

Supporting Information

Reductive sandmeyer-type reaction for the synthesis of sulfoxides from anilines under photocatalysis

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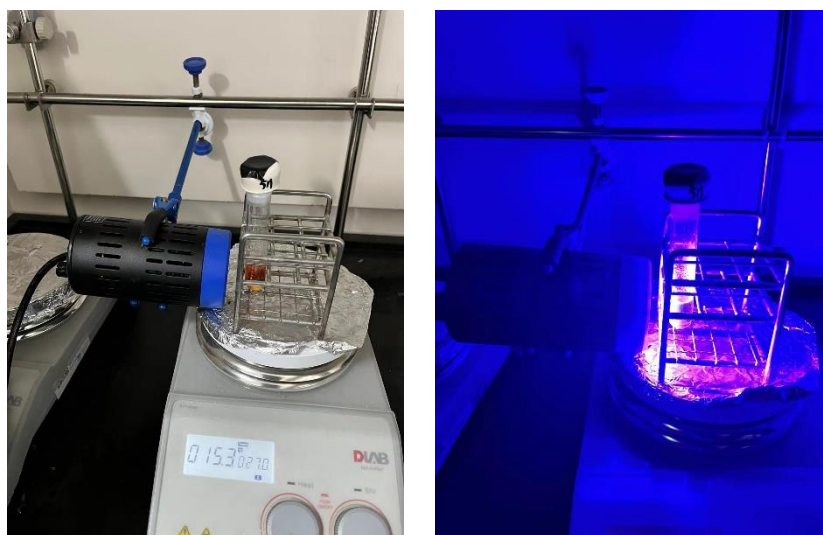
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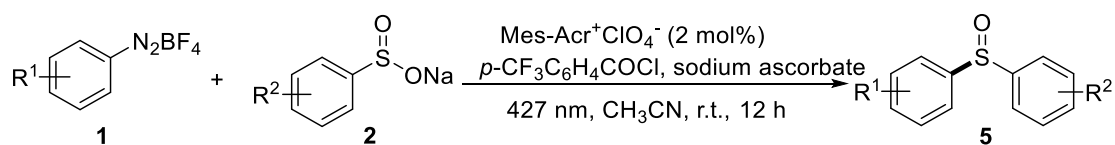
1. General experimental methods

All experiments were carried out under nitrogen atmosphere using anhydrous solvents. Unless otherwise noted, all commercially available reagents and solvents were purchased and used as received without further purification. All reactions were monitored by thin layer chromatography (TLC) carried out on silica gel plates, Visualisation was by ultraviolet fluorescence. Column chromatography was performed on silica gel (300-400 mesh). ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker Avance-400 spectrometer in CDCl_3 as solvents at room temperature. Chemical shifts are expressed in parts per million (ppm) and referenced to the residual solvent peak. Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; m, multiplet, q, quartet, with all coupling constants (J) reported in Hertz (Hz). The high-resolution mass spectra (HRMS) were recorded on an IonSpec FT-ICR mass spectrometer with ESI resource. GS-MS analysis was analyzed with GC-MS (Agilent 7890B-5977A, USA). All reactions irradiated with a 40 W Kessil blue LED lamp (PR160L-427nm). The aryldiazonium salts and sodium sulfinates were prepared according to the literature ^[1]. The photoreaction was set up as below:



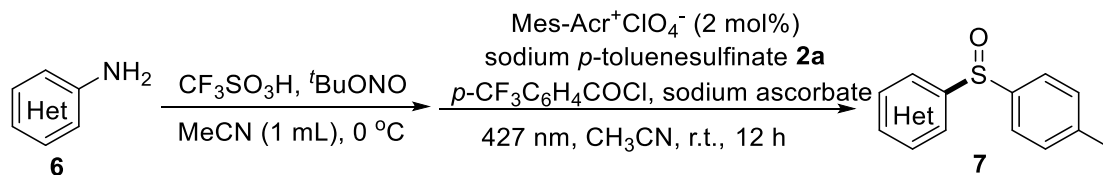
Supplementary Figure 1. Setup for the photoreactions

2. General experimental procedure for the synthesis of sulfoxides



A 10 mL glass tube equipped with a magnetic stirrer was charged with aryldiazonium salts **1** (0.15 mmol, 1.0 equiv.), sodium sulfinate **2** (0.375 mmol, 2.5 equiv.), sodium ascorbate **4a** (0.375 mmol, 2.5 equiv.) and 9-Mesityl-10-methylacridinium perchlorate (2 mol%). Then, the tube was carefully evacuated and backfilled with N₂ for three times. Afterwards, anhydrous MeCN (3.0 mL) and 4-trifluoromethylbenzoyl chloride (0.3 mmol, 2.0 equiv.) were added via syringe. After the reaction was stirred under a 40W Kessil 427 nm lamp for 12 hours, the mixture was extracted with EtOAc (3×5 mL) and dried over anhydrous Na₂SO₄. The organic solvent was evaporated and the crude product was purified by flash column chromatography on silica gel (EtOAc: Petroleum = 1:8 to 1:1) to give the diaryl sulfoxide product **5**.

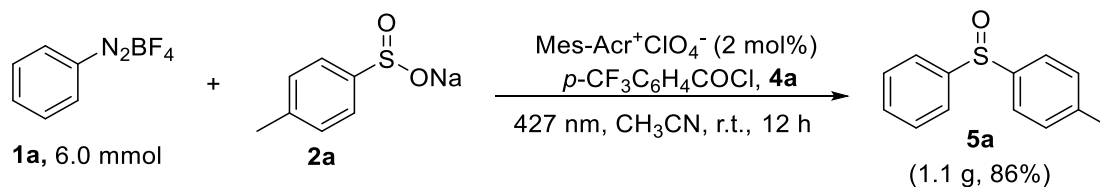
3. General procedure for the one-pot synthesis of sulfoxides from anilines



To a 10 mL glass tube equipped with a magnetic stirrer was charged with aniline **6** (0.15 mmol, 1.0 equiv.), CF₃SO₃H (20 μL, 0.24 mmol, 1.6 equiv.) and MeCN (1 mL). Then *t*-BuONO (24.7 μL, 0.24 mmol, 1.6 equiv.) was added dropwise at 0 °C. The mixture was stirred at 0 °C for 15 minutes and used in the next step. To a 10 mL glass tube equipped with a magnetic stirrer was charged with sodium *p*-toluenesulfinate **2a** (0.375 mmol, 2.5 equiv.), sodium ascorbate **4a** (0.375 mmol, 2.5 equiv.) and 9-Mesityl-10-methylacridinium perchlorate (2 mol%). Then, the tube was carefully evacuated and backfilled with N₂ for three times. Afterwards, 4-trifluoromethylbenzoyl chloride (0.3 mmol, 2.0 equiv.), the above diazonium salt mixture and anhydrous MeCN (2.0 mL) were added via syringe. The reaction mixture was then irradiated with a 40W Kessil 427 nm lamp. After 12 hours, the mixture was concentrated under reduced pressure to

give the crude product directly, which was next purified by flash chromatography on silica gel (EtOAc:Petroleum = 1:4 to 1:1) to give the desired product **7**.

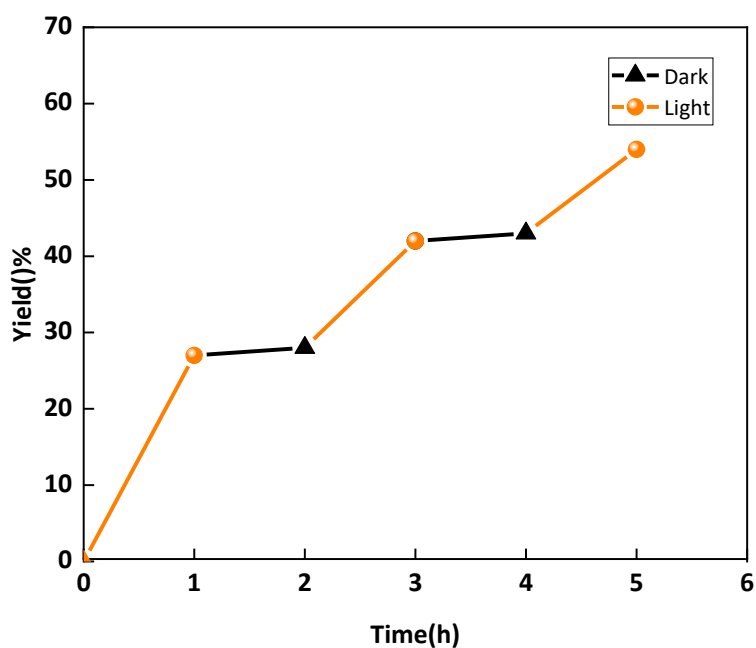
4. Gram-scale experiment



A 500 mL round-bottom flask equipped with a magnetic stir bar was charged with phenyl diazonium salt **1a** (6.0 mmol, 1.15 g), sodium *p*-toluenesulfinate **2a** (15.0 mmol, 2.73 g), sodium ascorbate **4a** (15.0 mmol, 3.0 g) and 9-Mesityl-10-methylacridinium perchlorate (0.12 mmol, 48.0mg). Then, the tube was carefully evacuated and backfilled with N₂ for three times. Afterwards, anhydrous MeCN (120 mL) and 4-trifluoromethylbenzoyl chloride (12 mmol) were added via syringe. The reaction mixture was stirred under irradiation of two 40W Kessil 427 nm lamps for 12 h, then diluted with ethyl acetate and washed with water. The organic layer was collected, dried over anhydrous sodium sulfate, concentrated under reduced pressure, and the remaining material was purified by flash chromatography on silica gel to give the desired product **5a** as a yellowish solid in 86% yield (1.1 g).

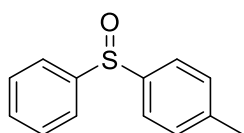
5. Light on-off experiment

According to standard conditions, the reaction was carried out under an atmosphere of nitrogen. Then, the reaction mixture was stirred with alternating intervals of 1.0-hour irradiation by a 40W Kessil 427 nm lamp and 1.0-hour dark, during a total of 5 hours. The experimental results show that the reaction rate decreases with increasing reaction time under light conditions, and the reaction is very slow under dark conditions.

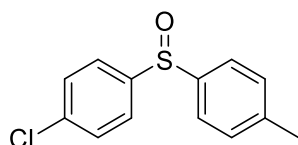


Supplementary Figure 2. Light on/off experiment.

6. Data of compounds

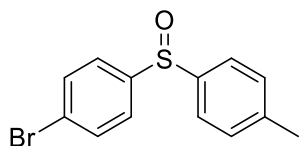


1-Methyl-4-(phenylsulfinyl)benzene (**5a**)^[2]: According to the General Procedure, **5a** (27.5 mg, 85%) was prepared as a yellowish solid; m.p. 65-66 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 7.7, 1.9 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.46 – 7.38 (m, 3H), 7.26 – 7.22 (m, 2H), 2.34 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 145.8, 142.5, 141.8, 131.0, 130.2, 129.4, 125.1, 124.8, 21.5.

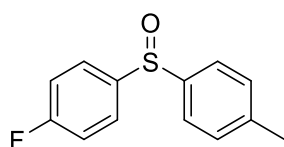


1-Chloro-4-(*p*-tolylsulfinyl)benzene (**5b**)^[2]: According to the General Procedure, **5b** (27.0 mg, 72%) was prepared as a yellow solid; m.p. 45-46 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.7 Hz,

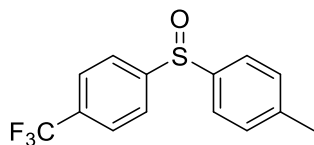
2H), 7.25 (d, $J = 7.9$ Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.4, 142.2, 142.1, 137.2, 130.3, 129.6, 126.1, 125.0, 21.6.



1-Bromo-4-(*p*-tolylsulfinyl)benzene (**5c**)^[2]: According to the General Procedure, **5c** (33.6 mg, 76%) was prepared as a yellowish solid; m.p. 60-61 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, $J = 8.5$ Hz, 2H), 7.52 – 7.45 (m, 4H), 7.25 (d, $J = 8.0$ Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.8, 142.2, 141.8, 132.5, 130.2, 126.2, 125.5, 125.0, 21.5.

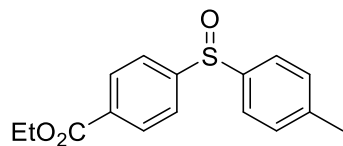


1-Fluoro-4-(*p*-tolylsulfinyl)benzene (**5d**)^[2]: According to the General Procedure, **5d** (27.0 mg, 77%) was prepared as a yellowish solid; m.p. 36-37 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.57 (m, 2H), 7.49 (d, $J = 8.2$ Hz, 2H), 7.25 (d, $J = 7.4$ Hz, 2H), 7.13 (t, $J = 8.6$ Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.2 (d, $J_{\text{C-F}} = 251.4$ Hz), 142.3, 142.0, 141.4 (d, $J_{\text{C-F}} = 3.0$ Hz), 130.2, 127.0 (d, $J_{\text{C-F}} = 9.0$ Hz), 124.9, 116.6 (d, $J_{\text{C-F}} = 22.7$ Hz), 21.5; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.5.

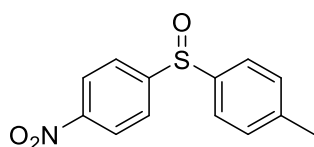


1-Methyl-4-([4-(trifluoromethyl)phenyl]sulfinyl)benzene (**5e**)^[3]: According to the General Procedure, **5e** (21.3 mg, 50%) was prepared as a yellowish oil; ^1H NMR (500 MHz, Chloroform-*d*) δ 7.80 (d, $J = 8.4$ Hz, 2H), 7.76 (d, $J = 8.4$ Hz, 2H), 7.60 (d, $J = 8.2$ Hz, 2H), 7.36 – 7.30 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.3, 142.5, 141.8, 131.6, 130.4, 126.3 (q, $J_{\text{C-F}} = 3.5$ Hz), 125.2, 124.8, 123.6 (q, $J_{\text{C-F}}$

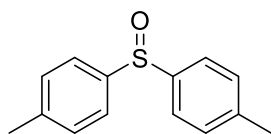
= 273.0 Hz), 21.5; ^{19}F NMR (470 MHz, CDCl_3) δ -62.8.



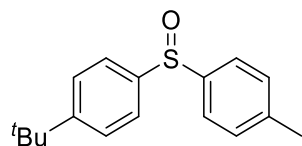
Ethyl 4-(*p*-tolylsulfinyl)benzoate (**5f**)^[4]: According to the General Procedure, **5f** (23.8 mg, 55%) was prepared as a yellow solid; m.p. 85-86 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, J = 8.5 Hz, 2H), 7.67 (d, J = 8.5 Hz, 2H), 7.52 (d, J = 8.2 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 4.35 (q, J = 7.1 Hz, 2H), 2.34 (s, 3H), 1.36 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.7, 150.7, 142.3, 142.0, 132.7, 130.4, 130.3, 125.2, 124.4, 61.5, 21.6, 14.4.



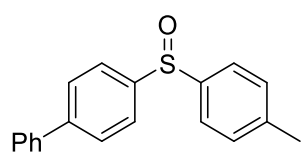
1-Methyl-4-[(4-nitrophenyl)sulfinyl]benzene (**5g**)^[3]: According to the General Procedure, **5g** (22.3 mg, 57%) was prepared as a yellow solid; m.p. 120-121 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, J = 8.7 Hz, 2H), 7.79 (d, J = 8.7 Hz, 2H), 7.54 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.3 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.1, 149.2, 143.0, 141.1, 130.6, 125.32, 125.25, 124.4, 21.5.



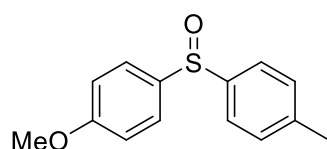
4,4'-Sulfinylbis(methylbenzene) (**5h**)^[2]: According to the General Procedure, **5h** (26.6 mg, 77%) was prepared as a yellowish solid; m.p. 92-93 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, J = 8.2 Hz, 4H), 7.23 (d, J = 7.8 Hz, 4H), 2.34 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.7, 141.5, 130.1, 124.9, 21.5.



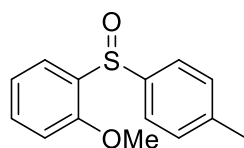
1-(*Tert*-butyl)-4-(*p*-tolylsulfinyl)benzene (**5i**)^[2]: According to the General Procedure, **5i** (27.3 mg, 67%) was prepared as a yellow solid; m.p. 83-85 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.50 (m, 4H), 7.46 – 7.42 (m, 2H), 7.26 – 7.23 (m, 2H), 2.35 (s, 3H), 1.28 (s, 9H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 154.6, 142.6, 142.5, 141.5, 130.1, 126.5, 125.0, 124.8, 35.0, 31.3, 21.5.



4-(*p*-Tolylsulfinyl)-1,1'-biphenyl (**5j**)^[5]: According to the General Procedure, **5j** (26.7 mg, 61%) was prepared as a yellowish solid; m.p. 140-141 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.63 (m, 4H), 7.55 (dd, *J* = 8.2, 6.6 Hz, 4H), 7.46 – 7.35 (m, 3H), 7.27 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 144.3, 144.1, 142.2, 141.8, 139.8, 130.2, 129.0, 128.12, 128.06, 127.3, 125.3, 125.1, 21.5.

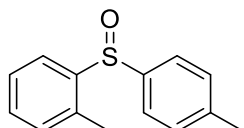


1-Methoxy-4-(*p*-tolylsulfinyl)benzene (**5k**)^[2]: According to the General Procedure, **5k** (31.7 mg, 86%) was prepared as an yellow oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.54-7.52 (m, 2H), 7.48-7.46 (m, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 6.95 – 6.91 (m, 2H), 3.79 (s, 3H), 2.35 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.0, 142.7, 141.4, 137.0, 130.0, 127.2, 124.8, 114.8, 55.6, 21.5.

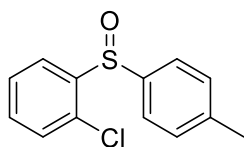


1-Methoxy-2-(*p*-tolylsulfinyl)benzene (**5l**)^[3]: According to the General Procedure, **5l**

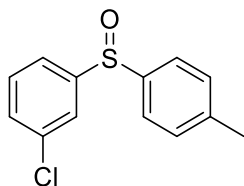
(26.6 mg, 72%) was prepared as a yellow solid; m.p. 86-87 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.90 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.38 (t, *J* = 8.1 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.13 (t, *J* = 7.8 Hz, 1H), 6.82 (d, *J* = 8.2 Hz, 1H), 3.77 (s, 3H), 2.33 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 155.6, 142.3, 141.4, 133.3, 132.1, 129.8, 125.5, 124.6, 121.7, 111.0, 55.8, 21.6.



1-Methyl-2-(*p*-tolylsulfinyl)benzene (**5m**)^[6]: According to the General Procedure, **5m** (24.2 mg, 70%) was prepared as a white solid; m.p. 90-91 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.5 Hz, 1H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.0 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 7.3 Hz, 1H), 2.34 (s, 3H), 2.30 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 143.1, 141.9, 141.4, 135.6, 131.0, 130.9, 130.1, 127.2, 126.3, 124.5, 21.6, 18.7.

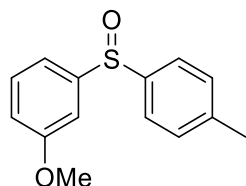


1-Chloro-2-(*p*-tolylsulfinyl)benzene (**5n**)^[6]: According to the General Procedure, **5n** (19.9 mg, 53%) was prepared as a yellow oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 143.2, 142.3, 141.0, 132.0, 131.1, 130.02, 129.98, 128.0, 126.2, 125.7, 21.5.

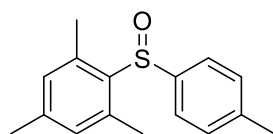


1-Chloro-3-(*p*-tolylsulfinyl)benzene (**5o**)^[7]: According to the General Procedure, **5o** (24.7 mg, 66%) was prepared as a colorless oil; ¹H NMR (500 MHz, Chloroform-*d*) δ

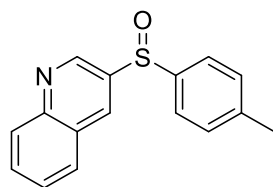
7.67 – 7.68 (m, 1H), 7.58 (d, $J = 8.2$ Hz, 2H), 7.55 – 7.51 (m, 1H), 7.44 – 7.41 (m, 2H), 7.32 (d, $J = 8.0$ Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, Chloroform- d) δ 148.0, 142.2, 141.9, 135.6, 131.0, 130.5, 130.3, 125.1, 124.5, 122.7, 21.5.



1-Methoxy-3-(*p*-tolylsulfinyl)benzene (**5p**)^[3]: According to the General Procedure, **5p** (27.0 mg, 73%) was prepared as a yellowish oil; ^1H NMR (400 MHz, Chloroform- d) δ 7.54 – 7.49 (m, 2H), 7.32 (t, $J = 7.9$ Hz, 1H), 7.27 – 7.19 (m, 3H), 7.12 (d, $J = 7.7$ Hz, 1H), 6.92 (dd, $J = 8.1, 2.3$ Hz, 1H), 3.80 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, Chloroform- d) δ 160.4, 147.1, 142.5, 141.8, 130.3, 130.2, 125.1, 117.3, 116.9, 109.0, 55.7, 21.5.

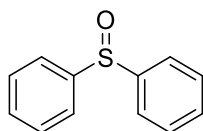


1,3,5-Trimethyl-2-(*p*-tolylsulfinyl)benzene (**5q**)^[2]: According to the General Procedure, **5q** (18.6 mg, 48%) was prepared as a yellow oil; ^1H NMR (400 MHz, Chloroform- d) δ 7.29 (d, $J = 8.2$ Hz, 2H), 7.21 (d, $J = 8.2$ Hz, 2H), 6.85 (s, 2H), 2.40 (s, 6H), 2.35 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (101 MHz, Chloroform- d) δ 142.2, 141.1, 140.0, 139.8, 136.7, 130.8, 129.7, 124.6, 21.4, 21.3, 19.5.

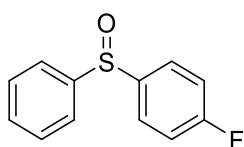


3-(*p*-Tolylsulfinyl)quinoline (**5r**)^[8]: According to the General Procedure, **5r** (18.8 mg, 47%) was prepared as a brown solid; m.p. 125-126 °C; ^1H NMR (400 MHz, Chloroform- d) δ 8.82 (d, $J = 2.2$ Hz, 1H), 8.59 (d, $J = 1.8$ Hz, 1H), 8.11 (d, $J = 8.5$ Hz,

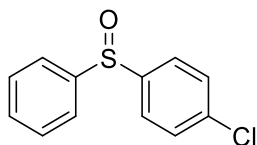
1H), 7.93 (s, 1H), 7.82 – 7.76 (m, 1H), 7.60 (dd, $J = 12.4, 7.7$ Hz, 3H), 7.27 (d, $J = 8.0$ Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 148.8, 145.9, 142.6, 141.3, 139.1, 132.9, 131.3, 130.5, 130.4, 129.6, 128.5, 128.0, 125.2, 21.5.



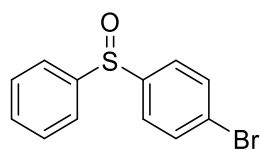
Sulfinyldibenzene (**5s**)^[2]: According to the General Procedure, **5s** (27.3 mg, 90%) was prepared as a yellow solid; m.p. 70-71 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.66 – 7.61 (m, 4H), 7.48 – 7.41 (m, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.6, 131.2, 129.5, 124.9.



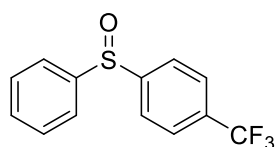
1-Fluoro-4-(phenylsulfinyl)benzene (**5t**)^[6]: According to the General Procedure, **5t** (27.4 mg, 83%) was prepared as a yellow oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.57 (m, 4H), 7.49 – 7.40 (m, 3H), 7.13 (t, $J = 8.6$ Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.4 (d, $J_{\text{C-F}} = 251.8$ Hz), 145.4, 141.2 (d, $J_{\text{C-F}} = 2.9$ Hz), 131.1, 129.4, 127.3 (d, $J_{\text{C-F}} = 9.0$ Hz), 124.6, 116.8 (d, $J_{\text{C-F}} = 22.5$ Hz); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.1.



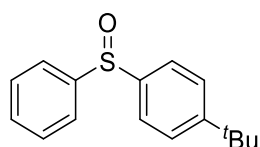
1-Chloro-4-(phenylsulfinyl)benzene (**5u**)^[2]: According to the General Procedure, **5u** (23.4 mg, 66%) was prepared as a yellow oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.59 (m, 2H), 7.59 – 7.54 (m, 2H), 7.49 – 7.43 (m, 3H), 7.43 – 7.39 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.3, 144.2, 137.4, 131.5, 129.7, 129.6, 126.2, 124.8.



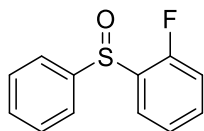
1-Bromo-4-(phenylsulfinyl)benzene (**5v**)^[2]: According to the General Procedure, **5v** (27.4 mg, 65%) was prepared as a yellow solid; m.p. 51-52 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.60 (m, 2H), 7.60 – 7.56 (m, 2H), 7.52 – 7.48 (m, 2H), 7.48 – 7.43 (m, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 145.2, 144.8, 132.6, 131.5, 129.6, 126.3, 125.7, 124.8.



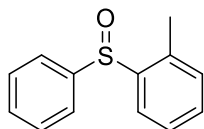
1-(Phenylsulfinyl)-4-(trifluoromethyl)benzene (**5w**)^[9]: According to the General Procedure, **5w** (25.5 mg, 63%) was prepared as a yellowish solid; m.p. 70-71 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 8.3 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.68 – 7.62 (m, 2H), 7.48 – 7.45 (m, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 149.8, 144.8, 132.9 (q, *J*_{C-F} = 33.7 Hz), 131.8, 130.4, 129.7, 126.4 (q, *J*_{C-F} = 3.8 Hz), 124.9, 123.5 (q, *J*_{C-F} = 273.6 Hz); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -62.8.



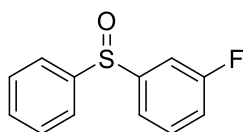
1-(*Tert*-butyl)-4-(phenylsulfinyl)benzene (**5x**)^[2]: According to the General Procedure, **5x** (26.3 mg, 68%) was prepared as a white solid; m.p. 87-88 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.64 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.54 (d, *J* = 8.7 Hz, 2H), 7.47 – 7.43 (m, 5H), 1.28 (s, 9H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 154.8, 145.6, 142.3, 131.0, 129.4, 126.5, 124.9, 124.9, 35.1, 31.3.



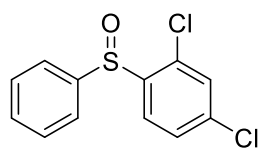
1-Fluoro-2-(phenylsulfinyl)benzene (**5y**): According to the General Procedure, **5y** (25.4 mg, 77%) was prepared as a white solid; m.p. 45-46 °C; ¹H NMR (500 MHz, Chloroform-*d*) δ 8.01 – 7.93 (m, 1H), 7.80 – 7.73 (m, 2H), 7.54 – 7.45 (m, 4H), 7.39 (m, 1H), 7.13 – 7.06 (m, 1H); ¹³C NMR (126 MHz, Chloroform-*d*) δ 158.3 (d, *J*_{C-F} = 248.1 Hz), 144.8, 133.2 (d, *J*_{C-F} = 15.6 Hz), 132.8 (d, *J*_{C-F} = 7.3 Hz), 131.4, 129.4, 125.4 (d, *J*_{C-F} = 3.3 Hz), 125.3, 124.9, 116.0 (d, *J*_{C-F} = 20.6 Hz); ¹⁹F NMR (470 MHz, CDCl₃) δ -113.9; HRMS (ESI): Calcd for [C₁₂H₉OFS+H]⁺: 221.0436, found: 221.0434.



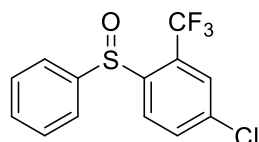
1-Methyl-2-(phenylsulfinyl)benzene (**5z**)^[2]: According to the General Procedure, **5z** (24.9 mg, 77%) was prepared as a yellow solid; m.p. 38-39 °C; ¹H NMR (500 MHz, Chloroform-*d*) δ 8.00 (d, *J* = 7.7 Hz, 1H), 7.64-7.67 (m, 2H), 7.51 – 7.41 (m, 5H), 7.22 (d, *J* = 7.4 Hz, 1H), 2.41 (s, 3H); ¹³C NMR (126 MHz, Chloroform-*d*) δ 144.7, 143.0, 135.8, 131.15, 131.05, 131.0, 129.4, 127.2, 126.0, 124.8, 18.6.



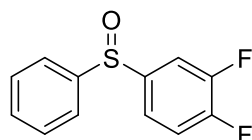
1-Fluoro-3-(phenylsulfinyl)benzene (**5aa**)^[10]: According to the General Procedure, **5aa** (27.4 mg, 83%) was prepared as a yellowish solid; m.p. 41-42 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.61 (m, 2H), 7.49 – 7.35 (m, 6H), 7.15 – 7.07 (m, 1H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 163.1 (d, *J*_{C-F} = 252.0 Hz), 148.2 (d, *J*_{C-F} = 5.5 Hz), 145.1, 131.6, 131.1 (d, *J*_{C-F} = 7.7 Hz), 129.6, 124.9, 120.4 (d, *J*_{C-F} = 3.2 Hz), 118.3 (d, *J*_{C-F} = 21.5 Hz), 111.8 (d, *J*_{C-F} = 24.0 Hz); ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -109.3.



2,4-Dichloro-1-(phenylsulfinyl)benzene (**5ab**): According to the General Procedure, **5ab** (21.9 mg, 54%) was prepared as a yellow solid; m.p. 47-48 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, $J = 8.4$ Hz, 1H), 7.74 – 7.67 (m, 2H), 7.50 – 7.43 (m, 4H), 7.34 (d, $J = 2.0$ Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.0, 142.1, 137.8, 131.9, 131.8, 130.0, 129.5, 128.6, 126.8, 126.0; HRMS (ESI): Calcd for $[\text{C}_{12}\text{H}_8\text{OSCl}_2+\text{H}]^+$: 270.9751, found: 270.9742.

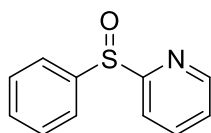


4-Chloro-1-(phenylsulfinyl)-2-(trifluoromethyl)benzene (**5ac**): According to the General Procedure, **5ac** (21.8 mg, 48%) was prepared as a yellow solid; m.p. 50-51 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, $J = 2.1$ Hz, 1H), 7.72 (dd, $J = 8.4, 2.2$ Hz, 1H), 7.67 – 7.62 (m, 2H), 7.59 (d, $J = 8.3$ Hz, 1H), 7.51 – 7.47 (m, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.2, 144.5, 135.3, 132.6, 132.0, 129.8, 128.8, 125.5 (q, $J_{\text{C-F}} = 3.6$ Hz), 124.8, 123.8 (q, $J_{\text{C-F}} = 5.4$ Hz), 122.2 (q, $J_{\text{C-F}} = 274.8$ Hz); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.9; HRMS (ESI): Calcd for $[\text{C}_{13}\text{H}_8\text{OF}_3\text{SCl}+\text{H}]^+$: 305.0015, found: 305.0012.

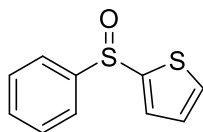


1,2-Difluoro-4-(phenylsulfinyl)benzene (**5ad**): According to the General Procedure, **5aa** (28.5 mg, 80%) was prepared as a colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.66 – 7.58 (m, 2H), 7.48 (dd, $J = 4.8, 2.1$ Hz, 4H), 7.39 (m, 1H), 7.27 – 7.24 (m, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.1 (dd, $J_{\text{C-F}} = 255.5, 12.1$ Hz), 151.0 (q,

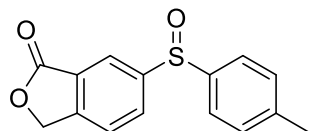
$J_{C-F} = 256.5, 13.1$ Hz), 145.0, 142.5, 131.7, 129.7, 124.7, 121.3 (dd, $J_{C-F} = 7.1, 4.0$ Hz), 118.5 (d, $J_{C-F} = 18.6$ Hz), 114.2 (d, $J_{C-F} = 19.3$ Hz). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -133.3, -132.5. HRMS (ESI): Calcd for $[\text{C}_{12}\text{H}_8\text{OF}_2\text{S}+\text{H}]^+$: 239.0342, found: 239.0345.



2-(Phenylsulfinyl)pyridine (**5ae**)^[2]: According to the General Procedure, **5ae** (9.1 mg, 30%) was prepared as a yellow solid; m.p. 61-62 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.53 (d, $J = 1.9$ Hz, 1H), 8.45 (d, $J = 4.7$ Hz, 1H), 7.59 (ddd, $J = 8.0, 2.3, 1.6$ Hz, 1H), 7.40 – 7.27 (m, 5H), 7.21 (ddd, $J = 8.0, 4.8, 0.8$ Hz, 1H).; ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.1, 148.0, 138.0, 134.0, 133.7, 131.9, 129.6, 128.0, 124.0.

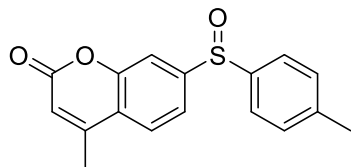


2-(Phenylsulfinyl) thiophene (**5af**)^[2]: According to the General Procedure, **5af** (16.5 mg, 53%) was prepared as a yellow oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.66 (m, 2H), 7.59 – 7.55 (m, 2H), 7.48 – 7.51 (m, 3H), 7.04 – 7.06 (m, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.1, 145.1, 132.6, 131.6, 131.3, 129.3, 127.4, 124.4.

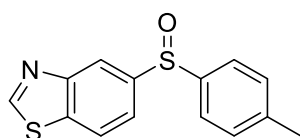


6-(*p*-Tolylsulfinyl) isobenzofuran-1(3*H*)-one (**7b**): According to the General Procedure, **7b** (30.3 mg, 74%) was prepared as a yellow solid; m.p. 132-133 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 8.05 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.62 (d, $J = 8.0$ Hz, 1H), 7.55 (d, $J = 8.2$ Hz, 2H), 7.29 (d, $J = 8.0$ Hz, 2H), 5.34 (s, 2H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.6, 148.8, 148.6, 142.5, 141.7, 130.4, 129.8,

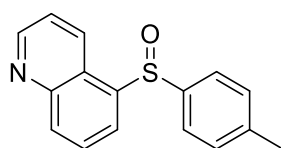
126.9, 124.9, 123.4, 122.4, 69.6, 21.5. HRMS (ESI): Calcd for $[C_{15}H_{12}O_3S+Na]^+$: 295.0405, found: 295.0408.



4-Methyl-7-(*p*-tolylsulfinyl)-2*H*-chromen-2-one (**7c**): According to the General Procedure, **7c** (29.0 mg, 65%) was prepared as a yellow solid; m.p. 138-139 °C; 1H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, $J = 8.2$ Hz, 1H), 7.60 – 7.53 (m, 4H), 7.29 (d, $J = 8.0$ Hz, 2H), 6.34 (s, 1H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.8, 153.6, 151.6, 150.2, 142.6, 141.7, 130.4, 125.7, 125.0, 121.8, 119.6, 116.5, 113.2, 21.5, 18.7. HRMS (ESI): Calcd for $[C_{17}H_{14}O_3S+Na]^+$: 321.0561, found: 321.0558.

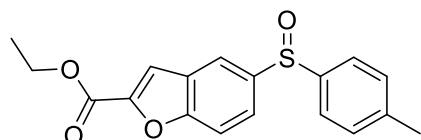


5-(*p*-Tolylsulfinyl)benzo[d]thiazole (**7d**): According to the General Procedure, **7d** (23.9 mg, 58%) was prepared as a white solid; m.p. 95-96 °C; 1H NMR (400 MHz, Chloroform-*d*) δ 9.08 (s, 1H), 8.42 (d, $J = 1.4$ Hz, 1H), 8.04 (d, $J = 8.4$ Hz, 1H), 7.70 (dd, $J = 8.4, 1.6$ Hz, 1H), 7.58 (d, $J = 8.2$ Hz, 2H), 7.28 – 7.25 (m, 2H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.9, 153.3, 144.8, 142.4, 141.9, 136.5, 130.2, 124.9, 123.1, 121.3, 120.3, 21.4. HRMS (ESI): Calcd for $[C_{14}H_{11}NO_2S+H]^+$: 274.0360, found: 274.0369.

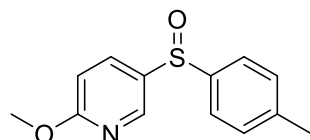


5-(*p*-Tolylsulfinyl)quinoline (**7e**): According to the General Procedure, **7e** (29.2 mg, 73%) was prepared as a yellow solid; m.p. 103-104 °C; 1H NMR (500 MHz,

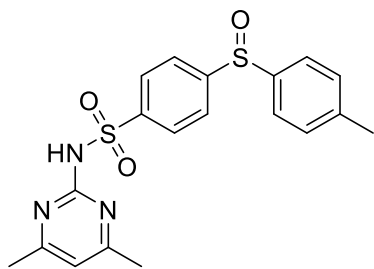
Chloroform-*d*) δ 9.03 (dd, $J = 4.2, 1.3$ Hz, 1H), 8.67 (d, $J = 8.5$ Hz, 1H), 8.34 – 8.29 (m, 2H), 7.99 – 7.92 (m, 1H), 7.78 (d, $J = 8.2$ Hz, 1H), 7.58 (d, $J = 8.2$ Hz, 2H), 7.27 (d, $J = 8.1$ Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.8, 147.9, 142.1, 132.8, 131.5, 130.4, 130.3, 129.2, 125.5, 125.4, 125.2, 124.9, 122.0, 21.4. HRMS (ESI): Calcd for $[\text{C}_{16}\text{H}_{13}\text{NOS}+\text{H}]^+$: 268.0796, found: 268.0802.



Ethyl 5-(*p*-tolylsulfinyl)benzofuran-2-carboxylate (**7f**): According to the General Procedure, **7f** (26.1 mg, 53%) was prepared as a yellow solid; m.p. 96-97 °C; ^1H NMR (500 MHz, Chloroform-*d*) δ 8.17 – 8.13 (m, 1H), 7.71 – 7.62 (m, 2H), 7.59 (d, $J = 8.4$ Hz, 3H), 7.32 – 7.30 (m, 2H), 4.49 (q, $J = 7.1$ Hz, 2H), 2.41 (s, 3H), 1.47 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.1, 156.7, 147.4, 142.5, 141.9, 141.7, 130.2, 127.7, 125.0, 124.0, 120.1, 113.61, 113.58, 61.9, 21.5, 14.3. HRMS (ESI): Calcd for $[\text{C}_{18}\text{H}_{16}\text{O}_4\text{S}+\text{Na}]^+$: 351.0667, found: 351.0670.

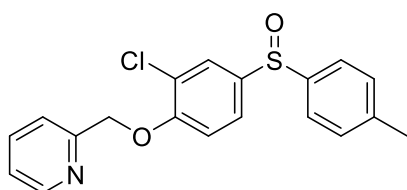


2-Methoxy-5-(*p*-tolylsulfinyl) pyridine (**7g**): According to the General Procedure, **7g** (22.6 mg, 61%) was prepared as a yellow oil; ^1H NMR (500 MHz, Chloroform-*d*) δ 8.46 (d, $J = 2.1$ Hz, 1H), 7.76 (dd, $J = 8.7, 2.4$ Hz, 1H), 7.55 (d, $J = 8.2$ Hz, 2H), 7.33 (d, $J = 8.0$ Hz, 2H), 6.83 (d, $J = 8.7$ Hz, 1H), 4.00 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.1, 145.6, 141.7, 138.9, 135.6, 134.7, 130.2, 124.6, 112.6, 54.1, 21.4. HRMS (ESI): Calcd for $[\text{C}_{13}\text{H}_{13}\text{NO}_2\text{S}+\text{H}]^+$: 248.0745, found: 248.0753.

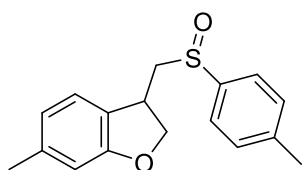


N-(4,6-dimethylpyrimidin-2-yl)-4-(p-tolylsulfinyl)benzenesulfonamide (**7h**):

According to the General Procedure, **7h** (37.3 mg, 62%) was prepared as a white solid; m.p. 70-71 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 8.5 Hz, 2H), 7.73 (d, *J* = 8.6 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.9 Hz, 2H), 6.66 (s, 1H), 2.36 (s, 9H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 168.4, 156.0, 151.1, 142.7, 142.2, 141.5, 130.5, 129.8, 125.3, 124.4, 115.0, 23.5, 21.6. HRMS (ESI): Calcd for [C₁₉H₁₉N₃O₃S₂+Na]⁺: 424.0766, found: 424.0764.



2-{[2-Chloro-4-(*p*-tolylsulfinyl)phenoxy]methyl}pyridine (**7i**): According to the General Procedure, **7i** (30.0 mg, 56%) was prepared as a yellow solid; m.p. 75-76 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.58 (d, *J* = 5.4 Hz, 1H), 7.74 (td, *J* = 7.7, 1.7 Hz, 1H), 7.66 (d, *J* = 2.2 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.53 – 7.43 (m, 3H), 7.28 (d, *J* = 8.5 Hz, 3H), 7.04 (d, *J* = 8.6 Hz, 1H), 5.29 (s, 2H), 2.38 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 156.0, 153.7, 149.2, 142.0, 141.9, 138.6, 137.2, 130.2, 127.0, 125.0, 124.8, 124.4, 123.0, 121.2, 113.9, 71.4, 21.4. HRMS (ESI): Calcd for [C₁₉H₁₆NO₂SCl+H]⁺: 358.0669, found: 358.0676.



6-Methyl-3-((*p*-tolylsulfinyl)methyl)-2,3-dihydrobenzofuran (**9**): According to the

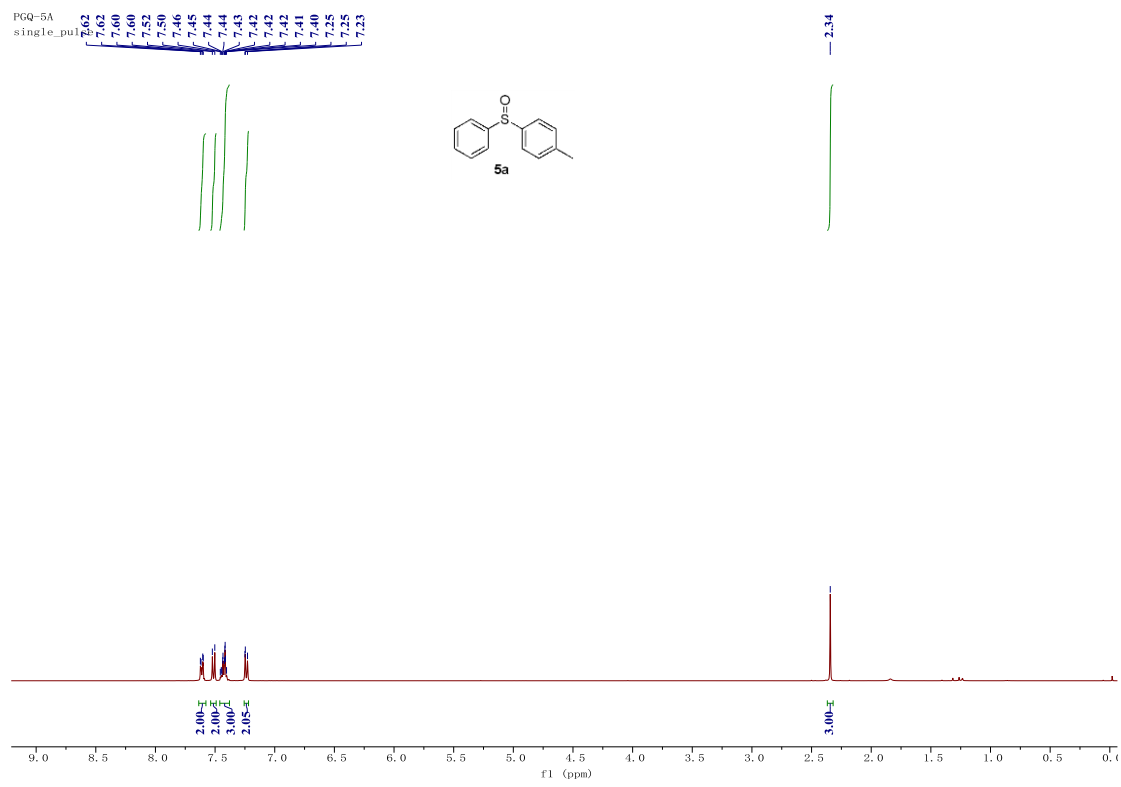
General Procedure, **9** (19.3 mg, 45%, dr = 1:1) was prepared as a yellow oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 8.1 Hz, 2H), 7.33 (dd, *J* = 8.2, 2.6 Hz, 2H), 7.10 and 6.82 (s, 1H), 6.92 (dd, *J* = 14.6, 8.0 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 4.70 – 4.75 and 4.12 – 4.1 (m, 1H), 4.54 – 4.49 (m, 1H), 4.00 – 3.79 (m, 1H), 3.15 – 2.92 (m, 2H), 2.40 (s, 3H), 2.27 and 2.21 (s, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 157.6, 142.0, 141.9, 140.4, 140.0, 130.28, 130.27, 129.6, 129.5, 128.4, 128.3, 125.4, 124.8, 124.0, 109.6, 76.3, 75.9, 62.2, 62.0, 37.1, 36.9, 21.6, 21.5, 20.9, 20.8. HRMS (ESI): Calcd for [C₁₇H₁₈O₂S+Na]⁺: 309.0925, found: 309.0928.

References

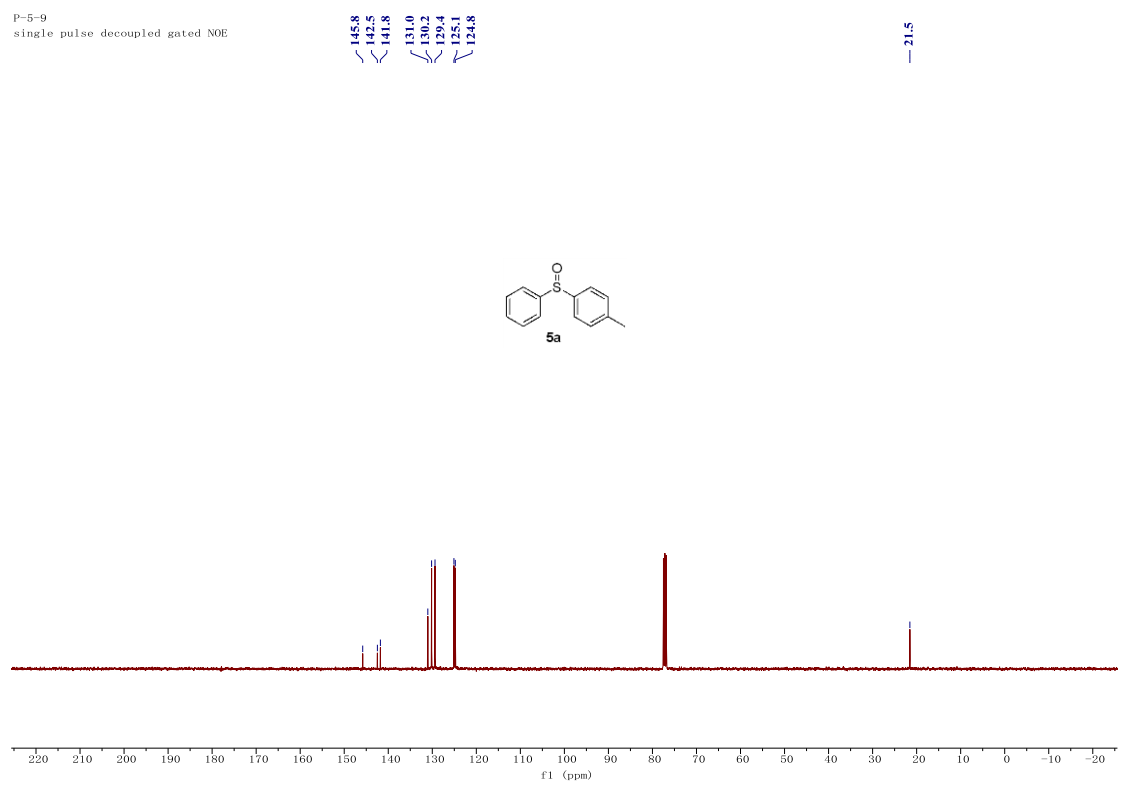
- [1] T. Zhong, M.-K. Pang, Z.-D. Chen, B. Zhang, J. Weng, and G. Lu, *Org. Lett.*, **2020**, 22 (8), 3072-3078.
- [2] H. Yu, Zh. Li, and C. Bolm, *Org. Lett.*, **2018**, 20 (22), 7104-7106.
- [3] G. Maitro, S. Vogel, G. Prestat, D. Madec, and G. Poli, *Org. Lett.*, **2006**, 8 (26), 5951-5954.
- [4] L. Wang, M.Chen, J. Zhang, *Org. Chem. Front.*, **2019**, 6(1), 32-35.
- [5] J. Wang, F. Shi, D. Dai, L. Xiong, Y. Yang, *Phosphorus, Sulfur Silicon Relat. Elem.*, **2021**, 196(5), 439-443.
- [6] H.-J. Xu, Y.-C. Lin, X. Wan, C.-Y. Yang, Y.-S. Feng, *Tetrahedron*, **2010**, 66 (46), 8823.
- [7] D. Augros, B. Yalcouye, A. Berthelot-Brehier, M. Chesse, S. Choppin, A. Panossian, F. R. Leroux, *Tetrahedron*, **2016**, 72(34), 5208-5220.
- [8] S. Dumouchel, F. Mongin, F. Trécourt, G. Quéguiner, *Tetrahedron*, **2003**, 59(43), 8629-8640.
- [9] T. Jia, A. Bellomo, S. Montel, M. Zhang, K. EL Baina, B. Zheng, P. J. Walsh, *Angew. Chem. Int. Ed.*, **2014** 53 (1), 260-264.
- [10] M. Shigeno, K. Hanasaka, I. Tohara, K. Izumi, H. Yamakoshi, E. Kwon, K. Nozawa-Kumada, and Y. Kondo, *Org. Lett.*, **2022**, 24 (3), 809-814.

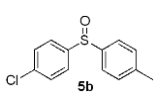
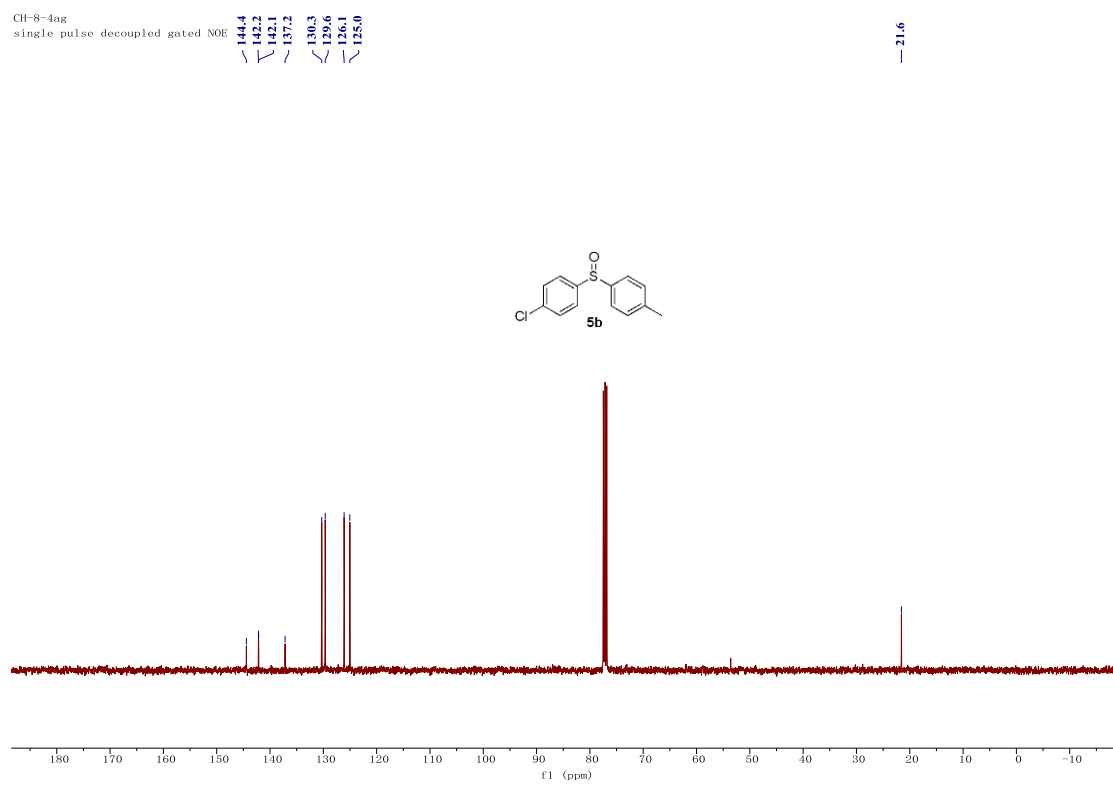
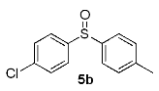
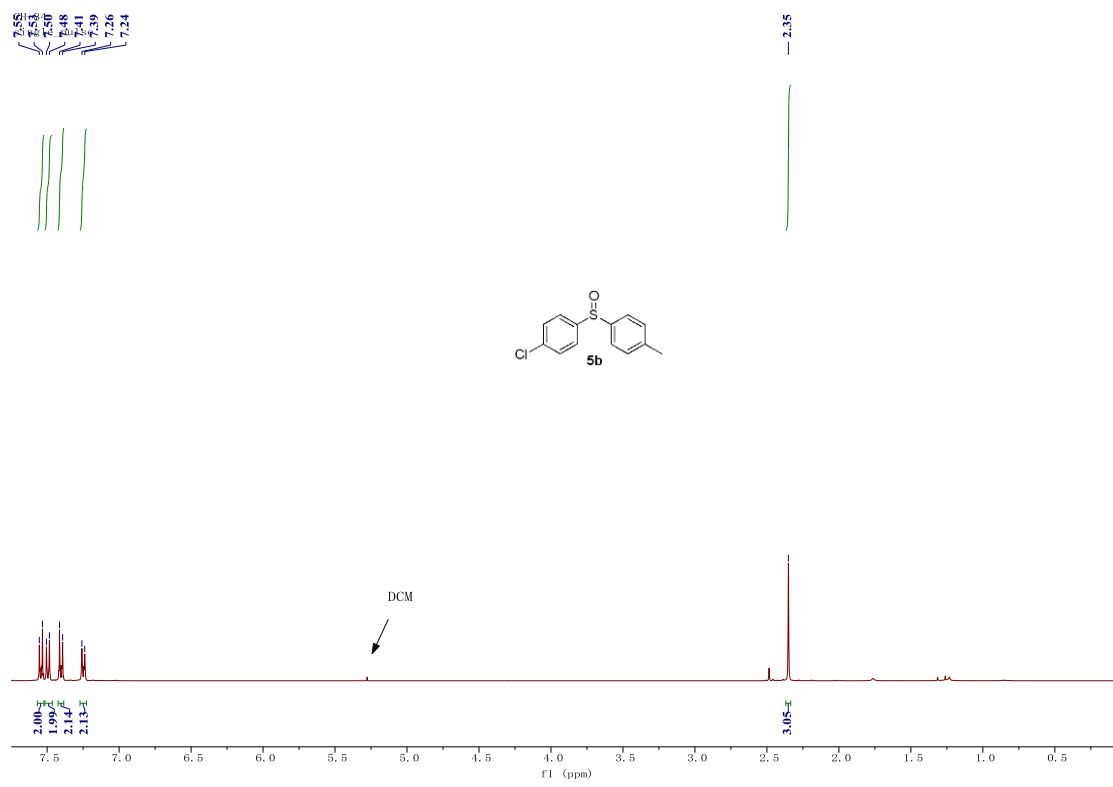
7. NMR spectra for all compounds

PGQ-5A
single_pulse

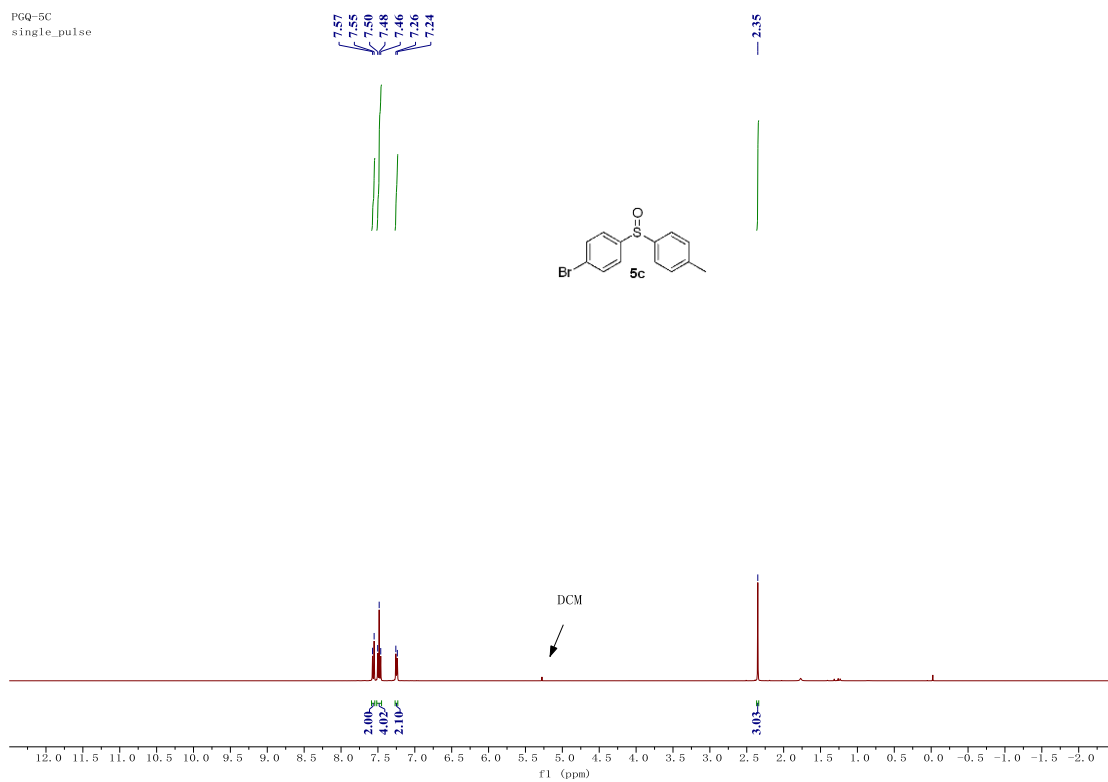


P-5-9
single pulse decoupled gated NOE

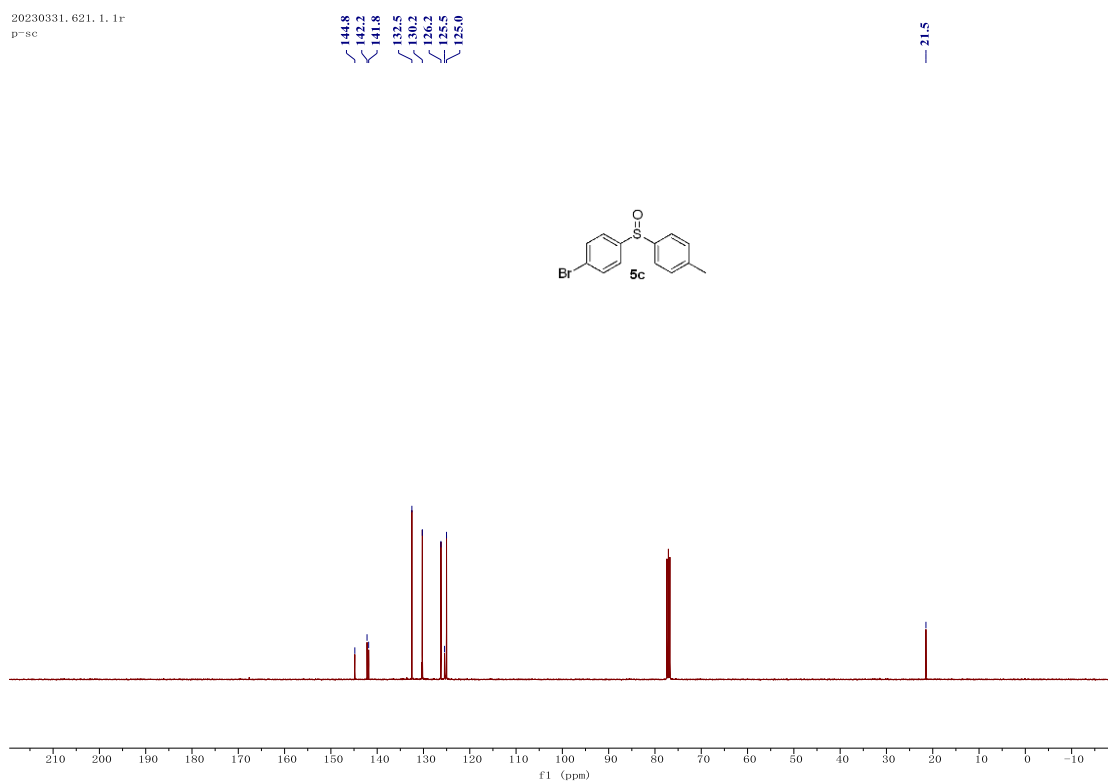




PGQ-5C
single_pulse



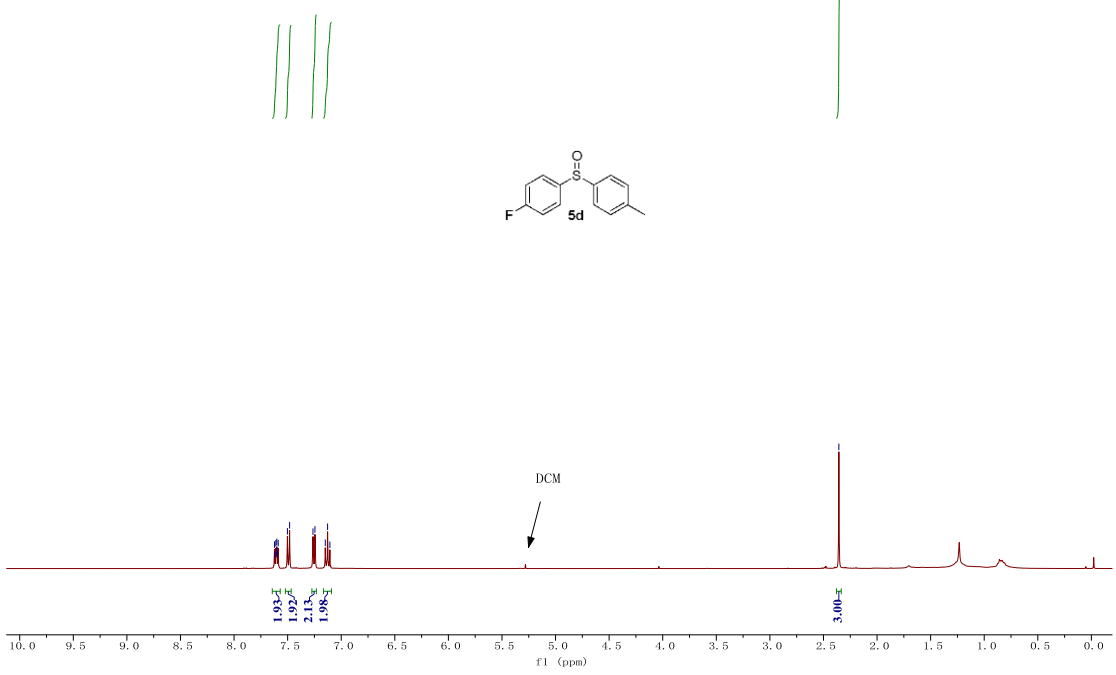
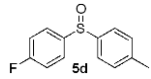
20230331.621.1.1r
p=sc



CH-83
single_pulse

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7.62
7.61
7.60
7.59
7.50
7.48
7.26
7.25
7.15
7.11

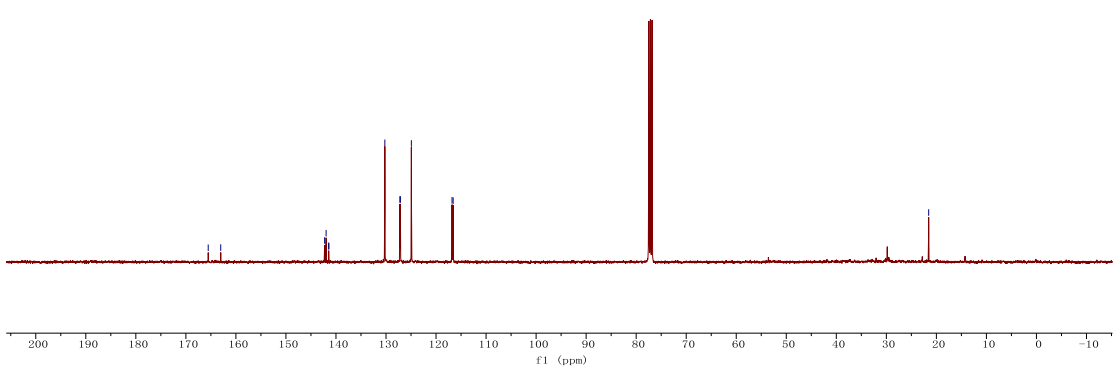
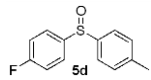
2.36



CH-8-3
single pulse decoupled gated

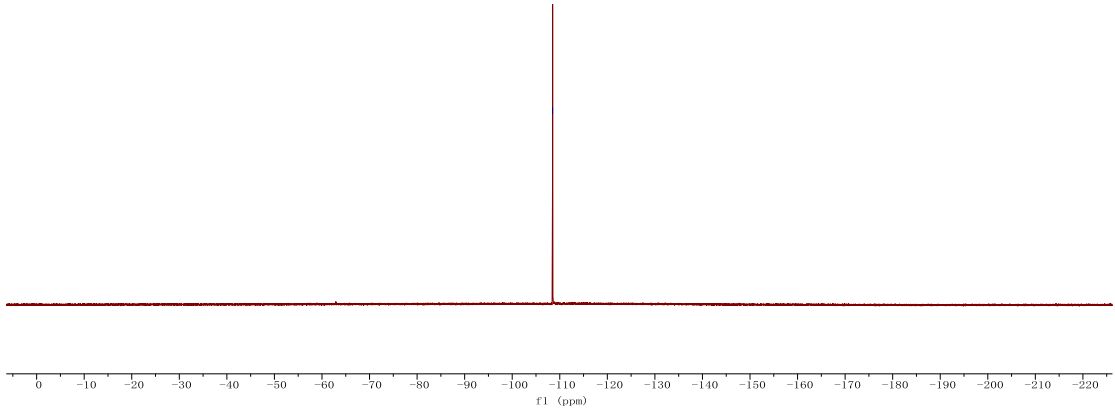
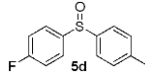
165.5
163.0
142.3
142.0
141.5
141.4
130.2
127.2
127.1
124.9
116.8
116.6

21.5



GH-8-3
single_pulse

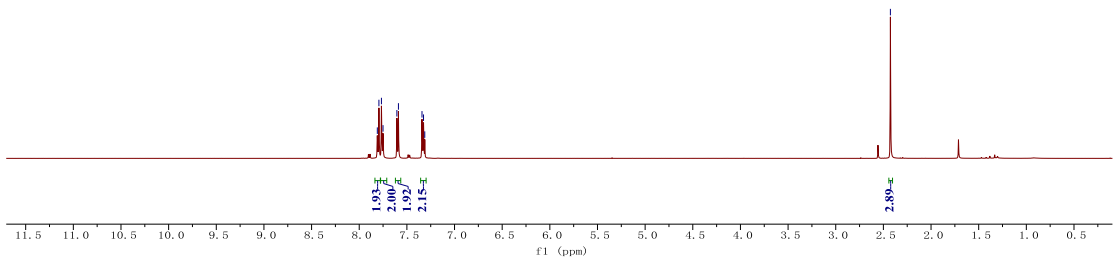
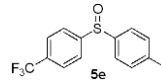
-108.5



0106-H.526.1.1r
2023-01-06 1H-526 CDCL3 WDH-526 (ZDQ-P-11-7)

7.81
7.79
7.77
7.75
7.60
7.59
7.34
7.33
7.31

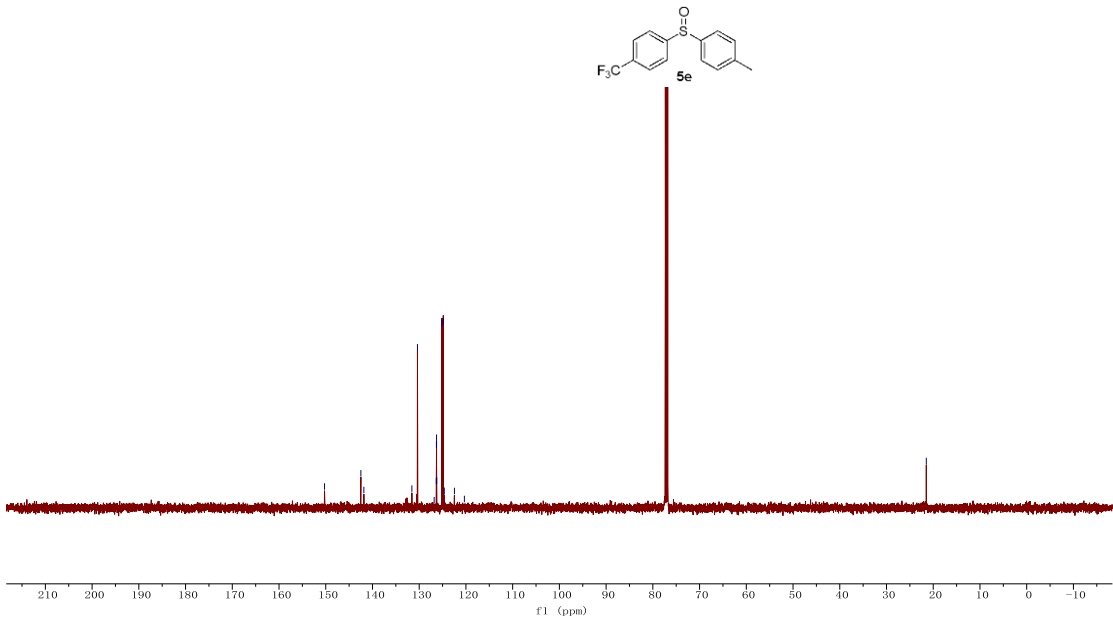
2.43



0106_20.1.1r
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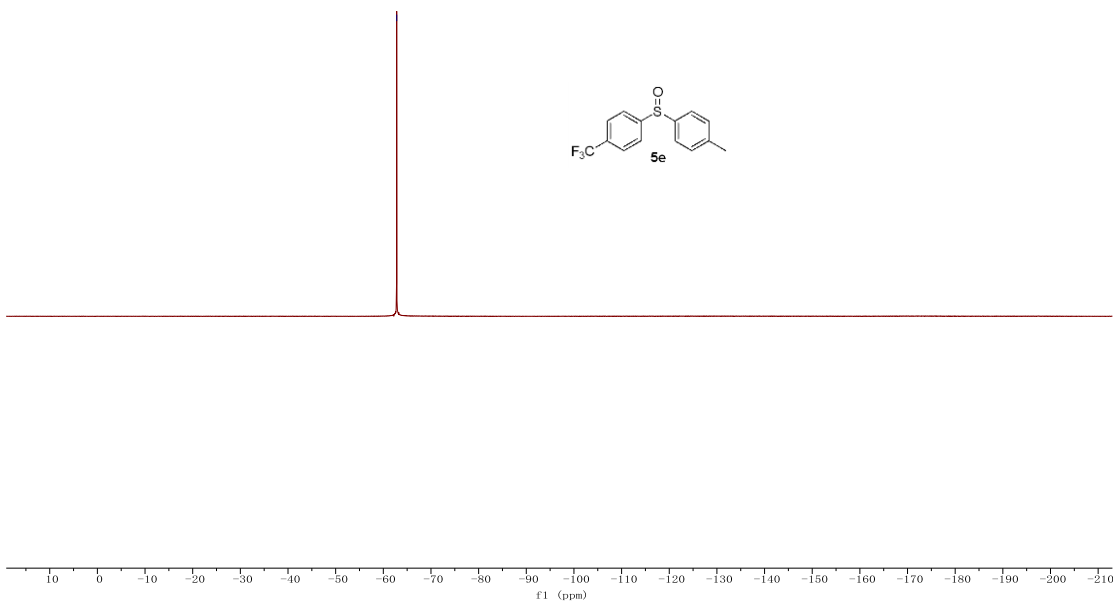
150.3
142.5
141.8
131.6
130.4
126.8
126.3
126.3
125.2
124.8
124.6
122.5
120.3

21.5

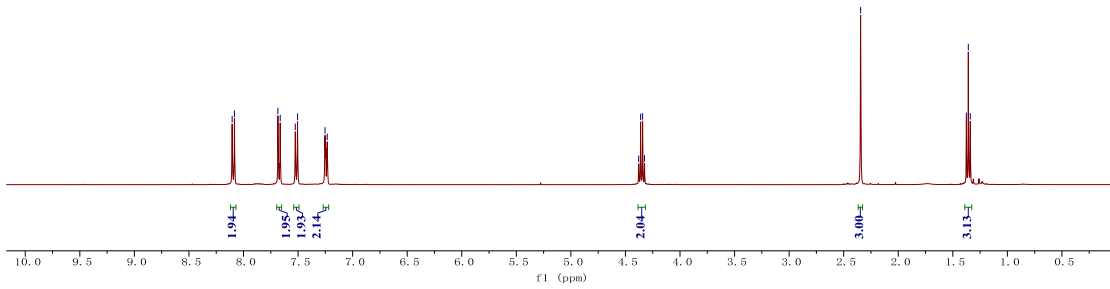
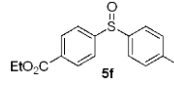
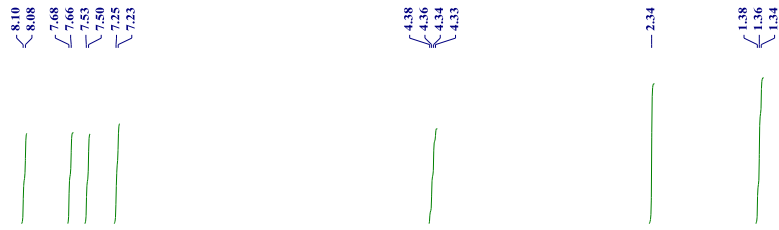


0106_10.2.1r
2023-01-06 19F-9 CDCL3 (ZDQ-P-11-7)

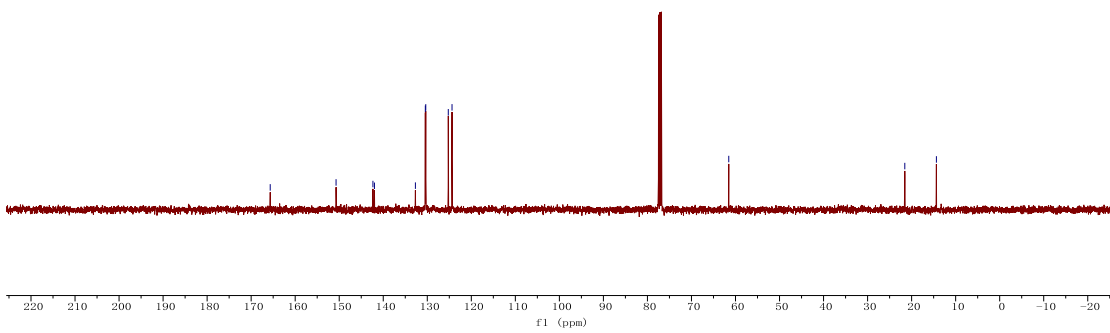
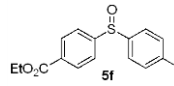
-62.8



CXY-91-G
single_pulse

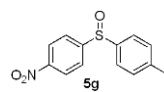
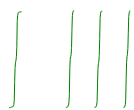


CXY-91-G
single_pulse decoupled gated NOE

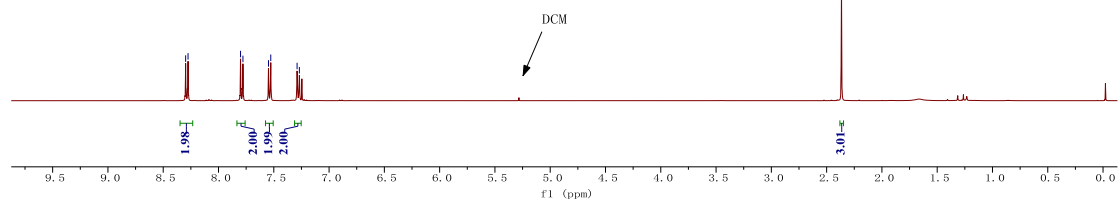


PGQ-5G
single_pulse

8.30
8.28
7.80
7.78
7.55
7.53
7.29
7.27

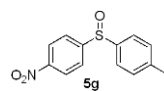


2.37

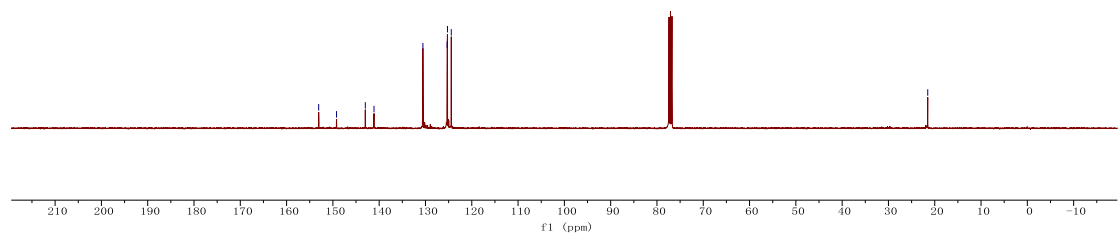


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p=s8

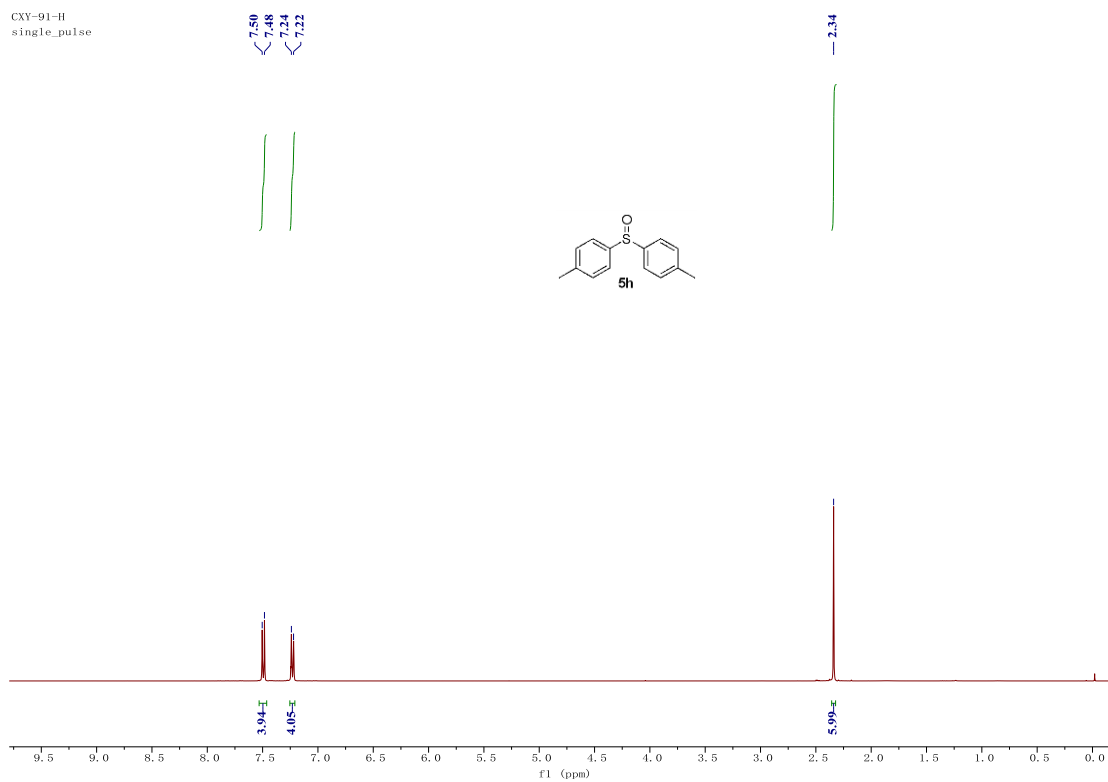
153.1
149.2
143.0
141.1
130.6
125.3
125.3
124.4



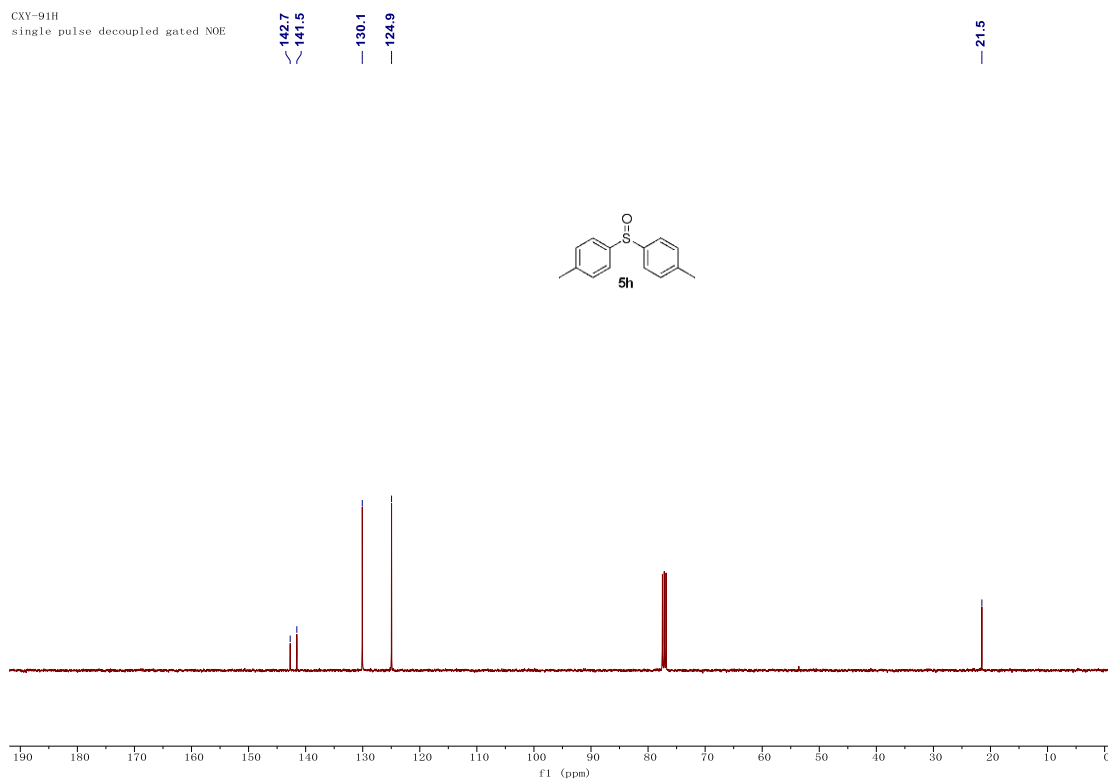
21.5

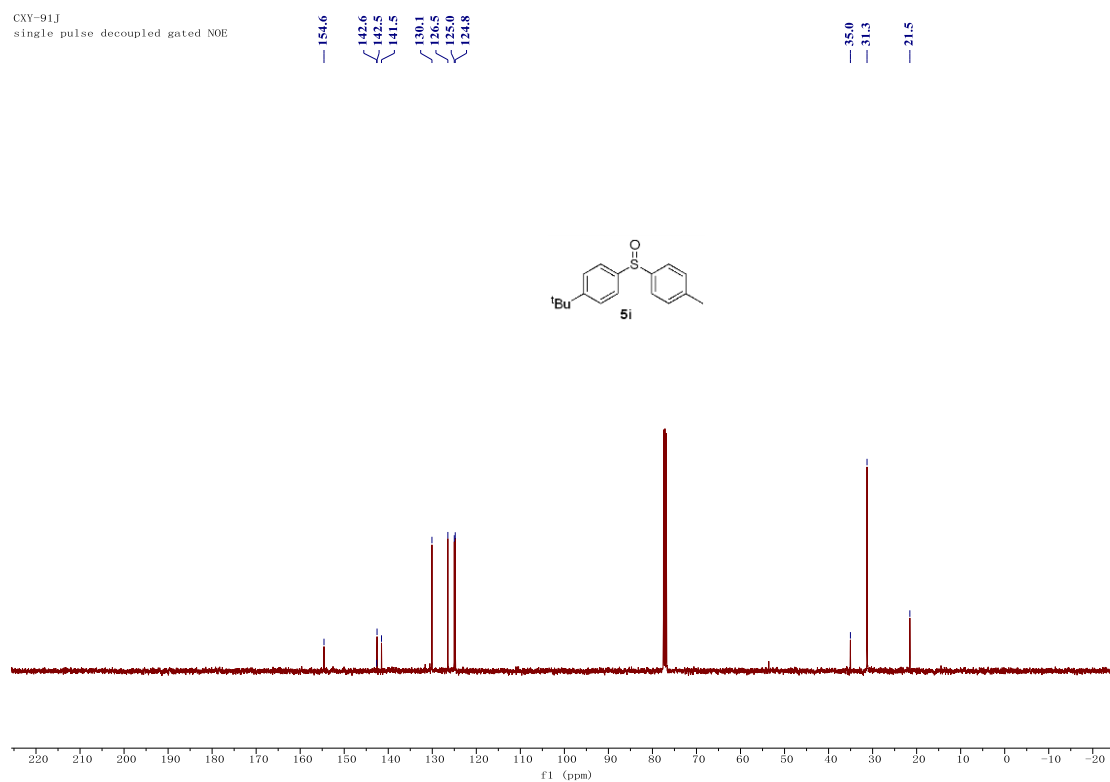
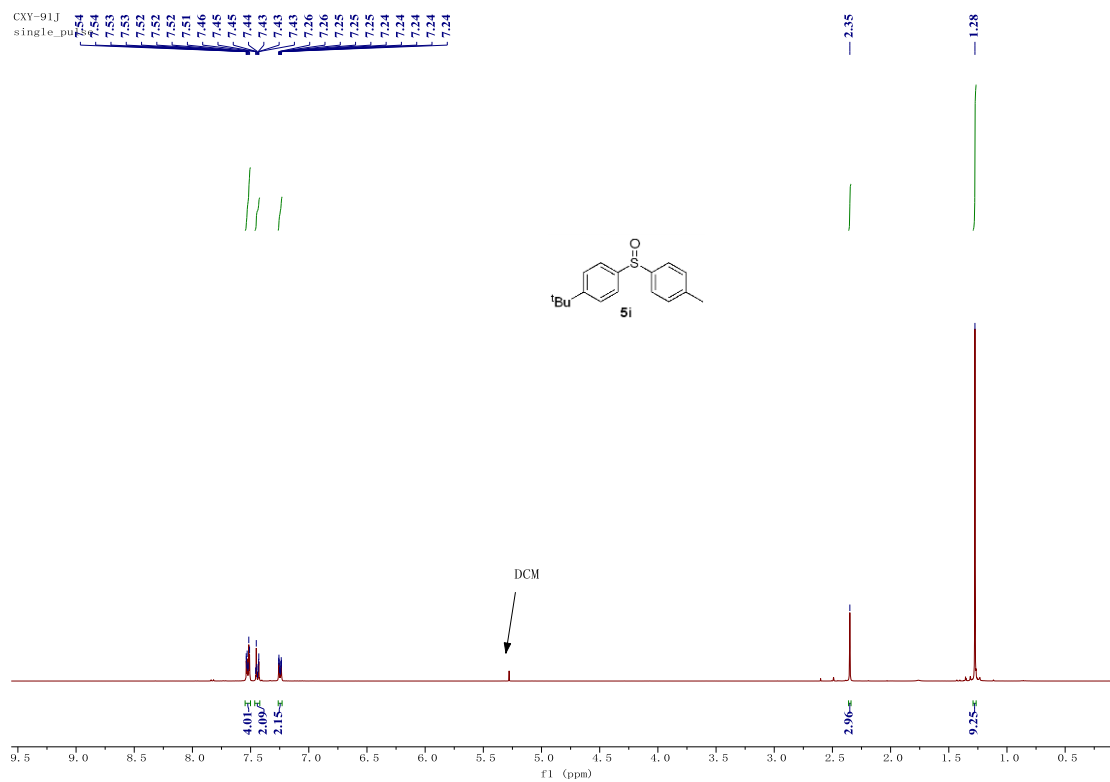


CXY-91-H
single_pulse



CXY-91H
single pulse decoupled gated NOE

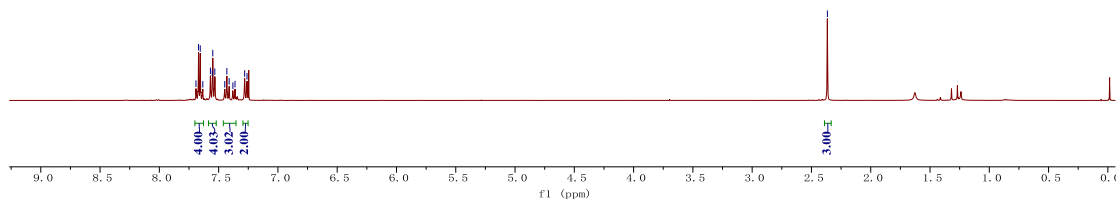
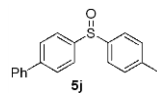




PGQ-5J
single_pulse

7.69
7.67
7.66
7.63
7.57
7.55
7.53
7.45
7.43
7.41
7.38
7.36
7.28
7.26

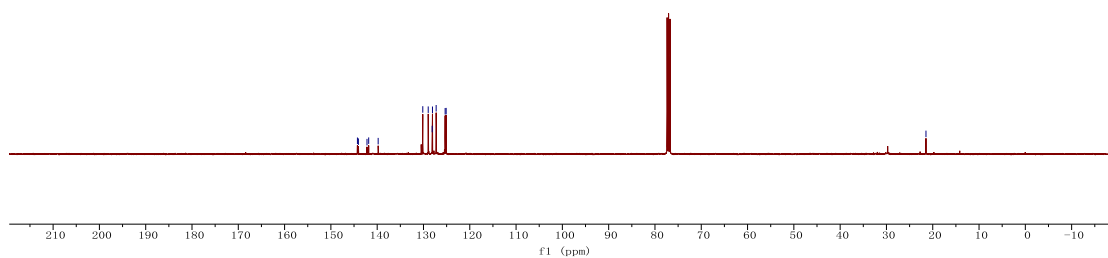
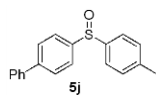
2.37

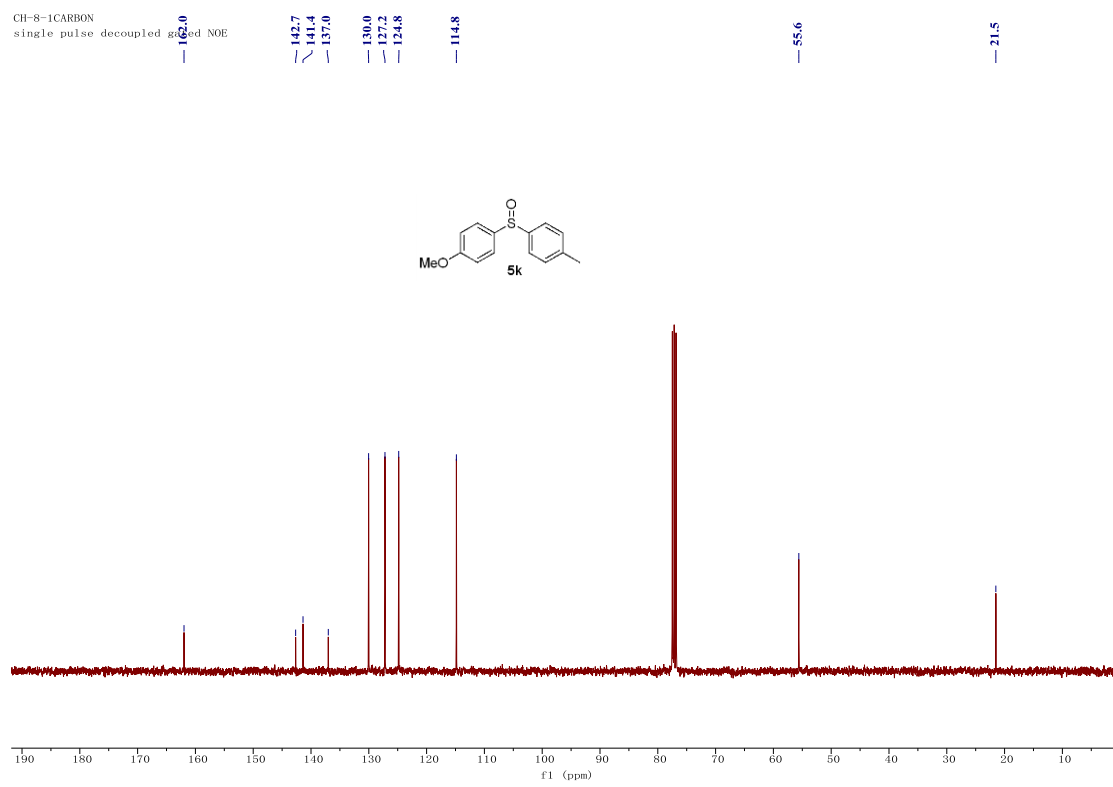
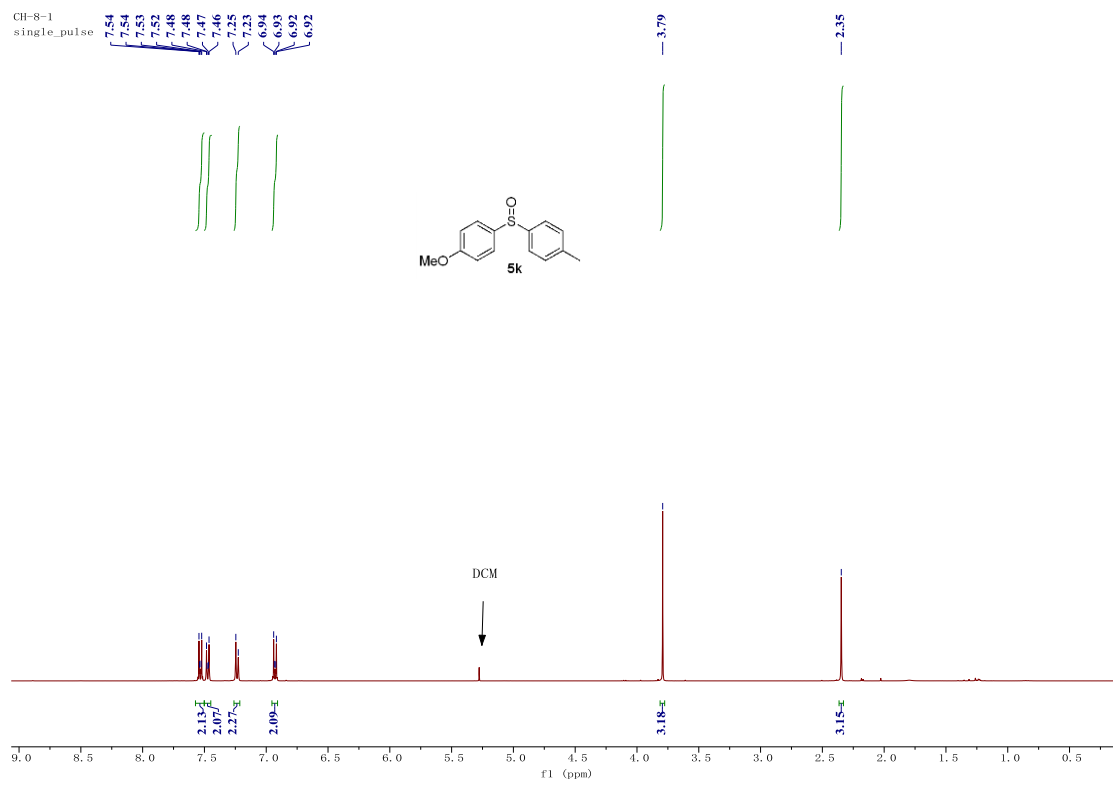


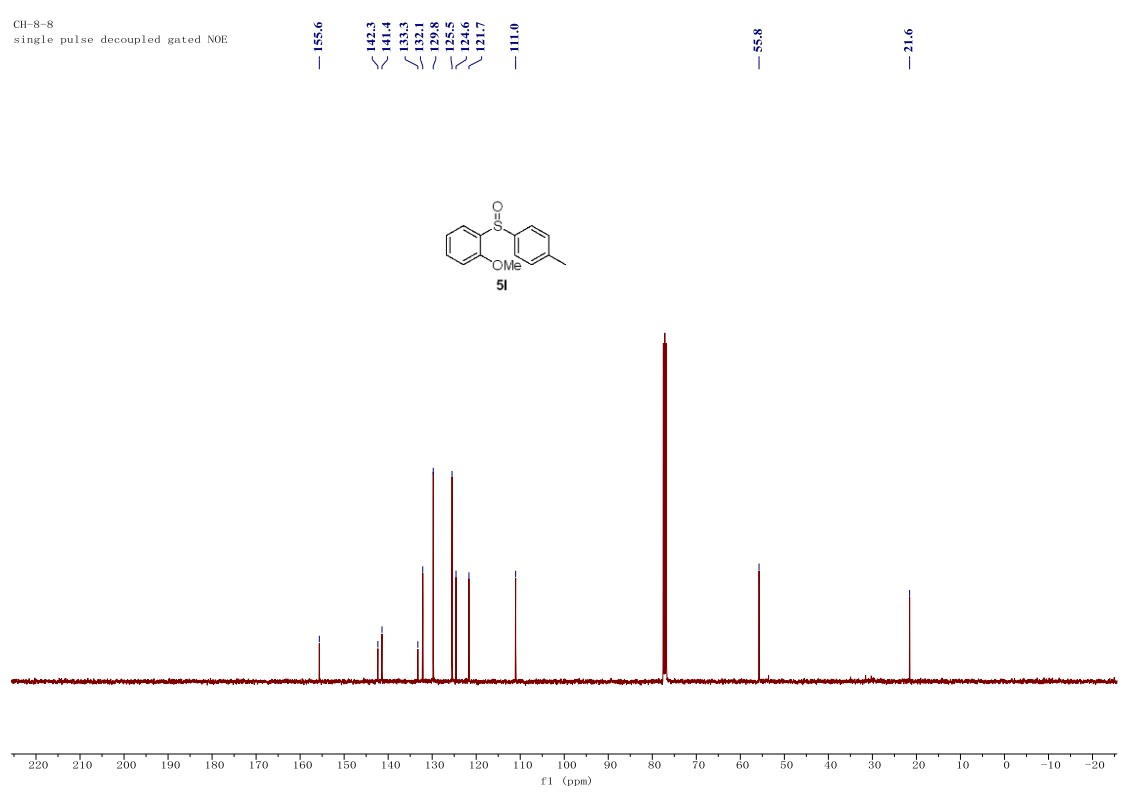
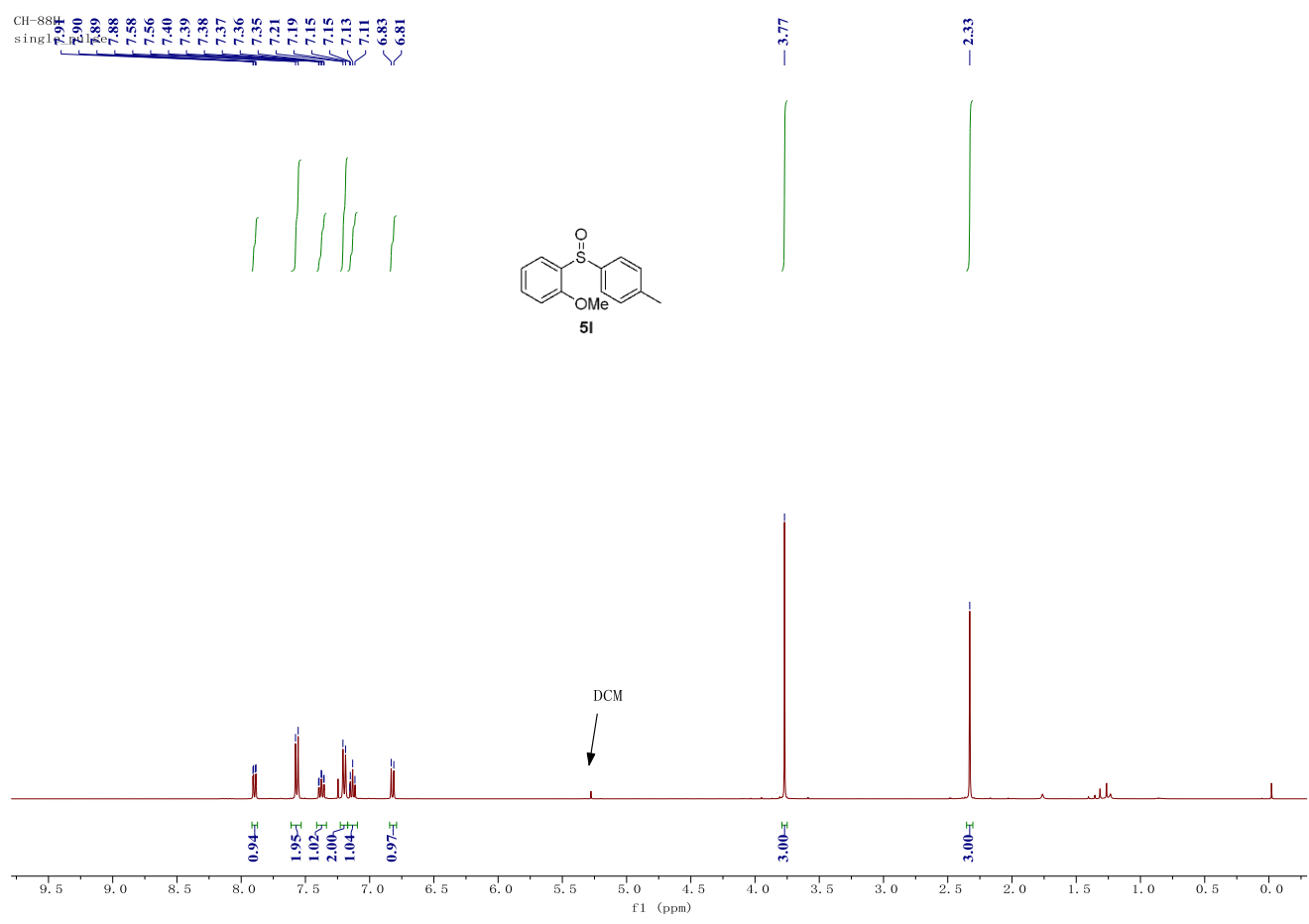
20230331.641.1.1r
p=s.j

144.3
144.1
142.2
141.8
139.8
130.2
129.0
128.1
128.1
125.3
125.1

21.5



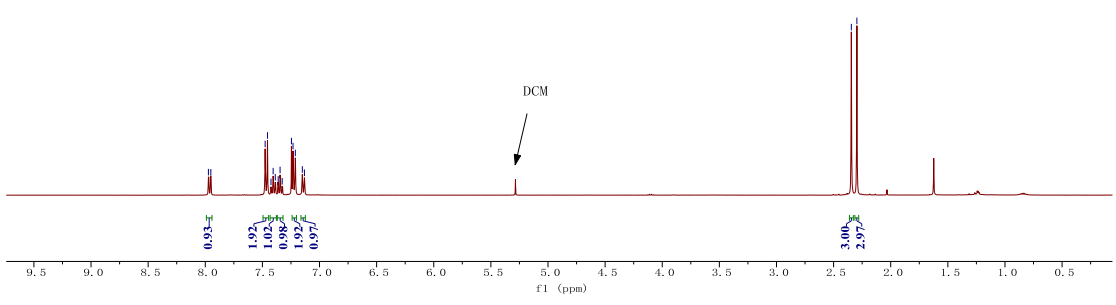
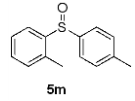
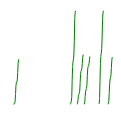




HY-11-2
single_pulse

7.97
7.95
7.48
7.46
7.42
7.41
7.39
7.36
7.35
7.35
7.35
7.33
7.31
7.15
7.13

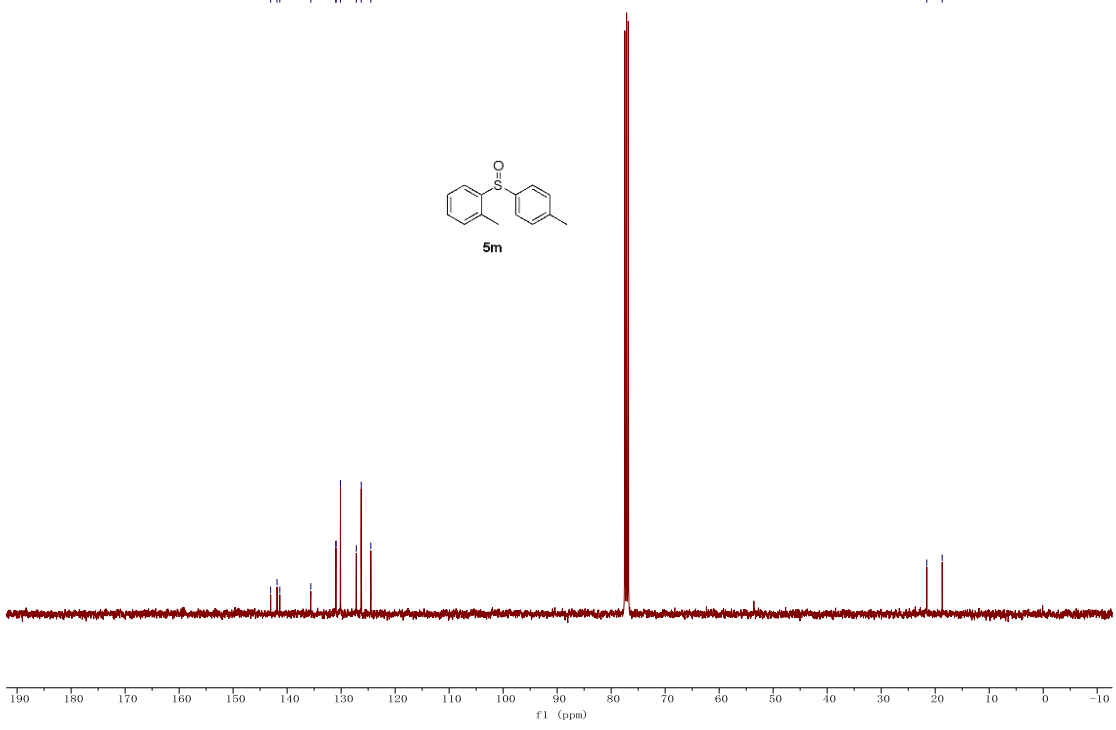
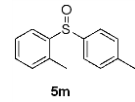
2.34
2.30



HY-11-2
single pulse decoupled gated NOE

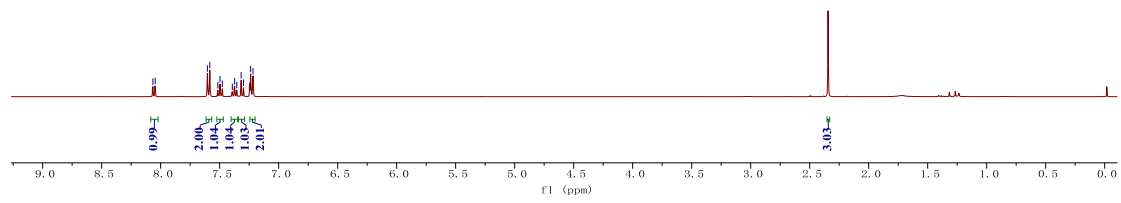
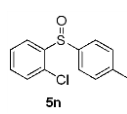
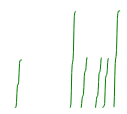
143.1
141.9
141.4
135.6
131.0
130.9
130.1
127.2
126.3
124.5

21.6
18.7



PGQ-5Q
single_pulse

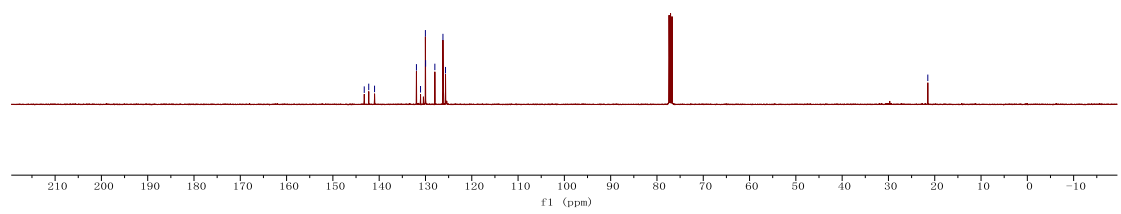
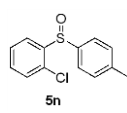
8.07
8.05
7.60
7.58
7.52
7.50
7.48
7.39
7.37
7.35
7.32
7.30
7.24
7.22

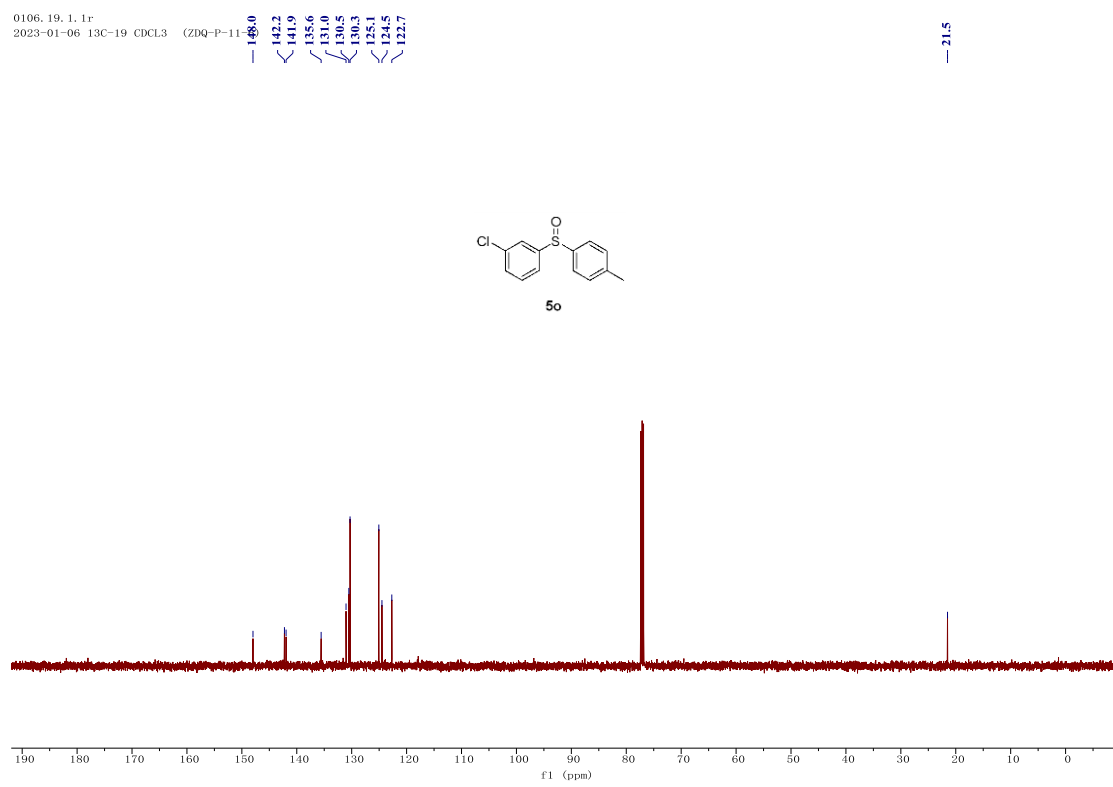
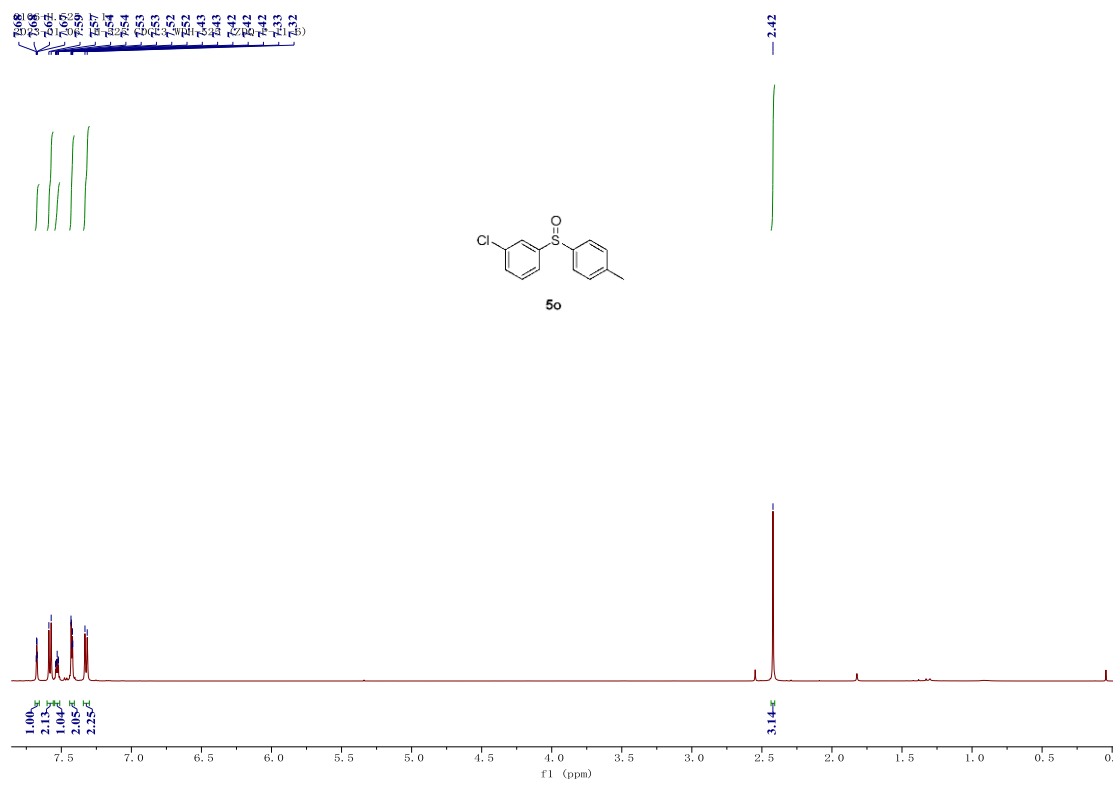


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p=sq

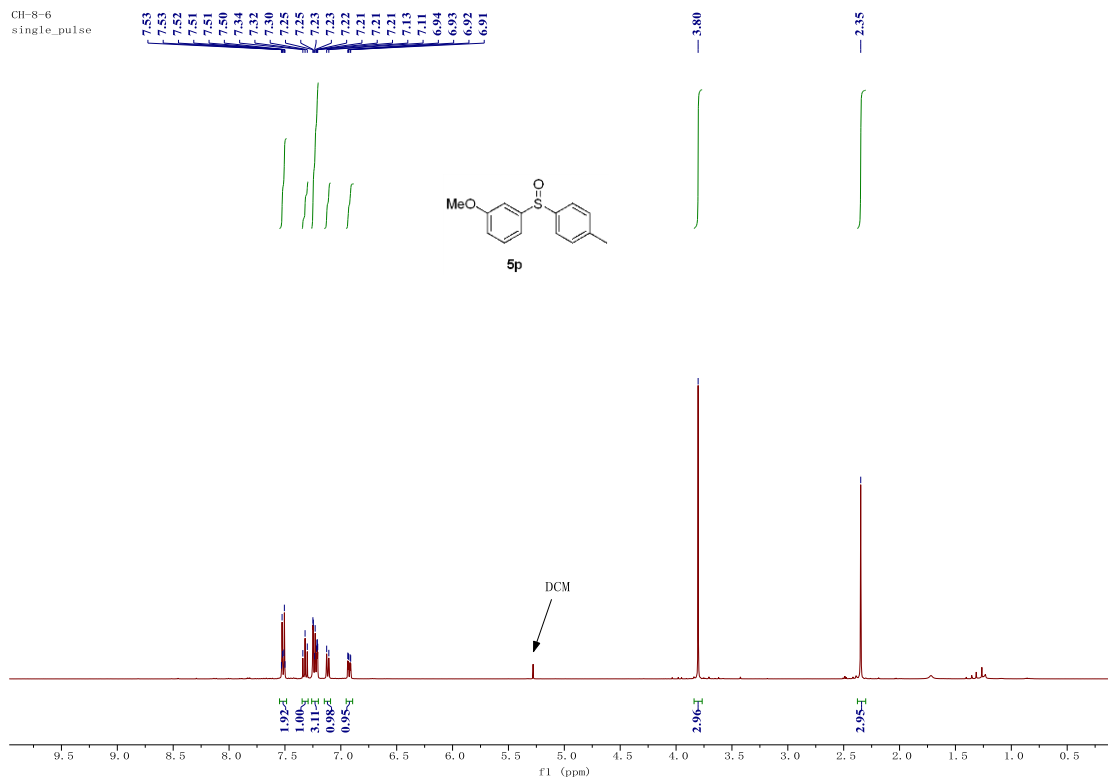
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142.3
141.0
132.0
131.1
130.0
128.0
126.2
125.7

21.5

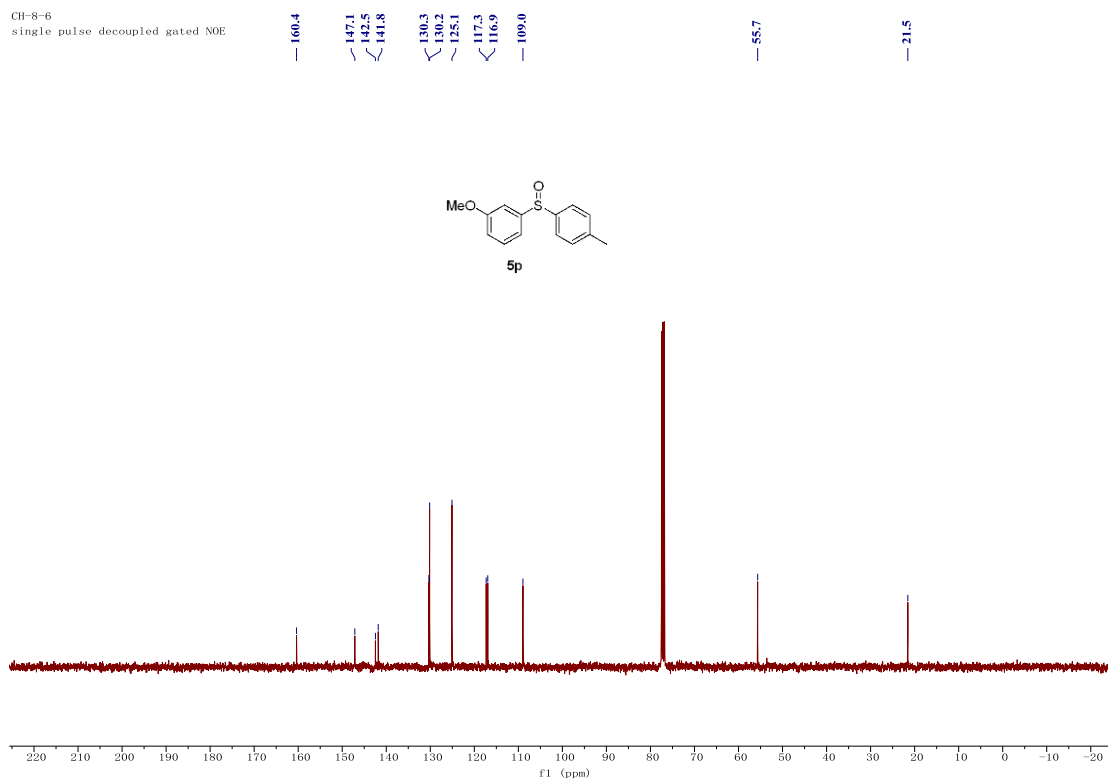




CH-8-6
single_pulse



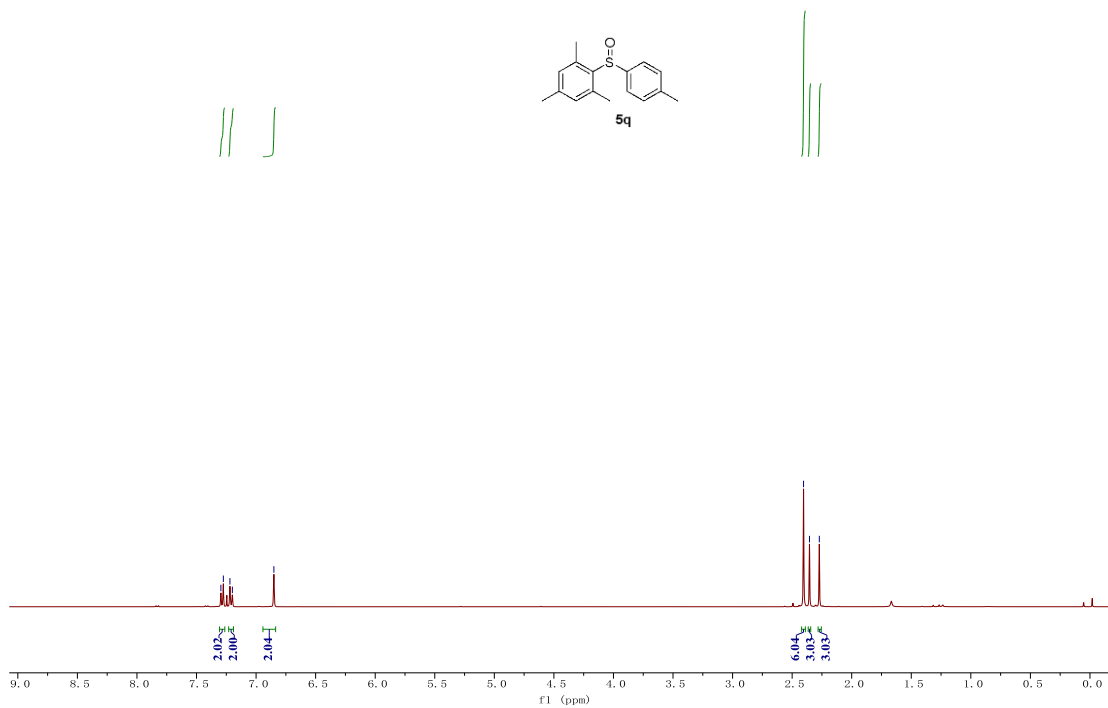
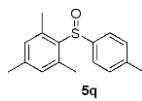
CH-8-6
single pulse decoupled gated NOE



PGQ-5N 1
single_pulse

7.30
7.27
7.22
7.20
6.85

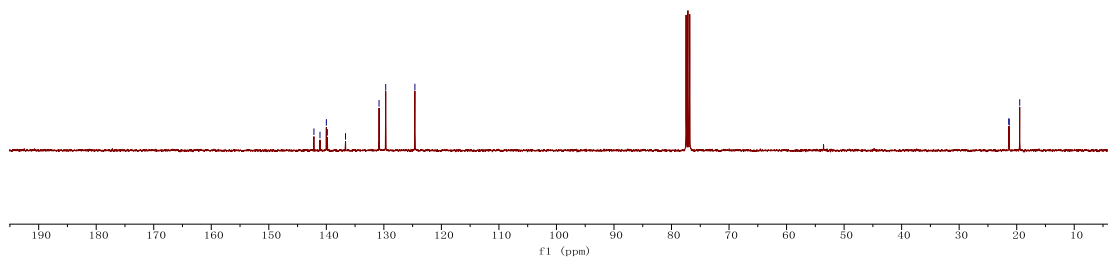
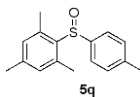
2.40
2.35
2.27



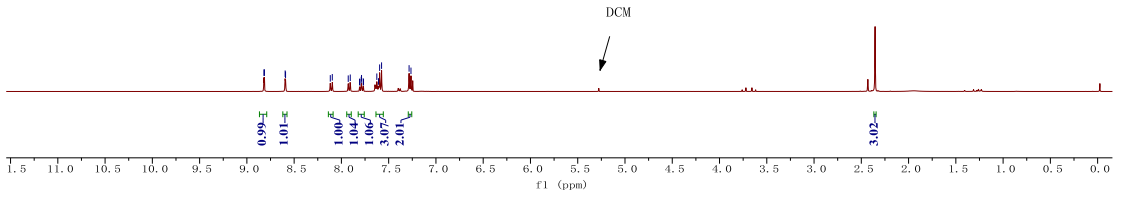
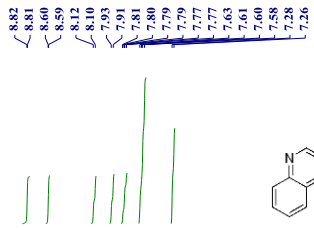
HY-10-6 1
single pulse decoupled gated NOE

142.2
141.1
140.0
139.8
136.7
130.8
129.7
124.6

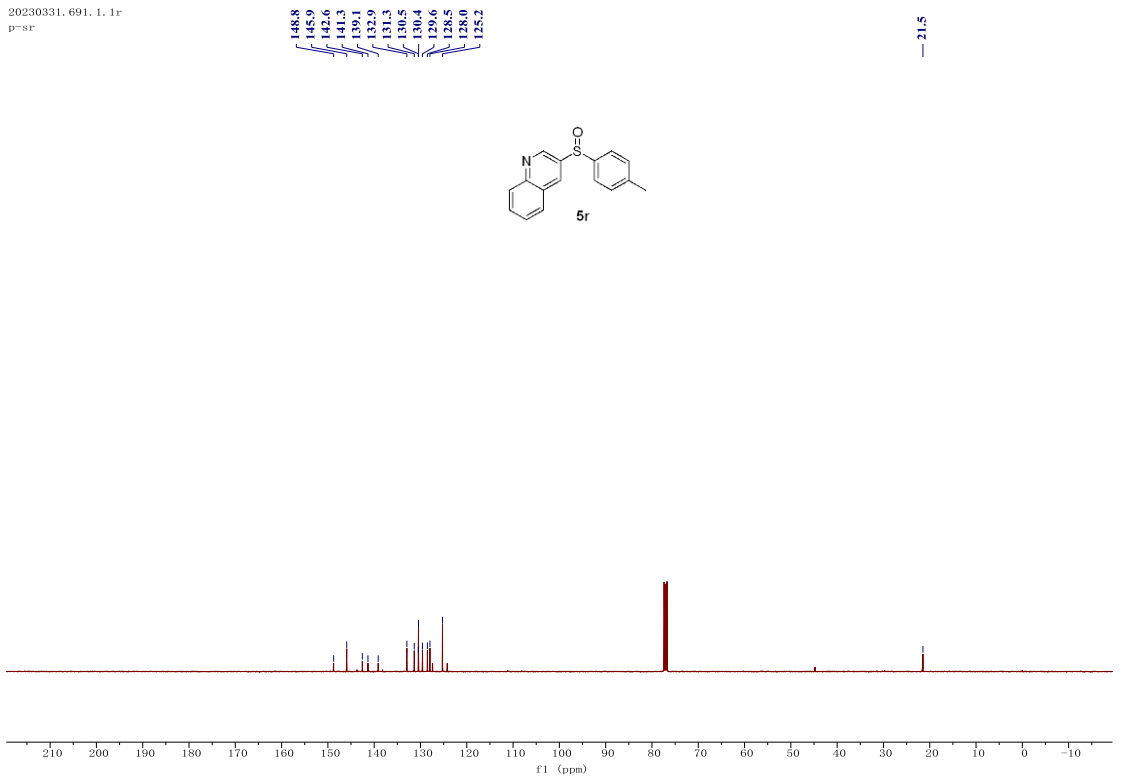
21.4
21.3
19.5



PGQ-11-9
single_pulse

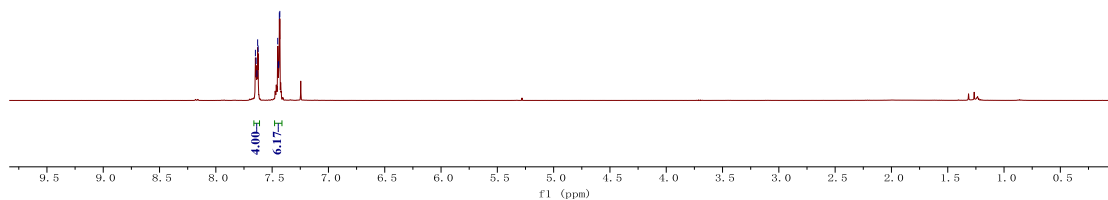
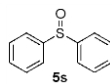
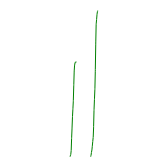


20230331.691.1.1r
p-sr



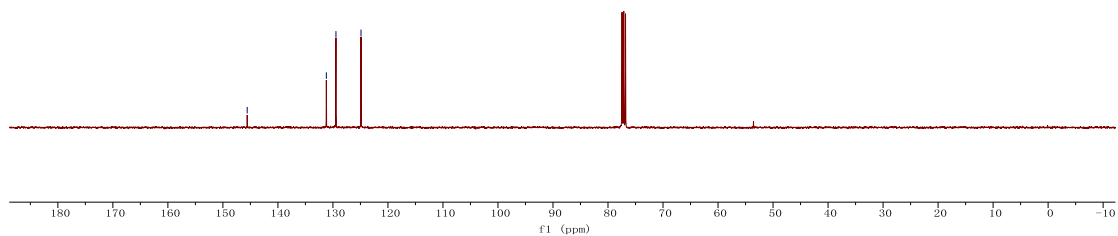
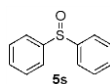
HY-8-3
single_pulse

7.65
7.64
7.64
7.63
7.62
7.45
7.44
7.44
7.43



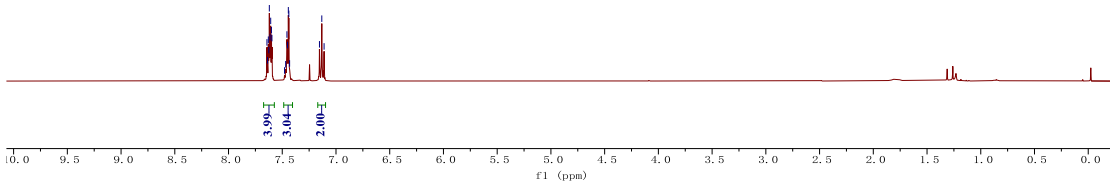
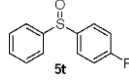
HY-8-3
single pulse decoupled gated NOE

145.6
131.2
129.5
124.9



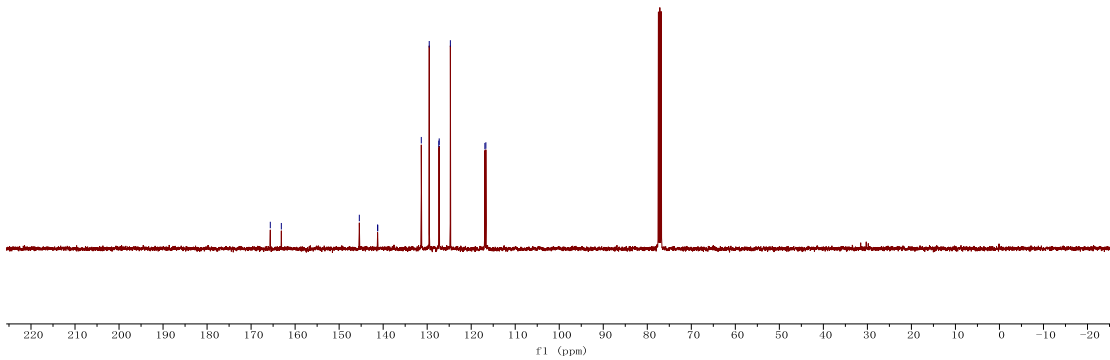
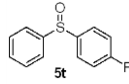
CH-7-1
single_pulse

7.64
7.64
7.63
7.62
7.61
7.60
7.48
7.47
7.46
7.45
7.44
7.44
7.43
7.15
7.11



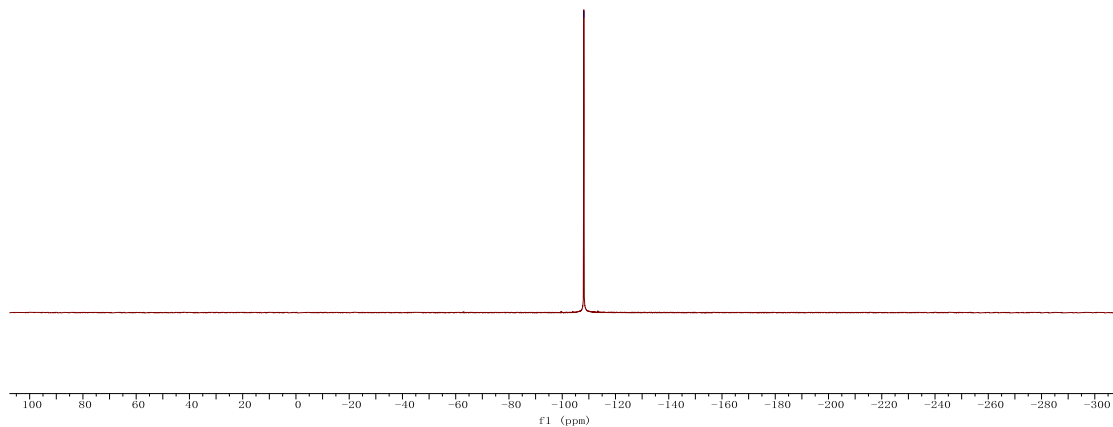
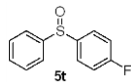
CH-7-1
single pulse decoupled gated NOE

165.6
163.1
145.4
141.3
141.2
131.3
129.5
127.4
127.3
124.7
116.9
116.7



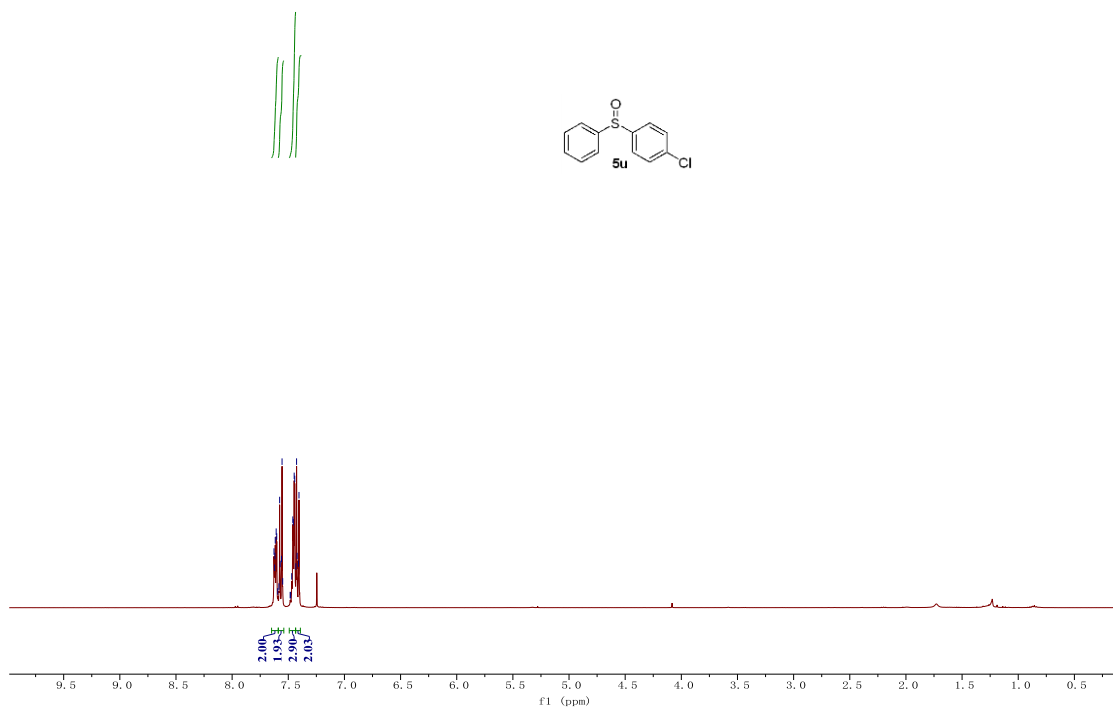
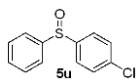
CH-7-1
single_pulse

-108.1



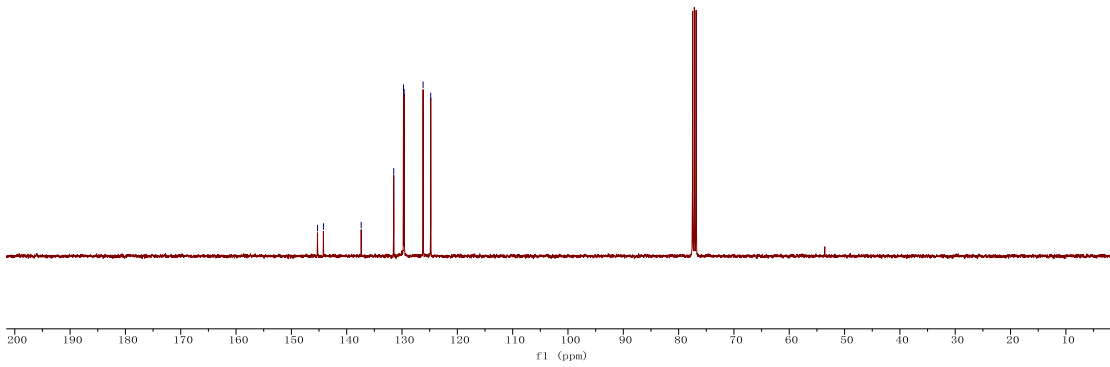
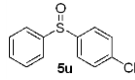
CH-7-2ag
single_pulse

7.63
7.62
7.62
7.61
7.60
7.59
7.58
7.57
7.56
7.55
7.48
7.47
7.46
7.45
7.44
7.43
7.42
7.41
7.40



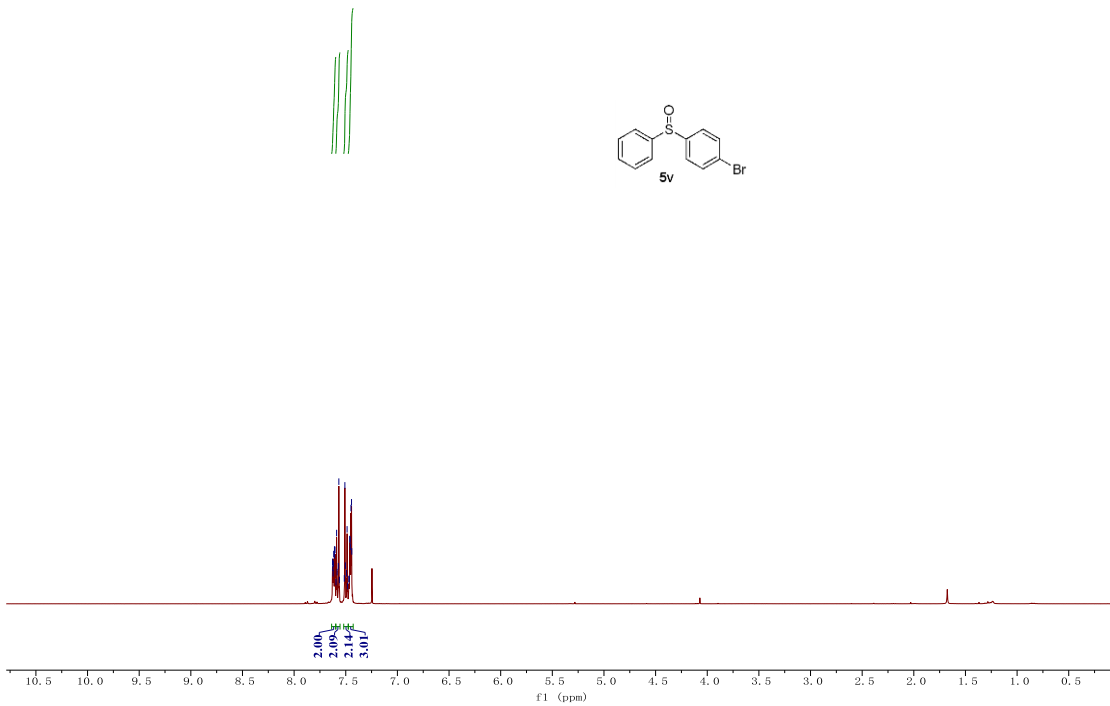
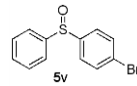
CH-7-2ag
single pulse decoupled gated NOE

145.3
144.2
137.4
131.5
129.7
129.6
126.2
124.8



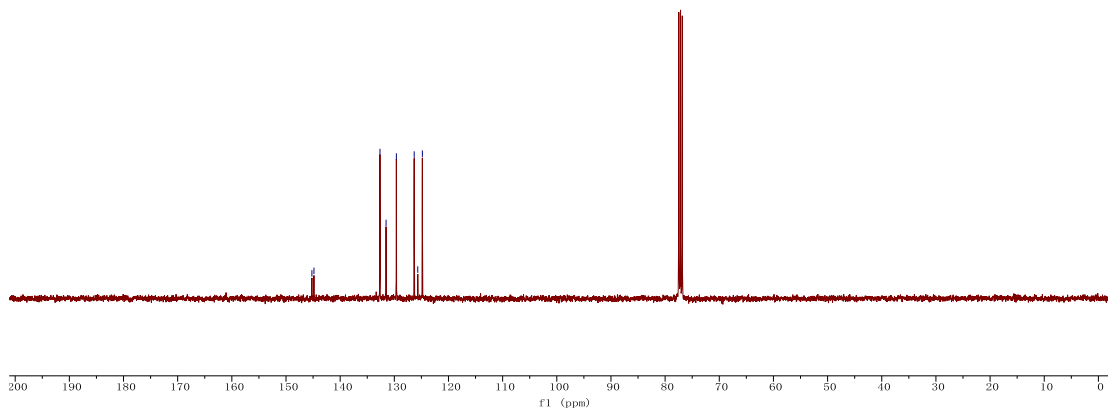
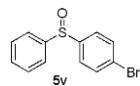
CH-73
single_pulse

7.63
7.63
7.62
7.62
7.61
7.61
7.60
7.59
7.58
7.57
7.56
7.56
7.51
7.51
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.45
7.44
7.44



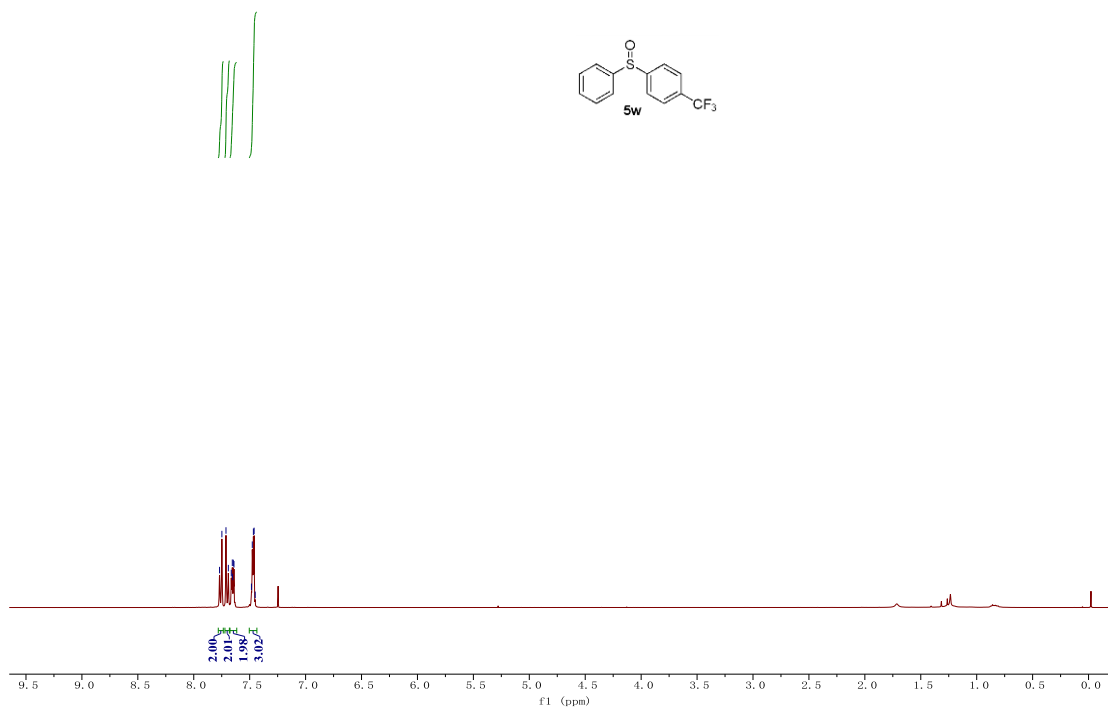
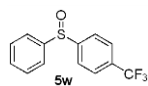
CH-7-3
single pulse decoupled gated NOE

145.2
144.8
132.6
131.5
129.6
126.3
125.7
124.8



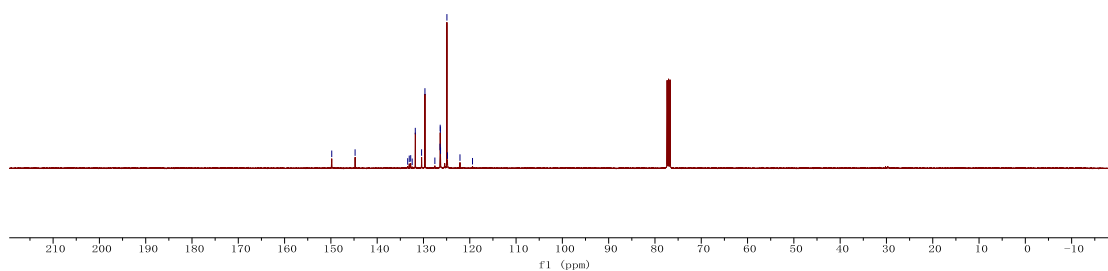
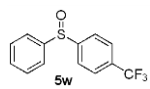
PGQ-5E
single_pulse

7.77
7.75
7.71
7.69
7.66
7.65
7.64
7.48
7.47
7.46
7.45



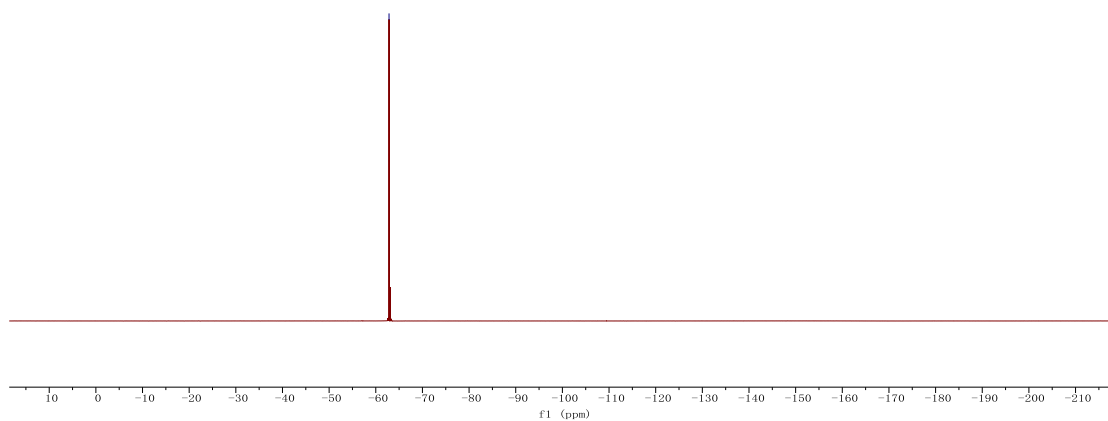
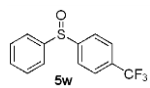
20230331.652.1.1r
p=sab

149.8
144.8
133.4
133.1
132.8
132.4
131.8
130.4
129.7
127.5
126.4
126.4
126.3
124.9
124.6
122.1
119.4



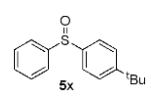
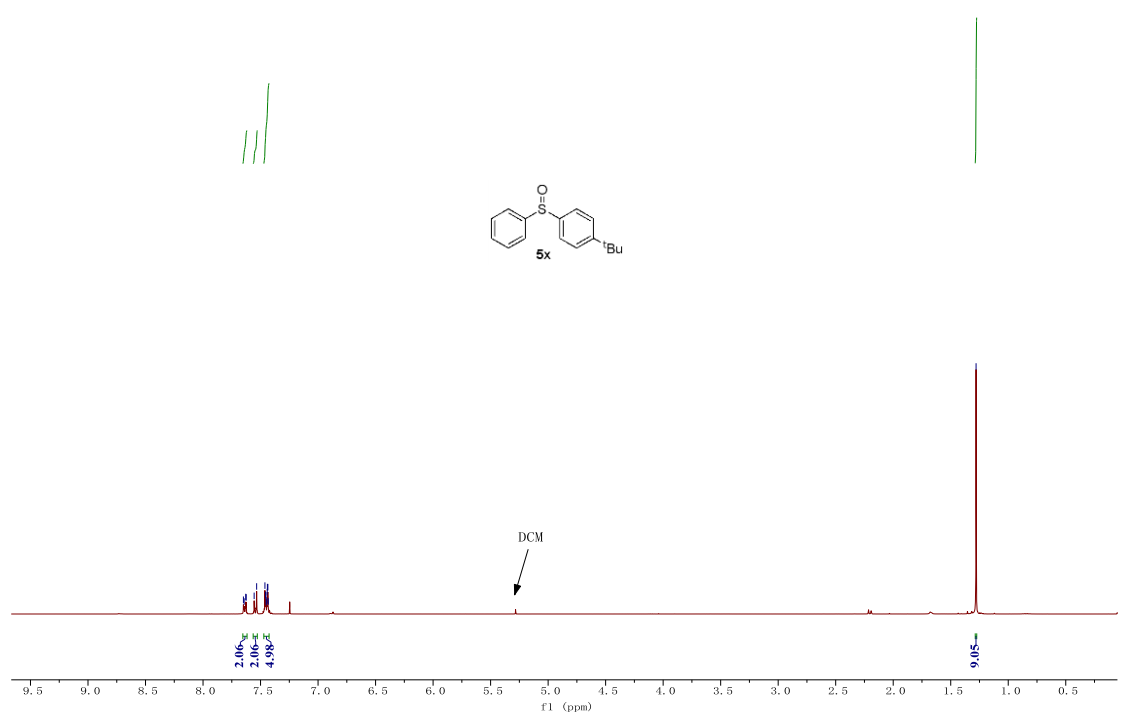
20230331.651.1.1r
p=sab

-62.8



HY-8-4
single_pulse

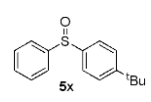
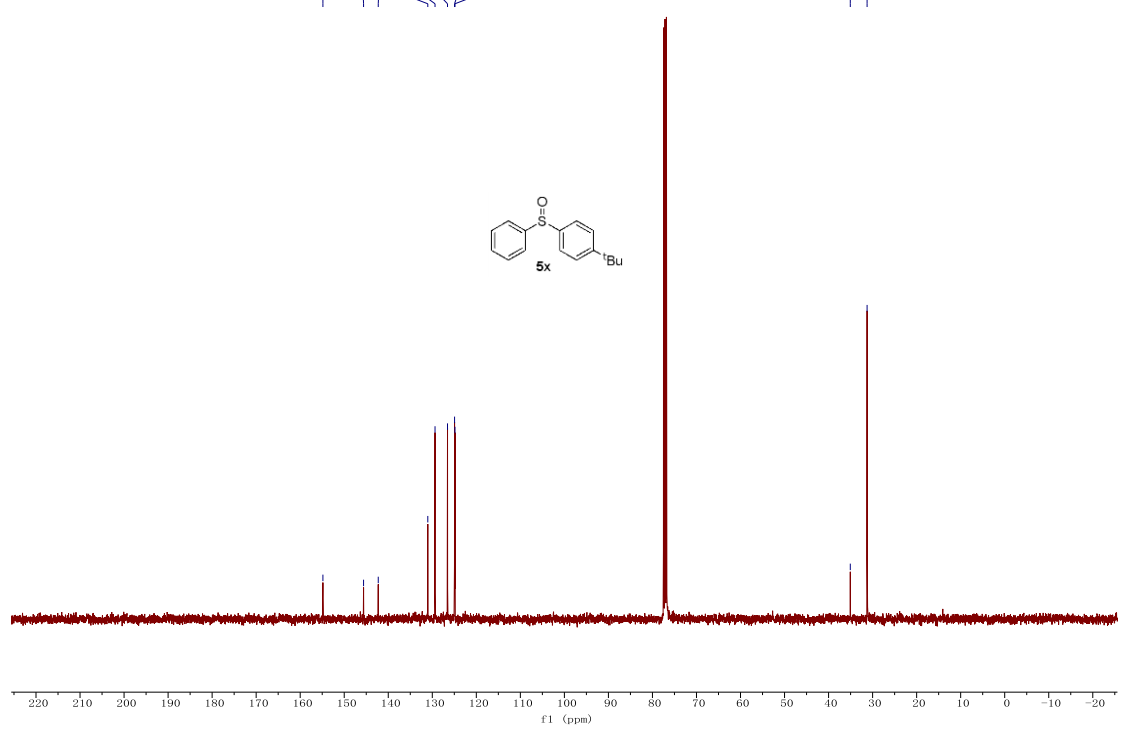
7.65
7.64
7.63
7.62
7.56
7.53
7.46
7.45
7.44
7.44
7.44
7.43



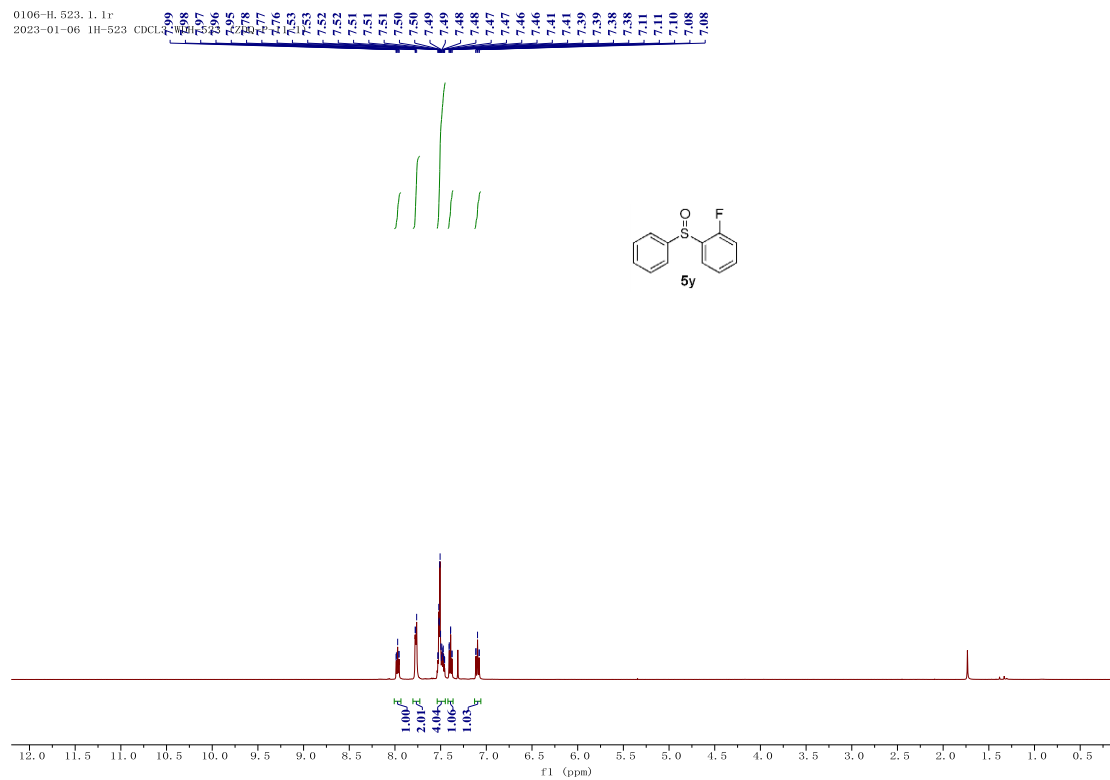
HY-8-4CARBON
single pulse decoupled gated NOE

154.8
145.6
142.3
131.0
129.4
126.5
124.9
124.9

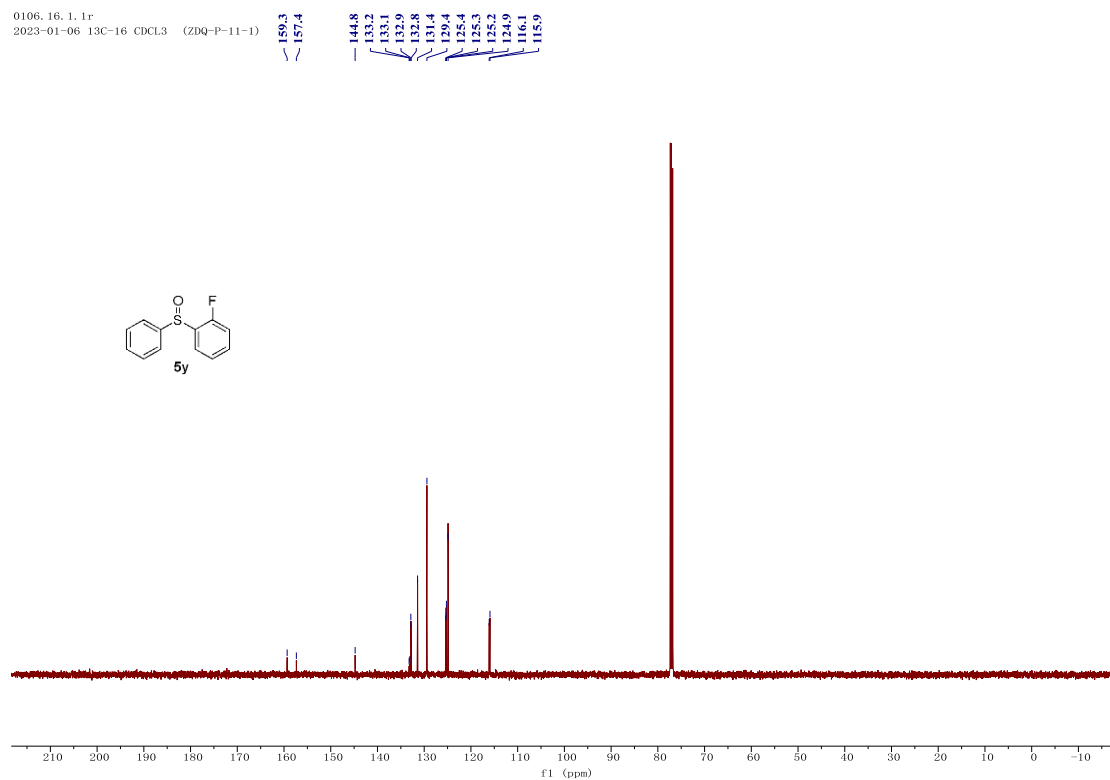
35.1
31.3



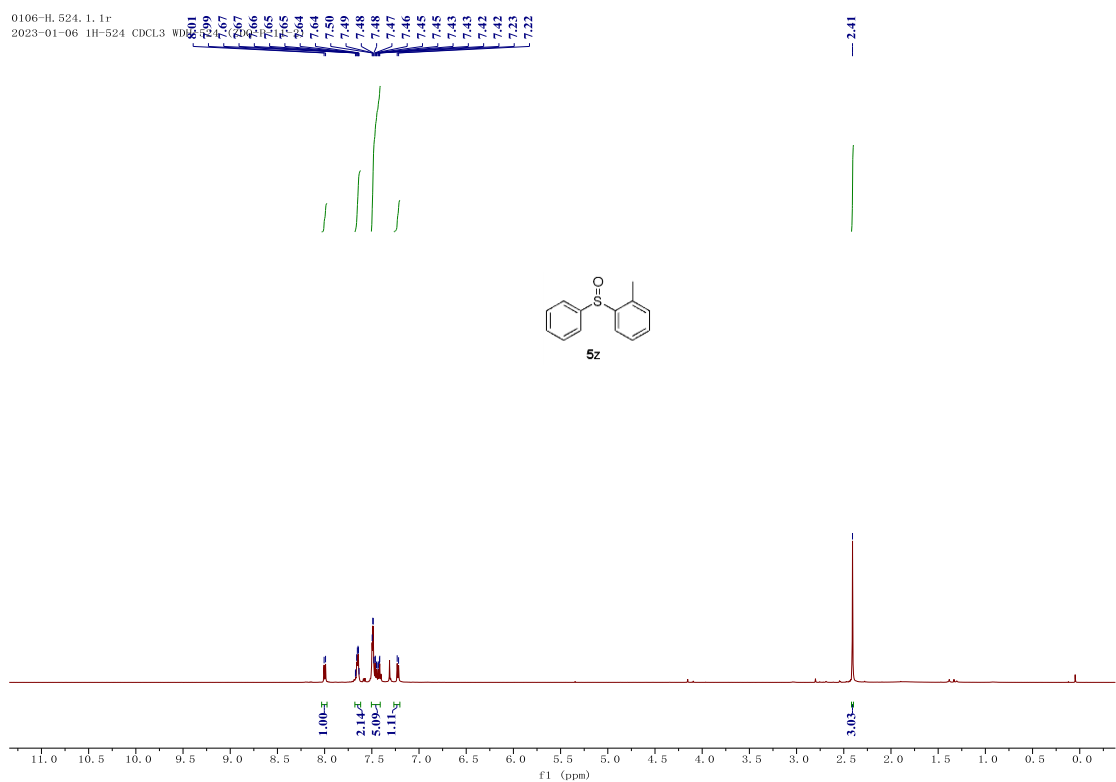
0106-H. 523. 1. 1r
2023-01-06 1H-523 CDCL3



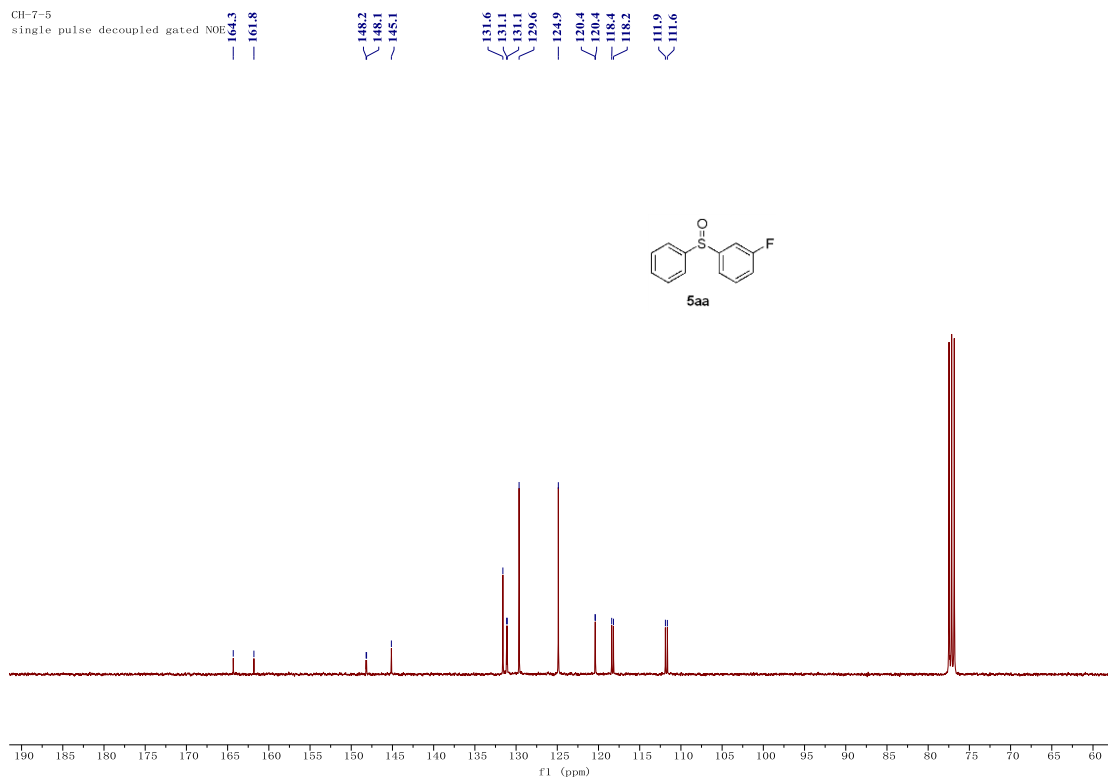
0106. 16. 1. 1r
2023-01-06 13C-16 CDCL3 (ZDQ-P-11-1)



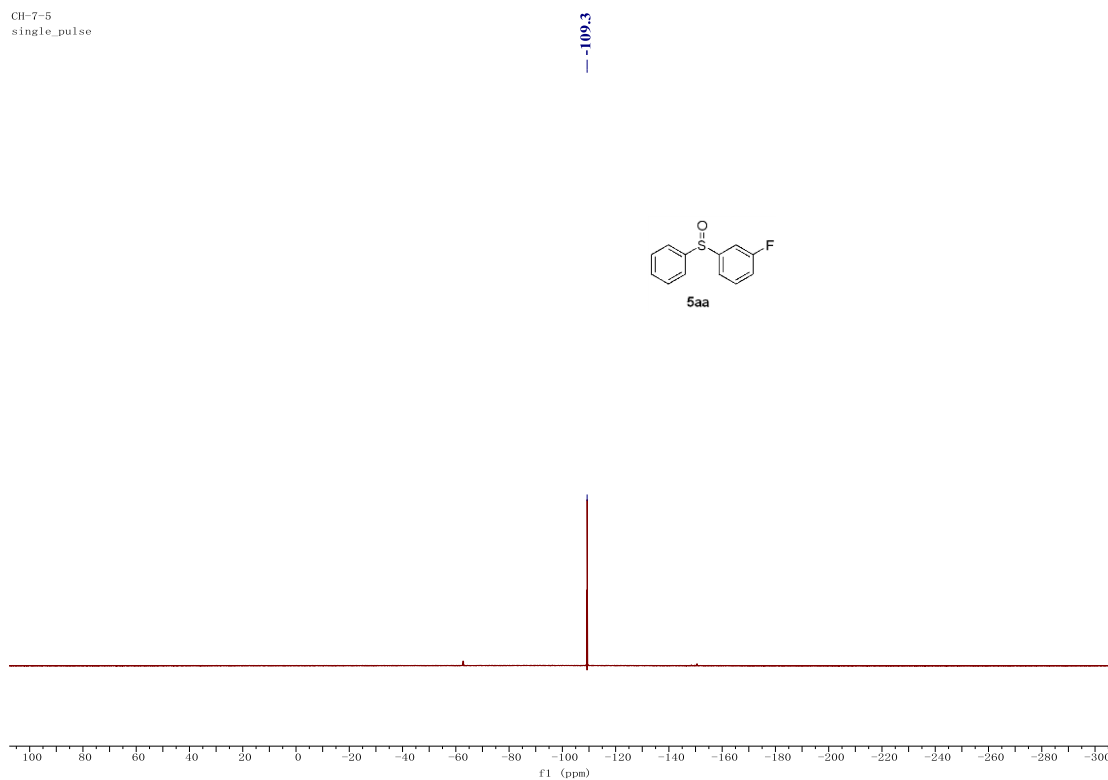
0106_9.2.1r
2023-01-06 19F-9 CDCL3 (ZDQ-P-11-1)



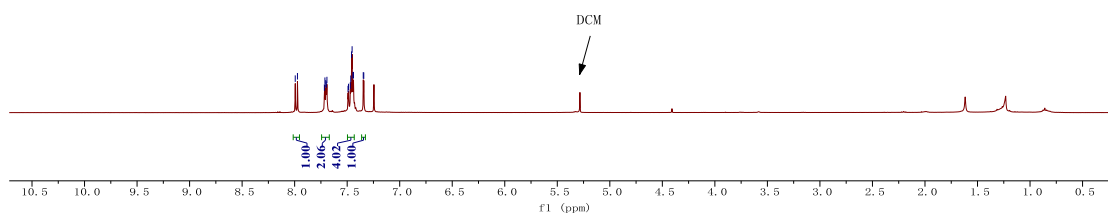
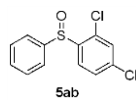
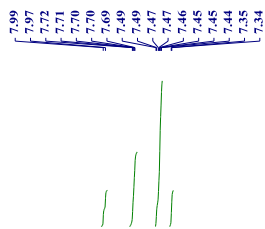
CH-7-5
single pulse decoupled gated NOE



CH-7-5
single_pulse

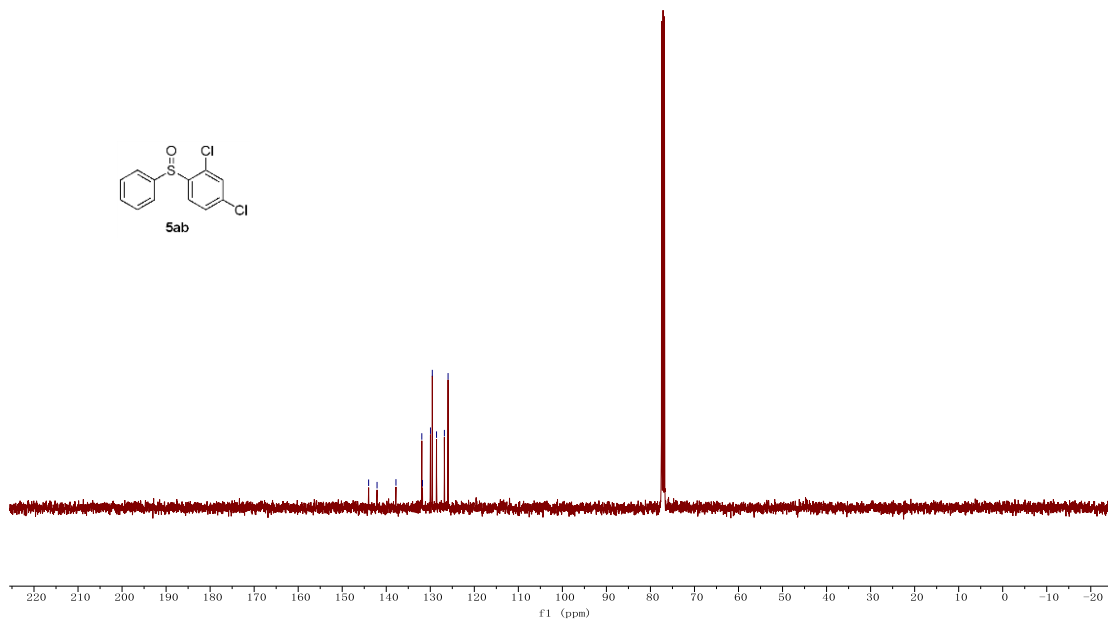
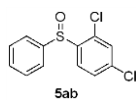


CH-77
single_pulse

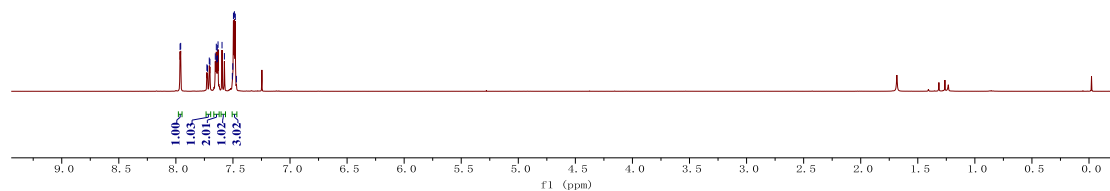
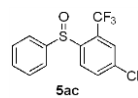
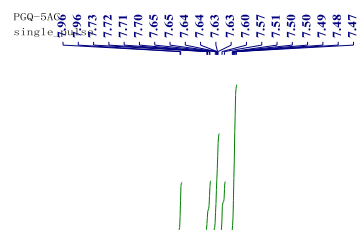


CH-7-7
single pulse decoupled gated NOE

144.0
142.1
137.8
131.9
131.8
130.0
129.5
128.6
126.0

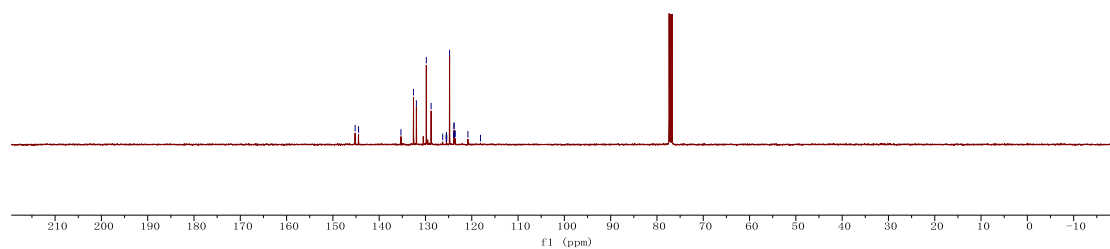
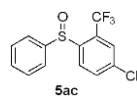


PGQ-5Ac
single



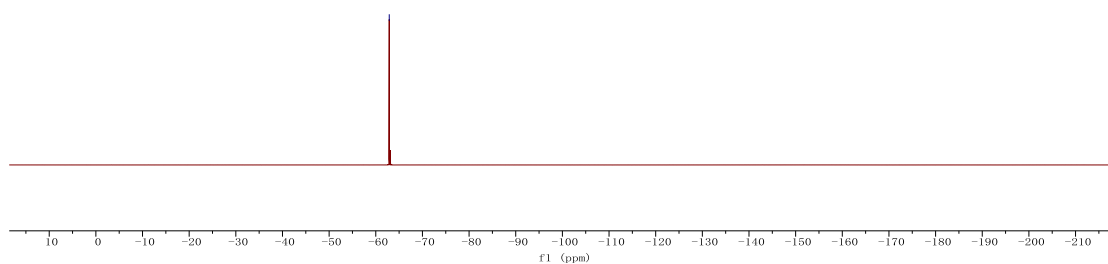
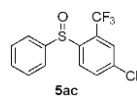
20230331.672.1.1r
p=sac

145.2
144.5
135.3
132.6
132.0
129.8
128.8
126.3
125.2
125.1
125.0
124.8
123.9
123.8
123.8
123.6
120.8
118.1



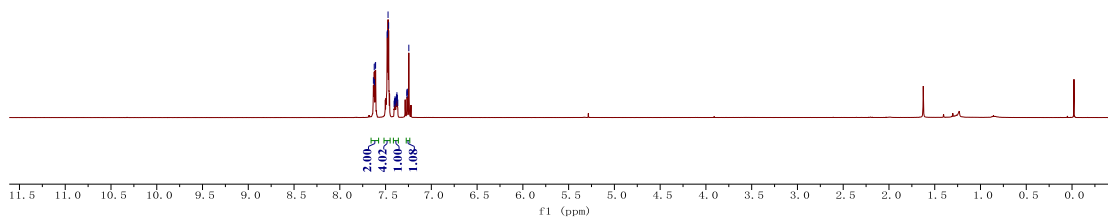
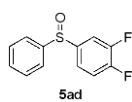
20230331.671.1.1r
p-sac

-62.9



CH-76PH
single_pulse

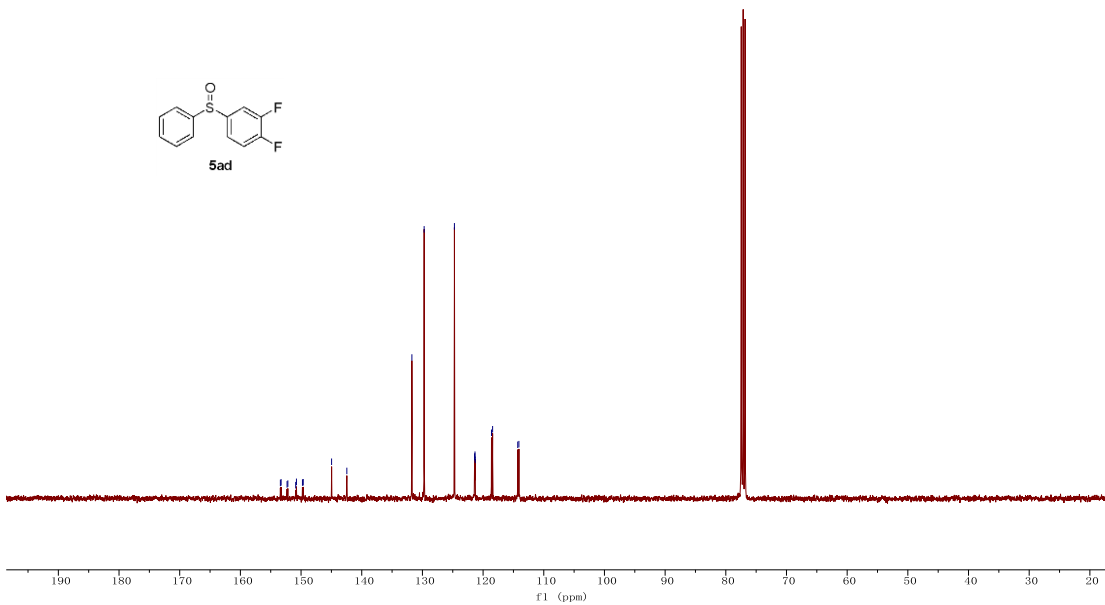
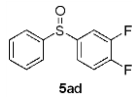
7.63
7.62
7.62
7.61
7.61
7.48
7.48
7.47
7.47
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.27
7.26
7.25



PGQ-7-6

single pulse decoupled gated NOE

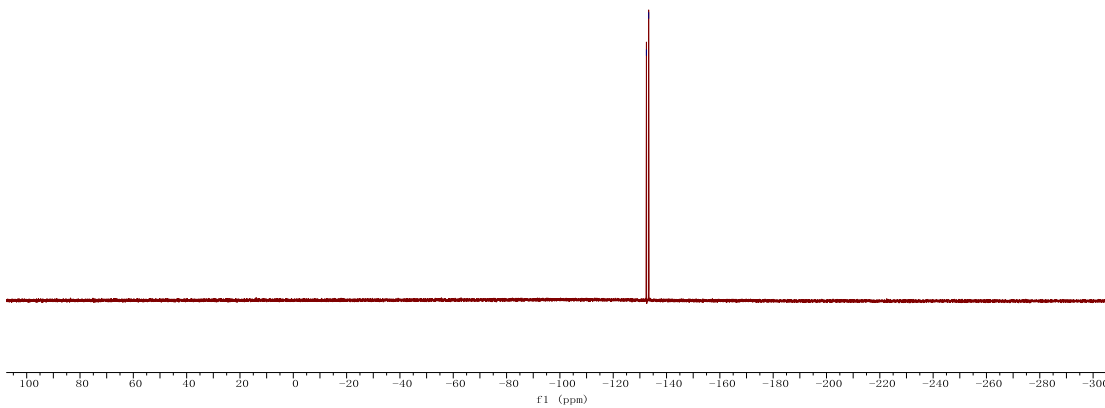
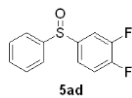
153.4
153.3
152.3
152.2
150.9
150.8
149.8
149.6
145.0
142.5
131.7
129.7
124.7
121.4
121.3
121.3
118.6
118.4
114.3
114.1



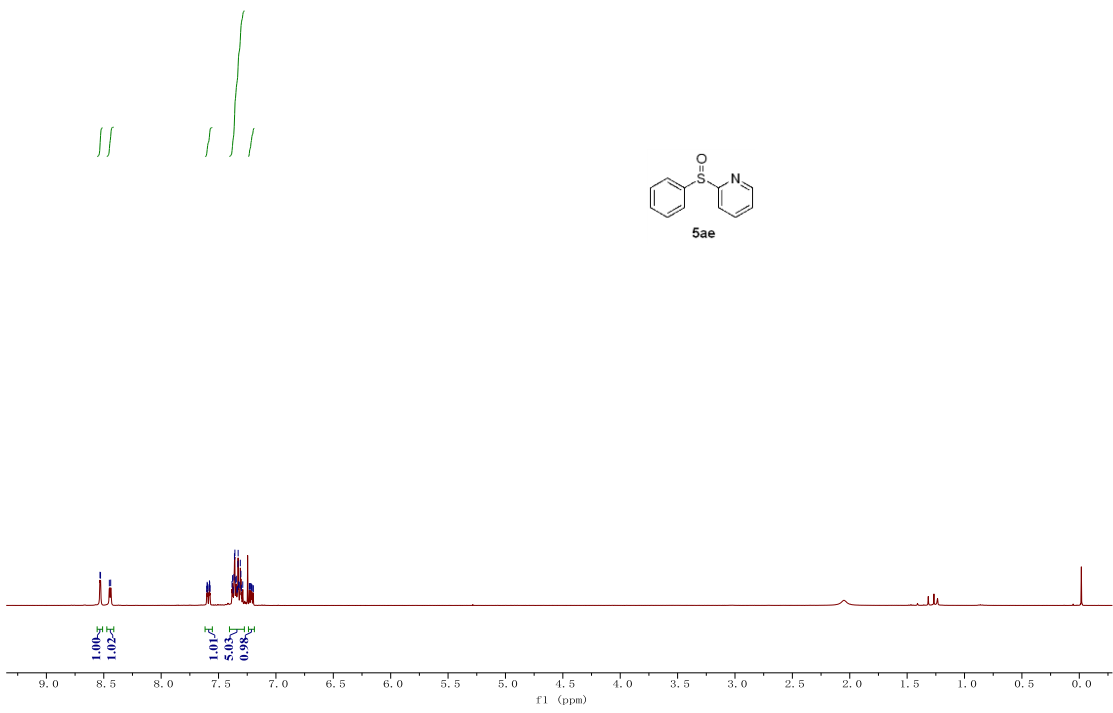
CH-7-6

single_pulse

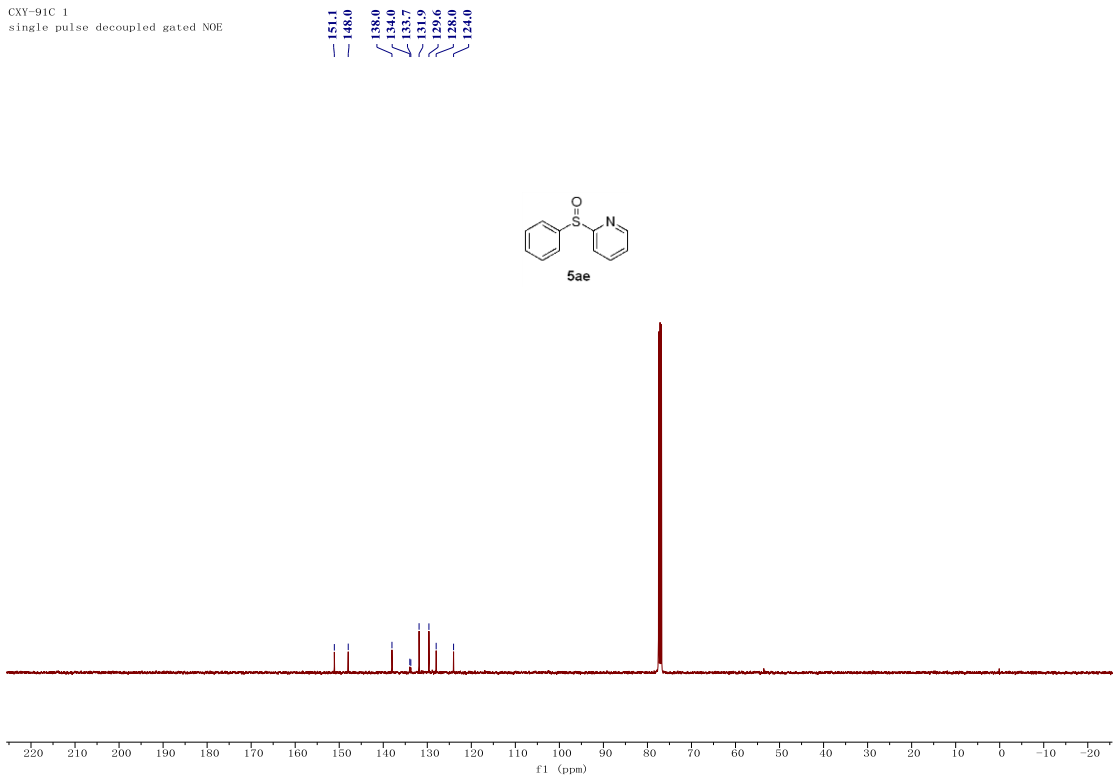
132.5
133.3



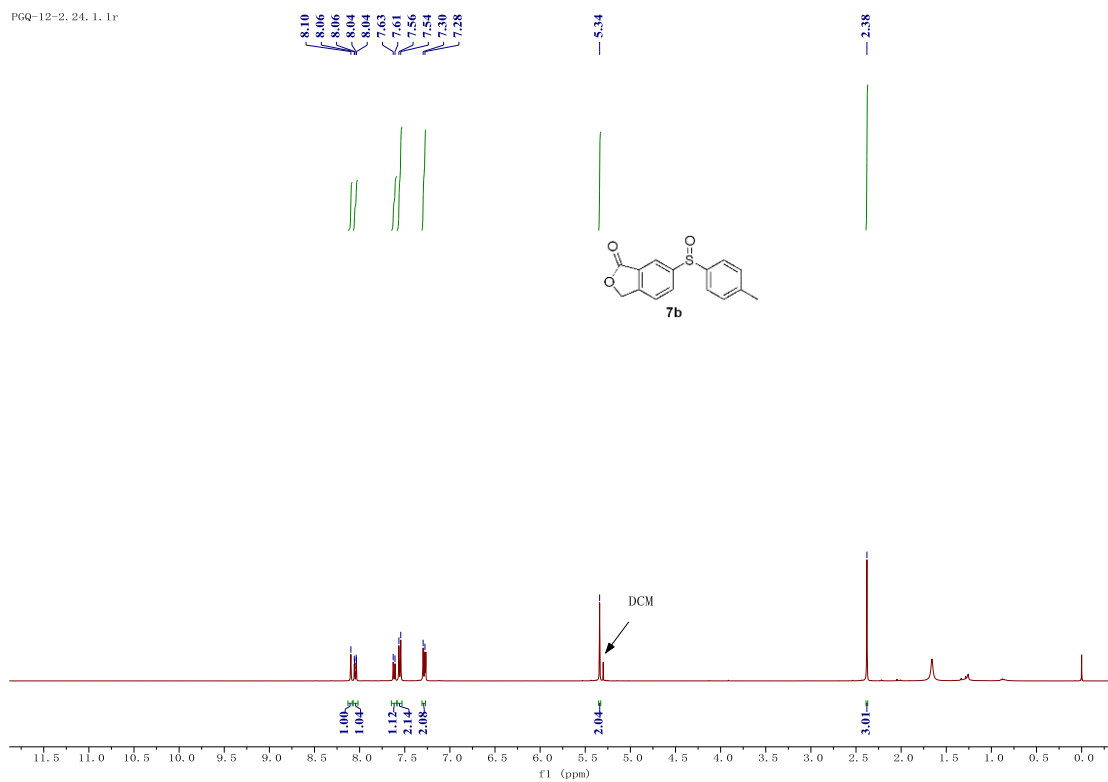
PGQ-5AE
single_pulse



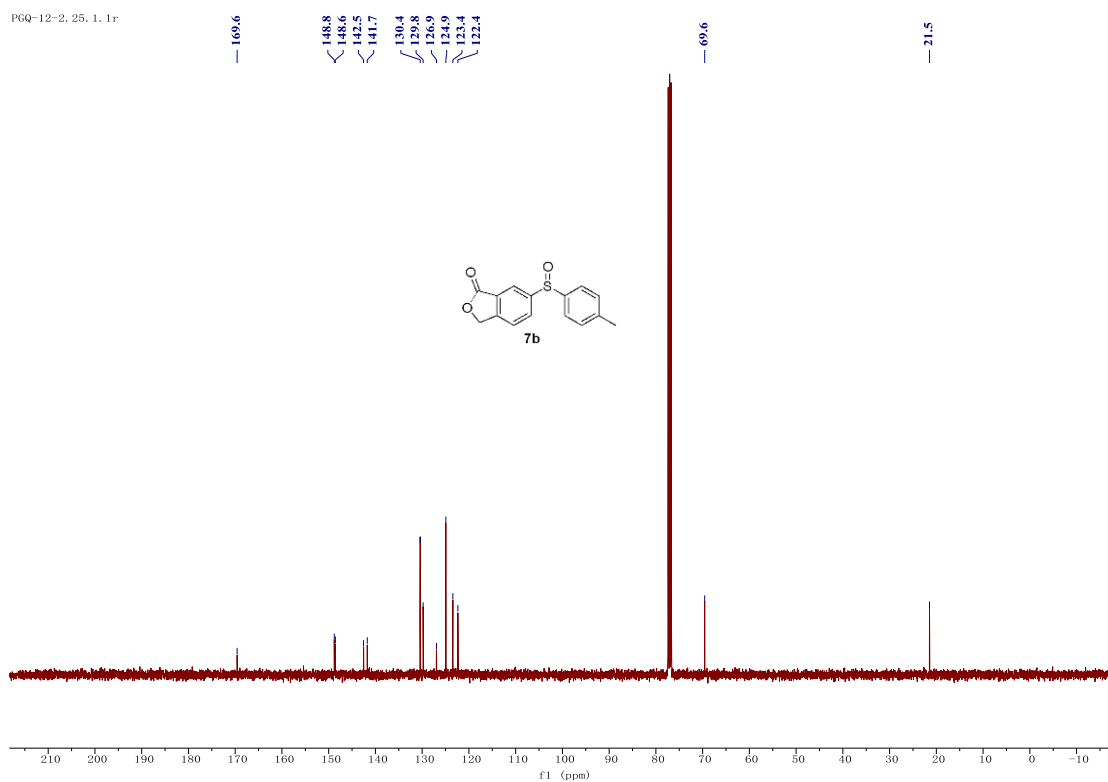
CXY-91C 1
single pulse decoupled gated NOE



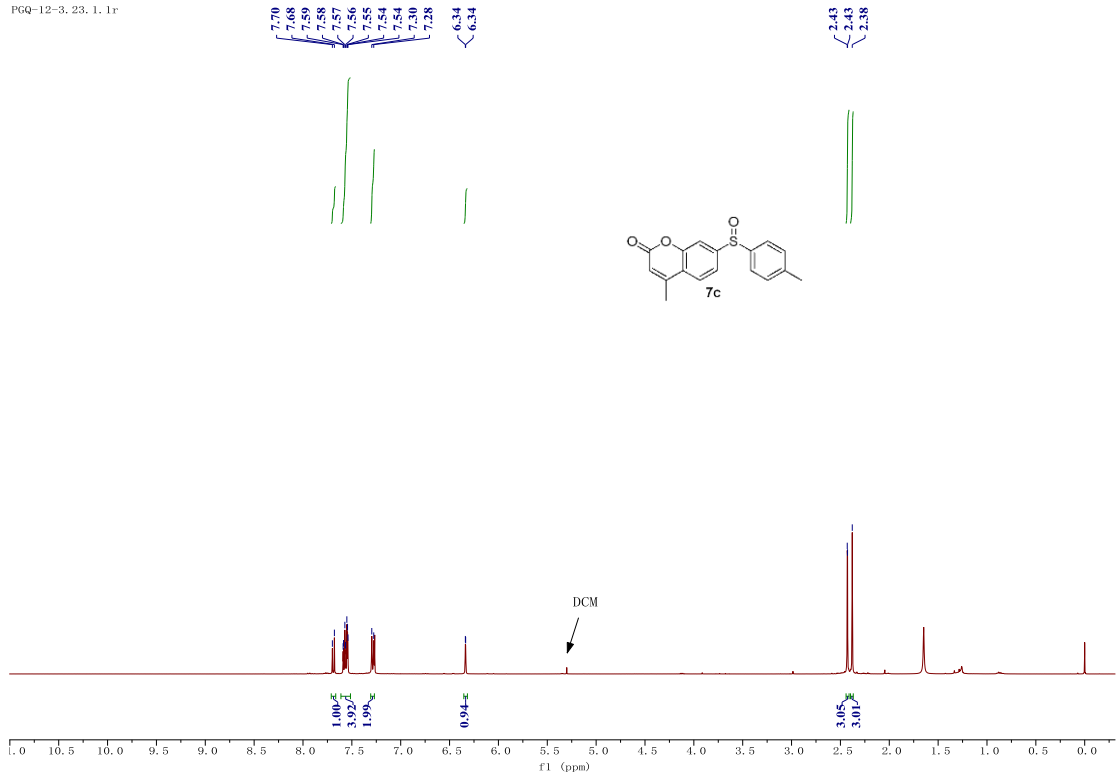
PGQ-12-2.24.1.1r



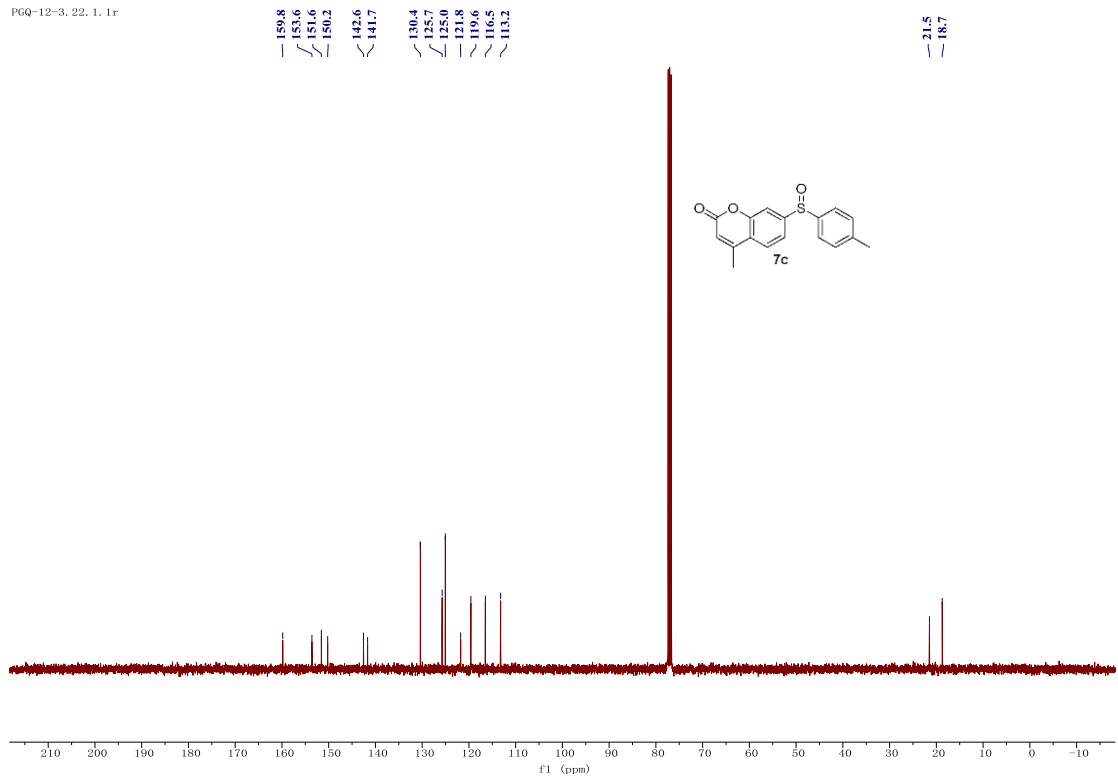
PGQ-12-2.25.1.1r



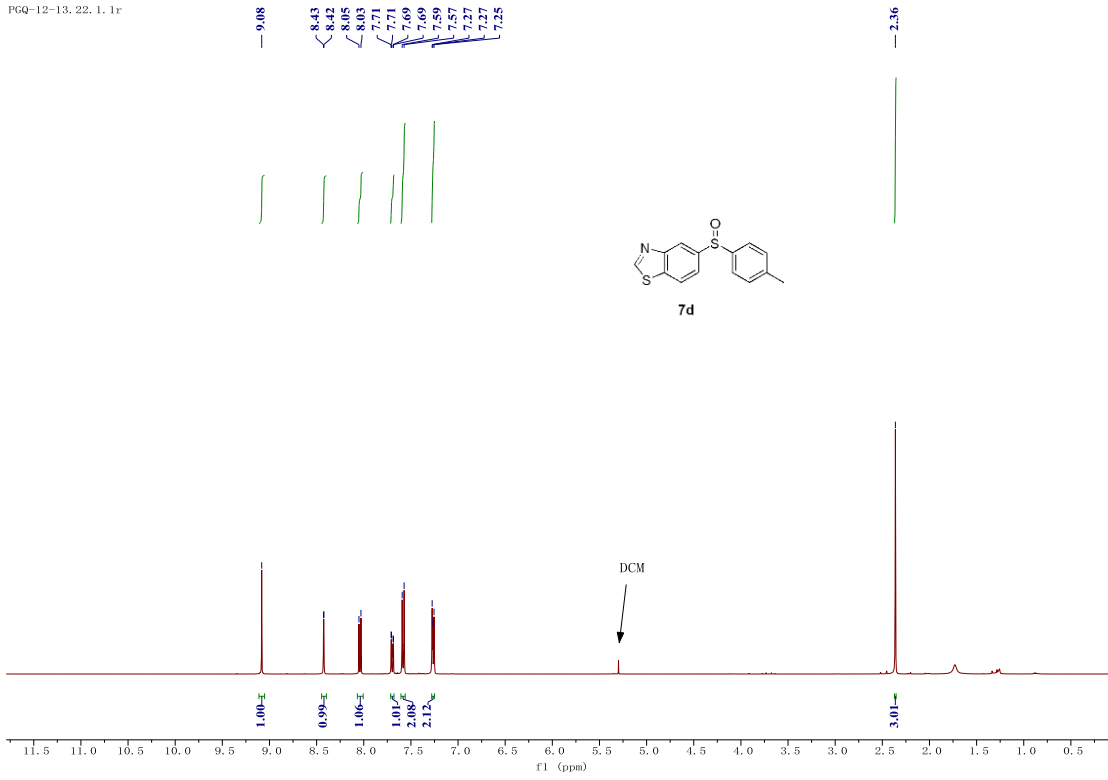
PGQ-12-3, 23, 1, 1r



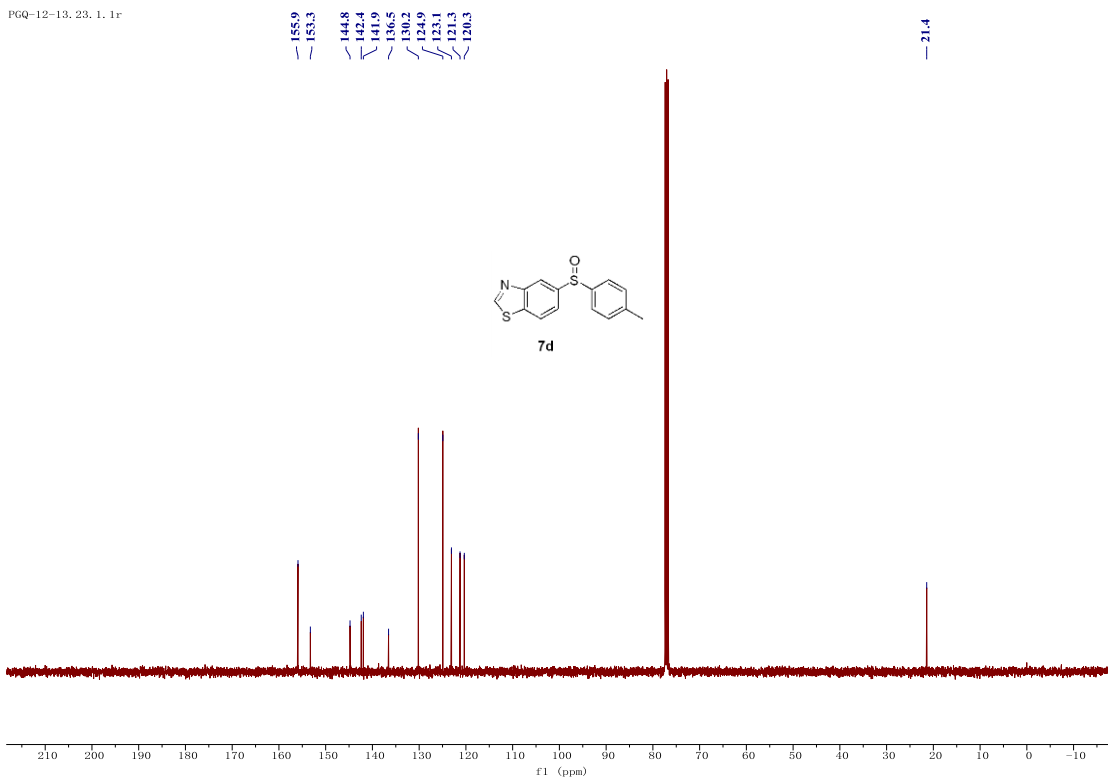
PGQ-12-3, 22, 1, 1r



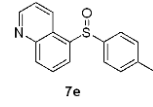
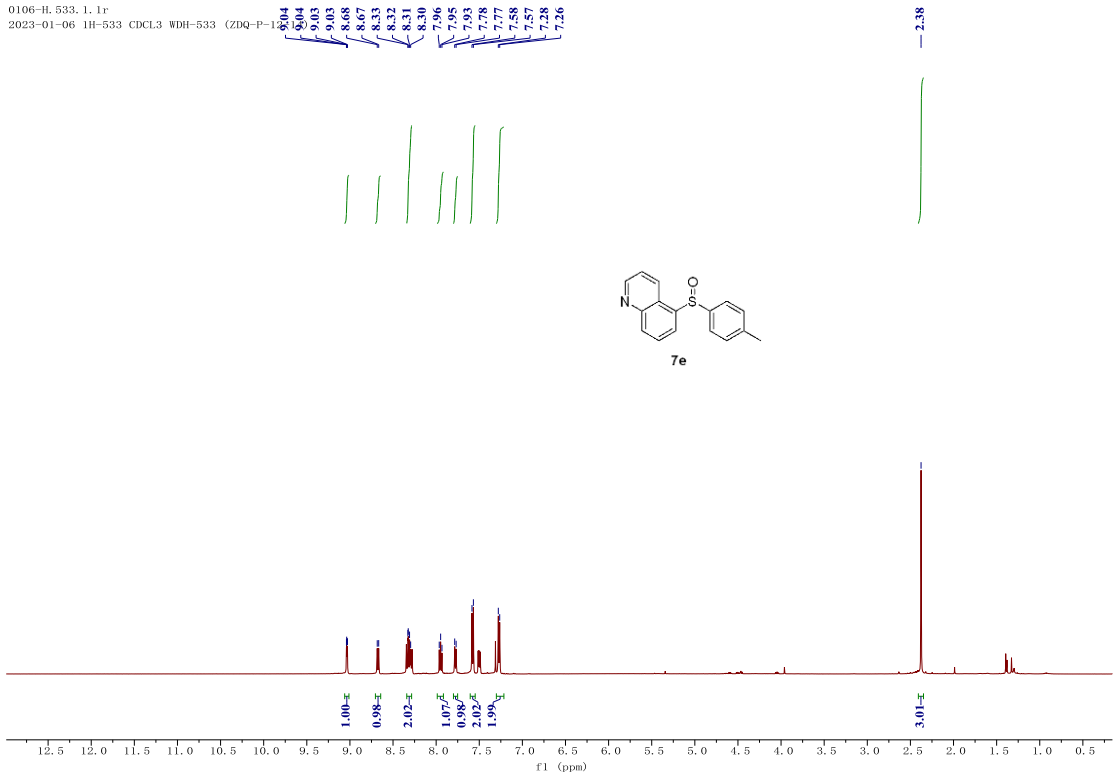
PGQ-12-13. 22. 1. 1r



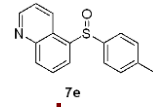
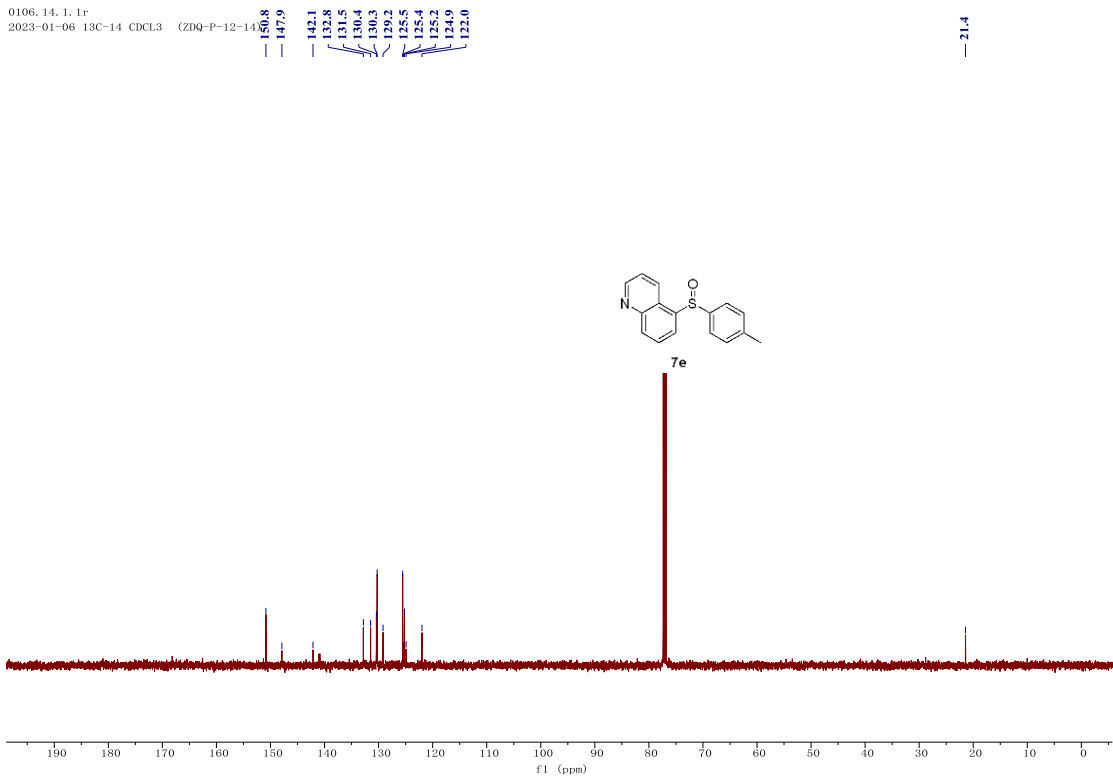
PGQ-12-13. 23. 1. 1r



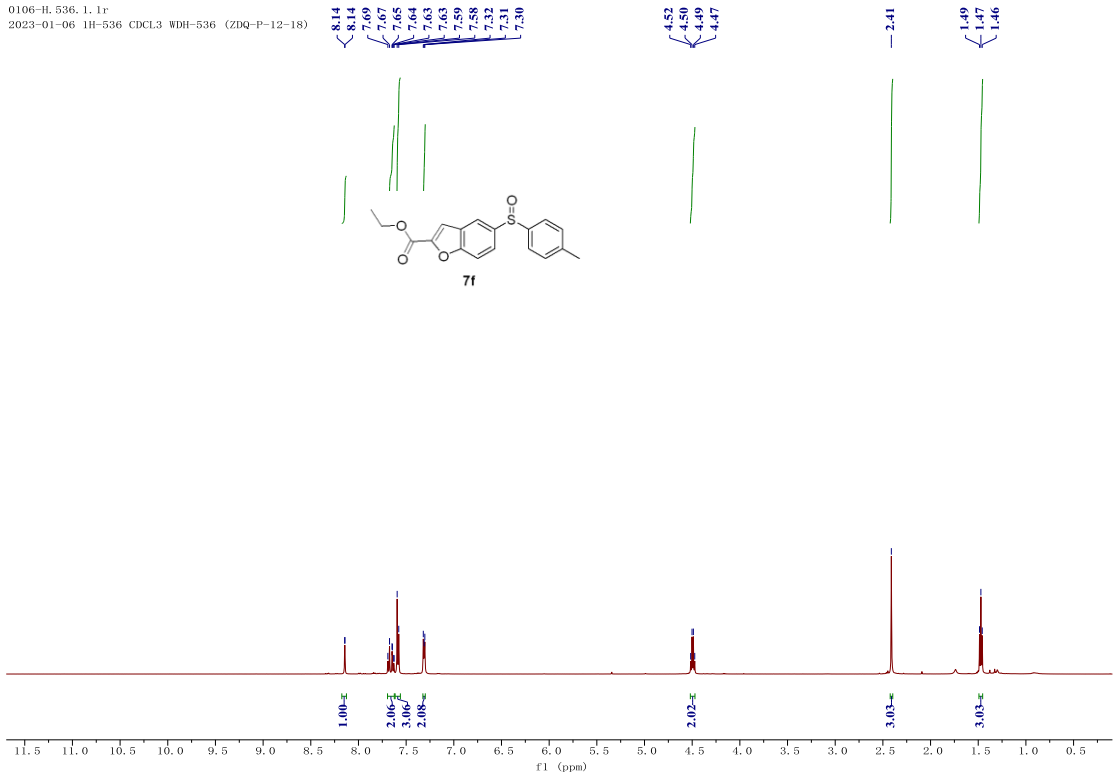
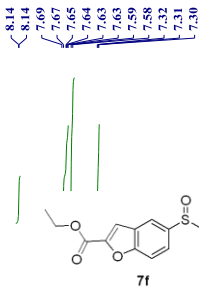
0106-H. 533. 1. 1r
2023-01-06 1H-533 CDCL3 WDH-533 (ZDQ-P-1



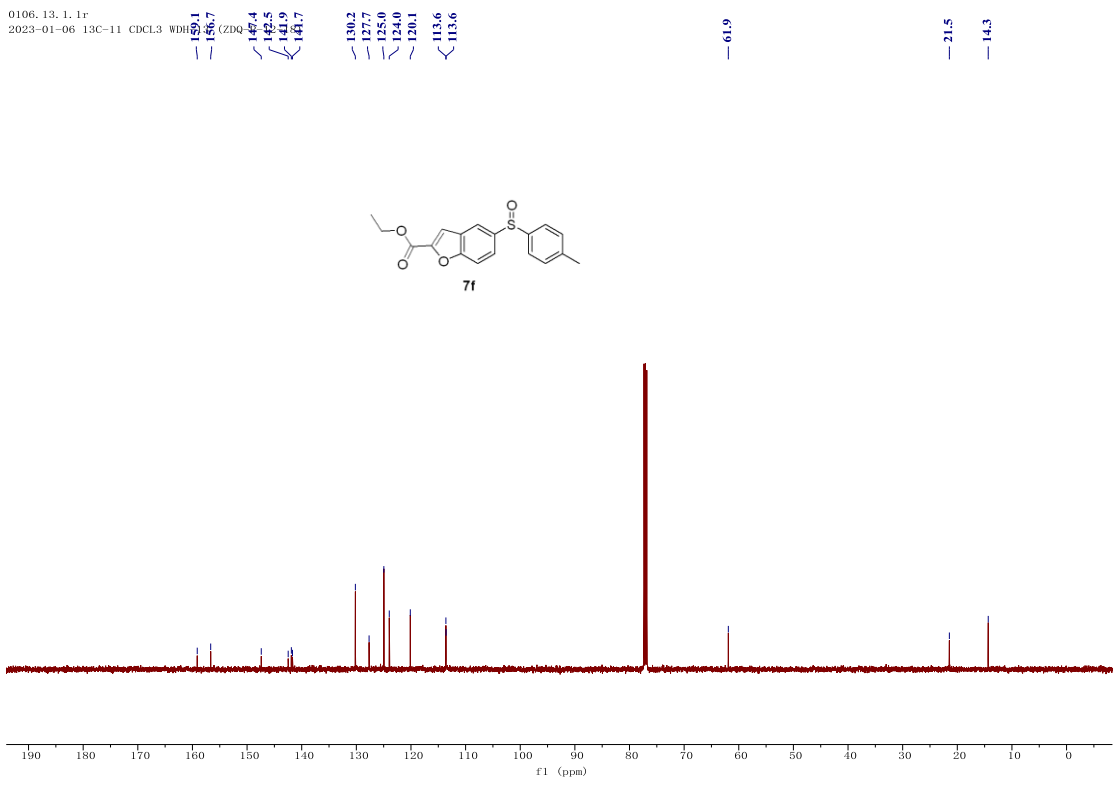
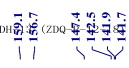
0106. 14. 1. 1r
2023-01-06 13C-14 CDCL3 (ZDQ-P-12-14



0106-H-536, 1, 1r
2023-01-06 1H-536 CDCL3 WDH-536 (ZDQ-P-12-18)

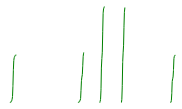


0106, 13, 1, 1r
2023-01-06 13C-11 CDCL3 WDH-536 (ZDQ-P-12-18)



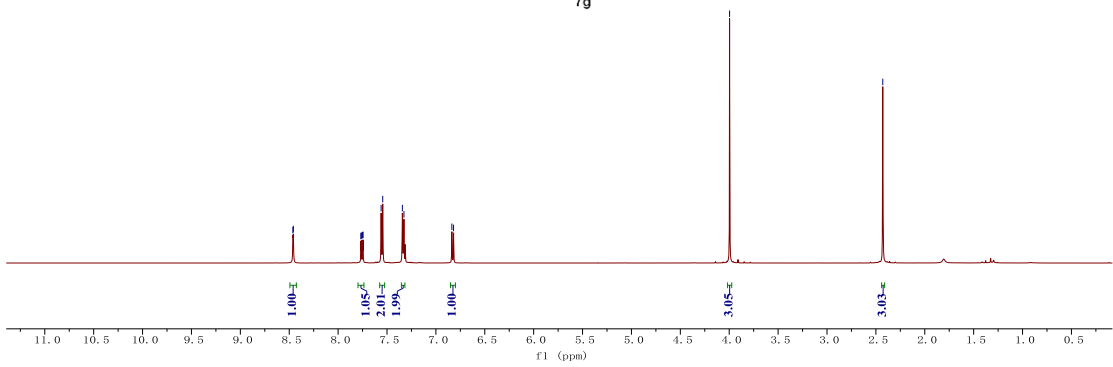
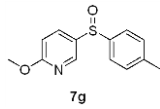
0106-H. 531. 1. 1r
2023-01-06 1H-531 CDCL3 WDH-531 (ZDQ-P-12)

8.46
8.46
7.77
7.76
7.75
7.74
7.56
7.54
7.33
6.84
6.82



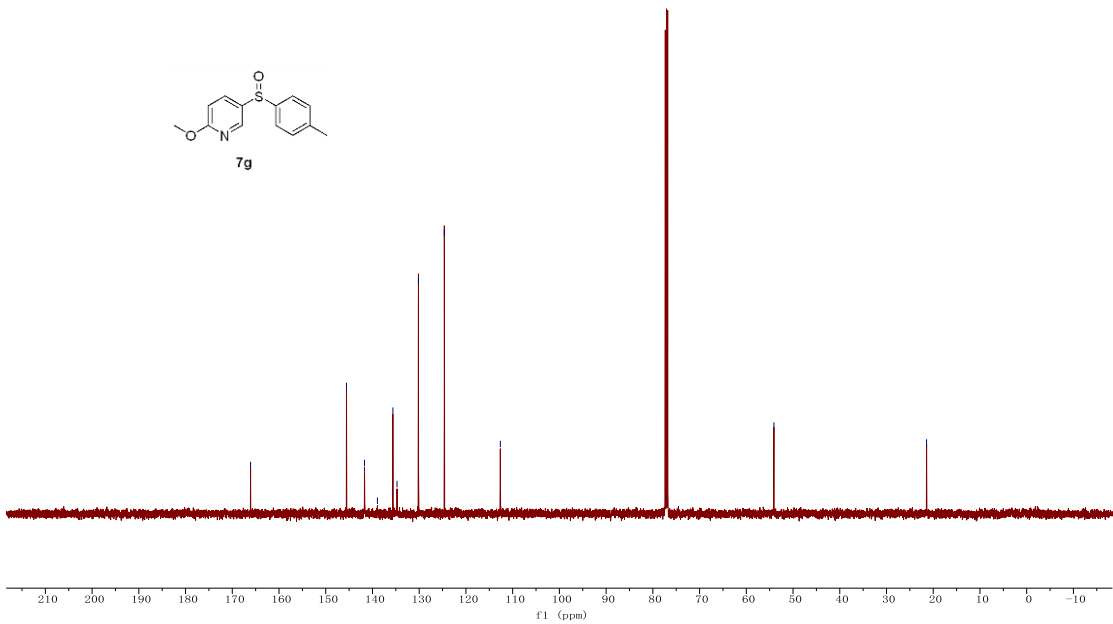
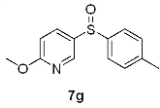
4.00

2.43



0106. 15. 1. 1r
2023-01-06 13C-15 CDCL3 (ZDQ-P-12)

166.1
145.6
141.7
138.9
135.6
134.7
130.2
124.6
112.6
54.1
21.4

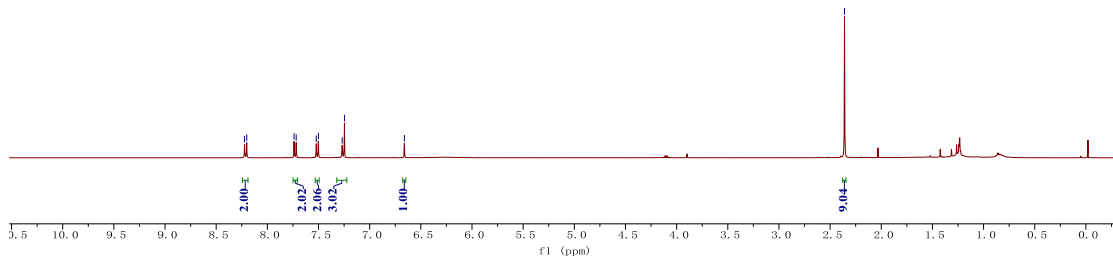
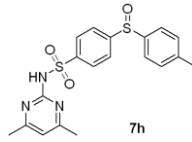


P12-1S
single_pulse

8.22
8.20
7.74
7.72
7.52
7.50
7.27
7.25

6.66

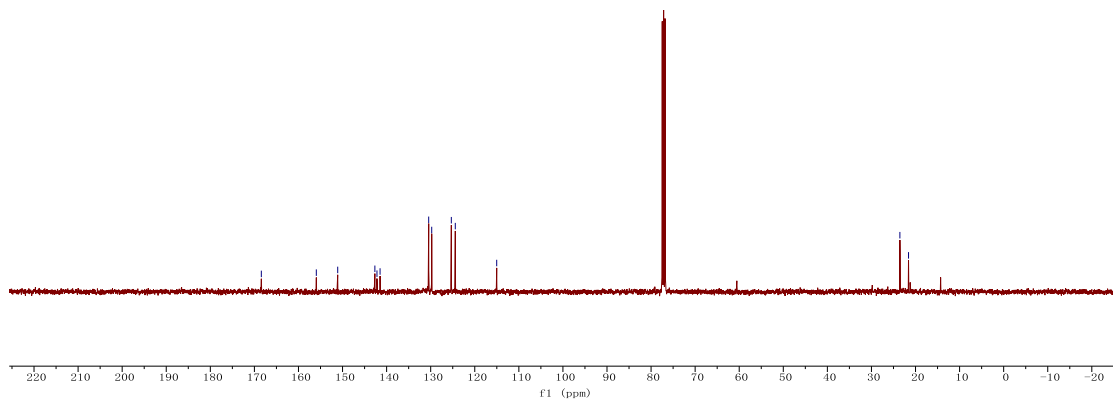
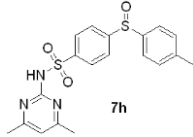
2.36



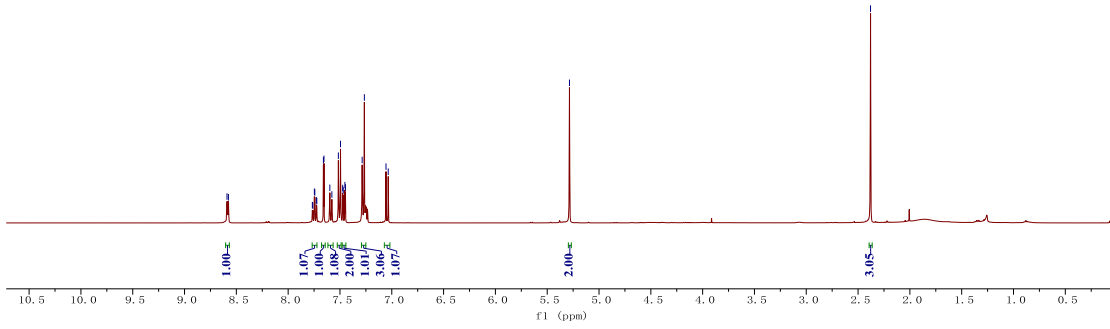
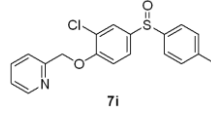
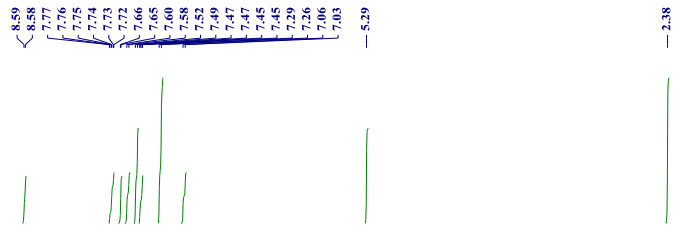
P-12-15
single pulse decoupled gated NOE

168.4
156.0
151.1
142.7
142.2
141.5
130.5
129.8
125.3
124.4
115.0

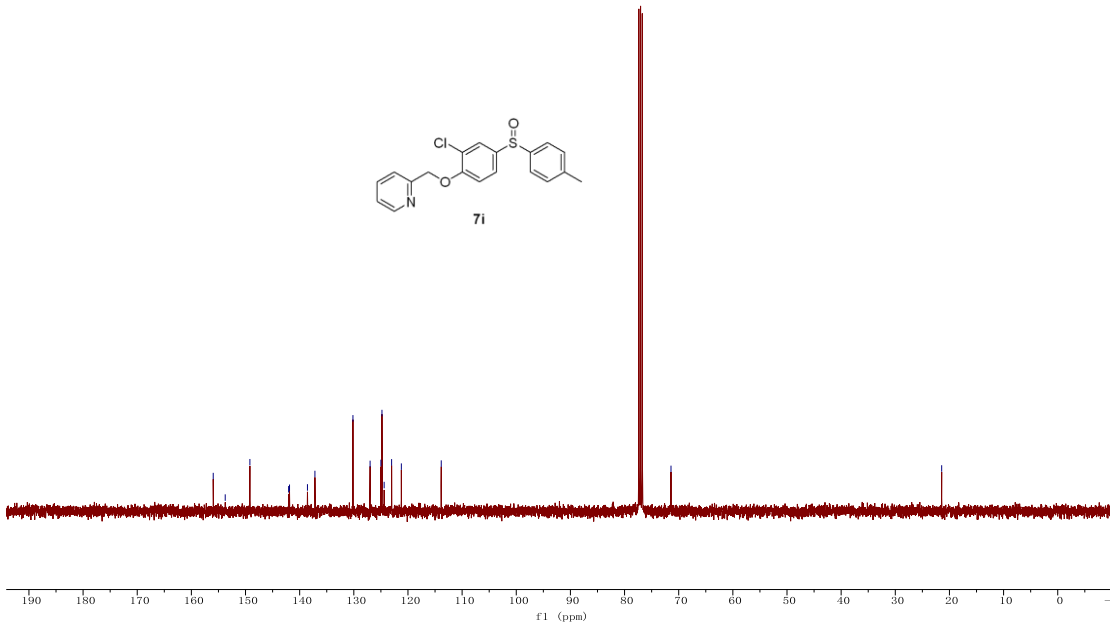
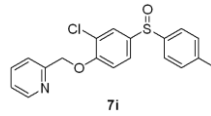
21.5
21.6



PGQ-12-16. 24. 1. 1r

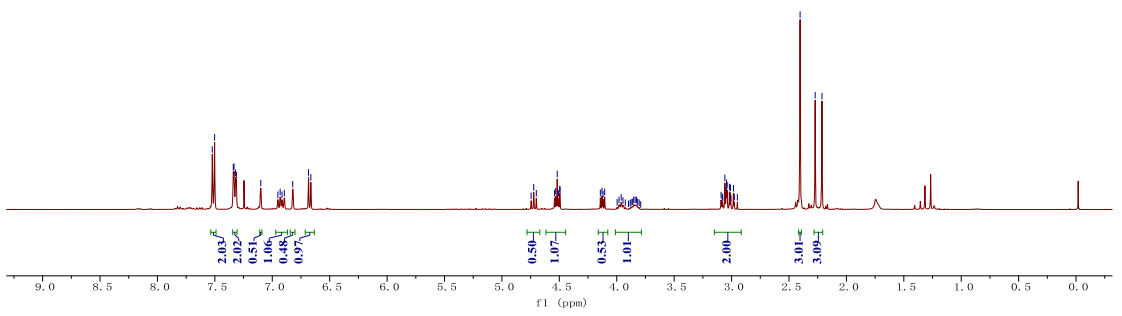
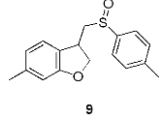
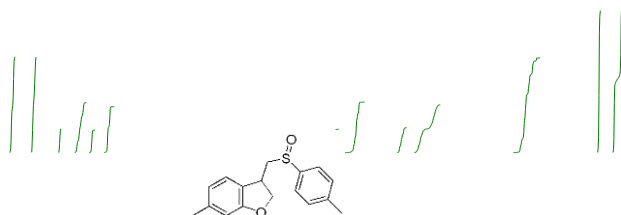


PGQ-12-16. 25. 1. 1r



PGQ-P-13-2
single_pulse

7.52
7.50
7.34
7.33
7.32
7.31
7.10
6.95
6.93
6.92
6.89
6.82
6.68
6.66
4.75
4.72
4.70
4.54
4.53
4.52
4.51
4.50
4.49
4.14
4.13
4.12
4.11
4.00
3.98
3.96
3.95
3.93
3.90
3.88
3.87
3.86
3.85
3.84
3.83
3.82
3.80
3.09
3.08
3.06
3.05
3.04
3.04
3.02
3.01
3.01
2.98
2.95
2.40
2.27
2.21



P-12
single pulse decoupled gated NOE

157.6
142.0
141.9
140.4
140.0
130.3
129.6
129.5
128.4
128.3
125.4
124.8
124.0
109.6
76.3
75.9
62.2
62.0
37.1
36.9
21.6
21.5
20.9
20.8

