Supporting Information

Direct intramolecular C(sp^3)-H bond sulfonamidation to synthesize benzosultam derivatives under metal-free conditions

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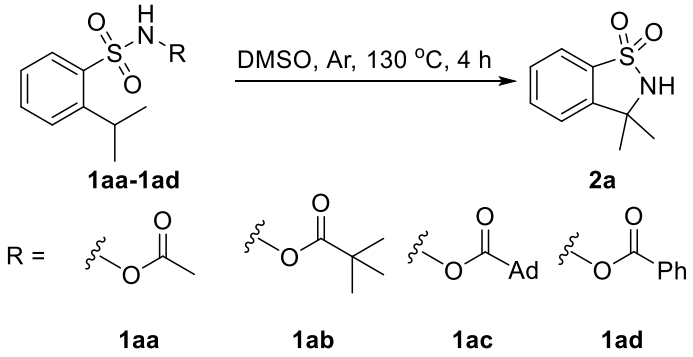
General Information

^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded at 600 MHz, 151 MHz, and 565 MHz respectively on a Bruker DPX instrument using Me_4Si as an internal standard. New compounds for HRMS were tested on a Waters Q-Tof Micro MS/MS System ESI spectrometer. Melting points were measured on a WC-1 instrument and uncorrected. Chemical shift multiplicities are represented as follows: (s = singlet, d = doublet, m = multiplet, dd = double doublet). Unless otherwise mentioned, all materials were commercially obtained and used without further purification, and all procedures were performed under the argon atmosphere. All substrates **1** were synthesized according to literature procedures.[1-8] **3**, **4** were synthesized according to literature procedures.[1,9] Abbreviations for the solvents are PE, petroleum ether; EA, ethyl acetate.

Experimental Section

1. Optimization of reaction conditions

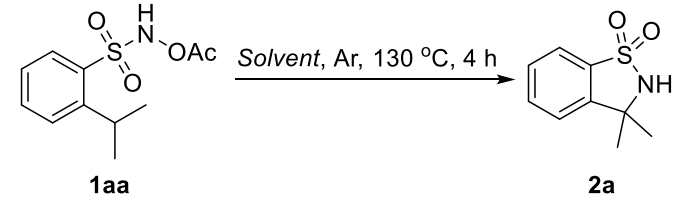
Table S1. Optimization of the leaving group[a]



Entry	Substrate	**2a** (%)
1	**1aa**	**89**
2	**1ab**	77
3	**1ac**	80
4	**1ad**	51

[a] Reaction condition: **1aa-1ad** (0.1 mmol), DMSO (1 mL), 130 °C, Ar atmosphere, 4 h, Isolated yields. Ad= adamantine.

Table S2. Optimization of solvents[a]

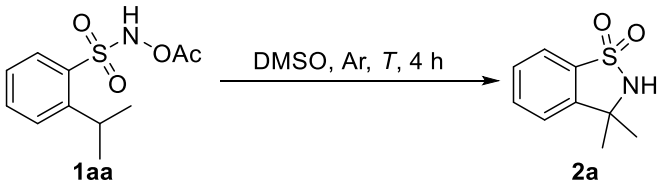


Entry	Solvent	**2a** (%)
1	**DMSO**	**89**
2	DMF	78
3	DMPU	84
4	HFIP	70
5	$PhCF_3$	75
6	DCE	69

[a] Reaction condition: **1aa** (0.1 mmol), solvent (1 mL), 130 °C, Ar atmosphere, 4 h, isolated yields. DMSO = Dimethyl sulfoxide; DMF = N,N-Dimethylformamide; DMPU =

1,3-Dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone; HFIP = 1,1,1,3,3,3-Hexafluoroisopropanol; DCE = 1,2-Dichloroethane.

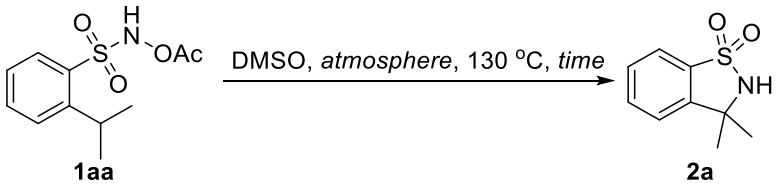
Table S3. Optimization of temperature[a]



Entry	T (°C)	**2a** (%)
1	**130**	**89**
2	120	85
3	110	83
4	100	79
5	90	61
6	80	42

[a] Reaction condition: **1aa** (0.1 mmol), DMSO (1 mL), 80-130 °C, Ar atmosphere, 4 h, isolated yield.

Table S4. Optimization of dosage and atmosphere[a]



Entry	Solvent (mL)	Time	**2a** (%)
1	1	4	79
2	1.5	4	83
3	**2**	**4**	**89[b]**
4	2	4	76[c]
5	2	4	56[d]
6	2.5	4	85
7	3	4	82
8	2	2	65
7	2	6	83
9	2	8	84
10	2	10	81

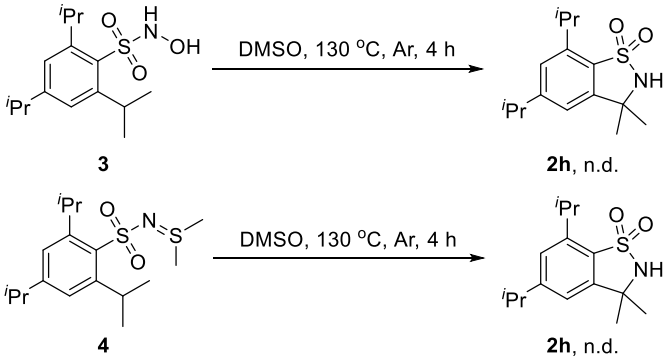
[a] Reaction condition: **1aa** (0.1 mmol), DMSO (1-3 mL), 130 °C, Ar atmosphere, 4-10 h, isolated yields. [b] **1aa** (0.2 mmol), DMSO (2 mL). [c] **1aa** (0.2 mmol), DMSO (2 mL), air. [d] **1aa** (0.2 mmol), DMSO (2 mL), O_2.

2. General Procedure for Synthesis of 2.

A 15 mL oven-dried pressure tube was equipped with a magnetic stir bar and charged with the substrate **1** (0.2 mmol), DMSO (2.0 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 4 h, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. The product was purified by preparative TLC on silica gel.

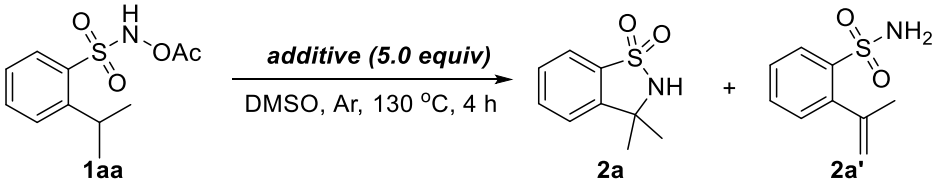
3. Control experiments and mechanistic studies

Control experiments



A 15 mL oven-dried pressure tube was equipped with a magnetic stir bar and charged with substrate **3** or **4** (0.2 mmol), DMSO (2.0 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 4 h, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. No desired product **2h** was detected by TLC.

The reaction at the presence of radical scavenger.

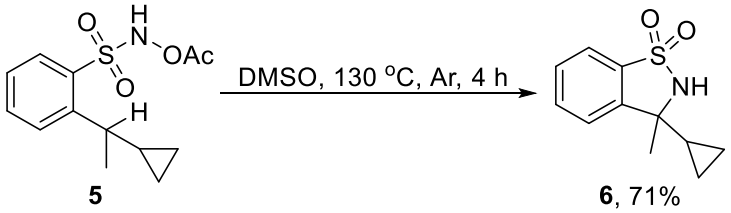


Entry	Additive	Yield of **2a** (%)[a]	Yield of **2a'** (%)[a]
1	TEMPO	0	63
2	BHT	73	0
3	1,1-diphenylethylene	81	0

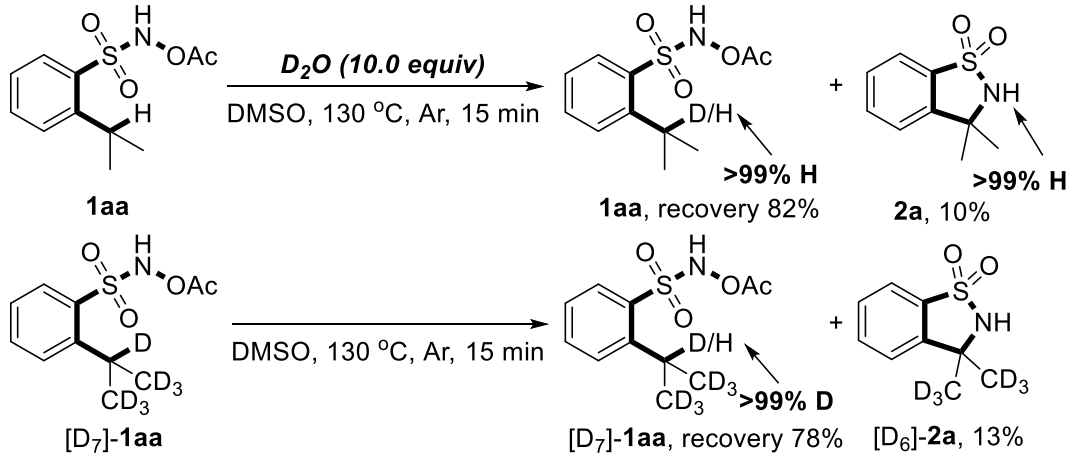
[a]Reaction condition: **1aa** (0.2 mmol), additive (5.0 equiv), DMSO (2 mL), 130 °C, Ar atmosphere, 4 h, isolated yields.

A 15 mL oven-dried pressure tube was equipped with a magnetic stir bar and charged with *N*-acetoxy-2-isopropylbenzenesulfonamide **1aa** (0.2 mmol), additive (5.0 equiv), DMSO (2.0 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 4 h, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. The product was purified by preparative TLC on silica gel.

The radical clock experiment



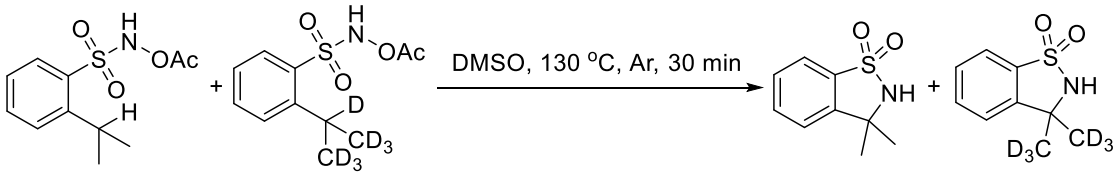
H/D exchange experiment



A 15 mL oven-dried pressure tube was equipped with a magnetic stir bar and charged with **1aa** (0.2 mmol), D_2O (10.0 equiv), or [D_7]-**1aa** (0.2 mmol), DMSO (2.0 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 4 h, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. The product was purified by preparative TLC on silica gel. ^{1}HNMR analysis showed that the H contents in the recovered **1aa** and the D contents in the recovered [D_7]-**1aa** were greater than 99%.

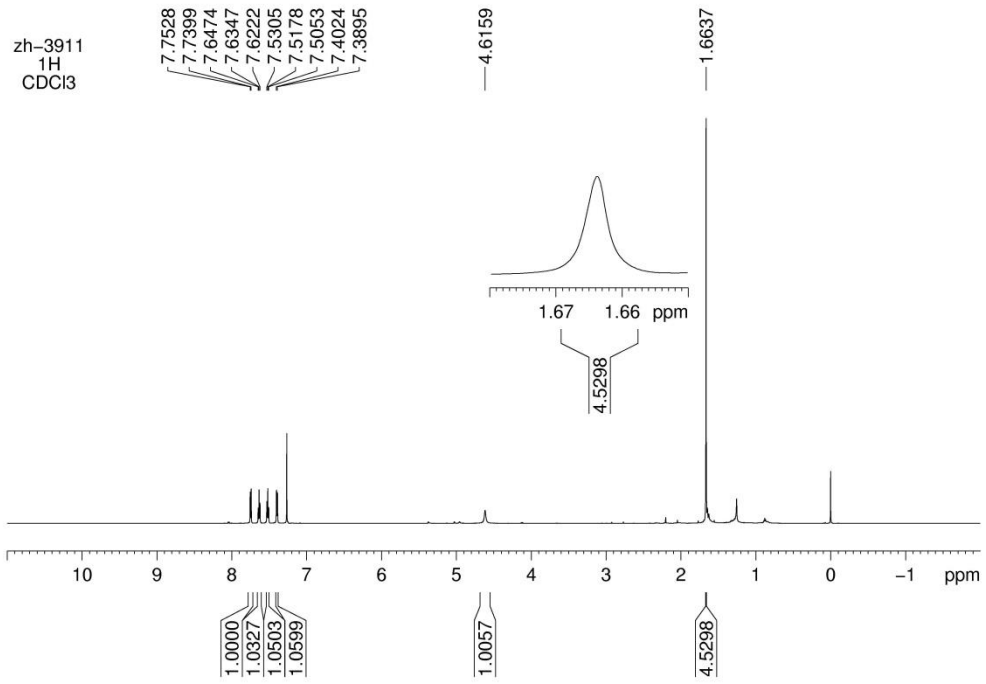
Kinetic isotope effect experiments

Competitive KIE experiment

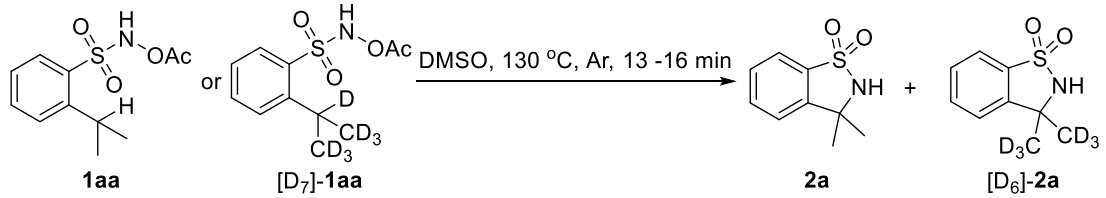


1aa [D7]-**1aa** **2a** [D6]-**2a**

A 15 mL oven-dried pressure tube was equipped with a magnetic stir bar and charged with *N*-acetoxy-2-isopropylbenzenesulfonamide **1aa** (0.1 mmol) and [D_7]-**1aa** (0.1 mmol), DMSO (2.0 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 4 h, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. The product was purified by preparative TLC on silica gel (petroleumether/ethyl acetate = 3/1), affording the target products of **2a** and [D_6]-**2a**. A mixture of **2a** and [D_6]-**2a** was determined on the basis of ^{1}H NMR analysis. Based on the integrations related to different hydrogen resonances, the kinetic isotope effect is calculated to be $k_H/k_D \approx 3.1$.



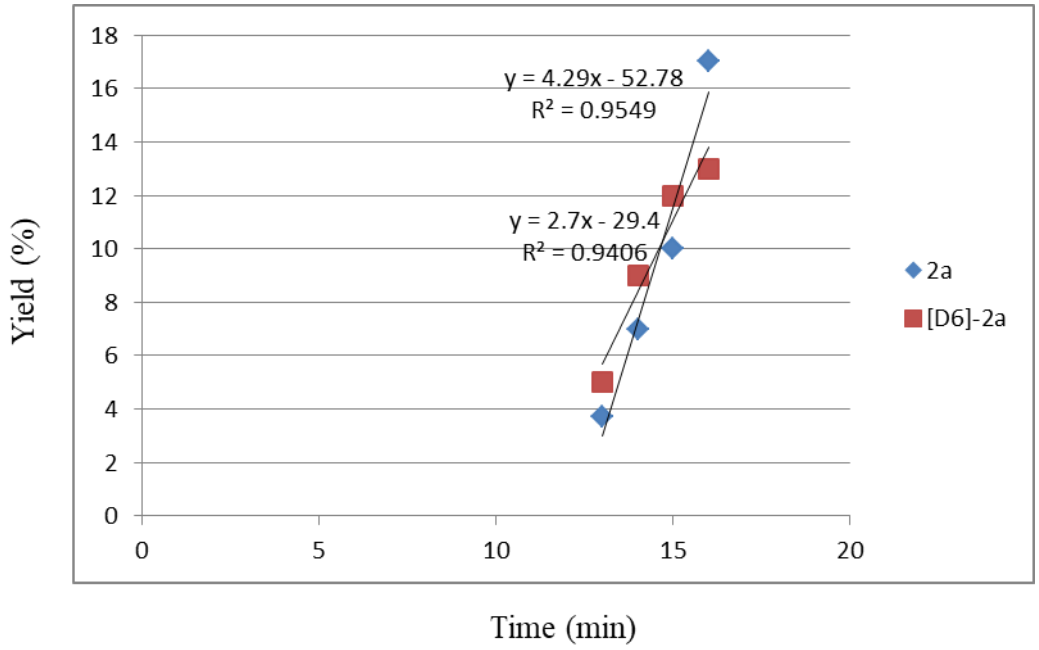
Parallel KIE experiments



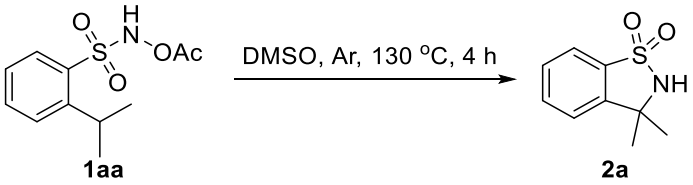
1aa [D7]-**1aa** **2a** [D6]-**2a**

A 15 mL oven-dried pressure tube was equipped with a magnetic stir bar and

charged with **1aa** (0.1 mmol) or [D_7]-**1aa** (0.1 mmol), DMSO (1.0 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 13-16 min, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. ^{1}H NMR was taken using Anisole (10.8 mg) as the internal standard. The KIE was determined as k_H/k_D = 4.29/2.7 ≈ 1.6.



Gram scale experiments.



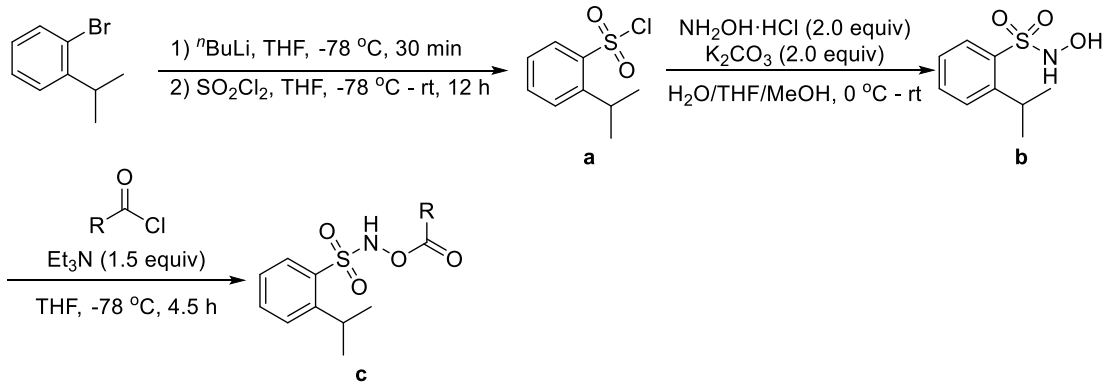
1aa
4 mmol, 1.028 g

2a
0.63 g, 80%

A 250 mL oven-dried pressure tube was equipped with a magnetic stir bar and charged with *N*-acetoxy-2-isopropylbenzenesulfonamide **1aa** (4 mmol), DMSO (40 mL) were added under the argon atmosphere, then, the reaction system was closed with a stopcock. The container was stirred at 130 °C for 4 h, and cooled down to room temperature. Next, the reaction mixture was diluted with H_2O. The resulting aqueous suspension was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. the residue was purified by column chromatography on silica gel using a mixture of PE/EA (50/1 to 10/1) as eluent to give the desired product **2a** (yellow solid, 0.63 g) in 80% yield.

4. General Procedure for Synthesis of substrates.

Route A:



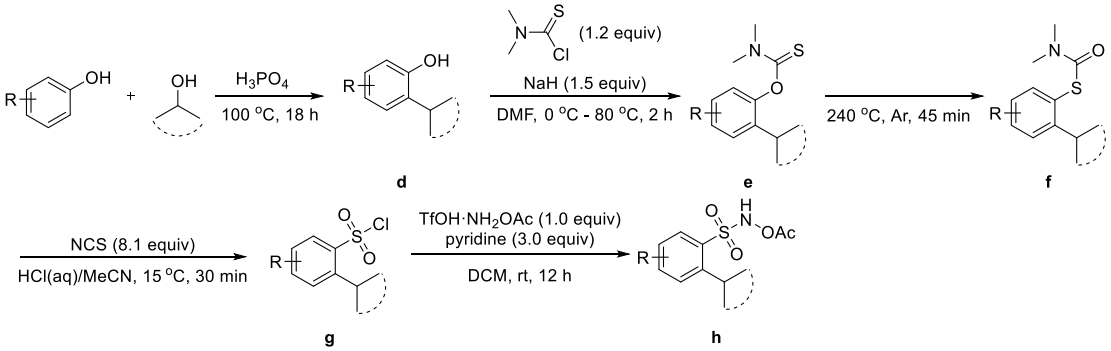
1) n-Butyllithium (1.1 equiv) was added dropwise to a stirred solution of the requisite 1-Bromo-2-(1-methylethyl)benzene (1.0 equiv) in THF (0.4 M) at -78 °C. The reaction was stirred at this temperature for the time specified, then sulfuryl chloride (1.5 equiv) was added dropwise, and the mixture was allowed to warm to room temperature and was stirred overnight. The reaction was quenched with H_2O, then the aqueous phase was separated and extracted three times with EA; the combined organic portions were dried (Na_2SO_4), filtered and concentrated in vacuum to give the crude product. Which was used for the next synthetic step without further purification.[7]

2) (10 mmol, 2.0 equiv) hydroxylamine hydrochloride was dissovled in 1 mL water at 0 °C. A solution of (10 mmol, 2.0 equiv) K_2CO_3 dissolved in 0.75 mL water was added to the hydroxylamine hydrochloride solution dropwise while maintaining the internal reaction temperature between 5 and 15 °C. After stirring the solution for 15 minutes, 5 mL tetrahydrofuran and 1.25 mL methanol were added; subsequently, 2.29 g (12 mmol, 1.0 equiv) 2 -isopropylbenzenesulfonyl chloride was added portion wise while maintaining the internal reaction temperature between 5 and 15 °C. Upon complete addition, the reaction was allowed to rise to room temperature. After stirring for 4 hours at room temperature, the organic solvents were removed under reduced pressure. The resulting aqueous suspension was extracted with EtOAc. The combined organic layers were dried over Na_2SO_4. The solvent of the mixture was then removed under reduced pressure to afford the N-hydroxy-2 -isopropylbenzenesulfonamide, which was used for the next synthetic step without further purification.[1]

2) The *N*-hydroxy-2 -isopropylbenzenesulfonamide (5 mmol, 1.0 equiv) was dissolved in 10 mL tetrahydrofuran at -78 °C. Then triethylamine(6 mmol, 1.2 equiv) was added dropwise. After stirring the mixture for 15 minutes at this temperature, Acyl Chloride (6 mmol, 1.2 equiv) was added dropwise. The reaction mixture was stirred for 4 hours at -78 °C. The reaction mixture was allowed to warm to room temperature; the white solid formed in the reaction was filtered. The filtrate was

evaporated and the residue was purified by column chromatography on silica gel using a mixture of PE/EA (50/1 to 10/1) as eluent to give the desired product **c**.[6]

Route B:



1) A mixture of Phenols (30 mmol, 1.0 equiv) and Alcohols (60mmol, 2.0 equiv) in H_3PO_4 (45 mL) was stirred at 100 °C overnight. After cooling to room temperature, the mixture was diluted with water and extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate and concentrated under vacuum. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (100/1 to 80/1) as eluent to give the desired product **d**.[2]

2) To a solution of **d** (10 mmol, 1.0 equiv) in DMF (20 mL) was added NaH (20 mmol, 2.0 equiv, 60% in mineral oil) and the mixture was stirred at 0 °C for 30 min. Then dimethylcarbamothioic chloride (15 mmol, 1.5 equiv) was added to the reaction. The mixture was heated to 80 °C and stirred at this temperature for 2 h. After cooling to room temperature, the mixture was diluted with water and extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under vacuum. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (100/1 to 10/1) as eluent to give the desired product **e**.[3]

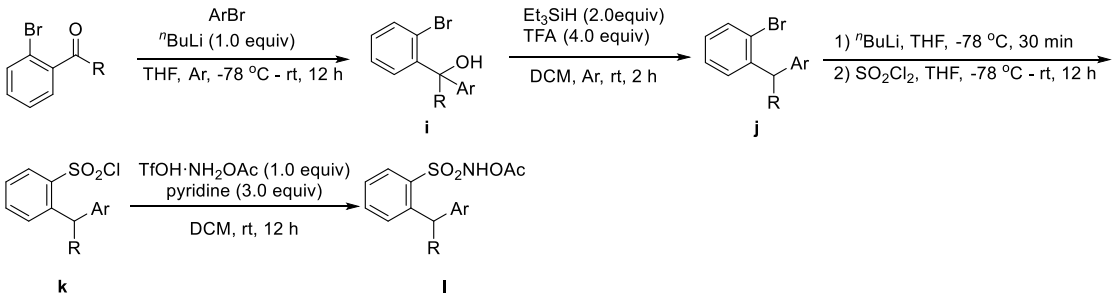
3) A 25 mL single-necked round bottom flask fitted with air condenser and argon balloon that containing the requisite substrate **e** was heated to 240 °C. The reaction was kept at 240 °C for 30 min and cooled down to room temperature. The resulting brown solid was dissolved in CH_2Cl_2 and the residue was purified by column chromatography on silica gel using a mixture of PE/EA (50/1 to 5/1) as eluent to give the desired product **f**.[4]

4) The **f** (5 mmol, 1.0 equiv) was partially dissolved in HCl(aq)/MeCN (1/5, 10 mL). After cooling to 0 °C, *N*-chlorosuccinimide (40.5 mmol, 8.1 equiv) was added in small portions, and the mixture became slightly green-yellow. The mixture was warmed to room temperature and kept at this temperature for 30 min. During the suspension became a solution and later a colorless solid separated. The mixture was extracted with EtOAc, and the organic phase was washed with brine. After evaporating the solvent the residue was purified by column chromatography (PE/EA = 100:1) to afford the desired product arenesulfonyl chlorides **g**.[5]

5) TfOH·NH_2OAc (1.05 mmol, 1.0 equiv) was dissolved in CH_2Cl_2 (5.0 mL) and

Pyridine (1.0 equiv) was added. Arenesulfonyl chlorides (1.05 mmol, 1.0 equiv) was added and the mixture was stirred at room temperature for 12 h. The mixture was quenched with HCl (1 mol/L), extracted with CH_2Cl_2 (10 mL x 3), dried over anhydrous sodium sulfate and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (50/1 to 10/1) to afford the desired sulfonamide **h**.[6]

Route C:



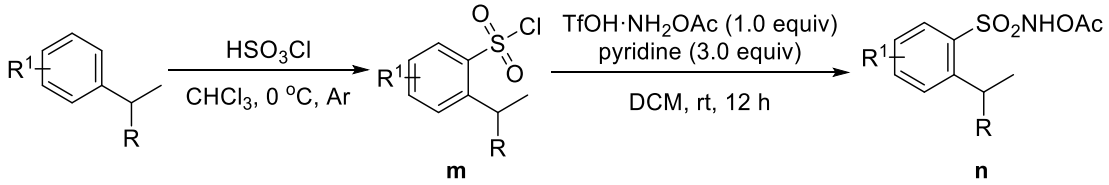
1) n-Butyllithium (0.98 – 1.0 equiv) was added dropwise to a stirred solution of the requisite aryl bromide (1.0 – 1.03 equiv) in THF (0.4 M) at -78 °C. The reaction was stirred at this temperature for 1 h, then the requisite starting materials (1.0 equiv) was added dropwise, and the mixture was allowed to warm to room temperature and was stirred for the time specified. The reaction was quenched with H_2O, then the aqueous phase was separated and extracted with EA, and the combined organic portions were dried over anhydrous sodium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (100/1 to 50/1) to afford the desired **i**.[7]

2) A Schlenk flask containing the requisite aryl alcohols (1.0 equiv) was evacuated and back-filled with Ar three times, then CH_2Cl_2 (0.3 M) was added. The solution was cooled to 0 °C, then TFA (4.0 equiv) was added dropwise. After 2 min, Et_3SiH (2.0 equiv) was added dropwise, and the reaction stirred at room temperature overnight. The mixture was quenched with saturated $NaHCO_3$ and extracted with EtOAc, and the organic phase was washed with brine. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (100/1 to 50/1) to afford the desired aryl bromide **j**.[7]

3) n-Butyllithium (1.1 equiv) was added dropwise to a stirred solution of the requisite aryl bromide (1.0 equiv) in THF (0.4 M) at -78 °C. The reaction was stirred at this temperature for the time specified, then sulfuryl chloride (1.5 equiv) was added dropwise, and the mixture was allowed to warm to room temperature and was stirred overnight. The reaction was quenched with H_2O, then the aqueous phase was separated and extracted three times with EA; the combined organic portions were dried over anhydrous sodium sulfate, filtered and concentrated in vacuum to give the crude product. Which was used for the next synthetic step without further purification.[7]

4) TfOH·NH_2OAc (1.0 equiv) was dissolved in CH_2Cl_2 (5.0 mL) and Pyridine (1.0 equiv) was added. Arenesulfonyl chlorides (1.0 equiv) was added and the mixture was stirred at room temperature for 12 h. The mixture was quenched with HCl (1 mol/L), extracted with CH_2Cl_2, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (50/1 to 10/1) to afford the desired sulfonamide **k**.[7]

Route D:



1) A round bottom flaskwas purged with Ar and charged with the substituted benzene and chloroform (2.0 ml/mmol sub. benzene). The resulting solution was cooled in an ice bath to 0 °C. Chlorosulfonic acid (4.5 equiv) was added to the flask via a syringe over 10 minutes and was stirred under Ar atmosphere until the reaction was complete. Upon reaction completion, the mixture was carefully poured over crushed ice and the aqueous layer was extracted with chloroform. The combined organic layers were then washed with brine, dried over anhydrous sodium sulfate, and concentrated by rotary evaporation to give the crude product **m**. The resulting oil was then purified by flash column chromatography (PE/EA = 100/1).[8]

2) TfOH·NH_2OAc (1.0 equiv) was dissolved in CH_2Cl_2 (5.0 mL) and Pyridine (1.0 equiv) was added. Arenesulfonyl chlorides (1.0 equiv) was added and the mixture was stirred at room temperature for 12 h. The mixture was quenched with HCl (1 mol/L), extracted with CH_2Cl_2, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using a mixture of PE/EA (50/1 to 10/1) to afford the desired sulfonamide **n**.[6]

Characterization Data

Characterization of substrates

***N*-acetoxy-2-isopropylbenzenesulfonamide (1aa):** Following Route A. white solid, mp 49-50 °C, R_f = 0.47 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.64 (t, J = 7.6 Hz, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 3.91 – 3.79 (m, 1H), 2.07 (s, 3H), 1.32 (d, J = 6.8 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 150.6, 134.8, 132.8, 131.2, 128.3, 126.0, 77.2, 77.0, 76.8, 29.9, 24.1, 18.2. HRMS (ESI) m/z calcd for $C_{11}H_{15}NO_4S+H^+$: 258.0800 $[M+H]^+$; found: 258.0797.

2-isopropyl-*N*-(pivaloyloxy)benzenesulfonamide (1ab): Following Route A. white solid, mp 50-52 °C, R_f = 0.51 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.02 (d, *J* = 7.9 Hz, 1H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.54 (d, *J* = 7.8 Hz ,1H), 7.33 (t, *J* = 7.5 Hz, 1H), 3.81 (m, 1H), 1.31 (d, *J* = 12.6 Hz, 6H), 1.10 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.9, 150.6, 134.7, 132.6, 131.6, 128.2, 125.9, 38.3, 30.1, 26.7, 24.1. HRMS (ESI) m/z calcd for $C_{14}H_{21}NO_4S+H^+$: 300.1264 $[M + H^+]$; found: 300.1260.

***N*-(((3s)-adamantane-1-carbonyl)oxy)-2-isopropylbenzenesulfonamide (1ac):** Following Route A. white solid, mp 83-85 °C, R_f = 0.43 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 3.88 – 3.73 (m, 1H), 1.95 (d, *J* = 19.7 Hz, 3H), 1.73 (s, 6H), 1.69 (d, *J* = 12.4 Hz, 3H), 1.62 (d, *J* = 12.2 Hz, 3H), 1.32 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.9, 150.59, 134.7, 132.6, 131.7, 128.2, 125.8, 40.3, 38.2, 36.1, 30.1, 27.5, 24.1. HRMS (ESI) m/z calcd for $C_{20}H_{27}NO_4S+H^+$: 378.1734 $[M + H^+]$; found: 378.1739.

***N*-(benzoyloxy)-2-isopropylbenzenesulfonamide (1ad):** Following Route A. white solid, mp 80-82 °C, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 2H), 7.61 (dd, *J* = 15.5, 7.7 Hz, 2H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 3.99 – 3.88 (m, 1H), 1.33 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.3, 150.7, 134.8, 134.5, 132.8, 131.3, 129.8, 128.7, 128.2, 126.1, 125.9, 29.9, 24.1. HRMS (ESI) m/z calcd for $C_{16}H_{17}NO_4S+H^+$: 320.0951 $[M + H^+]$; found: 320.0950.

***N*-acetoxy-2-(*sec*-butyl)benzenesulfonamide (1b):** Following Route B. yellow oil, R_f = 0.52 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 1H), 8.04 – 8.02 (m, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.53 Hz, 1H), 3.66 – 3.59 (m, 1H), 2.10 (s, 3H), 1.74 – 1.69 (m, 1H), 1.65-1.60 (m, 1H), 1.28 (d, *J* = 6.8 Hz, 3H), 0.89 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 149.8, 134.7, 133.4, 131.1, 128.5, 125.9, 36.5, 31.2, 21.8, 18.2, 12.1. HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_4S+Na^+$: 294.0770 $[M + Na^+]$; found: 294.0774.

***N*-acetoxy-2-isopropyl-4-methylbenzenesulfonamide (1c):** Following Route B.

colourless oil, R_f = 0.45 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.32 (s, 1H), 7.13 (d, *J* = 8.1 Hz, 1H), 3.84-3.80 (m, 1H), 2.42 (s, 3H), 2.06 (s, 3H), 1.31 (t, *J* = 11.3 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 150.5, 145.8, 131.4, 129.7, 128.9, 126.8, 29.7, 24.1, 21.7, 18.2. HRMS (ESI) m/z calcd for $C_{12}H_{17}NO_4S+H^+$: 272.0951 [M + H^+]; found: 272.0953.

***N*-acetoxy-4-ethyl-2-isopropylbenzenesulfonamide (1d):** Following Route B. colourless oil, R_f = 0.46 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.35 (s, 1H), 7.17 (d, *J* = 8.2 Hz, 1H), 3.92 – 3.76 (m, 1H), 2.72 (q, *J* = 7.6 Hz, 3H), 2.07 (s, 3H), 1.31 (d, *J* = 6.8 Hz, 6H), 1.27 (t, *J* = 7.7 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 151.9, 150.6, 131.5, 129.8, 127.7, 125.5, 29.8, 28.9, 24.1, 18.2, 14.9. HRMS (ESI) m/z calcd for $C_{13}H_{19}NO_4S+H^+$: 286.1108 [M + H^+]; found: 286.1111.

***N*-acetoxy-4-fluoro-2-isopropylbenzenesulfonamide (1e):** Following Route B. yellow oil, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.04 (dd, J = 8.7, 5.8 Hz, 1H), 7.21 (d, J = 10.1 Hz, 1H), 7.02 (t, J = 7.5 Hz, 1H), 3.85 (m, 1H), 2.09 (s, 3H), 1.30 (d, J = 6.8 Hz, 6H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -102.32. ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 166.6 ($^1J_{C-F}$ = 257.0 Hz), 154.6 ($^3J_{C-F}$ = 8.5 Hz), 134.2 ($^3J_{C-F}$ = 9.9 Hz), 128.7 ($^4J_{C-F}$ = 2.6 Hz), 115.5 ($^2J_{C-F}$ = 22.5 Hz), 113.4 ($^2J_{C-F}$ = 22.4 Hz), 30.2, 23.9, 18.2. HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_4S+H^+$:276.0701 [M + H^+]; found: 276.0705.

***N*-acetoxy-4-chloro-2-isopropylbenzenesulfonamide (1f):** Following Route B. colourless oil, R_f = 0.55 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.50 (s, 1H), 7.31 (d, *J* = 8.6 Hz, 1H), 3.89 – 3.78 (m, 1H), 2.10 (s, 3H), 1.30 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 152.6, 141.5, 132.7, 131.4, 128.7, 126.4, 30.1, 23.9, 18.2. HRMS (ESI) m/z calcd for $C_{11}H_{14}ClNO_4S+H^+$: 292.0405 [M + H^+]; found: 292.0408.

***N*-acetoxy-2,6-diisopropylbenzenesulfonamide (1g):** Following Route D. colourless oil, R_f = 0.42 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (s, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 2H), 4.10 – 3.97 (m, 2H), 2.00 (s, 3H), 1.19 (d, *J* = 7.3 Hz, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.1, 151.3, 132.8, 130.3, 125.0, 29.1, 23.7, 17.1. HRMS (ESI) m/z calcd for $C_{14}H_{21}NO_4S+Na^+$: 322.1083 [M + Na^+]; found: 322.1086.

***N*-acetoxy-2,4,6-triisopropylbenzenesulfonamide (1h):** Following Route D. colourless oil, R_f = 0.52 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (s, 2H), 4.16 – 4.05 (m, 2H), 2.95-2.90 (m, 1H), 2.13 (s, 3H), 1.28 (dd, *J* = 15.0, 7.0 Hz, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 154.7, 152.4, 128.6, 124.2, 34.3, 30.1, 24.9, 23.5, 18.3. HRMS (ESI) m/z calcd for $C_{17}H_{27}NO_4S+Na^+$: 364.1553 [M + Na^+]; found: 364.1557.

***N*-acetoxy-2,5-diisopropylbenzenesulfonamide (1i):** Following Route D. colourless oil, R_f = 0.46 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.49 (dd, *J* = 17.8, 8.1 Hz, 2H), 3.87 – 3.77 (m, 1H), 3.04 – 2.88 (m, 1H), 2.05 (s, 3H), 1.30 (d, *J* = 6.9 Hz, 6H), 1.26 (d, *J* = 7.1 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 147.7, 146.9, 133.0, 132.4, 128.9, 128.3, 33.6, 29.6, 24.1, 23.7, 18.1. HRMS (ESI) m/z calcd for $C_{14}H_{21}NO_4S+H^+$: 300.1264 [M + H^+]; found: 300.1269.

***N*-acetoxy-2-isopropyl-5-methylbenzenesulfonamide (1j):** Following Route D. colourless oil, R_f = 0.44 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.00 (s, 1H), 7.82 (s, 1H), 7.44 (s, 2H), 3.85-3.80 (m, 1H), 2.38 (s, 3H), 2.07 (s, 3H), 1.29 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 147.4, 136.1, 135.7, 132.4, 131.2, 128.2, 29.4, 24.1, 20.7, 18.2. HRMS (ESI) m/z calcd for $C_{12}H_{17}NO_4S+H^+$: 272.0951 [M + H^+]; found: 272.0953.

methyl 3-(*N*-acetoxysulfamoyl)-4-isopropylbenzoate (1k): Following Route D. white solid. mp 62-63 °C, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.67 (t, *J* = 4.2 Hz, 1H), 8.27 (d, *J* = 8.2, 1H), 7.64 (d, *J* = 8.2 Hz, 1H), 3.95 (s, 3H), 3.93-3.90 (m, 1H) 2.11 (s, 3H), 1.33 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 165.3, 155.6, 135.4, 132.4, 128.7, 128.4, 52.5, 30.2, 23.9, 18.2. HRMS (ESI) m/z calcd for $C_{13}H_{17}NO_6S+H^+$: 316.0850 [M + H^+]; found: 316.0854.

***N*-acetoxy-2-cyclopentyl-4-methylbenzenesulfonamide (1l):** Following Route B. colourless oil, R_f = 0.48 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.31 (s, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 3.87 – 3.79 (m, 1H), 2.41 (s, 3H), 2.20 (m, 2H), 1.86 (m, 2H), 1.80 – 1.69 (m, 2H), 1.59 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 148.9, 145.7, 131.3, 130.5, 129.5, 126.7, 41.4, 36.0, 26.2, 21.6, 18.2. HRMS (ESI) m/z calcd for $C_{14}H_{19}NO_4S+Na^+$: 320.0927 [M + Na^+]; found: 320.0929.

***N*-acetoxy-2-cyclohexyl-4-methylbenzenesulfonamide (1m):** Following Route B. colourless oil, R_f = 0.52 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.31 (s, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 3.42-3.39 (m, 1H), 2.42 (s, 3H), 2.08 (s, 3H), 1.91 (d, *J* = 9.9 Hz, 2H), 1.85 (d, *J* = 11.7 Hz, 2H), 1.79 (d, *J* = 13.2 Hz, 1H), 1.49 – 1.38 (m, 4H), 1.35 – 1.20 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 149.3, 145.6, 131.5, 129.9, 129.6, 126.7, 40.5, 34.4, 26.8, 26.1, 21.7, 18.2. HRMS (ESI) m/z calcd for $C_{15}H_{21}NO_4S+Na^+$: 334.1083 [M + Na^+]; found: 334.1085.

***N*-acetoxy-2-cycloheptyl-4-methylbenzenesulfonamide (1n):** Following Route B. light yellow oil, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 – 7.86 (m, 1H), 7.25 (s, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 3.56 – 3.43 (m, 1H), 2.40 (s, 3H), 2.05 (s, 3H), 1.94 – 1.92 (m, 2H), 1.80 – 1.79 (m, 2H), 1.72 – 1.71 (m, 2H), 1.64 – 1.59 (m, 6 H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.7, 151.3, 145.3, 131.0, 129.7, 126.6, 126.4, 41.7, 36.8, 27.7, 27.5, 21.7, 18.4. HRMS (ESI) m/z calcd for $C_{16}H_{23}NO_4S+Na^+$: 348.1240 [M + Na^+]; found: 348.1244.

***N*-acetoxy-2-cyclohexylbenzenesulfonamide (1o):** Following Route B. colourless oil, R_f = 0.47 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 3.51 – 3.38 (m, 1H), 2.08 (s, 3H), 1.93 (d, *J* = 9.5 Hz, 2H), 1.85 (t, *J* = 11.7 Hz, 2H), 1.80 (d, *J* = 13.2 Hz, 1H), 1.51 – 1.38 (m, 4H), 1.35 – 1.22 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 149.4, 134.6, 132.9, 131.3, 128.9, 125.9, 40.6, 34.4, 26.8, 26.1, 18.2. HRMS (ESI) m/z calcd for $C_{14}H_{19}NO_4S$ +Na^+: 320.0927 [M + Na^+]; found: 320.0925.

***N*-acetoxy-2-cyclohexyl-4-ethylbenzenesulfonamide (1p)** Following Route B. colourless oil, R_f = 0.47 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H),

7.92 (d, *J* = 8.2 Hz, 1H), 7.32 (s, 1H), 7.15 (d, *J* = 8.2 Hz, 1H), 3.43 (t, *J* = 9.3 Hz, 1H), 2.71 (q, *J* = 7.6 Hz, 2H), 2.08 (s, 3H), 1.92 (d, *J* = 8.5 Hz, 2H), 1.85 (d, *J* = 9.7 Hz, 2H), 1.79 (d, *J* = 12.9 Hz, 1H), 1.48-1.40 (m, 4H), 1.31-1.30 (m, 1H) 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 151.6, 149.3, 131.5, 130.1, 128.5, 125.5, 40.5, 34.4, 28.9, 26.8, 26.1, 18.2, 14.9. HRMS (ESI) m/z calcd for $C_{16}H_{23}NO_4S+H^+$: 326.1421 [M + H^+]; found: 326.1425.

***N*-acetoxy-2-cyclohexyl-4-fluorobenzenesulfonamide (1q)** Following Route B. colourless oil, R_f = 0.52 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.05 (dd, *J* = 8.7, 5.8 Hz, 1H), 7.19 (t, *J* = 15.0 Hz, 1H), 7.02 (dd, *J* = 11.8, 4.4 Hz, 1H), 3.45 (t, *J* = 11.3 Hz, 1H), 2.10 (s, 3H), 1.97 – 1.74 (m, 6H), 1.51 – 1.23 (m, 6H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -102.56. ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 166.5 ($^1J_{C-F}$ = 256.8 Hz), 153.3 ($^2J_{C-F}$ = 8.6 Hz), 134.2 ($^3J_{C-F}$ = 9.9 Hz), 128.9 ($^4J_{C-F}$ = 2.7 Hz), 116.2 ($^2J_{C-F}$ = 22.6 Hz), 113.3 ($^2J_{C-F}$ = 22.3 Hz), 40.8, 34.3, 26.6, 25.9, 18.2. HRMS (ESI) m/z calcd for $C_{14}H_{18}FNO_4S+H^+$: 316.1014 [M + H^+]; found: 316.1017.

***N*-acetoxy-2,5-dicyclohexylbenzenesulfonamide (1r)** Following Route D. yellow oil, R_f = 0.54 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.44 (q, *J* = 8.2 Hz, 2H), 3.40 (t, *J* = 9.6 Hz, 1H), 2.55 (t, *J* = 9.8 Hz, 1H), 2.05 (s, 3H), 1.92-1.82 (m, 8H), 1.76 (t, *J* = 12.7 Hz, 2H), 1.45 – 1.38 (m, 8H), 1.28 – 1.23 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 146.5, 146.0, 133.2, 132.5, 129.4, 128.9, 43.8, 40.3, 34.4, 34.2, 26.8, 26.7, 26.1, 25.9, 18.1. HRMS (ESI) m/z calcd for $C_{20}H_{29}NO_4S+Na^+$: 402.1709 [M + Na^+]; found: 402.1709.

***N*-acetoxy-2-benzhydrylbenzenesulfonamide (1s)** Following Route C. colourless oil, R_f = 0.57 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, J = 8.0 Hz, 1H), 7.78 (s, 1H), 7.57 (t, J = 7.5 Hz, 1H), 7.41 (dd, J = 16.4, 9.1 Hz, 1H), 7.30 (t, J = 7.5 Hz, 4H), 7.25 (d, J = 7.1 Hz, 3H), 7.10 (d, J = 7.5 Hz, 4H), 6.74 (s, 1H), 1.98 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.4, 144.2, 142.3, 134.2, 133.0, 132.0, 129.6, 128.8, 128.6, 127.7, 126.9, 51.1, 18.2. HRMS (ESI) m/z calcd for $C_{21}H_{19}NO_4S+H^+$: 382.1108 [M + H^+]; found: 382.1109.

***N*-acetoxy-2-(phenyl(*p*-tolyl)methyl)benzenesulfonamide (1t)** Following Route C. colourless oil, R_f = 0.61 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.68 (s, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.24 (dd, *J* = 9.0, 4.9 Hz, 1H), 7.14 – 7.07 (m, 4H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.70 (s, 1H), 2.33 (s, 3H), 2.00 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.3, 144.4, 142.5, 139.2, 136.7, 134.2, 133.9, 132.9, 132.1, 129.6, 129.5, 129.4, 128.6, 126.9, 126.8, 50.8, 21.0, 18.3. HRMS (ESI) m/z calcd for $C_{22}H_{21}NO_4S$ +Na^+: 418.1083 [M + Na^+]; found: 418.1085.

***N*-acetoxy-2-(phenyl(4-(trifluoromethyl)phenyl)methyl)benzenesulfonamide (1u):** Following Route C. colourless oil, R_f = 0.61 (PE/EA = 5/1). 1H NMR (600 MHz, CDCl3) δ 8.26 (s, 1H), 8.13 (d, J = 8.0 Hz, 1H), 7.64 – 7.60 (m, 1H), 7.55 (d, J = 8.2 Hz, 2H), 7.46 (t, J = 7.7 Hz, 1H), 7.32 (t, J = 7.4 Hz, 2H), 7.28 (d, J = 7.2 Hz, 1H), 7.24 (d, J = 7.9 Hz, 1H), 7.21 (d, J = 8.1 Hz, 2H), 7.09 (d, J = 7.5 Hz, 2H), 6.77 (s, 1H), 2.04 (s, 3H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.46. 13C NMR (151 MHz, CDCl3) δ 168.7, 146.8, 143.4, 141.7, 134.4, 133.1, 132.0, 129.9, 129.5, 128.9 ($^2J_{C-F}$ = 32.1 Hz), 128.8, 127.3, 127.2, 125.5 ($^4J_{C-F}$ = 3.3 Hz), 123.3 ($^1J_{C-F}$ = 273.2 Hz), 50.9,

18.2. HRMS (ESI) m/z calcd for $C_{22}H_{18}F_3NO_4S+H^+$: 450.0982 [M + H^+]; found: 450.0979.

***N*-acetoxy-2-((4-fluorophenyl)(phenyl)methyl)benzenesulfonamide (1v):** Following Route C. colourless oil, R_f = 0.60 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.0 Hz, 1H), 8.04 (s, 1H), 7.60 (t, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.7, 1H), 7.31 (t, *J* = 7.3 Hz, 2H), 7.26-7.23 (m, 2H), 7.10 – 7.03 (m, 5H), 6.99 (t, *J* = 8.4 Hz, 2H), 6.71 (s, 1H), 2.02 (s, 3H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -115.76. ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.6, 161.7 ($^1J_{C\text{-}F}$ = 246.0 Hz), 144.1, 142.3, 138.2 ($^4J_{C\text{-}F}$ = 3.2 Hz), 134.3, 134.1, 132.9, 131.9, 131.1 ($^3J_{C\text{-}F}$ = 8.0 Hz), 129.5, 128.7, 127.1, 115.4 ($^2J_{C\text{-}F}$ = 21.3 Hz), 50.4, 18.2. HRMS (ESI) m/z calcd for $C_{21}H_{18}FNO_4S+Na^+$: 422.0833 [M + Na^+]; found: 422.0832.

***N*-acetoxy-2-((4-chlorophenyl)(phenyl)methyl)benzenesulfonamide (1w):** Following Route C. colourless oil, R_f = 0.58 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, J = 8.6 Hz, 2H), 7.60 (t, J = 7.6 Hz, 1H), 7.44 (t, J = 7.7 Hz, 1H), 7.31 (t, J = 7.5 Hz, 2H), 7.26 (d, J = 7.7 Hz, 2H), 7.24 (d, J = 7.9 Hz, 1H), 7.08 (d, J = 7.6 Hz, 2H), 7.02 (d, J = 8.1 Hz, 2H), 6.69 (s, 1H), 2.03 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.6, 143.8, 142.0, 141.1, 134.3, 134.1, 132.9, 132.7, 131.9, 130.8, 129.5, 128.7, 128.6, 127.1, 127.1, 50.6, 18.2. HRMS (ESI) m/z calcd for $C_{21}H_{18}ClNO_4S+Na^+$: 438.0537 [M + Na^+]; found: 438.0540.

***N*-acetoxy-2-(1-phenylethyl)benzenesulfonamide (1x):** Following Route C. colourless oil, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.06 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.38 – 7.29 (m, 6H), 7.22 (t, *J* = 6.8 Hz, 1H), 5.28 (q, *J* = 7.0 Hz, 1H), 2.12 (s, 3H), 1.69 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 148.3, 144.5, 134.7, 133.2, 131.2, 130.8, 128.5, 127.8, 126.5, 126.3, 39.3, 22.0, 18.3. HRMS (ESI) m/z calcd for $C_{16}H_{17}NO_4S+Na^+$: 342.0770 [M + Na^+]; found: 342.0774.

***N*-acetoxy-2-(1-(p-tolyl)ethyl)benzenesulfonamide (1y):** Following Route C. colourless oil, R_f = 0.51 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61 (s, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 5.22 (q, *J* = 6.9 Hz, 1H), 2.31 (s, 3H), 2.11 (s, 3H), 1.67 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.1, 148.5, 141.5, 136.1, 134.7, 133.2, 131.2, 130.7, 129.2, 127.7, 126.3, 38.9, 22.1, 20.9, 18.3. HRMS (ESI) m/z calcd for $C_{17}H_{19}NO_4S+H^+$: 334.1108 [M + H^+]; found: 334.1109.

***N*-acetoxy-2-(1-(4-(trifluoromethyl)phenyl)ethyl)benzenesulfonamide (1z):** Following Route C. colourless oil, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.55 (s, 2H), 8.07 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 8.2 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 7.38 (t, J = 7.7 Hz, 1H), 5.32 (dd, J = 13.7, 6.7 Hz, 1H), 2.15 (s, 3H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.46. ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.4, 134.9, 133.5, 131.6, 131.2, 128.2, 126.7, 125.3 ($^4J_{C\text{-}F}$ = 3.3 Hz), 51.4, 24.7, 18.3. HRMS (ESI) m/z calcd for $C_{17}H_{16}F_3NO_4S+Na^+$: 410.0644 [M + Na^+]; found: 410.0647

***N*-acetoxy-2-(1-(4-fluorophenyl)ethyl)benzenesulfonamide (1ba):** Following Route C. colourless oil, R_f = 0.53 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.82 (s 1H), 8.05 (d, J = 8.0 Hz, 1H), 7.57 (t, J = 7.8 Hz, 1H), 7.36 (t, J = 7.4 Hz, 1H), 7.30 – 7.28

(m, 3H), 5.23 (q, J = 7.1 Hz, 1H), 2.14 (s, 3H), 1.66 (d, J = 7.0 Hz, 3H). ^{19}F NMR (565 MHz, CDCl3) δ -116.57. ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 134.8, 133.3, 131.4, 130.6, 129.5, 129.4, 126.5, 115.1 ($^2J_{C-F}$ = 29.1 Hz), 51.3, 24.9, 18.3.
HRMS (ESI) m/z calcd for $C_{16}H_{16}FNO_4S$+Na^+: 360.0676 [M + Na^+]; found: 360.0675.

***N*-acetoxy-2-(1-(4-chlorophenyl)ethyl)benzenesulfonamide (1bb):** Following Route C. colourless oil, R_f = 0.54 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.05 (d, J = 8.0 Hz, 1H), 7.57 (t, J = 7.6 Hz, 1H), 7.36 (dd, J = 15.0, 7.7 Hz, 1H), 7.32 – 7.26 (m, 5H), 5.23 (q, J = 7.0 Hz, 1H), 2.15 (s, 3H), 1.66 (d, J = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 148.0, 143.0, 134.8, 132.3, 131.2, 130.8, 129.2, 128.6, 128.1, 126.5, 38.8, 21.9, 18.3. HRMS (ESI) m/z calcd for +Na^+: 376.0381 [M + Na^+]; found: 376.0382.

***N*-acetoxy-2-benzylbenzenesulfonamide (1bc):** Following Route C. colourless oil, R_f = 0.48 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.28 – 7.21 (m, 5H), 4.48 (s, 2H), 2.04 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.9, 142.0, 138.9, 134.6, 133.5, 132.6, 131.7, 129.5, 128.8, 126.8, 126.7, 38.4, 18.2. HRMS (ESI) m/z calcd for +Na^+: 328.0614 [M + Na^+]; found: 328.0619.

***N*-acetoxy-2-phenethylbenzenesulfonamide (1bd):** Following Route C. colourless oil, R_f = 0.43 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 2H), 7.26 (d, *J* = 7.9 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 3.37 – 3.27 (m, 2H), 3.03 – 2.94 (m, 2H), 2.03 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 143.1, 141.2, 134.5, 133.5, 132.3, 131.6, 128.6, 128.5, 126.6, 126.2, 38.0, 35.9, 18.1. HRMS (ESI) m/z calcd for $C_{16}H_{17}NO_4S$+H^+: 320.0951 [M + H^+]; found: 320.0951.

***N*-acetoxy-2,4,6-triethylbenzenesulfonamide (1be):** Following Route D. colourless oil, R_f = 0.48 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.06 (s, 2H), 3.08 (q, *J* = 7.4 Hz, 4H), 2.71-2.57 (m, 2H), 2.05 (s, 3H), 1.30 (t, *J* = 7.5 Hz, 6H), 1.25 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 150.6, 147.6, 129.7, 28.7, 28.5, 18.1, 16.9, 14.8. HRMS (ESI) m/z calcd for $C_{14}H_{21}NO_4S$+Na^+: 322.1083 [M + Na^+]; found: 322.1087.

***N*-hydroxy-2,4,6-triisopropylbenzenesulfonamide (3):** White solid, mp 110-112 °C, R_f = 0.2 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.21 (s, 2H), 4.11 (dq, J = 13.5, 6.6 Hz, 2H), 2.91 (dq, J = 13.5, 6.8 Hz, 1H), 1.29 (d, J = 6.8 Hz, 12H), 1.26 (d, J = 6.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.2, 152.0, 145.8, 124.1, 34.3, 30.0, 24.9, 23.5. HRMS (ESI) m/z calcd for $C_{15}H_{25}NO_3S$+H^+: 300.1628 [M + H^+]; found: 300.1630.

***N*-(dimethyl-λ^4-sulfanylidene)-2,4,6-triisopropylbenzenesulfonamide(4):** White solid, mp 80-82 °C, R_f = 0.2 (EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.10 (s, 2H), 4.43 (hept, *J* = 6.7 Hz, 2H), 2.91 – 2.82 (m, 1H), 2.70 (s, 6H), 1.25 (dd, *J* = 9.7, 6.9 Hz, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.1, 149.0, 137.2, 123.2, 36.3, 34.1, 29.4, 24.9, 23.7. HRMS (ESI) m/z calcd for $C_{17}H_{29}NO_2S_2$+H^+: 344.1713 [M + H^+]; found: 344.1716

***N*-acetoxy-2-(1-cyclopropylethyl)benzenesulfonamide (5):** Following Route B

(ArOH is prepared according to literature 14). colourless oil, R_f = 0.48 (PE/EA = 5/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.00 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.67 (dtd, *J* = 8.9, 7.9, 1.3 Hz, 1H), 7.35 (ddd, *J* = 8.4, 7.1, 1.6 Hz, 1H), 3.07 (dq, *J* = 13.8, 6.9 Hz, 1H), 2.11 (s, 1H), 1.34 (d, *J* = 6.9 Hz, 1H), 1.11-1.03 (m, 1H), 0.65-0.55 (m, 1H), 0.37-0.27 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.3, 149.9, 134.7, 132.9, 130.9, 129.4, 126.0, 39.5, 22.4, 18.2, 18.1, 5.2, 3.6. HRMS (ESI) m/z calcd for $C_{13}H_{17}NO_4S+Na^+$: 306.0776 [M + Na^+]; found: 306.0778.

Characterization of products

3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2a): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.3; yellow solid (35.1mg, 89%), mp 113-115 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 4.79 (s, 1H), 1.65 (s, 7H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.1, 135.2, 133.4, 129.1, 122.8, 121.2, 60.9, 29.7. HRMS (ESI) m/z calcd for $C_9H_{11}NO_2S+H^+$: 198.0583 [M + H^+]; found: 198.0587.

2-(prop-1-en-2-yl)benzenesulfonamide (2a'): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.41 (q, *J* = 8.3 Hz, 1H), 7.25 (s, 1H), 5.38 (s, 1H), 5.03 (s, 1H), 4.90 (s, 2H), 2.21 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.6, 142.5, 139.6, 132.5, 130.1, 129.1, 127.7, 127.4, 116.2, 25.6. HRMS (ESI) m/z calcd for $C_9H_{11}NO_2S+H^+$: 198.0583 [M + H^+]; found: 198.0587.

3-ethyl-3-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2b): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.4; white solid (34.2 mg, 81%), mp 117-119 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 1H), 4.67 (s, 1H), 1.97-1.87 (m, 2H), 1.62 (s, 3H), 0.87 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.6, 135.5, 133.3, 129.2, 123.0, 121.3, 64.4, 34.7, 27.9, 8.5. HRMS (ESI) m/z calcd for $C_{10}H_{13}NO_2S+H^+$: 212.0740 [M + H^+]; found: 212.0744.

3,3,5-trimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2c): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.4; white solid (34.2 mg, 81%), mp 113-114 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.16 (s, 1H), 4.64 (s, 1H), 2.46 (s, 3H), 1.63 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.4, 144.3, 132.5, 130.0, 123.0, 120.9, 60.7, 29.7, 21.8. HRMS (ESI) m/z calcd for $C_{10}H_{13}NO_2S+H^+$: 212.0740 [M + H^+]; found: 212.0744.

5-ethyl-3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2d): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.3; white solid (33.8 mg, 72%), mp 105-107 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.16 (s, 1H), 4.68 (s, 1H), 2.75 (q, *J* = 7.6 Hz, 2H), 1.64 (s, 6H), 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.6, 146.5, 132.7, 128.9, 121.8, 121.0, 60.7, 29.7, 29.1, 15.3. HRMS (ESI) m/z

calcd for $C_{11}H_{15}NO_2S+H^+$: 226.0896 [M + H^+]; found: 226.0899.

5-fluoro-3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2e): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.3; white solid (27.1 mg, 63%), mp 131-132 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 8.3, 4.7 Hz, 1H), 7.20 (t, *J* = 8.3 Hz, 1H), 7.05 (d, *J* = 8.1 Hz, 1H), 4.72 (s, 1H), 1.65 (s, 6H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -104.11. ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.8 ($^1J_{C-F}$ = 255.1 Hz), 149.4, 131.4, 123.6 ($^3J_{C-F}$ = 9.9 Hz), 117.1 ($^2J_{C-F}$ = 24.2 Hz), 110.0 ($^2J_{C-F}$ = 23.8 Hz), 60.5 ($^4J_{C-F}$ = 2.1 Hz), 29.5. HRMS (ESI) m/z calcd for $C_9H_{10}FNO_2S+H^+$: 216.0489 [M + H^+]; found: 216.0492.

5-chloro-3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2f): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.35; white solid (35.3 mg, 76%), white solid. mp 125-127 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2, , 1H), 7.48 (d, *J* = 8.2, 1H), 7.36 (s, 1H), 4.62 (s, 1H), 1.65 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.2, 139.8, 133.9, 129.6, 123.3, 122.5, 60.6, 29.5. HRMS (ESI) m/z calcd for $C_9H_{10}ClNO_2S+H^+$: 232.0194 [M + H^+]; found: 232.0190.

7-isopropyl-3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2g): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.4; white solid (40.2 mg, 84%), mp 120-122 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (t, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 7.7 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 1.64 (s, 6H), 1.35 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.3, 145.6, 133.7, 133.2, 125.9, 120.1, 59.7, 29.84 (s), 29.4, 23.6. HRMS (ESI) m/z calcd for $C_{12}H_{17}NO_2S$ +H^+: 240.1053 [M + H^+]; found: 240.1054.

5,7-diisopropyl-3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2h): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (48.9 mg, 87%),white solid, mp 121-122 °C, R_f = 0.5 (PE/EA = 3:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (s, 1H), 6.98 (s, 1H), 4.48 (s, 1H), 3.65 – 3.55 (m, 1H), 3.05 – 2.90 (m, 1H), 1.63 (s, 6H), 1.35 (d, *J* = 6.8 Hz, 6H), 1.27 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.5, 146.7, 145.3, 130.9, 124.3, 117.7, 59.7, 34.6, 29.9, 29.4, 23.8, 23.6. HRMS (ESI) m/z calcd for $C_{15}H_{23}NO_2S+H^+$: 282.1522 [M + H^+]; found: 282.1523.

6-isopropyl-3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2i): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.45; white solid (36.8 mg, 77%), mp 123-125 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 4.68 (s, 1H), 3.05 – 2.97 (m, 1H), 1.63 (s, 6H), 1.27 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.6, 143.6, 135.2, 132.2), 122.6, 118.5, 60.6, 33.9, 29.7, 23.7. HRMS (ESI) m/z calcd for $C_{12}H_{17}NO_2S+H^+$: 240.1053 [M + H^+]; found: 240.1054.

3,3,6-trimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2j): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.4; white solid (36.3 mg, 86%), mp 98-100 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.26 (d, *J* = 7.6 Hz, 1H), 4.53 (s, 1H), 2.44 (s, 3H), 1.63 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3, 139.6, 135.3, 134.4, 122.5, 121.1, 60.7, 29.8, 21.2. HRMS (ESI) m/z calcd for $C_{10}H_{13}NO_2S$ +H^+: 212.0740 [M + H^+]; found:

212.0740.

methyl 3,3-dimethyl-2,3-dihydrobenzo[*d*]isothiazole-6-carboxylate 1,1-dioxide (2k): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (37.7 mg, 74%), mp 108-110 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.27 (d, *J* = 8.1 Hz, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 5.02 (d, *J* = 15.8 Hz, 1H), 3.95 (s, 3H), 1.67 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.1, 150.5, 135.9, 134.5, 131.5, 123.1, 122.9, 60.9, 52.7, 29.4. HRMS (ESI) m/z calcd for $C_{11}H_{13}NO_4S+H^+$: 256.0638 [M + H^+]; found: 256.0641.

5-methyl-2*H*-spiro[benzo[*d*]isothiazole-3,1'-cyclopentane] 1,1-dioxide (2l): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.4; white solid (27 mg, 57%) white solid. mp 93-95 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, J = 7.9 Hz, 1H), 7.29 (d, J = 7.9 Hz, 1H), 7.15 (s, 1H), 4.45 (s, 1H), 2.46 (s, 3H), 2.12-2.04 (m, 4H), 1.99-1.94 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.4, 144.2, 133.8, 129.9, 123.1, 120.8, 709, 53.4, 41.7, 24.6, 21.8. HRMS (ESI) m/z calcd for $C_{12}H_{15}NO_2S+Na^+$: 260.0715 [M + Na^+]; found: 260.0718.

5-methyl-2*H*-spiro[benzo[*d*]isothiazole-3,1'-cyclohexane] 1,1-dioxide (2m): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (41.2 mg, 82%), mp 95-97 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 1H), 7.16 (s, 1H), 4.58 (s, 1H), 2.46 (s, 3H), 1.79-1.88 (m, 7H), 1.57-1.64 (m, 2H), 1.36-1.26 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.5, 144.1, 132.8, 130.2, 123.4, 121.1, 63.6, 37.7, 24.8, 22.6, 21.9. HRMS (ESI) m/z calcd for $C_{13}H_{17}NO_2S+H^+$: 252.1053 [M + H^+]; found: 252.1051.

5-methyl-2*H*-spiro[benzo[*d*]isothiazole-3,1'-cycloheptane] 1,1-dioxide (2n): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.6; white solid (42.9 mg, 81%), mp 105-106 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 1H), 7.45 – 7.28 (m, 1H), 7.23 – 7.18 (m, 1H), 4.5 (s, 1H), 2.46 (s, 3H), 2.14 – 1.53 (m, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.1, 144.3, 132.8, 130.0, 123.2, 120.9, 66.6, 41.7, 28.5, 23.3, 21.9. HRMS (ESI) m/z calcd for $C_{14}H_{19}NO_2S+H^+$: 266.1209 [M + H^+]; found: 266.1207.

2*H*-spiro[benzo[*d*]isothiazole-3,1'-cyclohexane] 1,1-dioxide (2o): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (34.6 mg, 73%), mp 112-114 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 1.89-1.84 (m, 3H), 1.83-1.79 (m, 4H), 1.66-1.59(m, 2H), 1.37-1.33 (m, 1H).^{13}C NMR (151 MHz, $CDCl_3$) δ 146.2, 135.5, 133.2, 129.2, 123.1, 121.3, 63.8, 37.7, 24.8, 22.5. HRMS (ESI) m/z calcd for $C_{12}H_{15}NO_2S+H^+$: 238.0896 [M + H^+]; found: 238.0902.

5-ethyl-2*H*-spiro[benzo[*d*]isothiazole-3,1'-cyclohexane] 1,1-dioxide (2p): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.6; white solid (39.8 mg, 75%), mp 132-134 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.17 (s, 1H), 4.69 (s, 1H), 2.74 (q, *J* = 7.6 Hz, 2H), 1.89-1.79 (m, 8H), 1.67 – 1.55 (m, 2H), 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.4, 146.6, 132.9, 129.2, 122.2, 121.2, 63.7, 37.8, 29.2, 24.8, 22.6, 15.4. HRMS (ESI) m/z calcd for $C_{14}H_{19}NO_2S+H^+$: 266.1209 [M + H^+];

found: 266.1211.

5-fluoro-2*H*-spiro[benzo[*d*]isothiazole-3,1'-cyclohexane] 1,1-dioxide (2q): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.55; white solid (35.7 mg, 70%), mp 130-131 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 8.4, 4.8 Hz, 1H), 7.20 (t, *J* = 8.4 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 4.69 (s, 1H), 1.91 (d, *J* = 13.0 Hz, 2H), 1.84-1.80 (m, 4H), 1.78-1.75 (m, 1H), 1.63 – 1.56 (m, 2H), 1.38 – 1.33 (m, 1H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -104.42. ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.7 ($^1J_{C\text{-}F}$ = 254.6 Hz), 149.5 ($^3J_{C\text{-}F}$ = 8.4 Hz), 131.6, 123.7 ($^3J_{C\text{-}F}$ = 10.0 Hz), 117.2 ($^2J_{C\text{-}F}$ = 24.1 Hz), 110.3 ($^2J_{C\text{-}F}$ = 23.9 Hz), 63.4, 37.6, 24.7, 22.4. HRMS (ESI) m/z calcd for $C_{12}H_{14}FNO_2S+H^+$: 256.0802 [M + H^+]; found: 256.0803.

6-cyclohexyl-2*H*-spiro[benzo[*d*]isothiazole-3,1'-cyclohexane] 1,1-dioxide (2r): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (36.4 mg, 57%), mp 145-147 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 4.54 (s, 1H), 2.61 (d, *J* = 8.2 Hz, 1H), 1.90 – 1.75 (m, 12H), 1.61 – 1.55 (m, 2H), 1.43-1.33 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.9, 143.6, 135.4, 132.4, 122.8, 119.1, 63.5, 44.3, 37.8, 34.3, 26.7, 25.9, 24.8, 22.6. HRMS (ESI) m/z calcd for $C_{18}H_{25}NO_2S+H^+$: 320.1679 [M + H^+]; found: 320.1683.

3,3-diphenyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2s): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (55.9 mg, 87%), mp 189-190 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.7 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.32 (m, 10H), 4.93 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.1, 143.0, 135.2, 133.3, 129.6, 128.8, 128.5, 127.8, 126.7, 121.5, 72.5. HRMS (ESI) m/z calcd for $C_{19}H_{15}NO_2S+H^+$: 322.0896 [M + H^+]; found: 322.0896.

3-phenyl-3-(*p*-tolyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2t): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.55; white solid (46.9 mg, 70%), mp 180-182 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.55 (dd, *J* = 13.6, 6.3 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 7.2 Hz, 2H), 7.33 (q, *J* = 5.7 Hz, 3H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 7.9 Hz, 2H), 4.92 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3, 143.1, 140.2, 138.4, 135.2, 133.2, 129.5, 129.4, 128.7, 128.3, 127.7, 127.6, 126.7, 121.5, 72.4, 21.0. HRMS (ESI) m/z calcd for $C_{20}H_{17}NO_2S+H^+$: 336.1503 [M + H^+]; found: 336.1053.

3-phenyl-3-(4-(trifluoromethyl)phenyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2u): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.55; white solid (58.4 mg, 75%), mp 182-184 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.7 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.63 – 7.59 (m, 5H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.38-7.37 (m, 3H), 7.23-7.23 (m, 2H), 4.98 (s, 1H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.69. ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.7, 142.4, 142.2, 135.3, 133.5, 130.5 ($^2J_{C\text{-}F}$ = 32.6 Hz), 130.0, 129.2, 129.1, 128.1, 127.8, 126.5, 125.69 ($^3J_{C\text{-}F}$ = 3.7 Hz), 123.8 ($^1J_{C\text{-}F}$ = 292.2 Hz), 72.1. HRMS (ESI) m/z calcd for $C_{20}H_{14}F_3NO_2S+H^+$: 390.0770 [M + H^+]; found: 390.0773.

3-(4-fluorophenyl)-3-phenyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2v):

purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (54.9 mg, 81%), mp 188-189 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.7 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.6Hz, 1H), 7.41-7.35 (m, 6H), 7.32 – 7.29 (m, 2H), 7.03 (t, *J* = 8.5 Hz, 2H), 4.95 (s, 1H).^{19}F NMR (565 MHz, $CDCl_3$) δ -113.45.^{13}C NMR (151 MHz, $CDCl_3$) δ 162.5 ($^1J_{C\text{-}F}$ = 248.6 Hz), 142.9 ($^2J_{C\text{-}F}$ = 12.7 Hz), 138.89, 135.2, 133.4, 129.8, 129.7 ($^3J_{C\text{-}F}$ = 8.3 Hz), 128.9, 128.7, 127.7, 126.5, 121.6, 115.6 ($^2J_{C\text{-}F}$ = 21.7 Hz), 71.9. HRMS (ESI) m/z calcd for $C_{19}H_{14}FNO_2S+H^+$: 340.0802 [M + H^+]; found: 340.0804.

3-(4-chlorophenyl)-3-phenyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2w): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (41.9 mg, 59%), mp 178-180 °C.^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.7 Hz, 1H), 7.63 (q, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 7.8 Hz, 5H), 7.32 (d, *J* = 7.7 Hz, 2H), 7.28 (d, *J* = 3.0 Hz, 2H), 4.95 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.7, 142.6, 141.5, 135.3, 134.5, 133.4, 129.8, 129.2, 129.0, 128.9, 128.8, 127.7, 126.5, 121.6, 72.0. HRMS (ESI) m/z calcd for $C_{19}H_{14}ClNO_2S+H^+$: 356.0507 [M + H^+]; found: 356.0511.

3-methyl-3-phenyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2x): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (43 mg, 83%), mp 160-162 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 4.92 (s, 1H), 2.06 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.3, 142.8, 134.6, 133.6, 129.4, 129.1, 128.4, 126.3, 124.6, 121.3, 65.5, 28.7. HRMS (ESI) m/z calcd for $C_{14}H_{13}NO_2S+H^+$: 260.0740 [M + H^+]; found: 260.0742.

3-methyl-3-(*p*-tolyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2y): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (44.7 mg, 82%), mp 161-163 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.7 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 4.74 (s, 1H), 2.33 (s, 3H), 2.04 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.5, 139.7, 138.4, 134.6, 133.5, 129.6,129.3, 126.1, 124.5, 121.2, 65.3, 28.6, 20.9. HRMS (ESI) m/z calcd for $_{15}H_{15}NO_2S+H^+$: 274.0896 [M + H^+]; found: 274.0900.

3-methyl-3-(4-(trifluoromethyl)phenyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2z): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (42.5 mg, 65%), mp 156-158 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.67 – 7.64 (m, 2H), 7.63 – 7.60 (m, 3H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.27 (s, 1H), 4.83 (s, 1H), 2.09 (s, 3H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.76. ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.7, 144.1, 134.6, 133.7, 130.5 ($^2J_{C\text{-}F}$ = 32.9 Hz), 129.7, 126.6, 125.9 ($^3J_{C\text{-}F}$ = 3.7 Hz), 124.3, 121.5, 64.9, 28.8. HRMS (ESI) m/z calcd for $C_{15}H_{12}F_3NO_2S+H^+$: 328.0614 [M + H^+]; found: 328.0617.

3-(4-fluorophenyl)-3-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2ba): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (37.7 mg, 68%), mp 161-162 °C. ^{1}H NMR (600 MHz,

$CDCl_3$) δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.46 (dt, *J* = 16.6, 8.3 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.04 (t, *J* = 8.5 Hz, 2H), 4.77 (s, 1H), 2.06 (s, 3H). ^{19}F NMR (565 MHz, CDCl3) δ -113.50. ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.5 ($^1J_{C-F}$ = 248.6 Hz), 144.9, 138.5, 134.5, 133.6, 129.5, 128.17 ($^3J_{C-F}$ = 8.4 Hz), 124.4, 121.4, 115.8 ($^2J_{C-F}$ = 21.6 Hz), 64.9, 28.9. HRMS (ESI) m/z calcd for $C_{14}H_{12}FNO_2S+H^+$: 278.0646 [M + H^+]; found: 278.0644.

3-(4-chlorophenyl)-3-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2bb): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (32.8 mg, 56%), mp 165-167 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.7 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 1H), 4.81 (s, 1H), 2.05 (s, 3H).^{13}C NMR (151 MHz, $CDCl_3$) δ 144.6, 141.3, 134.5, 133.6, 129.6, 129.1, 127.7, 124.3, 121.4, 64.8, 28.7. HRMS (ESI) m/z calcd for $C_{14}H_{12}ClNO_2S+H^+$: 294.0350 [M + H^+]; found: 294.0351.

3-phenyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2bc): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.6; white solid (37.2 mg, 76%), mp 89-91 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81 (t, *J* = 7.1 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.41 – 7.33 (m, 5H), 7.14 (d, *J* = 7.2 Hz, 1H), 5.72 (d, *J* = 3.4 Hz, 1H), 5.10 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.8, 138.7, 134.8, 133.3, 129.5, 129.3, 129.1, 127.6, 125.4, 121.1, 61.4. HRMS (ESI) m/z calcd for $C_{13}H_{11}NO_2S+H^+$: 246.0583 [M + H^+]; found: 246.0587.

3-benzyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2bd): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; white solid (31.6 mg, 61%), mp 81-82 °C.^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.46 – 7.38 (m, 5H), 7.36 (t, *J* = 6.9 Hz, 1H), 7.28 (d, *J* = 7.7 Hz, 1H), 4.97 (td, *J* = 10.4, 5.4 Hz, 1H), 4.84 (d, *J* = 10.2 Hz, 1H), 3.31–3.22 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.6, 137.9, 134.9, 132.3, 129.4, 129.0, 128.4, 127.9, 126.2, 123.8, 56.8, 35.6. HRMS (ESI) m/z calcd for $C_{14}H_{13}NO_2S+H^+$: 260.0740 [M + H^+]; found: 260.0742.

5,7-diethyl-3-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (2be): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.6; colourless oil (33.5 mg, 70%), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.12 (s, 1H), 6.98 (s, 1H), 4.75 (s, 1H), 4.69 (q, *J* = 6.5 Hz, 1H), 2.98 (q, *J* = 7.6 Hz, 2H), 2.71 (q, *J* = 7.6 Hz, 2H), 1.58 (d, *J* = 6.7 Hz, 3H), 1.34 (t, *J* = 7.5 Hz, 3H), 1.25 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.6, 142.5, 140.2, 131.4, 128.7, 120.3, 52.7, 29.0, 24.3, 21.6, 15.4, 14.6. HRMS (ESI) m/z calcd for $C_{12}H_{17}NO_2S+H^+$: 240.1053 [M + H^+]; found: 240.1052.

3-cyclopropyl-3-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (6): purified by analytical TLC on silica gel with petroleum ether/ethyl acetate (3/1) as an eluent R_f = 0.5; colourless oil (32 mg, 71%), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, J = 7.8 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.45 (d, J = 7.8 Hz, 1H), 4.59 (s, 1H), 1.57 (s, 3H), 1.24 (tt, J = 7.9, 5.9 Hz, 1H), 0.62-0.54 (m, 2H), 0.47-0.37 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.1, 134.7, 133.3, 129.2, 123.4, 121.2, 63.3, 26.8, 21.5, 2.1, 0.9. HRMS (ESI) m/z calcd for $C_{11}H_{13}NO_2S+H^+$: 246.0565 [M + H^+]; found:

246.0566.

DFT calculations

Computational details

The DFT calculations were performed using the Gaussian 09 program[10]. All the optimizations were performed at B3LYP[11, 12]/6-31G(d, p) level in DMSO solvent using the IEF-PCM model[13]. All geometry optimization calculations were followed by frequency calculations to verify that intermediate structures are real minima in the potential energy surface by confirming that their frequencies are real. Transition states that connect these intermediates bear only one imaginary frequency. Moreover, we further refined the energy by employing the single-point energy calculations at the B3LYP-D3(BJ)/6-311++G(2df, 2pd)//IEF-PCM$_{DMSO}$ level based on the B3LYP/6-31G(d, p)//IEF-PCM$_{DMSO}$ optimized structures.

Computational results of the other possible pathways

As shown in Figure S1, other possible radical formation pathway and nitrene formation pathway have been studied in theory herein. The formation of both radical and nitrene intermediates need extremely high energies in thermodynamic, so we can exclude the two pathways. As shown in Figure S2, the solvent DMSO- and base anion-assisted S_N2 pathways and the PTS_N2 pathway with the participation of solvent DMSO were also considered, and the free energy barriers of TS1', TS1'' and TS1''' are 42.1, 53.4 and 72.8 kcal/mol, respectively. The free energy barriers of the three possible pathways are much higher than that of pathway through transition state TS1, indicating that three possible pathways can be safely excluded. Moreover, two possible pathways associated with C-H deprotonation coupled with dissociation of AcOH were calculated in Figure S3, the free energy barriers of TS1h and TS1h' are 62.7 and 63.5 kcal/mol respectively, which are higher than that of pathway through transition state TS1, so the two pathways can also be excluded.

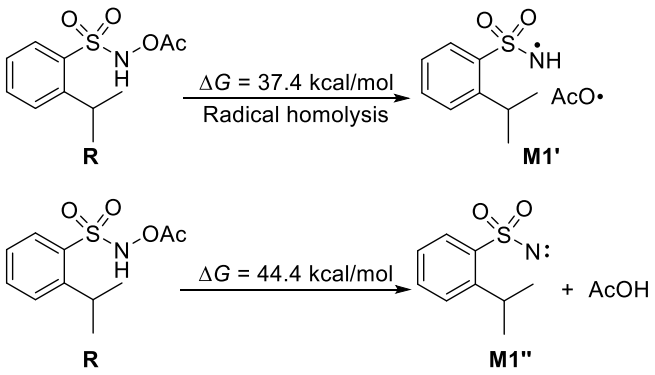


Figure S1. Relative Gibbs free energies of the radical formation pathway and nitrene formation pathway.

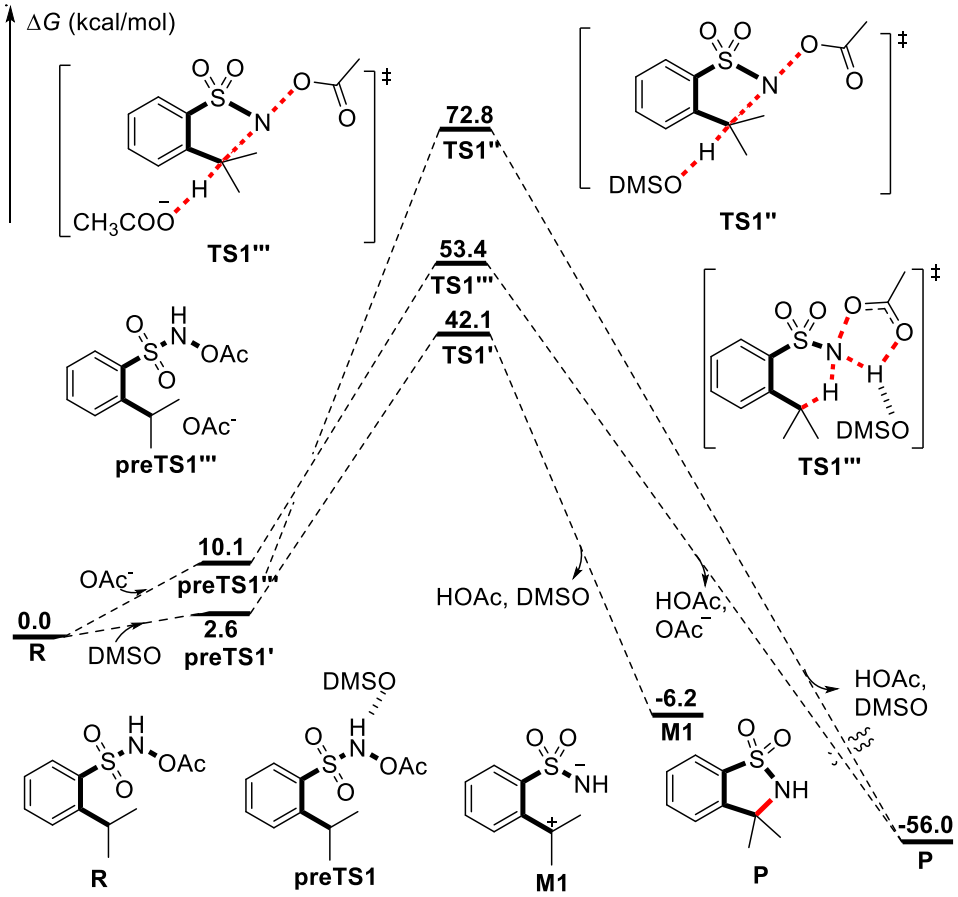


Figure S2. Relative Gibbs free energy profiles for the solvent DMSO- and base anion-assisted S_N2 pathways and the PTS_N2 pathway with the participation of solvent DMSO.

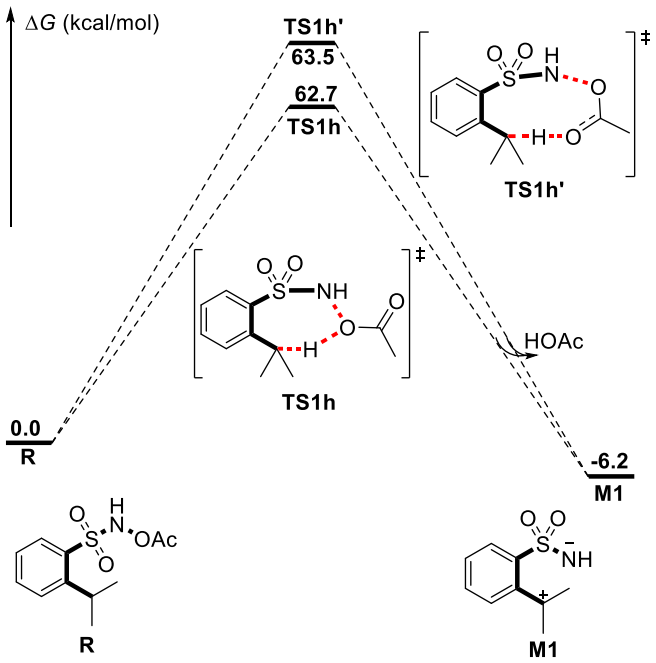


Figure S3. Relative Gibbs free energy profiles for the pathways associated with C-H deprotonation coupled with dissociation of AcOH.

Scanning results of N-O distance in R

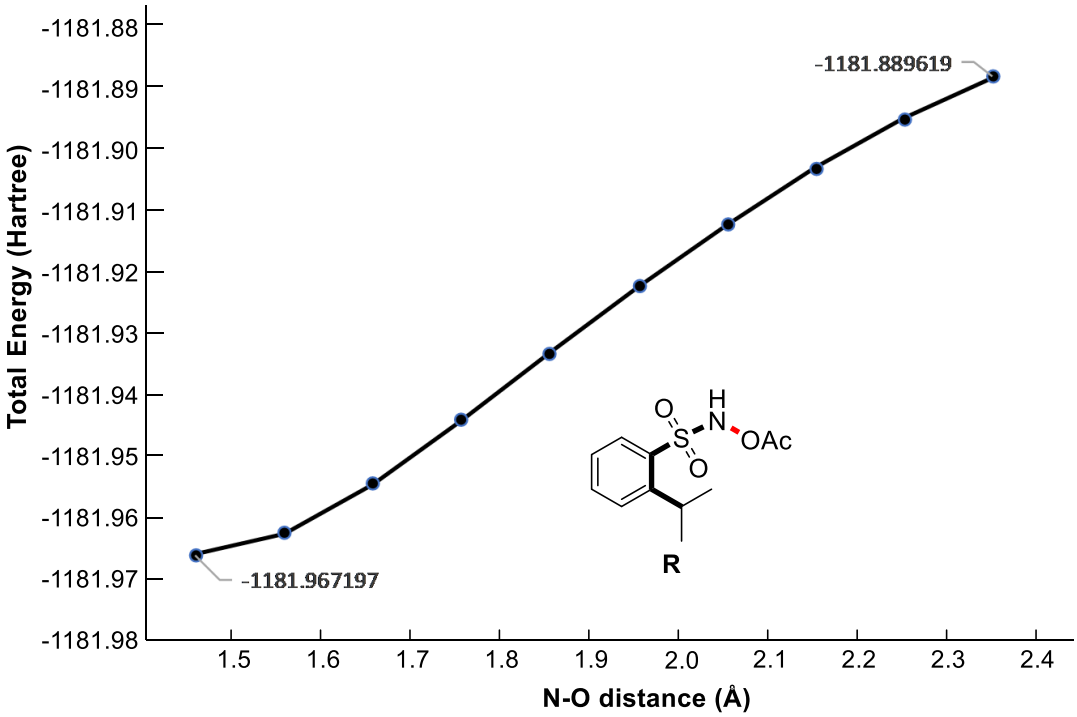


Figure S4. Scanning results of N-O distance in R

The energies of all the optimized structures

Table S5. The single-point energies (E), Gibbs free energy corrections (GFEC), Gibbs free energies (GFE) and number of imaginary frequencies (NF) of the stationary points (SP). (energy in a.u.)

SP	GFEC (6-31G(d,p))	E (6-311++G(2df,2pd))	GFE	NF
R	0.205724	-1182.353935	-1182.148211	0
TS1	0.19893	-1182.290858	-1182.091928	1
M1	0.147364	-953.147038	-952.999674	0
HOAc	0.034512	-229.19293	-229.158418	0
TS2	0.148864	-953.140412	-952.991548	1
P	0.15128	-953.230253	-953.078973	0
M1'	0.190865	-1182.279441	-1182.088576	0
M1''	0.198274	-1182.275726	-1182.077452	0
preTS1'	0.276208	-1735.694528	-1735.41832	0
DMSO	0.05132	-553.325635	-553.274315	0
TS1'	0.272637	-1735.628132	-1735.355495	1
AcO-	0.022445	-228.723713	-228.701268	0
TS1''	0.273735	-1735.580193	-1735.306458	1
preTS1'''	0.246865	-1411.080219	-1410.833354	0
TS1'''	0.242511	-1411.006825	-1410.764314	1
TS1h	0.197636	-1182.245976	-1182.04834	1
TS1h'	0.197638	-1182.24471	-1182.047072	1

Cartesian coordinates of all the stationary points

R1

C	-3.957287	-0.237782	-0.579012
C	-3.077244	0.815569	-0.339344
C	-1.723368	0.608564	-0.030605
C	-1.305689	-0.738873	0.029070
C	-2.178033	-1.809735	-0.212130
C	-3.510388	-1.558302	-0.519253
H	-4.995623	-0.024749	-0.813735
H	-3.451132	1.832707	-0.391363
C	-0.825889	1.814817	0.233739
H	-1.803737	-2.824388	-0.154028
H	-4.188996	-2.383495	-0.706668
C	-0.880516	2.832375	-0.920932
C	-1.190263	2.471388	1.580040

H	-2.218912	2.847657	1.578019
H	-1.089435	1.758704	2.403726
H	-0.523344	3.317021	1.777486
H	-0.170674	3.643142	-0.728647
H	-0.610047	2.364837	-1.872571
H	-1.871883	3.282795	-1.032802
N	1.221689	-0.572429	-0.916680
H	0.207666	1.478528	0.302542
S	0.364693	-1.216945	0.473842
O	0.870812	-0.466421	1.629096
O	0.448505	-2.685567	0.504327
O	2.621535	-0.754756	-0.673141
C	3.293248	0.431303	-0.418414
O	2.773665	1.515903	-0.407263
C	4.739472	0.110152	-0.156680
H	4.828874	-0.388814	0.813116
H	5.130534	-0.567684	-0.918583
H	5.312662	1.036138	-0.142384
H	1.036753	-1.204394	-1.701834

TS1

C	-3.732723	-0.814019	-1.162870
C	-3.143909	0.403819	-0.818137
C	-1.881584	0.435884	-0.209681
C	-1.241239	-0.785889	0.023494
C	-1.810489	-2.009241	-0.325636
C	-3.070630	-2.018571	-0.922459
H	-4.709792	-0.816485	-1.634833
H	-3.668062	1.331384	-1.021875
C	-1.247005	1.740934	0.178525
H	-1.267309	-2.931299	-0.152756
H	-3.524571	-2.961182	-1.208363
C	-1.108020	2.774677	-0.915151
C	-1.615968	2.265882	1.551546
H	-2.670564	2.575320	1.524833

H	-1.513377	1.498413	2.321630
H	-1.016329	3.139749	1.817575
H	-0.453790	3.592012	-0.602228
H	-0.739127	2.341584	-1.846812
H	-2.096961	3.211064	-1.114391
N	1.032104	0.743228	0.451120
H	0.040946	1.434288	0.430571
S	0.340296	-0.816500	0.884550
O	0.114306	-0.738827	2.334153
O	1.119509	-1.927969	0.335884
O	3.048094	0.106875	0.565764
C	3.407078	0.184258	-0.665469
O	2.646745	0.490422	-1.610610
C	4.866453	-0.163765	-0.937526
H	5.491810	0.045435	-0.068748
H	4.931691	-1.233517	-1.161297
H	5.220318	0.394034	-1.806390
H	1.344645	0.712770	-0.568894

M1

C	-2.370299	2.031018	0.076271
C	-2.349884	0.659479	-0.071923
C	-1.131105	-0.095683	-0.041132
C	0.106908	0.644905	0.034957
C	0.052538	2.030414	0.162206
C	-1.159800	2.719763	0.204007
H	-3.315110	2.562101	0.092621
H	-3.294614	0.136159	-0.128838
C	-1.292144	-1.506853	0.045411
H	0.984065	2.581654	0.183542
H	-1.155655	3.800338	0.305774
C	-2.535019	-2.186708	-0.420215
C	-0.296293	-2.405028	0.654182
H	-0.752926	-3.339190	0.984810
H	0.453207	-2.628854	-0.121383

H	0.251340	-1.913911	1.463018
H	-3.131937	-1.616815	-1.128679
H	-2.254296	-3.143224	-0.873147
H	-3.151264	-2.442099	0.453734
N	2.234973	-0.449455	1.336563
H	2.302216	-1.466847	1.366923
S	1.812685	-0.039540	-0.128178
O	1.701795	-1.151285	-1.118276
O	2.581679	1.138995	-0.602481

AcOH

H	1.725763	-0.820117	0.000147
O	0.641064	1.206527	-0.000045
C	0.092367	0.122226	0.000107
O	0.778596	-1.042931	0.000007
C	-1.394251	-0.112588	-0.000064
H	-1.917341	0.842559	-0.001446
H	-1.677001	-0.695723	-0.881136
H	-1.677395	-0.693316	0.882478

TS2

C	2.284833	2.076286	0.023699
C	2.277264	0.705727	0.228750
C	1.087274	-0.061489	0.033330
C	-0.145076	0.638748	-0.201128
C	-0.107756	2.013750	-0.381464
C	1.095313	2.727046	-0.307301
H	3.212516	2.629739	0.114735
H	3.216210	0.201163	0.418266
C	1.313059	-1.459688	-0.113678
H	-1.044706	2.536216	-0.531146
H	1.090230	3.800678	-0.466445
C	2.253670	-2.187887	0.769256
C	0.745326	-2.241467	-1.236842
H	0.462102	-3.252143	-0.926784
H	-0.075003	-1.747185	-1.748532

H	1.595345	-2.372082	-1.927872
H	2.839673	-1.558614	1.436024
H	1.599556	-2.808446	1.404303
H	2.885891	-2.886890	0.214431
N	-2.104159	-1.387462	-0.662402
H	-1.751826	-2.180287	-0.123836
S	-1.811926	-0.092704	0.170320
O	-1.660342	-0.301320	1.642458
O	-2.731347	0.997219	-0.247357

P

C	-2.936501	0.938197	0.000000
C	-1.694182	1.575647	0.000000
C	-0.532434	0.802645	0.000000
C	-0.653658	-0.582946	0.000000
C	-1.879416	-1.243902	0.000000
C	-3.032466	-0.460016	0.000000
H	-3.842246	1.536052	0.000000
H	-1.633585	2.659109	0.000000
C	0.896048	1.327142	0.000000
H	-1.933198	-2.327220	0.000000
H	-4.007256	-0.936144	0.000000
C	1.182863	2.148593	1.269260
C	1.182863	2.148593	-1.269260
H	2.230904	2.462782	-1.283752
H	0.980082	1.554215	-2.163401
H	0.557986	3.045946	-1.292378
H	0.980082	1.554215	2.163401
H	2.230904	2.462782	1.283752
H	0.557986	3.045946	1.292378
N	1.713225	0.096980	0.000000
H	2.723903	0.121041	0.000000
S	0.939834	-1.366436	0.000000
O	1.182863	-2.119895	1.246845
O	1.182863	-2.119895	-1.246845

M1’

C	2.272330	-2.162847	-1.789958
C	1.643810	-2.195634	-0.547145
C	1.293444	-1.026433	0.145751
C	1.614580	0.189523	-0.492179
C	2.243569	0.240352	-1.741530
C	2.574312	-0.942271	-2.394870
H	2.525809	-3.094388	-2.286756
H	1.417728	-3.156809	-0.096809
C	0.614237	-1.141404	1.507664
H	2.465463	1.201683	-2.187989
H	3.062034	-0.908625	-3.363141
C	-0.686906	-1.962128	1.427375
C	1.585322	-1.720152	2.556227
H	1.897987	-2.736577	2.292177
H	2.482443	-1.100510	2.645935
H	1.098631	-1.762014	3.535847
H	-1.174898	-1.976373	2.406222
H	-1.384286	-1.527968	0.704148
H	-0.496802	-2.999975	1.138197
N	-0.373802	1.802852	0.439297
S	1.298975	1.782279	0.266623
O	1.889597	1.835769	1.618098
O	1.652634	2.845279	-0.692281
H	-0.584892	2.730715	0.842723
H	0.337719	-0.142233	1.849519
O	-4.098099	1.172069	0.139737
C	-4.334698	0.076057	-0.444864
O	-3.274976	-0.392919	-0.954845
C	-5.676361	-0.558142	-0.549893
H	-6.294595	-0.270652	0.303887
H	-6.160606	-0.210320	-1.468943
H	-5.573808	-1.645505	-0.601197

M1”

C	2.683602	-1.414735	-1.921433
C	2.671809	-0.158712	-1.318422
C	1.806745	0.167004	-0.262392
C	0.923159	-0.861809	0.139739
C	0.926039	-2.134122	-0.452545
C	1.810841	-2.411997	-1.486939
H	3.377665	-1.612445	-2.732275
H	3.356708	0.600344	-1.679140
C	1.832778	1.582387	0.308317
H	0.233629	-2.889519	-0.104157
H	1.813420	-3.394360	-1.946423
C	3.262337	2.087353	0.575869
C	1.067843	2.538295	-0.631324
H	1.568292	2.618512	-1.602669
H	0.046064	2.188298	-0.800215
H	1.022834	3.539928	-0.191157
H	3.214663	3.059949	1.075586
H	3.813540	1.400401	1.225376
H	3.839998	2.223681	-0.343770
N	0.207288	0.106704	2.783146
H	1.318961	1.577338	1.268166
S	-0.238203	-0.688763	1.487193
O	-0.851350	0.751302	1.538419
O	-1.115090	-1.860132	1.513898
O	-3.892966	1.232627	-1.849591
C	-3.211417	0.416216	-1.019221
O	-2.011784	0.236829	-1.126039
C	-4.108351	-0.215287	0.010047
H	-4.883961	-0.804638	-0.487579
H	-3.521091	-0.851457	0.669688
H	-4.611603	0.563604	0.590024
H	-3.251661	1.601078	-2.482228

preTS1’

C	-3.176141	2.120776	-1.112359
C	-3.266168	1.294688	0.005409
C	-2.442738	0.169797	0.176151
C	-1.509739	-0.074424	-0.852279
C	-1.405716	0.747927	-1.982673
C	-2.243090	1.850131	-2.114677
H	-3.836788	2.977785	-1.200226
H	-3.997396	1.527297	0.772758
C	-2.593506	-0.672893	1.440004
H	-0.673871	0.511200	-2.745163
H	-2.168324	2.486661	-2.989945
C	-2.228023	0.153845	2.688610
C	-4.006869	-1.274931	1.550376
H	-4.776216	-0.500056	1.630624
H	-4.240312	-1.895289	0.679664
H	-4.074996	-1.904056	2.443787
H	0.943864	-0.221051	0.524874
H	-2.265560	-0.479697	3.580914
H	-1.219959	0.568480	2.598849
H	-2.925911	0.984163	2.840178
N	0.530704	-1.183746	0.555946
H	-1.892714	-1.505561	1.388117
S	-0.419573	-1.501520	-0.864026
O	-1.163556	-2.741789	-0.592672
O	0.408827	-1.467385	-2.082426
O	1.568574	-2.167821	0.595931
C	2.785054	-1.789654	0.072803
O	3.007898	-0.680113	-0.350295
C	3.742987	-2.944777	0.142517
H	4.752718	-2.585383	-0.051577
H	3.692039	-3.429741	1.119559
H	3.467773	-3.685573	-0.614450
S	1.859019	2.690081	0.665676

O	0.936473	1.514808	1.031351
C	2.175594	2.578108	-1.125327
H	2.895794	3.350095	-1.405552
H	2.548507	1.579933	-1.360724
H	1.223969	2.759256	-1.627438
C	3.534203	2.260187	1.242878
H	4.224345	3.047982	0.932221
H	3.492906	2.215777	2.332448
H	3.823241	1.292743	0.829337

DMSO

S	0.000269	0.230942	-0.441090
O	0.004027	1.515578	0.381839
C	1.361057	-0.817723	0.184269
H	1.322076	-1.791468	-0.310173
H	2.296951	-0.313276	-0.062855
H	1.267449	-0.927463	1.267728
C	-1.364825	-0.811655	0.184575
H	-1.331347	-1.784340	-0.312464
H	-1.270421	-0.924698	1.267603
H	-2.298626	-0.302180	-0.060177

TS1’

C	-3.580661	1.243434	-0.656995
C	-3.211050	0.453656	0.435104
C	-2.090764	-0.380108	0.357582
C	-1.366970	-0.393312	-0.834471
C	-1.717936	0.385776	-1.932808
C	-2.837004	1.215334	-1.838139
H	-4.448562	1.890527	-0.578198
H	-3.793784	0.490685	1.349748
C	-1.652788	-1.257494	1.498237
H	-1.112215	0.357460	-2.832047
H	-3.118404	1.841461	-2.678443
C	-1.543086	-0.561796	2.845094
C	-2.340542	-2.614886	1.521812

H	-3.407627	-2.469782	1.731333
H	-2.243584	-3.118301	0.556981
H	-1.921996	-3.251651	2.305847
H	1.852005	0.401880	0.816646
H	-1.088520	-1.225753	3.585568
H	-0.953439	0.351591	2.752735
H	-2.547370	-0.305694	3.206121
N	0.630865	-1.598898	0.595800
H	-0.474207	-1.511031	1.275798
S	0.030731	-1.527525	-0.983247
O	-0.522278	-2.829041	-1.443001
O	1.000021	-0.885365	-1.904487
O	2.604874	-1.872918	0.086202
C	3.292091	-0.863395	0.298631
O	2.853037	0.302778	0.695858
C	4.784373	-0.902685	0.095330
H	5.045047	-0.223453	-0.721780
H	5.286448	-0.546505	0.998470
H	5.108362	-1.913650	-0.146415
S	0.196221	2.539933	0.215968
O	0.506261	1.322737	1.112350
C	1.278780	2.398255	-1.243538
H	1.096191	3.256927	-1.893124
H	2.320444	2.362277	-0.918619
H	1.016236	1.465589	-1.744593
C	1.029515	3.965147	0.992008
H	0.937359	4.831566	0.332825
H	0.522524	4.160328	1.938225
H	2.078752	3.716195	1.166321

AcO^-

O	-0.810484	-1.103322	0.000216
C	-0.200133	0.000204	-0.000842
O	-0.706413	1.156626	0.000212
C	1.352232	-0.050513	0.000075

H	1.734678	-1.075585	-0.001061
H	1.744569	0.476774	-0.877879
H	1.743335	0.474234	0.880115

TS1”

C	2.227658	2.005765	1.507340
C	1.642740	0.769093	1.739283
C	0.636929	0.239844	0.867489
C	0.144665	1.181885	-0.082991
C	0.750290	2.413661	-0.345267
C	1.836623	2.816346	0.424579
H	3.015902	2.347781	2.173216
H	2.003915	0.155349	2.559200
H	0.320698	3.078734	-1.087914
H	2.316937	3.771635	0.244541
C	-0.097243	-2.011540	-0.268380
C	0.058941	-1.827074	2.265091
H	0.176611	-1.149933	3.115458
H	-0.924097	-2.308931	2.369148
H	0.803367	-2.632852	2.369906
H	-1.113971	-2.429284	-0.315887
H	0.083276	-1.505414	-1.217456
H	0.568091	-2.888504	-0.223394
N	-2.111898	-0.049111	0.638668
S	-1.489054	0.904112	-0.713591
O	-2.174848	2.209549	-0.747646
O	-1.549813	0.116445	-1.968277
O	-3.793096	0.359935	0.421561
C	-4.481130	-0.704491	0.039134
O	-3.991074	-1.803505	-0.208338
C	-5.963087	-0.402910	-0.070331
H	-6.133361	0.270752	-0.915315
H	-6.511837	-1.331894	-0.228023
H	-6.317421	0.098428	0.833232
H	-2.273141	-1.003698	0.288756

S	3.452828	-0.488061	-0.683003
O	2.898668	-1.665071	0.288977
C	4.955290	0.011419	0.182220
H	5.500783	0.691076	-0.475724
H	4.632654	0.534728	1.081698
H	5.546757	-0.873489	0.419720
C	4.128552	-1.471998	-2.038311
H	4.656684	-0.788644	-2.706656
H	4.798360	-2.234200	-1.638032
H	3.279236	-1.921668	-2.553392
C	0.137183	-1.106794	0.937235
H	1.950309	-1.411063	0.548991

preTS1’’’

C	1.977495	2.543451	-0.605334
C	1.811667	1.172407	-0.412255
C	0.561515	0.620497	-0.079261
C	-0.508098	1.534788	0.048271
C	-0.350377	2.915273	-0.146710
C	0.900756	3.422598	-0.475835
H	2.961256	2.927204	-0.860669
H	2.678204	0.518167	-0.521677
C	0.444001	-0.885422	0.138354
H	-1.205476	3.570785	-0.036820
H	1.030440	4.489140	-0.627658
C	1.021408	-1.678964	-1.049853
C	1.114693	-1.294694	1.466983
H	2.195087	-1.115352	1.450649
H	0.677033	-0.746736	2.307689
H	0.952745	-2.364181	1.645140
H	0.862277	-2.750176	-0.884323
H	0.518368	-1.407298	-1.984043
H	2.095248	-1.511509	-1.172688
N	-2.587634	0.084840	-0.902217
H	-0.610643	-1.148971	0.208631

S	-2.164241	1.033631	0.516144
O	-2.173795	0.086940	1.638331
O	-3.019361	2.228481	0.610835
O	-3.870231	-0.502836	-0.648600
C	-3.814818	-1.871534	-0.438967
O	-2.805498	-2.524498	-0.479318
C	-5.206367	-2.363964	-0.146763
H	-5.494345	-2.049543	0.861279
H	-5.926547	-1.938445	-0.848684
H	-5.218099	-3.451709	-0.202479
H	-2.782676	0.750885	-1.656238
O	4.571188	-0.526449	-0.933189
C	5.201546	-0.935405	0.087537
O	4.735556	-1.168308	1.234195
C	6.717342	-1.173096	-0.122438
H	6.873084	-1.935241	-0.894952
H	7.196151	-0.255952	-0.484137
H	7.211741	-1.495274	0.797799

TS1'''

C	2.316574	2.321741	1.428800
C	1.867946	1.035457	1.668075
C	0.897841	0.402330	0.820463
C	0.281152	1.300755	-0.109860
C	0.745137	2.595684	-0.370581
C	1.802864	3.104568	0.372183
H	3.096133	2.733314	2.065584
H	2.320098	0.454742	2.466492
H	0.225666	3.217812	-1.093105
H	2.173832	4.107700	0.191199
C	0.368738	-1.893256	-0.281381
C	0.666328	-1.705138	2.228434
H	0.655967	-1.031434	3.090850
H	-0.167730	-2.409688	2.358895
H	1.585625	-2.314048	2.292742

H	-0.599047	-2.418295	-0.325576
H	0.499760	-1.370896	-1.228519
H	1.127227	-2.693083	-0.236597
N	-1.879727	-0.104243	0.659885
S	-1.320857	0.871972	-0.716014
O	-2.128645	2.107525	-0.776178
O	-1.341648	0.050756	-1.952553
O	-3.535376	0.145188	0.457329
C	-4.152955	-0.974498	0.094137
O	-3.589808	-2.040119	-0.130204
C	-5.649003	-0.766865	-0.018112
H	-5.860679	-0.129010	-0.881423
H	-6.140541	-1.731368	-0.148299
H	-6.032275	-0.262390	0.871758
H	-1.914484	-1.081827	0.344706
O	3.475662	-1.419897	0.372004
C	0.522533	-0.969524	0.915972
H	2.545786	-1.091656	0.438119
C	3.957274	-1.088929	-0.837921
O	3.301356	-0.507016	-1.682957
C	5.391195	-1.525964	-1.004984
H	5.745290	-1.264031	-2.001231
H	6.014902	-1.041339	-0.248079
H	5.470206	-2.606016	-0.851357

TS1h

C	3.791354	0.801967	-0.493456
C	2.585014	1.483830	-0.427463
C	1.378912	0.843767	-0.040573
C	1.460770	-0.570970	0.094749
C	2.679271	-1.260414	0.056422
C	3.850904	-0.572661	-0.226774
H	4.699238	1.349878	-0.725539
H	2.582649	2.556354	-0.577201
C	0.212665	1.696879	0.290978

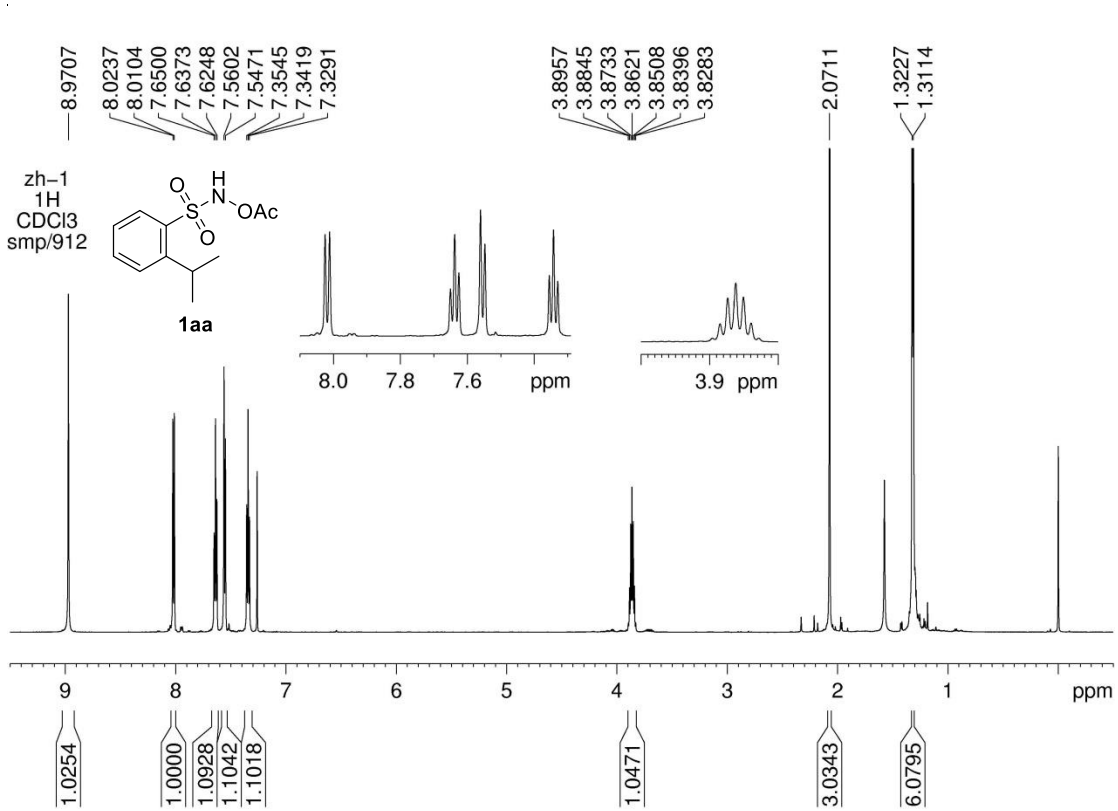
H	2.677927	-2.336472	0.183766
H	4.794246	-1.105344	-0.283601
C	-0.035917	1.916388	1.789386
C	0.089970	2.991438	-0.501057
H	0.798591	3.754102	-0.148305
H	0.254473	2.838821	-1.570883
H	-0.910466	3.412051	-0.364412
H	-1.086970	2.152458	1.982019
H	0.229855	1.042010	2.380789
H	0.561537	2.776544	2.124325
N	-0.923791	-0.858022	1.136836
H	-0.997985	1.080998	-0.032543
S	-0.009855	-1.594340	-0.025248
O	-0.601414	-1.344864	-1.351523
O	0.359440	-2.987838	0.300367
O	-2.960154	-0.945429	0.462701
C	-3.058131	0.133278	-0.139656
O	-2.174657	1.047208	-0.363373
C	-4.418418	0.478731	-0.751908
H	-4.326905	0.398217	-1.838380
H	-5.184686	-0.205806	-0.394118
H	-4.673759	1.510147	-0.504404
H	-0.997603	-1.514389	1.925345

TS1h’

C	-3.201031	1.498991	-1.068063
C	-2.001774	1.925014	-0.503395
C	-1.053909	1.038370	0.054497
C	-1.362455	-0.354239	-0.051129
C	-2.564064	-0.773082	-0.624062
C	-3.490898	0.142046	-1.126736
H	-3.898615	2.233215	-1.457747
H	-1.808865	2.988858	-0.453405
C	0.131387	1.681932	0.713908
H	-2.766674	-1.834303	-0.688455

H	-4.414351	-0.214315	-1.570367
C	0.550529	3.050801	0.214575
C	0.281225	1.514327	2.214219
H	-0.473396	2.149533	2.702870
H	0.127579	0.487795	2.539758
H	1.264060	1.862008	2.544808
H	1.590937	3.233378	0.495455
H	0.465698	3.145469	-0.869865
H	-0.052215	3.841233	0.683791
N	0.789275	-1.946808	-0.734691
H	1.105799	0.896270	0.231918
S	-0.338603	-1.788292	0.481111
O	0.236882	-1.535635	1.817452
O	-1.204365	-2.989021	0.377937
O	1.664410	-0.045574	-0.267467
C	2.925677	0.276506	-0.677334
O	3.385595	1.382189	-0.465418
C	3.646748	-0.841735	-1.381347
H	3.033392	-1.238535	-2.193081
H	4.593123	-0.461702	-1.765981
H	3.840402	-1.656807	-0.677674
H	1.457068	-2.641026	-0.367785

NMR Spectra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3.8957
3.8845
3.8733
3.8621
3.8508
3.8396
3.8283
2.0711
1.3227
1.3114
zh–1
1H
CDCl3
smp/912
1aa
8.0
7.8
7.6
ppm
3.9 ppm
9
8
7
6
5
4
3
2
1
ppm
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1.0000
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1.1042
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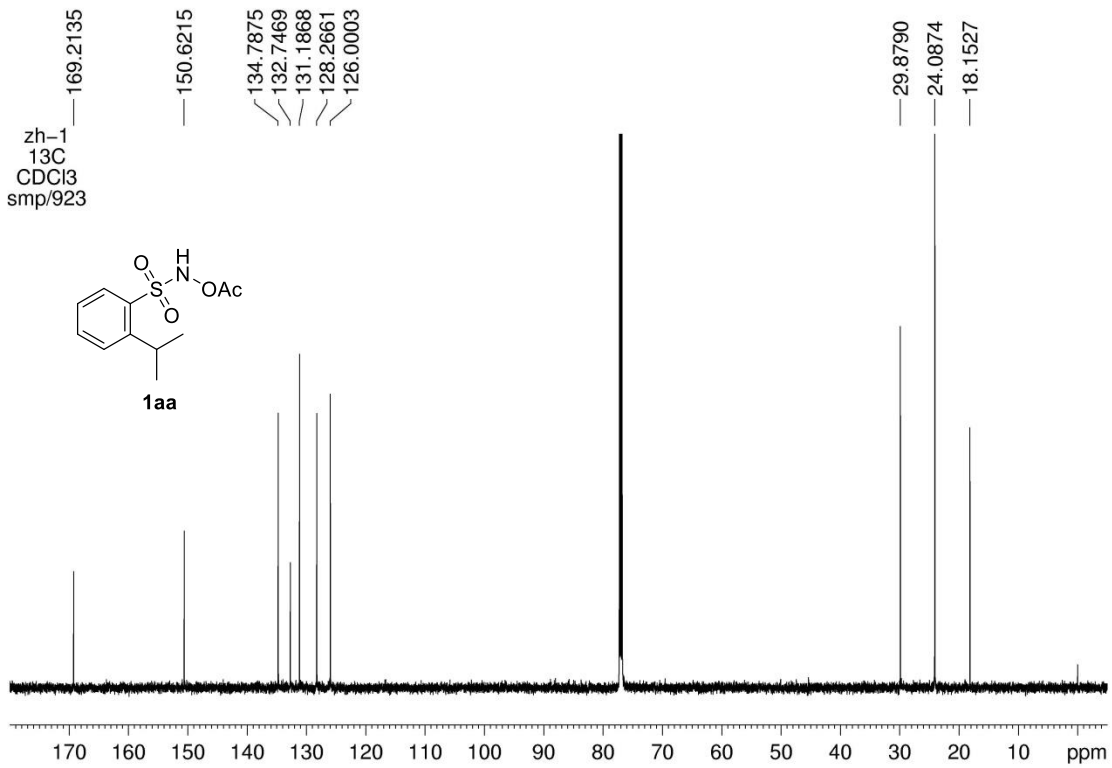
3.0343
6.0795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150.6215
134.7875
132.7469
131.1868
128.2661
126.0003
29.8790
24.0874
18.1527
zh–1
13C
CDCl3
smp/923
1aa
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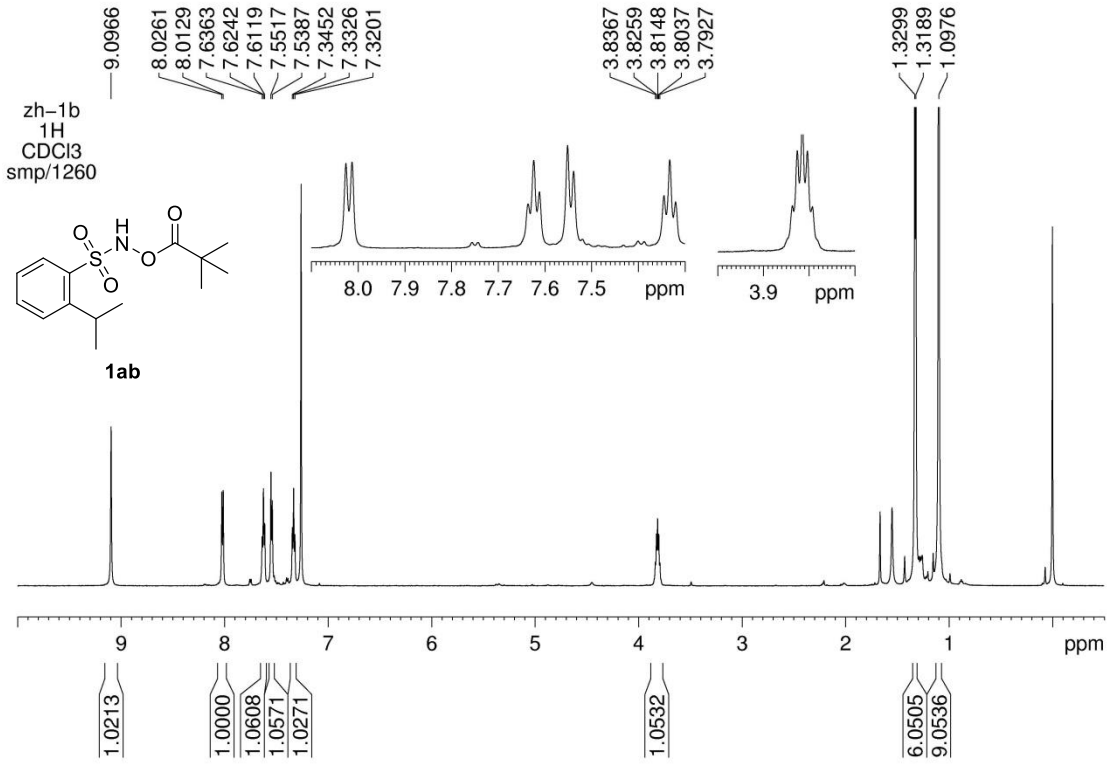
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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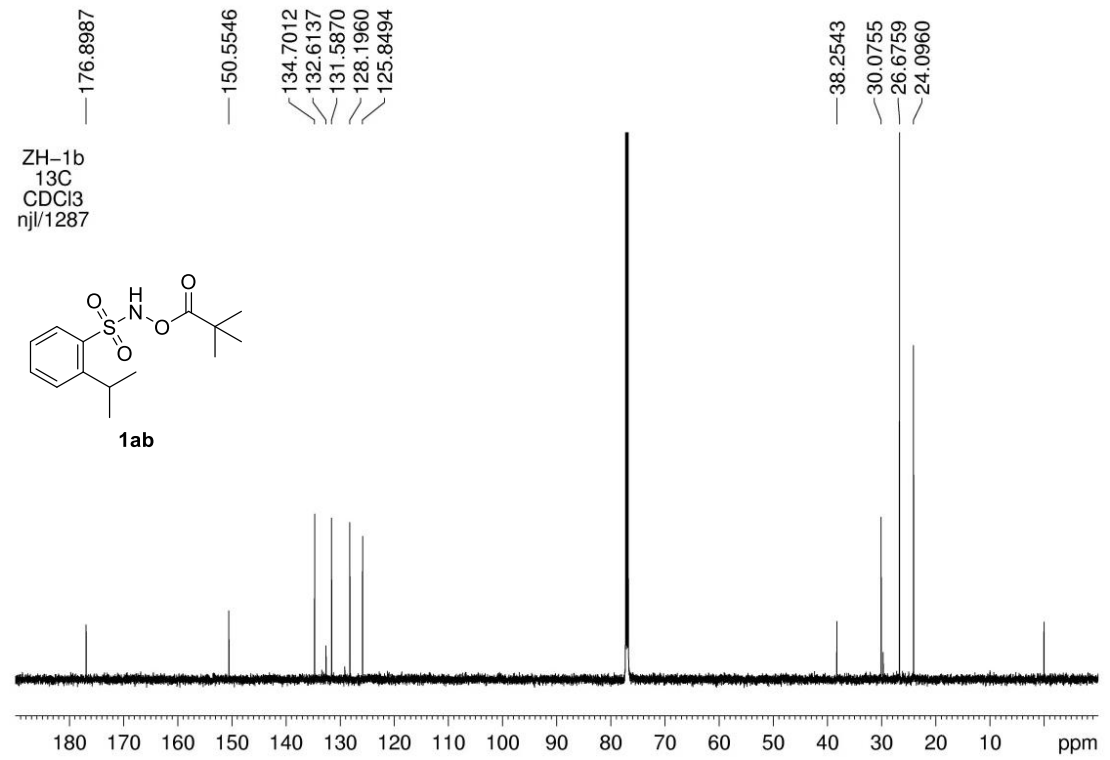
7.3201
3.8367
3.8259
3.8148
3.8037
3.7927
1.3299
1.3189
1.0976
zh-1b
1H
CDCl3
smp/1260
1ab
8.0 7.9 7.8 7.7 7.6 7.5 ppm
3.9 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0213
1.0000
1.0608
1.0571
1.0271
1.0532
6.0505
9.0536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30.0755
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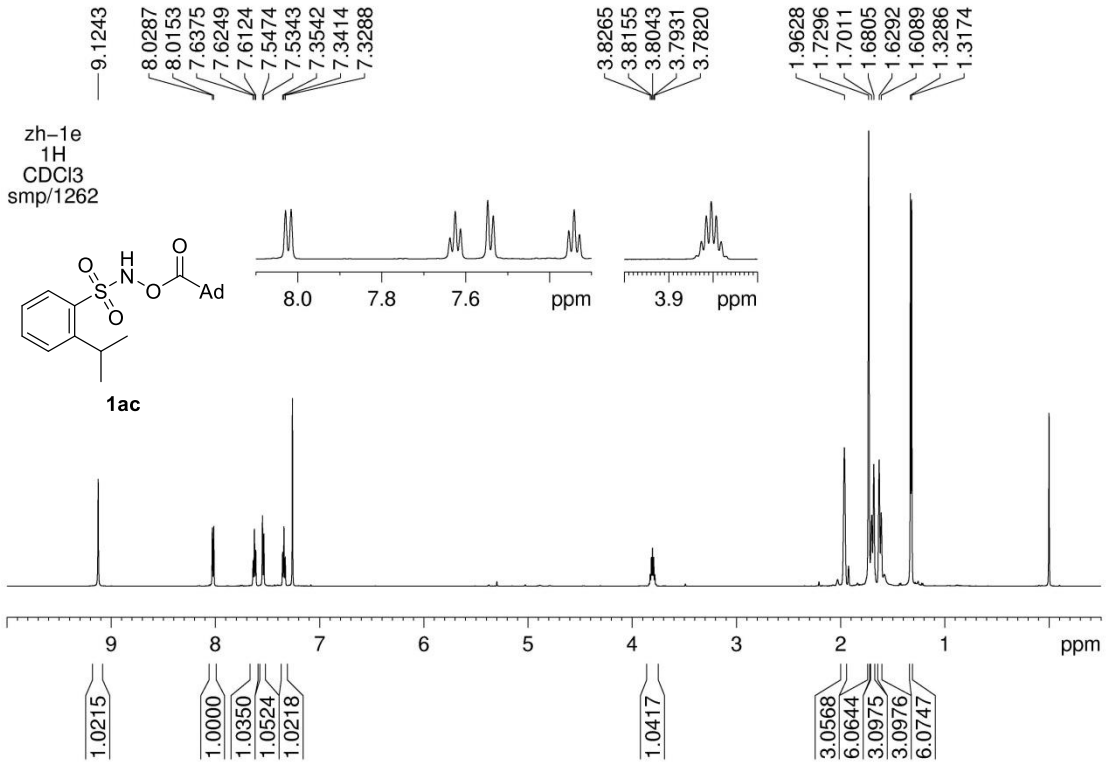
ZH-1b
13C
CDCl3
njl/1287
1ab
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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3.8265
3.8155
3.8043
3.7931
3.7820
1.9628
1.7296
1.7011
1.6805
1.6292
1.6089
1.3286
1.3174
zh-1e
1H
CDCl3
smp/1262
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7.8
7.6
ppm
3.9
ppm
1ac
9
8
7
6
5
4
3
2
1
ppm
1.0215
1.0000
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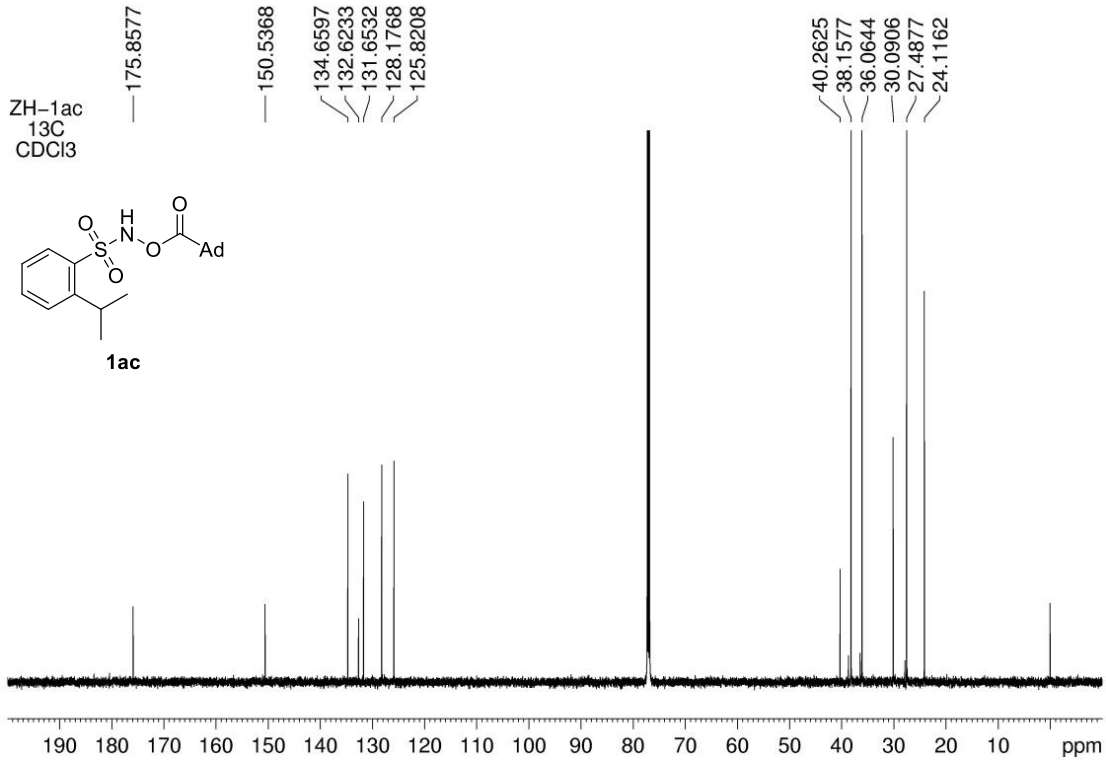
1.0524
1.0218
1.0417
3.0568
6.0644
3.0975
3.0976
6.0747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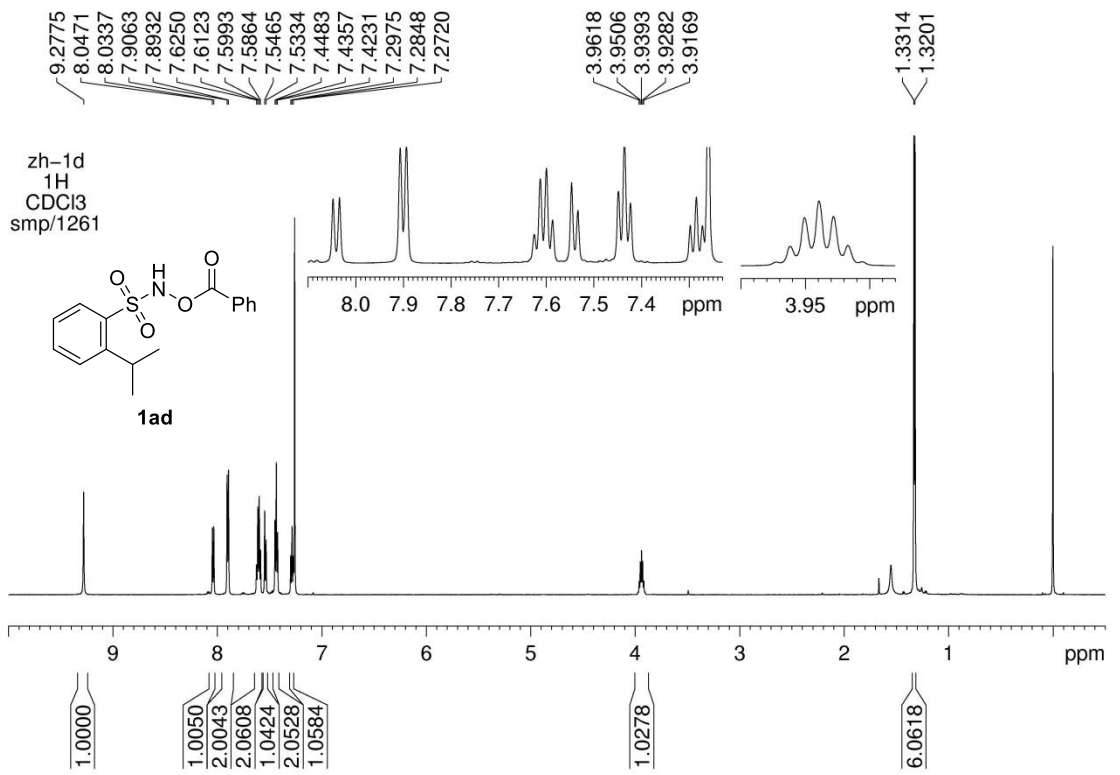
134.6597
132.6233
131.6532
128.1768
125.8208
40.2625
38.1577
36.0644
30.0906
27.4877
24.1162
ZH-1ac
13C
CDCl3
1ac
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.5465
7.5334
7.4483
7.4357
7.4231
7.2975
7.2848
7.2720
3.9618
3.9506
3.9393
3.9282
3.9169
1.3314
1.3201
zh-1d
1H
CDCl3
smp/1261
1ad
8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
3.95 ppm
9 8 7 6 5 4 3 2 1 ppm
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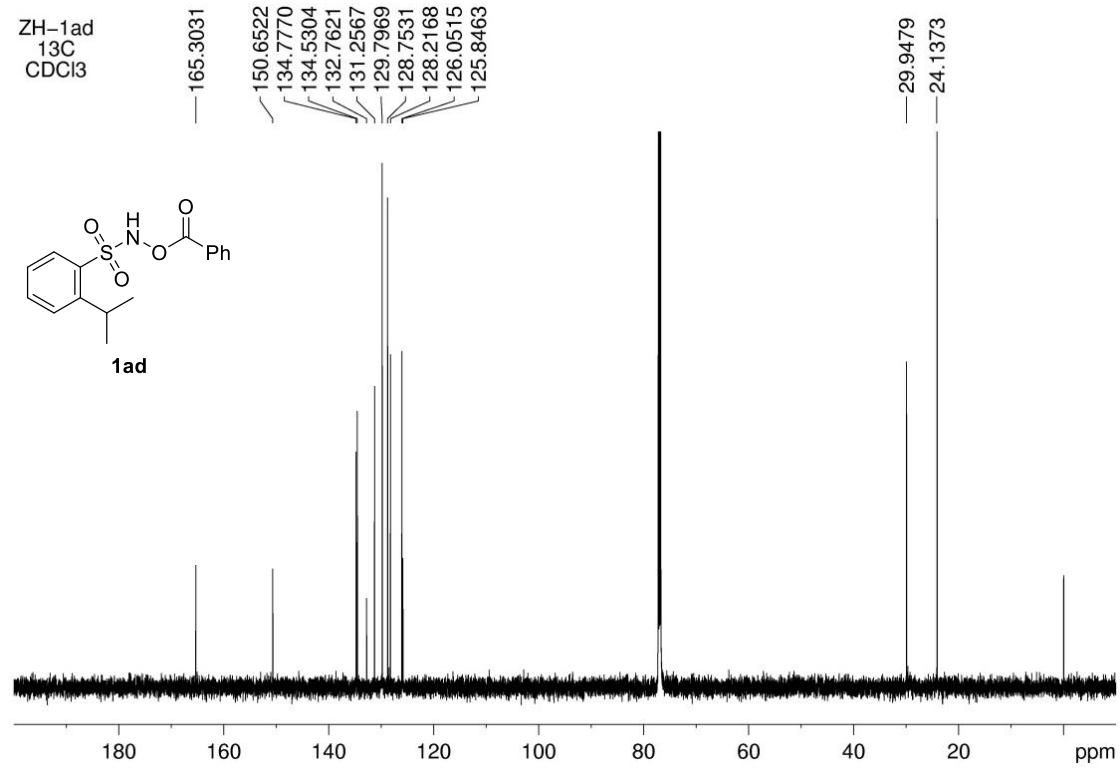
1.0050
2.0043
2.0608
1.0424
2.0528
1.0584
1.0278
6.0618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CDCl3
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134.5304
132.7621
131.2567
129.7969
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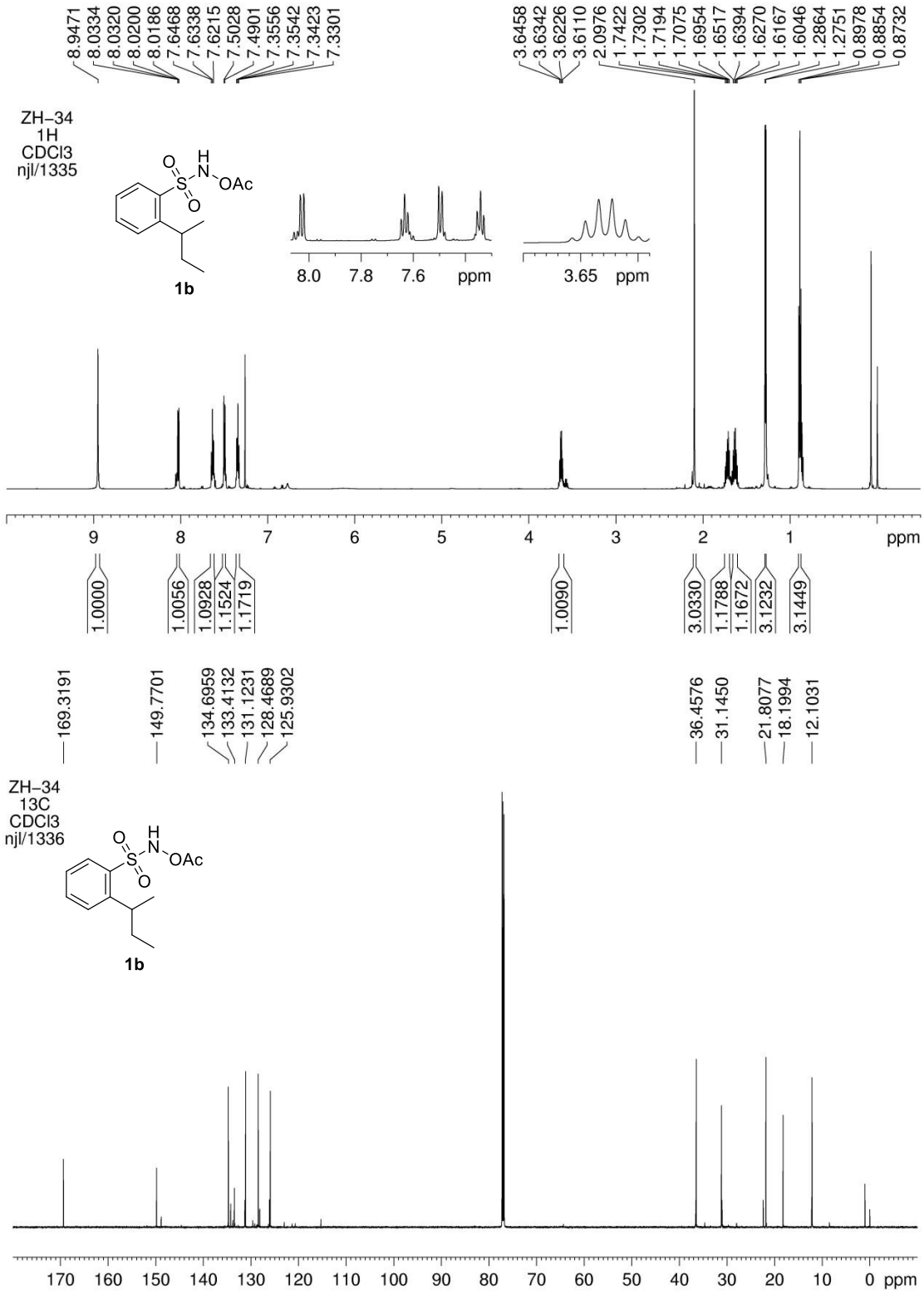
128.2168
126.0515
125.8463
29.9479
24.1373
1ad
180 160 140 120 100 80 60 40 20 ppm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7.3542
7.3423
7.3301
3.6458
3.6342
3.6226
3.6110
2.0976
1.7422
1.7302
1.7194
1.7075
1.6954
1.6517
1.6394
1.6270
1.6167
1.6046
1.2864
1.2751
0.8978
0.8854
0.8732
ZH–34
1H
CDCl3
njl/1335
1b
8.0 7.8 7.6 ppm
3.65 ppm
9 8 7 6 5 4 3 2 1 ppm
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1.0056
1.0928
1.1524
1.1719
1.0090
3.0330
1.1788
1.1672
3.1232
3.1449
169.3191
149.7701
134.6959
133.4132
131.1231
128.4689
125.9302
36.4576
31.1450
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13C
CDCl3
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1b
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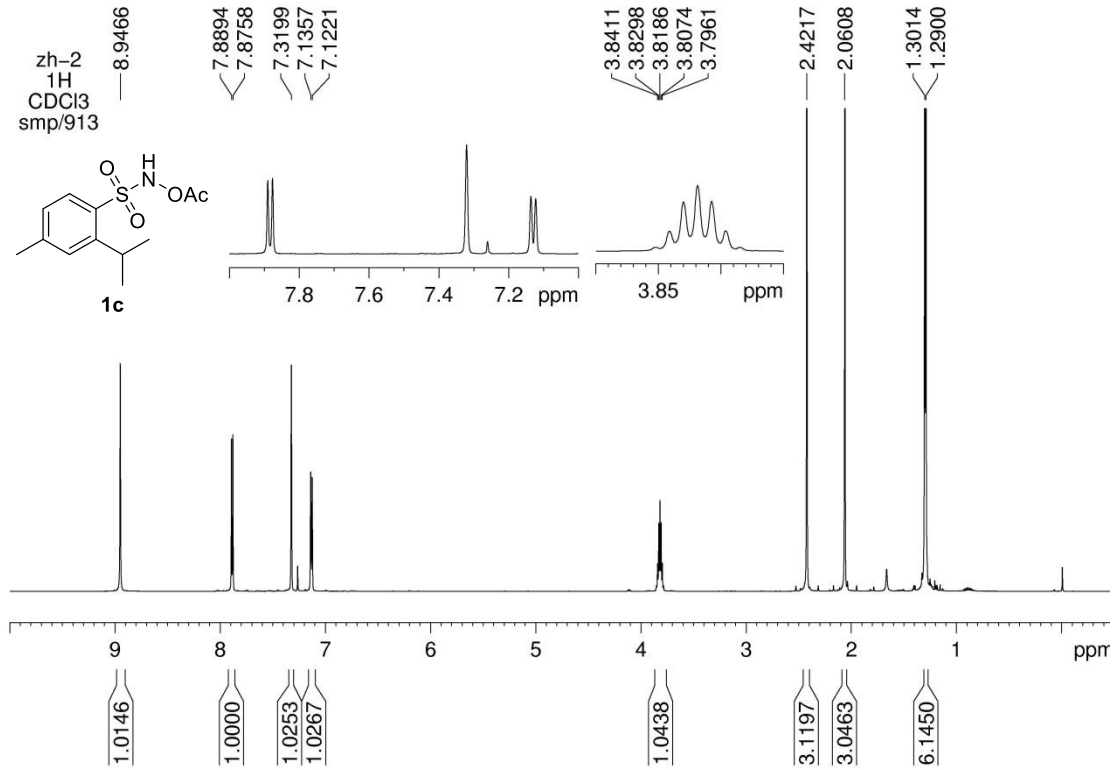
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7.3199
7.1357
7.1221
3.8411
3.8298
3.8186
3.8074
3.7961
2.4217
2.0608
1.3014
1.2900
1c
7.8
7.6
7.4
7.2 ppm
3.85 ppm
9
8
7
6
5
4
3
2
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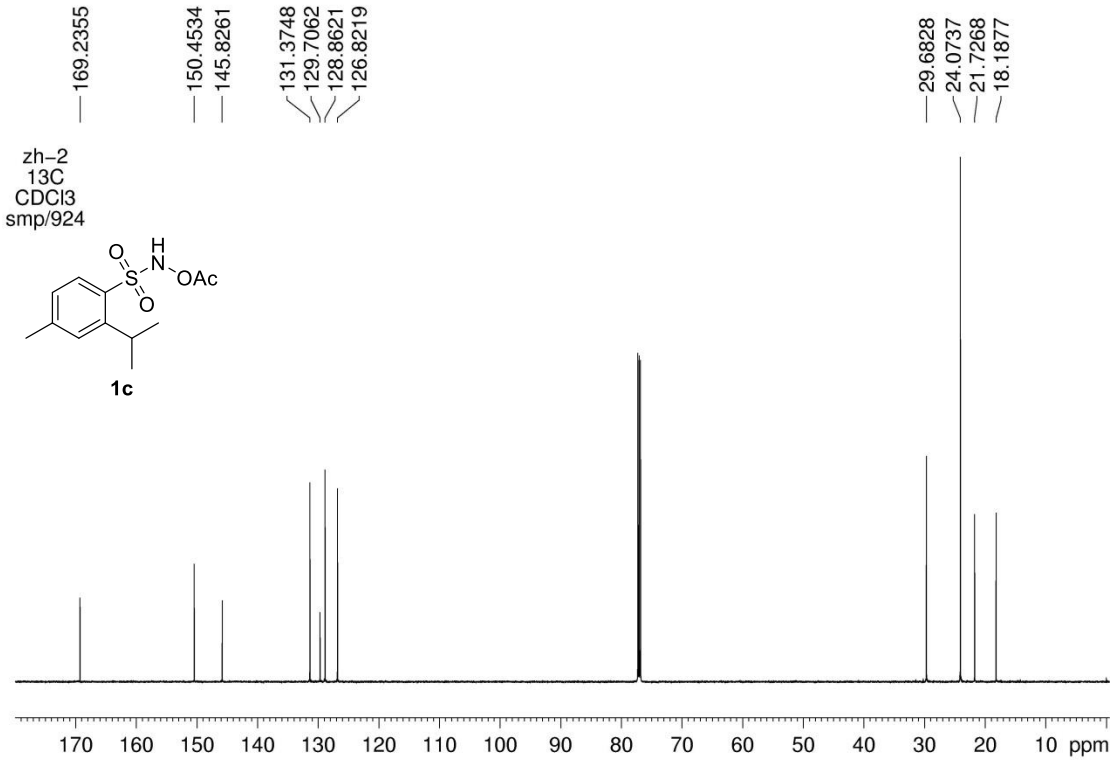
1.0267
1.0438
3.1197
3.0463
6.1450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24.0737
21.7268
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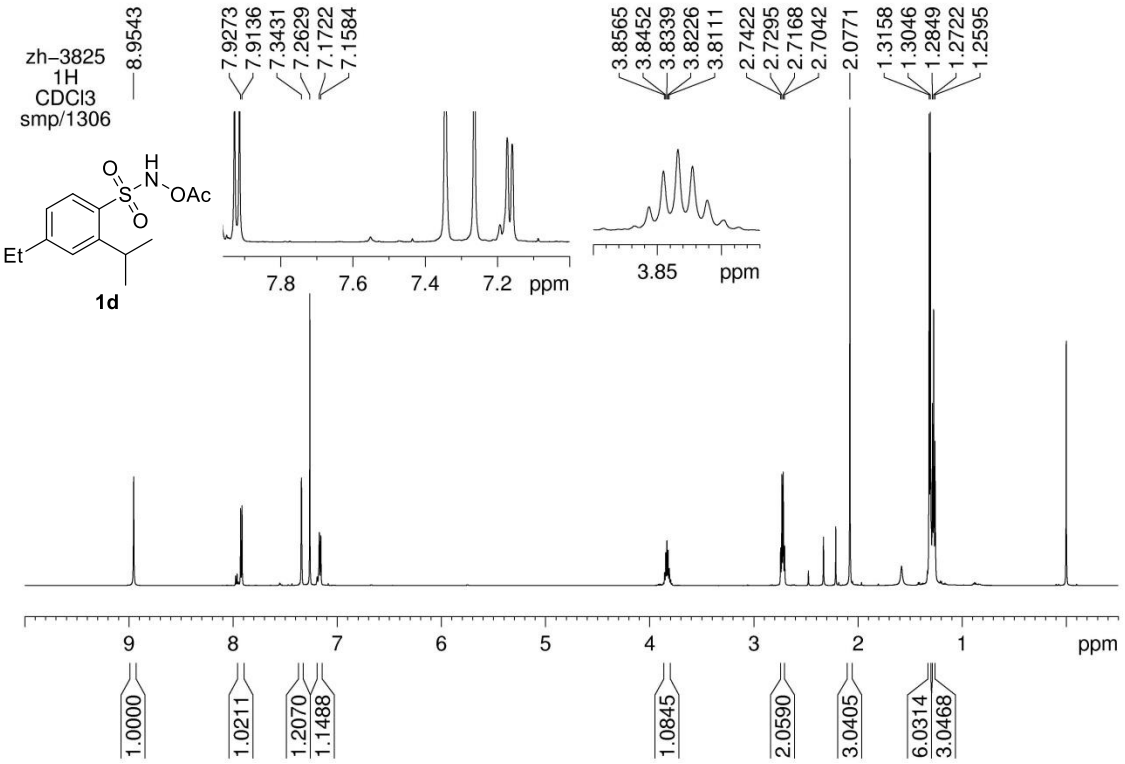
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm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3.8452
3.8339
3.8226
3.8111
2.7422
2.7295
2.7168
2.7042
2.0771
1.3158
1.3046
1.2849
1.2722
1.2595
Et
OAc
1d
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7.6
7.4
7.2
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3.85
ppm
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8
7
6
5
4
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2
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ppm
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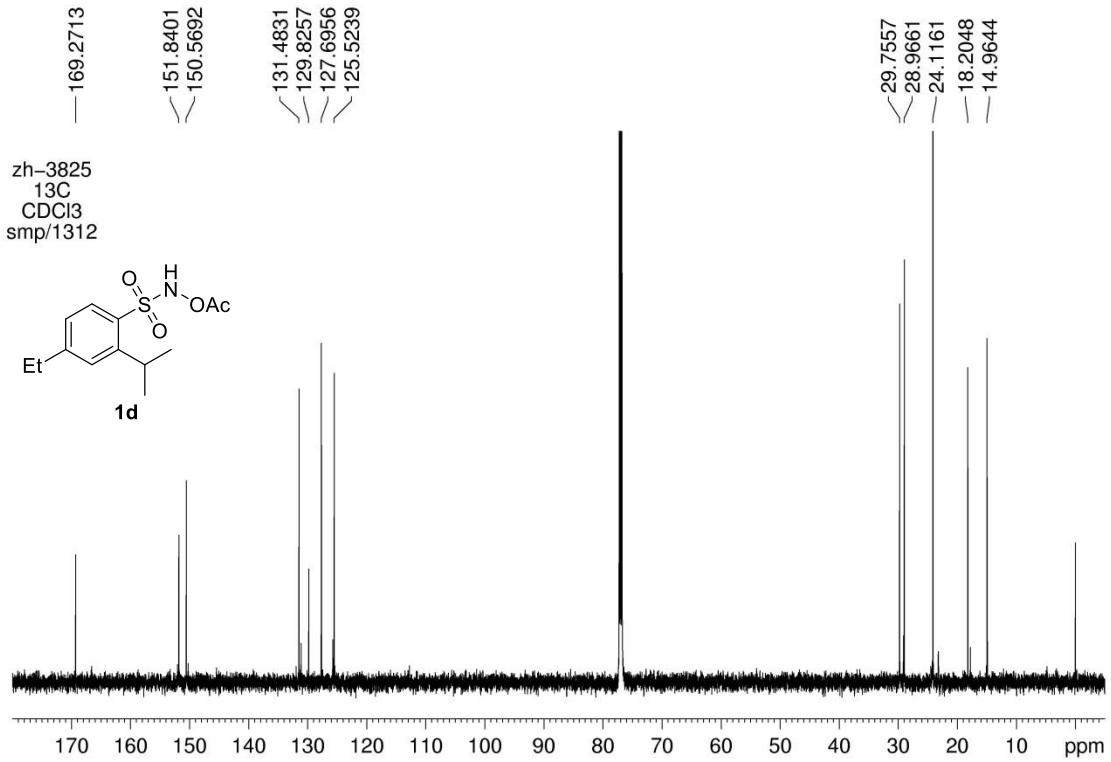
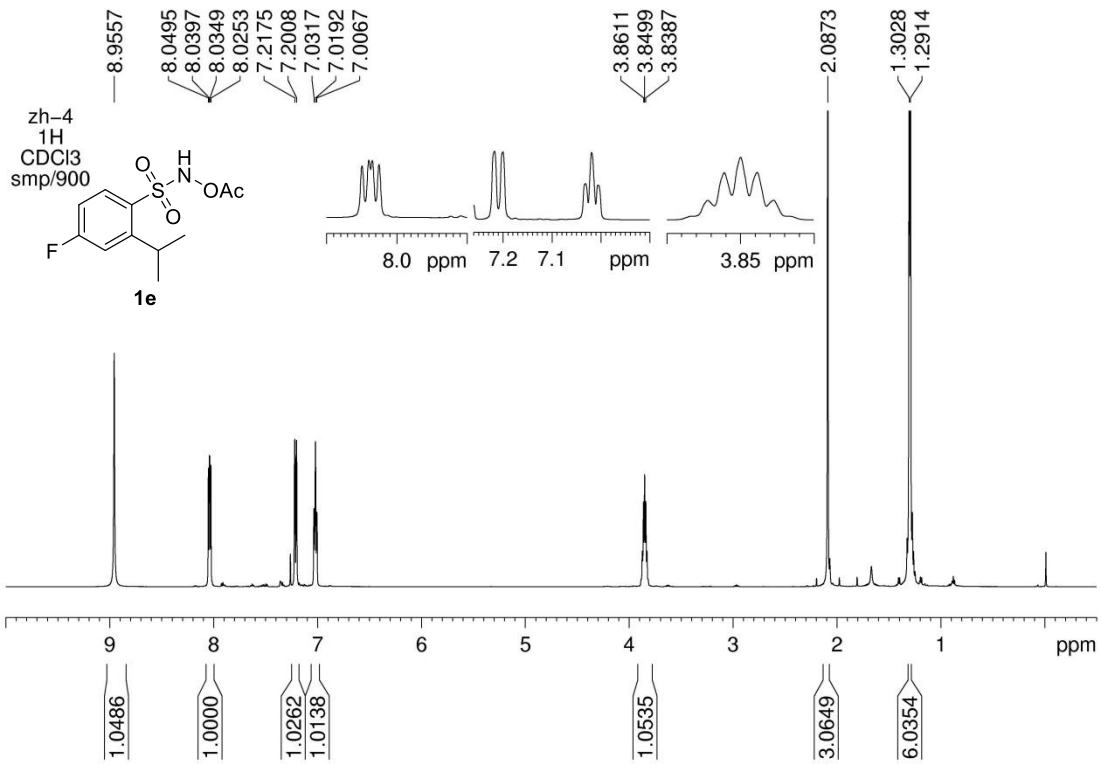
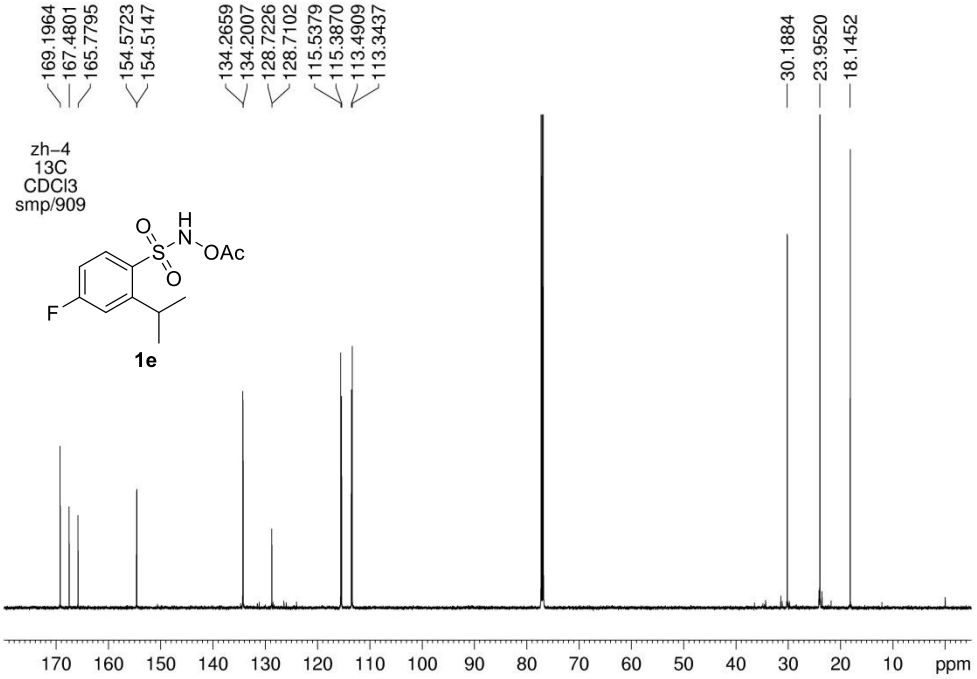
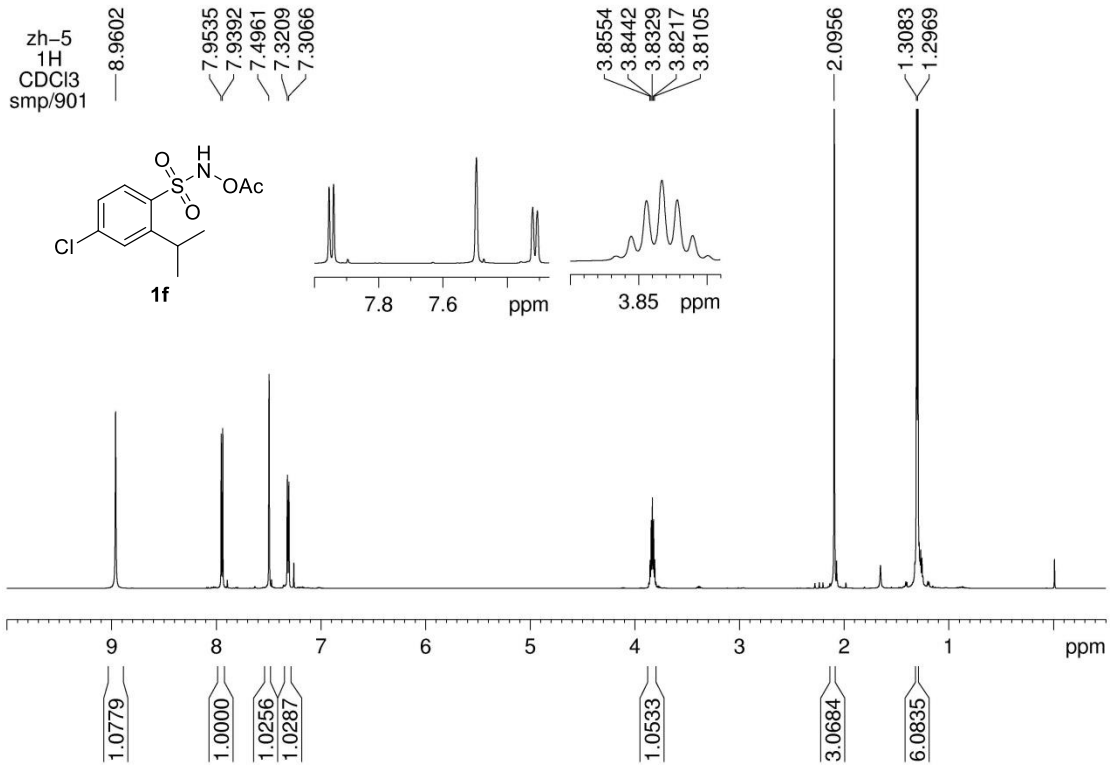
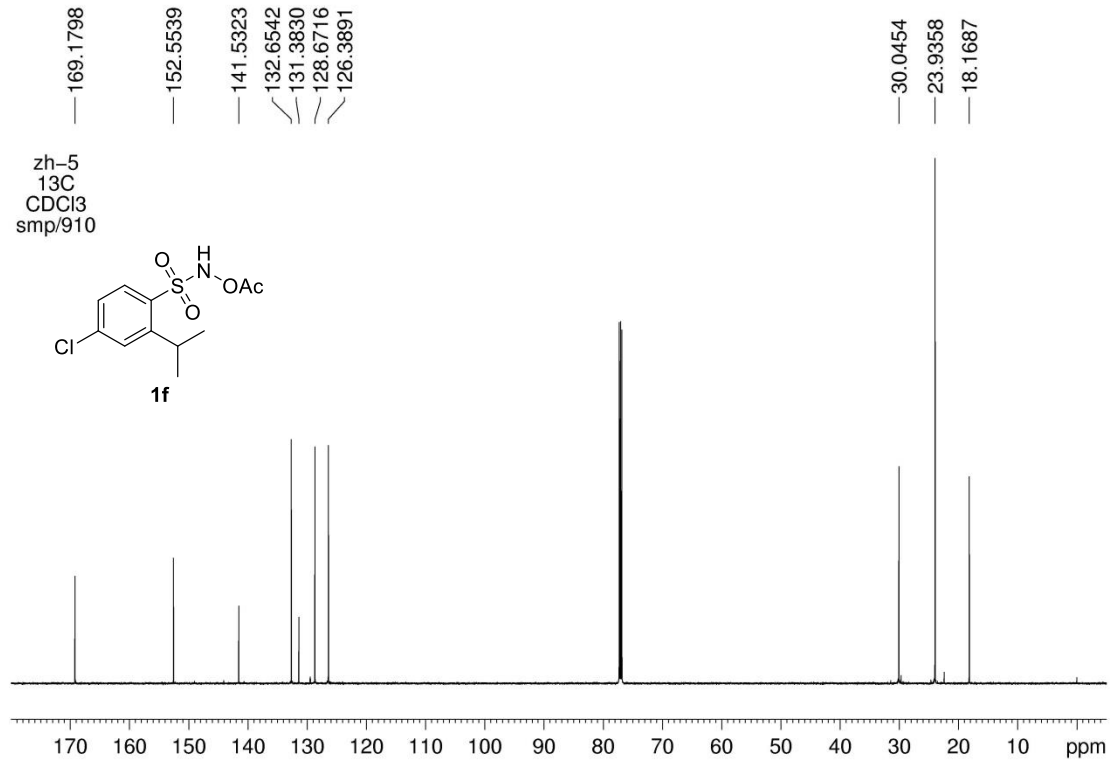
2.0590
3.0405
6.0314
3.0468

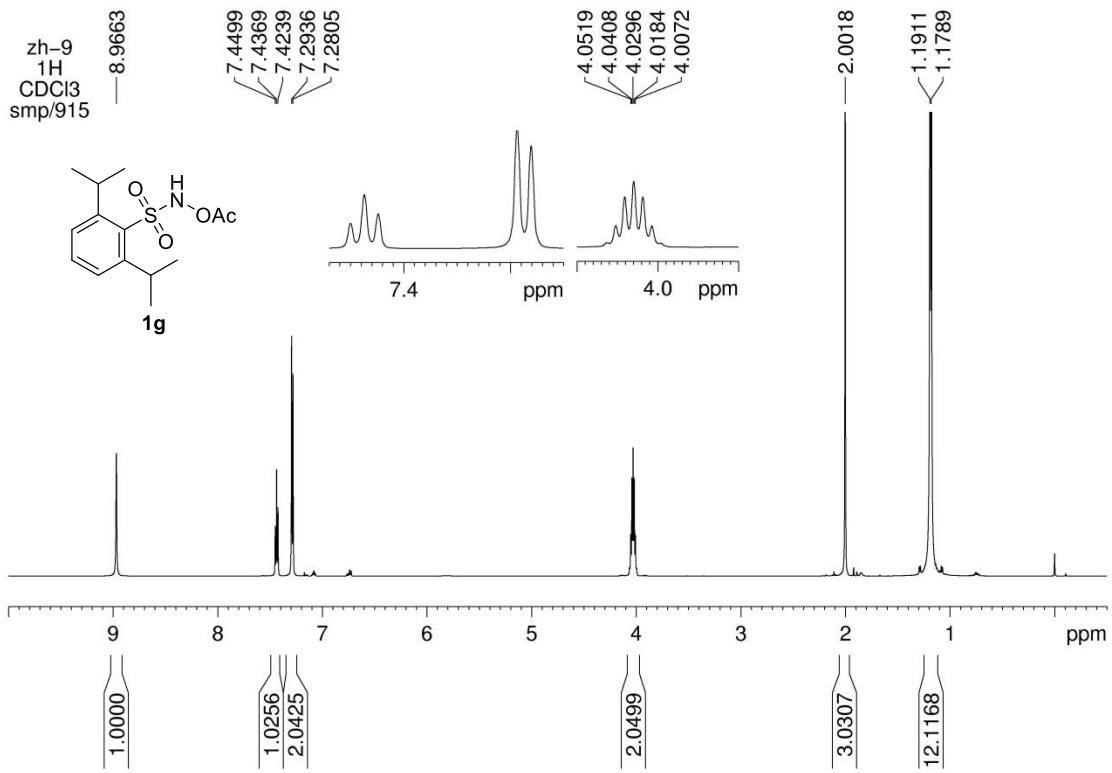

zh–3825
13C
CDCl3
smp/1312
169.2713
151.8401
150.5692
131.4831
129.8257
127.6956
125.5239
29.7557
28.9661
24.1161
18.2048
14.9644
Et
OAc
1d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

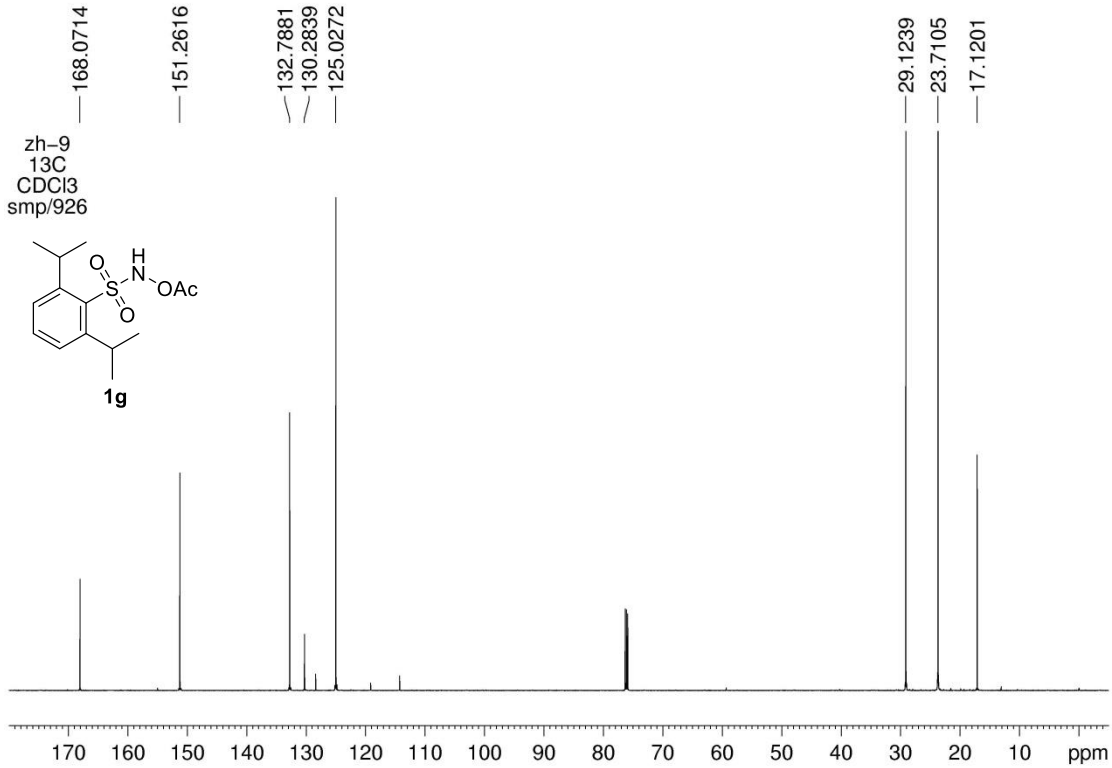

8.9557
8.0495
8.0397
8.0349
8.0253
7.2175
7.2008
7.0317
7.0192
7.0067
3.8611
3.8499
3.8387
2.0873
1.3028
1.2914
zh–4
1H
CDCl3
smp/900
1e
8.0 ppm
7.2 7.1 ppm
3.85 ppm
1.0486
1.0000
1.0262
1.0138
1.0535
3.0649
6.0354
ppm

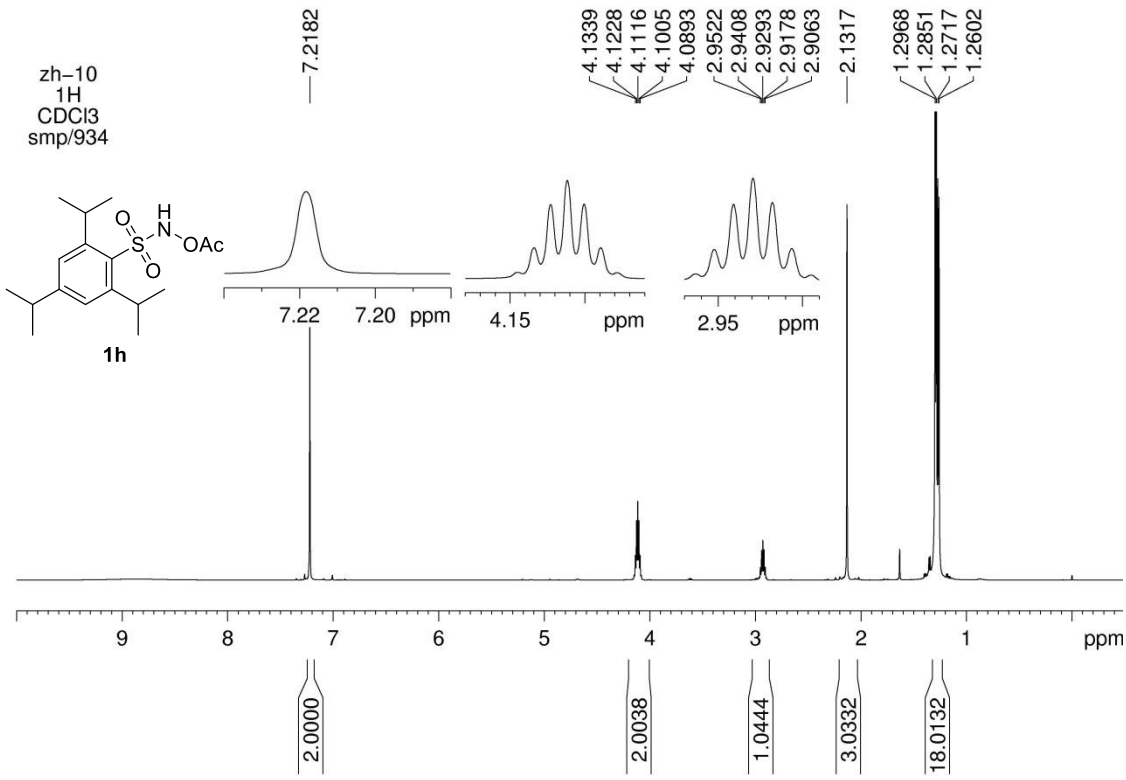

169.1964
167.4801
165.7795
154.5723
154.5147
134.2659
134.2007
128.7226
128.7102
115.5379
115.3870
113.4909
113.3437
30.1884
23.9520
18.1452
zh–4
13C
CDCl3
smp/909
1e
ppm

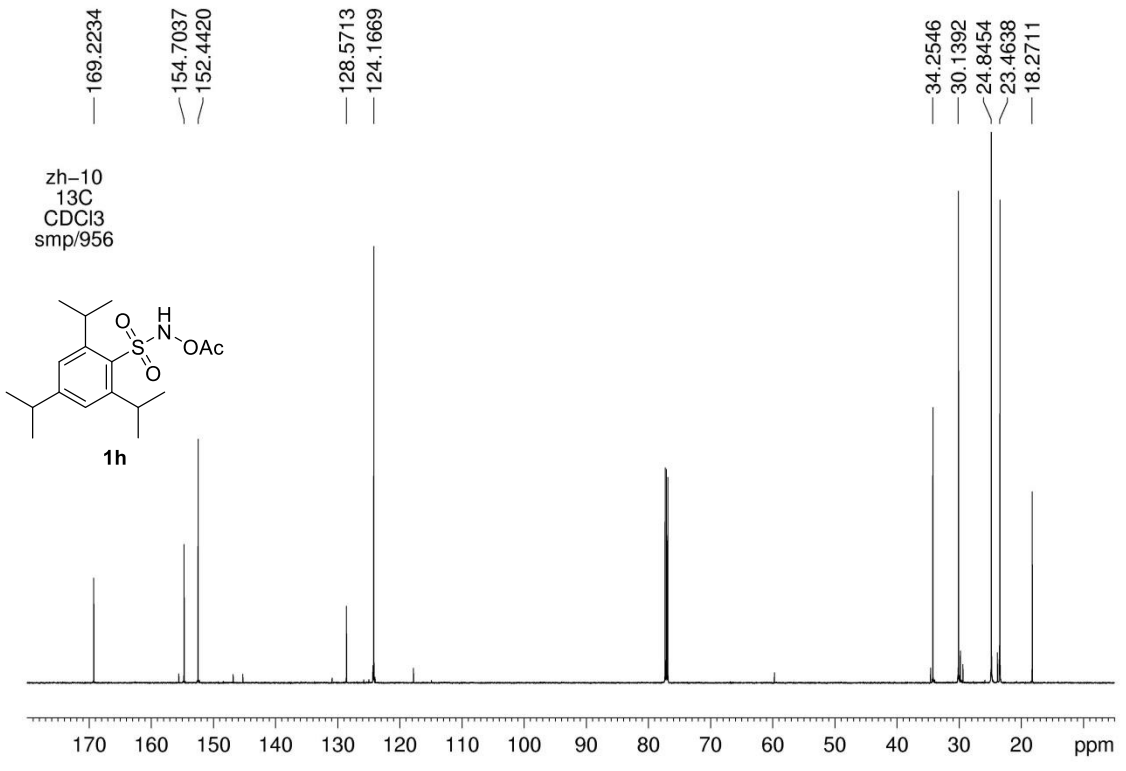

zh–5
1H
CDCl3
smp/901
8.9602
7.9535
7.9392
7.4961
7.3209
7.3066
3.8554
3.8442
3.8329
3.8217
3.8105
2.0956
1.3083
1.2969
1f
7.8
7.6
ppm
3.85
ppm
9
8
7
6
5
4
3
2
1
ppm
1.0779
1.0000
1.0256
1.0287
1.0533
3.0684
6.0835

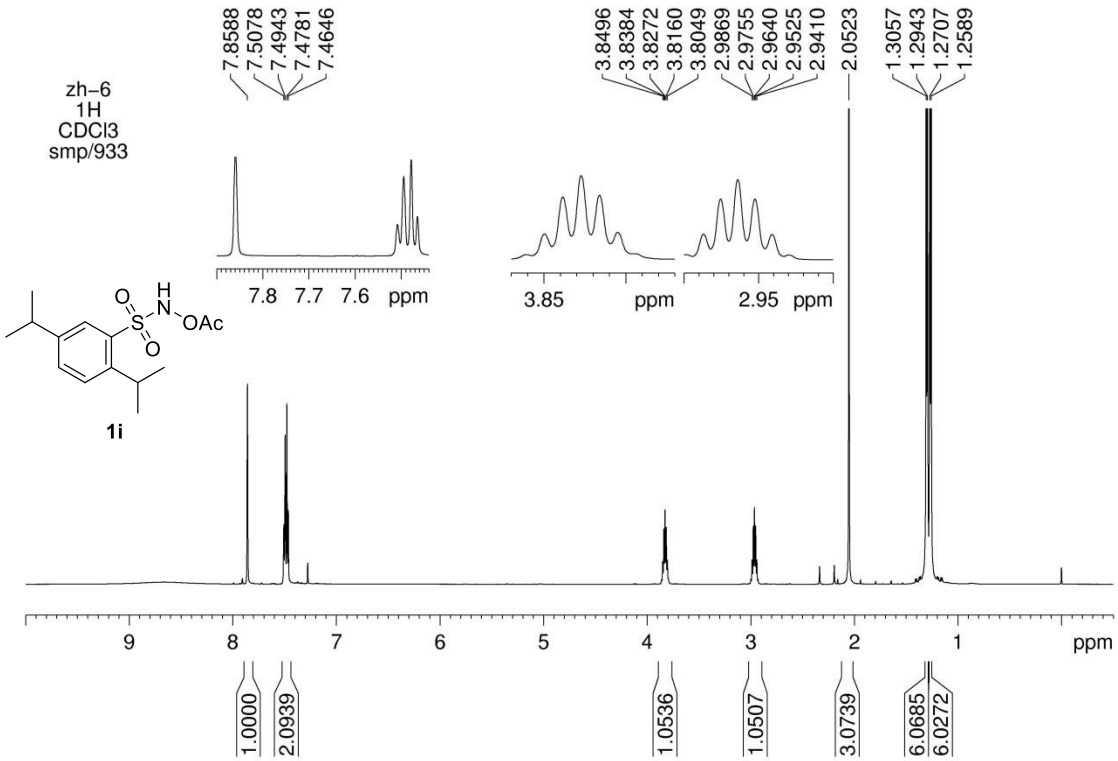

169.1798
152.5539
141.5323
132.6542
131.3830
128.6716
126.3891
30.0454
23.9358
18.1687
zh–5
13C
CDCl3
smp/910
1f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

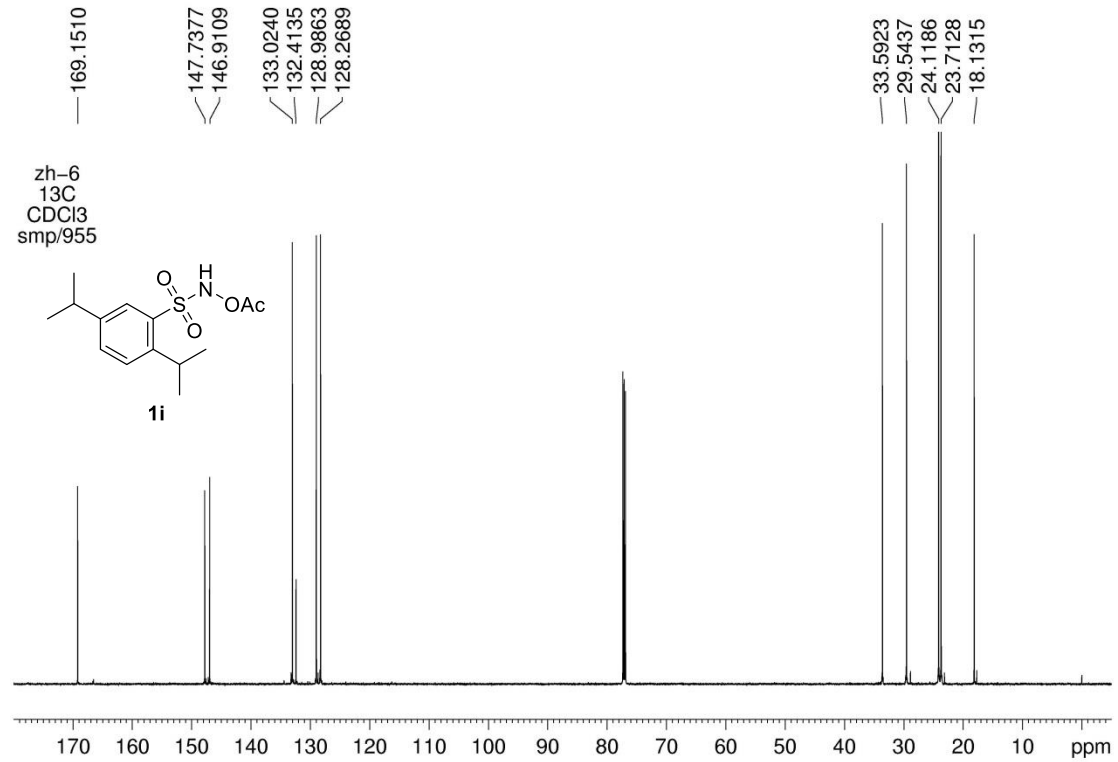

zh–9
1H
CDCl3
smp/915
8.9663
7.4499
7.4369
7.4239
7.2936
7.2805
4.0519
4.0408
4.0296
4.0184
4.0072
2.0018
1.1911
1.1789
1g
7.4 ppm
4.0 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0000
1.0256
2.0425
2.0499
3.0307
12.1168

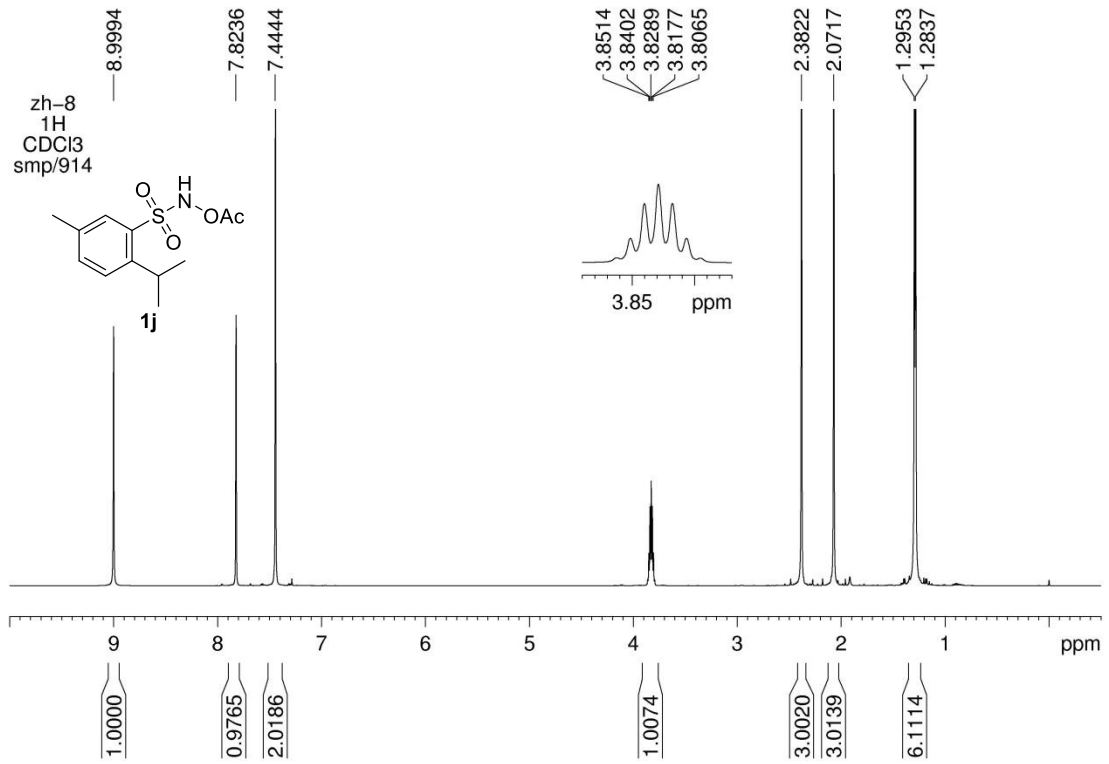

zh–9
13C
CDCl3
smp/926
168.0714
151.2616
132.7881
130.2839
125.0272
29.1239
23.7105
17.1201
1g
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

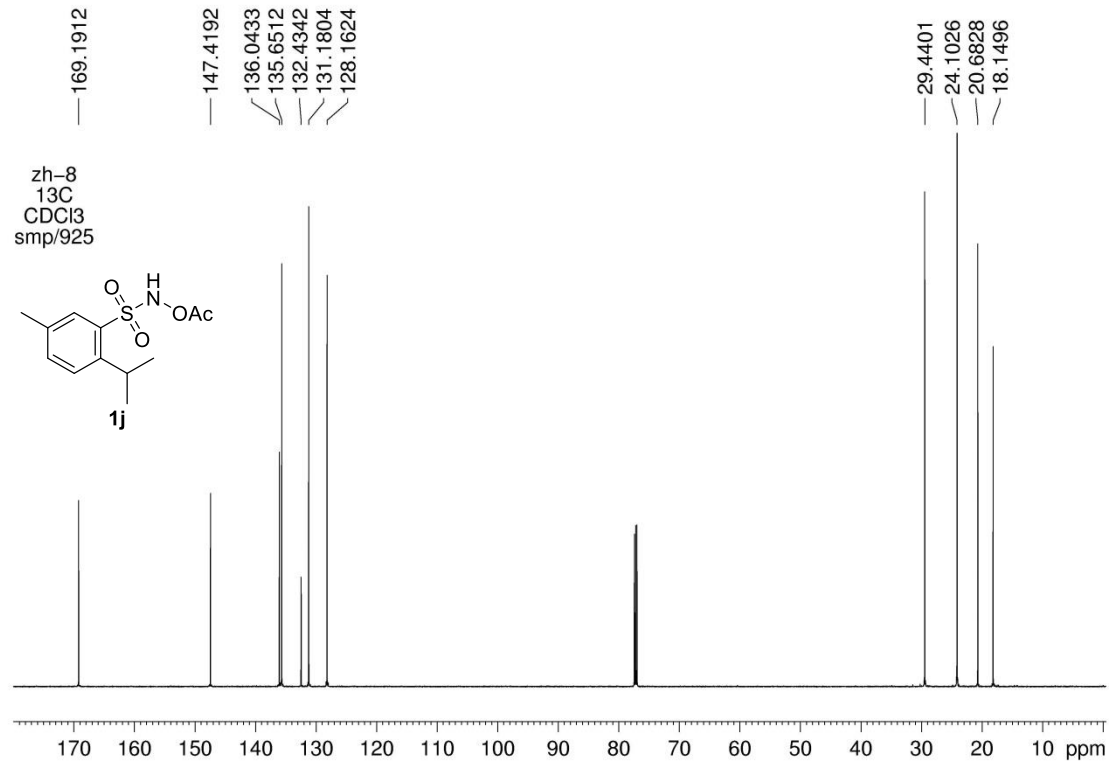

zh–10
1H
CDCl3
smp/934
7.2182
4.1339
4.1228
4.1116
4.1005
4.0893
2.9522
2.9408
2.9293
2.9178
2.9063
2.1317
1.2968
1.2851
1.2717
1.2602
7.22
7.20
ppm
4.15
ppm
2.95
ppm
1h
9
8
7
6
5
4
3
2
1
ppm
2.0000
2.0038
1.0444
3.0332
18.0132

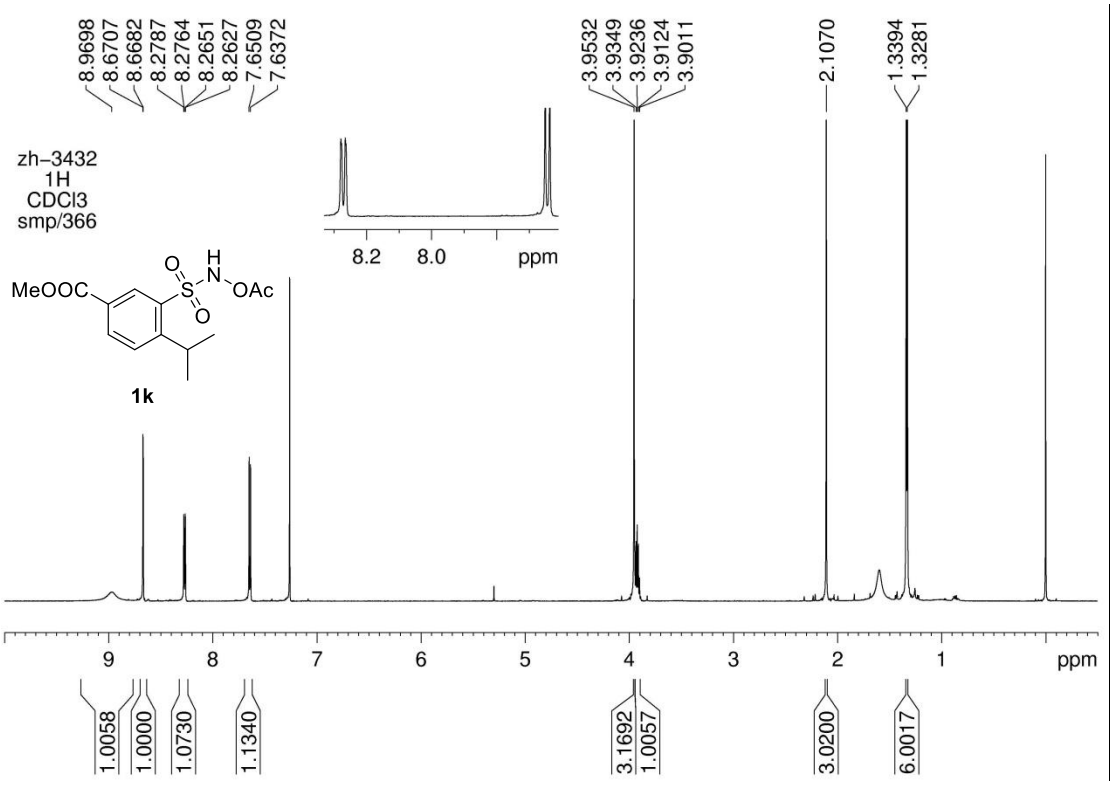

169.2234
154.7037
152.4420
128.5713
124.1669
34.2546
30.1392
24.8454
23.4638
18.2711
zh–10
13C
CDCl3
smp/956
1h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

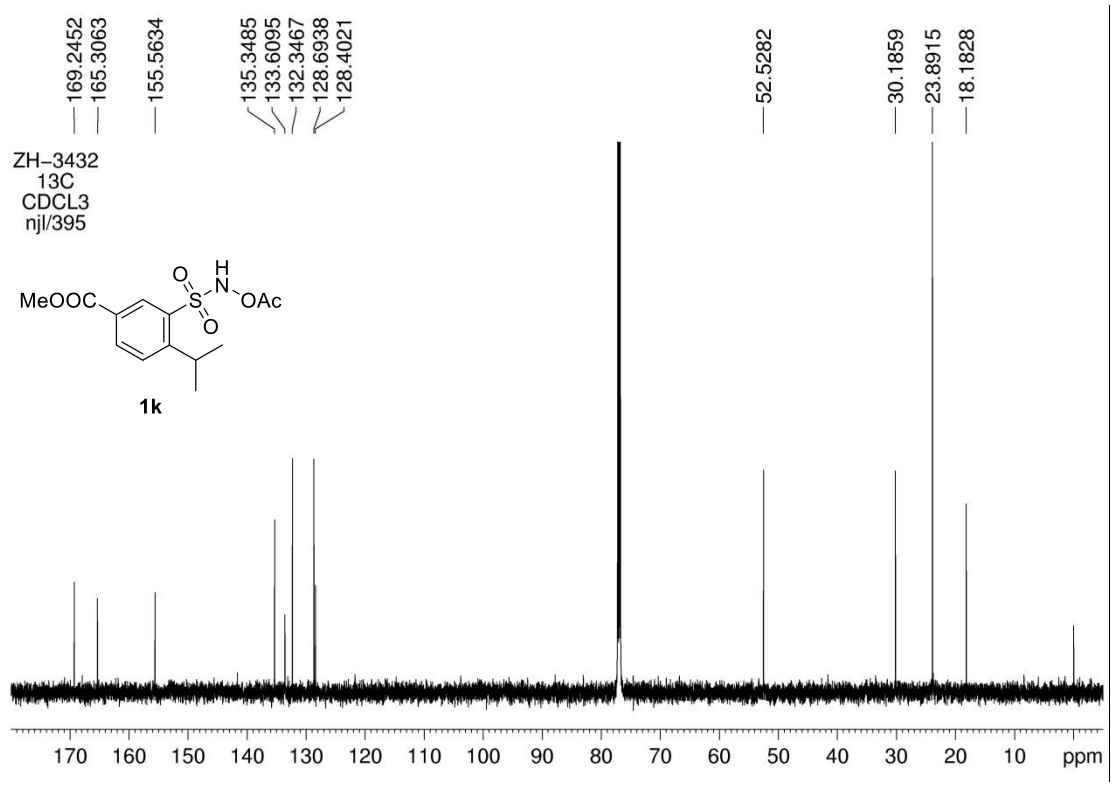

zh–6
1H
CDCl3
smp/933
7.8588
7.5078
7.4943
7.4781
7.4646
3.8496
3.8384
3.8272
3.8160
3.8049
2.9869
2.9755
2.9640
2.9525
2.9410
2.0523
1.3057
1.2943
1.2707
1.2589
7.8 7.7 7.6 ppm
3.85 ppm
2.95 ppm
1i
9 8 7 6 5 4 3 2 1 ppm
1.0000
2.0939
1.0536
1.0507
3.0739
6.0685
6.0272

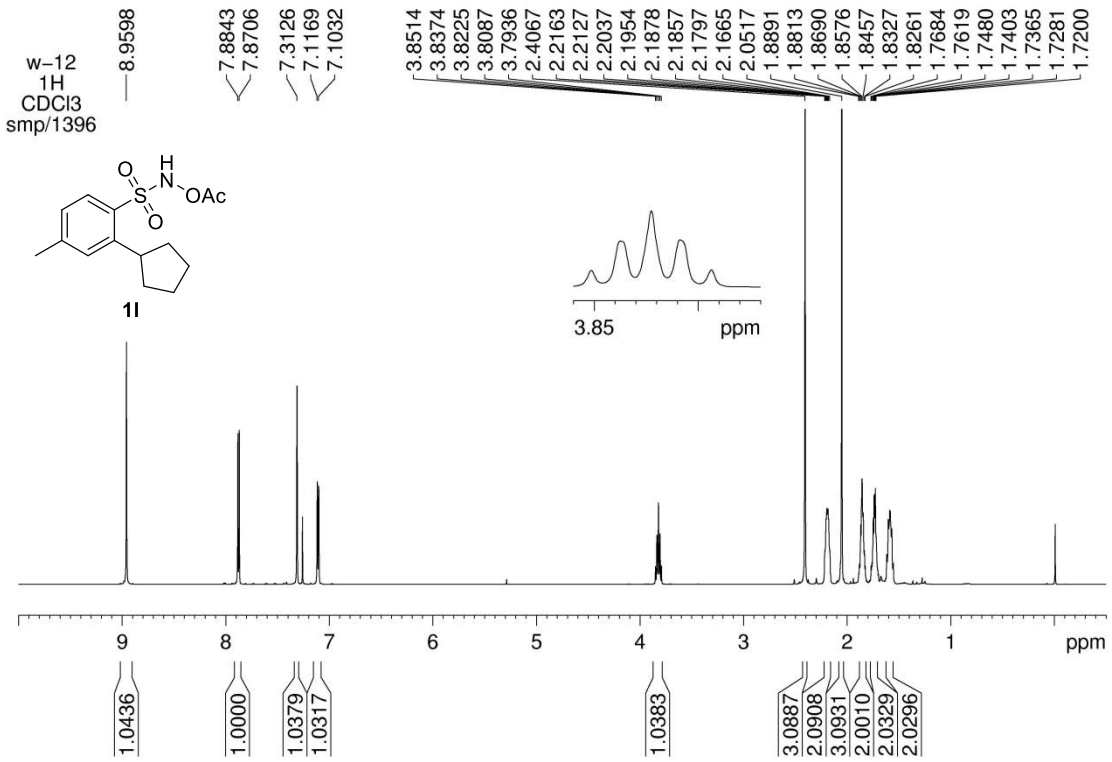

169.1510
147.7377
146.9109
133.0240
132.4135
128.9863
128.2689
33.5923
29.5437
24.1186
23.7128
18.1315
zh–6
13C
CDCl3
smp/955
1i
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

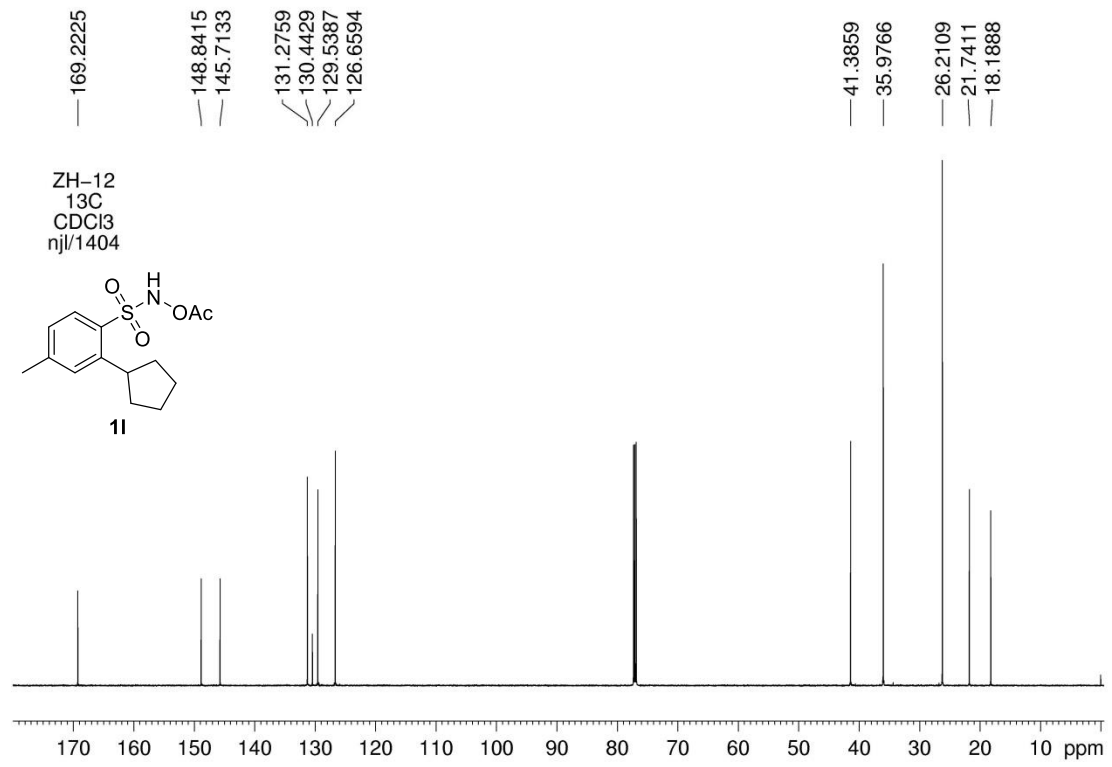

8.9994
7.8236
7.4444
3.8514
3.8402
3.8289
3.8177
3.8065
2.3822
2.0717
1.2953
1.2837
zh–8
1H
CDCl3
smp/914
1j
3.85 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0000
0.9765
2.0186
1.0074
3.0020
3.0139
6.1114

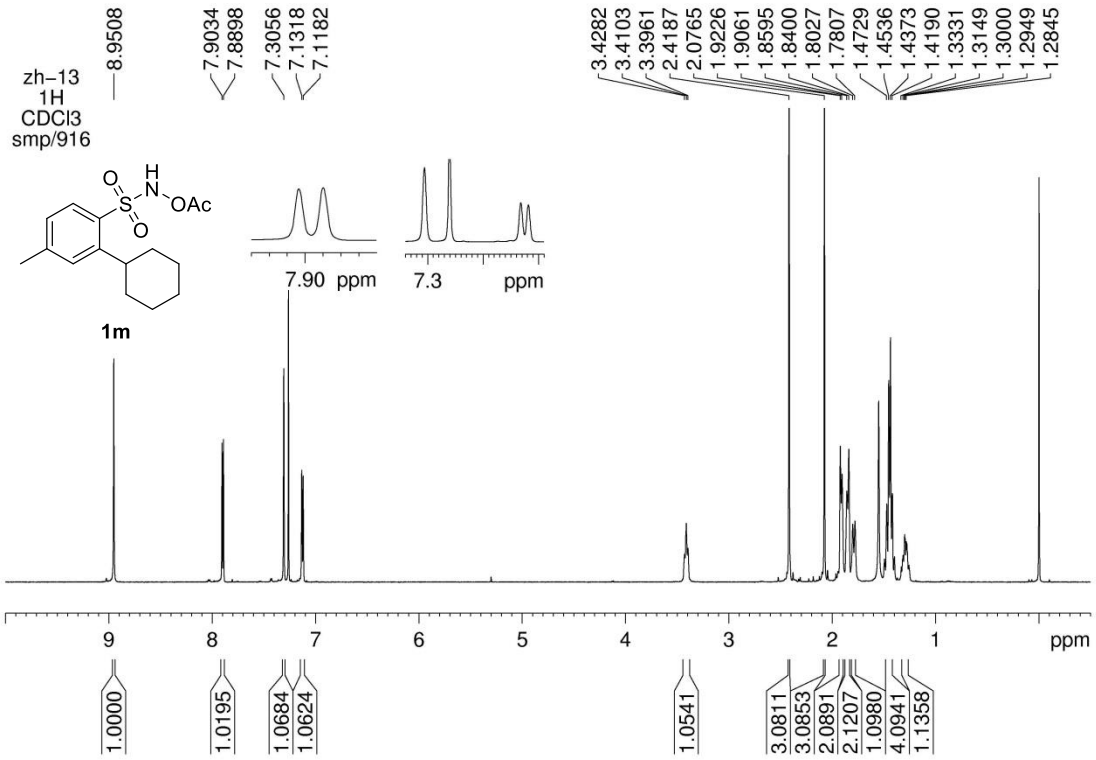

169.1912
147.4192
136.0433
135.6512
132.4342
131.1804
128.1624
29.4401
24.1026
20.6828
18.1496
zh–8
13C
CDCl3
smp/925
1j
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

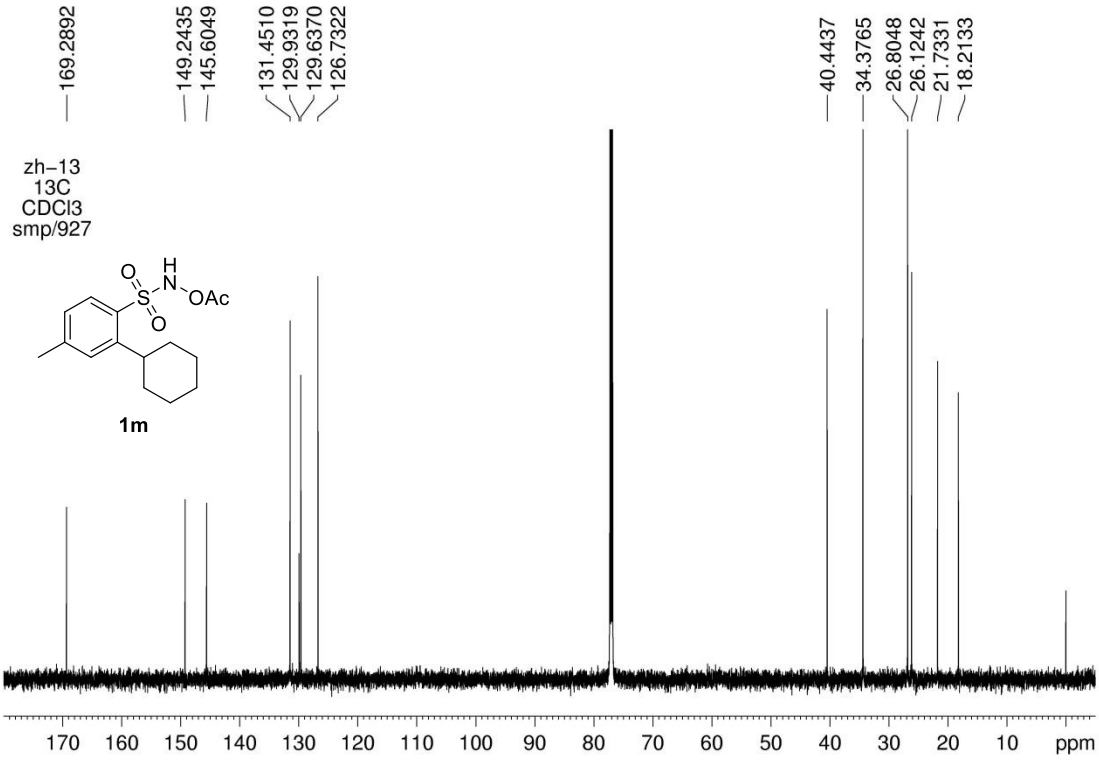

8.9698
8.6707
8.6682
8.2787
8.2764
8.2651
8.2627
7.6509
7.6372
3.9532
3.9349
3.9236
3.9124
3.9011
2.1070
1.3394
1.3281
zh–3432
1H
CDCl3
smp/366
8.2
8.0
ppm
MeOOC
O
S
O
H
N
OAc
1k
9
8
7
6
5
4
3
2
1
ppm
1.0058
1.0000
1.0730
1.1340
3.1692
1.0057
3.0200
6.0017

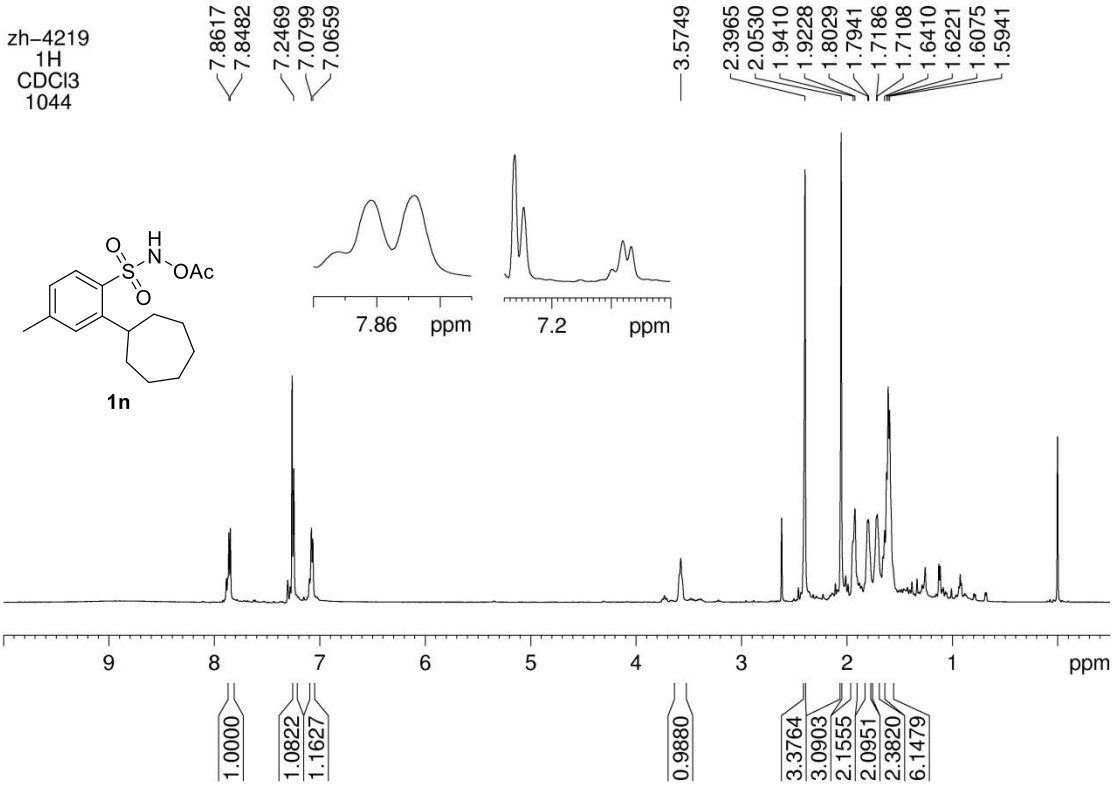

169.2452
165.3063
155.5634
135.3485
133.6095
132.3467
128.6938
128.4021
52.5282
30.1859
23.8915
18.1828
ZH–3432
13C
CDCL3
njl/395
MeOOC
O
S
O
H
N
OAc
1k
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

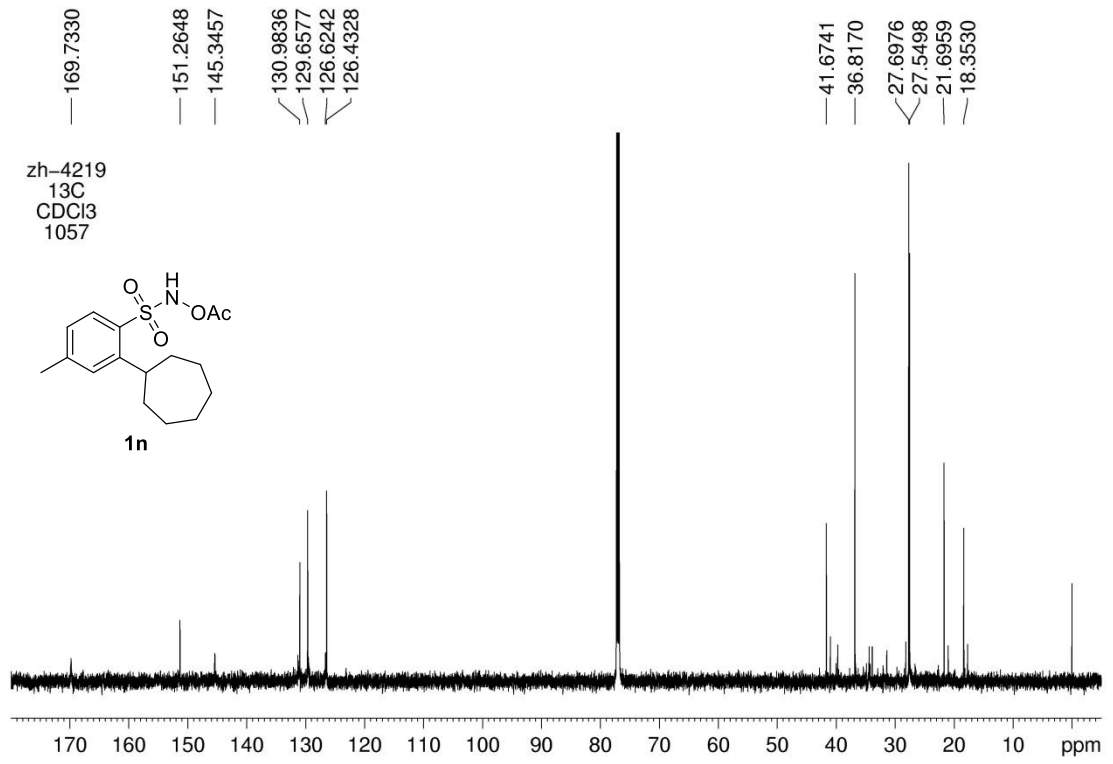

w–12
1H
CDCl3
smp/1396
8.9598
7.8843
7.8706
7.3126
7.1169
7.1032
3.8514
3.8374
3.8225
3.8087
3.7936
2.4067
2.2163
2.2127
2.2037
2.1954
2.1878
2.1857
2.1797
2.1665
2.0517
1.8891
1.8813
1.8690
1.8576
1.8457
1.8327
1.8261
1.7684
1.7619
1.7480
1.7403
1.7365
1.7281
1.7200
1I
3.85
ppm
9
8
7
6
5
4
3
2
1
ppm
1.0436
1.0000
1.0379
1.0317
1.0383
3.0887
2.0908
3.0931
2.0010
2.0329
2.0296

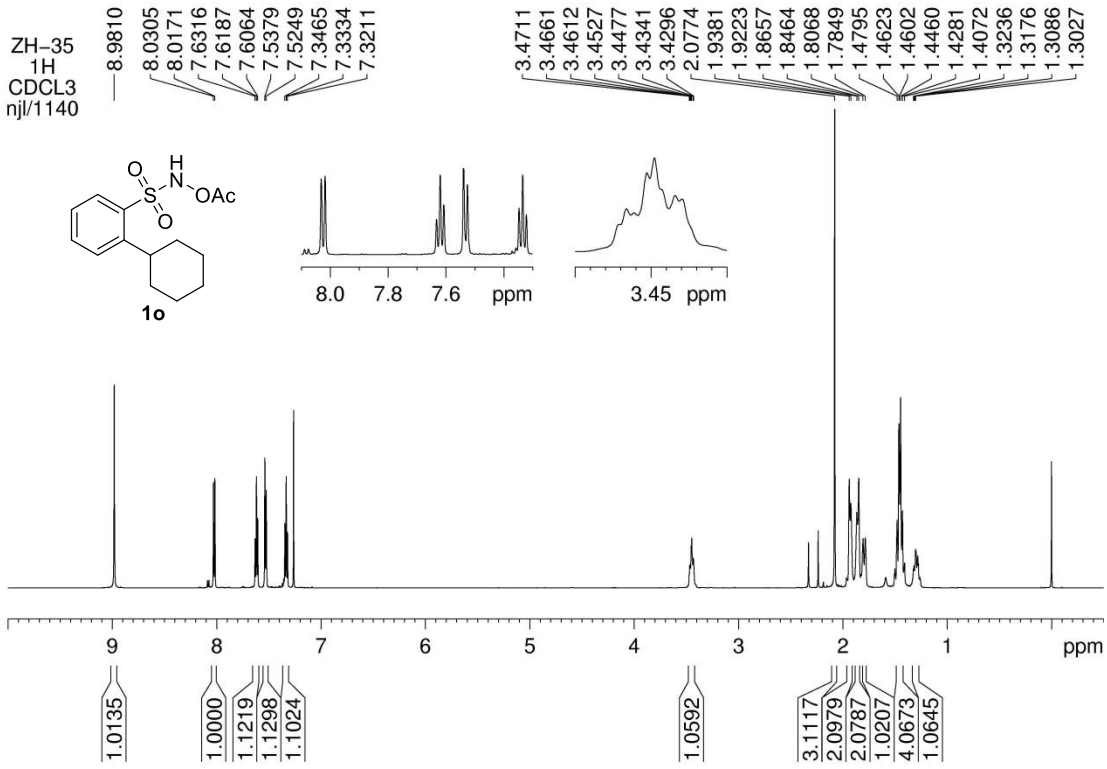

169.2225
148.8415
145.7133
131.2759
130.4429
129.5387
126.6594
41.3859
35.9766
26.2109
21.7411
18.1888
ZH–12
13C
CDCl3
njl/1404
1I
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

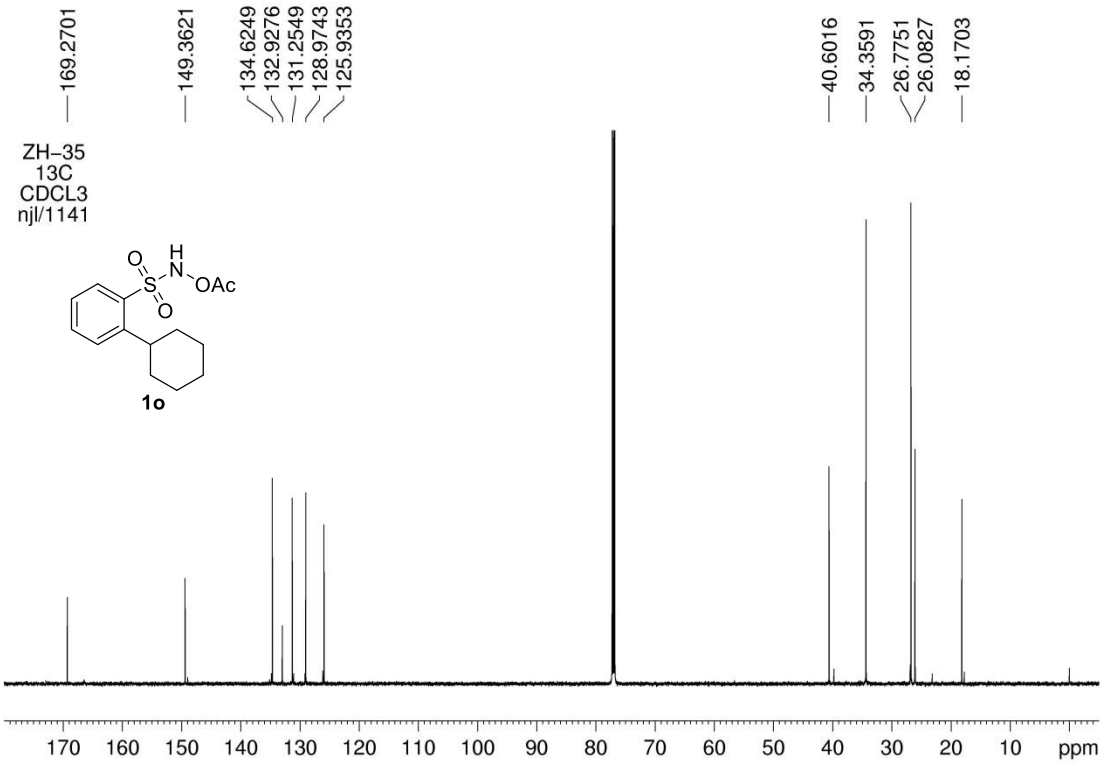

zh–13
1H
CDCl3
smp/916
8.9508
7.9034
7.8898
7.3056
7.1318
7.1182
3.4282
3.4103
3.3961
2.4187
2.0765
1.9226
1.9061
1.8595
1.8400
1.8027
1.7807
1.4729
1.4536
1.4373
1.4190
1.3331
1.3149
1.3000
1.2949
1.2845
7.90 ppm
7.3 ppm
1m
ppm
1.0000
1.0195
1.0684
1.0624
1.0541
3.0811
3.0853
2.0891
2.1207
1.0980
4.0941
1.1358

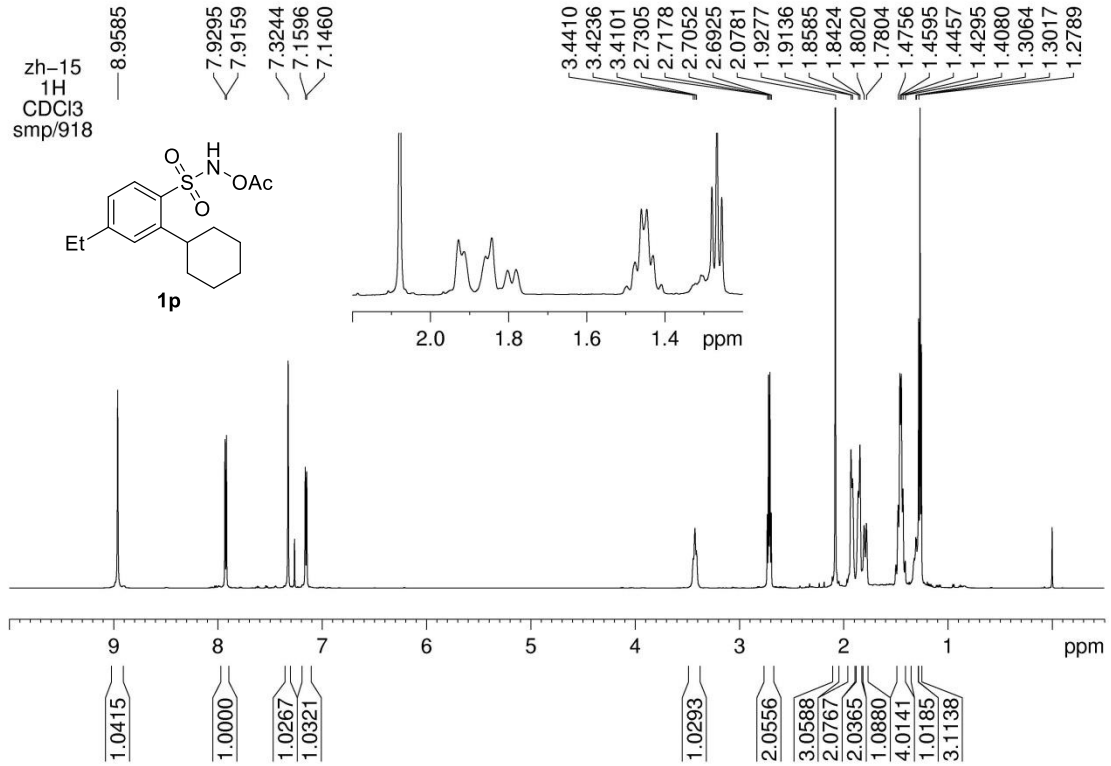

zh–13
13C
CDCl3
smp/927
169.2892
149.2435
145.6049
131.4510
129.9319
129.6370
126.7322
40.4437
34.3765
26.8048
26.1242
21.7331
18.2133
1m
ppm

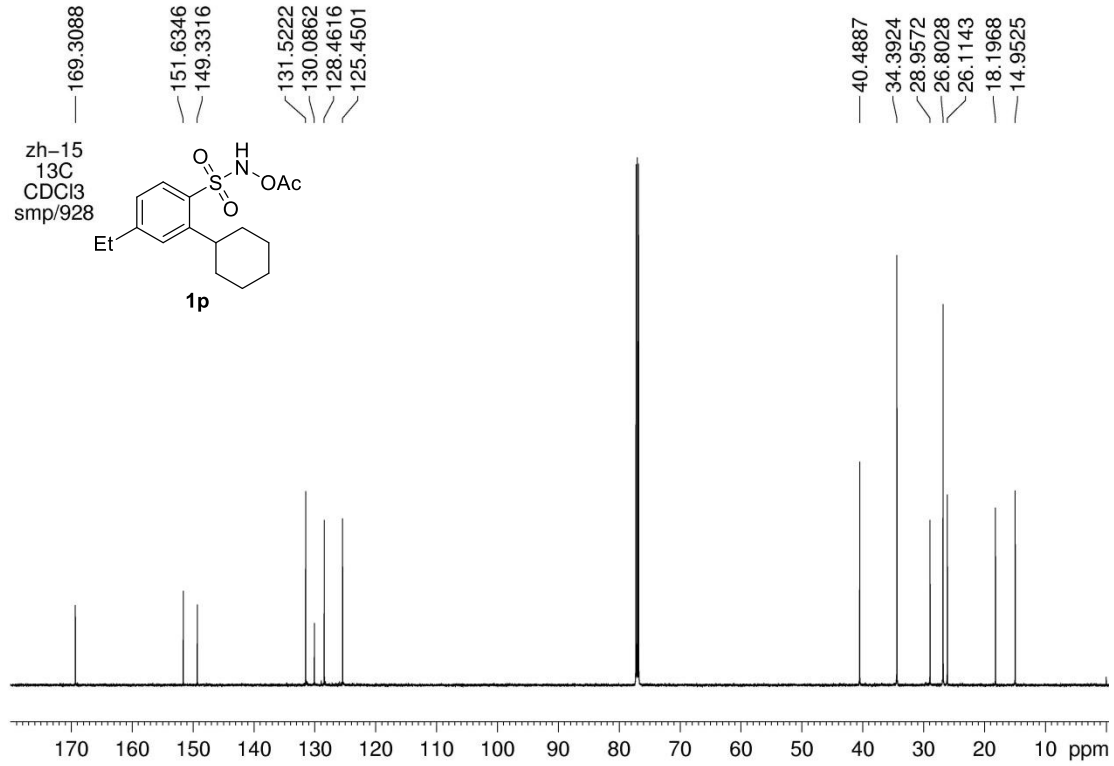

zh–4219
1H
CDCl3
1044
7.8617
7.8482
7.2469
7.0799
7.0659
3.5749
2.3965
2.0530
1.9410
1.9228
1.8029
1.7941
1.7186
1.7108
1.6410
1.6221
1.6075
1.5941
7.86 ppm
7.2 ppm
1n
9 8 7 6 5 4 3 2 1 ppm
1.0000
1.0822
1.1627
0.9880
3.3764
3.0903
2.1555
2.0951
2.3820
6.1479

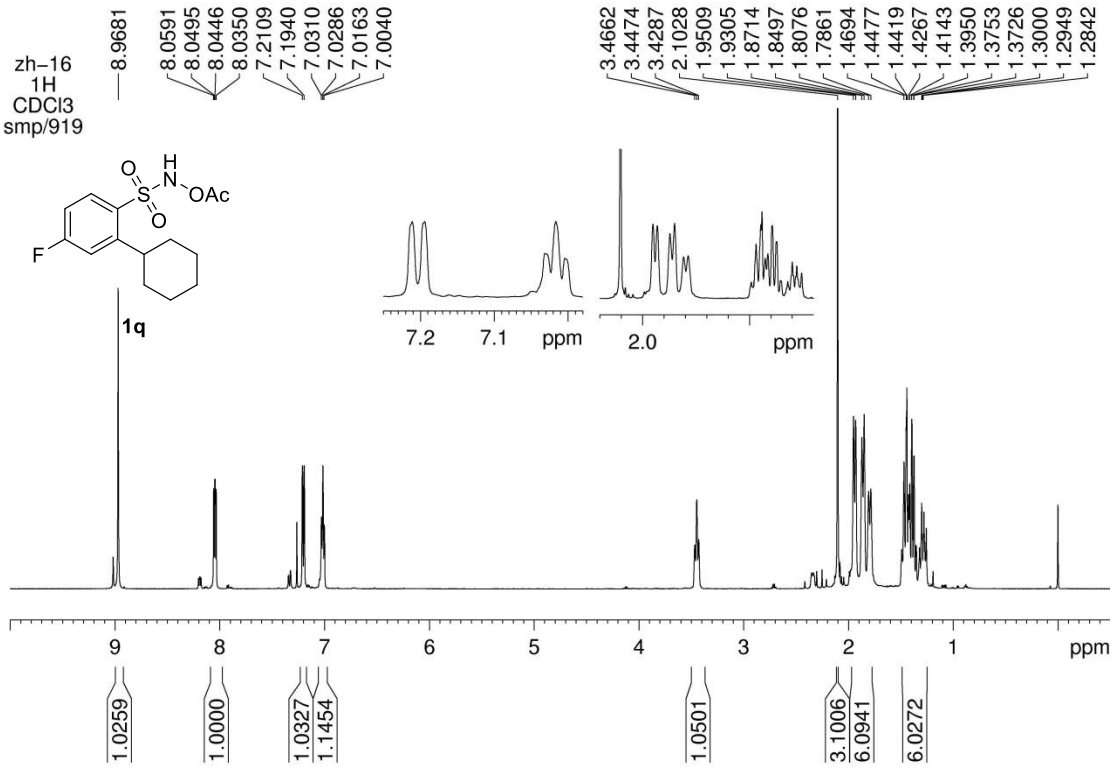

169.7330
151.2648
145.3457
130.9836
129.6577
126.6242
126.4328
41.6741
36.8170
27.6976
27.5498
21.6959
18.3530
zh–4219
13C
CDCl3
1057
1n
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ZH–35
1H
CDCL3
njl/1140
8.9810
8.0305
8.0171
7.6316
7.6187
7.6064
7.5379
7.5249
7.3465
7.3334
7.3211
3.4711
3.4661
3.4612
3.4527
3.4477
3.4341
3.4296
2.0774
1.9381
1.9223
1.8657
1.8464
1.8068
1.7849
1.4795
1.4623
1.4602
1.4460
1.4281
1.4072
1.3236
1.3176
1.3086
1.3027
OAc
1o
8.0
7.8
7.6
ppm
3.45 ppm
9
8
7
6
5
4
3
2
1
ppm
1.0135
1.0000
1.1219
1.1298
1.1024
1.0592
3.1117
2.0979
2.0787
1.0207
4.0673
1.0645


169.2701
149.3621
134.6249
132.9276
131.2549
128.9743
125.9353
40.6016
34.3591
26.7751
26.0827
18.1703
ZH–35
13C
CDCL3
njl/1141
OAc
1o
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


zh-15
1H
CDCl3
smp/918
8.9585
7.9295
7.9159
7.3244
7.1596
7.1460
3.4410
3.4236
3.4101
2.7305
2.7178
2.7052
2.6925
2.0781
1.9277
1.9136
1.8585
1.8424
1.8020
1.7804
1.4756
1.4595
1.4457
1.4295
1.4080
1.3064
1.3017
1.2789
1p
2.0 1.8 1.6 1.4 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0415
1.0000
1.0267
1.0321
1.0293
2.0556
3.0588
2.0767
2.0365
1.0880
4.0141
1.0185
3.1138


zh-15
13C
CDCl3
smp/928
169.3088
151.6346
149.3316
131.5222
130.0862
128.4616
125.4501
40.4887
34.3924
28.9572
26.8028
26.1143
18.1968
14.9525
1p
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


zh–16
1H
CDCl3
smp/919
8.9681
8.0591
8.0495
8.0446
8.0350
7.2109
7.1940
7.0310
7.0286
7.0163
7.0040
3.4662
3.4474
3.4287
2.1028
1.9509
1.9305
1.8714
1.8497
1.8076
1.7861
1.4694
1.4477
1.4419
1.4267
1.4143
1.3950
1.3753
1.3726
1.3000
1.2949
1.2842
1q
7.2
7.1
ppm
2.0
ppm
9
8
7
6
5
4
3
2
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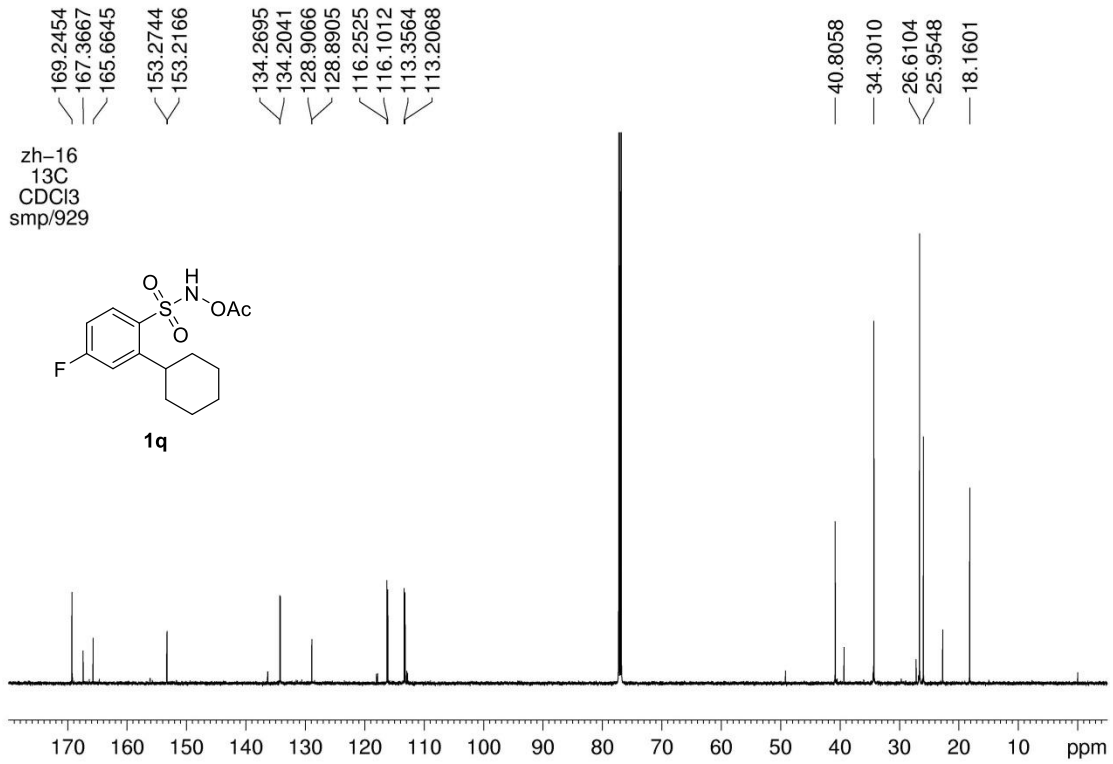
ppm
1.0259
1.0000
1.0327
1.1454
1.0501
3.1006
6.0941
6.02721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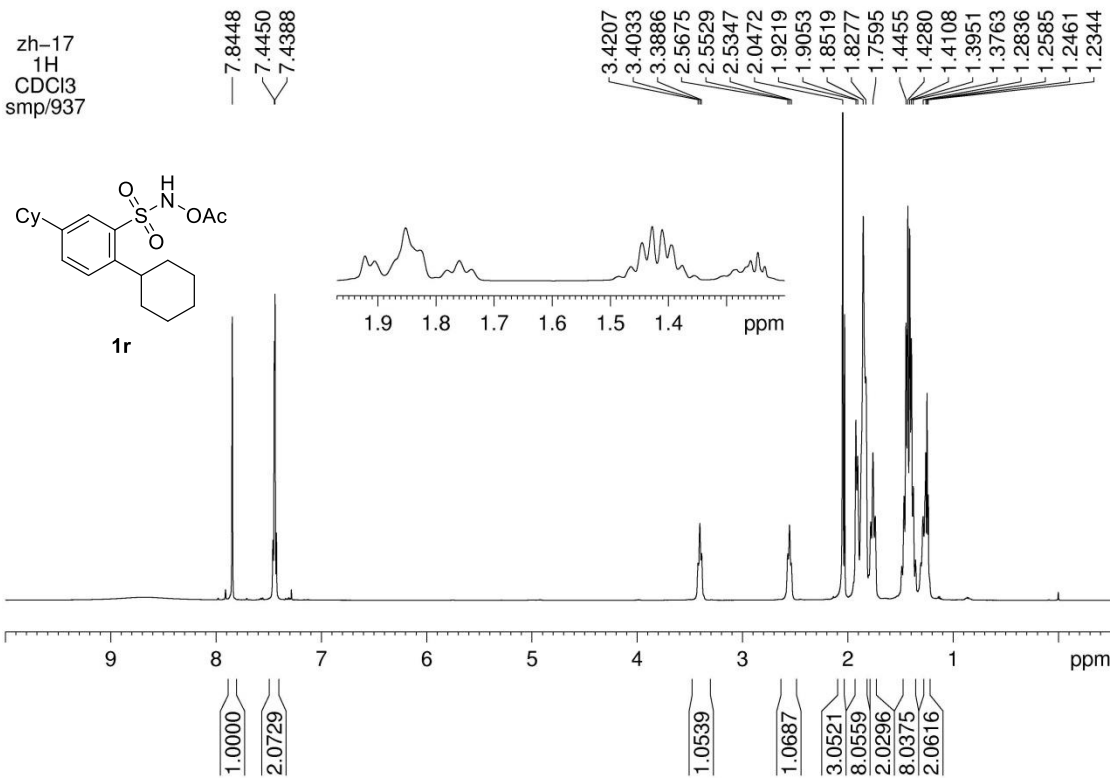
153.2744
153.2166
134.2695
134.2041
128.9066
128.8905
116.2525
116.1012
113.3564
113.2068
40.8058
34.3010
26.6104
25.9548
18.1601
zh–16
13C
CDCl3
smp/929
1q
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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CDCl3
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7.4450
7.4388
3.4207
3.4033
3.3886
2.5675
2.5529
2.5347
2.0472
1.9219
1.9053
1.8519
1.8277
1.7595
1.4455
1.4280
1.4108
1.3951
1.3763
1.2836
1.2585
1.2461
1.2344
Cy
O
S
O
H
N
OAc
1r
1.9 1.8 1.7 1.6 1.5 1.4 ppm
9 8 7 6 5 4 3 2 1 ppm
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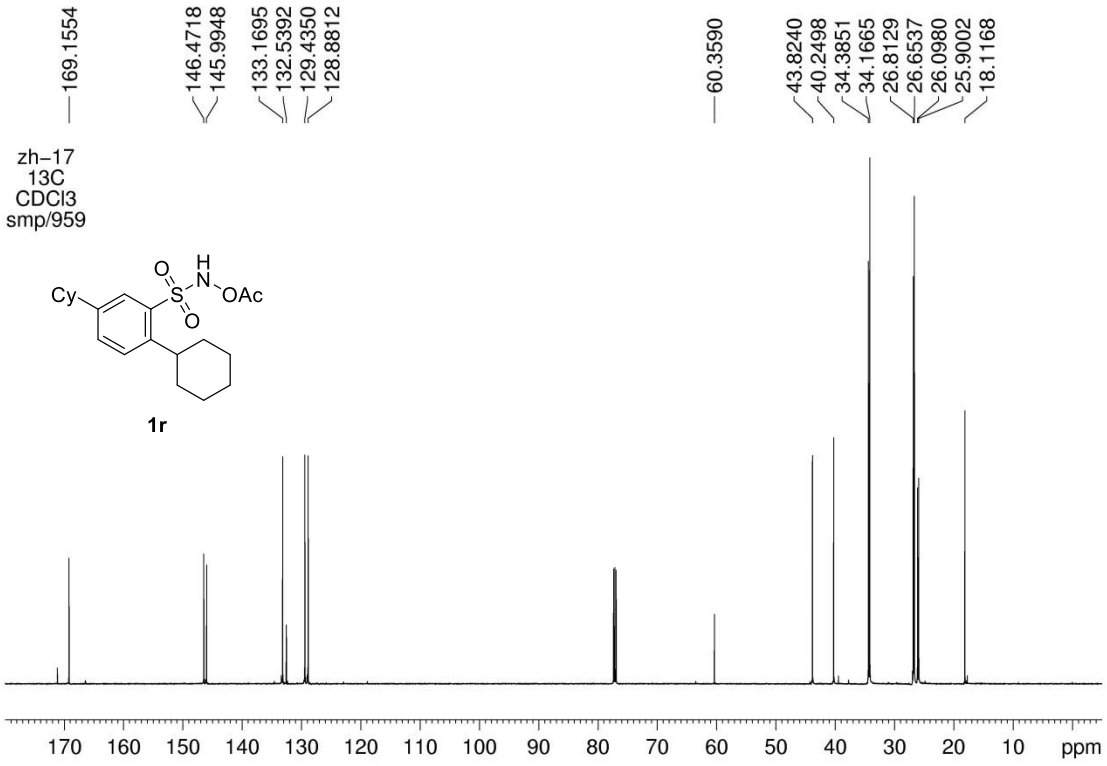
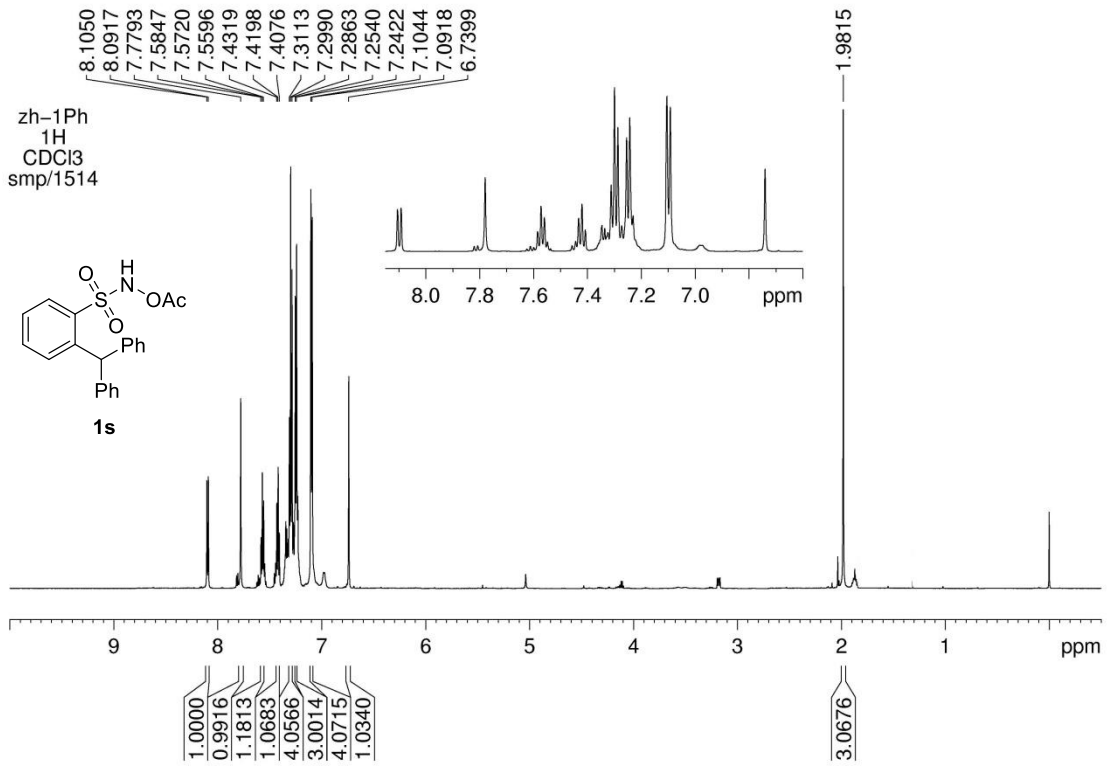
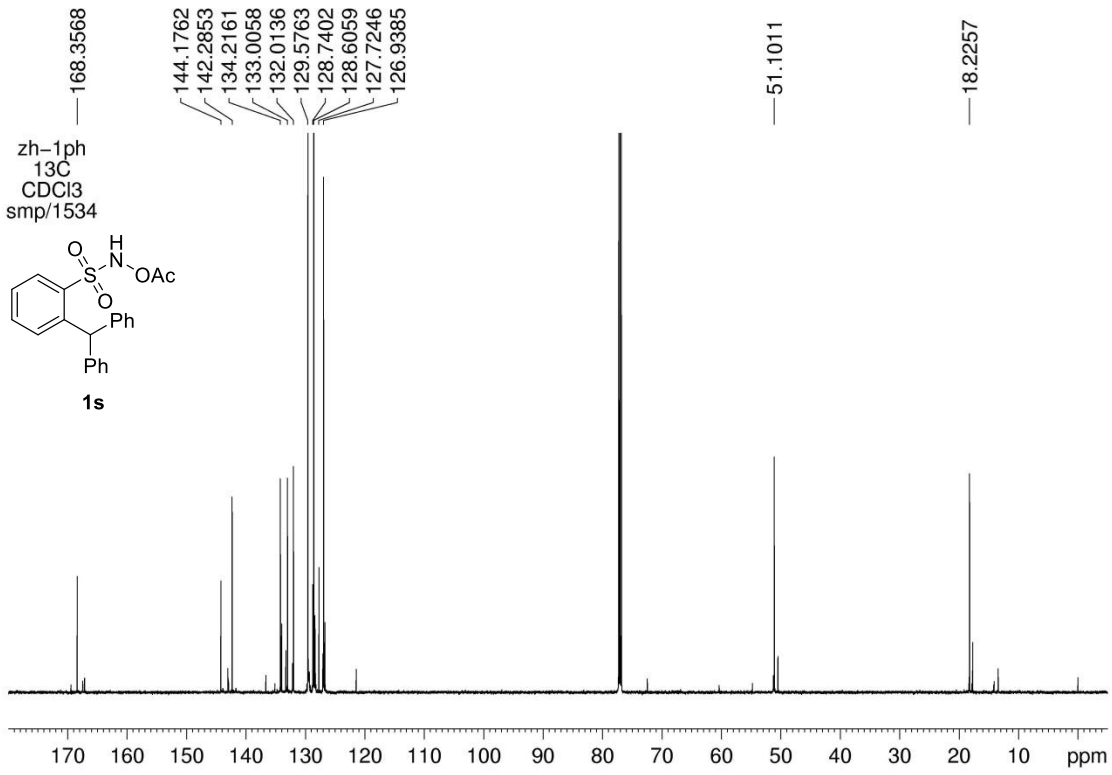
2.0729
1.0539
1.0687
3.0521
8.0559
2.0296
8.0375
2.0616


zh–17
13C
CDCl3
smp/959
169.1554
146.4718
145.9948
133.1695
132.5392
129.4350
128.8812
60.3590
43.8240
40.2498
34.3851
34.1665
26.8129
26.6537
26.0980
25.9002
18.1168
Cy
O
S
O
H
N
OAc
1r
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.1050
8.0917
7.7793
7.5847
7.5720
7.5596
7.4319
7.4198
7.4076
7.3113
7.2990
7.2863
7.2540
7.2422
7.1044
7.0918
6.7399
1.9815
zh–1Ph
1H
CDCl3
smp/1514
1s
8.0 7.8 7.6 7.4 7.2 7.0 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0000
0.9916
1.1813
1.0683
4.0566
3.0014
4.0715
1.0340
3.0676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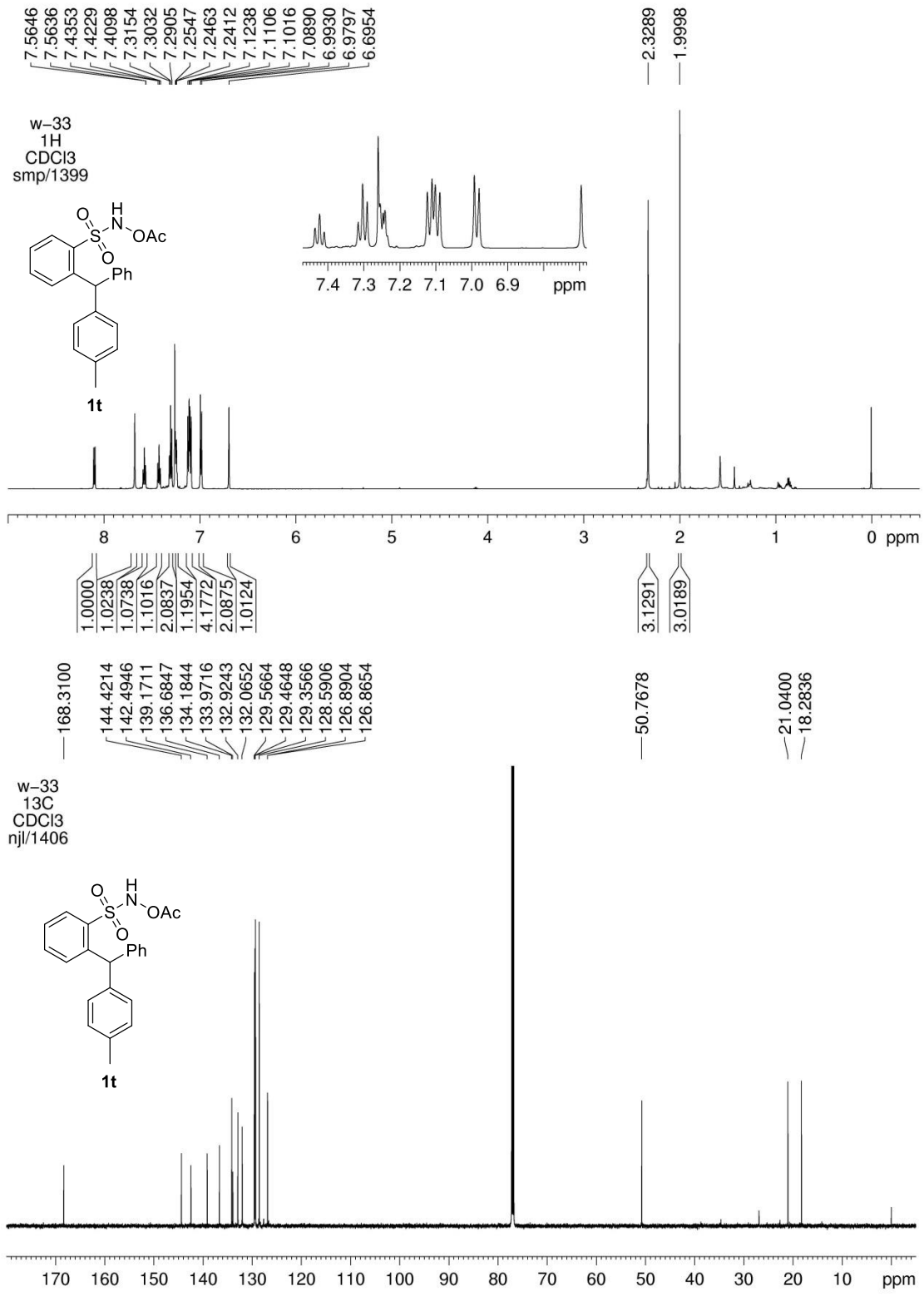
144.1762
142.2853
134.2161
133.0058
132.0136
129.5763
128.7402
128.6059
127.7246
126.9385
51.1011
18.2257
zh–1ph
13C
CDCl3
smp/1534
1s
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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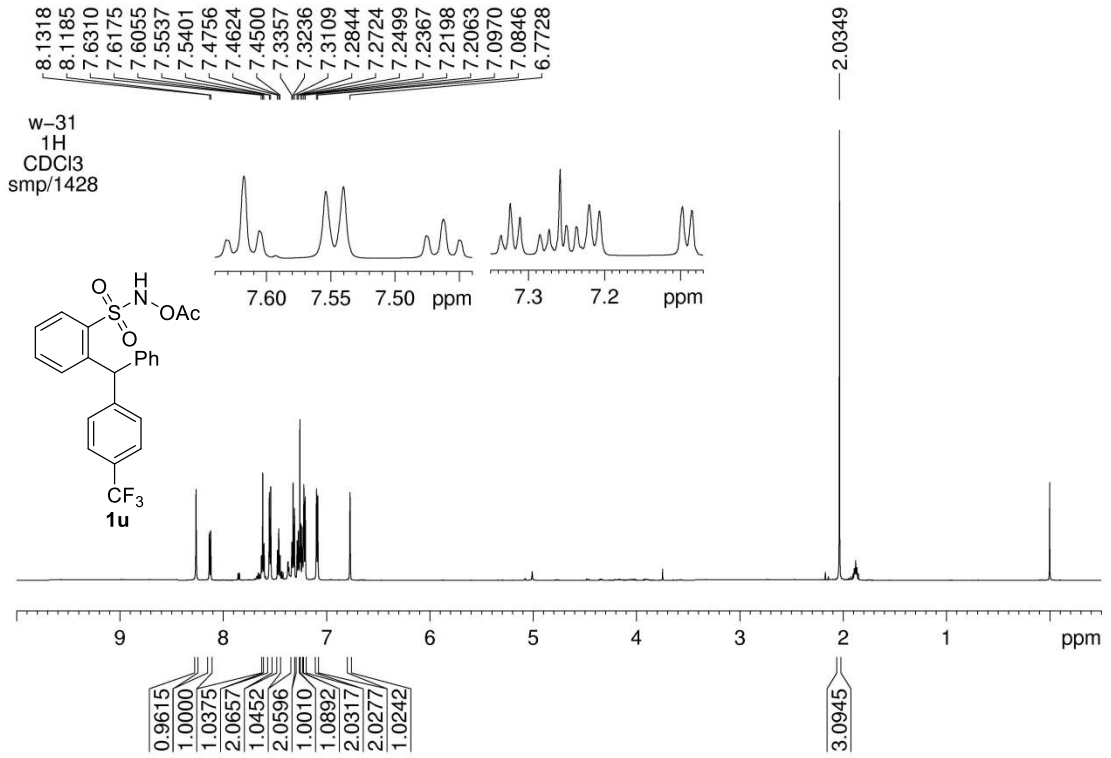
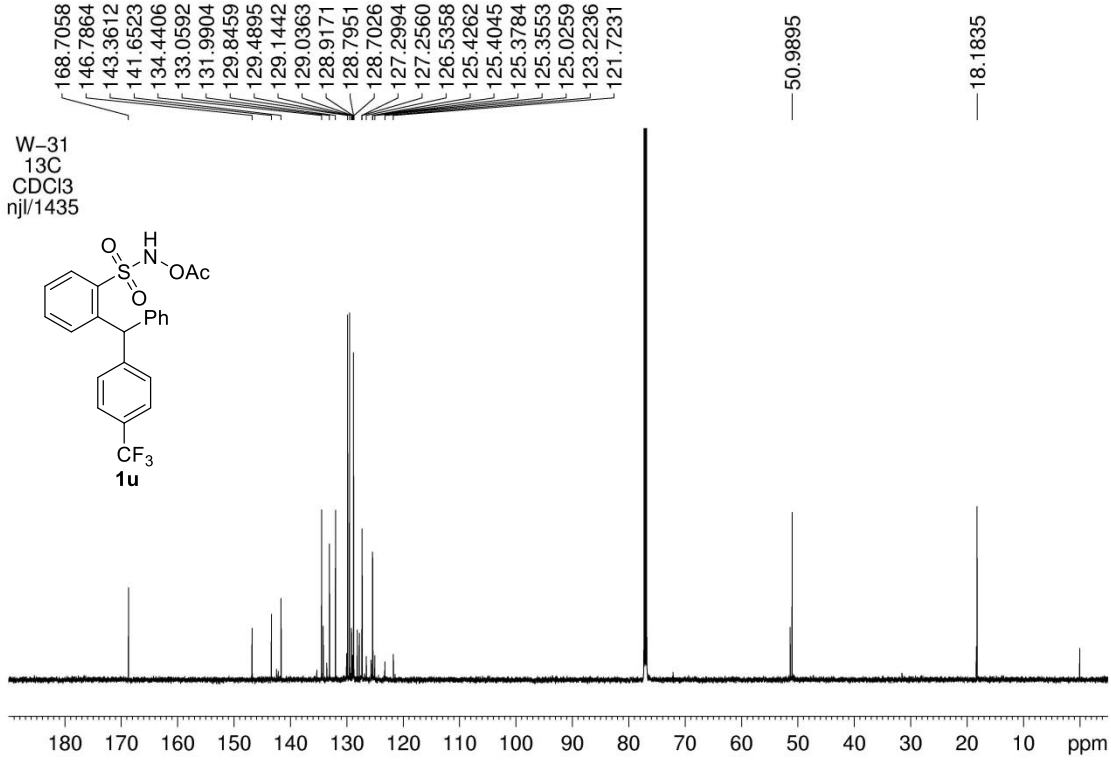
7.5636
7.4353
7.4229
7.4098
7.3154
7.3032
7.2905
7.2547
7.2463
7.2412
7.1238
7.1106
7.1016
7.0890
6.9930
6.9797
6.6954
2.3289
1.9998
w–33
1H
CDCl3
smp/1399
O
H
N
OAc
S
O
Ph
1t
7.4 7.3 7.2 7.1 7.0 6.9 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0238
1.0738
1.1016
2.0837
1.1954
4.1772
2.0875
1.0124
3.1291
3.0189
168.3100
144.4214
142.4946
139.1711
136.6847
134.1844
133.9716
132.9243
132.0652
129.5664
129.4648
129.3566
128.5906
126.8904
126.8654
50.7678
21.0400
18.2836
w–33
13C
CDCl3
njl/1406
1t
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.1318
8.1185
7.6310
7.6175
7.6055
7.5537
7.5401
7.4756
7.4624
7.4500
7.3357
7.3236
7.3109
7.2844
7.2724
7.2499
7.2367
7.2198
7.2063
7.0970
7.0846
6.7728
2.0349
w–31
1H
CDCl3
smp/1428
7.60 7.55 7.50 ppm
7.3 7.2 ppm
OAc
Ph
CF3
1u
9 8 7 6 5 4 3 2 1 ppm
0.9615
1.0000
1.0375
2.0657
1.0452
2.0596
1.0010
1.0892
2.0317
2.0277
1.0242
3.0945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146.7864
143.3612
141.6523
134.4406
133.0592
131.9904
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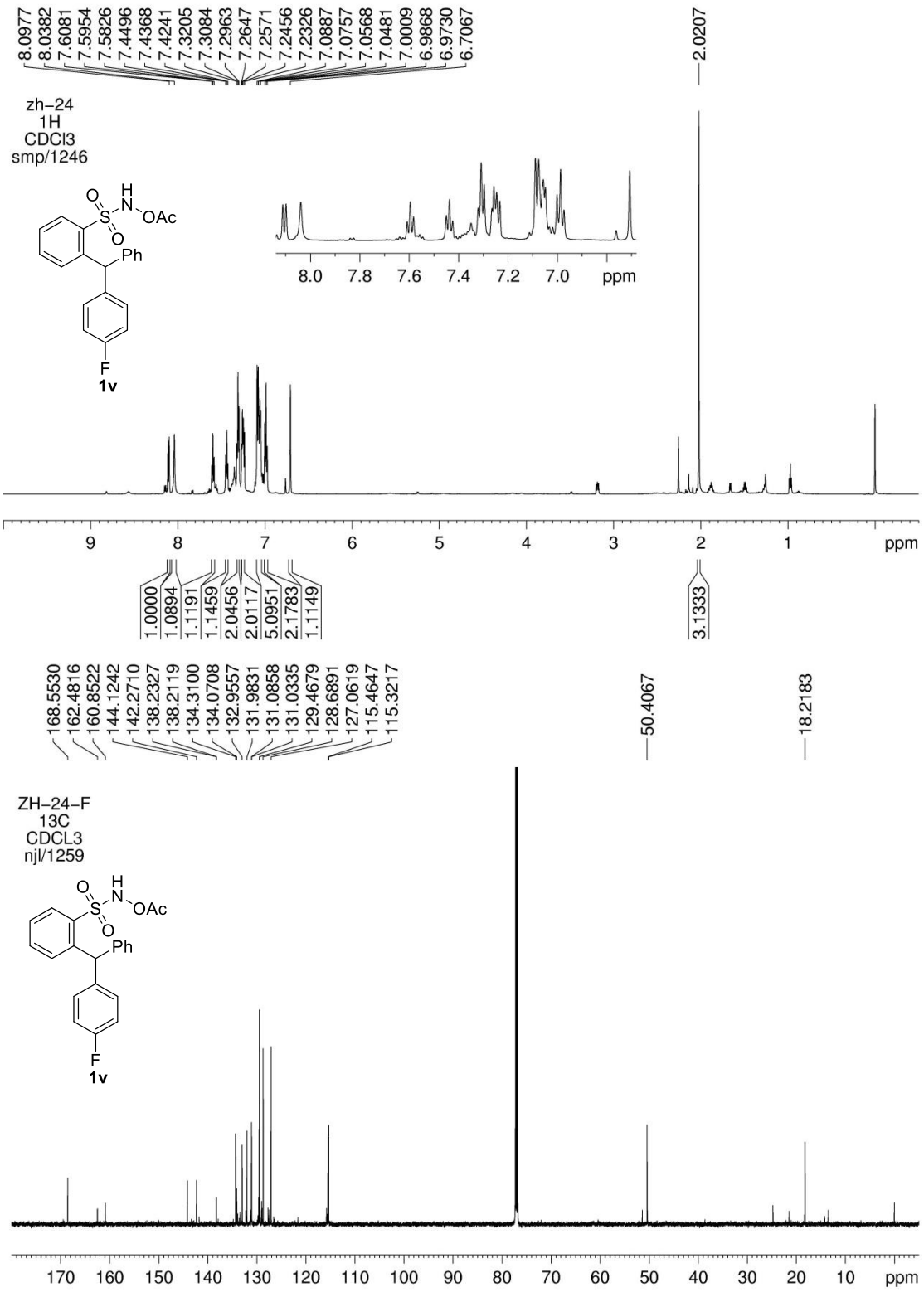
129.4895
129.1442
129.0363
128.9171
128.7951
128.7026
127.2994
127.2560
126.5358
125.4262
125.4045
125.3784
125.3553
125.0259
123.2236
121.7231
50.9895
18.1835
W–31
13C
CDCl3
njl/1435
OAc
Ph
CF3
1u
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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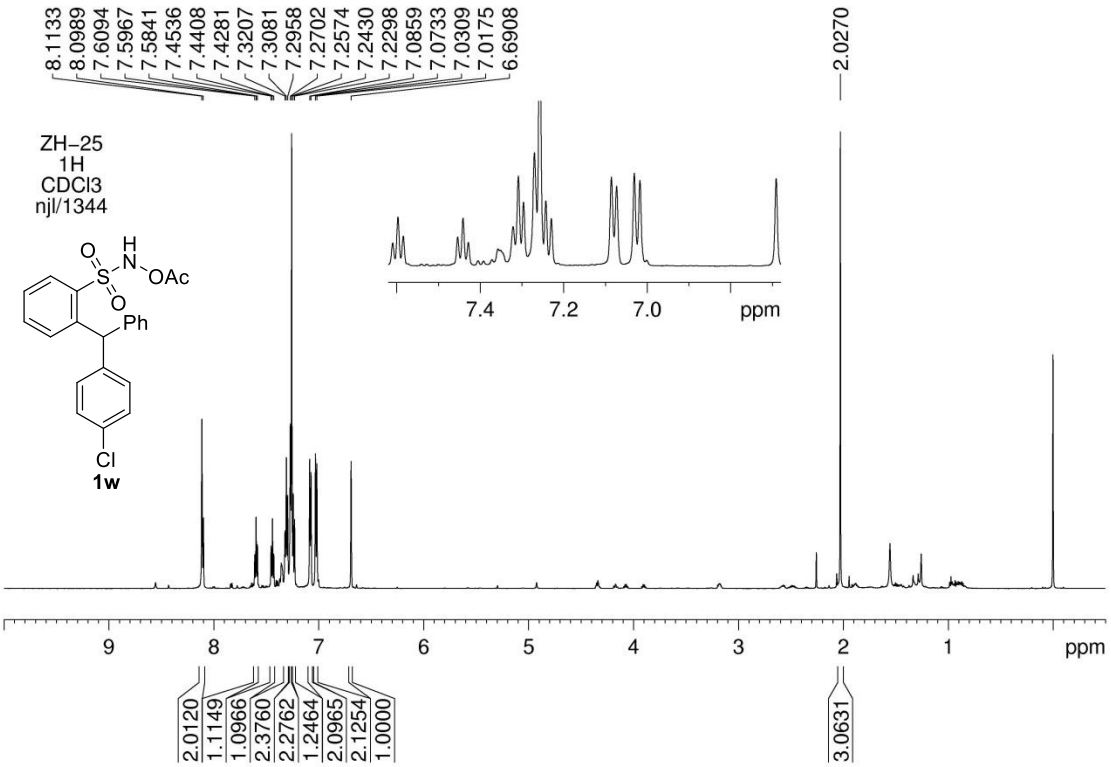
8.0382
7.6081
7.5954
7.5826
7.4496
7.4368
7.4241
7.3205
7.3084
7.2963
7.2647
7.2571
7.2456
7.2326
7.0887
7.0757
7.0568
7.0481
7.0009
6.9868
6.9730
6.7067
2.0207
zh–24
1H
CDCl3
smp/1246
H
N
OAc
O
S
O
Ph
F
1v
8.0
7.8
7.6
7.4
7.2
7.0
ppm
9
8
7
6
5
4
3
2
1
ppm
1.0000
1.0894
1.1191
1.1459
2.0456
2.0117
5.0951
2.1783
1.1149
3.1333
168.5530
162.4816
160.8522
144.1242
142.2710
138.2327
138.2119
134.3100
134.0708
132.9557
131.9831
131.0858
131.0335
129.4679
128.6891
127.0619
115.4647
115.3217
50.4067
18.2183
ZH–24–F
13C
CDCL3
njl/1259
H
N
OAc
O
S
O
Ph
F
1v
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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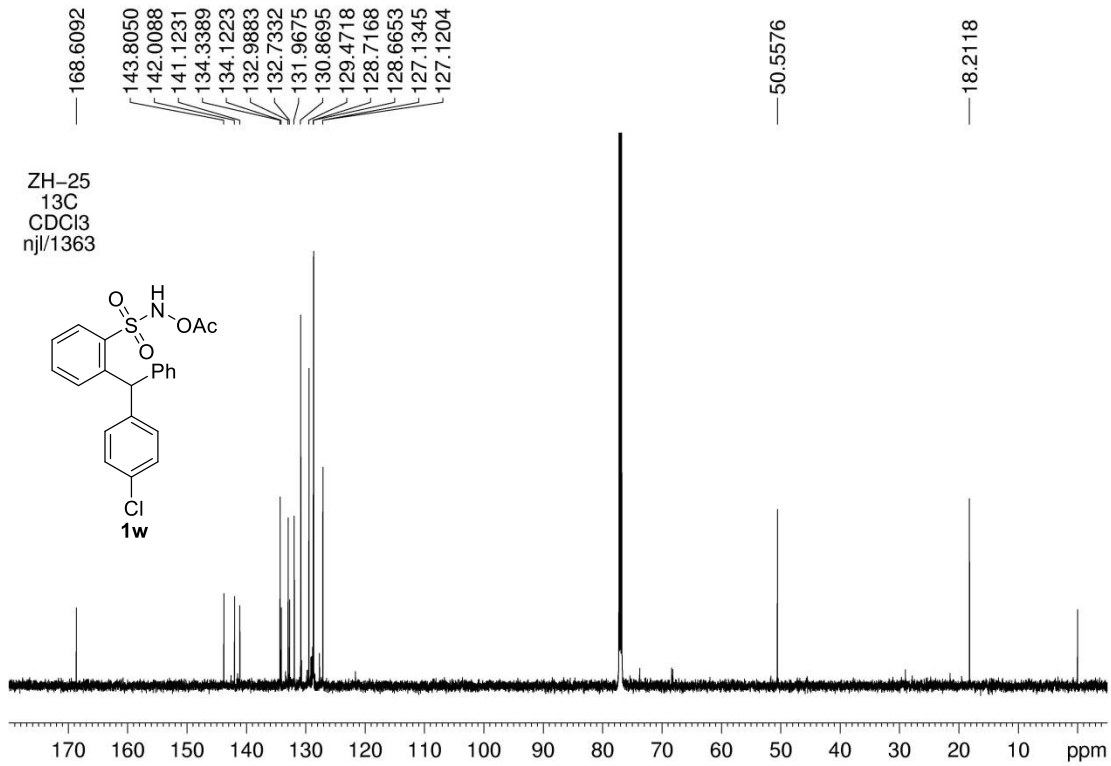
7.5967
7.5841
7.4536
7.4408
7.4281
7.3207
7.3081
7.2958
7.2702
7.2574
7.2430
7.2298
7.0859
7.0733
7.0309
7.0175
6.6908
2.0270
ZH–25
1H
CDCl3
njl/1344
O
H
N
OAc
S
O
Ph
Cl
1w
7.4
7.2
7.0
ppm
9
8
7
6
5
4
3
2
1
ppm
2.0120
1.1149
1.0966
2.3760
2.2762
1.2464
2.0965
2.1254
1.0000
3.0631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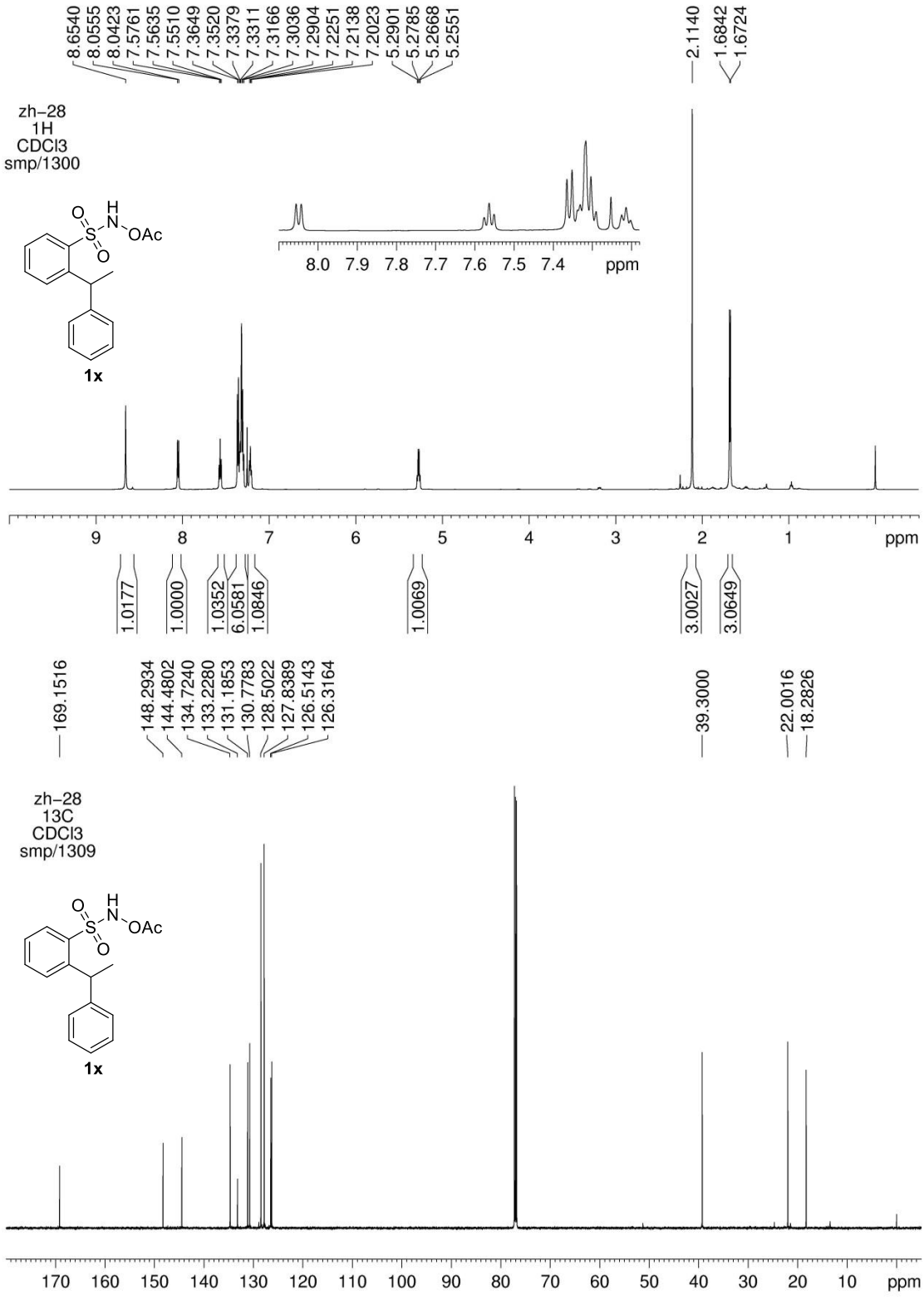
143.8050
142.0088
141.1231
134.3389
134.1223
132.9883
132.7332
131.9675
130.8695
129.4718
128.7168
128.6653
127.1345
127.1204
50.5576
18.2118
ZH–25
13C
CDCl3
njl/1363
O
H
N
OAc
S
O
Ph
Cl
1w
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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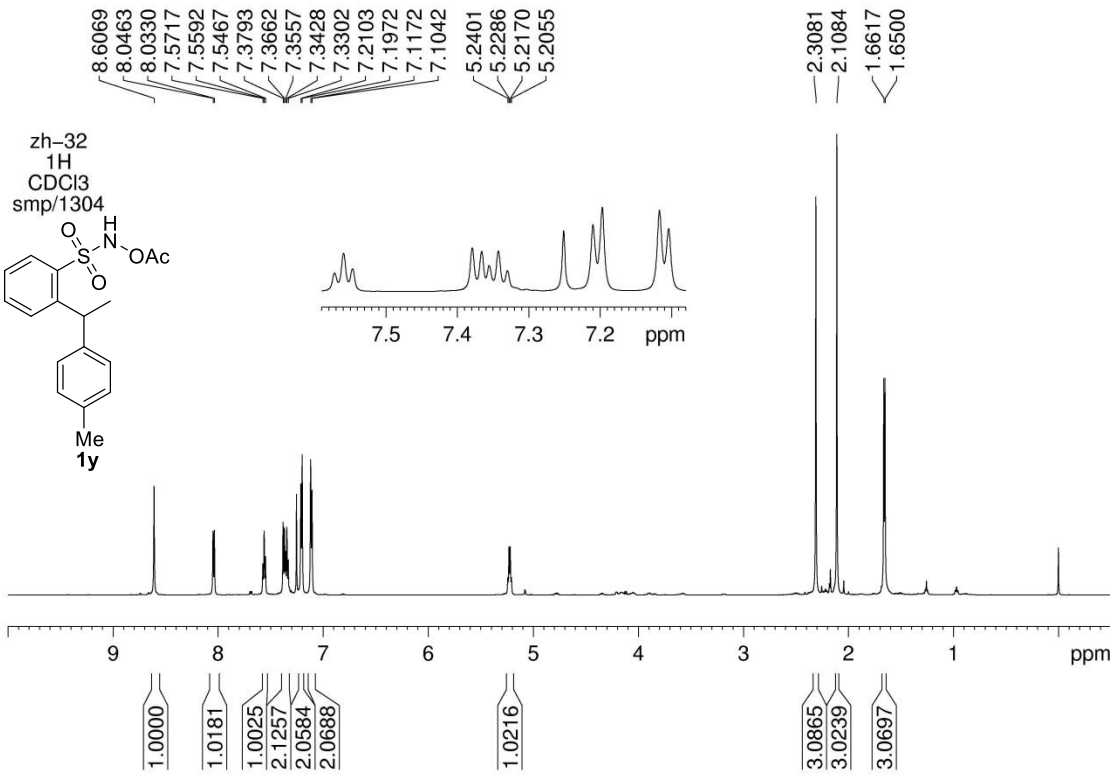
8.0555
8.0423
7.5761
7.5635
7.5510
7.3649
7.3520
7.3379
7.3311
7.3166
7.3036
7.2904
7.2251
7.2138
7.2023
5.2901
5.2785
5.2668
5.2551
2.1140
1.6842
1.6724
zh–28
1H
CDCl3
smp/1300
1x
8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0177
1.0000
1.0352
6.0581
1.0846
1.0069
3.0027
3.0649
169.1516
148.2934
144.4802
134.7240
133.2280
131.1853
130.7783
128.5022
127.8389
126.5143
126.3164
39.3000
22.0016
18.2826
zh–28
13C
CDCl3
smp/1309
1x
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.0330
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7.5592
7.5467
7.3793
7.3662
7.3557
7.3428
7.3302
7.2103
7.1972
7.1172
7.1042
5.2401
5.2286
5.2170
5.2055
2.3081
2.1084
1.6617
1.6500
zh–32
1H
CDCl3
smp/1304
OAc
Me
1y
7.5
7.4
7.3
7.2
ppm
9
8
7
6
5
4
3
2
1
ppm
1.0000
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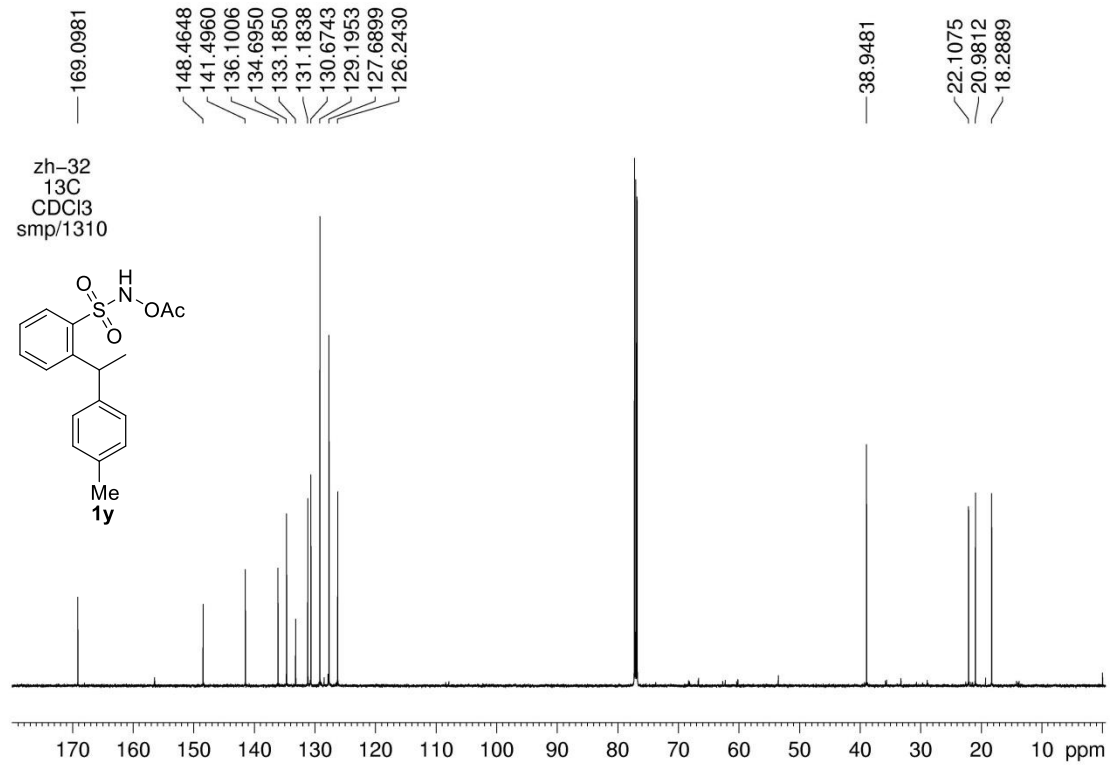
1.0025
2.1257
2.0584
2.0688
1.0216
3.0865
3.0239
3.0697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136.1006
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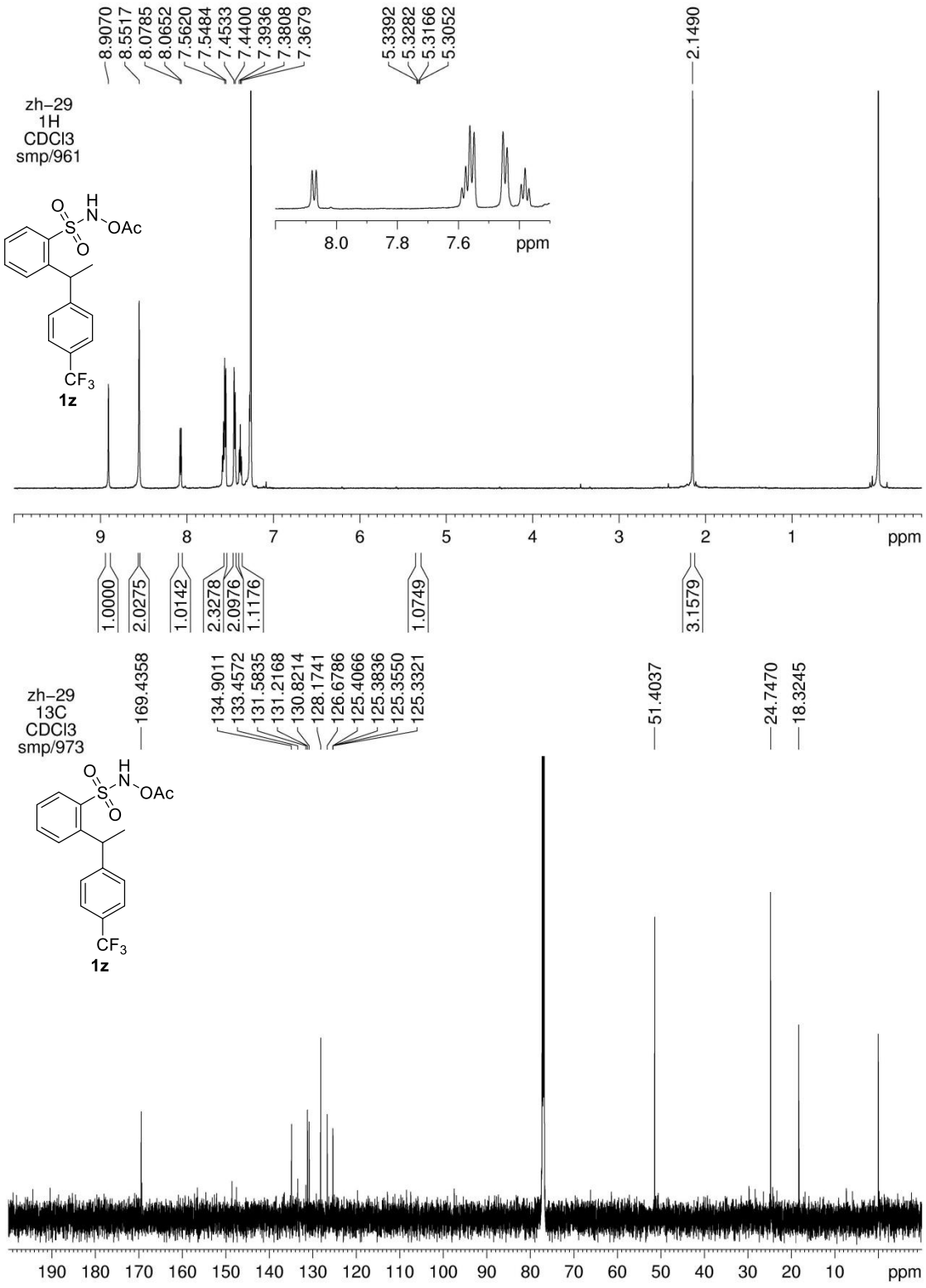
133.1850
131.1838
130.6743
129.1953
127.6899
126.2430
38.9481
22.1075
20.9812
18.2889
zh–32
13C
CDCl3
smp/1310
OAc
Me
1y
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.0652
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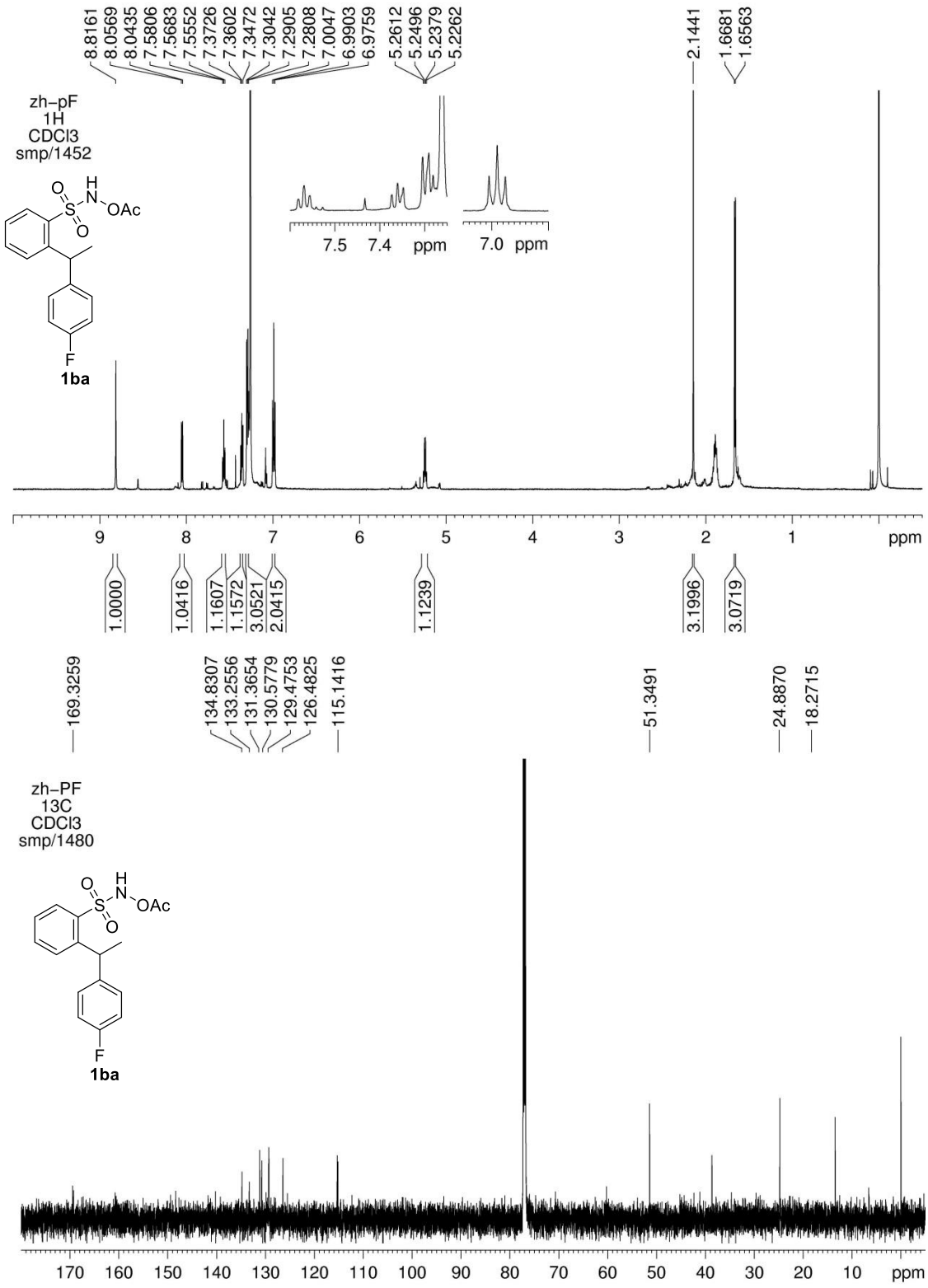
7.5484
7.4533
7.4400
7.3936
7.3808
7.3679
5.3392
5.3282
5.3166
5.3052
2.1490
zh–29
1H
CDCl3
smp/961
8.0
7.8
7.6
ppm
1z
9
8
7
6
5
4
3
2
1
ppm
1.0000
2.0275
1.0142
2.3278
2.0976
1.1176
1.0749
3.1579
169.4358
134.9011
133.4572
131.5835
131.2168
130.8214
128.1741
126.6786
125.4066
125.3836
125.3550
125.3321
51.4037
24.7470
18.3245
zh–29
13C
CDCl3
smp/973
1z
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.3726
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7.3472
7.3042
7.2905
7.2808
7.0047
6.9903
6.9759
5.2612
5.2496
5.2379
5.2262
2.1441
1.6681
1.6563
zh–pF
1H
CDCl3
smp/1452
1ba
7.5 7.4 ppm
7.0 ppm
1.0000
1.0416
1.1607
1.1572
3.0521
2.0415
1.1239
3.1996
3.0719
169.3259
134.8307
133.2556
131.3654
130.5779
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126.4825
115.1416
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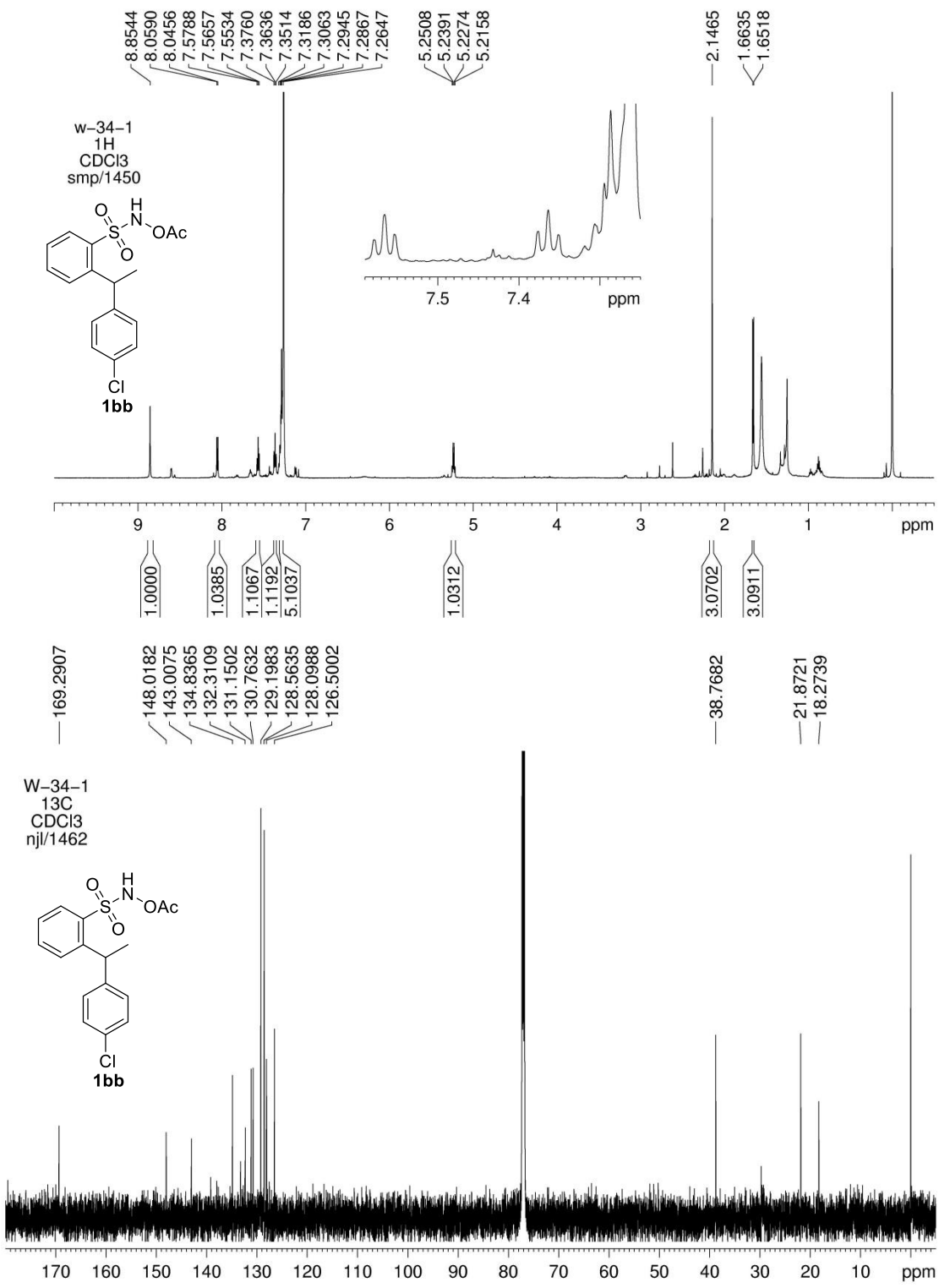
24.8870
18.2715
zh–PF
13C
CDCl3
smp/1480
1ba


w–34–1
1H
CDCl3
smp/1450
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8.0590
8.0456
7.5788
7.5657
7.5534
7.3760
7.3636
7.3514
7.3186
7.3063
7.2945
7.2867
7.2647
5.2508
5.2391
5.2274
5.2158
2.1465
1.6635
1.6518
1.0000
1.0385
1.1067
1.1192
5.1037
1.0312
3.0702
3.0911
W–34–1
13C
CDCl3
njl/1462
1bb
169.2907
148.0182
143.0075
134.8365
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130.7632
129.1983
128.5635
128.0988
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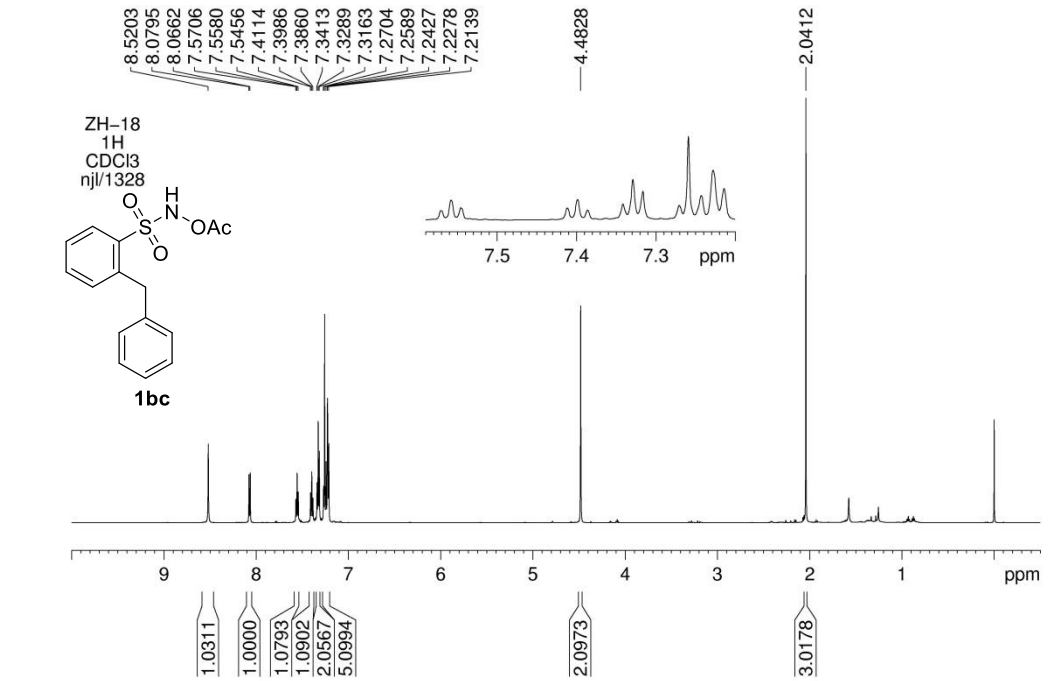
ppm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8.0662
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7.5456
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7.3986
7.3860
7.3413
7.3289
7.3163
7.2704
7.2589
7.2427
7.2278
7.2139
4.4828
2.0412
ZH–18
1H
CDCl3
njl/1328
O
H
N
S
O
OAc
O
1bc
7.5
7.4
7.3
ppm
9
8
7
6
5
4
3
2
1
ppm
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1.0793
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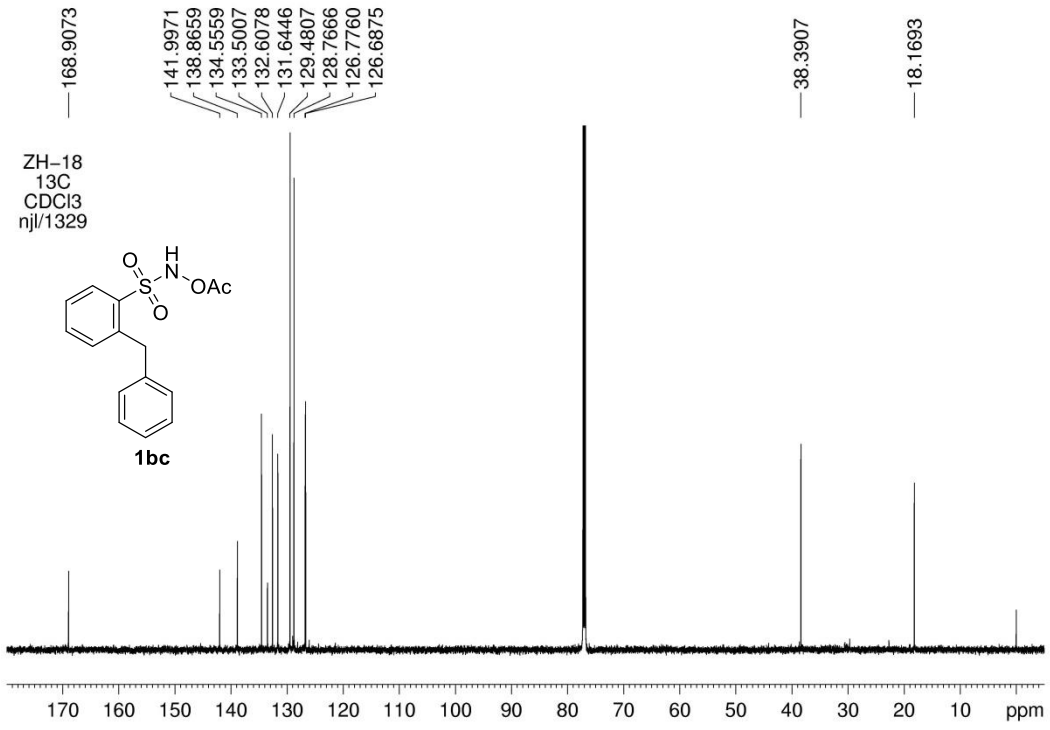
3.0178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134.5559
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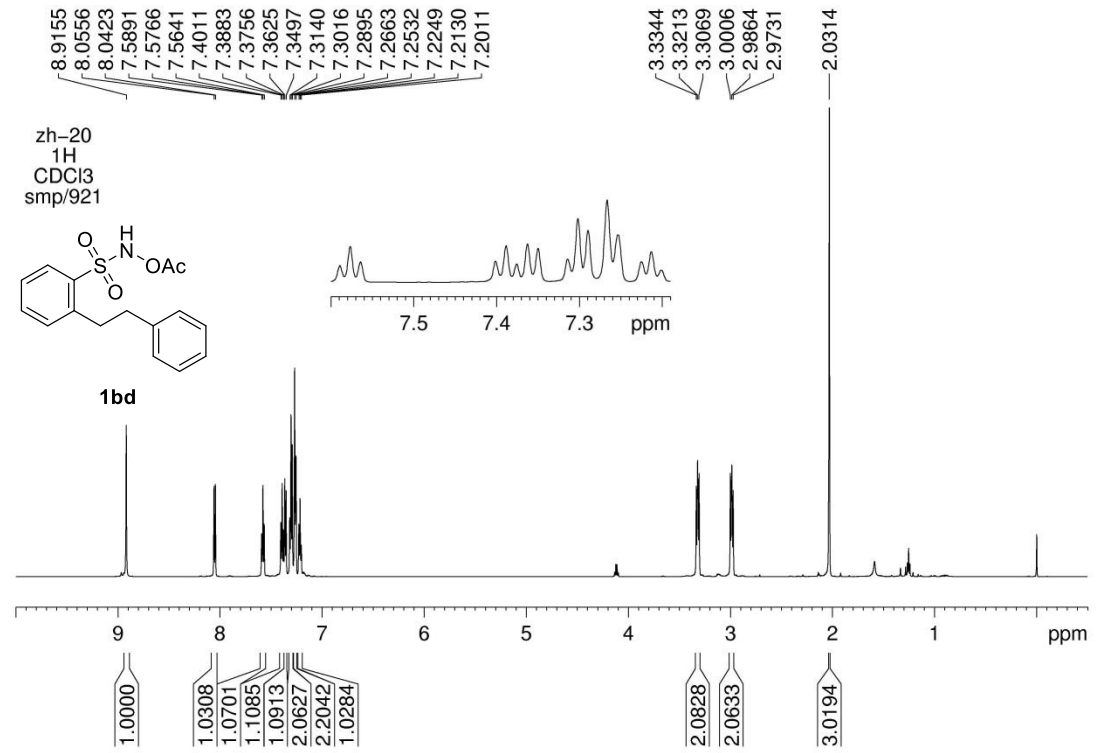
132.6078
131.6446
129.4807
128.7666
126.7760
126.6875
38.3907
18.1693
ZH–18
13C
CDCl3
njl/1329
O
H
N
S
O
OAc
O
1bc
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.3140
7.3016
7.2895
7.2663
7.2532
7.2249
7.2130
7.2011
3.3344
3.3213
3.3069
3.0006
2.9864
2.9731
2.0314
zh–20
1H
CDCl3
smp/921
1bd
7.5
7.4
7.3
ppm
9
8
7
6
5
4
3
2
1
ppm
1.0000
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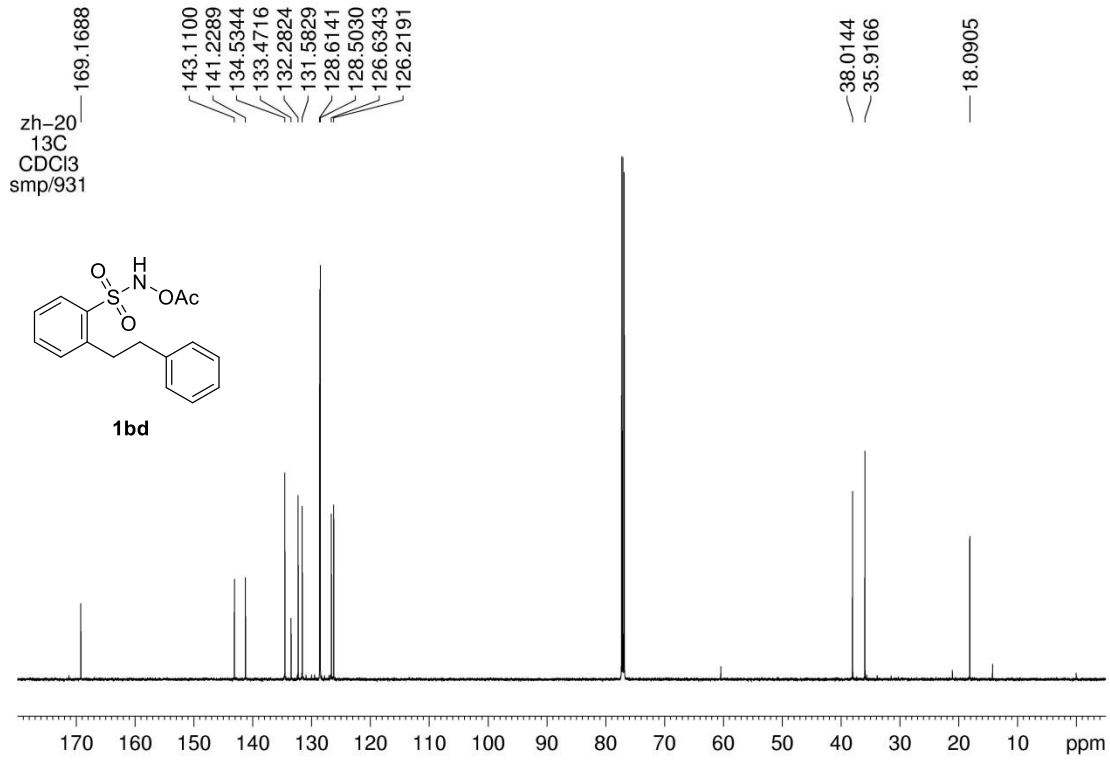
1.1085
1.0913
2.0627
2.2042
1.0284
2.0828
2.0633
3.0194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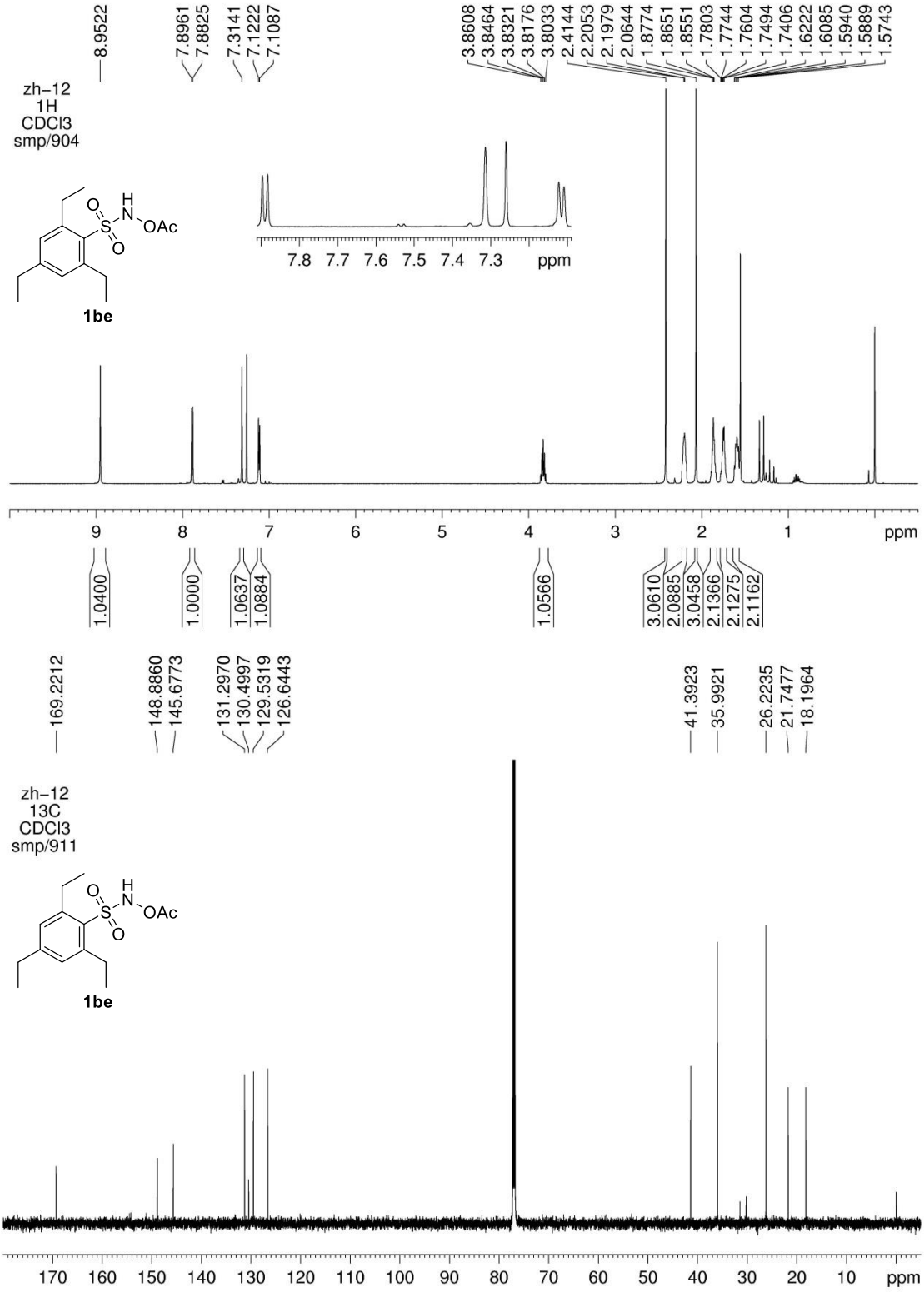
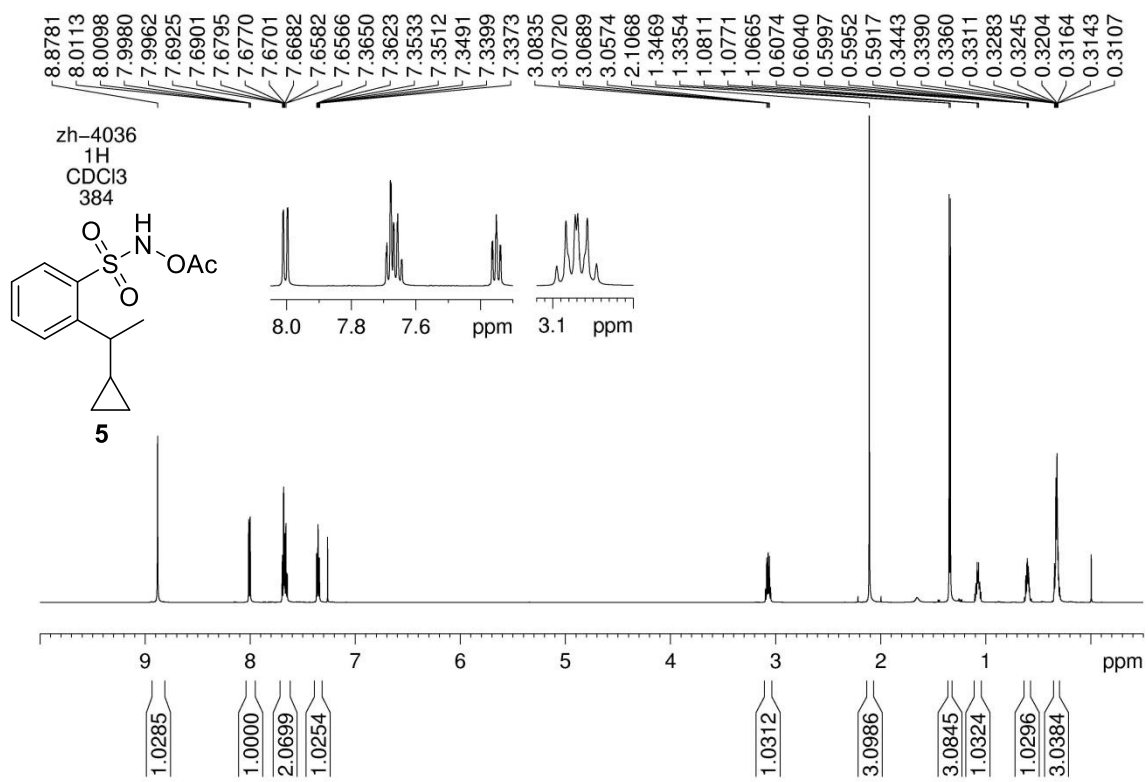
141.2289
134.5344
133.4716
132.2824
131.5829
128.6141
128.5030
126.6343
126.2191
38.0144
35.9166
18.0905
zh–20
13C
CDCl3
smp/931
1bd
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.9522
7.8961
7.8825
7.3141
7.1222
7.1087
3.8608
3.8464
3.8321
3.8176
3.8033
2.4144
2.2053
2.1979
2.0644
1.8774
1.8651
1.8551
1.7803
1.7744
1.7604
1.7494
1.7406
1.6222
1.6085
1.5940
1.5889
1.5743
zh−12
1H
CDCl3
smp/904
1be
7.8 7.7 7.6 7.5 7.4 7.3 ppm
9 8 7 6 5 4 3 2 1 ppm
1.0400
1.0000
1.0637
1.0884
1.0566
3.0610
2.0885
3.0458
2.1366
2.1275
2.1162
169.2212
148.8860
145.6773
131.2970
130.4997
129.5319
126.6443
41.3923
35.9921
26.2235
21.7477
18.1964
zh−12
13C
CDCl3
smp/911
1be
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.0098
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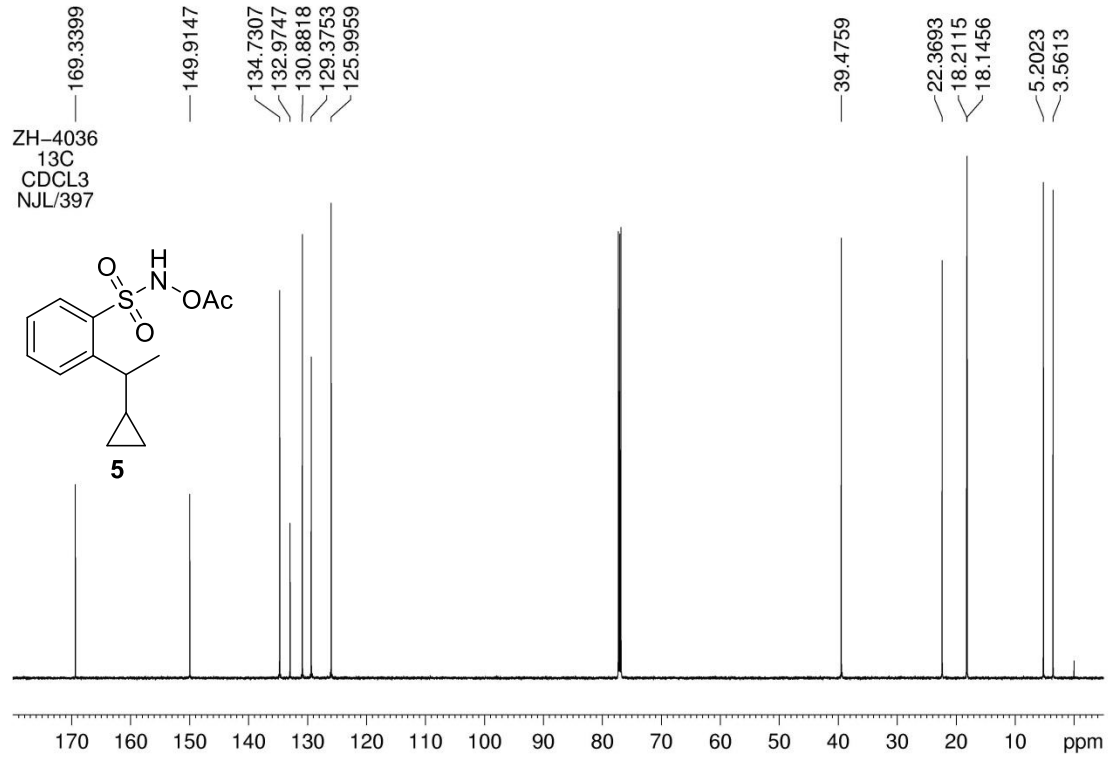
7.9962
7.6925
7.6901
7.6795
7.6770
7.6701
7.6682
7.6582
7.6566
7.3650
7.3623
7.3533
7.3512
7.3491
7.3399
7.3373
3.0835
3.0720
3.0689
3.0574
2.1068
1.3469
1.3354
1.0811
1.0771
1.0665
0.6074
0.6040
0.5997
0.5952
0.5917
0.3443
0.3390
0.3360
0.3311
0.3283
0.3245
0.3204
0.3164
0.3143
0.3107
zh–4036
1H
CDCl3
384
O
H
N
S
OAc
O
O
5
8.0
7.8
7.6
ppm
3.1
ppm
9
8
7
6
5
4
3
2
1
ppm
1.0285
1.0000
2.0699
1.0254
1.0312
3.0986
3.0845
1.0324
1.0296
3.0384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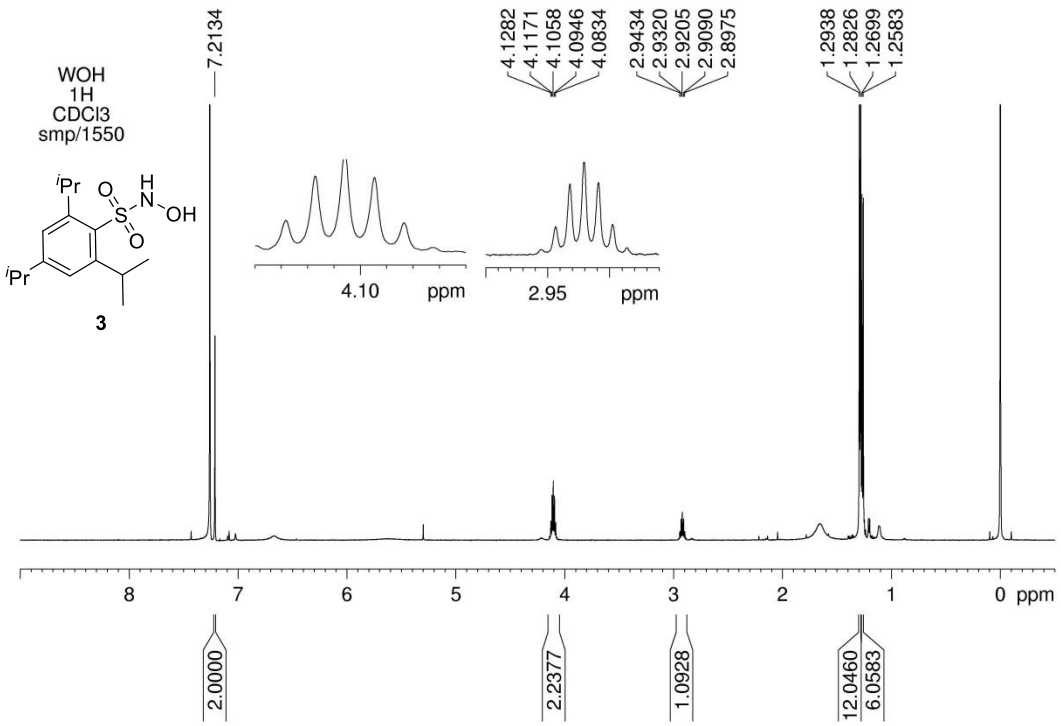
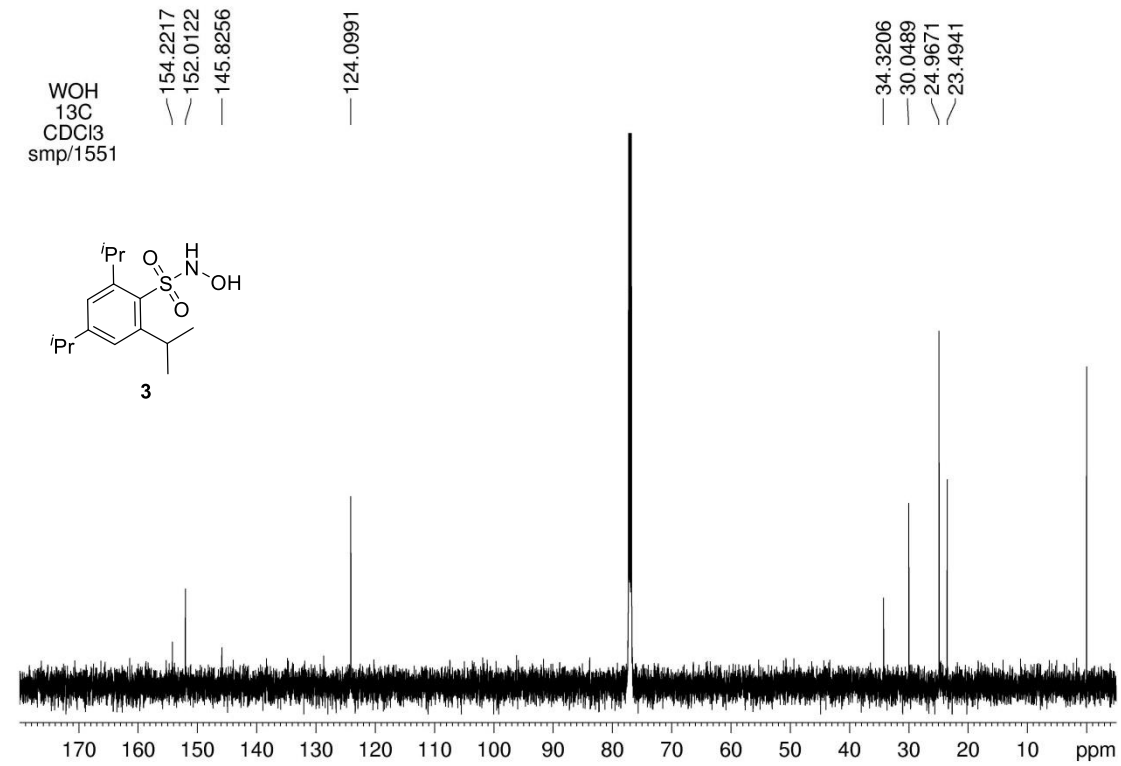
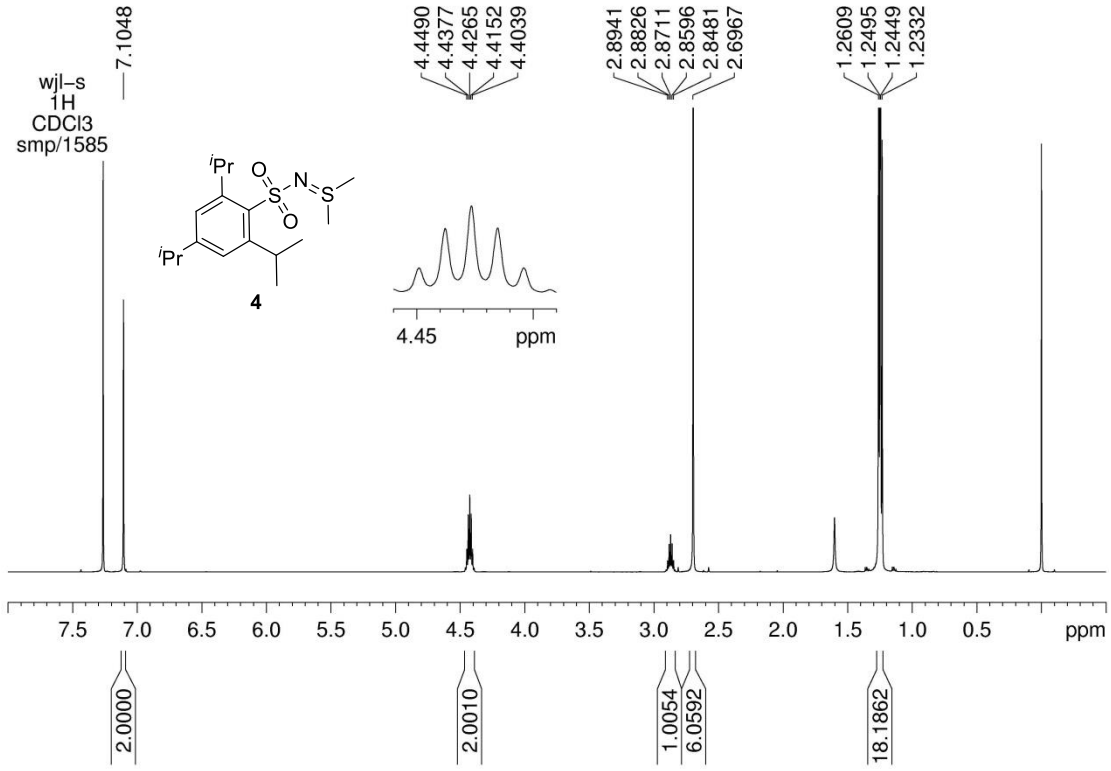
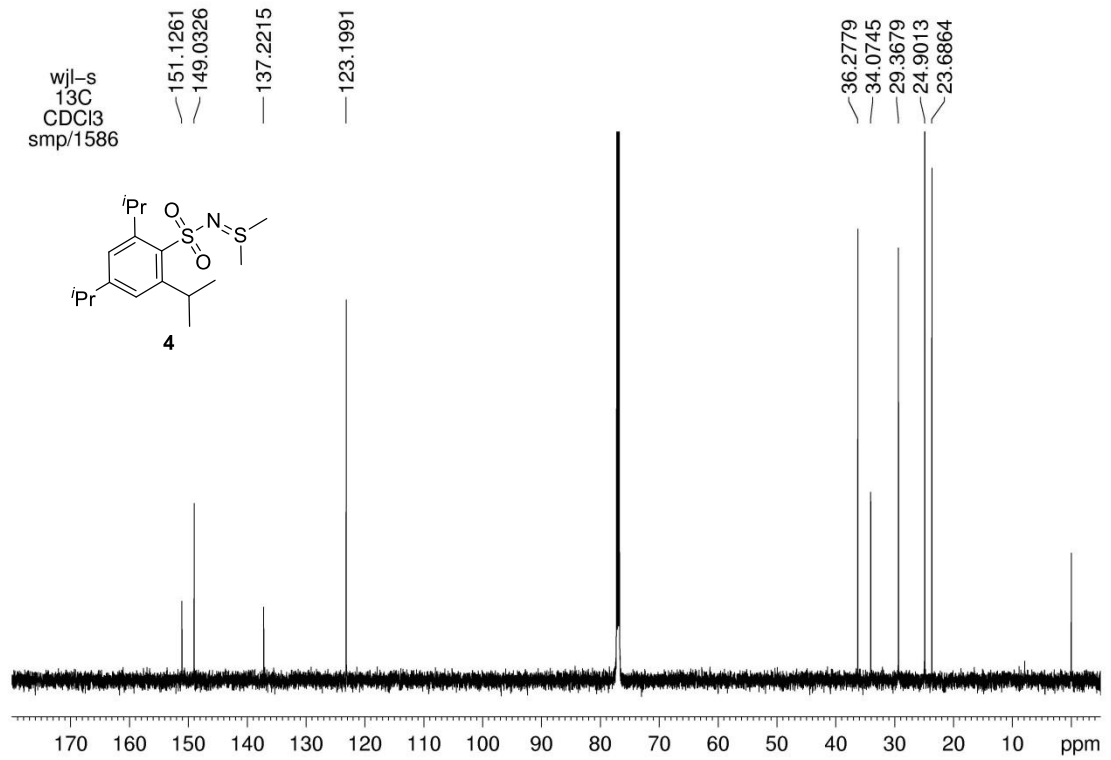
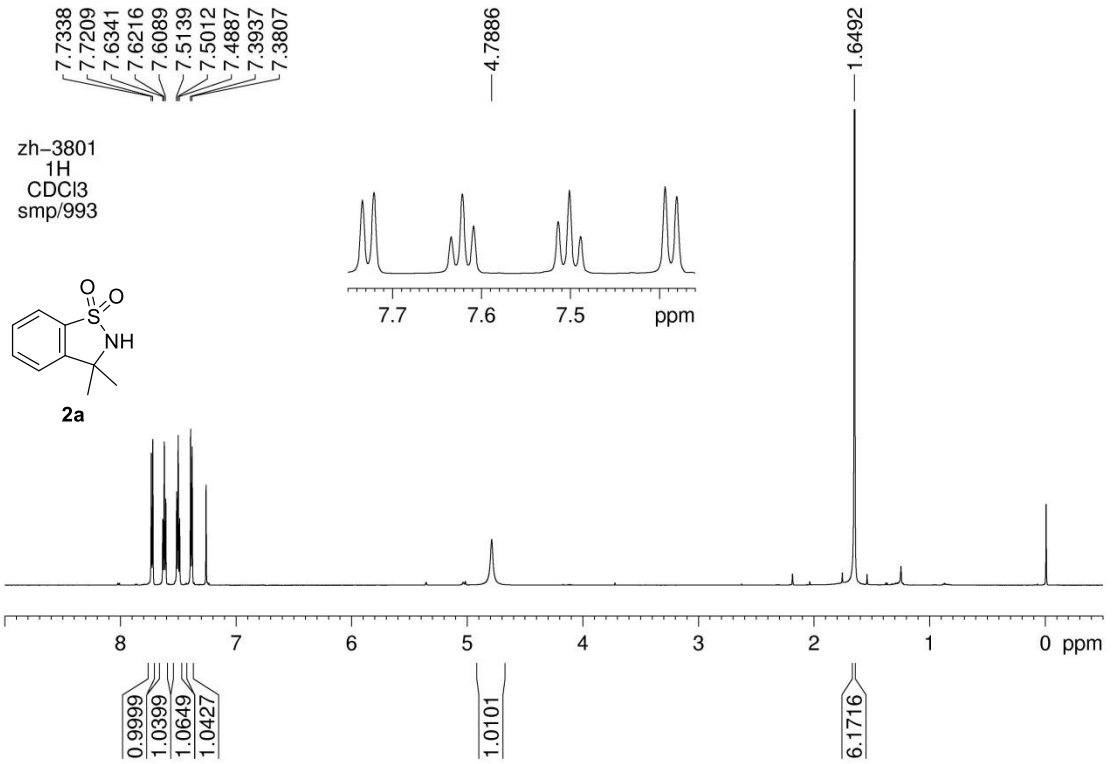
149.9147
134.7307
132.9747
130.8818
129.3753
125.9959
39.4759
22.3693
18.2115
18.1456
5.2023
3.5613
ZH–4036
13C
CDCL3
NJL/397
O
H
N
S
OAc
O
5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

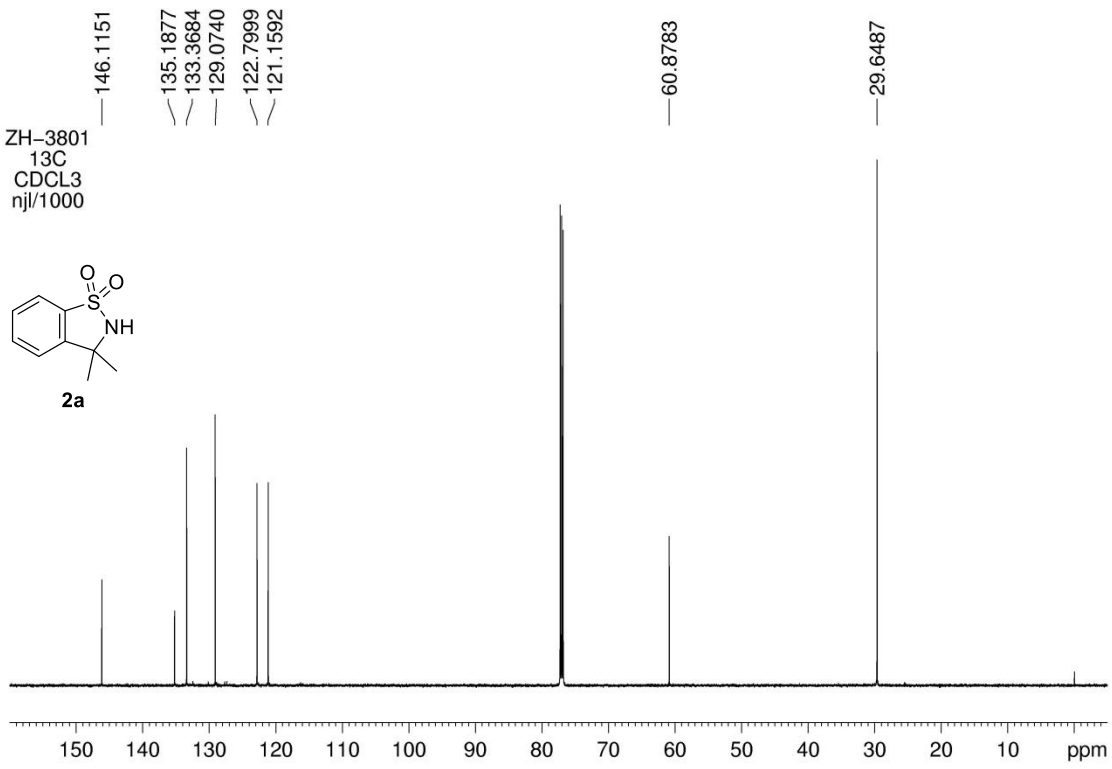

WOH
1H
CDCl3
smp/1550
7.2134
4.1282
4.1171
4.1058
4.0946
4.0834
2.9434
2.9320
2.9205
2.9090
2.8975
1.2938
1.2826
1.2699
1.2583
4.10 ppm
2.95 ppm
3
8 7 6 5 4 3 2 1 0 ppm
2.0000
2.2377
1.0928
12.0460
6.0583

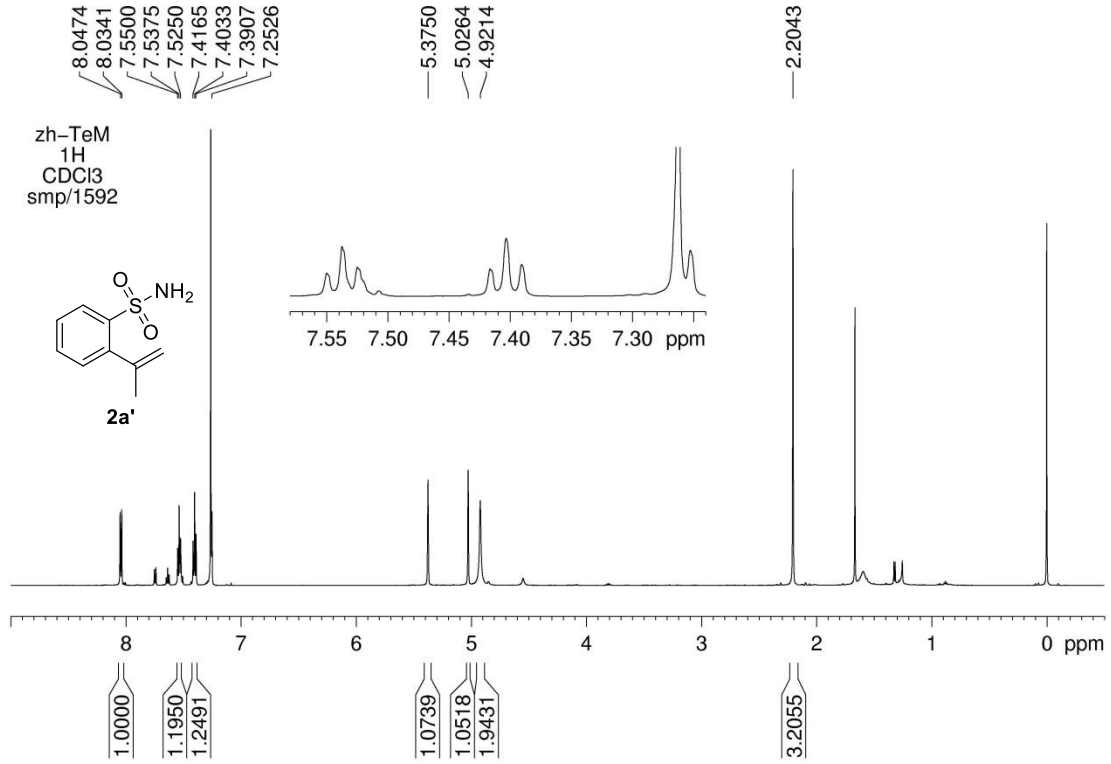

WOH
13C
CDCl3
smp/1551
154.2217
152.0122
145.8256
124.0991
34.3206
30.0489
24.9671
23.4941
3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

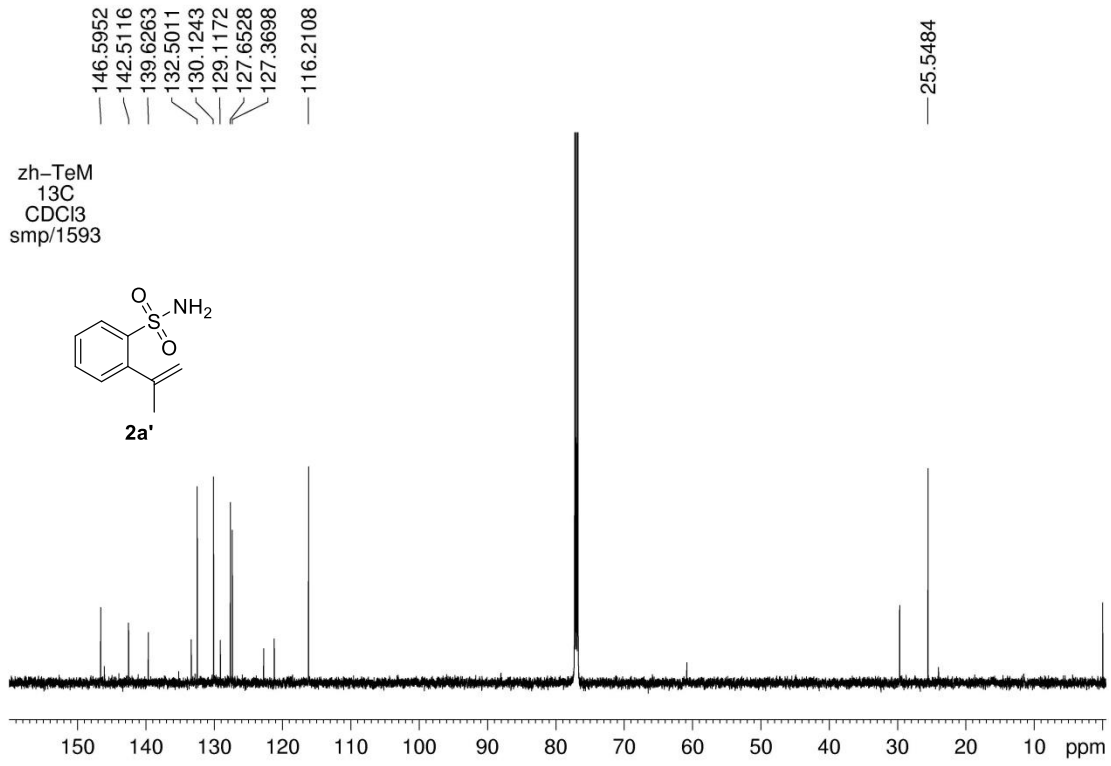

wjl-s
1H
CDCl3
smp/1585
7.1048
4.4490
4.4377
4.4265
4.4152
4.4039
2.8941
2.8826
2.8711
2.8596
2.8481
2.6967
1.2609
1.2495
1.2449
1.2332
4
4.45
ppm
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.0000
2.0010
1.0054
6.0592
18.1862

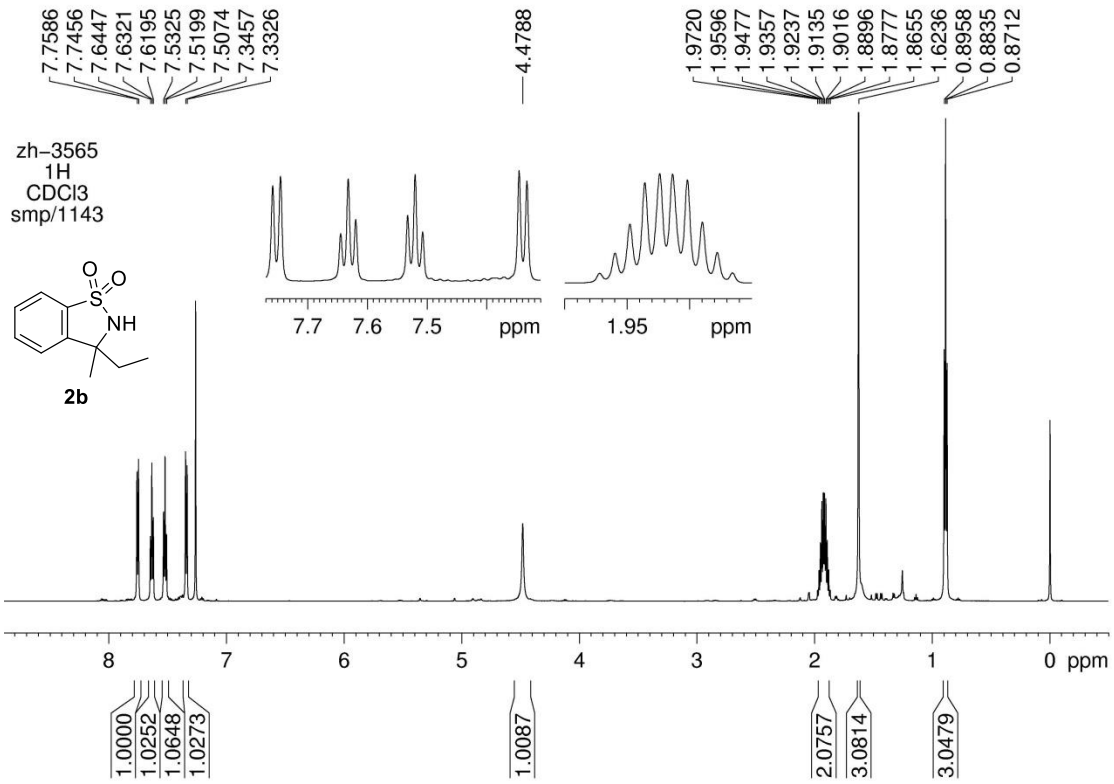

wjl-s
13C
CDCl3
smp/1586
151.1261
149.0326
137.2215
123.1991
36.2779
34.0745
29.3679
24.9013
23.6864
4
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

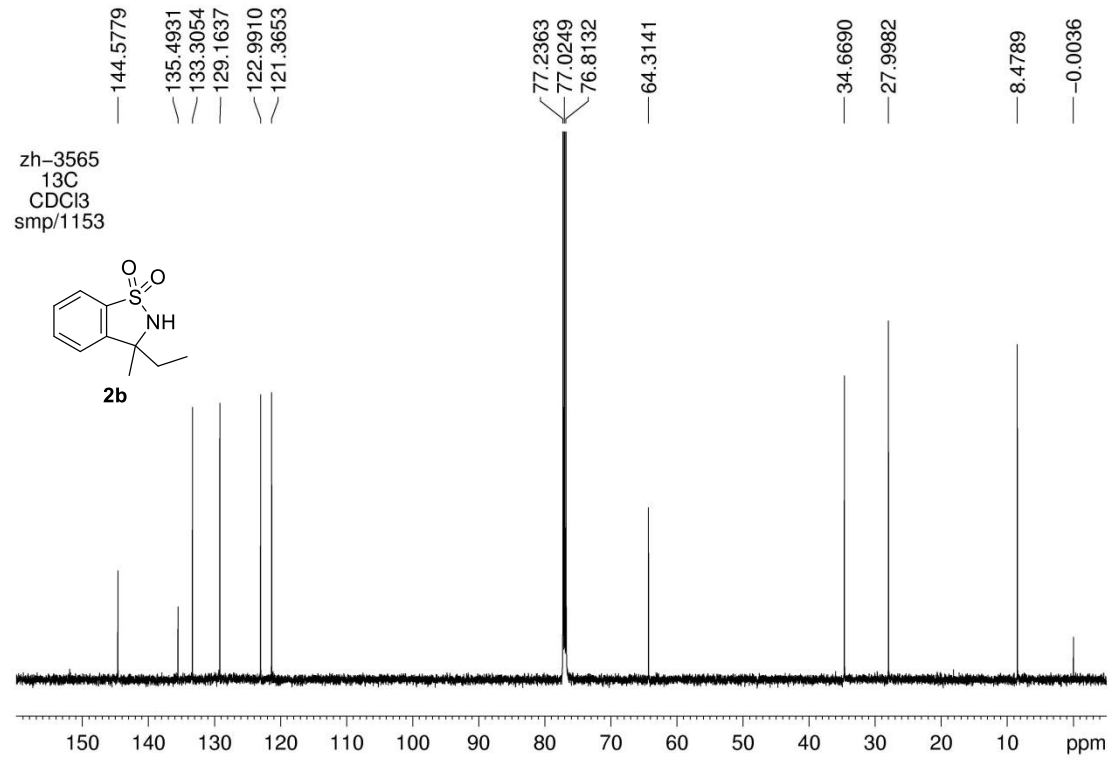

7.7338
7.7209
7.6341
7.6216
7.6089
7.5139
7.5012
7.4887
7.3937
7.3807
4.7886
1.6492
zh–3801
1H
CDCl3
smp/993
7.7
7.6
7.5
ppm
2a
8
7
6
5
4
3
2
1
0 ppm
0.9999
1.0399
1.0649
1.0427
1.0101
6.1716

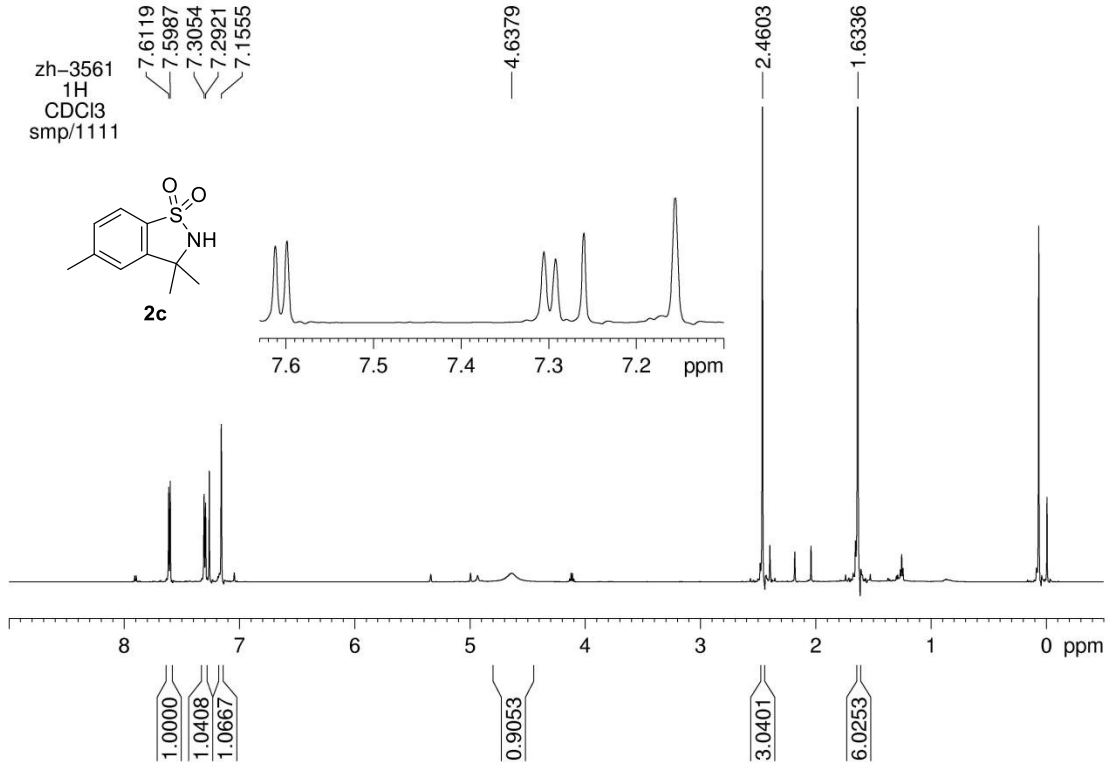

146.1151
135.1877
133.3684
129.0740
122.7999
121.1592
60.8783
29.6487
ZH–3801
13C
CDCL3
njl/1000
2a
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

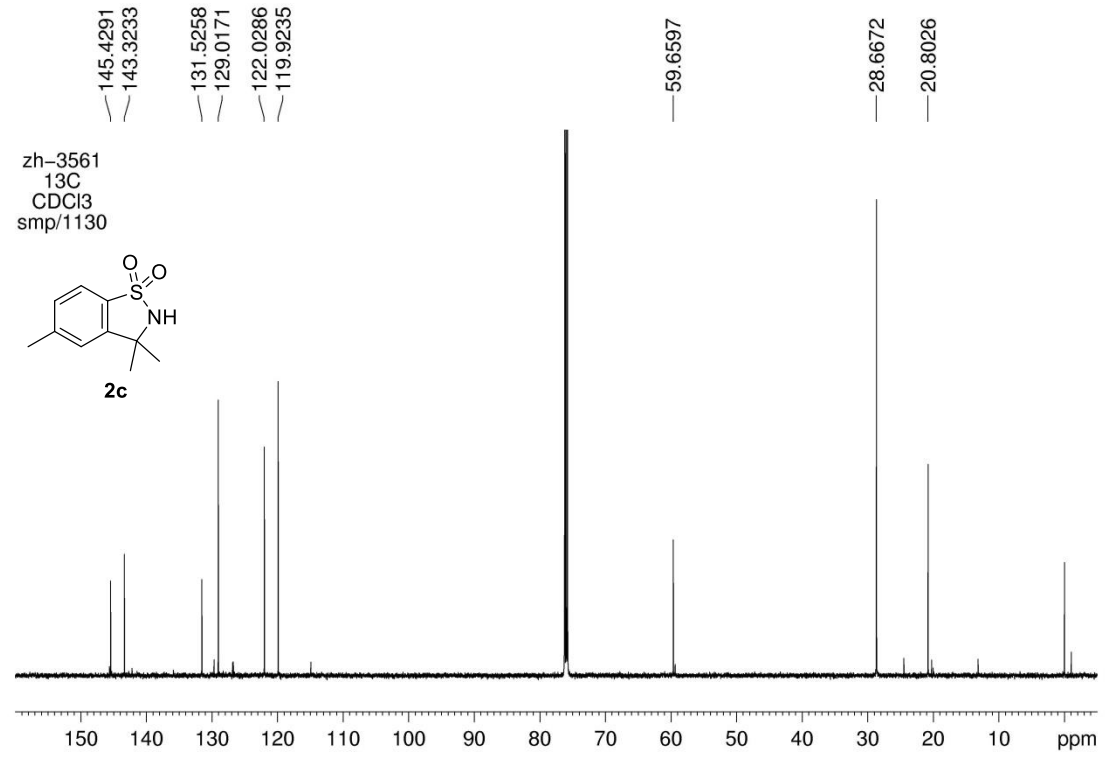

8.0474
8.0341
7.5500
7.5375
7.5250
7.4165
7.4033
7.3907
7.2526
5.3750
5.0264
4.9214
2.2043
zh–TeM
1H
CDCl3
smp/1592
O
NH2
S
O
2a'
7.55 7.50 7.45 7.40 7.35 7.30 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.1950
1.2491
1.0739
1.0518
1.9431
3.2055

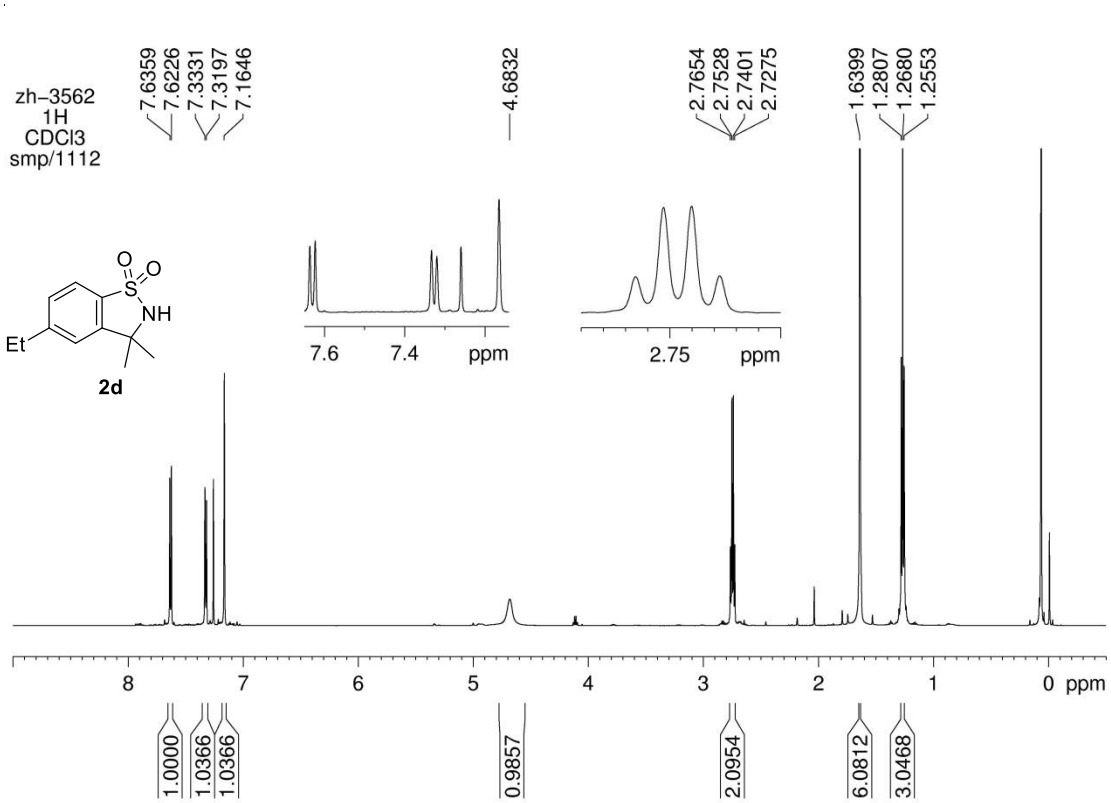

146.5952
142.5116
139.6263
132.5011
130.1243
129.1172
127.6528
127.3698
116.2108
25.5484
zh–TeM
13C
CDCl3
smp/1593
O
NH2
S
O
2a'
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

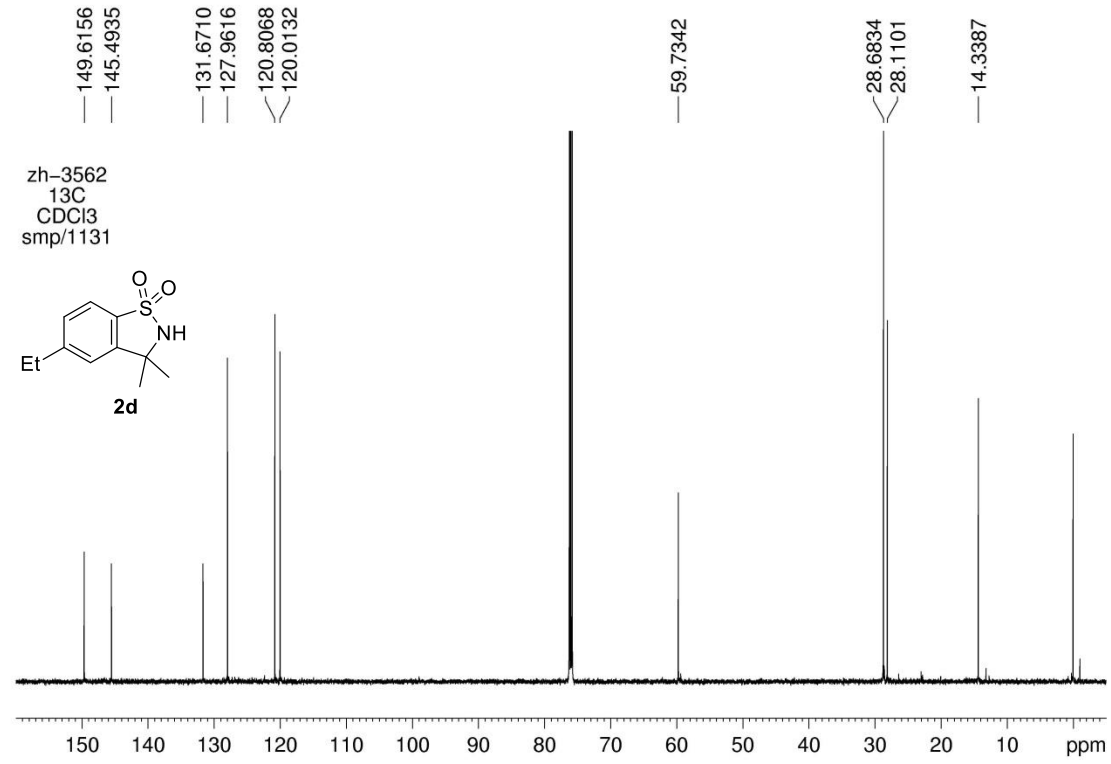

7.7586
7.7456
7.6447
7.6321
7.6195
7.5325
7.5199
7.5074
7.3457
7.3326
4.4788
1.9720
1.9596
1.9477
1.9357
1.9237
1.9135
1.9016
1.8896
1.8777
1.8655
1.6236
0.8958
0.8835
0.8712
zh–3565
1H
CDCl3
smp/1143
2b
7.7 7.6 7.5 ppm
1.95 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0252
1.0648
1.0273
1.0087
2.0757
3.0814
3.0479

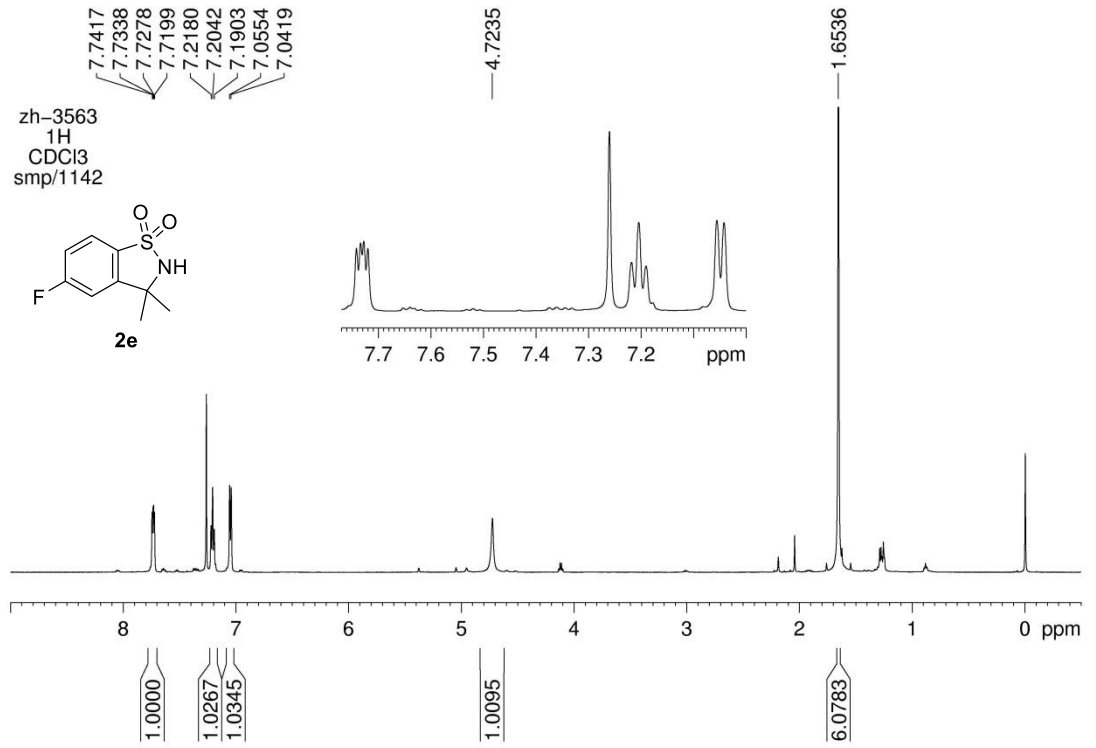

144.5779
135.4931
133.3054
129.1637
122.9910
121.3653
77.2363
77.0249
76.8132
64.3141
34.6690
27.9982
8.4789
–0.0036
zh–3565
13C
CDCl3
smp/1153
2b
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

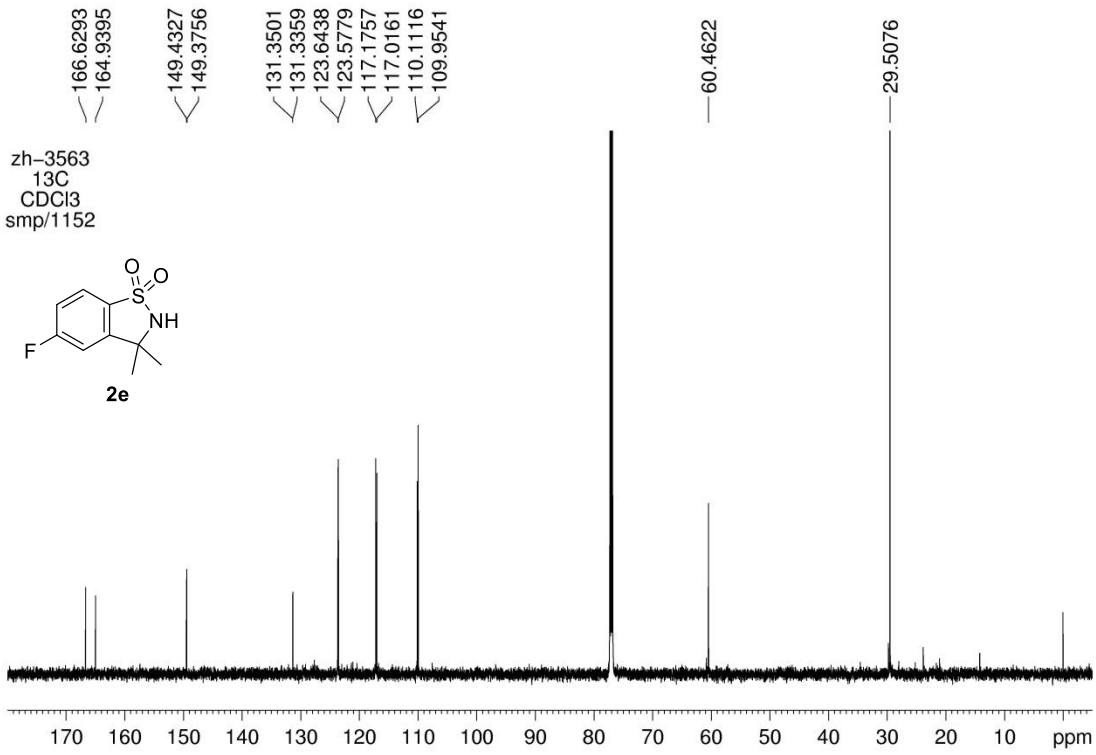

zh–3561
1H
CDCl3
smp/1111
7.6119
7.5987
7.3054
7.2921
7.1555
4.6379
2.4603
1.6336
2c
7.6
7.5
7.4
7.3
7.2
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0408
1.0667
0.9053
3.0401
6.0253

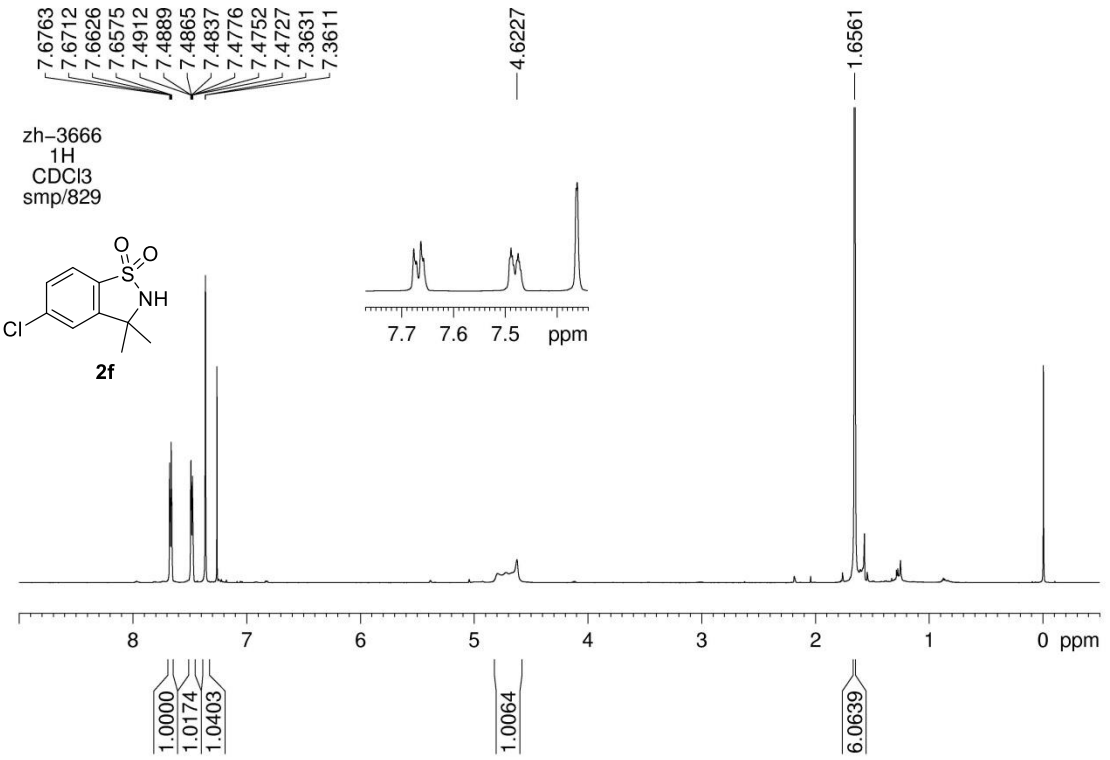

zh–3561
13C
CDCl3
smp/1130
145.4291
143.3233
131.5258
129.0171
122.0286
119.9235
59.6597
28.6672
20.8026
2c
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

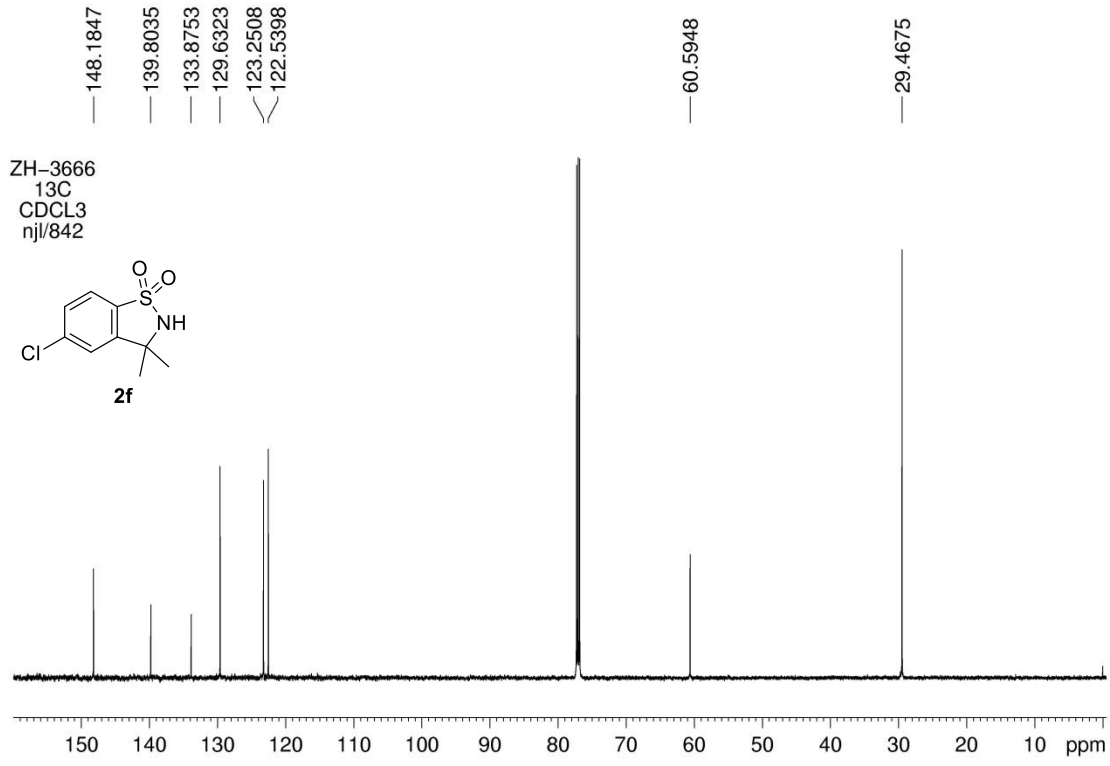

zh–3562
1H
CDCl3
smp/1112
7.6359
7.6226
7.3331
7.3197
7.1646
4.6832
2.7654
2.7528
2.7401
2.7275
1.6399
1.2807
1.2680
1.2553
Et
NH
2d
7.6
7.4
ppm
2.75
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0366
1.0366
0.9857
2.0954
6.0812
3.0468


149.6156
145.4935
131.6710
127.9616
120.8068
120.0132
59.7342
28.6834
28.1101
14.3387
zh–3562
13C
CDCl3
smp/1131
Et
NH
2d
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.7417
7.7338
7.7278
7.7199
7.2180
7.2042
7.1903
7.0554
7.0419
4.7235
1.6536
zh–3563
1H
CDCl3
smp/1142
O
O
S
NH
F
2e
7.7 7.6 7.5 7.4 7.3 7.2 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0267
1.0345
1.0095
6.0783


166.6293
164.9395
149.4327
149.3756
131.3501
131.3359
123.6438
123.5779
117.1757
117.0161
110.1116
109.9541
60.4622
29.5076
zh–3563
13C
CDCl3
smp/1152
O
O
S
NH
F
2e
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.6763
7.6712
7.6626
7.6575
7.4912
7.4889
7.4865
7.4837
7.4776
7.4752
7.4727
7.3631
7.3611
4.6227
1.6561
zh–3666
1H
CDCl3
smp/829
O
O
S
NH
Cl
2f
7.7 7.6 7.5 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0174
1.0403
1.0064
6.0639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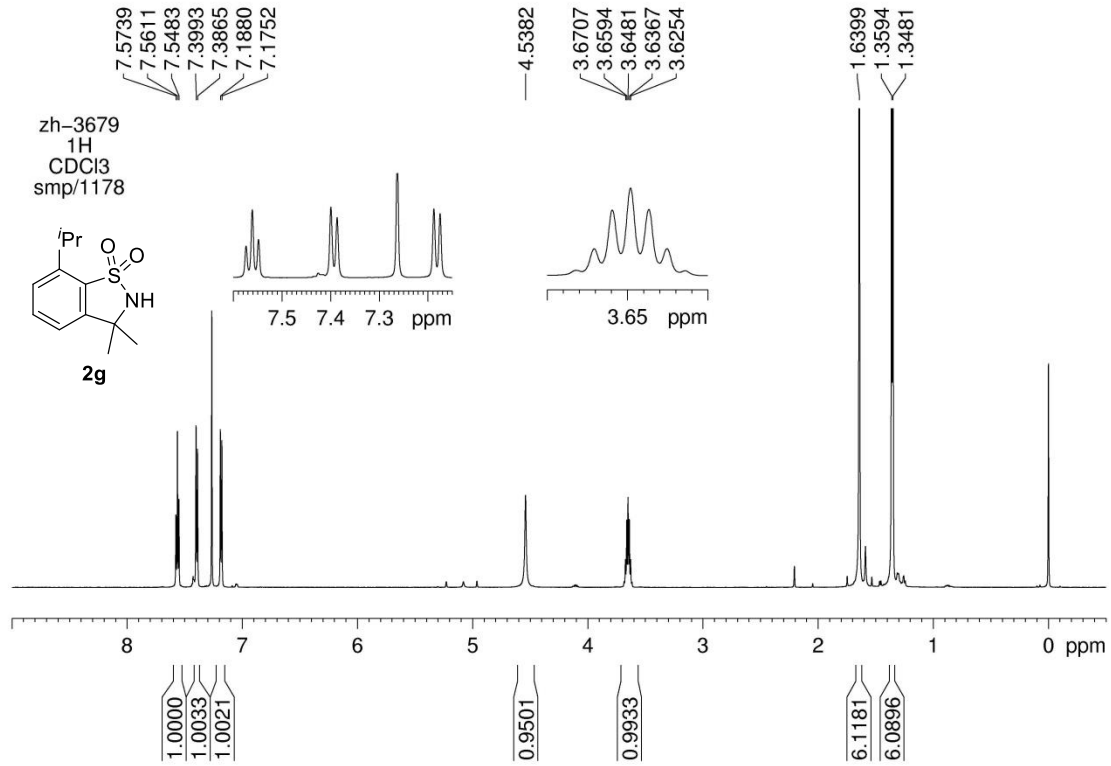
139.8035
133.8753
129.6323
123.2508
122.5398
60.5948
29.4675
ZH–3666
13C
CDCL3
njl/842
O
O
S
NH
Cl
2f
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.5739
7.5611
7.5483
7.3993
7.3865
7.1880
7.1752
4.5382
3.6707
3.6594
3.6481
3.6367
3.6254
1.6399
1.3594
1.3481
zh–3679
1H
CDCl3
smp/1178
iPr
O
O
S
NH
2g
7.5 7.4 7.3 ppm
3.65 ppm
8 7 6 5 4 3 2 1 0 ppm
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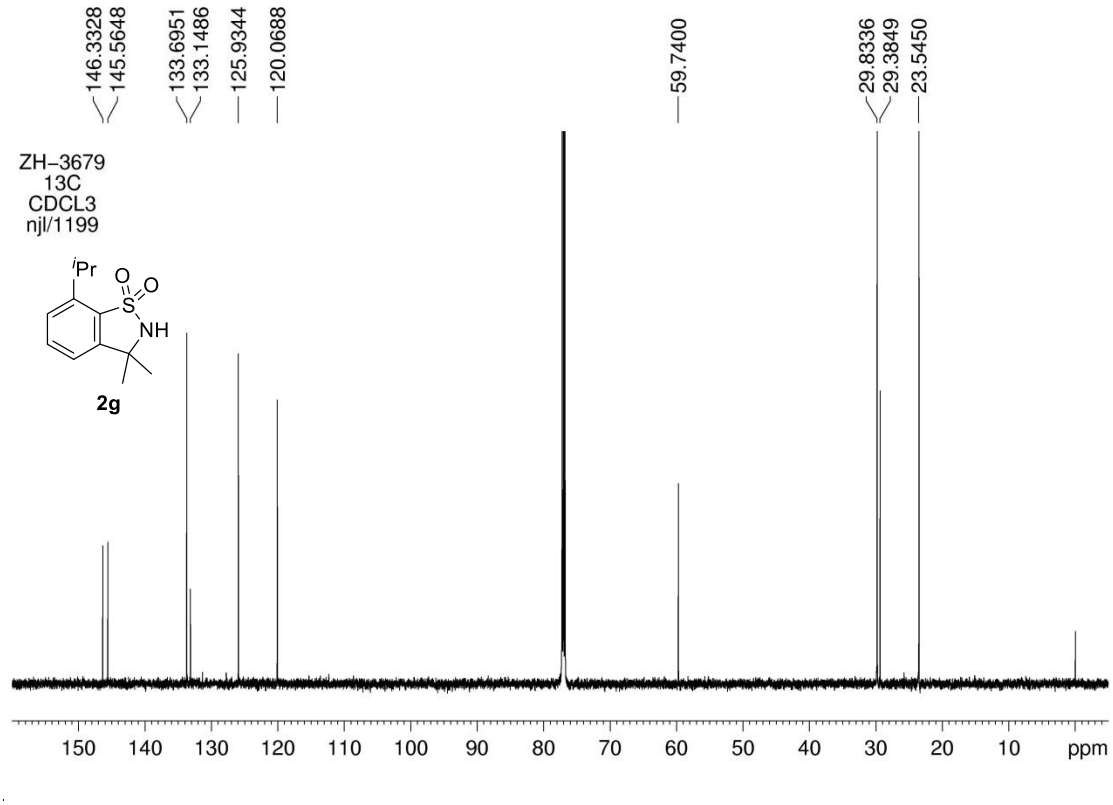
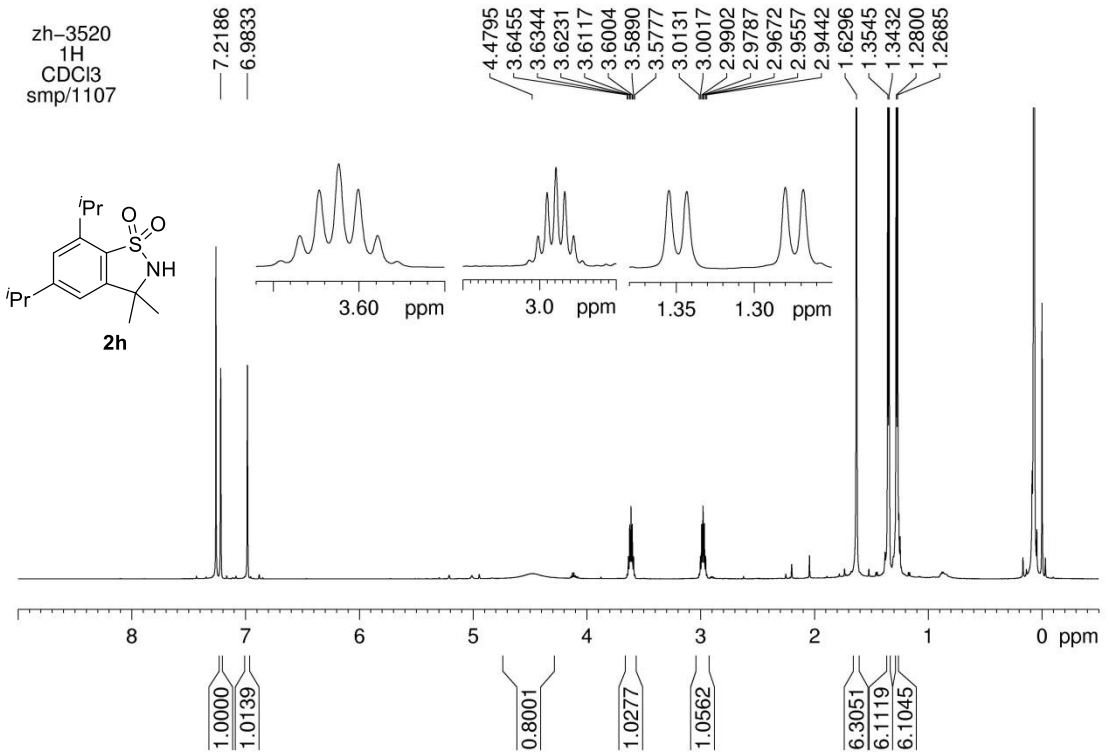
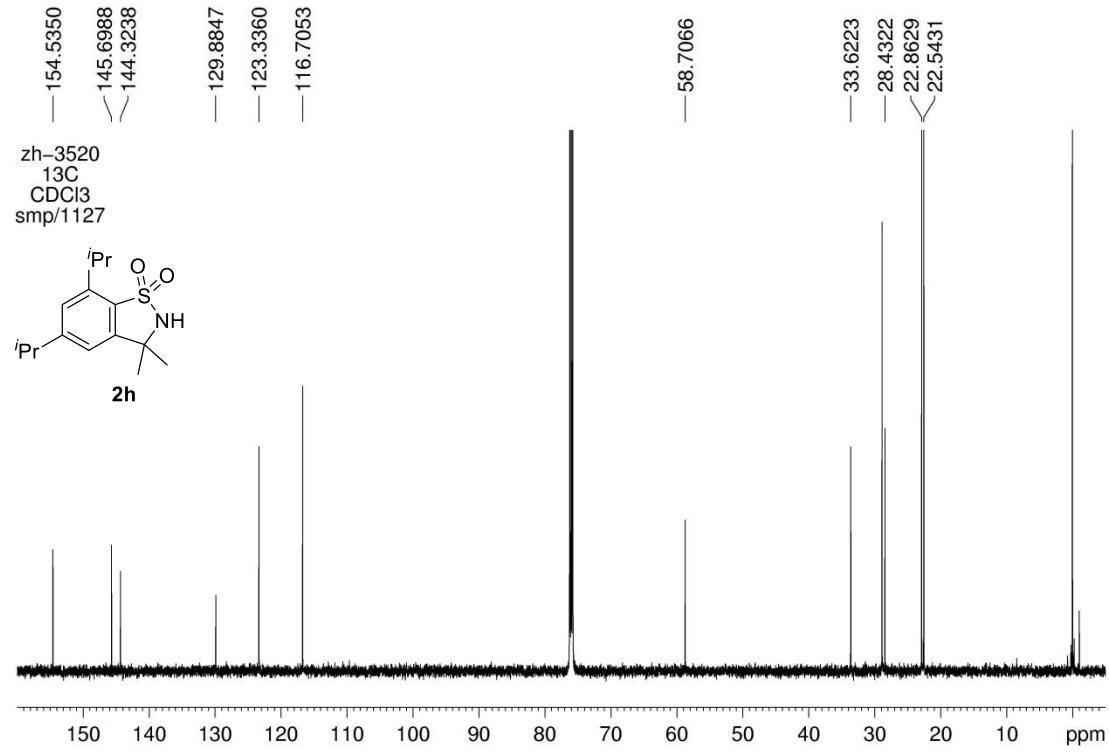
1.0033
1.0021
0.9501
0.9933
6.1181
6.0896


146.3328
145.5648
133.6951
133.1486
125.9344
120.0688
59.7400
29.8336
29.3849
23.5450
ZH–3679
13C
CDCL3
njl/1199
iPr
O
O
S
NH
2g
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


zh–3520
1H
CDCl3
smp/1107
7.2186
6.9833
4.4795
3.6455
3.6344
3.6231
3.6117
3.6004
3.5890
3.5777
3.0131
3.0017
2.9902
2.9787
2.9672
2.9557
2.9442
1.6296
1.3545
1.3432
1.2800
1.2685
3.60 ppm
3.0 ppm
1.35
1.30 ppm
2h
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0139
0.8001
1.0277
1.0562
6.3051
6.1119
6.1045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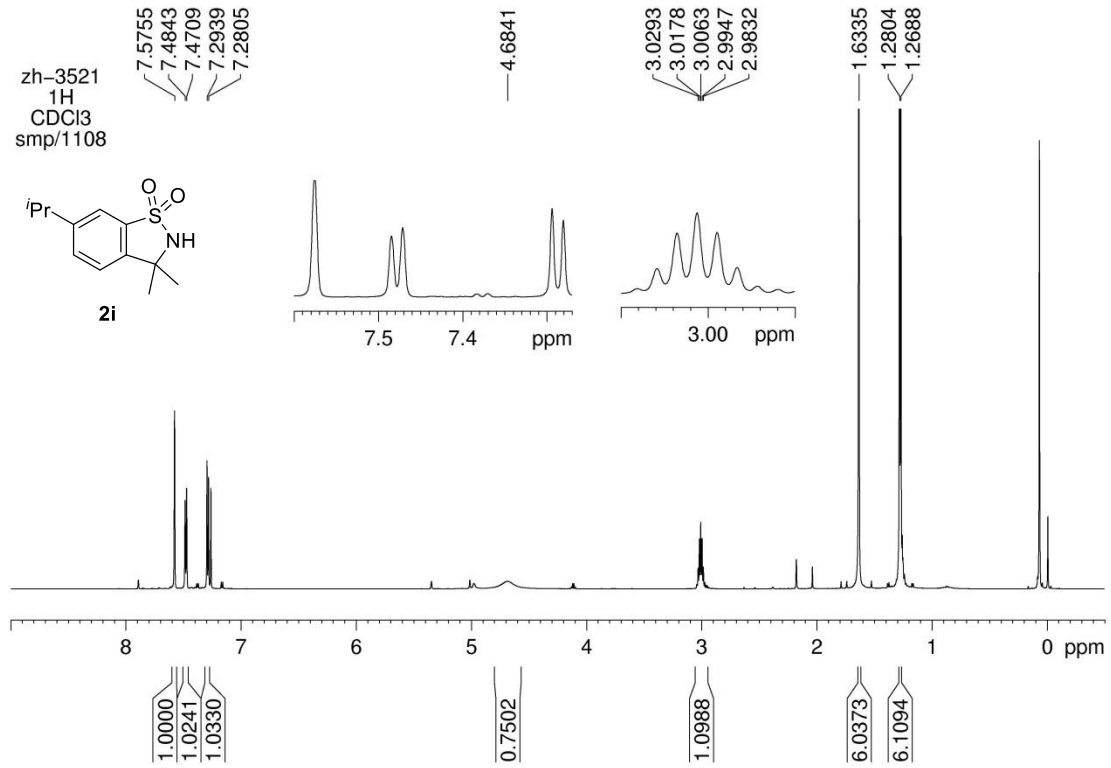
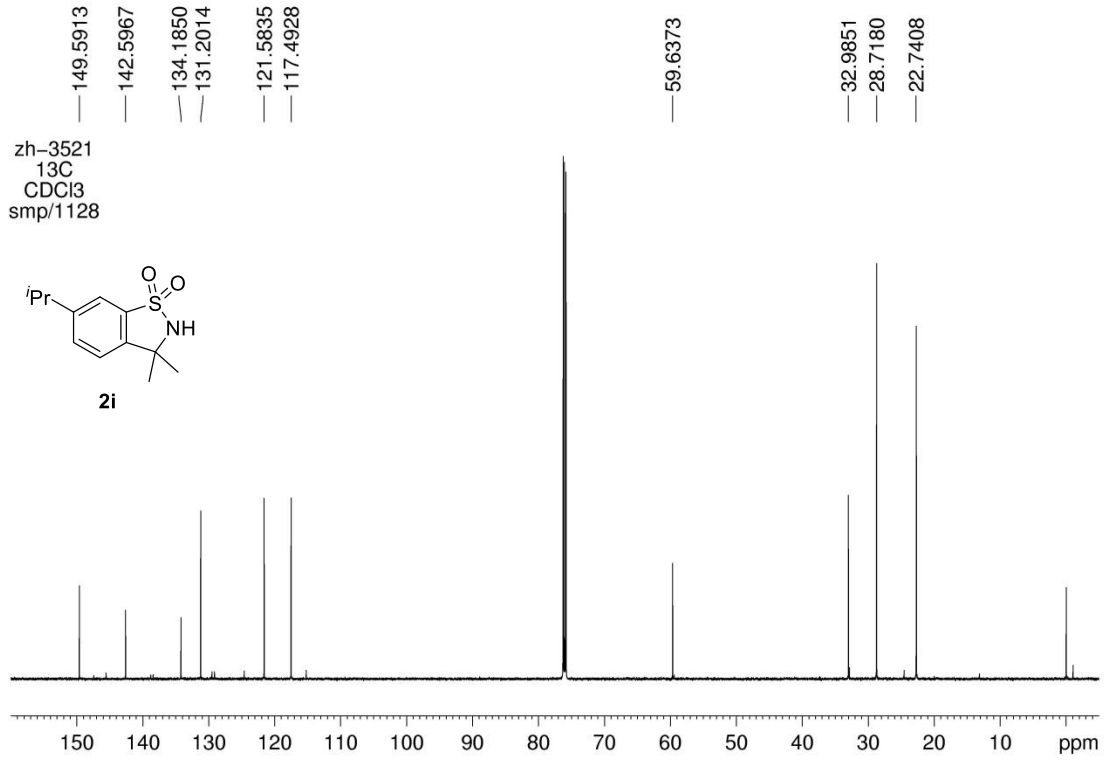
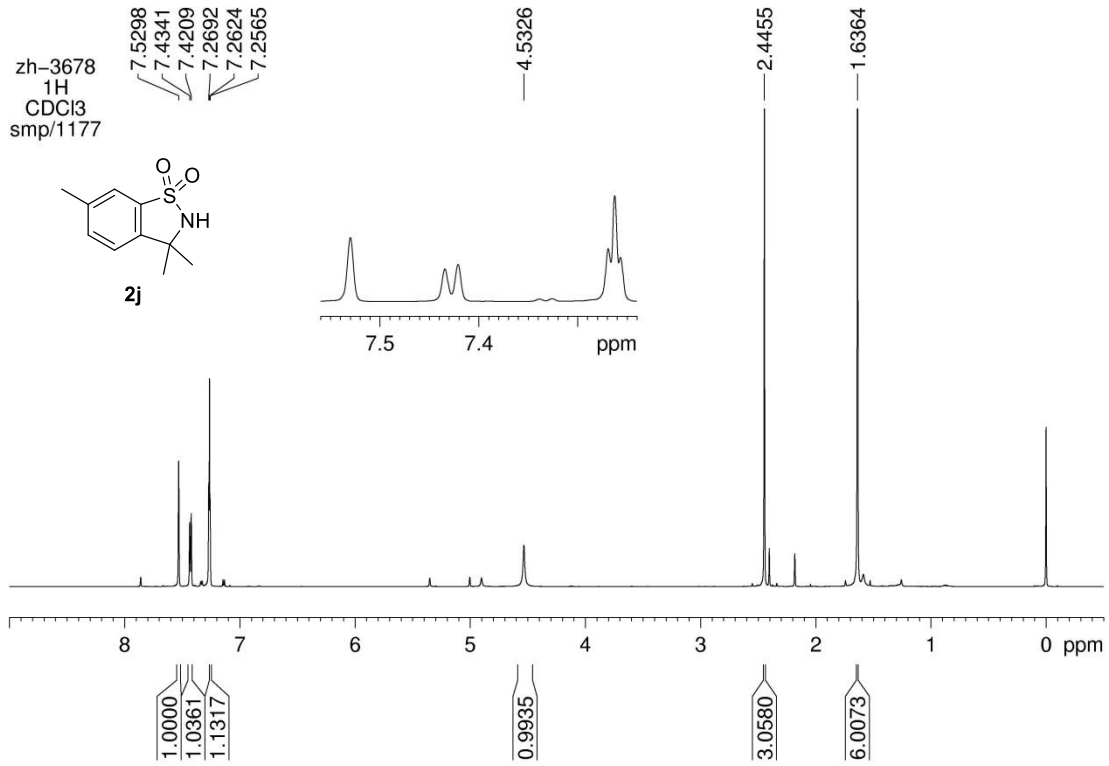
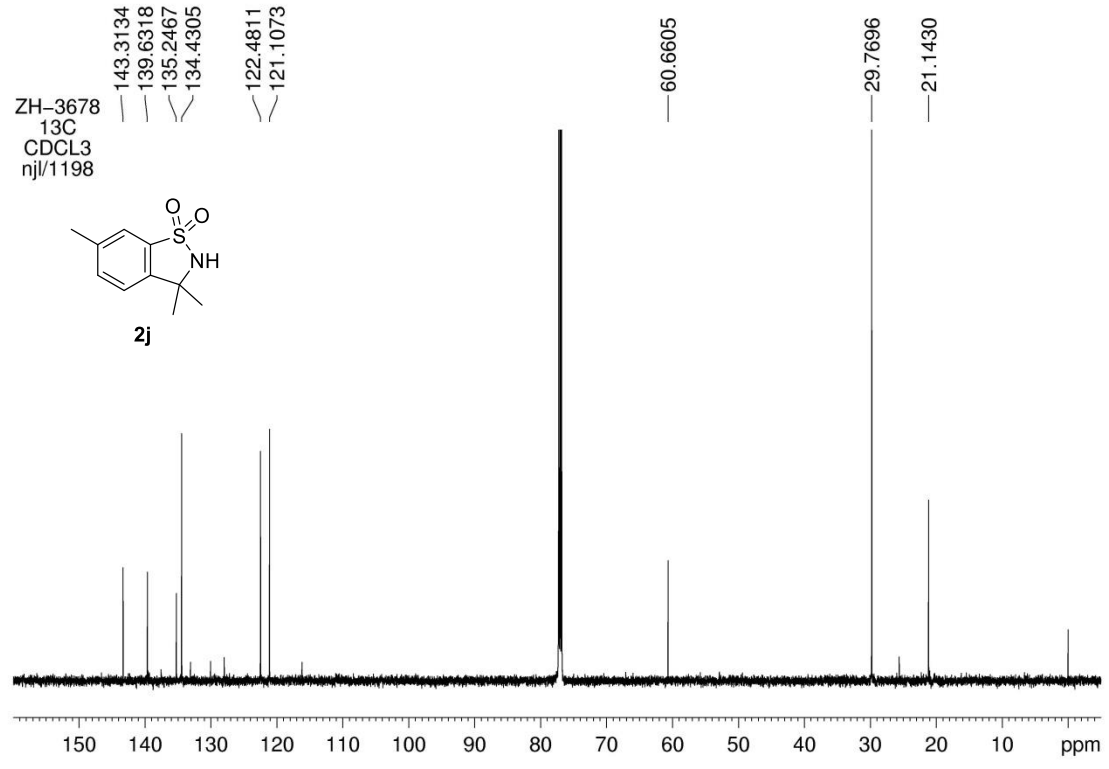
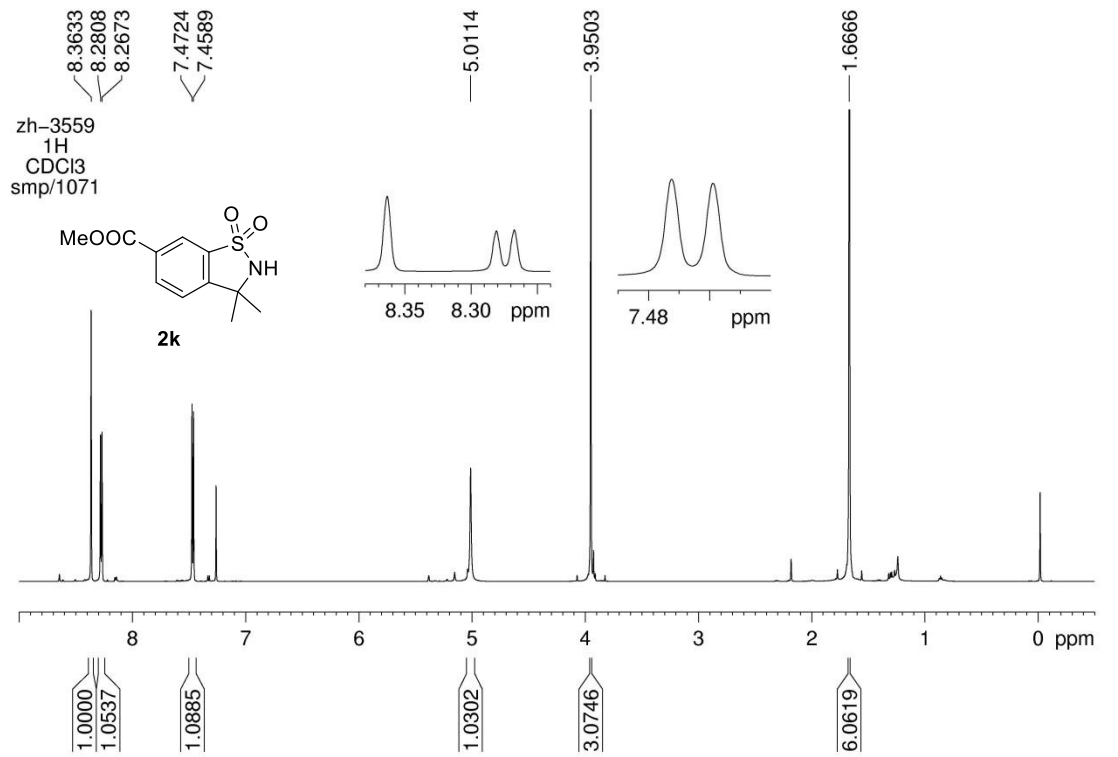
145.6988
144.3238
129.8847
123.3360
116.7053
58.7066
33.6223
28.4322
22.8629
22.5431
zh–3520
13C
CDCl3
smp/1127
2h
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

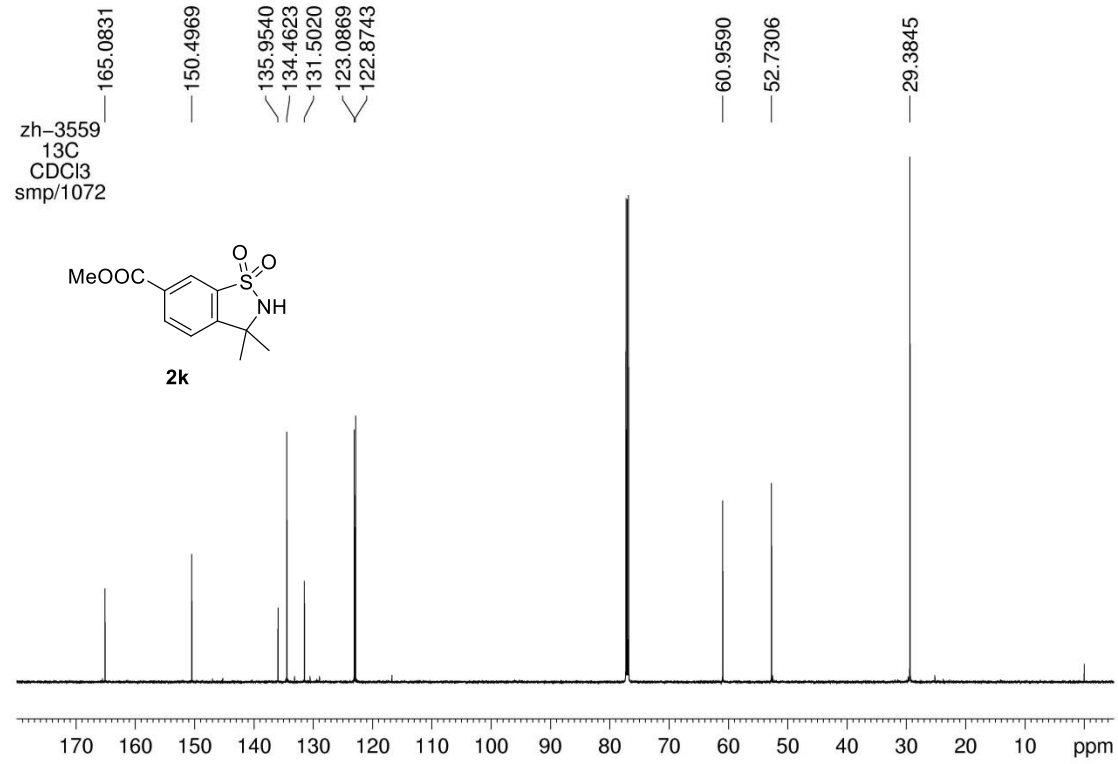

zh–3521
1H
CDCl3
smp/1108
7.5755
7.4843
7.4709
7.2939
7.2805
4.6841
3.0293
3.0178
3.0063
2.9947
2.9832
1.6335
1.2804
1.2688
iPr
O
S
O
NH
2i
7.5
7.4
ppm
3.00
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0241
1.0330
0.7502
1.0988
6.0373
6.1094


149.5913
142.5967
134.1850
131.2014
121.5835
117.4928
59.6373
32.9851
28.7180
22.7408
zh–3521
13C
CDCl3
smp/1128
iPr
O
S
O
NH
2i
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


zh–3678
1H
CDCl3
smp/1177
7.5298
7.4341
7.4209
7.2692
7.2624
7.2565
4.5326
2.4455
1.6364
2j
7.5
7.4
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0361
1.1317
0.9935
3.0580
6.0073


ZH–3678
13C
CDCL3
njl/1198
143.3134
139.6318
135.2467
134.4305
122.4811
121.1073
60.6605
29.7696
21.1430
2j
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.3633
8.2808
8.2673
7.4724
7.4589
5.0114
3.9503
1.6666
zh–3559
1H
CDCl3
smp/1071
MeOOC
O
O
S
NH
2k
8.35
8.30
ppm
7.48
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0537
1.0885
1.0302
3.0746
6.0619


165.0831
150.4969
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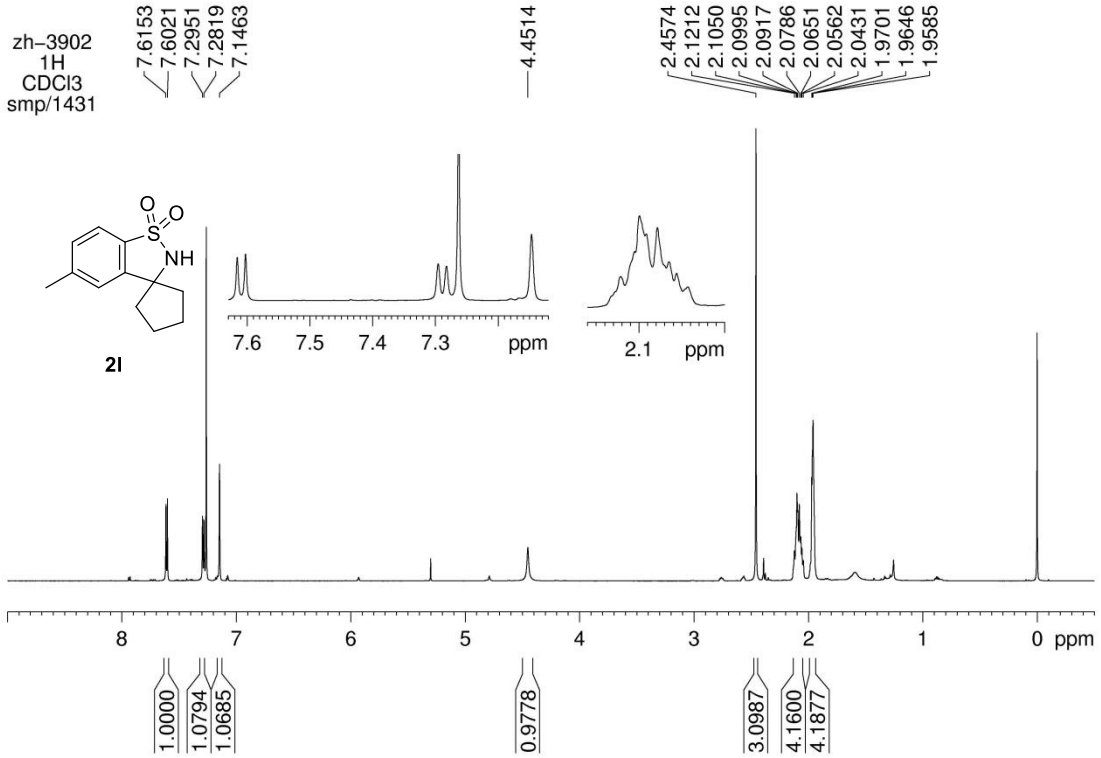
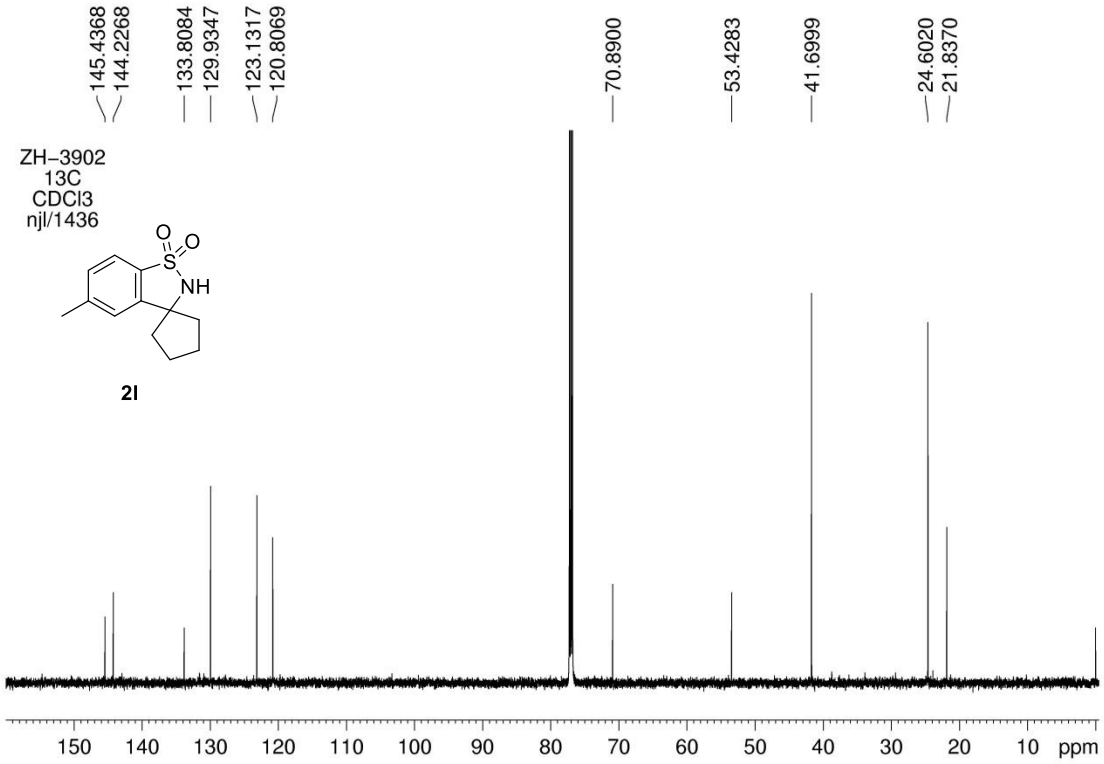
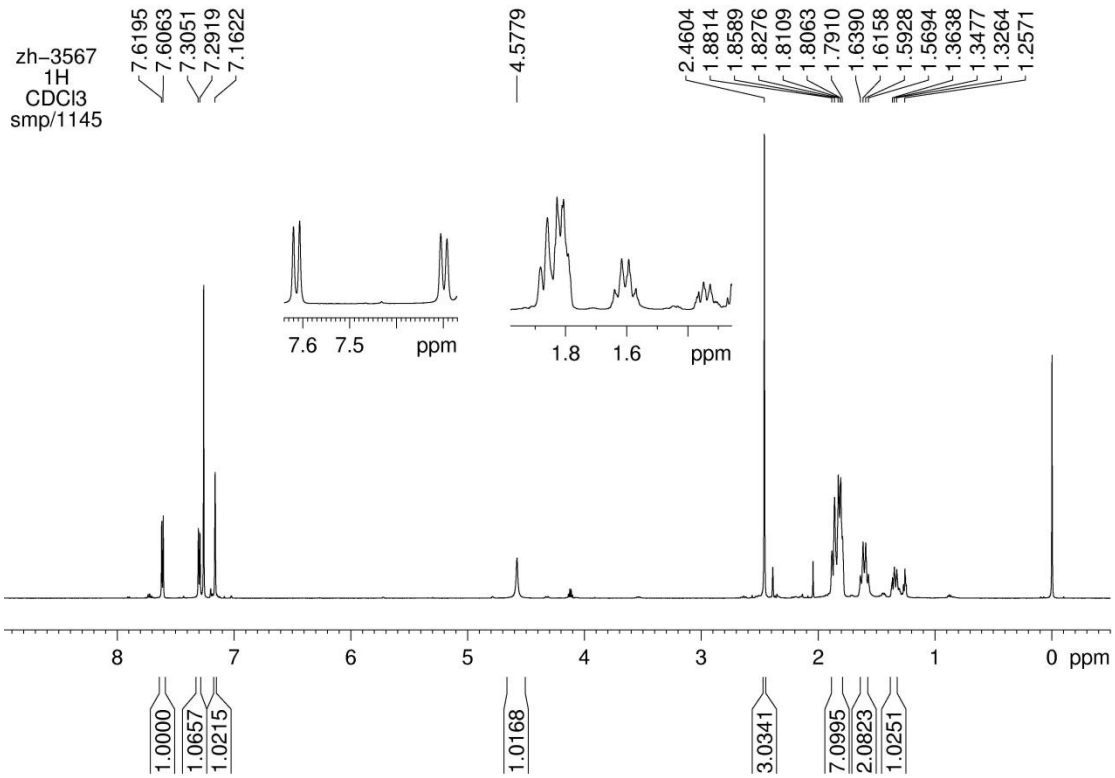
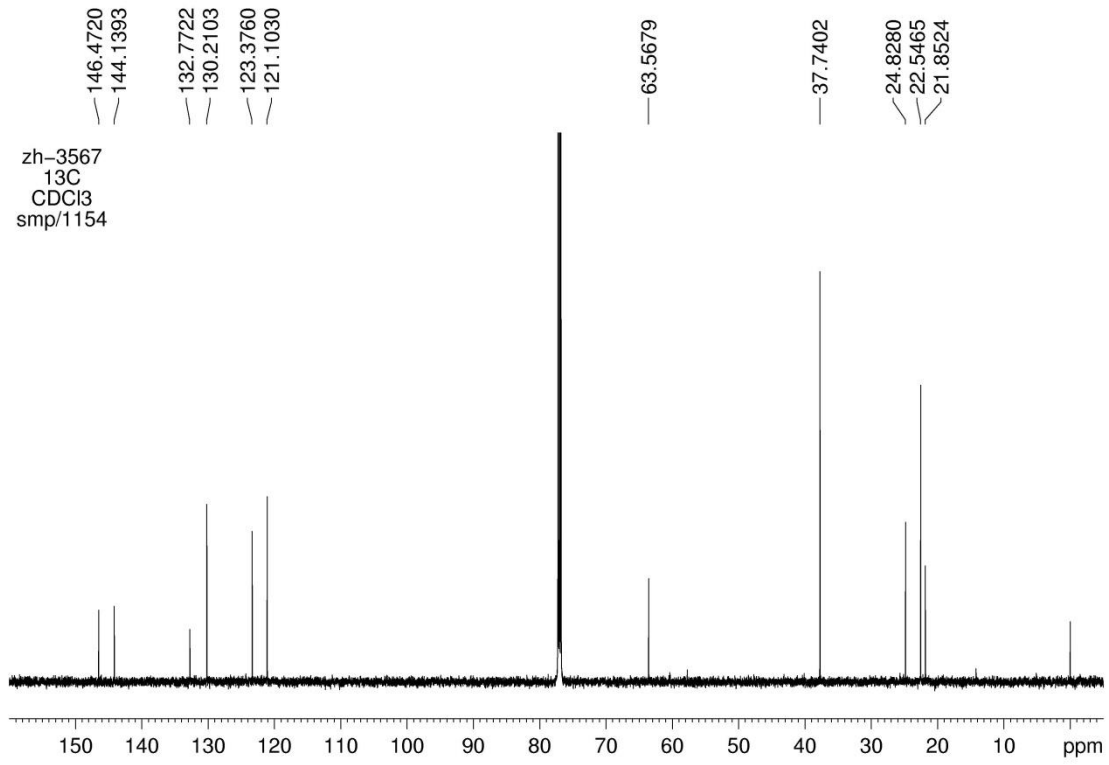
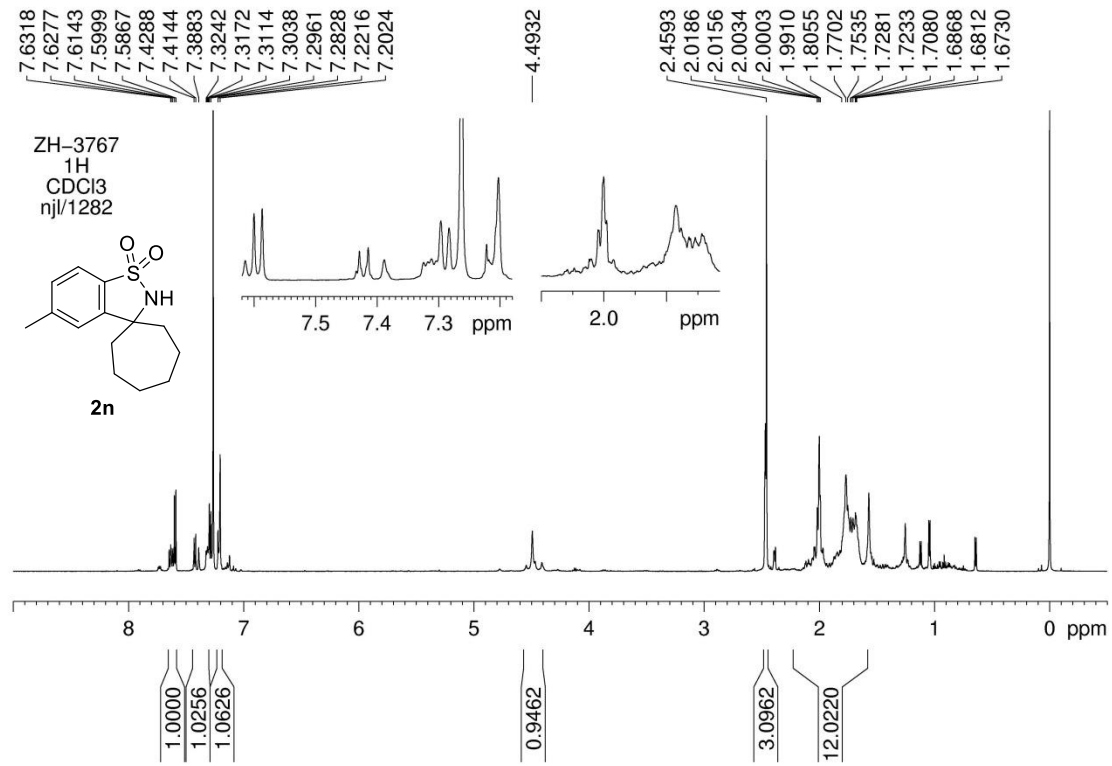
134.4623
131.5020
123.0869
122.8743
60.9590
52.7306
29.3845
zh–3559
13C
CDCl3
smp/1072
MeOOC
O
O
S
NH
2k
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

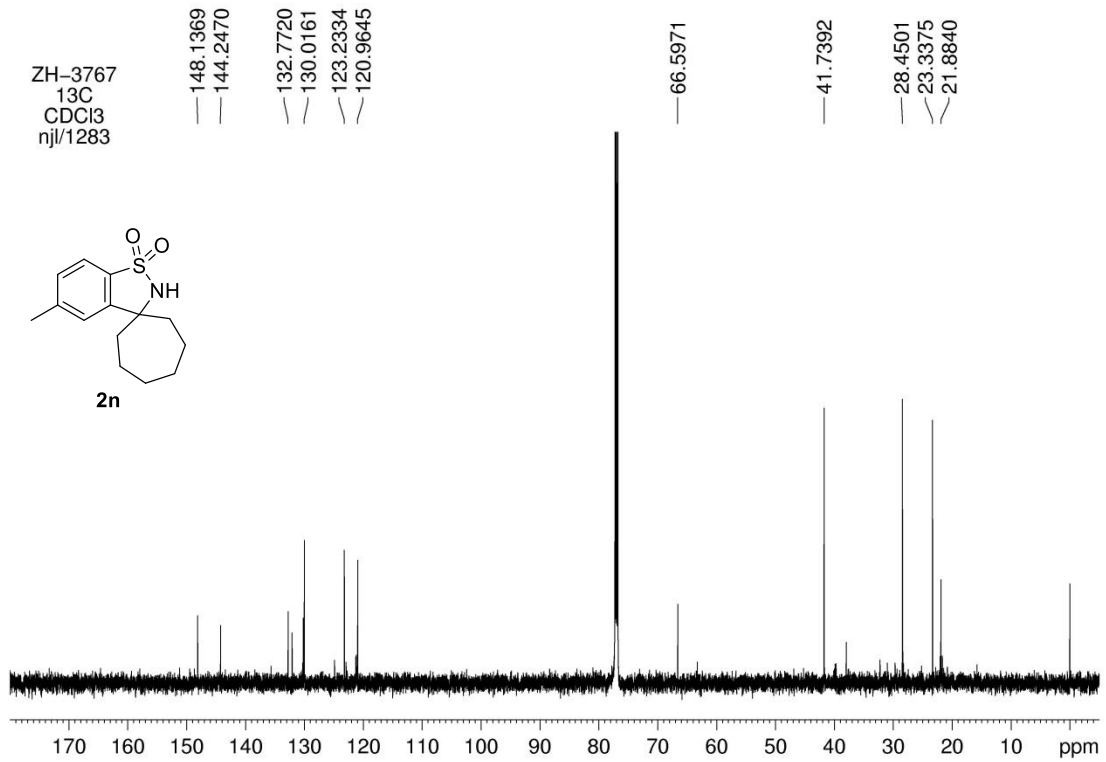

zh–3902
1H
CDCl3
smp/1431
7.6153
7.6021
7.2951
7.2819
7.1463
4.4514
2.4574
2.1212
2.1050
2.0995
2.0917
2.0786
2.0651
2.0562
2.0431
1.9701
1.9646
1.9585
O
O
S
NH
2l
7.6 7.5 7.4 7.3 ppm
2.1 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0794
1.0685
0.9778
3.0987
4.1600
4.1877

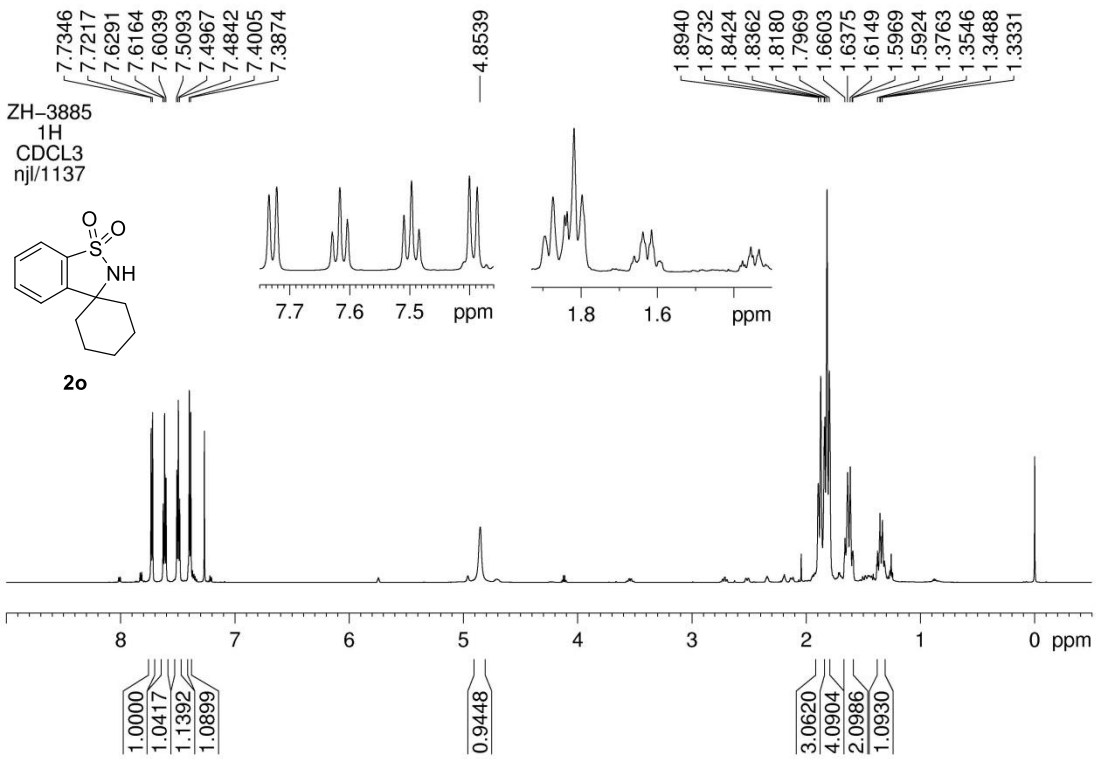

145.4368
144.2268
133.8084
129.9347
123.1317
120.8069
70.8900
53.4283
41.6999
24.6020
21.8370
ZH–3902
13C
CDCl3
njl/1436
O
O
S
NH
2l
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

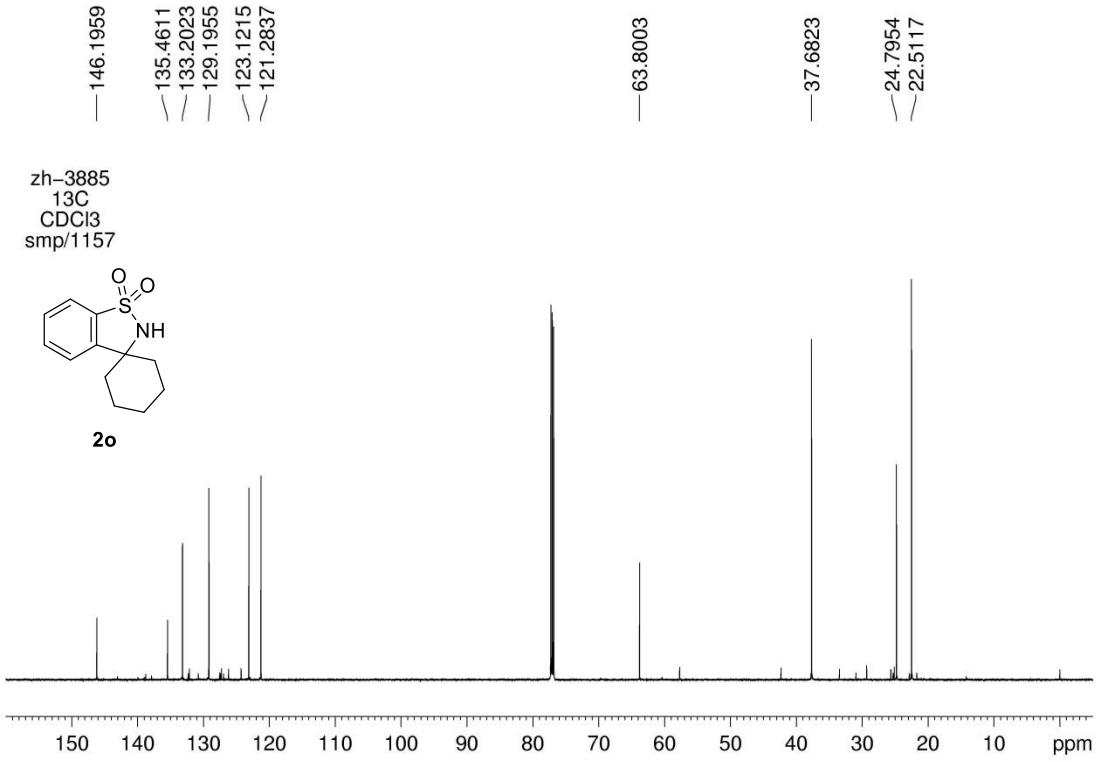

zh–3567
1H
CDCl3
smp/1145
7.6195
7.6063
7.3051
7.2919
7.1622
4.5779
2.4604
1.8814
1.8589
1.8276
1.8109
1.8063
1.7910
1.6390
1.6158
1.5928
1.5694
1.3638
1.3477
1.3264
1.2571
7.6 7.5 ppm
1.8 1.6 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0657
1.0215
1.0168
3.0341
7.0995
2.0823
1.0251

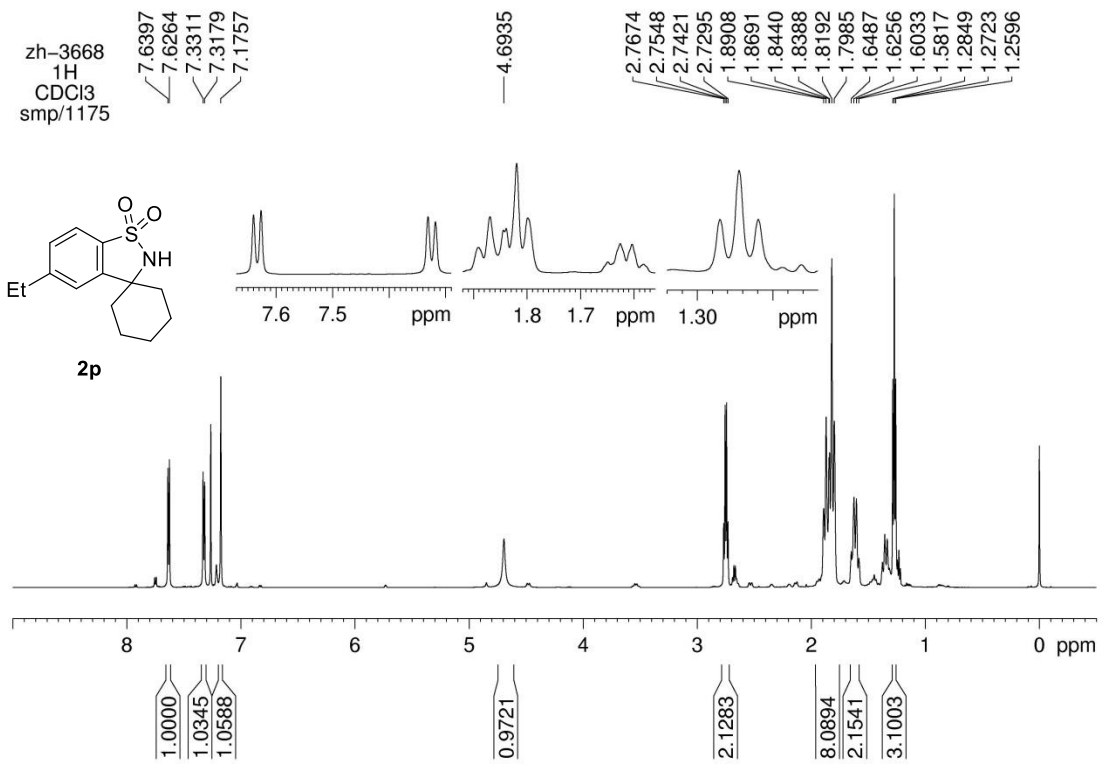

146.4720
144.1393
132.7722
130.2103
123.3760
121.1030
63.5679
37.7402
24.8280
22.5465
21.8524
zh–3567
13C
CDCl3
smp/1154
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.6318
7.6277
7.6143
7.5999
7.5867
7.4288
7.4144
7.3883
7.3242
7.3172
7.3114
7.3038
7.2961
7.2828
7.2216
7.2024
4.4932
2.4593
2.0186
2.0156
2.0034
2.0003
1.9910
1.8055
1.7702
1.7535
1.7281
1.7233
1.7080
1.6868
1.6812
1.6730
ZH–3767
1H
CDCl3
njl/1282
7.5 7.4 7.3 ppm
2.0 ppm
2n
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0256
1.0626
0.9462
3.0962
12.0220


148.1369
144.2470
132.7720
130.0161
123.2334
120.9645
66.5971
41.7392
28.4501
23.3375
21.8840
ZH–3767
13C
CDCl3
njl/1283
2n
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.7346
7.7217
7.6291
7.6164
7.6039
7.5093
7.4967
7.4842
7.4005
7.3874
4.8539
1.8940
1.8732
1.8424
1.8362
1.8180
1.7969
1.6603
1.6375
1.6149
1.5969
1.5924
1.3763
1.3546
1.3488
1.3331
ZH-3885
1H
CDCL3
njl/1137
O
O
S
NH
2o
7.7
7.6
7.5
ppm
1.8
1.6
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0417
1.1392
1.0899
0.9448
3.0620
4.0904
2.0986
1.0930


146.1959
135.4611
133.2023
129.1955
123.1215
121.2837
63.8003
37.6823
24.7954
22.5117
zh-3885
13C
CDCl3
smp/1157
O
O
S
NH
2o
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


zh-3668
1H
CDCl3
smp/1175
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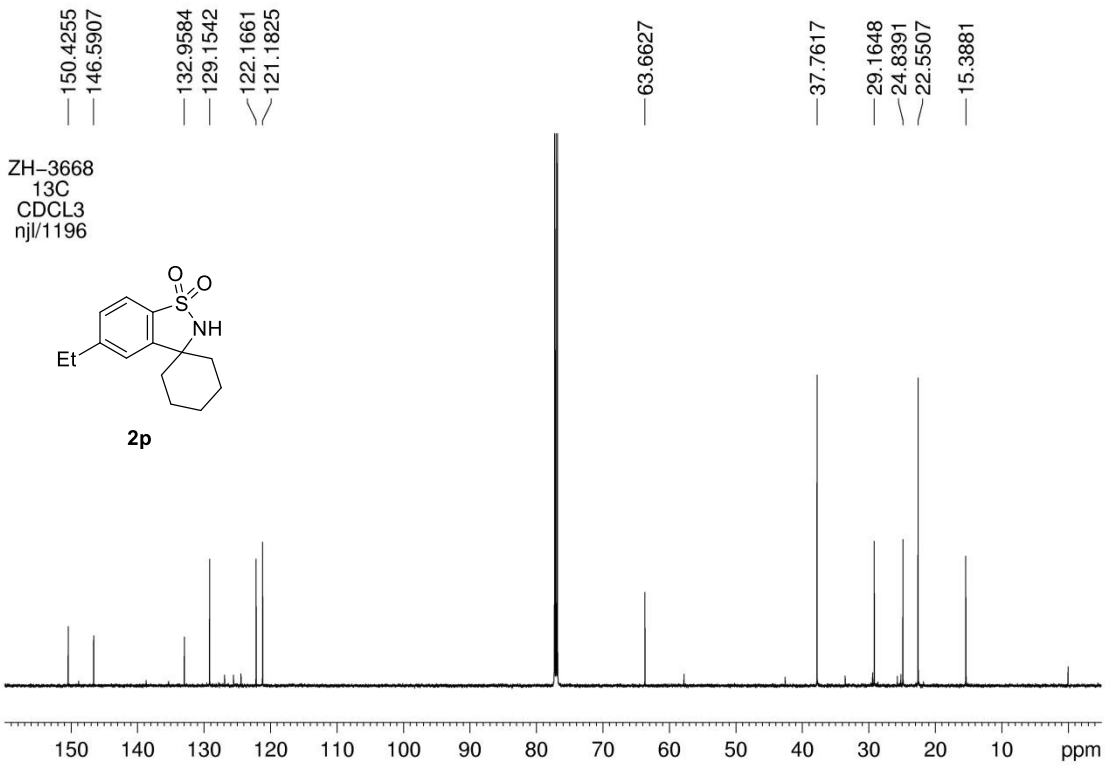
7.6264
7.3311
7.3179
7.1757
4.6935
2.7674
2.7548
2.7421
2.7295
1.8908
1.8691
1.8440
1.8388
1.8192
1.7985
1.6487
1.6256
1.6033
1.5817
1.2849
1.2723
1.2596
Et
NH
2p
7.6 7.5 ppm
1.8 1.7 ppm
1.30 ppm
8 7 6 5 4 3 2 1 0 ppm
1.0000
1.0345
1.0588
0.9721
2.1283
8.0894
2.1541
3.1003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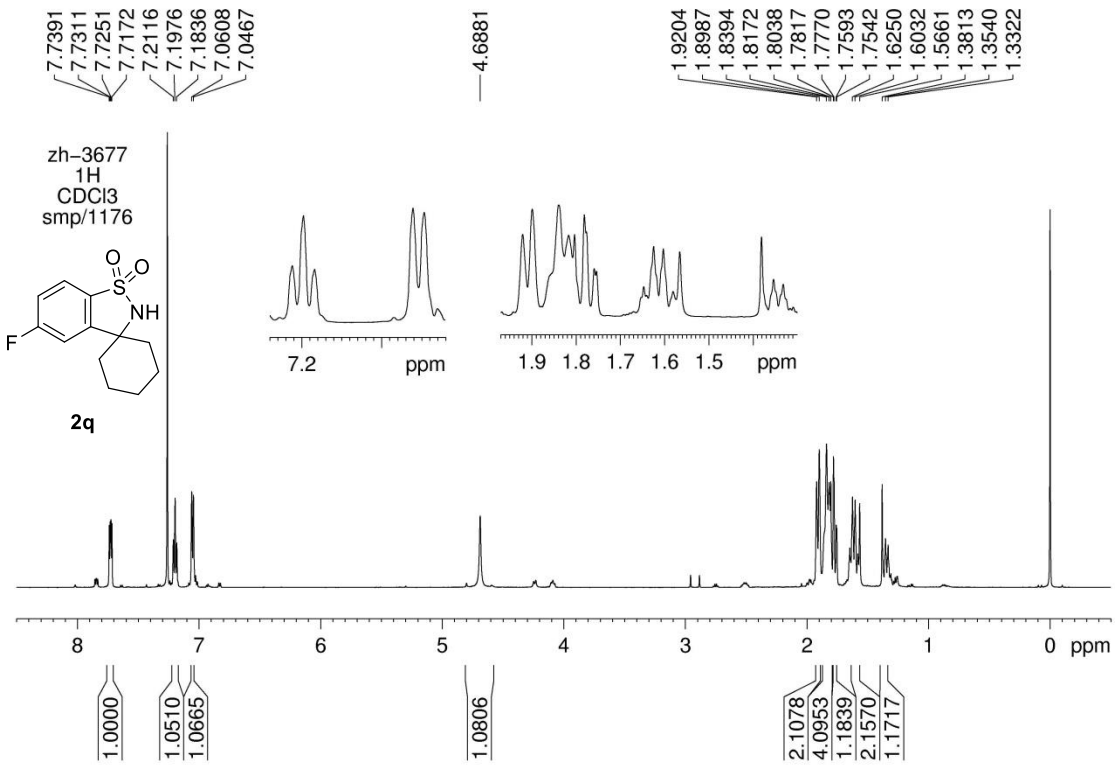
132.9584
129.1542
122.1661
121.1825
63.6627
37.7617
29.1648
24.8391
22.5507
15.3881
ZH-3668
13C
CDCL3
njl/1196
Et
NH
2p
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.7391
7.7311
7.7251
7.7172
7.2116
7.1976
7.1836
7.0608
7.0467
4.6881
1.9204
1.8987
1.8394
1.8172
1.8038
1.7817
1.7770
1.7593
1.7542
1.6250
1.6032
1.5661
1.3813
1.3540
1.3322
zh–3677
1H
CDCl3
smp/1176
O
O
S
NH
F
2q
7.2
ppm
1.9 1.8 1.7 1.6 1.5
ppm
8
7
6
5
4
3
2
1
0 ppm
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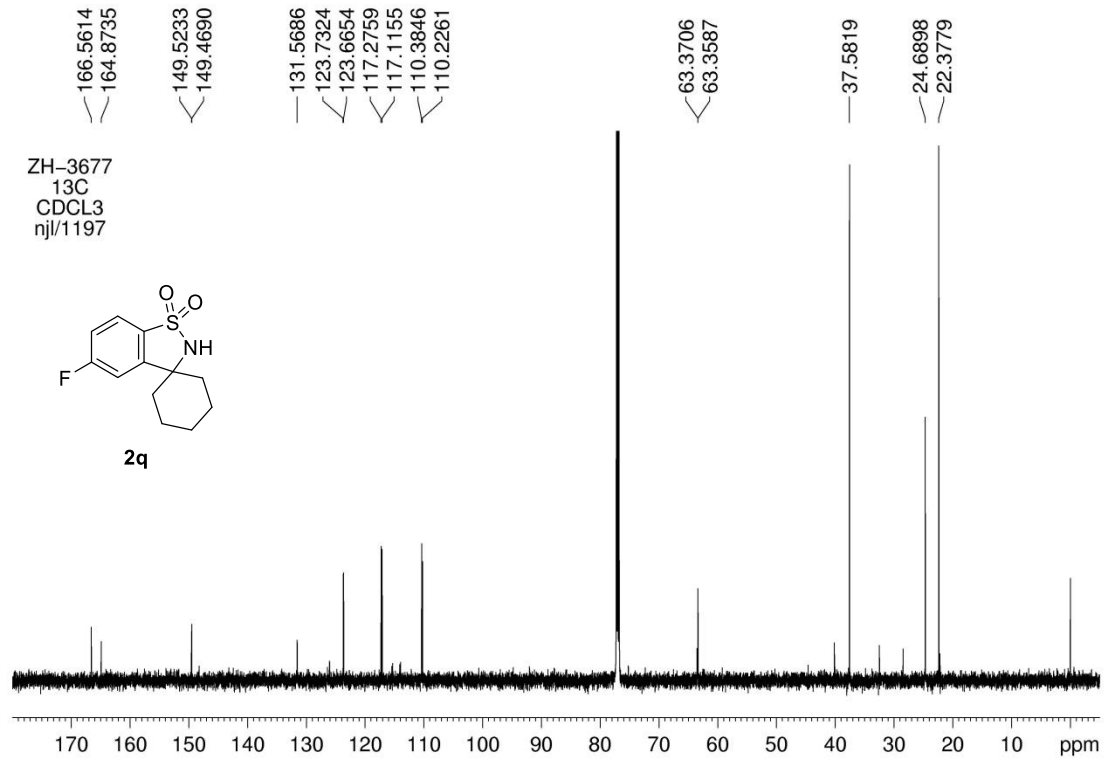
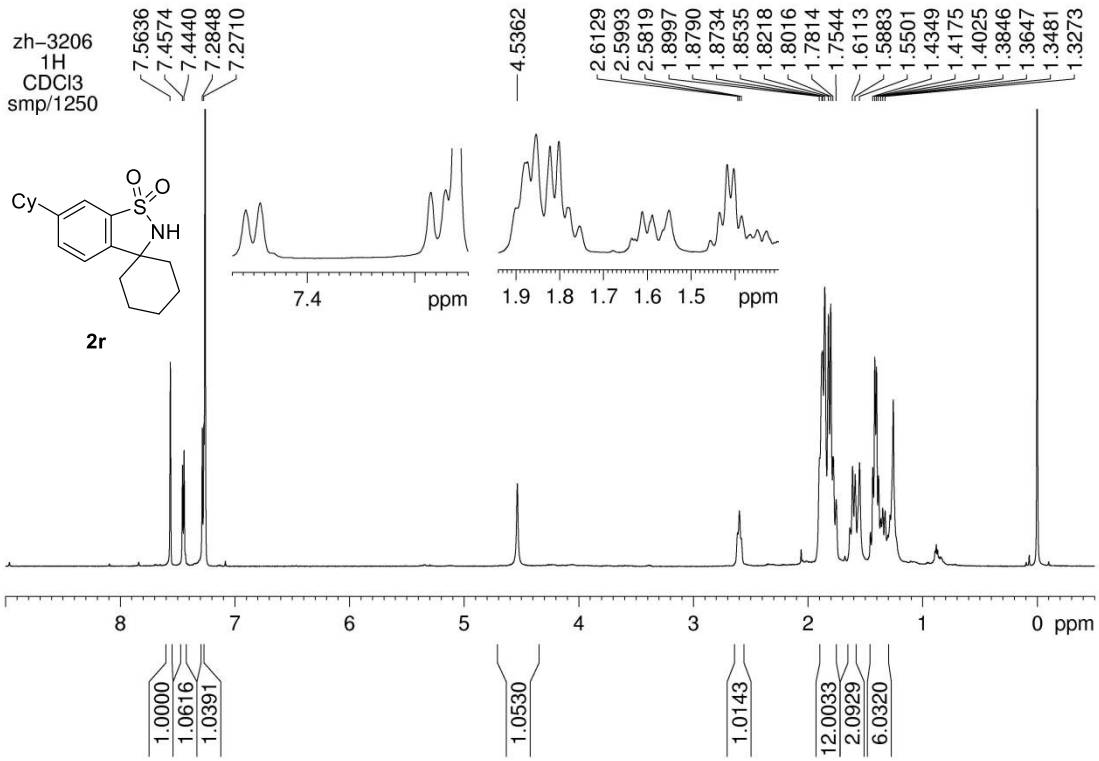
1.0510
1.0665
1.0806
2.1078
4.0953
1.1839
2.1570
1.1717


166.5614
164.8735
149.5233
149.4690
131.5686
123.7324
123.6654
117.2759
117.1155
110.3846
110.2261
63.3706
63.3587
37.5819
24.6898
22.3779
ZH–3677
13C
CDCL3
njl/1197
O
O
S
NH
F
2q
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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CDCl3
smp/1250
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7.4440
7.2848
7.2710
4.5362
2.6129
2.5993
2.5819
1.8997
1.8790
1.8734
1.8535
1.8218
1.8016
1.7814
1.7544
1.6113
1.5883
1.5501
1.4349
1.4175
1.4025
1.3846
1.3647
1.3481
1.3273
Cy
O
O
S
NH
2r
7.4
ppm
1.9 1.8 1.7 1.6 1.5
ppm
8 7 6 5 4 3 2 1 0 ppm
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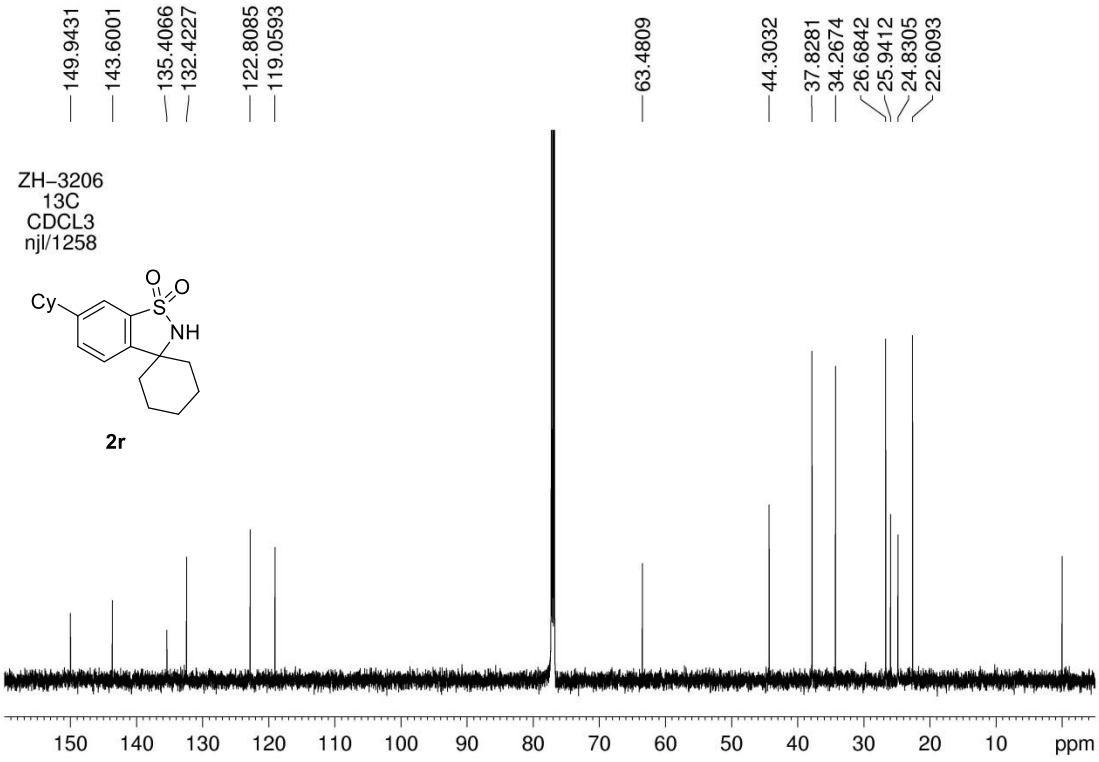
1.0391
1.0530
1.0143
12.0033
2.0929
6.0320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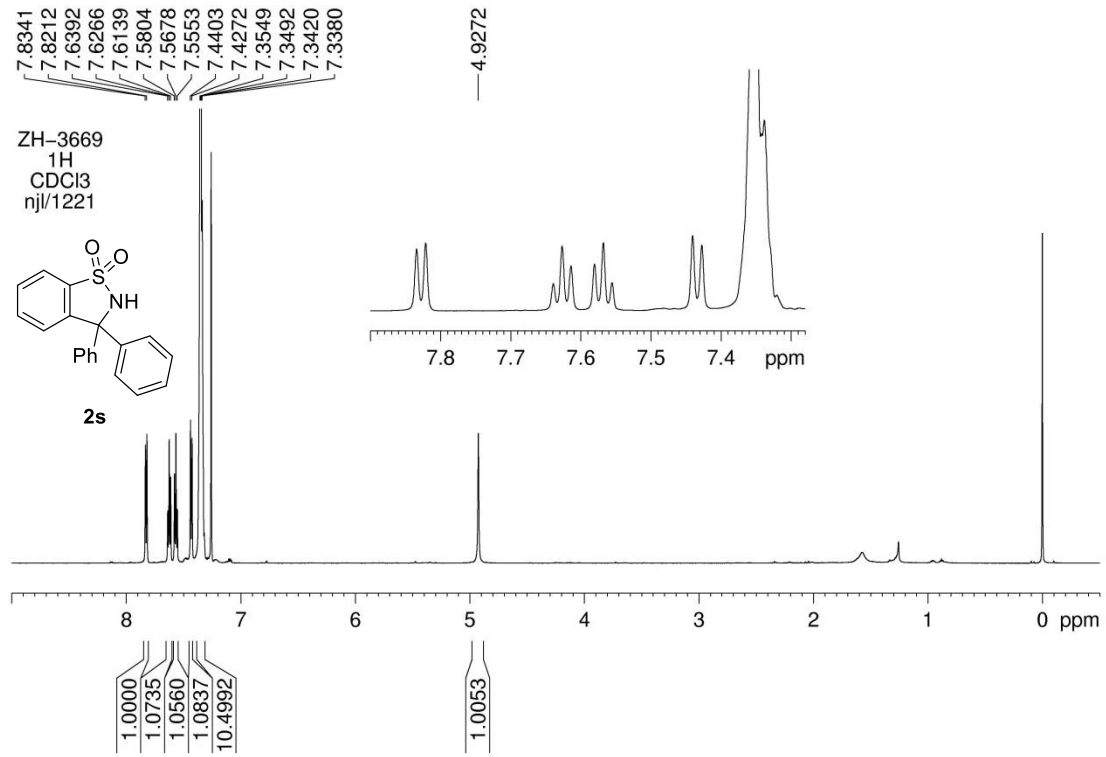
143.6001
135.4066
132.4227
122.8085
119.0593
63.4809
44.3032
37.8281
34.2674
26.6842
25.9412
24.8305
22.6093
ZH–3206
13C
CDCL3
njl/1258
Cy
O
O
S
NH
2r
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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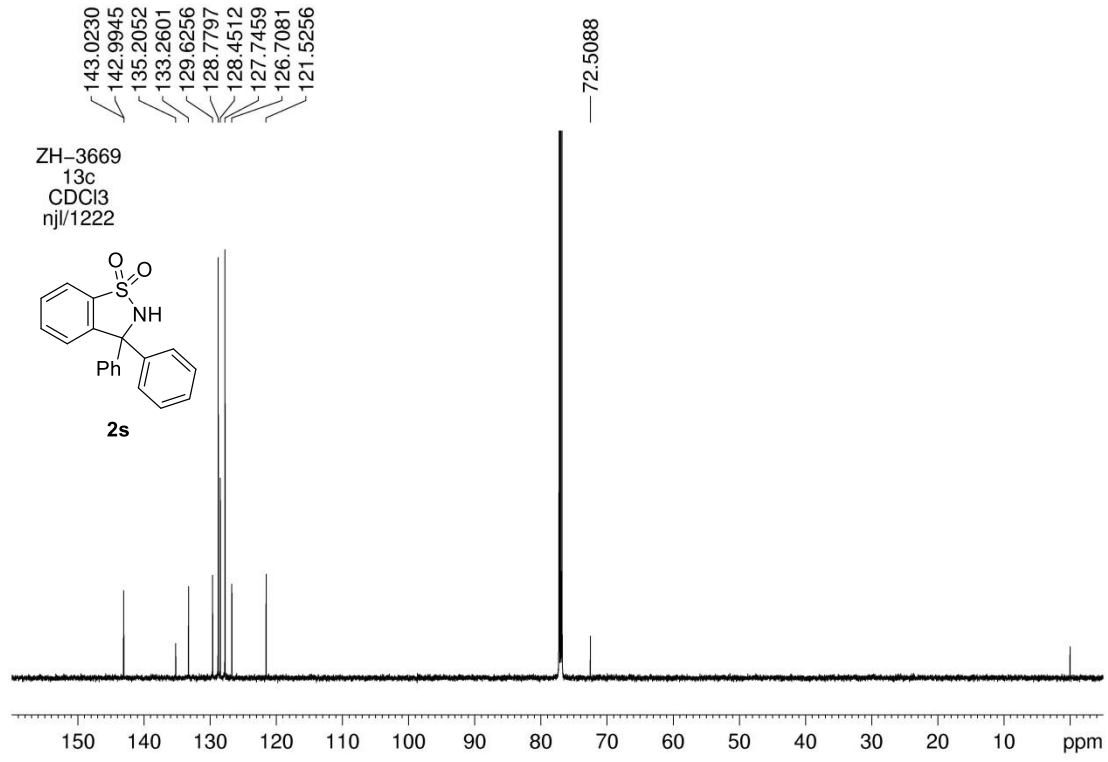
7.8212
7.6392
7.6266
7.6139
7.5804
7.5678
7.5553
7.4403
7.4272
7.3549
7.3492
7.3420
7.3380
4.9272
ZH–3669
1H
CDCl3
njl/1221
O
O
S
NH
Ph
2s
7.8
7.7
7.6
7.5
7.4
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
1.0735
1.0560
1.0837
10.4992
1.0053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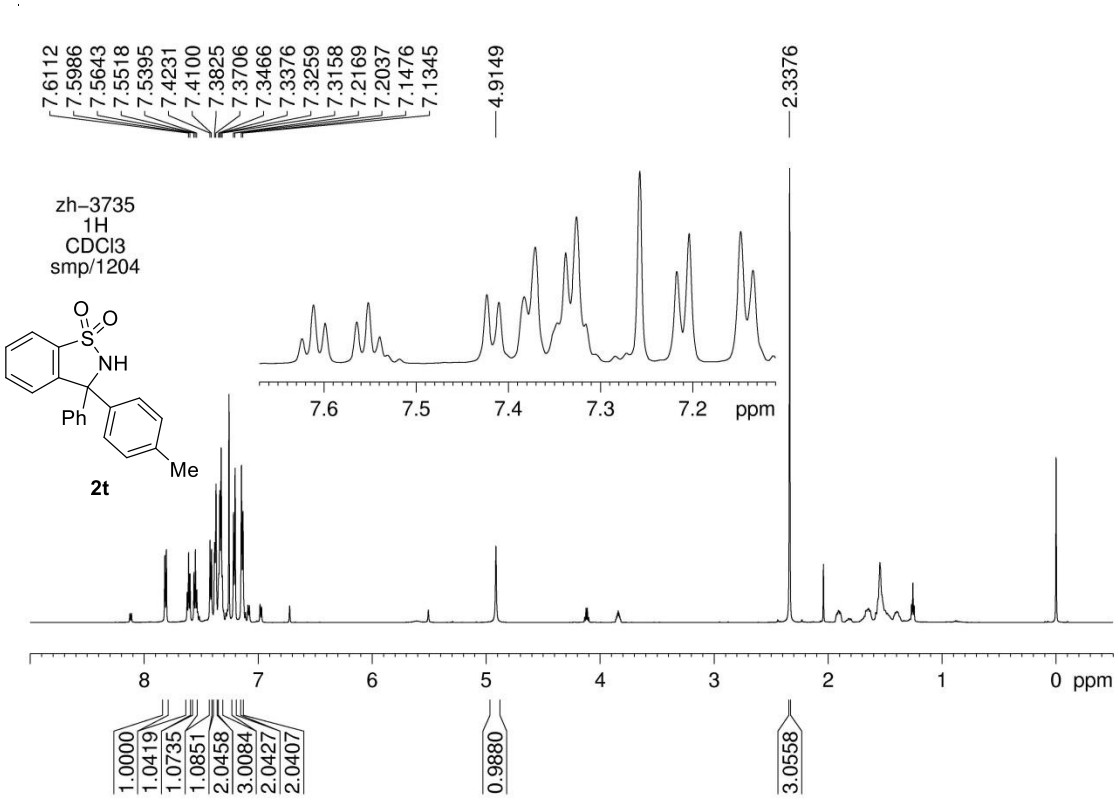
142.9945
135.2052
133.2601
129.6256
128.7797
128.4512
127.7459
126.7081
121.5256
72.5088
ZH–3669
13c
CDCl3
njl/1222
O
O
S
NH
Ph
2s
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.6112
7.5986
7.5643
7.5518
7.5395
7.4231
7.4100
7.3825
7.3706
7.3466
7.3376
7.3259
7.3158
7.2169
7.2037
7.1476
7.1345
4.9149
2.3376
zh–3735
1H
CDCl3
smp/1204
O
O
S
NH
Ph
Me
2t
7.6
7.5
7.4
7.3
7.2
ppm
8
7
6
5
4
3
2
1
0 ppm
1.0000
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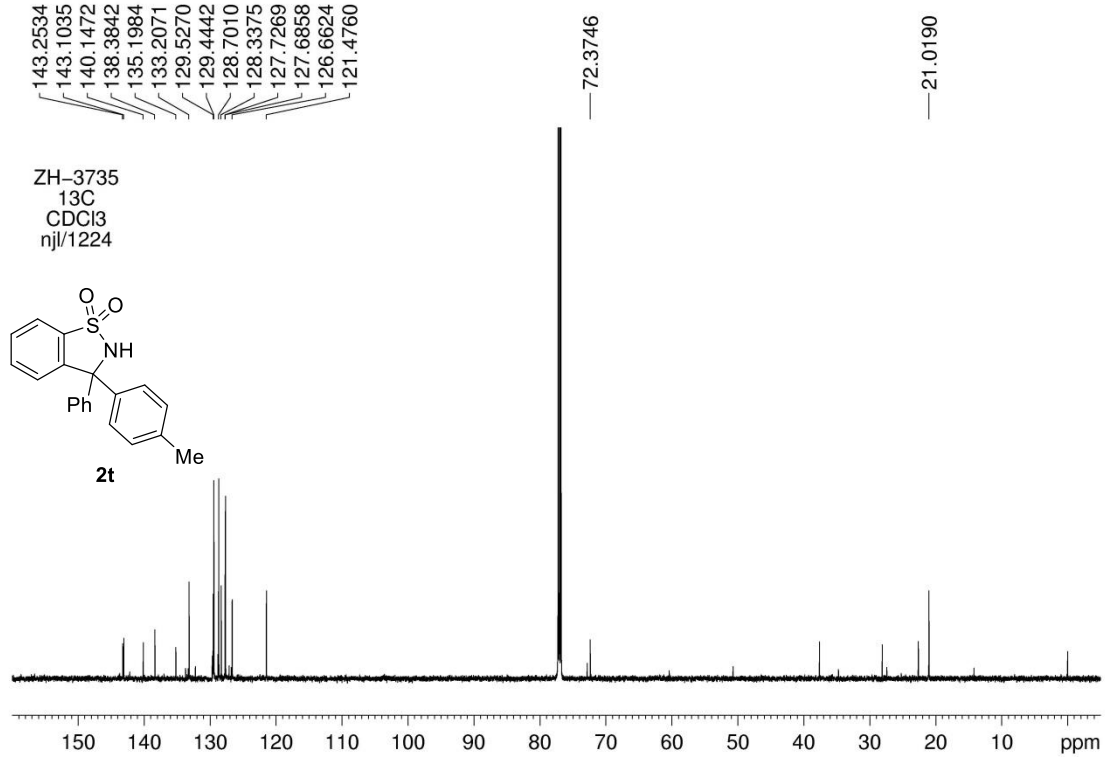
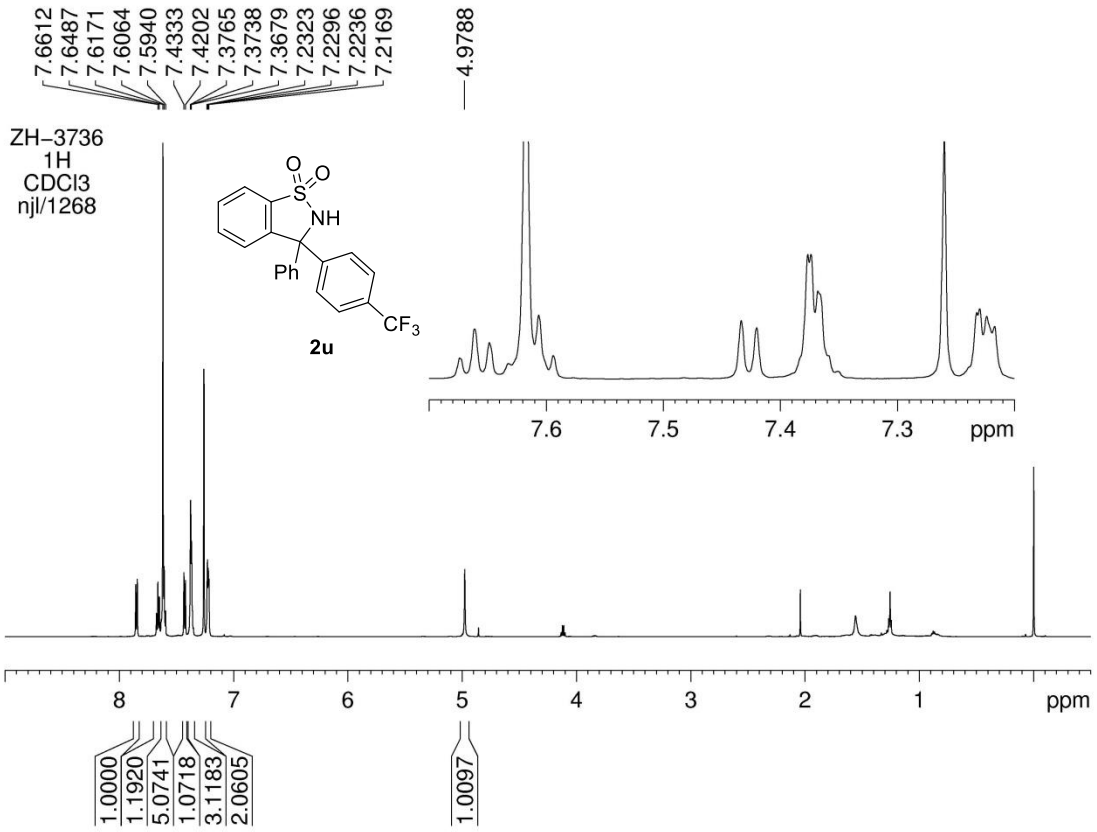
1.0735
1.0851
2.0458
3.0084
2.0427
2.0407
0.9880
3.0558


143.2534
143.1035
140.1472
138.3842
135.1984
133.2071
129.5270
129.4442
128.7010
128.3375
127.7269
127.6858
126.6624
121.4760
72.3746
21.0190
ZH–3735
13C
CDCl3
njl/1224
O
O
S
NH
Ph
Me
2t
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.6612
7.6487
7.6171
7.6064
7.5940
7.4333
7.4202
7.3765
7.3738
7.3679
7.2323
7.2296
7.2236
7.2169
4.9788
ZH–3736
1H
CDCl3
njl/1268
O
O
S
NH
Ph
CF3
2u
7.6
7.5
7.4
7.3
ppm
8
7
6
5
4
3
2
1
ppm
1.0000
1.1920
5.0741
1.0718
3.1183
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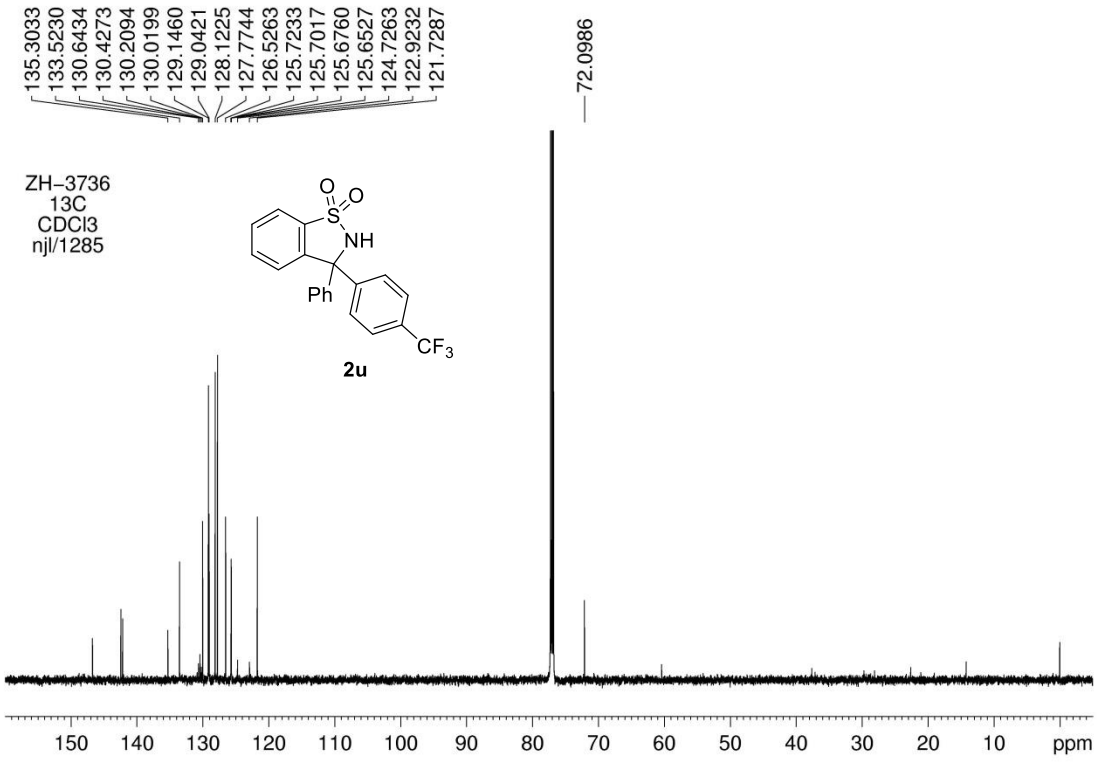
1.0097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128.1225
127.7744
126.5263
125.7233
125.7017
125.6760
125.6527
124.7263
122.9232
121.7287
72.0986
ZH–3736
13C
CDCl3
njl/1285
O
O
S
NH
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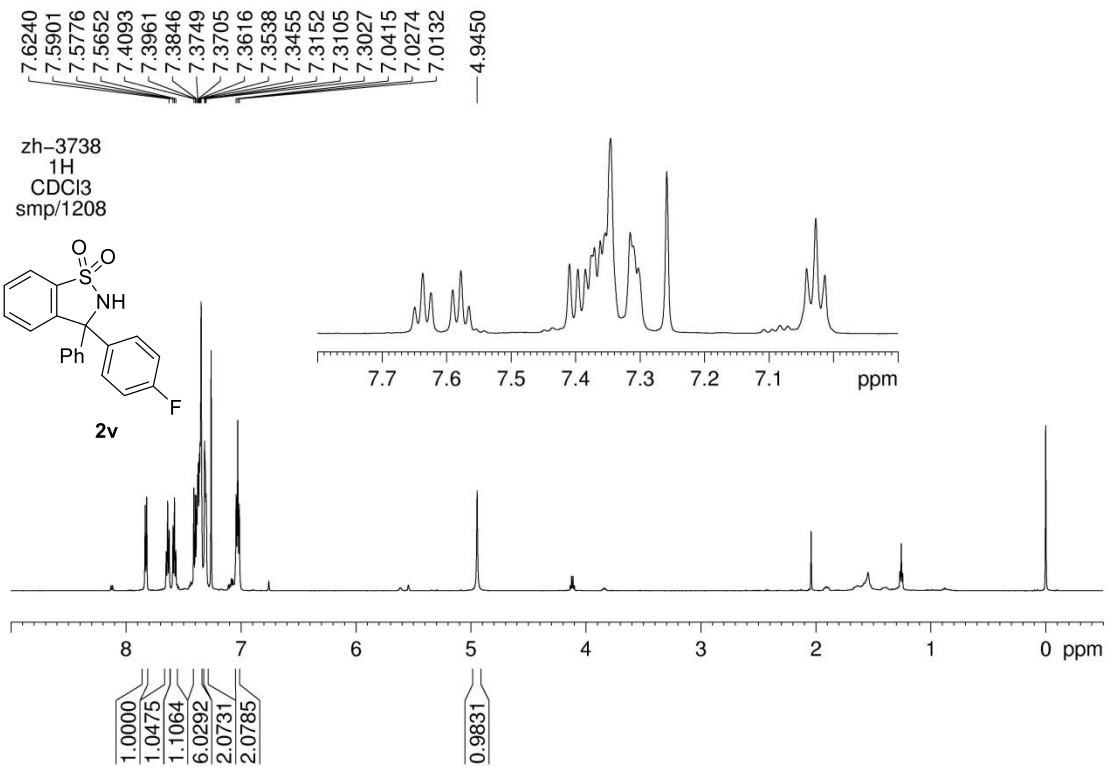
ppm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7.3538
7.3455
7.3152
7.3105
7.3027
7.0415
7.0274
7.0132
4.9450
zh–3738
1H
CDCl3
smp/1208
O
O
S
NH
Ph
F
2v
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
8
7
6
5
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1
0 ppm
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6.0292
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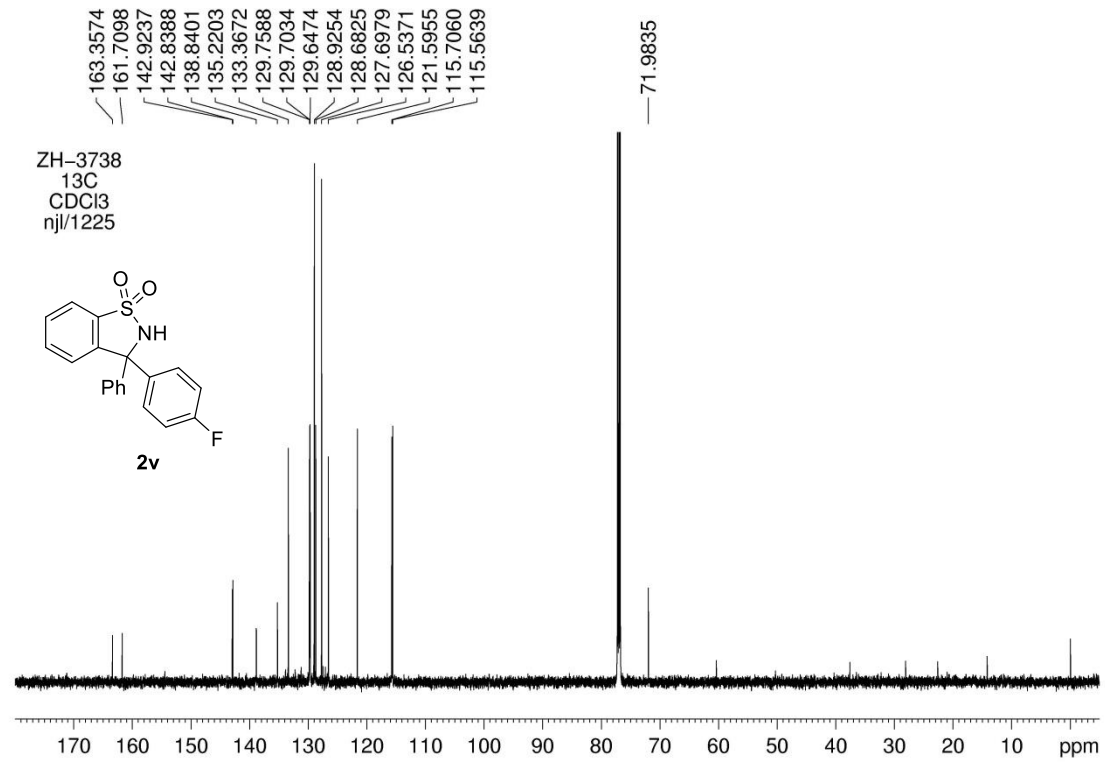
0.9831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126.5371
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115.7060
115.5639
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ZH–3738
13C
CDCl3
njl/1225
O
O
S
NH
Ph
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140
130
120
110
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80
70
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30
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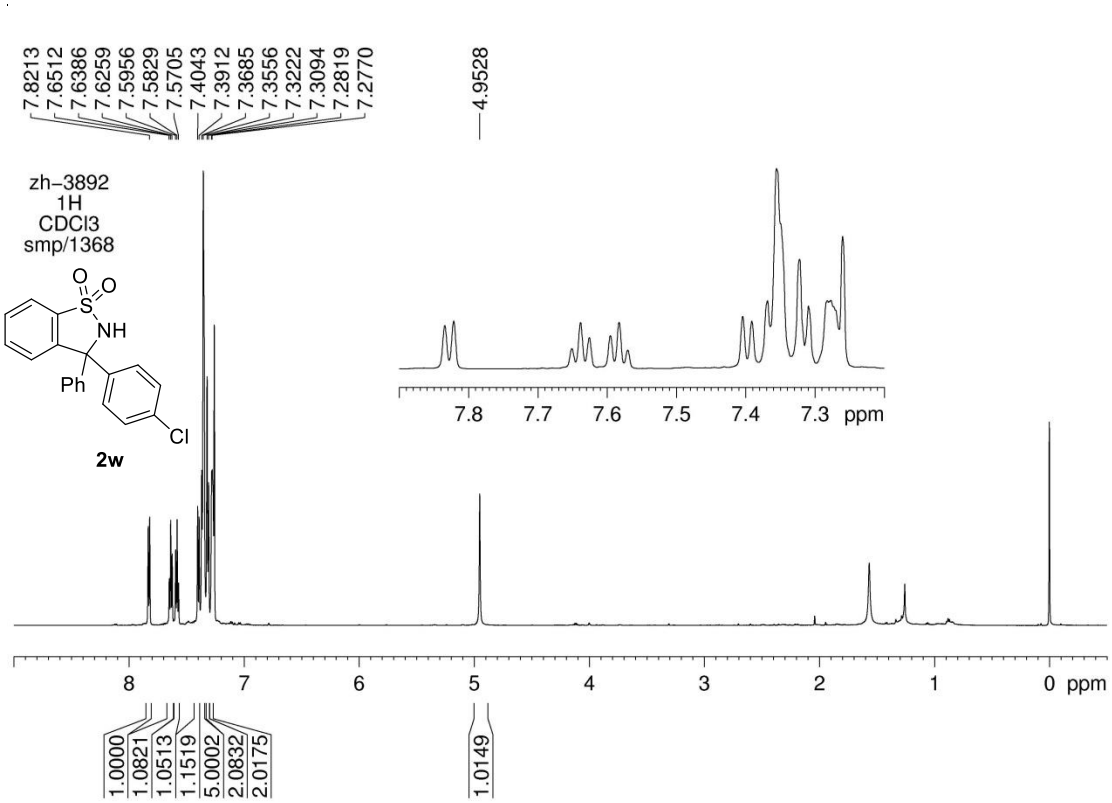
10
ppm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7.5705
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7.3556
7.3222
7.3094
7.2819
7.2770
4.9528
zh–3892
1H
CDCl3
smp/1368
O
O
S
NH
Ph
Cl
2w
7.8
7.7
7.6
7.5
7.4
7.3 ppm
8
7
6
5
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5.0002
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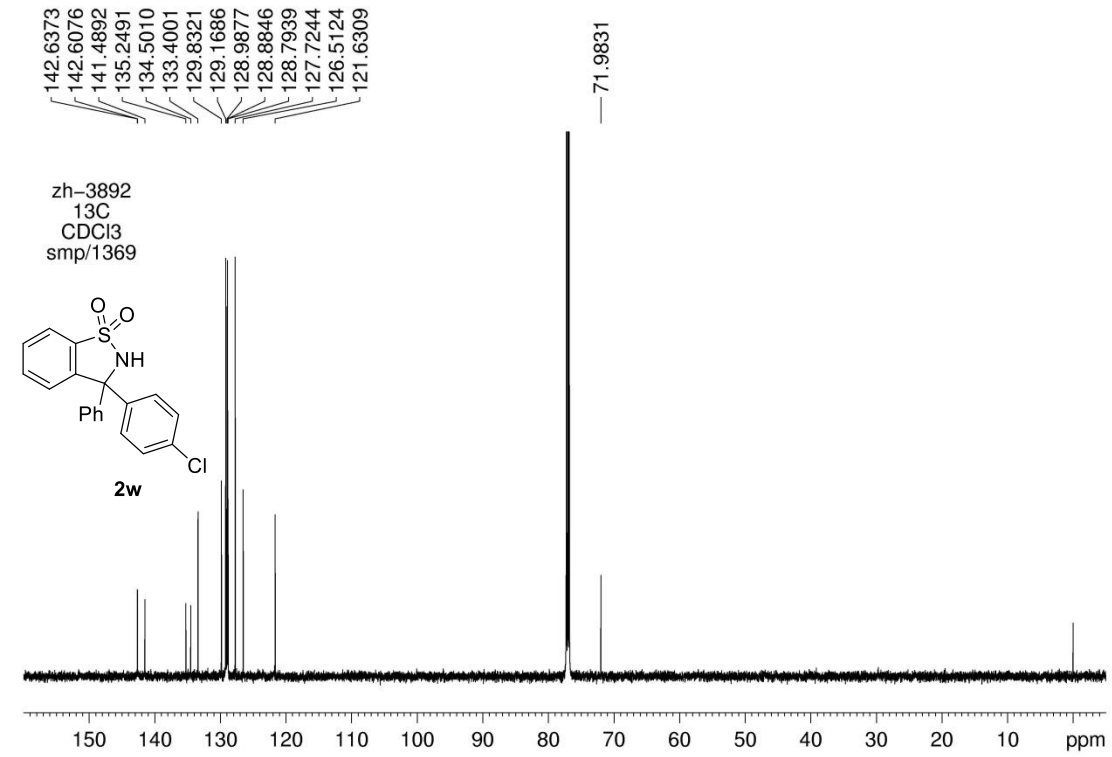
2.0175
1.0149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127.7244
126.5124
121.6309
71.9831
zh–3892
13C
CDCl3
smp/1369
O
O
S
NH
Ph
Cl
2w
150
140
130
120
110
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90
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70
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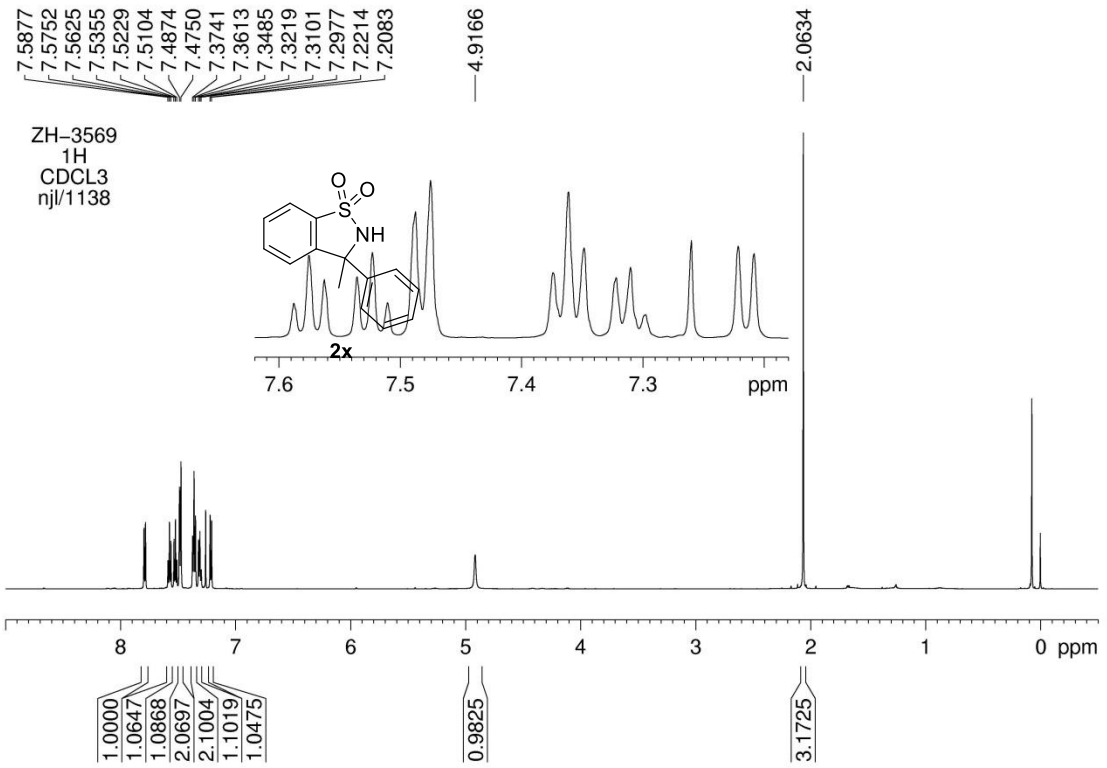
50
40
30
20
10
ppm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7.3485
7.3219
7.3101
7.2977
7.2214
7.2083
4.9166
2.0634
ZH–3569
1H
CDCL3
njl/1138
2x
7.6
7.5
7.4
7.3
ppm
8
7
6
5
4
3
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1.1019
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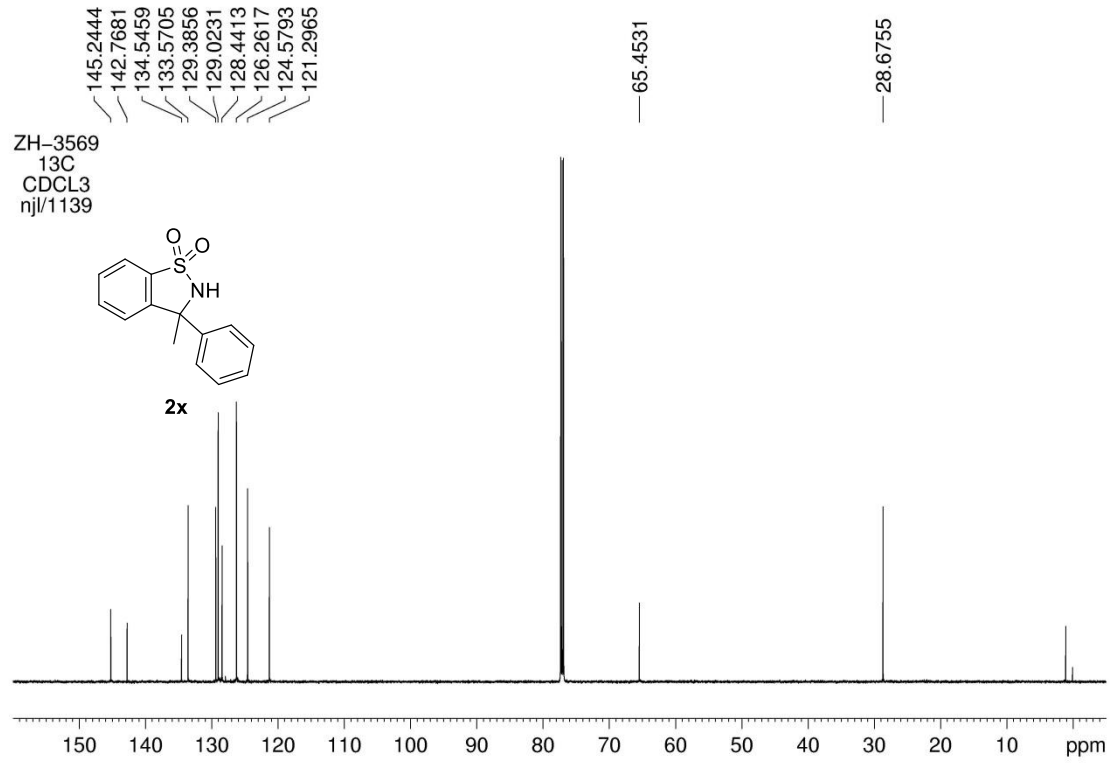
3.1725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128.4413
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65.4531
28.6755
ZH–3569
13C
CDCL3
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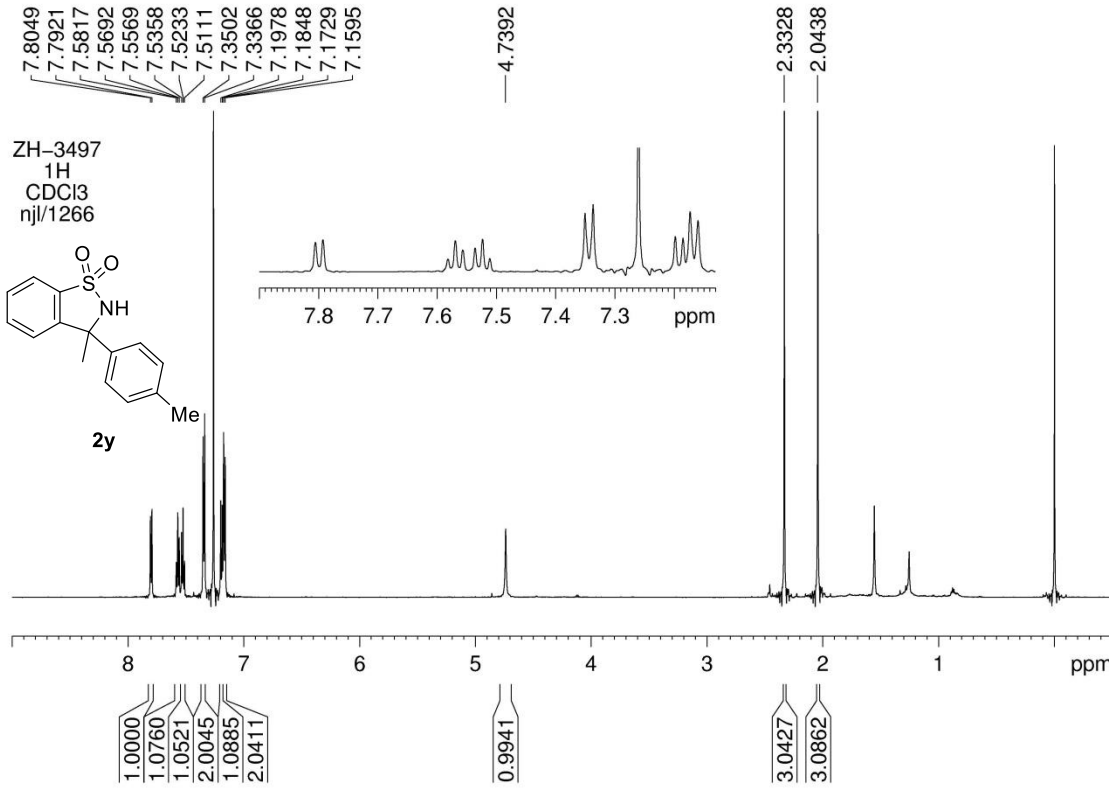
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.5817
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7.5358
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7.3502
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7.1978
7.1848
7.1729
7.1595
4.7392
2.3328
2.0438
ZH–3497
1H
CDCl3
njl/1266
O
O
S
NH
Me
2y
7.8 7.7 7.6 7.5 7.4 7.3 ppm
8 7 6 5 4 3 2 1 ppm
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1.0760
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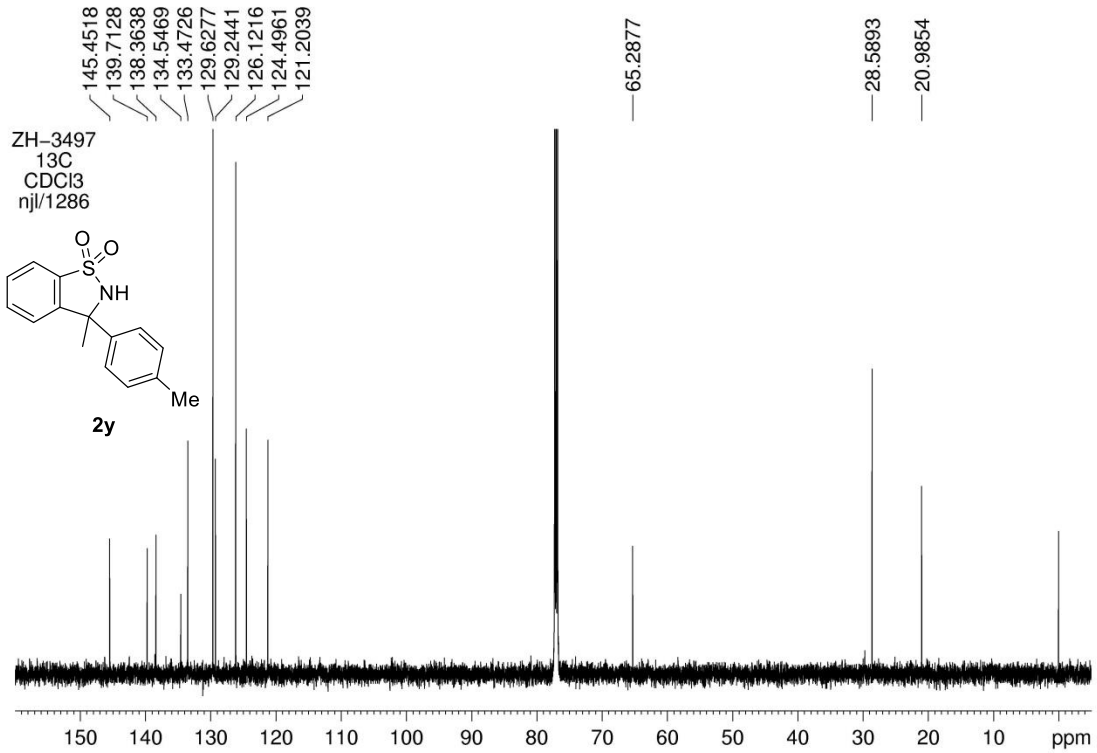
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65.2877
28.5893
20.9854
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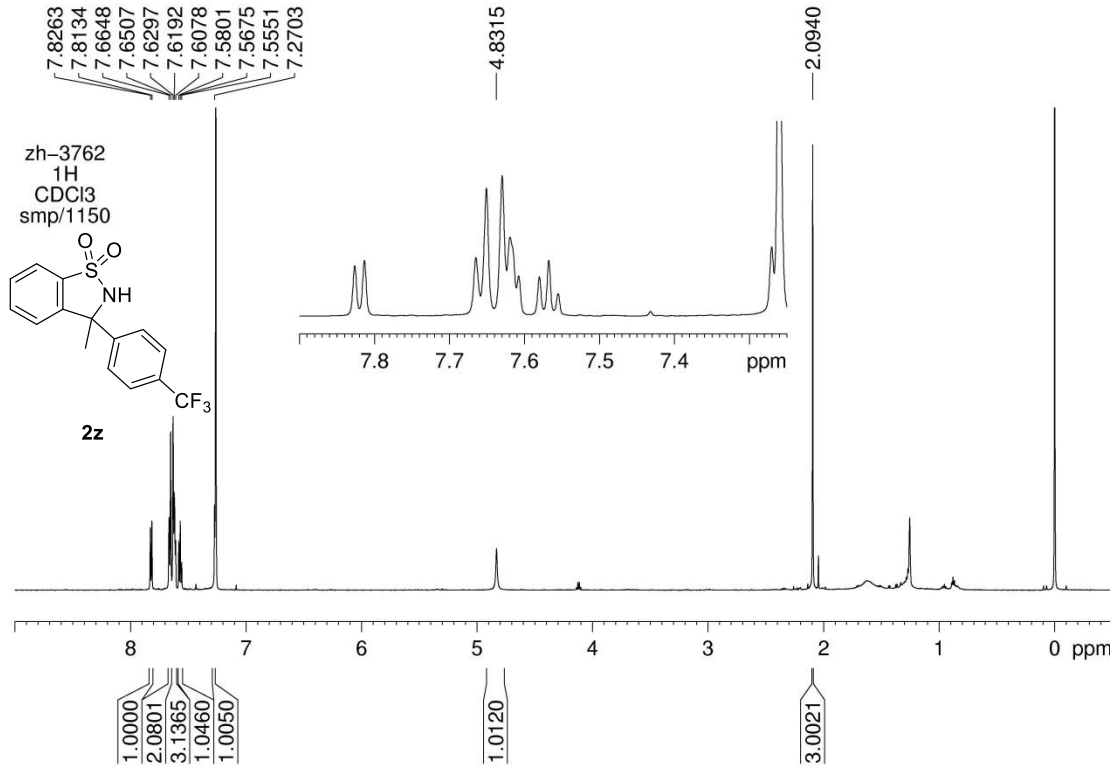
CDCl3
njl/1286
O
O
S
NH
Me
2y
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.6078
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7.5675
7.5551
7.2703
4.8315
2.0940
zh–3762
1H
CDCl3
smp/1150
O
O
S
NH
CF3
2z
7.8
7.7
7.6
7.5
7.4
ppm
8
7
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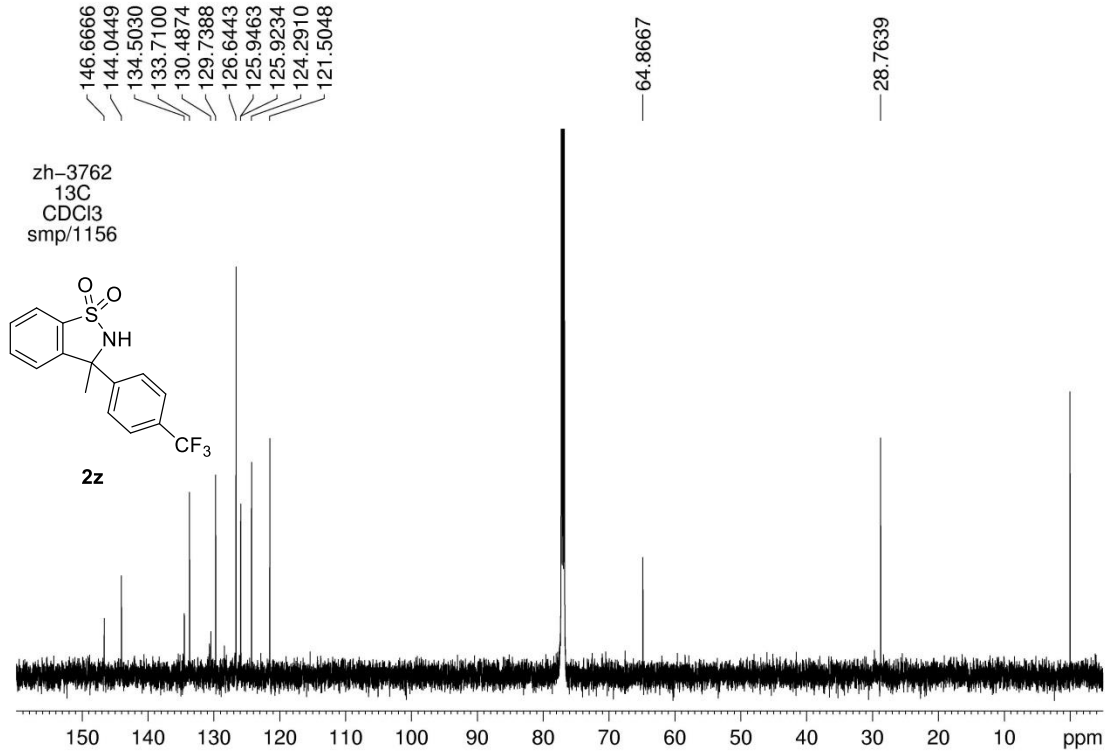
3.0021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121.5048
64.8667
28.7639
zh–3762
13C
CDCl3
smp/1156
O
O
S
NH
CF3
2z
150
140
130
120
110
100
90
80
70
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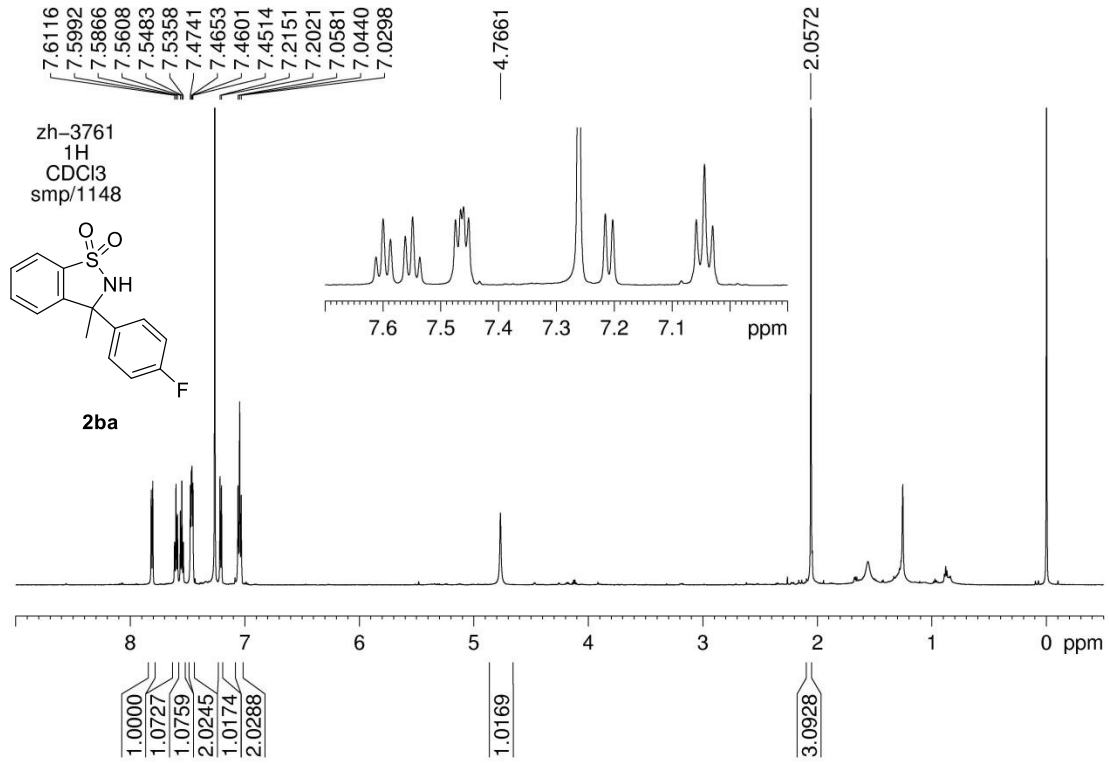
50
40
30
20
10
ppm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7.4741
7.4653
7.4601
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7.2151
7.2021
7.0581
7.0440
7.0298
4.7661
2.0572
zh–3761
1H
CDCl3
smp/1148
O
O
S
NH
F
2ba
7.6 7.5 7.4 7.3 7.2 7.1 ppm
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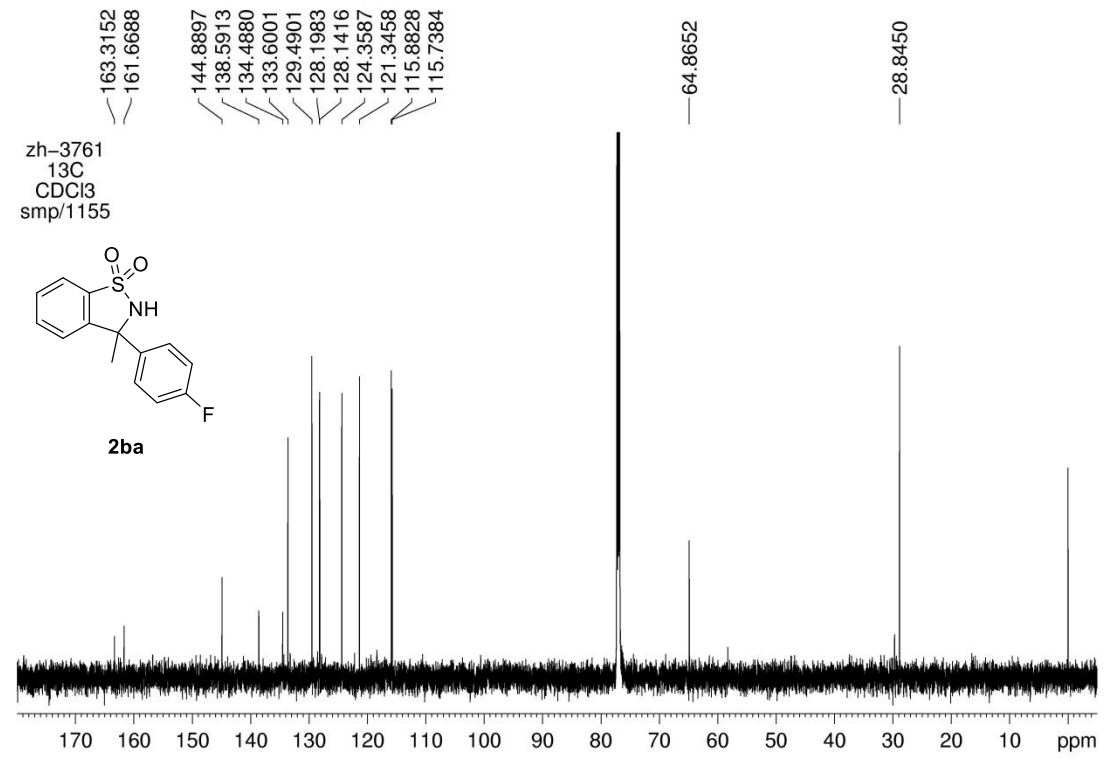
1.0174
2.0288
1.0169
3.0928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129.4901
128.1983
128.1416
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121.3458
115.8828
115.7384
64.8652
28.8450
zh–3761
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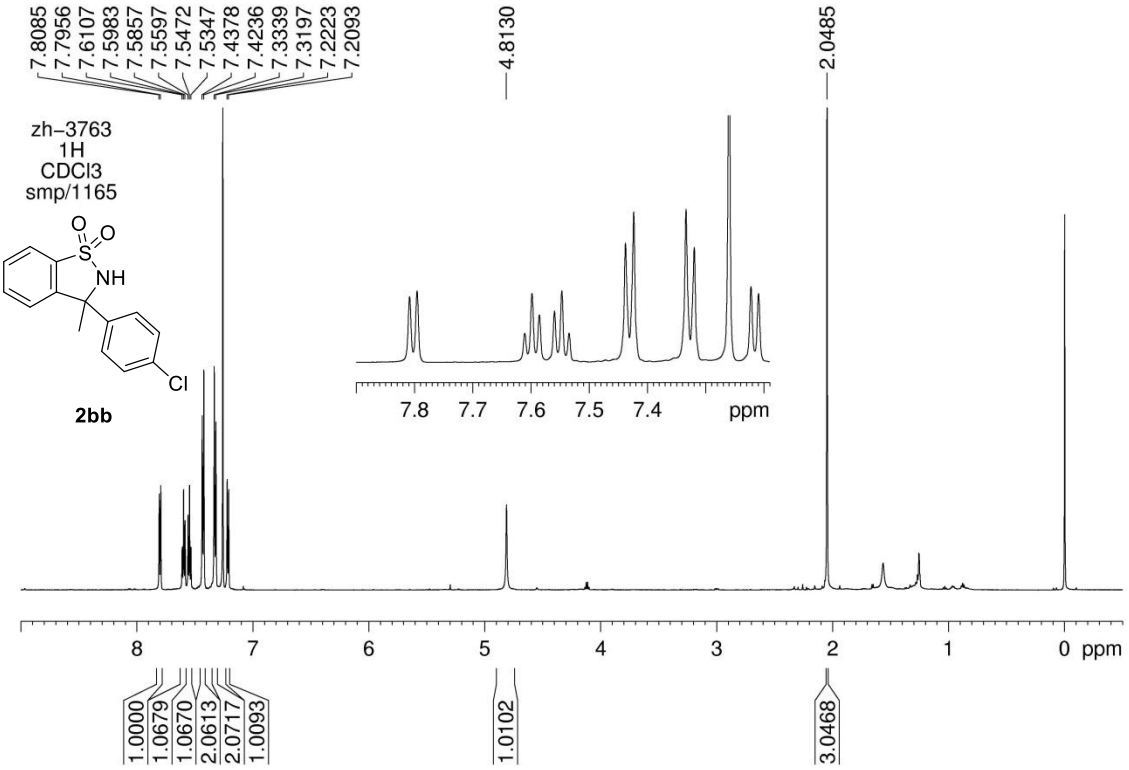
smp/1155
O
O
S
NH
F
2ba
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.6107
7.5983
7.5857
7.5597
7.5472
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7.4378
7.4236
7.3339
7.3197
7.2223
7.2093
4.8130
2.0485
zh–3763
1H
CDCl3
smp/1165
O
O
S
NH
Cl
2bb
7.8 7.7 7.6 7.5 7.4 ppm
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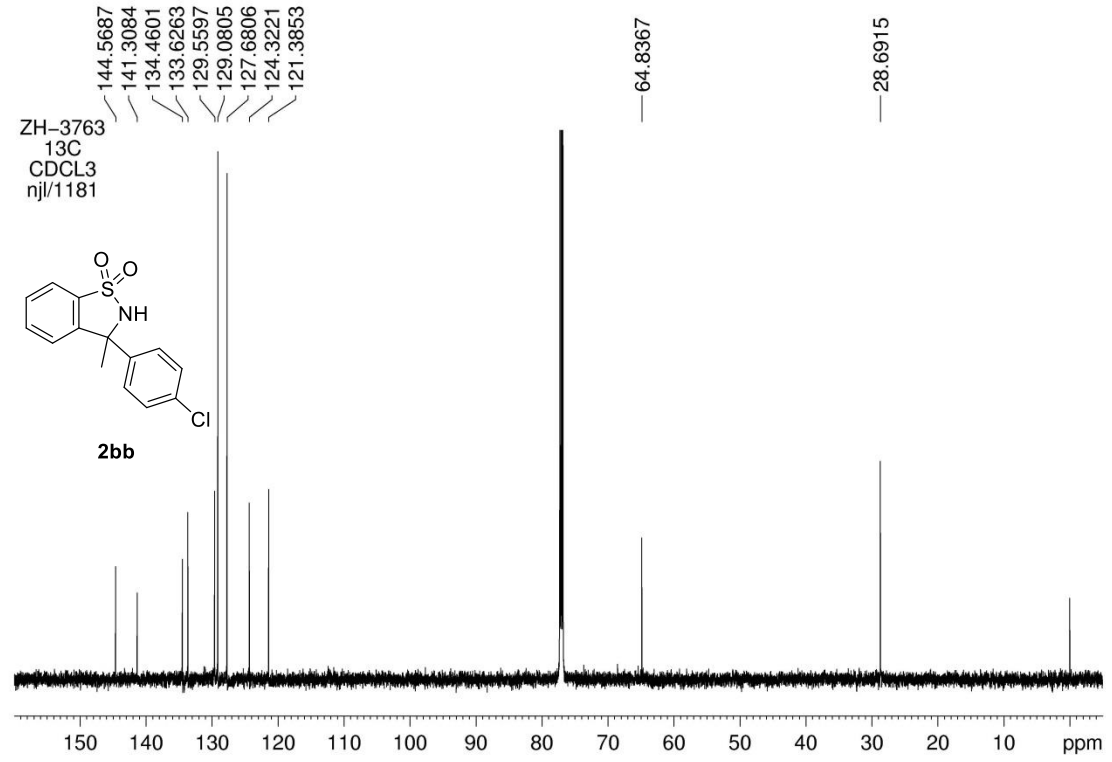
3.0468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28.6915
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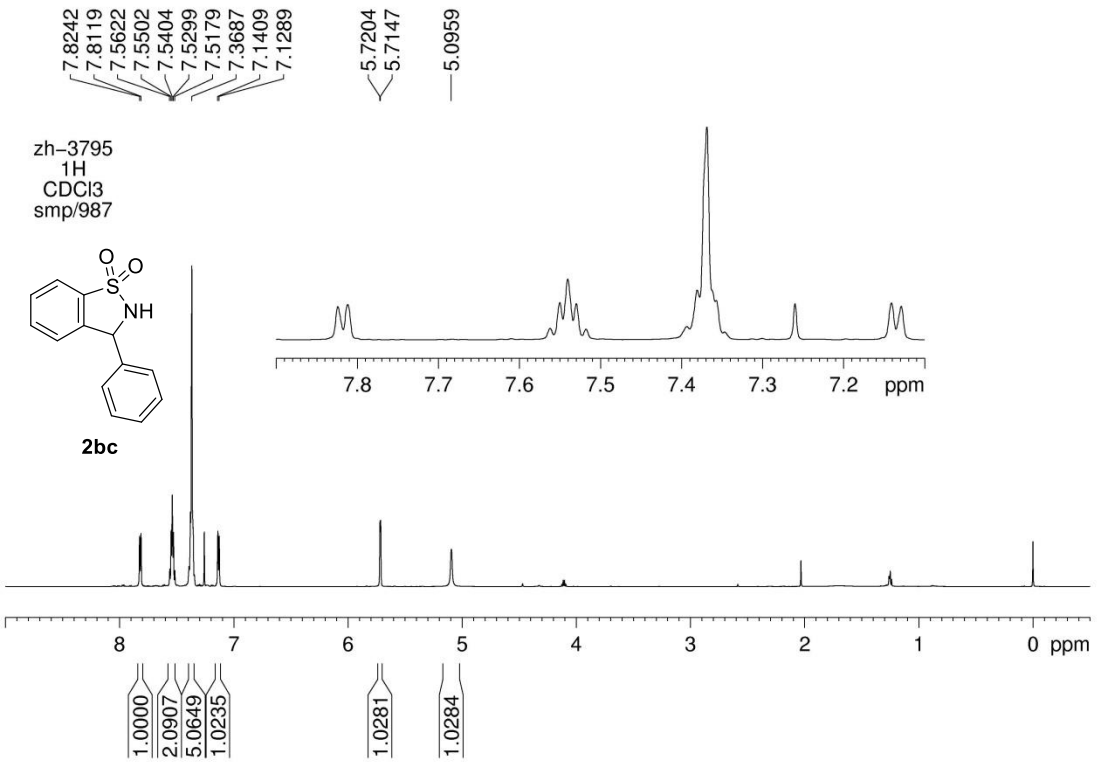
njl/1181
O
O
S
NH
Cl
2bb
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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5.7204
5.7147
5.0959
zh–3795
1H
CDCl3
smp/987
O
O
S
NH
2bc
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
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7
6
5
4
3
2
1
0 ppm
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5.0649
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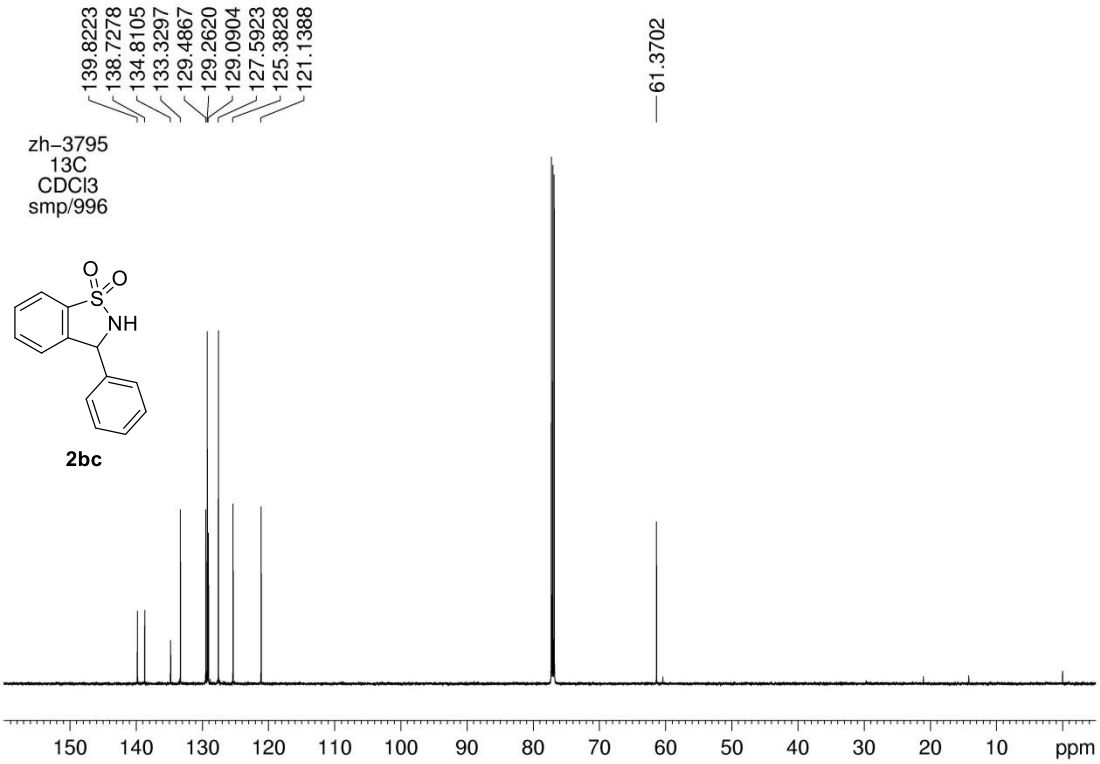
1.0284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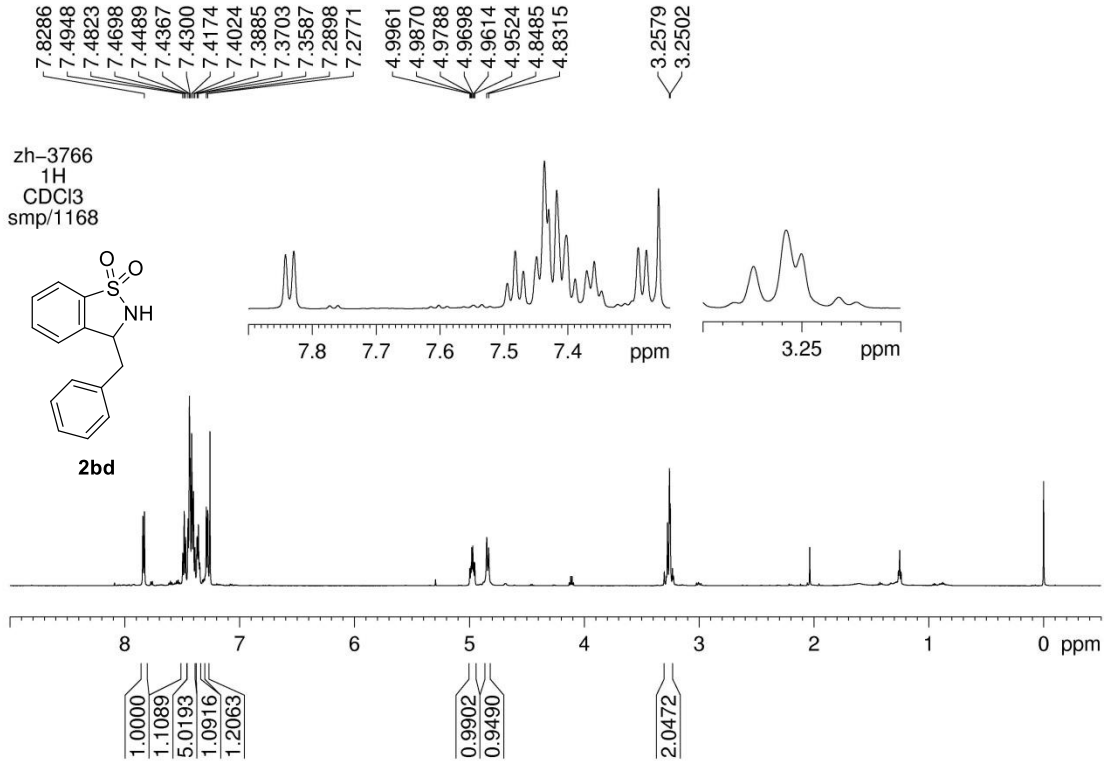
125.3828
121.1388
61.3702
zh–3795
13C
CDCl3
smp/996
O
O
S
NH
2bc
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.4300
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7.3703
7.3587
7.2898
7.2771
4.9961
4.9870
4.9788
4.9698
4.9614
4.9524
4.8485
4.8315
3.2579
3.2502
zh–3766
1H
CDCl3
smp/1168
O
O
S
NH
2bd
7.8
7.7
7.6
7.5
7.4
ppm
3.25
ppm
8
7
6
5
4
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2
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1.2063
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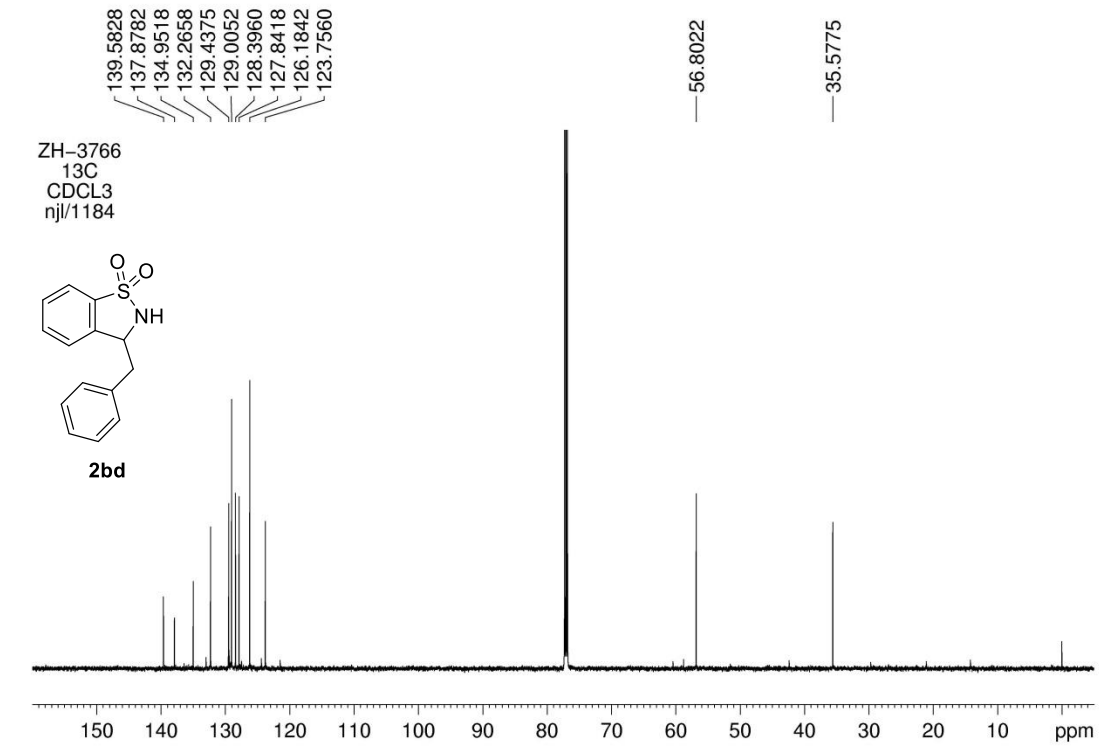
0.9490
2.0472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35.5775
ZH–3766
13C
CDCL3
njl/1184
O
O
S
NH
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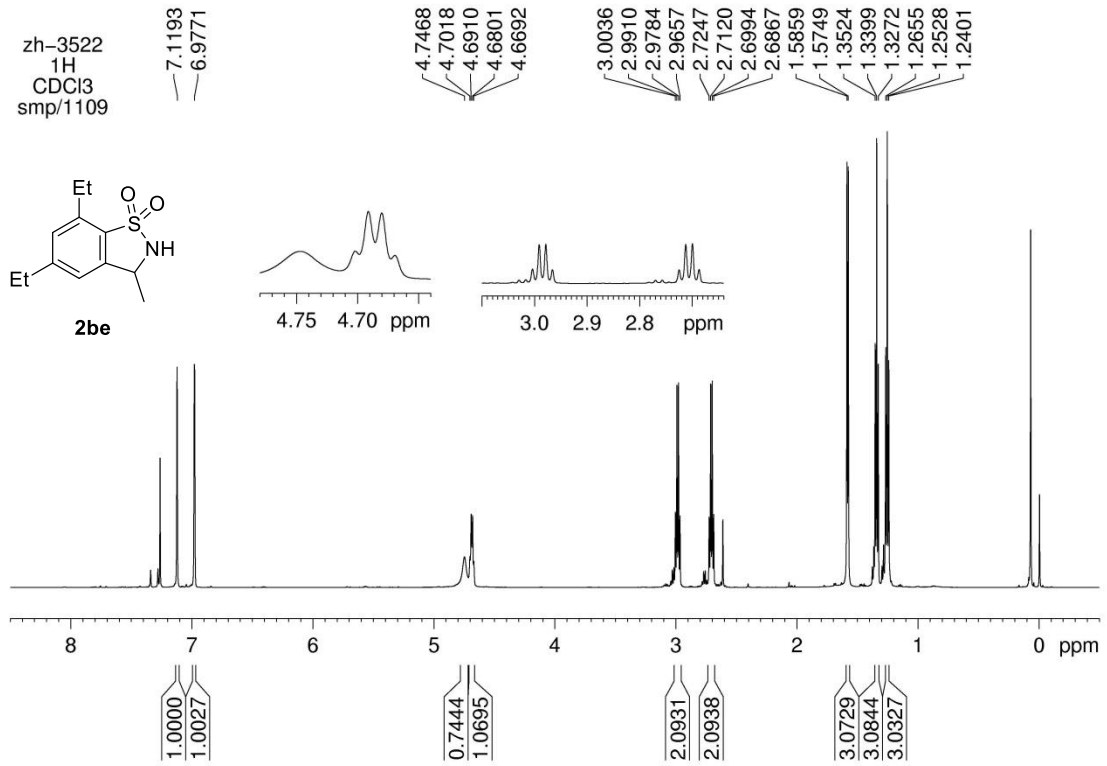
80
70
60
50
40
30
20
10
ppm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4.6692
3.0036
2.9910
2.9784
2.9657
2.7247
2.7120
2.6994
2.6867
1.5859
1.5749
1.3524
1.3399
1.3272
1.2655
1.2528
1.2401
Et
O
O
S
NH
Et
2be
4.75 4.70 ppm
3.0 2.9 2.8 ppm
8 7 6 5 4 3 2 1 0 ppm
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1.0027
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1.0695
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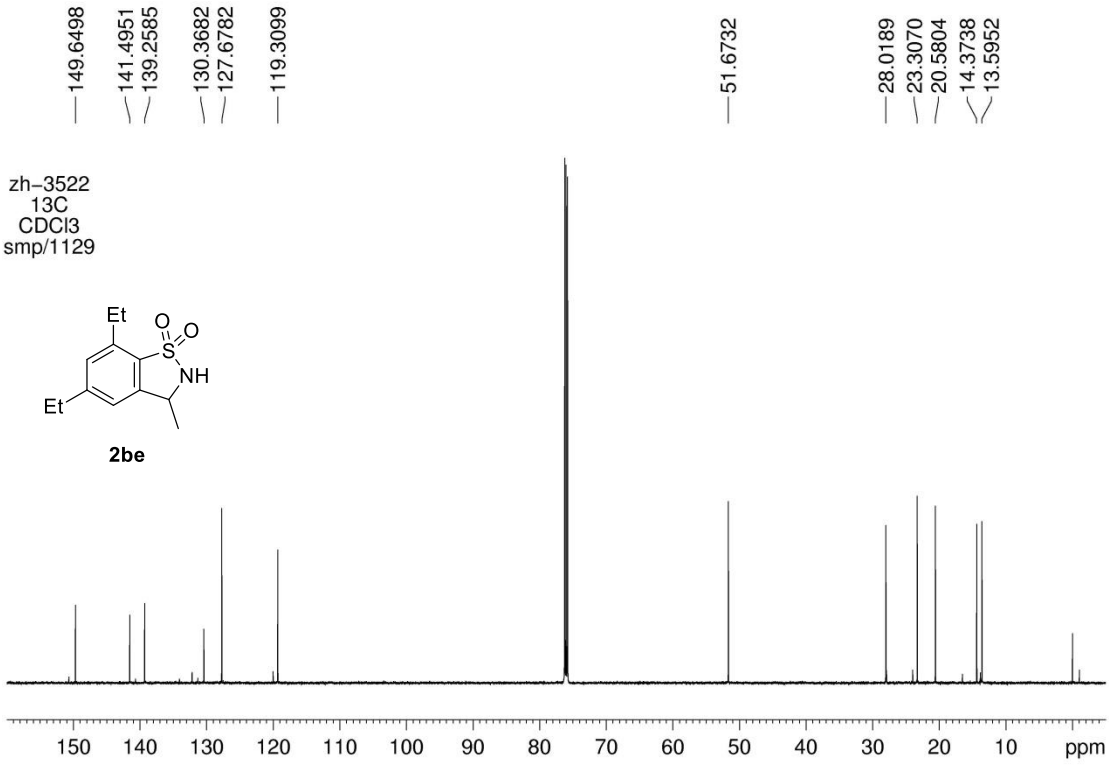
2.0938
3.0729
3.0844
3.0327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139.2585
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23.3070
20.5804
14.3738
13.5952
zh–3522
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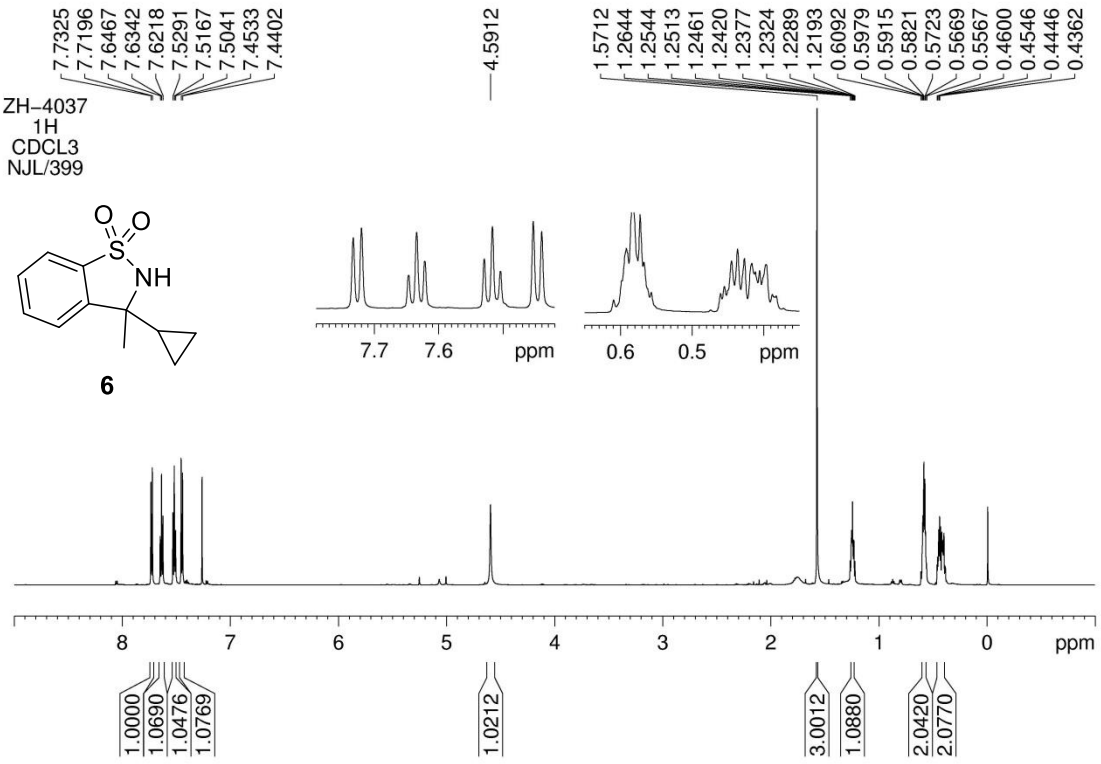
CDCl3
smp/1129
Et
O
O
S
NH
Et
2be
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.4533
7.4402
4.5912
1.5712
1.2644
1.2544
1.2513
1.2461
1.2420
1.2377
1.2324
1.2289
1.2193
0.6092
0.5979
0.5915
0.5821
0.5723
0.5669
0.5567
0.4600
0.4546
0.4446
0.4362
ZH–4037
1H
CDCL3
NJL/399
O
O
S
NH
6
7.7
7.6
ppm
0.6
0.5
ppm
8
7
6
5
4
3
2
1
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ppm
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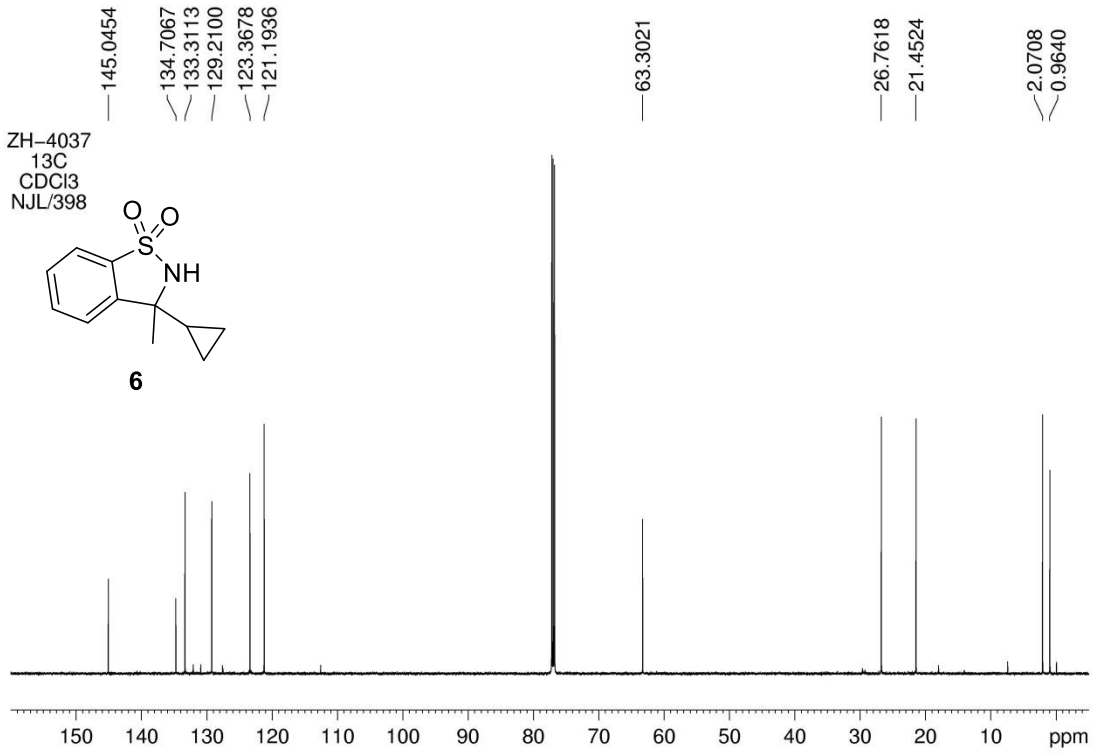
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121.1936
63.3021
26.7618
21.4524
2.0708
0.9640
ZH–4037
13C
CDCl3
NJL/398
O
O
S
NH
6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

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