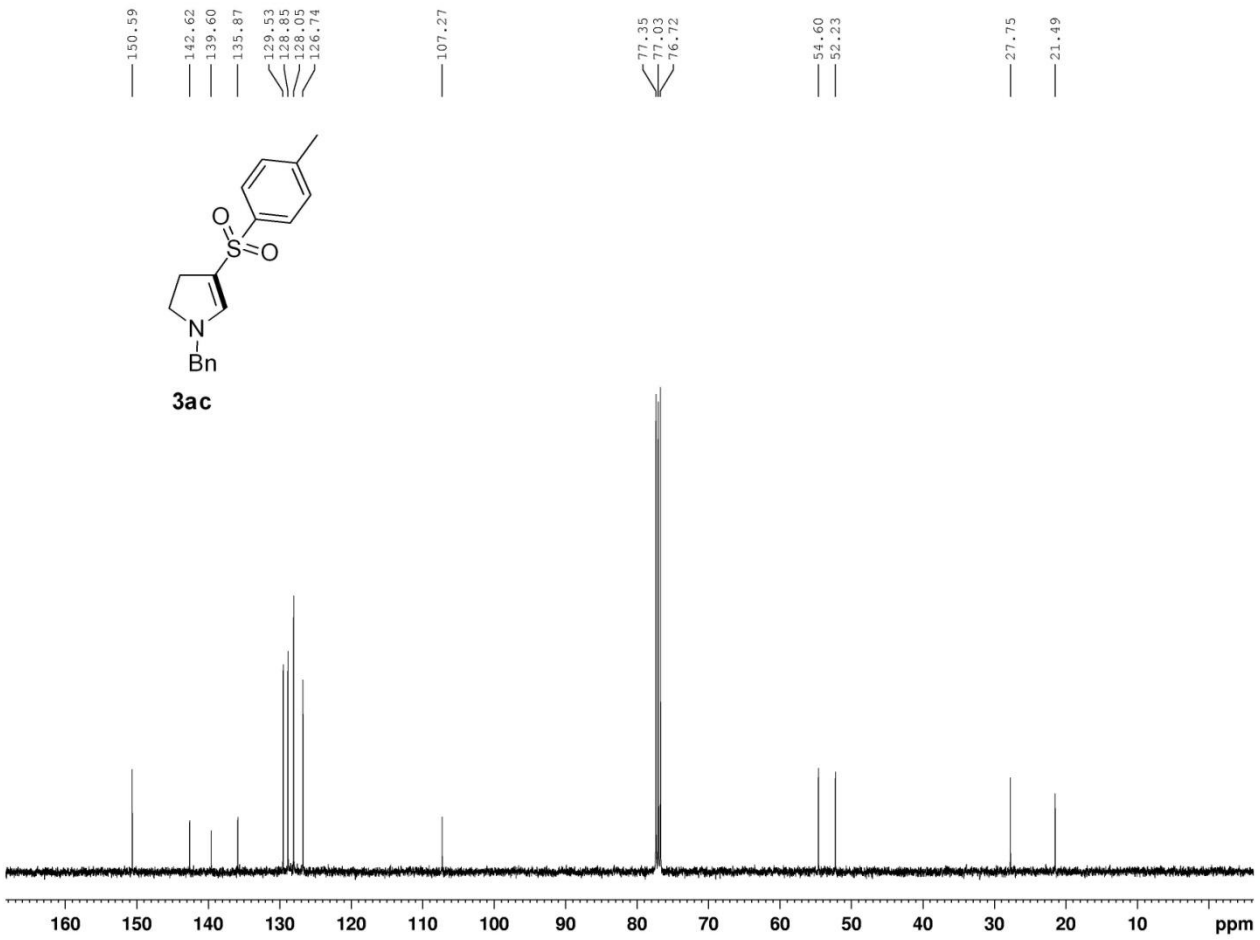
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77.03
76.72
54.60
52.23
27.75
21.49
O
S
O
N
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140
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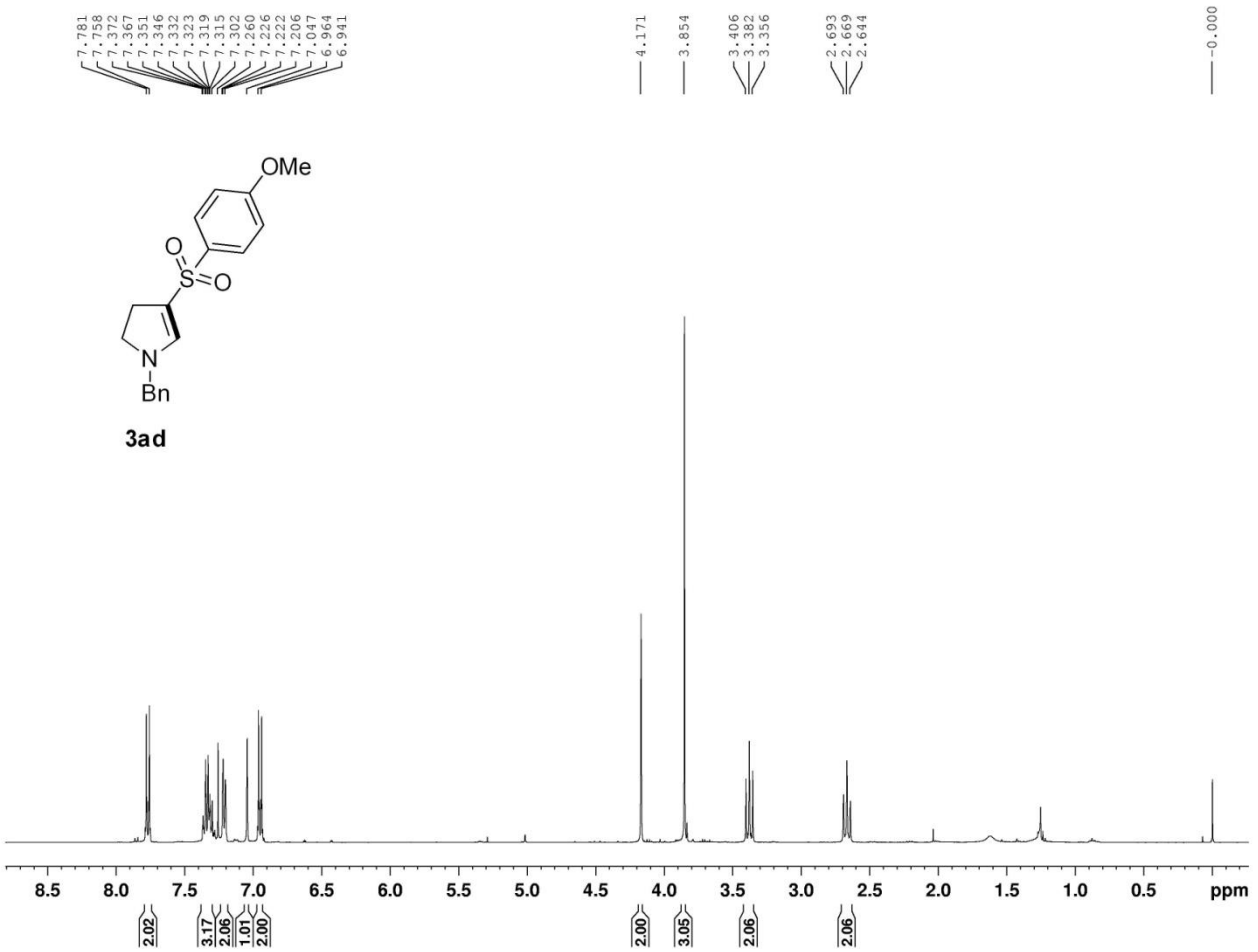
40
30
20
10
ppm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7.047
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6.941
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3.406
3.382
3.356
2.693
2.669
2.644
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O
S
O
N
Bn
3ad
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4.0
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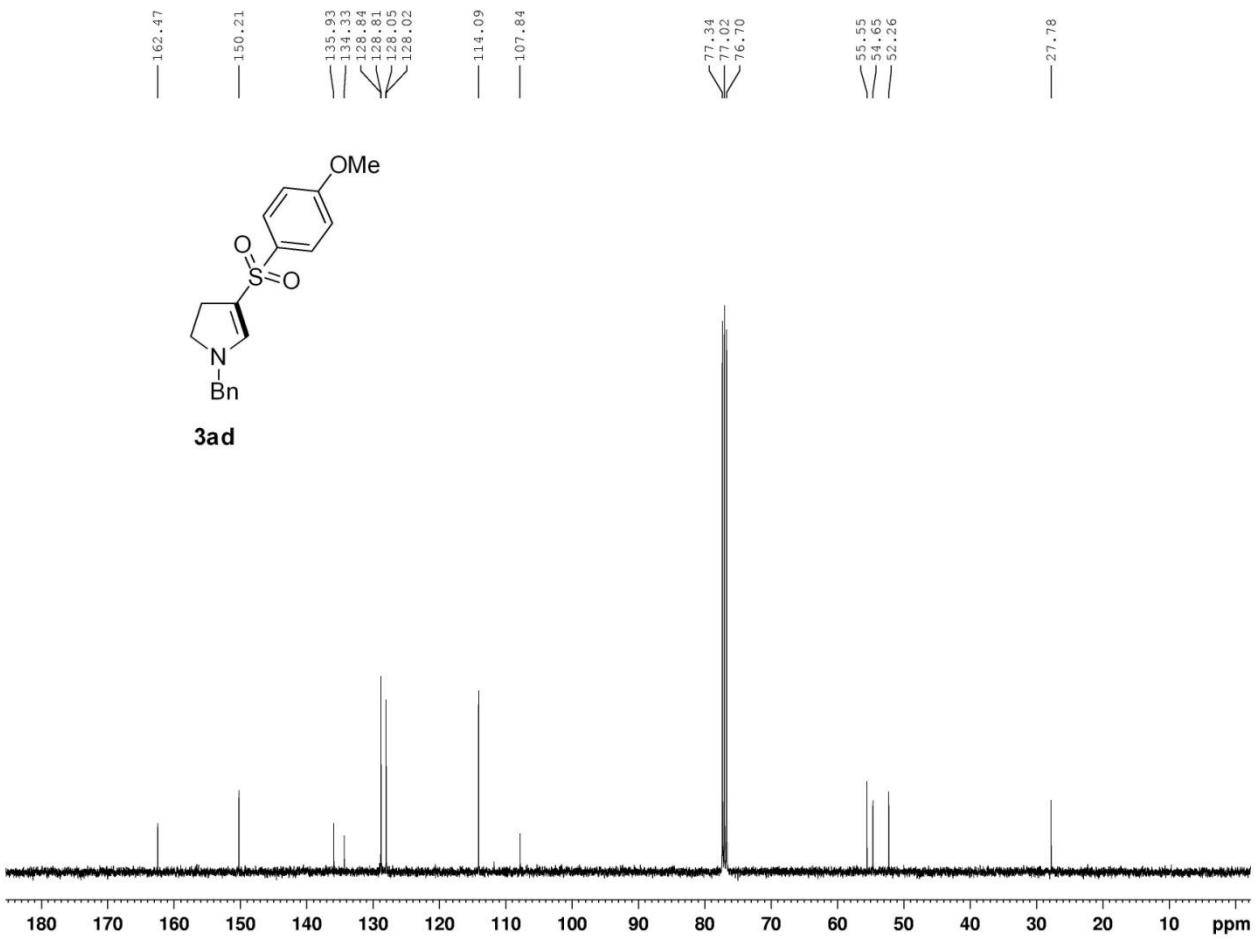
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54.65
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27.78
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O
S
O
N
Bn
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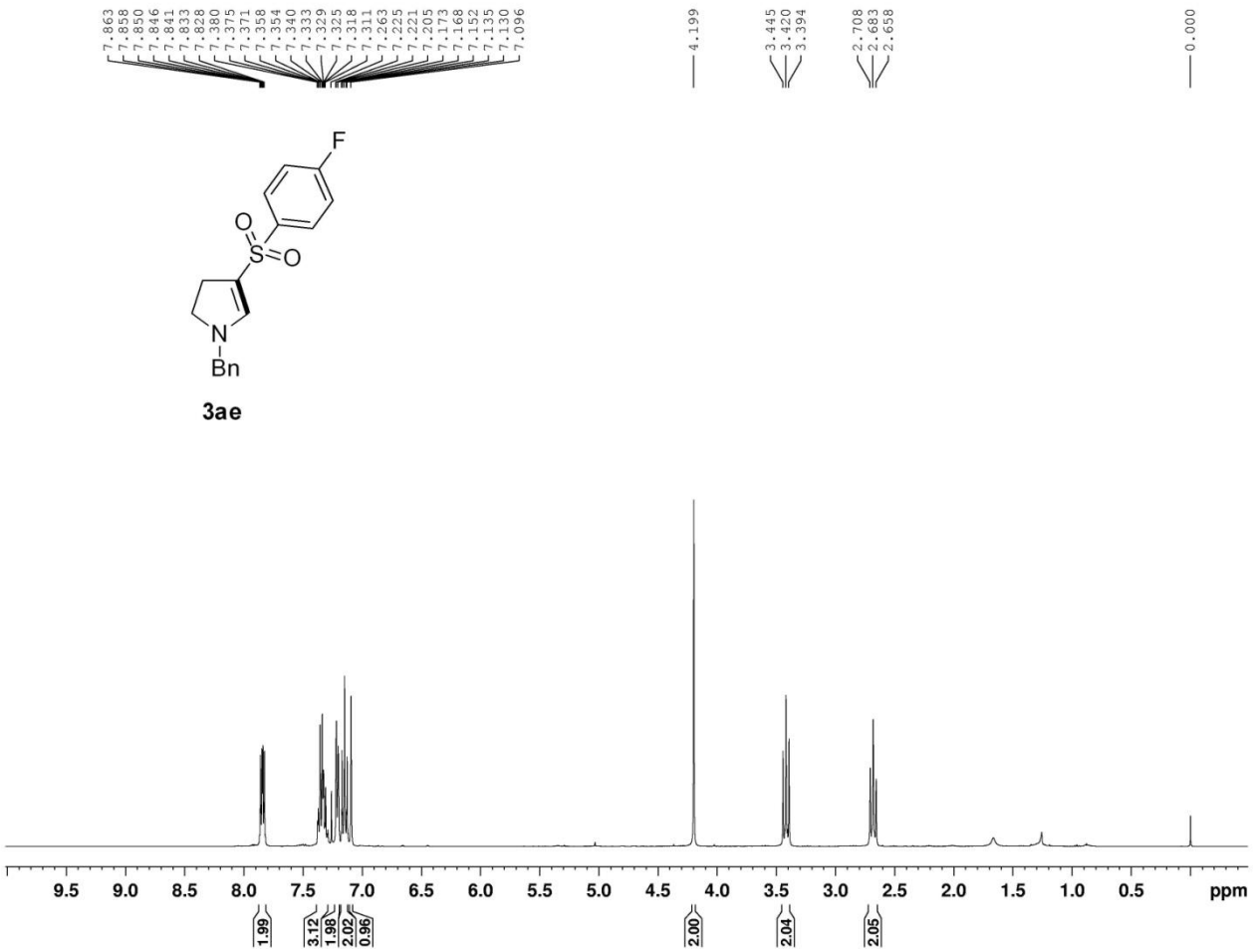
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O
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Bn
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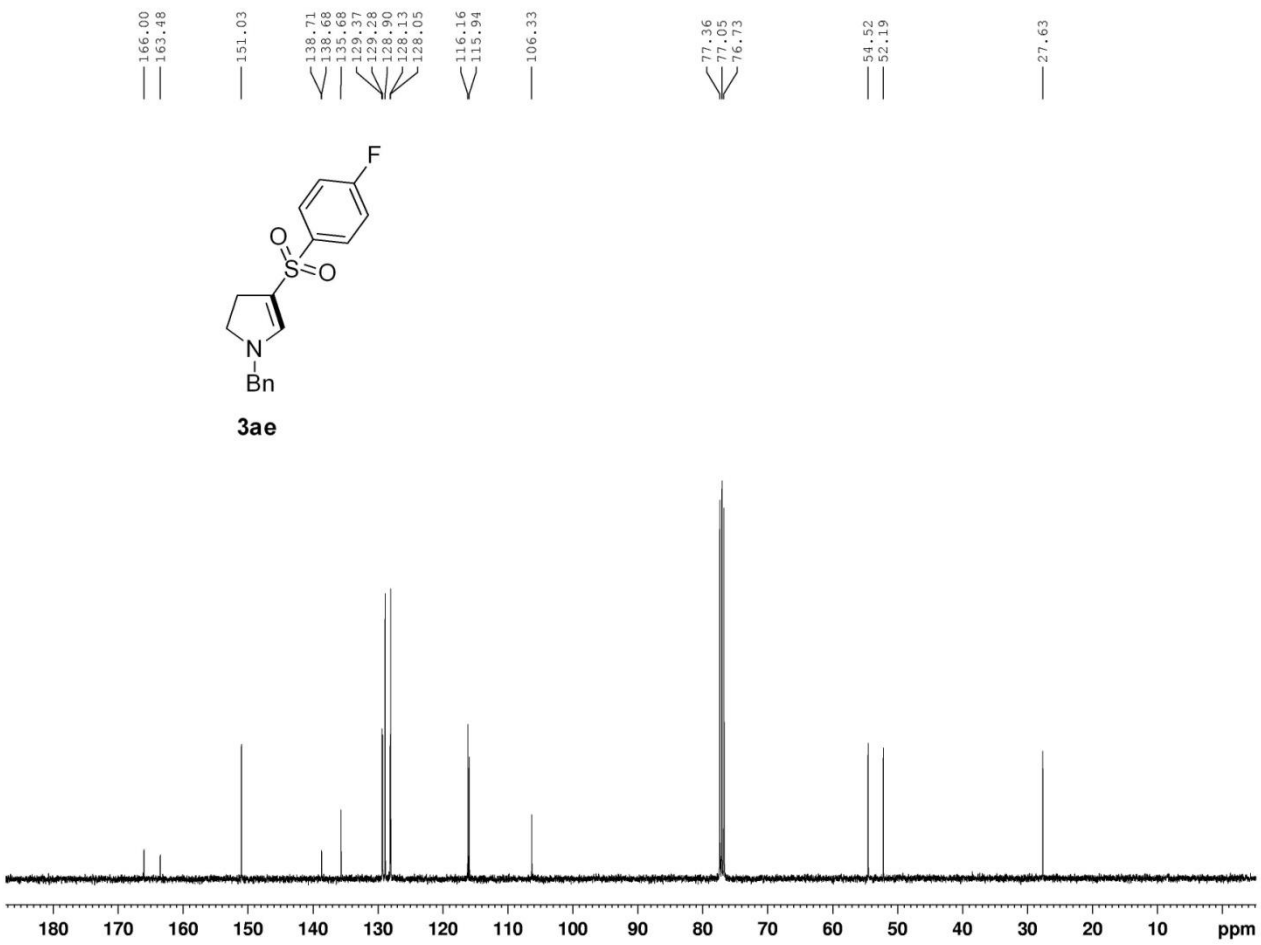
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77.05
76.73
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O
S
O
N
Bn
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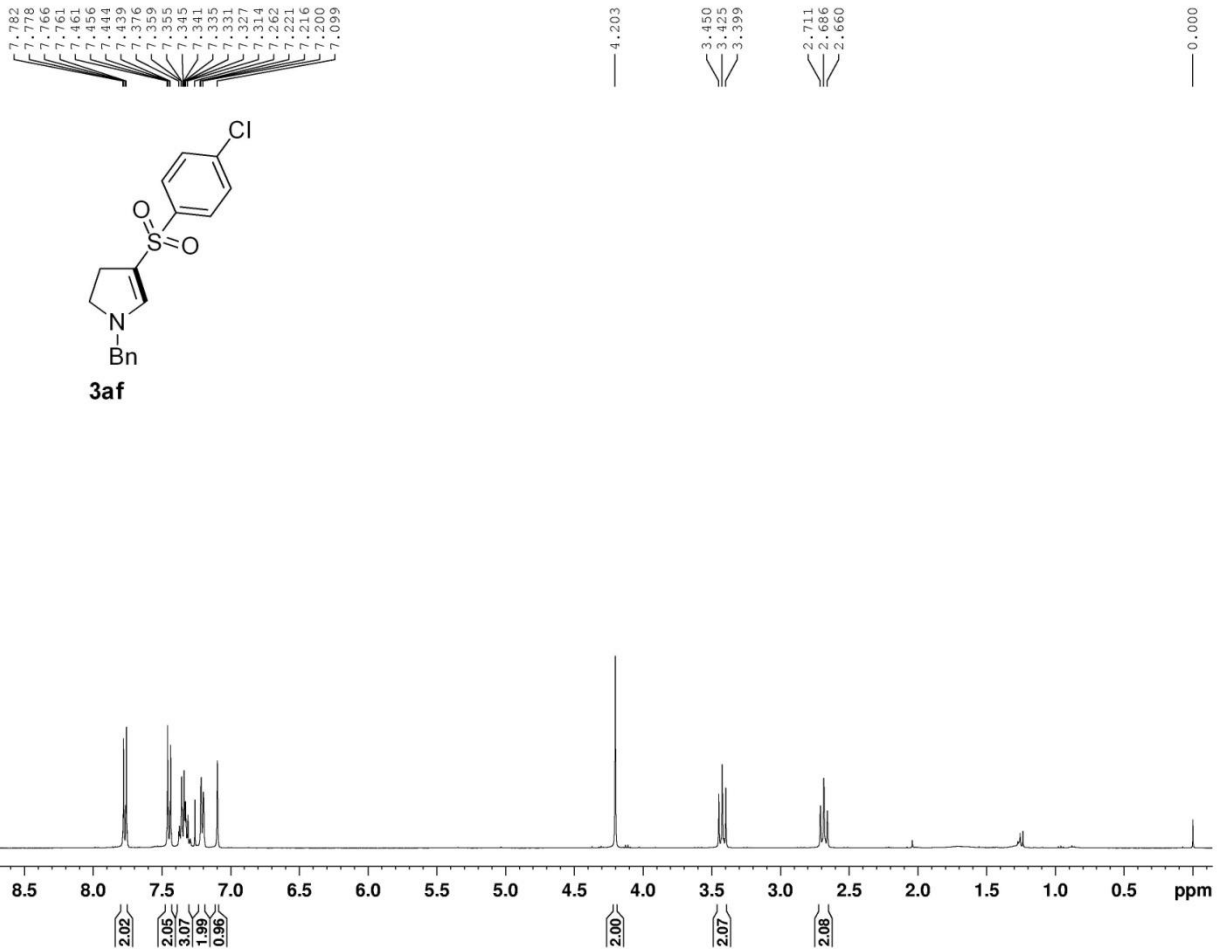
ppm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7.099
4.203
3.450
3.425
3.399
2.711
2.686
2.660
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S
O
N
Bn
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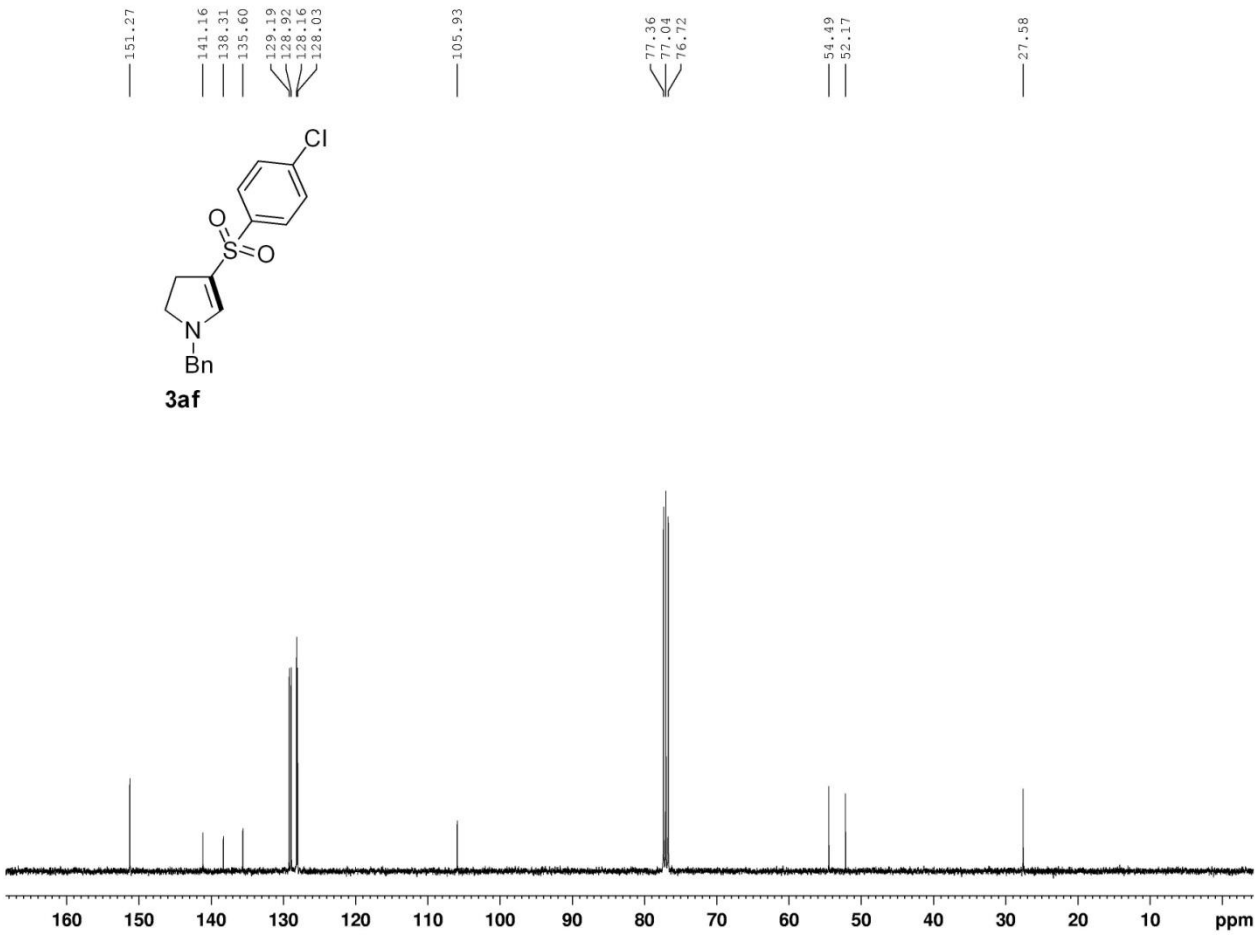
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77.04
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54.49
52.17
27.58
Cl
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S
O
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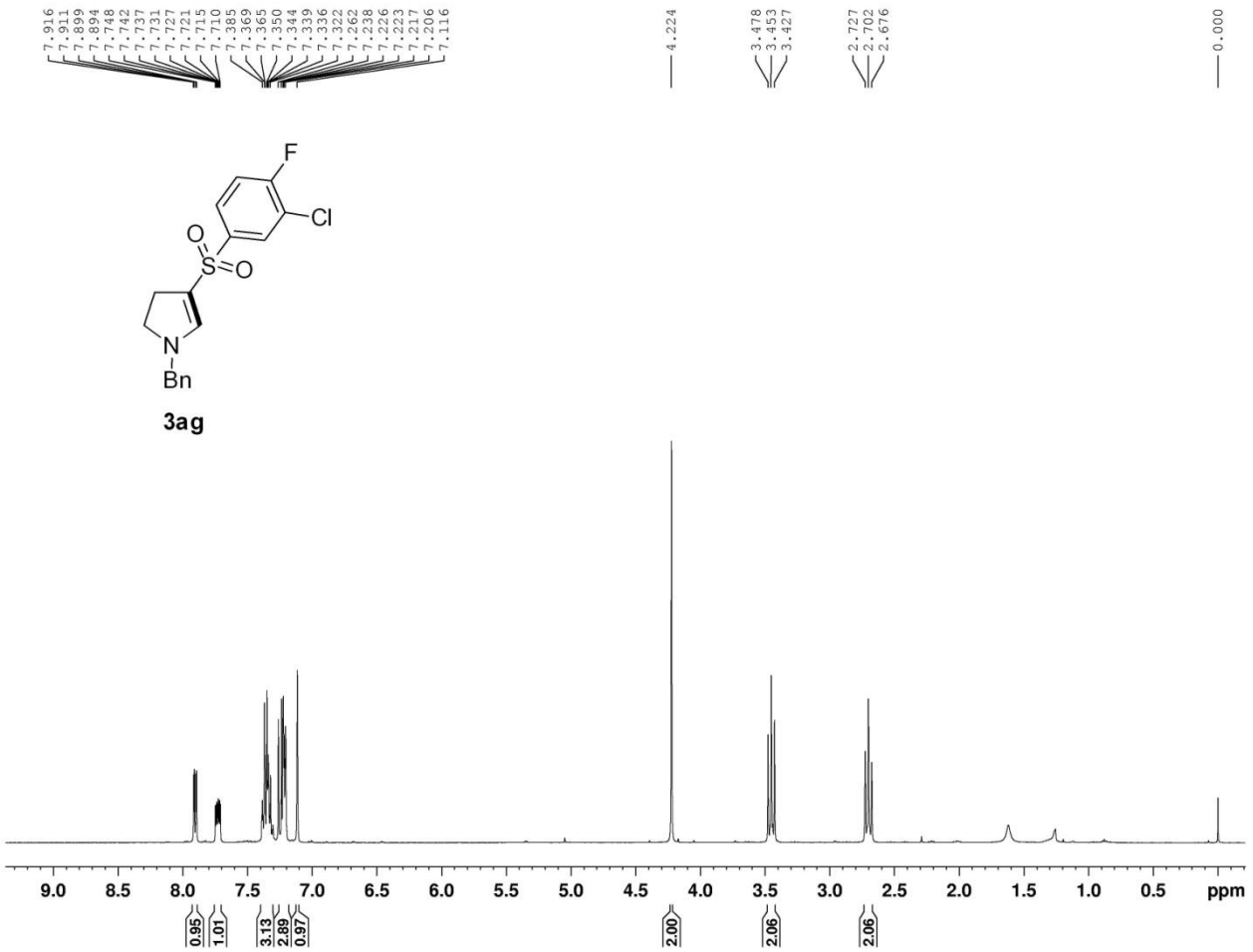
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Bn
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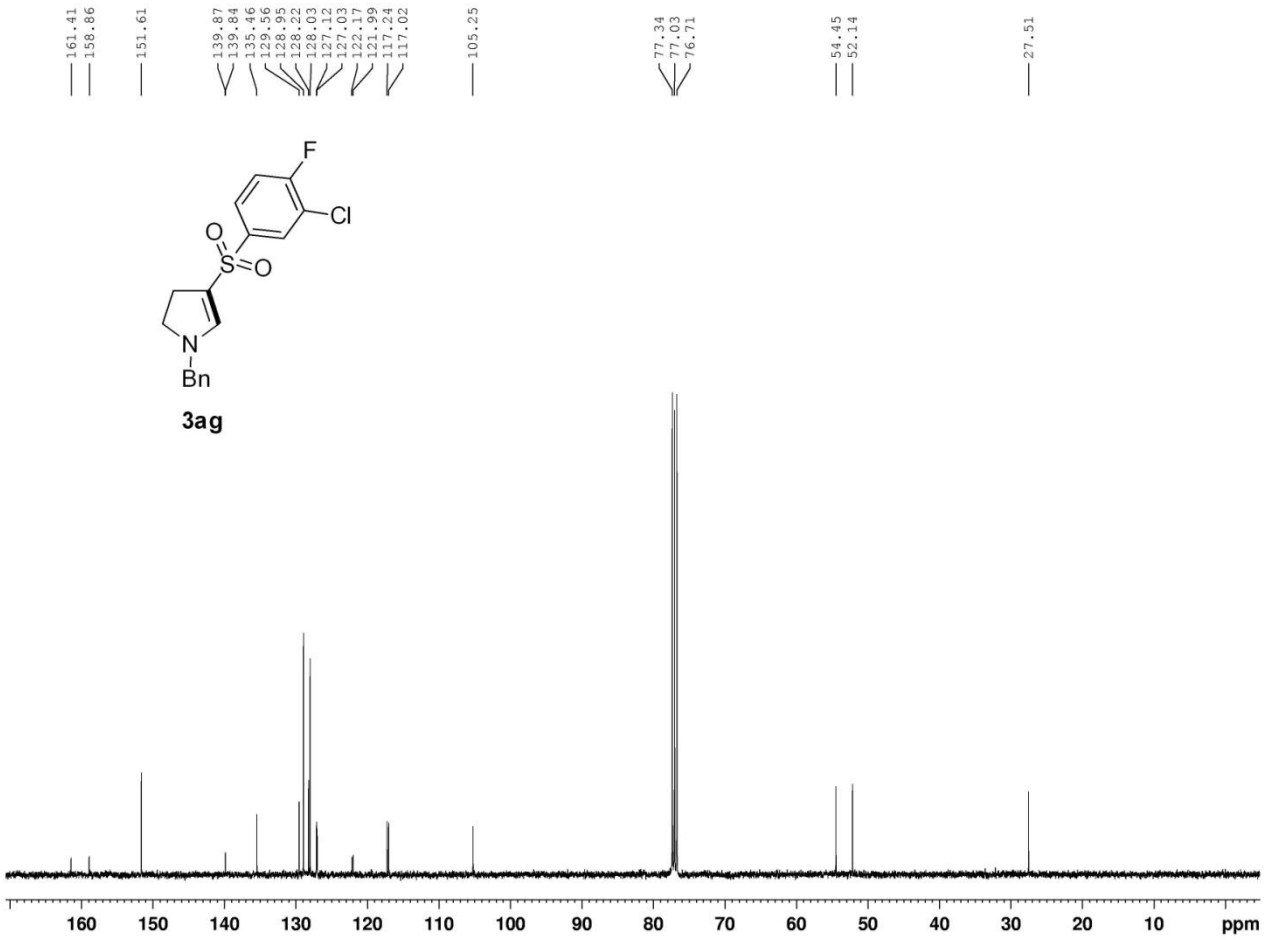
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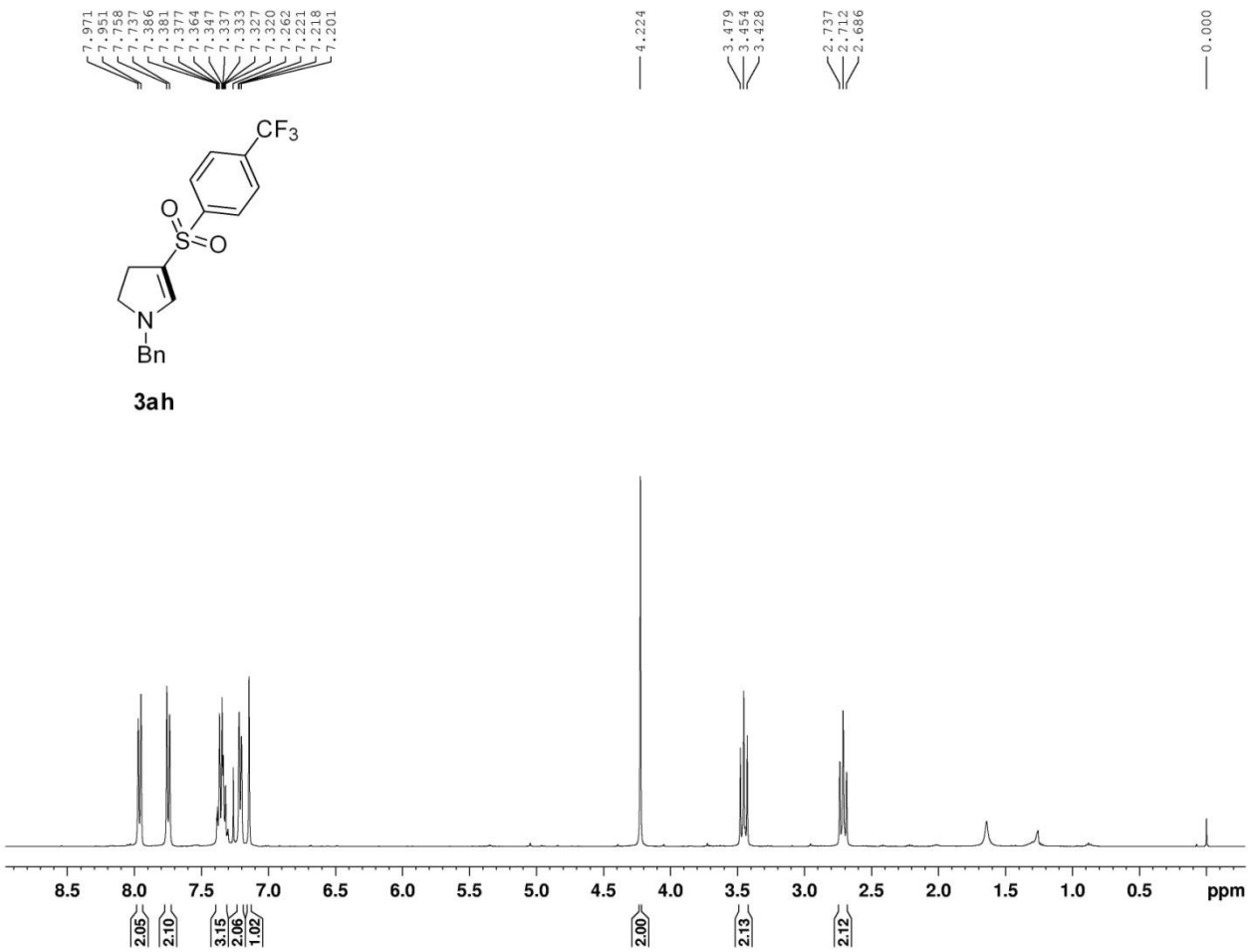
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7.218
7.201
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Bn
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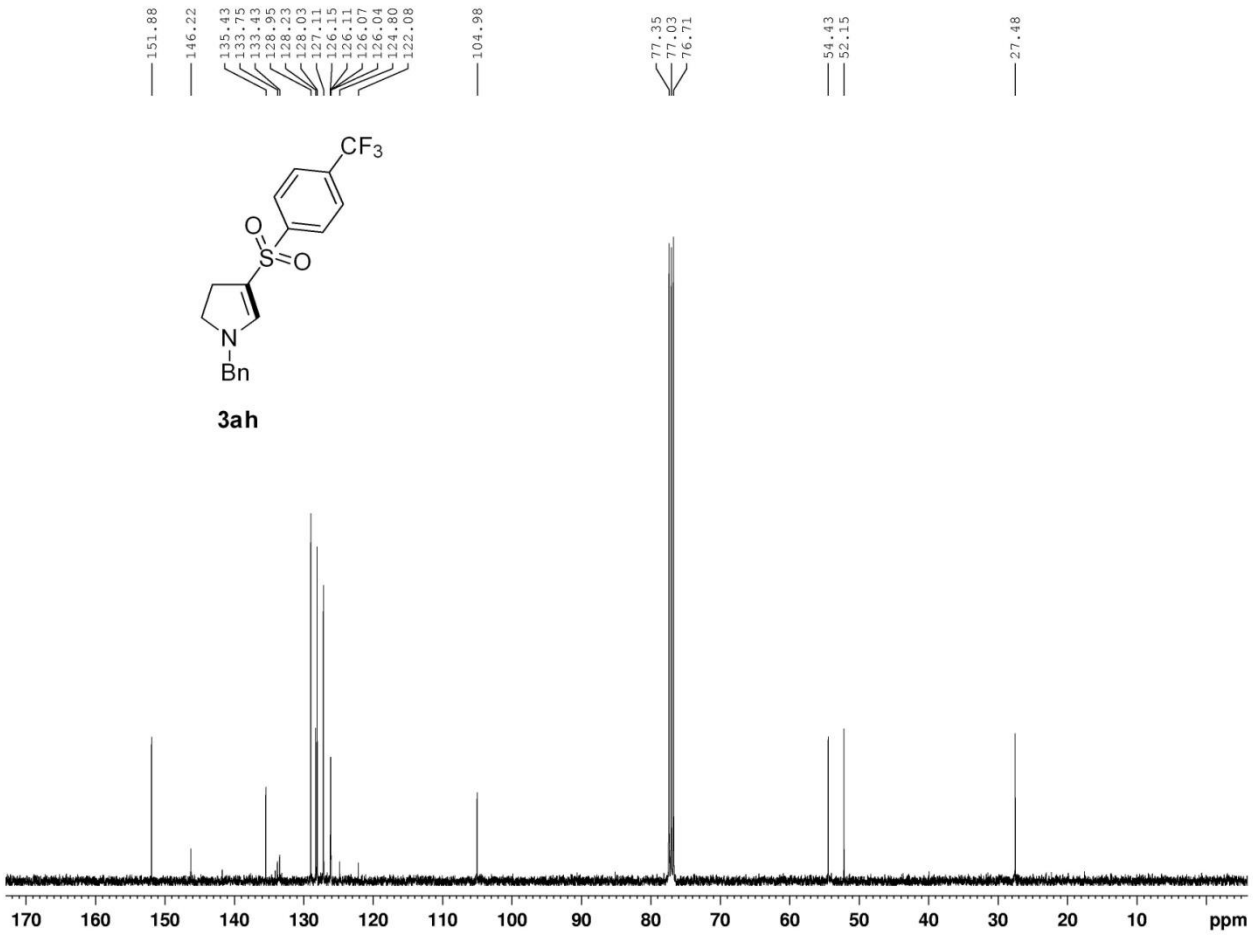
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20
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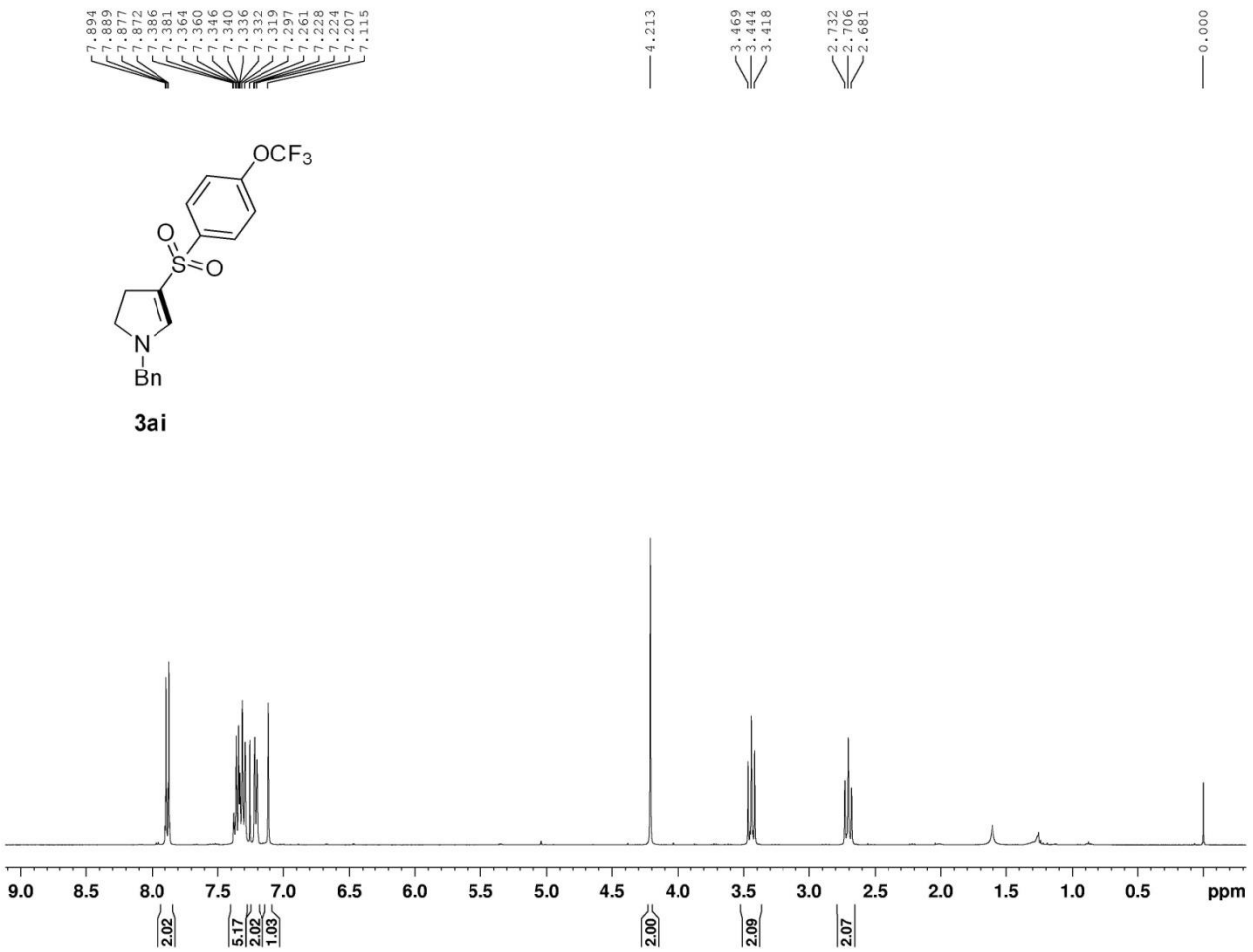
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7.297
7.261
7.228
7.224
7.207
7.115
4.213
3.469
3.444
3.418
2.732
2.706
2.681
0.000
OCF3
O
S
O
N
Bn
3ai
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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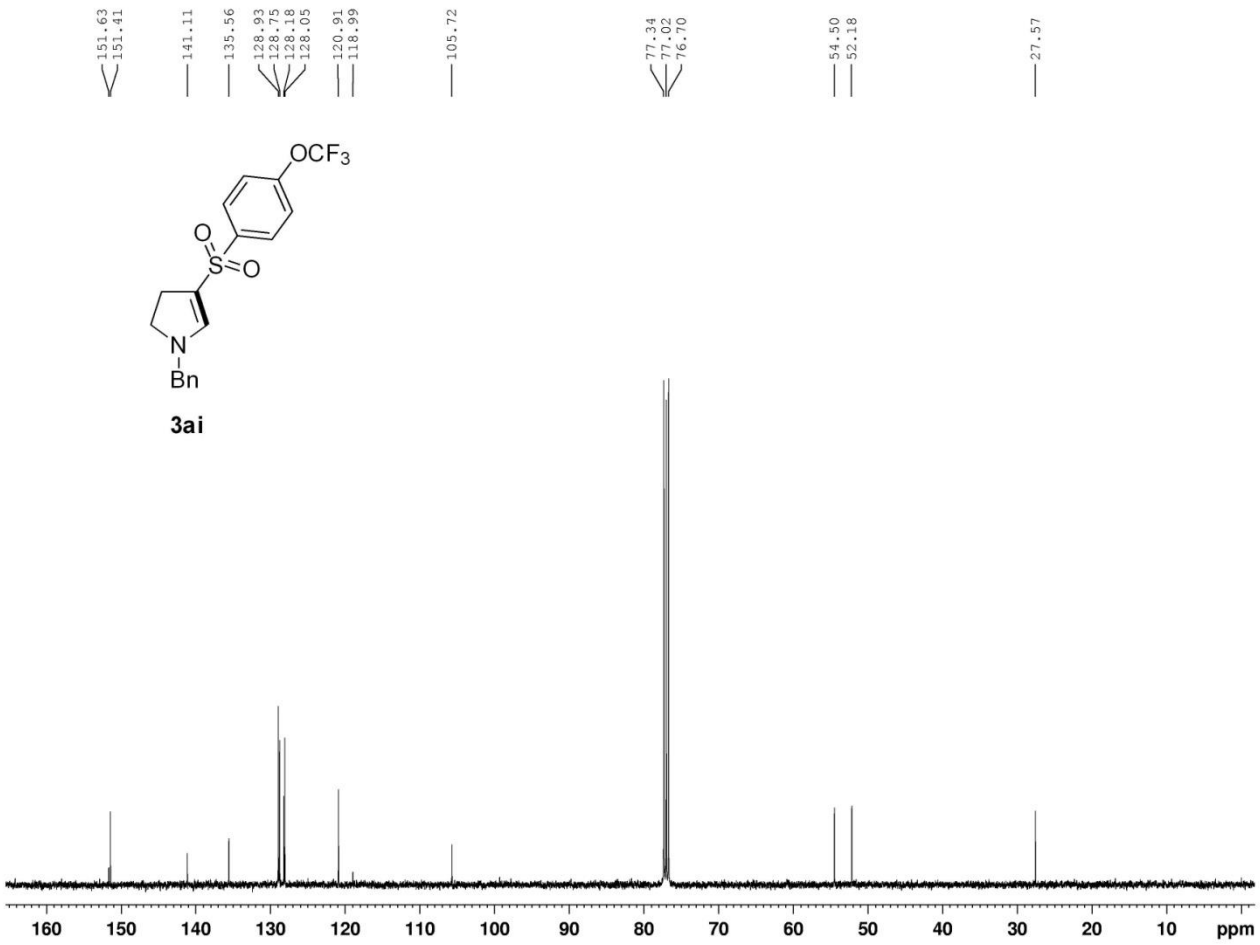
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76.70
54.50
52.18
27.57
OCF3
O
S
O
N
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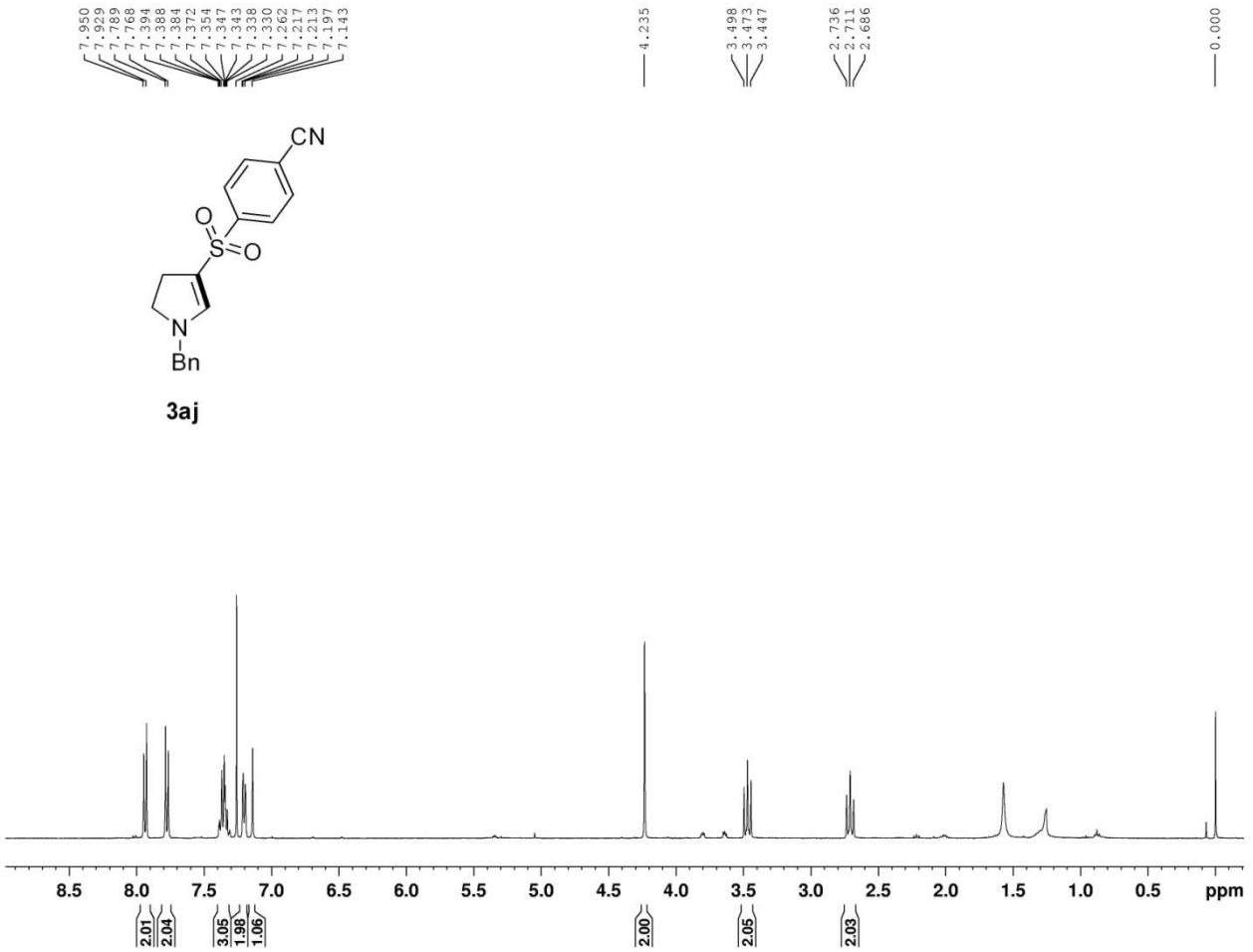
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7.330
7.262
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7.213
7.197
7.143
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3.473
3.447
2.736
2.711
2.686
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CN
O
S
O
N
Bn
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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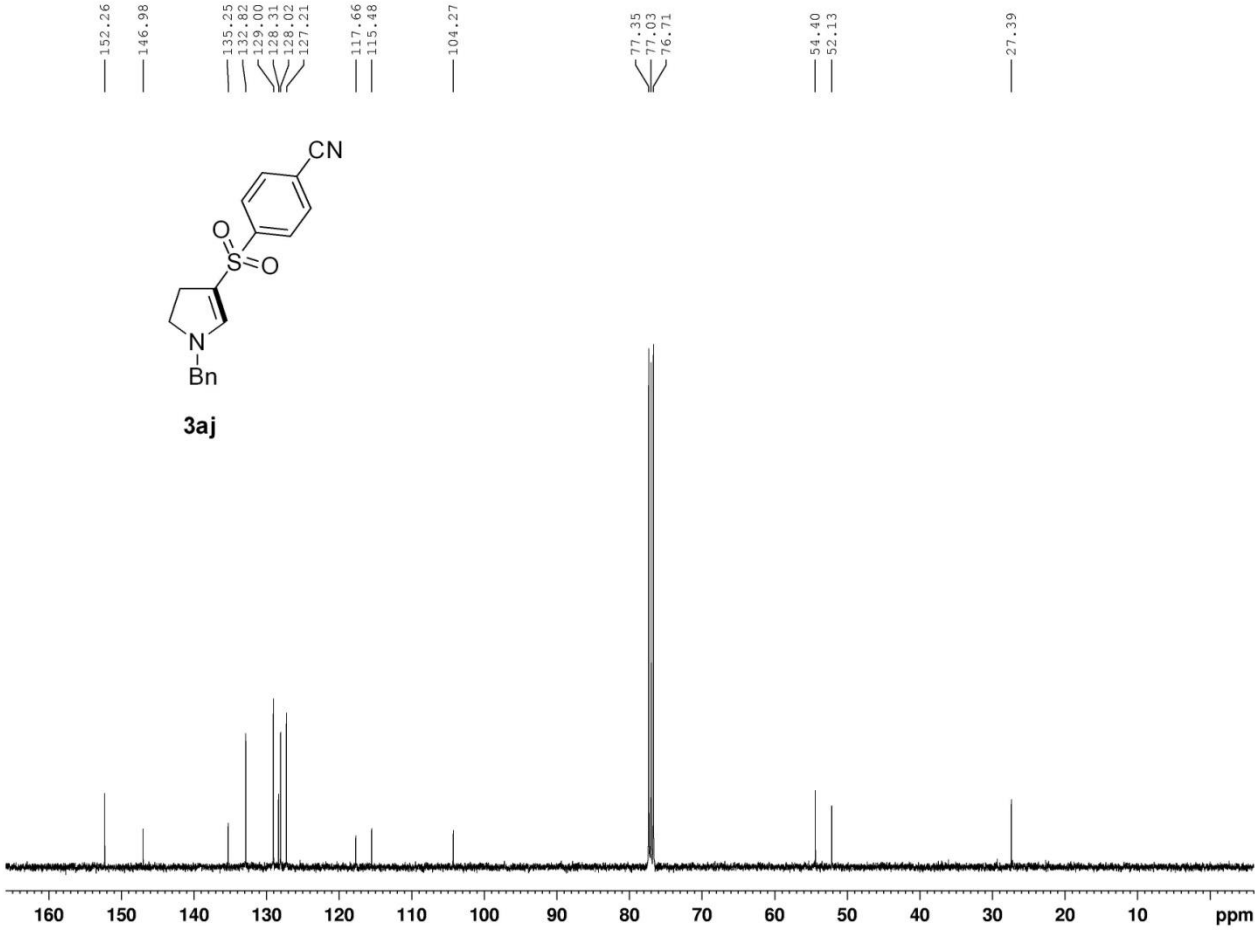
2.03

3aj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76.71
54.40
52.13
27.39
CN
O
S
O
N
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30
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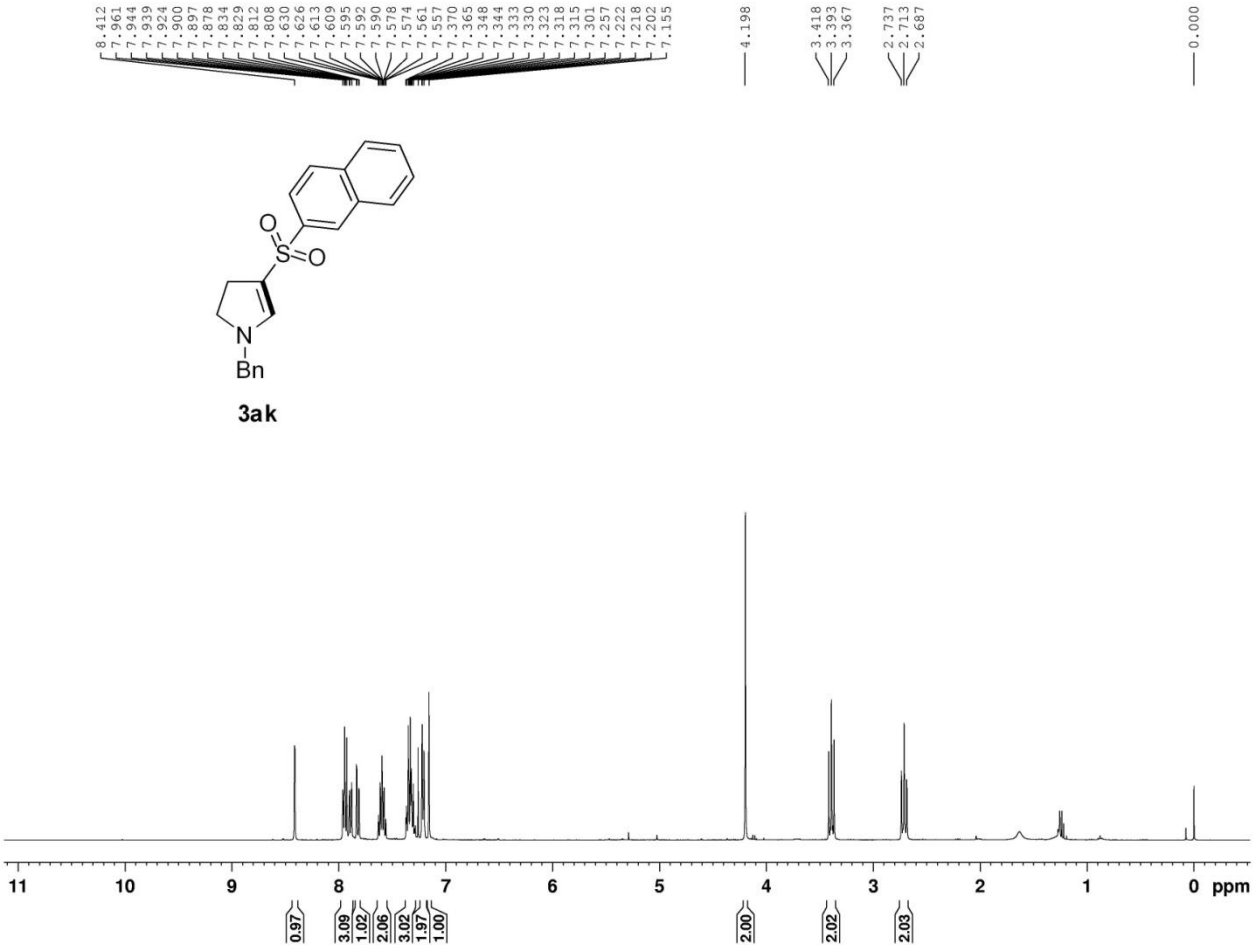
ppm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7.829
7.812
7.808
7.630
7.626
7.613
7.609
7.595
7.592
7.590
7.578
7.574
7.561
7.557
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7.365
7.348
7.344
7.333
7.330
7.323
7.318
7.315
7.301
7.257
7.222
7.218
7.202
7.155
4.198
3.418
3.393
3.367
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S
O
N
Bn
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9
8
7
6
5
4
3
2
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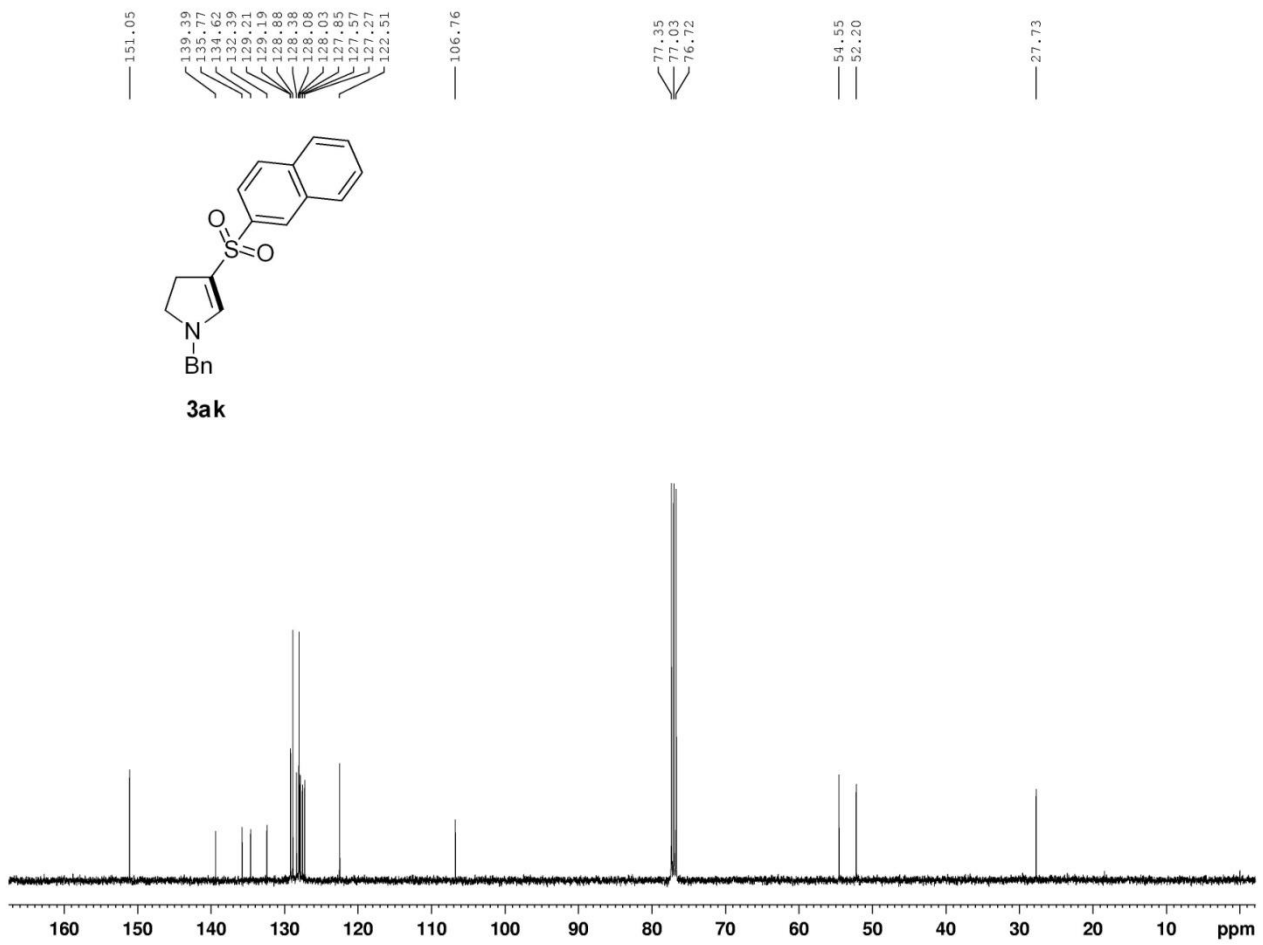
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127.57
127.27
122.51
106.76
77.35
77.03
76.72
54.55
52.20
27.73
O
S
O
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130
120
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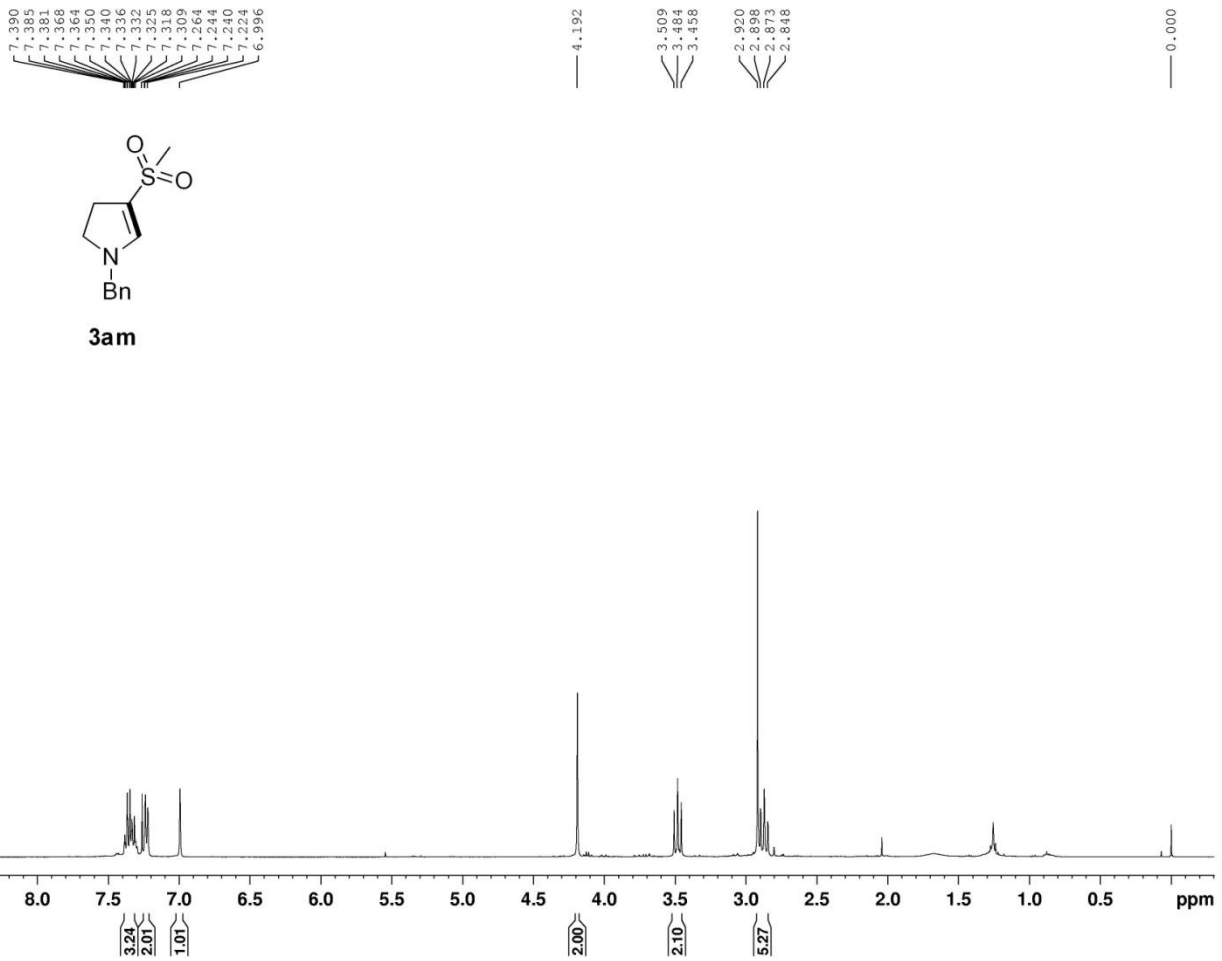
20
10
ppm

3ak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7.325
7.318
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7.244
7.240
7.224
6.996
4.192
3.509
3.484
3.458
2.920
2.898
2.873
2.848
0.000
O
S
O
N
Bn
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
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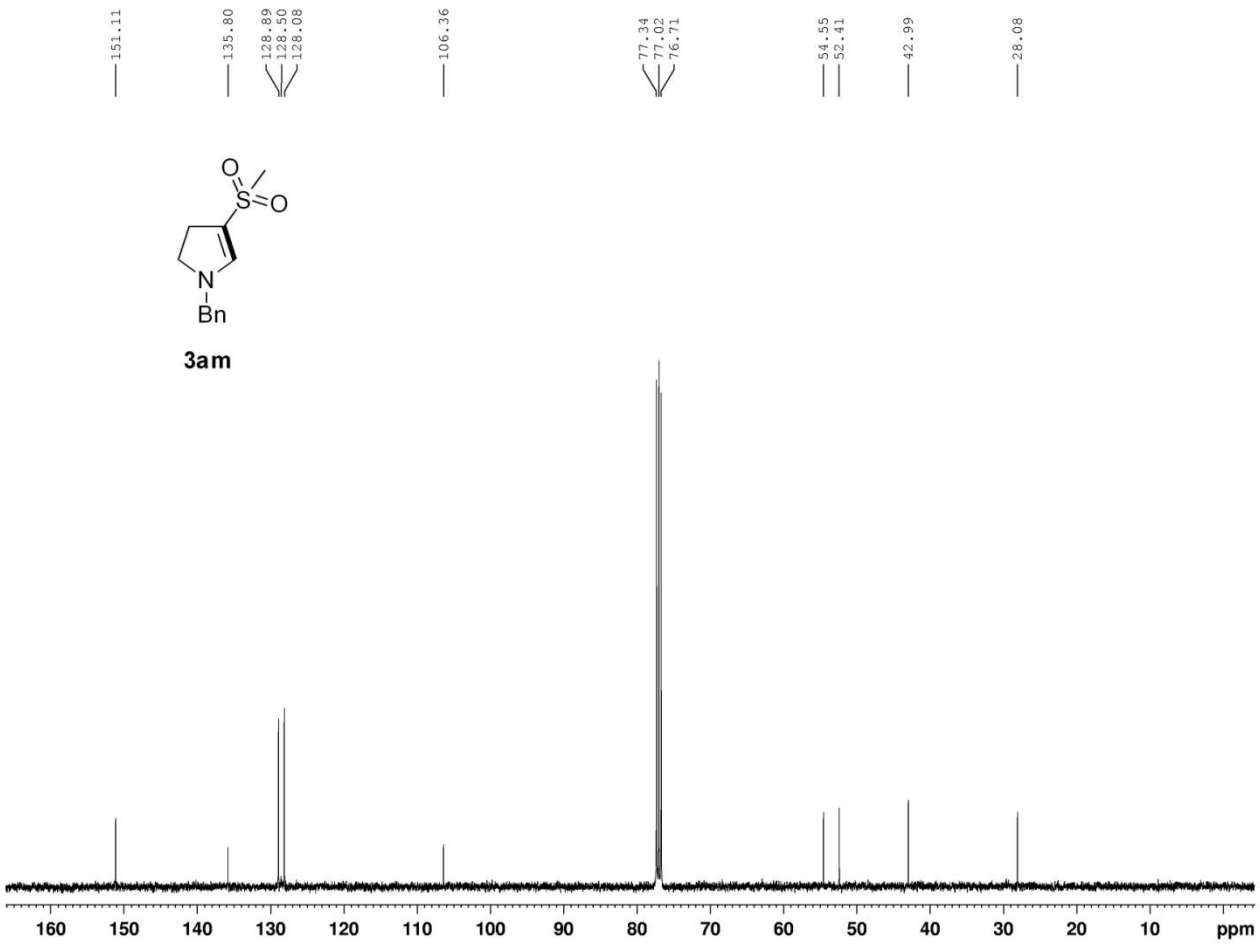
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52.41
42.99
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O
S
O
N
Bn
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140
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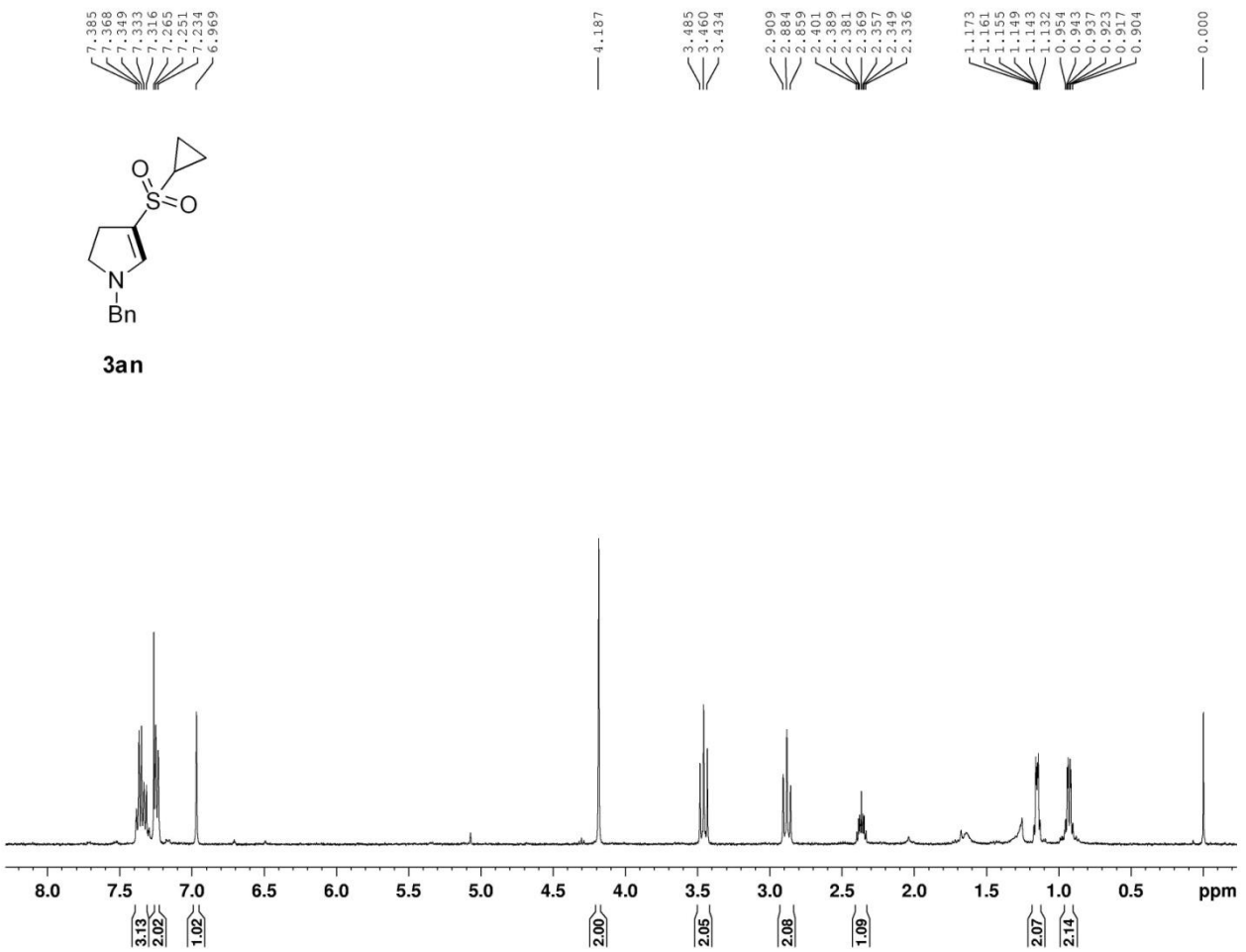
ppm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3.460
3.434
2.909
2.884
2.859
2.401
2.389
2.381
2.369
2.357
2.349
2.336
1.173
1.161
1.155
1.149
1.143
1.132
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0.943
0.937
0.923
0.917
0.904
0.000
O
S
O
N
Bn
3an
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7.0
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6.0
5.5
5.0
4.5
4.0
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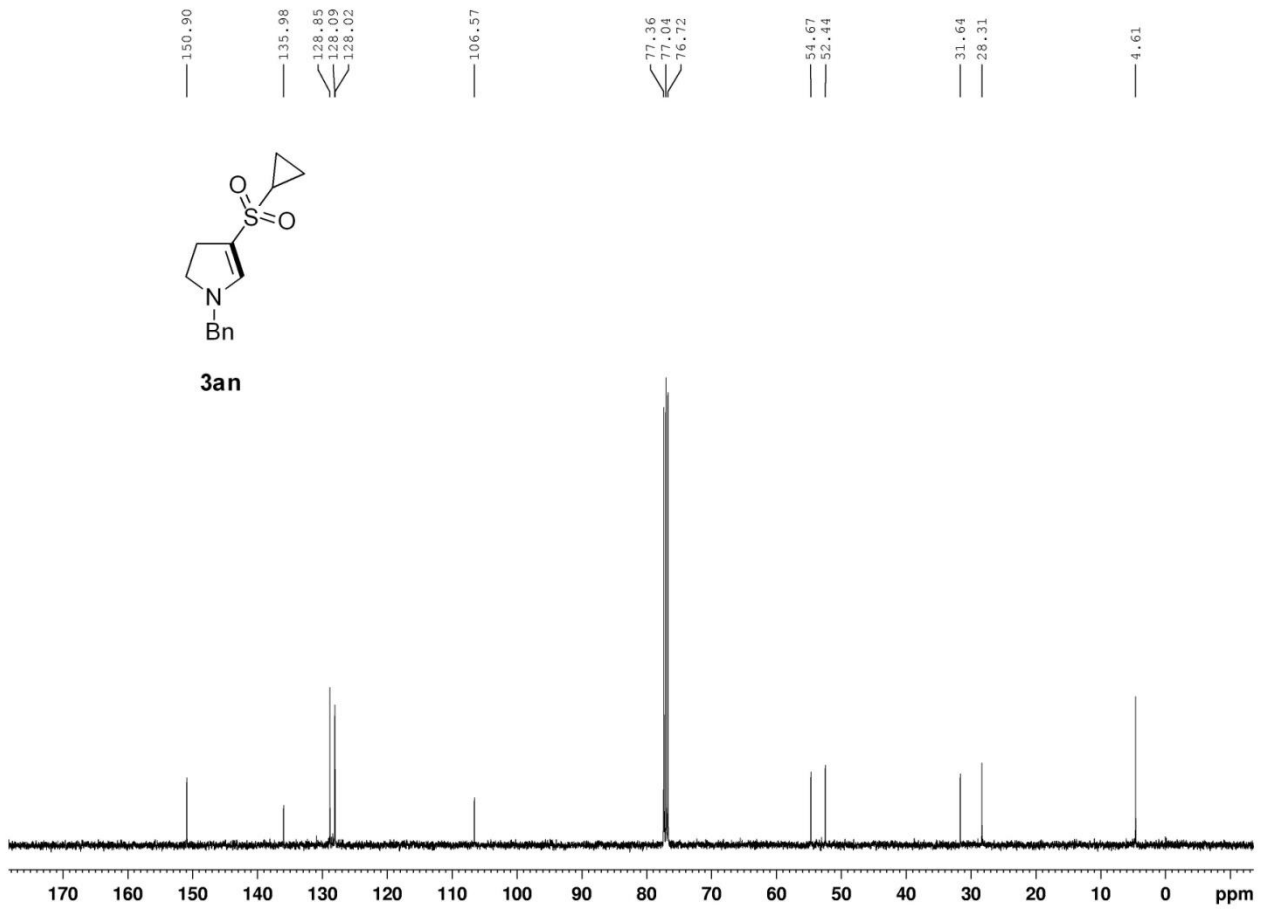
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54.67
52.44
31.64
28.31
4.61
O
S
O
N
Bn
3an
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140
130
120
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60
50
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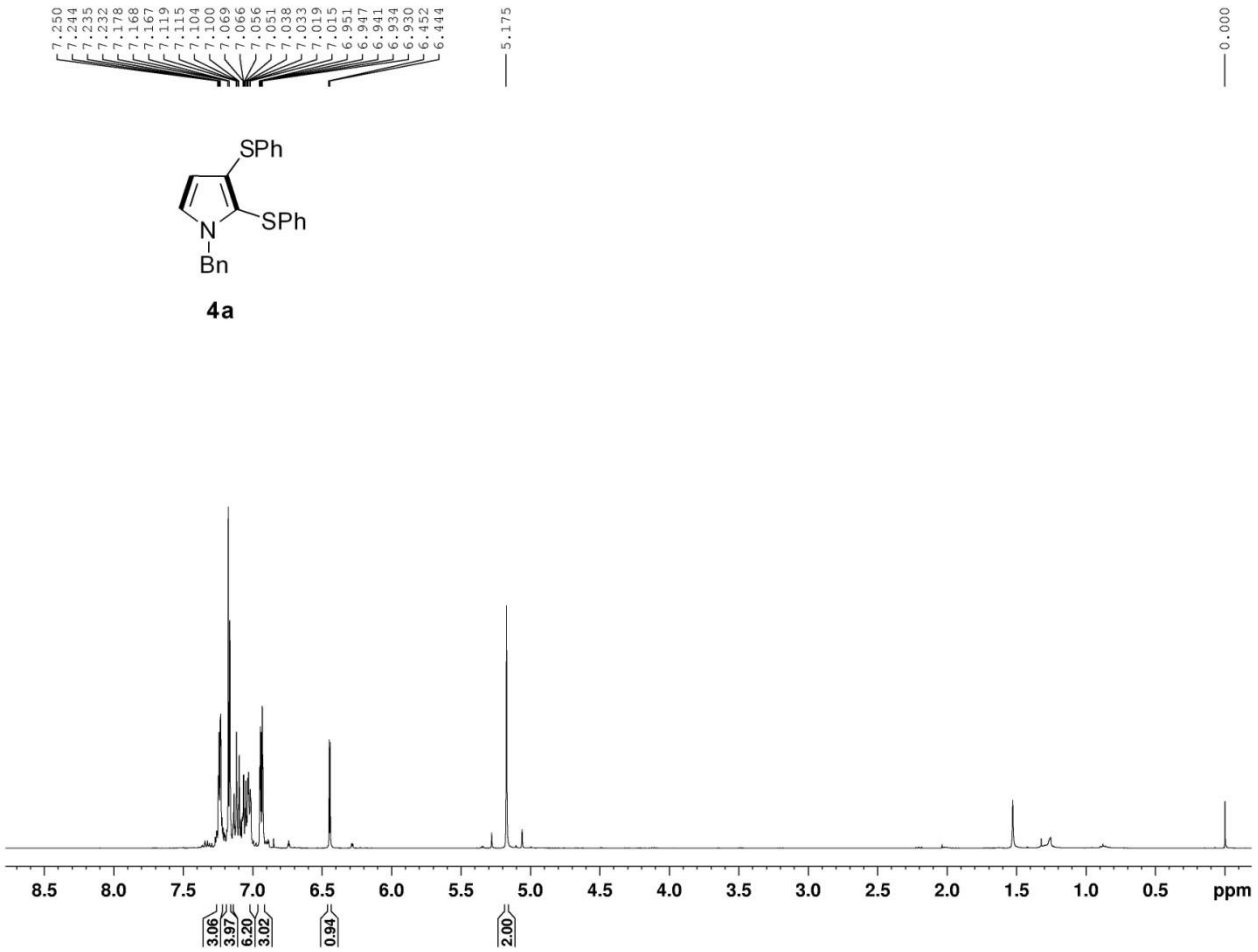
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7.069
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7.056
7.051
7.038
7.033
7.019
7.015
6.951
6.947
6.941
6.934
6.930
6.452
6.444
5.175
0.000
SPh
SPh
N
Bn
4a
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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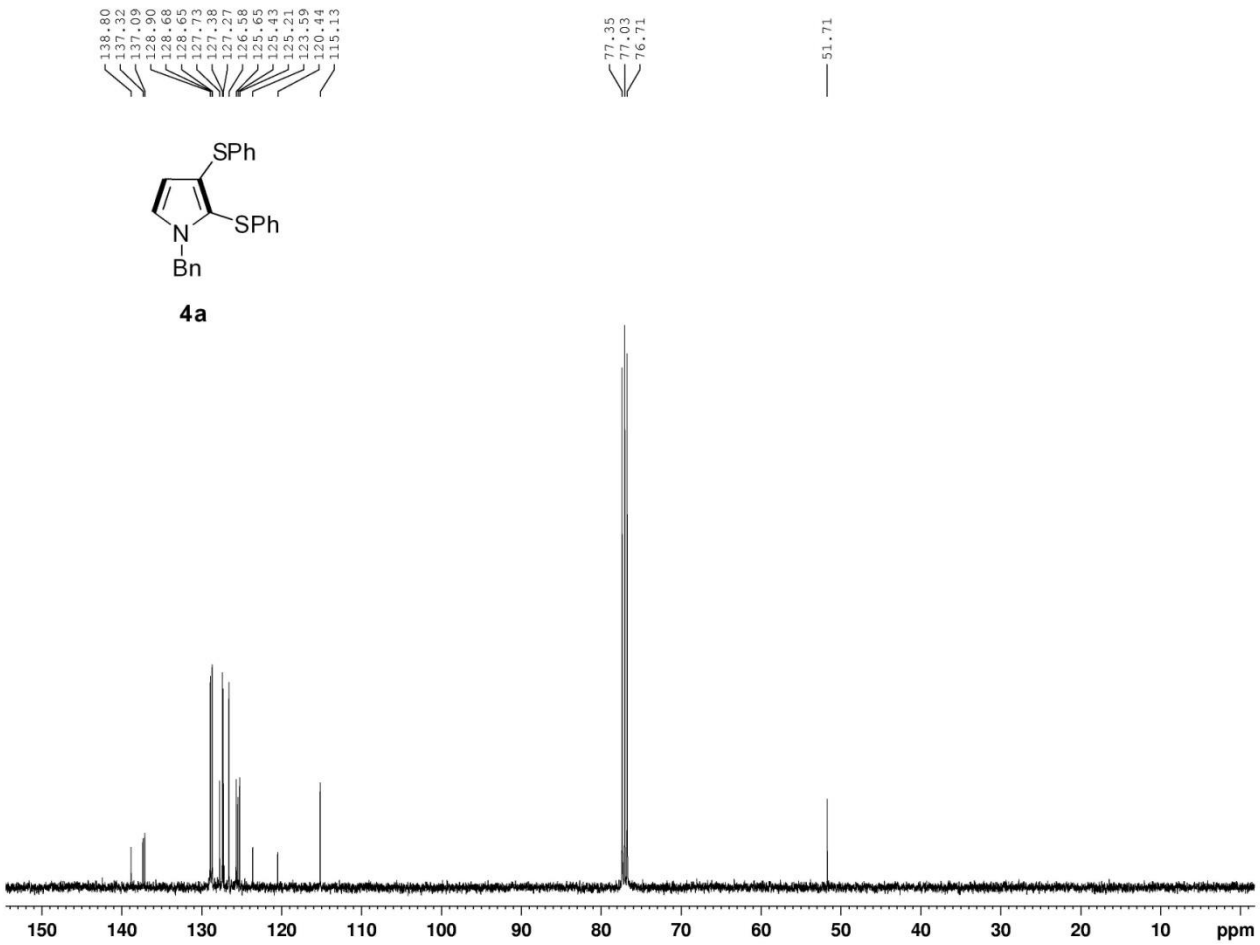
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125.43
125.21
123.59
120.44
115.13
77.35
77.03
76.71
51.71
SPh
SPh
N
Bn
4a
150
140
130
120
110
100
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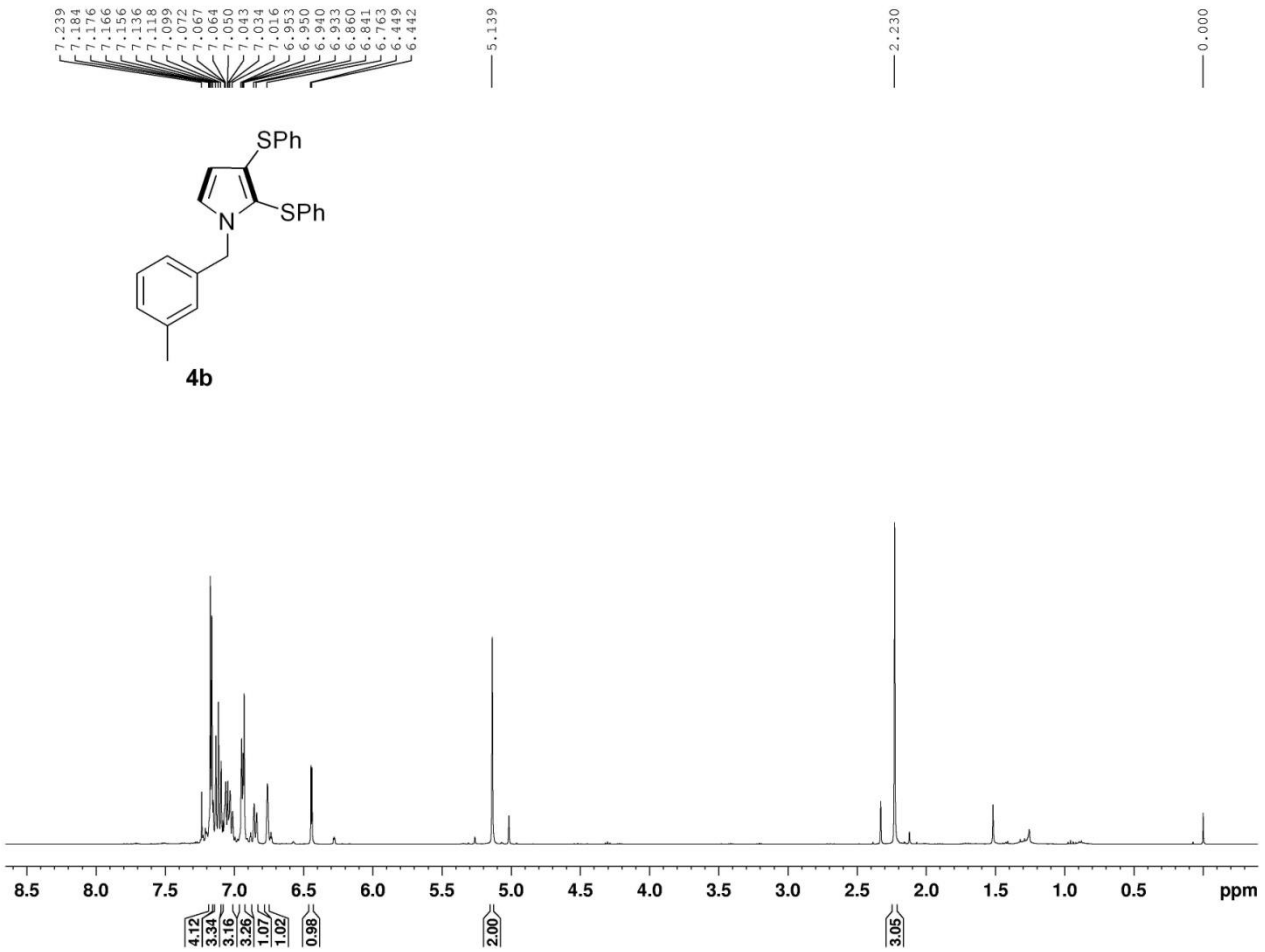
80
70
60
50
40
30
20
10
ppm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7.043
7.034
7.016
6.953
6.950
6.940
6.933
6.860
6.841
6.763
6.449
6.442
5.139
2.230
0.000
SPh
SPh
N
4b
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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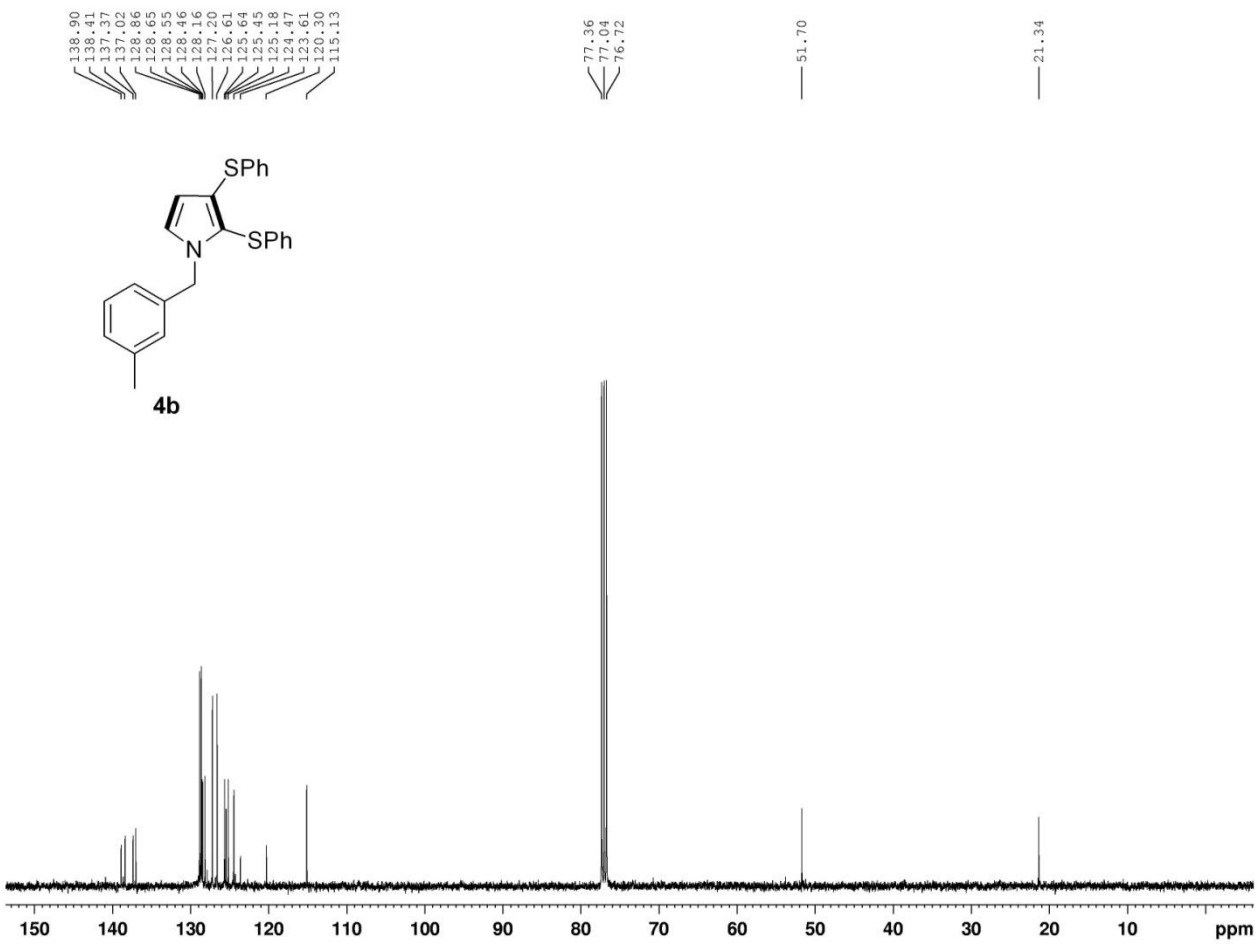
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125.18
124.47
123.61
120.30
115.13
77.36
77.04
76.72
51.70
21.34
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SPh
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130
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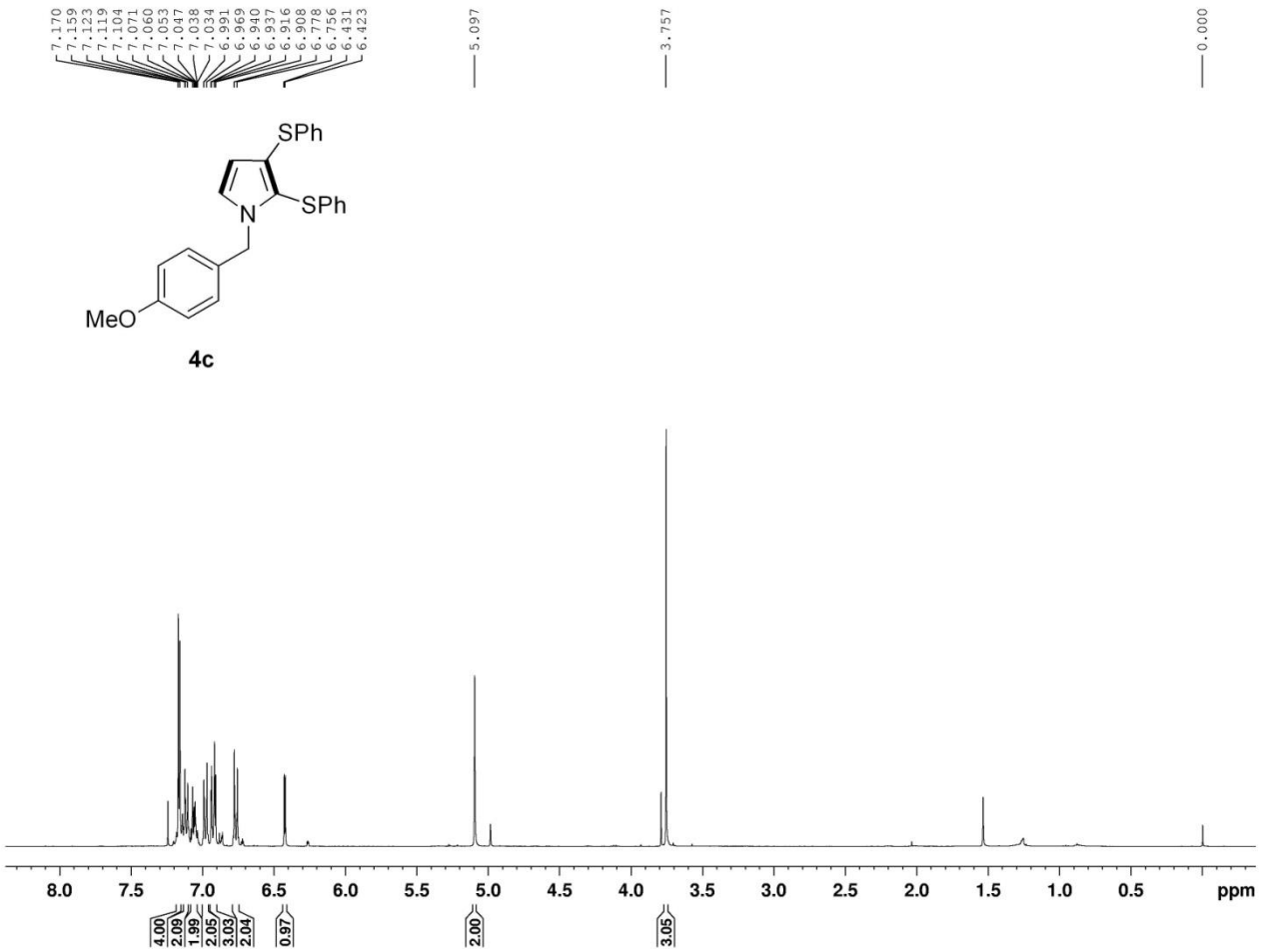
30
20
10
ppm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6.940
6.937
6.916
6.908
6.778
6.756
6.431
6.423
5.097
3.757
0.000
SPh
SPh
N
MeO
4c
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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3.03
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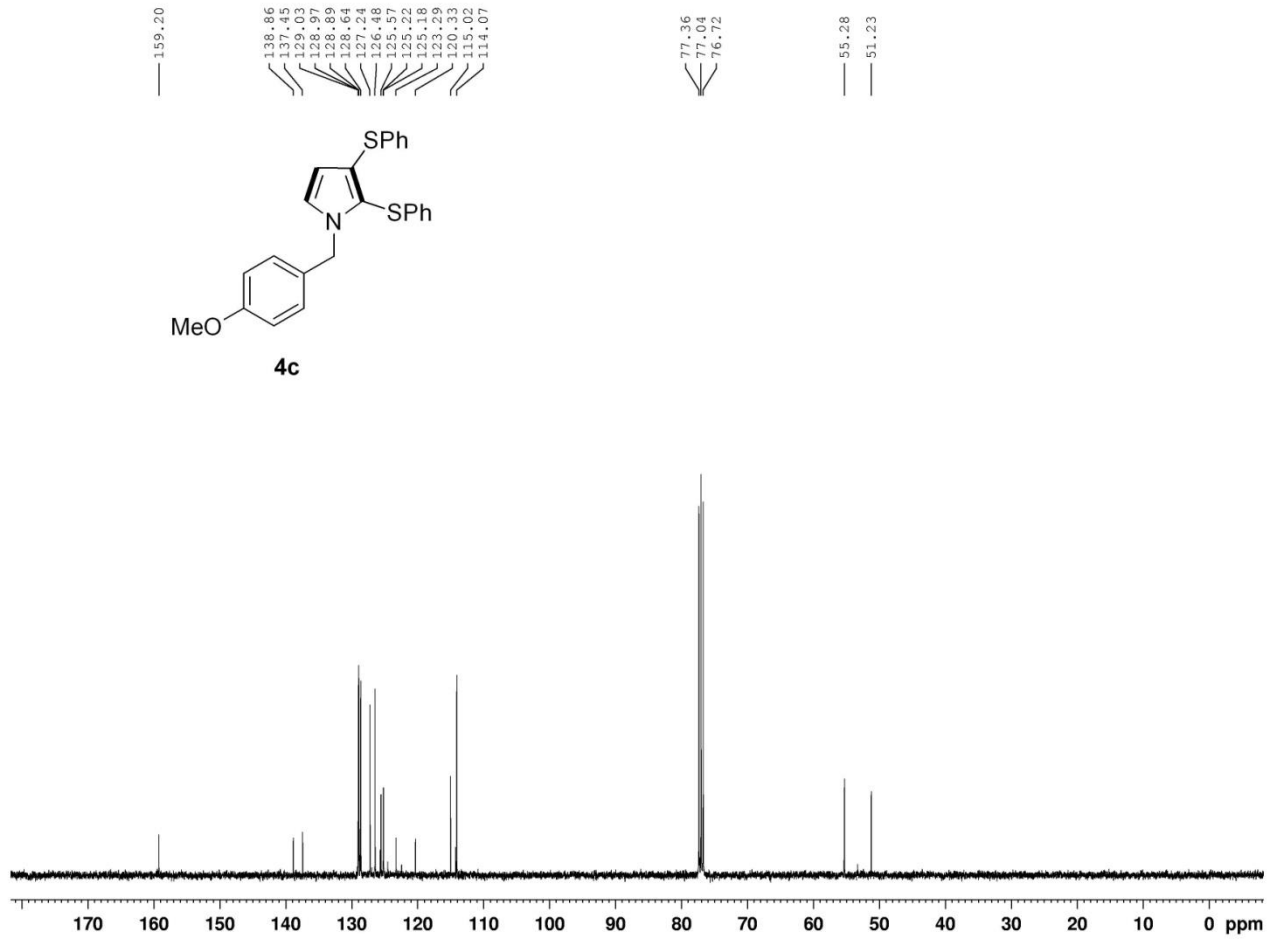
3.05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125.18
123.29
120.33
115.02
114.07
77.36
77.04
76.72
55.28
51.23
SPh
SPh
N
MeO
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60
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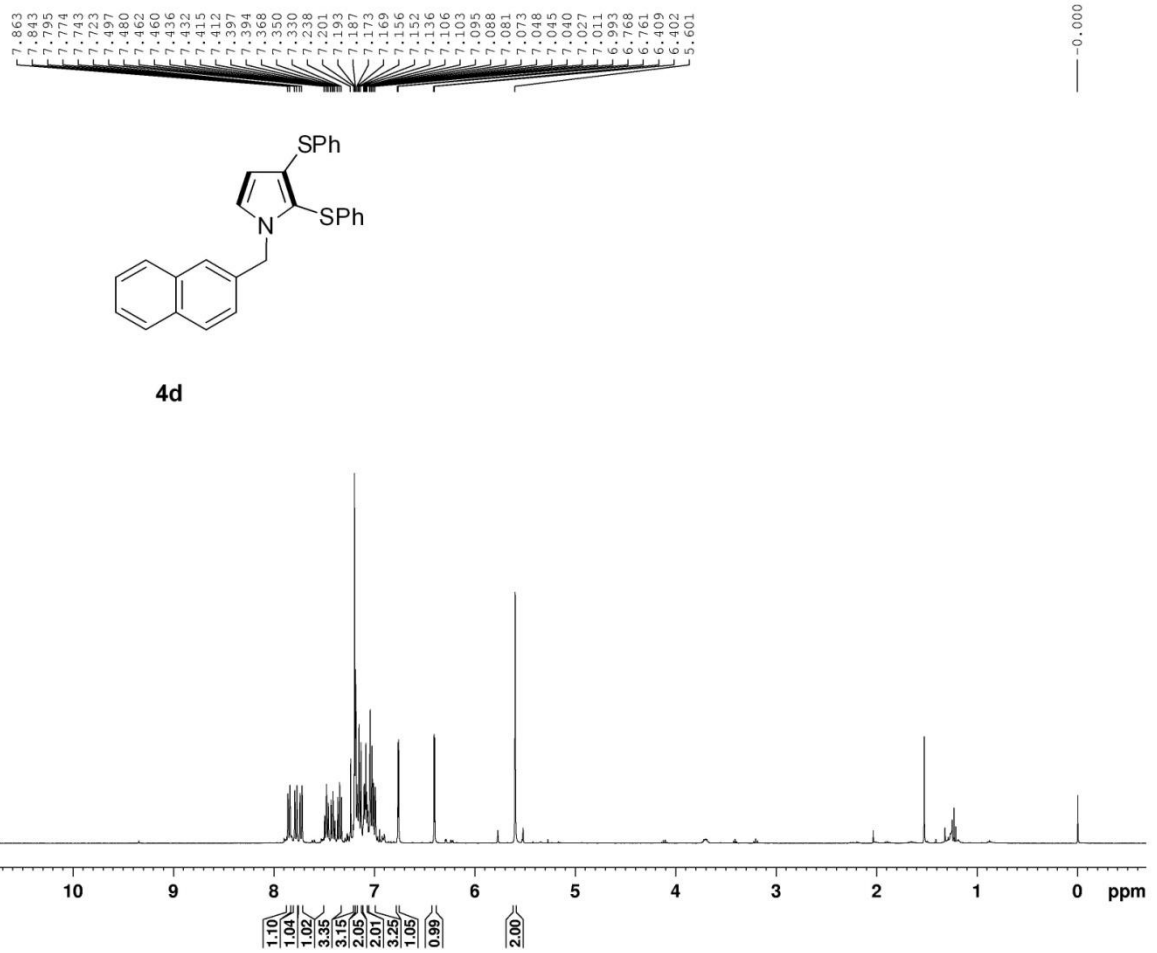
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7.169
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7.136
7.106
7.103
7.095
7.088
7.081
7.073
7.048
7.045
7.040
7.027
7.011
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6.768
6.761
6.409
6.402
5.601
0.000
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SPh
N
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10
9
8
7
6
5
4
3
2
1
0
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3.25
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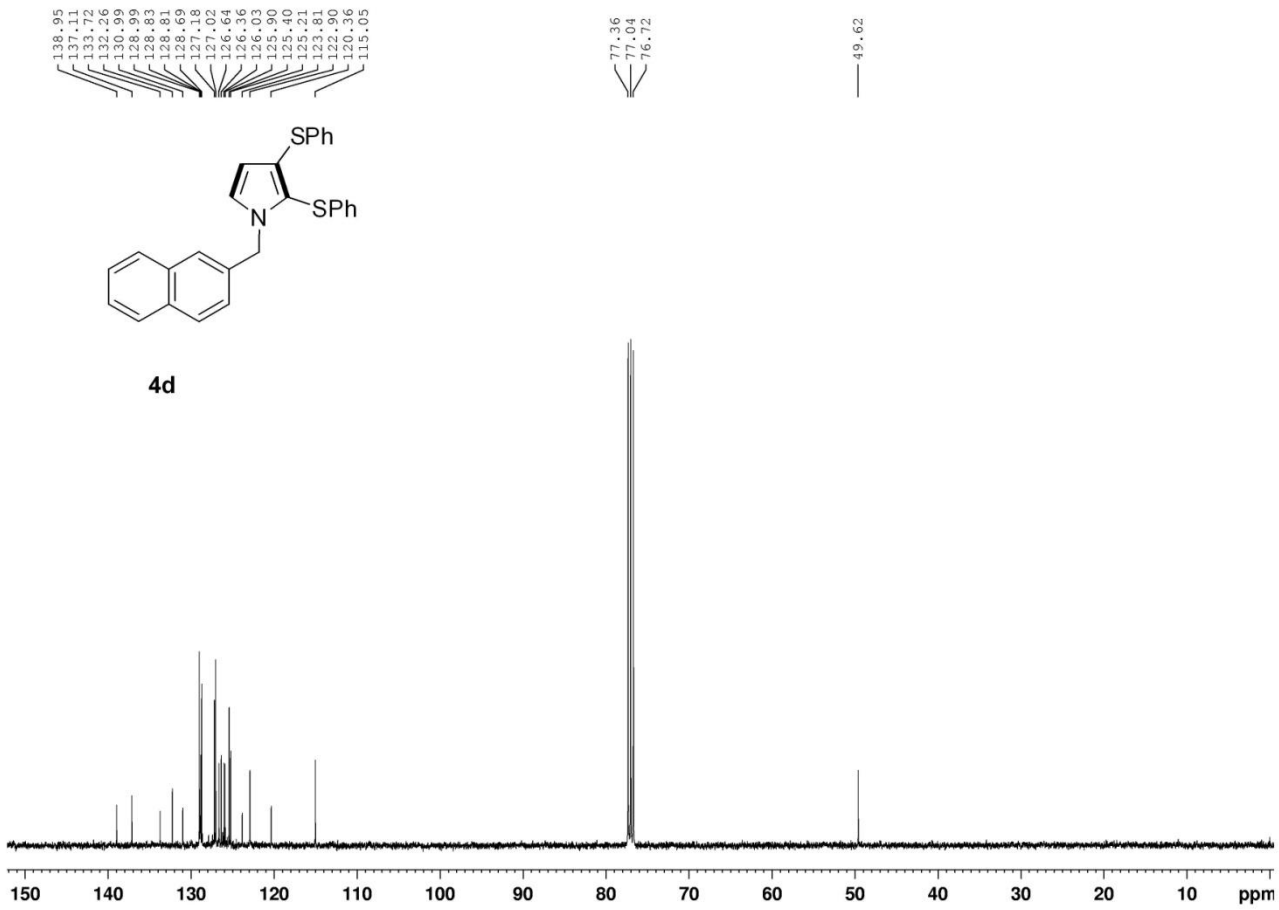
4d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49.62
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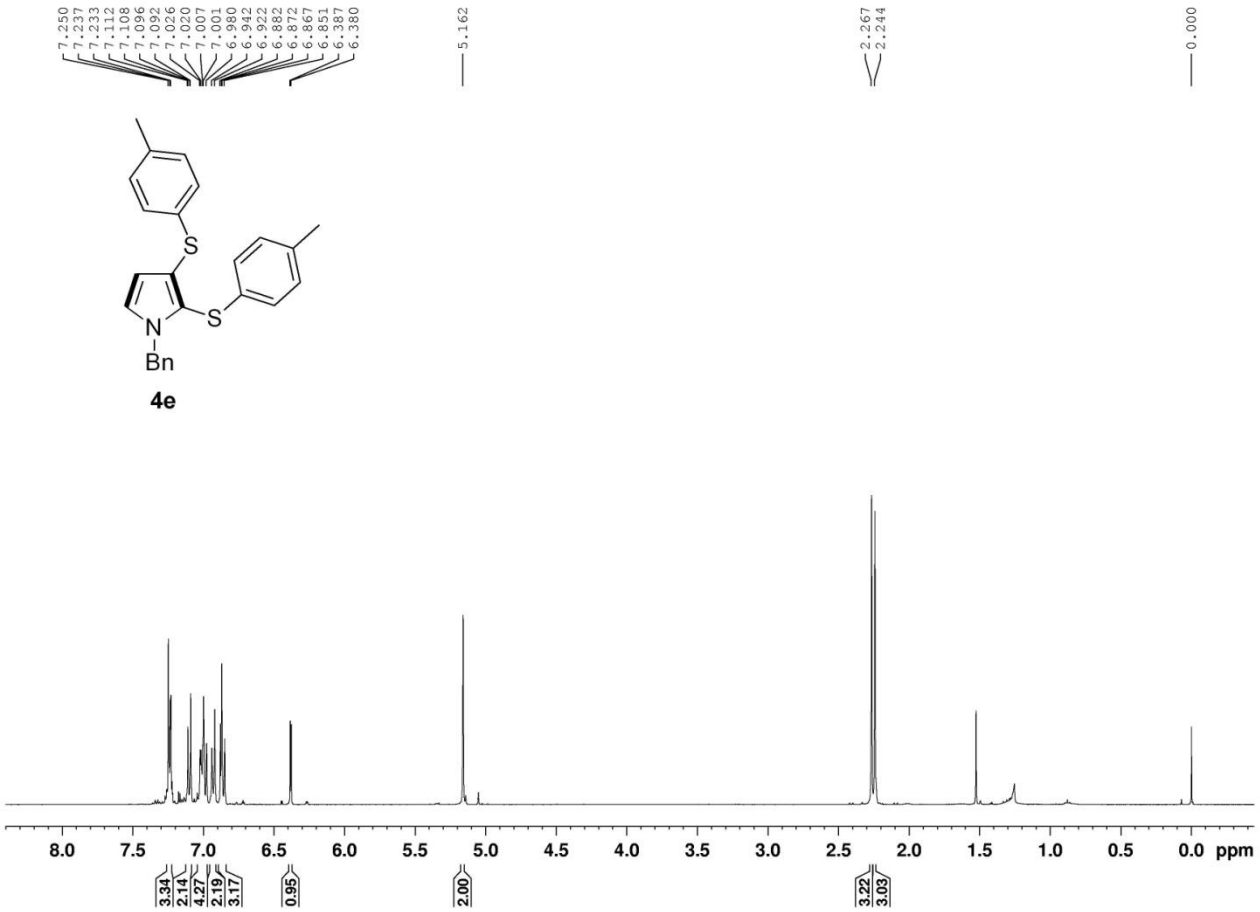
10
ppm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6.922
6.882
6.872
6.867
6.851
6.387
6.380
5.162
2.267
2.244
0.000
S
S
N
Bn
4e
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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4.27
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2.00
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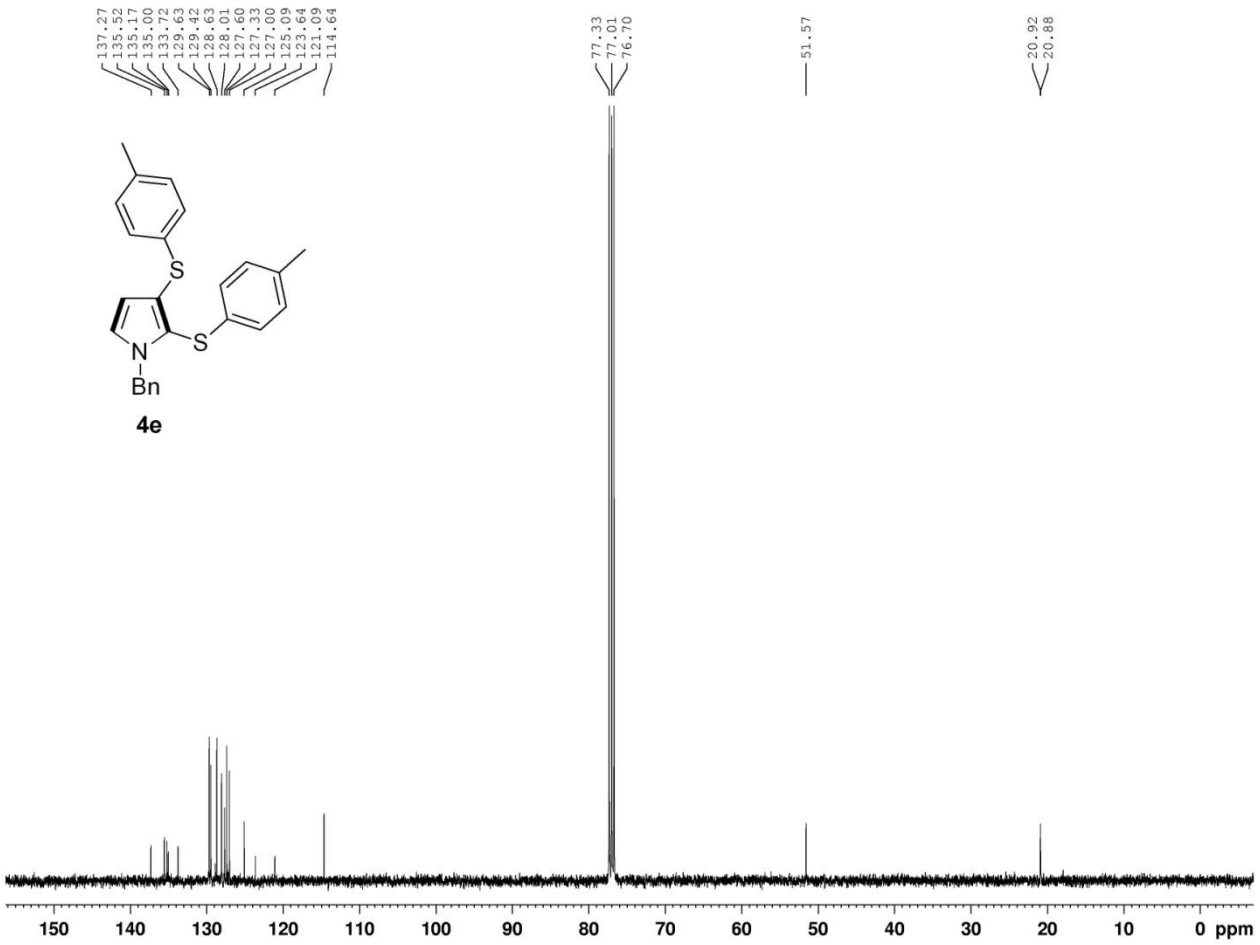
3.03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127.33
127.00
125.09
123.64
121.09
114.64
77.33
77.01
76.70
51.57
20.92
20.88
S
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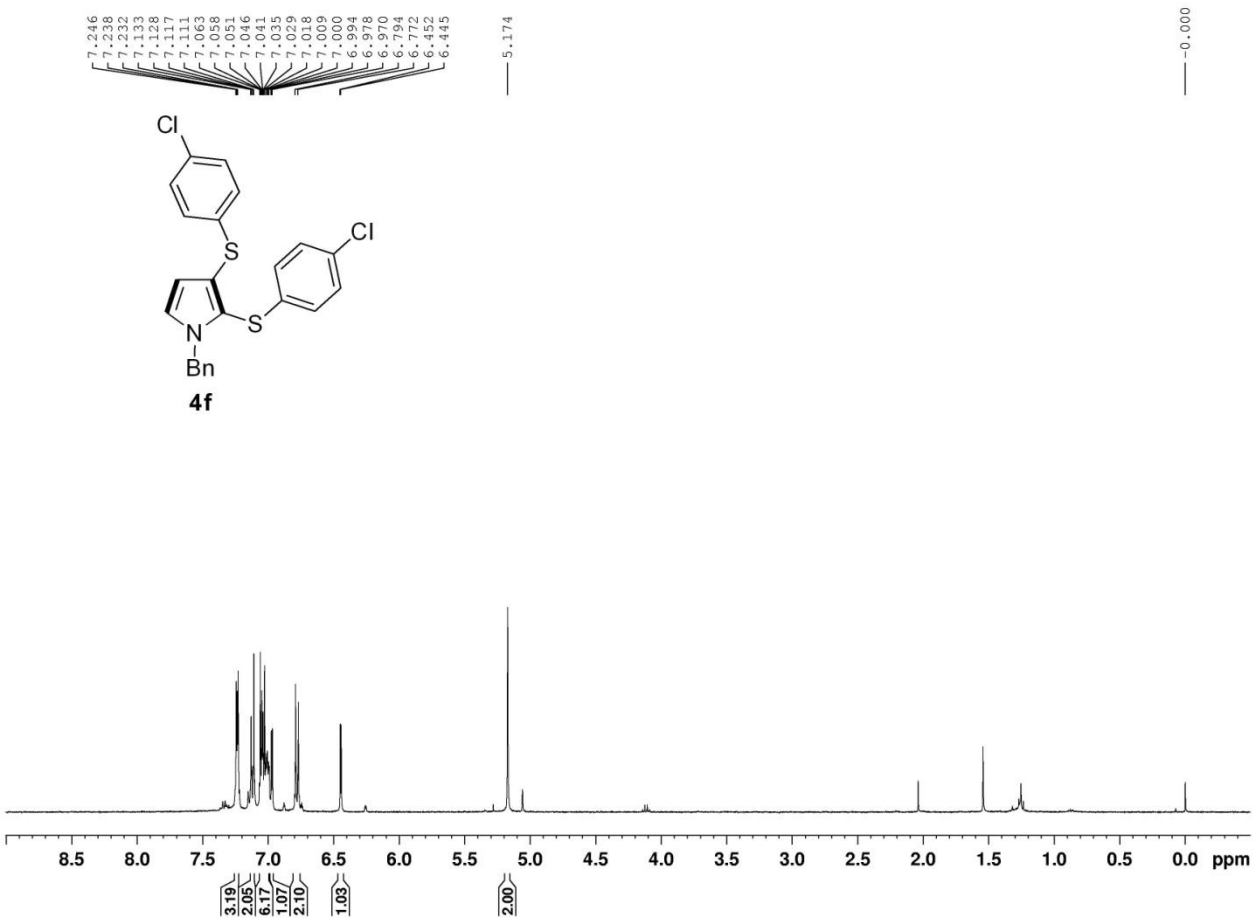
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7.029
7.018
7.009
7.000
6.994
6.978
6.970
6.794
6.772
6.452
6.445
5.174
0.000
Cl
S
Cl
S
N
Bn
4f
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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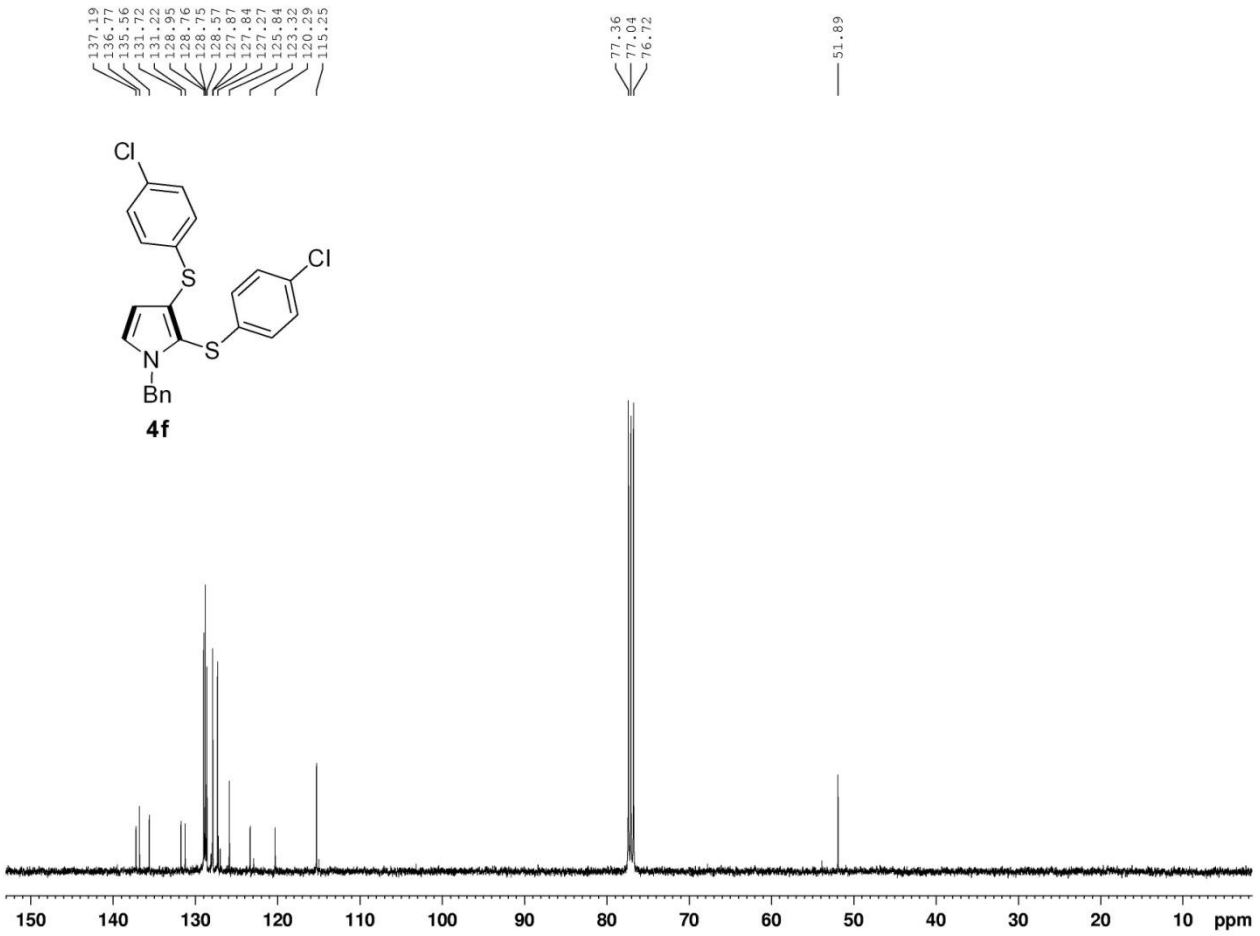
1.03
2.00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115.25
77.36
77.04
76.72
51.89
Cl
S
Cl
S
N
Bn
4f
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20
10
ppm