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Photoredox/Cu dual catalyzed 1,4-cyanosulfonylation enabled by remote cyano migration

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Table of Contents

1. General information

All commercially available reagents were used without further purification. Column chromatography was performed on silica gel (200-300 mesh). ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on Bruker 400 MHz and JOEL 500 MHz NMR spectrometers. Chemical shifts (δ) were reported in ppm, and coupling constants (J) were given in Hertz (Hz). Data were reported as s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, br = broad, m = multiplet. High-resolution mass spectra (HRMS) were recorded on an AB SCIEX Triple ESI-TOF 5600+ mass spectrometer. The electrochemical measurements were carried out on a CS2350M electrochemical workstation (Wuhan Corrtest Instrument Co., Ltd). The 30 W blue LED lamp (λ_{max} = 445 nm) was manufactured by Hongye Photoelectricity Co., Ltd. Photo reactions were carried out in 20 mL reaction tubes at the distance of 2.0 cm from the LED lamp. In addition, an electronic fan was also equipped to maintain the reaction temperature in a range of 25−30 °C.

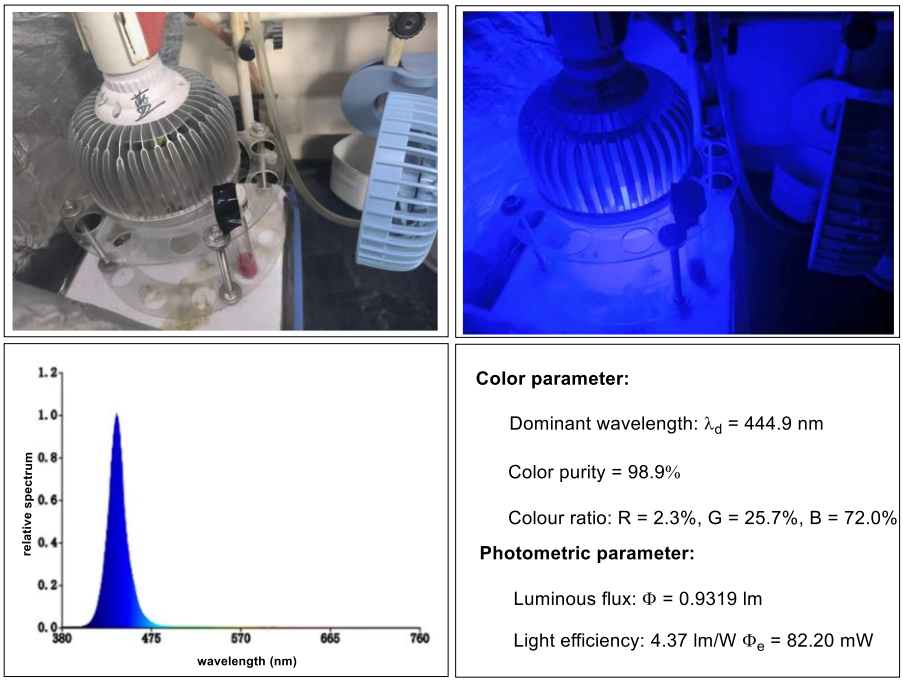
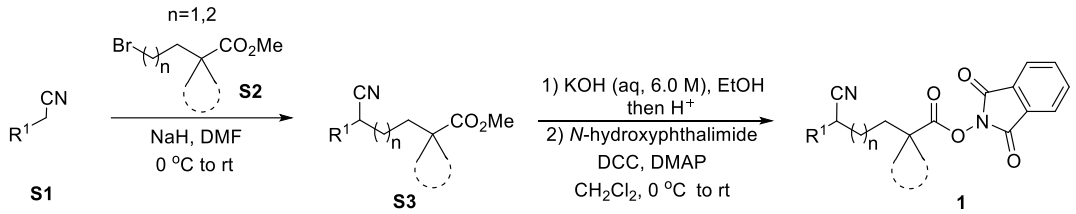


Figure S1. The spectrum of the lamp and the visible-light irradiation instrument

2. General procedures for photoredox/Cu dual catalyzed 1,4-cyanosulfonylation enabled by remote cyano migration

2.1 General procedure for the preparation of substrates 1[1]



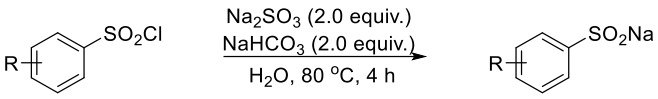
Under nitrogen atmosphere, to the suspension of NaH (15 mmol, 1.5 equiv,) in dry DMF (10 mL) **S1** was added dropwise (10 mmol, in 5.0 mL DMF, 1.0 equiv.) at 0 ℃ in an ice-water bath. After stirring for 1 h at the same temperature, **S2** (20 mmol, 2.0 equiv.) was added dropwise *via* a syringe at 0 ℃. Then the reaction mixture was warmed to room temperature, stirred for 16 h, quenched with saturated aq. NH_4Cl (10 mL), and extracted with ethyl acetate (15 mL×3). The combined organic layers were washed with brine (20 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The resulting residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford **S3** for the next step reaction.

To a round-bottomed flask equipped with a magnetic stir bar were added **S3** (5.0 mmol) and EtOH (10 mL). Then the KOH solution (2.5 mL, aq. 6.0 M, 3.0 equiv) was added dropwise, and the reaction mixture was stirred at rt for 12 h. After that, the reaction mixture was brought to pH = 2~4 with HCl (1.0 M), and extracted with EtOAc (10 mL×3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the corresponding alkyl carboxylic acid.

To a solution of alkyl carboxylic acid (1.0 equiv.), *N*,*N*-dimethylpyridin-4-amine (DMAP, 10 mol%), and *N*-hydroxyphthalimide (1.5 equiv.) in dry CH_2Cl_2 (0.1 M) was added a solution of *N*,*N*-dicyclohexylcarbodiimide (DCC, 1.5 equiv.) in CH_2Cl_2 (0.4 M) in an ice-water bath. Then, the reaction mixture was stirred for 12 h at room temperature. After the completion of reaction, the organic solvent was removed by rotary evaporator under vacuum, and the residue was purified by flash column chromatography on silica

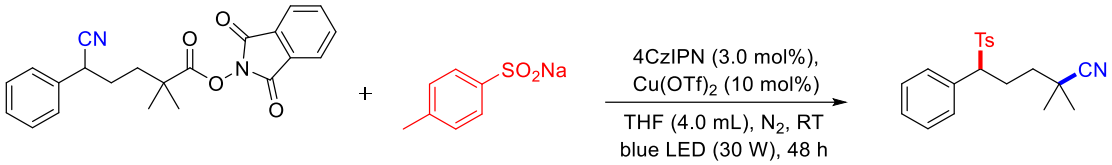
gel (petroleum ether/ethyl acetate = 5:1, V/V) to afford substrates **1**.

2.2 General procedure for the synthesis of sodium arylsulfinates[2]



To a 100 mL oven-dried round-bottomed flask equipped with a stirring bar was charged with aromatic (heteroaromatic) sulfonyl chloride (5.0 mmol), sodium sulfite (10 mmol), sodium bicarbonate (10 mmol) and H_2O (10 mL). After refluxing for 4 hours, the reaction mixture was concentrated in *vacuo*. The observed white solid was stirred with EtOH (10 mL) for 1 h, then the mixture was filtered through a pad of silica gel and rinsed with EtOH. The filtrate was concentrated under reduced pressure to afford substrates **2** without further purification.

2.3 General procedure for photoredox/Cu dual catalyzed 1,4-cyanosulfonylation of NHPI esters



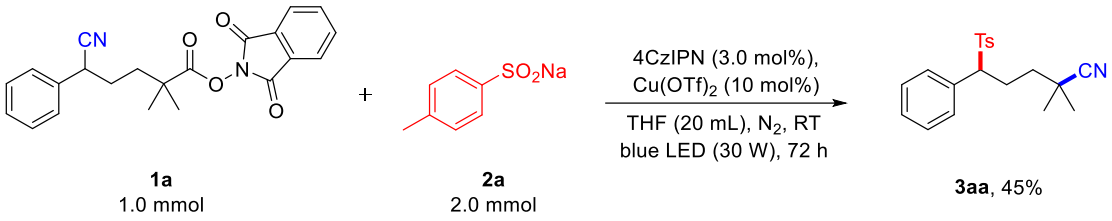
1a
0.2 mmol

2a
0.4 mmol

3aa, 68%

To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (0.2 mmol, 75.3 mg), 4CzIPN (3.0 mol%, 4.8 mg), $Cu(OTf)_2$ (10 mol%, 7.2 mg) and **2a** (0.4 mmol, 77.7 mg). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, dry THF (4.0 mL) was added in one portion *via* a syringe. The reaction mixture was irradiated with a 30 W blue LED lamp and stirred at room temperature under nitrogen atmosphere for 48 h. After removed the solvent in *vacuo*, the mixture was dissolved in EtOH (2.0 mL) with 0.2 mmol hydrazinium hydroxide solution and refluxed for 2 h. Then the residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 10:1, V/V) to give the product **3aa** (46.5 mg, 68%).

2.4 Procedure for a 1.0 mmol scale reaction



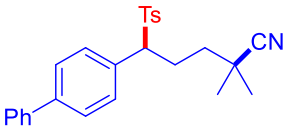
1a
1.0 mmol

2a
2.0 mmol

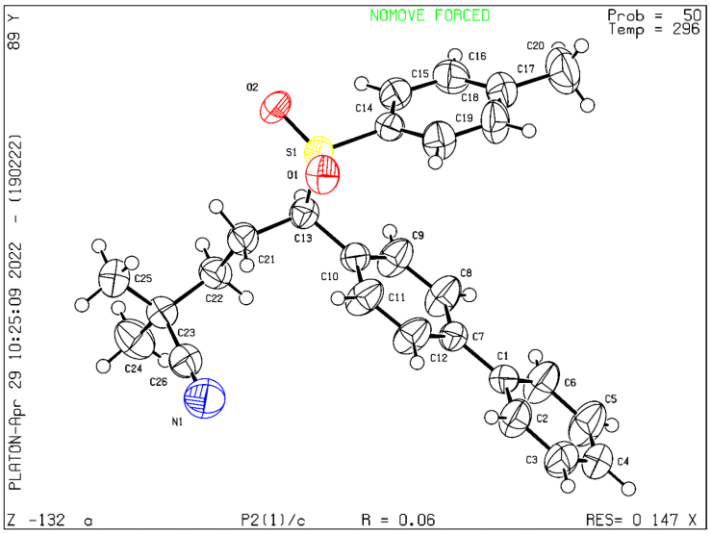
3aa, 45%

To a 20 mL test tube flask equipped with a stirring bar was charged with **1a** (1.0 mmol, 346.4 mg), 4CzIPN (3.0 mol%, 23.7 mg), $Cu(OTf)_2$ (10 mol%, 36.2 mg) and **2a** (2.0 mmol, 178.2 mg). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, dry THF (10 mL) was added in one portion *via* a syringe. The reaction mixture was irradiated with a 30 W blue LED lamp and stirred at room temperature under nitrogen atmosphere for 72 h. After removed the solvent in vacuo, the mixture was dissolved in EtOH (2.0 mL) with 0.2 mmol hydrazinium hydroxide solution and refluxed for 2 h. Then the residue was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 10:1, V/V) to give the product **3aa** (154.0 mg, 45%).

3. X-Ray single crystal diffraction analysis of the product 3ea (CCDC: 2348540)



3ea



checkCIF/PLATON report

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THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

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                 Calculated                 Reported
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Hall group       -P 2ybc                    ?
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Z                4                          4
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F000'            888.84
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Tmin'            0.954

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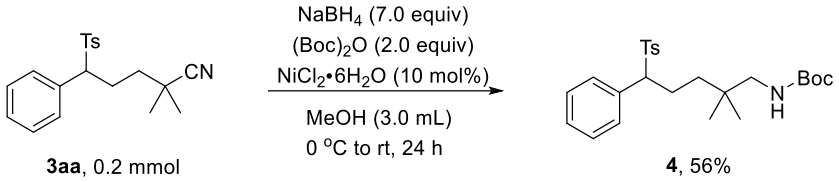
4. Derivatizations of product 3aa

4.1 The procedure for the 3aa to a Boc-protected amine 4[3]

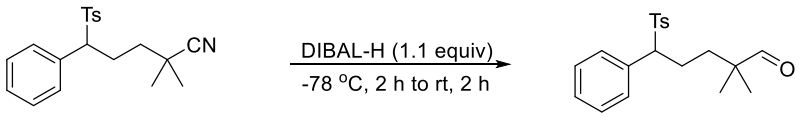


3aa, 0.2 mmol

4, 56%

To a reaction tube equipped with a magnetic stir bar were added **3aa** (68.3 mg, 0.20 mmol) and dry methanol (3.0 mL). The reaction was cooled to 0 °C, and Boc_2O (87.3 mg, 0.40 mmol) and $NiCl_2•6H_2O$ (3.0 mg, 10 mol%) were added. $NaBH_4$ (53.0 mg, 1.4 mmol) was then added in small portions. The resulting reaction mixture was allowed to warm to room temperature and stirred for 24 h. The reaction was quenched with H_2O and washed with ethyl acetate (5.0 mL×3). The combined organic layers were washed with brine (10 mL), dry over Na_2SO_4, and then concentrated in *vacuo*. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1) to give **4** (50.0 mg, 56%).

4.2 The procedure for the reduction of 3aa to aldehyde 5[4]



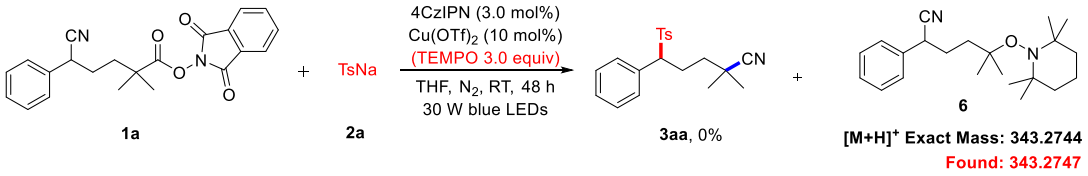
3aa, 0.2 mmol

5, 87%

The **3aa** (68.3 mg, 0.20 mmol) was dissolved in DCM (2.0 mL), the DIBAL-H (1.0 M in cyclohexane; 1.2 equiv) was added dropwise at -78 °C. The reaction mixture was stirred at -78 °C for 2 h and room temperature for another 2 h. Then the reaction mixture was cooled to 0 °C before the slow addition of 15% aqueous HCl and stirred overnight. The mixture was extracted three times with DCM (5.0 mL). The combined extracts were washed with brine (10 mL) and dried over anhydrous Na_2SO_4. The solvents were removed in *vacuo* and the crude residue was purified by flash column chromatography (eluent: petroleum ether/ethyl acetate = 10:1) to give **5** (60.0 mg, 87%).

5. Mechanistic studies

5.1 Radical-trapping experiment



To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (75.3 mg, 0.20 mmol), **2a** (77.7 mg, 0.4 mmol), 4CzIPN (4.8 mg, 3.0 mol%), $Cu(OTf)_2$ (7.2 mg, 10 mol%) and TEMPO (93.8 mg, 0.6 mmol). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, dry THF (2.0 mL) was added in one portion *via* a syringe. The reaction mixture was irradiated with a 30 W blue LED lamp and stirred at room temperature under nitrogen atmosphere for 48 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **3aa** was not observed, and their corresponding adduct was detected by HRMS analysis (Figure S2).

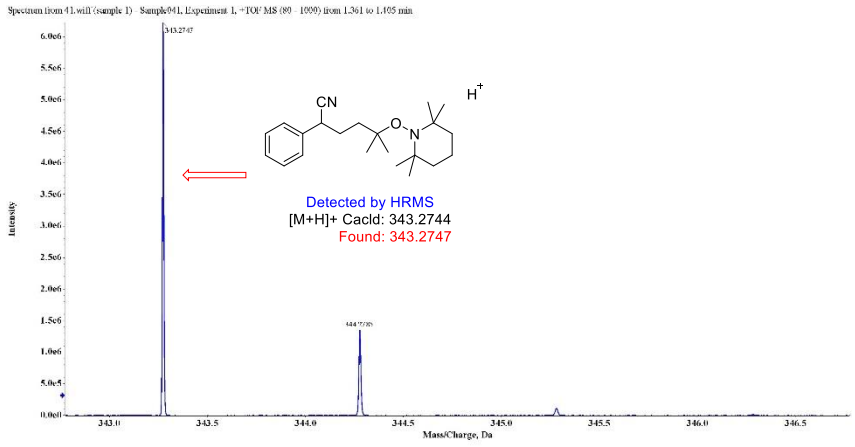


Figure S2. HRMS analysis of the adduct with TEMPO

5.2 Light on/off experiment

To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (0.20 mmol), **2a** (0.40 mmol), 4CzIPN (4.8 mg, 0.0060 mmol). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, THF (4.0 mL) was added in one portion *via* a syringe. The reaction mixture was stirred at rt under nitrogen atmosphere with the light turned on and off at intervals, and the yields were

determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as an internal standard.

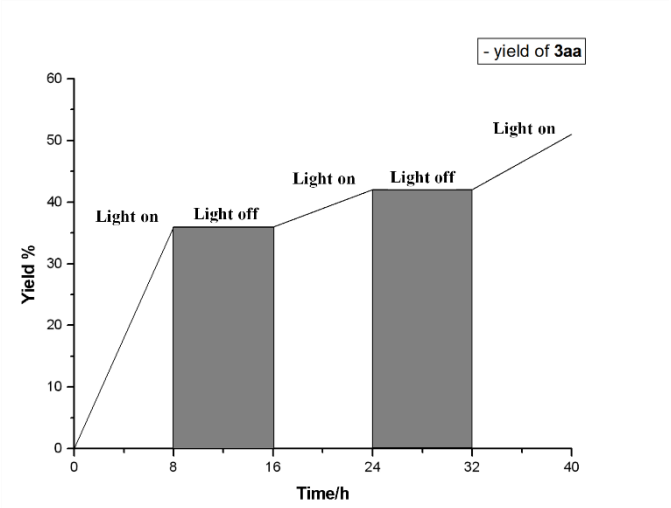


Figure S3. Reaction profile with the light on/off over time.

5.3 Cyclic voltammetry experiment

Cyclic Voltammetry was performed on a CS2350M electrochemical workstation (Wuhan Corrtest Instrument Co., Ltd). CV measurement of substrate **1a** (1.0 mM) was carried out in 0.10 M of Bu_4NPF_6/MeCN at a scan rate of 50 mV/s with the protection of N_2. The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is Ag/AgCl (3.5 M KCl). The reduction peak of **1a** ($E_{1/2}$(**1a**/**1a**$^{\bullet-}$) = -1.21 V vs SCE) was showed in Figure S4.

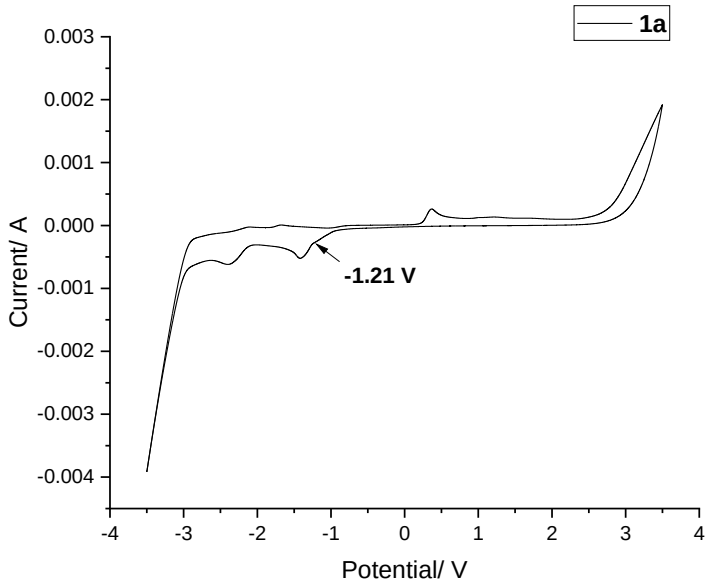


Figure S4. Cyclic voltammogram of **1a**

5.4 Stern-Volmer fluorescence quenching experiments

The luminescence quenching experiment was taken using a FluoroMax-4 Spectrophotometer. The experiments were carried out in 6.25×10^{-4} mol/L of 4CzIPN in THF at rt. The excitation wavelength was 384 nm and the emission intensity was collected at 560 nm (Note: Due to the poor solubility of sodium 4-methylbenzenesulfinate in THF, 4-methylbenzenesulfinic acid (4-$MeC_6H_4SO_2H$) was used as the quencher instead).

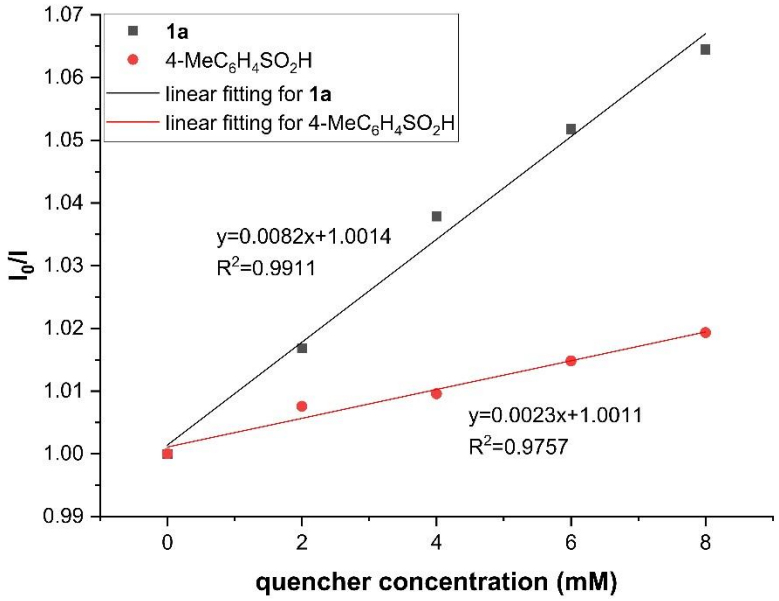
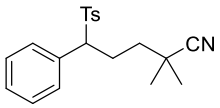


Figure S5 Emission quenching experiments with **1a** and 4-$MeC_6H_4SO_2H$ as quenchers

6. Characterization data

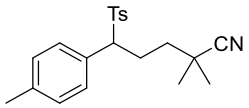
2,2-Dimethyl-5-phenyl-5-tosylpentanenitrile (3aa)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.35 (m, 2H), 7.32 – 7.29 (m, 1H), 7.25 – 7.23 (m, 2H), 7.17 – 7.15 (m, 2H), 7.09 – 7.07 (m, 2H), 4.00 (dd, J = 11.0, 3.5 Hz, 1H), 2.65 – 2.60 (m, 1H), 2.38 (s, 3H), 2.33 – 2.25 (m, 1H), 1.53 (td, J = 12.5, 4.5 Hz, 1H), 1.38 (td, J = 13.0, 4.0 Hz, 1H), 1.33 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 133.8, 131.8, 129.7, 129.3, 129.1, 129.0, 128.6, 124.4, 71.0, 38.1, 32.0, 26.6, 26.2, 23.5, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{24}NO_2S$ 342.1522,

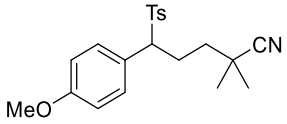
found 342.1520.

2,2-Dimethyl-5-(*p*-tolyl)-5-tosylpentanenitrile (3ba)



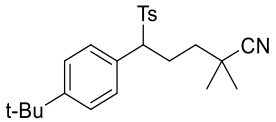
White solid, m.p. 152.9 – 154.6 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.40 (m, 2H), 7.29 – 7.26 (m, 1H), 7.22 – 7.20 (m, 2H), 7.10 – 7.08 (m, 2H), 7.00 – 6.98 (m, 2H), 4.00 (dd, *J* = 11.2, 4.0 Hz, 1H), 2.66 – 2.57 (m, 1H), 2.42 (s, 3H), 2.35 (s, 3H), 2.33 – 2.23 (m, 1H), 1.53 (td, *J* = 13.2, 4.8 Hz, 1H), 1.41 (td, *J* = 12.8, 4.0 Hz, 1H), 1.35 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 138.9, 133.9, 129.6, 129.34, 129.28, 129.1, 128.3, 124.0, 70.7, 38.0, 32.0, 26.5, 26.2, 23.6, 21.6, 21.2. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{21}H_{26}NO_2S$ 356.1679, found 356.1684.

5-(4-Methoxyphenyl)-2,2-dimethyl-5-tosylpentanenitrile (3ca)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.36 (m, 2H), 7.19 – 7.17 (m, 2H), 7.00 – 6.98 (m, 2H), 6.78 – 6.76 (m, 2H), 3.95 (dd, *J* = 11.5, 4.0 Hz, 1H), 3.78 (s, 3H), 2.62 – 2.55 (m, 1H), 2.38 (s, 3H), 2.26 – 2.18 (m, 1H), 1.50 (td, *J* = 13.5, 5.0 Hz, 1H), 1.38 (td, *J* = 12.5, 4.0 Hz, 1H), 1.32 (s, 3H), 1.29 (s, 3H) ; ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.0, 144.6, 133.9, 130.9, 129.3, 129.1, 127.1, 124.4, 114.0, 70.3, 55.3, 38.0, 32.0, 26.6, 26.2, 23.6, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{21}H_{26}NO_3S$ 372.1628, found 372.1636.

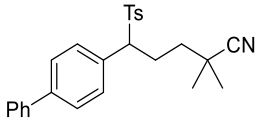
5-(4-(Tert-butyl)phenyl)-2,2-dimethyl-5-tosylpentanenitrile (3da)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.33 (m, 2H), 7.26 – 7.24 (m, 2H), 7.15 – 7.13 (m, 2H), 7.00 – 6.98 (m, 2H), 3.98 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.60 – 2.53 (m, 1H), 2.38 (s, 3H), 2.31 – 2.23 (m, 1H), 1.50 (td, *J* = 13.5, 5.0 Hz, 1H), 1.38 (td, *J* = 12.5, 4.0 Hz, 1H), 1.33 (s, 3H), 1.30 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.2, 144.5, 133.9, 129.3, 129.2, 129.1, 128.5, 125.5, 124.4, 70.8, 38.0, 34.6, 32.0,

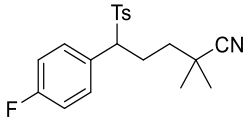
31.2, 26.5, 26.2, 23.4, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{24}H_{32}NO_2S$ 398.2148, found 398.2155.

5-([1,1'-Biphenyl]-4-yl)-2,2-dimethyl-5-tosylpentanenitrile (3ea)



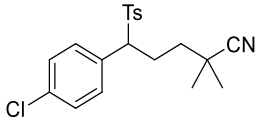
White solid, m.p. 146.9 – 148.5 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.57 (m, 2H), 7.51 – 7.49 (m, 2H), 7.46 – 7.41 (m, 4H), 7.38 – 7.35 (m, 1H), 7.19 – 7.15 (m, 4H), 4.07 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.68 – 2.61 (m, 1H), 2.39 (s, 3H), 2.36 – 2.28 (m, 1H), 1.59 – 1.53 (m, 1H), 1.47 – 1.41 (m, 1H), 1.35 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 141.7, 140.0, 134.7, 133.8, 130.7, 130.1, 129.4, 129.1, 128.9, 127.7, 127.2, 124.4, 70.7, 38.0, 32.1, 26.6, 26.2, 23.6, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{26}H_{28}NO_2S$ 418.1835, found 418.1841.

5-(4-Fluorophenyl)-2,2-dimethyl-5-tosylpentanenitrile (3fa)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.36 (m, 2H), 7.20 – 7.18 (m, 2H), 7.08 – 7.04 (m, 2H), 6.97 – 6.93 (m, 2H), 4.00 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.66 – 2.59 (m, 1H), 2.39 (s, 3H), 2.27 – 2.19 (m, 1H), 1.56 – 1.49 (m, 1H), 1.39 – 1.36 (m, 1H), 1.33 (s, 3H), 1.30 (s, 3H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.8; ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.1 (d, *J* = 247.8 Hz), 145.0, 133.8, 131.6 (d, *J* = 8.3 Hz), 129.6, 129.2, 127.9 (d, *J* = 3.0 Hz), 124.4, 115.9 (d, *J* = 21.5 Hz), 70.3, 38.2, 32.2, 26.8, 26.3, 23.8, 21.8. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{23}FNO_2S$ 360.1428, found 360.1425.

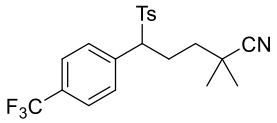
5-(4-Chlorophenyl)-2,2-dimethyl-5-tosylpentanenitrile (3ga)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.38 (m, 2H), 7.24 – 7.23 (m, 2H), 7.21 – 7.19 (m, 2H), 7.04 – 7.02 (m, 2H), 3.99 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.64 – 2.57 (m, 1H), 2.40 (s, 3H), 2.26 – 2.18 (m, 1H), 1.51 (td, *J* = 12.5, 5.0 Hz, 1H), 1.34 (td, *J* =

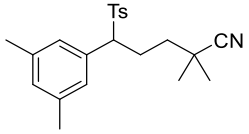
13.0, 4.0 Hz, 1H), 1.32 (s, 3H), 1.29 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.0, 135.1, 133.6, 130.9, 130.5, 129.5, 129.0, 128.9, 124.2, 70.2, 38.0, 32.0, 26.6, 26.2, 23.7, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{23}ClNO_2S$ 376.1133, found 376.1135.

2,2-Dimethyl-5-tosyl-5-(4-(trifluoromethyl)phenyl)pentanenitrile (3ha)



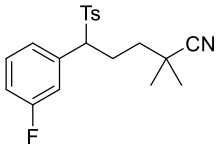
White solid, m.p. 135.4 – 137.1 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 – 7.52 (m, 2H), 7.40 – 7.38 (m, 2H), 7.25 – 7.23 (m, 2H), 7.21 – 7.19 (m, 2H), 4.09 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.67 – 2.60 (m, 1H), 2.40 (s, 3H), 2.33 – 2.24 (m, 1H), 1.57 – 1.51 (m, 1H), 1.37 – 1.34 (m, 1H), 1.33 (s, 3H), 1.30 (s, 3H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.8; ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.2, 136.1, 133.6, 131.2 (q, *J* = 32.9 Hz), 130.1, 129.5, 129.0, 125.6 (q, *J* = 3.7 Hz), 124.2, 123.7 (q, *J* = 273.0 Hz), 70.5, 38.0, 32.0, 26.5, 26.2, 23.8, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{21}H_{23}F_3NO_2S$ 410.1396, found 410.1398.

5-(3,5-Dimethylphenyl)-2,2-dimethyl-5-tosylpentanenitrile (3ia)



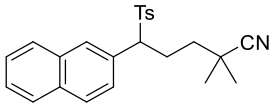
White solid, m.p. 144.1 – 145.7 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.37 (m, 2H), 7.18 – 7.16 (m, 2H), 6.90 (br, 1H), 6.64 (br, 2H), 3.91 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.57 – 2.50 (m, 1H), 2.37 (s, 3H), 2.28 – 2.22 (m, 1H), 2.19 (s, 6H), 1.50 (td, *J* = 13.5, 5.0 Hz, 1H), 1.39 (td, *J* = 13.0, 4.5 Hz, 1H), 1.30 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.4, 138.0, 133.9, 131.4, 130.5, 129.09, 129.06, 127.4, 124.3, 71.0, 38.0, 32.0, 26.5, 26.1, 23.5, 21.4, 21.0. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{22}H_{28}NO_2S$ 370.1835, found 370.1838.

5-(3-Fluorophenyl)-2,2-dimethyl-5-tosylpentanenitrile (3ja)



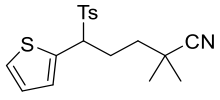
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.39 (m, 2H), 7.24 – 7.21 (m, 1H), 7.20 – 7.19 (m, 2H), 7.02 – 6.98 (m, 1H), 6.88 – 6.87 (m, 1H), 6.84 – 6.81 (m, 1H), 4.00 (dd, J_1 = 11.0, 4.0 Hz, 1H), 2.65 – 2.58 (m, 1H), 2.39 (s, 3H), 2.28 – 2.20 (m, 1H), 1.57 – 1.51 (m, 1H), 1.42 – 1.35 (m, 1H), 1.33 (s, 3H), 1.31 (s, 3H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.7; ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.6 (d, J = 248.1 Hz), 145.0, 134.4 (d, J = 7.4 Hz), 133.6, 130.2 (d, J = 8.2 Hz), 129.5, 129.0, 125.4 (d, J = 2.8 Hz), 124.3, 116.6 (d, J = 22.4 Hz), 116.0 (d, J = 21.0 Hz), 70.5, 38.0, 32.0, 26.5, 26.2, 23.7, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{23}FNO_2S$ 360.1428, found 360.1432.

2,2-Dimethyl-5-(naphthalen-2-yl)-5-tosylpentanenitrile (3ka)



White wax; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.81 (m, 1H), 7.76 – 7.74 (m, 1H), 7.71 – 7.70 (m, 1H), 7.52 – 7.51 (m, 1H), 7.50 – 7.46 (m, 2H), 7.39 – 7.37 (m, 2H), 7.25 – 7.23 (m, 1H), 7.13 – 7.11 (m, 2H), 4.18 (dd, J = 11.0, 4.0 Hz, 1H), 2.73 – 2.66 (m, 1H), 2.44 – 2.39 (m, 1H), 2.35 (s, 3H), 1.57 – 1.52 (m, 1H), 1.42 – 1.35 (m, 1H), 1.32 (s, 3H), 1.29 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.9, 134.1, 133.5, 133.1, 129.9, 129.51, 129.46, 129.3, 128.7, 128.2, 127.8, 126.9, 126.6, 126.5, 123.9, 71.4, 38.3, 32.2, 26.7, 26.4, 24.0, 21.7. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{24}H_{26}NO_2S$ 392.1679, found 392.1681.

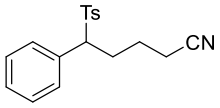
2,2-Dimethyl-5-(thiophen-2-yl)-5-tosylpentanenitrile (3la)



Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.44 (m, 2H), 7.28 – 7.27 (m, 1H), 7.21 – 7.20 (m, 2H), 6.91 – 6.89 (m, 1H), 6.81 – 6.80 (m, 1H), 4.29 (dd, J = 11.0, 4.0 Hz, 1H), 2.69 – 2.62 (m, 1H), 2.40 (s, 3H), 2.23 – 2.15 (m, 1H), 1.62 – 1.48 (m, 2H), 1.33 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.9, 134.0, 133.4,

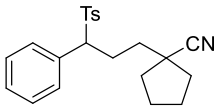
129.4, 129.2, 129.0, 127.1, 127.0, 124.3, 66.5, 37.9, 32.0, 26.4, 26.3, 25.2, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{18}H_{22}NO_2S_2$ 348.1086, found 348.1082.

5-Phenyl-5-tosylpentanenitrile (3ma)



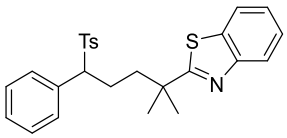
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.36 (m, 2H), 7.32 – 7.29 (m, 1H), 7.26 – 7.23 (m, 2H), 7.17 – 7.16 (m, 2H), 7.10 – 7.08 (m, 2H), 4.02 (dd, J = 11.0, 4.0 Hz, 1H), 2.58 – 2.51 (m, 1H), 2.38 (s, 3H), 2.35 – 2.31 (m, 2H), 2.30 – 2.24 (m, 1H), 1.73 – 1.63 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 133.9, 131.7, 129.6, 129.3, 129.1, 129.0, 128.7, 118.9, 70.7, 26.9, 23.1, 21.6, 17.0. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{18}H_{20}NO_2S$ 314.1209, found 314.1215.

1-(3-Phenyl-3-tosylpropyl)cyclopentane-1-carbonitrile (3na)



White solid, m.p. 142.8 – 144.1 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.35 (m, 2H), 7.32 – 7.29 (m, 1H), 7.25 – 7.23 (m, 2H), 7.17 – 7.16 (m, 2H), 7.10 – 7.08 (m, 2H), 4.02 (dd, J = 11.0, 4.5 Hz, 1H), 2.67 – 2.60 (m, 1H), 2.38 (s, 3H), 2.36 – 2.28 (m, 1H), 2.15 – 2.09 (m, 2H), 1.84 – 1.80 (m, 2H), 1.72 – 1.68 (m, 2H), 1.57 – 1.51 (m, 2H), 1.49 – 1.43 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.6, 133.8, 131.9, 129.7, 129.3, 129.1, 128.9, 128.6, 124.6, 71.0, 42.8, 38.1, 37.8, 35.7, 24.7, 24.1, 24.0, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{22}H_{26}NO_2S$ 368.1679, found 368.1681.

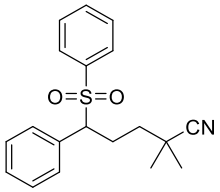
2-(2-methyl-5-phenyl-5-tosylpentan-2-yl)benzo[d]thiazole (3pa)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 – 7.93 (m, 1H), 7.85 – 7.83 (m, 1H), 7.48 – 7.44 (m, 1H), 7.37 – 7.34 (m, 1H), 7.30 – 7.28 (m, 3H), 7.22 – 7.19 (m, 2H), 7.06 – 7.04 (m, 2H), 7.02 – 7.01 (m, 2H), 3.93 (dd, J = 11.5, 3.5 Hz, 1H), 2.38 – 2.35 (m, 1H), 2.32 (s, 3H), 2.16 – 2.07 (m, 1H), 1.78 (td, J = 13.0, 4.5 Hz, 1H), 1.46 (s, 3H),

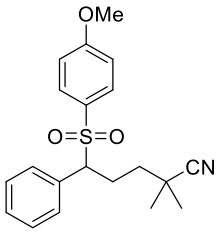
1.44 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.8, 153.0, 144.3, 134.8, 134.1, 131.9, 129.9, 129.1, 128.9, 128.7, 128.4, 125.8, 124.7, 122.7, 121.5, 71.6, 41.2, 40.6, 28.4, 22.9, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{26}H_{27}NO_2S_2$ 450.1556, found 450.1561.

2,2-Dimethyl-5-phenyl-5-(phenylsulfonyl)pentanenitrile (3ab)



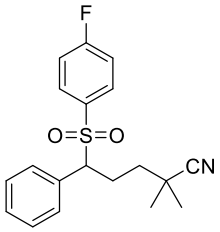
White solid, m.p. 123.5 – 125.2 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.52 (m, 1H), 7.50 – 7.49 (m, 2H), 7.39 – 7.35 (m, 2H), 7.31 – 7.28 (m, 1H), 7.25 – 7.22 (m, 2H), 7.08 – 7.07 (m, 2H), 4.03 (dd, J = 11.0, 4.5 Hz, 1H), 2.68 – 2.61 (m, 1H), 2.35 – 2.27 (m, 1H), 1.58 – 1.52 (m, 1H), 1.43 – 1.37 (m, 1H), 1.33 (s, 3 H), 1.31 (s, 3 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.1, 133.8, 131.9, 129.8, 129.2, 128.84, 128.82, 124.5, 71.2, 38.2, 32.2, 26.7, 26.4, 23.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{19}H_{22}NO_2S$ 328.1366, found 328.1371.

5-((4-Methoxyphenyl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3ac)



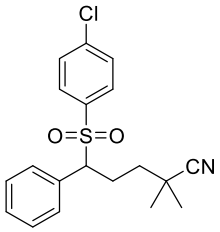
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.37 (m, 2H), 7.32 – 7.29 (m, 1H), 7.27 – 7.24 (m, 2H), 7.09 – 7.07 (m, 2H), 6.83 – 6.81 (m, 2H), 3.99 (dd, J = 11.0, 4.5 Hz, 1H), 3.83 (s, 3H), 2.67 – 2.60 (m, 1H), 2.32 – 2.24 (m, 1H), 1.57 – 1.49 (m, 1H), 1.42 – 1.41 (m, 1H), 1.33 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.8, 132.2, 131.4, 129.8, 129.1, 128.8, 128.4, 124.5, 114.0, 71.3, 55.7, 38.2, 32.2, 26.7, 26.4, 23.7. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{24}NO_3S$ 358.1471, found 358.1476.

5-((4-Fluorophenyl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3ad)



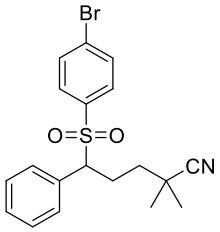
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 2H), 7.32 – 7.29 (m, 1H), 7.27 – 7.24 (m, 2H), 7.08 – 7.01 (m, 4H), 4.02 (dd, *J* = 11.0, 4.5 Hz, 1H), 2.69 – 2.62 (m, 1H), 2.35 – 2.27 (m, 1H), 1.59 – 1.52 (m, 1H), 1.43 – 1.36 (m, 1H), 1.34 (s, 3H), 1.31 (s, 3H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -103.2; ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.7 (d, *J* = 257.2 Hz), 132.9 (d, *J* = 2.8 Hz), 131.8 (d, *J* = 9.7 Hz), 131.6, 129.6, 129.2, 128.8, 124.3, 116.0 (d, *J* = 22.7 Hz), 71.2, 38.0, 32.0, 26.5, 26.2, 23.3. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{19}H_{21}FNO_2S$ 346.1272, found 346.1275.

5-((4-Chlorophenyl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3ae)



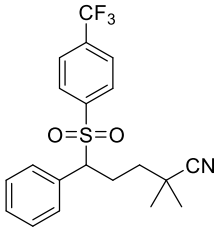
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.38 (m, 2H), 7.34 – 7.30 (m, 3H), 7.27 – 7.25 (m, 2H), 7.08 – 7.07 (m, 2H), 4.03 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.69 – 2.62 (m, 1H), 2.35 – 2.27 (m, 1H), 1.55 (td, *J* = 13.0, 4.5 Hz, 1H), 1.39 (td, *J* = 13.0, 3.5 Hz, 1H), 1.34 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.4, 135.3, 131.5, 130.4, 129.6, 129.2, 128.9, 128.8, 124.3, 71.1, 37.9, 32.0, 26.5, 26.2, 23.3. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{19}H_{21}ClNO_2S$ 362.0976, found 362.0982.

5-((4-Bromophenyl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3af)



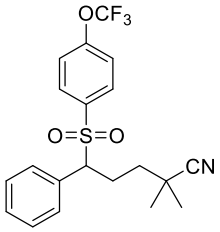
White solid, m.p. 117.2 – 119.7 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.49 (m, 2H), 7.34 – 7.30 (m, 1H), 7.28 – 7.25 (m, 2H), 7.09 – 7.07 (m, 4H), 4.02 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.69 – 2.62 (m, 1H), 2.35 – 2.27 (m, 1H), 1.58 – 1.53 (m, 1H), 1.43 – 1.37 (m, 1H), 1.34 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.9, 132.0, 131.5, 130.5, 129.6, 129.3, 129.1, 128.9, 124.3, 71.1, 38.0, 32.0, 26.5, 26.2, 23.3. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{19}H_{21}BrNO_2S$ 406.0471, found 406.0473.

2,2-Dimethyl-5-phenyl-5-((4-(trifluoromethyl)phenyl)sulfonyl)pentanenitrile (3ag)



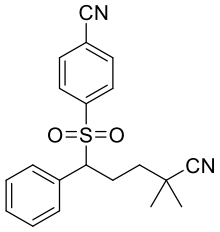
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 4H), 7.33 – 7.30 (m, 1H), 7.27 – 7.24 (m, 2H), 7.08 – 7.06 (m, 2H), 4.06 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.72 – 2.65 (m, 1H), 2.39 – 2.31 (m, 1H), 1.57 (td, *J* = 12.5, 5.0 Hz, 1H), 1.41 (td, *J* = 12.5, 4.0 Hz, 1H), 1.35 (s, 3H), 1.32 (s, 3H); ^{9}F NMR (471 MHz, $CDCl_3$) δ -63.1; ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.5, 140.6, 135.2 (q, *J* = 33.0 Hz), 131.3, 129.6, 129.4, 128.9, 125.7 (q, *J* = 3.6 Hz), 124.3, 123.0 (q, *J* = 271.6 Hz), 71.2, 38.0, 32.0, 26.5, 26.3, 23.3. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{21}F_3NO_2S$ 396.1240, found 396.1243.

2,2-Dimethyl-5-phenyl-5-((4-(trifluoromethoxy)phenyl)sulfonyl)pentanenitrile (3ah)



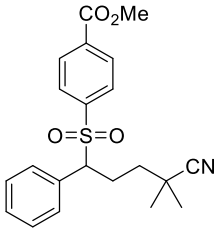
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.49 (m, 2H), 7.32 – 7.30 (m, 1H), 7.26 – 7.23 (m, 2H), 7.18 – 7.16 (m, 2H), 7.07 – 7.06 (m, 2H), 4.04 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.70 – 2.63 (m, 1H), 2.37 – 2.29 (m, 1H), 1.56 (td, *J* = 13.5, 5.0 Hz, 1H), 1.41 (td, *J* = 12.5, 4.0 Hz, 1H), 1.34 (s, 3H), 1.31 (s, 3H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -57.6; ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.9, 135.1, 131.5, 131.2, 129.6, 129.3, 128.8, 124.3, 120.3, 120.0 (q, *J* = 249.4 Hz), 71.2, 38.0, 32.0, 26.5, 26.2, 23.2. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{21}F_3NO_3S$ 412.1189, found 412.1202.

4-((4-Cyano-4-methyl-1-phenylpentyl)sulfonyl)benzonitrile (3ai)



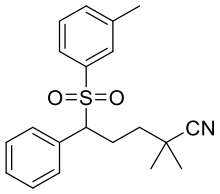
White solid, m.p. 140.2 – 141.5 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 – 7.63 (m, 2H), 7.58 – 7.56 (m, 2H), 7.34 – 7.31 (m, 1H), 7.27 – 7.24 (m, 2H), 7.07 – 7.05 (m, 2H), 4.07 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.71 – 2.64 (m, 1H), 2.38 – 2.30 (m, 1H), 1.57 (td, *J* = 13.5, 5.0 Hz, 1H), 1.41 (td, *J* = 12.5, 4.0 Hz, 1H), 1.34 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.3, 132.3, 131.1, 129.64, 129.58, 129.5, 129.0, 124.2, 117.3, 117.0, 71.2, 37.9, 32.0, 26.5, 26.3, 23.2. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{21}N_2O_2S$ 353.1318, found 353.1323.

Methyl 4-((4-cyano-4-methyl-1-phenylpentyl)sulfonyl)benzoate (3aj)



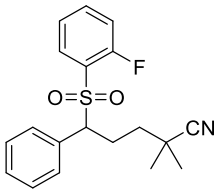
Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 – 8.00 (m, 2H), 7.56 – 7.54 (m, 2H), 7.32 – 7.29 (m, 1H), 7.25 – 7.22 (m, 2H), 7.07 – 7.06 (m, 2H), 4.06 (dd, *J* = 11.0, 4.0 Hz, 1H), 3.94 (s, 3H), 2.71 – 2.64 (m, 1H), 2.38 – 2.29 (m, 1H), 1.56 (td, *J* = 12.5, 4.5 Hz, 1H), 1.41 (td, *J* = 12.5, 4.0 Hz, 1H), 1.34 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5, 141.0, 134.6, 131.3, 129.7, 129.6, 129.3, 129.1, 128.9, 124.2, 71.9, 52.7, 38.0, 32.1, 26.6, 26.2, 23.3. HRMS (ESI) m/z: $[M+K]^+$ calcd. for $C_{21}H_{23}KNO_4S$ 424.0979, found 424.0988.

2,2-Dimethyl-5-phenyl-5-(m-tolylsulfonyl)pentanenitrile (3ak)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.35 (m, 2H), 7.30 – 7.29 (m, 1H), 7.26 – 7.23 (m, 2H), 7.17 – 7.15 (m, 2H), 7.09 – 7.07 (m, 2H), 4.00 (dd, *J* = 11.0, 4.5 Hz, 1H), 2.66 – 2.59 (m, 1H), 2.38 (s, 3H), 2.33 – 2.25 (m, 1H), 1.56 – 1.50 (m, 1H), 1.41 – 1.35 (m, 1H), 1.33 (s, 3 H), 1.30 (s, 3 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 139.6, 133.8, 131.8, 129.7, 129.3, 129.1, 129.0, 128.6, 125.8, 124.4, 71.0, 38.0, 32.0, 26.6, 26.2, 23.5, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{24}NO_2S$ 342.1522, found 345.1525.

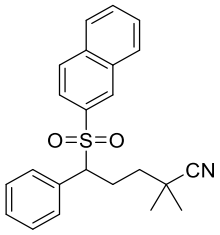
5-((2-Fluorophenyl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3al)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.47 (m, 2H), 7.25 – 7.21 (m, 5H),

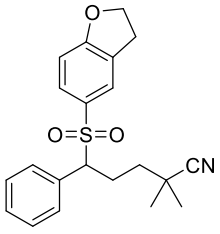
7.17 – 7.13 (m, 1H), 7.11 – 7.07 (m, 1H), 4.37 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.67 – 2.60 (m, 1H), 2.42 – 2.34 (m, 1H), 1.63 – 1.57 (m, 1H), 1.47 – 1.40 (m, 1H), 1.34 (s, 3 H), 1.32 (s, 3 H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -108.3; ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.5 (d, *J* = 255.3 Hz), 136.1 (d, *J* = 8.4 Hz), 134.1, 131.4, 131.3, 129.3, 129.2, 128.8, 124.5 (d, *J* = 3.3 Hz), 124.3, 116.7 (d, *J* = 21.7 Hz), 70.2, 38.0, 32.1, 26.6, 24.1, 23.2. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{19}H_{21}FNO_2S$ 358.1471, found 358.1470.

2,2-Dimethyl-5-(naphthalen-2-ylsulfonyl)-5-phenylpentanenitrile (3am)



White solid, m.p. 204.9 – 206.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (br, 1H), 7.87 – 7.86 (m, 1H), 7.83 – 7.79 (m, 2H), 7.66 – 7.62 (m, 1H), 7.59 – 7.56 (m, 1H), 7.44 – 7.42 (m, 1H), 7.29 – 7.27 (m, 1H), 7.21 – 7.18 (m, 2H), 7.09 – 7.07 (m, 2H), 4.11 (dd, *J* = 11.0, 4.0 Hz, 1H), 2.75 – 2.68 (m, 1H), 2.40 – 2.32 (m, 1H), 1.61 – 1.55 (m, 1H), 1.42 (td, *J* = 13.0, 4.0 Hz, 1H), 1.34 (s, 3 H), 1.31 (s, 3 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.2, 133.9, 131.9, 131.1, 129.8, 129.4, 129.2, 129.1, 128.71, 128.68, 127.9, 127.5, 124.3, 123.6, 71.2, 38.1, 32.1, 29.7, 26.6, 26.3, 23.6. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{23}H_{24}NO_2S$ 378.1522, found 378.1528.

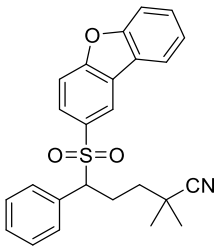
5-((2,3-Dihydrobenzofuran-5-yl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3an)



Light yellow solid, m.p. 127.2 – 128.5 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 1H), 7.27 – 7.23 (m, 4H), 7.10 – 7.08 (m, 2H), 6.69 – 6.67 (m, 1H), 4.63 (t, *J* = 9.0

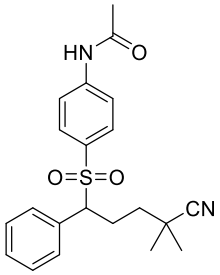
Hz, 2H), 3.98 (dd, *J* = 11.0, 4.5 Hz, 1H), 3.18 – 3.06 (m, 2H), 2.64 – 2.58 (m, 1H), 2.31 – 2.23 (m, 1H), 1.54 (td, *J* = 13.5, 5.0 Hz, 1H), 1.38 (td, *J* = 12.5, 4.0 Hz, 1H), 1.32 (s, 3 H), 1.29 (s, 3 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.6, 132.2, 130.7, 129.7, 128.9, 128.5, 128.3, 127.9, 126.3, 124.3, 109.1, 72.3, 71.3, 38.1, 32.0, 28.6, 26.5, 26.2, 23.6. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{21}H_{24}NO_3S$ 370.1471, found 370.1478.

5-(Dibenzo[b,d]furan-2-ylsulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3ao)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.08 (m, 1H), 7.88 – 7.86 (m, 1H), 7.62 – 7.60 (m, 1H), 7.55 – 7.52 (m, 2H), 7.51 – 7.49 (m, 1H), 7.42 – 7.39 (m, 1H), 7.29 – 7.26 (m, 1H), 7.23 – 7.20 (m, 2H), 7.09 – 7.08 (m, 2H), 4.11 (dd, *J* = 11.0, 4.5 Hz, 1H), 2.76 – 2.09 (m, 1H), 2.41 – 2.33 (m, 1H), 1.59 (td, *J* = 13.5, 5.0 Hz, 1H), 1.43 (td, *J* = 12.5, 4.0 Hz, 1H), 1.35 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.6, 156.9, 131.9, 131.3, 129.7, 129.1, 128.7, 128.6, 128.0, 124.7, 124.4, 123.7, 122.9, 122.7, 121.1, 112.1, 111.8, 71.5, 38.1, 32.1, 26.6, 26.3, 23.5. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{25}H_{24}NO_3S$ 418.1471, found 418.1482.

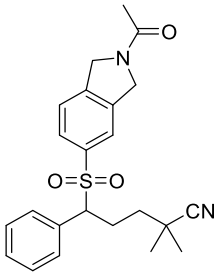
***N*-(4-((4-cyano-4-methyl-1-phenylpentyl)sulfonyl)phenyl)acetamide (3ap)**



White solid, m.p. 154.9 – 156.2 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (br, 1H), 7.54 – 7.52 (m, 2H), 7.40 – 7.38 (m, 2H), 7.32 – 7.29 (m, 1H), 7.26 – 7.23 (m, 2H), 7.09 – 7.07 (m, 2H), 4.01 (dd, *J* = 11.0, 4.5 Hz, 1H), 2.65 – 2.58 (m, 1H), 2.33 – 2.25 (m, 1H), 2.18 (s, 3H), 1.53 (td, *J* = 13.5, 5.0 Hz, 1H), 1.37 (td, *J* = 13.0, 4.0 Hz, 1H), 1.32 (s,

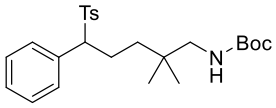
3H), 1.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.2, 142.9, 131.6, 131.2, 130.3, 129.7, 129.1, 128.7, 124.4, 118.6, 71.1, 38.0, 32.1, 26.5, 26.3, 24.7, 23.5. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{21}H_{25}N_2O_3S$ 385.1580, found 385.1587.

5-((2-Acetylisoindolin-5-yl)sulfonyl)-2,2-dimethyl-5-phenylpentanenitrile (3aq)



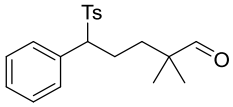
White solid, m.p. 170.1 – 171.5 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 – 8.14 (m, 1H), 7.32 – 7.28 (m, 2H), 7.26 – 7.23 (m, 2H), 7.18 (br, 1H), 7.09 – 7.08 (m, 2H), 4.09 (t, *J* = 8.5 Hz, 2H), 3.99 (dd, *J* = 11.0, 4.0 Hz, 1H), 3.16 – 3.03 (m, 2H), 2.65 – 2.58 (m, 1H), 2.32 – 2.27 (m, 1H), 2.23 (s, 3H), 1.53 (td, *J* = 13.5, 5.0 Hz, 1H), 1.38 (td, *J* = 12.5, 4.0 Hz, 1H), 1.32 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.5, 147.3, 131.9, 131.7, 130.9, 129.8, 129.7, 129.0, 128.6, 125.4, 124.3, 116.1, 71.1, 49.1, 38.0, 32.0, 27.2, 26.5, 26.2, 24.3, 23.5. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{23}H_{27}N_2O_3S$ 411.1737, found 411.1745.

***tert*-Butyl (2,2-dimethyl-5-phenyl-5-tosylpentyl)carbamate (4)**



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.34 (m, 2H), 7.28 – 7.25 (m, 1H), 7.23 – 7.20 (m, 2H), 7.15 – 7.13 (m, 2H), 7.05 – 7.04 (m, 2H), 4.44 (br, 1H), 3.92 (dd, *J* = 11.5, 3.5 Hz, 1H), 2.92 – 2.82 (m, 2H), 2.46 – 2.40 (m, 1H), 2.37 (s, 3H), 2.13 – 2.04 (m, 1H), 1.39 (s, 9H), 1.14 (td, *J* = 13.0, 4.5 Hz, 1H), 0.97 (td, *J* = 13.0, 4.0 Hz, 1H), 0.83 (s, 3H), 0.81 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 144.3, 134.3, 132.4, 129.7, 129.2, 129.0, 128.7, 128.4, 79.0, 72.0, 50.2, 36.6, 34.4, 28.3, 24.5, 24.4, 22.0, 21.6. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{25}H_{36}NO_4S$: 446.2360, Found: 446.2364.

2,2-Dimethyl-5-phenyl-5-tosylpentanal (5)



Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.34 (br, 1H), 7.33 – 7.32 (m, 2H), 7.30 – 7.27 (m, 1H), 7.24 – 7.21 (m, 2H), 7.15 – 7.13 (m, 2H), 7.05 – 7.04 (m, 2H), 3.94 (dd, J = 11.0, 3.5 Hz, 1H), 2.43 – 2.38 (m, 1H), 2.37 (s, 3H), 2.09 – 2.01 (m, 1H), 1.42 (td, J = 13.0, 4.5 Hz, 1H), 1.27 (td, J = 13.5, 4.0 Hz, 1H), 1.02 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 205.4, 144.5, 134.0, 132.0, 129.7, 129.2, 129.0, 128.8, 128.5, 71.7, 45.6, 33.8, 22.3, 21.6, 21.3, 21.0. HRMS(ESI) m/z: $[M+H]^+$ calcd. for $C_{20}H_{25}O_3S$: 345.1519, Found: 345.1520.

7. References

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3. S. Caddick, D. B. Judd, A. K. de K Lewis, M. T. Reich and M. R. Williams, A Generic Approach for the Catalytic Reduction of Nitriles, *Tetrahedron*, 2003, **59**, 5417−5423.

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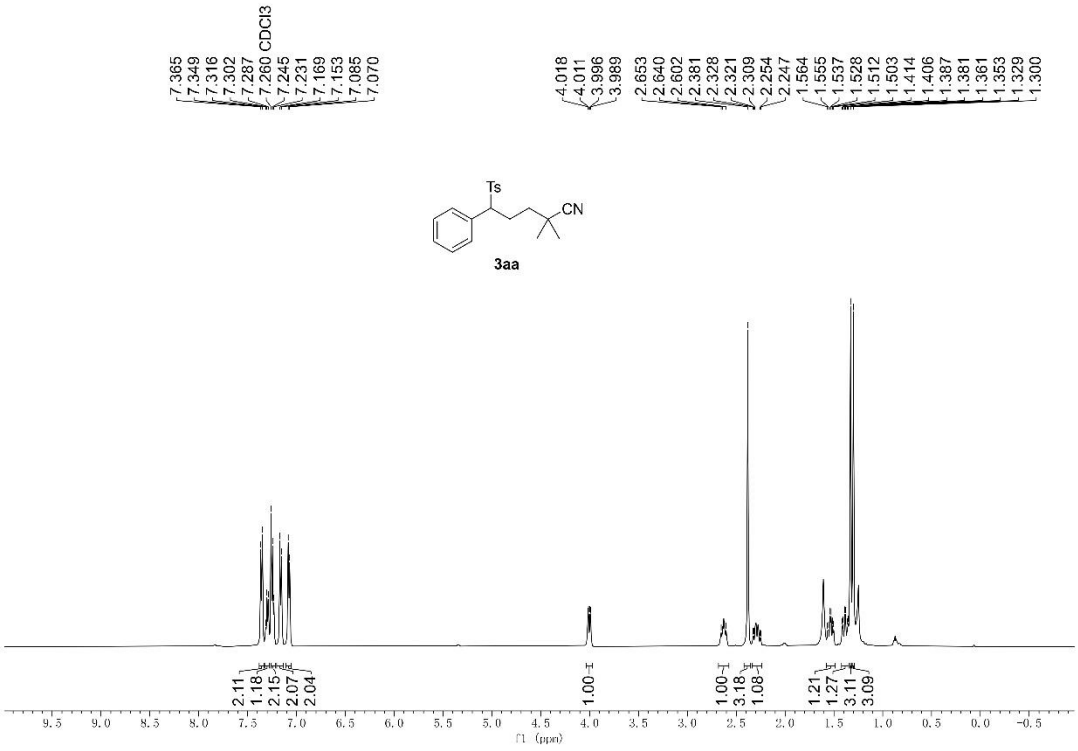
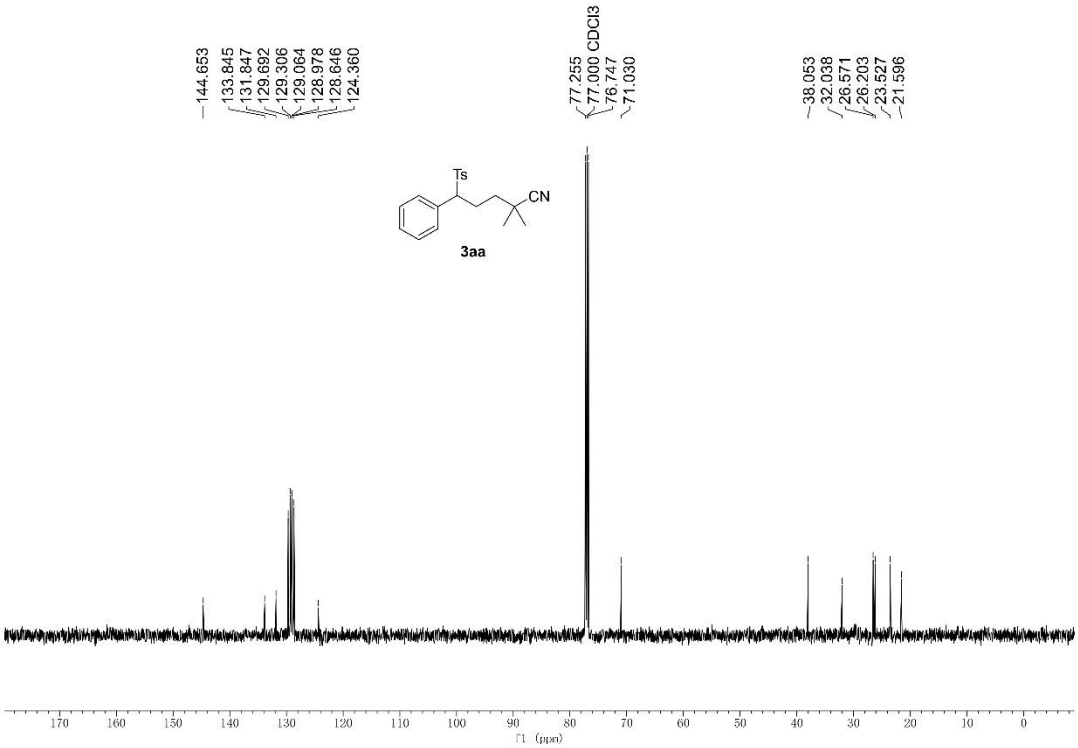
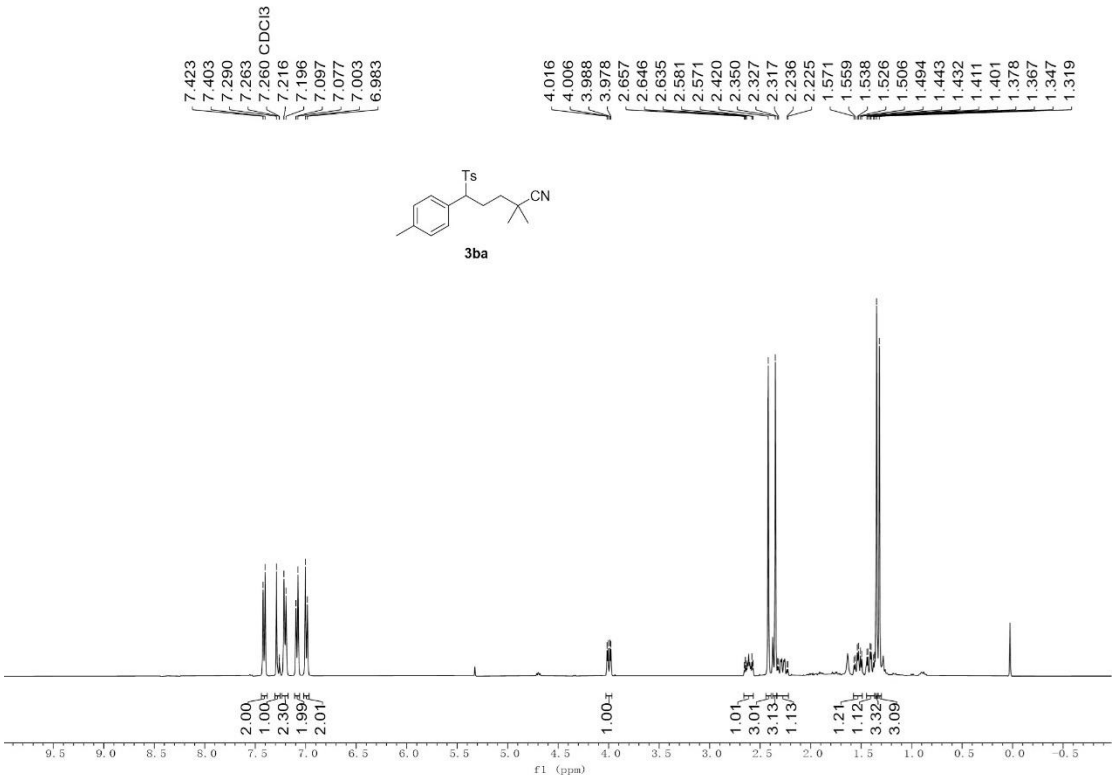
8. NMR spectra



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7.403
7.290
7.263
7.260 CDCl3
7.216
7.196
7.097
7.077
7.003
6.983
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4.006
3.988
3.978
2.657
2.646
2.635
2.581
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1.538
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1.506
1.494
1.443
1.432
1.411
1.401
1.378
1.367
1.347
1.319
Ts
CN
3ba
2.00
1.00
2.30
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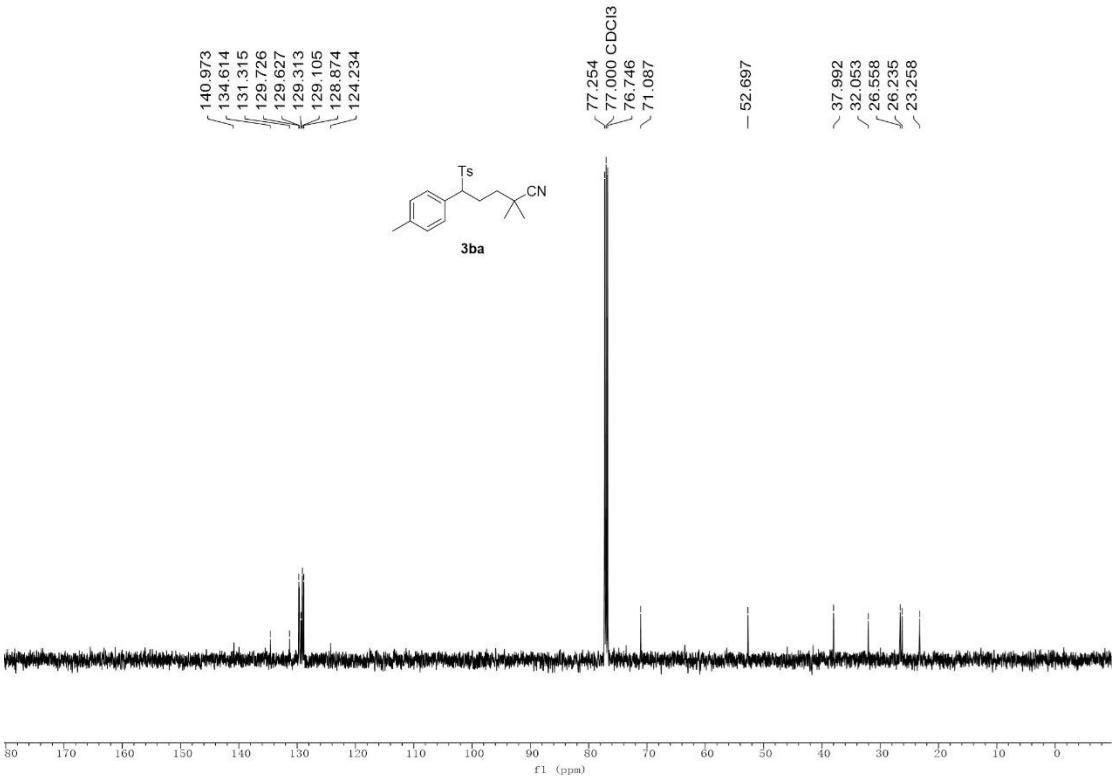
3.13
1.13
1.21
1.12
3.32
3.09
f1 (ppm)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26.235
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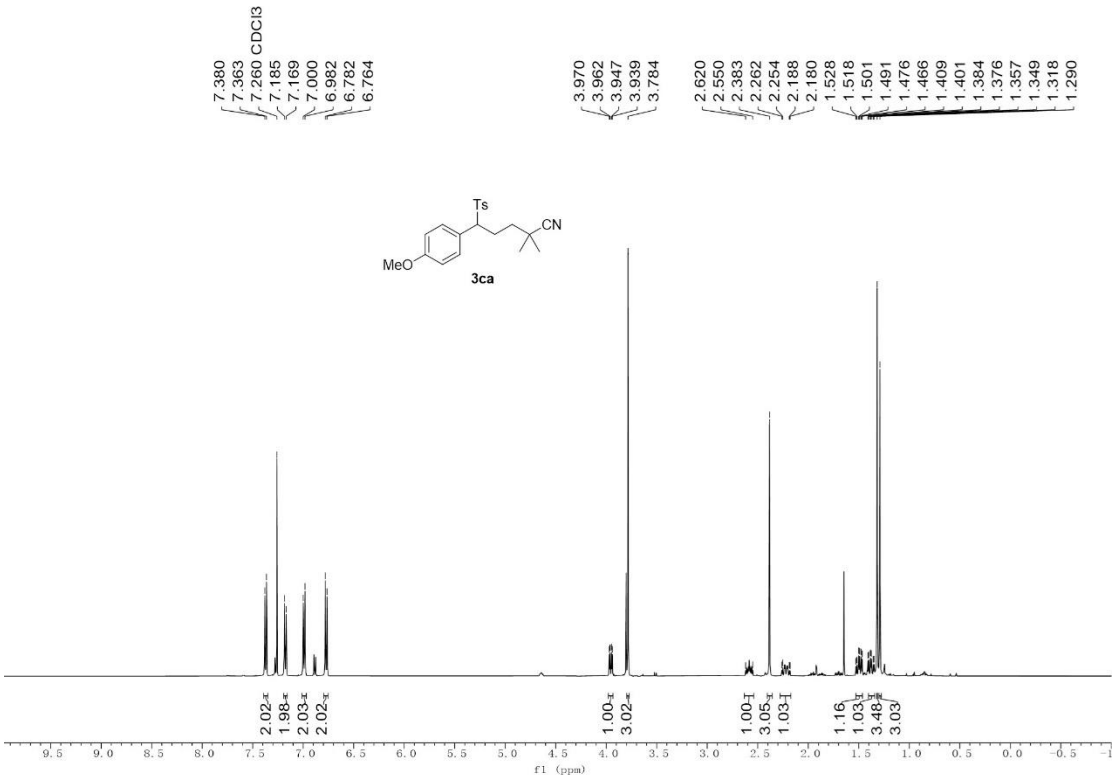
3ba
f1 (ppm)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6.782
6.764
3.970
3.962
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3.939
3.784
2.620
2.550
2.383
2.262
2.254
2.188
2.180
1.528
1.518
1.501
1.491
1.476
1.466
1.409
1.401
1.384
1.376
1.357
1.349
1.318
1.290
Ts
CN
MeO
3ca
2.02
1.98
2.03
2.02
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3.05
1.03
1.16
1.03
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3.03
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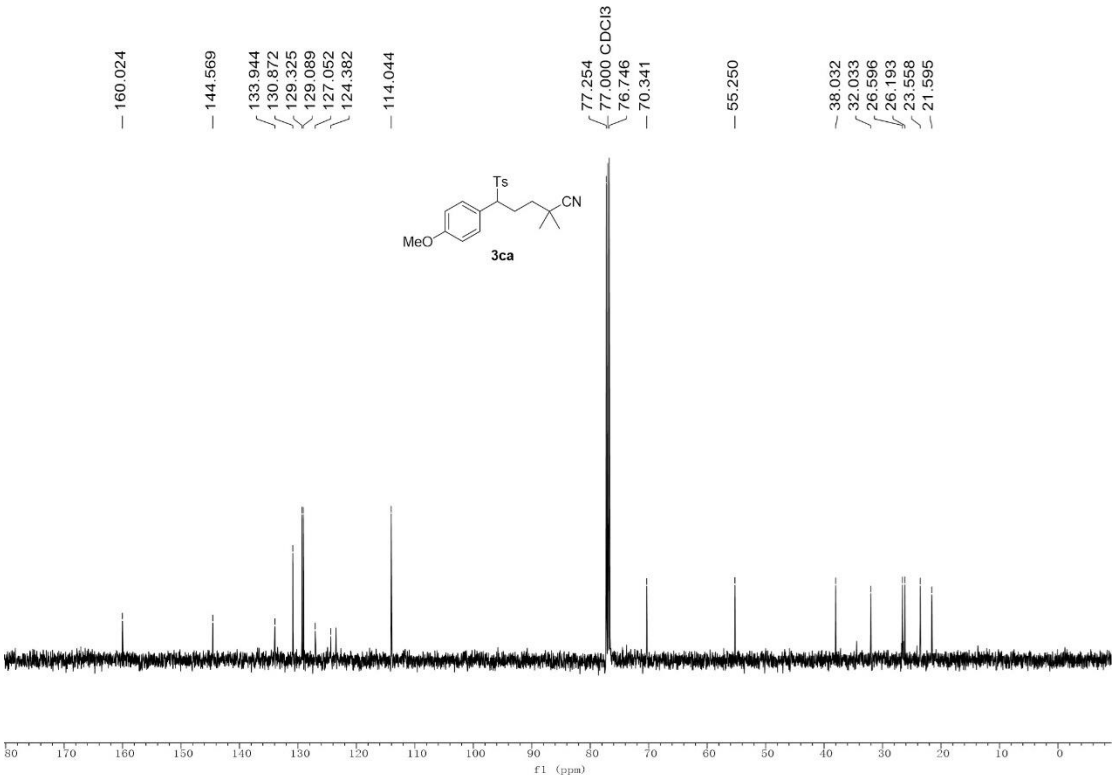
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32.033
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26.193
23.558
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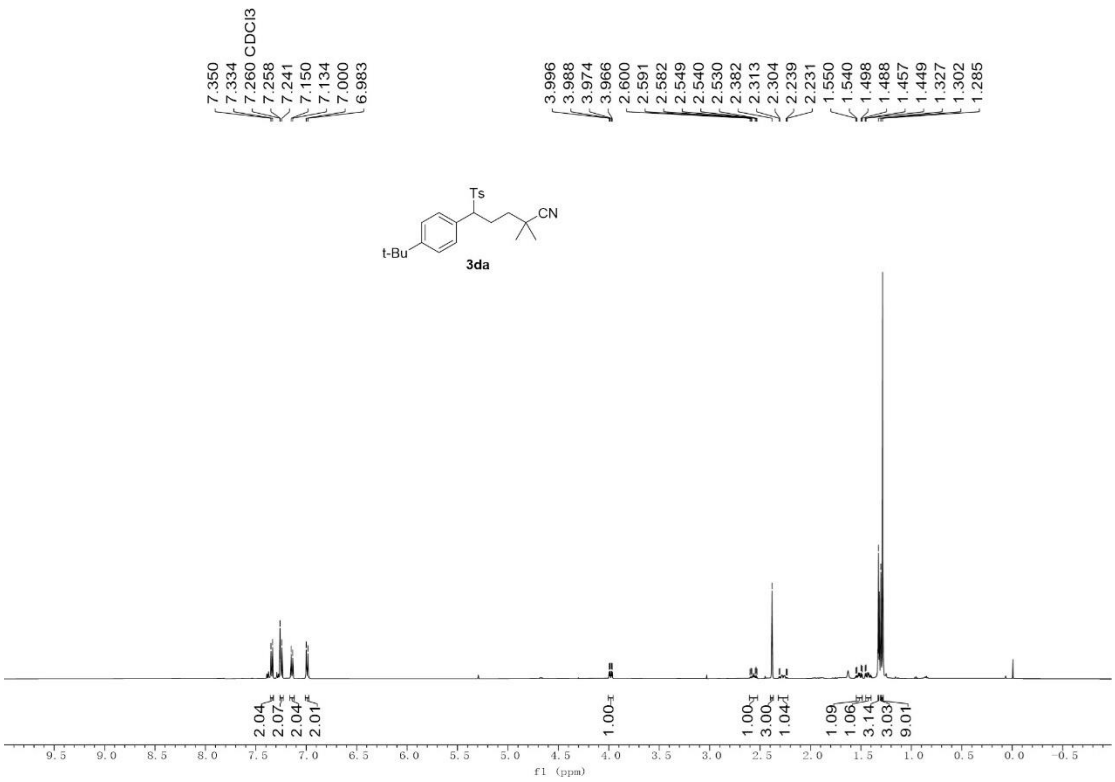
Ts
CN
MeO
3ca
f1 (ppm)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3.966
2.600
2.591
2.582
2.549
2.540
2.530
2.382
2.313
2.304
2.239
2.231
1.550
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1.498
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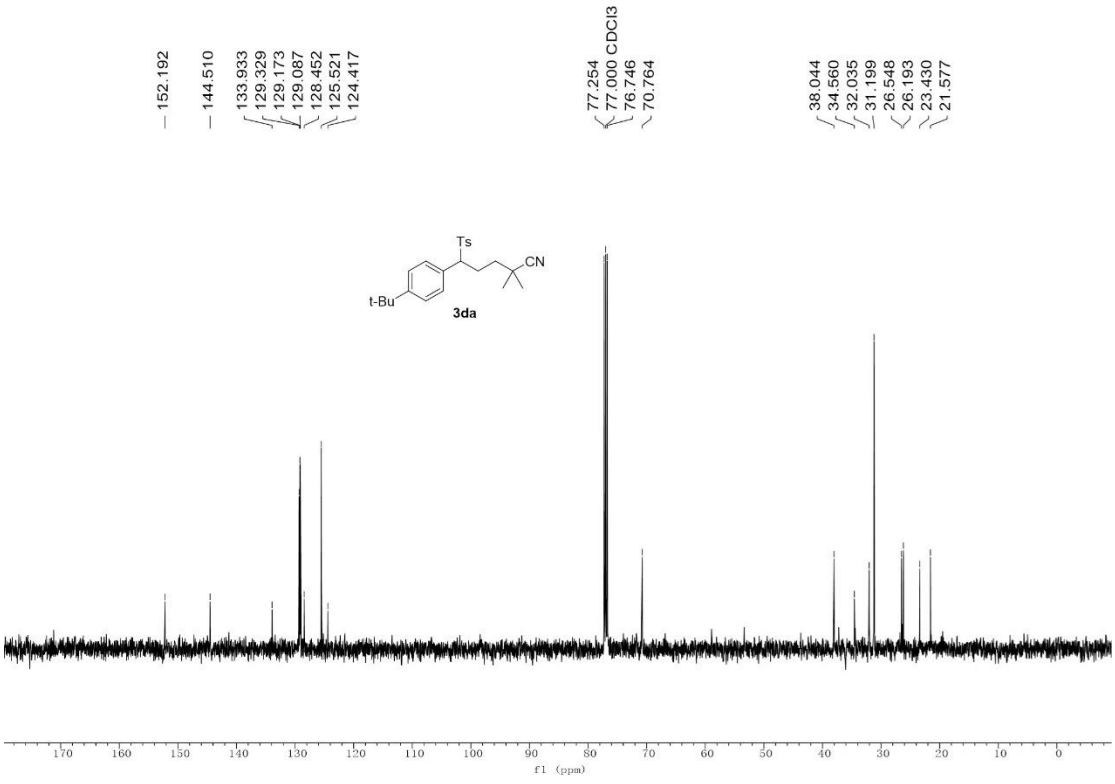
1.457
1.449
1.327
1.302
1.285
Ts
CN
t-Bu
3da
2.04
2.07
2.04
2.01
1.00
1.00
3.00
1.04
1.09
1.06
3.14
3.03
9.01
f1 (ppm)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125.521
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77.000 CDCl3
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70.764
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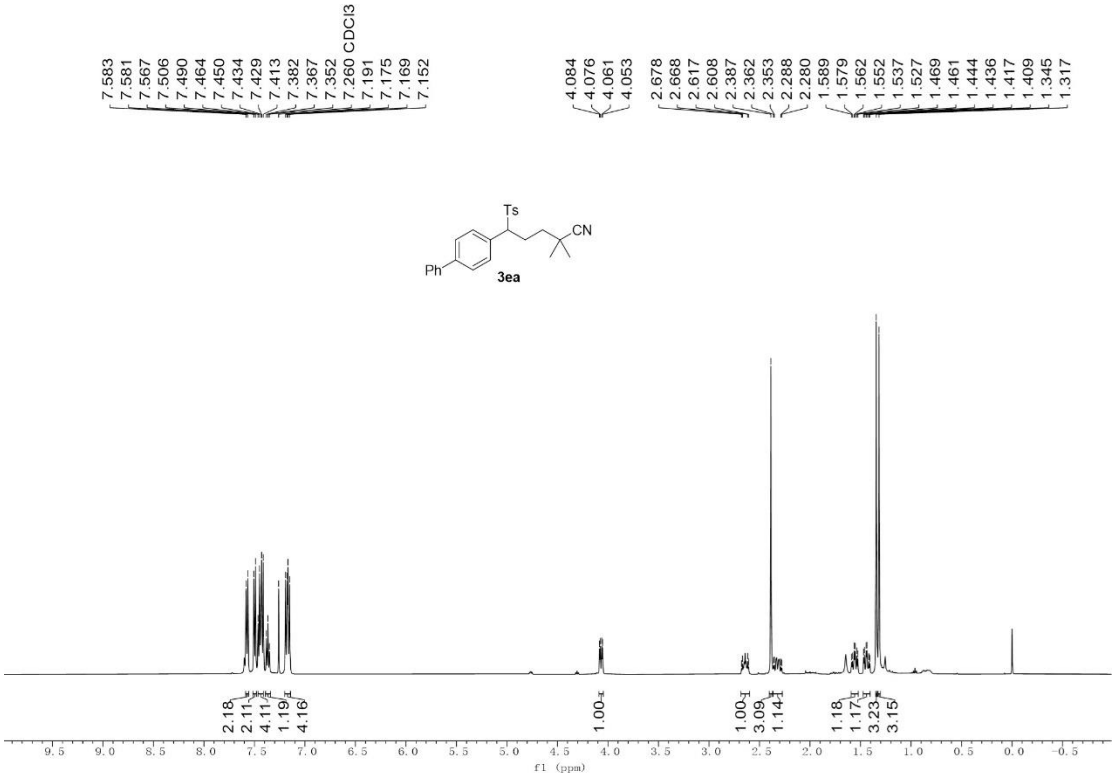
26.193
23.430
21.577
Ts
CN
t-Bu
3da
f1 (ppm)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7.352
7.260 CDCl3
7.191
7.175
7.169
7.152
4.084
4.076
4.061
4.053
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2.668
2.617
2.608
2.387
2.362
2.353
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2.280
1.589
1.579
1.562
1.552
1.537
1.527
1.469
1.461
1.444
1.436
1.417
1.409
1.345
1.317
Ts
CN
Ph
3ea
2.18
2.11
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1.18
1.17
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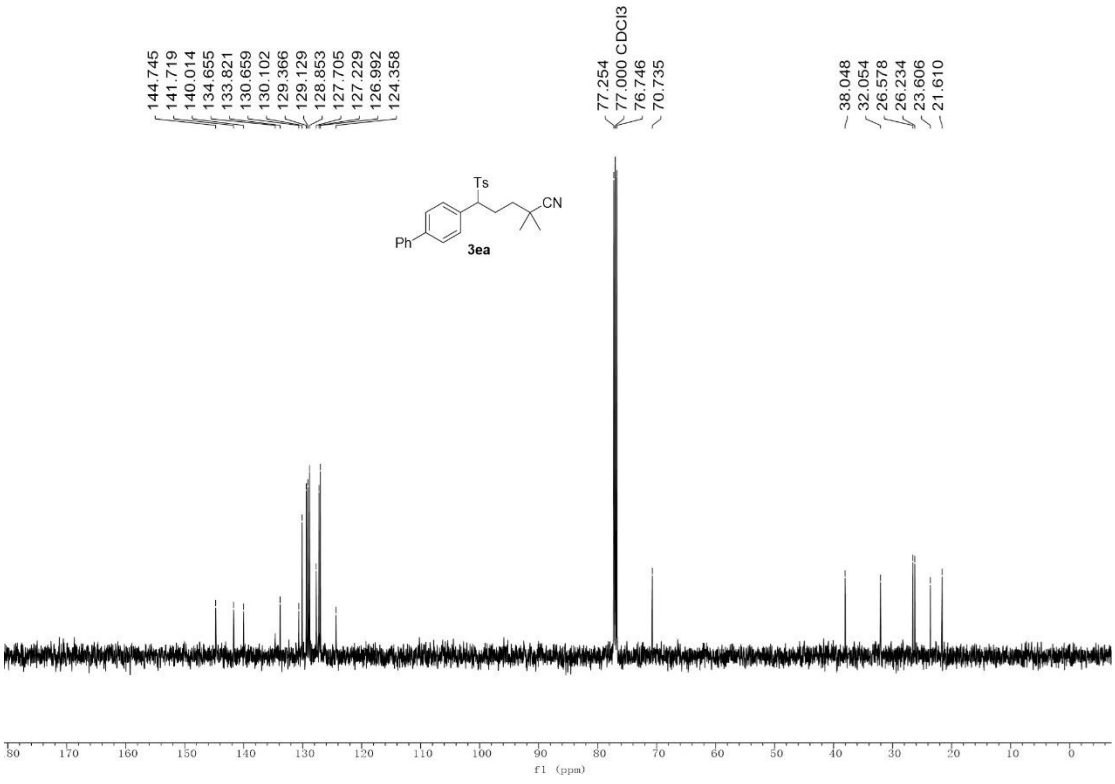
f1 (ppm)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77.000 CDCl3
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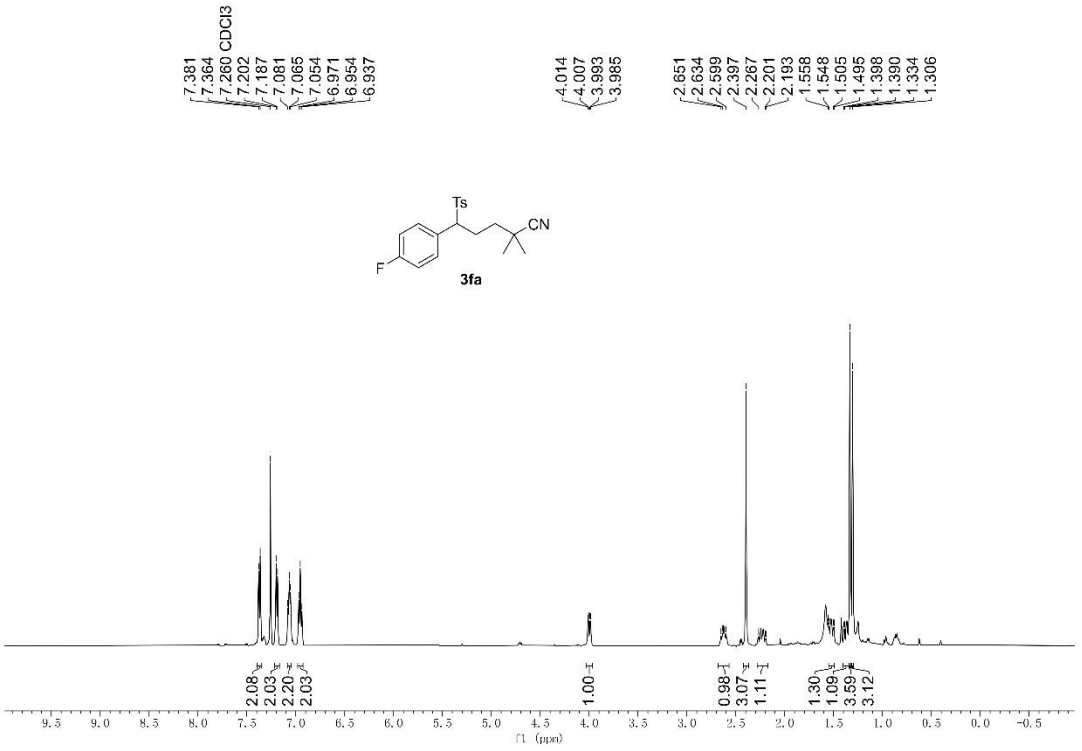
21.610
Ts
CN
Ph
3ea
f1 (ppm)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7.187
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7.054
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6.954
6.937
4.014
4.007
3.993
3.985
2.651
2.634
2.599
2.397
2.267
2.201
2.193
1.558
1.548
1.505
1.495
1.398
1.390
1.334
1.306
Ts
CN
F
3fa
2.08
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1.09
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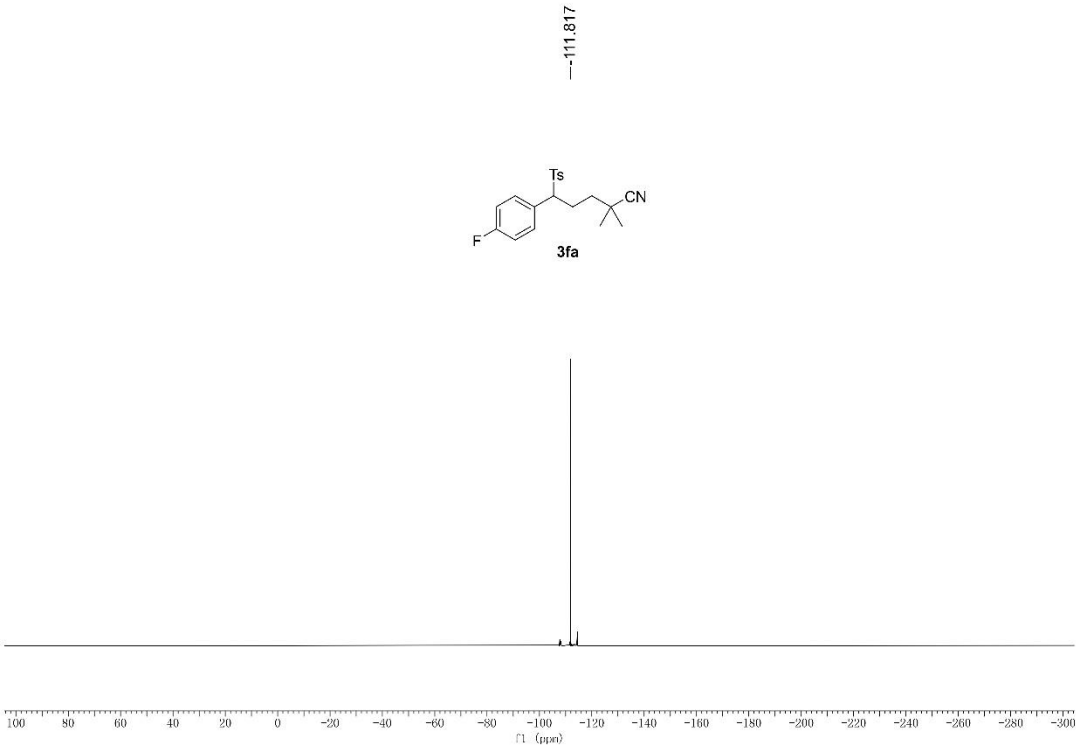
3.12
f1 (ppm)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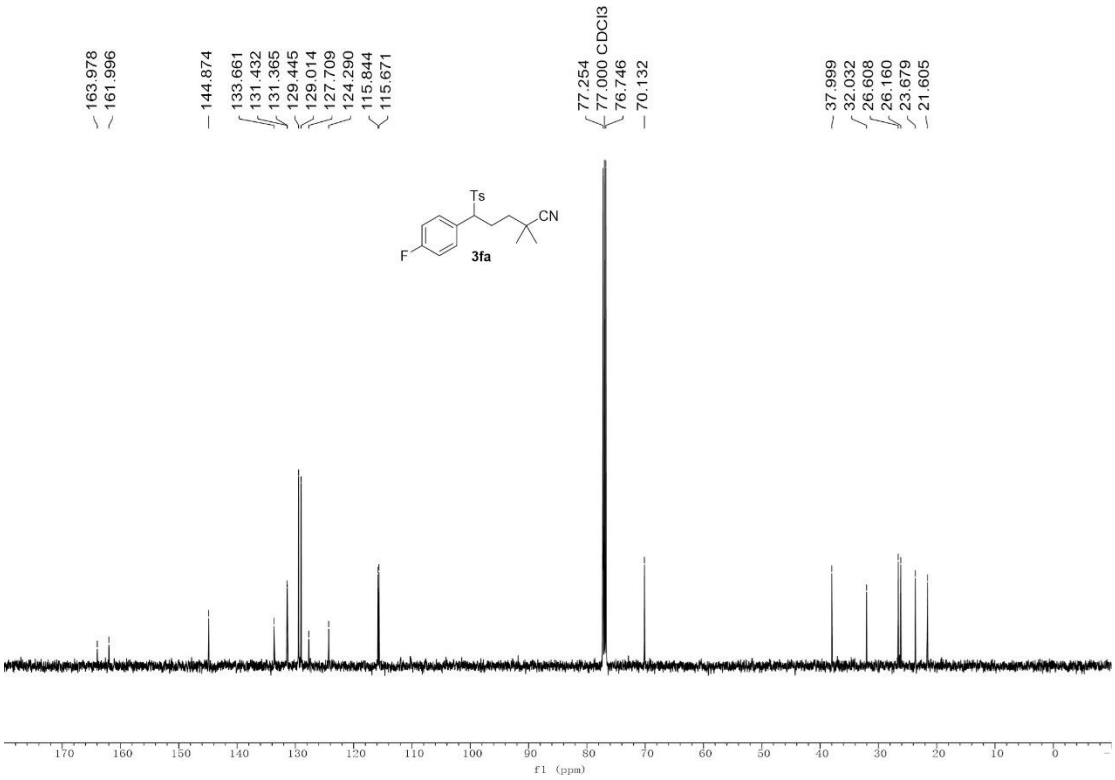
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115.671
77.254
77.000 CDCl3
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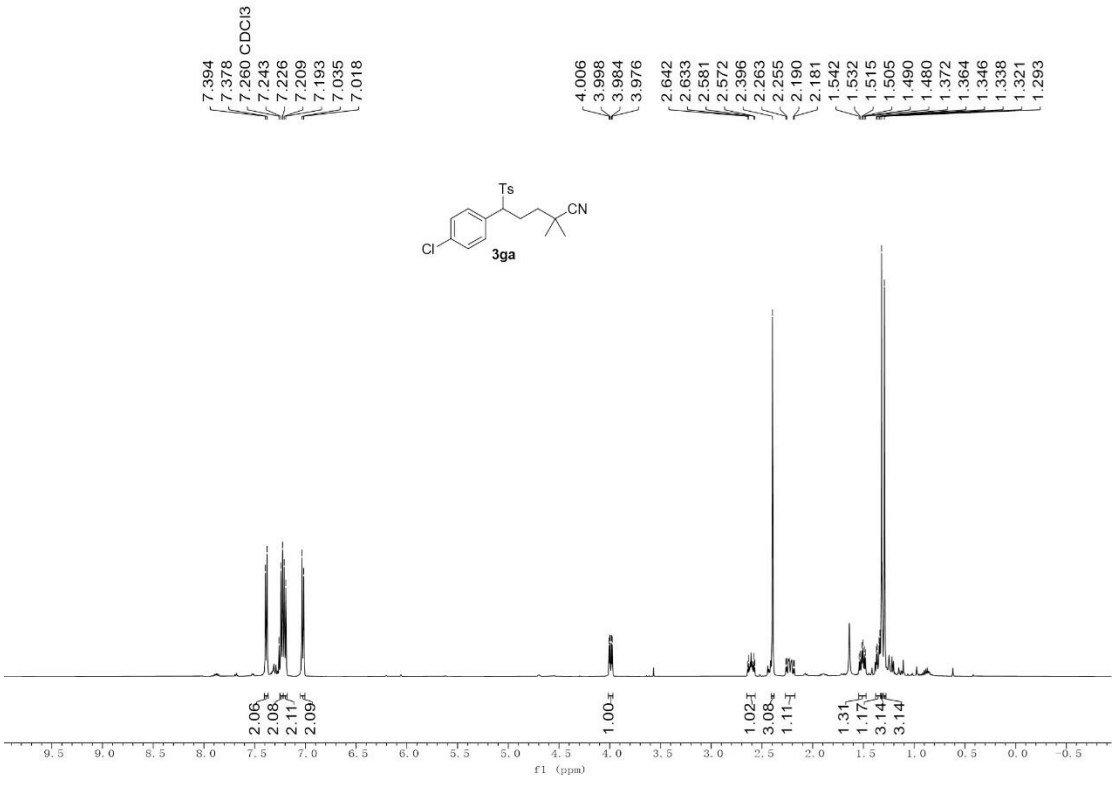
Ts
CN
F
3fa
f1 (ppm)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7.209
7.193
7.035
7.018
4.006
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3.984
3.976
2.642
2.633
2.581
2.572
2.396
2.263
2.255
2.190
2.181
1.542
1.532
1.515
1.505
1.490
1.480
1.372
1.364
1.346
1.338
1.321
1.293
Ts
CN
Cl
3ga
2.06
2.08
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1.17
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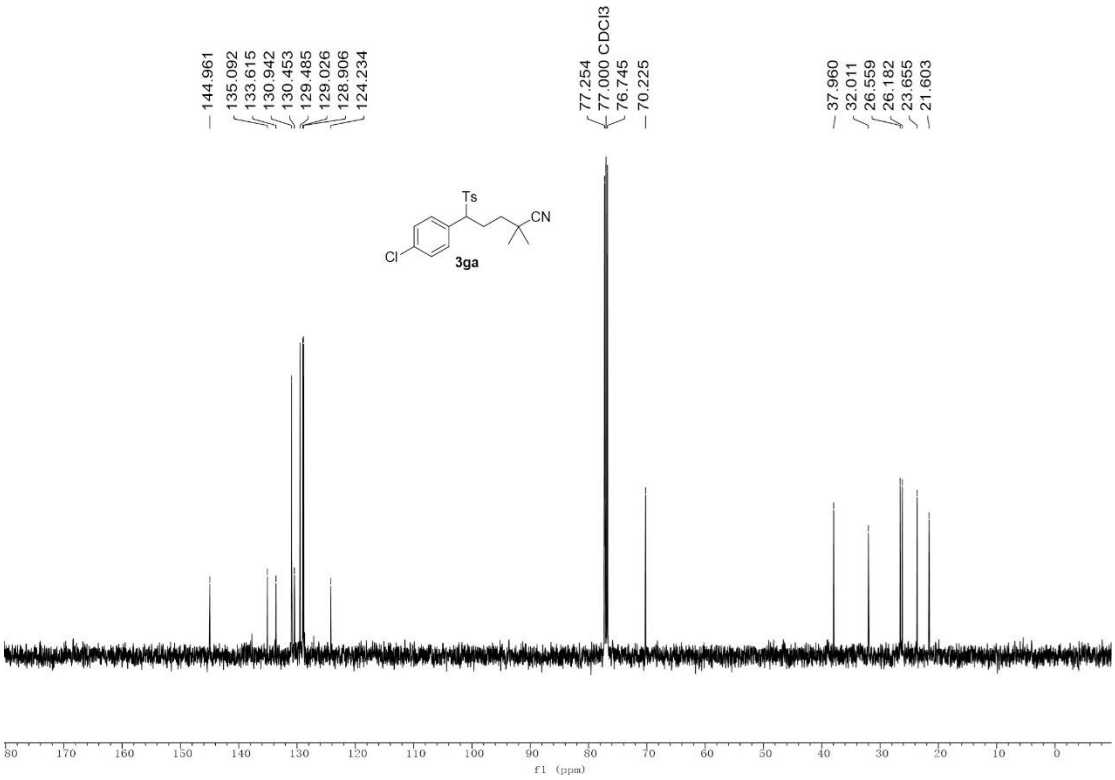
3.14
f1 (ppm)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77.000 CDCl3
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37.960
32.011
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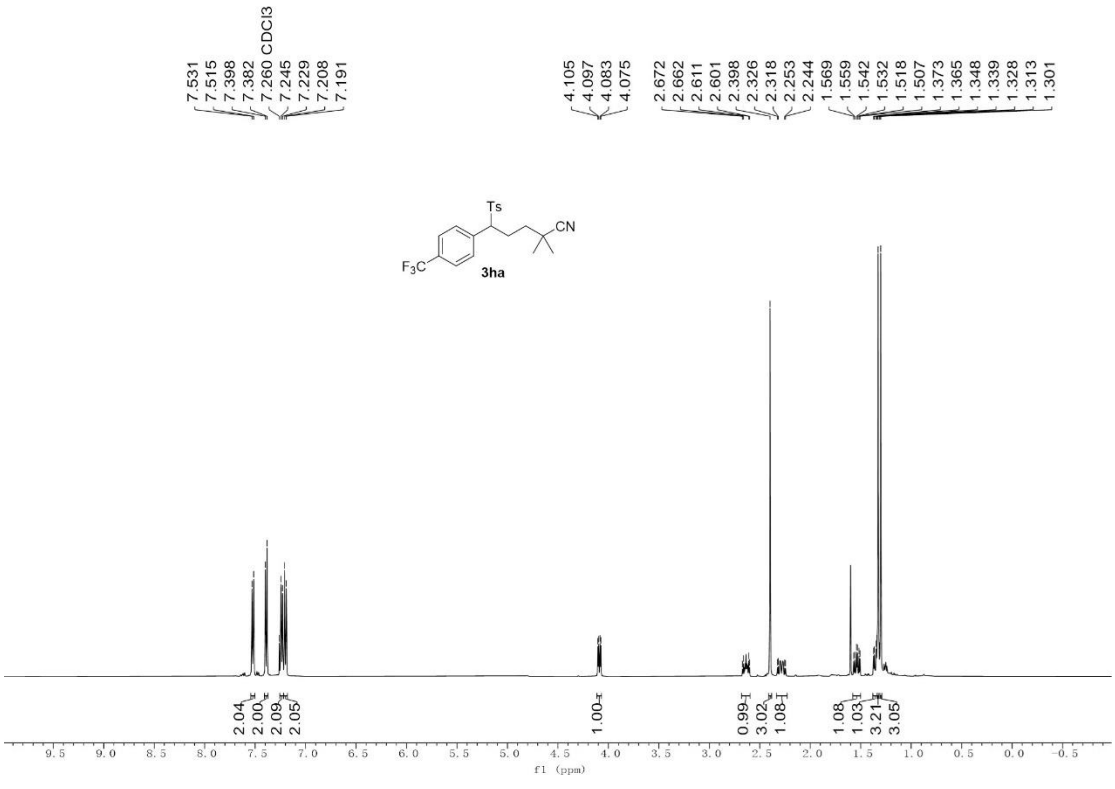
26.182
23.655
21.603
Ts
CN
Cl
3ga
f1 (ppm)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7.245
7.229
7.208
7.191
4.105
4.097
4.083
4.075
2.672
2.662
2.611
2.601
2.398
2.326
2.318
2.253
2.244
1.569
1.559
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1.532
1.518
1.507
1.373
1.365
1.348
1.339
1.328
1.313
1.301
Ts
CN
F3C
3ha
2.04
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3.02
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1.08
1.03
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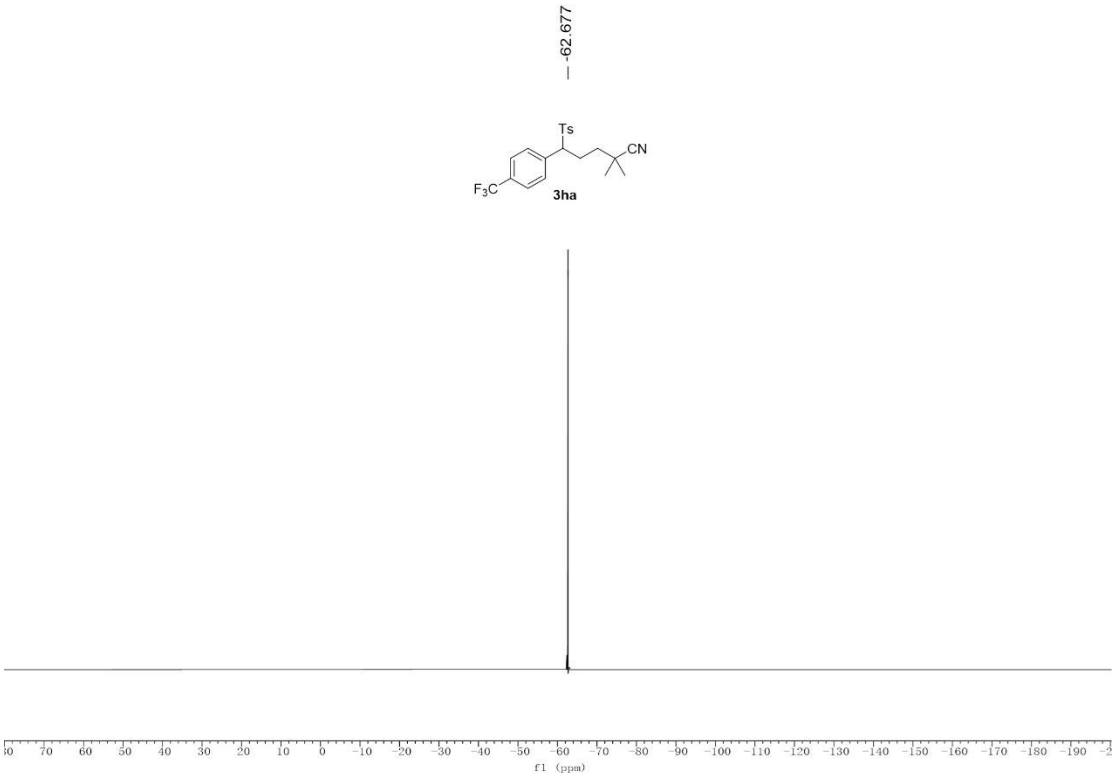
3.05
f1 (ppm)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F3C
3ha
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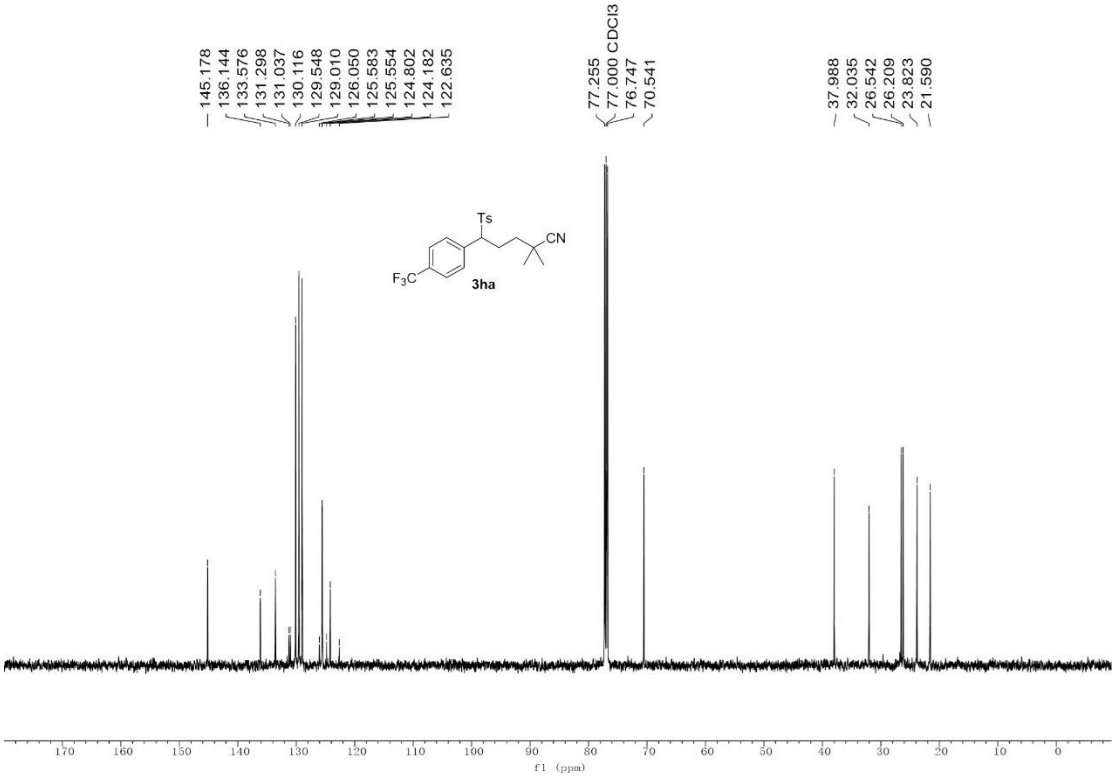
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122.635
77.255
77.000 CDCl3
76.747
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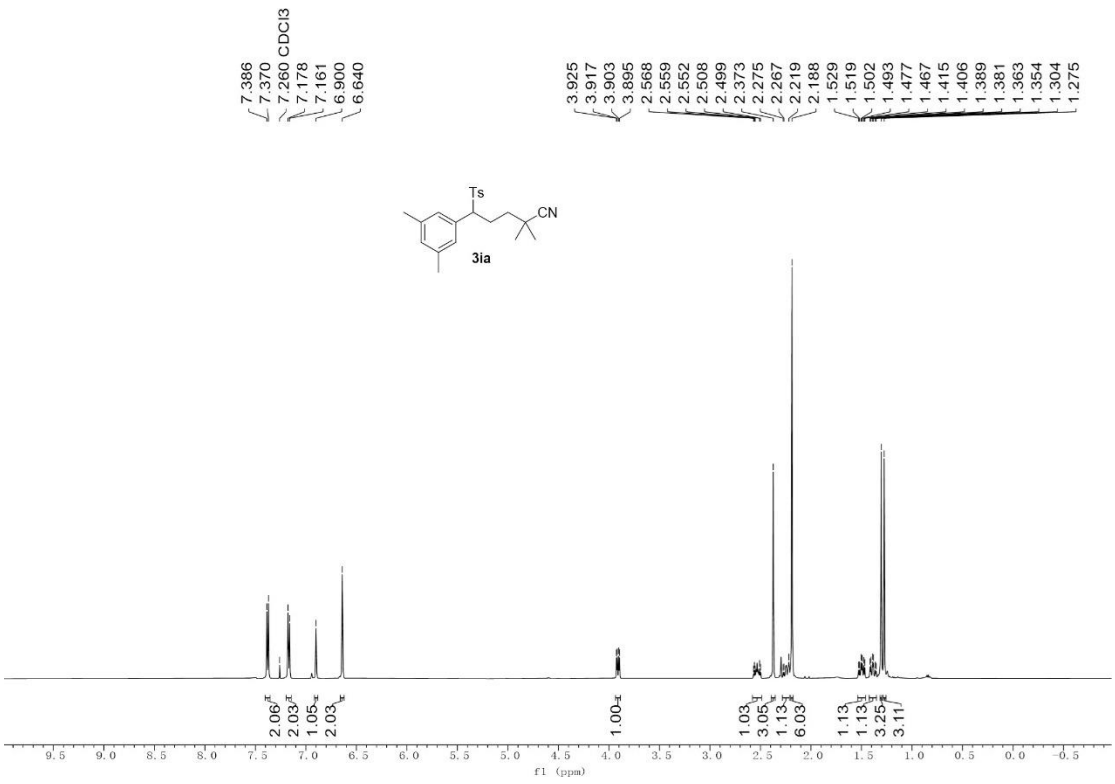
Ts
CN
F3C
3ha
f1 (ppm)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3.903
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2.559
2.552
2.508
2.499
2.373
2.275
2.267
2.219
2.188
1.529
1.519
1.502
1.493
1.477
1.467
1.415
1.406
1.389
1.381
1.363
1.354
1.304
1.275
Ts
CN
3ia
2.06
2.03
1.05
2.03
1.00
1.03
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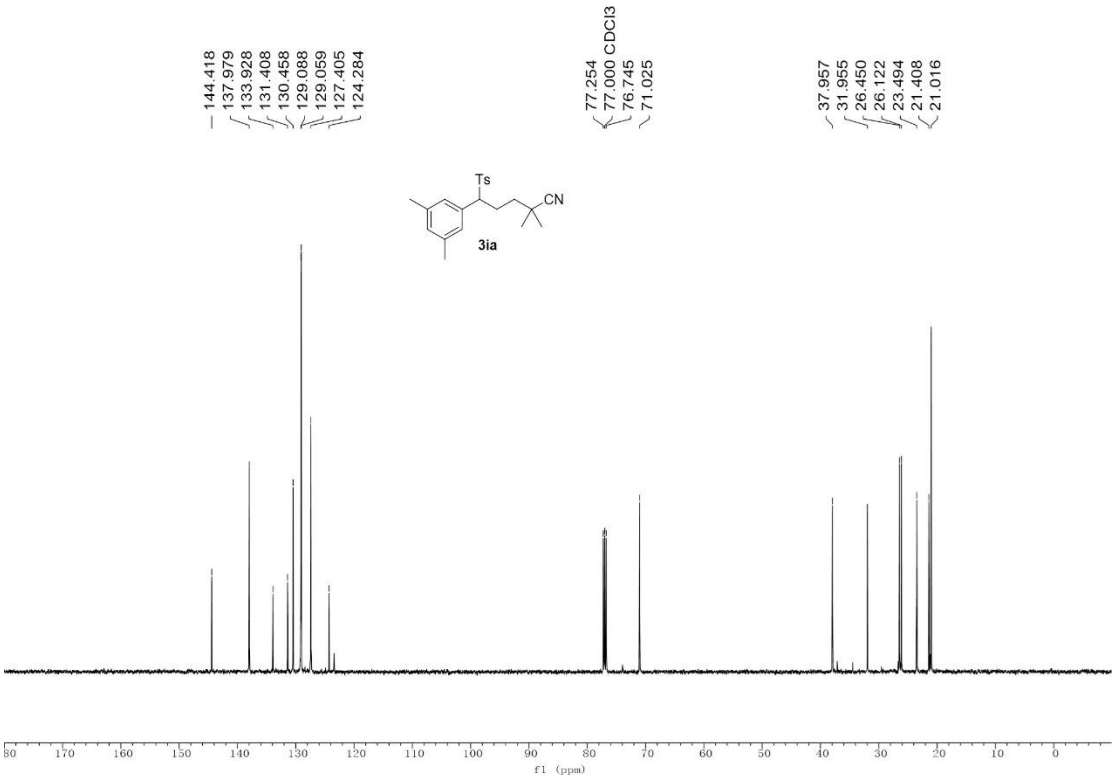
1.13
6.03
1.13
1.13
3.25
3.11
f1 (ppm)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127.405
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77.254
77.000 CDCl3
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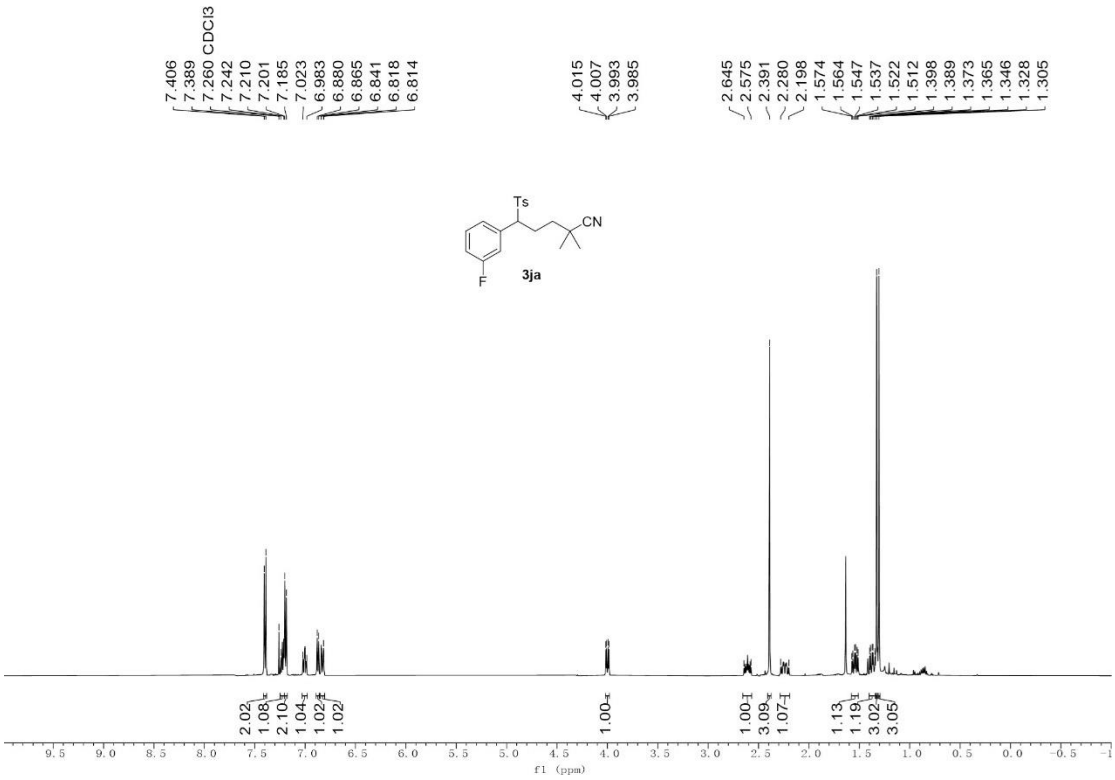
21.016
Ts
CN
3ia
f1 (ppm)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6.814
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4.007
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3.985
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2.575
2.391
2.280
2.198
1.574
1.564
1.547
1.537
1.522
1.512
1.398
1.389
1.373
1.365
1.346
1.328
1.305
Ts
CN
F
3ja
2.02
1.08
2.10
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1.00
1.00
3.09
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1.13
1.19
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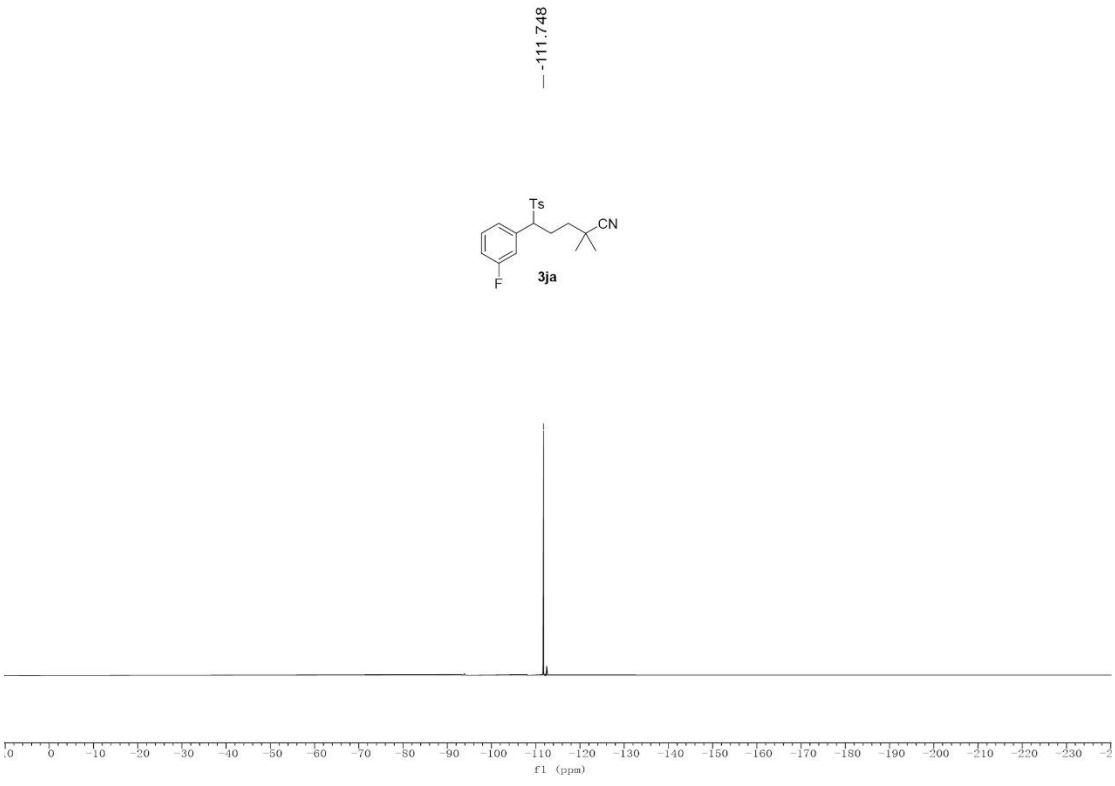
3.05
f1 (ppm)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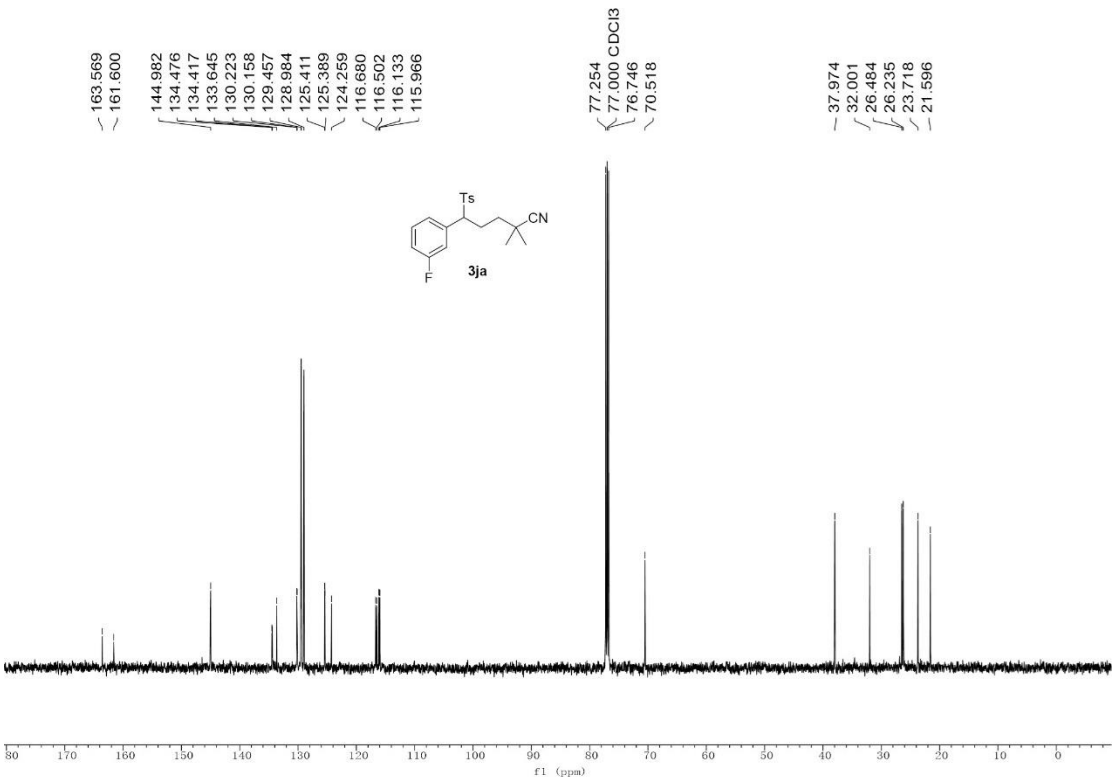
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125.389
124.259
116.680
116.502
116.133
115.966
77.254
77.000 CDCl3
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21.596
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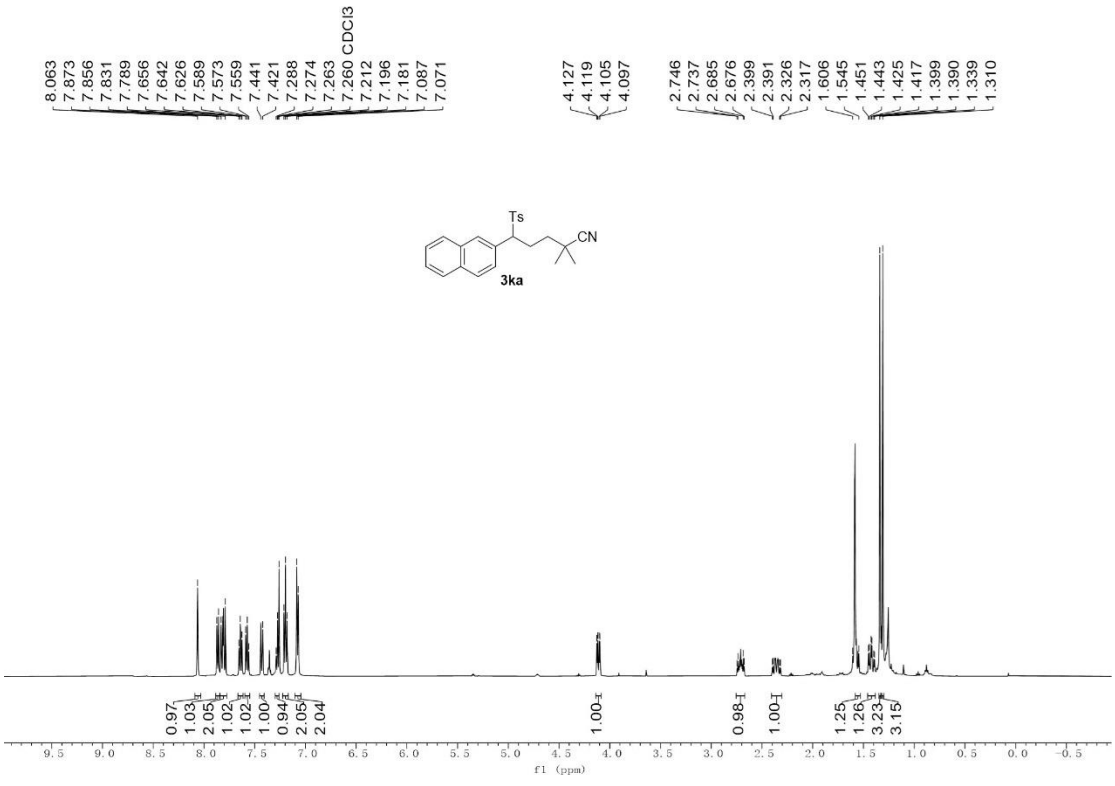
CN
F
3ja
f1 (ppm)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7.421
7.288
7.274
7.263
7.260 CDCl3
7.212
7.196
7.181
7.087
7.071
4.127
4.119
4.105
4.097
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1.425
1.417
1.399
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1.310
Ts
CN
3ka
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2.05
1.02
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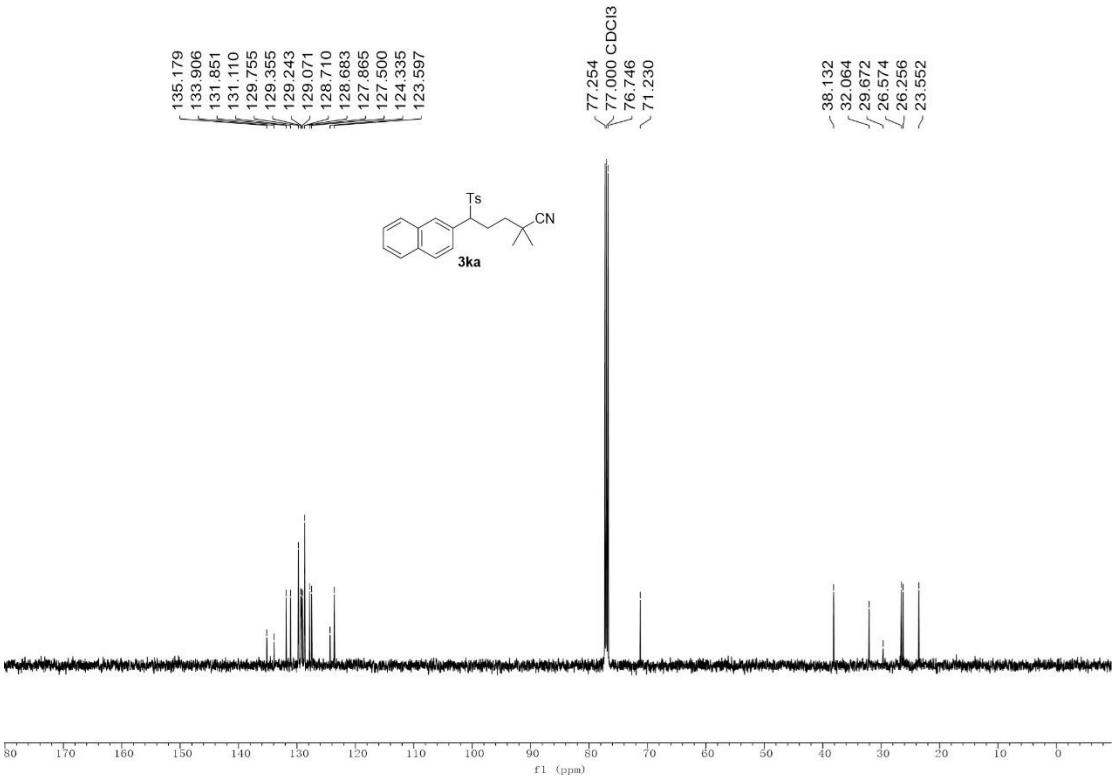
3.15
f1 (ppm)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123.597
77.254
77.000 CDCl3
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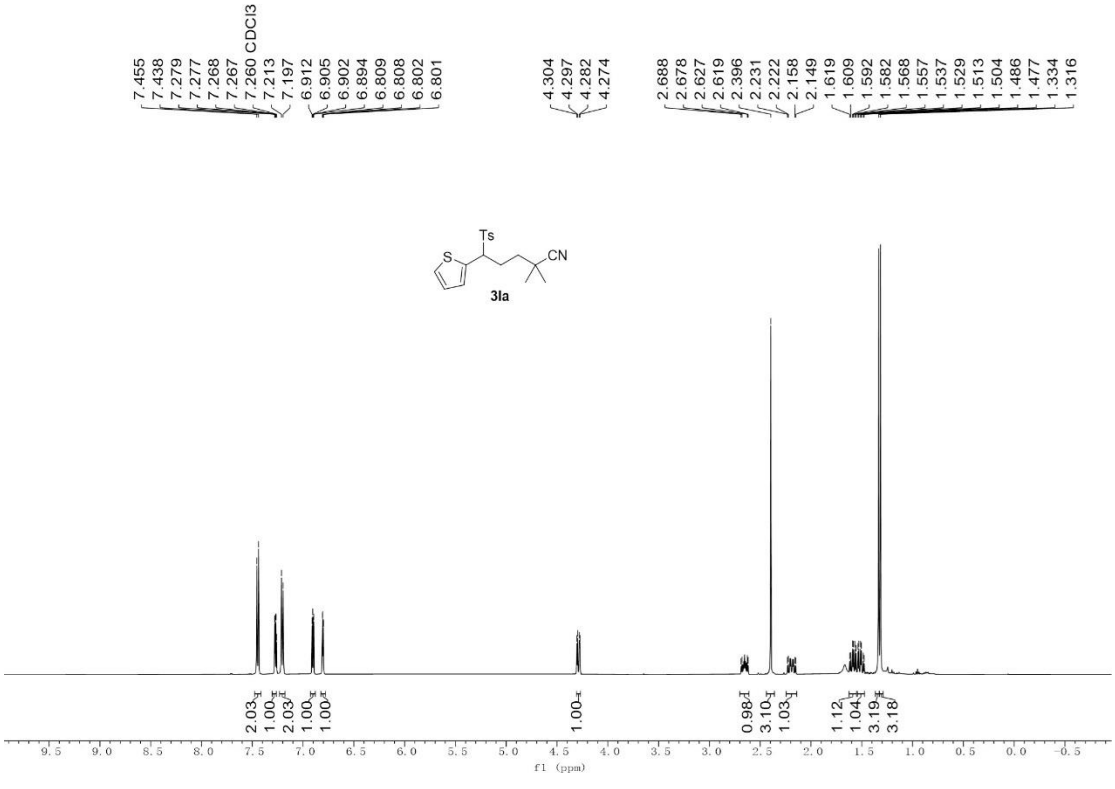
f1 (ppm)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6.802
6.801
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4.297
4.282
4.274
2.688
2.678
2.627
2.619
2.396
2.231
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2.158
2.149
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1.609
1.592
1.582
1.568
1.557
1.537
1.529
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1.504
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Ts
S
CN
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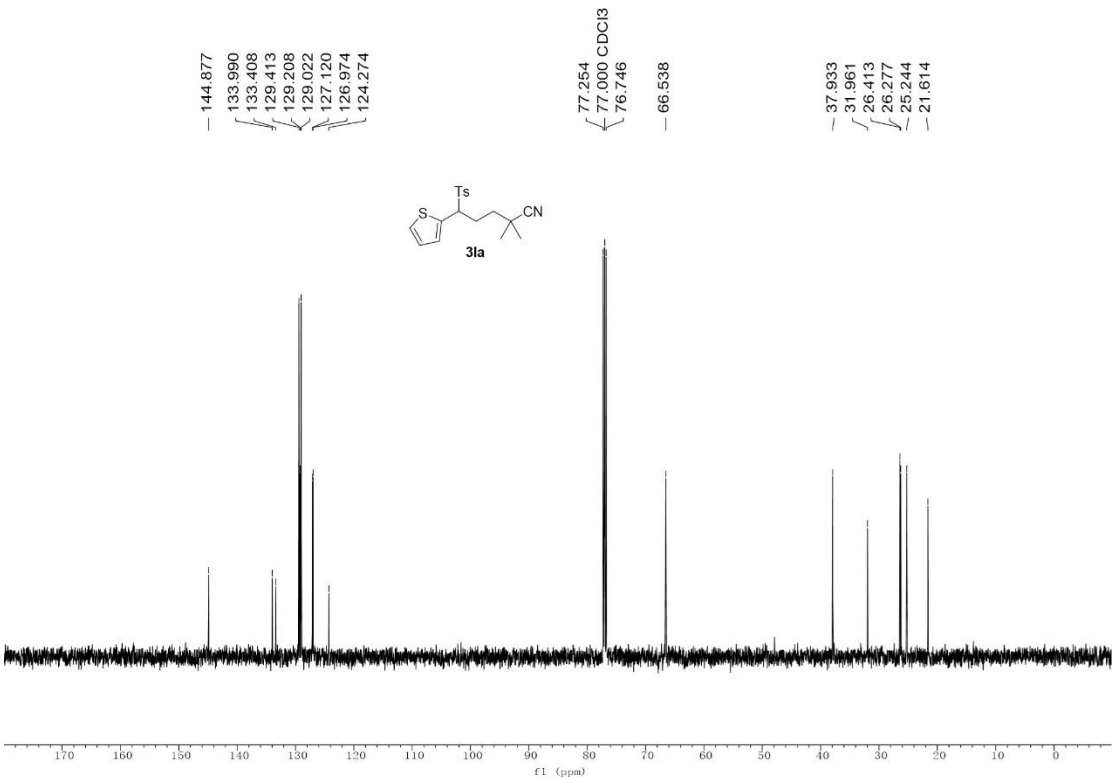
f1 (ppm)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77.000 CDCl3
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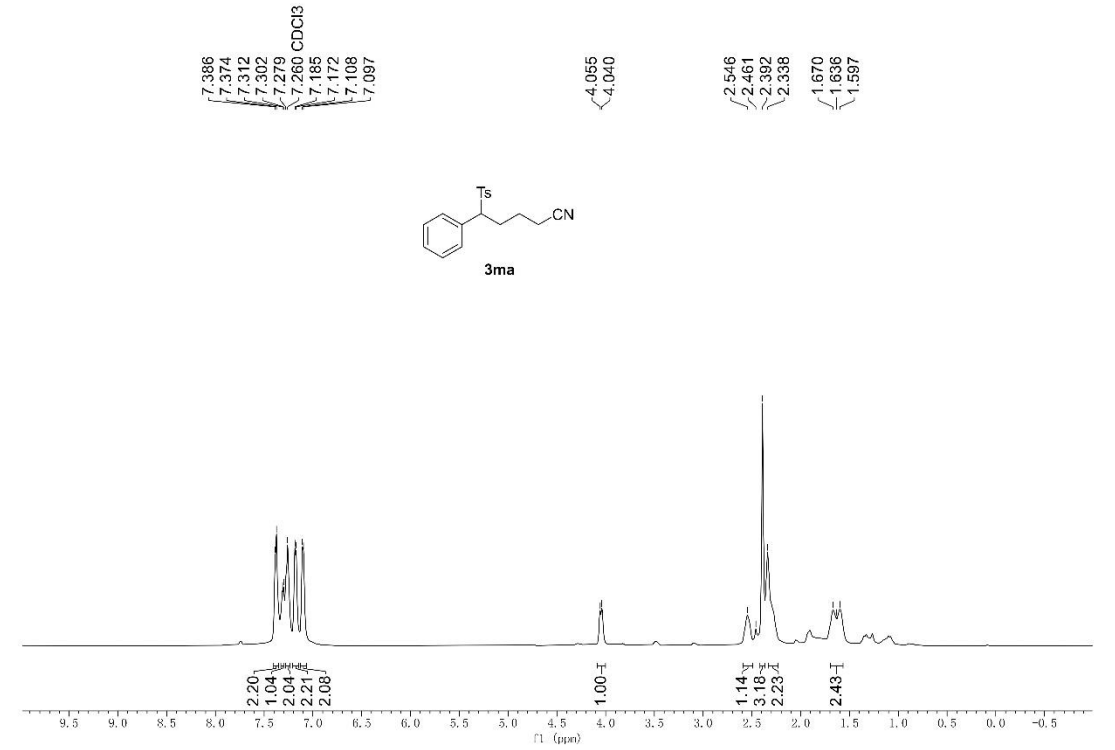
25.244
21.614
Ts
S
CN
3la
f1 (ppm)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2.461
2.392
2.338
1.670
1.636
1.597
Ts
CN
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2.08
1.00
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3.18
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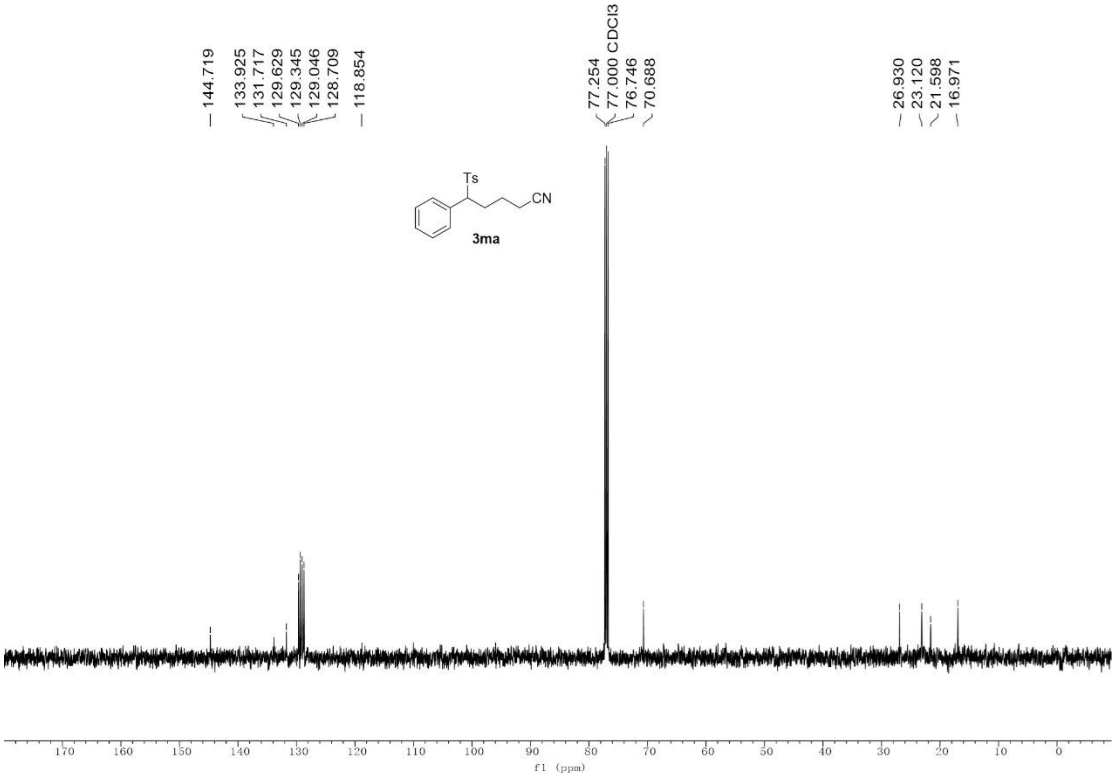
2.43
f1 (ppm)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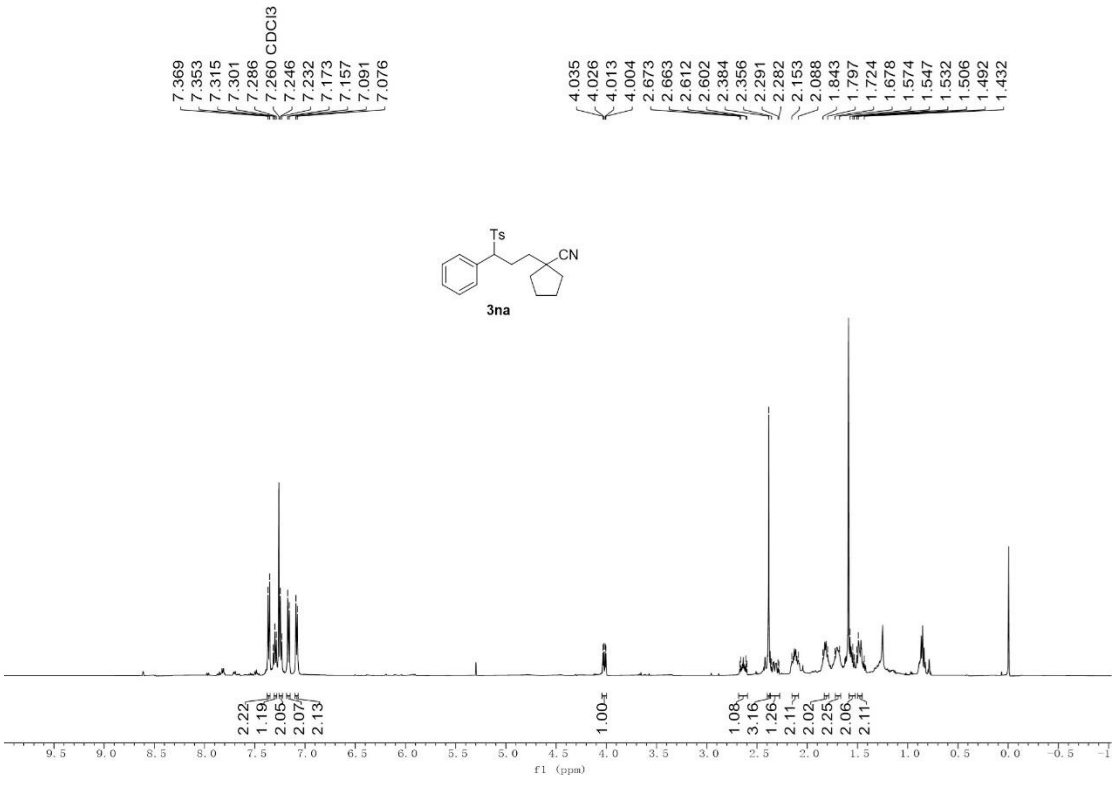
Ts
CN
3ma
f1 (ppm)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1.492
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Ts
CN
3na
2.22
1.19
2.05
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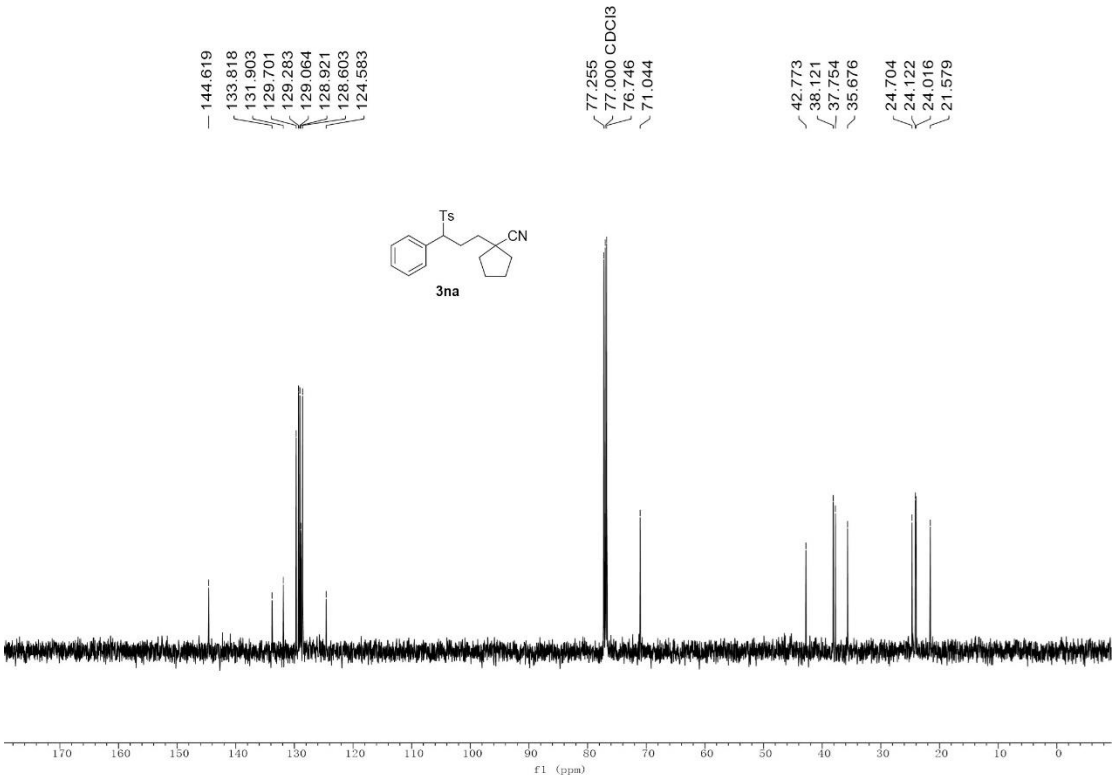
2.11
f1 (ppm)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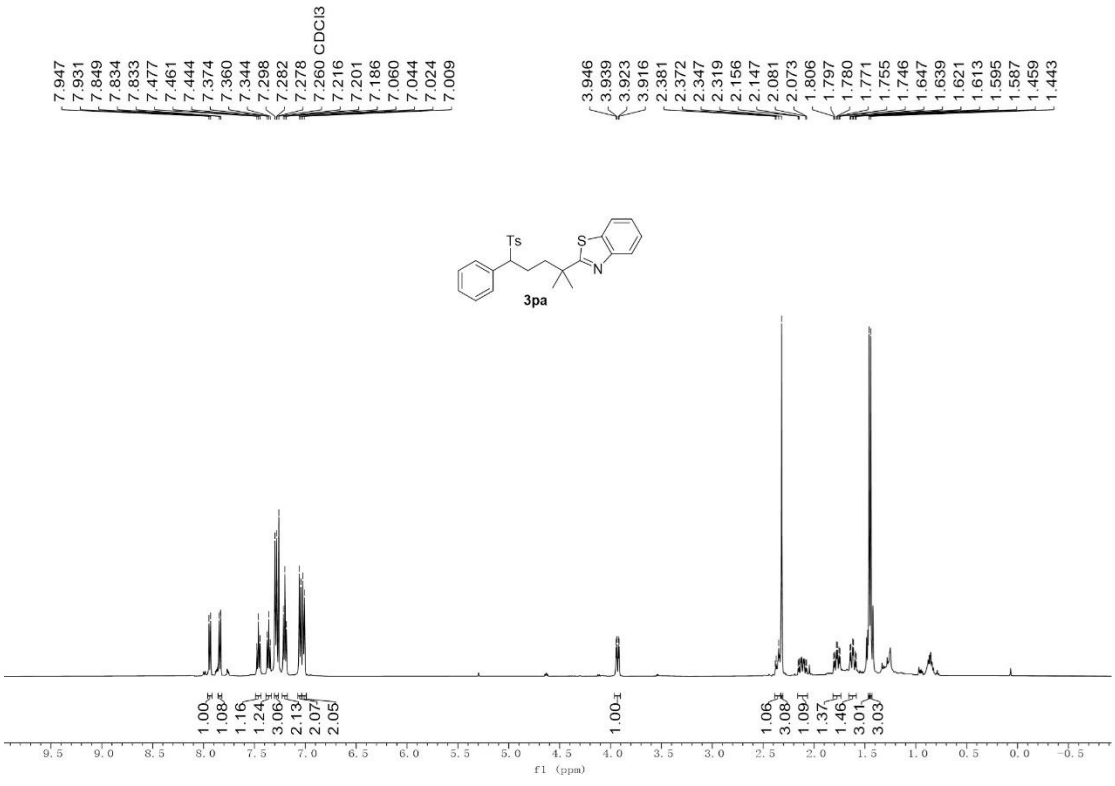
71.044
42.773
38.121
37.754
35.676
24.704
24.122
24.016
21.579
Ts
CN
3na
f1 (ppm)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7.477
7.461
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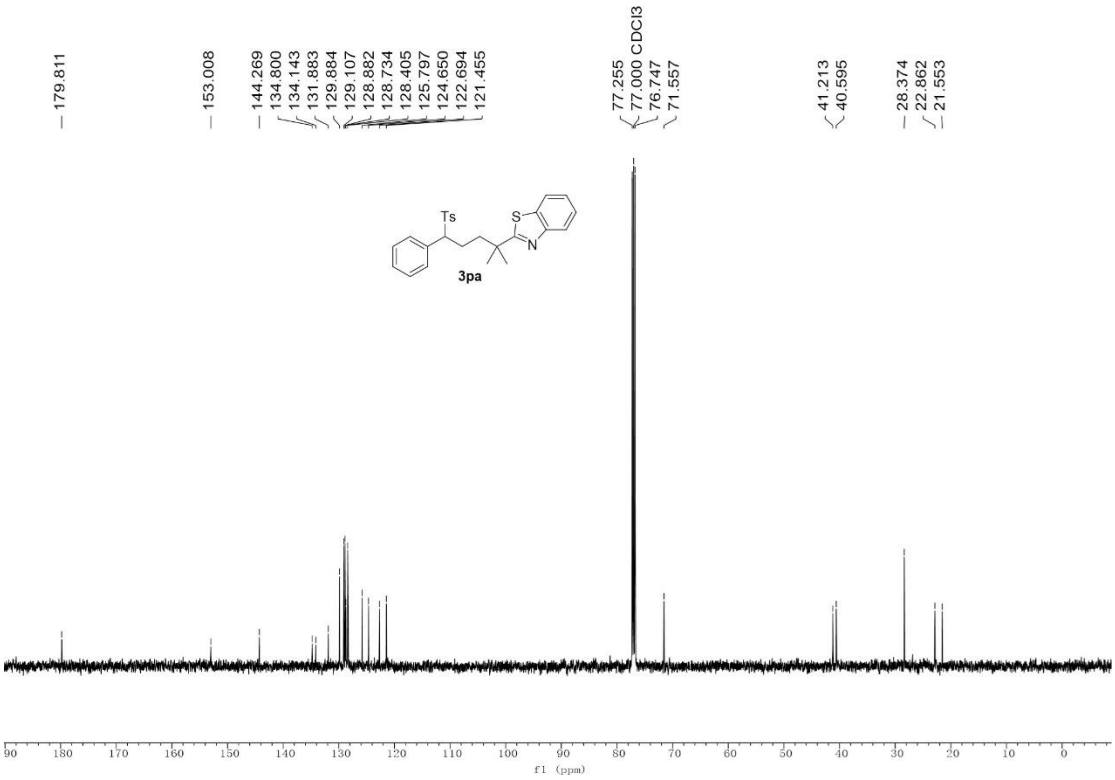
7.374
7.360
7.344
7.298
7.282
7.278
7.260 CDCl3
7.216
7.201
7.186
7.060
7.044
7.024
7.009
3.946
3.939
3.923
3.916
2.381
2.372
2.347
2.319
2.156
2.147
2.081
2.073
1.806
1.797
1.780
1.771
1.755
1.746
1.647
1.639
1.621
1.613
1.595
1.587
1.459
1.443
Ts
S
N
3pa
1.00
1.08
1.16
1.24
3.06
2.13
2.07
2.05
1.00
1.06
3.08
1.09
1.37
1.46
3.01
3.03
f1 (ppm)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129.107
128.882
128.734
128.405
125.797
124.650
122.694
121.455
77.255
77.000 CDCl3
76.747
71.557
41.213
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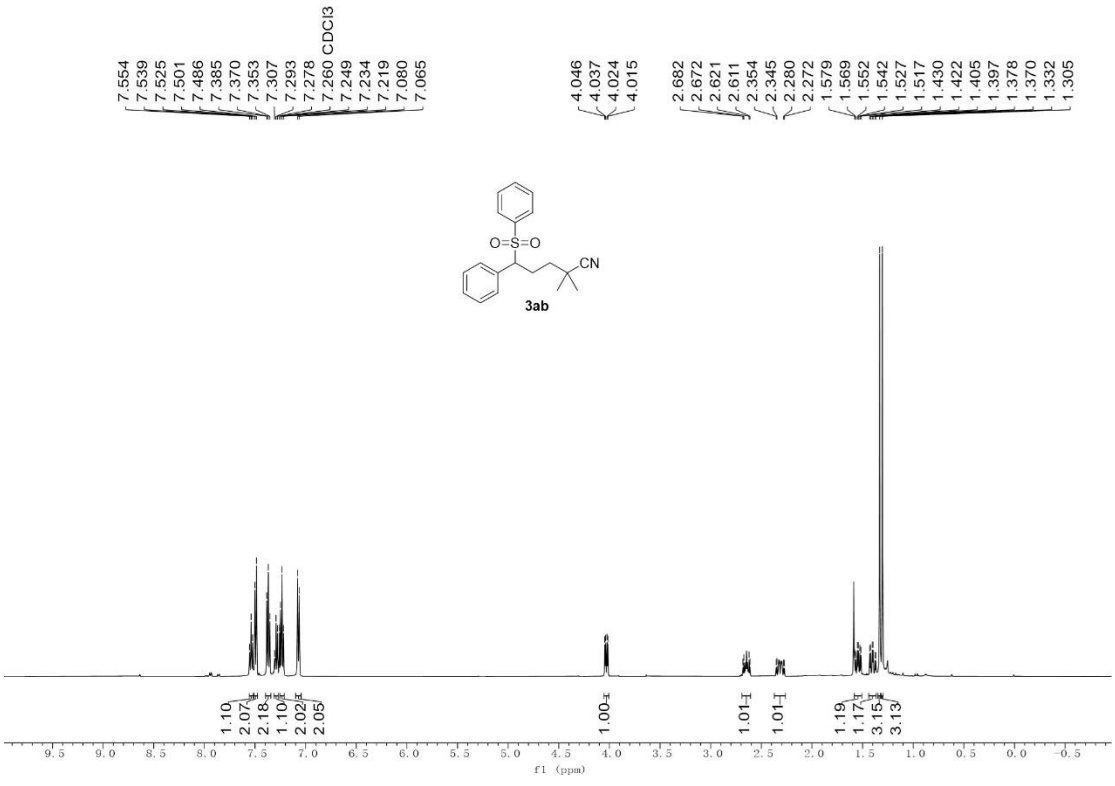
22.862
21.553
Ts
S
N
3pa
f1 (ppm)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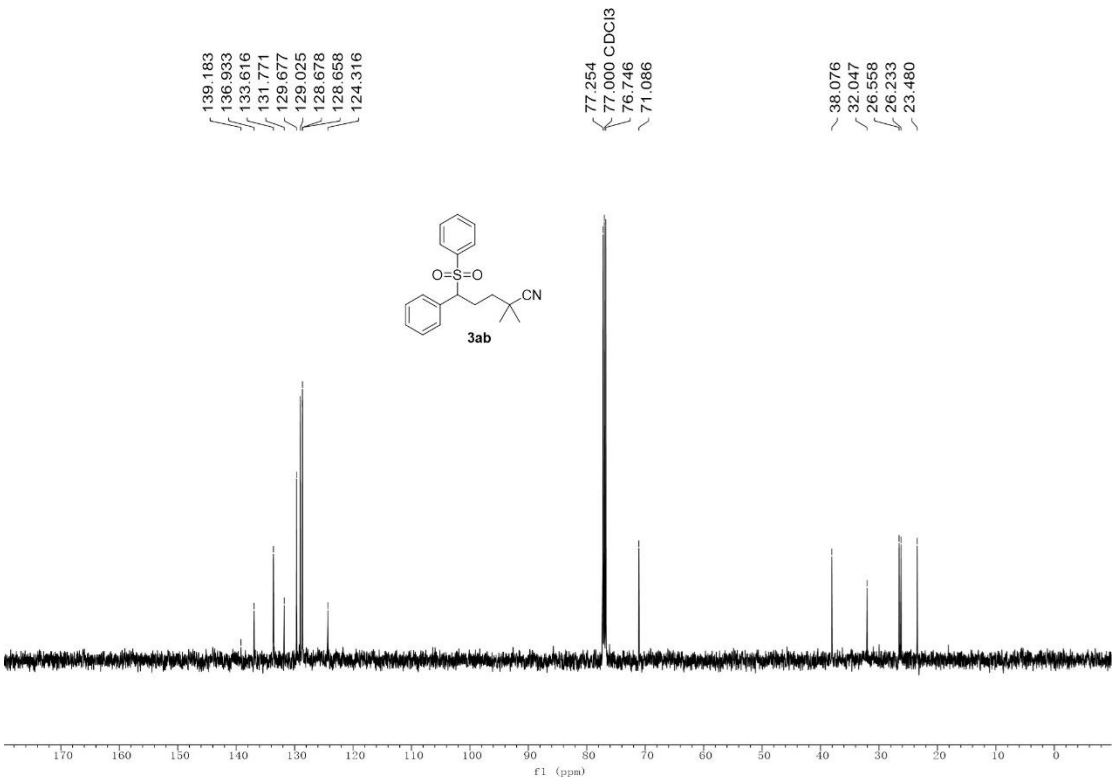
7.385
7.370
7.353
7.307
7.293
7.278
7.260 CDCl3
7.249
7.234
7.219
7.080
7.065
4.046
4.037
4.024
4.015
2.682
2.672
2.621
2.611
2.354
2.345
2.280
2.272
1.579
1.569
1.552
1.542
1.527
1.517
1.430
1.422
1.405
1.397
1.378
1.370
1.332
1.305
O=S=O
CN
3ab
1.10
2.07
2.18
1.10
2.02
2.05
1.00
1.01
1.01
1.19
1.17
3.15
3.13
f1 (ppm)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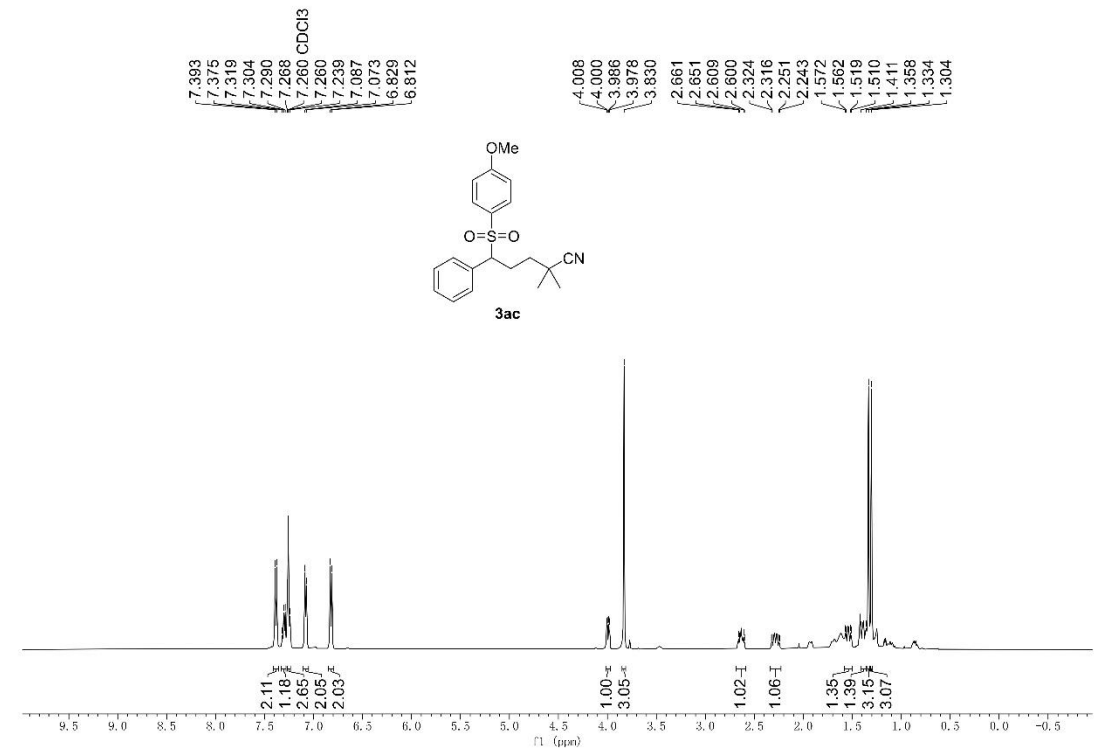
136.933
133.616
131.771
129.677
129.025
128.678
128.658
124.316
77.254
77.000 CDCl3
76.746
71.086
38.076
32.047
26.558
26.233
23.480
O=S=O
CN
3ab
f1 (ppm)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7.319
7.304
7.290
7.268
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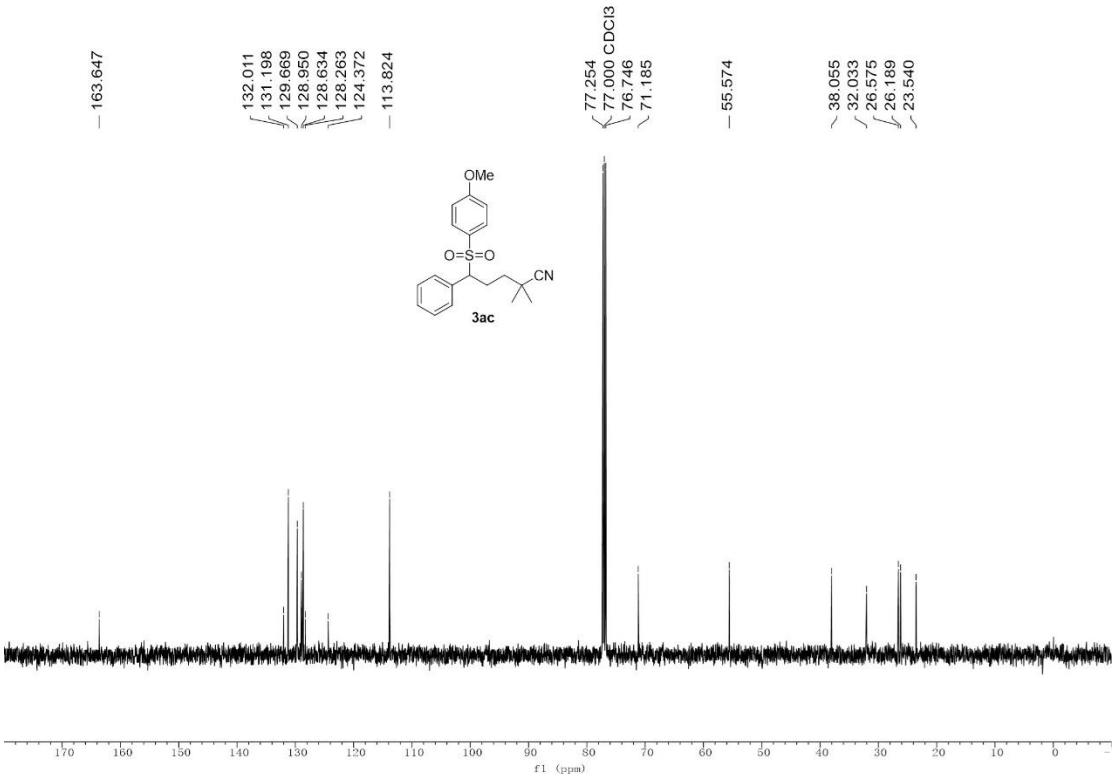
7.260
7.239
7.087
7.073
6.829
6.812
4.008
4.000
3.986
3.978
3.830
2.661
2.651
2.609
2.600
2.324
2.316
2.251
2.243
1.572
1.562
1.519
1.510
1.411
1.358
1.334
1.304
OMe
O=S=O
CN
3ac
2.11
1.18
2.65
2.05
2.03
1.00
3.05
1.02
1.06
1.35
1.39
3.15
3.07
f1 (ppm)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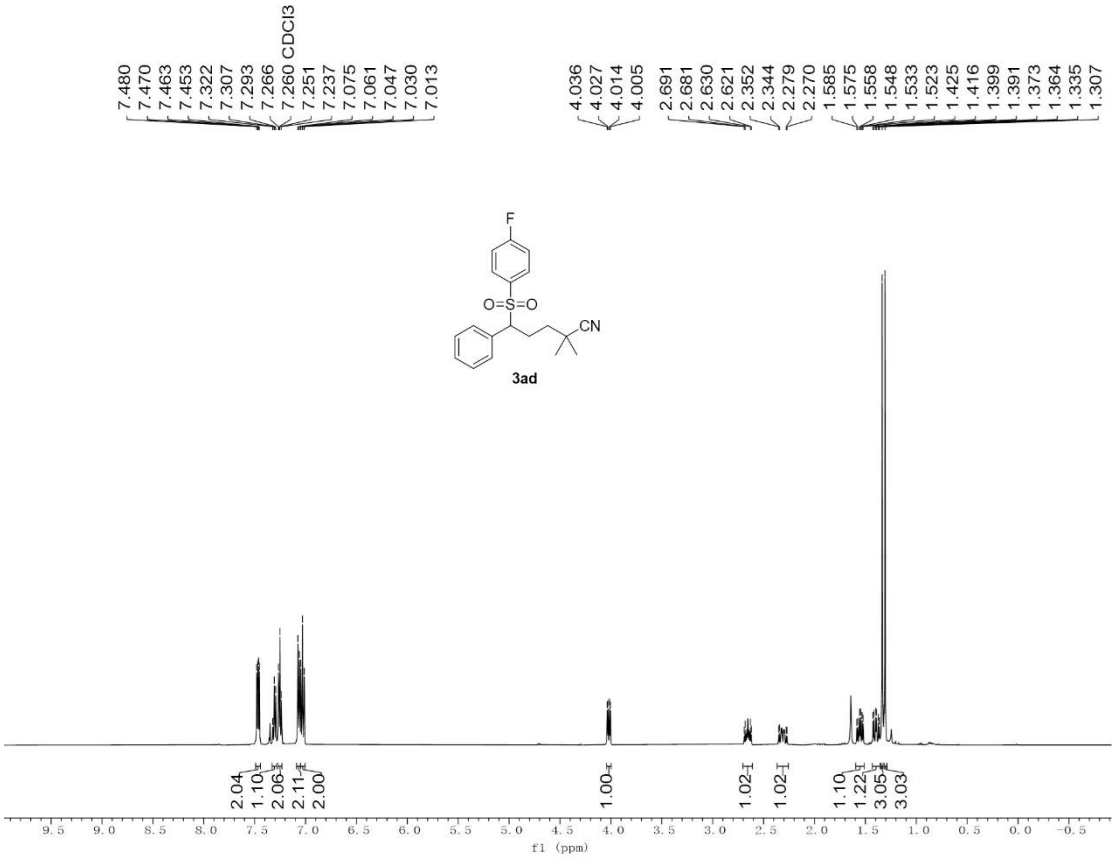
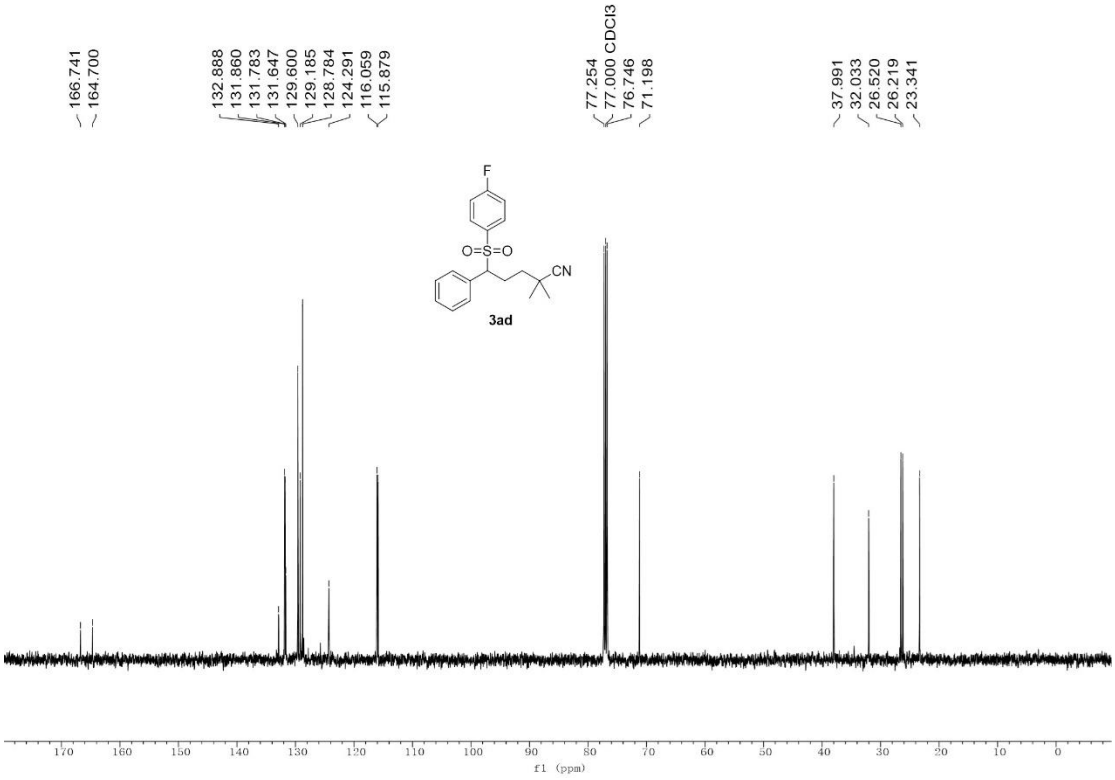
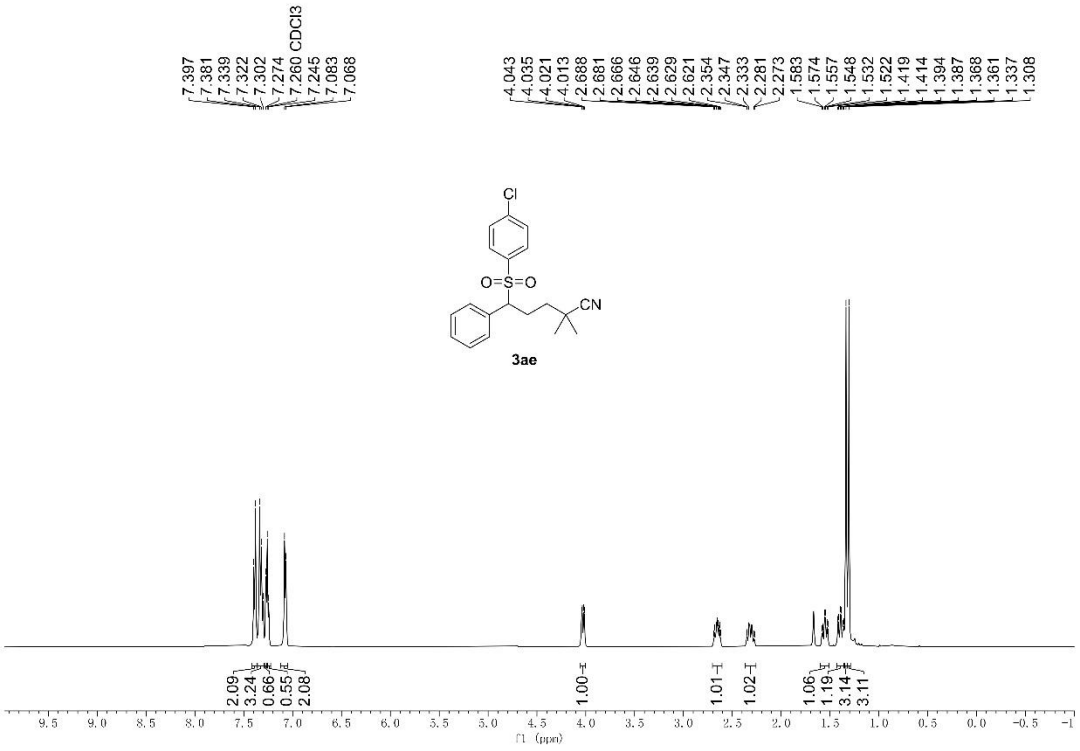
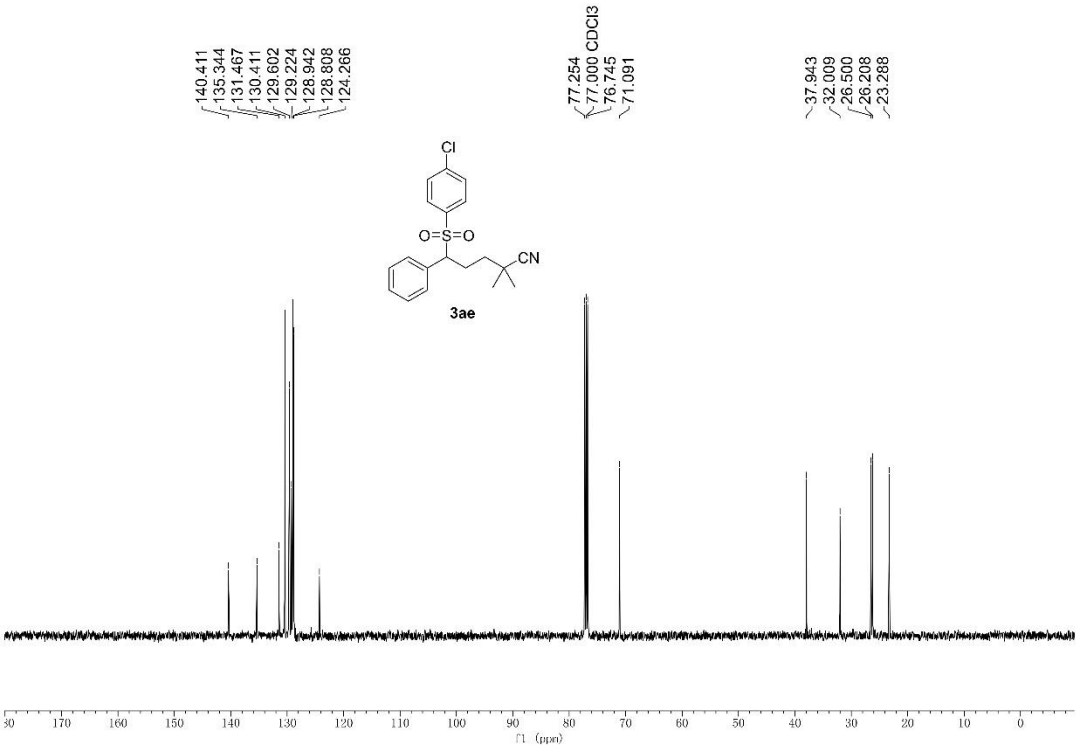
132.011
131.198
129.669
128.950
128.634
128.263
124.372
113.824
77.254
77.000 CDCl3
76.746
71.185
55.574
38.055
32.033
26.575
26.189
23.540
OMe
O=S=O
CN
3ac
f1 (ppm)

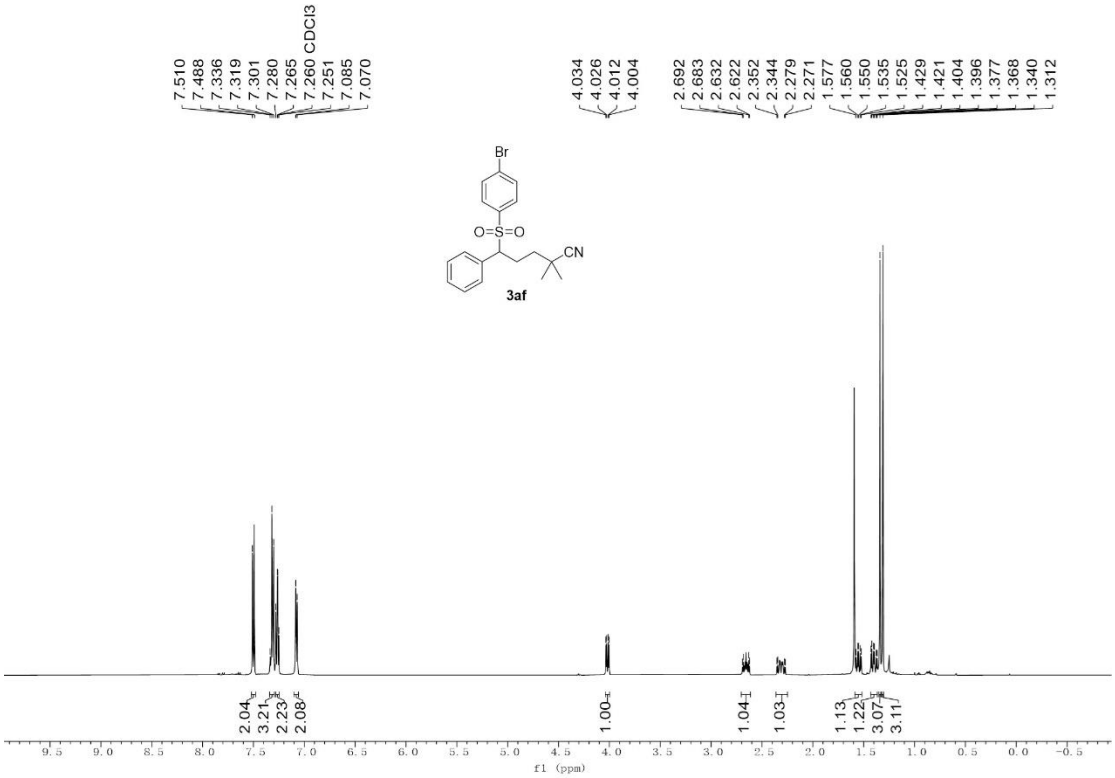

7.480
7.470
7.463
7.453
7.322
7.307
7.293
7.266
7.260 CDCl3
7.251
7.237
7.075
7.061
7.047
7.030
7.013
4.036
4.027
4.014
4.005
2.691
2.681
2.630
2.621
2.352
2.344
2.279
2.270
1.585
1.575
1.558
1.548
1.533
1.523
1.425
1.416
1.399
1.391
1.373
1.364
1.335
1.307
F
O=S=O
CN
3ad
2.04
1.10
2.06
2.11
2.00
1.00
1.02
1.02
1.10
1.22
3.05
3.03
f1 (ppm)

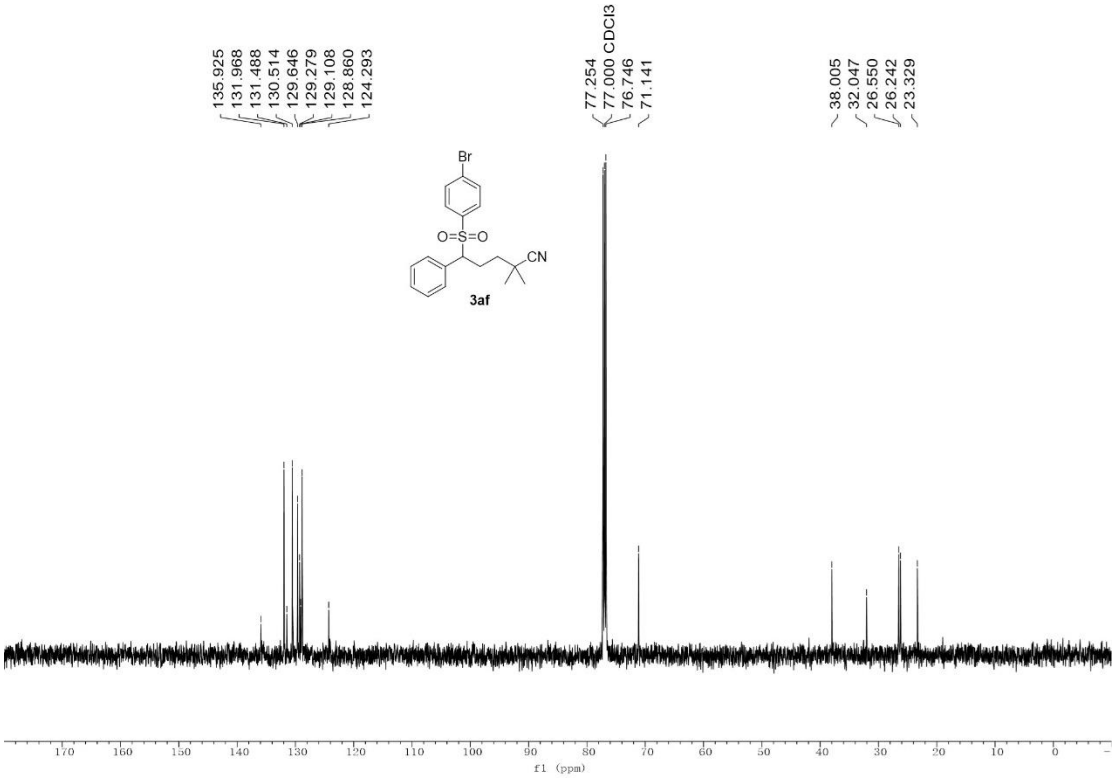

-103.152
F
O=S=O
CN
3ad
f1 (ppm)


166.741
164.700
132.888
131.860
131.783
131.647
129.600
129.185
128.784
124.291
116.059
115.879
77.254
77.000 CDCl3
76.746
71.198
37.991
32.033
26.520
26.219
23.341
F
O=S=O
CN
3ad
f1 (ppm)


7.397
7.381
7.339
7.322
7.302
7.274
7.260 CDCl3
7.245
7.083
7.068
4.043
4.035
4.021
4.013
2.688
2.681
2.666
2.646
2.639
2.629
2.621
2.354
2.347
2.333
2.281
2.273
1.583
1.574
1.557
1.548
1.532
1.522
1.419
1.414
1.394
1.387
1.368
1.361
1.337
1.308
Cl
O=S=O
CN
3ae
2.09
3.24
0.66
0.55
2.08
1.00
1.01
1.02
1.06
1.19
3.14
3.11
f1 (ppm)


140.411
135.344
131.467
130.411
129.602
129.224
128.942
128.808
124.266
77.254
77.000 CDCl3
76.745
71.091
37.943
32.009
26.500
26.208
23.288
Cl
O=S=O
CN
3ae
f1 (ppm)


7.510
7.488
7.336
7.319
7.301
7.280
7.265
7.260 CDCl3
7.251
7.085
7.070
4.034
4.026
4.012
4.004
2.692
2.683
2.632
2.622
2.352
2.344
2.279
2.271
1.577
1.560
1.550
1.535
1.525
1.429
1.421
1.404
1.396
1.377
1.368
1.340
1.312
Br
O=S=O
CN
3af
2.04
3.21
2.23
2.08
1.00
1.04
1.03
1.13
1.22
3.07
3.11
f1 (ppm)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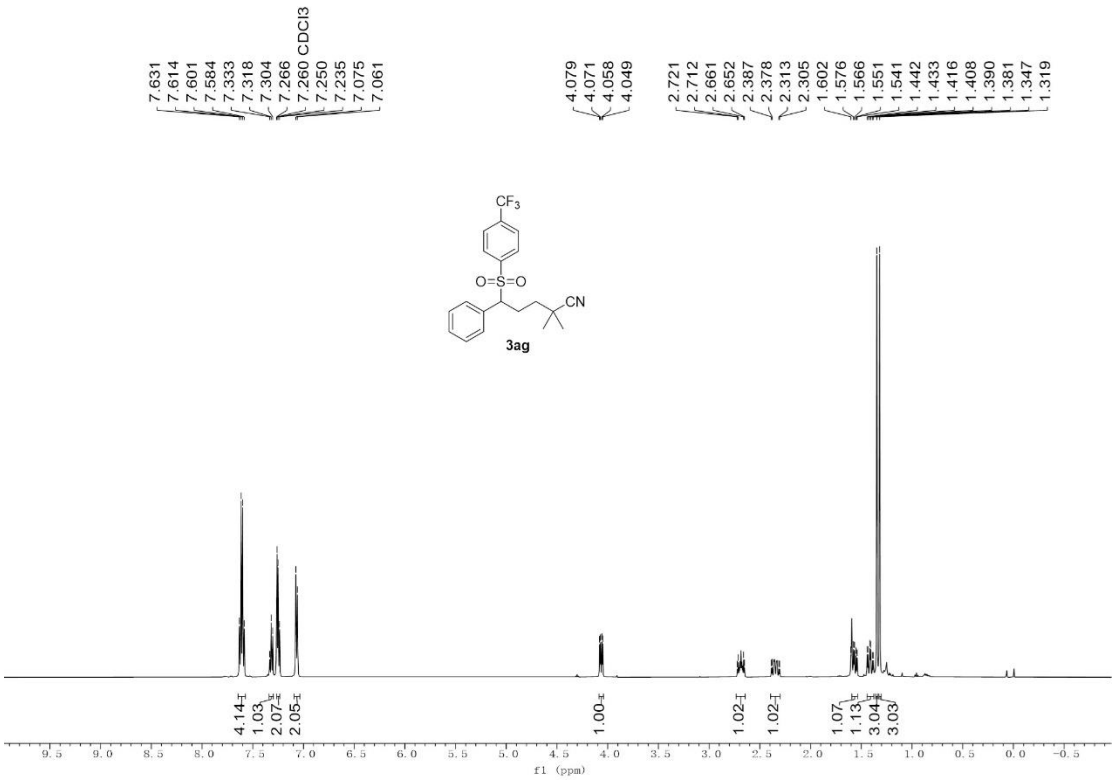
131.488
130.514
129.646
129.279
129.108
128.860
124.293
77.254
77.000 CDCl3
76.746
71.141
38.005
32.047
26.550
26.242
23.329
Br
O=S=O
CN
3af
f1 (ppm)


7.631
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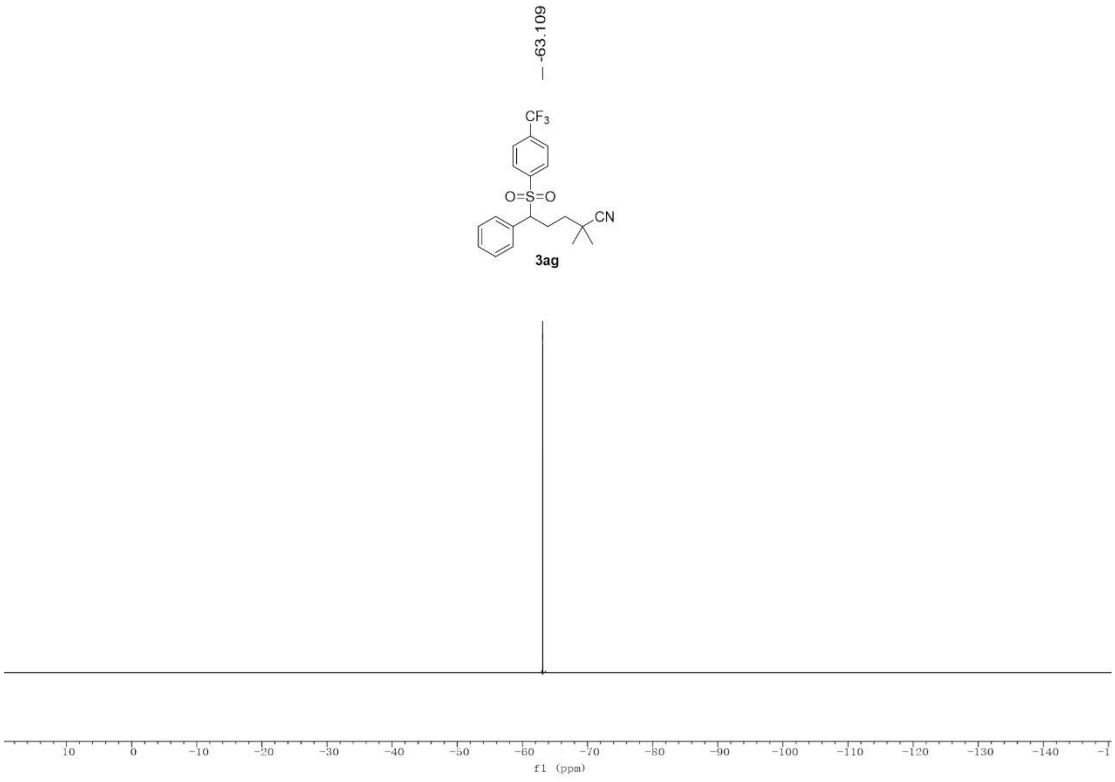
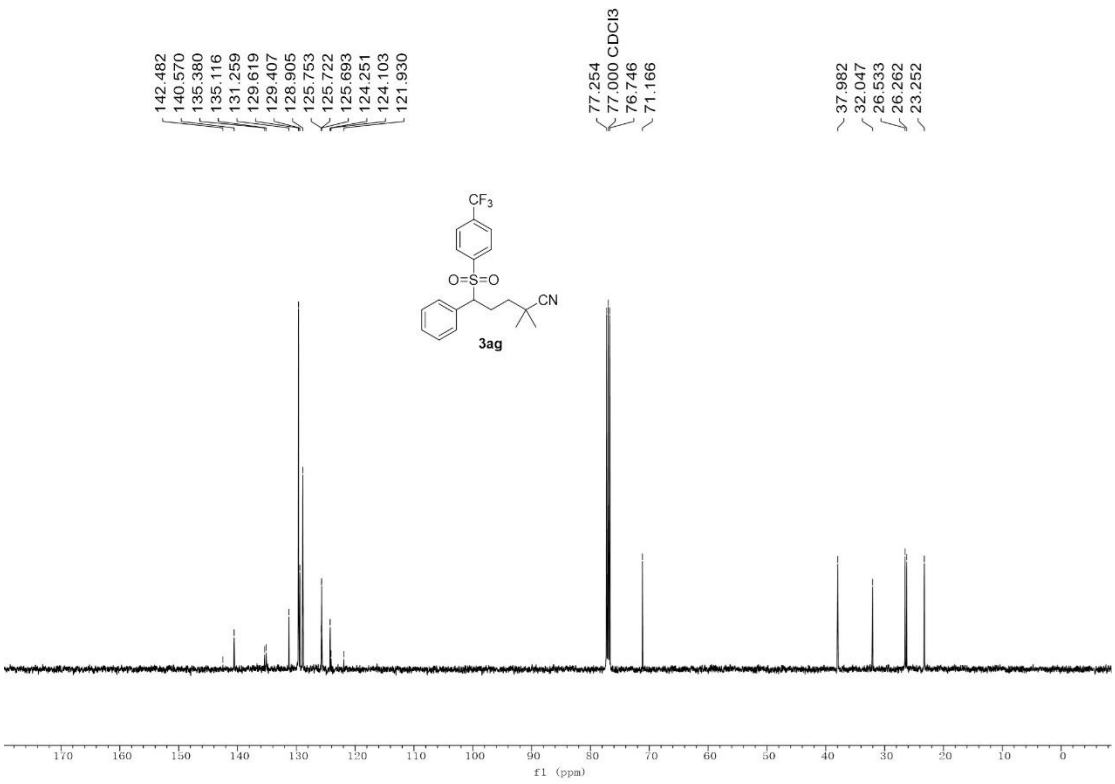
7.601
7.584
7.333
7.318
7.304
7.266
7.260 CDCl3
7.250
7.235
7.075
7.061
4.079
4.071
4.058
4.049
2.721
2.712
2.661
2.652
2.387
2.378
2.313
2.305
1.602
1.576
1.566
1.551
1.541
1.442
1.433
1.416
1.408
1.390
1.381
1.347
1.319
CF3
O=S=O
CN
3ag
4.14
1.03
2.07
2.05
1.00
1.02
1.02
1.07
1.13
3.04
3.03
f1 (ppm)


-63.109
CF3
O=S=O
CN
3ag
f1 (ppm)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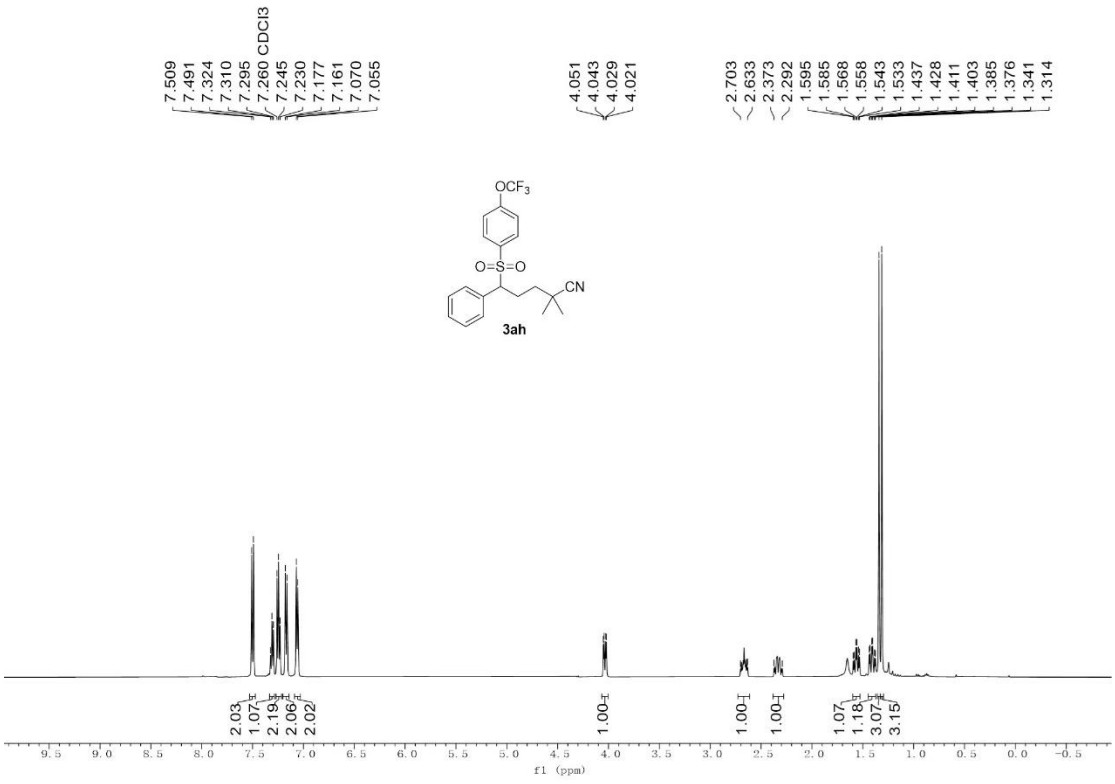
135.116
131.259
129.619
129.407
128.905
125.753
125.722
125.693
124.251
124.103
121.930
77.254
77.000 CDCl3
76.746
71.166
37.982
32.047
26.533
26.262
23.252
CF3
O=S=O
CN
3ag
f1 (ppm)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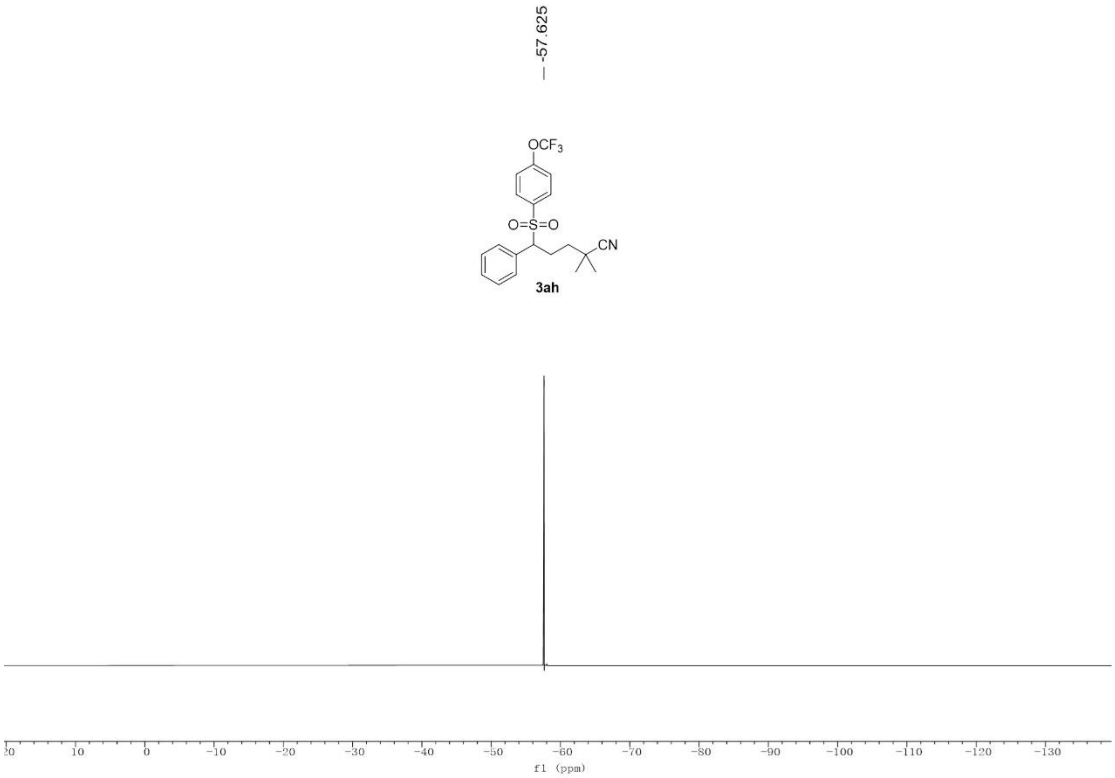
7.310
7.295
7.260 CDCl3
7.245
7.230
7.177
7.161
7.070
7.055
4.051
4.043
4.029
4.021
2.703
2.633
2.373
2.292
1.595
1.585
1.568
1.558
1.543
1.533
1.437
1.428
1.411
1.403
1.385
1.376
1.341
1.314
OCF3
O=S=O
CN
3ah
2.03
1.07
2.19
2.06
2.02
1.00
1.00
1.00
1.07
1.18
3.07
3.15
f1 (ppm)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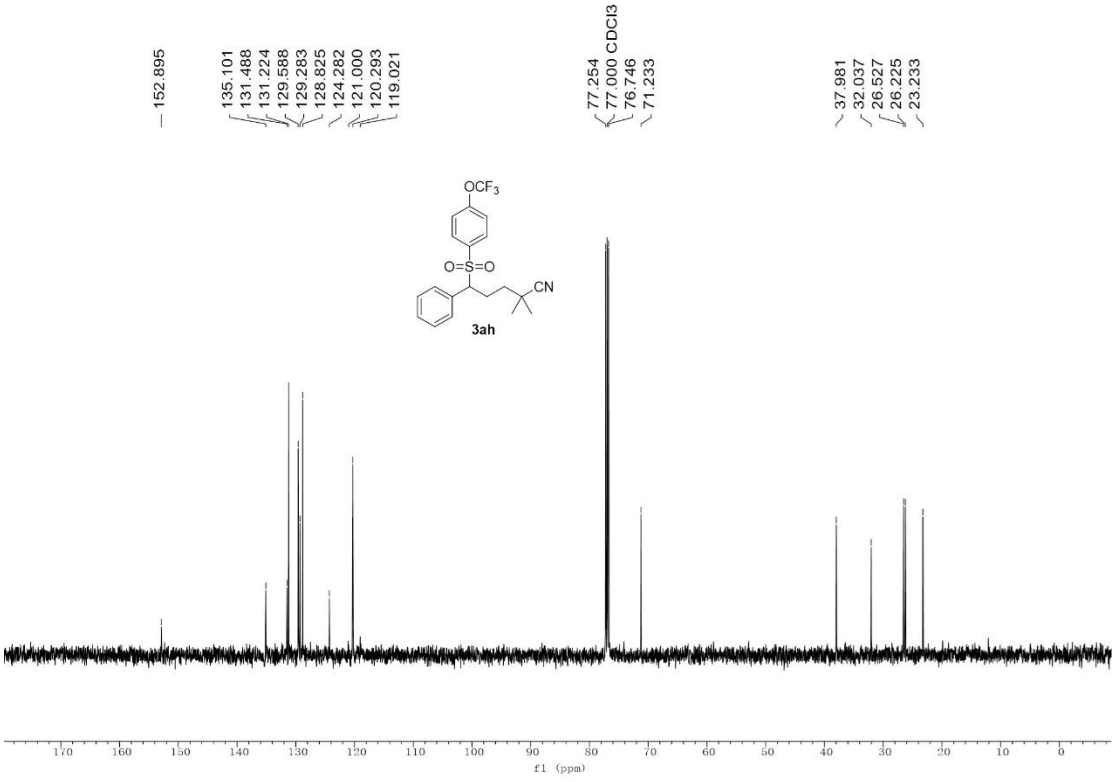
OCF3
O=S=O
CN
3ah
f1 (ppm)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131.224
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129.283
128.825
124.282
121.000
120.293
119.021
77.254
77.000 CDCl3
76.746
71.233
37.981
32.037
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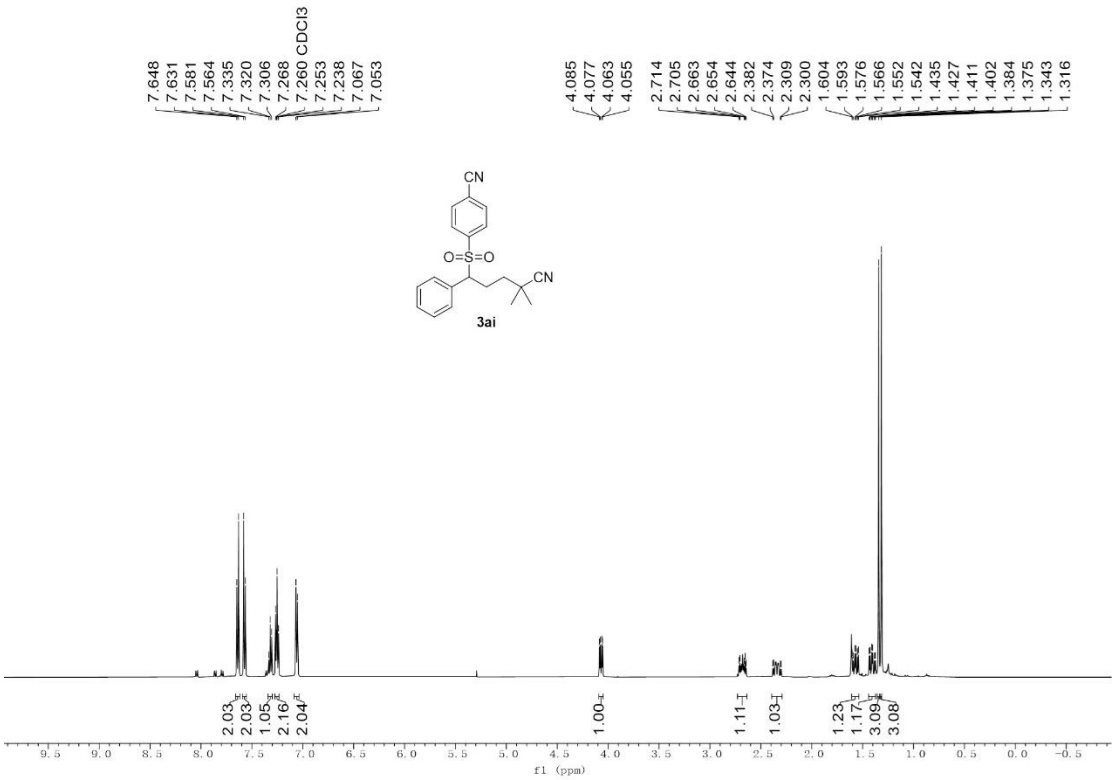
26.225
23.233
OCF3
O=S=O
CN
3ah
f1 (ppm)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7.564
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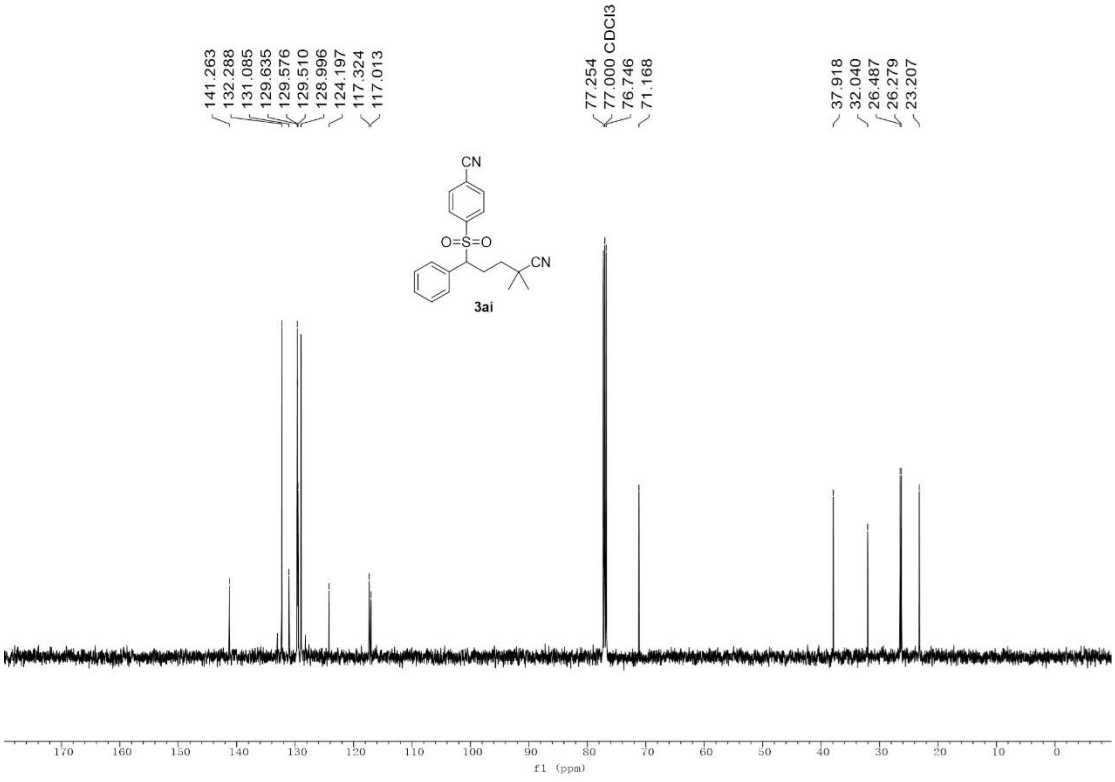
7.306
7.268 CDCl3
7.253
7.238
7.067
7.053
4.085
4.077
4.063
4.055
2.714
2.705
2.663
2.654
2.644
2.382
2.374
2.309
2.300
1.604
1.593
1.576
1.566
1.552
1.542
1.435
1.427
1.411
1.402
1.384
1.375
1.343
1.316
CN
O=S=O
CN
3ai
2.03
2.03
1.05
2.16
2.04
1.00
1.11
1.03
1.23
1.17
3.09
3.08
f1 (ppm)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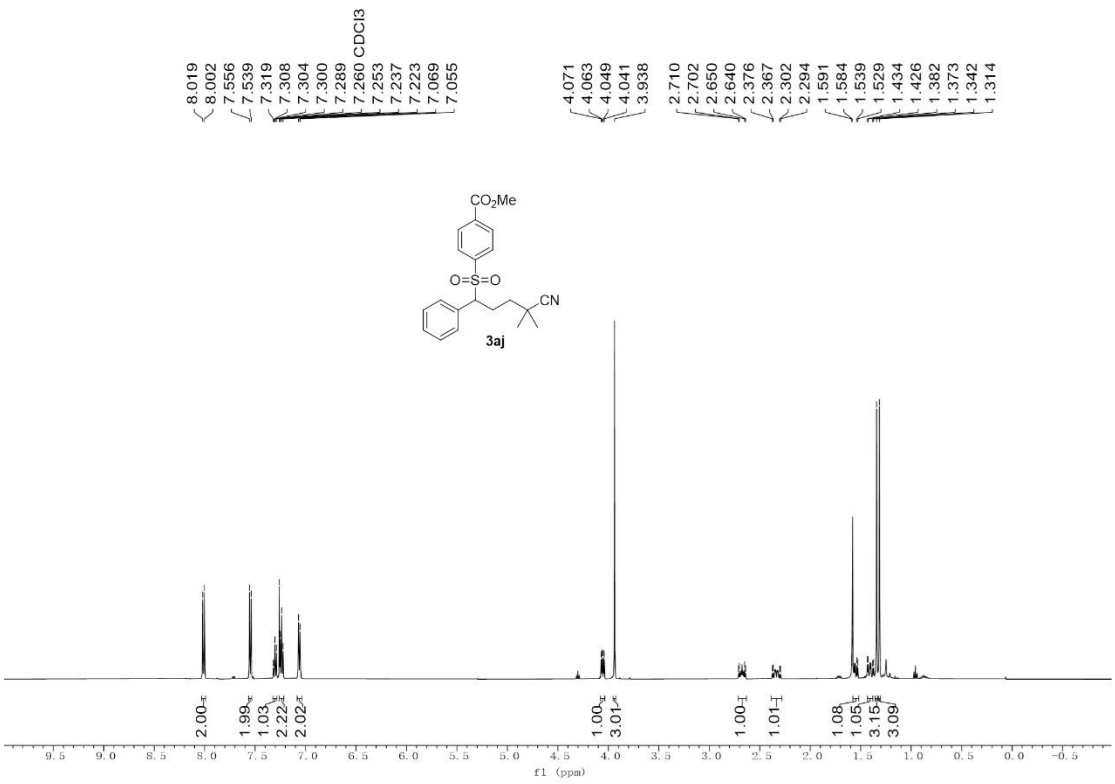
129.510
128.996
124.197
117.324
117.013
77.254
77.000 CDCl3
76.746
71.168
37.918
32.040
26.487
26.279
23.207
CN
O=S=O
CN
3ai
f1 (ppm)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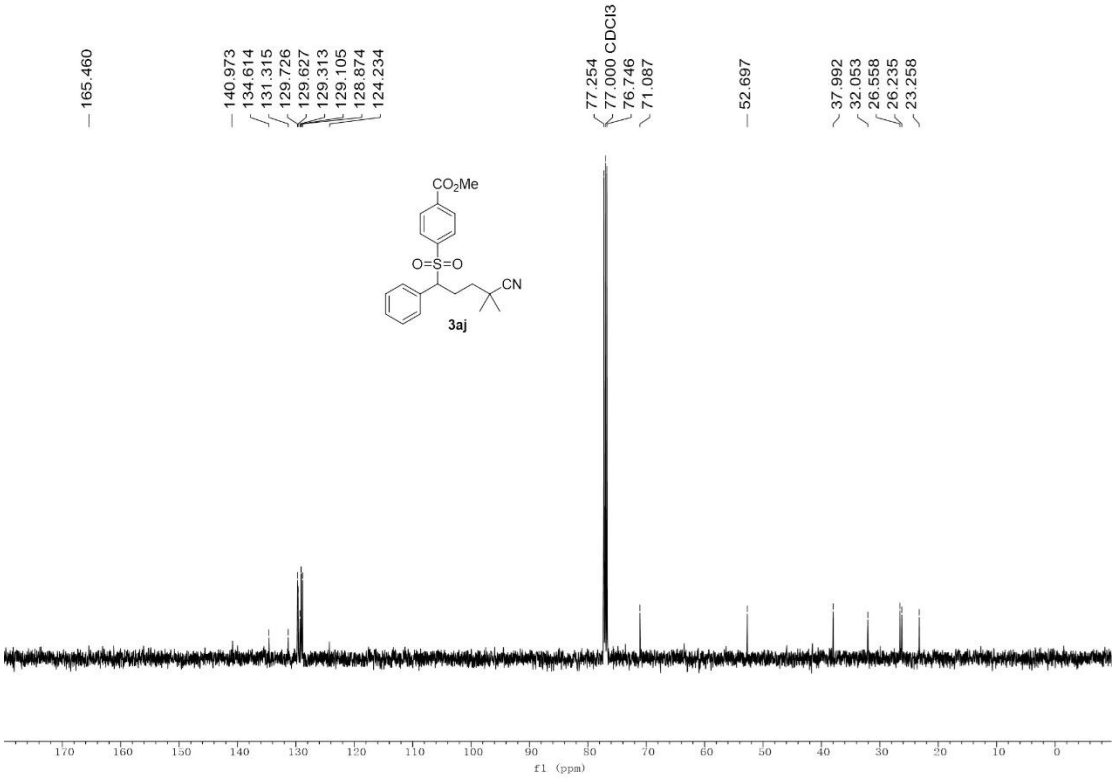
7.319
7.308
7.304
7.300
7.289
7.260 CDCl3
7.253
7.237
7.223
7.069
7.055
4.071
4.063
4.049
4.041
3.938
2.710
2.702
2.650
2.640
2.376
2.367
2.302
2.294
1.591
1.584
1.539
1.529
1.434
1.426
1.382
1.373
1.342
1.314
CO2Me
O=S=O
CN
3aj
2.00
1.99
1.03
2.22
2.02
1.00
3.01
1.00
1.01
1.08
1.05
3.15
3.09
f1 (ppm)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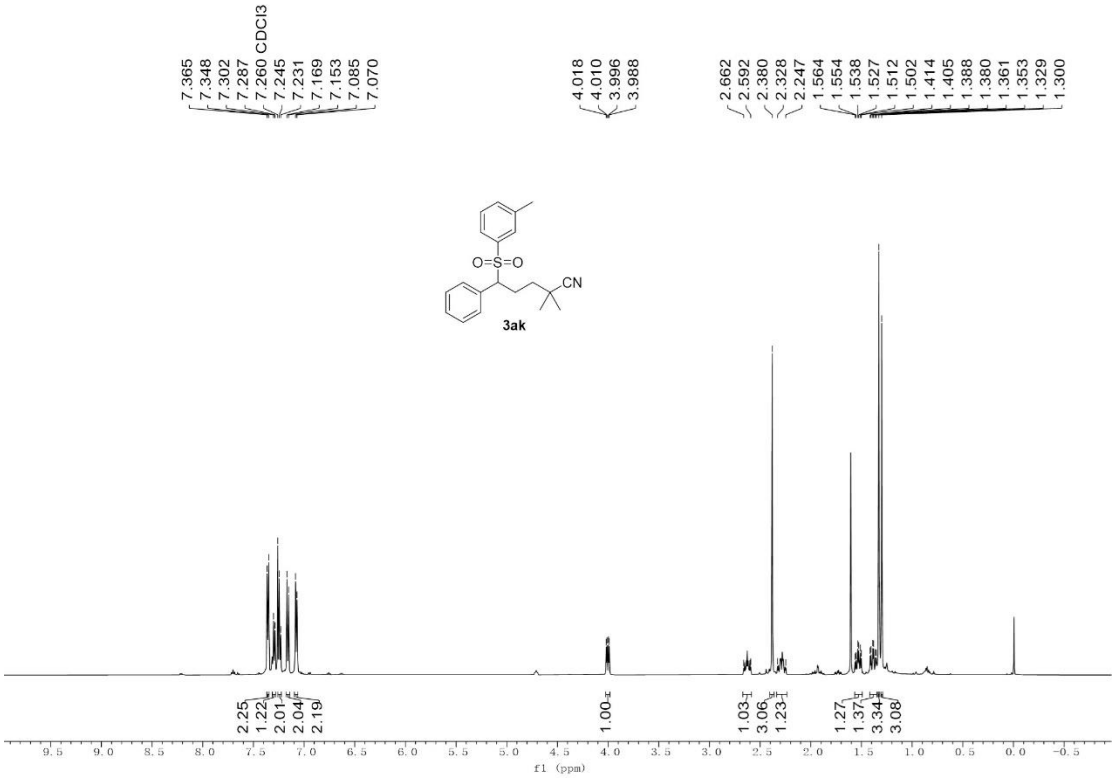
129.627
129.313
129.105
128.874
124.234
77.254
77.000 CDCl3
76.746
71.087
52.697
37.992
32.053
26.558
26.235
23.258
CO2Me
O=S=O
CN
3aj
f1 (ppm)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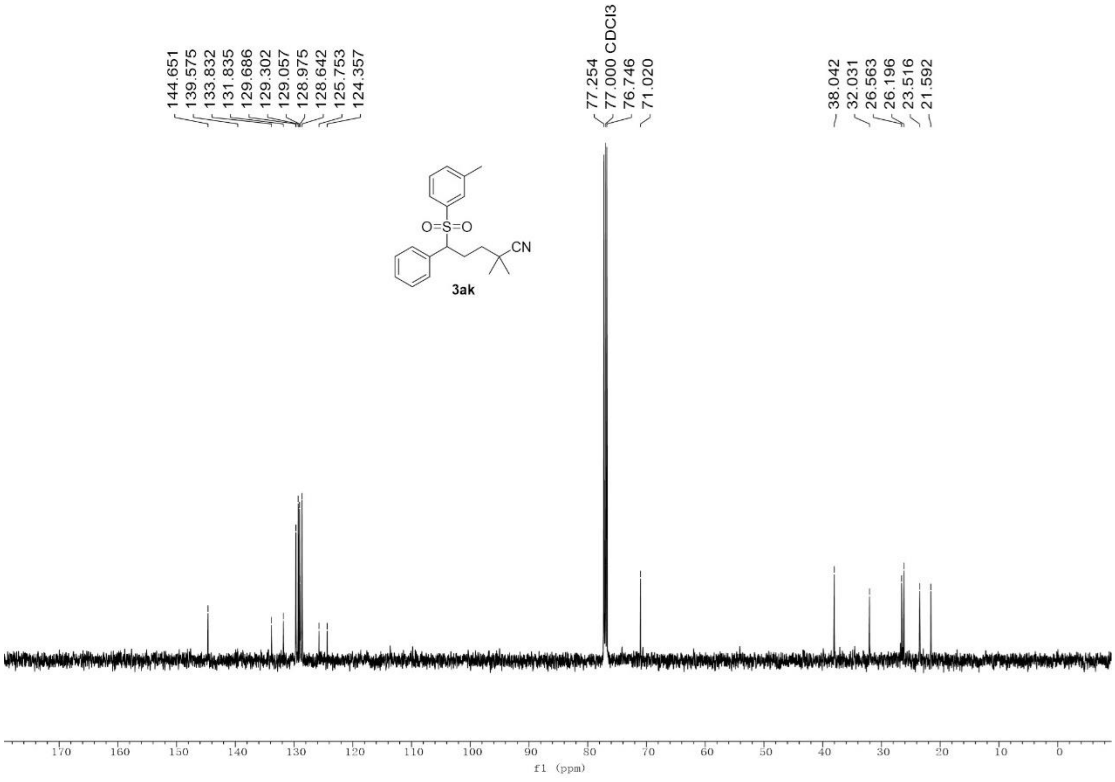
7.287
7.260 CDCl3
7.245
7.231
7.169
7.153
7.085
7.070
4.018
4.010
3.996
3.988
2.662
2.592
2.380
2.328
2.247
1.564
1.554
1.538
1.527
1.512
1.502
1.414
1.405
1.388
1.380
1.361
1.353
1.329
1.300
O=S=O
CN
3ak
2.25
1.22
2.01
2.04
2.19
1.00
1.03
3.06
1.23
1.27
1.37
3.34
3.08
f1 (ppm)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129.302
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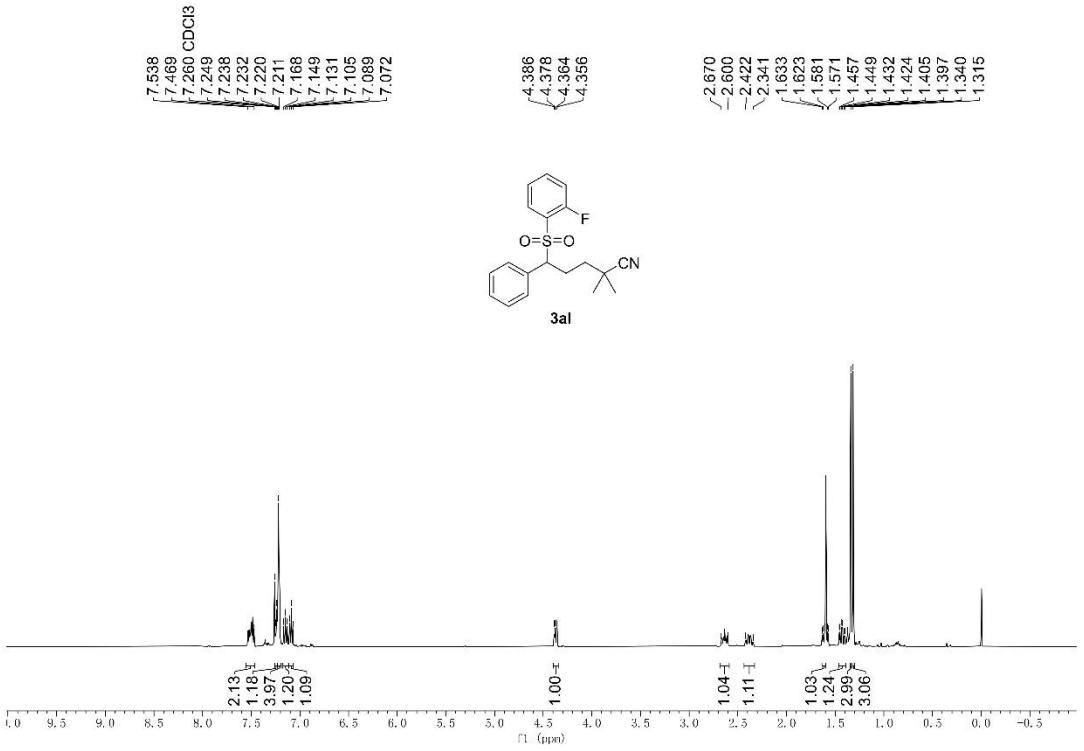
128.975
128.642
125.753
124.357
77.254
77.000 CDCl3
76.746
71.020
38.042
32.031
26.563
26.196
23.516
21.592
O=S=O
CN
3ak
f1 (ppm)


7.538
7.469
7.260 CDCl3
7.249
7.238
7.232
7.220
7.211
7.168
7.149
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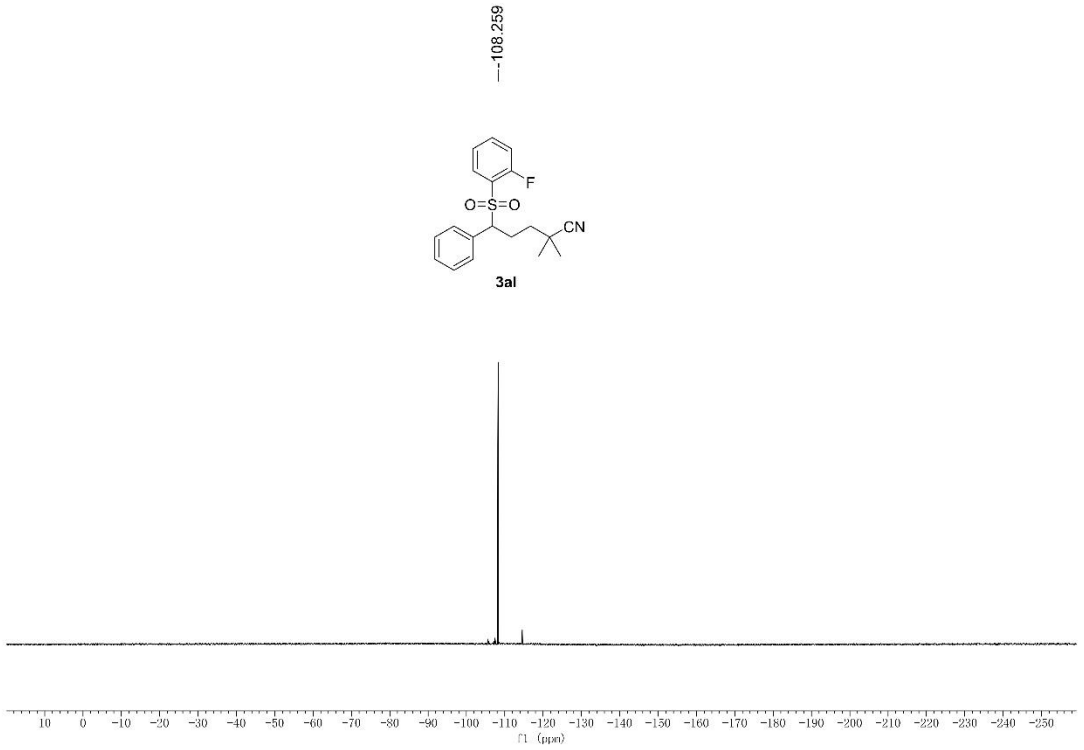
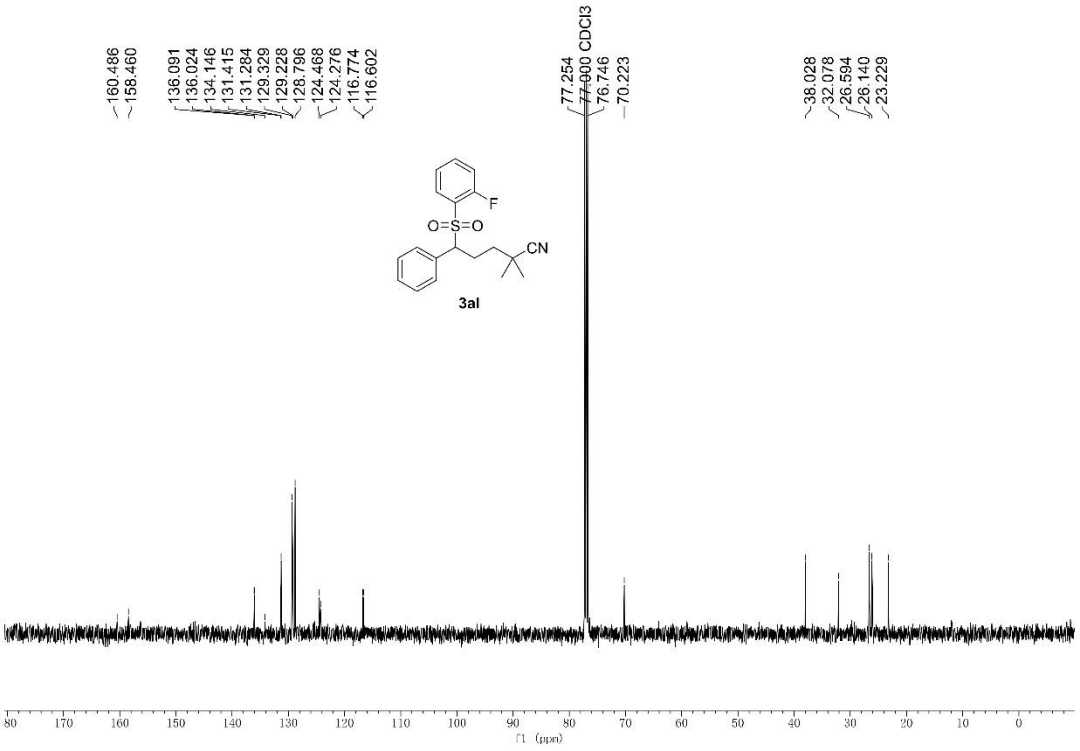
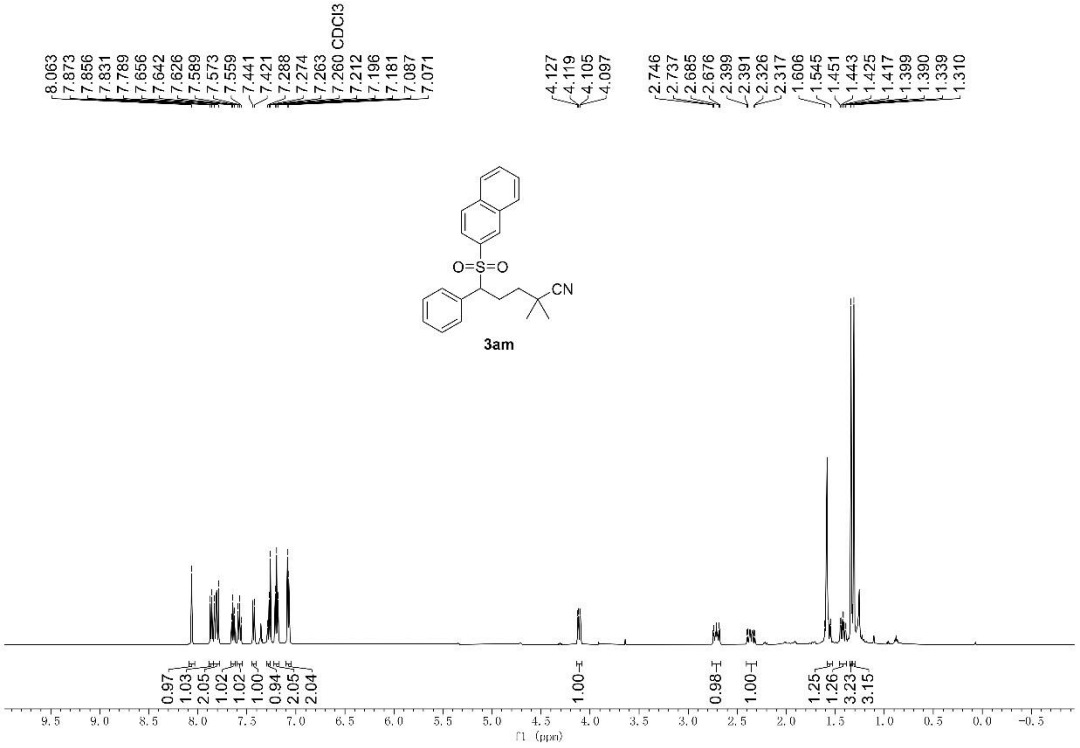
7.105
7.089
7.072
4.386
4.378
4.364
4.356
2.670
2.600
2.422
2.341
1.633
1.623
1.581
1.571
1.457
1.449
1.432
1.424
1.405
1.397
1.340
1.315
F
O=S=O
CN
3al
2.13
1.18
3.97
1.20
1.09
1.00
1.04
1.11
1.03
1.24
2.99
3.06
f1 (ppm)


-108.259
F
O=S=O
CN
3al
f1 (ppm)


160.486
158.460
136.091
136.024
134.146
131.415
131.284
129.329
129.228
128.796
124.468
124.276
116.774
116.602
77.254
77.000 CDCl3
76.746
70.223
38.028
32.078
26.594
26.140
23.229
F
O=S=O
CN
3al
f1 (ppm)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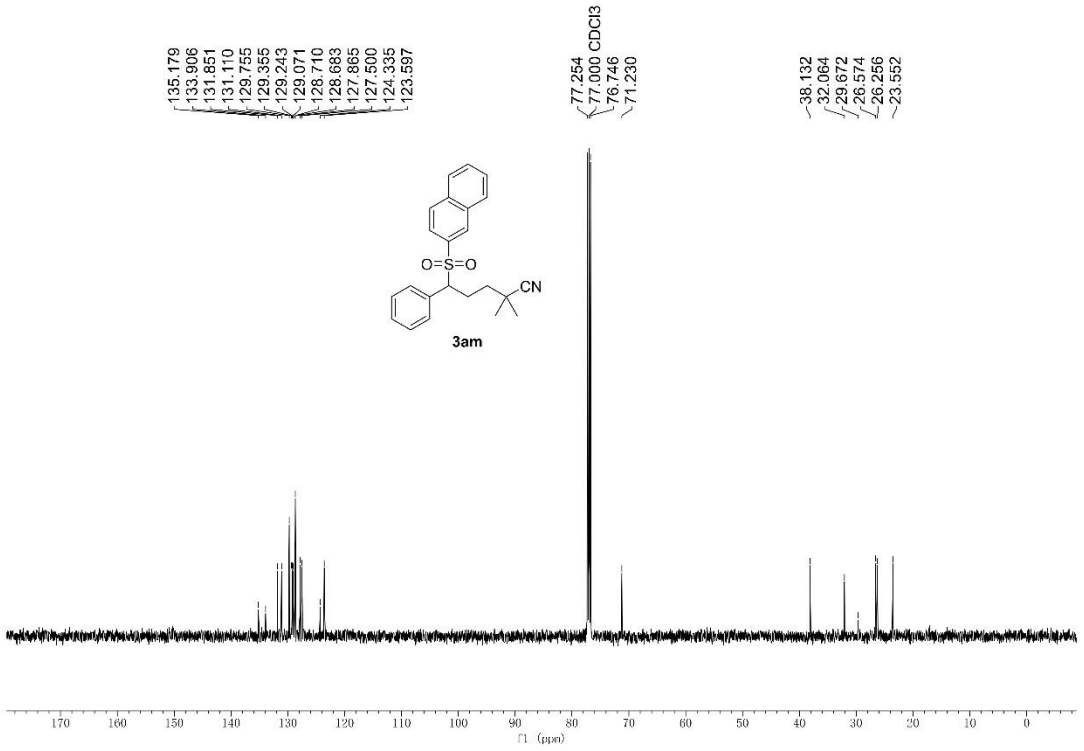
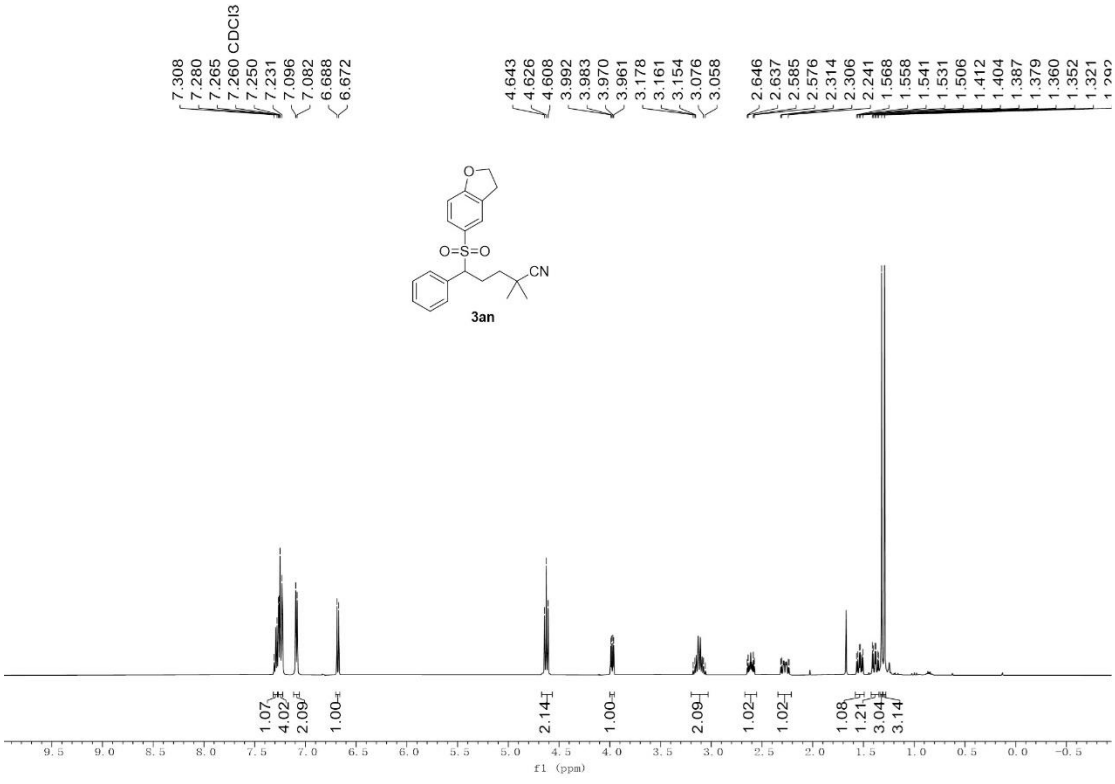
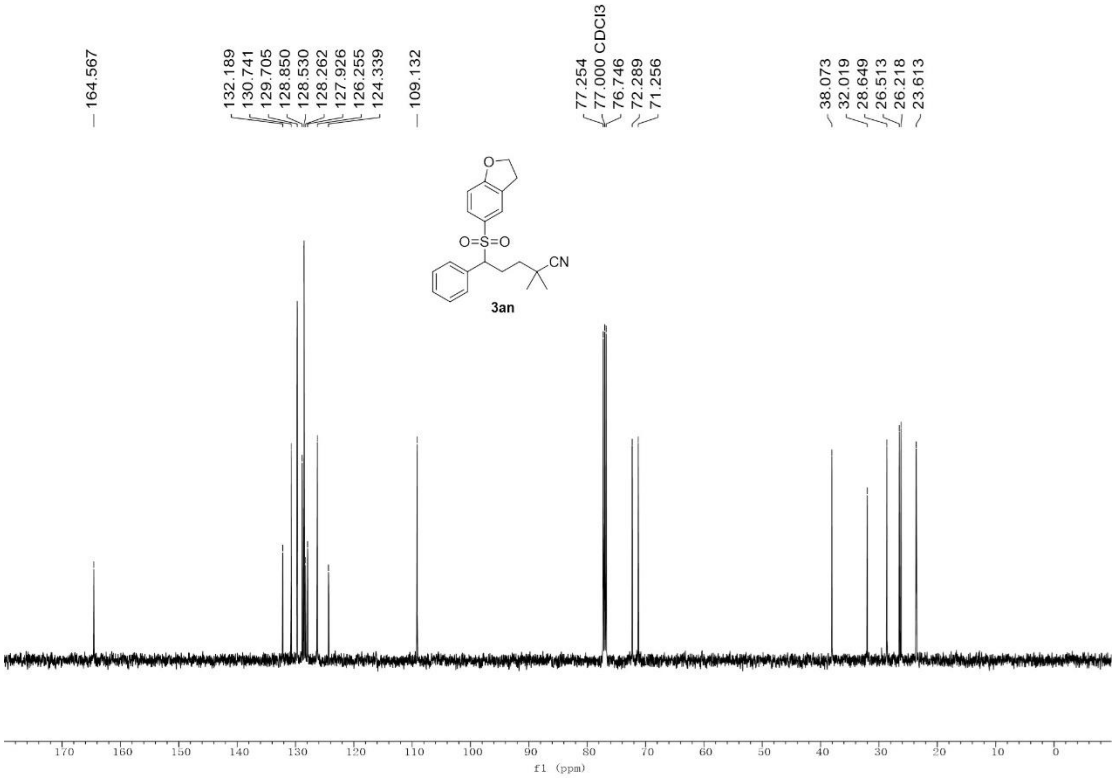
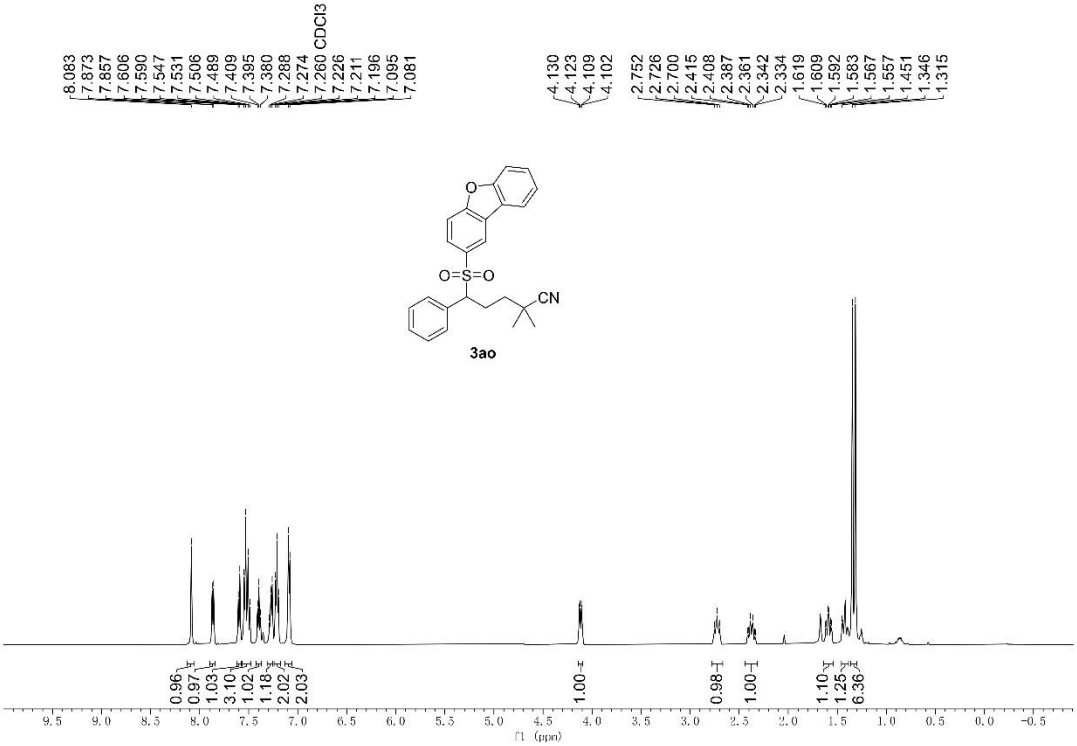
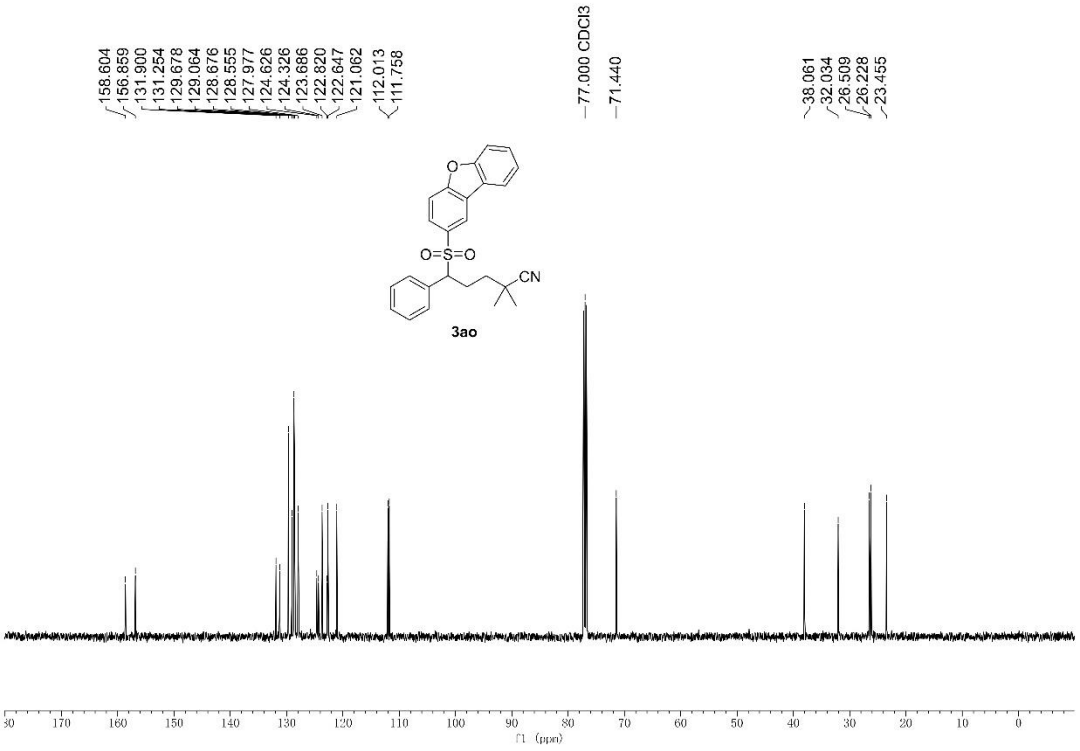
7.873
7.856
7.831
7.789
7.656
7.642
7.626
7.589
7.573
7.559
7.441
7.421
7.288
7.274
7.263
7.260 CDCl3
7.212
7.196
7.181
7.087
7.071
4.127
4.119
4.105
4.097
2.746
2.737
2.685
2.676
2.399
2.391
2.326
2.317
1.606
1.545
1.451
1.443
1.425
1.417
1.399
1.390
1.339
1.310
O=S=O
CN
3am
0.97
1.03
2.05
1.02
1.02
1.00
0.94
2.05
2.04
1.00
0.98
1.00
1.25
1.26
3.23
3.15
f1 (ppm)

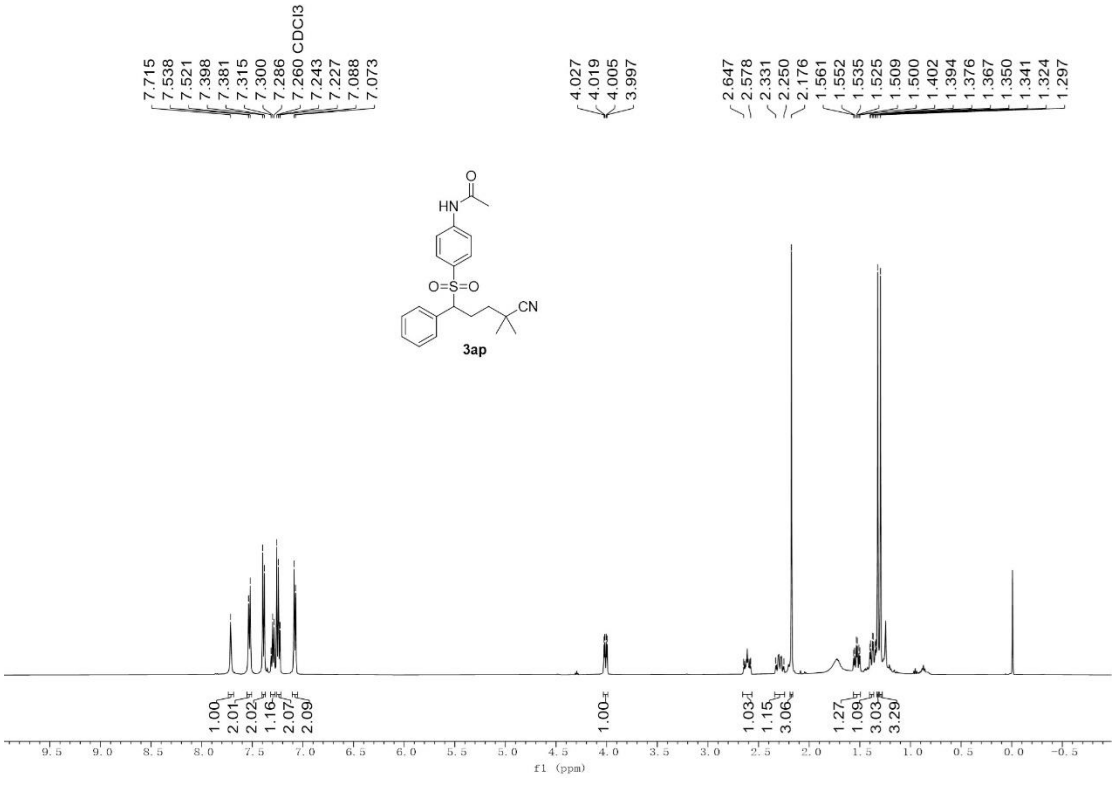

135.179
133.906
131.851
131.110
129.755
129.355
129.243
129.071
128.710
128.683
127.865
127.500
124.335
123.597
77.254
77.000 CDCl3
76.746
71.230
38.132
32.064
29.672
26.574
26.256
23.552
O=S=O
CN
3am
f1 (ppm)

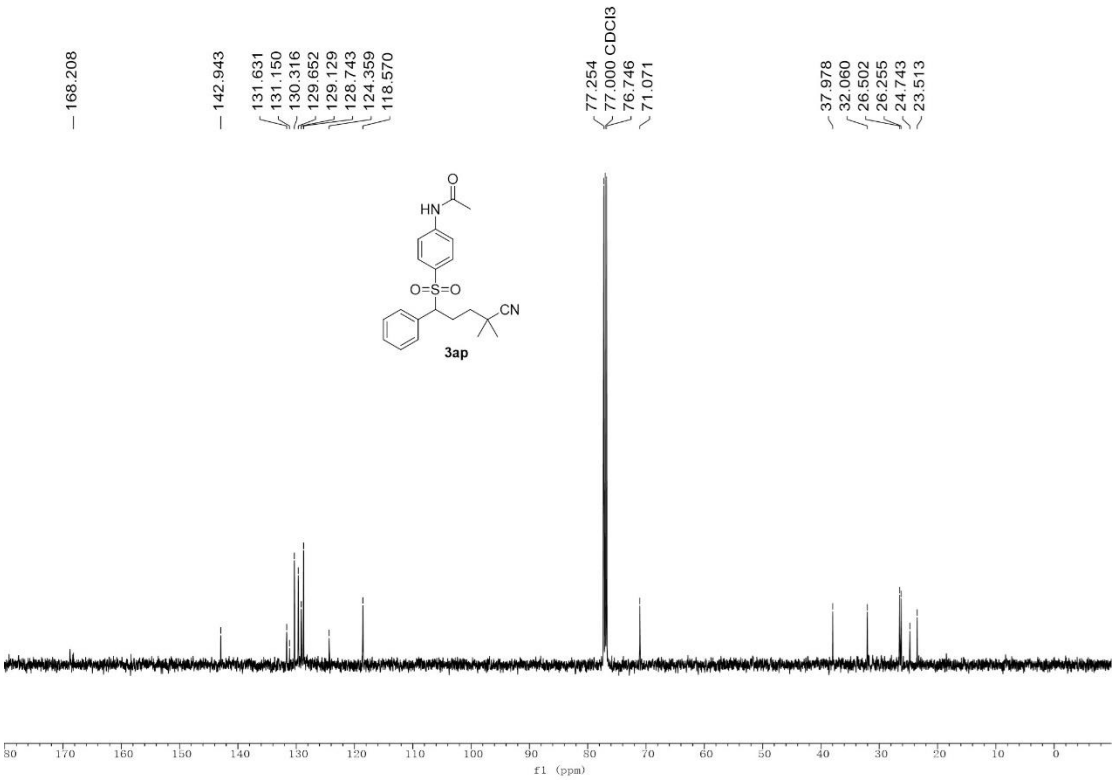

7.308
7.280
7.265
7.260 CDCl3
7.250
7.231
7.096
7.082
6.688
6.672
4.643
4.626
4.608
3.992
3.983
3.970
3.961
3.178
3.161
3.154
3.076
3.058
2.646
2.637
2.585
2.576
2.314
2.306
2.241
1.568
1.558
1.541
1.531
1.506
1.412
1.404
1.387
1.379
1.360
1.352
1.321
O=S=O
CN
3an
1.07
4.02
2.09
1.00
2.14
1.00
2.09
1.02
1.02
1.08
1.21
3.04
3.14
f1 (ppm)

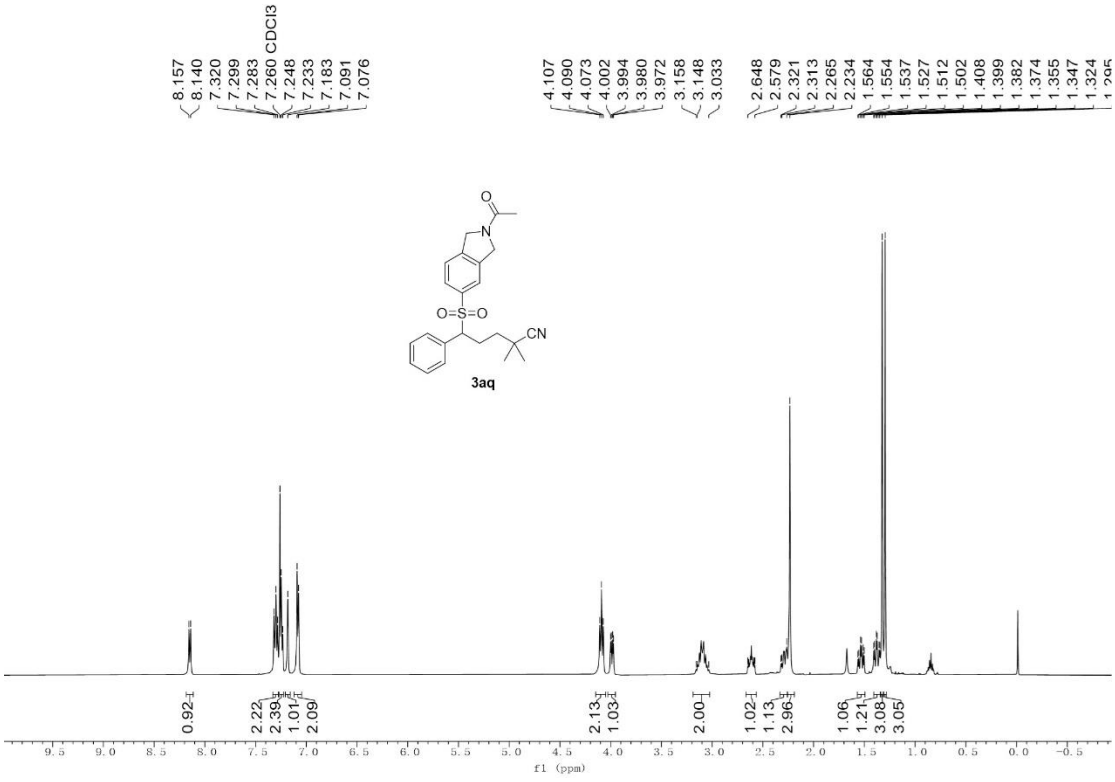

164.567
132.189
130.741
129.705
128.850
128.530
128.262
127.926
126.255
124.339
109.132
77.254
77.000 CDCl3
76.746
72.289
71.256
38.073
32.019
28.649
26.513
26.218
23.613
O=S=O
CN
3an
f1 (ppm)

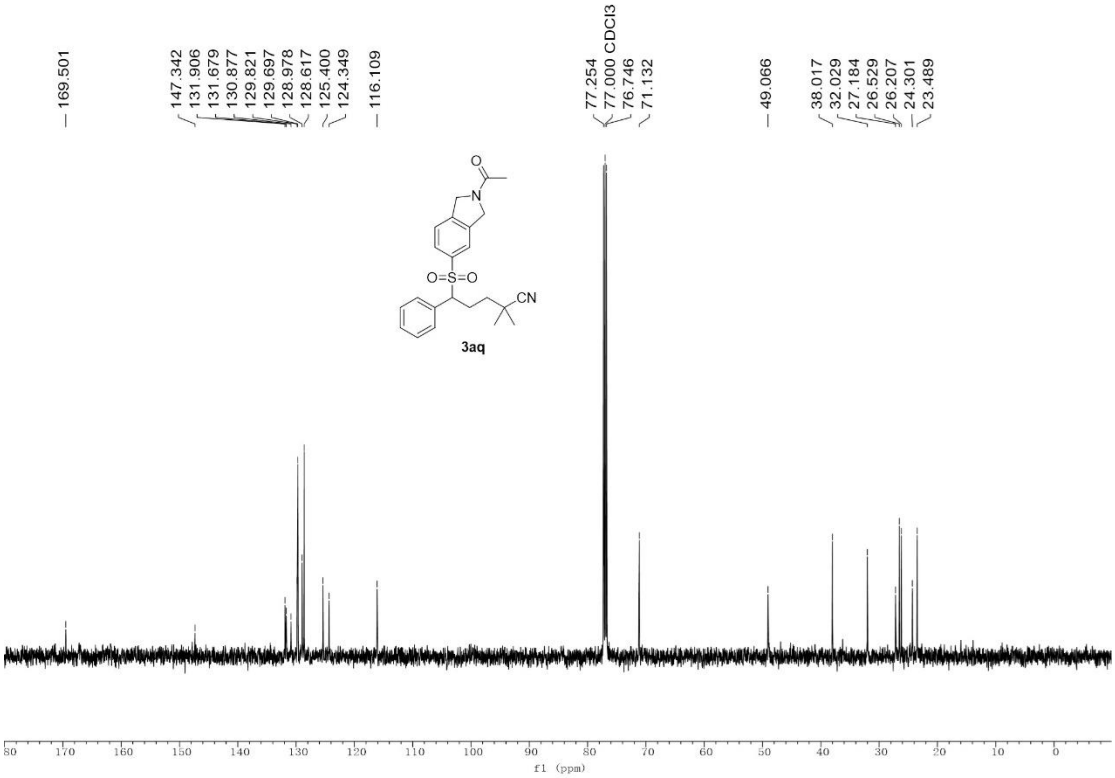

8.083
7.873
7.857
7.606
7.590
7.547
7.531
7.506
7.489
7.409
7.395
7.380
7.288
7.274
7.260 CDCl3
7.226
7.211
7.196
7.095
7.081
4.130
4.123
4.109
4.102
2.752
2.726
2.700
2.415
2.408
2.387
2.361
2.342
2.334
1.619
1.609
1.592
1.583
1.567
1.557
1.451
1.346
1.315
O=S=O
CN
3ao
0.96
0.97
1.03
3.10
1.02
1.18
2.02
2.03
1.00
0.98
1.00
1.10
1.25
6.36
f1 (ppm)

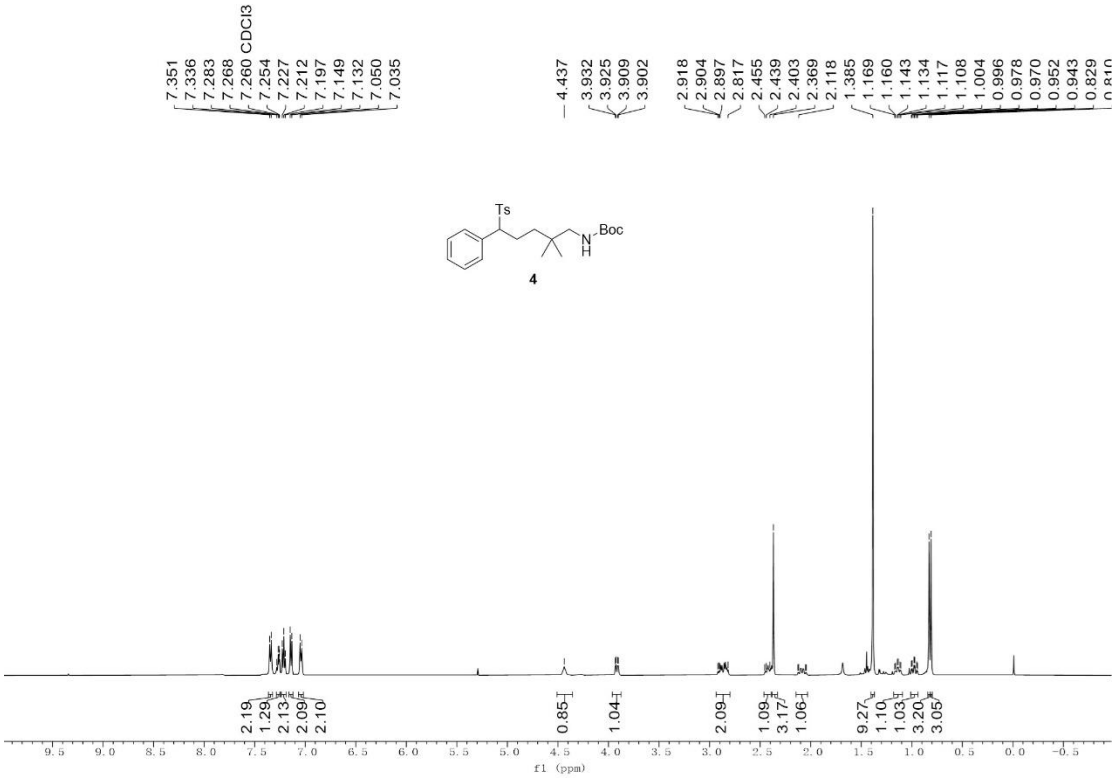

158.604
156.859
131.900
131.254
129.678
129.064
128.676
128.555
127.977
124.626
124.326
123.686
122.820
122.647
121.062
112.013
111.758
77.000 CDCl3
71.440
38.061
32.034
26.509
26.228
23.455
O=S=O
CN
3ao
f1 (ppm)

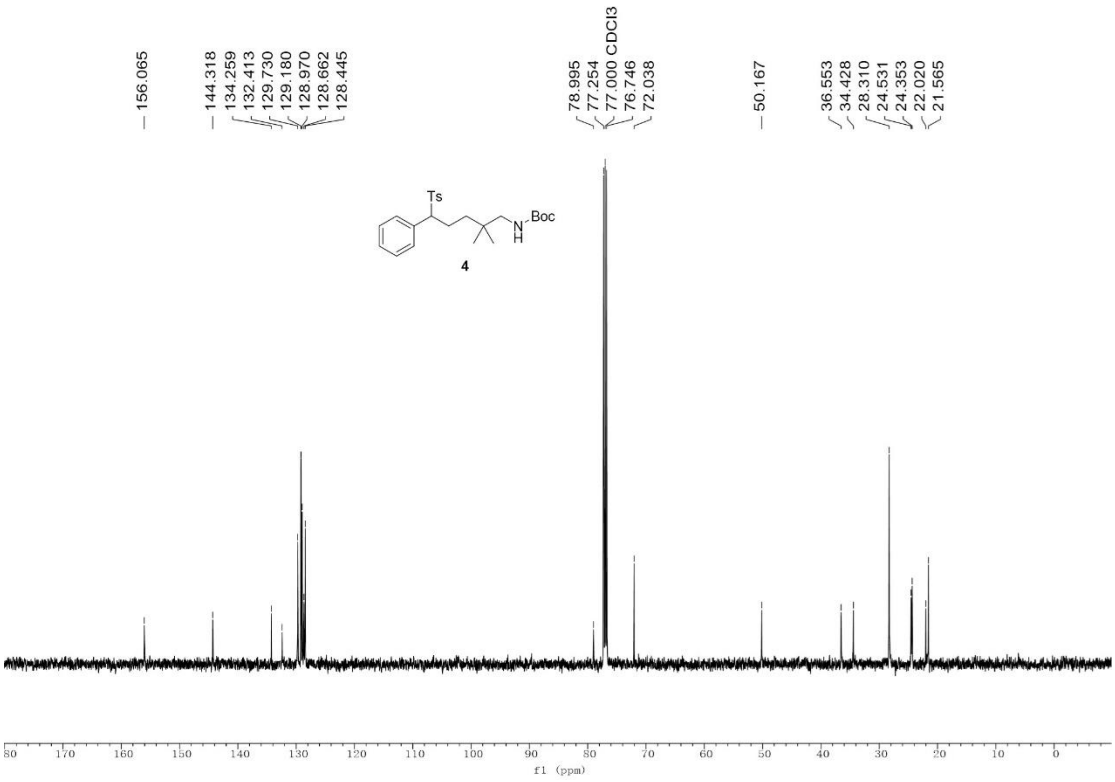

7.715
7.538
7.521
7.398
7.381
7.315
7.300
7.286
7.260 CDCl3
7.243
7.227
7.088
7.073
4.027
4.019
4.005
3.997
2.647
2.578
2.331
2.250
2.176
1.561
1.552
1.535
1.525
1.509
1.500
1.402
1.394
1.376
1.367
1.350
1.341
1.324
1.297
HN
O=S=O
CN
3ap
1.00
2.01
2.02
1.16
2.07
2.09
1.00
1.03
1.15
3.06
1.27
1.09
3.03
3.29
f1 (ppm)

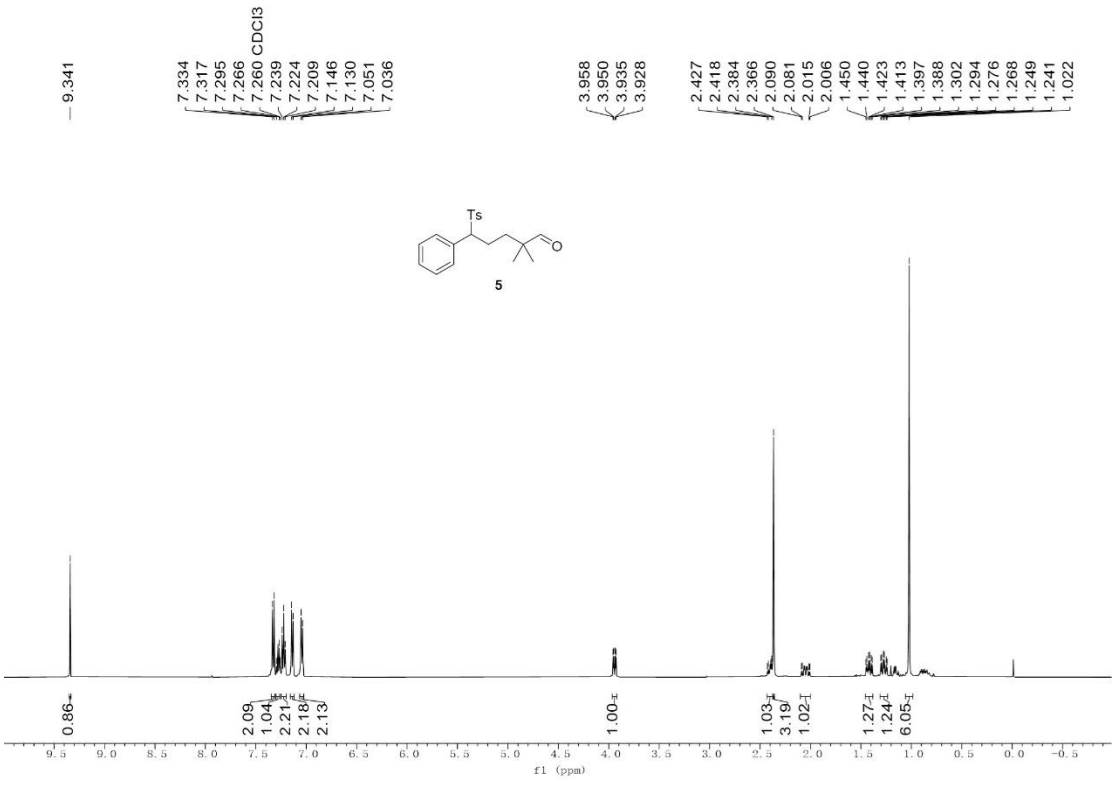

168.208
142.943
131.631
131.150
130.316
129.652
129.129
128.743
124.359
118.570
77.254
77.000 CDCl3
76.746
71.071
37.978
32.060
26.502
26.255
24.743
23.513
HN
O
O=S=O
CN
3ap
f1 (ppm)

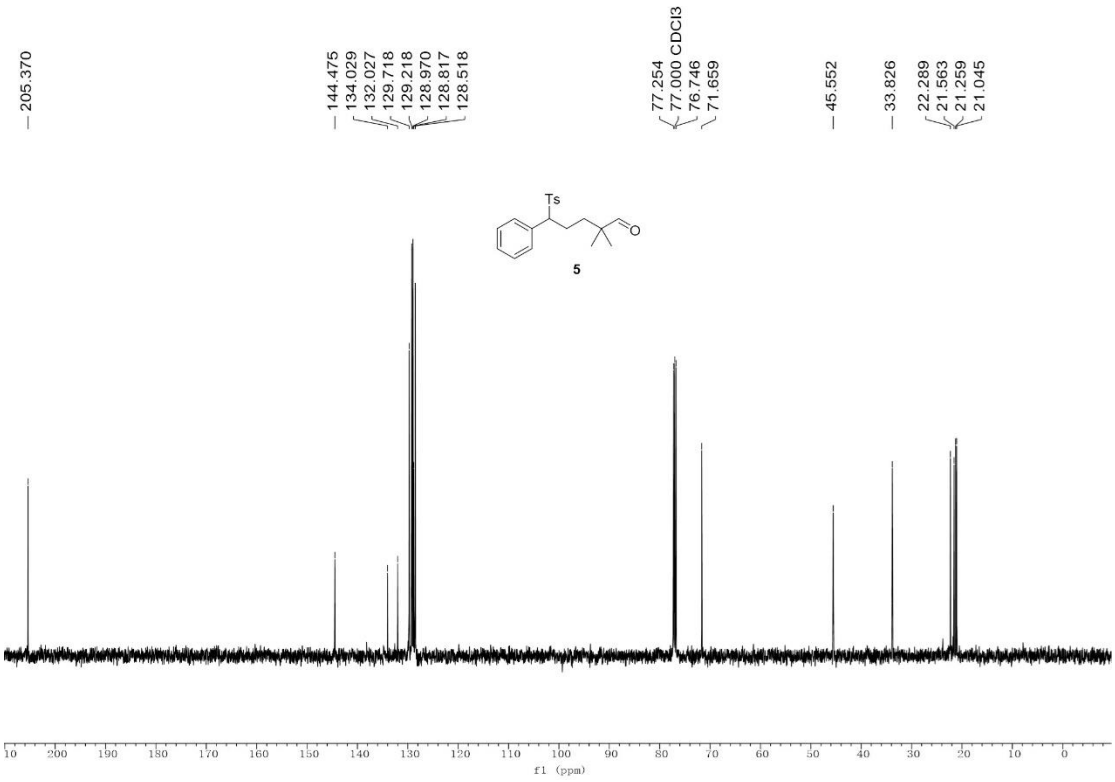

8.157
8.140
7.320
7.299
7.283
7.260 CDCl3
7.248
7.233
7.183
7.091
7.076
4.107
4.090
4.073
4.002
3.994
3.980
3.972
3.158
3.148
3.033
2.648
2.579
2.321
2.313
2.265
2.234
1.564
1.554
1.537
1.527
1.512
1.502
1.408
1.399
1.382
1.374
1.355
1.347
1.324
0.92
2.22
2.39
1.01
2.09
2.13
1.03
2.00
1.02
1.13
2.96
1.06
1.21
3.08
3.05
O=S=O
CN
3aq
f1 (ppm)


169.501
147.342
131.906
131.679
130.877
129.821
129.697
128.978
128.617
125.400
124.349
116.109
77.254
77.000 CDCl3
76.746
71.132
49.066
38.017
32.029
27.184
26.529
26.207
24.301
23.489
O=S=O
CN
3aq
f1 (ppm)


7.351
7.336
7.283
7.268
7.260 CDCl3
7.254
7.227
7.212
7.197
7.149
7.132
7.050
7.035
4.437
3.932
3.925
3.909
3.902
2.918
2.904
2.897
2.817
2.455
2.439
2.403
2.369
2.118
1.385
1.169
1.160
1.143
1.134
1.117
1.108
1.004
0.996
0.978
0.970
0.952
0.943
0.829
Ts
Boc
N
H
4
2.19
1.29
2.13
2.09
2.10
0.85
1.04
2.09
1.09
3.17
1.06
9.27
1.10
1.03
3.20
3.05
f1 (ppm)


156.065
144.318
134.259
132.413
129.730
129.180
128.970
128.662
128.445
78.995
77.254
77.000 CDCl3
76.746
72.038
50.167
36.553
34.428
28.310
24.531
24.353
22.020
21.565
Ts
Boc
4
f1 (ppm)


9.341
7.334
7.317
7.295
7.266
7.260 CDCl3
7.239
7.224
7.209
7.146
7.130
7.051
7.036
3.958
3.950
3.935
3.928
2.427
2.418
2.384
2.366
2.090
2.081
2.015
2.006
1.450
1.440
1.423
1.413
1.397
1.388
1.302
1.294
1.276
1.268
1.249
1.241
1.022
Ts
O
5
0.86
2.09
1.04
2.21
2.18
2.13
1.00
1.03
3.19
1.02
1.27
1.24
6.05
f1 (ppm)


205.370
144.475
134.029
132.027
129.718
129.218
128.970
128.817
128.518
77.254
77.000 CDCl3
76.746
71.659
45.552
33.826
22.289
21.563
21.259
21.045
Ts
O
5
f1 (ppm)