

Palladium-Catalyzed Directing Group Assisted and Regioselectivity Reversed Cyclocarbonylation of Aryllallenes with 2-Iodoanilines

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Supporting Information

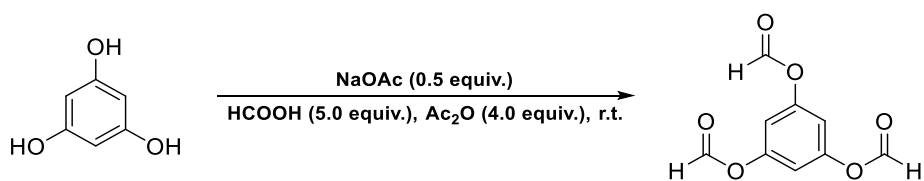
Table of Contents

1. General experimental information	S1
2. Preparation of benzene-1,3,5-triyl triformate (TFBen).....	S1
3. General procedure for the synthesis of (<i>N</i> -SO ₂ Py)-2-iodoanilines (1a-1l).....	S2
4. General procedure for the synthesis of allenes (2a-2w).....	S3
5. General procedure for the synthesis of 2,3-dihydroquinolin-4(<i>1H</i>)-ones.....	S4
5.1 General procedure for the synthesis of 2,3-dihydroquinolin-4(<i>1H</i>)-ones (3aa-3aw).....	S4
5.2 General procedure for the synthesis of 2,3-dihydroquinolin-4(<i>1H</i>)-ones (3ba-3la).....	S5
6. Transformation 3aa into compounds 4-6.....	S5
7. Removal of the <i>N</i> -SO ₂ Py directing group of 6.....	S7
8. Preparation of compound 17	S8
9. Characterization data of compounds 1a-1l and 2a-2w	S8
10. Characterization data of products 3aa-3aw and 3ba-3la.....	S17
11. Characterization data of compounds 4-6, 7, 12, 17 and 18	S31
12. References.....	S35
13. X-ray crystal data for compound 3aa	S36
14. ¹ H, ¹³ C spectra of 1a-1l, 2a-2w, 3aa-3aw, 3ba-3la, 4-6, 7, 12, 15/15', 17 and 18.....	S37
15. Computational Methods	S115

1. General experimental information

Unless otherwise noted, all reactions were carried out under a nitrogen atmosphere. All commercially available reagents were used without further purification. All of the solvents were treated according to known methods. Column chromatography was performed on silica gel (200-400 mesh). ^1H NMR (400 MHz) chemical shifts were reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard. ^{13}C NMR (100 MHz) chemical shifts were reported in ppm (δ) from tetramethylsilane (TMS) with the solvent resonance as the internal standard. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, qd = quartet of doublets, m = multiplet), coupling constants (Hz) and integration. HRMS measurements were obtained on a TOF analyzer.

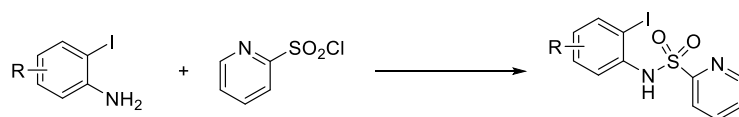
2. Preparation of benzene-1,3,5-triyl triformate (TFBen)¹



Formic acid (8.4 mL, 222.8 mmol, 5.0 equiv.) was added to acetic anhydride (16.8 mL, 178.2 mmol, 4.0 equiv.) at rt. The mixture was stirred at 60 °C for 1 h and cooled to rt. The resulting solution was poured into a flask containing 1,3,5-trihydroxybenzene (5.62 g, 44.6 mmol, 1.0 equiv.) and AcONa (1.83 g, 22.3 mmol, 0.5 equiv.). The mixture was stirred for 4 h in a water bath and then diluted with toluene (100 mL), washed with H₂O (50 mL) twice. Keep the organic phase in fridge (2-8 °C) for overnight. Then filtered and dried in vacuo to afford the desired product benzene-1,3,5-triyl triformate (TFBen) as a white solid (5.1 g, 55% yield).

3. General procedure for the synthesis of (*N*-SO₂Py)-2-iodoanilines (**1a-1l**)

The (*N*-SO₂Py)-2-iodoanilines **1a-1d** and **1h-1l** were prepared according to a general procedure reported by Carretero.²



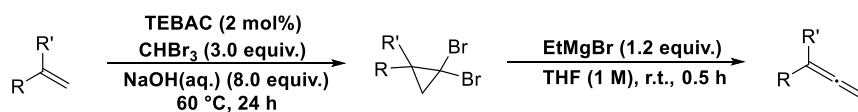
To a solution of 2-iodoaniline (4.0 mmol, 1.0 equiv.) in THF (40 mL), pyridine (379.7 mg, 4.8 mmol, 1.2 equiv.) and 2-pyridylsulfonyl chloride (852.5 mg, 4.8 mmol, 1.2 equiv.) were successively added dropwise at 0 °C under N₂ atmosphere. The mixture was warmed to room temperature and stirred overnight. During this time, a gradual formation of a precipitate was observed. The resulting mixture was then suction filtered through a 6-cm fritted glass funnel (coarse) into a round-bottomed flask, and the filter cake was rinsed with THF (3 × 10 mL). To the resulting filtrate and the washes, water (20 mL) was added and the THF was removed by evaporation at reduced pressure, yielding a suspension of a white solid in the aqueous medium. This solid was collected by filtration, washed sequentially with toluene (2 × 5 mL) and diethyl ether (2 × 5 mL). Then it was transferred to a round-bottomed flask, and dried over anhydrous Na₂SO₄, filtered, and concentrated. The crude mixture was purified by silica gel column chromatography to obtain (*N*-SO₂Py)-2-iodoanilines **1a-1d** and **1h-1l**.

The (*N*-SO₂Py)-2-iodoanilines **1e-1g** were prepared according to a general procedure reported by Chan.³

To a solution of 2-iodoaniline (5.0 mmol, 1.0 equiv.) in pyridine (5 mL) was added pyridine-2-sulfonyl chloride (1.33 g, 7.5 mmol, 1.5 equiv.) at 0 °C under N₂ atmosphere and the resulting reaction mixture was stirred at room temperature for 2 h. The reaction mixture was quenched with the addition of DCM (30 mL) followed by HCl (50 mL, 1M). The organic layer was extracted and washed with water (2 × 10 mL), brine (10 mL), dried over Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by flash column chromatography to obtain (*N*-SO₂Py)-2-iodoanilines **1e-1g**.

4. General procedure for the synthesis of allenes (2a-2w)

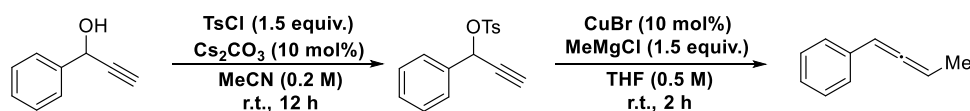
The allenes **2a-2v** were prepared according to a general procedure reported by Baird.⁴



To a mixture of alkene (20.0 mmol, 1.0 equiv.), bromoform (15.2 g, 60.0 mmol, 3.0 equiv.), and TEBAC (91.1 mg, 0.4 mmol, 0.02 equiv.) was added dropwise a solution of NaOH (6.4 g) in water (6.4 mL) over 1 h. The resulting mixture was stirred vigorously at 60 °C for 24 h, then cooled to room temperature, and quenched with water (50 mL). The mixture was extracted with dichloromethane and the organic phase was separated, dried over Na₂SO₄, and concentrated. The residue was purified by column chromatography over silica gel with petroleum ether as eluent to give 1,1-dibromocyclopropanes.

To a stirred solution of 1,1-dibromocyclopropane (10.0 mmol) in dry THF (10 mL) at rt was added dropwise EtMgBr (12 mL, 12.0 mmol, 1.0 M in THF) under N₂ over 0.5 h. Then the mixture was quenched with NH₄Cl(sat.) (20 mL) and diluted with petroleum ether (50 mL). The organic phase was washed with water (50 mL), dried over anhydrous Na₂SO₄, and concentrated. The residue was purified by column chromatography over silica gel with petroleum ether as eluent to give the allenes **2a-2v**.

The allene **2w** was prepared according to a procedure reported by van Dam and Tsuji.^{5,6}



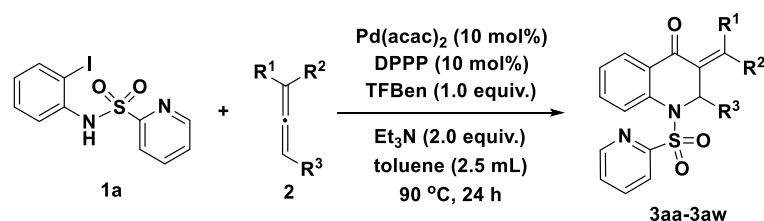
To a solution of alcohol (20.0 mmol) in MeCN (100 mL) *p*-toluenesulfonyl chloride (5.7 g, 30.0 mmol, 1.5 equiv.), and Cs₂CO₃ (651.6 mg, 2.0 mmol 10 mol%) were added. The reaction mixture was stirred rapidly at rt for 12 h. The progress of the reaction was monitored by thin-layer chromatography (TLC). After completion of the reaction, the mixture was diluted with water (100 mL) and the product was extracted with diethyl ether (2×100 mL). The organic extract was then washed with saturated solution of NaHCO₃ (2×100 mL), saline (2×100 mL) and water (100 mL). After drying over anhydrous Na₂SO₄, volatiles were evaporated under reduced pressure, residue

was dissolved in a mixture of ethyl acetate: petroleum ether 1:5 and purified *via* flash chromatography over silica gel.

A mixture of CuBr (143.5 mg, 1.0 mmol), THF (0.5 M) and the tosylate (10.0 mmol) was cooled to 0 °C. MeMgCl (5.0 mL, 15.0 mmol, 3.0 M in THF) was added dropwise. The reaction mixture was allowed to warm to room temperature and stirred for 2 h. It was quenched by addition of a saturated aqueous solution of NH₄Cl followed by extraction with Et₂O. The combined organic phases were washed with brine and dried over Na₂SO₄. The solvents were removed under reduced pressure and the residue was purified by column chromatography over silica gel with petroleum ether as eluent to give the allene **2w**.

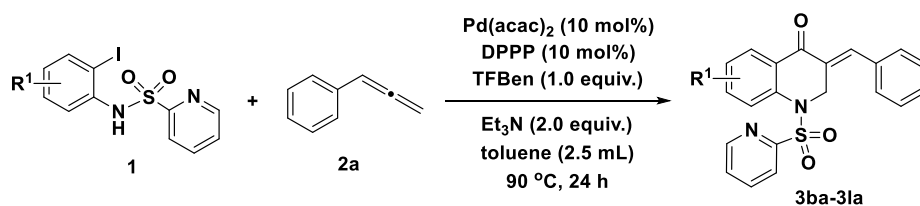
5. General procedure for the synthesis of 2,3-dihydroquinolin-4(1*H*)-ones

5.1 General procedure for the synthesis of 2,3-dihydroquinolin-4(1*H*)-ones (**3aa-3aw**)



1a (180.1 mg, 0.5 mmol, 1.0 equiv.), Pd(acac)₂ (15.2 mg, 0.05 mmol, 10 mol%), DPPP (20.6 mg, 0.05 mmol, 10 mol%), and a 2.5 mL vial containing TFBen (105.1 mg, 0.5 mmol, 1.0 equiv.) were added to an oven-dried tube (15 mL) which was then placed under vacuum and refilled with nitrogen three times. **2** (2.5 equiv.), Et₃N (101.2 mg, 1.0 mmol, 2.0 equiv.) and toluene (2.5 mL) were added into the tube via syringe. The tube was sealed and stirred at 90 °C for 24 h. Upon the reaction was completed, the resulting mixture was concentrated under vacuum and purified by silica gel column using chromatography (petroleum ether/ ethyl acetate = 5:1) to obtain the products **3aa-3aw**.

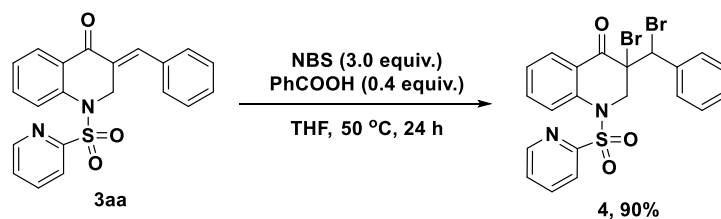
5.2 General procedure for the synthesis of 2,3-dihydroquinolin-4(1*H*)-ones (3ba-3la)



1 (0.5 mmol, 1.0 equiv.), Pd(acac)₂ (15.2 mg, 0.05 mmol, 10 mol%), DPPP (20.6 mg, 0.05 mmol, 10 mol%), and a 2.5 mL vial containing TFBen (105.1 mg, 0.5 mmol, 1.0 equiv.) were added to an oven-dried tube (15 mL) which was then placed under vacuum and refilled with nitrogen three times. **2a** (145.2 mg, 1.25 mmol, 2.5 equiv.), Et₃N (101.2 mg, 1.0 mmol, 2.0 equiv.) and toluene (2.5 mL) were added into the tube *via* syringe. The tube was sealed and stirred at 90 °C for 24 h. Upon the reaction was completed, the resulting mixture was concentrated under vacuum and purified by silica gel column using chromatography (petroleum ether/ ethyl acetate = 5:1) to obtain the products **3ba-3la**.

6. Transformation 3aa into compounds 4-6

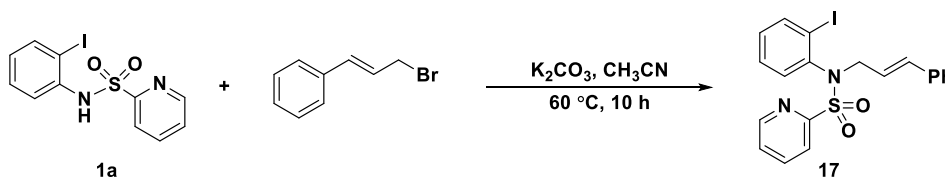
Compound **4** was prepared according to a general procedure reported by Zhao.⁷



To a solution of **3aa** (0.5 mmol, 1.0 equiv.) in THF (3 mL) was added NBS (267.0 mg, 1.5 mmol, 3.0 equiv.) and benzoic acid (24.4 mg, 0.2 mmol, 0.4 equiv.). The mixture was stirred for 24 h at room temperature. Upon the reaction was completed, the mixture was poured into water (10 mL) and extracted with CH₂Cl₂ (3 × 10 mL). The combined organic phase was washed with water (3 × 10 mL), and dried over anhydrous Na₂SO₄. The solvent was removed under reduced pressure, and the residue was purified by silica gel column using chromatography to obtain compound **4** (241.3 mg, 90% yield).

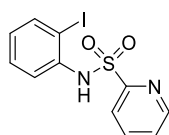
8. Preparation of compound 17

Compound 17 was prepared according to a general procedure reported by Zi.¹¹

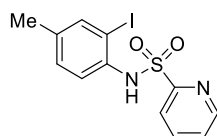


The allylic bromide (394.2 mg, 2.0 mmol, 2.0 equiv.) was added to a solution of 2-iodoaniline (1.0 mmol, 1.0 equiv.) and anhydrous K₂CO₃ (207.3 mg, 1.5 mmol, 1.5 equiv.) in CH₃CN (10 mL, 0.2 M) at 60 °C. The reaction mixture was stirred at 60 °C overnight then it was poured into cold water and extracted with ethyl acetate. The combined organic extracts were washed with water, aqueous KOH solution (10%), Na₂S₂O₃ solution (10%) and brine. Then it was dried over Na₂SO₄, filtered and concentrated under reduced pressure. The residue was eluted through a silica column to obtain compound 17 (381.1 mg, 80% yield).

9. Characterization data of compounds 1a-1l and 2a-2w

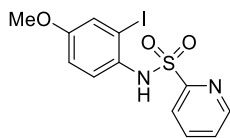


N-(2-iodophenyl)pyridine-2-sulfonamide (1a). White solid in 75% yield, mp 178.9 – 180.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.69 (d, *J* = 4.2 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.85 (td, *J* = 7.7, 1.7 Hz, 1H), 7.67 (dd, *J* = 8.1, 1.1 Hz, 2H), 7.48 (ddd, *J* = 7.5, 4.7, 1.2 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.09 (s, 1H), 6.82 (td, *J* = 7.9, 1.5 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 156.5, 150.5, 139.4, 138.1, 137.6, 129.6, 127.3, 127.0, 122.8, 122.5, 92.0.

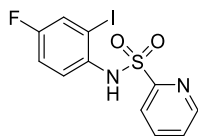


N-(2-iodo-4-methylphenyl)pyridine-2-sulfonamide (1b). White solid in 70% yield, mp 144.3 – 145.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.68 (d, *J* = 4.6 Hz, 1H), 7.86 – 7.81 (m, 2H), 7.50 – 7.45 (m, 3H), 7.07 (d, *J* = 10.3 Hz, 2H), 2.21 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 156.4, 150.4, 139.6,

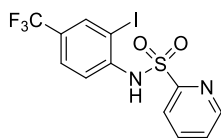
138.1, 137.5, 134.9, 130.3, 127.3, 123.2, 122.8, 92.8, 20.4.



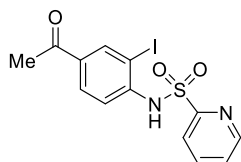
***N*-(2-iodo-4-methoxyphenyl)pyridine-2-sulfonamide (1c)**. White solid in 69% yield, mp 155.4–156.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.70 (d, *J* = 4.6 Hz, 1H), 7.85 – 7.79 (m, 2H), 7.50 – 7.47 (m, 2H), 7.18 (d, *J* = 2.8 Hz, 1H), 6.94 (s, 1H), 6.84 (dd, *J* = 8.9, 2.8 Hz, 1H), 3.73 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 158.1, 156.6, 150.4, 138.1, 130.5, 127.2, 125.8, 124.3, 122.9, 115.1, 94.8, 55.8.



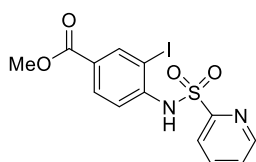
***N*-(4-fluoro-2-iodophenyl)pyridine-2-sulfonamide (1d)**. White solid in 73% yield, mp 143.8 – 145.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.70 (dt, *J* = 4.7, 1.2 Hz, 1H), 7.86 (dd, *J* = 4.9, 1.2 Hz, 2H), 7.61 (dd, *J* = 9.0, 5.3 Hz, 1H), 7.50 (dd, *J* = 8.8, 4.7 Hz, 1H), 7.39 (dd, *J* = 7.6, 2.9 Hz, 1H), 7.09 (s, 1H), 7.03 (ddd, *J* = 9.0, 7.8, 2.9 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 161.1, 157.5 (d, *J* = 222.8 Hz, 1C), 150.4, 138.2, 134.0, 127.4, 126.0 (d, *J* = 24.8 Hz, 1C), 124.9 (d, *J* = 8.0 Hz, 1C), 122.8, 116.5 (d, *J* = 22.1 Hz, 1C), 93.0 (d, *J* = 8.0 Hz, 1C).



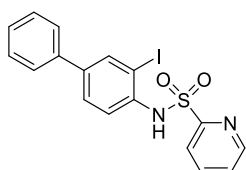
***N*-(2-iodo-4-(trifluoromethyl)phenyl)pyridine-2-sulfonamide (1e)**. White solid in 81% yield, mp 118.7 – 120.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.67 (d, *J* = 4.5 Hz, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.92 – 7.88 (m, 2H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.51 (dd, *J* = 7.2, 5.4 Hz, 2H), 7.35 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 156.2, 150.5, 140.9, 138.4, 136.3 (q, *J* = 3.7 Hz, 1C), 128.2 (q, *J* = 33.4 Hz, 1C), 127.7, 126.7 (q, *J* = 3.4 Hz, 1C), 122.8 (q, *J* = 272.4 Hz, 1C), 122.7, 120.7, 90.1.



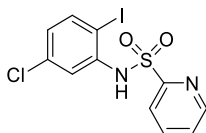
***N*-(4-acetyl-2-iodophenyl)pyridine-2-sulfonamide (1f).** White solid in 86% yield, mp 164.3 – 166.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.67 (d, *J* = 4.5 Hz, 1H), 8.28 (d, *J* = 1.8 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.90 (td, *J* = 7.8, 1.5 Hz, 1H), 7.83 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.50 (dd, *J* = 7.3, 4.9 Hz, 1H), 7.37 (s, 1H), 2.51 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 195.5, 156.2, 150.6, 141.7, 139.6, 138.3, 134.7, 129.8, 127.6, 122.8, 119.8, 90.3, 26.5.



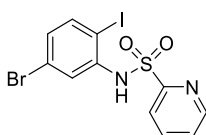
methyl 3-iodo-4-(pyridine-2-sulfonamido)benzoate (1g). White solid in 71% yield, mp 152.8 – 154.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.67 (d, *J* = 4.5 Hz, 1H), 8.35 (s, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.89 (dd, *J* = 15.4, 8.1 Hz, 2H), 7.74 (d, *J* = 8.2 Hz, 1H), 7.49 (dd, *J* = 7.6, 4.7 Hz, 1H), 7.35 (s, 1H), 3.87 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 165.0, 156.1, 150.4, 141.5, 140.6, 138.1, 130.8, 127.7, 127.5, 122.7, 119.6, 89.6, 52.4.



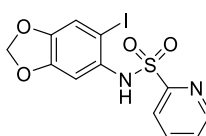
***N*-(3-iodo-[1,1'-biphenyl]-4-yl)pyridine-2-sulfonamide (1h).** White solid in 77% yield, mp 133.8 – 135.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.71 (d, *J* = 4.2 Hz, 1H), 7.95 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 2.0 Hz, 1H), 7.87 (td, *J* = 7.8, 1.6 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.52 – 7.49 (m, 2H), 7.48 – 7.46 (m, 2H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.35 – 7.32 (m, 1H), 7.19 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 156.4, 150.5, 140.1, 138.6, 138.2, 137.7, 136.6, 129.0, 128.2, 128.0, 127.4, 126.9, 122.8, 122.7, 92.7.



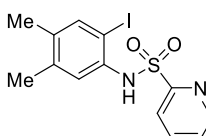
***N*-(5-chloro-2-iodophenyl)pyridine-2-sulfonamide (1i).** White solid in 65% yield, mp 171.5 – 172.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.70 (dd, *J* = 4.6, 0.6 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.89 (td, *J* = 7.7, 1.7 Hz, 1H), 7.70 (d, *J* = 2.4 Hz, 1H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.51 (ddd, *J* = 7.5, 4.7, 1.1 Hz, 1H), 7.11 (s, 1H), 6.82 (dd, *J* = 8.5, 2.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 156.2, 150.6, 139.9, 138.7, 138.3, 135.7, 127.5, 127.0, 122.8, 122.0, 88.6.



***N*-(5-bromo-2-iodophenyl)pyridine-2-sulfonamide (1j).** White solid in 55% yield, mp 179.1 – 180.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.70 (d, *J* = 4.6 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.89 (td, *J* = 7.7, 1.6 Hz, 1H), 7.84 (d, *J* = 2.2 Hz, 1H), 7.53 – 7.49 (m, 2H), 7.09 (s, 1H), 6.96 (dd, *J* = 8.4, 2.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 156.2, 150.6, 140.2, 138.9, 138.3, 129.9, 127.5, 124.9, 123.4, 122.9, 89.5.

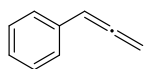


***N*-(6-iodobenzo[d][1,3]dioxol-5-yl)pyridine-2-sulfonamide (1k).** White solid in 90% yield, mp 178.2 – 181.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.71 – 8.69 (m, 1H), 7.88 – 7.83 (m, 2H), 7.51 – 7.48 (m, 1H), 7.23 (s, 1H), 7.04 (s, 1H), 6.82 (s, 1H), 5.97 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 156.6, 150.5, 149.2, 146.8, 138.2, 131.7, 127.3, 122.9, 117.6, 106.0, 102.4, 81.9.

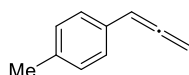


***N*-(2-iodo-4,5-dimethylphenyl)pyridine-2-sulfonamide (1l).** White solid in 76% yield, mp 209.8 – 211.5 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.82 (s, 1H), 8.75 (d, *J* = 4.0 Hz, 1H), 8.06 – 8.03 (m,

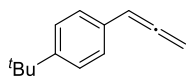
1H), 7.81 (d, $J = 7.8$ Hz, 1H), 7.68 (dd, $J = 6.9, 4.9$ Hz, 1H), 7.58 (s, 1H), 6.83 (s, 1H), 2.12 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 157.5, 150.0, 139.6, 138.6, 137.6, 137.1, 135.7, 129.5, 127.2, 122.2, 95.8, 19.0, 18.2.



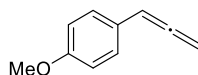
propa-1,2-dien-1-ylbenzene (2a). Colorless oil in 65% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.45 – 7.44 (m, 4H), 7.36 – 7.33 (m, 1H), 6.31 (td, $J = 6.7, 2.0$ Hz, 1H), 5.28 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.9, 134.0, 128.7, 127.0, 126.8, 94.1, 78.9.



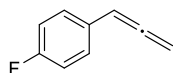
1-methyl-4-(propa-1,2-dien-1-yl)benzene (2b). Colorless oil in 68% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.32 (d, $J = 8.1$ Hz, 2H), 7.24 (d, $J = 8.0$ Hz, 2H), 6.27 (t, $J = 6.8$ Hz, 1H), 5.25 (d, $J = 6.8$ Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.7, 136.7, 131.0, 129.5, 126.7, 93.9, 78.8, 21.3.



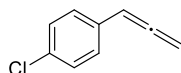
1-(tert-butyl)-4-(propa-1,2-dien-1-yl)benzene (2c). Colorless oil in 71% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.41 (m, 2H), 7.32 (d, $J = 8.4$ Hz, 2H), 6.23 (t, $J = 6.8$ Hz, 1H), 5.20 (d, $J = 6.8$ Hz, 2H), 1.40 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.9, 150.1, 131.1, 126.5, 125.7, 93.7, 78.7, 34.7, 31.5.



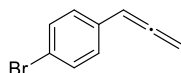
1-methoxy-4-(propa-1,2-dien-1-yl)benzene (2d). Colorless oil in 73% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.36 (d, $J = 8.4$ Hz, 2H), 6.98 (d, $J = 8.5$ Hz, 2H), 6.26 (t, $J = 6.8$ Hz, 1H), 5.25 (d, $J = 6.8$ Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.4, 158.8, 127.9, 126.2, 114.2, 93.5, 78.9, 55.3.



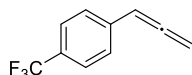
1-fluoro-4-(propa-1,2-dien-1-yl)benzene (2e). Colorless oil in 72% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.33 – 7.30 (m, 2H), 7.06 (t, $J = 8.7$ Hz, 2H), 6.20 (t, $J = 6.8$ Hz, 1H), 5.21 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.7, 162.0 (d, $J = 245.8$ Hz, 1C), 130.0 (d, $J = 3.0$ Hz, 1C), 128.2 (d, $J = 7.9$ Hz, 1C), 115.7 (d, $J = 21.7$ Hz, 1C), 93.2, 79.1.



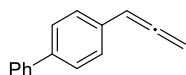
1-chloro-4-(propa-1,2-dien-1-yl)benzene (2f). Colorless oil in 74% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.30 – 7.28 (m, 2H), 7.24 – 7.22 (m, 2H), 6.14 (t, $J = 6.8$ Hz, 1H), 5.18 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.9, 132.6, 132.5, 128.9, 128.0, 93.3, 79.3.



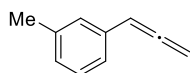
1-bromo-4-(propa-1,2-dien-1-yl)benzene (2g). Colorless oil in 76% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.47 (m, 2H), 7.21 (d, $J = 8.4$ Hz, 2H), 6.17 (t, $J = 6.8$ Hz, 1H), 5.21 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.9, 133.1, 131.8, 128.3, 120.6, 93.3, 79.4.



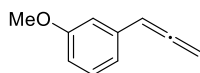
1-(propa-1,2-dien-1-yl)-4-(trifluoromethyl)benzene (2h). Colorless oil in 75% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, $J = 8.2$ Hz, 2H), 7.39 (d, $J = 8.1$ Hz, 2H), 6.20 (t, $J = 6.8$ Hz, 1H), 5.22 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.6, 138.1, 128.9 (q, $J = 32.5$ Hz, 1C), 126.9, 125.7 (q, $J = 3.0$ Hz, 1C), 123.0, 93.4, 79.5.



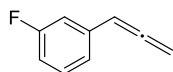
4-(propa-1,2-dien-1-yl)-1,1'-biphenyl (2i). Yellow solid in 80% yield, mp 54.1 – 55.6 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 7.4$ Hz, 2H), 7.56 (d, $J = 8.2$ Hz, 2H), 7.45 (t, $J = 7.6$ Hz, 2H), 7.39 – 7.33 (m, 3H), 6.22 (t, $J = 6.8$ Hz, 1H), 5.19 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.0, 140.8, 139.7, 133.0, 128.8, 127.4, 127.2, 127.1, 126.9, 93.6, 79.0.



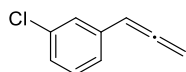
1-methyl-3-(propa-1,2-dien-1-yl)benzene (2j). Colorless oil in 80% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.38 (t, $J = 7.5$ Hz, 1H), 7.31 – 7.28 (m, 2H), 7.21 – 7.19 (m, 1H), 6.32 (t, $J = 6.8$ Hz, 1H), 5.31 (d, $J = 6.8$ Hz, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.0, 138.3, 133.9, 128.6, 127.9, 127.5, 124.0, 94.1, 78.7, 21.4.



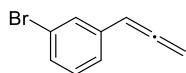
1-methoxy-3-(propa-1,2-dien-1-yl)benzene (2k). Colorless oil in 85% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.30 (t, $J = 7.9$ Hz, 1H), 7.00 – 6.92 (m, 2H), 6.84 (dd, $J = 8.2, 2.4$ Hz, 1H), 6.23 (t, $J = 6.8$ Hz, 1H), 5.23 (d, $J = 6.8$ Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.9, 160.0, 135.5, 129.7, 119.4, 112.8, 111.9, 94.1, 79.0, 55.2.



1-fluoro-3-(propa-1,2-dien-1-yl)benzene (2l). Colorless oil in 88% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.32 (dd, $J = 14.2, 7.7$ Hz, 1H), 7.10 (dd, $J = 15.7, 8.9$ Hz, 2H), 6.96 (t, $J = 8.4$ Hz, 1H), 6.20 (t, $J = 6.8$ Hz, 1H), 5.24 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.1, 163.3 (d, $J = 245.2$ Hz, 1C), 136.6 (d, $J = 7.8$ Hz, 1C), 130.1 (d, $J = 8.4$ Hz, 1C), 122.6 (d, $J = 2.5$ Hz, 1C), 113.9 (d, $J = 21.5$ Hz, 1C), 113.4 (d, $J = 22.3$ Hz, 1C), 93.5 (d, $J = 2.5$ Hz, 1C), 79.4.

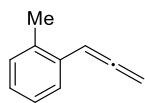


1-chloro-3-(propa-1,2-dien-1-yl)benzene (2m). Colorless oil in 85% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.36 (s, 1H), 7.31 – 7.27 (m, 1H), 7.24 – 7.21 (dd, $J = 8.8, 4.5$ Hz, 2H), 6.17 (t, $J = 6.8$ Hz, 1H), 5.25 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.0, 136.1, 134.7, 129.9, 127.0, 126.7, 125.0, 93.2, 79.5.

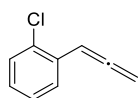


1-bromo-3-(propa-1,2-dien-1-yl)benzene (2n). Colorless oil in 83% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.52 (s, 1H), 7.38 (d, $J = 7.6$ Hz, 1H), 7.23 (dt, $J = 15.3, 7.7$ Hz, 2H), 6.16 (t, $J = 6.8$ Hz,

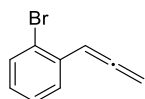
1H), 5.25 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.0, 136.4, 130.1, 129.9, 129.6, 125.4, 122.9, 93.1, 79.5.



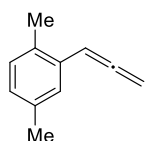
1-methyl-2-(propa-1,2-dien-1-yl)benzene (2o). Colorless oil in 60% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, $J = 7.6$ Hz, 1H), 7.39–7.29 (m, 3H), 6.56 (t, $J = 6.9$ Hz, 1H), 5.31 (d, $J = 6.9$ Hz, 2H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.6, 135.0, 132.3, 130.6, 127.4, 127.0, 126.3, 91.4, 78.1, 20.0.



1-chloro-2-(propa-1,2-dien-1-yl)benzene (2p). Colorless oil in 72% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.40 (dd, $J = 8.0, 1.1$ Hz, 1H), 7.27 (dd, $J = 10.8, 4.2$ Hz, 1H), 7.20–7.16 (m, 1H), 6.70 (t, $J = 6.8$ Hz, 1H), 5.25 (d, $J = 6.9$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.6, 132.0, 131.8, 129.8, 128.3, 128.0, 126.9, 90.5, 79.1.

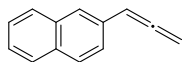


1-bromo-2-(propa-1,2-dien-1-yl)benzene (2q). Colorless oil in 76% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.59 (dd, $J = 8.0, 0.8$ Hz, 1H), 7.55 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.31 (t, $J = 7.5$ Hz, 1H), 7.12–7.08 (m, 1H), 6.71 (t, $J = 6.8$ Hz, 1H), 5.25 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.7, 133.6, 133.0, 128.5, 128.3, 127.5, 122.5, 93.2, 79.1.

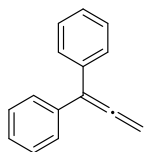


1,4-dimethyl-2-(propa-1,2-dien-1-yl)benzene (2r). Colorless oil in 58% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.32 (s, 1H), 7.14 (d, $J = 7.7$ Hz, 1H), 7.03 (d, $J = 7.6$ Hz, 1H), 6.44 (t, $J = 6.8$ Hz,

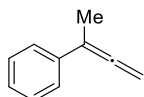
1H), 5.22 (d, $J = 6.9$ Hz, 2H), 2.42 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.4, 135.6, 131.9, 131.8, 130.5, 127.8, 127.7, 91.3, 78.0, 21.0, 19.4.



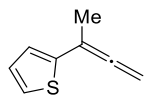
2-(propa-1,2-dien-1-yl)naphthalene (2s). Yellow solid in 85% yield, mp 42.5–44.7 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82–7.78 (m, 3H), 7.67 (s, 1H), 7.52 (dd, $J = 8.6, 1.5$ Hz, 1H), 7.49–7.42 (m, 2H), 6.36 (t, $J = 6.8$ Hz, 1H), 5.24 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.4, 133.8, 132.7, 131.5, 128.4, 127.9, 127.8, 126.4, 125.8, 125.5, 124.8, 94.5, 79.3.



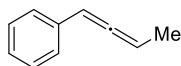
propa-1,2-diene-1,1-diyl dibenzene (2t). Colorless oil in 87% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.40–7.34 (m, 8H), 7.31–7.26 (m, 2H), 5.29 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 210.0, 136.4, 128.6, 127.4, 109.3, 78.2.



buta-2,3-dien-2-yl benzene (2u). Colorless oil in 69% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, $J = 7.6$ Hz, 2H), 7.45 (t, $J = 7.7$ Hz, 2H), 7.32 (t, $J = 7.3$ Hz, 1H), 5.15 (dd, $J = 6.2, 3.1$ Hz, 2H), 2.23 (t, $J = 3.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 209.1, 136.8, 128.4, 126.7, 125.8, 99.9, 77.0, 16.8.

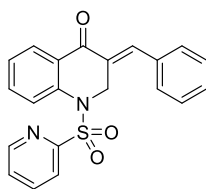


2-(buta-2,3-dien-2-yl)thiophene (2v). Colorless oil in 64% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.19 (d, $J = 5.1$ Hz, 1H), 6.99–6.97 (m, 1H), 6.92 (d, $J = 3.2$ Hz, 1H), 5.05 (d, $J = 3.0$ Hz, 2H), 2.12 (t, $J = 3.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 208.3, 142.1, 127.5, 124.6, 123.2, 96.3, 77.6, 17.8.

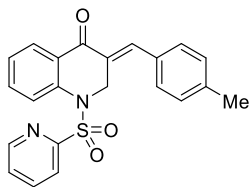


buta-1,2-dien-1-ylbenzene (2w). Colorless oil in 35% yield; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.47 – 7.46 (m, 4H), 7.38 – 7.32 (m, 1H), 6.28 (dq, $J = 6.4, 3.2$ Hz, 1H), 5.70 (p, $J = 7.0$ Hz, 1H), 1.96 (dd, $J = 7.1, 3.2$ Hz, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 206.1, 135.2, 128.7, 126.8, 94.2, 89.7, 14.2.

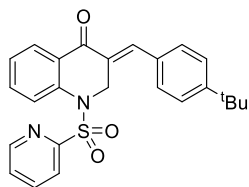
10. Characterization data of products 3aa–3aw and 3ba–3la



(E)-3-benzylidene-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3aa). Yellow solid, 163.7 mg, 87% yield, mp 151.3 – 152.6 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.37 (d, $J = 4.0$ Hz, 1H), 7.96 (d, $J = 7.7$ Hz, 1H), 7.76 (d, $J = 8.2$ Hz, 1H), 7.64 – 7.56 (m, 2H), 7.50 (d, $J = 6.3$ Hz, 2H), 7.45 – 7.39 (m, 3H), 7.37 – 7.32 (m, 2H), 7.29 (d, $J = 7.3$ Hz, 2H), 5.10 (s, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 183.0, 156.1, 150.0, 141.6, 138.0, 137.6, 134.2, 130.4, 130.0, 129.8, 128.9, 128.7, 128.3, 127.0, 126.9, 126.2, 122.8, 48.2; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{17}\text{N}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 377.0954; found: 377.0960.

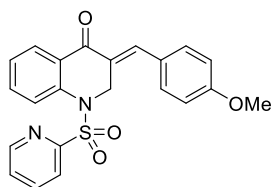


(E)-3-(4-methylbenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ab). Yellow solid, 162.0 mg, 83% yield, mp 179.8 – 180.9 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.36 – 8.35 (m, 1H), 7.95 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.75 (dd, $J = 8.2, 0.5$ Hz, 1H), 7.63 – 7.55 (m, 2H), 7.48 (d, $J = 7.8$ Hz, 1H), 7.44 (s, 1H), 7.36 – 7.32 (m, 2H), 7.26 – 7.23 (m, 2H), 7.18 (d, $J = 8.1$ Hz, 2H), 5.09 (d, $J = 1.4$ Hz, 2H), 2.39 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 183.0, 156.1, 150.1, 141.6, 140.3, 137.9, 137.8, 137.7, 134.0, 131.3, 130.2, 129.7, 129.5, 128.8, 128.2, 126.9, 126.2, 122.7, 48.3, 21.5; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 391.1111; found: 391.1115.



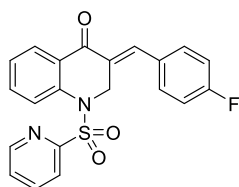
(E)-3-(4-(tert-butyl)benzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one

(3ac). Yellow solid, 160.0 mg, 74% yield, mp 188.9 – 190.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.42 (dd, *J* = 4.6, 0.7 Hz, 1H), 7.99 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.67 (td, *J* = 7.8, 1.7 Hz, 1H), 7.64 – 7.60 (m, 1H), 7.56 – 7.49 (m, 4H), 7.41 – 7.36 (m, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 5.17 (d, *J* = 1.5 Hz, 2H), 1.39 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 183.1, 156.1, 153.4, 150.1, 141.6, 137.9, 137.8, 137.7, 134.1, 131.4, 130.1, 129.6, 129.0, 128.3, 127.0, 126.3, 126.0, 122.8, 48.4, 35.0, 31.3; HRMS (ESI-TOF) Calcd. for C₂₅H₂₅N₂O₃S⁺ [M+H]⁺: 433.1580; found: 433.1586.



(E)-3-(4-methoxybenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ad).

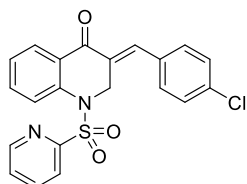
Yellow solid, 140.2 mg, 69% yield, mp 153.1 – 154.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.37 (dd, *J* = 4.6, 0.6 Hz, 1H), 7.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.64 – 7.57 (m, 2H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.43 (s, 1H), 7.36 (ddd, *J* = 7.6, 4.1, 2.4 Hz, 2H), 7.28 (d, *J* = 8.7 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 5.11 (d, *J* = 1.4 Hz, 2H), 3.87 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 183.1, 161.0, 156.1, 150.2, 141.5, 137.9, 137.7, 134.1, 132.2, 129.0, 128.3, 128.2, 127.0, 126.9, 126.8, 126.3, 122.8, 114.6, 55.5, 48.3; HRMS (ESI-TOF) Calcd. for C₂₂H₁₉N₂O₄S⁺ [M+H]⁺: 407.1060; found: 407.1058.



(E)-3-(4-fluorobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ae).

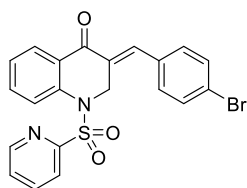
Yellow solid, 171.6 mg, 87% yield, mp 160.3 – 161.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 (dd, *J* = 4.6, 0.7 Hz, 1H), 7.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.78 – 7.74 (m, 1H), 7.66 (td, *J* = 7.7, 1.7 Hz,

1H), 7.62 – 7.56 (m, 1H), 7.54 (d, $J = 7.8$ Hz, 1H), 7.48 (s, 1H), 7.40 – 7.30 (m, 4H), 7.14 (t, $J = 8.6$ Hz, 2H), 5.09 (d, $J = 1.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 183.0, 163.4 (d, $J = 251.9$ Hz, 1C), 156.2, 150.1, 141.6, 138.0, 136.4, 136.3, 134.3, 132.1 (d, $J = 8.4$ Hz, 1C), 130.4 (d, $J = 2.9$ Hz, 1C), 130.3, 128.7, 128.4, 127.1, 127.0, 126.1, 122.8, 116.3 (d, $J = 21.8$ Hz, 1C), 48.3; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{16}\text{FN}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 395.0860; found: 395.0868.



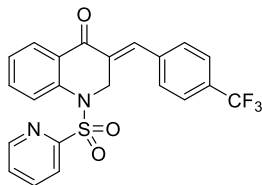
(E)-3-(4-chlorobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3af).

Yellow solid, 154.1 mg, 75% yield, mp 177.6 – 178.9 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.44 (dd, $J = 4.6, 0.7$ Hz, 1H), 8.01 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.82 – 7.80 (m, 1H), 7.71 (td, $J = 7.7, 1.7$ Hz, 1H), 7.66 – 7.62 (m, 1H), 7.59 (d, $J = 7.8$ Hz, 1H), 7.51 (s, 1H), 7.47 (d, $J = 8.5$ Hz, 2H), 7.44 – 7.38 (m, 2H), 7.32 (d, $J = 8.5$ Hz, 2H), 5.13 (d, $J = 1.6$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.9, 156.2, 150.1, 150.0, 141.6, 138.0, 136.2, 136.1, 135.9, 134.3, 132.7, 131.3, 131.0, 129.3, 128.6, 128.4, 127.1, 127.0, 126.1, 122.8, 48.3; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{16}\text{ClN}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 411.0565; found: 411.0566.

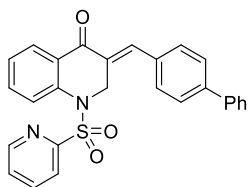


(E)-3-(4-bromobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ag).

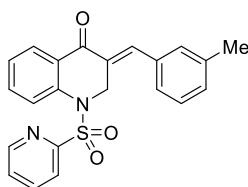
Yellow solid, 216.3 mg, 95% yield, mp 167.7 – 169.8 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.38 (dd, $J = 4.6, 0.7$ Hz, 1H), 7.95 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.75 (d, $J = 8.2$ Hz, 1H), 7.66 (td, $J = 7.8, 1.7$ Hz, 1H), 7.60 – 7.53 (m, 4H), 7.44 (s, 1H), 7.38 – 7.32 (m, 2H), 7.19 (d, $J = 8.4$ Hz, 2H), 5.06 (d, $J = 1.5$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.8, 156.1, 150.1, 141.6, 138.0, 136.1, 134.3, 133.1, 132.3, 131.4, 131.1, 128.6, 128.4, 127.1, 127.0, 126.1, 124.2, 122.8, 48.3; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{16}\text{BrN}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 455.0060; found: 455.0050.



(E)-1-(pyridin-2-ylsulfonyl)-3-(4-(trifluoromethyl)benzylidene)-2,3-dihydroquinolin-4(1H)-one (3ah). Yellow solid, 186.7 mg, 84% yield, mp 171.4 – 172.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 – 8.39 (m, 1H), 7.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.77 – 7.75 (m, 1H), 7.71 – 7.66 (m, 3H), 7.60 – 7.55 (m, 3H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.38 (ddd, *J* = 7.6, 4.7, 1.0 Hz, 1H), 7.34 (td, *J* = 7.7, 1.0 Hz, 1H), 5.10 (d, *J* = 1.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 182.7, 156.1, 150.1, 150.0, 141.6, 138.1, 137.8, 135.5, 135.4, 134.5, 132.5, 131.2 (q, *J* = 32.8 Hz, 1C), 130.0, 128.5, 128.4, 127.2, 127.0, 125.9, 123.86 (q, *J* = 272.4 Hz, 1C), 122.8, 48.3; HRMS (ESI-TOF) Calcd. for C₂₂H₁₆F₃N₂O₃S⁺ [M+H]⁺: 445.0828; found: 445.0827.

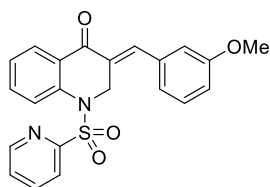


(E)-3-([1,1'-biphenyl]-4-ylmethylene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ai). Yellow solid, 203.6 mg, 90% yield, mp 170.7 – 172.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (dd, *J* = 4.6, 0.6 Hz, 1H), 7.99 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.70 – 7.59 (m, 6H), 7.56 – 7.54 (m, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 3H), 7.38 – 7.36 (m, 2H), 5.17 (d, *J* = 1.5 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 183.0, 156.1, 150.2, 142.6, 141.6, 140.0, 138.0, 137.3, 134.2, 133.1, 130.7, 130.3, 129.1, 128.8, 128.3, 128.1, 127.6, 127.2, 127.1, 126.3, 122.8, 48.4; HRMS (ESI-TOF) Calcd. for C₂₇H₂₁N₂O₃S⁺ [M+H]⁺: 453.1267; found: 453.1285.



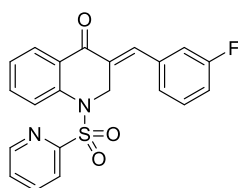
(E)-3-(3-methylbenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3aj). Yellow solid, 167.9 mg, 86% yield, mp 147.9 – 149.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, *J* = 4.4 Hz, 1H), 7.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.65 – 7.56 (m, 2H), 7.51 (d,

$J = 7.8$ Hz, 1H), 7.46 (s, 1H), 7.37 – 7.30 (m, 3H), 7.21 (d, $J = 7.6$ Hz, 1H), 7.09 (d, $J = 8.6$ Hz, 2H), 5.09 (d, $J = 1.5$ Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 183.0, 156.1, 150.1, 150.0, 141.6, 138.6, 137.9, 137.8, 134.1, 130.7, 130.6, 130.2, 128.8, 128.7, 128.2, 127.1, 127.0, 126.2, 122.8, 48.3, 21.5; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 391.1111; found: 391.1118.



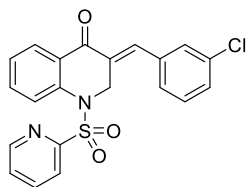
(*E*)-3-(3-methoxybenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one (3ak).

Yellow solid, 172.7 mg, 85% yield, mp 152.7 – 154.2 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.39 (dd, $J = 4.6, 0.6$ Hz, 1H), 7.96 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.76 (d, $J = 7.8$ Hz, 1H), 7.65 (td, $J = 7.8, 1.7$ Hz, 1H), 7.60 – 7.56 (m, 1H), 7.53 (d, $J = 7.8$ Hz, 1H), 7.47 (s, 1H), 7.36 (ddd, $J = 13.6, 9.2, 4.3$ Hz, 3H), 6.96 – 6.93 (m, 1H), 6.88 (d, $J = 7.7$ Hz, 2H), 5.10 (d, $J = 1.4$ Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 183.0, 159.8, 156.1, 150.1, 141.7, 138.0, 137.6, 135.4, 134.2, 130.6, 130.0, 128.7, 128.3, 127.0, 126.9, 126.1, 122.8, 122.3, 115.4, 115.3, 55.4, 48.3; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_4\text{S}^+$ $[\text{M}+\text{H}]^+$: 407.1060; found: 407.1064.



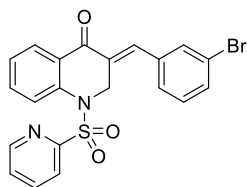
(*E*)-3-(3-fluorobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one (3al).

Yellow solid, 171.6 mg, 87% yield, mp 162.7 – 164.3 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.39 (d, $J = 4.0$ Hz, 1H), 7.95 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.76 (d, $J = 7.9$ Hz, 1H), 7.67 (td, $J = 7.8, 1.6$ Hz, 1H), 7.60 – 7.56 (m, 1H), 7.54 (d, $J = 7.8$ Hz, 1H), 7.46 (s, 1H), 7.42 – 7.32 (m, 3H), 7.12 – 7.08 (m, 2H), 6.99 (d, $J = 9.5$ Hz, 1H), 5.08 (d, $J = 1.5$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.8, 162.75 (d, $J = 247.5$ Hz, 1C), 156.1, 150.1, 141.6, 138.0, 136.3 (d, $J = 7.7$ Hz, 1C), 136.0, 134.3, 131.6, 130.6 (d, $J = 8.3$ Hz, 1C), 128.5, 128.3, 127.1, 127.0, 126.1, 125.6 (d, $J = 2.7$ Hz, 1C), 122.8, 116.8 (d, $J = 7.1$ Hz, 1C), 116.5 (d, $J = 7.9$ Hz, 1C), 48.2; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{16}\text{FN}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 395.0860; found: 395.0861.



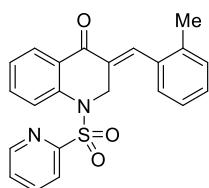
(E)-3-(3-chlorobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3am).

Yellow solid, 186.9 mg, 91% yield, mp 176.5 – 177.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (d, *J* = 4.4 Hz, 1H), 7.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.69 (td, *J* = 7.7, 1.6 Hz, 1H), 7.62 – 7.58 (m, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.45 (s, 1H), 7.41 – 7.34 (m, 4H), 7.25 (d, *J* = 6.2 Hz, 1H), 7.22 – 7.20 (m, 1H), 5.07 (d, *J* = 1.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 182.8, 156.2, 150.2, 141.7, 138.0, 136.0, 135.8, 134.9, 134.4, 131.8, 130.3, 129.9, 129.7, 128.6, 128.4, 127.7, 127.1, 127.0, 126.2, 122.9, 48.3; HRMS (ESI-TOF) Calcd. for C₂₁H₁₆ClN₂O₃S⁺ [M+H]⁺: 411.0565; found: 411.0565.



(E)-3-(3-bromobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3an).

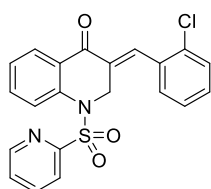
Yellow solid, 204.9 mg, 90% yield, mp 172.5 – 174.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.45 – 8.44 (m, 1H), 8.00 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.73 (td, *J* = 7.7, 1.6 Hz, 1H), 7.63 (td, *J* = 8.2, 1.5 Hz, 1H), 7.58 (t, *J* = 7.9 Hz, 2H), 7.47 (s, 1H), 7.43 (dd, *J* = 9.2, 3.1 Hz, 2H), 7.38 (dd, *J* = 16.7, 7.9 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 1H), 5.10 (d, *J* = 1.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 182.7, 156.1, 150.1, 141.7, 138.0, 136.2, 135.7, 134.4, 132.8, 132.6, 131.8, 130.5, 128.5, 128.4, 128.0, 127.1, 127.0, 126.1, 123.0, 122.8, 48.2; HRMS (ESI-TOF) Calcd. for C₂₁H₁₆BrN₂O₃S⁺ [M+H]⁺: 455.0060; found: 455.0063.



(E)-3-(2-methylbenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ao).

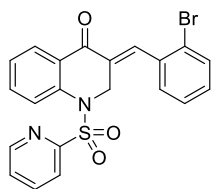
Yellow solid, 167.9 mg, 86% yield, mp 141.1 – 142.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.48 (dd,

$J = 4.6, 0.7$ Hz, 1H), 8.03 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.83 – 7.81 (m, 1H), 7.78 (s, 1H), 7.74 (td, $J = 7.7, 1.7$ Hz, 1H), 7.62 (dd, $J = 10.6, 4.8$ Hz, 2H), 7.43 (ddd, $J = 7.6, 4.7, 1.1$ Hz, 1H), 7.39 (td, $J = 7.7, 1.0$ Hz, 1H), 7.37 – 7.33 (m, 1H), 7.32 – 7.29 (m, 2H), 7.25 (t, $J = 7.3$ Hz, 1H), 5.07 (d, $J = 1.6$ Hz, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 183.1, 156.4, 150.0, 141.8, 138.0, 136.7, 134.2, 133.2, 130.7, 130.6, 129.8, 128.8, 128.7, 128.4, 127.1, 126.8, 126.2, 125.9, 122.8, 48.5, 20.1; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_3\text{S}^+ [\text{M}+\text{H}]^+$: 391.1111; found: 391.1117.



(E)-3-(2-chlorobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ap).

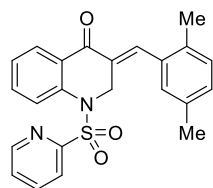
Yellow solid, 164.3 mg, 80% yield, mp 114.5 – 115.8 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.43 – 8.42 (m, 1H), 7.97 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.78 (d, $J = 8.1$ Hz, 1H), 7.73 – 7.68 (m, 2H), 7.61 – 7.57 (m, 1H), 7.54 (d, $J = 7.9$ Hz, 1H), 7.47 – 7.43 (m, 1H), 7.41 – 7.37 (m, 1H), 7.35 – 7.33 (m, 3H), 7.31 – 7.29 (m, 1H), 5.01 (d, $J = 1.7$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.5, 155.9, 150.1, 141.7, 138.2, 135.0, 134.5, 134.4, 132.6, 131.8, 130.9, 130.2, 130.1, 128.6, 128.4, 127.3, 127.1, 127.0, 126.2, 122.7, 48.4; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{16}\text{ClN}_2\text{O}_3\text{S}^+ [\text{M}+\text{H}]^+$: 411.0565; found: 411.0567.



(E)-3-(2-bromobenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3aq).

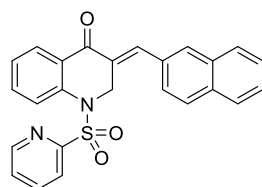
Yellow solid, 193.5 mg, 85% yield, mp 142.1 – 143.7 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.44 (dd, $J = 4.6, 0.7$ Hz, 1H), 7.97 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.78 (d, $J = 8.2$ Hz, 1H), 7.72 (td, $J = 7.8, 1.7$ Hz, 1H), 7.68 (s, 1H), 7.64 (dd, $J = 8.0, 0.8$ Hz, 1H), 7.61 – 7.55 (m, 2H), 7.41 – 7.36 (m, 2H), 7.34 – 7.31 (m, 2H), 7.28 – 7.23 (m, 1H), 5.01 (d, $J = 1.6$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.5, 155.8, 150.1, 141.6, 138.2, 136.6, 134.3, 133.4, 131.5, 130.9, 130.2, 128.6, 128.4, 127.7, 127.3,

127.0, 126.0, 125.7, 122.6, 48.4; HRMS (ESI-TOF) Calcd. for $C_{21}H_{16}BrN_2O_3S^+$ $[M+H]^+$: 455.0060; found: 455.0052.



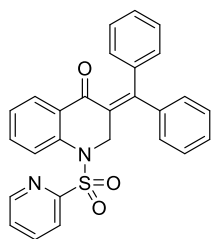
(*E*)-3-(2,5-dimethylbenzylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one

(3ar). Yellow solid, 178.0 mg, 88% yield, mp 117.3 – 118.7 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.42 (dd, $J = 4.6, 0.7$ Hz, 1H), 7.99 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.79 – 7.77 (m, 1H), 7.72 – 7.67 (m, 2H), 7.61 – 7.55 (m, 2H), 7.38 (ddd, $J = 7.7, 4.8, 1.1$ Hz, 1H), 7.34 (td, $J = 7.8, 1.0$ Hz, 1H), 7.11 (s, 2H), 6.98 (s, 1H), 5.02 (d, $J = 1.6$ Hz, 2H), 2.34 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.1, 156.4, 150.0, 149.9, 141.8, 137.9, 137.0, 136.9, 135.6, 134.8, 134.1, 133.0, 130.5, 129.2, 128.8, 128.4, 127.0, 126.8, 125.8, 122.7, 48.5, 21.1, 19.5; HRMS (ESI-TOF) Calcd. for $C_{23}H_{21}N_2O_3S^+$ $[M+H]^+$: 405.1267; found: 405.1273.

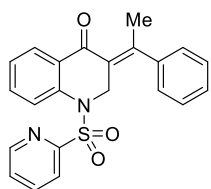


(*E*)-3-(naphthalen-2-ylmethylene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one

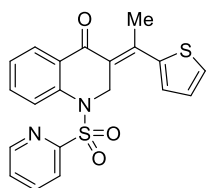
(3as). Yellow solid, 198.3 mg, 93% yield, mp 155.4 – 156.8 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, $J = 4.0$ Hz, 1H), 8.01 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.90 – 7.85 (m, 3H), 7.80 – 7.77 (m, 2H), 7.65 (s, 1H), 7.63 – 7.59 (m, 2H), 7.58 – 7.53 (m, 2H), 7.48 (d, $J = 7.8$ Hz, 1H), 7.39 – 7.34 (m, 3H), 5.20 (d, $J = 1.3$ Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.0, 156.2, 150.1, 141.7, 137.9, 137.7, 134.2, 133.6, 133.1, 131.7, 130.5, 130.4, 128.8, 128.7, 128.6, 128.3, 127.9, 127.6, 127.0, 126.9, 126.7, 126.2, 122.8, 48.4; HRMS (ESI-TOF) Calcd. for $C_{25}H_{18}N_2O_3SNa^+$ $[M+Na]^+$: 449.0930; found: 449.0931.



3-(diphenylmethylene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3at). Yellow solid, 210.4 mg, 93% yield, mp 158.1 – 160.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.64 – 8.63 (m, 1H), 7.92 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.85 – 7.80 (m, 2H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.49 (ddd, *J* = 7.6, 4.7, 1.0 Hz, 1H), 7.41 – 7.40 (m, 3H), 7.29 – 7.20 (m, 4H), 7.02 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.71 – 6.69 (m, 2H), 4.98 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 184.5, 157.1, 154.8, 150.3, 141.6, 141.4, 140.1, 138.2, 134.3, 129.6, 129.4, 129.1, 128.7, 128.5, 128.3, 128.0, 127.9, 127.1, 126.7, 126.1, 124.3, 123.0, 52.1; HRMS (ESI-TOF) Calcd. for C₂₇H₂₁N₂O₃S⁺ [M+H]⁺: 453.1267; found: 453.1277.

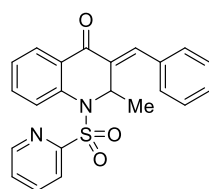


(E)-3-(1-phenylethylidene)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3au). Yellow solid, 165.9 mg, 85% yield, mp 128.5 – 130.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.57 (s, 1H), 8.07 – 8.04 (m, 1H), 7.90 – 7.86 (m, 1H), 7.77 – 7.70 (m, 2H), 7.57 – 7.56 (m, 1H), 7.49 – 7.42 (m, 4H), 7.37 – 7.34 (m, 1H), 7.16 (d, *J* = 6.2 Hz, 2H), 4.74 (d, *J* = 1.2 Hz, 2H), 2.44 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 185.3, 156.7, 154.7, 149.9, 141.9, 141.5, 137.8, 133.7, 129.3, 128.6, 128.5, 128.3, 127.1, 126.9, 126.2, 125.8, 124.6, 122.9, 51.4, 24.1; HRMS (ESI-TOF) Calcd. for C₂₂H₁₉N₂O₃S⁺ [M+H]⁺: 391.1111; found: 391.1113.



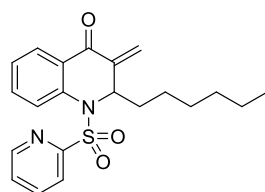
(E)-1-(pyridin-2-ylsulfonyl)-3-(1-(thiophen-2-yl)ethylidene)-2,3-dihydroquinolin-4(1H)-one (3av). Yellow solid, 144.7 mg, 73% yield, mp 136.8 – 138.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.48

(dd, $J = 4.6, 0.7$ Hz, 1H), 7.98 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.83 (td, $J = 7.8, 1.7$ Hz, 1H), 7.75 – 7.73 (m, 1H), 7.65 (d, $J = 7.8$ Hz, 1H), 7.56 (td, $J = 7.8, 1.6$ Hz, 1H), 7.50 (dd, $J = 5.1, 1.0$ Hz, 1H), 7.42 (ddd, $J = 7.6, 4.7, 1.0$ Hz, 1H), 7.36 – 7.32 (m, 1H), 7.10 (dd, $J = 5.1, 3.7$ Hz, 1H), 6.97 (dd, $J = 3.6, 1.0$ Hz, 1H), 5.00 (d, $J = 1.0$ Hz, 2H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 185.2, 157.0, 150.1, 146.6, 143.7, 141.5, 138.0, 134.0, 129.6, 129.4, 128.9, 128.4, 127.7, 126.9, 126.7, 126.0, 125.4, 123.0, 51.9, 25.3; HRMS (ESI-TOF) Calcd. for $\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}_3\text{S}_2^+$ $[\text{M}+\text{H}]^+$: 397.0675; found: 397.0676.



(*E*)-3-benzylidene-2-methyl-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one (3aw).

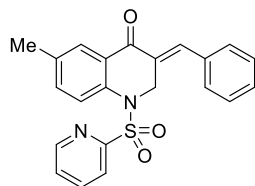
Yellow solid, 160.1 mg, 82% yield, mp 167.1 – 168.8 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.33 – 8.32 (m, 1H), 7.99 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.79 (d, $J = 8.1$ Hz, 1H), 7.61 (td, $J = 7.9, 1.5$ Hz, 1H), 7.54 (td, $J = 7.7, 1.7$ Hz, 1H), 7.44 (d, $J = 7.6$ Hz, 3H), 7.37 – 7.29 (m, 6H), 5.88 (q, $J = 6.9$ Hz, 1H), 1.50 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.9, 156.0, 150.0, 139.3, 137.8, 136.7, 135.0, 134.5, 134.0, 129.9, 129.8, 129.0, 128.0, 127.8, 127.5, 126.9, 126.8, 122.7, 53.0, 21.0; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$: 391.1111; found: 391.1116.



2-hexyl-3-methylene-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one (3ax).

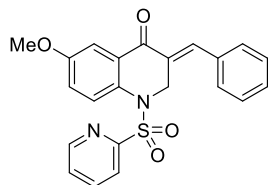
Yellow oil in 74% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.46 (dd, $J = 4.6, 0.6$ Hz, 1H), 7.92 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.80 (d, $J = 8.1$ Hz, 1H), 7.74 (td, $J = 7.7, 1.7$ Hz, 1H), 7.66 (d, $J = 7.8$ Hz, 1H), 7.63 – 7.58 (m, 1H), 7.38 – 7.32 (m, 2H), 5.98 (s, 1H), 5.21 (s, 1H), 5.11 – 5.07 (m, 1H), 1.74 – 1.66 (m, 1H), 1.47 – 1.35 (m, 3H), 1.29 – 1.21 (m, 6H), 0.84 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.4, 156.3, 150.1,

142.2, 139.8, 138.0, 134.6, 128.1, 128.0, 127.8, 127.1, 127.0, 123.3, 123.1, 61.8, 35.1, 31.7, 28.6, 25.9, 22.6, 14.1.



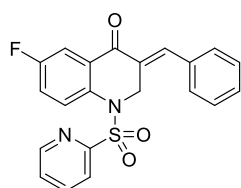
(E)-3-benzylidene-6-methyl-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ba).

Yellow solid, 165.9 mg, 85% yield, mp 153.2 – 154.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.42 (d, *J* = 4.5 Hz, 1H), 7.79 (s, 1H), 7.70 – 7.65 (m, 2H), 7.52 (d, *J* = 7.9 Hz, 2H), 7.46 (dd, *J* = 10.1, 7.7 Hz, 4H), 7.40 (dd, *J* = 7.6, 4.7 Hz, 1H), 7.32 (d, *J* = 7.5 Hz, 2H), 5.11 (s, 2H), 2.42 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 183.1, 156.1, 150.0, 139.2, 137.9, 137.5, 137.1, 135.1, 134.2, 130.5, 130.0, 129.8, 128.9, 128.5, 128.3, 126.9, 126.2, 122.8, 48.2, 21.0; HRMS (ESI-TOF) Calcd. for C₂₂H₁₉N₂O₃S⁺ [M+H]⁺: 391.1111; found: 391.1117



(E)-3-benzylidene-6-methoxy-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ca).

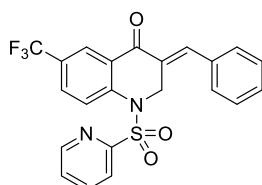
Yellow solid, 162.6 mg, 80% yield, mp 131.7 – 133.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 4.0 Hz, 1H), 7.69 (d, *J* = 8.9 Hz, 1H), 7.62 (td, *J* = 7.8, 1.6 Hz, 1H), 7.47 – 7.45 (m, 3H), 7.43 – 7.40 (m, 3H), 7.38 – 7.35 (m, 1H), 7.29 (d, *J* = 6.6 Hz, 2H), 7.16 (dd, *J* = 8.9, 3.1 Hz, 1H), 5.07 (d, *J* = 1.4 Hz, 2H), 3.85 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 182.9, 158.6, 156.0, 150.1, 137.9, 137.8, 134.9, 134.2, 130.4, 130.1, 130.0, 129.9, 129.0, 128.2, 126.9, 123.0, 121.8, 110.6, 55.8, 48.3; HRMS (ESI-TOF) Calcd. for C₂₂H₁₉N₂O₄S⁺ [M+H]⁺: 407.1060; found: 407.1065.



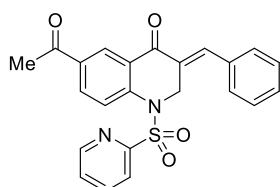
(E)-3-benzylidene-6-fluoro-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3da).

Yellow solid, 177.5 mg, 90% yield, mp 153.3 – 154.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.42 (d, *J*

= 4.6 Hz, 1H), 7.82 (dd, $J = 8.9, 4.6$ Hz, 1H), 7.71 – 7.65 (m, 2H), 7.55 – 7.52 (m, 2H), 7.49 – 7.46 (m, 3H), 7.42 (dd, $J = 7.6, 4.7$ Hz, 1H), 7.36 – 7.31 (m, 3H), 5.12 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.1, 161.2 (d, $J = 248.6$ Hz, 1C), 156.0, 150.1, 138.3, 138.1, 137.8 (d, $J = 2.3$ Hz, 1C), 134.0, 130.5 (d, $J = 7.1$ Hz, 1C), 130.1, 130.0, 129.8, 129.0, 128.6 (d, $J = 7.7$ Hz, 1C), 127.1, 122.9, 121.4 (d, $J = 23.4$ Hz, 1C), 114.2 (d, $J = 23.6$ Hz, 1C), 48.2; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{16}\text{FN}_2\text{O}_3\text{S}^+ [\text{M}+\text{H}]^+$: 395.0860; found: 395.0865.

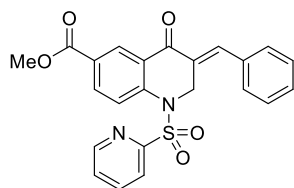


(E)-3-benzylidene-1-(pyridin-2-ylsulfonyl)-6-(trifluoromethyl)-2,3-dihydroquinolin-4(1H)-one (3ea). Yellow solid, 202.2 mg, 91% yield, mp 164.5 – 166.2 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.40 – 8.39 (m, 1H), 8.27 (d, $J = 1.5$ Hz, 1H), 7.92 (d, $J = 8.6$ Hz, 1H), 7.80 (dd, $J = 8.6, 2.0$ Hz, 1H), 7.68 (td, $J = 7.7, 1.6$ Hz, 1H), 7.59 (d, $J = 7.8$ Hz, 1H), 7.55 (s, 1H), 7.44 (d, $J = 7.2$ Hz, 3H), 7.42 – 7.38 (m, 1H), 7.29 – 7.27 (m, 2H), 5.13 (d, $J = 1.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.1, 156.2, 150.2, 144.6, 138.7, 138.3, 133.8, 130.5 (q, $J = 3.1$ Hz, 1C), 130.2, 130.1, 129.5, 129.1, 128.8 (q, $J = 33.7$ Hz, 1C), 128.4, 127.3, 126.3, 125.8 (q, $J = 3.7$ Hz, 1C), 123.6 (q, $J = 272.5$ Hz, 1C), 122.8, 48.1; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_3\text{S}^+ [\text{M}+\text{H}]^+$: 445.0828; found: 445.0830.

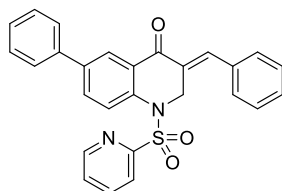


(E)-6-acetyl-3-benzylidene-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3fa). Yellow solid, 194.6 mg, 93% yield, mp 193.3 – 194.7 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.55 (d, $J = 2.1$ Hz, 1H), 8.40 (d, $J = 4.0$ Hz, 1H), 8.16 (dd, $J = 8.6, 2.2$ Hz, 1H), 7.87 (d, $J = 8.6$ Hz, 1H), 7.68 (td, $J = 7.7, 1.6$ Hz, 1H), 7.61 (d, $J = 7.8$ Hz, 1H), 7.58 (s, 1H), 7.45 (d, $J = 7.6$ Hz, 3H), 7.43 – 7.37 (m, 1H), 7.32 – 7.29 (m, 2H), 5.14 (d, $J = 1.4$ Hz, 2H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.5, 182.6, 156.3, 150.2, 145.6, 138.5, 138.2, 135.0, 134.0, 133.3, 130.1, 129.7, 129.1, 129.0,

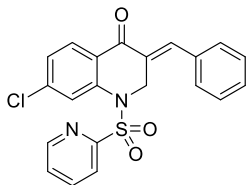
127.9, 127.3, 125.7, 122.8, 48.2, 26.8; HRMS (ESI-TOF) Calcd. for $C_{23}H_{19}N_2O_4S^+$ $[M+H]^+$: 419.1060; found: 419.1069.



methyl (E)-3-benzylidene-4-oxo-1-(pyridin-2-ylsulfonyl)-1,2,3,4-tetrahydroquinoline-6-carboxylate (3ga). Yellow solid, 178.1 mg, 82% yield, mp 147.7 – 149.5 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, $J = 2.0$ Hz, 1H), 8.39 (dd, $J = 4.6, 0.6$ Hz, 1H), 8.21 (dd, $J = 8.6, 2.1$ Hz, 1H), 7.85 (d, $J = 8.6$ Hz, 1H), 7.67 (td, $J = 7.7, 1.7$ Hz, 1H), 7.60 – 7.57 (m, 2H), 7.48 – 7.42 (m, 3H), 7.39 (ddd, $J = 7.5, 4.7, 1.1$ Hz, 1H), 7.33 – 7.28 (m, 2H), 5.14 (d, $J = 1.4$ Hz, 2H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.5, 165.9, 156.2, 150.2, 145.4, 138.4, 138.2, 134.8, 134.0, 130.1, 130.0, 129.7, 129.1, 128.4, 128.0, 127.2, 125.6, 122.8, 52.5, 48.2; HRMS (ESI-TOF) Calcd. for $C_{23}H_{19}N_2O_5S^+$ $[M+H]^+$: 435.1009; found: 435.1011.

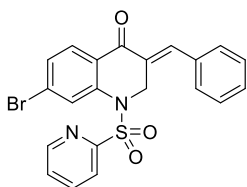


(E)-3-benzylidene-6-phenyl-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ha). Yellow solid, 196.8 mg, 87% yield, mp 145.8 – 147.2 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, $J = 4.1$ Hz, 1H), 8.22 (d, $J = 1.8$ Hz, 1H), 7.87 – 7.81 (m, 2H), 7.66 – 7.61 (m, 3H), 7.55 (d, $J = 8.6$ Hz, 2H), 7.47 – 7.41 (m, 5H), 7.39 – 7.35 (m, 2H), 7.30 (d, $J = 6.7$ Hz, 2H), 5.13 (d, $J = 1.1$ Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.0, 156.1, 150.1, 140.7, 139.8, 139.2, 138.0, 137.8, 134.1, 132.6, 130.3, 130.0, 129.8, 129.0, 128.9, 128.8, 128.0, 127.0, 126.6, 126.5, 122.8, 48.2; HRMS (ESI-TOF) Calcd. for $C_{27}H_{20}N_2O_3SNa^+$ $[M+Na]^+$: 475.1087; found: 475.1091.



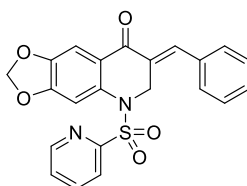
(E)-3-benzylidene-7-chloro-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ia).

Yellow solid, 180.8 mg, 88% yield, mp 186.4 – 187.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 4.1 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 1.9 Hz, 1H), 7.65 (td, *J* = 7.7, 1.6 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.49 (s, 1H), 7.46 – 7.42 (m, 3H), 7.40 – 7.36 (m, 1H), 7.31 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.27 – 7.25 (m, 2H), 5.07 (d, *J* = 1.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 182.2, 156.1, 150.2, 142.6, 140.3, 138.1, 138.0, 134.0, 130.0, 129.9, 129.8, 129.5, 129.0, 127.3, 127.2, 126.9, 126.0, 122.8, 48.2; HRMS (ESI-TOF) Calcd. for C₂₁H₁₆ClN₂O₃S⁺ [M+H]⁺: 411.0565; found: 411.0571.



(E)-3-benzylidene-7-bromo-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ja).

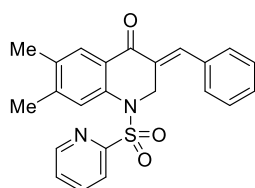
Yellow solid, 211.7 mg, 93% yield, mp 183.1 – 184.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.43 (dd, *J* = 4.6, 0.7 Hz, 1H), 8.00 (d, *J* = 1.7 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.69 (td, *J* = 7.7, 1.7 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.53 – 7.51 (m, 2H), 7.48 – 7.46 (m, 2H), 7.45 – 7.41 (m, 2H), 7.31 – 7.29 (m, 2H), 5.11 (d, *J* = 1.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 182.3, 156.0, 150.2, 142.5, 138.1, 138.0, 133.9, 130.3, 130.0, 129.9, 129.8, 129.5, 129.0, 128.9, 127.3, 127.2, 122.8, 48.2; HRMS (ESI-TOF) Calcd. for C₂₁H₁₆BrN₂O₃S⁺ [M+H]⁺: 455.0060; found: 455.0063.



(E)-7-benzylidene-5-(pyridin-2-ylsulfonyl)-6,7-dihydro-[1,3]dioxolo[4,5-g]quinolin-8(5H)-one (3ka).

Yellow solid, 172.4 mg, 82% yield, mp 144.3 – 145.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, *J* = 4.3 Hz, 1H), 7.62 (td, *J* = 7.7, 1.6 Hz, 1H), 7.46 – 7.35 (m, 6H), 7.31 (s, 1H), 7.24 – 7.21 (m,

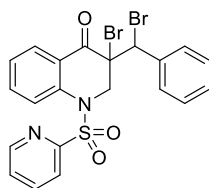
3H), 6.04 (s, 2H), 5.01 (d, $J = 1.2$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 181.5, 155.6, 152.5, 150.1, 147.1, 138.3, 137.9, 137.2, 134.2, 129.9, 129.7, 128.9, 127.0, 123.7, 122.9, 107.2, 106.3, 102.5, 48.3; HRMS (ESI-TOF) Calcd. for $\text{C}_{22}\text{H}_{17}\text{N}_2\text{O}_5\text{S}^+ [\text{M}+\text{H}]^+$: 421.0853; found: 421.0858.



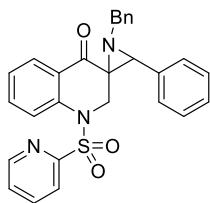
(*E*)-3-benzylidene-6,7-dimethyl-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one (31a).

Yellow solid, 165.8 mg, 82% yield, mp 160.8 – 161.5 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.42 (d, $J = 4.5$ Hz, 1H), 7.76 (s, 1H), 7.66 (td, $J = 7.7, 1.5$ Hz, 1H), 7.58 (s, 1H), 7.53 (s, 1H), 7.50 – 7.44 (m, 4H), 7.40 (dd, $J = 7.6, 4.7$ Hz, 1H), 7.31 – 7.30 (m, 2H), 5.08 (d, $J = 1.1$ Hz, 2H), 2.40 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 182.9, 156.1, 150.1, 144.5, 139.5, 137.9, 137.2, 136.2, 134.3, 130.5, 130.0, 129.7, 128.9, 128.8, 127.3, 126.9, 126.6, 122.9, 48.3, 20.7, 19.4; HRMS (ESI-TOF) Calcd. for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_3\text{S}^+ [\text{M}+\text{H}]^+$: 405.1267; found: 405.1270.

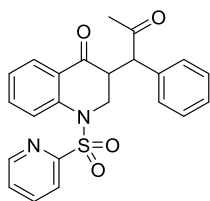
11. Characterization data of compounds 4-6, 7, 12, 17 and 18



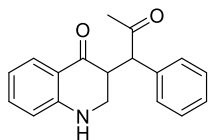
3-bromo-3-(bromo(phenyl)methyl)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1*H*)-one (4). Yellow oil, 241.3 mg, 90% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.71 (d, $J = 4.4$ Hz, 1H), 8.18 (dd, $J = 7.9, 1.4$ Hz, 1H), 8.13 (d, $J = 7.9$ Hz, 1H), 8.00 (td, $J = 7.8, 1.5$ Hz, 1H), 7.61 – 7.54 (m, 3H), 7.52 (d, $J = 8.2$ Hz, 1H), 7.47 (dd, $J = 7.1, 1.5$ Hz, 1H), 7.41 (ddd, $J = 8.8, 6.4, 2.3$ Hz, 3H), 7.21 (t, $J = 7.2$ Hz, 1H), 6.12 (s, 1H), 5.00 (q, $J = 14.3$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 185.2, 157.8, 150.5, 142.0, 138.6, 135.6, 135.4, 130.6, 130.2, 129.5, 128.6, 127.6, 124.5, 122.5, 121.5, 119.6, 65.5, 54.4, 52.4; HRMS (ESI-TOF) Calcd. for $\text{C}_{21}\text{H}_{17}\text{Br}_2\text{N}_2\text{O}_3\text{S}^+ [\text{M}+\text{H}]^+$: 534.9321; found: 534.9321.



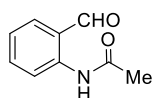
1-benzyl-3-phenyl-1'-(pyridin-2-ylsulfonyl)-1',2'-dihydro-4'H-spiro[aziridine-2,3'-quinolin]-4'-one (5). Yellow solid, 108.4 mg, 75% yield, mp 125.8 – 127.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.52 (d, *J* = 4.1 Hz, 1H), 8.01 (dd, *J* = 12.0, 4.6 Hz, 2H), 7.83 (td, *J* = 7.8, 1.6 Hz, 1H), 7.77 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.41 – 7.39 (m, 1H), 7.37 – 7.35 (m, 6H), 7.31 (dd, *J* = 10.6, 3.9 Hz, 2H), 7.28 – 7.26 (m, 2H), 7.21 (dd, *J* = 15.0, 7.8 Hz, 1H), 4.19 (d, *J* = 14.7 Hz, 1H), 4.03 (d, *J* = 13.8 Hz, 1H), 3.94 (s, 1H), 3.86 (d, *J* = 14.7 Hz, 1H), 3.49 (d, *J* = 13.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 189.6, 157.6, 149.9, 142.7, 138.8, 138.3, 135.1, 134.7, 128.5, 128.4, 128.3, 128.0, 127.9, 127.8, 127.4, 127.1, 127.0, 125.1, 122.8, 122.6, 54.9, 53.8, 51.3, 50.3; HRMS (ESI-TOF) Calcd. for C₂₈H₂₄N₃O₃S⁺ [M+H]⁺: 482.1533; found: 482.1536.



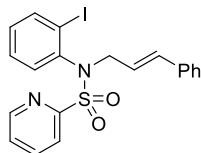
3-(2-oxo-1-phenylpropyl)-1-(pyridin-2-ylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (6). Yellow solid, 109.7 mg, 87% yield, mp 139.2 – 140.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.66 (d, *J* = 4.3 Hz, 1H), 7.90 (t, *J* = 6.6 Hz, 1H), 7.86 (ddd, *J* = 15.5, 7.9, 1.6 Hz, 2H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.45 (ddd, *J* = 7.5, 4.7, 1.1 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.35 – 7.28 (m, 3H), 7.22 (d, *J* = 7.1 Hz, 2H), 7.13 – 7.09 (m, 1H), 4.24 (dd, *J* = 13.7, 4.8 Hz, 1H), 4.15 (ddd, *J* = 14.3, 9.7, 4.8 Hz, 1H), 3.90 (d, *J* = 9.7 Hz, 1H), 3.47 (t, *J* = 13.9 Hz, 1H), 2.24 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 205.8, 194.8, 156.7, 150.6, 142.4, 138.2, 134.8, 134.2, 129.4, 128.9, 128.3, 128.1, 127.5, 124.9, 124.4, 123.3, 122.3, 56.6, 50.0, 48.0, 29.3; HRMS (ESI-TOF) Calcd. for C₂₃H₂₁N₂O₄S⁺ [M+H]⁺: 421.1217; found: 421.1222.



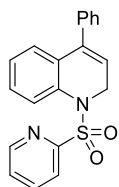
3-(2-oxo-1-phenylpropyl)-2,3-dihydroquinolin-4(1H)-one (7). Yellow solid, 21.8 mg, 78% yield, mp 126.9–128.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.41–7.30 (m, 6H), 6.76 (t, *J* = 7.5 Hz, 1H), 6.65 (d, *J* = 8.2 Hz, 1H), 4.41 (s, 1H), 4.05 (d, *J* = 10.0 Hz, 1H), 3.81 (ddd, *J* = 14.5, 10.0, 6.1 Hz, 1H), 3.12 (dd, *J* = 14.4, 11.9 Hz, 1H), 3.05 (dd, *J* = 11.7, 6.1 Hz, 1H), 2.36 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 206.6, 194.9, 151.6, 135.4, 135.3, 129.2, 128.9, 128.0, 127.9, 118.8, 118.0, 115.6, 56.7, 48.8, 45.4, 29.8; HRMS (ESI-TOF) Calcd. for C₁₈H₁₈NO₂⁺ [M+H]⁺: 280.1332; found: 280.1341.



N-(2-formylphenyl)acetamide (12). Yellow solid, 65.3 mg, 80% yield, mp 128.3–129.8 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.04 (s, 1H), 8.45 (d, *J* = 8.3 Hz, 1H), 7.96 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.59–7.55 (m, 1H), 7.15–7.11 (m, 1H), 2.13 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 169.4, 168.4, 140.8, 133.9, 131.0, 122.5, 119.9, 116.5, 25.0.



N-cinnamyl-N-(2-iodophenyl)pyridine-2-sulfonamide (17). Yellow oil, 381.1 mg, 80% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.84 (d, *J* = 4.6 Hz, 1H), 7.92–7.88 (m, 3H), 7.55 (dd, *J* = 8.8, 4.6 Hz, 1H), 7.33–7.30 (m, 4H), 7.28–7.24 (m, 2H), 7.10 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.02 (td, *J* = 7.7, 1.5 Hz, 1H), 6.39 (dt, *J* = 15.7, 6.8 Hz, 1H), 6.30 (d, *J* = 15.9 Hz, 1H), 4.70 (dd, *J* = 14.8, 6.7 Hz, 1H), 4.59 (dd, *J* = 14.8, 6.9 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 158.2, 150.1, 141.1, 140.3, 138.0, 136.3, 134.5, 131.7, 130.1, 128.9, 128.5, 127.9, 126.9, 126.5, 123.8, 123.2, 102.8, 55.3.



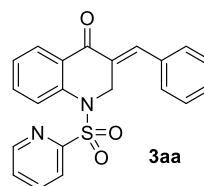
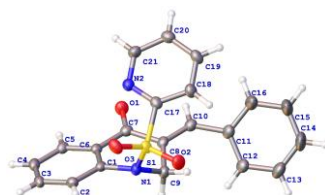
4-phenyl-1-(pyridin-2-ylsulfonyl)-1,2-dihydroquinoline (18). Yellow solid, 139.4 mg, 80% yield, mp 162.9–164.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.62 (d, *J* = 4.4 Hz, 1H), 8.08 (d, *J* = 7.9 Hz, 1H), 7.89 (td, *J* = 7.8, 1.5 Hz, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.49–7.45

(m, 3H), 7.39 (d, $J = 7.5$ Hz, 2H), 7.35 – 7.31 (m, 1H), 7.24 (t, $J = 7.7$ Hz, 1H), 7.07 (t, $J = 7.5$ Hz, 1H), 6.90 (t, $J = 2.9$ Hz, 1H), 5.36 (d, $J = 2.9$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.2, 150.4, 142.9, 138.0, 136.4, 132.7, 131.3, 129.7, 128.9, 128.5, 127.3, 123.9, 123.0, 120.4, 118.6, 114.3, 56.2.

12. References

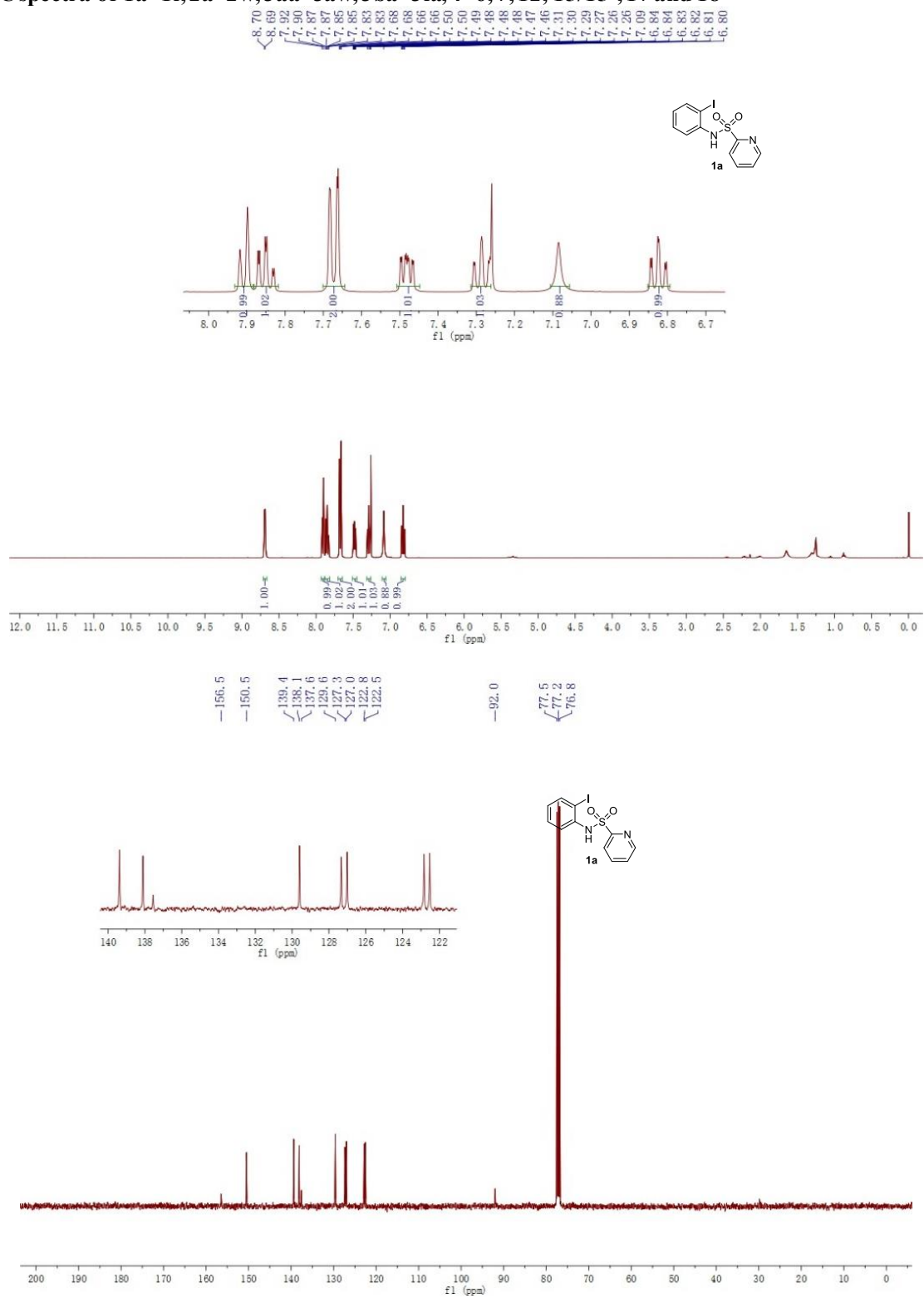
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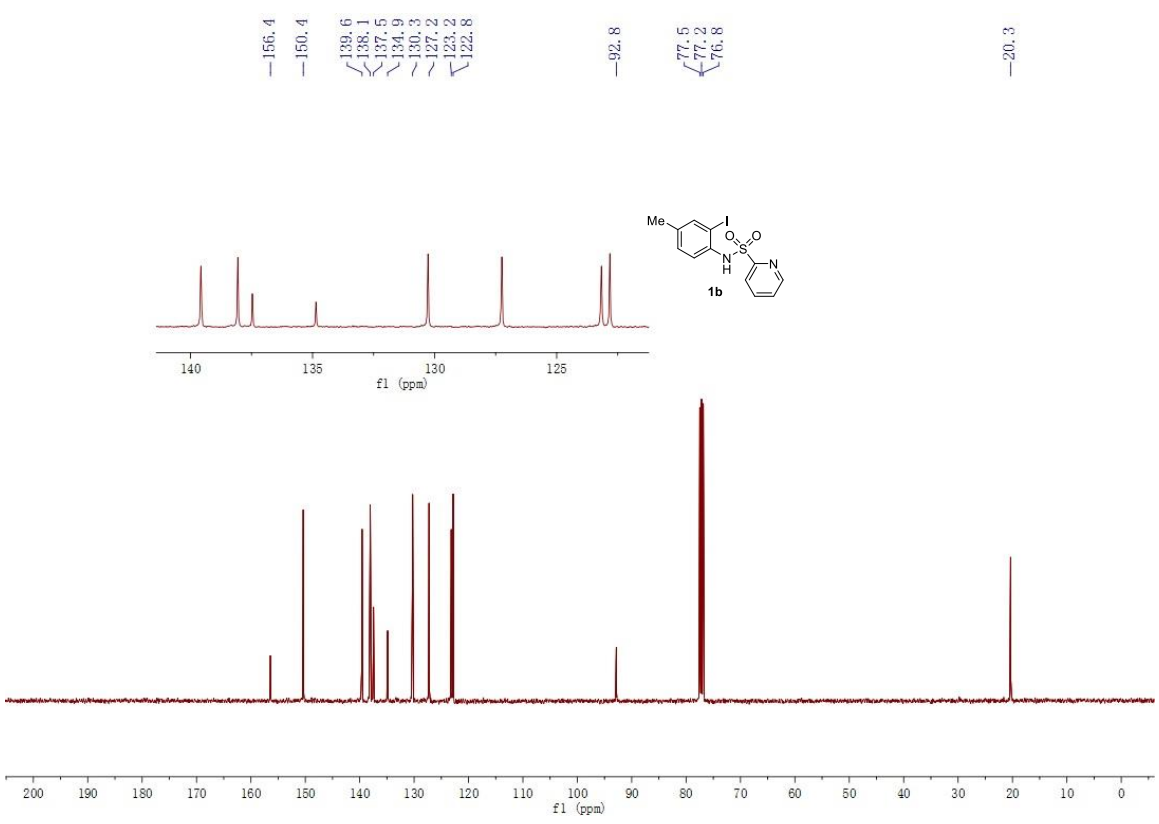
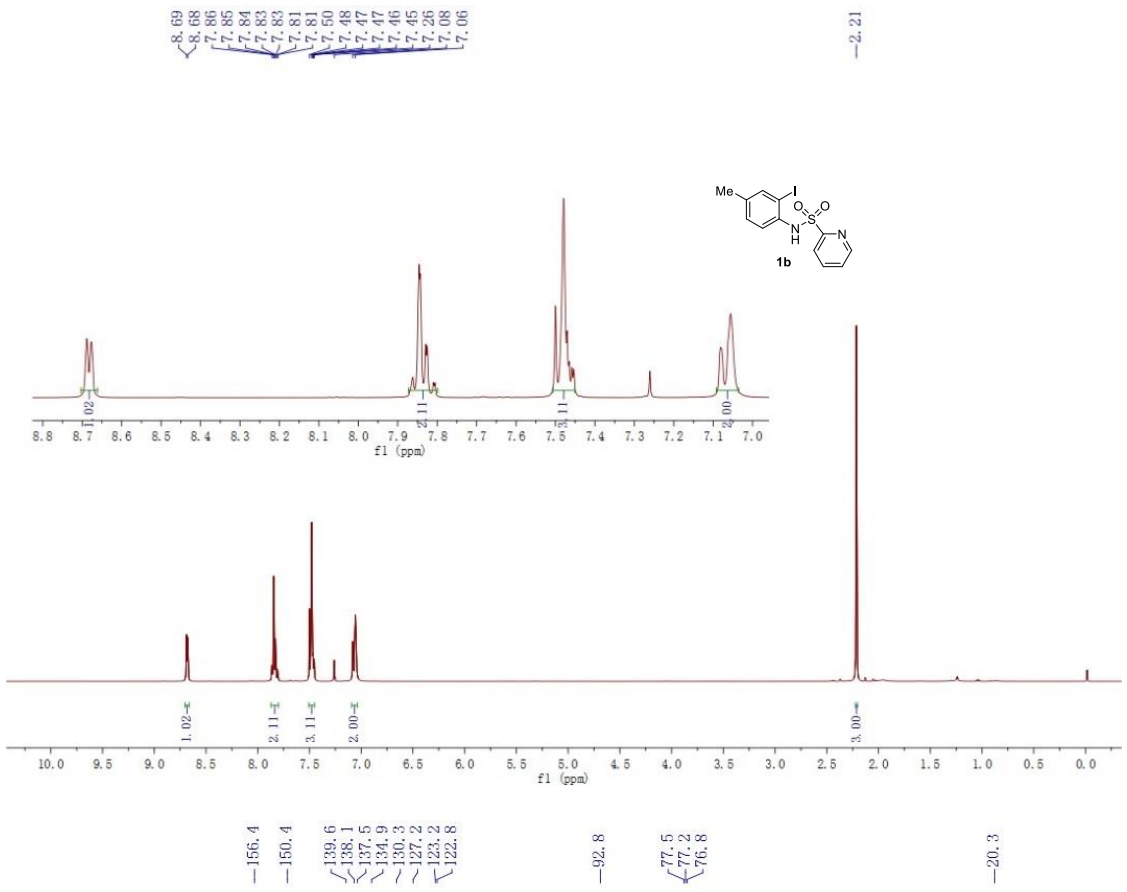
13. X-ray crystal data for compound 3aa

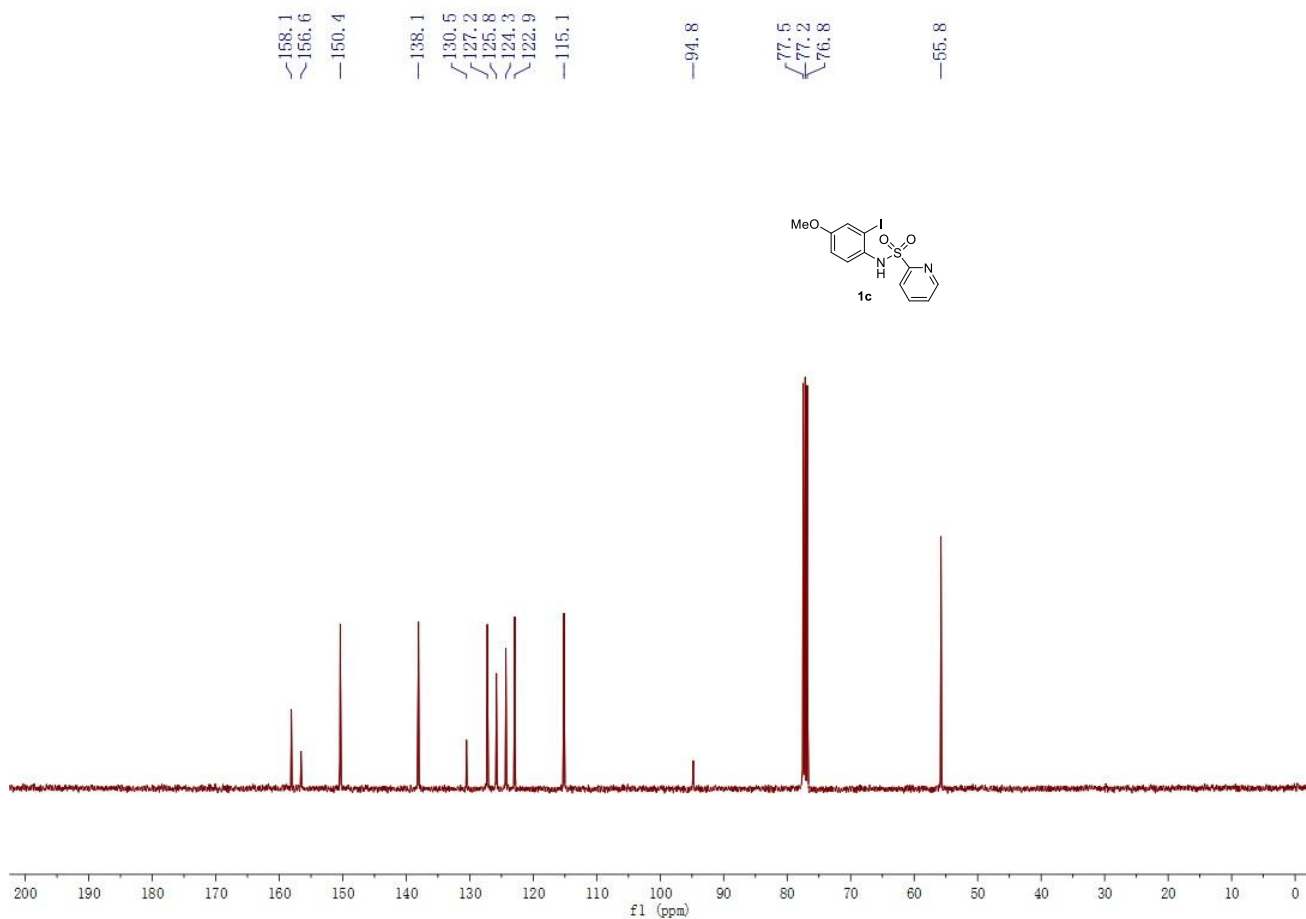
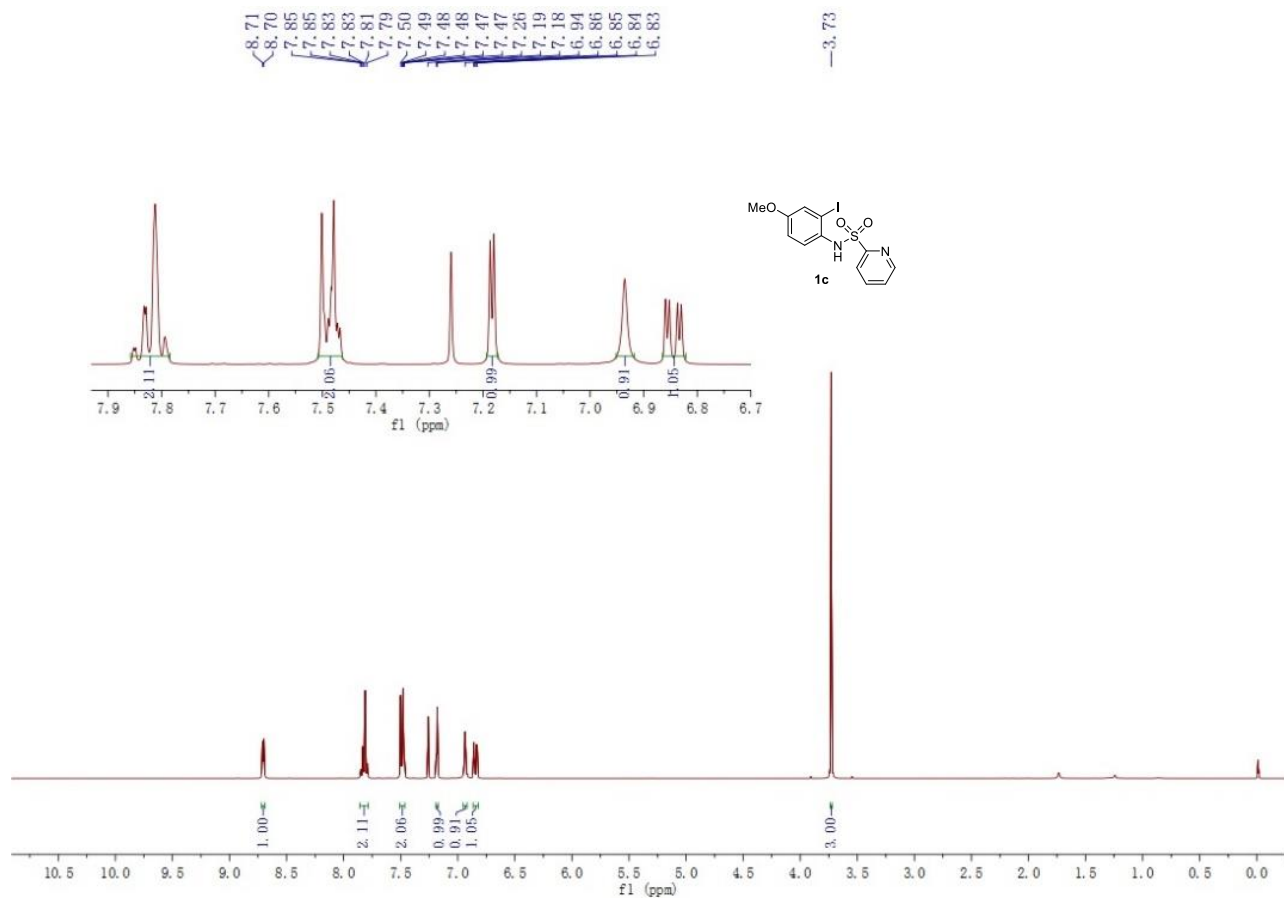


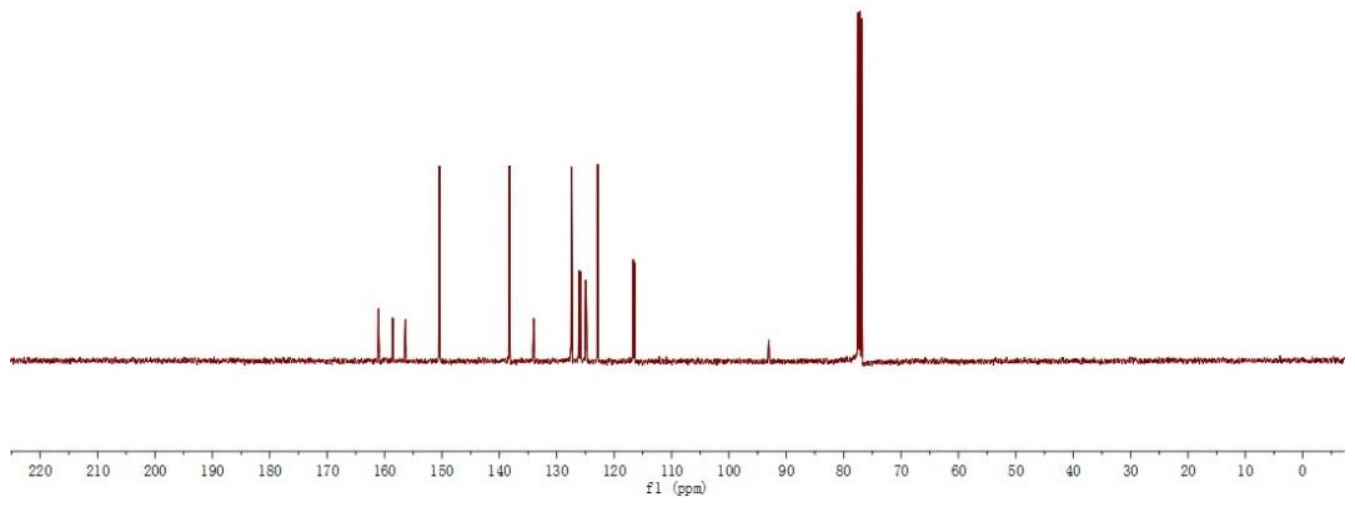
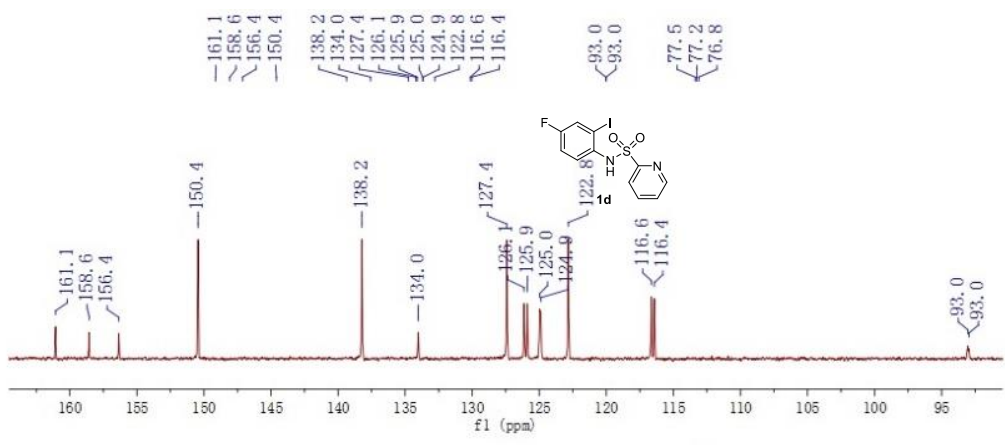
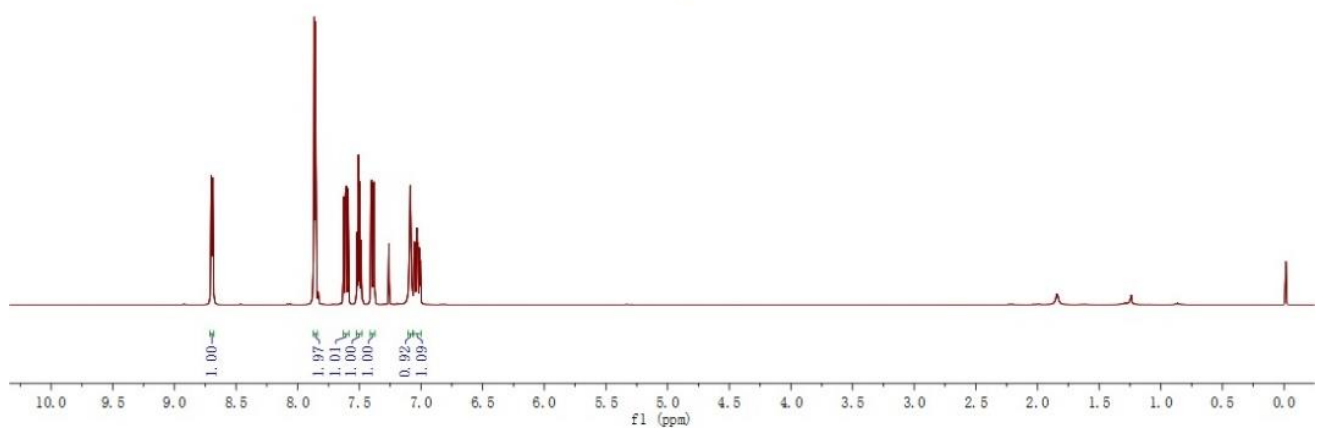
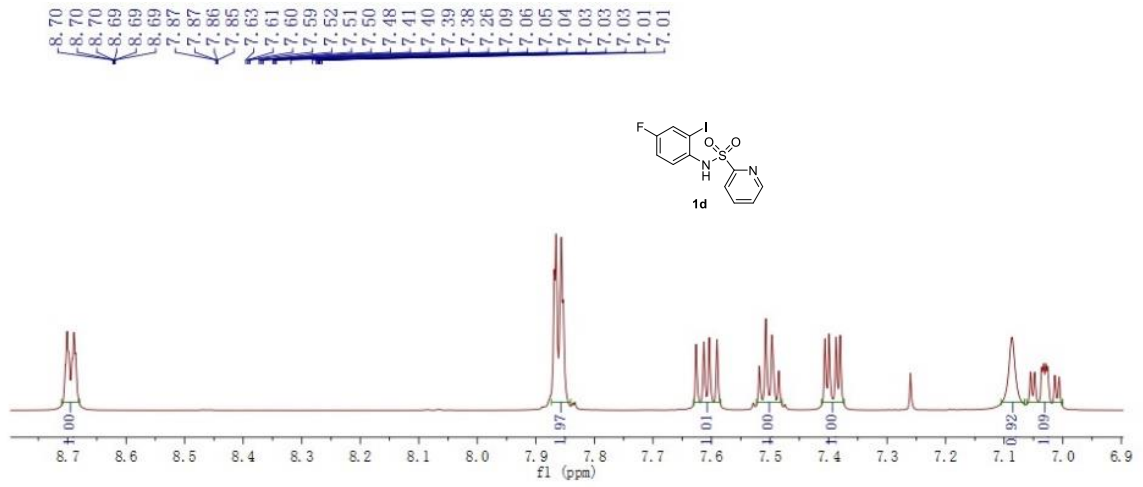
Compound	3aa
Empirical formula	C ₂₁ H ₁₆ N ₂ O ₃ S
Formula weight	376.42
Temperature/K	99.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	6.9424(6)
b/Å	8.1632(6)
c/Å	17.1903(15)
α/°	88.645(7)
β/°	89.576(7)
γ/°	73.503(7)
Volume/Å ³	933.85(14)
Z	2
ρ _{calc} /cm ³	1.339
μ/mm ⁻¹	0.197
F(000)	392.0
Crystal size/mm ³	0.12 × 0.11 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection /°	4.74 to 49.998
Index ranges	-8 ≤ h ≤ 7, -8 ≤ k ≤ 9, -20 ≤ l ≤ 20
Reflections collected	5946
Independent reflections	3289 [R _{int} =0.0279, R _{sigma} =0.0518]
Data/restraints/parameters	3289/0/245
Goodness-of-fit on F ²	1.055
Final R indexes [I ≥ 2σ(I)]	R ₁ = 0.0609, wR ₂ = 0.1369
Final R indexes [all data]	R ₁ = 0.0700, wR ₂ = 0.1419
Largest diff. peak/hole / e Å ⁻³	0.71/-0.44

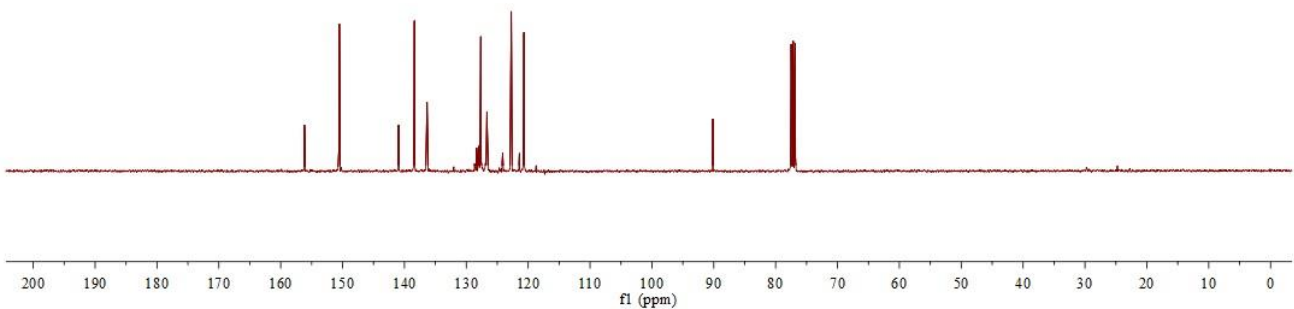
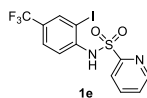
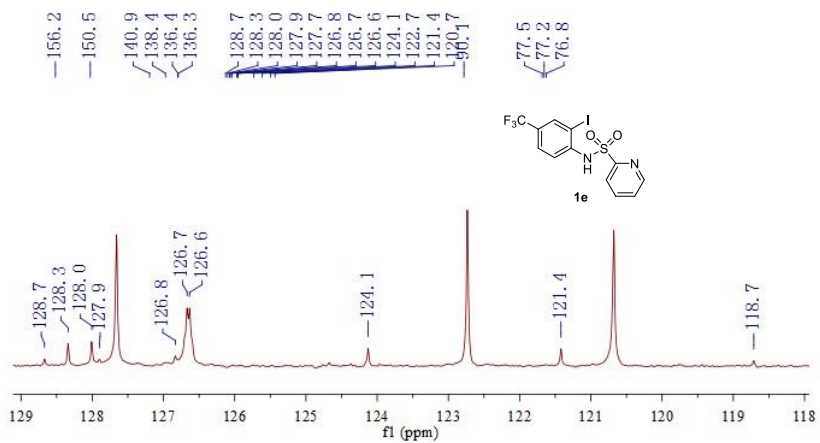
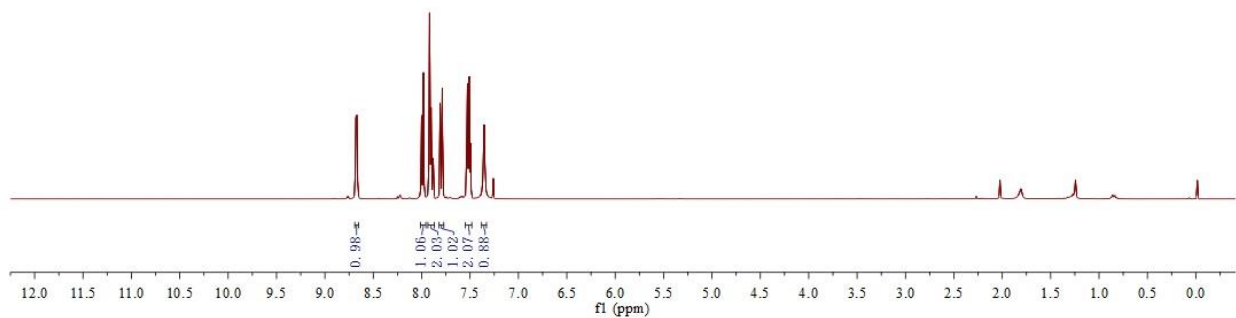
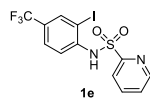
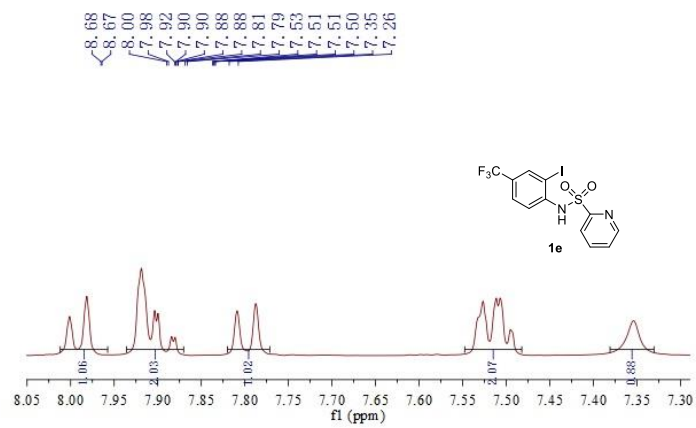
14. ^1H , ^{13}C spectra of 1a–1l, 2a–2w, 3aa–3aw, 3ba–3la, 4–6, 7, 12, 15/15', 17 and 18

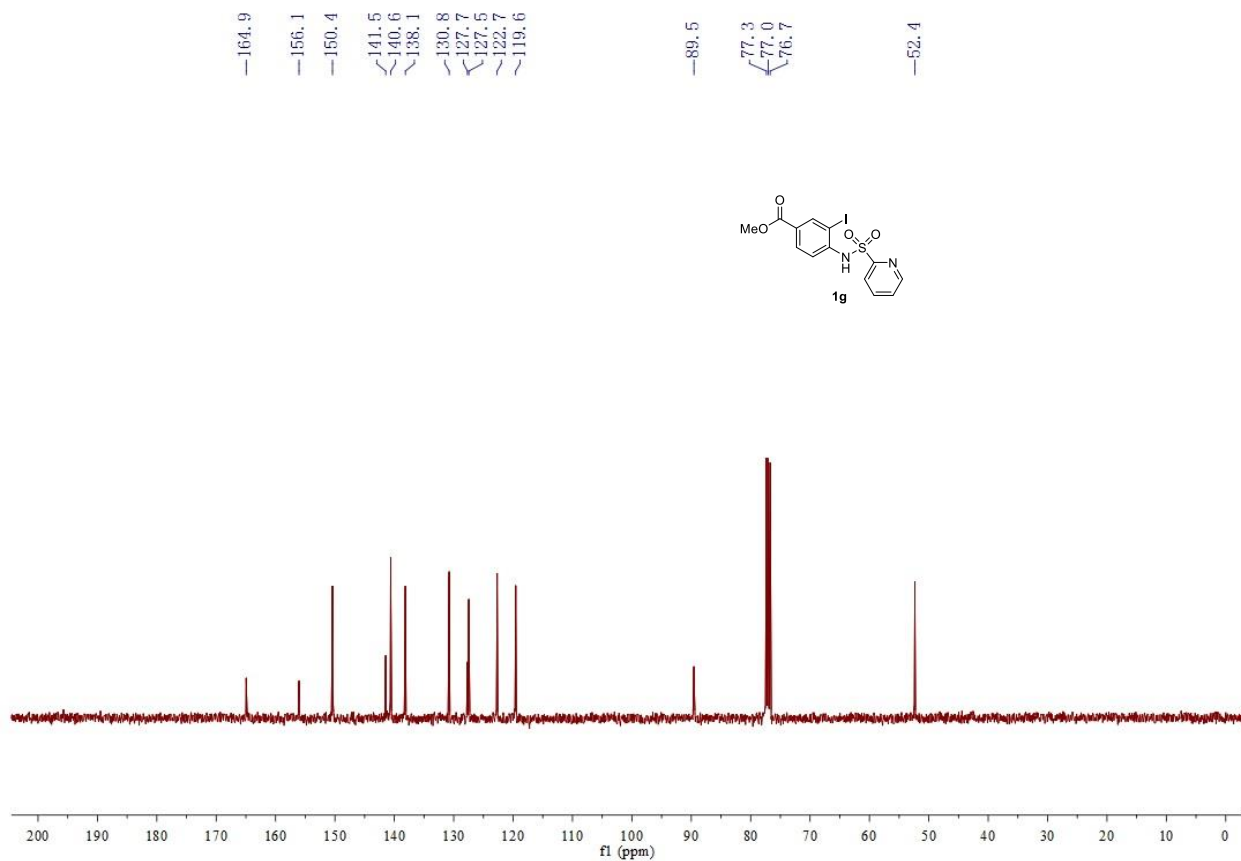
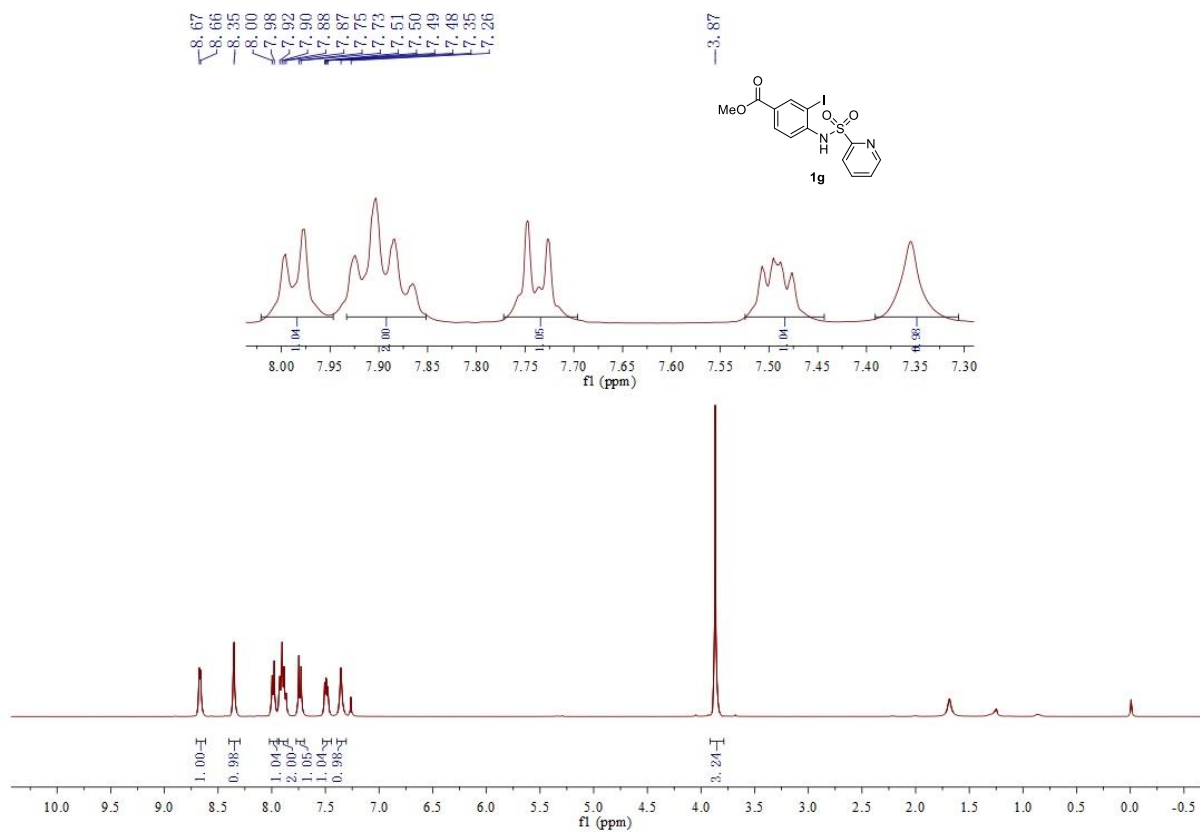




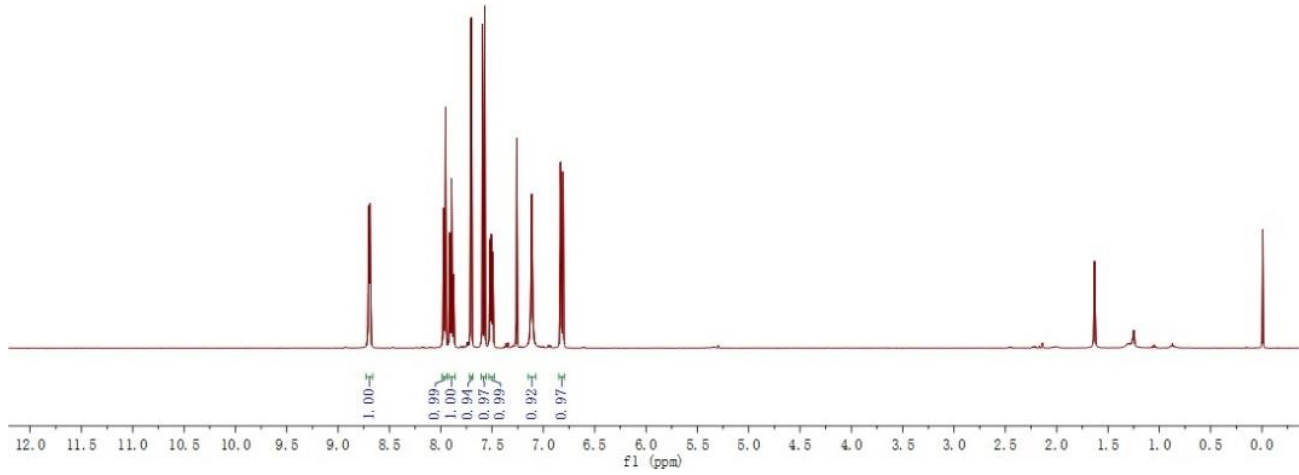
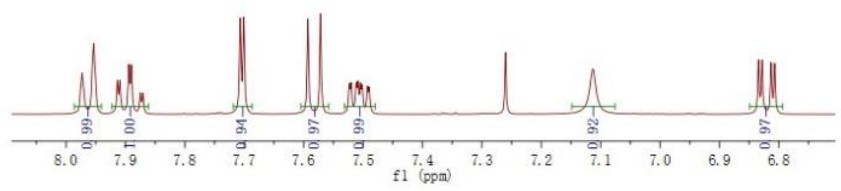
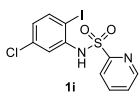




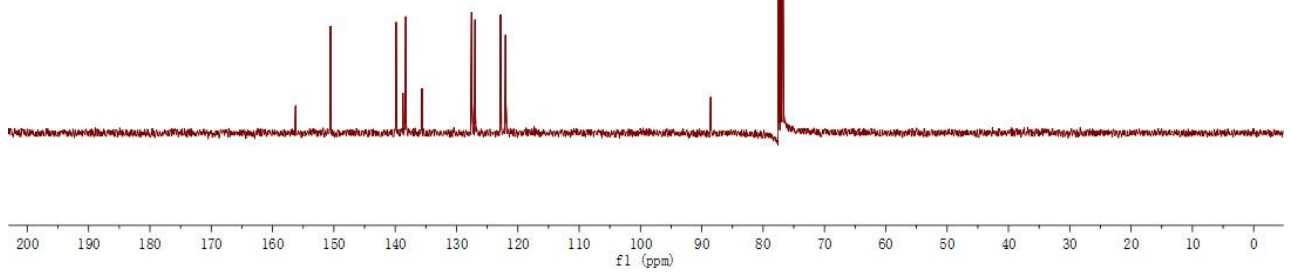
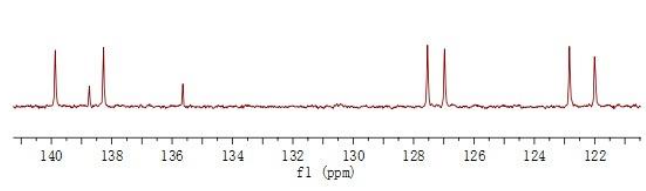
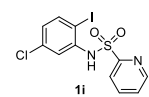




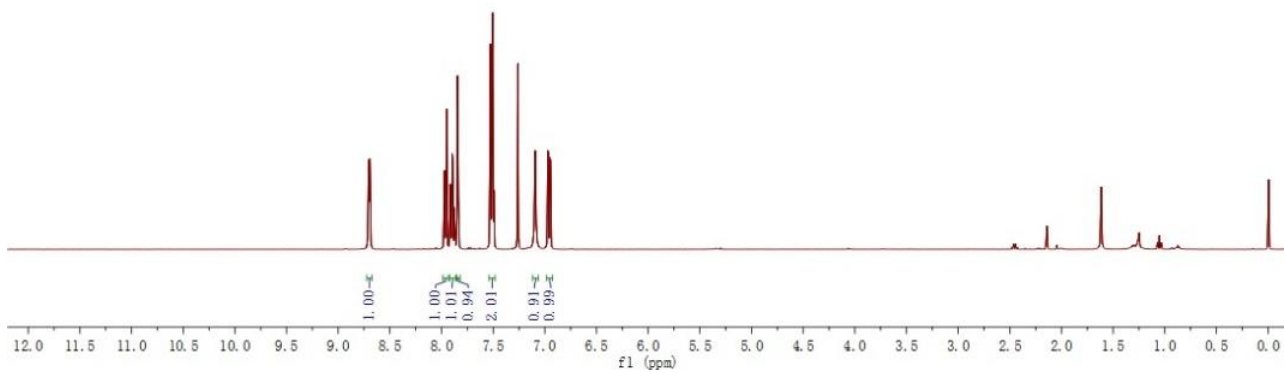
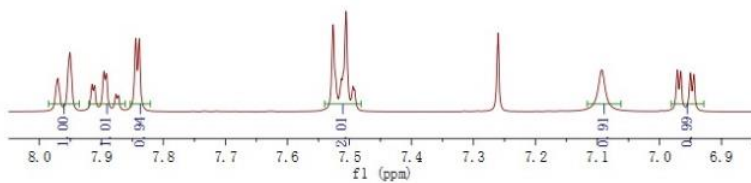
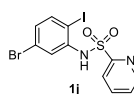
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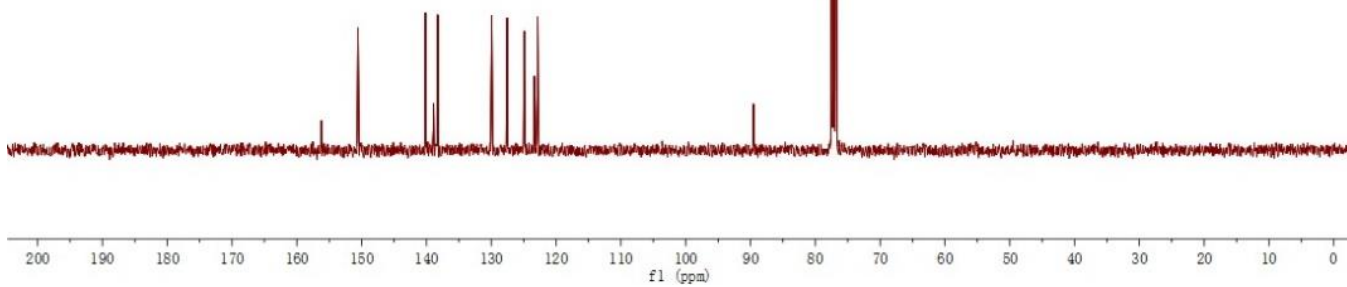
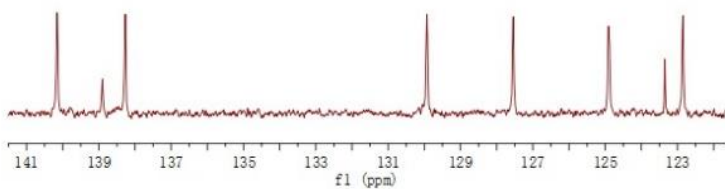
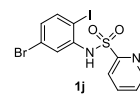
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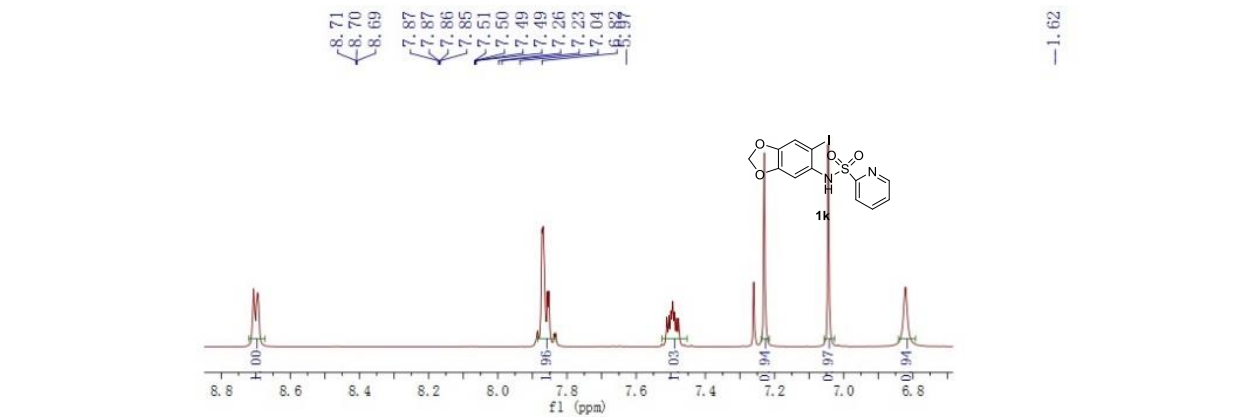


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6.94

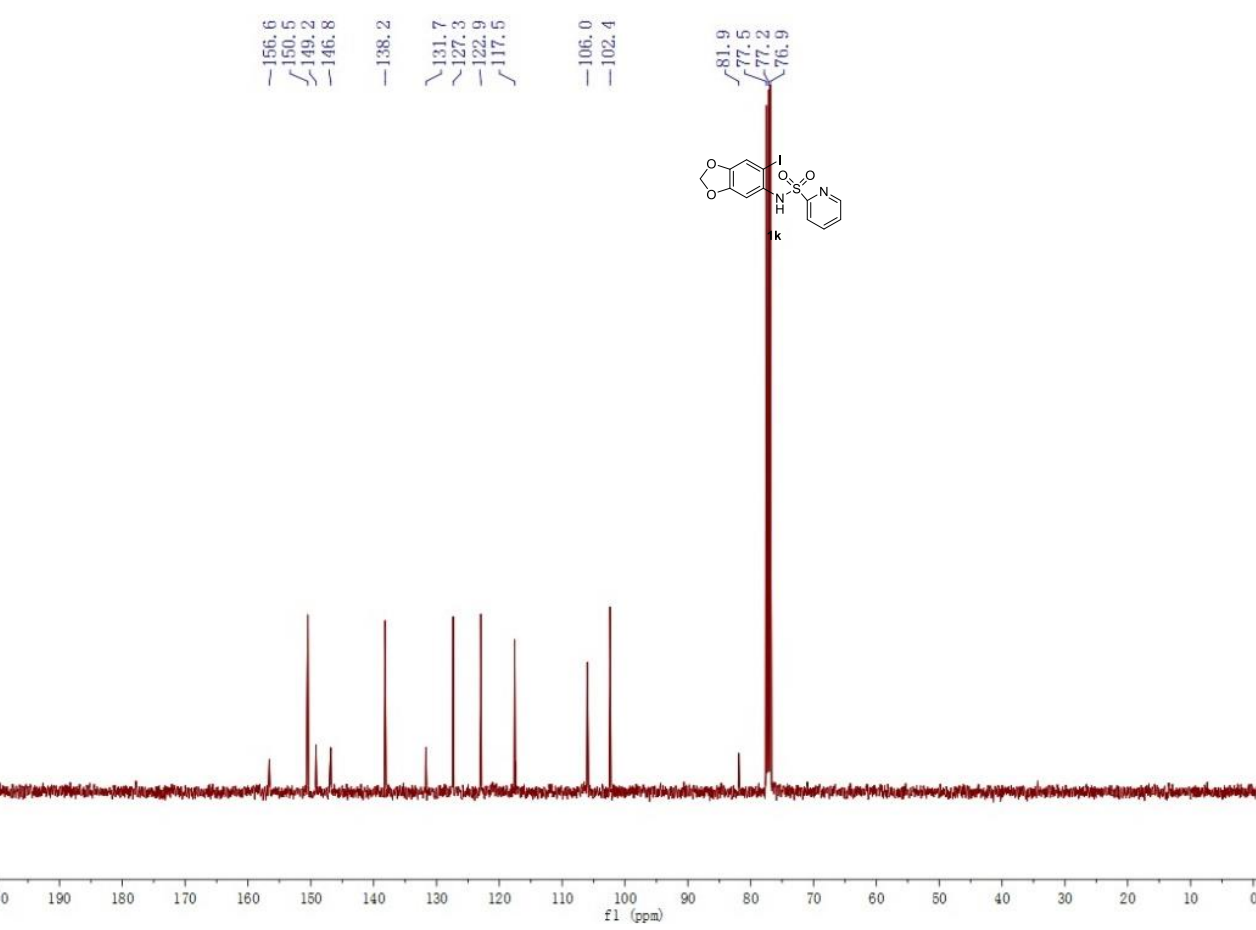
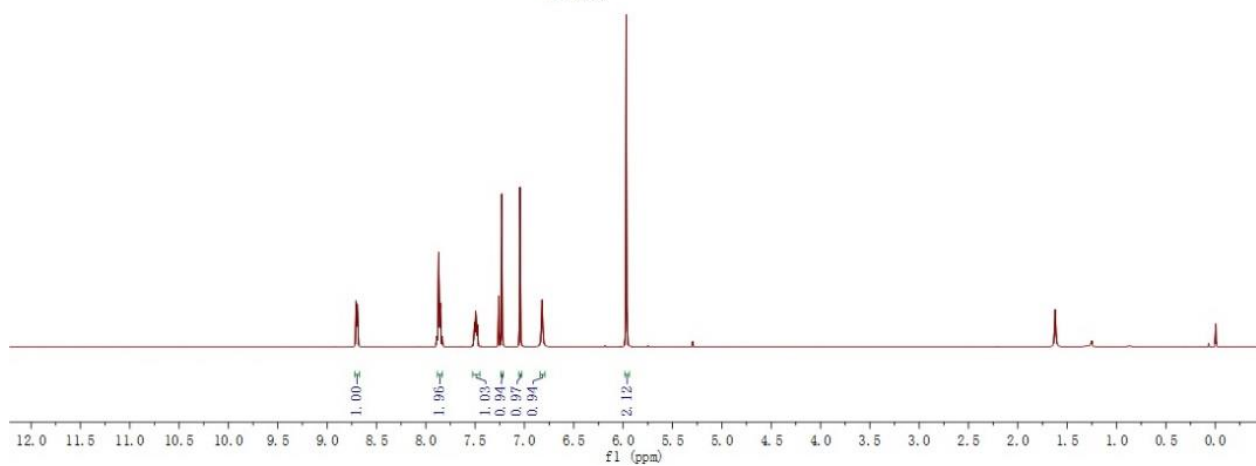


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77.2
76.8

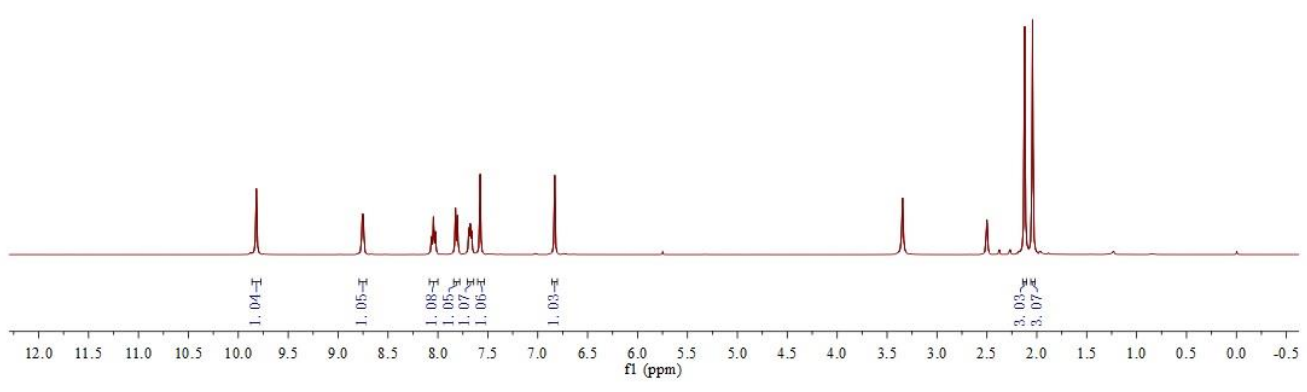
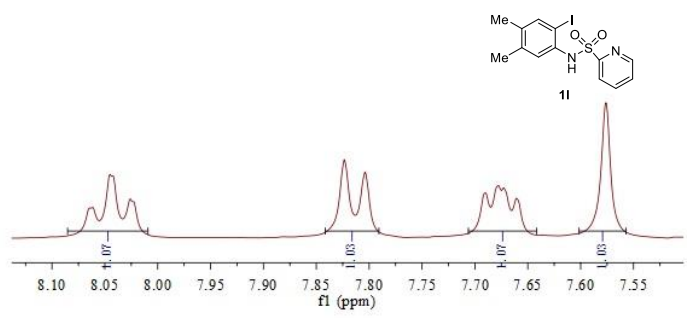




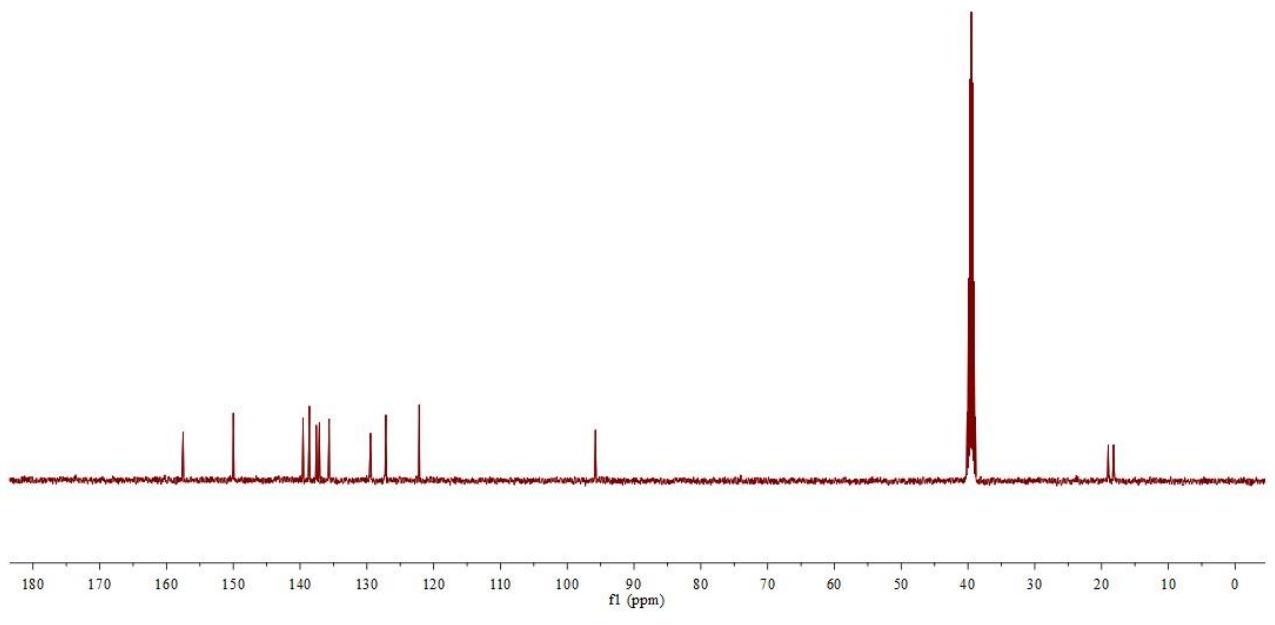
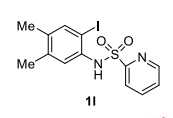
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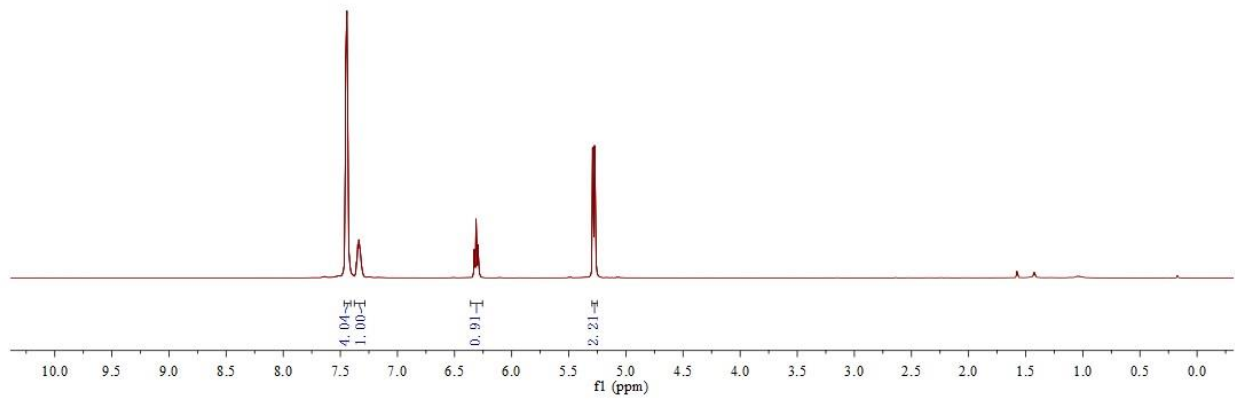
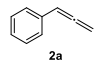
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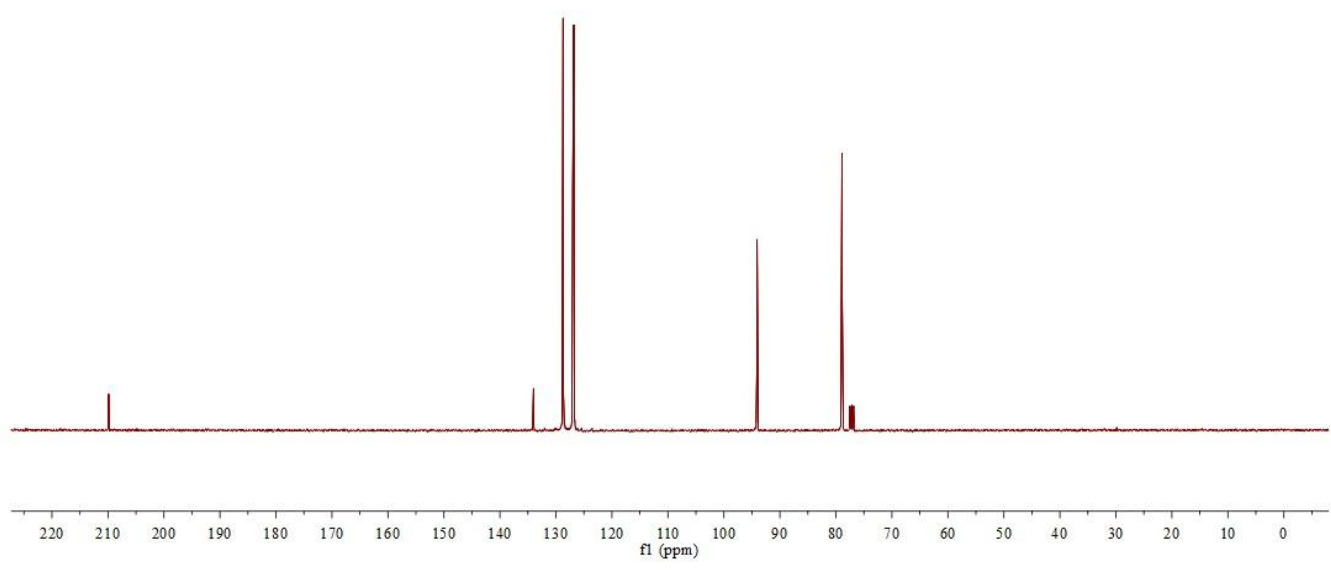
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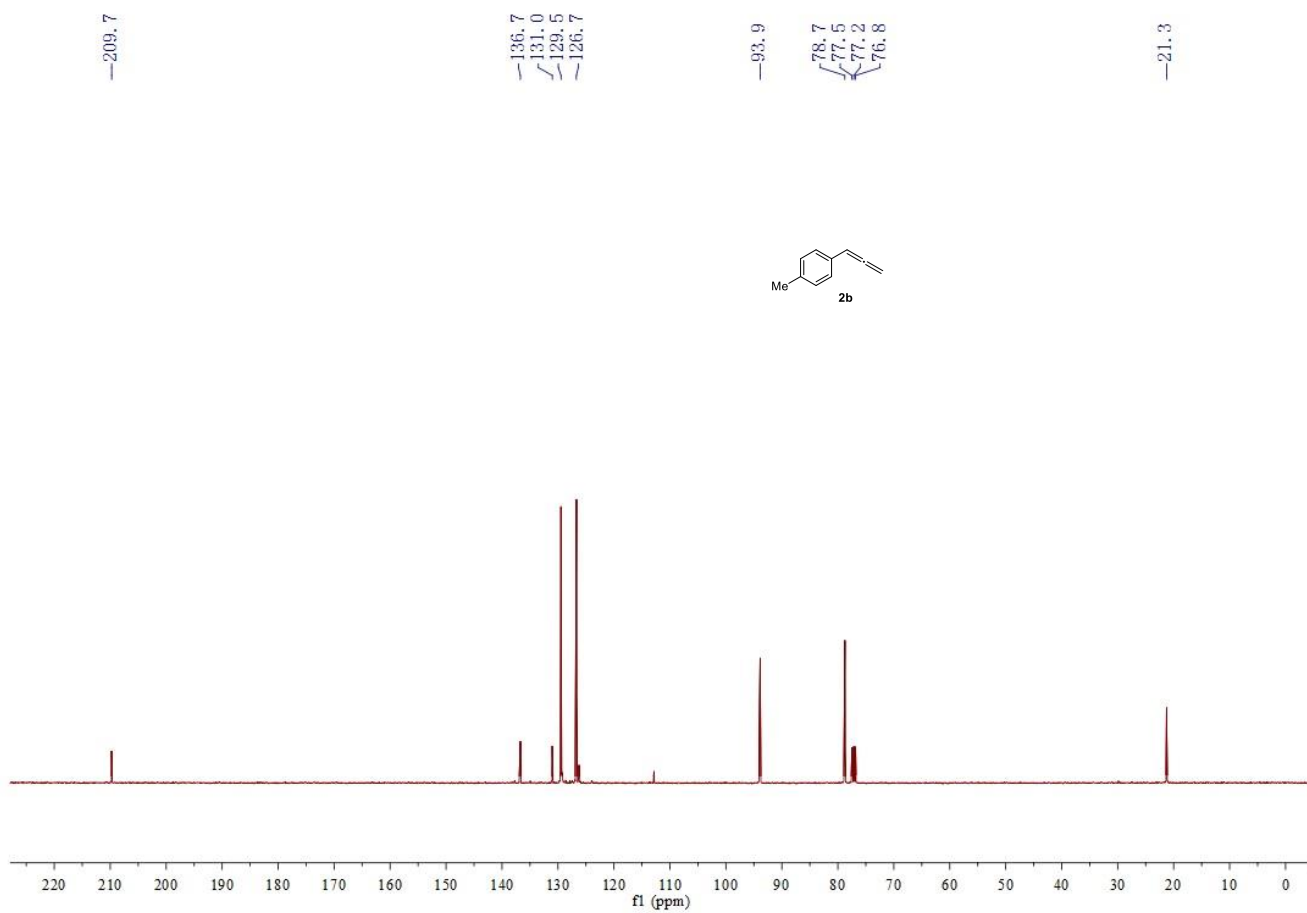
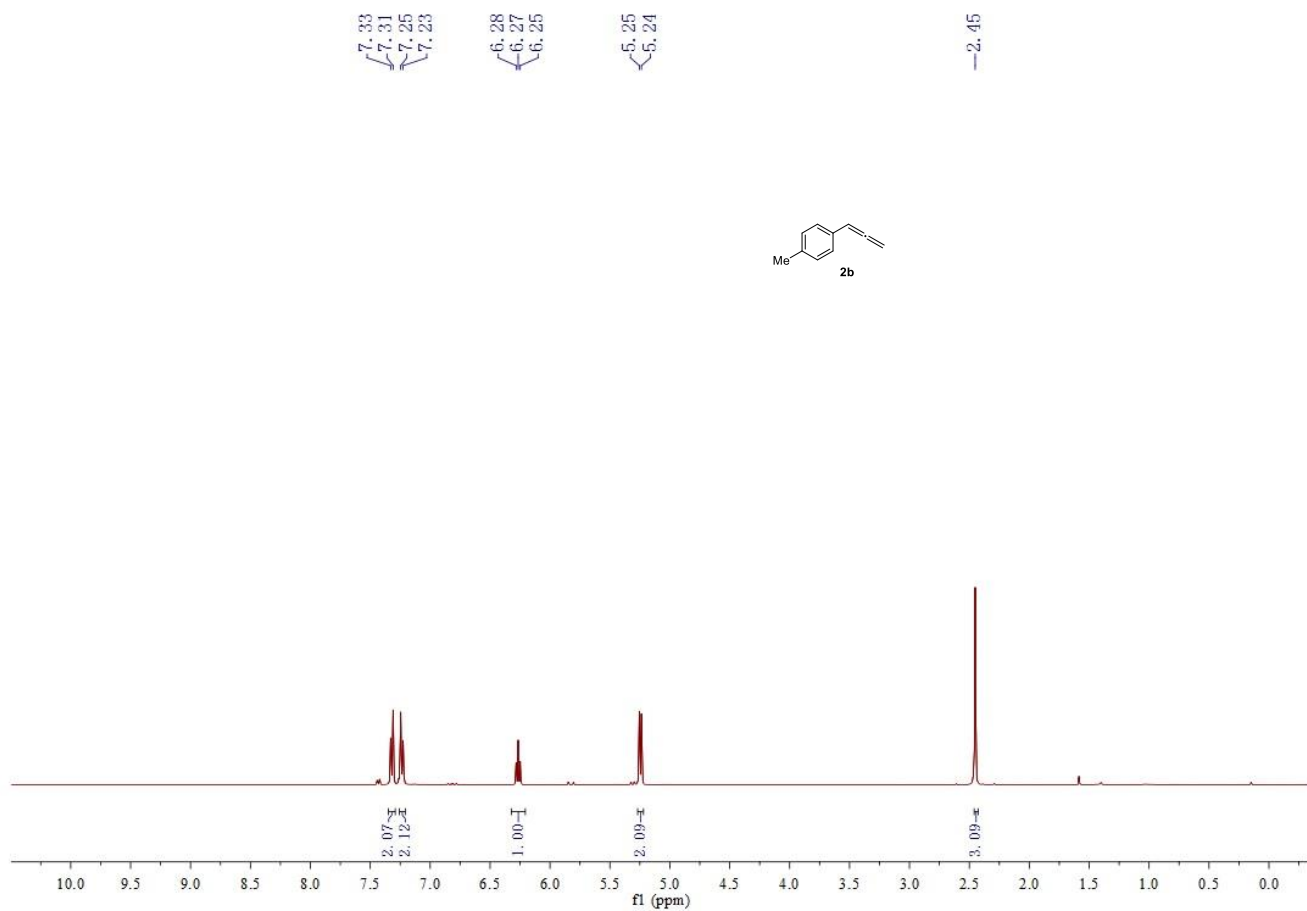


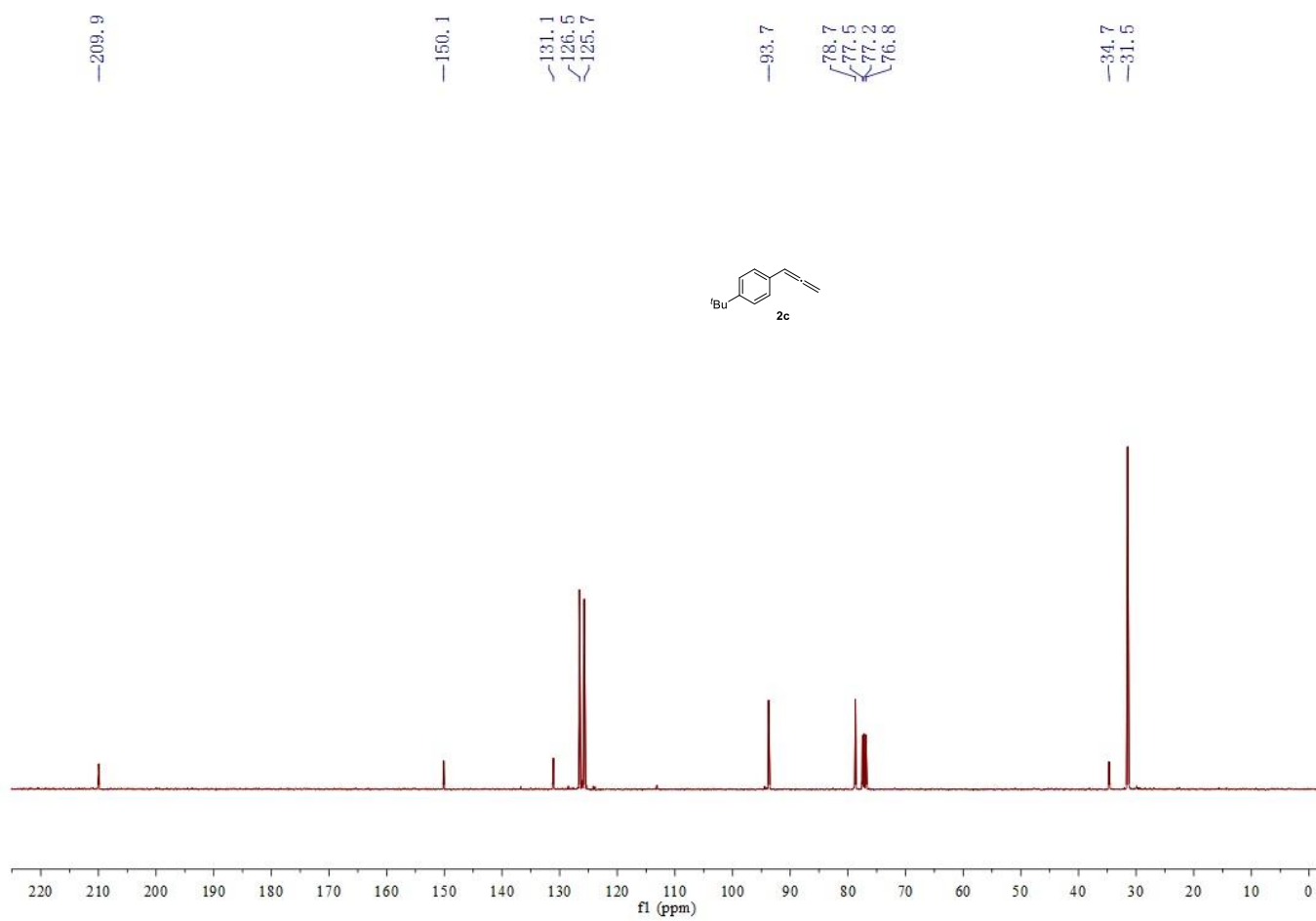
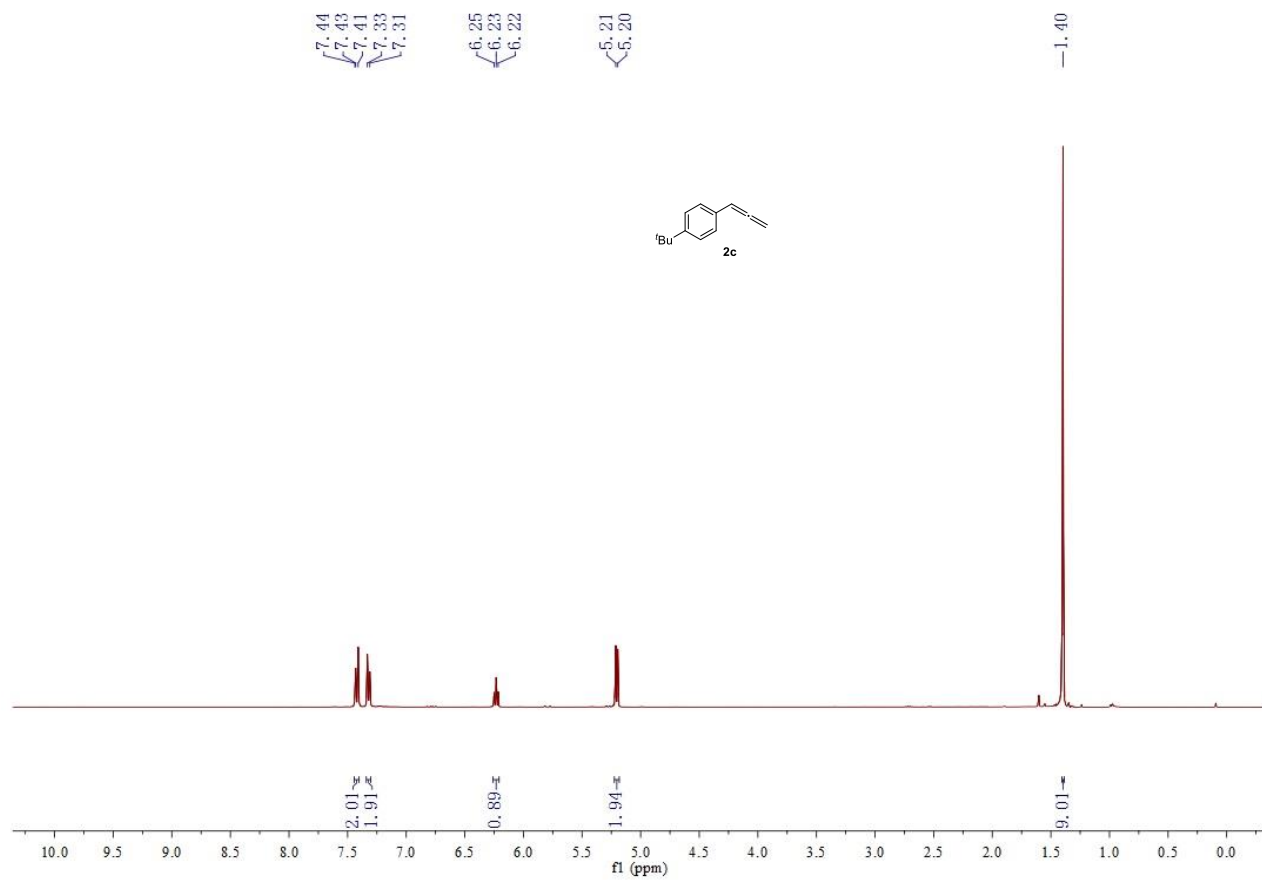
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5.27

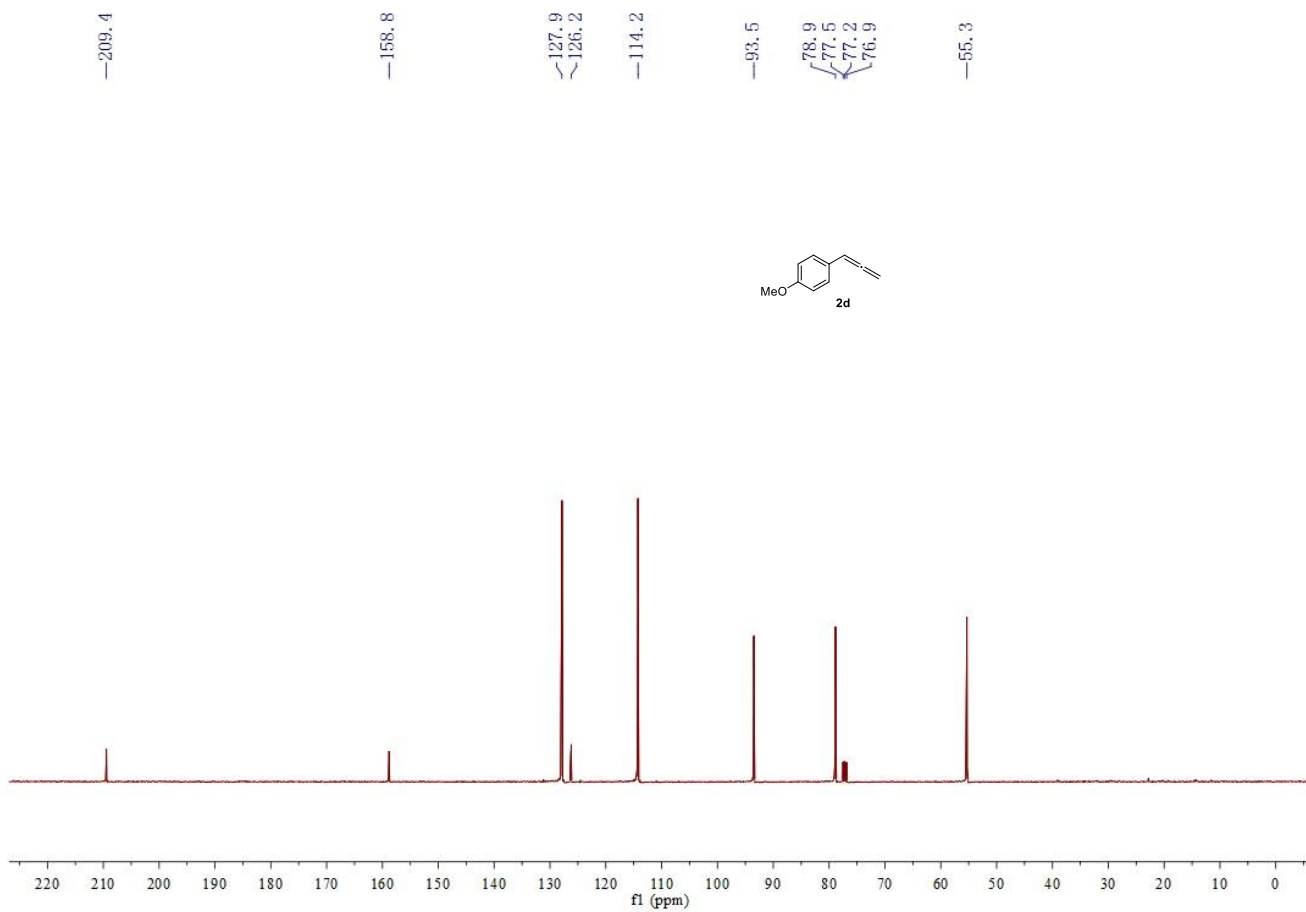
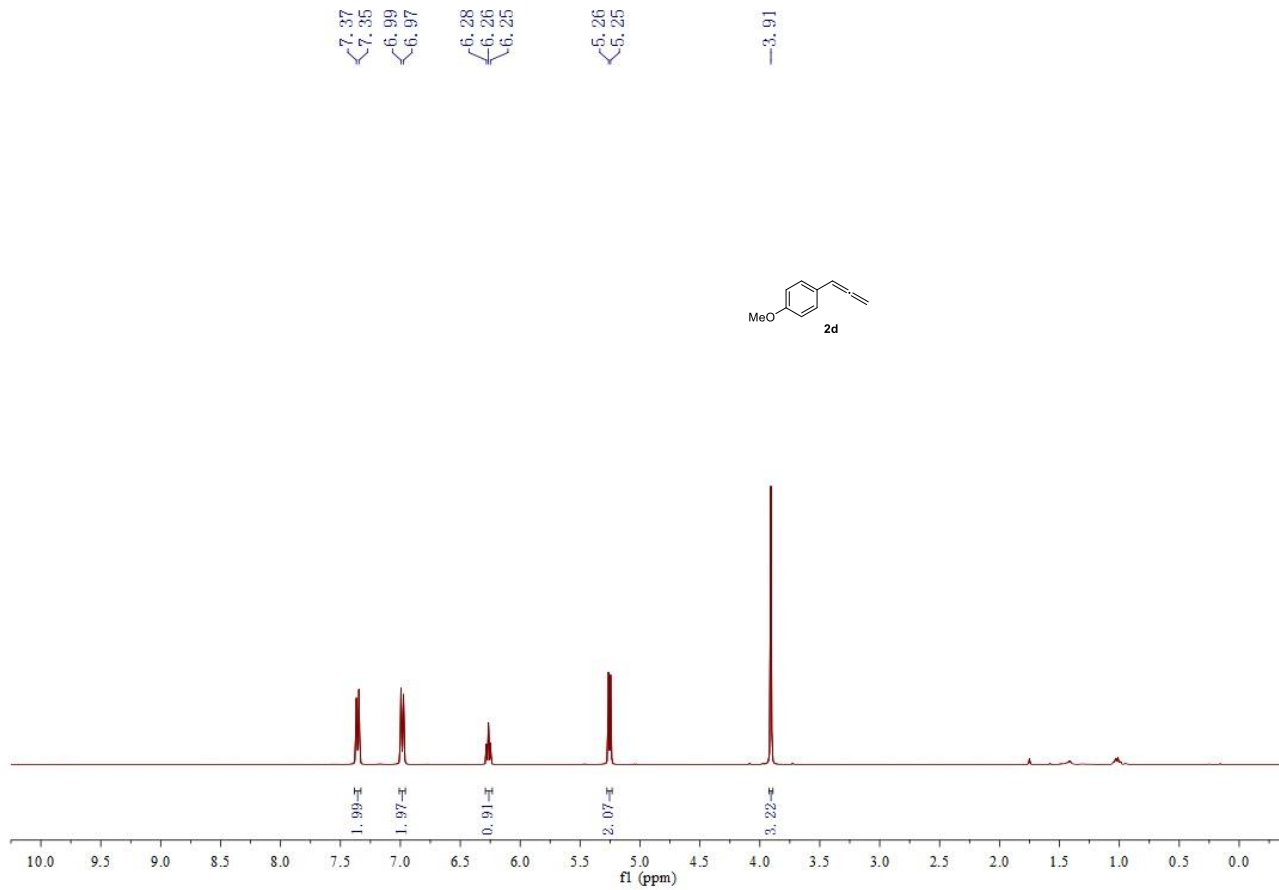


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127.0
126.8
94.1
78.9
77.5
77.2
76.8

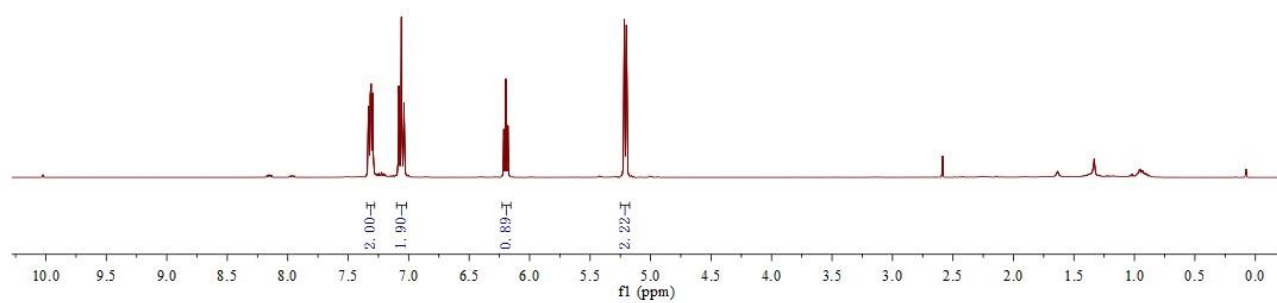
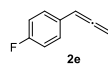








7.33
7.32
7.31
7.30
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7.04
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6.18
5.22
5.20



209.7

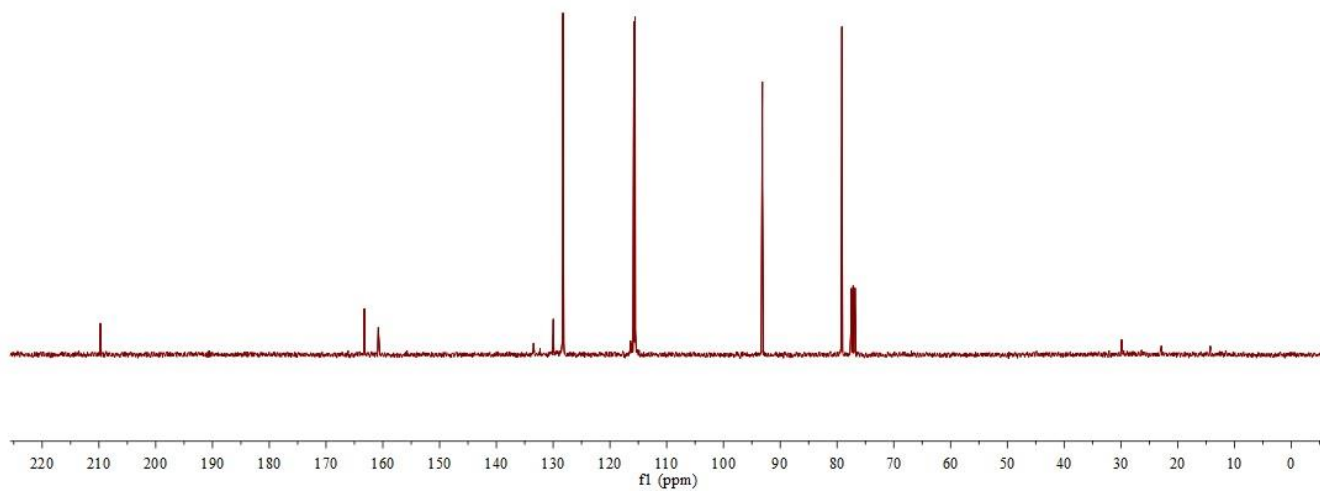
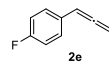
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128.2

115.8
115.6

93.2

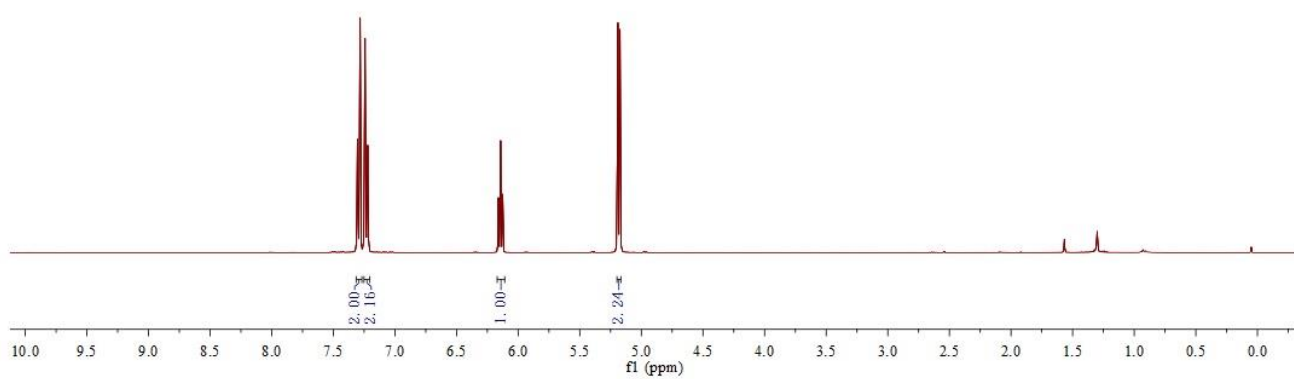
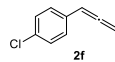
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77.5
77.2
76.8



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7.22

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6.14
6.13

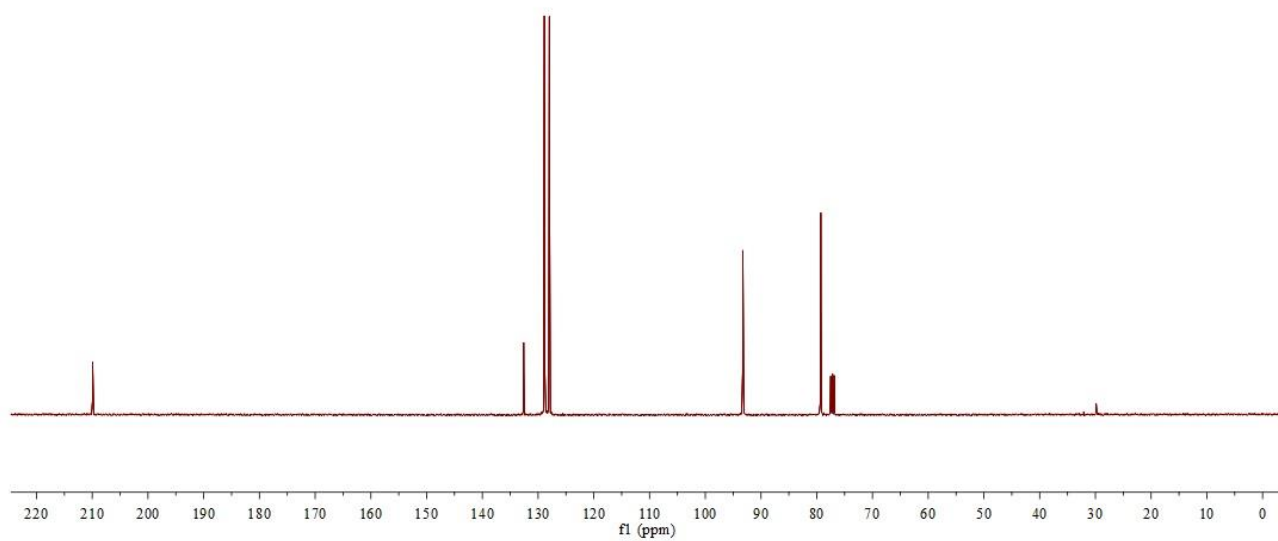
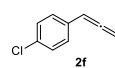
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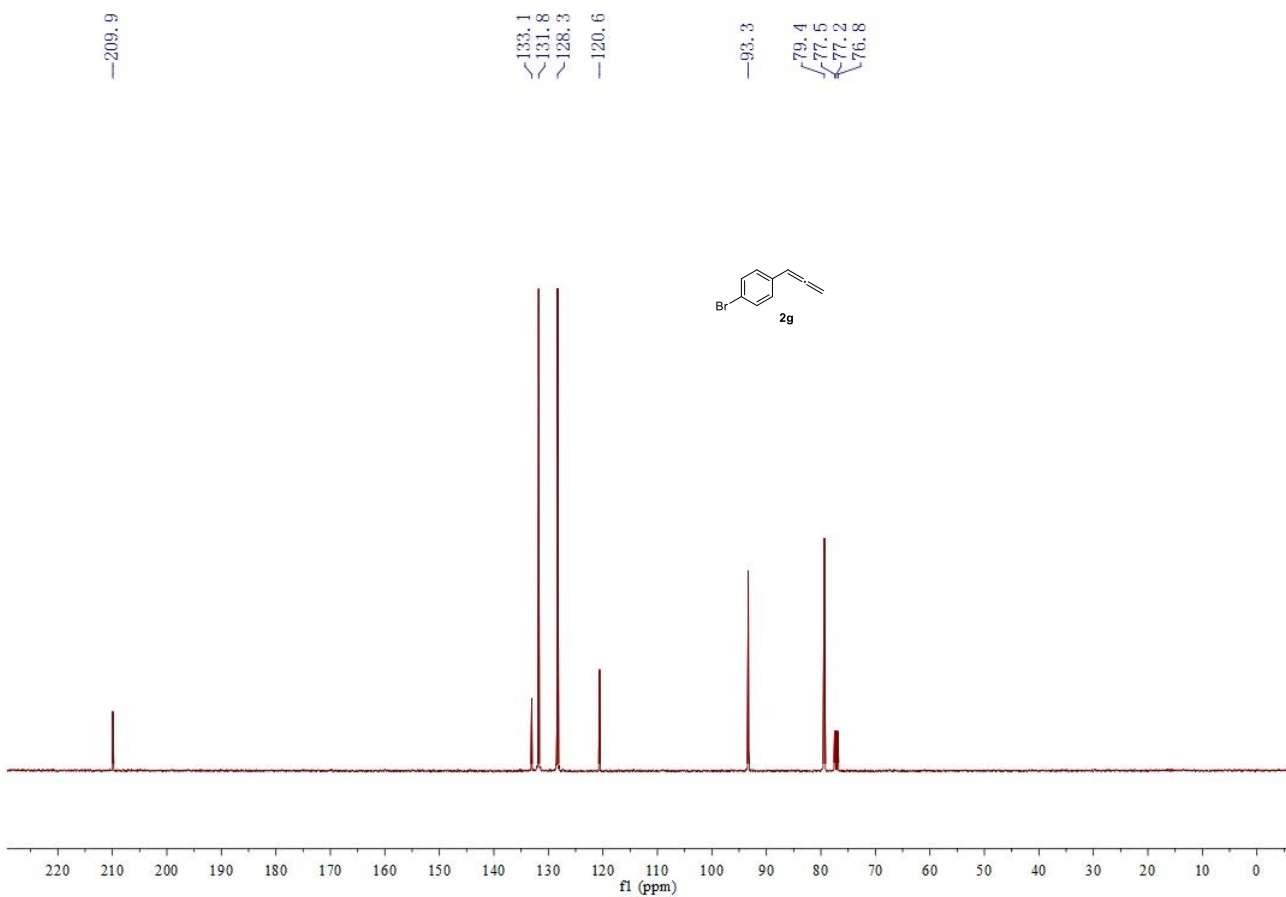
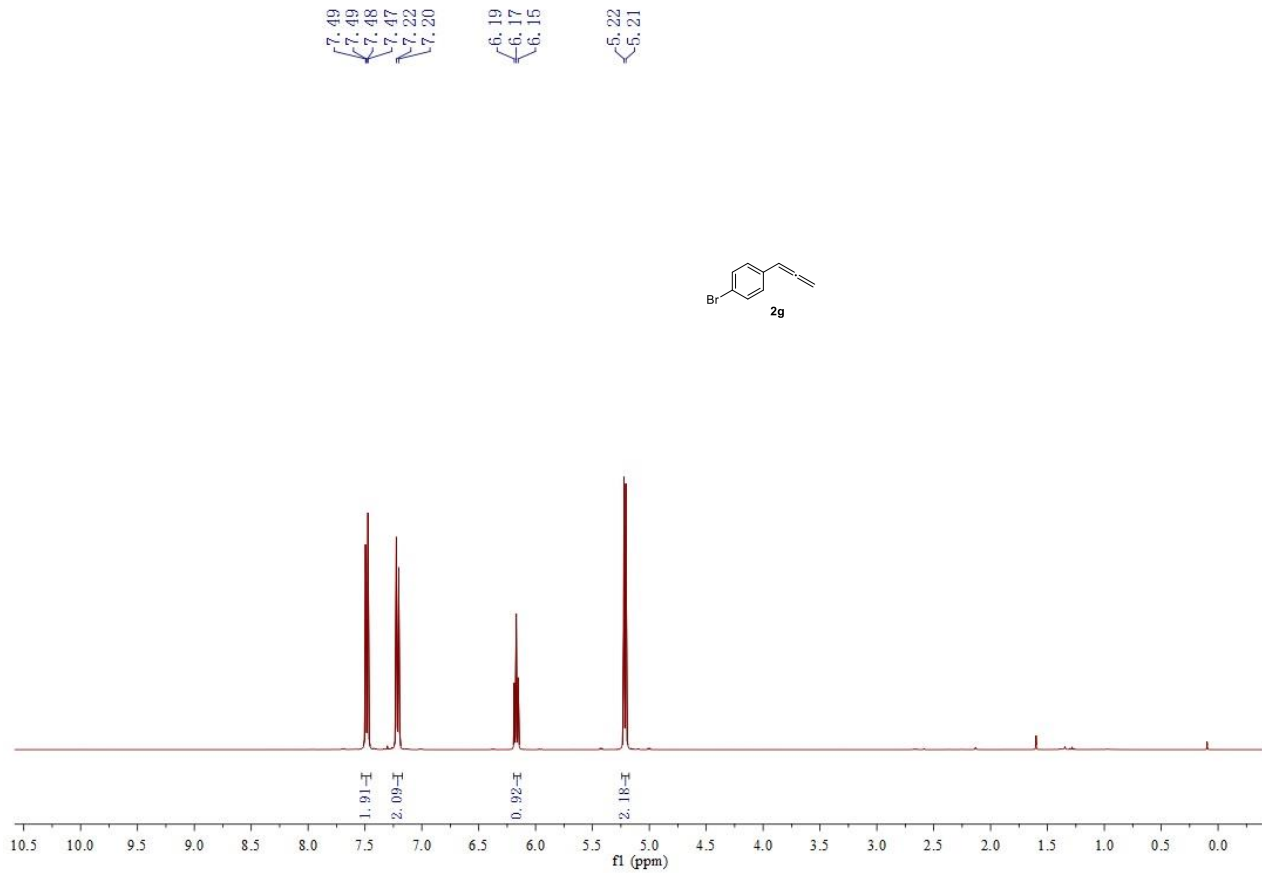


209.9

132.6
132.6
128.9
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93.3
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77.5
77.2
76.8

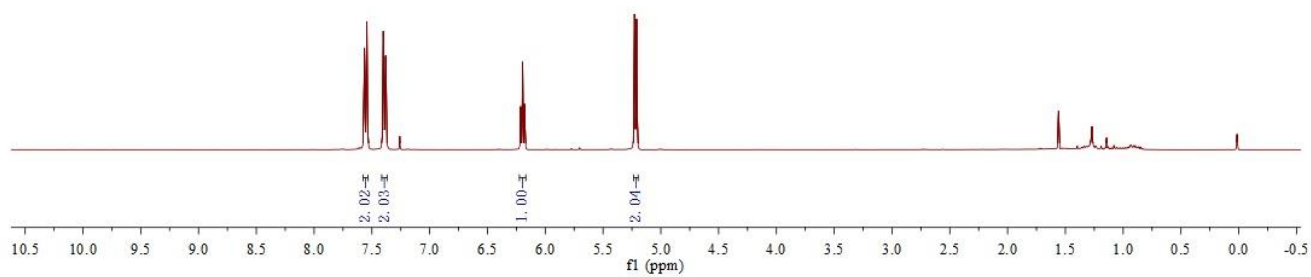
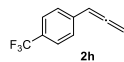




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6.18

5.23
5.21

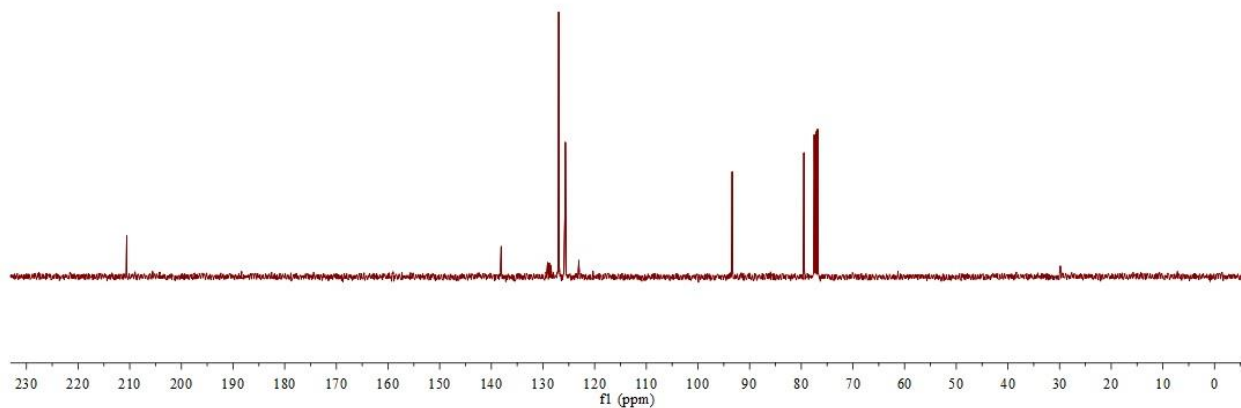
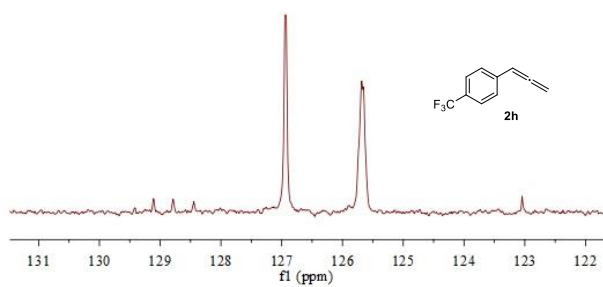
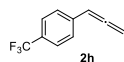


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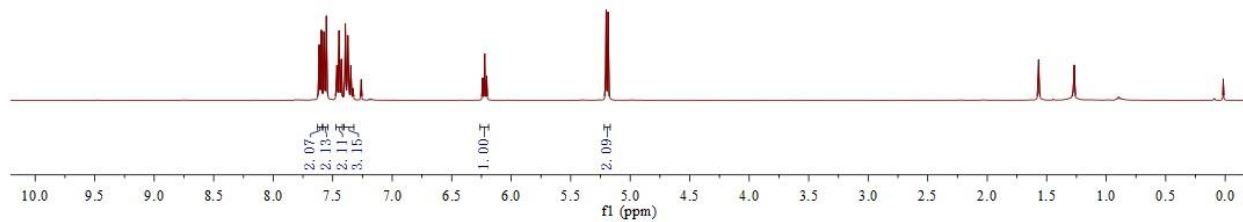
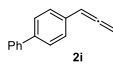
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76.8



7.61
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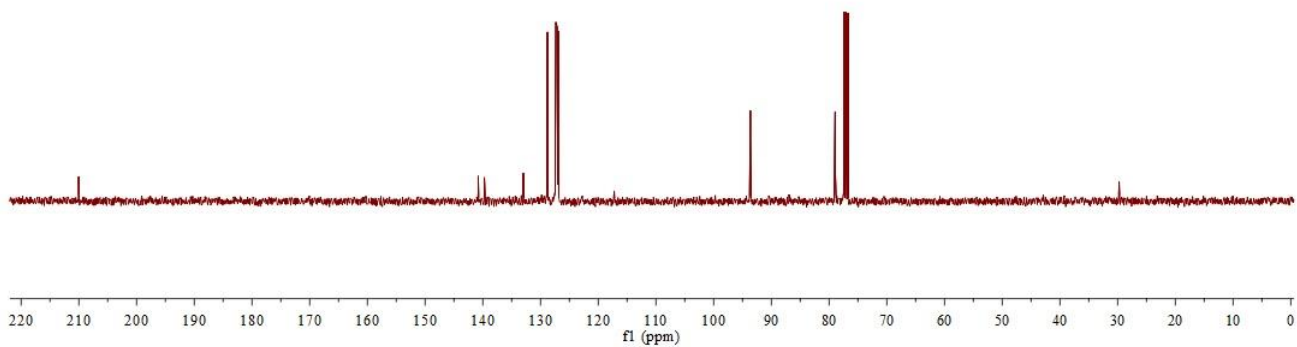
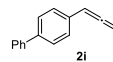


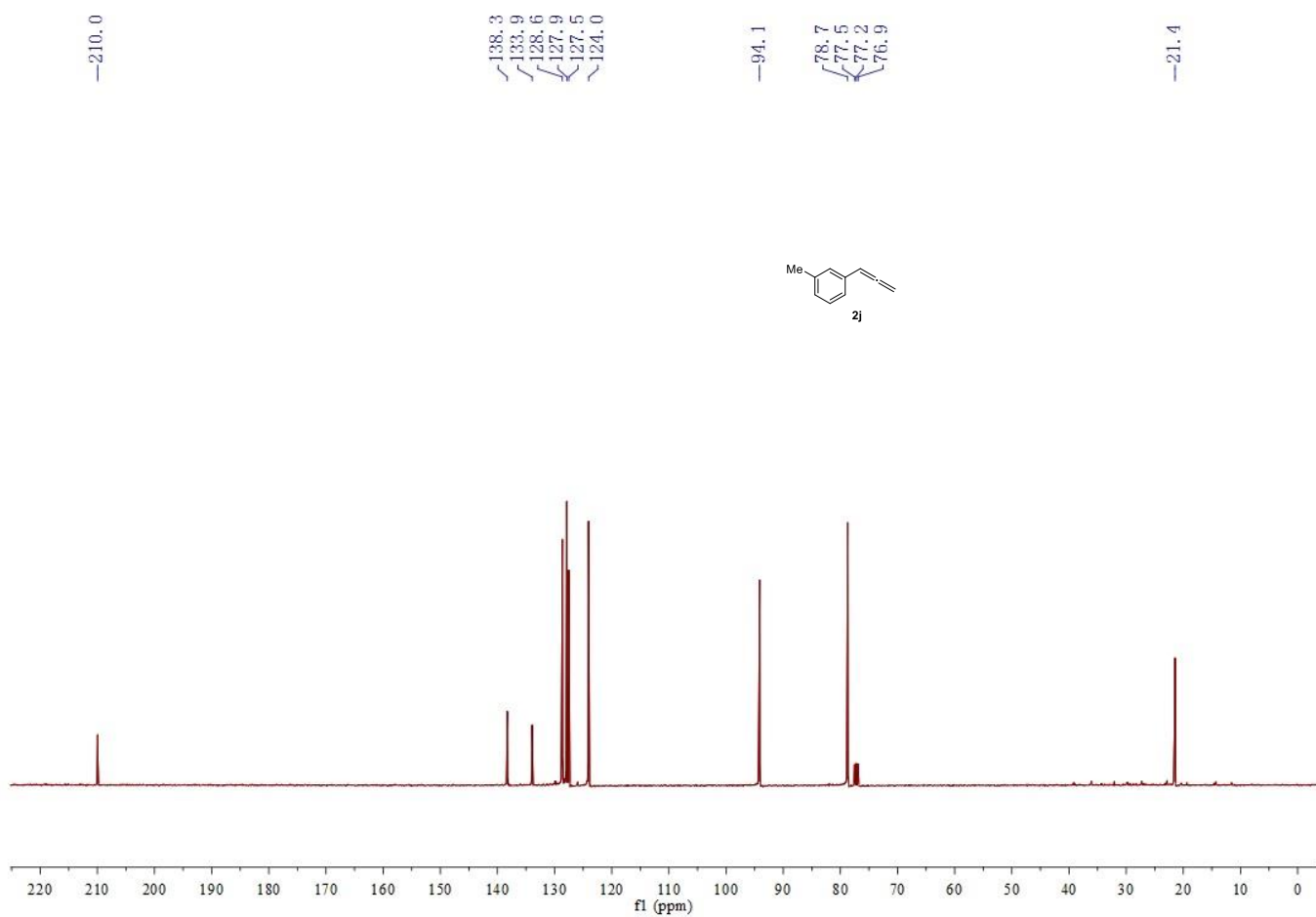
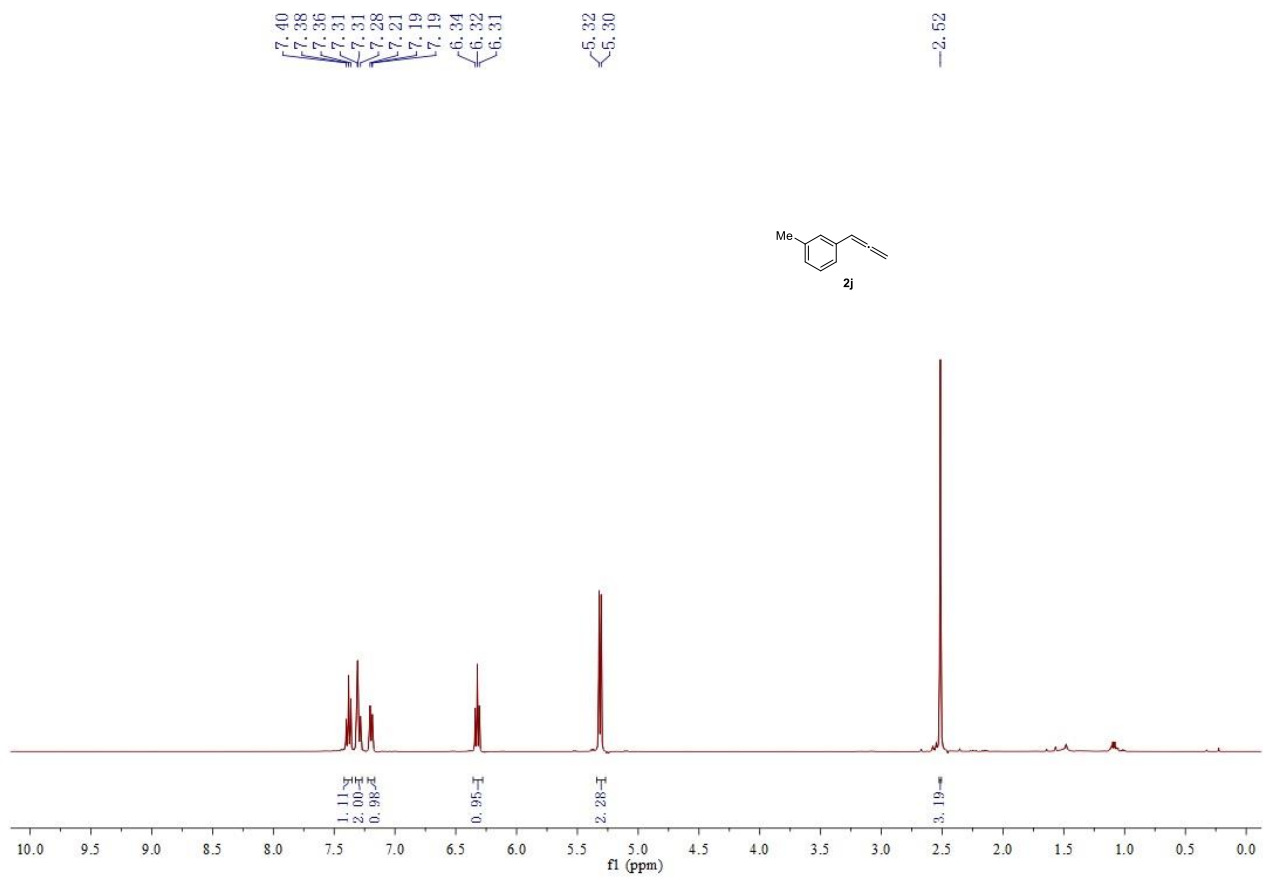
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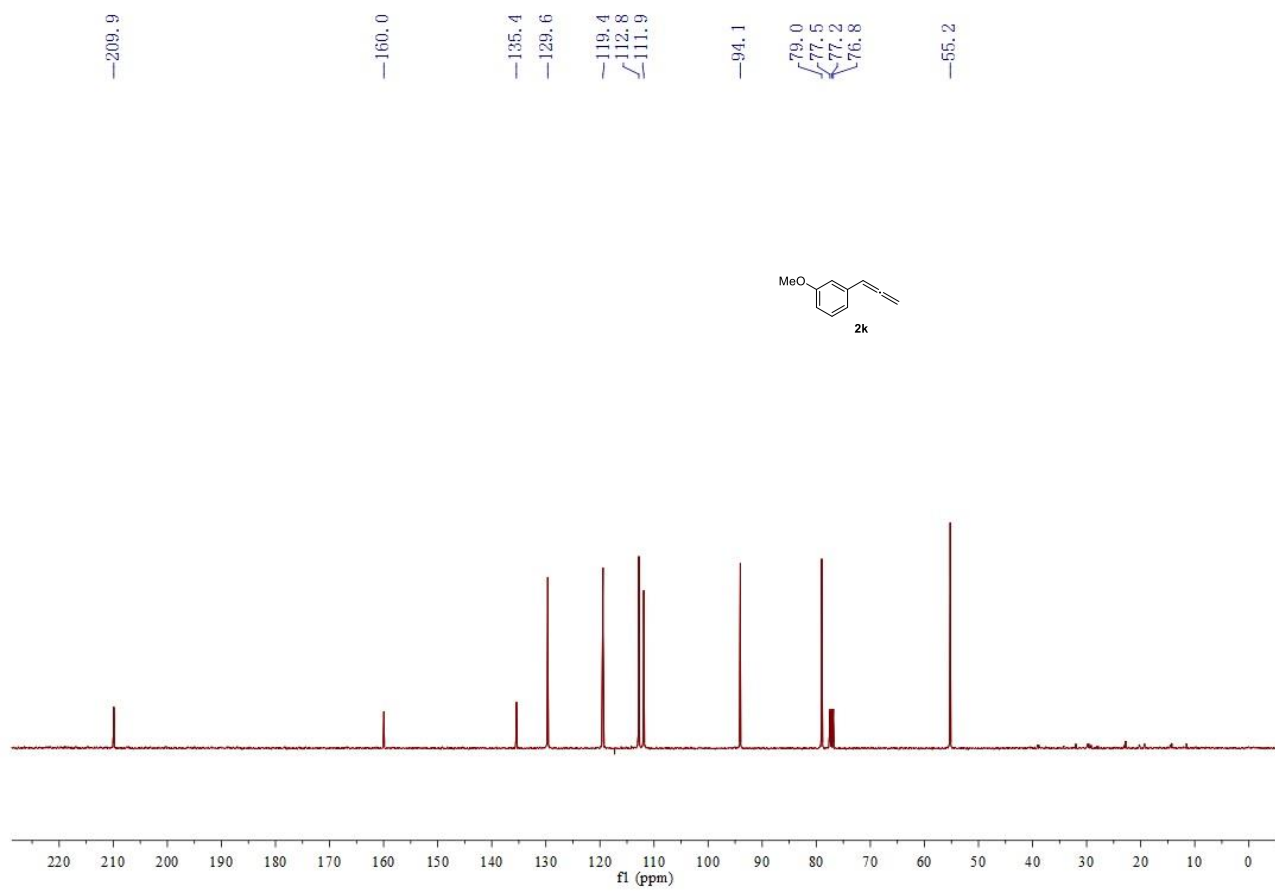
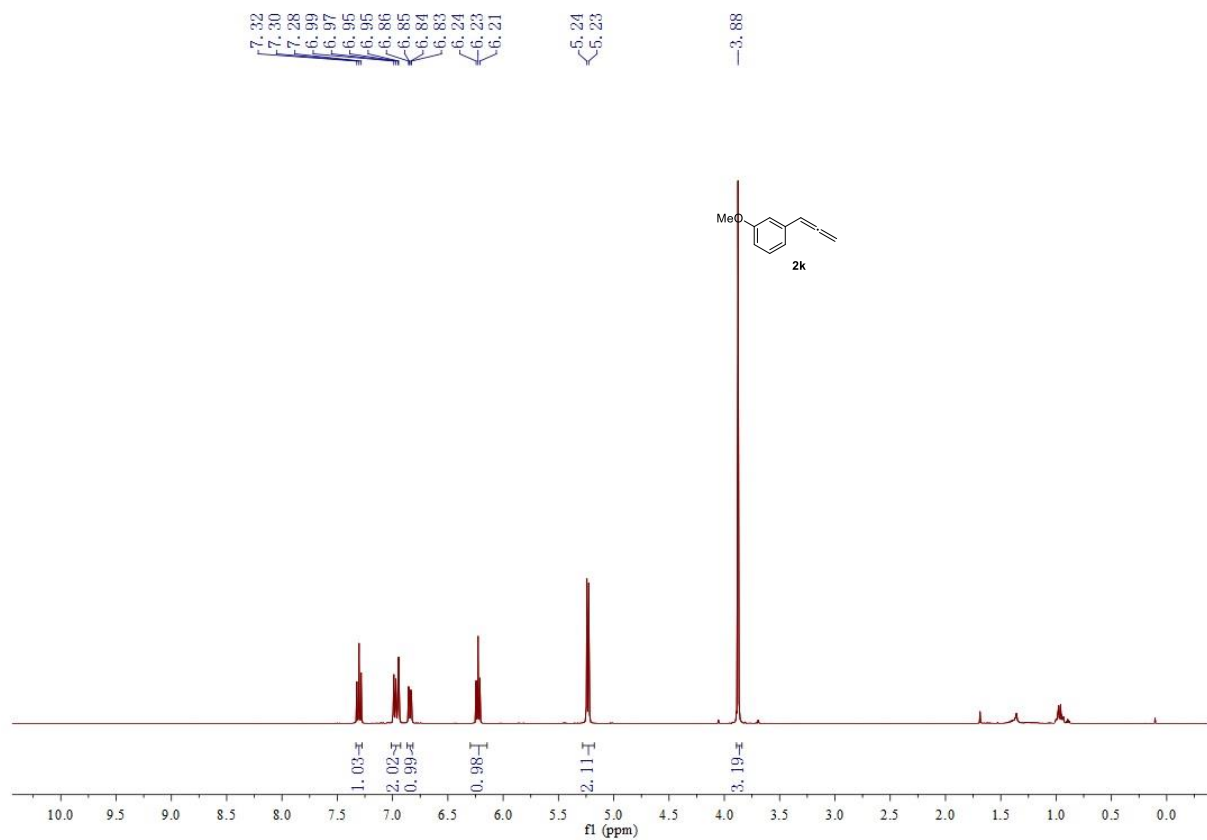
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93.6

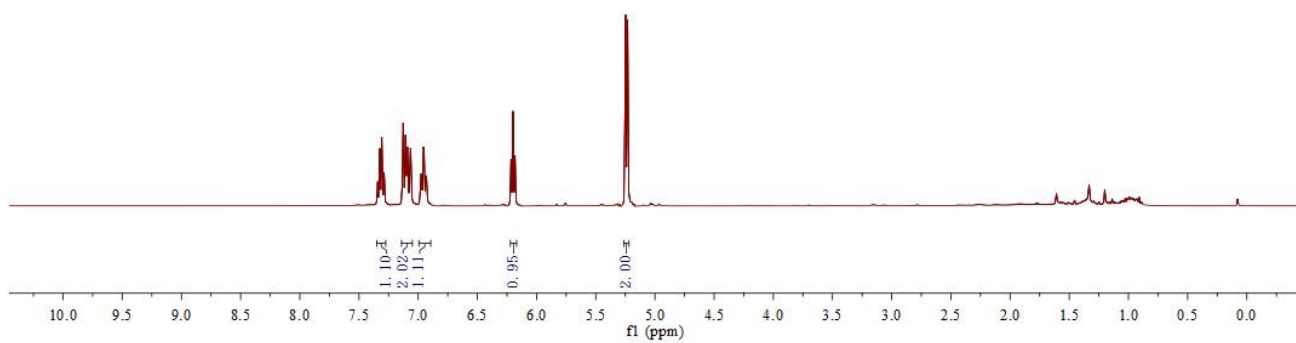
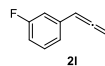
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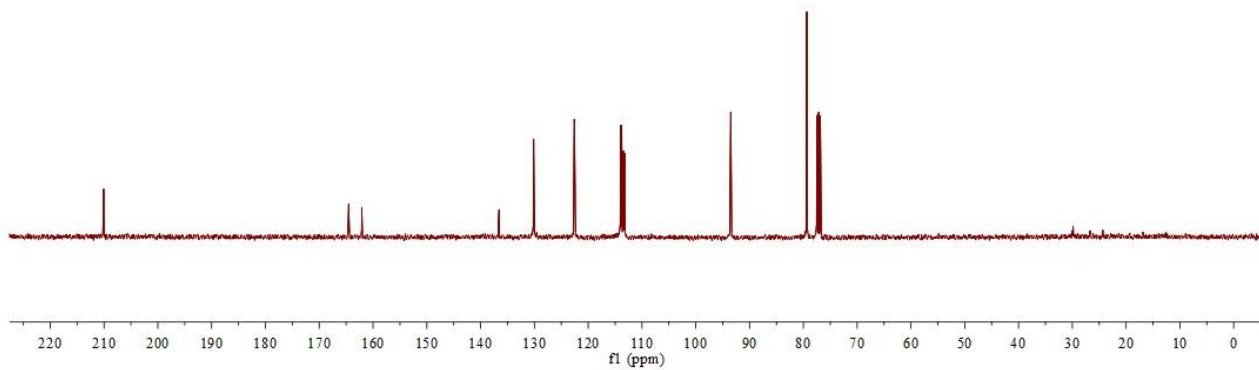
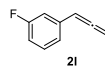


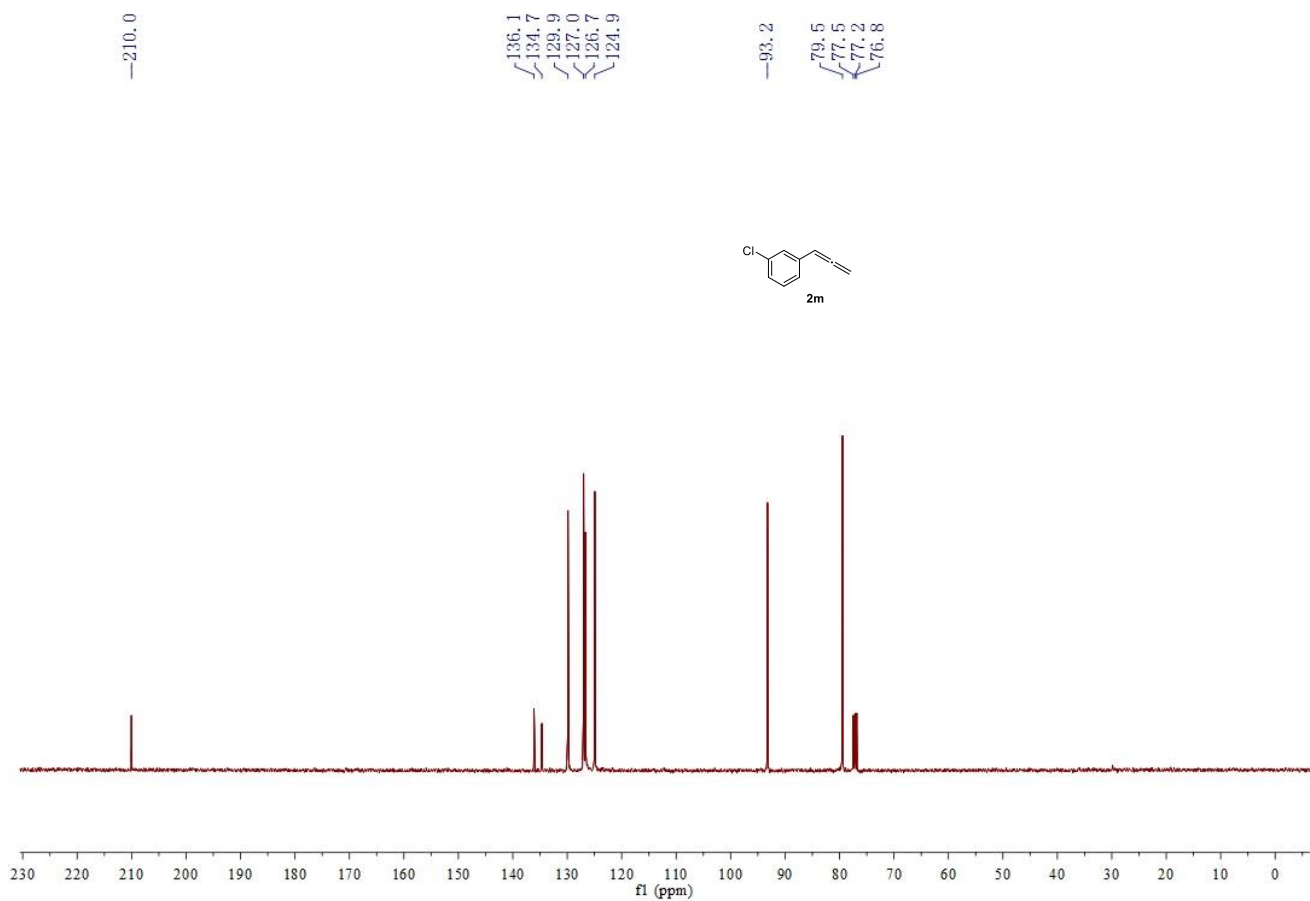
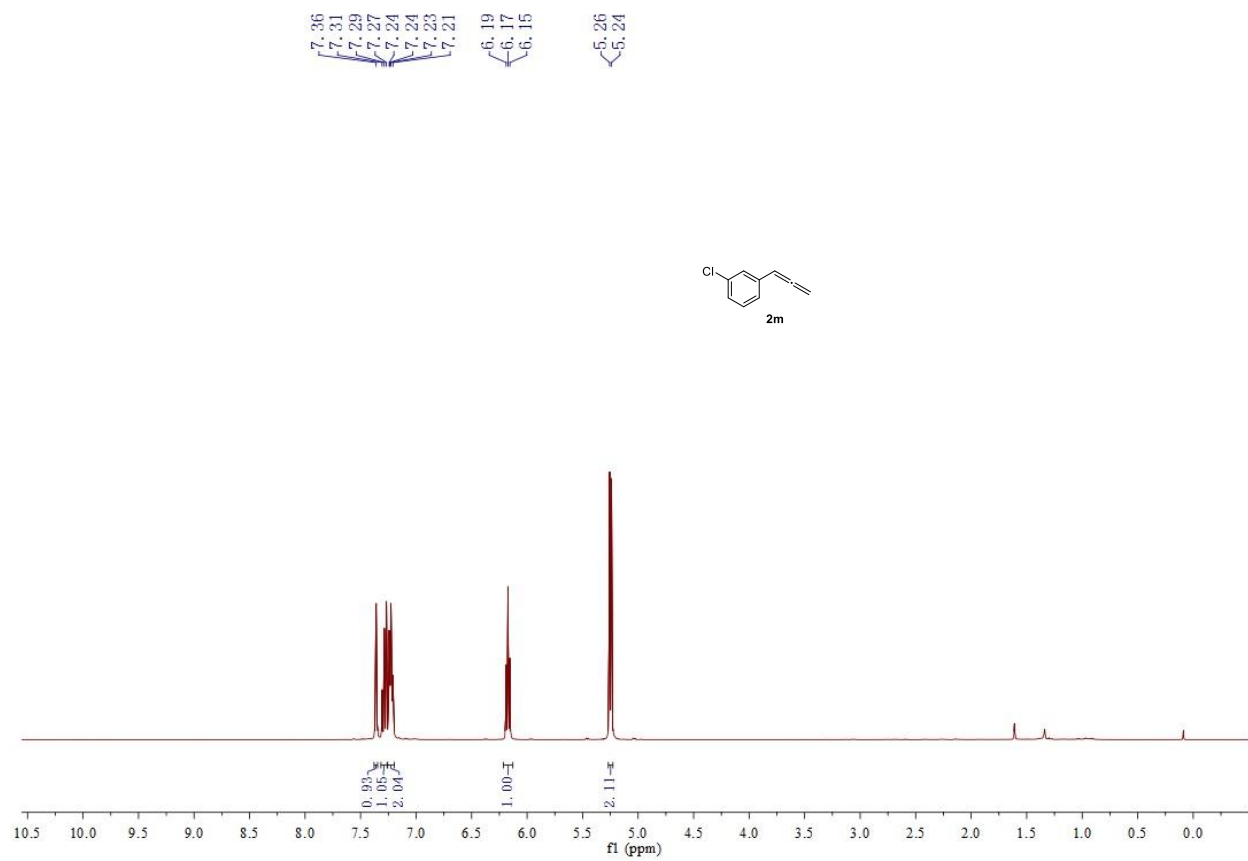
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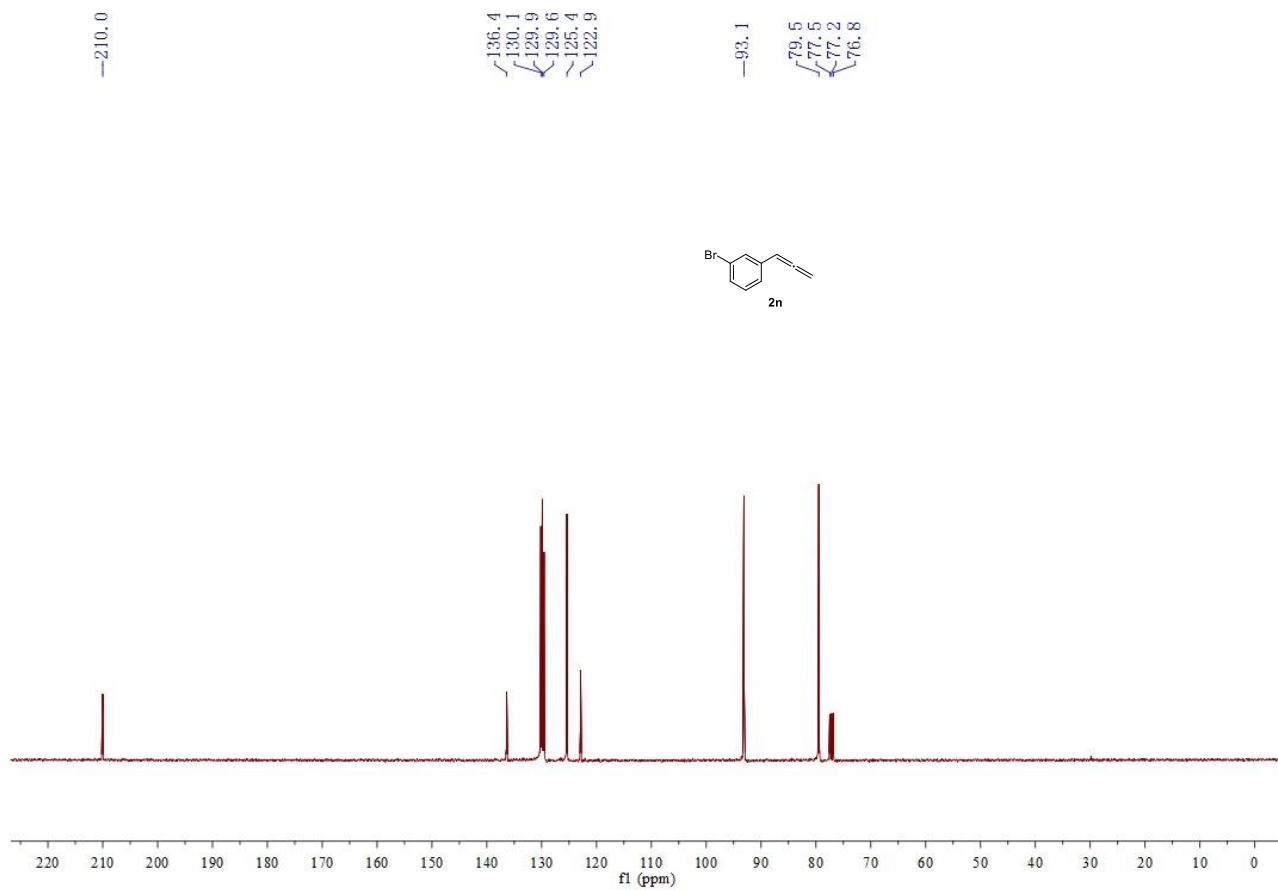
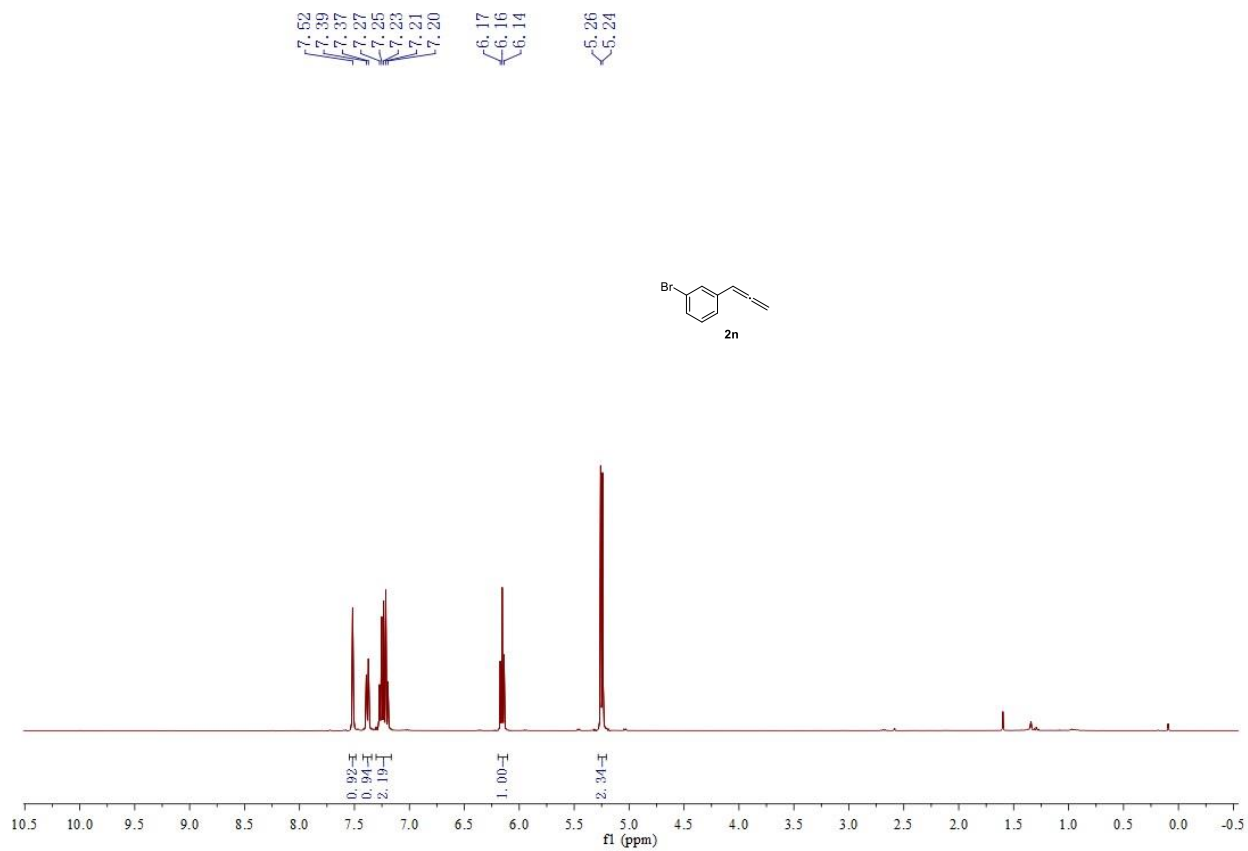
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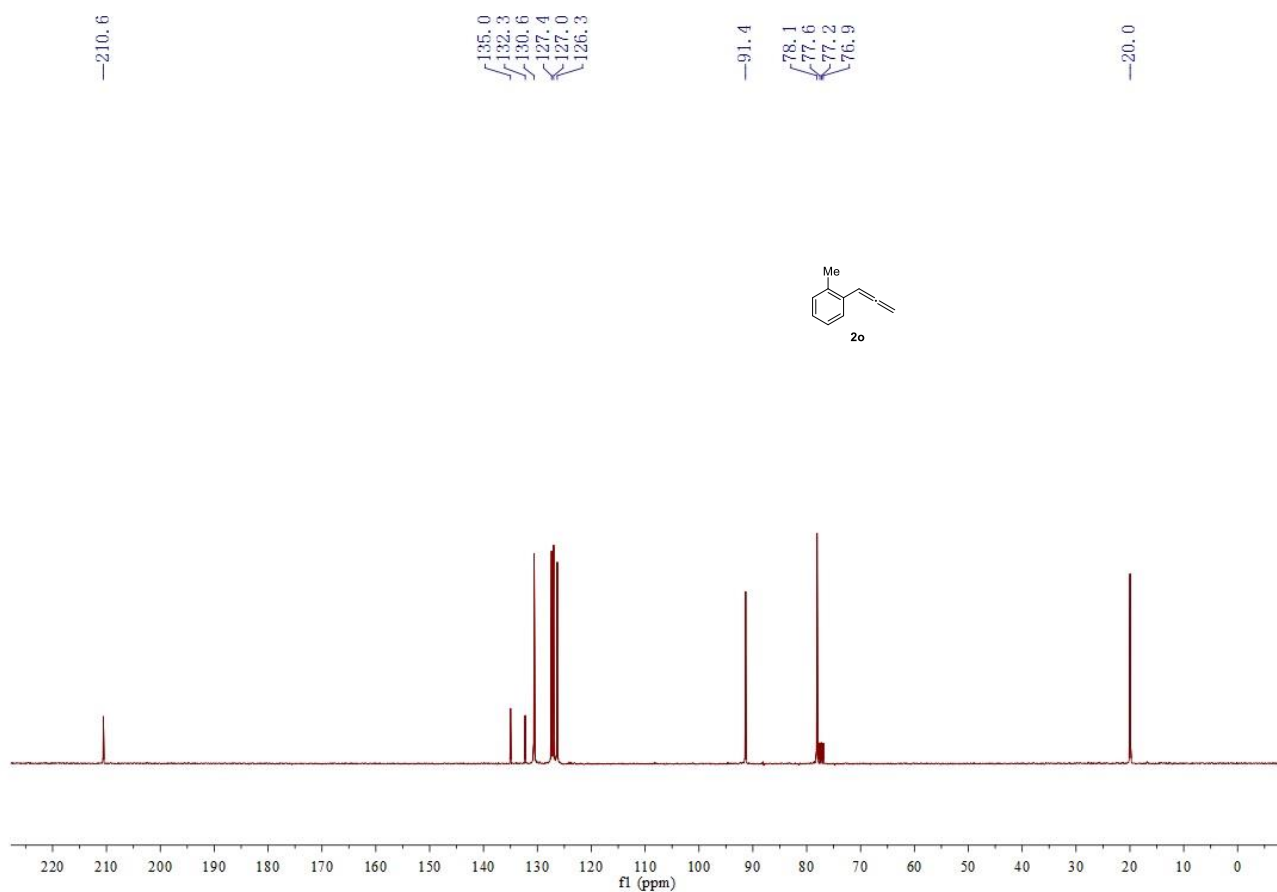
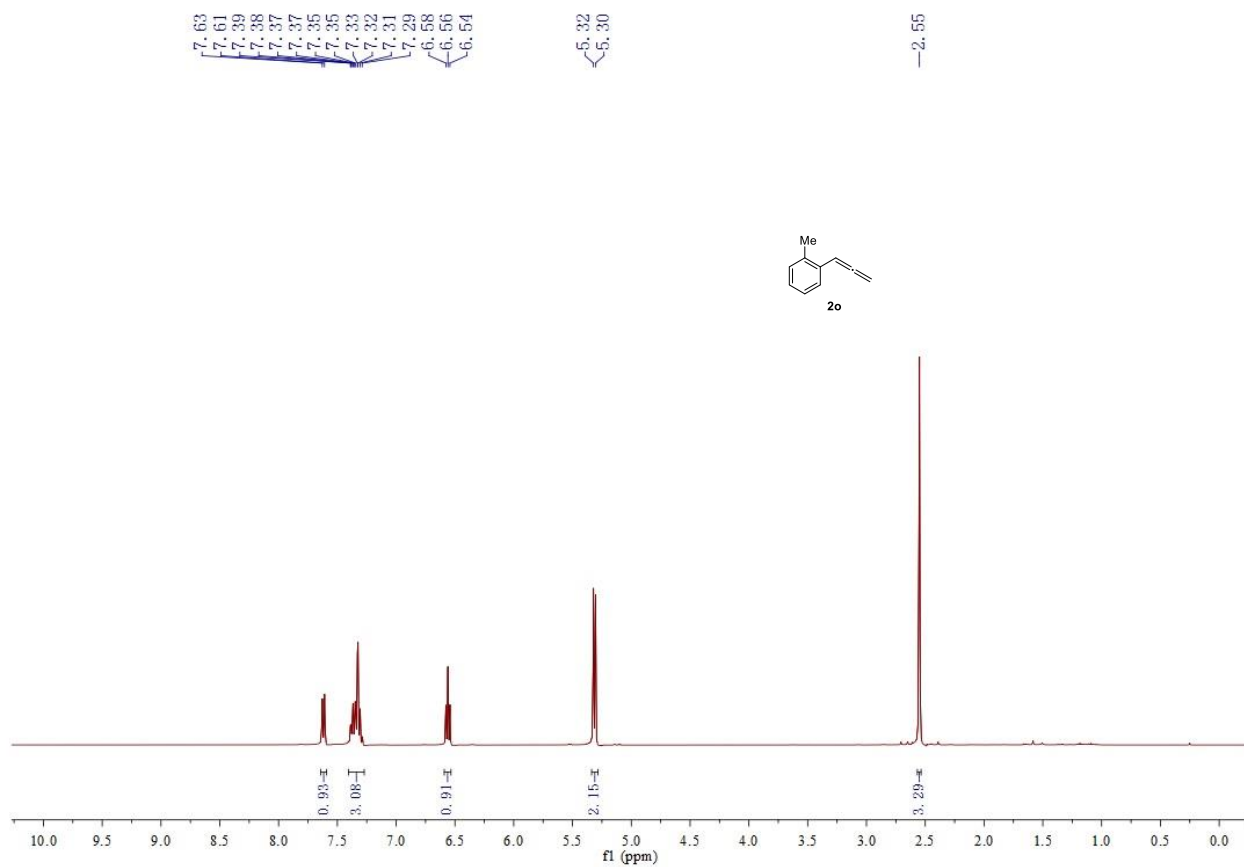
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113.2

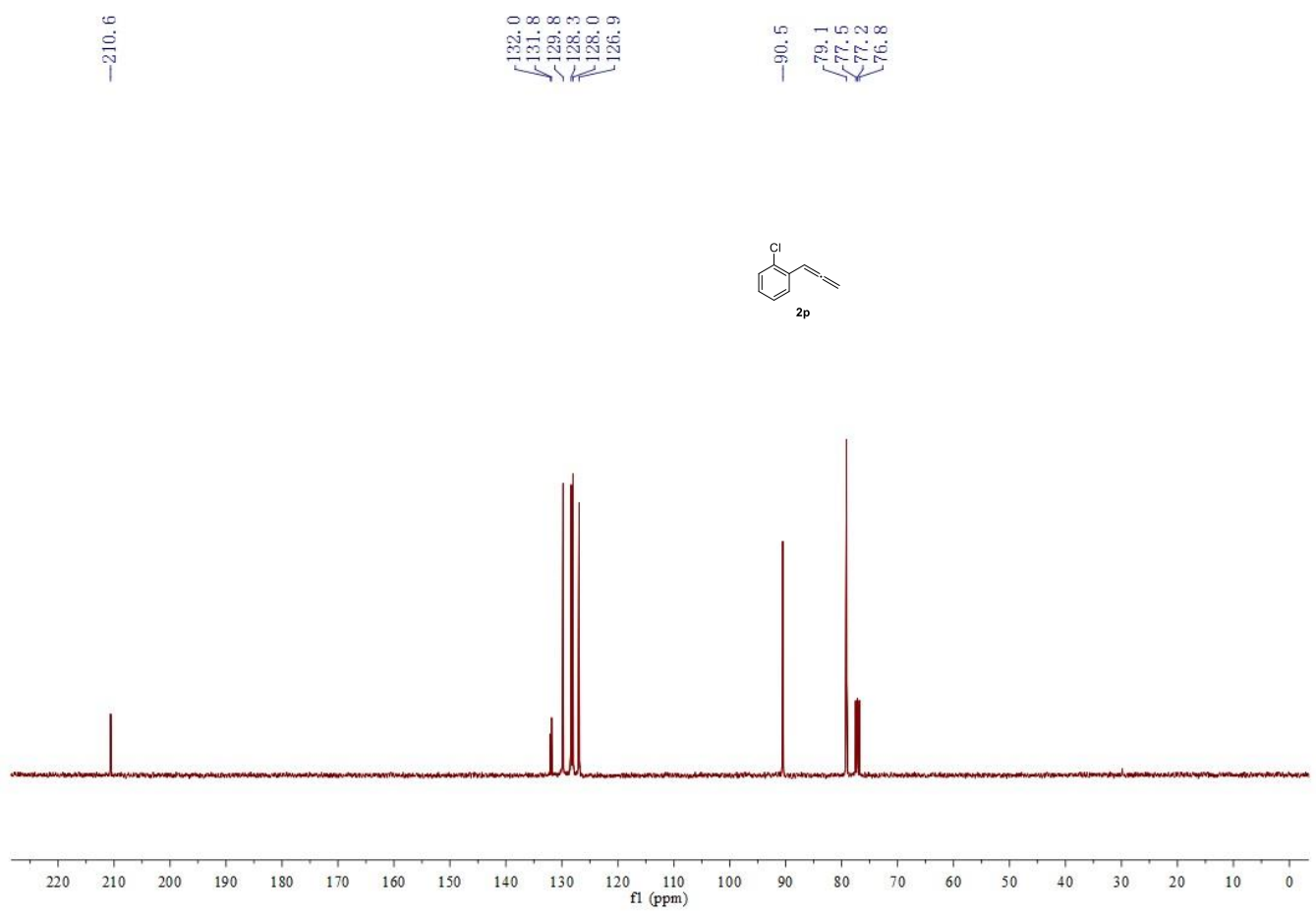
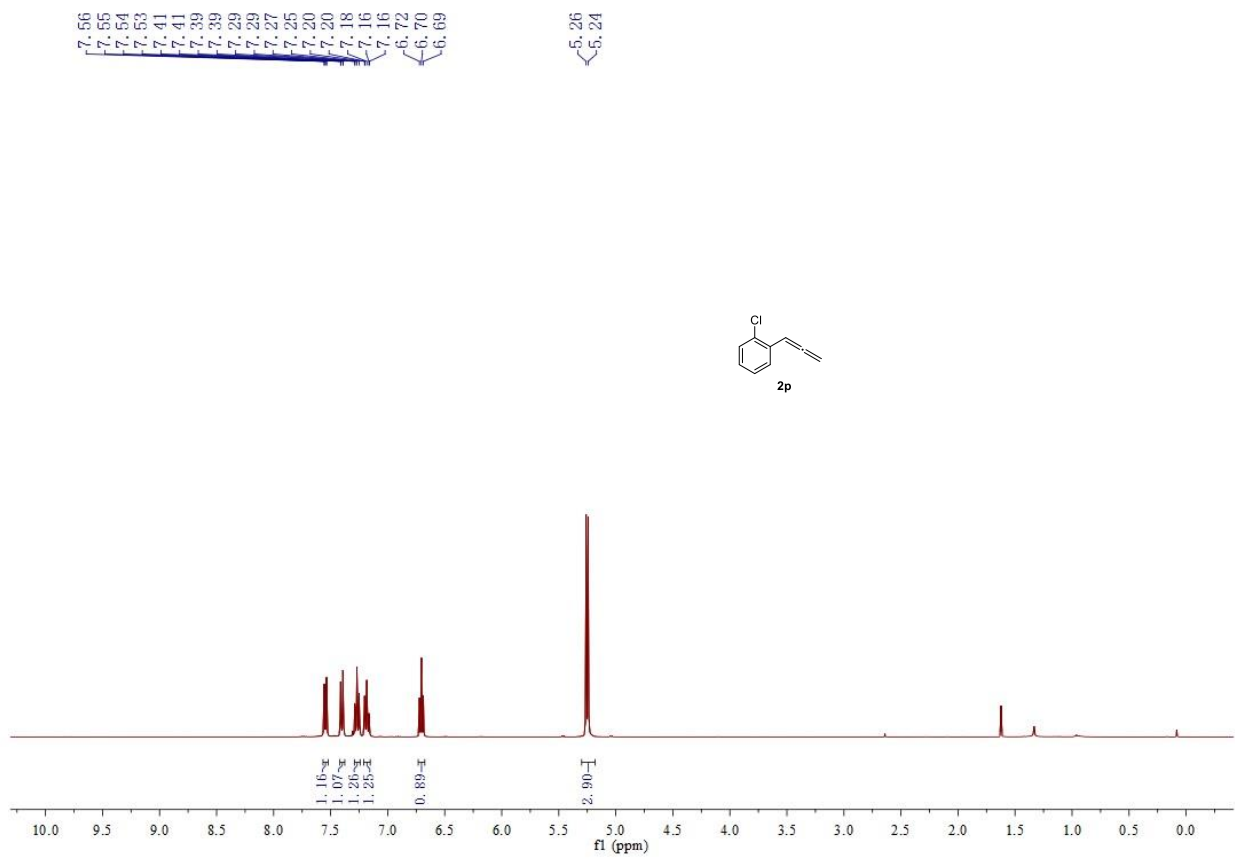
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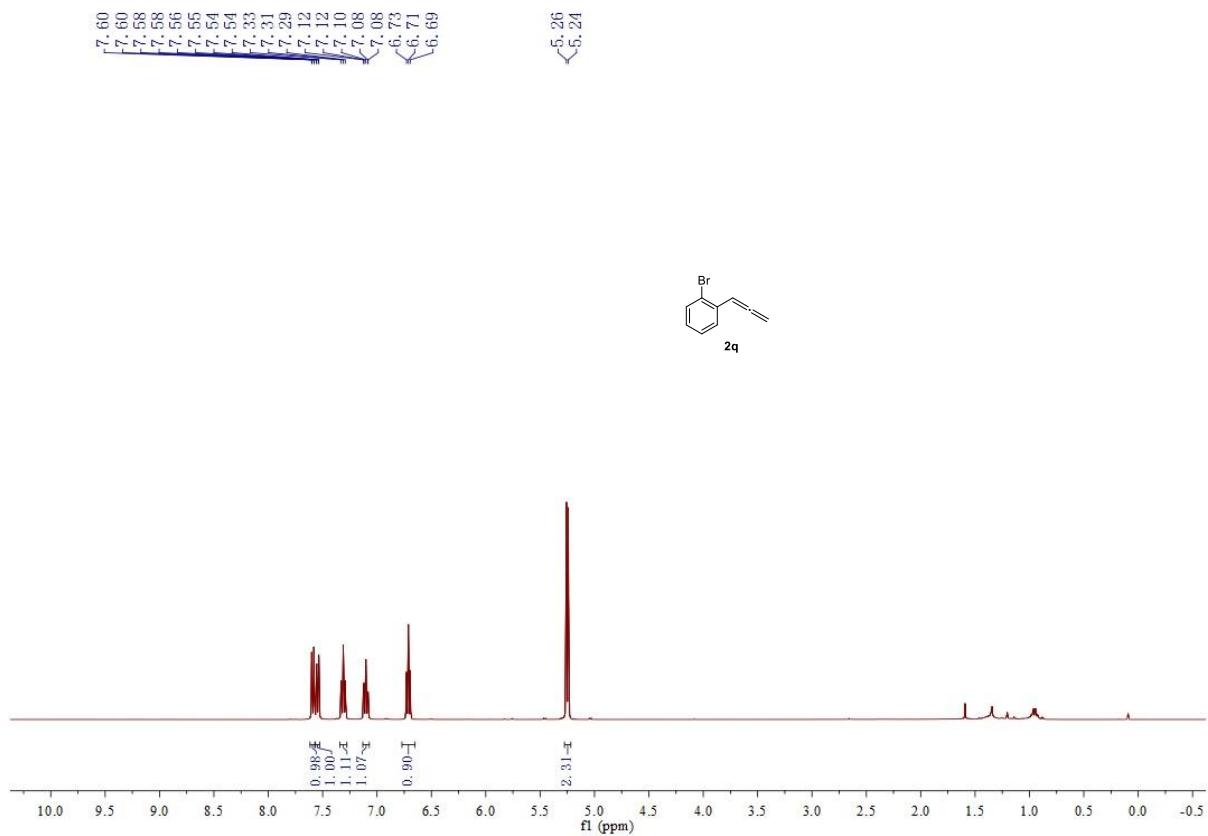


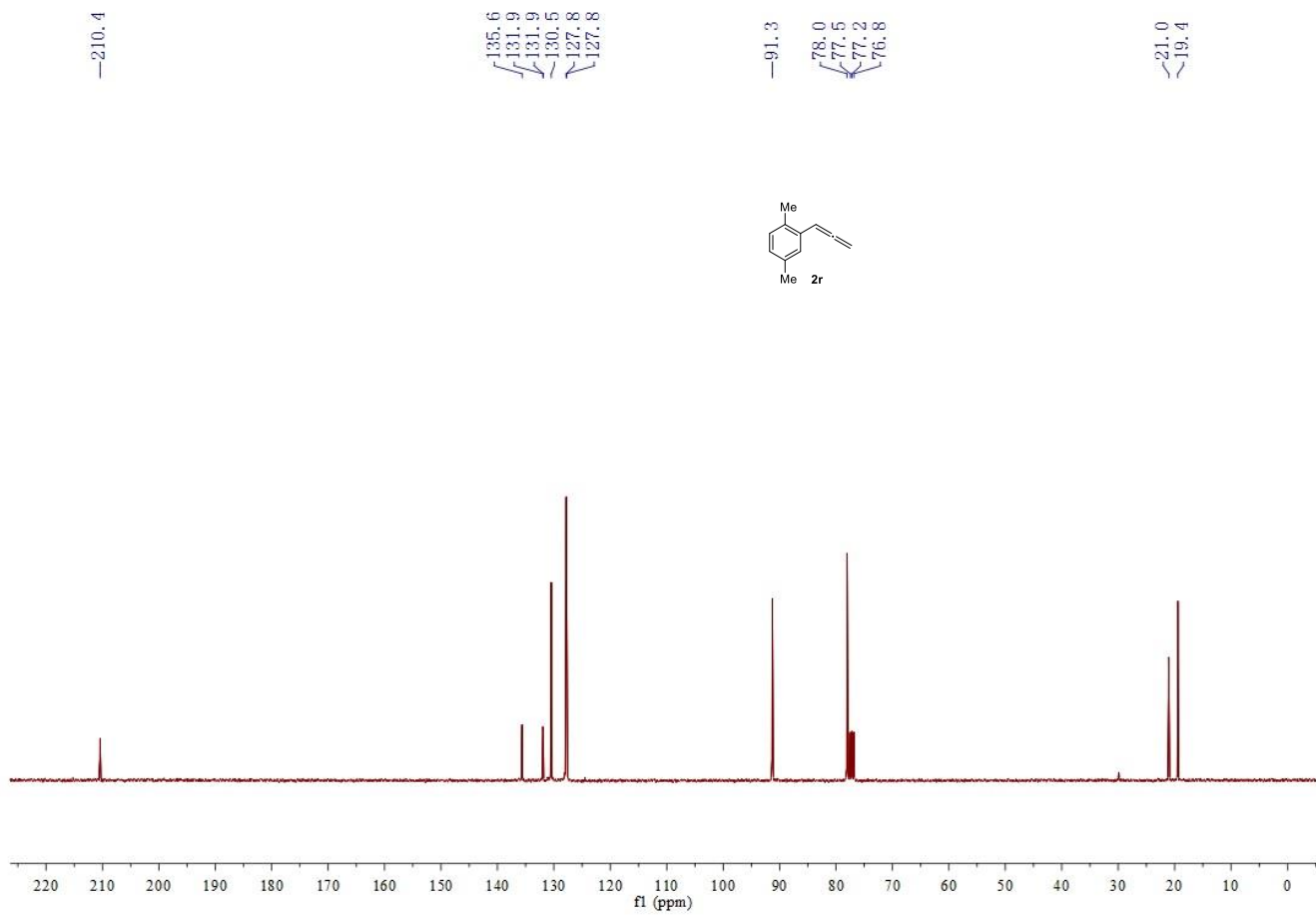
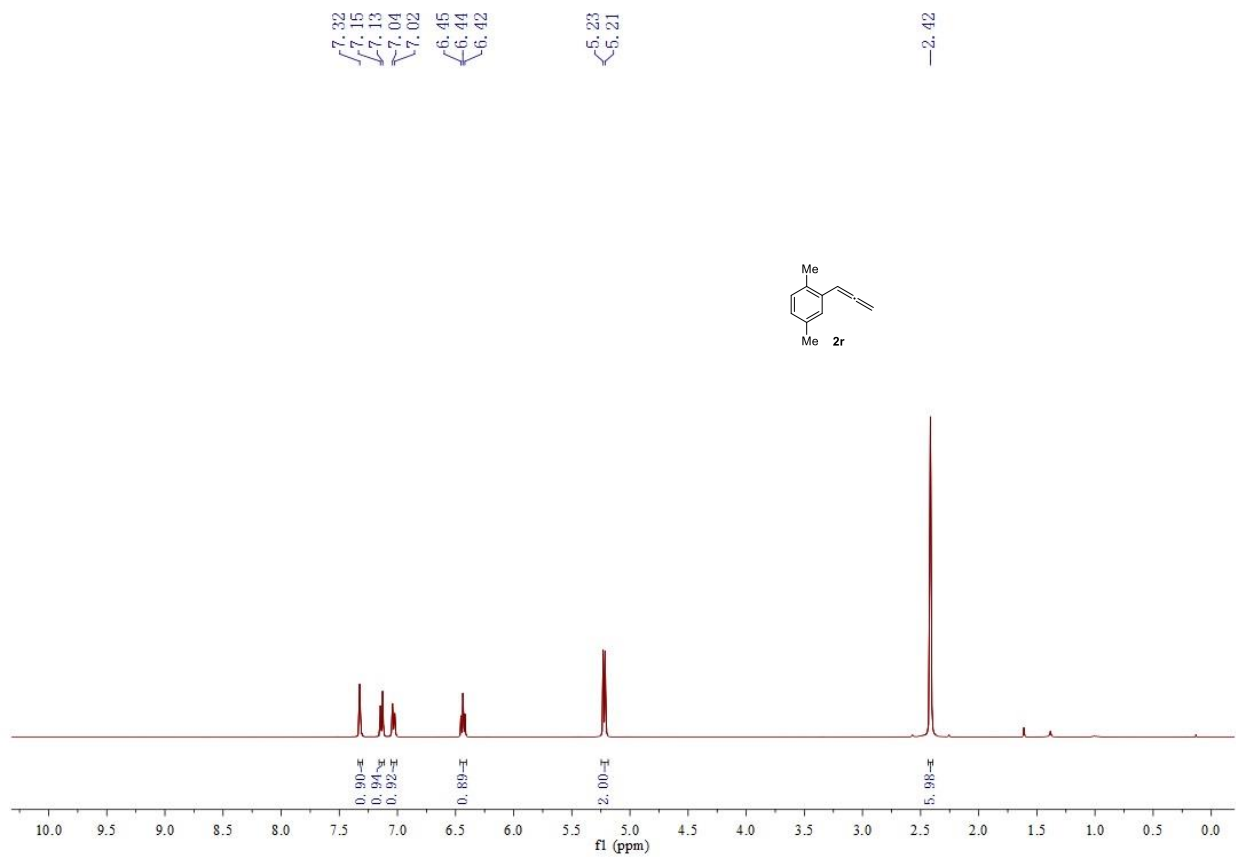


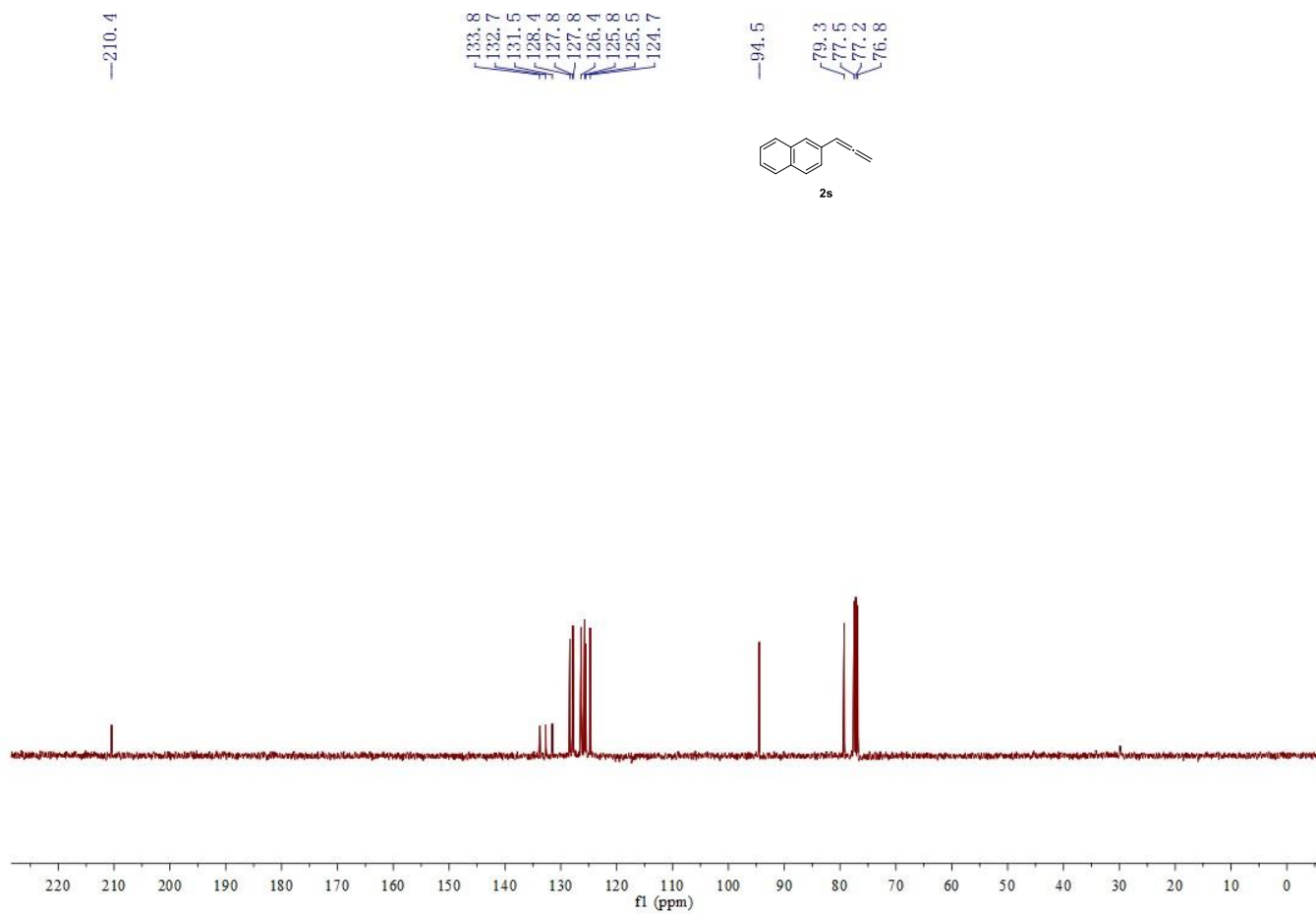
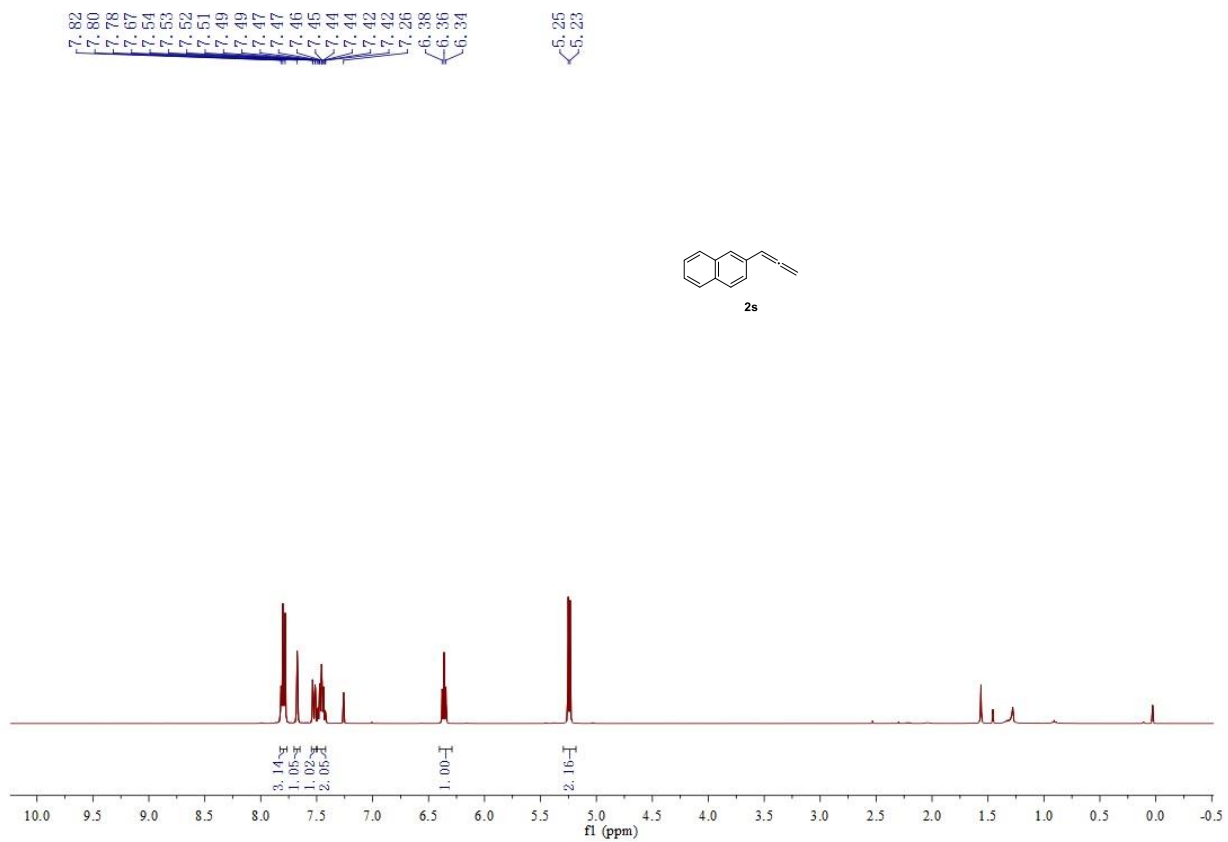


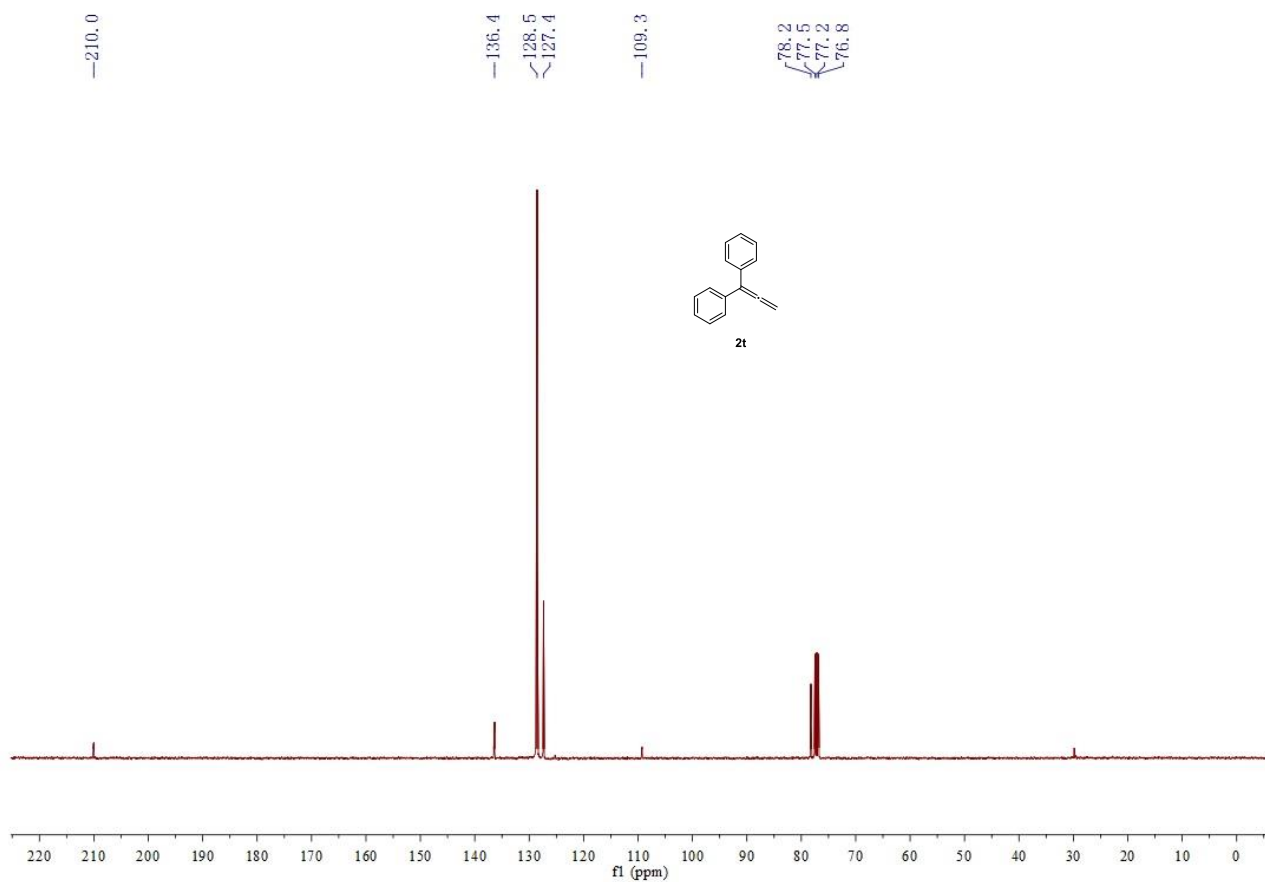
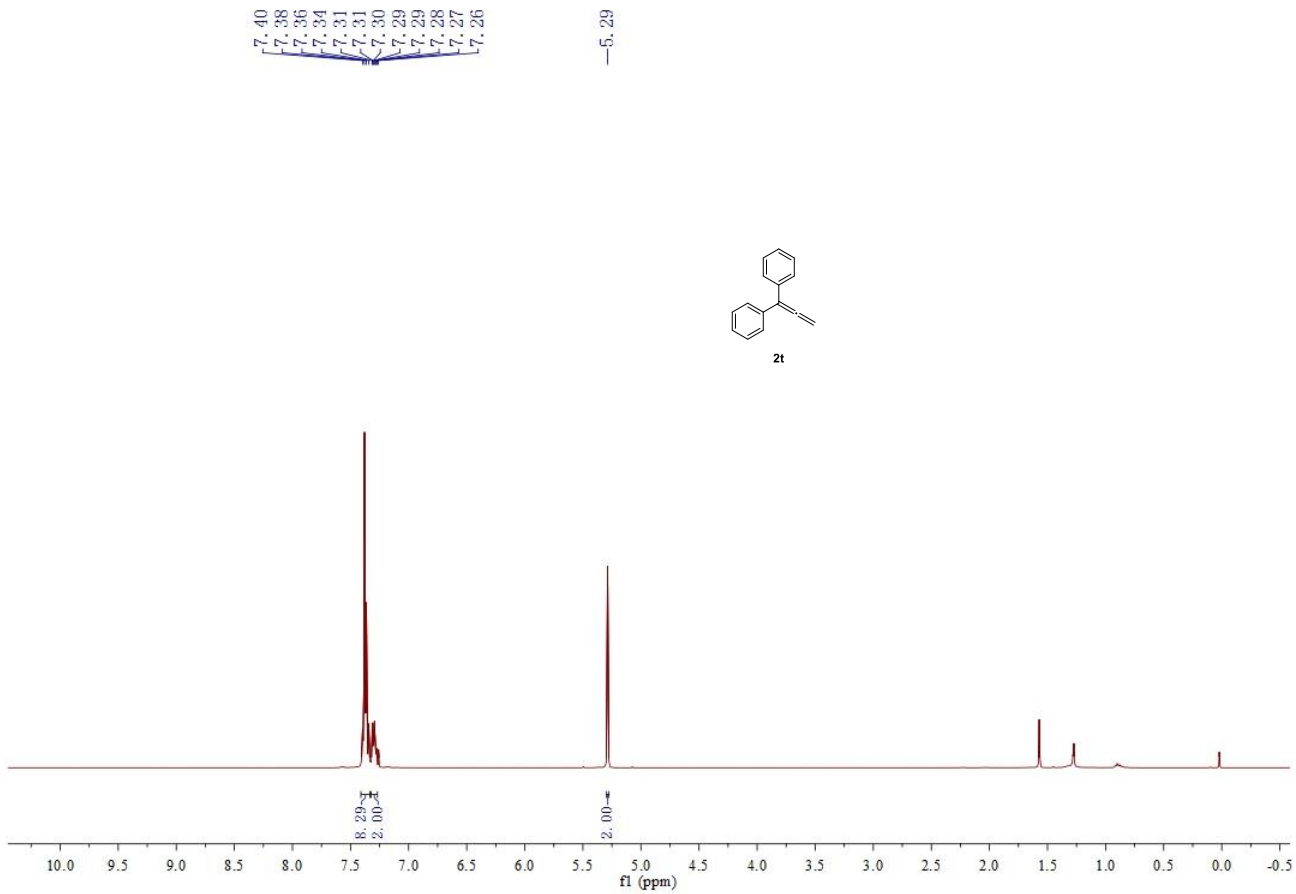


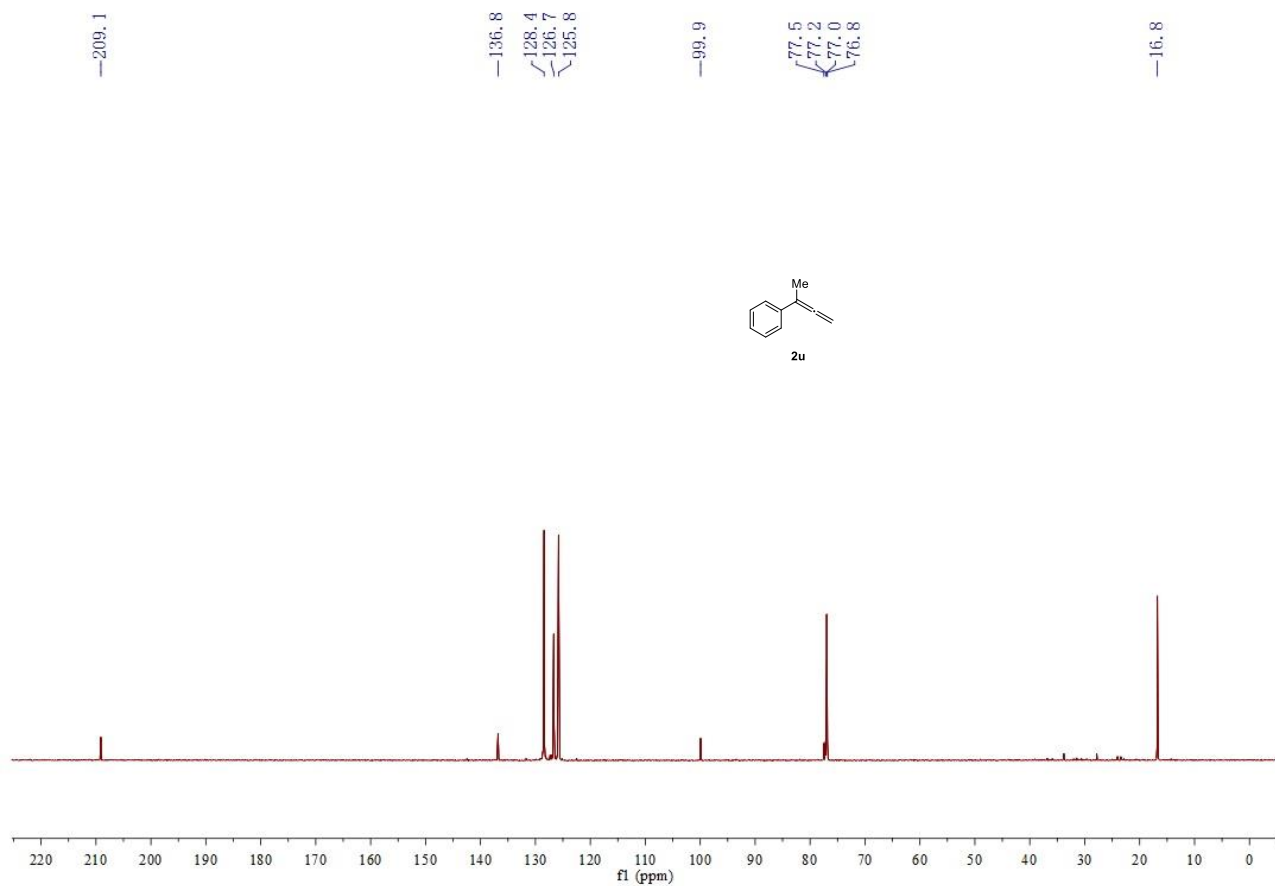
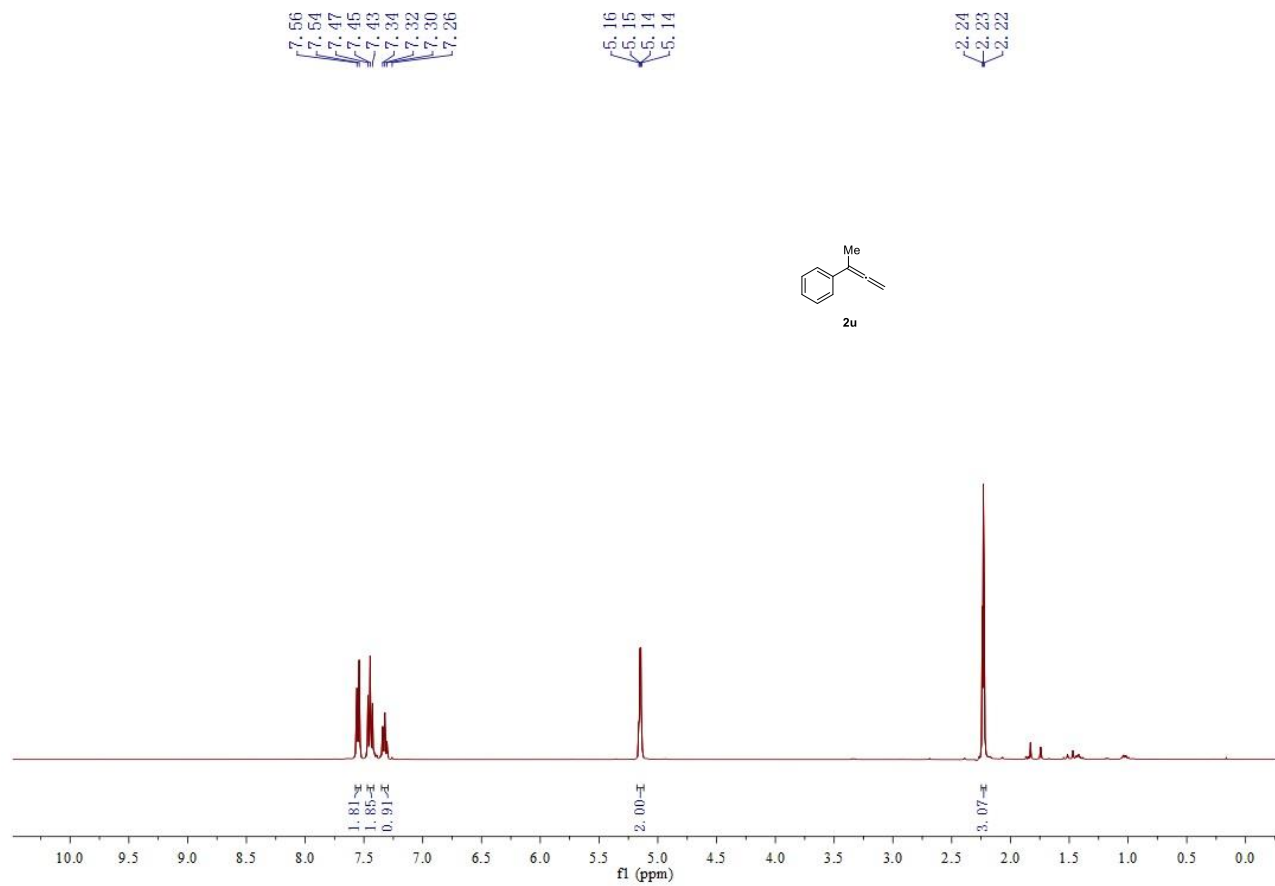


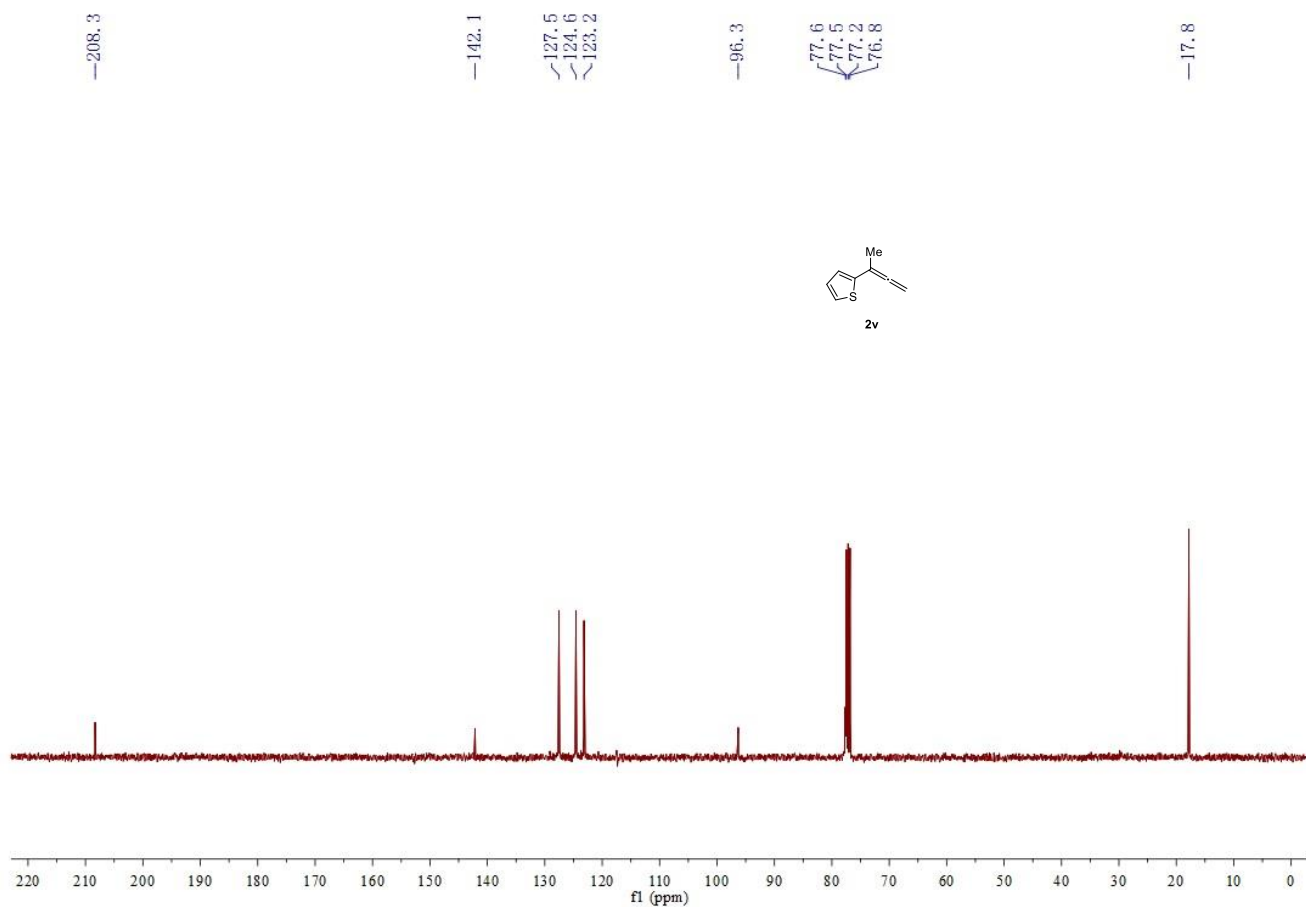
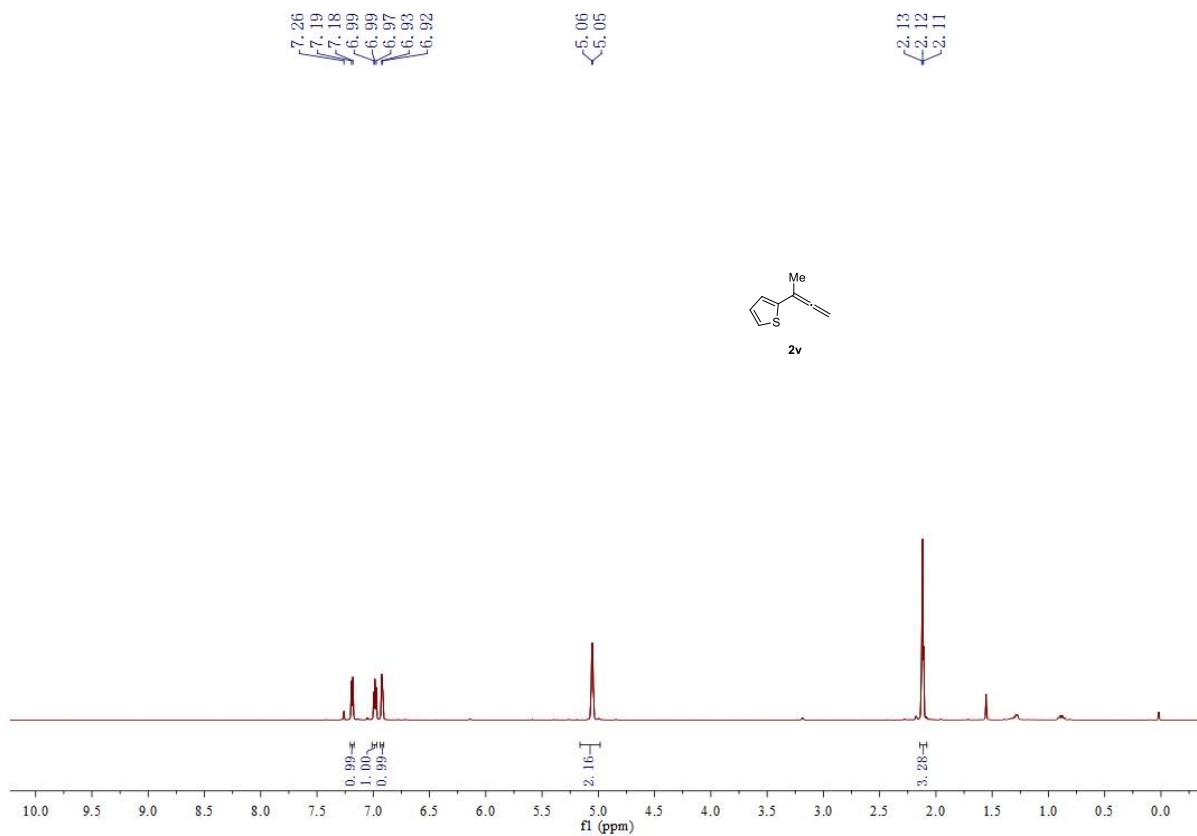


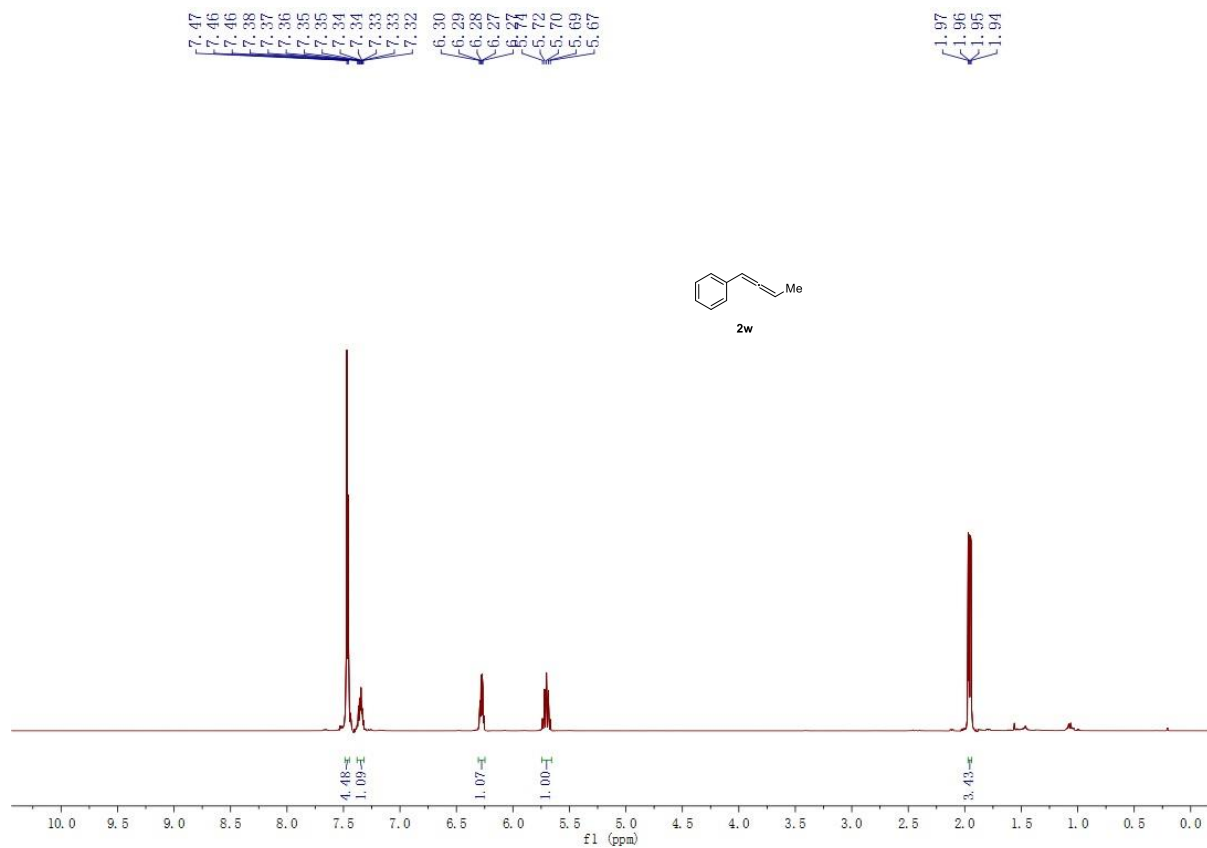










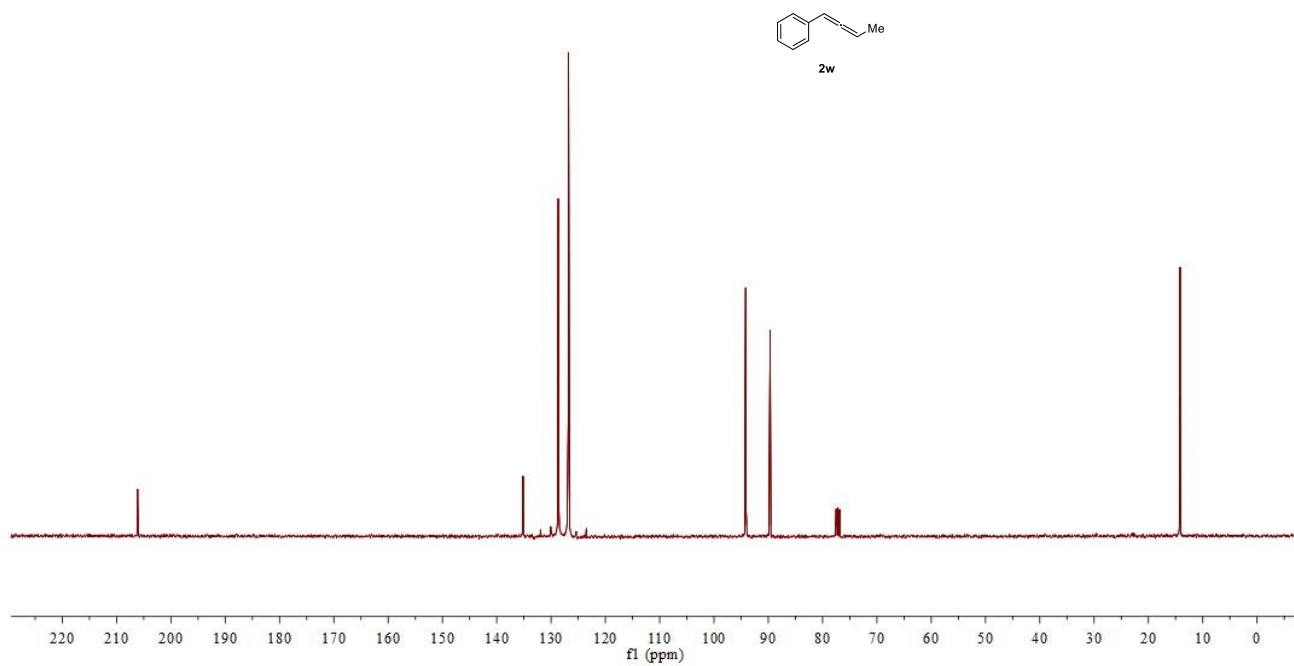


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—126.8

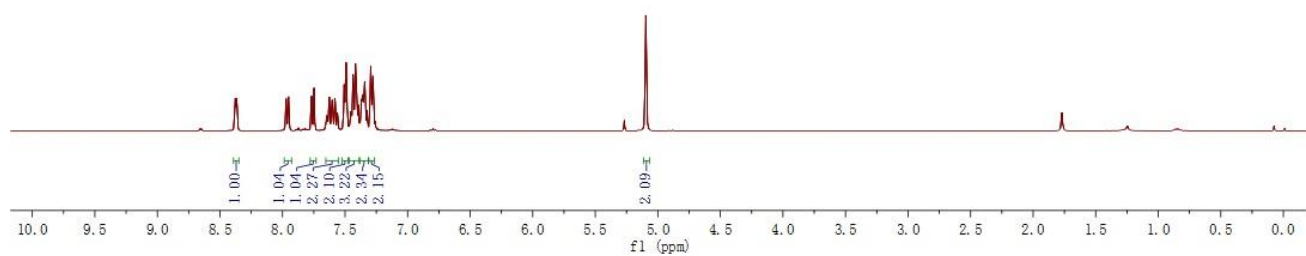
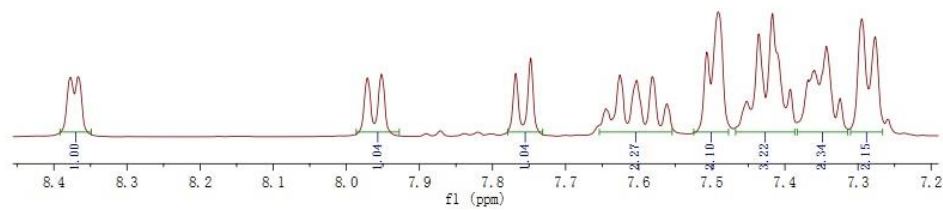
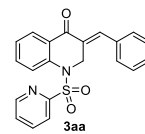
—94.2
—89.7
77.5
77.2
76.9

—14.2



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-1.77



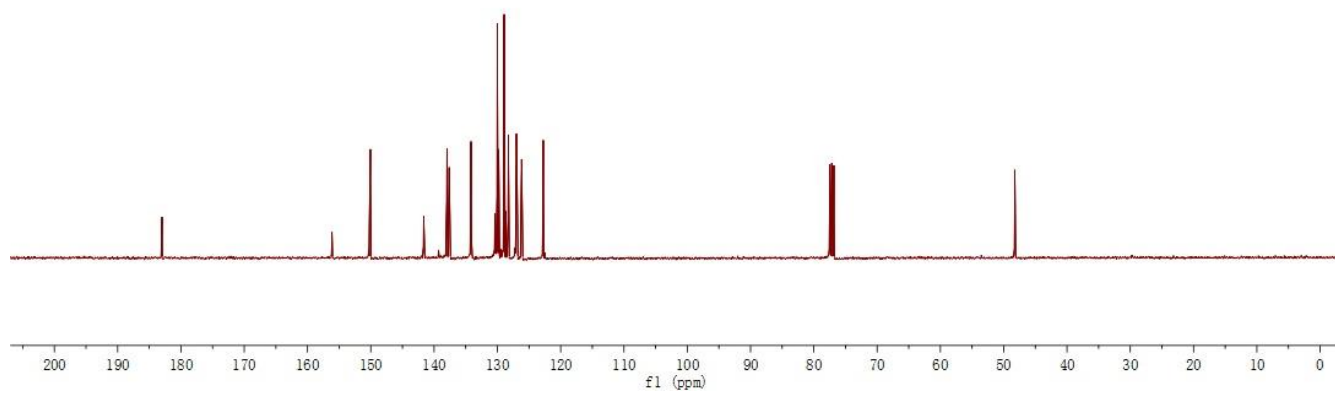
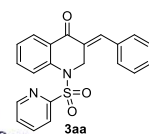
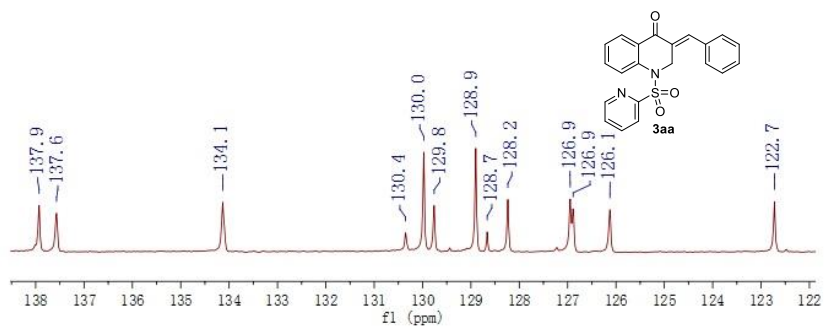
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122.8

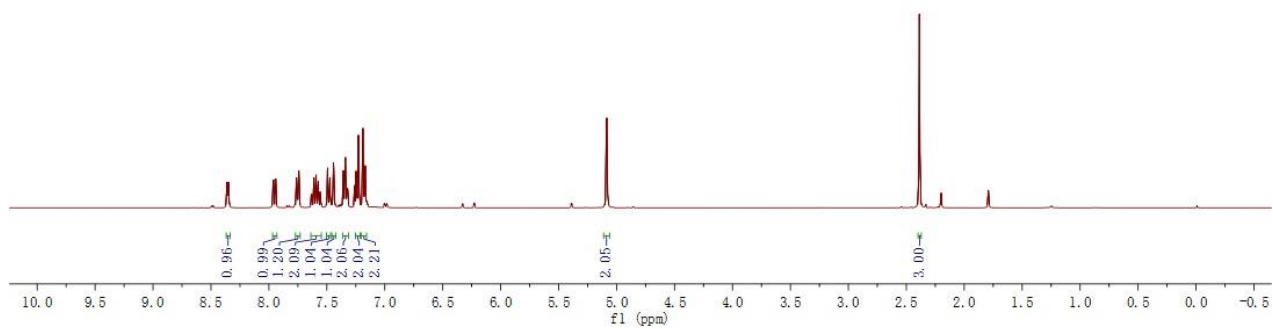
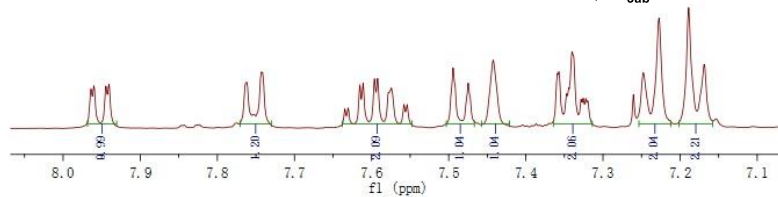
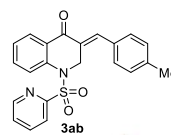
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76.8

-48.2



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7.19
7.09
5.08

2.39



183.0

156.1

150.8

140.3

137.9

137.8

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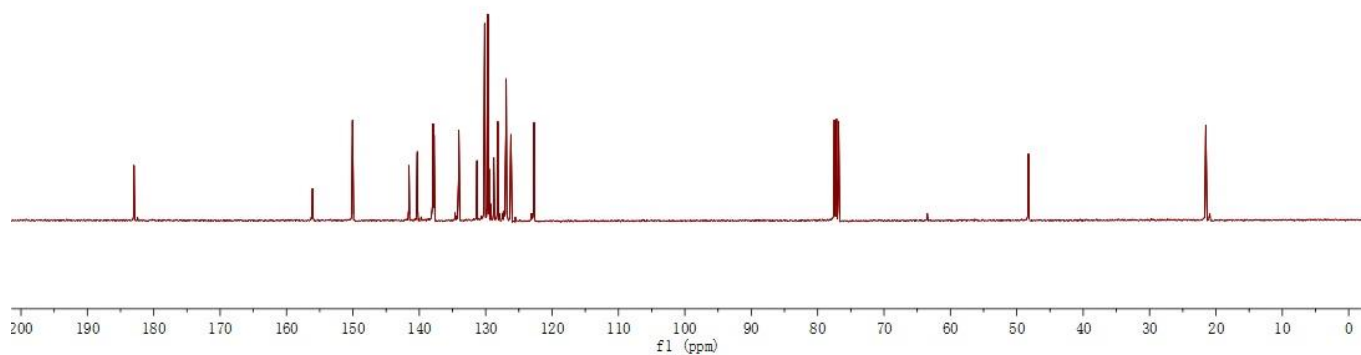
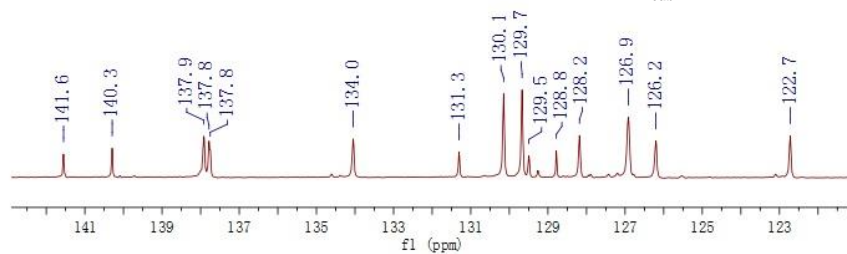
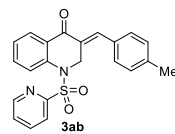
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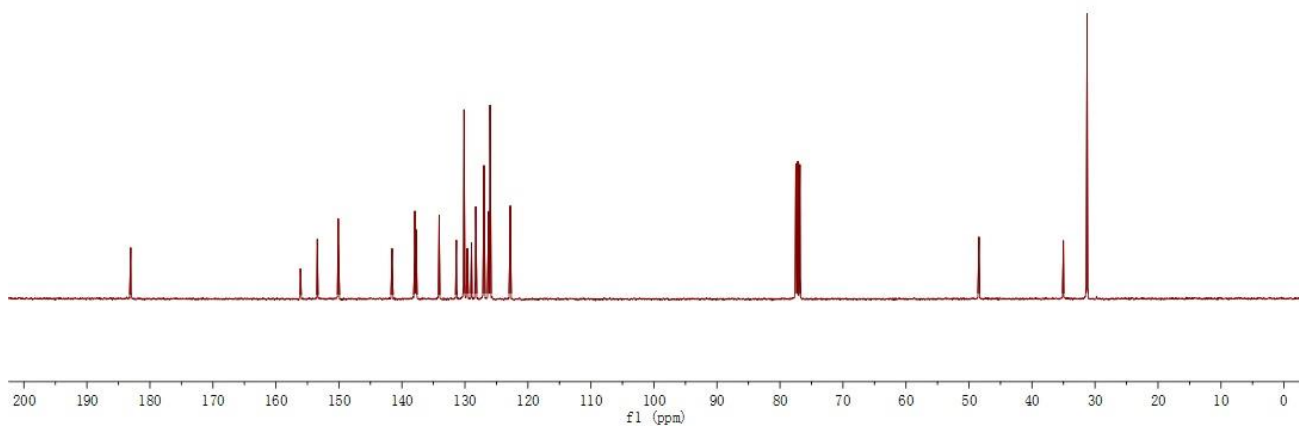
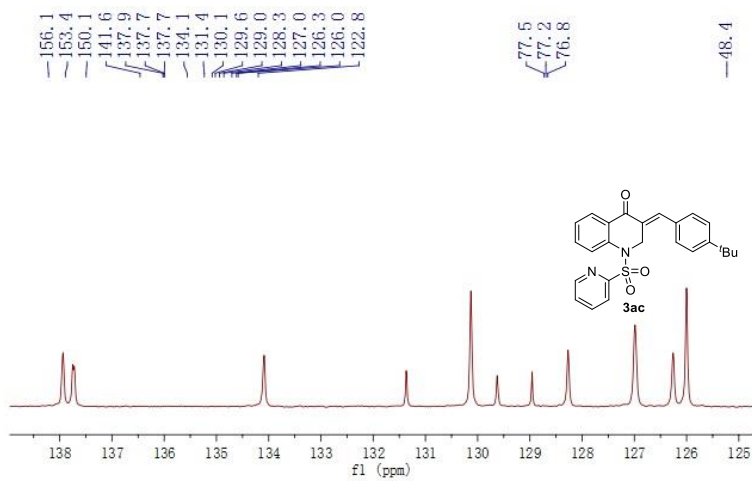
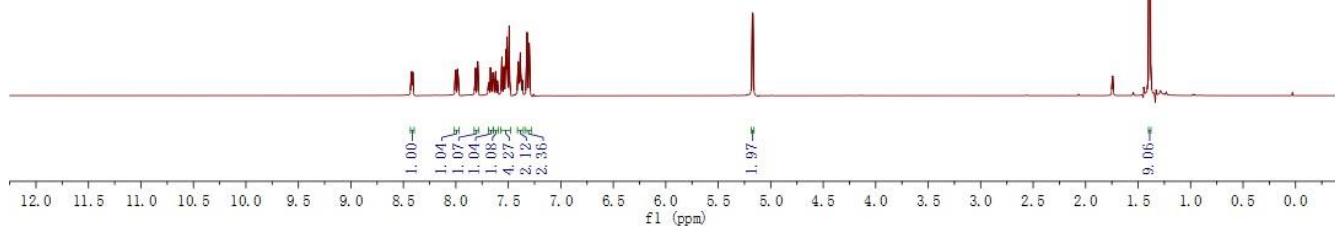
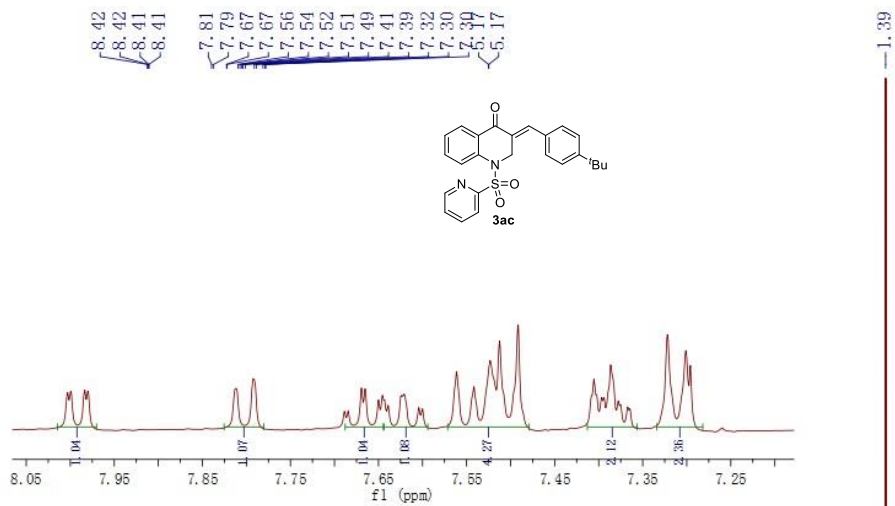
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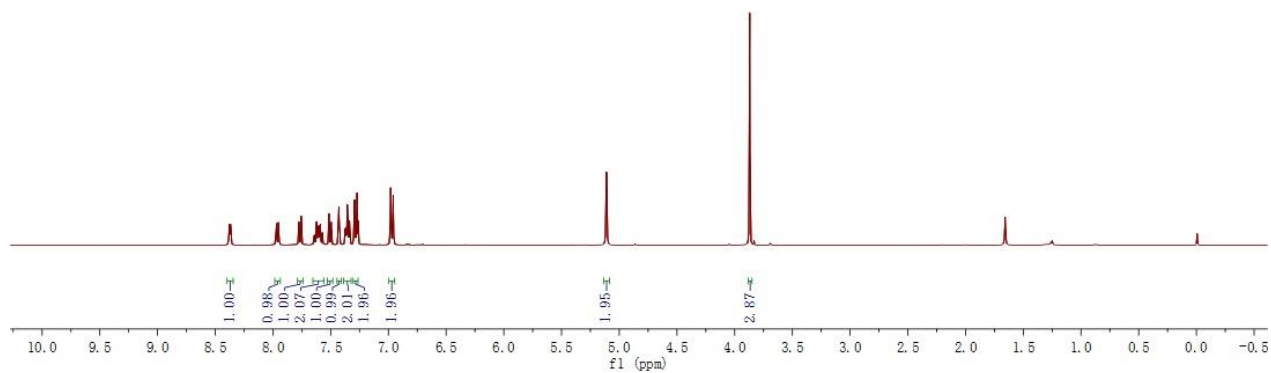
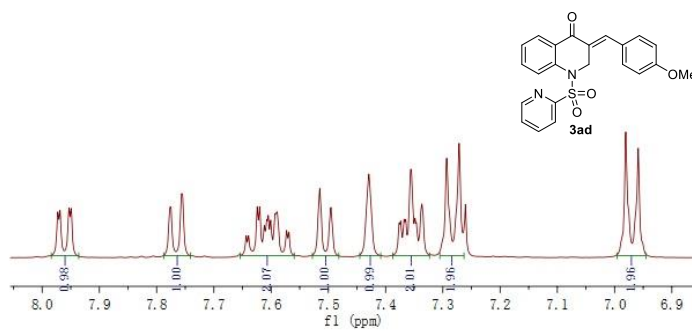
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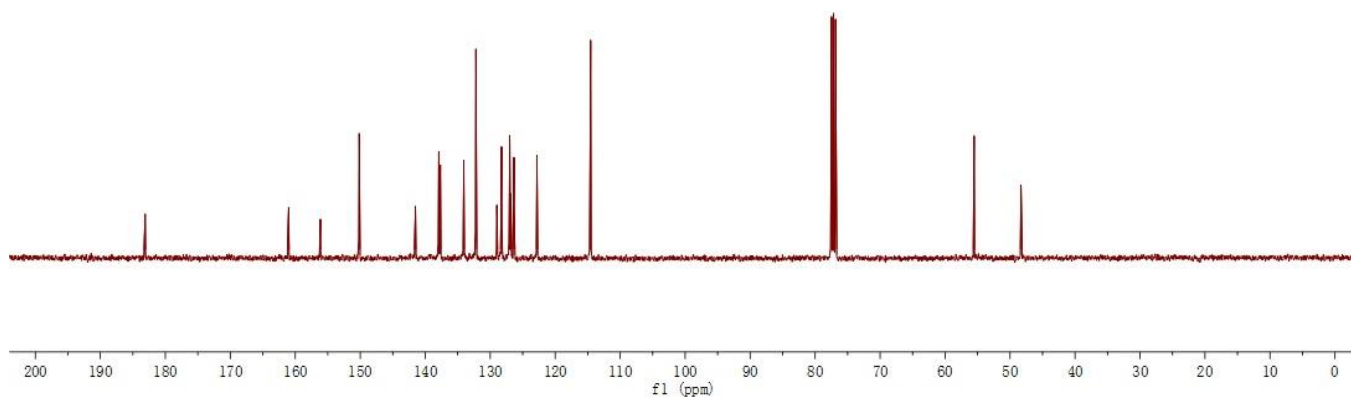
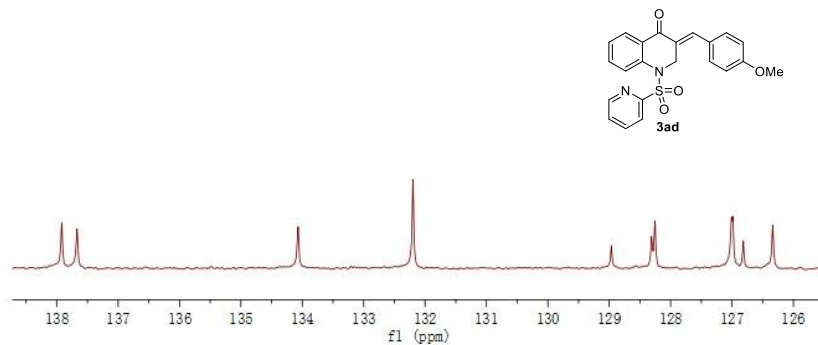


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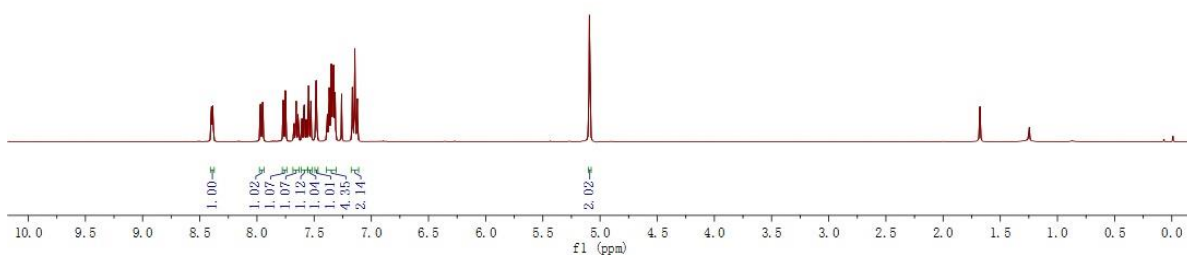
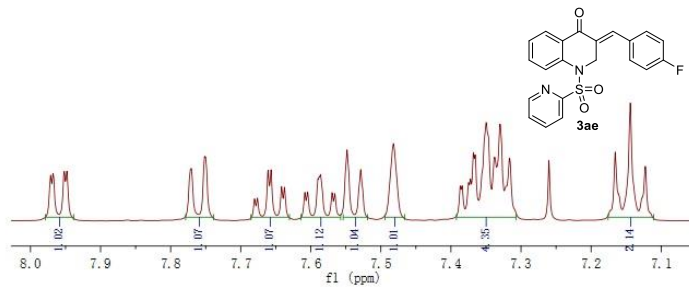
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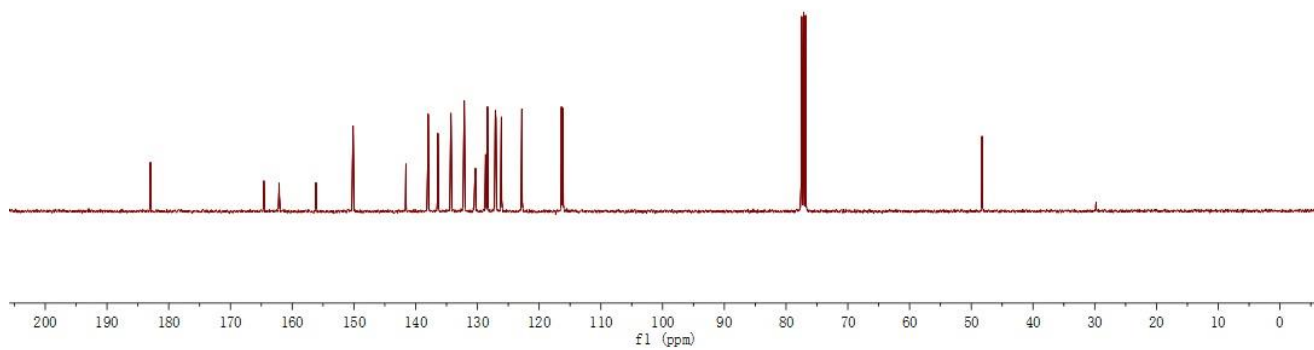
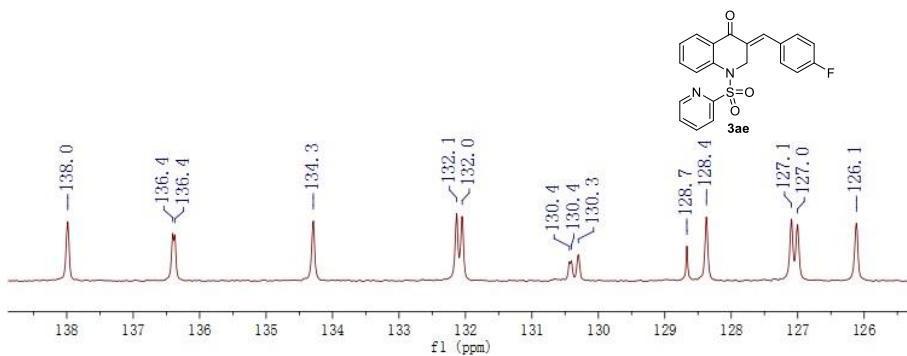


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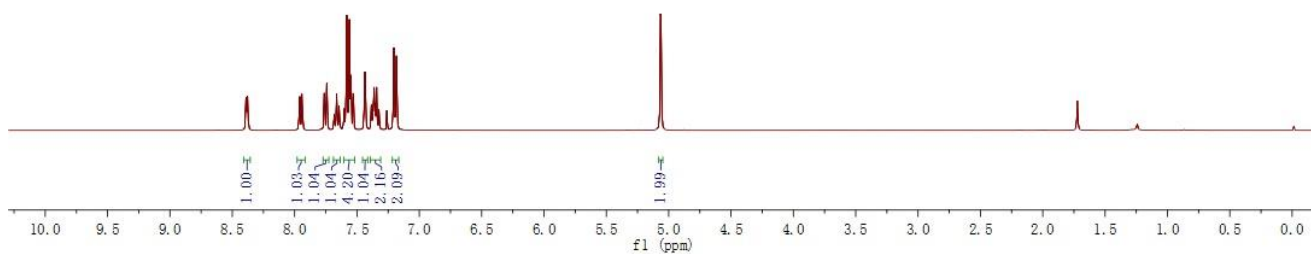
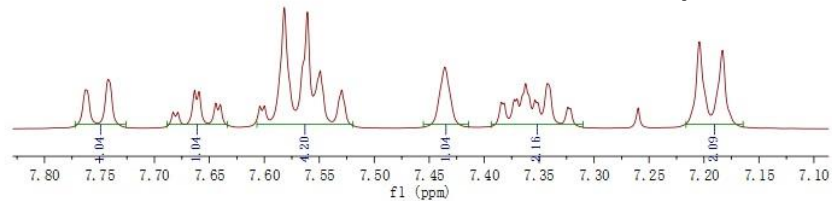
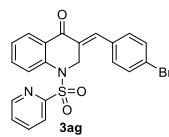
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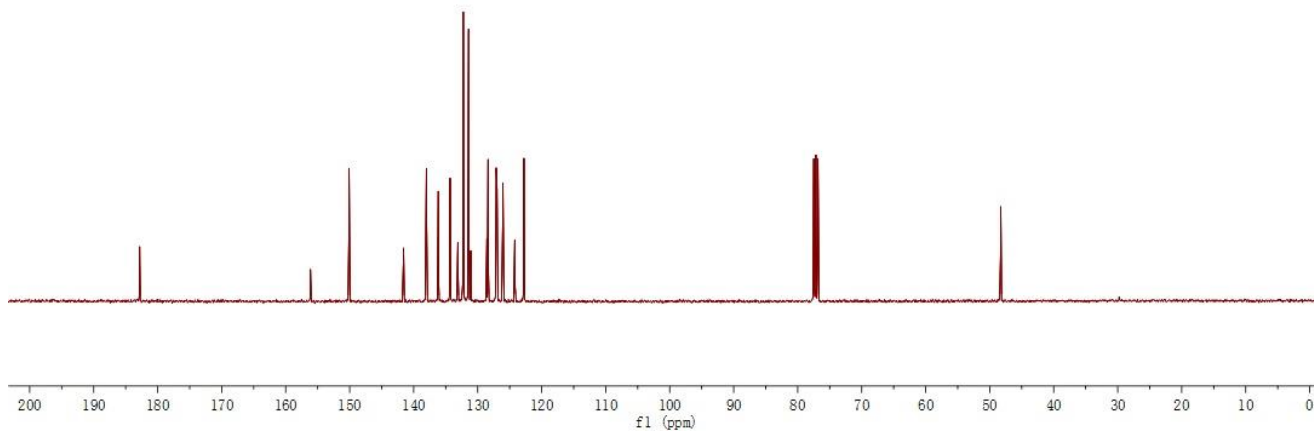
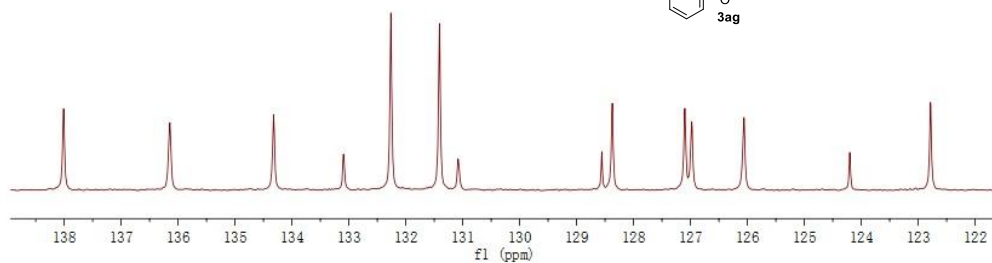
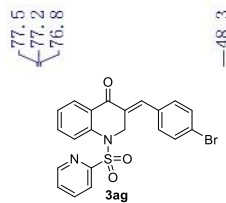
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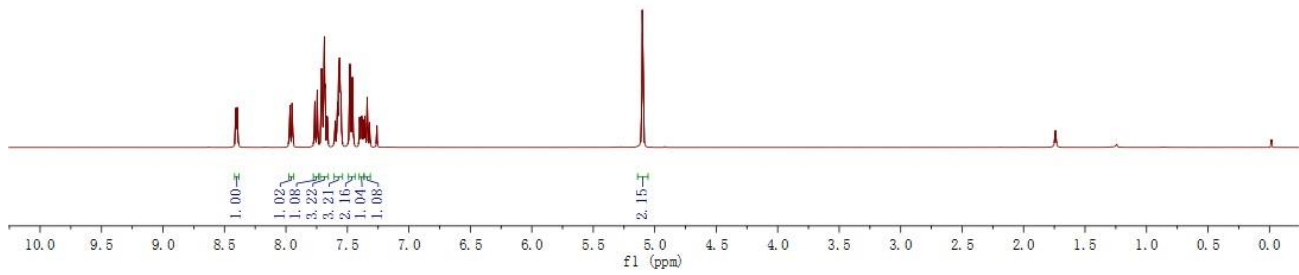
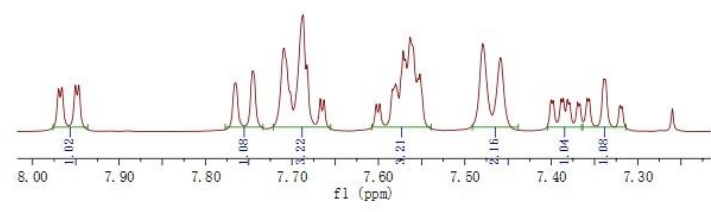
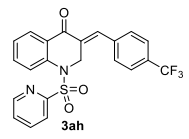
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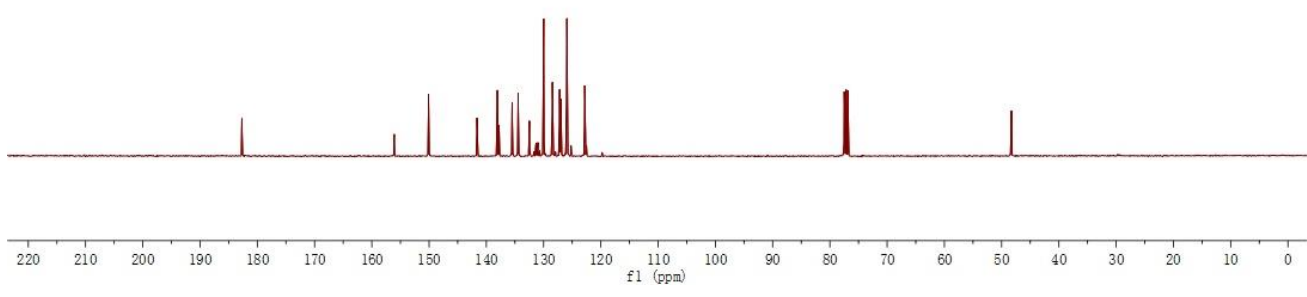
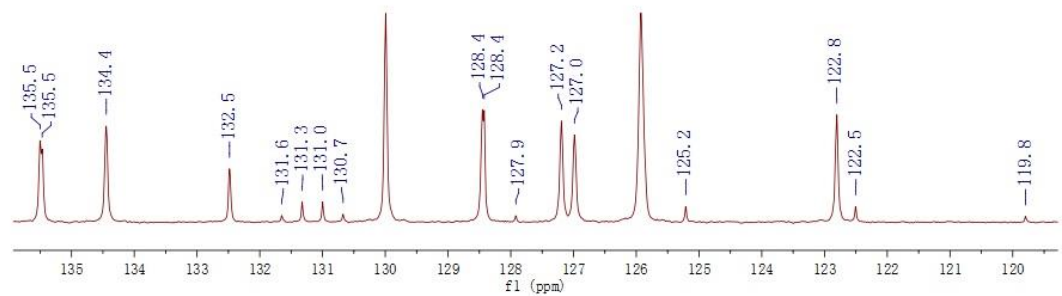
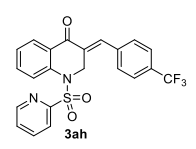
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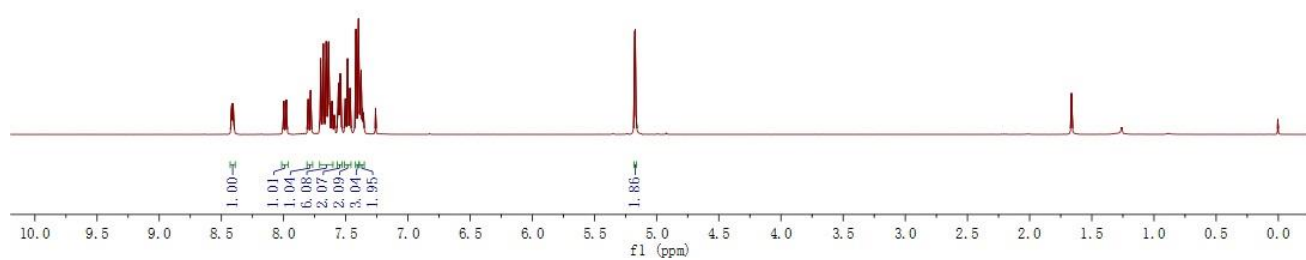
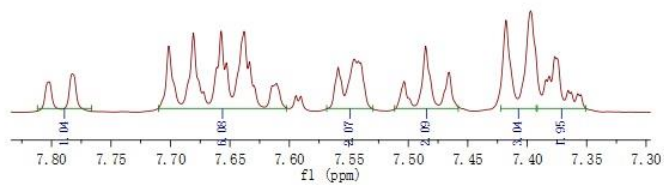
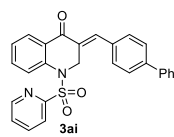
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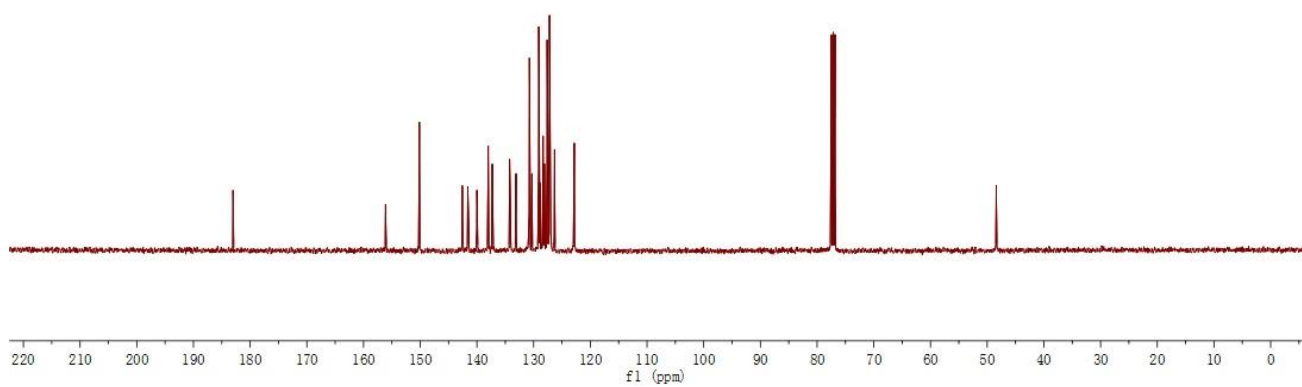
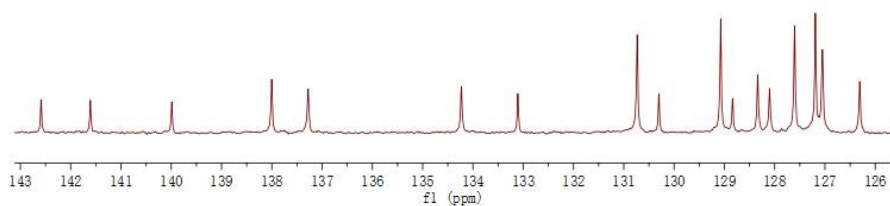
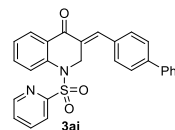
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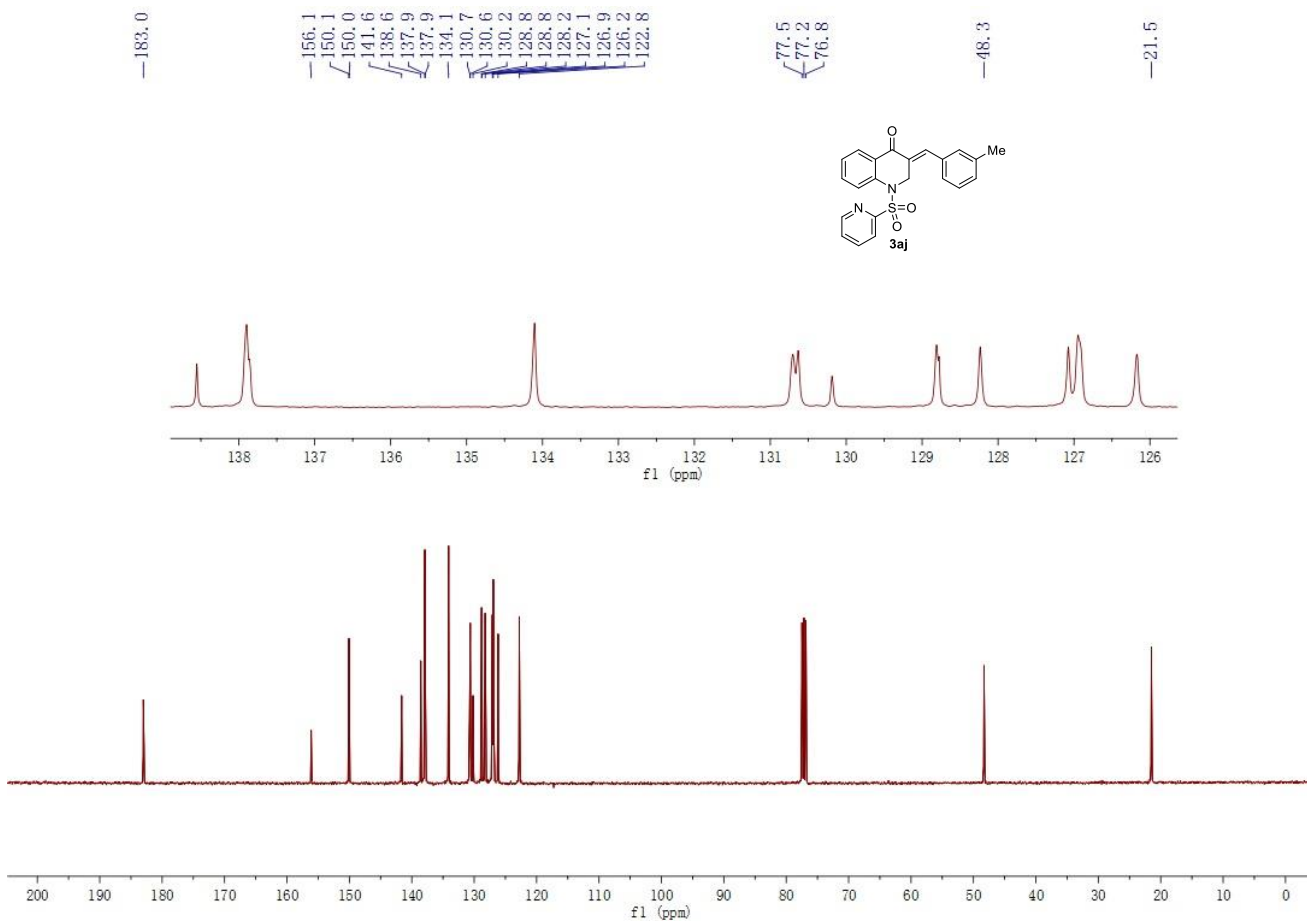
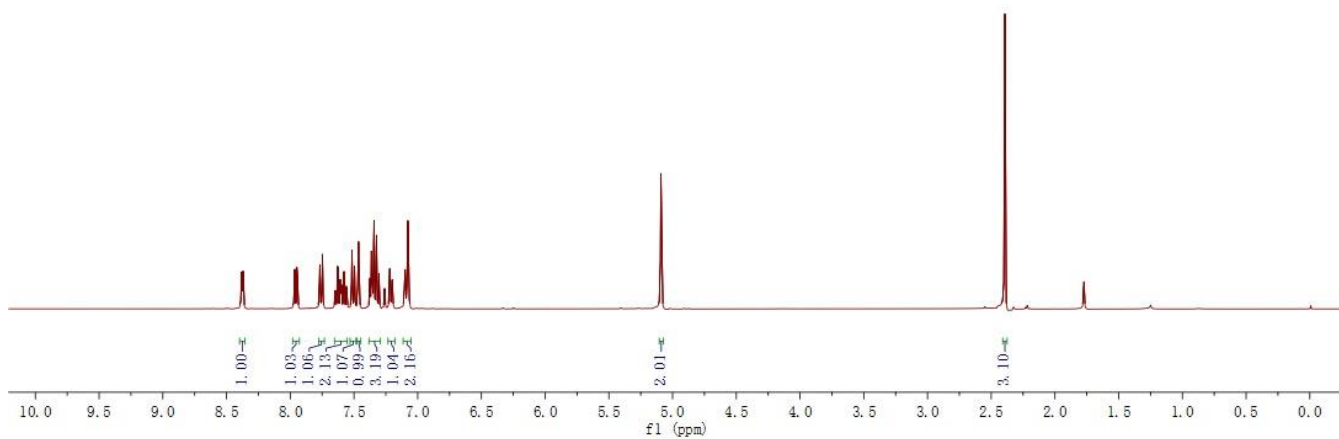
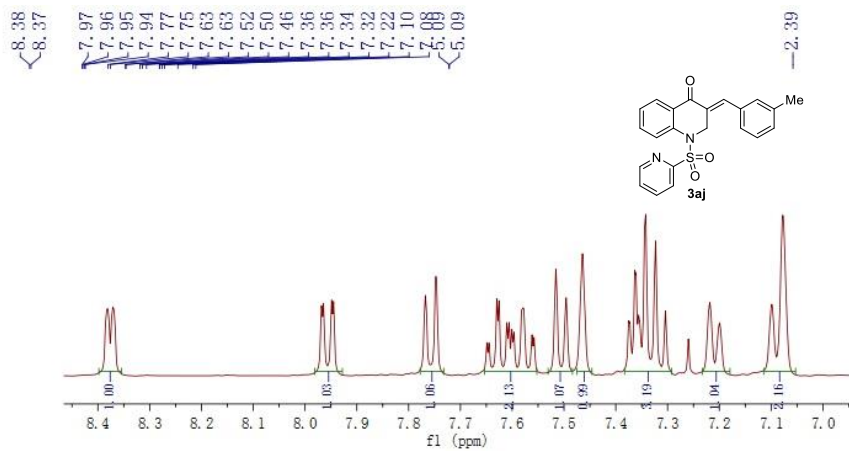


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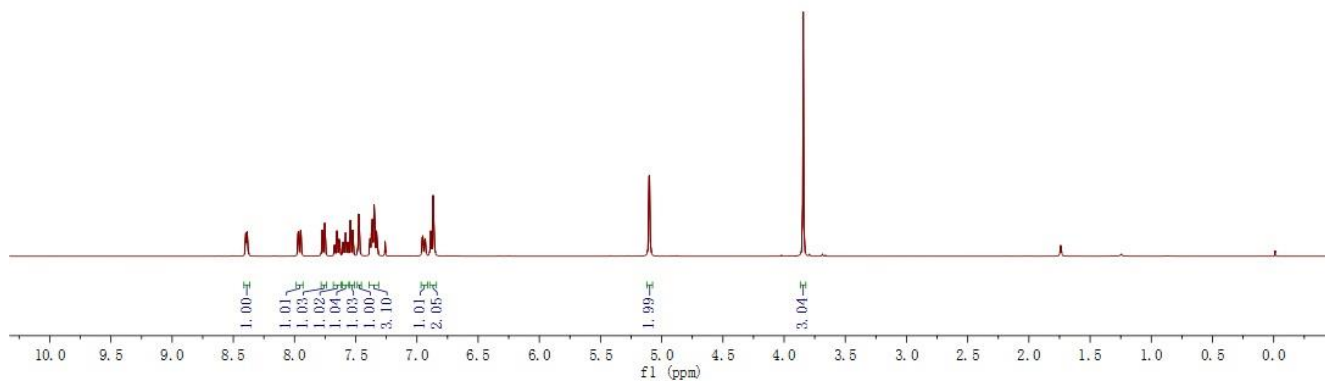
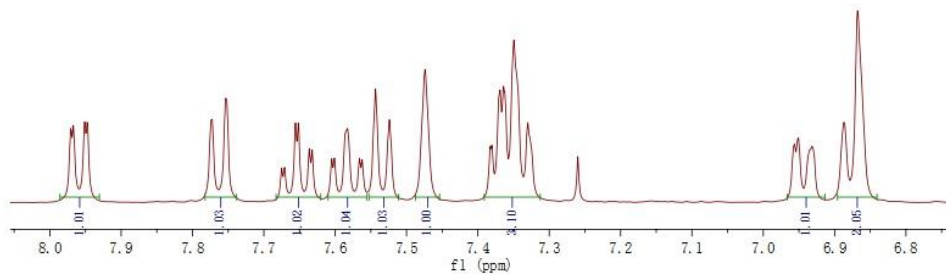
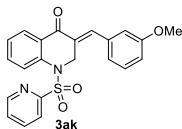


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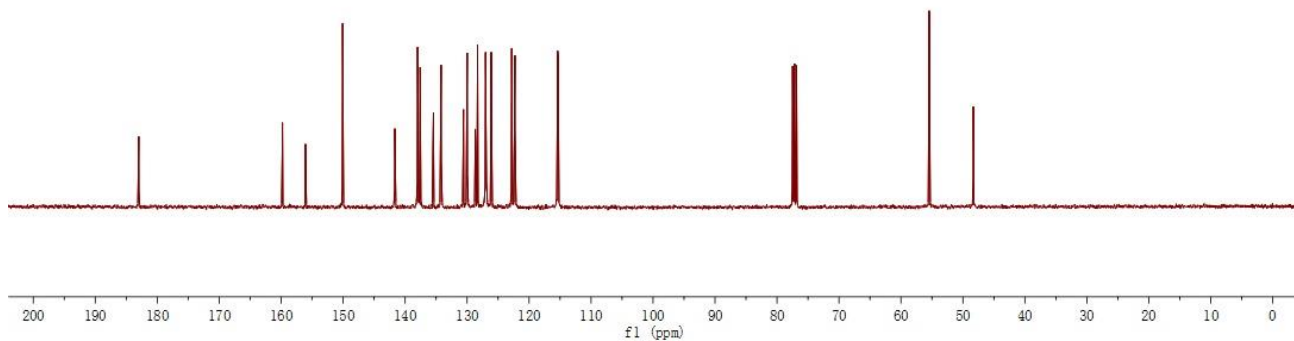
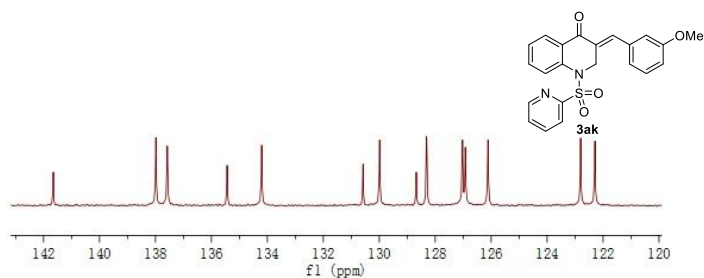




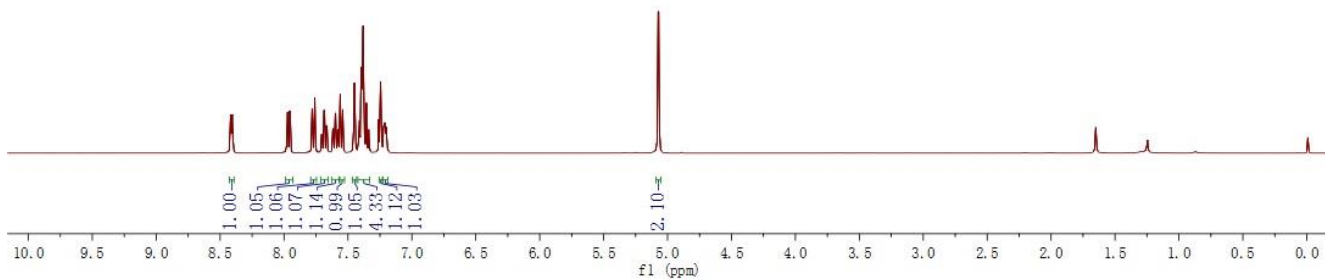
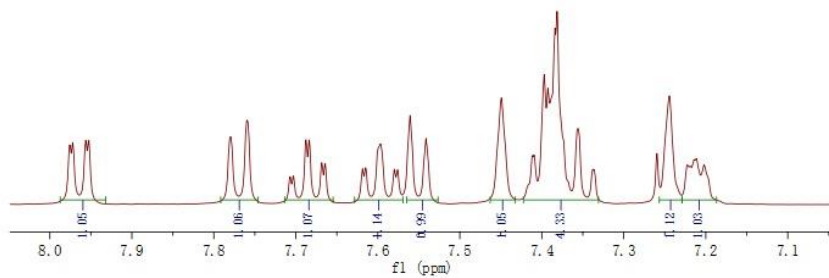
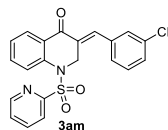
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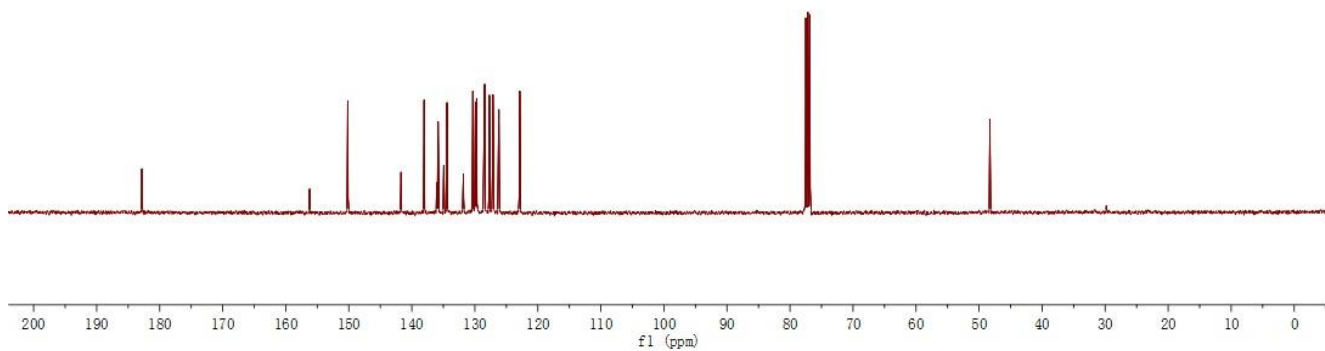
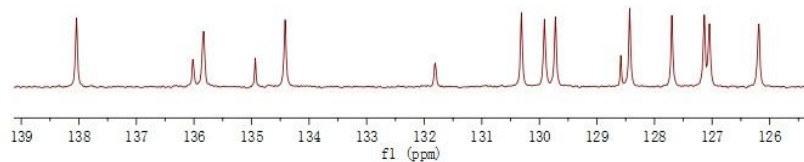
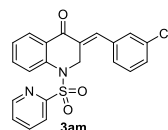


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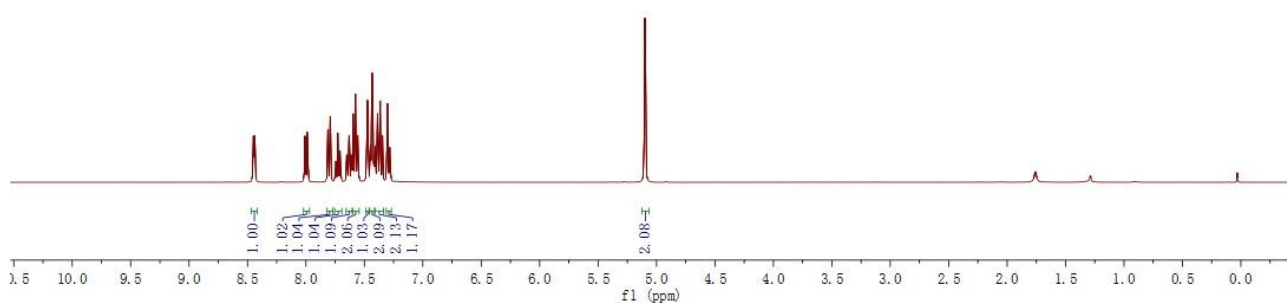
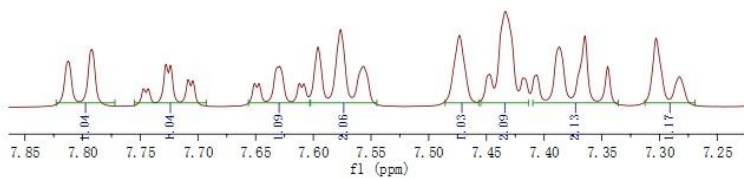
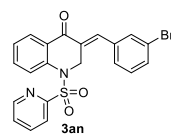
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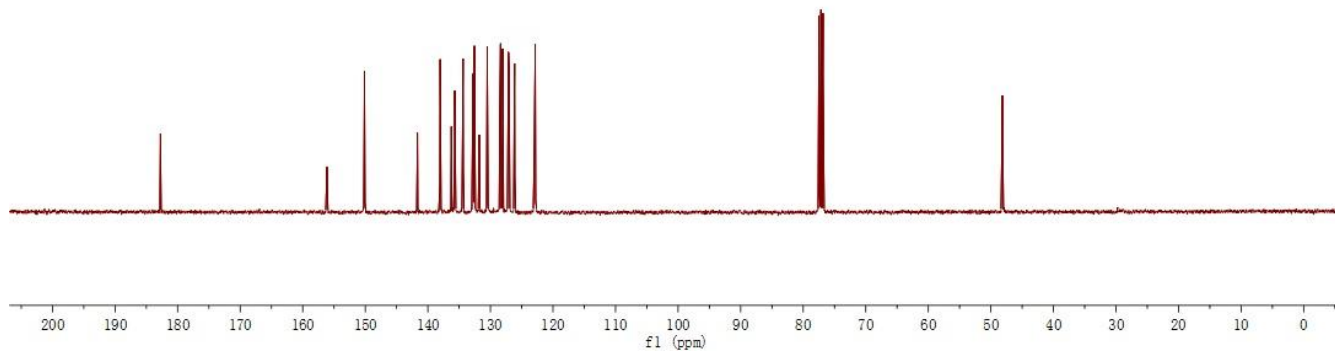
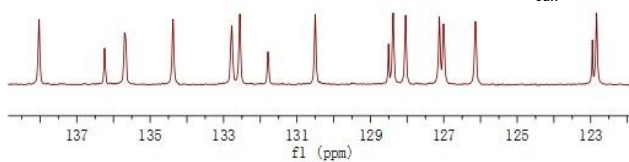
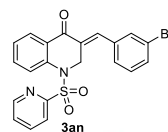
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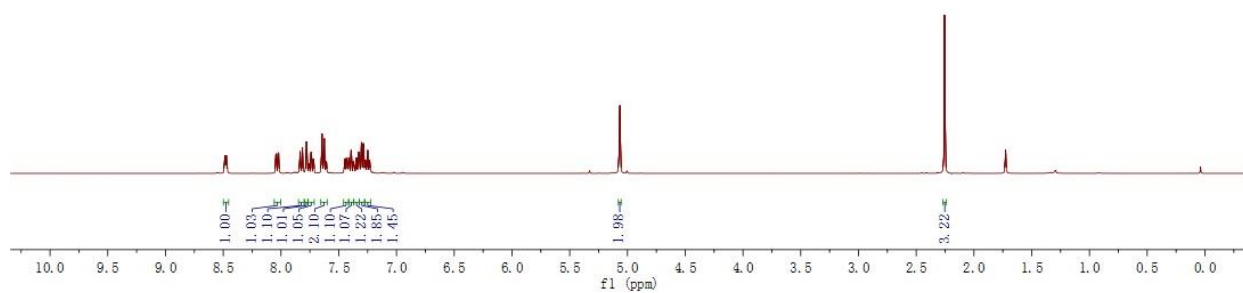
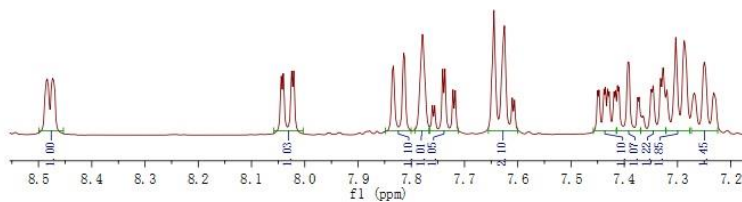
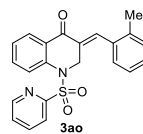
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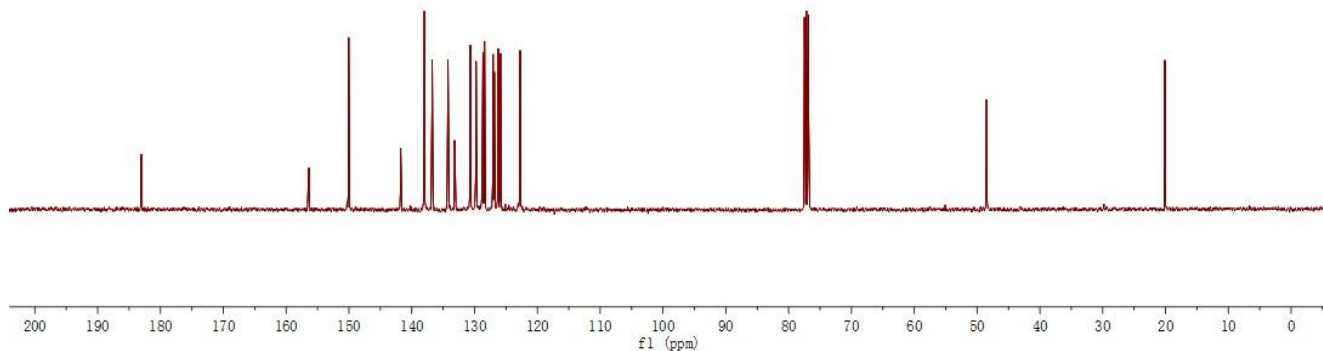
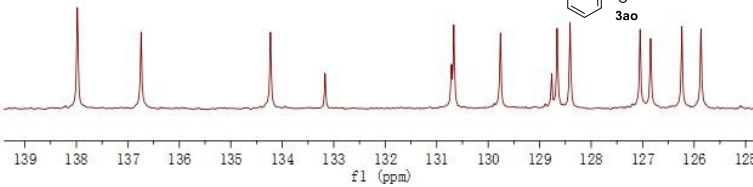
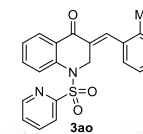
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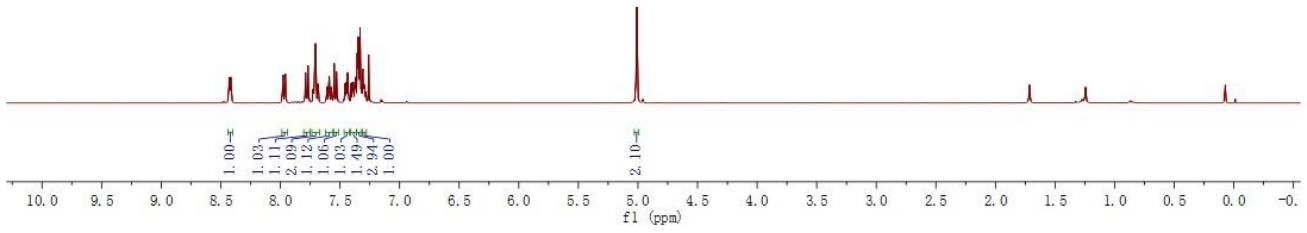
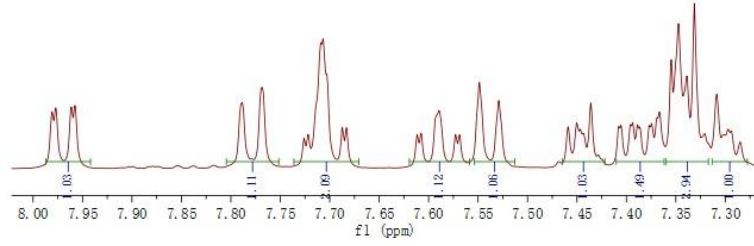
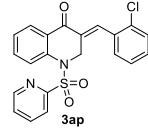
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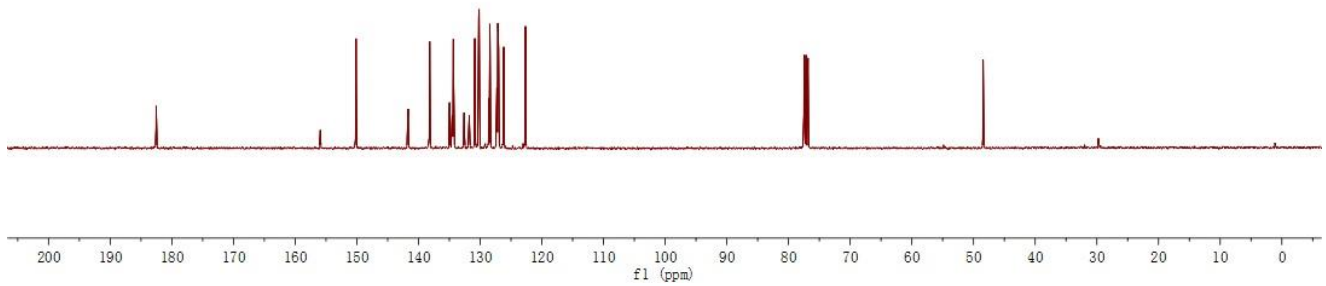
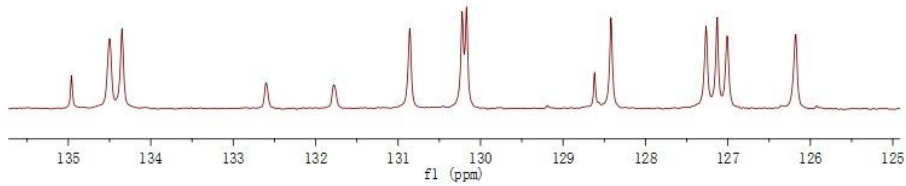
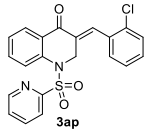
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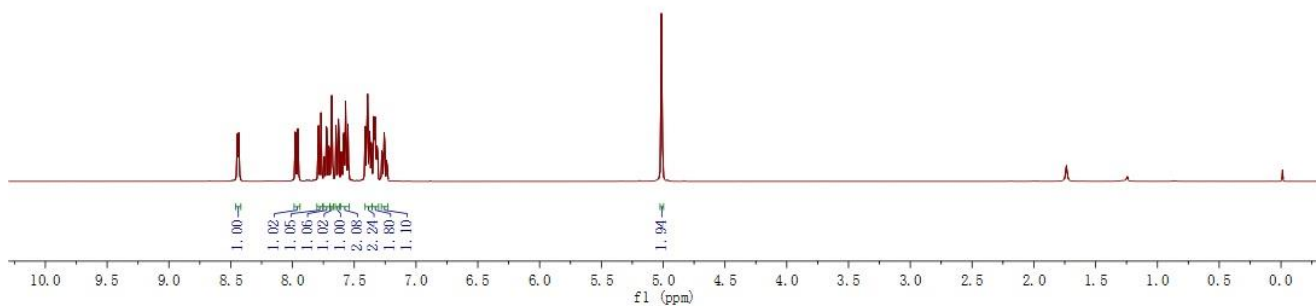
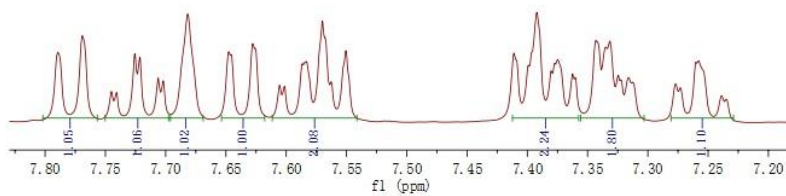
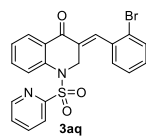
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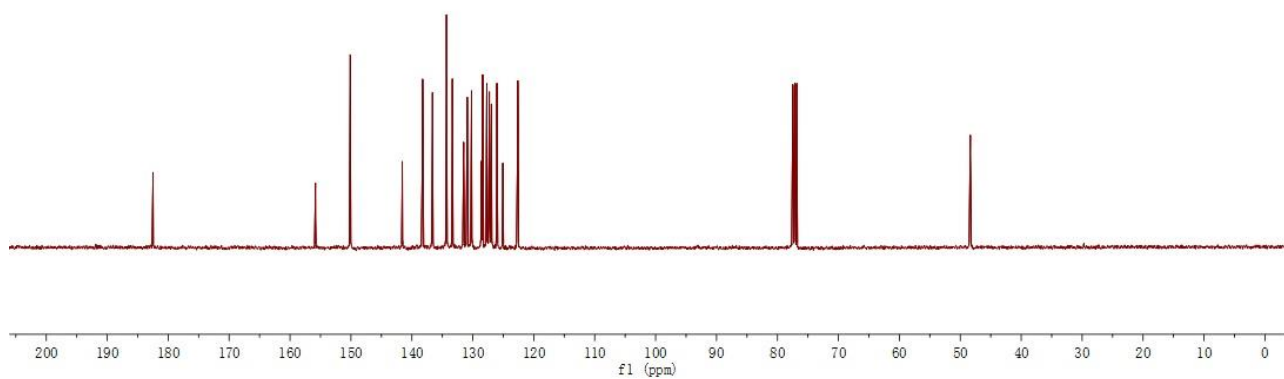
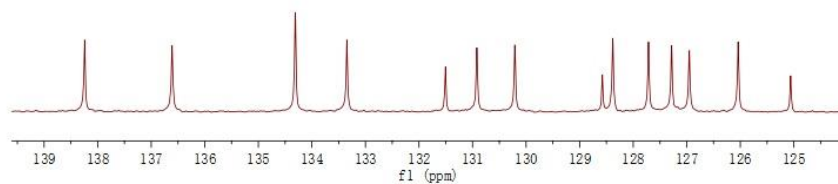
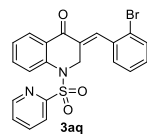
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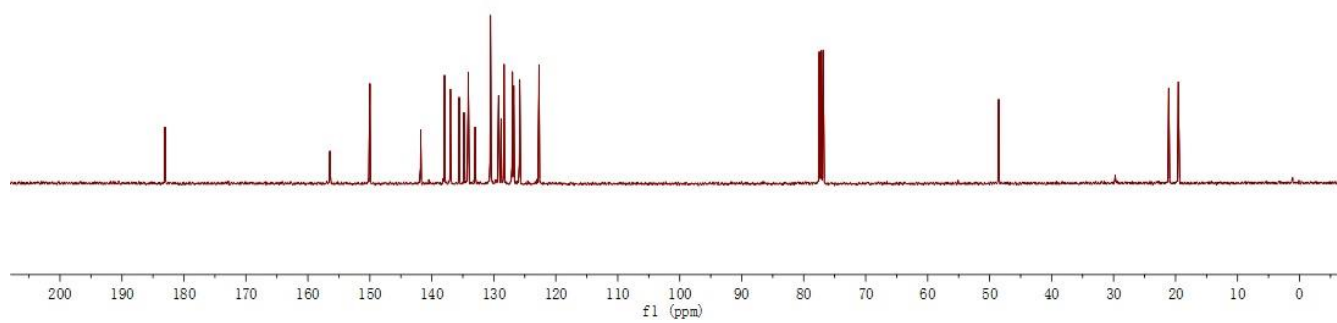
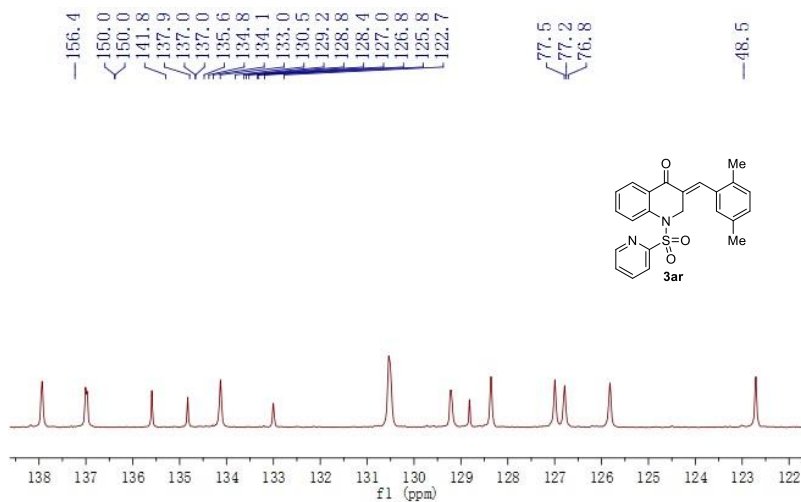
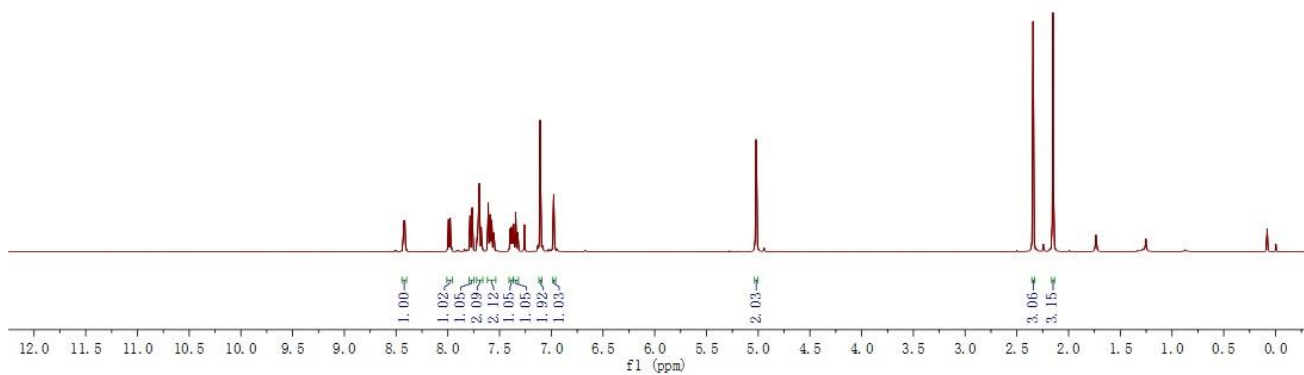
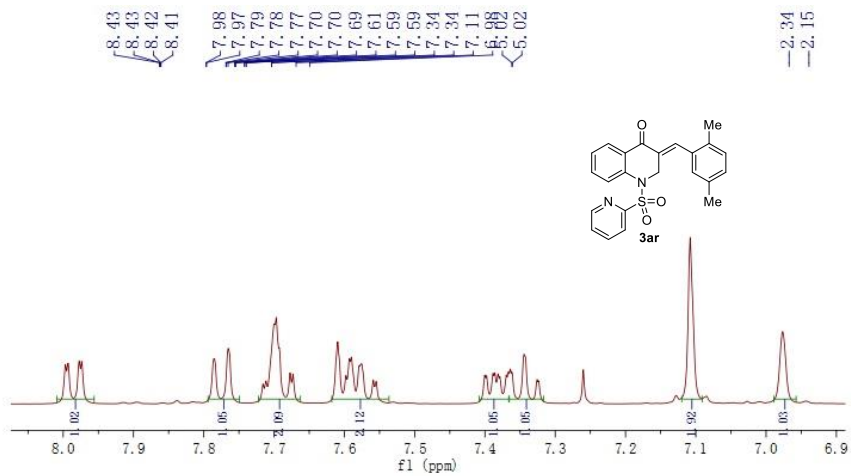


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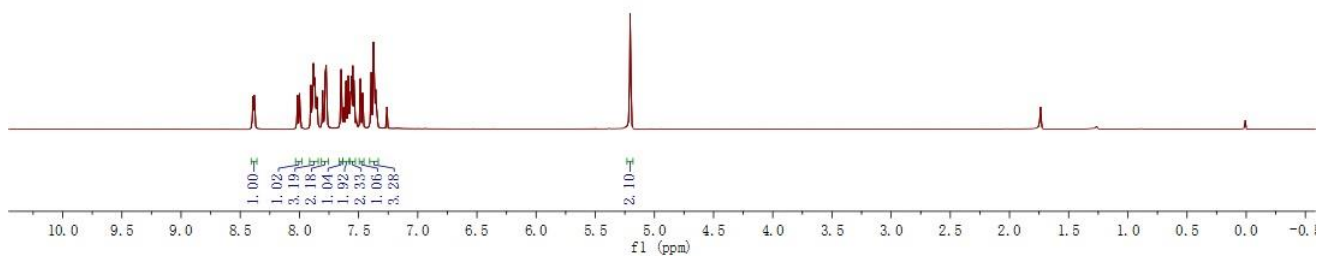
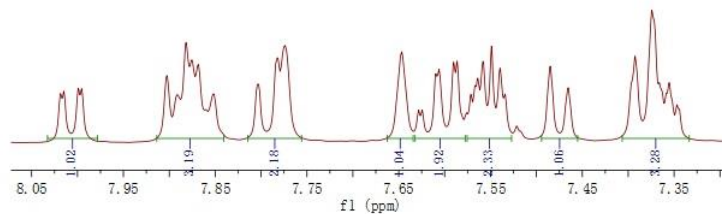
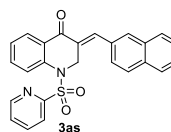


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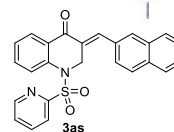
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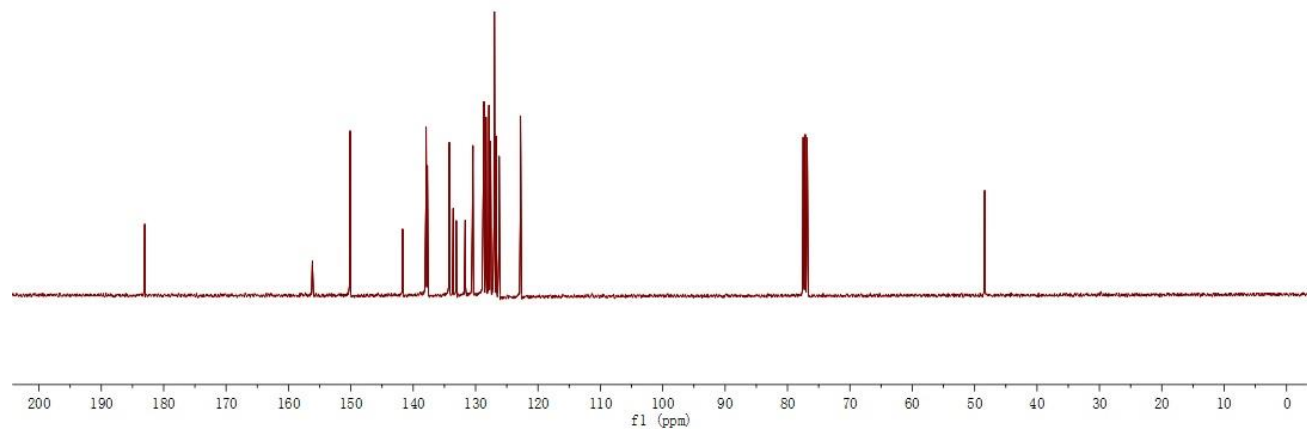
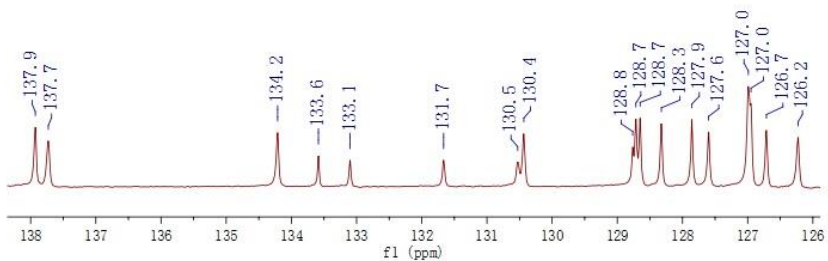
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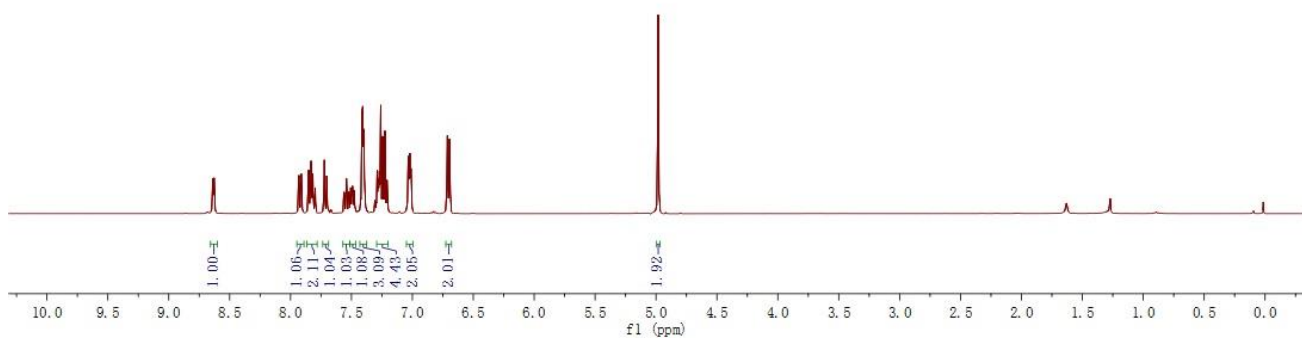
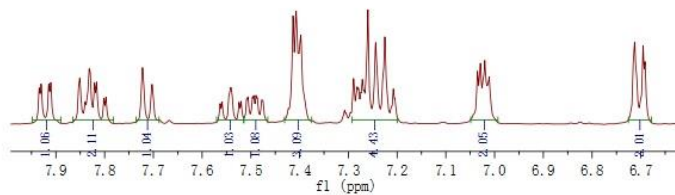
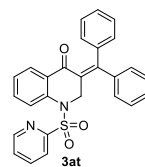
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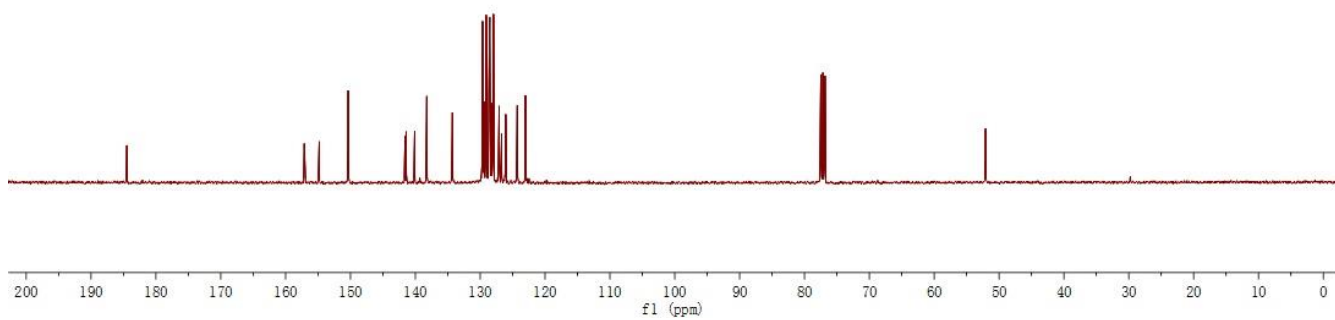
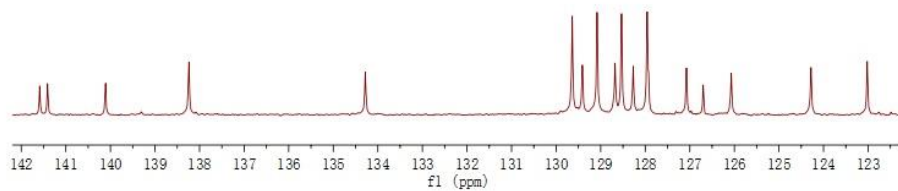
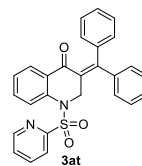


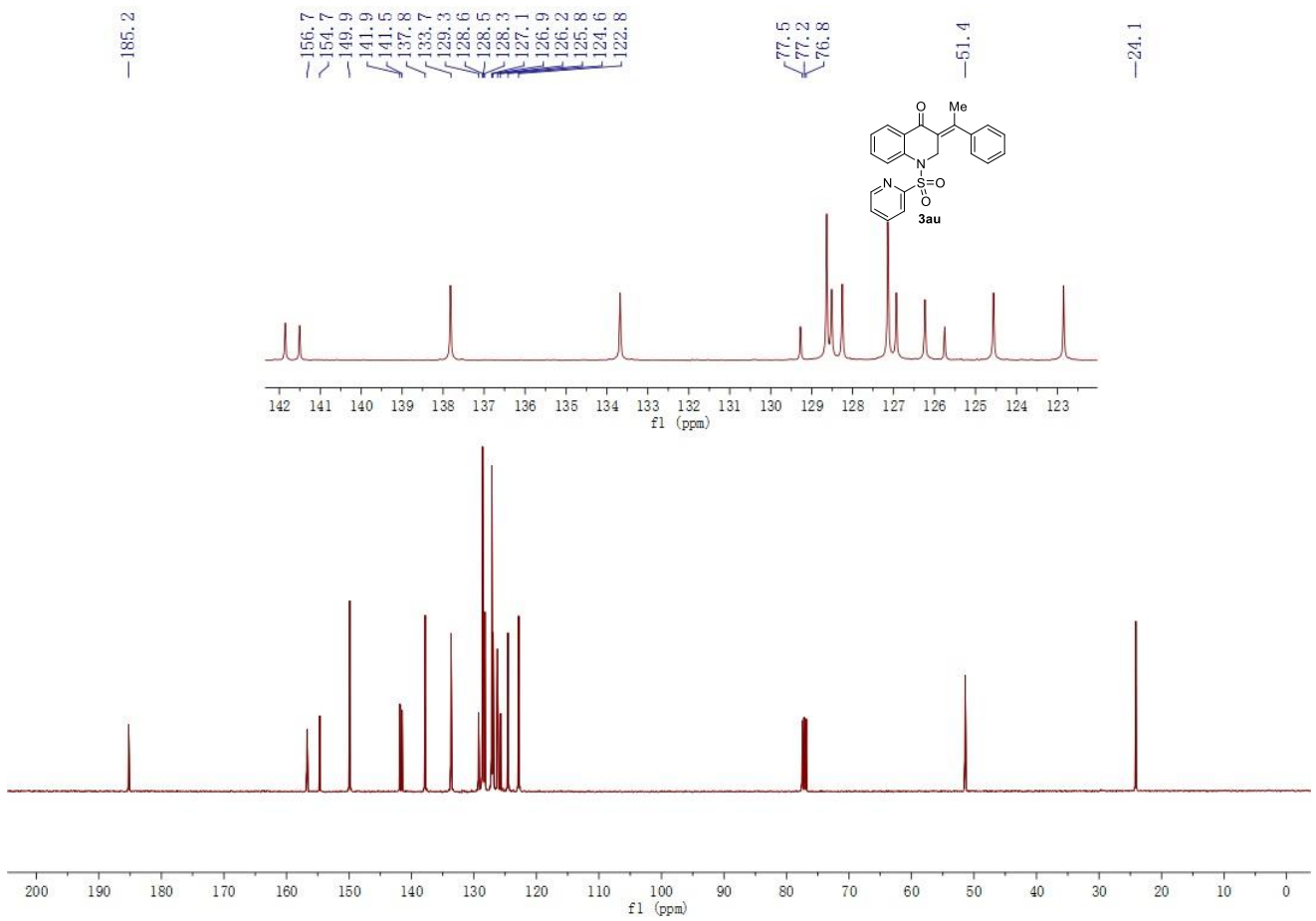
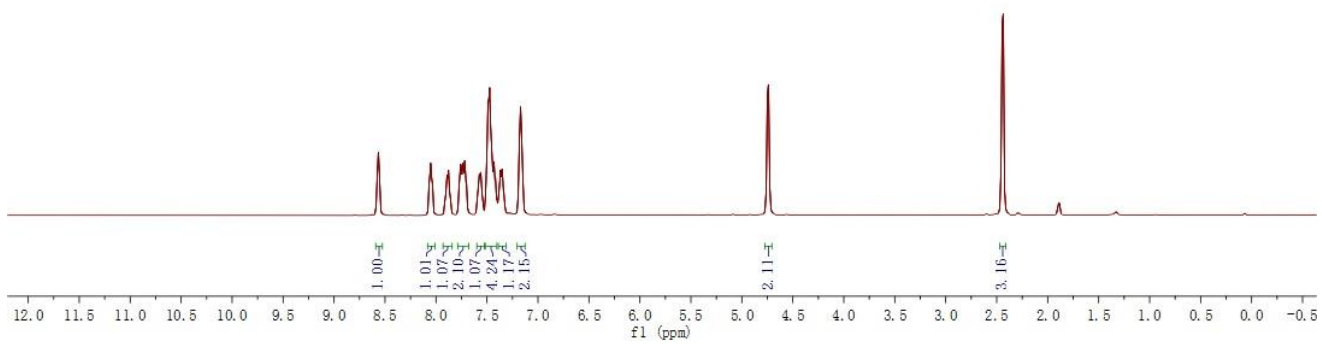
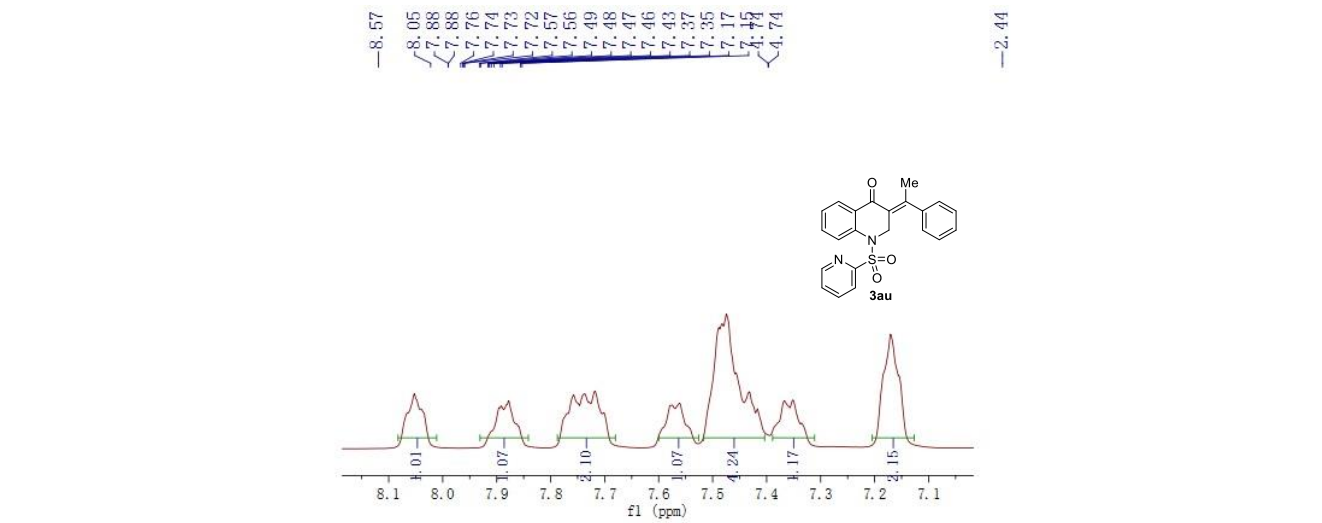
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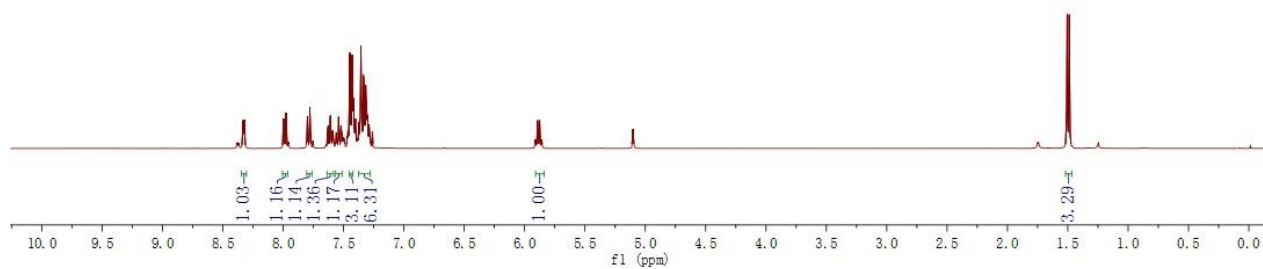
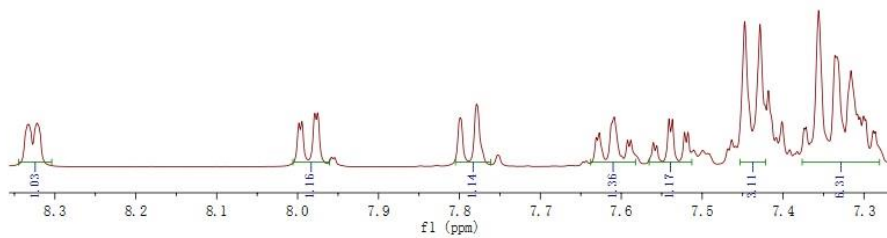
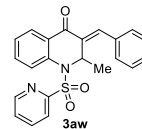
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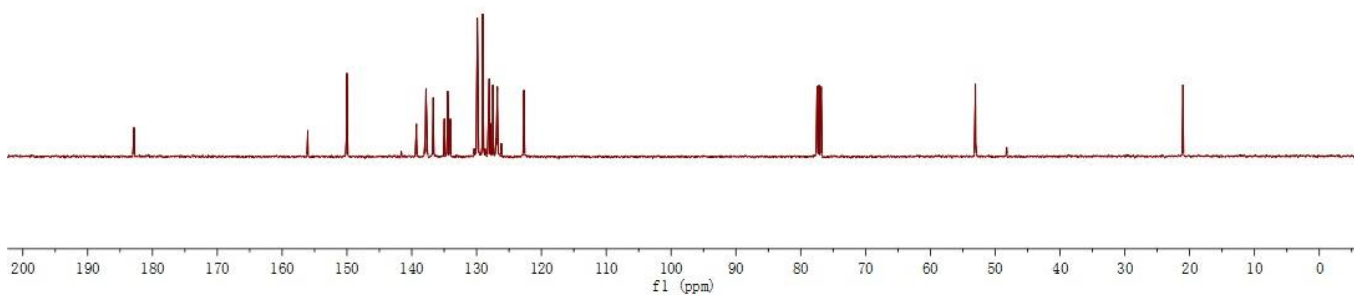
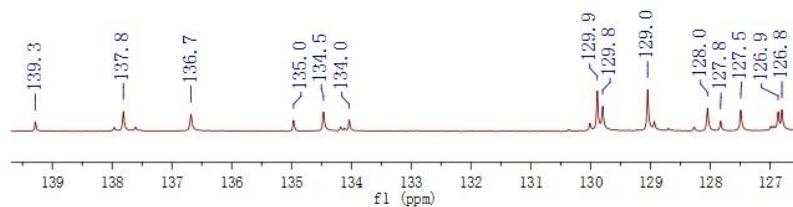
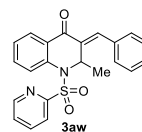


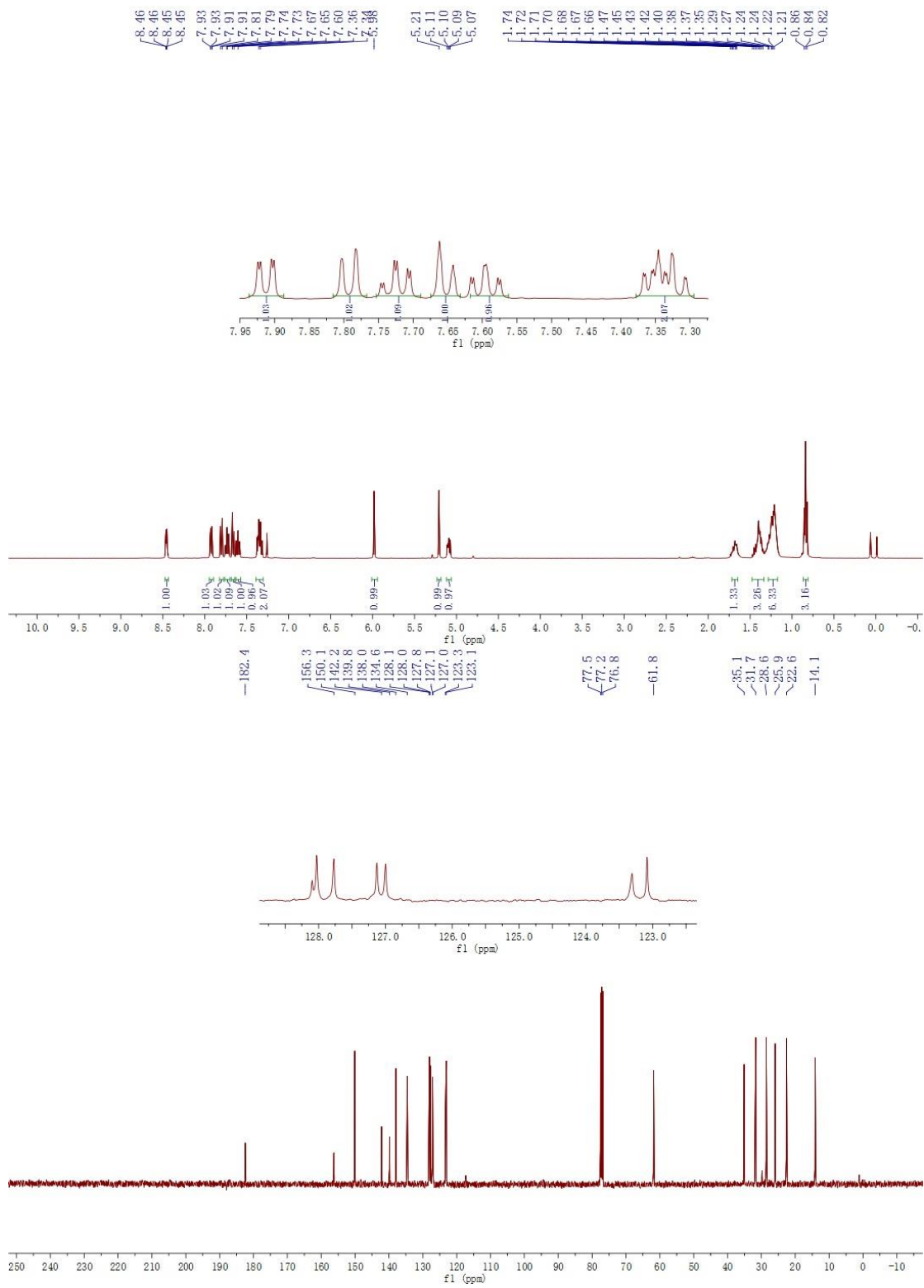


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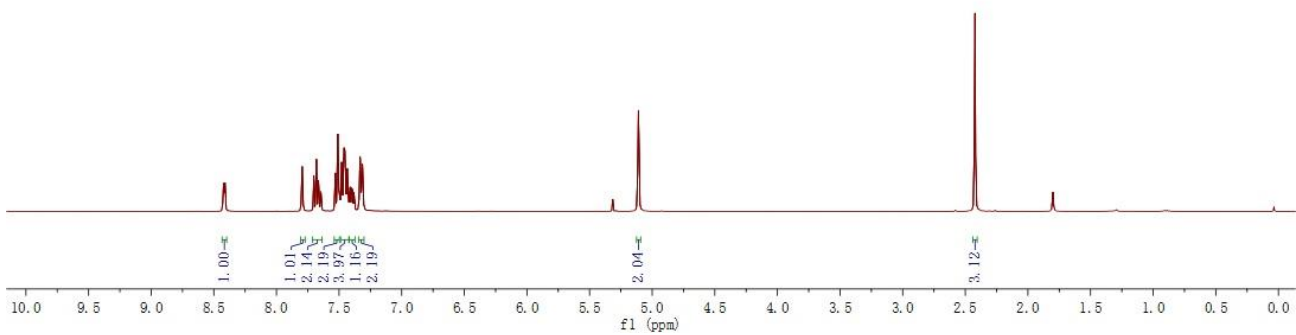
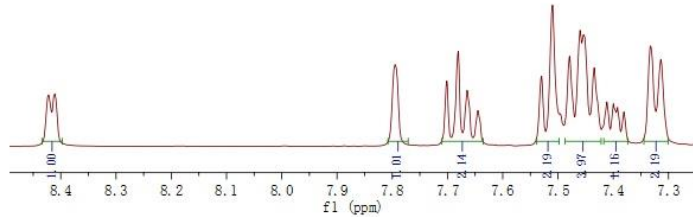
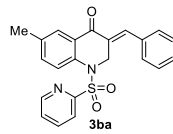




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-2.42



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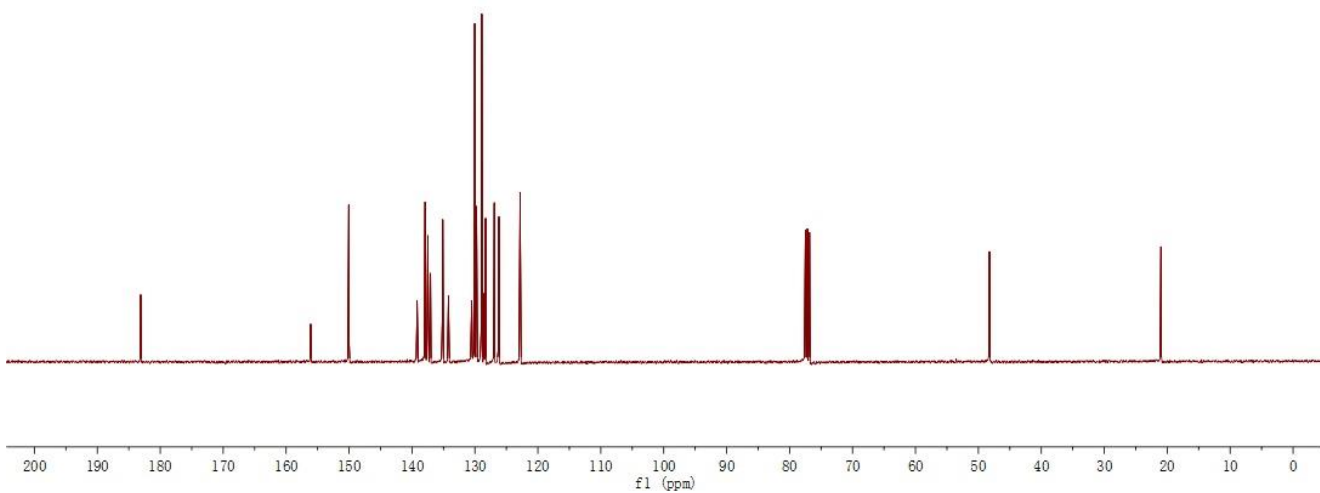
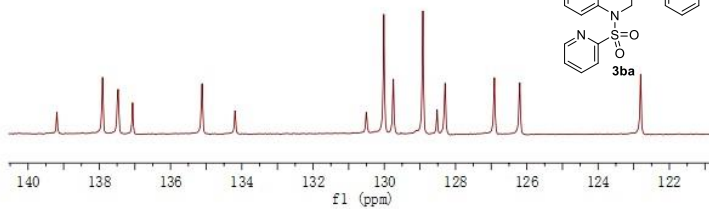
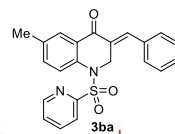
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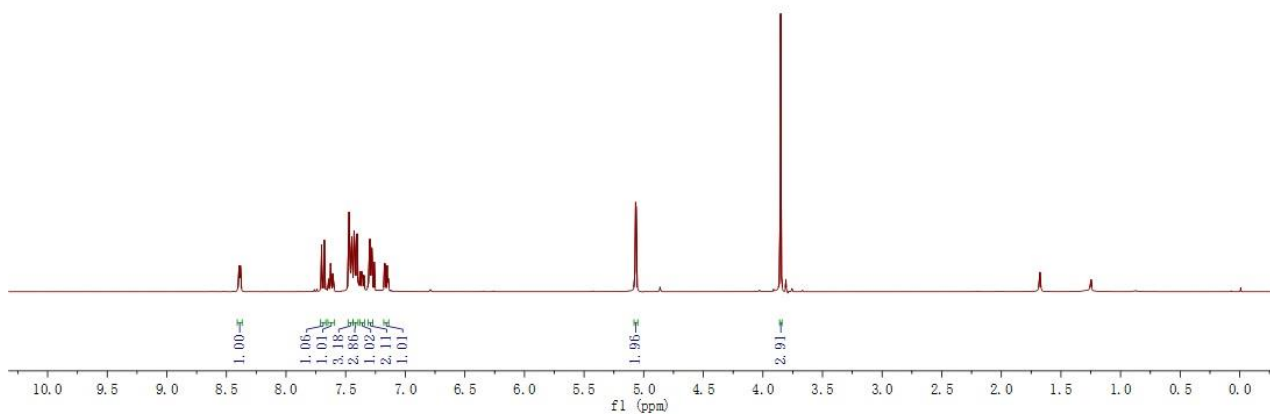
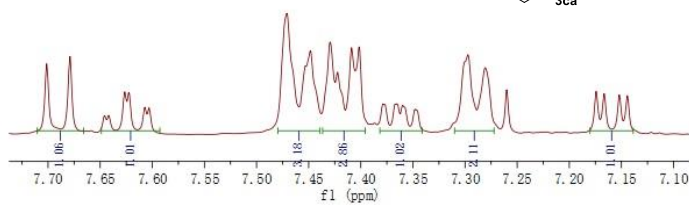
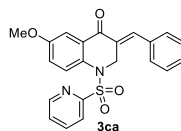
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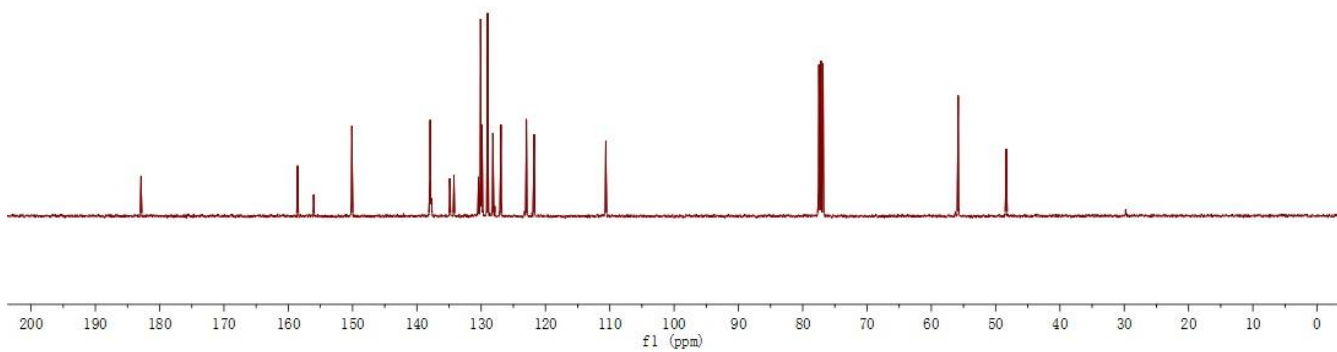
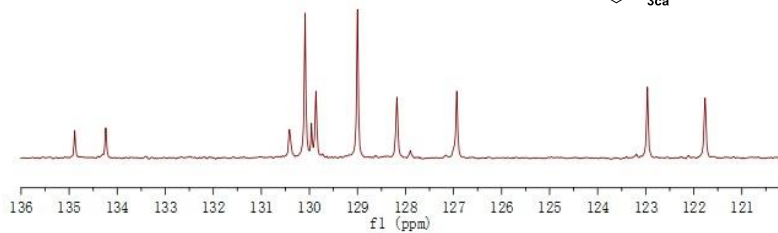
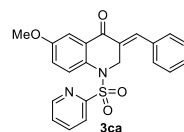
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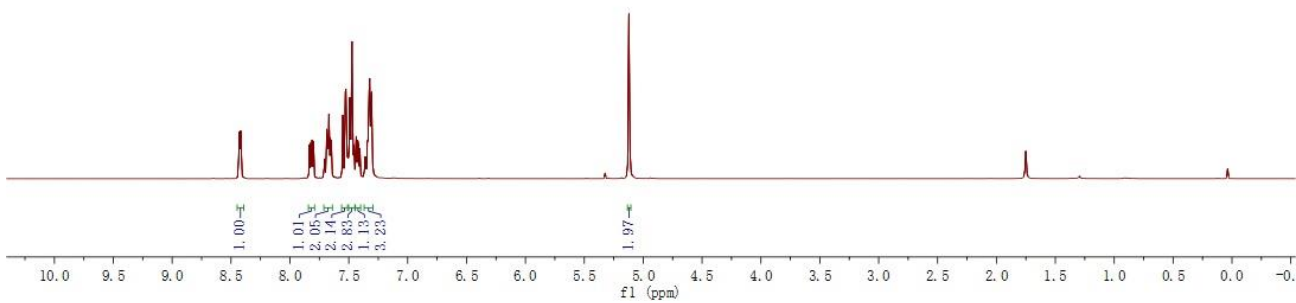
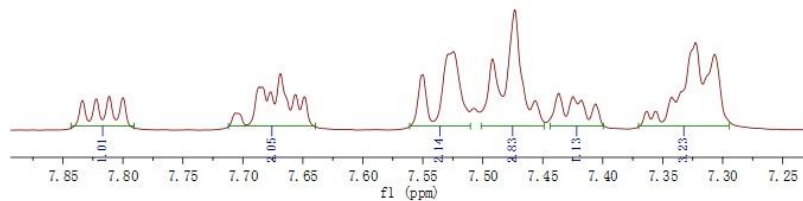
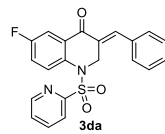
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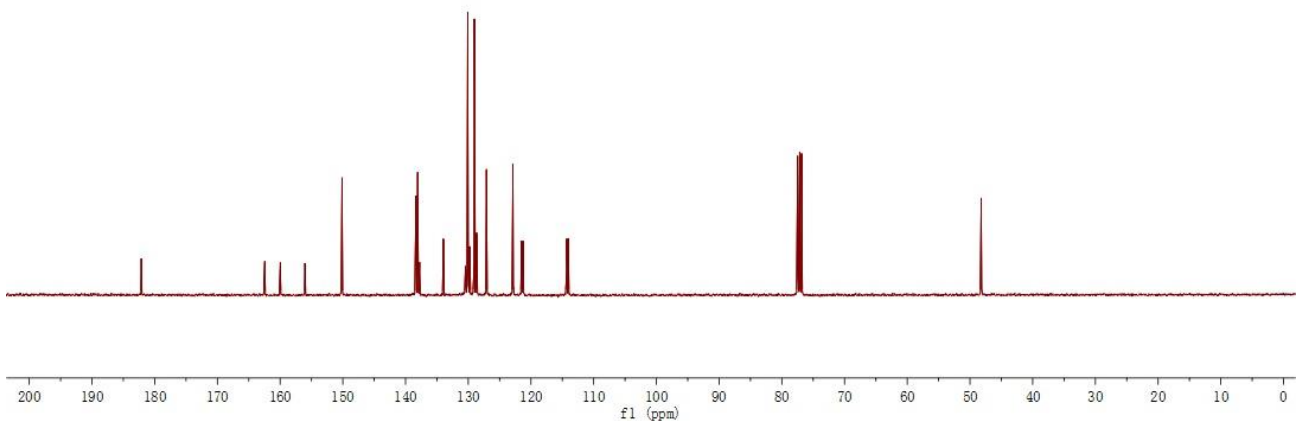
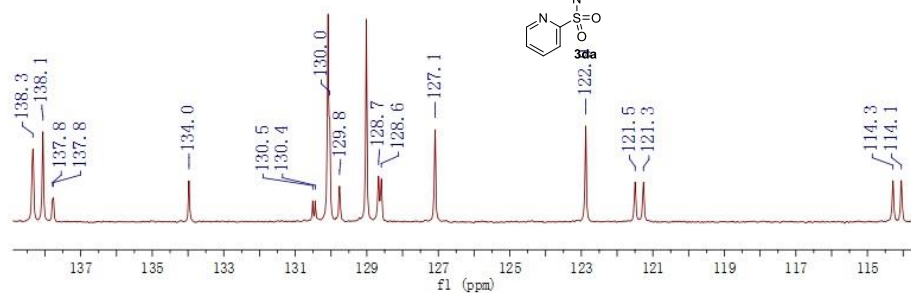
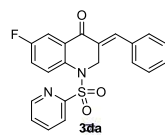
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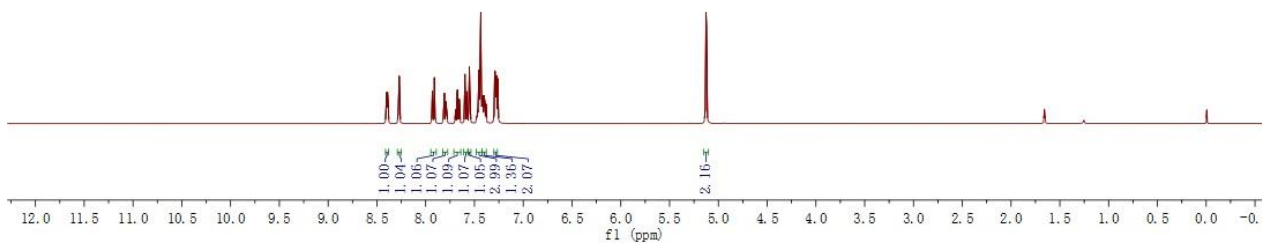
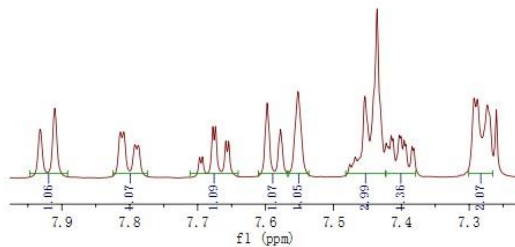
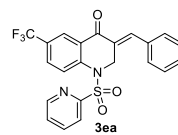
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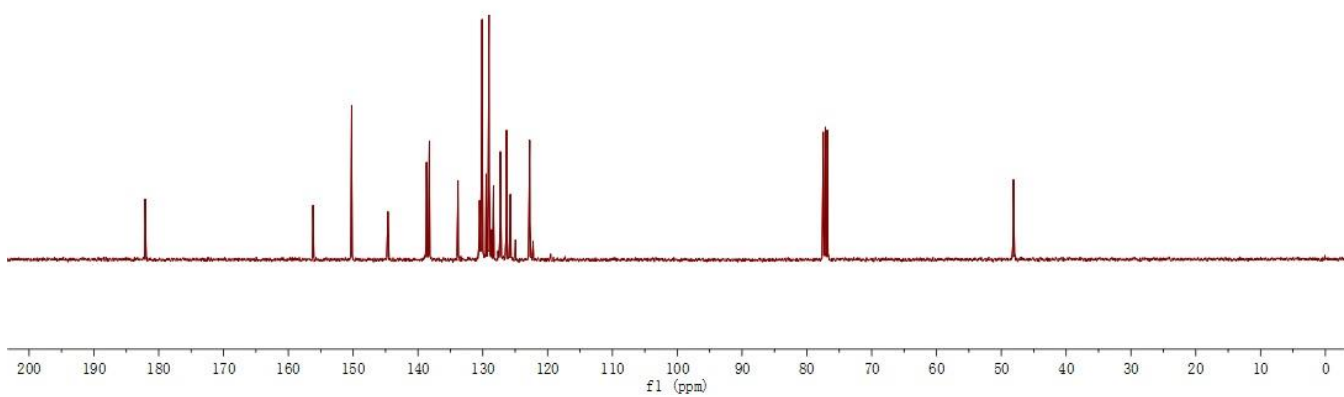
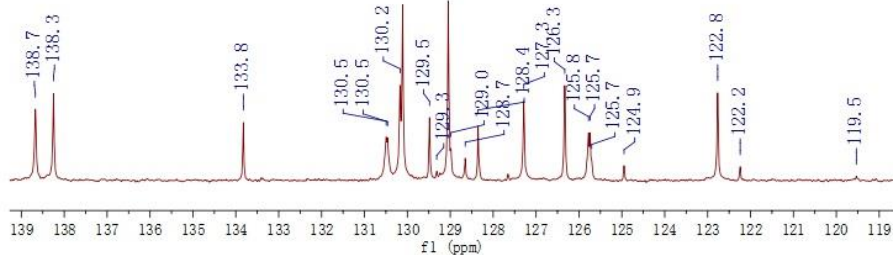
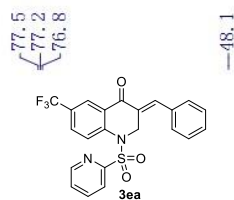
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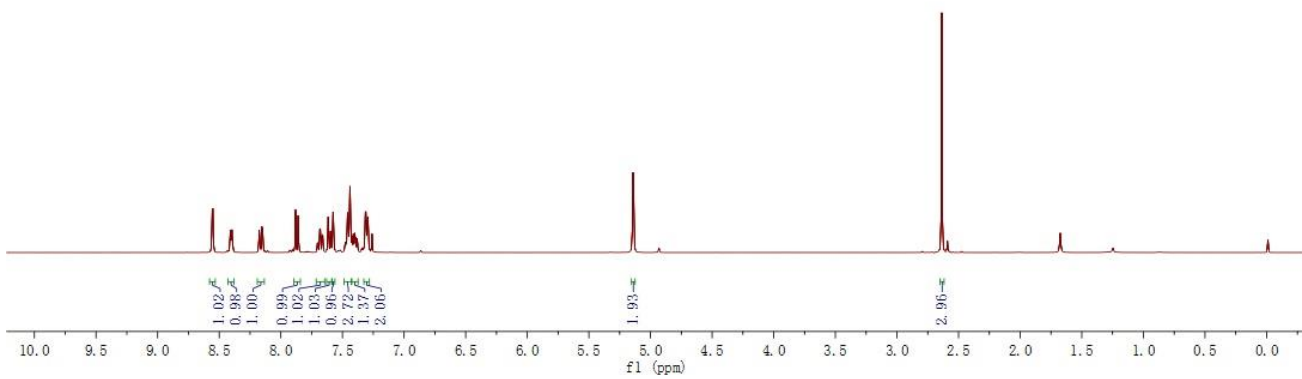
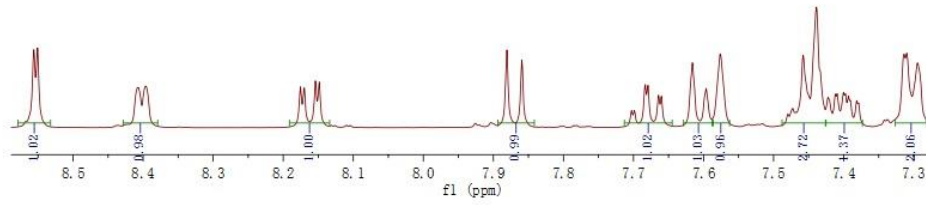
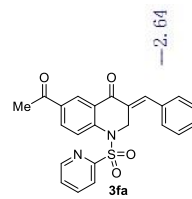
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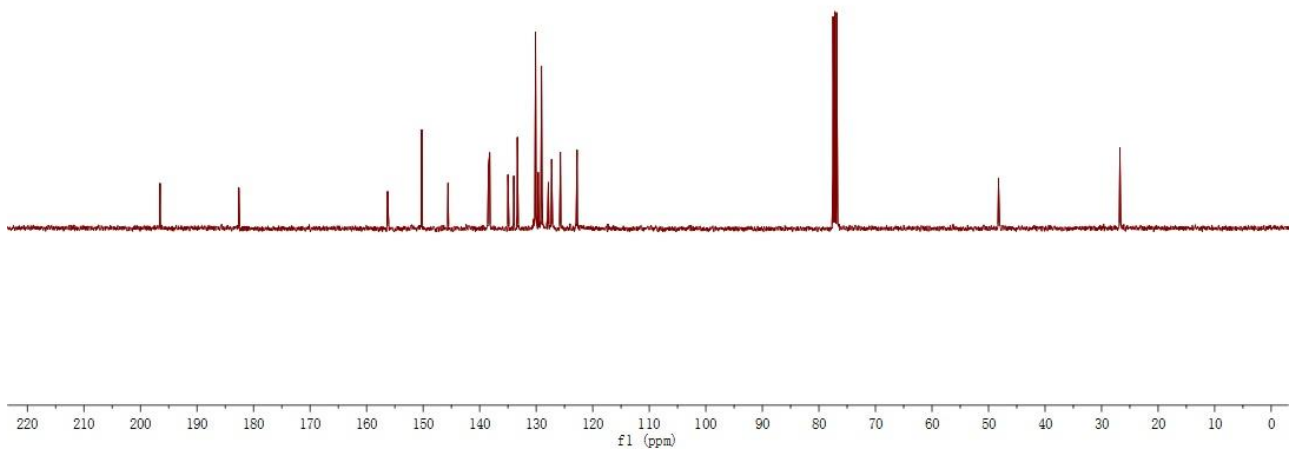
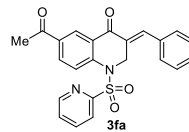
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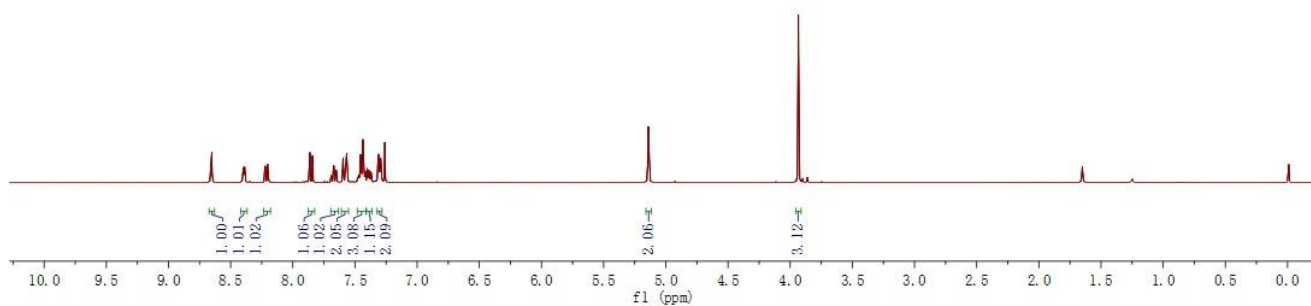
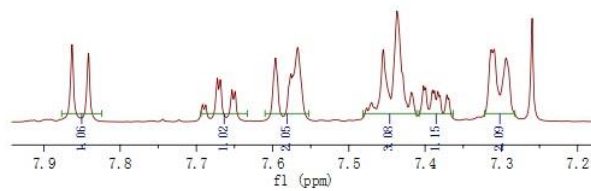
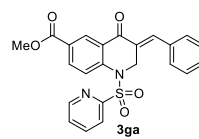
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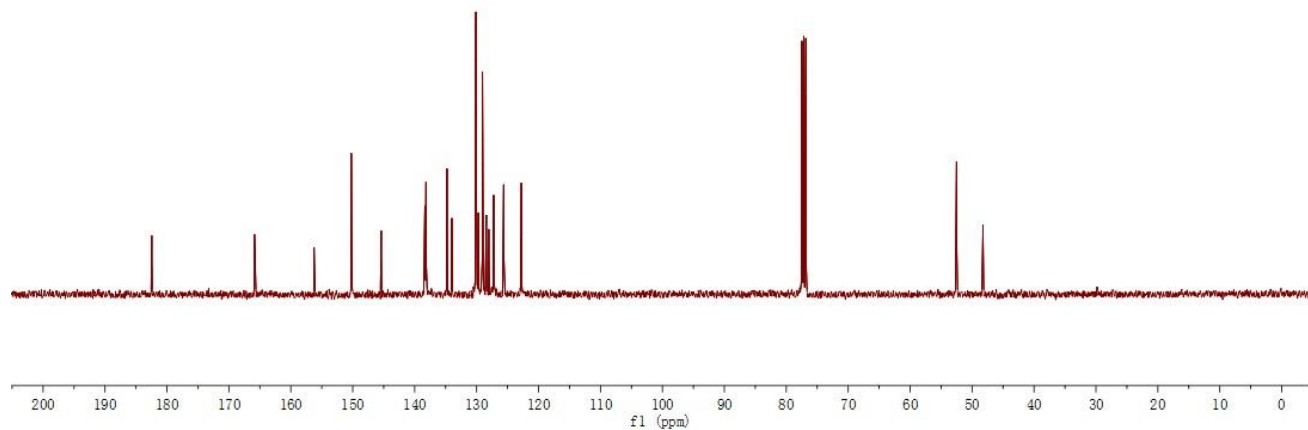
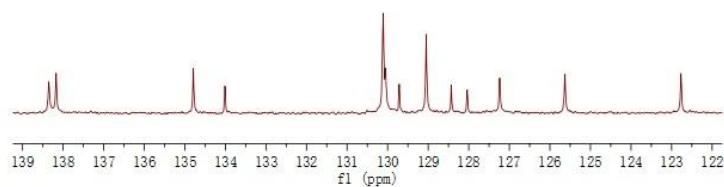
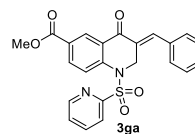
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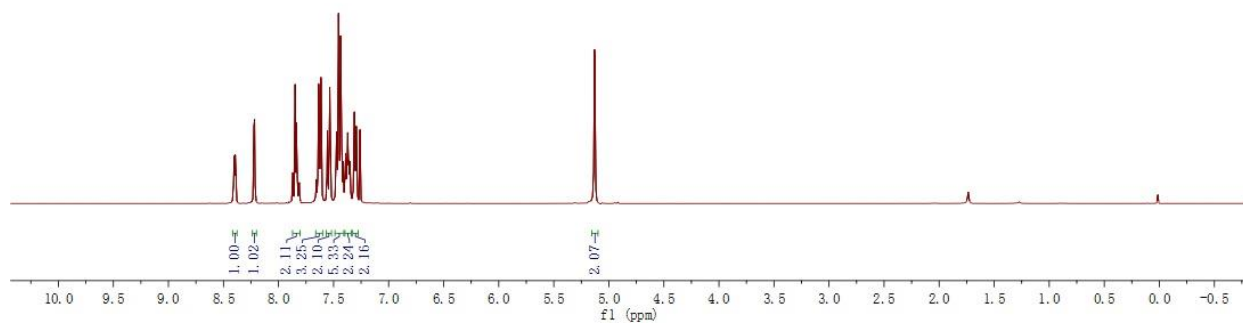
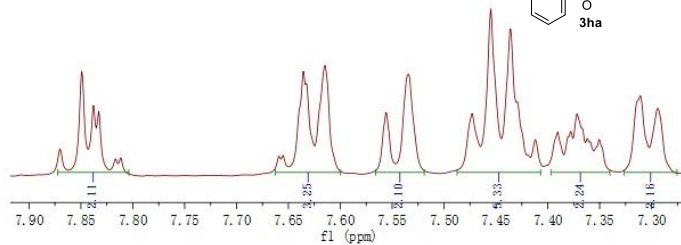
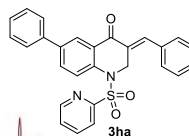
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77.5
77.2
76.8

-52.5
-48.2



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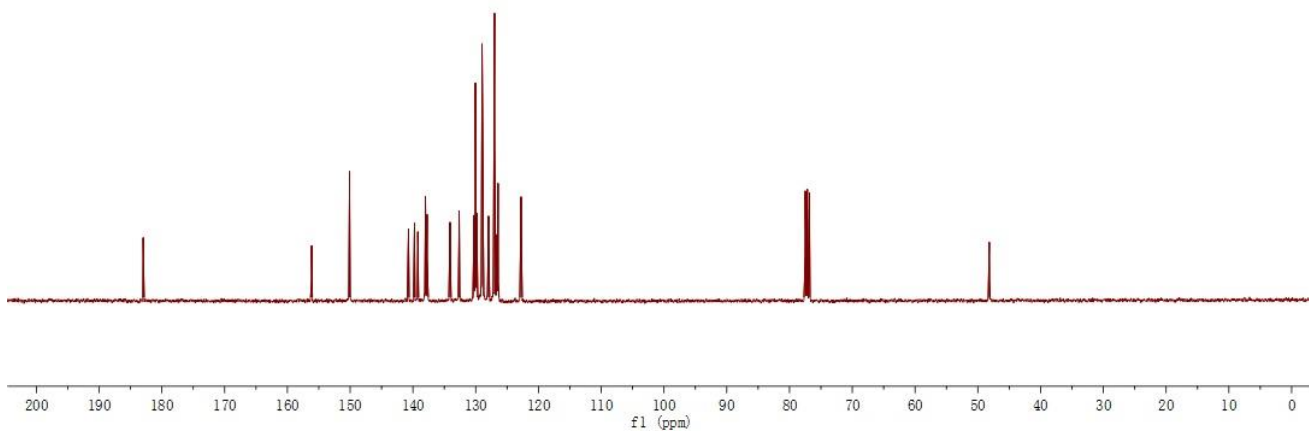
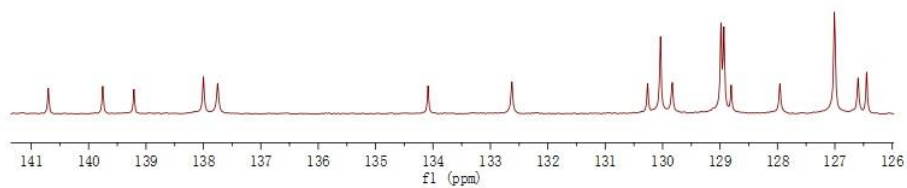
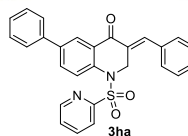
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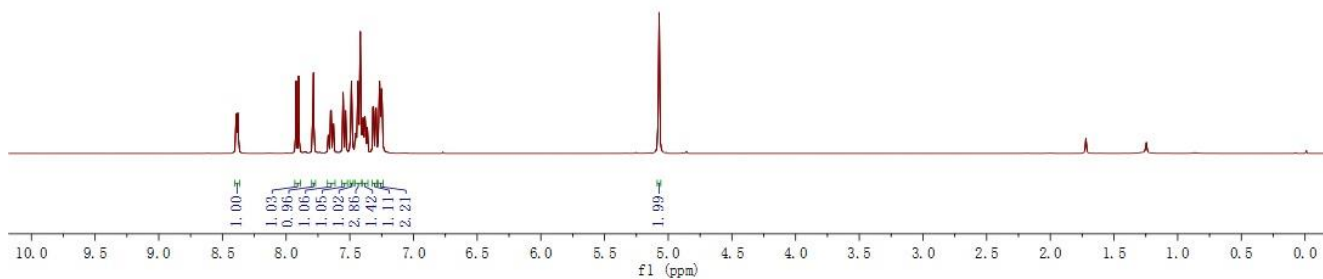
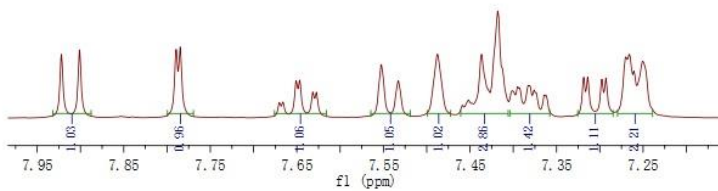
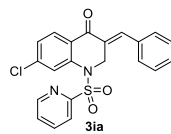
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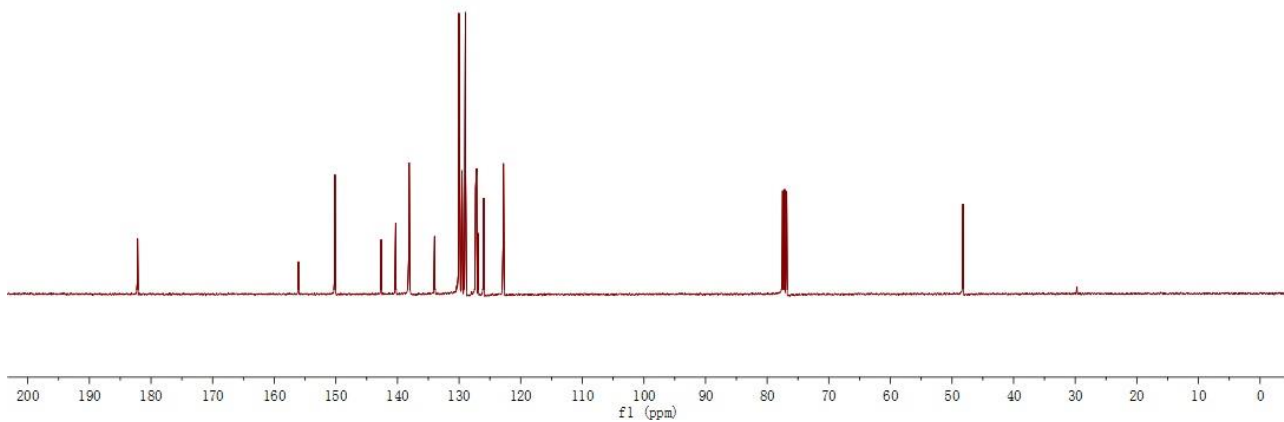
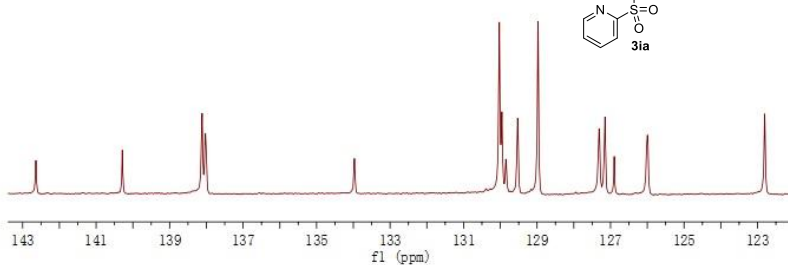
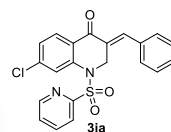


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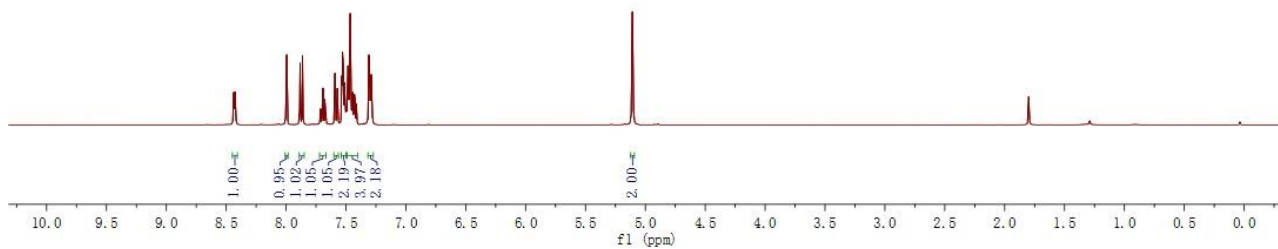
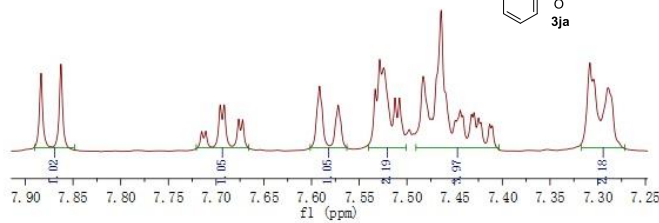
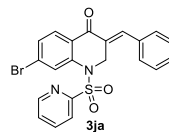
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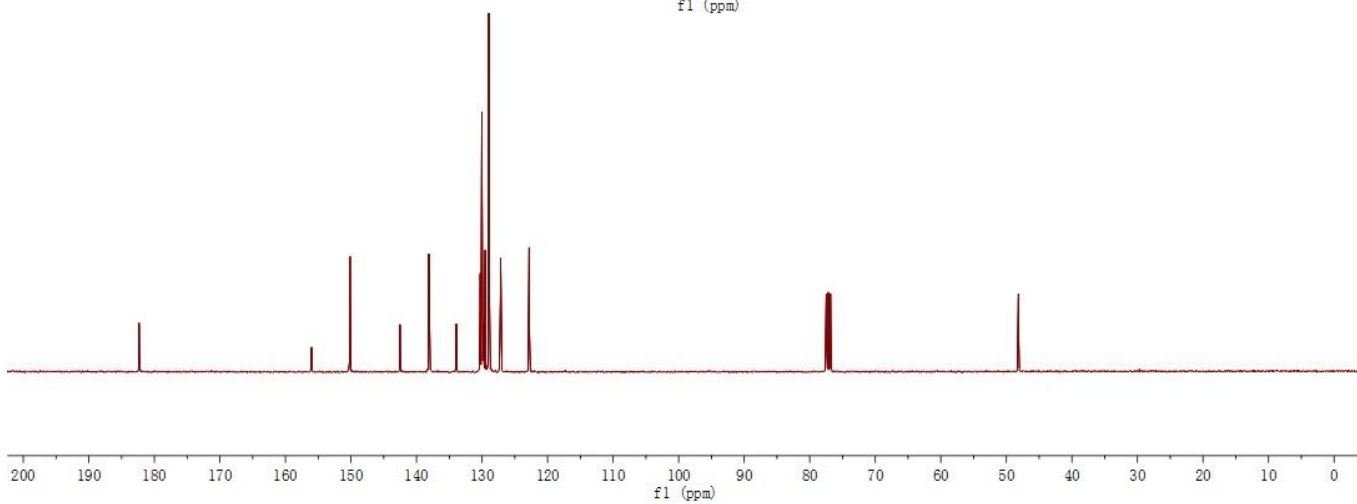
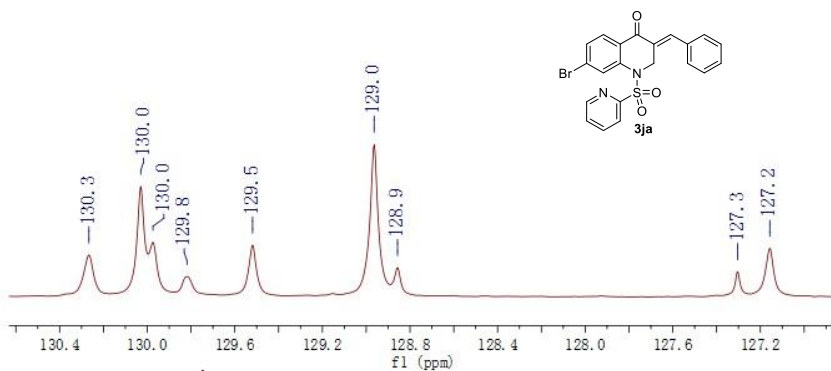
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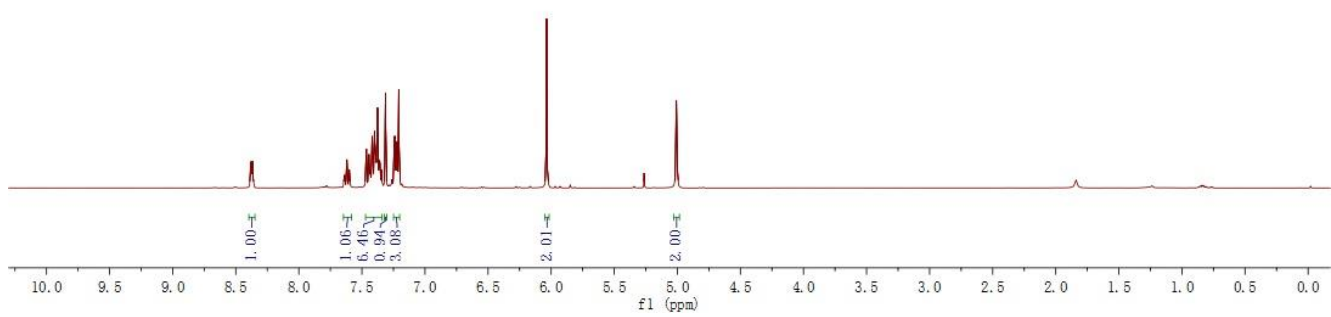
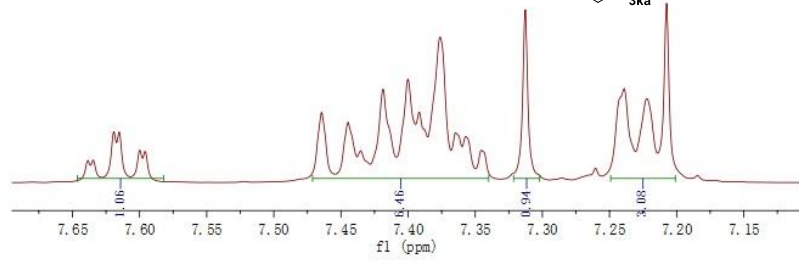
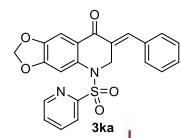
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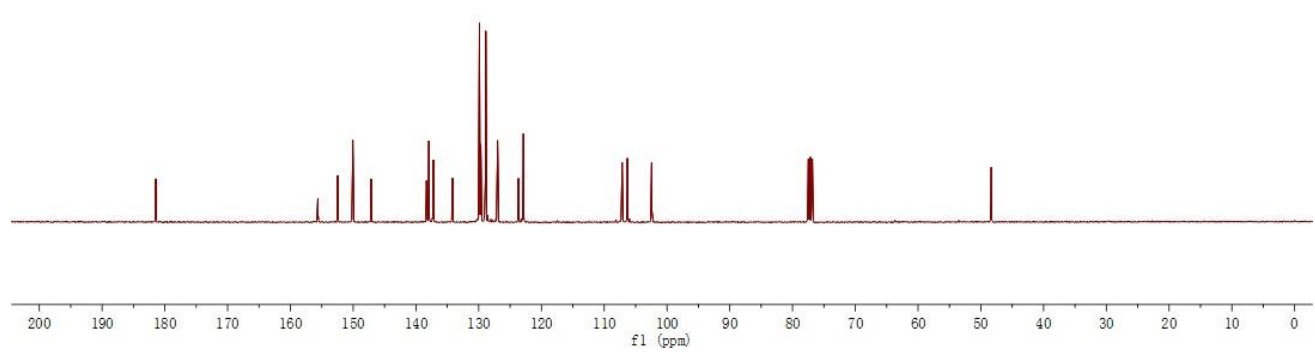
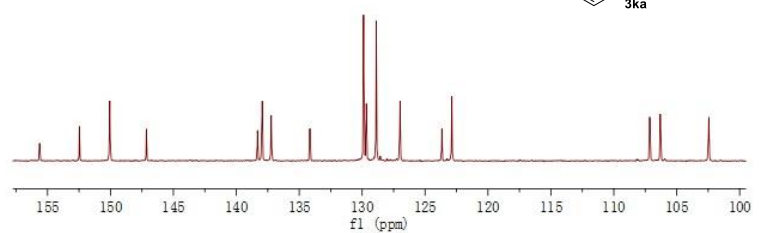
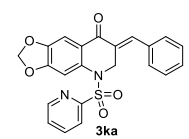
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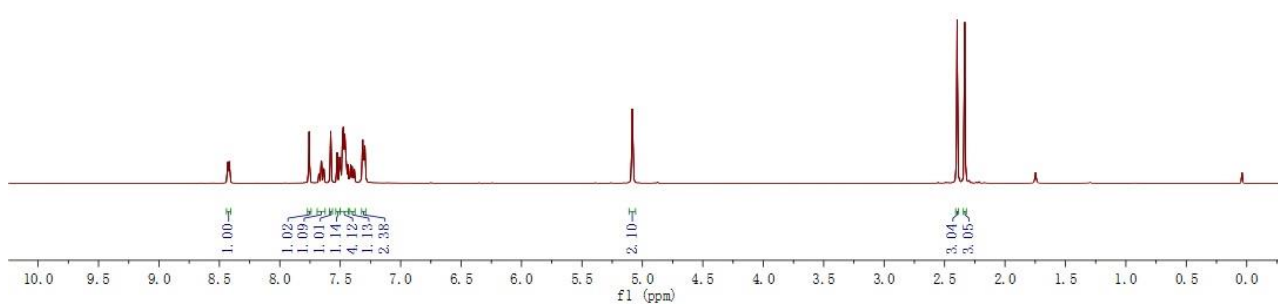
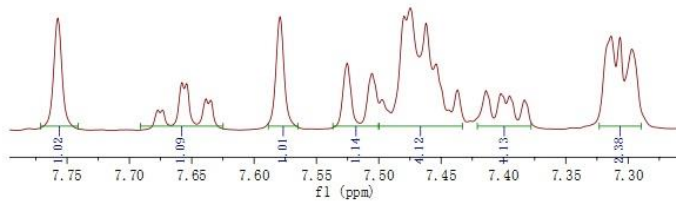
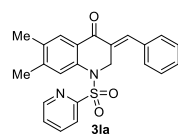


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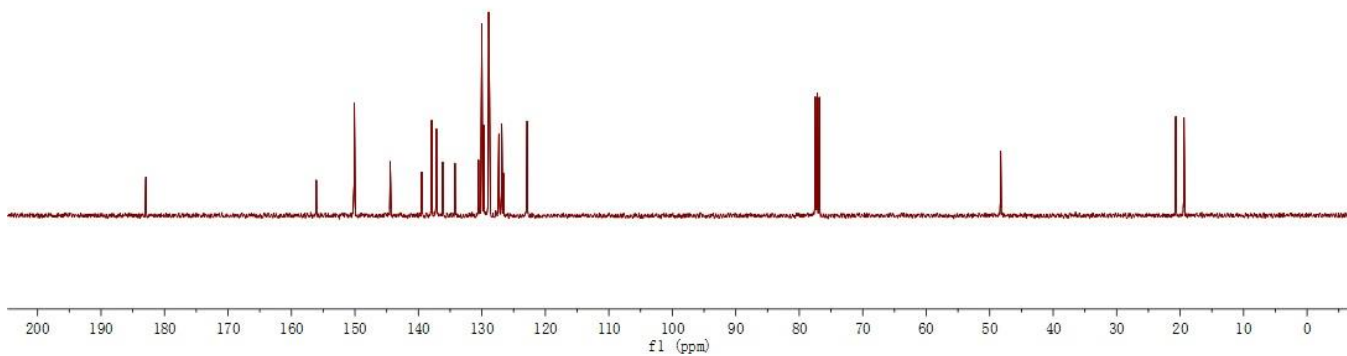
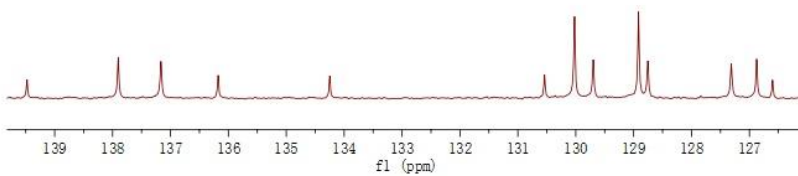
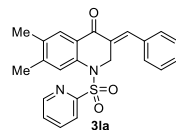
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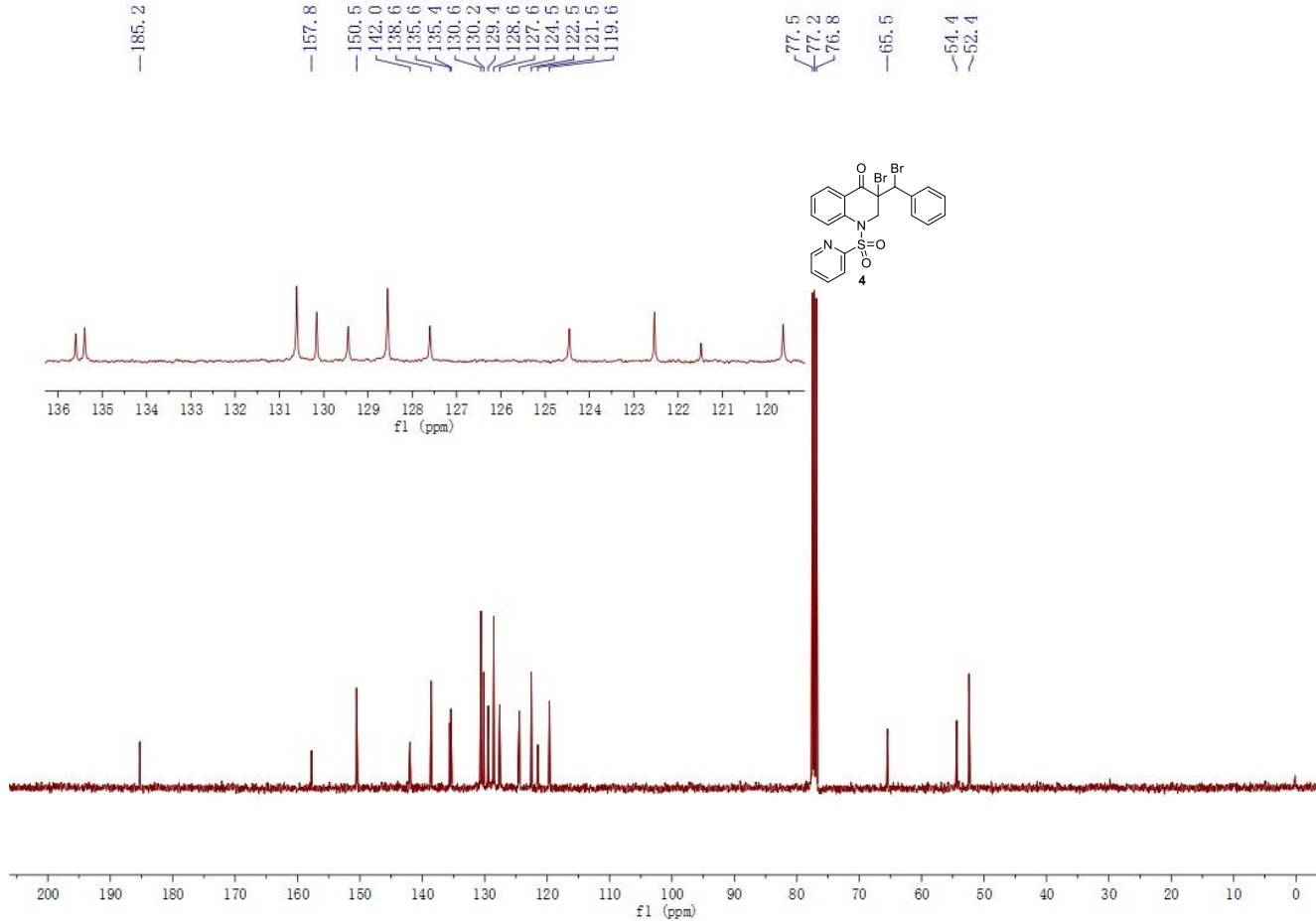
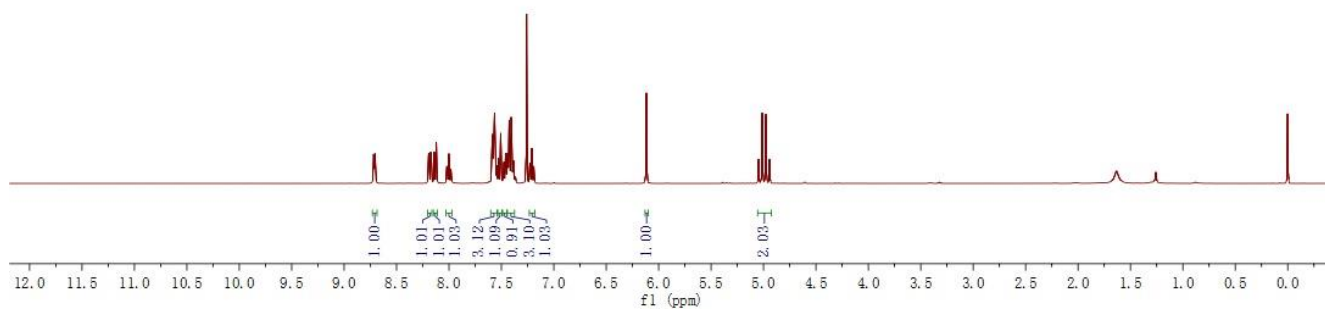
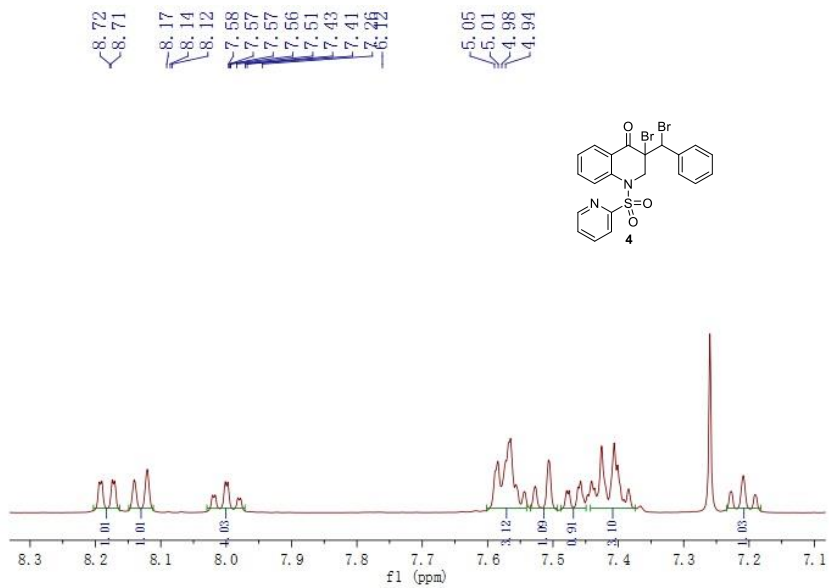
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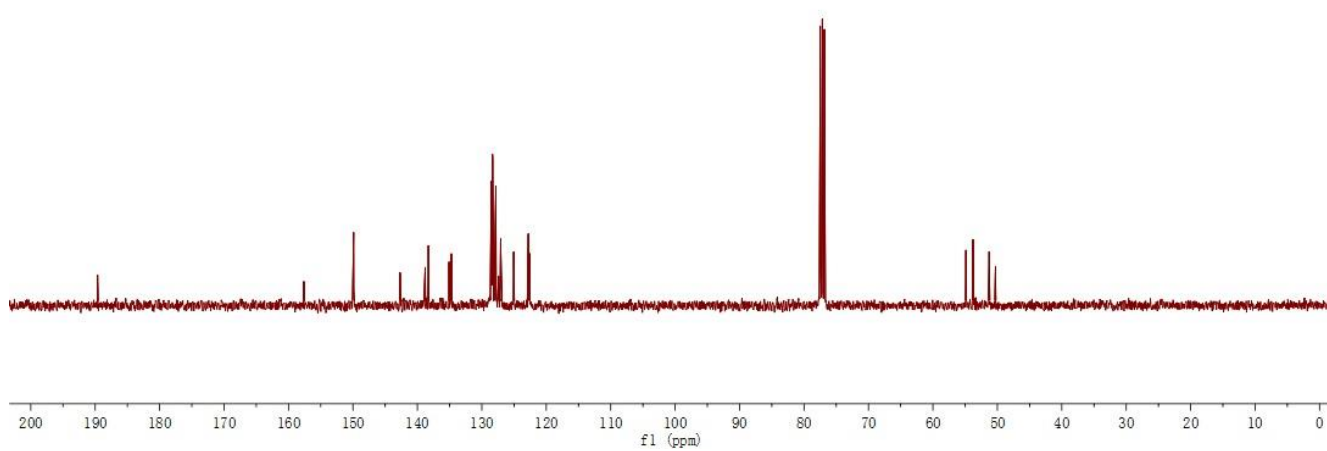
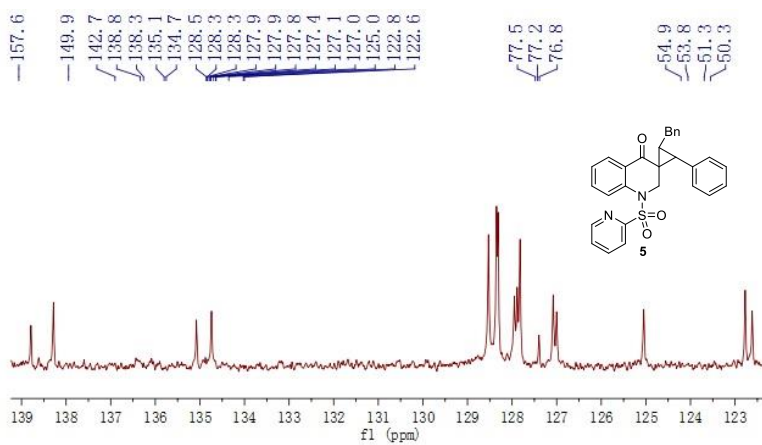
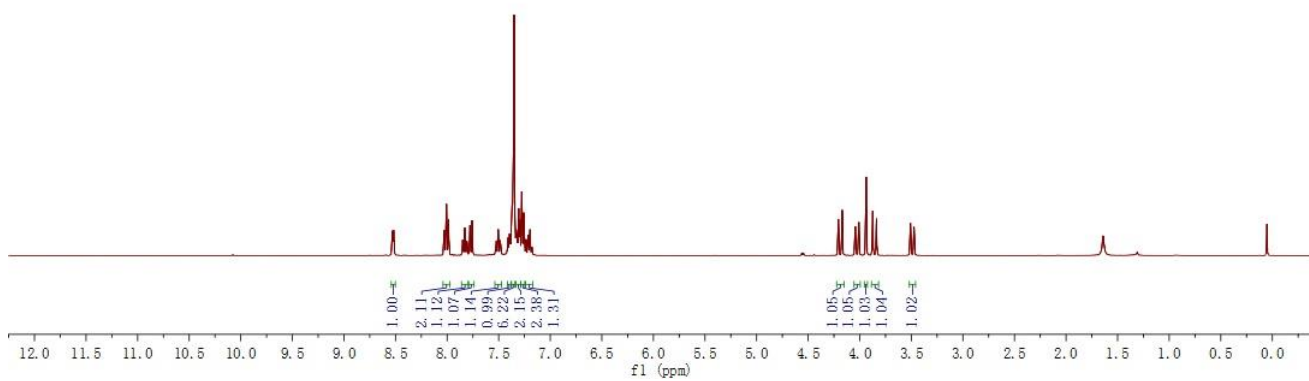
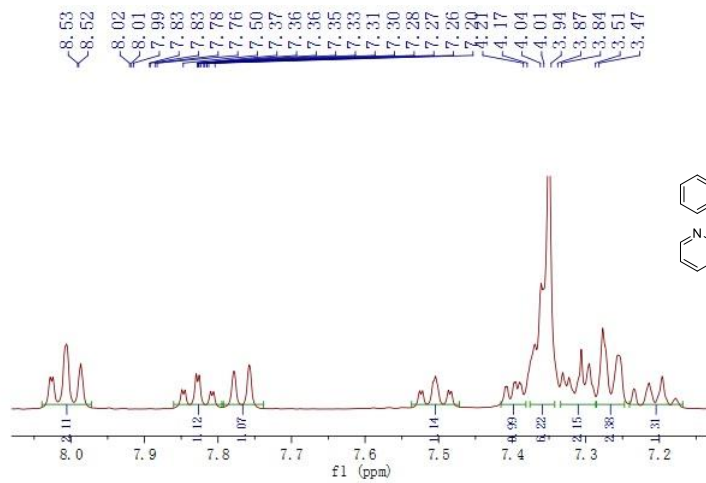
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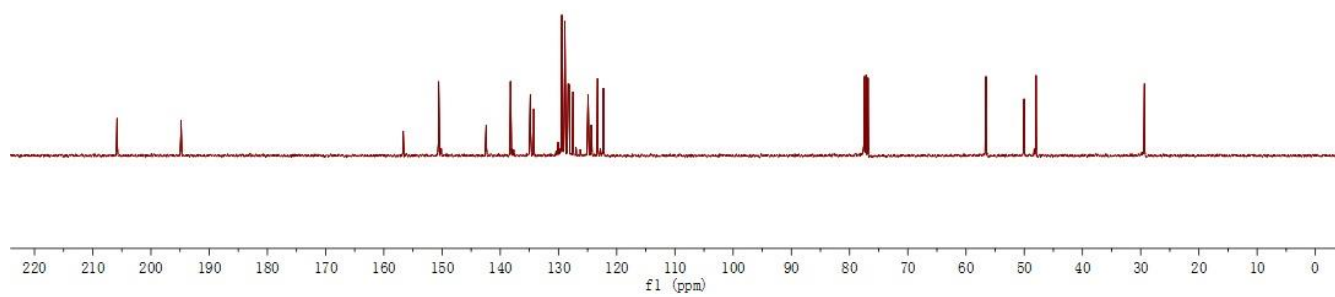
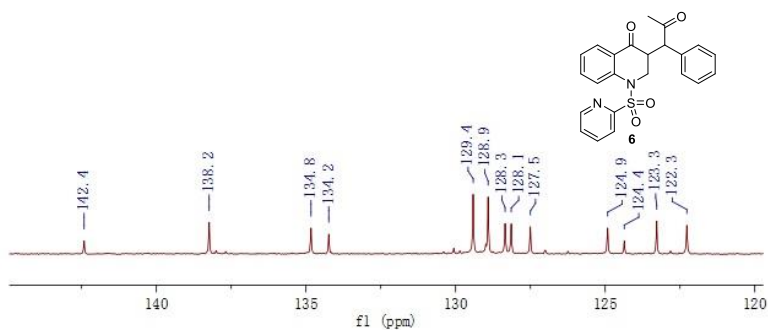
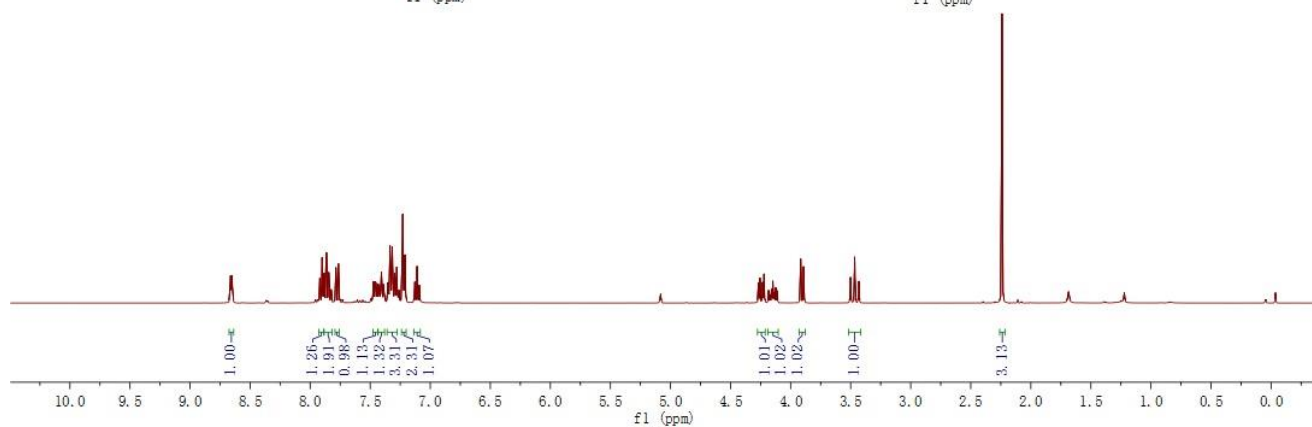
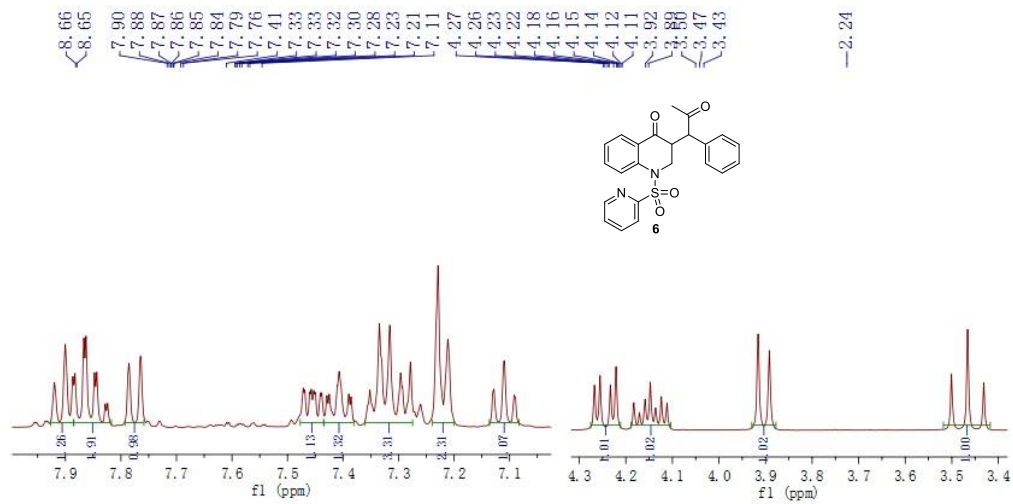
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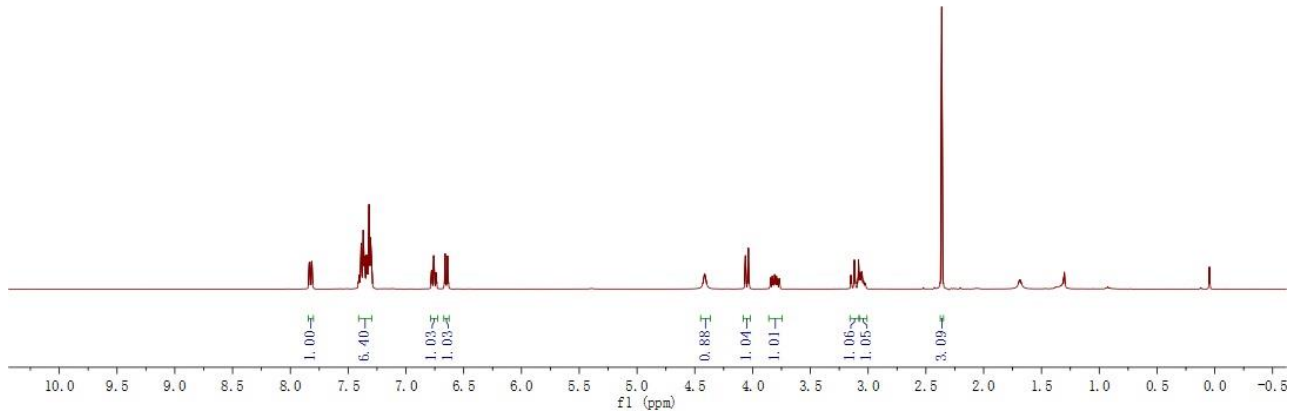
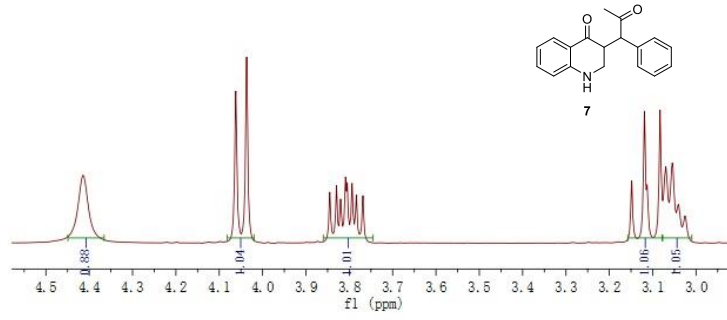






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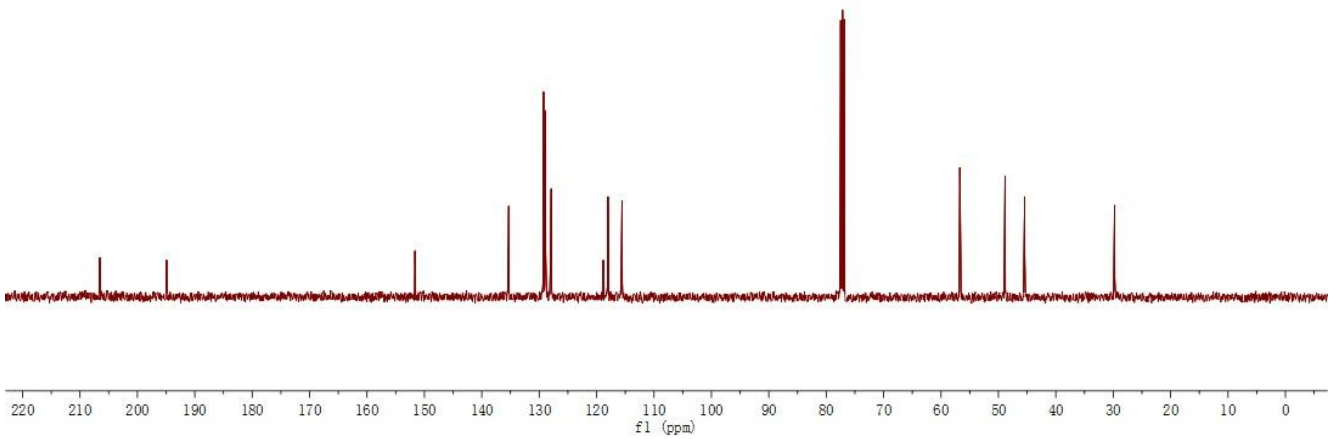
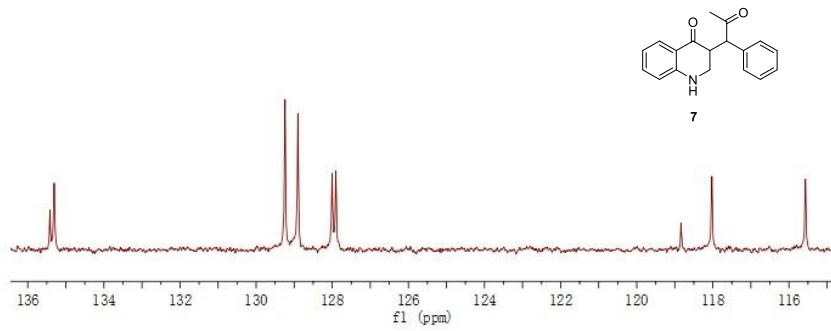
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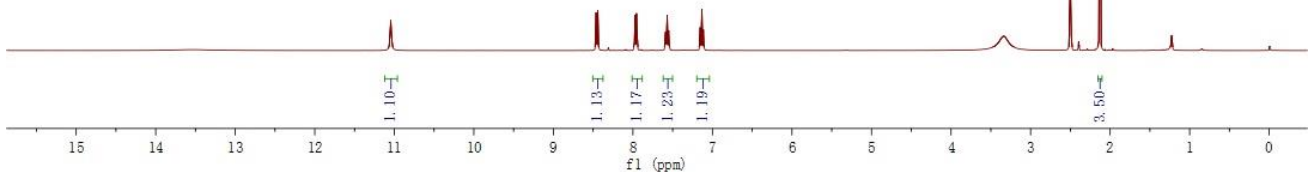
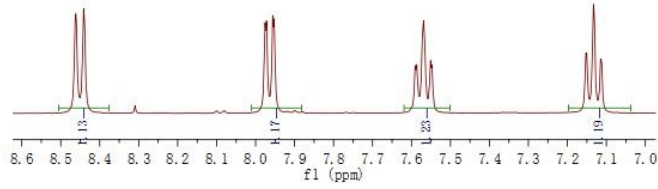
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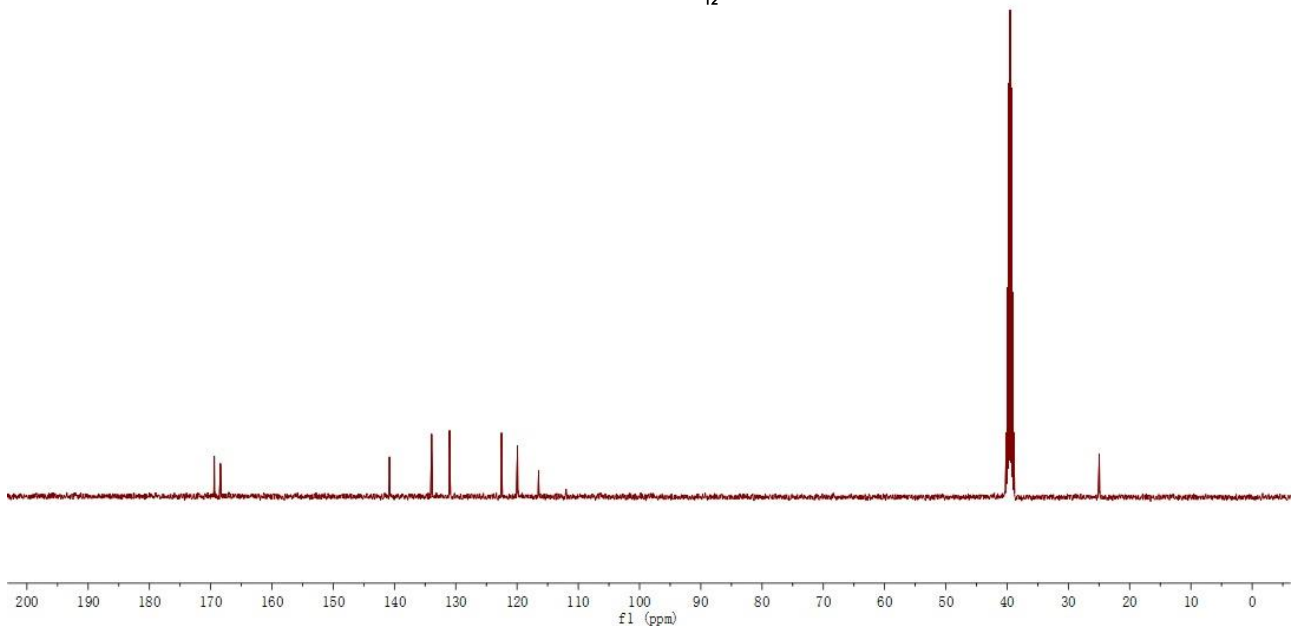
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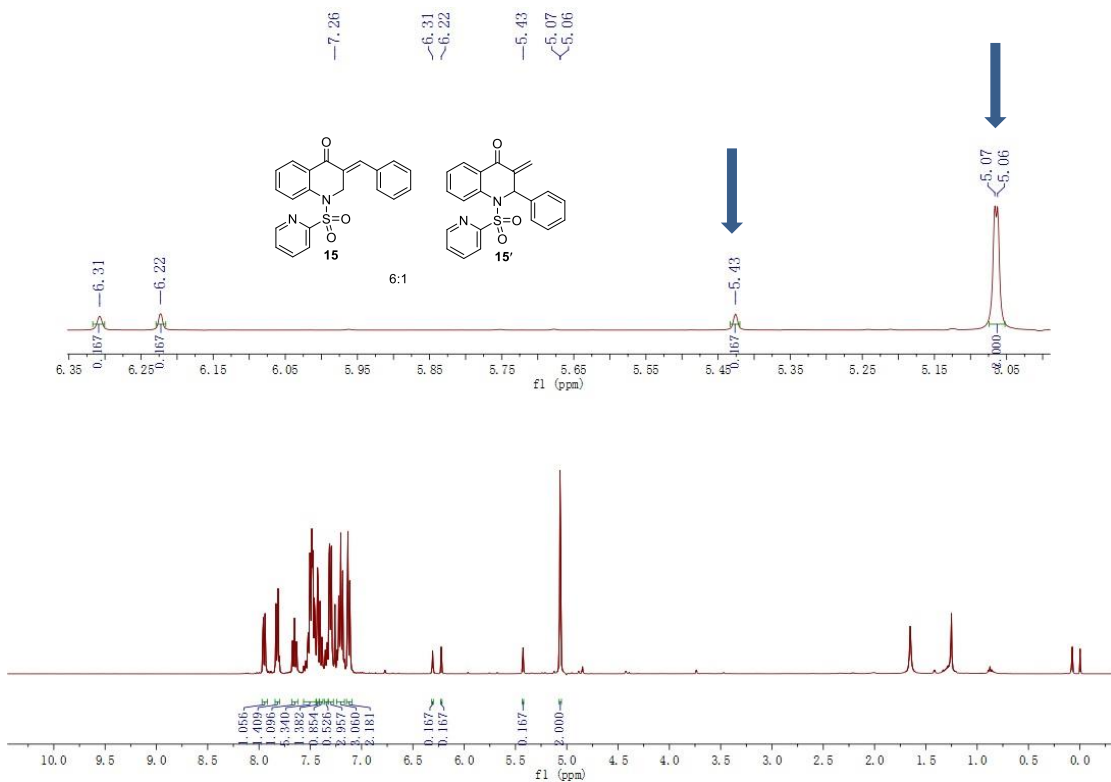
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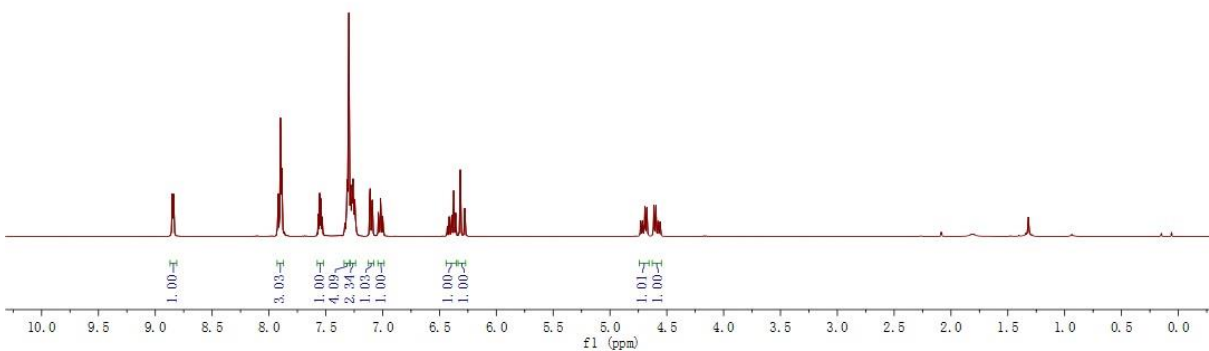
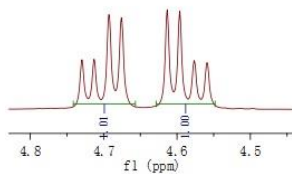
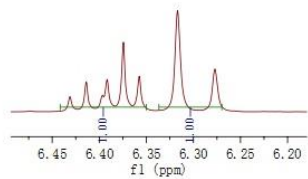
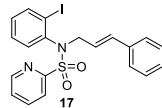
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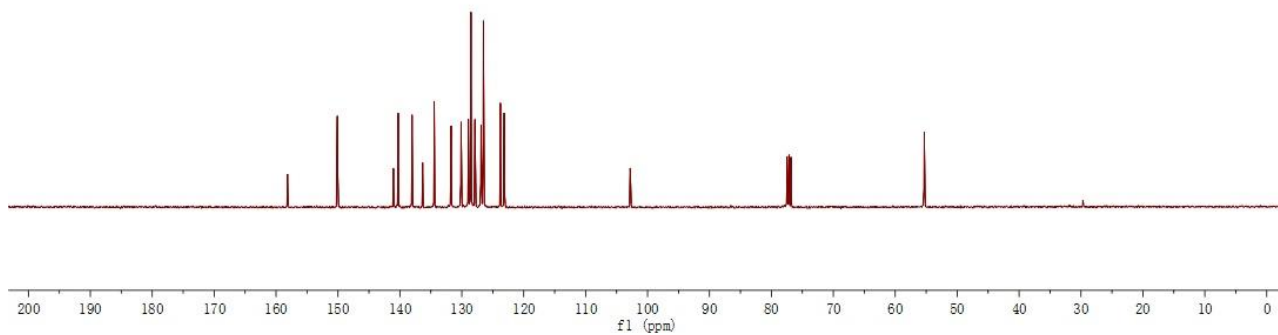
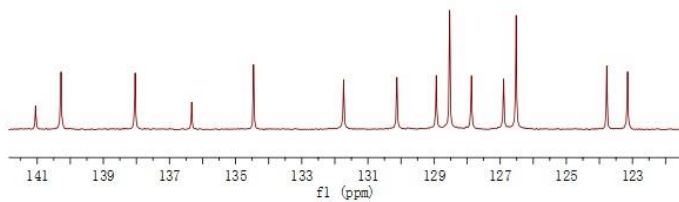
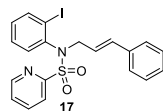
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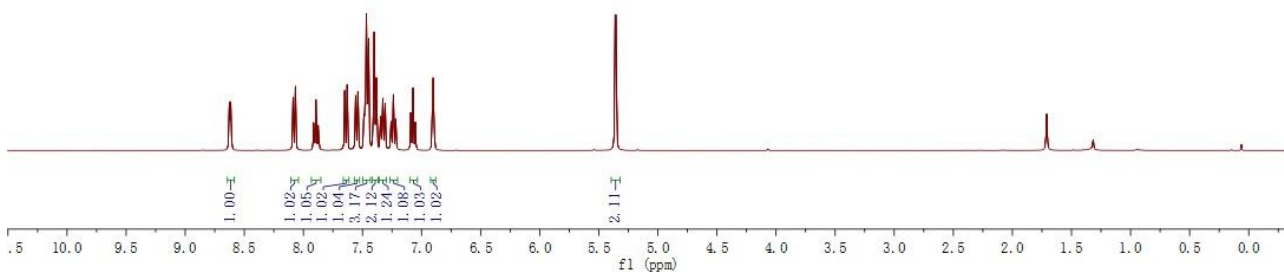
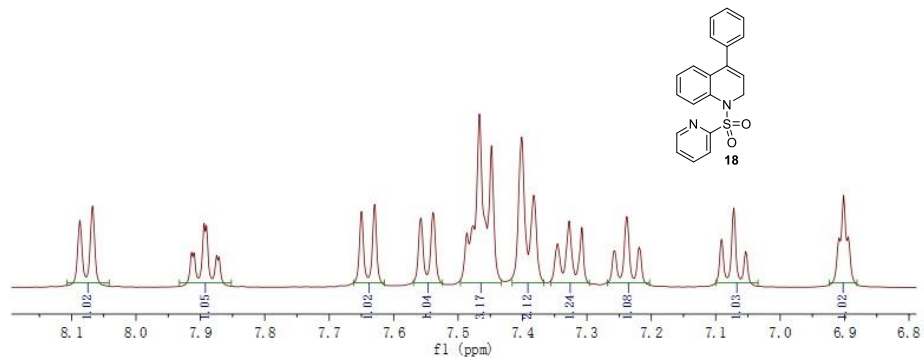
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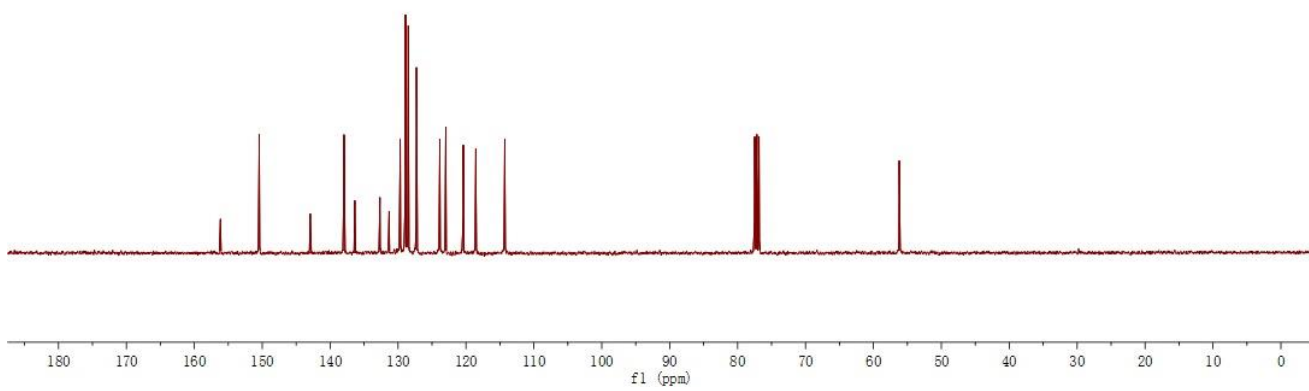
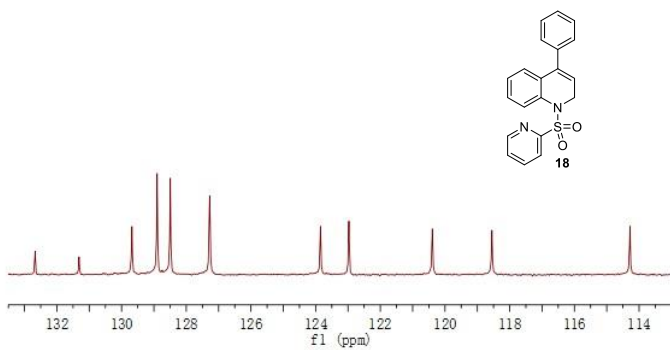
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15. Computational Methods

All of the calculations were performed with the Gaussian 09 program.¹ The geometries of the different structures were optimized at the DFT level using the B3LYP²⁻³ hybrid functional with a mixed basis set (BS1) of SDD⁴⁻⁵ for Pd and I and 6-31G(d) for the other atoms. Harmonic vibrational frequency calculations were performed at the same level to determine whether the optimized structures are local minima or transition states and to derive thermochemical corrections for the enthalpy and free energy. The solvent effects were taken into consideration by single point calculations of the gas-phase stationary points with the SMD⁶⁻⁸ continuum solvation model with toluene solvent. To obtain more accurate energy information, solvation single-point energy calculations were performed at the M06-L⁹ level of theory using a larger basis set (BS2) of LANL08(f) for Pd, LANL08(d)¹⁰⁻¹¹ for I and 6-311+G(d,p) for the other atoms. The free energies ($\Delta G_{M06-L(Toluene)}$) in the reported profiles were obtained by

$$\Delta G_{M06-L(Toluene)} = \Delta E_{M06-L(Toluene)} + \Delta G_{\text{correction}}$$

where $\Delta G_{\text{correction}}$ is the thermochemical correction for the Gibbs free energy calculated at the B3-LYP/BS1 level in the gas phase and $\Delta E_{M06-L(Toluene)}$ is the single-point energy calculated at the M06-L/BS2 level in toluene based on the gas-phase stationary point.

All of the three-dimensional molecular diagrams of the molecules were generated with CYLView.¹²

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For carbonylpalladium compound **25**, deprotonation can occur before allene insertion followed by reductive elimination. As shown in Figure S1, deprotonation occurs in the presence of NEt_3 via transition state **34-ts** with a free energy barrier of only 12.6 kcal/mol. With the dissociation of Et_3NHI , five-membered palladacycle **35** is generated and undergoes allene insertion via transition state **36-ts** to give seven-membered palladacycle **37**. The activation free energy for allene insertion is 25.1 kcal/mol. Although it is 4.2 kcal/mol lower than that of the allene insertion in path I via transition state **27-ts**, the followed reductive elimination step is difficult to occur as the barrier via transition state **38-ts** is calculated to be high by 41.2 kcal/mol. Therefore, this path can be excluded.

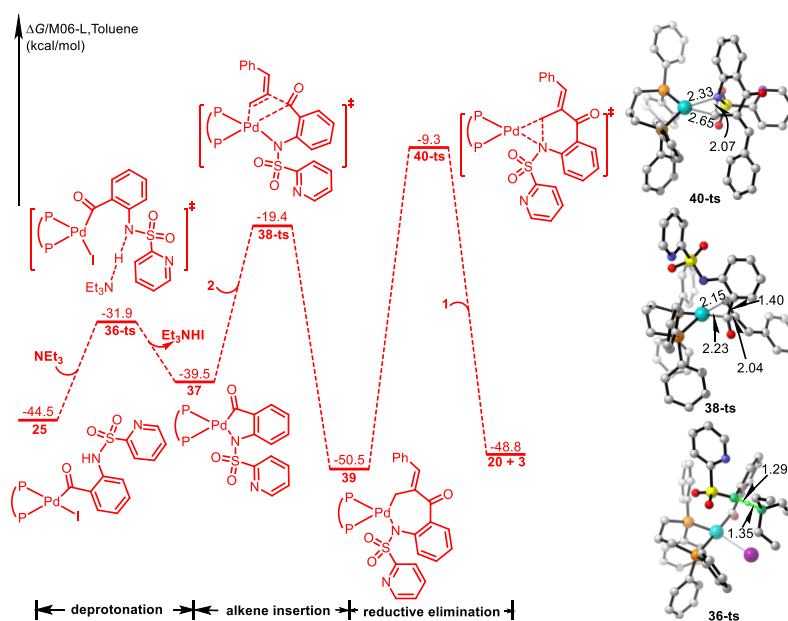


Figure S1 Free energy profiles of unfavored pathway of Palladium catalyzed regiospecific cyclocarbonylation of 2-iodoanilines and allenes. The energies are in kcal/mol and represent the relative free energies calculated with the DFT/M06-L method in toluene. The bond distances are in angstrom. The C-H bonds are omitted for clarity.

Absolute calculated electronic energies, correction of enthalpies, and free Energies.

Geometry	$E_{(\text{elec-B3LYP})}^1$	$G_{(\text{corr-B3LYP})}^2$	$H_{(\text{corr-B3LYP})}^3$	$E_{(\text{Toluene, M06-L})}^4$	IF^5
1	-1094.04585	0.141189	0.202376	-1094.150881	
2	-347.710453	0.105438	0.146662	-347.761035	
3	-1543.12512	0.275142	0.352243	-1543.343014	
19	-1855.18949	0.389572	0.482948	-1854.227652	
20	-2949.252123	0.550432	0.686853	-2948.411929	
21-ts	-2949.232941	0.551198	0.685536	-2948.396056	-168.82
22	-2949.299016	0.555441	0.687984	-2948.463157	
23	-3062.61024	0.561259	0.698499	-3061.805962	
24-ts	-3062.59432	0.560598	0.697435	-3061.78661	-249.47
25	-3062.647255	0.563972	0.70007	-3061.836185	
26	-3410.326356	0.692085	0.849333	-3409.584886	
27-ts	-3410.315058	0.6953	0.848277	-3409.576396	-319.62
28	-3410.360757	0.696669	0.850442	-3409.613827	
29	-3410.364598	0.698516	0.851333	-3409.621627	
30-ts	-3702.780414	0.895083	1.067745	-3702.084507	-988.58
31	-3398.316976	0.687909	0.835254	-3397.604115	
32-ts	-3398.307137	0.688678	0.834412	-3397.590055	-347.53
33-ts	-3410.302856	0.69714	0.847869	-3409.574246	-270.66
34	-3410.356157	0.697337	0.851063	-3409.602665	
35	-1543.114199	0.274669	0.351497	-1543.331779	
36-ts	-3355.047551	0.761403	0.916477	-3354.291514	-1177.73
37	-3050.582443	0.55557	0.684164	-3049.804921	
38-ts	-3398.272753	0.688512	0.832311	-3397.561315	-331.97
39	-3398.318145	0.692517	0.83528	-3397.6149	
40-ts	-3398.256864	0.686964	0.833319	-3397.543729	-437.39
NEt₃	-292.409811	0.172806	0.217442	-292.450777	
Et₃NHI	-304.464015	0.182558	0.234484	-304.475541	
CO	-113.306914	-0.014102	0.008341	-113.325765	

¹The electronic energy calculated by B3-LYP in gas phase. ² The thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. ³ The thermal correction to enthalpy calculated by B3-LYP in gas phase ⁴The electronic energy calculated by M06-L in toluene. ⁵The B3-LYP calculated imaginary frequencies for the transition states.

6 B3-LYP Geometries for All the Optimized Compounds and Transition State.

1

S	-1.44734100	-0.66782000	1.03463800
O	-1.37703200	-2.12514700	1.17775000
O	-1.41149900	0.23421900	2.18043100
N	-0.19911300	-0.28378400	-0.05823300
H	0.30351800	-1.14157000	-0.27525100
C	-2.95491700	-0.31765500	0.08101400
C	-3.81093900	-1.37045000	-0.23314300
C	-4.97549700	-1.05085400	-0.93421400
H	-3.56661100	-2.38329900	0.06360500
C	-4.27685100	1.24666100	-0.90601500
C	-5.21411200	0.27892700	-1.27797300
H	-5.68235700	-1.82963100	-1.20560500
H	-4.42652200	2.29427900	-1.15703700
H	-6.10723100	0.56754000	-1.82318400
C	0.59777800	0.88210300	0.02391600
C	-0.00223800	2.14240300	0.18433000
C	1.99521500	0.83065400	-0.10695100
C	0.77146900	3.29633400	0.23543500
H	-1.08305700	2.19419000	0.25700200
C	2.77079200	1.98855900	-0.08245900
C	2.15873400	3.22789600	0.09938800
H	0.28212100	4.25673400	0.36961400
H	3.84723600	1.92103700	-0.19384400
H	2.76566800	4.12786200	0.13102400
I	3.02437600	-1.05342000	-0.37859200
N	-3.16025900	0.95652700	-0.23041800

2

C	1.54575200	1.44932800	-0.00002000
C	0.23226100	0.98939300	-0.00003800
C	-0.04384600	-0.38950600	0.00004600
C	1.03510500	-1.28822800	0.00001100
C	2.35136700	-0.82633900	0.00002100
C	2.61272200	0.54445600	0.00003400
H	1.74031400	2.51877400	-0.00005700
H	-0.59424700	1.69482900	-0.00010700
H	0.83646200	-2.35762600	-0.00002500
H	3.17219200	-1.53878200	0.00001000
H	3.63717300	0.90665900	0.00004600
C	-1.42170200	-0.91633800	-0.00007200
H	-1.51542700	-2.00350900	-0.00014500
C	-2.52783000	-0.20447900	-0.00003200
C	-3.62657500	0.50165000	0.00004600
H	-4.11008000	0.81017200	-0.92631400
H	-4.10991800	0.80985800	0.92662100

3

S	-1.13158500	1.19916300	-1.55574300
O	0.09599300	1.82917400	-2.04188000
O	-2.36946000	1.27370500	-2.33584600
C	-1.52885800	1.87001900	0.08826500
C	-2.69215800	2.61624100	0.26240600
C	-2.91863800	3.14104500	1.53636600
H	-3.37820100	2.76719500	-0.56240100
C	-0.86615100	2.11407900	2.24826900
C	-1.99170900	2.88737500	2.54680800
H	-3.80717000	3.73366700	1.73463200
H	-0.12619500	1.88428500	3.01136800
H	-2.13551200	3.27400800	3.55087600
N	-0.63182700	1.61200700	1.03161600
C	-3.91945000	-2.31633400	-0.68145500
C	-2.99860600	-1.46038100	-1.28249200
C	-1.72696200	-1.29937300	-0.71487900
C	-1.38359400	-2.01440000	0.45189600
C	-2.32376600	-2.87636500	1.03368500
C	-3.58743200	-3.02951300	0.47604200
H	-4.90082700	-2.43790400	-1.13213800
H	-3.25048400	-0.91572200	-2.18340700
C	-0.04917200	-1.85888300	1.09819400
H	-2.03048500	-3.40690500	1.93387400
H	-4.30944500	-3.70097000	0.93172900
C	0.66055800	-0.82394700	-1.13458200
H	1.26593900	0.01118200	-1.48462400
O	0.14520200	-2.26793700	2.24094300
C	1.02197000	-1.21863800	0.27894500
C	2.23812300	-1.08349800	0.85605000
H	2.27304700	-1.41150500	1.89447600
N	-0.75524200	-0.43837200	-1.30157900
H	0.82901500	-1.66445000	-1.82418500
C	3.49608100	-0.55024800	0.33337500
C	3.84686200	-0.52130100	-1.03168500
C	4.43578400	-0.06214800	1.26546900
C	5.06967400	0.00546300	-1.44343800
H	3.18247400	-0.94636800	-1.77515700
C	5.65172800	0.47384600	0.85276500
H	4.19203900	-0.09834300	2.32434000
C	5.97231600	0.51336400	-0.50680500
H	5.32067400	0.01243200	-2.50055000
H	6.35306400	0.85409200	1.59052100
H	6.92344900	0.92531000	-0.83265400

19

P	-1.93302400	-0.21181300	0.04614700
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C	-1.31775900	-0.37107200	1.81800100
H	-1.18990400	-1.44950800	1.97351500
H	-2.11369000	-0.06191900	2.50799700
C	-0.00024200	0.36407300	2.17054300
H	-0.00035700	0.50684400	3.26011800
H	-0.00038700	1.37251500	1.73806200
C	1.31753800	-0.37065500	1.81821500
H	1.19011400	-1.44909500	1.97408300
H	2.11342400	-0.06096000	2.50803900
P	1.93287500	-0.21183300	0.04628400
C	3.36927800	-1.38570700	0.11376800
C	4.56969100	-1.09310200	0.78030200
C	3.22947200	-2.63498500	-0.50911300
C	5.60191500	-2.03105900	0.82662500
H	4.70384900	-0.12444200	1.25458500
C	4.25901000	-3.57715800	-0.45617700
H	2.30830100	-2.86033800	-1.04222800
C	5.44763500	-3.27596200	0.21093900
H	6.52829800	-1.78946900	1.34183000
H	4.13553800	-4.54090800	-0.94358900
H	6.25342000	-4.00458200	0.24620500
C	2.77175200	1.43935900	0.00285200
C	3.23215700	1.88936700	-1.24739400
C	2.94953500	2.27421600	1.11655900
C	3.86942200	3.12198700	-1.37623200
H	3.08049200	1.26615500	-2.12567600
C	3.57595900	3.51741100	0.98583700
H	2.59973000	1.96705100	2.09711400
C	4.04102900	3.94289900	-0.25809300
H	4.22221700	3.44750700	-2.35138700
H	3.69961600	4.15119500	1.86042000
H	4.52761400	4.90942200	-0.35864200
C	-3.36944800	-1.38560500	0.11321500
C	-3.22972100	-2.63461100	-0.51017700
C	-4.56977700	-1.09325200	0.77994400
C	-4.25926600	-3.57680200	-0.45754500
H	-2.30860900	-2.85979900	-1.04345600
C	-5.60202700	-2.03118700	0.82599400
H	-4.70392200	-0.12479700	1.25462200
C	-5.44784100	-3.27585800	0.20979900
H	-4.13586100	-4.54036200	-0.94535500
H	-6.52836800	-1.78979300	1.34136800
H	-6.25363500	-4.00448600	0.24484000
C	-2.77156600	1.43950500	0.00302700
C	-3.22982200	1.89081700	-1.24750100
C	-2.95128900	2.27313400	1.11730700

C	-3.86694200	3.12355800	-1.37612800
H	-3.07656600	1.26860200	-2.12620500
C	-3.57754600	3.51642800	0.98689300
H	-2.60313600	1.96496600	2.09813000
C	-4.04053200	3.94325400	-0.25737900
H	-4.21804100	3.45015200	-2.35154400
H	-3.70274900	4.14926900	1.86194000
H	-4.52700200	4.90986700	-0.35772000
Pd	-0.00004000	-0.46396400	-1.13930500
20			
P	-2.74039300	-0.76609000	0.83751500
C	-2.61652900	-0.03335700	2.55789700
H	-1.77833400	-0.56196300	3.02908300
H	-3.50633400	-0.30431100	3.14013200
C	-2.37720000	1.49206700	2.62675600
H	-2.70940900	1.82979000	3.61760800
H	-3.01898000	2.01488600	1.90595400
C	-0.91280000	1.95684600	2.46284600
H	-0.25291000	1.27997200	3.02086400
H	-0.80516300	2.95466200	2.90660400
P	-0.29369400	2.01247100	0.69212700
C	1.43745300	2.65301600	0.90565000
C	2.20754000	2.81201100	-0.26027700
C	2.03505700	2.94759300	2.14095300
C	3.52103800	3.27127100	-0.19706200
H	1.77095600	2.56495700	-1.22535700
C	3.35857400	3.39505700	2.20686400
H	1.47608600	2.83583100	3.06445800
C	4.10327800	3.56325200	1.04010700
H	4.09492700	3.38867400	-1.11247100
H	3.80188300	3.61781900	3.17447800
H	5.13048100	3.91493700	1.09186500
C	-1.16558200	3.52901100	0.06925400
C	-2.14244600	3.38936300	-0.92789000
C	-0.89474500	4.81136000	0.57372100
C	-2.84052500	4.50284100	-1.40301100
H	-2.34731000	2.40002800	-1.33043000
C	-1.58847000	5.92368600	0.09721000
H	-0.12800600	4.94515500	1.33267600
C	-2.56495800	5.77130200	-0.89131300
H	-3.59468900	4.37680200	-2.17551300
H	-1.36464800	6.91064300	0.49442200
H	-3.10345800	6.63924700	-1.26305800
C	-2.87570800	-2.56256400	1.27091100
C	-1.69332900	-3.32179400	1.27537200
C	-4.08464800	-3.18730700	1.61460200

C	-1.72018500	-4.67250300	1.62787500
H	-0.74799900	-2.86025400	0.99974800
C	-4.11035700	-4.54140300	1.95393500
H	-5.01088800	-2.61944000	1.60948900
C	-2.92881000	-5.28615100	1.96375700
H	-0.79528200	-5.24300900	1.62682300
H	-5.05528000	-5.01433300	2.21030100
H	-2.95166500	-6.34070800	2.22654900
C	-4.45537000	-0.33040000	0.28875500
C	-4.76970300	-0.54910000	-1.06430300
C	-5.44289800	0.22425400	1.11779500
C	-6.03361000	-0.24439300	-1.56740800
H	-4.00841400	-0.95643900	-1.72547600
C	-6.70577100	0.54489900	0.61142700
H	-5.23880200	0.41307900	2.16705700
C	-7.00635000	0.30841700	-0.73005700
H	-6.25594200	-0.42838500	-2.61536200
H	-7.45426900	0.97849900	1.26989600
H	-7.98871000	0.55763900	-1.12244400
Pd	-0.94622300	0.07461300	-0.39187200
S	3.04012700	-2.16231300	0.49688900
O	1.86691400	-2.62177400	1.25249200
O	3.87170500	-3.08150700	-0.27575200
N	2.50911300	-0.92126200	-0.50311500
H	1.54504000	-0.64704300	-0.28546500
C	4.10917800	-1.32577200	1.70962600
C	3.82675100	-1.46640200	3.06683500
C	4.69875100	-0.84785100	3.96480500
H	2.96268900	-2.03446700	3.38975800
C	5.96334500	-0.06284100	2.08167100
C	5.78546900	-0.13158200	3.46598000
H	4.52899400	-0.92571800	5.03499000
H	6.79881100	0.48689600	1.65398700
H	6.48562100	0.36506300	4.13051600
C	2.94603400	-0.74768100	-1.84119300
C	4.29579300	-0.46565700	-2.10090600
C	2.05819800	-0.81098900	-2.92814800
C	4.74049300	-0.25888400	-3.40322400
H	4.97502400	-0.41241200	-1.25612500
C	2.49307400	-0.56652400	-4.22989400
C	3.84111000	-0.29644900	-4.47022200
H	5.79193600	-0.05257300	-3.58248000
H	1.78826800	-0.60491500	-5.05421900
H	4.18101400	-0.12160500	-5.48715900
N	5.14124100	-0.65549100	1.21060800
I	-0.02316900	-1.33083500	-2.61462300

21-ts

P	2.29339200	-1.14278100	-0.95428800
C	2.27367700	-0.52219900	-2.71853100
H	1.34753300	-0.92054500	-3.15219400
H	3.09304300	-0.98775400	-3.28060400
C	2.31324500	1.01151100	-2.89581200
H	2.62951400	1.20858700	-3.92897600
H	3.09045300	1.45482400	-2.26057800
C	0.97513400	1.75372200	-2.68916000
H	0.16437100	1.16699400	-3.13994400
H	1.01601200	2.71220800	-3.22171000
P	0.49780000	2.09025800	-0.90471000
C	-1.02813000	3.12112600	-1.11418400
C	-1.57280400	3.70967700	0.04075700
C	-1.69559700	3.30844100	-2.33497800
C	-2.73085500	4.48064600	-0.02691900
H	-1.08992600	3.55334900	1.00167700
C	-2.86387300	4.07373500	-2.40049800
H	-1.31156800	2.86642800	-3.24842600
C	-3.38211300	4.66631500	-1.24965600
H	-3.13197000	4.92689500	0.87914100
H	-3.36342100	4.20867500	-3.35677100
H	-4.28872000	5.26350800	-1.30207900
C	1.74980200	3.38136000	-0.45036900
C	2.72527400	3.07343200	0.50992000
C	1.76922100	4.65194400	-1.04889600
C	3.70415100	4.00818800	0.85774000
H	2.70847800	2.09516100	0.98536800
C	2.74350600	5.58666400	-0.69911100
H	1.01099400	4.91788000	-1.78096200
C	3.71474000	5.26590200	0.25382000
H	4.45288900	3.75237100	1.60284600
H	2.74337600	6.56766600	-1.16762000
H	4.47214900	5.99633800	0.52624600
C	2.12221800	-2.96439800	-1.24506400
C	0.86533500	-3.55270700	-1.03497600
C	3.18195100	-3.77310000	-1.68807000
C	0.66537400	-4.91382600	-1.27690600
H	0.03607400	-2.95388300	-0.67082200
C	2.98356600	-5.13415100	-1.92253100
H	4.16728100	-3.34155700	-1.84260800
C	1.72470000	-5.70699900	-1.71980500
H	-0.31679700	-5.34495500	-1.10432800
H	3.81351900	-5.74890900	-2.26222200
H	1.57457200	-6.76841500	-1.89996000
C	4.06534500	-0.97879700	-0.44520000

C	4.37121500	-1.25818100	0.89966000
C	5.10716600	-0.57107700	-1.29269400
C	5.67759600	-1.15500900	1.37448600
H	3.57463300	-1.55421600	1.57770000
C	6.41542800	-0.45504500	-0.81354400
H	4.91196500	-0.33965700	-2.33505300
C	6.70558600	-0.75006900	0.51832800
H	5.89194800	-1.38319900	2.41533300
H	7.20715000	-0.13544500	-1.48648400
H	7.72337100	-0.66147700	0.88882700
Pd	0.74167600	0.12165600	0.32881100
S	-3.42848400	-2.08984400	0.36538600
O	-2.63656700	-3.15112700	-0.27339300
O	-4.12190500	-2.29007500	1.63472800
N	-2.41026600	-0.75600900	0.47274300
H	-1.49754700	-0.94488400	0.04998700
C	-4.66891000	-1.59144900	-0.87143000
C	-4.81876400	-2.36205400	-2.02276200
C	-5.81061400	-1.97210500	-2.92473400
H	-4.18182700	-3.22183100	-2.19143300
C	-6.33918400	-0.15755100	-1.44522500
C	-6.58559900	-0.85064900	-2.63340000
H	-5.97253200	-2.53671300	-3.83860500
H	-6.92041100	0.72381300	-1.18319100
H	-7.36608200	-0.51415400	-3.30873500
C	-2.37573400	0.15364000	1.56430800
C	-3.46861500	0.98790900	1.82438800
C	-1.20768800	0.30152900	2.33324300
C	-3.40246500	1.95397000	2.82602100
H	-4.35824200	0.86415900	1.21484600
C	-1.12200300	1.30292400	3.30642100
C	-2.21795200	2.13199500	3.54624200
H	-4.26730200	2.57917400	3.02810000
H	-0.21874200	1.40638900	3.89812100
H	-2.14879300	2.89644000	4.31578200
N	-5.39634900	-0.52169000	-0.57055100
I	0.16998900	-1.45721000	2.65927300
22			
P	2.34688200	-0.90494900	-0.99815800
C	2.22091100	-0.38740300	-2.78724500
H	1.33476900	-0.90768000	-3.17275800
H	3.07241100	-0.80530500	-3.33609800
C	2.09411000	1.12333700	-3.05384000
H	2.30588500	1.29650700	-4.11702900
H	2.85786600	1.68358000	-2.50061500
C	0.70030400	1.70510900	-2.76568100

H	-0.06370200	1.05949900	-3.21360400
H	0.60081600	2.68930200	-3.23758800
P	0.27274900	1.91813000	-0.96035400
C	-1.39721500	2.68793100	-1.06253300
C	-1.74860600	3.76091200	-0.22887800
C	-2.36260900	2.16842500	-1.93945100
C	-3.02770400	4.31372700	-0.28867300
H	-1.02755400	4.16167800	0.47483500
C	-3.63957800	2.72623900	-1.99974200
H	-2.13554100	1.31519700	-2.57125700
C	-3.97444300	3.80272400	-1.17744600
H	-3.28369000	5.14128200	0.36698500
H	-4.37374300	2.31165800	-2.68509700
H	-4.97030800	4.23508700	-1.22253600
C	1.39621000	3.28920900	-0.45670600
C	2.32224300	3.08321900	0.57645600
C	1.37570500	4.53132700	-1.11478200
C	3.21093800	4.09663100	0.94467100
H	2.34501200	2.12743100	1.09304200
C	2.26279300	5.54125300	-0.74551400
H	0.65524600	4.71907000	-1.90628700
C	3.18274000	5.32503100	0.28484100
H	3.92177300	3.92128700	1.74718000
H	2.23456300	6.49812300	-1.25978800
H	3.87244900	6.11415600	0.57182800
C	2.33607000	-2.73520700	-1.21068100
C	1.12703500	-3.43244800	-1.06618500
C	3.49205400	-3.43559600	-1.58706300
C	1.07393100	-4.80546600	-1.31147900
H	0.22970500	-2.91905300	-0.73618500
C	3.43659700	-4.81006000	-1.82200800
H	4.43906600	-2.91251600	-1.68601900
C	2.22731400	-5.49595100	-1.68780200
H	0.13174700	-5.33116500	-1.18657800
H	4.33973100	-5.34459100	-2.10480200
H	2.18712200	-6.56721000	-1.86668000
C	4.07780400	-0.47735300	-0.51750200
C	4.42623000	-0.57456300	0.84172600
C	5.05431200	-0.05495600	-1.43413700
C	5.71938600	-0.26821900	1.26544600
H	3.68213500	-0.89696700	1.56465400
C	6.34601300	0.25960900	-1.00450000
H	4.82360600	0.03309000	-2.49072400
C	6.68241600	0.15196800	0.34510400
H	5.97097100	-0.35688700	2.31885600
H	7.08766700	0.58645000	-1.72866400

H	7.68827500	0.39440600	0.67756100
Pd	0.60591000	0.06492400	0.40647700
S	-3.39592500	-2.00267200	0.37219900
O	-2.69202300	-2.96171900	-0.49564600
O	-3.77153600	-2.32980400	1.74390900
N	-2.47077300	-0.58850400	0.27677600
H	-1.58484000	-0.85613700	-0.15667800
C	-4.91963500	-1.55618300	-0.52112300
C	-5.24504600	-2.24969600	-1.68578100
C	-6.44276700	-1.90884100	-2.31630800
H	-4.58310200	-3.01881600	-2.06522700
C	-6.80458600	-0.28433500	-0.58676800
C	-7.23794900	-0.90717400	-1.76024900
H	-6.74876700	-2.41967600	-3.22510200
H	-7.39696100	0.50001500	-0.12029600
H	-8.17708400	-0.61350400	-2.21907400
C	-2.25442500	0.32288100	1.36346600
C	-3.32196600	0.78852800	2.13738700
C	-0.94095900	0.77673800	1.58596800
C	-3.08216700	1.70067600	3.16445300
H	-4.32651400	0.43500600	1.93055900
C	-0.72975800	1.70090700	2.61366500
C	-1.78758200	2.15960200	3.40695200
H	-3.91197600	2.04958200	3.77361300
H	0.27818400	2.04932500	2.82456300
H	-1.59390500	2.86281300	4.21353600
N	-5.66327400	-0.60462000	0.03097700
I	0.95934400	-1.78278500	2.36693000
23			
P	0.28700800	2.22007200	0.42008600
C	1.64196700	3.30818600	1.09948000
H	1.57002100	3.23587000	2.19095100
H	1.38552000	4.34314800	0.84793600
C	3.08437700	3.00416100	0.65970100
H	3.70275400	3.85128000	0.98324200
H	3.15636300	2.97995000	-0.43391400
C	3.70204400	1.72764300	1.26085100
H	3.48664600	1.68559800	2.33545000
H	4.79141900	1.76235400	1.14687500
P	3.07255400	0.15180800	0.49219500
C	4.08275900	-1.16951400	1.28048700
C	4.04395100	-2.45374600	0.70802100
C	4.84855000	-0.95923700	2.43717100
C	4.76434500	-3.49967000	1.28271500
H	3.43477600	-2.63939800	-0.17337500
C	5.56736300	-2.01262400	3.00833100

H	4.89647700	0.02018000	2.90256000
C	5.52806900	-3.28257700	2.43246500
H	4.72162400	-4.48714600	0.83208000
H	6.15858200	-1.83565100	3.90290500
H	6.08691100	-4.10057100	2.87885900
C	3.76132400	0.24943700	-1.21236900
C	2.92544200	0.15691000	-2.33112100
C	5.14488700	0.42376300	-1.39771100
C	3.46247400	0.25729700	-3.61795700
H	1.86600300	-0.02849500	-2.20198600
C	5.67554900	0.52354600	-2.68164800
H	5.81311900	0.46336400	-0.54111400
C	4.83224500	0.44441600	-3.79487500
H	2.80264200	0.17901100	-4.47696400
H	6.74610900	0.65489700	-2.81474100
H	5.24792900	0.51826500	-4.79634300
C	-1.20773700	3.06113800	1.09086600
C	-2.29292700	3.37294300	0.26071600
C	-1.27792300	3.38471200	2.45642700
C	-3.42017200	4.00858500	0.78435100
H	-2.27484200	3.11060700	-0.79048800
C	-2.39940100	4.03123900	2.97179900
H	-0.46821800	3.11907200	3.12921800
C	-3.47330500	4.34641000	2.13558900
H	-4.25884600	4.22441800	0.12952600
H	-2.43821500	4.27802200	4.02933100
H	-4.35098800	4.84284900	2.54065800
C	0.24035400	2.56816800	-1.38306700
C	-0.33002700	1.61338700	-2.23827900
C	0.68756200	3.78758400	-1.92080400
C	-0.46321000	1.87611100	-3.60316100
H	-0.68427700	0.66691100	-1.84804000
C	0.57323200	4.03703700	-3.28807200
H	1.11806000	4.55295500	-1.28268500
C	-0.00539500	3.08365200	-4.13059100
H	-0.93305900	1.13127400	-4.23769900
H	0.92889600	4.98059000	-3.69327700
H	-0.10313700	3.28714100	-5.19363900
Pd	0.68698400	-0.03792300	1.01396000
S	-3.68868800	-0.18183200	-1.16499100
O	-4.47103900	0.97881300	-0.72321900
O	-3.12664100	-0.23495400	-2.51541900
N	-2.39042000	-0.38520300	-0.13629300
H	-1.70521000	-1.05668800	-0.51305000
C	-4.75892900	-1.64026000	-0.95992200
C	-6.14275700	-1.47515000	-0.91989000

C	-6.91404100	-2.63474700	-0.82311300
H	-6.58063100	-0.48437700	-0.95664600
C	-4.87414600	-3.90504000	-0.80948400
C	-6.27117900	-3.87137400	-0.76775500
H	-7.99814200	-2.57110000	-0.78941400
H	-4.33301600	-4.84707100	-0.76299000
H	-6.83630800	-4.79510900	-0.69021400
C	-2.40970100	-0.24536100	1.28334100
C	-3.60567700	-0.22781700	2.01738800
C	-1.17810600	-0.10501700	1.95416100
C	-3.58786800	-0.08840200	3.40361100
H	-4.55714700	-0.31243200	1.50671900
C	-1.18379500	-0.00730200	3.35137100
C	-2.37550900	0.01160800	4.08157400
H	-4.52773200	-0.07562900	3.94907200
H	-0.23980100	0.07019100	3.88590800
H	-2.35021500	0.10083600	5.16466000
N	-4.12372900	-2.80318500	-0.90687700
I	0.36456900	-2.60093100	-1.30067200
C	0.84783500	-1.85113200	1.79347900
O	0.91918000	-2.82826000	2.38207000
24-ts			
P	1.14415400	2.06843200	0.79684400
C	2.31851200	2.11830200	2.24197400
H	1.74185500	1.79134500	3.11619600
H	2.61259400	3.15613200	2.43315200
C	3.58713300	1.25039400	2.10646700
H	4.28924800	1.58749100	2.87964200
H	4.08408000	1.44454700	1.14800100
C	3.39237300	-0.26692900	2.30363300
H	2.77260500	-0.44836000	3.19043800
H	4.37018200	-0.72788100	2.48694600
P	2.58960800	-1.12641700	0.85576400
C	2.55748100	-2.90423000	1.32640500
C	2.05244700	-3.80944200	0.37573000
C	2.98471600	-3.38891800	2.57117200
C	1.98982000	-5.17098300	0.66544900
H	1.69830800	-3.44389300	-0.58570800
C	2.91260800	-4.75486200	2.85894900
H	3.37739700	-2.71342900	3.32486600
C	2.41886400	-5.64732800	1.90757400
H	1.59732800	-5.85882900	-0.07819300
H	3.24699900	-5.11779500	3.82734900
H	2.36472500	-6.70893500	2.13298700
C	3.93877600	-1.05973200	-0.40127800
C	3.75805300	-0.38280900	-1.61305200

C	5.17492400	-1.67590300	-0.13572900
C	4.80342900	-0.30728400	-2.53848700
H	2.79542200	0.05398900	-1.84997900
C	6.21360100	-1.59936500	-1.06080800
H	5.32318200	-2.23123200	0.78702700
C	6.02966700	-0.91059300	-2.26422200
H	4.64738800	0.21847600	-3.47611200
H	7.16369000	-2.08187600	-0.84690100
H	6.83955000	-0.85463600	-2.98682000
C	-0.16614800	3.28777900	1.24296200
C	-1.17410900	3.53520200	0.29611600
C	-0.20070900	3.97412800	2.46528800
C	-2.18714700	4.45409000	0.56316100
H	-1.17871300	3.00039800	-0.64928200
C	-1.21892100	4.89349200	2.73092900
H	0.55987800	3.80429700	3.22049900
C	-2.21143900	5.13666200	1.78181400
H	-2.96319800	4.62418400	-0.17753100
H	-1.23176600	5.41862500	3.68247200
H	-3.00325600	5.85076800	1.99122000
C	2.03952100	2.93604900	-0.56449600
C	1.71860300	2.61505300	-1.89223400
C	2.97265400	3.95667300	-0.31650700
C	2.32029300	3.30246100	-2.94918900
H	1.01144300	1.81775500	-2.10768400
C	3.57913900	4.63279800	-1.37479500
H	3.22814000	4.24000600	0.70022000
C	3.25271100	4.30812000	-2.69397500
H	2.05774700	3.04203600	-3.97081700
H	4.30231300	5.41727700	-1.16790400
H	3.72329800	4.83932700	-3.51704200
Pd	0.38167700	-0.20730100	0.52841000
S	-4.28821000	0.40571400	-1.43420900
O	-5.21664300	1.44694000	-0.97667300
O	-3.88902400	0.33608200	-2.83487700
N	-2.84846500	0.51252500	-0.56211700
H	-2.07529000	0.08287500	-1.08902000
C	-5.02246900	-1.18532500	-0.93923600
C	-6.40867700	-1.28851500	-0.83257700
C	-6.92555900	-2.54710000	-0.52273300
H	-7.03996500	-0.41993100	-0.97979400
C	-4.67194900	-3.37791500	-0.45026000
C	-6.04436100	-3.61117500	-0.32884500
H	-7.99832600	-2.69139700	-0.42982700
H	-3.94883800	-4.17470800	-0.29497700
H	-6.40852100	-4.60393000	-0.08298600

C	-2.75666600	0.47886400	0.84417600
C	-3.77622700	1.02415800	1.64814900
C	-1.60455000	-0.04374000	1.47814900
C	-3.67603200	1.01078500	3.03531700
H	-4.63870100	1.47274000	1.17168600
C	-1.53140100	-0.05104800	2.88200500
C	-2.55398000	0.47248300	3.66807100
H	-4.48590000	1.43260300	3.62475000
H	-0.66400500	-0.49717100	3.36076900
H	-2.47893700	0.45366100	4.75163800
N	-4.16406300	-2.17936400	-0.75702700
I	-0.03139300	-0.92329300	-2.46883900
C	-0.74838600	-1.71135700	0.81941400
O	-1.23336100	-2.75996700	0.91001100
25			
P	-3.45832500	0.45397400	0.36424300
C	-3.77356200	1.68891800	1.72775100
H	-3.81539200	1.09498200	2.64979600
H	-4.77647800	2.11270000	1.60205500
C	-2.72803700	2.80766300	1.87822300
H	-3.14938000	3.57320900	2.54260400
H	-2.55143000	3.30844100	0.91814800
C	-1.39540900	2.34765900	2.49647500
H	-1.60204800	1.67255500	3.33428800
H	-0.85678500	3.20907000	2.90701600
P	-0.22011900	1.48365800	1.32894900
C	1.22031200	1.13321700	2.42533900
C	2.52438200	1.17635400	1.90543300
C	1.04008600	0.73316700	3.75944400
C	3.61750000	0.84895400	2.70794600
H	2.69068100	1.45675400	0.86970400
C	2.13603900	0.40821300	4.55976100
H	0.04516800	0.66469900	4.18841500
C	3.42837000	0.46828300	4.03743900
H	4.61847000	0.88755100	2.28816300
H	1.97603000	0.10643400	5.59140800
H	4.28140100	0.21270100	4.66002800
C	0.34878900	2.87579300	0.26540400
C	0.13632800	2.82715700	-1.11970400
C	0.96391200	4.00992300	0.82532700
C	0.52495200	3.89852600	-1.92914200
H	-0.30534600	1.94320200	-1.56695600
C	1.34939900	5.07608700	0.01498600
H	1.15540100	4.05670700	1.89437600
C	1.12775200	5.02202100	-1.36500100
H	0.36229400	3.84480600	-3.00171500

H	1.82288500	5.94808700	0.45857000
H	1.43088900	5.85287400	-1.99652300
C	-4.83714100	-0.72247000	0.69772800
C	-4.57839600	-1.85880200	1.47840400
C	-6.14562100	-0.47841600	0.25547400
C	-5.61571700	-2.72480900	1.82722700
H	-3.56111600	-2.08199600	1.78544200
C	-7.17914000	-1.35174700	0.59767500
H	-6.35836800	0.38801100	-0.36425100
C	-6.91663000	-2.47328500	1.38713300
H	-5.40192000	-3.60623200	2.42550800
H	-8.18810800	-1.15700200	0.24377100
H	-7.72161500	-3.15456800	1.64961000
C	-3.93886900	1.34241300	-1.18133900
C	-3.58671100	0.75507200	-2.41038200
C	-4.61448400	2.57346800	-1.19290900
C	-3.91344200	1.37987000	-3.61397700
H	-3.05777200	-0.19368100	-2.42237000
C	-4.93214400	3.20055500	-2.40019700
H	-4.90072500	3.05856300	-0.26527800
C	-4.58395000	2.60514800	-3.61296400
H	-3.63618200	0.90805700	-4.55258400
H	-5.45294400	4.15448300	-2.38886300
H	-4.83177100	3.09387200	-4.55141400
Pd	-1.13566000	-0.32148000	0.15793600
S	4.91286400	-1.37212300	-2.09557600
O	5.69610200	-2.58578900	-1.84548000
O	4.74488000	-0.83665400	-3.44263600
N	3.36051600	-1.56401200	-1.51270000
H	2.69315000	-0.90477500	-1.92943600
C	5.67793300	-0.06744500	-1.07867100
C	6.94021900	-0.28671300	-0.52932200
C	7.52763600	0.77466600	0.16179400
H	7.42924300	-1.24601000	-0.64963400
C	5.56606000	2.07452100	-0.31984500
C	6.83244200	1.97914500	0.26575000
H	8.51226700	0.66172000	0.60680700
H	4.98902400	2.99454000	-0.25471800
H	7.25671300	2.83066000	0.78885100
C	2.93686300	-2.12165900	-0.29385000
C	3.72814200	-3.03332000	0.42441800
C	1.64091300	-1.78837900	0.20035700
C	3.25803000	-3.59083300	1.60931200
H	4.69559300	-3.31984000	0.03287400
C	1.19661600	-2.38767400	1.38908400
C	1.98884000	-3.27559300	2.10285900

H	3.88960500	-4.29652500	2.14306800
H	0.19615900	-2.14054600	1.73188800
H	1.62147700	-3.72857000	3.01859500
N	4.98993900	1.06626200	-0.98362000
I	-1.84056800	-2.67629900	-1.06183200
C	0.74639500	-0.82150000	-0.49380600
O	1.07115400	-0.24557700	-1.52780900
26			
P	-2.09996900	-0.07518000	1.84240000
C	-3.02712600	-1.66871800	2.05698400
H	-3.77975000	-1.67406100	1.25983500
H	-3.56215400	-1.63653600	3.01261600
C	-2.18448000	-2.95185100	1.95482200
H	-2.82941700	-3.78030200	2.27401100
H	-1.34464600	-2.93412800	2.66088600
C	-1.70124000	-3.29439200	0.53444000
H	-2.51209300	-3.12659400	-0.18435800
H	-1.41477000	-4.35148800	0.48575700
P	-0.22179800	-2.34293800	-0.07674300
C	0.18834300	-3.20240500	-1.64898200
C	1.50049300	-3.59423500	-1.95878200
C	-0.83592700	-3.41082900	-2.58948500
C	1.77950000	-4.21158300	-3.17888300
H	2.30522600	-3.42346700	-1.25067100
C	-0.54717800	-4.03038600	-3.80578100
H	-1.85054300	-3.06780700	-2.39682500
C	0.75617500	-4.43551100	-4.10189800
H	2.79817900	-4.51431400	-3.40634000
H	-1.34797100	-4.18617100	-4.52301600
H	0.97498800	-4.91767900	-5.05108100
C	1.07201200	-2.86835300	1.12578600
C	1.67568900	-1.95089500	1.99158400
C	1.38382700	-4.23579800	1.26013200
C	2.56244200	-2.38425500	2.98197800
H	1.45240900	-0.89430600	1.91216500
C	2.27490500	-4.66530600	2.24029900
H	0.93390300	-4.96599700	0.59384200
C	2.86200300	-3.73890900	3.10912000
H	3.01002300	-1.65211800	3.64641500
H	2.50594500	-5.72325400	2.33125500
H	3.54618800	-4.07815000	3.88277300
C	-3.43015700	1.18368600	2.10275700
C	-4.64171000	1.06915300	1.39581100
C	-3.24455600	2.27650900	2.96539800
C	-5.64654100	2.02315200	1.56788500
H	-4.80012500	0.25660200	0.68951900

C	-4.25357600	3.22752500	3.12781000
H	-2.31920200	2.38532600	3.52125700
C	-5.45801700	3.10207800	2.43350800
H	-6.57591000	1.91715000	1.01512700
H	-4.09539200	4.06507100	3.80214600
H	-6.24269400	3.84267300	2.56341300
C	-1.06508700	0.09862900	3.35782300
C	-1.35684400	-0.56223200	4.56226200
C	0.04336800	0.95824800	3.31274700
C	-0.55312700	-0.37193900	5.68721600
H	-2.21323100	-1.22501800	4.63460700
C	0.84389100	1.15393600	4.44014800
H	0.29874400	1.47466300	2.39306900
C	0.54757800	0.48651200	5.62967500
H	-0.79061300	-0.89331200	6.61078700
H	1.70031100	1.81791800	4.37221700
H	1.16984000	0.63286700	6.50869400
Pd	-0.81218600	-0.04725400	-0.33521700
S	3.33177200	1.72013800	0.39882200
O	3.70198900	2.84342900	-0.46855000
O	2.54348100	1.93728500	1.61575000
N	2.46285200	0.56050600	-0.45449400
H	1.53000700	0.41773300	-0.05554800
C	4.89062700	0.90698100	0.86270000
C	6.09389000	1.55493000	0.58781200
C	7.26286700	0.91803500	1.01091200
H	6.10298300	2.50424300	0.06551200
C	5.89572300	-0.85280400	1.88726800
C	7.16470700	-0.30760200	1.66810700
H	8.23145900	1.37342300	0.82630300
H	5.77383000	-1.80729800	2.39415200
H	8.05049000	-0.83558600	2.00701900
C	2.61114500	0.28103000	-1.83177400
C	3.89784400	0.26766000	-2.39324400
C	1.49616700	-0.01955000	-2.64795500
C	4.08925000	-0.02107700	-3.73877500
H	4.75728600	0.48239000	-1.76989400
C	1.72509800	-0.32375700	-4.00503200
C	2.99797700	-0.32465000	-4.55543400
H	5.09738500	-0.01864400	-4.14422000
H	0.85787600	-0.55667300	-4.61192800
H	3.13957500	-0.56056400	-5.60581500
N	4.76845700	-0.25126800	1.49579600
I	-4.40026900	-1.49995100	-1.68130000
C	0.04219700	-0.04859800	-2.23566600
O	-0.80695300	-0.08809500	-3.09720100

C	-0.96285800	2.32293900	-0.98529300
C	0.03529300	3.18526900	-1.00329400
H	1.01713900	2.88617300	-0.65548900
C	-2.15473100	1.72203400	-1.08077300
H	-2.91069100	1.86470500	-0.31263500
H	-2.47556900	1.19993700	-1.98310200
C	-0.06013100	4.57880600	-1.48593000
C	1.10152700	5.36930700	-1.47138000
C	-1.25840600	5.14202600	-1.95716700
C	1.06380500	6.69134900	-1.91404200
H	2.03373500	4.93748900	-1.11633500
C	-1.29150600	6.46177200	-2.39810900
H	-2.16337200	4.54120300	-1.97897000
C	-0.13147200	7.24295900	-2.37775600
H	1.97102600	7.28959600	-1.89710100
H	-2.22544800	6.88314600	-2.76040800
H	-0.16136500	8.27286500	-2.72314600

27-ts

P	-2.14240000	-0.43143800	1.80300100
C	-3.04410800	-2.04653600	1.68727900
H	-3.78656100	-1.90277200	0.89152000
H	-3.59537800	-2.20101700	2.62211800
C	-2.18540100	-3.28078000	1.35827300
H	-2.83859400	-4.15486900	1.47348600
H	-1.37810500	-3.40880700	2.09071500
C	-1.63420700	-3.32624600	-0.07867700
H	-2.41637200	-3.01899700	-0.78378200
H	-1.33970100	-4.35203000	-0.32806400
P	-0.14448500	-2.25566800	-0.40557100
C	0.31786900	-2.73865300	-2.11913700
C	1.63719100	-3.06993300	-2.46663100
C	-0.67461400	-2.71819900	-3.11490200
C	1.95414500	-3.40350700	-3.78433800
H	2.41713700	-3.07530200	-1.71158200
C	-0.34836600	-3.05577500	-4.42892300
H	-1.69505700	-2.41910800	-2.88281500
C	0.96154000	-3.40289900	-4.76621900
H	2.97789900	-3.66349300	-4.04073600
H	-1.12592900	-3.03908800	-5.18732500
H	1.20944800	-3.66618800	-5.79125600
C	1.11959800	-3.04406000	0.68200300
C	1.74016900	-2.32361200	1.70851100
C	1.40740500	-4.41642500	0.54808200
C	2.61678700	-2.95755500	2.59455400
H	1.54090800	-1.26660500	1.83477300
C	2.28829300	-5.04514400	1.42487300

H	0.94735600	-4.99466600	-0.24807300
C	2.89076400	-4.31671100	2.45628100
H	3.07597100	-2.37742000	3.38908700
H	2.49995400	-6.10465000	1.30795500
H	3.56739400	-4.81244100	3.14779300
C	-3.48269900	0.74946200	2.25986700
C	-4.60378700	0.86131200	1.41752800
C	-3.40153100	1.55620900	3.40637700
C	-5.62906200	1.75301100	1.73461700
H	-4.67768800	0.26787600	0.50711200
C	-4.43028600	2.45001100	3.71157600
H	-2.54369300	1.48632600	4.06714200
C	-5.54699900	2.54813000	2.87992300
H	-6.49066300	1.82306900	1.07638800
H	-4.35667800	3.06591100	4.60407100
H	-6.34742600	3.24243200	3.12177100
C	-1.09648800	-0.52263500	3.31395400
C	-1.36897800	-1.40588100	4.37105000
C	-0.00219100	0.34968500	3.42579800
C	-0.55954500	-1.41911700	5.50807400
H	-2.21331600	-2.08568600	4.31667200
C	0.80310500	0.34043900	4.56610200
H	0.23778700	1.03328300	2.61726700
C	0.52660300	-0.54634100	5.60842500
H	-0.78038100	-2.11127700	6.31624600
H	1.64977600	1.01795500	4.62161600
H	1.15415100	-0.55921600	6.49570900
Pd	-0.83770000	0.05415600	-0.17992300
S	3.33606400	1.65960900	0.69055800
O	3.71259600	2.89689700	-0.00343600
O	2.55060600	1.68860900	1.92775900
N	2.47162600	0.64048500	-0.33782800
H	1.55090700	0.42661600	0.05523500
C	4.89232600	0.78033600	1.02569300
C	6.10002300	1.44317700	0.81396500
C	7.26658700	0.74420400	1.13348600
H	6.11395400	2.45121200	0.41695700
C	5.88826000	-1.10676500	1.80241200
C	7.16128000	-0.55309900	1.63279400
H	8.23852400	1.20784300	0.99190900
H	5.76140700	-2.11676900	2.18530500
H	8.04456300	-1.13014300	1.88797600
C	2.56842300	0.66786700	-1.75113300
C	3.84165800	0.65985800	-2.33891800
C	1.42176000	0.66149400	-2.57951600
C	3.99365100	0.66852400	-3.72065000

H	4.71930000	0.63557300	-1.70320000
C	1.60629400	0.63693800	-3.97503700
C	2.86992600	0.65178700	-4.54907400
H	4.99303600	0.67062600	-4.14698800
H	0.71617800	0.61071300	-4.59327300
H	2.97803200	0.64433700	-5.62944600
N	4.76351000	-0.44759000	1.50942400
I	-4.43834100	-1.24507300	-1.96472200
C	-0.02152400	0.65383400	-2.14408400
O	-0.91604400	0.51620800	-2.94770800
C	-0.60339700	2.18006500	-0.87478200
C	0.31918900	3.15307600	-0.92489100
H	1.37218500	2.90345600	-0.96447700
C	-1.91119200	1.91396900	-0.51495600
H	-2.31297600	2.36287000	0.39030300
H	-2.63414300	1.51710500	-1.23129800
C	0.02937900	4.58961100	-0.99322600
C	1.10862200	5.48564200	-0.85873100
C	-1.26411500	5.11328200	-1.18025900
C	0.89586300	6.86179700	-0.88713000
H	2.10976500	5.08797700	-0.71411400
C	-1.47044300	6.48926900	-1.21296900
H	-2.10350500	4.43909300	-1.32053800
C	-0.39360600	7.36905900	-1.06391900
H	1.73790500	7.53932700	-0.77372600
H	-2.47390500	6.87782600	-1.36386200
H	-0.55917900	8.44261600	-1.09269000
28			
P	-2.24369000	2.26247600	-0.07790800
C	-4.10500500	2.32696500	-0.26768100
H	-4.29185700	2.38615200	-1.34625100
H	-4.43839400	3.28127800	0.15510600
C	-4.91146300	1.15638300	0.32241600
H	-5.95330000	1.48768500	0.42638900
H	-4.56620000	0.91453700	1.33526600
C	-4.89532500	-0.09458000	-0.57123900
H	-5.02944600	0.20864400	-1.61624500
H	-5.73754600	-0.75386700	-0.33447900
P	-3.32415800	-1.11628300	-0.53608700
C	-3.55601800	-2.02479100	-2.12723000
C	-4.53194100	-3.02495000	-2.25958400
C	-2.81255500	-1.64548300	-3.25372800
C	-4.75998500	-3.63064400	-3.49573700
H	-5.10733700	-3.34111100	-1.39428000
C	-3.04740700	-2.24766500	-4.49144900
H	-2.02873100	-0.90177600	-3.15241200

C	-4.01988500	-3.24130100	-4.61446400
H	-5.51370700	-4.40880200	-3.58325200
H	-2.45689100	-1.95093500	-5.35401900
H	-4.19567300	-3.71638100	-5.57599600
C	-3.68780100	-2.39485700	0.74778700
C	-2.92362200	-3.57426300	0.76895600
C	-4.69118500	-2.22591400	1.71450900
C	-3.17538000	-4.56315400	1.71884300
H	-2.12746100	-3.71660200	0.04564300
C	-4.93749900	-3.21675000	2.66797100
H	-5.29436200	-1.32412000	1.73652200
C	-4.18425000	-4.39064500	2.66923300
H	-2.57665100	-5.46980200	1.71548400
H	-5.72247400	-3.06870600	3.40516900
H	-4.37973900	-5.16446700	3.40692200
C	-1.75842600	3.42979600	-1.42383900
C	-1.26279600	2.91622200	-2.63205300
C	-1.96109100	4.81369000	-1.30266800
C	-0.98234800	3.76898100	-3.70131300
H	-1.08139300	1.84818800	-2.72296100
C	-1.67619600	5.66421800	-2.37168500
H	-2.33063600	5.23008600	-0.37011300
C	-1.18850800	5.14370600	-3.57259900
H	-0.59295200	3.35856500	-4.62894900
H	-1.83268900	6.73424600	-2.26437900
H	-0.96429500	5.80850200	-4.40243000
C	-1.94459000	3.21916200	1.47079400
C	-2.92820700	3.33580700	2.46764400
C	-0.67930200	3.78242200	1.70933900
C	-2.65276300	3.99788800	3.66591000
H	-3.91527900	2.90826200	2.32621100
C	-0.40391500	4.43679600	2.90893700
H	0.10593200	3.71127300	0.96766100
C	-1.38980000	4.54711600	3.89118000
H	-3.42750200	4.07785300	4.42380400
H	0.59228500	4.83633400	3.07169400
H	-1.17376800	5.05226500	4.82851600
Pd	-1.24949900	0.16219800	-0.28483700
S	4.62881100	-0.96217500	1.04718200
O	5.05111600	0.18754300	1.85143100
O	3.94761400	-2.11096300	1.64475100
N	3.64005400	-0.40573600	-0.16846300
H	3.06159600	-1.12930900	-0.59661700
C	6.13742400	-1.59006500	0.24105000
C	7.38162300	-1.25617000	0.77333900
C	8.50549500	-1.81613900	0.16403800

H	7.45052800	-0.58386800	1.62037000
C	7.02979800	-2.91376600	-1.37992000
C	8.32882900	-2.66253800	-0.93022100
H	9.50088100	-1.59206400	0.53729700
H	6.85167300	-3.56199600	-2.23535900
H	9.17685200	-3.11814500	-1.43215000
C	3.93737800	0.79263400	-0.88990500
C	4.68192600	0.72841200	-2.07286700
C	3.50779400	2.03846200	-0.39178400
C	5.01399500	1.89477200	-2.76200700
H	5.00518000	-0.24393100	-2.43171800
C	3.89575000	3.20307700	-1.06883600
C	4.63313300	3.13692000	-2.24918800
H	5.58513300	1.83335100	-3.68443900
H	3.59196400	4.15953500	-0.65504100
H	4.90774600	4.05060400	-2.76941100
N	5.94262300	-2.38717800	-0.80513200
I	0.22823800	-2.07672800	-1.01389800
C	2.62164200	2.20741300	0.82193000
O	2.78379400	3.18045900	1.54735300
C	1.45835700	1.25575300	1.01925000
C	1.38289100	0.66735600	2.22536000
H	2.20922700	0.88529000	2.90312200
C	0.60767900	1.17374400	-0.22480000
H	0.47070300	2.18943200	-0.61467800
H	1.16051300	0.64592100	-1.00553300
C	0.39077700	-0.28773900	2.77859200
C	0.80302200	-1.58967500	3.11246900
C	-0.91414600	0.10839800	3.10865200
C	-0.07610500	-2.47306900	3.73685900
H	1.81247100	-1.90621000	2.86696100
C	-1.78924000	-0.77678300	3.74454300
H	-1.22581200	1.12748900	2.91118300
C	-1.37554800	-2.07121700	4.05776500
H	0.25839300	-3.47888500	3.97869800
H	-2.79198300	-0.44680200	4.00645600
H	-2.05811000	-2.75985400	4.54780700
29			
P	-1.24305900	-0.97985500	-1.74954100
C	0.27199900	-0.46753700	-2.74038000
H	-0.03689300	-0.35988200	-3.78615300
H	0.99241300	-1.28805600	-2.69732100
C	0.98520700	0.80971900	-2.27011300
H	1.77443600	1.02078700	-3.00317500
H	1.50361200	0.59739900	-1.33138000
C	0.08781000	2.05706800	-2.13939100

H	-0.69523000	2.05175000	-2.90667300
H	0.67700900	2.96669400	-2.29830300
P	-0.78443800	2.20143200	-0.48941600
C	-2.13889500	3.40252200	-0.86234200
C	-1.91337300	4.48156100	-1.73673500
C	-3.38866200	3.27723900	-0.24294200
C	-2.92402500	5.40627300	-1.99265900
H	-0.94671700	4.61139700	-2.21474800
C	-4.39763500	4.21135100	-0.49819900
H	-3.58365800	2.44376800	0.42714800
C	-4.17026200	5.27284500	-1.37271100
H	-2.73768900	6.23346300	-2.67286200
H	-5.36190700	4.09684800	-0.01034000
H	-4.95670100	5.99618200	-1.57261200
C	0.35288000	3.26074600	0.51554900
C	-0.18219400	4.01475500	1.57484100
C	1.73834600	3.29792200	0.29730500
C	0.64533800	4.79253300	2.38388500
H	-1.25271400	4.00342300	1.75972600
C	2.56444800	4.08122200	1.10784500
H	2.18629600	2.71303700	-0.49963200
C	2.02262200	4.83060200	2.15186300
H	0.21123800	5.37384300	3.19300700
H	3.63498000	4.10239300	0.92111600
H	2.66675700	5.43962100	2.78033500
C	-2.64305000	-0.52583100	-2.86563800
C	-3.75213400	0.16052700	-2.35405500
C	-2.62318500	-0.86941100	-4.23057800
C	-4.81257800	0.51384400	-3.19516400
H	-3.80291300	0.39289600	-1.29435600
C	-3.68124100	-0.51584300	-5.06515500
H	-1.78824400	-1.42956800	-4.64331400
C	-4.77767400	0.18257700	-4.54843600
H	-5.66467000	1.04552000	-2.78118100
H	-3.65316200	-0.78849700	-6.11702200
H	-5.60243000	0.45829500	-5.20060100
C	-1.20173000	-2.82320400	-1.85963300
C	-0.00690900	-3.52528500	-1.61881700
C	-2.38087900	-3.55078200	-2.08921900
C	0.00580900	-4.92118400	-1.63075800
H	0.91300700	-2.99168000	-1.39919600
C	-2.36211700	-4.94695300	-2.09591400
H	-3.31564000	-3.02934900	-2.26841300
C	-1.16929400	-5.63661600	-1.87073700
H	0.93889100	-5.44715400	-1.44713900
H	-3.28369100	-5.49323500	-2.27883400

H	-1.15608600	-6.72326200	-1.87802800
Pd	-1.14174200	0.00539600	0.44431300
S	4.61485000	-1.13667100	-0.76062200
O	4.75512700	-2.21003500	0.22189600
O	3.86891500	-1.32250300	-2.00546200
N	4.08798900	0.32171100	-0.01499000
H	4.69745200	1.05158800	-0.39364500
C	6.30732200	-0.65479300	-1.25145300
C	7.26045200	-1.65603200	-1.42986700
C	8.52175900	-1.26173200	-1.87442100
H	7.01911700	-2.69113700	-1.21600100
C	7.73830800	1.00799700	-1.88036500
C	8.76591700	0.09290000	-2.10872000
H	9.30315000	-1.99986800	-2.03057200
H	7.89071600	2.07308400	-2.03783500
H	9.73525600	0.43801300	-2.45381700
C	3.96231600	0.39909400	1.40355900
C	4.95637900	1.06504100	2.13032500
C	2.80608300	-0.07291800	2.07265100
C	4.84251800	1.24281100	3.50773800
H	5.83219300	1.43486300	1.60308100
C	2.72212400	0.10302900	3.46352400
C	3.72784000	0.74489200	4.18195400
H	5.63124900	1.75513800	4.05166700
H	1.85361300	-0.27908300	3.98837200
H	3.63803200	0.85841800	5.25807700
N	6.52031800	0.64192500	-1.45710300
C	1.71793000	-0.78521100	1.33270800
O	1.97894100	-1.42390400	0.31836600
C	0.31324500	-0.77485600	1.89890700
C	-0.47519400	-1.93212100	1.62416700
H	-0.03374000	-2.60276700	0.89198100
C	-0.29878600	0.38879500	2.44088200
C	-1.46606800	-2.58487100	2.49055500
C	-2.20569100	-3.66109800	1.96196100
C	-1.63154800	-2.27200200	3.85275800
C	-3.09965200	-4.37350100	2.75425300
H	-2.08109200	-3.92415500	0.91581800
C	-2.51897200	-2.99299700	4.64690200
H	-1.04547000	-1.47688400	4.30055900
C	-3.26235900	-4.04183600	4.10154100
H	-3.66943800	-5.19074100	2.32045400
H	-2.62816100	-2.73620400	5.69719900
H	-3.95747200	-4.59988200	4.72299100
H	-1.18971000	0.32145800	3.05367900
H	0.28569100	1.29700700	2.54541000

I	-3.99856600	-0.05117100	1.56447300
30-ts			
P	1.52712100	-1.15088800	1.59709700
C	0.15906400	-0.39853900	2.63907700
H	0.48760500	-0.40122400	3.68452000
H	-0.71832100	-1.04481600	2.56809800
C	-0.27269800	1.02261700	2.23505800
H	-1.04505700	1.33566800	2.94845500
H	-0.76544700	0.99184800	1.25713500
C	0.86427000	2.06553800	2.23396800
H	1.59002800	1.83549700	3.02251900
H	0.47305800	3.06374800	2.45616000
P	1.83198100	2.12799100	0.63249600
C	3.44603600	2.86244500	1.16401300
C	3.49848700	3.78927500	2.22044400
C	4.62385800	2.55450100	0.47082900
C	4.70710200	4.38366100	2.58065000
H	2.59745000	4.06092200	2.76247800
C	5.83218700	3.15755100	0.83163400
H	4.60718900	1.82726500	-0.33689800
C	5.87824300	4.06932700	1.88562200
H	4.73283800	5.09581400	3.40152800
H	6.73602500	2.90283800	0.28452800
H	6.81939600	4.53501000	2.16675100
C	1.12611900	3.55663100	-0.30848300
C	1.86000700	4.04143200	-1.40582800
C	-0.09723300	4.16438600	0.00110400
C	1.38853100	5.11379300	-2.16118000
H	2.81056300	3.58338600	-1.66619600
C	-0.56480500	5.24460000	-0.75327900
H	-0.69874500	3.80108500	0.82784100
C	0.17406900	5.72295300	-1.83472100
H	1.97436700	5.47676800	-3.00141100
H	-1.50814700	5.71537900	-0.48832300
H	-0.19070100	6.56415100	-2.41807300
C	3.00392300	-1.06418500	2.70479300
C	4.23587200	-0.61865500	2.20984500
C	2.91527600	-1.47053400	4.04963200
C	5.35318400	-0.55814400	3.04937600
H	4.33169900	-0.34652000	1.16337600
C	4.03015700	-1.40929600	4.88265200
H	1.97854000	-1.85279500	4.44651800
C	5.25242500	-0.94632000	4.38386900
H	6.29970900	-0.20648500	2.64884200
H	3.94738000	-1.72645100	5.91905400
H	6.12150100	-0.89756200	5.03496800

C	1.15433400	-2.95956900	1.58102700
C	-0.15680700	-3.43109700	1.39598000
C	2.20627600	-3.88877300	1.64709900
C	-0.40459100	-4.80217700	1.29913400
H	-0.99357700	-2.74318300	1.32794300
C	1.95145700	-5.25746400	1.54732000
H	3.22753400	-3.54543800	1.77609500
C	0.64512400	-5.71953400	1.37490100
H	-1.42532200	-5.14992300	1.16230100
H	2.77803600	-5.96083100	1.60318200
H	0.44761700	-6.78550100	1.29796500
Pd	1.58550900	-0.00464100	-0.50126400
S	-3.92135300	-0.49987600	1.41927500
O	-2.81449900	-1.45070300	1.66426800
O	-4.03436200	0.69631600	2.27601200
N	-3.94088300	0.02302900	-0.10918400
H	-4.34251600	1.24852900	-0.28601600
C	-5.42342400	-1.48773700	1.76882000
C	-5.30059800	-2.68051200	2.48251500
C	-6.47199900	-3.37297700	2.79013900
H	-4.32051800	-3.03743600	2.77427400
C	-7.69605800	-1.65071100	1.65677700
C	-7.69537400	-2.85011500	2.37194500
H	-6.42816700	-4.30601400	3.34519200
H	-8.62962200	-1.21355100	1.30772100
H	-8.63034000	-3.35732100	2.58908700
C	-3.69790300	-0.87344100	-1.18300600
C	-4.69755800	-1.78899300	-1.55119100
C	-2.48723400	-0.85210100	-1.92978600
C	-4.52882600	-2.66986200	-2.61727800
H	-5.62712100	-1.78223600	-0.99238400
C	-2.34168000	-1.74938500	-3.00504800
C	-3.34544500	-2.64874900	-3.35395600
H	-5.32621200	-3.36170300	-2.87644800
H	-1.42896600	-1.73298900	-3.59031200
H	-3.20201800	-3.32086400	-4.19484300
N	-6.58101300	-0.97369700	1.35687000
C	-1.40587000	0.16743400	-1.70415800
O	-1.67695100	1.32577200	-1.39979100
C	0.01411000	-0.24657100	-2.03810700
C	0.48560400	-1.57485100	-1.78012000
H	-0.14984300	-2.15890300	-1.11739900
C	0.92630500	0.74721300	-2.47082000
C	1.30757100	-2.42347100	-2.66467800
C	1.73558000	-3.67733200	-2.18948400
C	1.57387000	-2.09696100	-4.00709500

C	2.42850500	-4.55733600	-3.01454700
H	1.52713200	-3.95377200	-1.16091800
C	2.25956100	-2.98343000	-4.83460300
H	1.23079800	-1.15104100	-4.41297200
C	2.69607000	-4.21459300	-4.34237100
H	2.75920400	-5.51459400	-2.62039400
H	2.45267600	-2.70988700	-5.86851800
H	3.23495600	-4.90246000	-4.98834900
H	1.81224100	0.49535300	-3.04113800
H	0.57504200	1.77221700	-2.52651500
I	4.39639600	-0.57395200	-1.72107100
N	-4.80110400	2.42859500	-0.48267900
C	-4.75289600	2.53001400	-1.97319600
C	-4.82146000	3.92182700	-2.60635000
H	-5.56474900	1.89791800	-2.34956700
H	-3.80884500	2.05979600	-2.26303000
H	-4.81127300	3.80547600	-3.69631100
H	-5.72486700	4.47516900	-2.33739700
H	-3.94927800	4.52654900	-2.33989600
C	-3.83238000	3.29901400	0.25361700
C	-4.28643400	4.71300200	0.62524800
H	-2.92625700	3.32349200	-0.35546900
H	-3.59010400	2.74914300	1.16784200
H	-3.46525600	5.21049000	1.15507200
H	-4.54391700	5.32811600	-0.24138800
H	-5.14233000	4.70163300	1.30748000
C	-6.16665000	2.33814600	0.12114100
C	-7.22345600	3.34908600	-0.32968800
H	-6.02027000	2.38186700	1.20371600
H	-6.52238800	1.32393500	-0.08577900
H	-8.14641000	3.15408500	0.22878200
H	-6.93473800	4.38662200	-0.14214800
H	-7.46181500	3.24537500	-1.39321700

31

S	4.59793700	0.17130500	-1.37612200
O	3.79384000	-0.42094700	-2.47138000
O	5.12376300	1.53414900	-1.58702800
C	6.04076400	-0.94023400	-1.22538100
C	6.08996900	-2.11123400	-1.98437600
C	7.20691500	-2.93214600	-1.83570500
H	5.27684500	-2.34489200	-2.66068500
C	8.05262700	-1.35881000	-0.23650600
C	8.21118600	-2.55185500	-0.94450700
H	7.29306700	-3.85269700	-2.40741300
H	8.81288100	-1.02719400	0.46895600
H	9.09821700	-3.16123100	-0.79870500

N	6.98881000	-0.56014100	-0.37118700
C	5.16623000	2.14949000	2.64959200
C	5.06260300	1.50749400	1.43285600
C	3.91435300	0.72121200	1.10530700
C	2.85612700	0.68894500	2.08073000
C	3.01683500	1.33366900	3.33354800
C	4.14748800	2.06588200	3.62482800
H	6.06707900	2.72103200	2.86461400
H	5.87415200	1.56065800	0.71987800
C	1.57653100	0.03164800	1.84989800
H	2.20603400	1.24250800	4.04971000
H	4.25683000	2.56551900	4.58342200
C	0.93987700	0.66936600	-0.52374900
H	0.83692900	0.42605000	-1.57651600
O	0.75524000	-0.17328200	2.76112200
C	1.14329300	-0.35255000	0.43211800
C	0.48999800	-1.60537800	0.27034400
H	0.39431200	-2.18546700	1.18610800
N	3.75063100	-0.04235500	-0.01086900
H	1.32856800	1.65988700	-0.31481000
C	0.35516400	-2.40473900	-0.97052100
C	1.13365600	-2.17252500	-2.12052200
C	-0.52783000	-3.50405200	-0.96874500
C	0.98621700	-2.98863600	-3.24365800
H	1.89905100	-1.40192400	-2.12739600
C	-0.66966800	-4.31359400	-2.09288300
H	-1.10498900	-3.71958600	-0.07258400
C	0.08052100	-4.05144200	-3.24347700
H	1.60620800	-2.79783600	-4.11572300
H	-1.35912500	-5.15377400	-2.06809200
H	-0.02343000	-4.68505900	-4.12060700
P	-2.98058600	-0.96363700	1.08665900
C	-3.93028600	0.17907600	2.21508100
H	-3.27732800	0.34817900	3.08039300
H	-4.80897700	-0.35467700	2.59509700
C	-4.35551000	1.52660800	1.60111200
H	-5.10751300	1.96744300	2.26835800
H	-4.86380800	1.36596400	0.64198200
C	-3.22519400	2.55928800	1.44227100
H	-2.63115700	2.60784200	2.36348400
H	-3.64623500	3.56151600	1.30156600
P	-1.99226900	2.24298300	0.07916600
C	-0.82503500	3.64470500	0.33706300
C	-0.80722900	4.78719600	-0.47450000
C	0.09374100	3.54177100	1.39633300
C	0.11248000	5.80944000	-0.22666600

H	-1.49956600	4.88058800	-1.30516900
C	1.00870400	4.56473600	1.64100400
H	0.11532600	2.64965100	2.01760100
C	1.01974900	5.70093800	0.82774700
H	0.12325800	6.68695800	-0.86749900
H	1.72842800	4.45501300	2.44694300
H	1.74280200	6.49146300	1.00773400
C	-2.88517200	2.60248600	-1.48692600
C	-3.93644200	3.52977900	-1.57749400
C	-2.47992300	1.92437700	-2.64832900
C	-4.56495700	3.77127400	-2.80009400
H	-4.26934200	4.07415900	-0.69885300
C	-3.10304000	2.17355200	-3.87174000
H	-1.67539700	1.19643500	-2.58900800
C	-4.14822400	3.09563000	-3.94904900
H	-5.37854900	4.48951100	-2.85415400
H	-2.77341600	1.64401300	-4.76114700
H	-4.63764200	3.28670700	-4.90007500
C	-2.76212500	-2.43865000	2.17212600
C	-1.72508800	-2.40031600	3.12160600
C	-3.58625400	-3.57190600	2.09896100
C	-1.53626100	-3.47345400	3.99396900
H	-1.04636100	-1.55104700	3.15947600
C	-3.38316700	-4.64592300	2.96860900
H	-4.38211000	-3.62419900	1.36261800
C	-2.36267900	-4.59708700	3.91973000
H	-0.73076100	-3.43358900	4.72204700
H	-4.02388100	-5.52108600	2.89925400
H	-2.20625100	-5.43483400	4.59394700
C	-4.20488300	-1.46083500	-0.19536500
C	-5.58432900	-1.55692300	0.05529700
C	-3.73057400	-1.76250900	-1.48247400
C	-6.46496700	-1.94382100	-0.95606600
H	-5.98193600	-1.33578300	1.04145800
C	-4.61162300	-2.15718900	-2.49072400
H	-2.66724800	-1.69621200	-1.69244500
C	-5.97991800	-2.24550400	-2.23066700
H	-7.52927100	-2.01031000	-0.74697000
H	-4.22561600	-2.39202400	-3.47868500
H	-6.66675100	-2.54699900	-3.01685000
Pd	-1.03400500	0.10636700	0.23134700
32-ts			
S	4.41309700	0.15069000	-1.35723300
O	3.50661600	-0.19049500	-2.47843700
O	5.11294700	1.44639900	-1.40515600
C	5.69041400	-1.15602600	-1.38258800

C	5.56904900	-2.21425100	-2.28521900
C	6.56620700	-3.18872100	-2.27308600
H	4.72642700	-2.24917300	-2.96460700
C	7.63793400	-1.96157900	-0.51380100
C	7.62252000	-3.06430900	-1.36995300
H	6.51995200	-4.03050700	-2.95901100
H	8.44438700	-1.82704300	0.20486800
H	8.41924300	-3.80091400	-1.32795300
N	6.69167500	-1.01661500	-0.51793300
C	5.35933500	1.32161800	2.92050100
C	5.10251600	0.90124800	1.62617100
C	3.85050500	0.33938200	1.26148400
C	2.85981800	0.21981000	2.30325300
C	3.17021900	0.64757100	3.61332700
C	4.39473000	1.20285800	3.93434400
H	6.33352800	1.74954700	3.14722900
H	5.87052700	0.99339300	0.87052300
C	1.51072100	-0.37399700	2.13704700
H	2.40135300	0.51622500	4.36814000
H	4.60887000	1.52914300	4.94809300
C	1.40168200	0.31053000	-0.24339900
H	1.29275700	0.15330300	-1.30699500
O	0.80008500	-0.67357600	3.10150700
C	1.01852100	-0.63152900	0.72887100
C	0.20482300	-1.77493300	0.49658200
H	-0.04470500	-2.32026800	1.40358200
N	3.54218800	-0.11837400	-0.00675900
H	1.69530200	1.30317000	0.06680800
C	0.07226400	-2.58214900	-0.74065700
C	0.90496200	-2.44600400	-1.86935600
C	-0.90399900	-3.60104200	-0.75940600
C	0.72707300	-3.26823700	-2.98378900
H	1.72402700	-1.73546900	-1.87627400
C	-1.07471400	-4.42018300	-1.87196900
H	-1.53496900	-3.74245800	0.11492900
C	-0.26454000	-4.25044200	-2.99879700
H	1.38477700	-3.14341900	-3.84018700
H	-1.83637300	-5.19571900	-1.85710400
H	-0.39279300	-4.88957500	-3.86847100
P	-3.22546200	-0.63102800	0.89783900
C	-4.09587100	0.68958200	1.89331000
H	-3.54056200	0.75871500	2.83704000
H	-5.09775000	0.33126600	2.15722500
C	-4.18879600	2.08047600	1.23436700
H	-4.95290800	2.64959200	1.78007600
H	-4.56100800	1.99304200	0.20562400

C	-2.89409500	2.91466300	1.26293900
H	-2.45059500	2.88205000	2.26615700
H	-3.12368500	3.96865300	1.06755300
P	-1.53881600	2.36864200	0.09871400
C	-0.21341000	3.58309900	0.51508800
C	0.10158000	4.69361700	-0.28098000
C	0.53422400	3.34887800	1.68281800
C	1.13822700	5.55388300	0.08933200
H	-0.45026100	4.88601400	-1.19555800
C	1.56561200	4.21157700	2.05159800
H	0.32716900	2.47461800	2.29598700
C	1.87020100	5.31670900	1.25324900
H	1.37834500	6.40545800	-0.54159100
H	2.14656100	4.00090800	2.94481700
H	2.68474300	5.98023100	1.52966200
C	-2.14000600	2.84131000	-1.57542800
C	-2.96761700	3.95051200	-1.81702800
C	-1.73617300	2.05247200	-2.66519600
C	-3.37742600	4.26180100	-3.11448400
H	-3.29360100	4.58407500	-0.99727100
C	-2.13969000	2.36871900	-3.96325700
H	-1.10551500	1.18438300	-2.49131900
C	-2.96299500	3.47275400	-4.18978200
H	-4.01875400	5.12248900	-3.28450600
H	-1.81249400	1.74994100	-4.79406800
H	-3.28180800	3.71773200	-5.19923500
C	-3.38770800	-2.07876000	2.03243300
C	-2.43571300	-2.21025600	3.05959100
C	-4.41492800	-3.02813500	1.92616900
C	-2.52794600	-3.26241700	3.97205500
H	-1.60668700	-1.50940300	3.13576100
C	-4.49454100	-4.08545400	2.83539300
H	-5.15091000	-2.94901100	1.13200200
C	-3.55540000	-4.20237200	3.86155500
H	-1.78500800	-3.35251800	4.75976100
H	-5.29201800	-4.81773200	2.73913100
H	-3.61879600	-5.02671200	4.56683800
C	-4.37200300	-0.97127000	-0.50456800
C	-5.75858400	-0.75261300	-0.44367400
C	-3.82118600	-1.47529100	-1.69465100
C	-6.57147000	-1.03055700	-1.54418400
H	-6.21617000	-0.36635600	0.46219100
C	-4.63626000	-1.76178900	-2.79069900
H	-2.75120100	-1.64911600	-1.75925700
C	-6.01210100	-1.53679300	-2.71921500
H	-7.64168900	-0.85209100	-1.48168000

H	-4.19233900	-2.15557200	-3.70080600
H	-6.64610500	-1.75243500	-3.57501800
Pd	-1.02727500	0.07649600	0.35078300
33-ts			
P	1.75851700	-0.95977000	1.34999100
C	2.41858000	0.10257000	2.72909400
H	3.22181800	0.68839600	2.26796300
H	2.88514700	-0.56404000	3.46298700
C	1.44193800	1.06175300	3.42533800
H	1.97332800	1.47691800	4.29155500
H	0.57700600	0.52379800	3.83272900
C	0.99086600	2.25107800	2.56400100
H	1.84627900	2.65736300	2.01210700
H	0.59359800	3.04757100	3.20296300
P	-0.33096000	1.86698300	1.30869200
C	-0.74214700	3.55789200	0.70147400
C	-2.05610000	4.05101200	0.68148400
C	0.30264300	4.36405500	0.21554800
C	-2.31726900	5.34054100	0.21460700
H	-2.87814800	3.43549300	1.03213300
C	0.03264300	5.65129700	-0.24926400
H	1.32284300	3.98921200	0.17377800
C	-1.27378100	6.14503700	-0.24617300
H	-3.33862500	5.71243900	0.21087100
H	0.85064400	6.26245000	-0.61996900
H	-1.47842900	7.14971700	-0.60711300
C	-1.74772500	1.39837100	2.39645200
C	-2.37794600	0.15460300	2.27099400
C	-2.16747200	2.26813300	3.42145700
C	-3.39931500	-0.21646800	3.15009300
H	-2.07836100	-0.53647400	1.49349400
C	-3.18970600	1.89916900	4.29314900
H	-1.70280100	3.24333200	3.53333300
C	-3.80688100	0.65155200	4.16092000
H	-3.86396600	-1.19067000	3.03652900
H	-3.50238800	2.58402200	5.07687900
H	-4.60013400	0.36222700	4.84539100
C	3.24835700	-2.01963500	1.06248600
C	4.50510900	-1.41012600	0.90042400
C	3.16866100	-3.42109100	1.08252100
C	5.65683300	-2.19212200	0.80641700
H	4.59051700	-0.32823800	0.83214500
C	4.32427700	-4.19604500	0.97443100
H	2.20989000	-3.91384100	1.20432500
C	5.57247800	-3.58454200	0.84793700
H	6.62100100	-1.70330700	0.69440400

H	4.24562700	-5.27988900	1.00012500
H	6.47252500	-4.19002700	0.77796200
C	0.58726100	-2.13091700	2.16448600
C	0.61794100	-2.40312200	3.54204900
C	-0.34927700	-2.80691800	1.36710700
C	-0.27417500	-3.31708100	4.10476900
H	1.34013500	-1.91071700	4.18487100
C	-1.23657800	-3.72779700	1.92810500
H	-0.39309600	-2.62645300	0.29752400
C	-1.20320900	-3.98100700	3.30024600
H	-0.23906200	-3.51237200	5.17340800
H	-1.95638000	-4.22510700	1.28591900
H	-1.89414500	-4.69416200	3.74259400
Pd	0.59622300	0.35853100	-0.39041800
S	-3.02847800	-1.97655300	-1.84209900
O	-3.42918600	-1.79882000	-3.24134100
O	-2.01071800	-2.95923400	-1.45697900
N	-2.49114600	-0.50775300	-1.18974300
H	-1.53157800	-0.60937100	-0.84244500
C	-4.55709100	-2.37048500	-0.93515300
C	-5.73266400	-2.54952900	-1.66268800
C	-6.87243600	-2.91929000	-0.94517000
H	-5.74030400	-2.40765800	-2.73667500
C	-5.53506100	-2.88398400	1.04870300
C	-6.77389700	-3.08998100	0.43434900
H	-7.81681500	-3.07401700	-1.45881300
H	-5.42052600	-3.01158800	2.12276900
H	-7.63482300	-3.37923600	1.02875500
C	-2.80096500	0.74509100	-1.78472200
C	-4.15156100	1.05152300	-2.00436300
C	-1.80764800	1.68983900	-2.14112600
C	-4.53041800	2.24985700	-2.59873300
H	-4.90894400	0.33853700	-1.69770100
C	-2.22220700	2.90429700	-2.71888800
C	-3.56014800	3.18581700	-2.96081600
H	-5.58455400	2.45534900	-2.76329200
H	-1.45051800	3.62294100	-2.96984100
H	-3.84386100	4.13035200	-3.41519100
N	-4.43462900	-2.52878200	0.37730100
I	4.01488400	2.45249000	-0.08799100
C	-0.31466500	1.57819400	-1.93540300
O	0.43429700	2.46741000	-2.27523800
C	0.54279400	-0.16510500	-2.57188800
C	1.88907600	-0.22028400	-2.21692100
H	2.43833400	0.71892300	-2.11001500
C	-0.21165700	-0.60891200	-3.57837500

H	0.28796800	-0.96137000	-4.48107100
H	-1.29266700	-0.58990500	-3.60532200
C	2.70433700	-1.42484600	-2.38701100
C	4.10181600	-1.26160200	-2.45063400
C	2.15302500	-2.70182600	-2.62070000
C	4.92125600	-2.33833600	-2.78182700
H	4.52814700	-0.28236300	-2.24883700
C	2.97949600	-3.77461500	-2.93574100
H	1.07853900	-2.84525200	-2.55742300
C	4.36465000	-3.59510700	-3.02576400
H	5.99645800	-2.19587400	-2.84166600
H	2.54464200	-4.75433200	-3.11464700
H	5.00589800	-4.43506800	-3.27953600
34			
P	-1.17596900	2.24042400	0.31636800
C	-2.41631500	3.43514600	1.07295300
H	-2.91452600	3.91364600	0.22228200
H	-1.82356300	4.21513700	1.56332800
C	-3.49117000	2.89201100	2.02682500
H	-3.93265100	3.75252900	2.54700200
H	-3.05754600	2.26054200	2.81222400
C	-4.61661700	2.14505300	1.29789700
H	-4.91292300	2.70936100	0.40531200
H	-5.49718000	2.07651200	1.94537600
P	-4.16505200	0.40513900	0.74962900
C	-5.45302400	0.12333300	-0.54288500
C	-6.76495300	0.61055100	-0.39718400
C	-5.10622600	-0.52741700	-1.73743700
C	-7.70585000	0.43986800	-1.41317600
H	-7.06242400	1.12644200	0.51105700
C	-6.04876800	-0.69244000	-2.75501600
H	-4.10303300	-0.91935300	-1.86451600
C	-7.34891800	-0.21234700	-2.59550800
H	-8.71586100	0.81885600	-1.28073000
H	-5.76085300	-1.20106200	-3.67087800
H	-8.08136300	-0.34332100	-3.38767600
C	-4.66406200	-0.53794500	2.25598900
C	-5.92680300	-1.12179200	2.42148400
C	-3.73210700	-0.62782600	3.30249600
C	-6.25463200	-1.76823900	3.61523300
H	-6.65174100	-1.09388700	1.61480300
C	-4.06624900	-1.26217200	4.49877300
H	-2.72849000	-0.23314700	3.16711200
C	-5.33013500	-1.83398000	4.65856100
H	-7.23383500	-2.22707000	3.72450900
H	-3.33144300	-1.32741200	5.29683900

H	-5.58751800	-2.33982300	5.58525700
C	-0.78079900	3.20735800	-1.20585900
C	-1.53870600	2.94501000	-2.35859000
C	0.13616400	4.26933500	-1.22291500
C	-1.38083900	3.72529100	-3.50491400
H	-2.24449300	2.11805600	-2.36021700
C	0.30060300	5.04034700	-2.37520100
H	0.73005000	4.49322200	-0.34296100
C	-0.45635600	4.77158200	-3.51672900
H	-1.97094700	3.50583200	-4.39055200
H	1.02350000	5.85153400	-2.37795600
H	-0.32418100	5.37245100	-4.41234400
C	0.28093500	2.43115300	1.42894100
C	0.08870400	2.66087800	2.80290700
C	1.59366200	2.31091600	0.94395900
C	1.17990100	2.78552900	3.66295200
H	-0.91153700	2.74911400	3.21476900
C	2.68531500	2.44920700	1.80420700
H	1.78604000	2.10482200	-0.10294300
C	2.48014700	2.68864200	3.16382200
H	1.01012100	2.96740000	4.72109900
H	3.68943300	2.36806000	1.39908900
H	3.33016200	2.79916100	3.83209300
Pd	-1.87349900	0.03223700	-0.01006500
S	6.06220700	0.72404200	-0.18482200
O	5.90567000	0.34977900	-1.58555500
O	5.85237900	2.09425800	0.28868700
N	5.08482700	-0.25983300	0.79201400
H	5.43865800	-0.18478400	1.74571800
C	7.75976400	0.27092600	0.29959400
C	8.75283300	0.18878100	-0.67352500
C	10.04762000	-0.09679700	-0.23770200
H	8.50751500	0.33431600	-1.71924700
C	9.19514500	-0.19561300	2.00577500
C	10.27537500	-0.28957200	1.12511200
H	10.86276800	-0.17250300	-0.95176000
H	9.33077600	-0.35115000	3.07384400
H	11.26745900	-0.51567300	1.50310600
C	4.78700700	-1.60863100	0.39193300
C	5.68110200	-2.64399500	0.68759900
C	3.54692700	-1.89799600	-0.21002200
C	5.37796100	-3.96237400	0.34999500
H	6.61533500	-2.40703100	1.18854900
C	3.25734900	-3.23016600	-0.53825700
C	4.16810400	-4.25359000	-0.28033100
H	6.08474200	-4.75537000	0.57843400

H	2.30613400	-3.45816900	-1.00723700
H	3.92465000	-5.27575000	-0.55588400
N	7.94868600	0.08216400	1.60381800
I	-2.56370800	-2.67093200	0.11710400
C	2.53144600	-0.82311300	-0.53167700
O	2.86370500	0.17604600	-1.15229100
C	1.10655300	-1.01701200	-0.06488000
C	0.90707600	-1.65210600	1.10136100
C	0.05937800	-0.35467500	-0.93314100
H	1.73340800	-2.08951400	1.65479000
H	-0.08245100	-1.74434300	1.53314800
C	-0.14758100	-1.04603900	-2.25661400
C	-0.07926800	-2.44415500	-2.40989400
C	-0.36690900	-0.27949900	-3.41762900
C	-0.23952700	-3.04408200	-3.65794900
H	0.07297500	-3.06539300	-1.53476600
C	-0.53830700	-0.87757000	-4.66540300
H	-0.38005700	0.80331000	-3.34018700
C	-0.47778500	-2.26678700	-4.79379900
H	-0.18453500	-4.12681600	-3.74121500
H	-0.69971900	-0.25466900	-5.54231100
H	-0.60307300	-2.73644100	-5.76604200
H	0.44809000	0.63582700	-1.17700200
35			
S	-1.01086900	-1.70131100	0.56358400
O	-0.65888000	-2.82711600	-0.30372000
O	-1.19804700	-1.90336600	2.00262600
C	-2.54922000	-0.94322300	-0.04398100
C	-3.68287400	-0.94809800	0.76543900
C	-4.84192400	-0.38375300	0.22866800
H	-3.64633400	-1.37076100	1.76225600
C	-3.59685200	0.10148700	-1.76848700
C	-4.80038100	0.14982700	-1.05894200
H	-5.75906900	-0.35901900	0.81017100
H	-3.52135900	0.51562700	-2.77128200
H	-5.67939400	0.60085800	-1.50860100
N	-2.48141900	-0.44174800	-1.27068000
C	-0.10340200	2.05249500	3.00260500
C	-0.02592800	0.80511500	2.38648500
C	0.11489200	0.72311400	0.99401200
C	0.20321200	1.90878000	0.23156500
C	0.13391300	3.15270100	0.87538700
C	-0.02370800	3.23166800	2.25308800
H	-0.20960100	2.10172200	4.08300800
H	-0.07195700	-0.10495000	2.96988500
C	0.35435600	1.87334000	-1.24779300

H	0.20185300	4.04269700	0.25794200
H	-0.07546700	4.19868300	2.74488300
C	1.02853800	-0.59387900	-0.91040300
H	0.77121800	-1.53845000	-1.39093900
O	0.22021100	2.88354100	-1.93124500
C	0.68190500	0.54291400	-1.85121800
C	0.68112900	0.40672500	-3.18182100
H	0.45578800	1.26035600	-3.81382100
N	0.19848300	-0.53501900	0.32865800
C	2.50742300	-0.66305200	-0.50615200
C	2.93955900	-1.77416400	0.23344100
C	3.43818800	0.31977100	-0.85489900
C	4.27213000	-1.89544400	0.61980200
H	2.22267900	-2.54525800	0.50356000
C	4.77538500	0.20119600	-0.46311700
H	3.13060400	1.17743000	-1.44451800
C	5.19583000	-0.90385800	0.27475900
H	4.59159000	-2.76500600	1.18810900
H	5.48541600	0.97626100	-0.73930500
H	6.23562700	-0.99671600	0.57686200
H	0.90357300	-0.54157500	-3.66331300
36-ts			
P	1.63870000	-1.46587900	-1.22689200
C	1.52780300	-0.70686800	-2.92795500
H	0.47415500	-0.45409400	-3.08913800
H	1.80171600	-1.46027800	-3.67532200
C	2.40008700	0.54936400	-3.12402600
H	2.47092100	0.73065100	-4.20490700
H	3.42373400	0.34952900	-2.78645800
C	1.86716300	1.85114600	-2.49363700
H	0.82456100	2.00371300	-2.79012900
H	2.43838400	2.70685800	-2.87341100
P	1.83898200	1.95444400	-0.63457500
C	1.31024300	3.71257700	-0.38252700
C	2.20701600	4.70053700	0.05287400
C	-0.02240400	4.07463600	-0.64234000
C	1.78291800	6.02056700	0.21804500
H	3.23854200	4.44603700	0.26888300
C	-0.43904500	5.39643900	-0.48047400
H	-0.73107100	3.31922600	-0.96267000
C	0.46007800	6.37364500	-0.04926800
H	2.49107600	6.77122400	0.55936200
H	-1.47429000	5.65961000	-0.68279000
H	0.13088100	7.40116800	0.08236000
C	3.60637100	1.97921000	-0.10650000
C	3.88587200	1.76317400 _{S153}	1.25530700

C	4.66993000	2.22791800	-0.98755500
C	5.20235800	1.79346900	1.71667700
H	3.06923300	1.58493700	1.94992300
C	5.98715300	2.24412000	-0.52275100
H	4.48352200	2.41446400	-2.04060700
C	6.25592300	2.02667100	0.82925600
H	5.40219800	1.62877000	2.77208900
H	6.80083800	2.42960400	-1.21909400
H	7.28119200	2.04190600	1.18983100
C	0.78978700	-3.09091000	-1.45229300
C	-0.25041900	-3.26547500	-2.37824900
C	1.18021200	-4.18275600	-0.65781400
C	-0.86734600	-4.51110600	-2.52215800
H	-0.60589700	-2.43365500	-2.97408900
C	0.56017400	-5.42367400	-0.80367200
H	1.97162600	-4.06328800	0.07451700
C	-0.46225600	-5.59407300	-1.74071300
H	-1.66638100	-4.62967600	-3.24964500
H	0.88121300	-6.25845000	-0.18608900
H	-0.93965100	-6.56349900	-1.85901800
C	3.40843100	-1.98070800	-1.10629000
C	4.11947700	-1.72398700	0.07384500
C	4.05730000	-2.64621300	-2.16087200
C	5.45557400	-2.11692100	0.19451200
H	3.62006500	-1.23323600	0.90247500
C	5.39138500	-3.03191000	-2.04132200
H	3.51802300	-2.87741700	-3.07576100
C	6.09372300	-2.76628500	-0.86172000
H	5.99218700	-1.91199900	1.11664200
H	5.88155400	-3.54476700	-2.86496700
H	7.13312400	-3.07031700	-0.76791400
Pd	0.80994200	0.13509000	0.46668700
S	-2.37116800	0.43599200	-1.38893100
O	-1.31242600	1.39253100	-1.78357200
O	-2.38881900	-0.87924700	-2.05574200
N	-2.38968300	0.15192200	0.21651000
H	-2.99829300	-0.92974900	0.55336500
C	-3.90544800	1.29873700	-1.93192100
C	-3.78888900	2.42790000	-2.74414500
C	-4.96568000	3.01367700	-3.21188300
H	-2.81006300	2.81618600	-2.99518600
C	-6.18624200	1.32491100	-2.02900300
C	-6.19017600	2.45321600	-2.85097000
H	-4.92420300	3.89361200	-3.84794500
H	-7.11996500	0.85914800	-1.71998800
H	-7.12905300	2.87718400	-3.19339500

C	-2.50582500	1.25986800	1.12556900
C	-3.80574500	1.74402900	1.37098400
C	-1.42691500	1.81617200	1.85898800
C	-4.05829600	2.76316300	2.28361700
H	-4.62590600	1.29230700	0.82362900
C	-1.71098800	2.84677600	2.77824600
C	-2.99682600	3.32531300	2.99272000
H	-5.07703700	3.10885700	2.44075200
H	-0.87258400	3.25561500	3.33037000
H	-3.16882000	4.12142600	3.71219100
N	-5.06492900	0.75283500	-1.57486200
C	0.05992500	1.44248100	1.80540500
O	0.81086000	1.98924000	2.59189200
N	-3.60746900	-2.08068300	0.91340600
C	-4.21969500	-1.89811100	2.26092000
C	-3.24126000	-1.48178000	3.35659600
H	-4.72956700	-2.82298200	2.55611900
H	-4.99285900	-1.13017500	2.14281700
H	-3.80024700	-1.34334500	4.28920100
H	-2.46754400	-2.23201100	3.53591600
H	-2.73755900	-0.54116200	3.12359400
C	-2.49460300	-3.08519000	0.87200000
C	-2.72346900	-4.44510400	1.53692600
H	-1.62892200	-2.61048000	1.33889300
H	-2.24472900	-3.21555700	-0.18372300
H	-1.79477200	-5.01683900	1.43963000
H	-2.93687700	-4.35650100	2.60709600
H	-3.52321600	-5.03036900	1.07556100
C	-4.65208400	-2.27680400	-0.14051000
C	-5.60303300	-3.47118900	-0.01047600
H	-4.11696100	-2.32174400	-1.09120800
H	-5.23119600	-1.34995200	-0.16510100
H	-6.36042800	-3.39086700	-0.79914800
H	-5.09701600	-4.43069900	-0.14314400
H	-6.13276400	-3.49130700	0.94752100
I	0.81338400	-1.72997600	2.54812700
37			
P	-2.23620400	0.52778200	-0.94871500
C	-2.89994700	-0.61960900	-2.26956900
H	-2.54787700	-0.18194700	-3.21292700
H	-3.99402900	-0.54296300	-2.29465500
C	-2.48003800	-2.09909900	-2.20638700
H	-3.02046500	-2.62306000	-3.00570900
H	-2.81767100	-2.55790500	-1.26978400
C	-0.97606900	-2.36711200	-2.41309000
H	-0.58150600	-1.68188800	-3.17233500

H	-0.82727600	-3.38510400	-2.79117000
P	0.06973800	-2.18681300	-0.87610000
C	1.73164400	-2.73493700	-1.45323500
C	2.58244000	-3.46522900	-0.60714300
C	2.20196800	-2.35432000	-2.72159100
C	3.86444500	-3.81860500	-1.03016800
H	2.24817500	-3.74243400	0.38522900
C	3.48338500	-2.71278400	-3.14114000
H	1.57666500	-1.77133400	-3.39091200
C	4.31789100	-3.44799800	-2.29713700
H	4.50994200	-4.38346600	-0.36300000
H	3.82721600	-2.41694800	-4.12883600
H	5.31571300	-3.72773600	-2.62443800
C	-0.55565600	-3.56019000	0.17529800
C	-1.23220000	-3.26724100	1.36765100
C	-0.42196100	-4.90130100	-0.22187800
C	-1.76625100	-4.29531300	2.14772900
H	-1.33624700	-2.23540400	1.68778700
C	-0.95280500	-5.92638500	0.56018400
H	0.11179700	-5.14864700	-1.13562000
C	-1.62645100	-5.62420000	1.74689300
H	-2.28639200	-4.05339700	3.07030700
H	-0.83793300	-6.96015700	0.24528700
H	-2.03776400	-6.42395200	2.35706600
C	-3.00810600	2.10972300	-1.52501800
C	-2.22248600	3.06332800	-2.18810700
C	-4.38417600	2.34690500	-1.36222800
C	-2.81028600	4.22911100	-2.68809500
H	-1.15259600	2.91142900	-2.28522200
C	-4.96378900	3.51227800	-1.86197900
H	-5.00423100	1.62675400	-0.83555700
C	-4.17705700	4.45564200	-2.52882900
H	-2.18882000	4.96521700	-3.19082600
H	-6.02845600	3.68566900	-1.72687900
H	-4.62890000	5.36639700	-2.91349700
C	-3.23114000	0.13250500	0.55960900
C	-2.87041500	0.79301800	1.74922700
C	-4.29497900	-0.78119200	0.59635000
C	-3.55981600	0.54848400	2.93650000
H	-2.04665800	1.50210600	1.74171200
C	-4.97850400	-1.03270300	1.78983000
H	-4.60545900	-1.30464800	-0.30245100
C	-4.61342400	-0.36947800	2.96148100
H	-3.26895400	1.07206700	3.84311700
H	-5.79926100	-1.74535000	1.79846200
H	-5.14666900	-0.56441200	3.88811000

Pd	0.10991600	-0.03395900	-0.00115700
S	1.36179300	2.92734100	-0.36459300
O	0.85277100	2.57581800	-1.70788900
O	1.27996100	4.32324600	0.08823400
N	0.63331600	1.89927600	0.69614600
C	3.13427500	2.48175300	-0.40819000
C	3.65581900	1.85874800	-1.54359900
C	5.01266800	1.53655600	-1.53102800
H	3.01507800	1.65048000	-2.39127100
C	5.13569800	2.46157400	0.67868500
C	5.76996700	1.84131400	-0.39976500
H	5.46986000	1.05455800	-2.39092900
H	5.69006000	2.71430100	1.58036200
H	6.82863600	1.60542300	-0.34947500
C	1.08370300	1.84825100	2.02916300
C	1.21614700	2.95443800	2.88780000
C	1.37140000	0.56066800	2.52528200
C	1.61213800	2.75287100	4.20624700
H	1.01961800	3.94883500	2.50496900
C	1.77323200	0.37139200	3.85717100
C	1.88691400	1.46783600	4.70231700
H	1.70453900	3.61262900	4.86563100
H	1.98910100	-0.63615400	4.19975400
H	2.18399100	1.33413300	5.73881300
N	3.83758400	2.78422900	0.67897200
C	1.26823700	-0.58060400	1.57049400
O	1.68778500	-1.69232700	1.82010200

38-ts

P	-1.05464700	-0.30046200	-2.16636000
C	0.03102500	0.57769100	-3.41055500
H	-0.59482000	0.90174400	-4.25001600
H	0.73364200	-0.16975100	-3.78388700
C	0.83563700	1.76375700	-2.84616500
H	1.30347000	2.27207200	-3.69920300
H	1.65514100	1.36910300	-2.23881300
C	0.00521400	2.79570900	-2.05590400
H	-1.00182400	2.87359500	-2.48062000
H	0.46397400	3.78816300	-2.12079700
P	-0.15797000	2.36336100	-0.23755500
C	-1.61941100	3.35709300	0.30365800
C	-2.15498600	4.40083400	-0.46870600
C	-2.21569600	3.05937900	1.54139700
C	-3.26525200	5.12112600	-0.02185000
H	-1.71132300	4.66645100	-1.42247200
C	-3.32256000	3.78397000	1.98543400
H	-1.80029400	2.26854400	-2.15769800

C	-3.85393900	4.81315600	1.20502700
H	-3.66639200	5.92403600	-0.63490000
H	-3.76946700	3.54247500	2.94648800
H	-4.71762700	5.37412600	1.55248600
C	1.27883400	3.24321300	0.51440900
C	2.49498900	2.55589800	0.64572600
C	1.20011000	4.58491900	0.92214800
C	3.61356300	3.20810300	1.16984700
H	2.57642800	1.51417800	0.34992000
C	2.31993900	5.22756600	1.45008700
H	0.26335400	5.12763900	0.84036700
C	3.52981300	4.54034300	1.57496100
H	4.54487500	2.65827600	1.27039000
H	2.24414400	6.26382700	1.76967100
H	4.39952500	5.04143600	1.99249800
C	-2.72761200	0.45833500	-2.39502500
C	-3.51427600	0.73323700	-1.26666300
C	-3.25920200	0.73188600	-3.66804200
C	-4.79405400	1.27775300	-1.40268700
H	-3.11404500	0.52857500	-0.27809000
C	-4.53522100	1.27792700	-3.80388500
H	-2.68643400	0.50345100	-4.56252700
C	-5.30519100	1.55404500	-2.67024600
H	-5.38255600	1.49234400	-0.51512800
H	-4.93017600	1.48410500	-4.79524600
H	-6.29877700	1.98101800	-2.77790100
C	-1.27825600	-1.99625800	-2.86572800
C	-0.14669600	-2.78392100	-3.14375000
C	-2.55499400	-2.55610400	-3.04010200
C	-0.29748600	-4.09045500	-3.60915200
H	0.84899400	-2.38565100	-2.97577100
C	-2.69714800	-3.86673200	-3.50153500
H	-3.44344300	-1.97215000	-2.82450700
C	-1.57004500	-4.63624300	-3.79151800
H	0.58805000	-4.68435100	-3.81834700
H	-3.69286900	-4.28193900	-3.63462700
H	-1.68205400	-5.65586400	-4.15081600
Pd	-0.27057500	-0.05321100	0.09767400
S	2.88640800	-1.56604700	-0.90611000
O	2.93630900	-3.04380500	-0.81480400
O	2.35300300	-0.99046600	-2.16225100
N	2.10320400	-0.84061500	0.31485800
C	4.63745600	-1.02489300	-0.86037100
C	5.64086400	-1.97669600	-1.04783800
C	6.95981300	-1.52417100	-1.08540300
H	5.37934900	-3.02260400	-1.15775800

C	6.12335200	0.69827500	-0.74990400
C	7.20931200	-0.16026500	-0.93419300
H	7.77742800	-2.22517500	-1.23047200
H	6.27551700	1.76904200	-0.62789400
H	8.22046200	0.23461400	-0.95699800
C	2.35288500	-1.18884400	1.63147800
C	3.41264100	-2.00502700	2.10678200
C	1.49821400	-0.60831400	2.61115600
C	3.66006700	-2.13605600	3.46537100
H	4.04136200	-2.53306700	1.40184500
C	1.79138900	-0.72536400	3.98396000
C	2.86667700	-1.48186400	4.42020900
H	4.49107000	-2.75876000	3.78905400
H	1.13044400	-0.23146900	4.68933400
H	3.07594500	-1.58619200	5.48072000
N	4.85299500	0.27941200	-0.71395800
C	0.24131800	0.08846700	2.26261200
O	-0.25619700	0.96397200	2.94681600
C	-1.14005800	-1.30416500	1.70567600
C	-2.13006200	-1.19648500	2.60756300
H	-2.23610200	-0.24319600	3.12171200
C	-0.72668700	-2.08910000	0.62555100
H	0.22227000	-2.61944000	0.64531800
H	-1.47965600	-2.50569400	-0.04158000
C	-3.04011700	-2.26137200	3.03840200
C	-4.08257800	-1.93038400	3.92708300
C	-2.93286500	-3.59971300	2.61045200
C	-4.99668000	-2.89071200	4.35366800
H	-4.17223800	-0.90432500	4.27619700
C	-3.84484500	-4.55890500	3.04132400
H	-2.11859100	-3.88792900	1.95348400
C	-4.88291000	-4.21053100	3.91110200
H	-5.79508200	-2.61024200	5.03567700
H	-3.74148100	-5.58652100	2.70286800
H	-5.59100900	-4.96337800	4.24657700
39			
S	0.00059300	2.60753300	-1.28997300
O	-1.14381900	2.20084500	-2.13445600
O	0.30733200	4.04748600	-1.19411900
C	1.46749700	1.84579500	-2.05491100
C	2.61483200	2.62357900	-2.20299100
C	3.71465200	2.03904600	-2.82870200
H	2.62611800	3.64242400	-1.83700100
C	2.41431100	0.03944000	-3.07310800
C	3.61510800	0.72134500	-3.27318700
H	4.63652600	2.59878500	-2.95151000

H	2.30110300	-0.99193600	-3.39899500
H	4.44885200	0.22661400	-3.76171200
N	1.34794100	0.58782400	-2.47632800
C	-1.68922900	4.42488200	2.42161600
C	-1.27408600	3.77862900	1.26300200
C	-0.42318200	2.65216300	1.31898300
C	-0.00007100	2.22090300	2.60734900
C	-0.48192100	2.85295000	3.76639900
C	-1.30934400	3.96391700	3.68779100
H	-2.34414200	5.28826600	2.33197900
H	-1.62860300	4.13482700	0.30519700
C	0.95789500	1.10522700	2.79568600
H	-0.15564000	2.46054700	4.72503800
H	-1.65234700	4.46573700	4.58814600
C	1.81108200	-0.35542200	0.95956200
H	2.46856400	-0.45041700	0.09439500
O	0.92055100	0.37721500	3.78801300
C	2.02918700	0.87522000	1.75638300
C	3.02710700	1.78684200	1.69470500
H	2.89691200	2.68615600	2.29806900
N	-0.05525800	1.89446700	0.19211400
H	1.90081800	-1.24464500	1.59043200
C	4.29048400	1.75848700	0.94453500
C	4.95163800	0.57464500	0.56110600
C	4.92362500	2.98312400	0.64808900
C	6.16896600	0.61874600	-0.11759100
H	4.52451700	-0.38609200	0.82731300
C	6.13984400	3.02779800	-0.03029500
H	4.44411700	3.90940100	0.95634400
C	6.76882100	1.84306900	-0.42311100
H	6.66092500	-0.31091700	-0.39381600
H	6.60243100	3.98834800	-0.24414200
H	7.72288100	1.87346000	-0.94307000
P	-2.54949500	-0.27240000	-0.47051700
C	-3.31945700	-1.73936200	0.40714200
H	-4.40886100	-1.62978100	0.43990200
H	-2.96674000	-1.67445800	1.44252400
C	-2.96853900	-3.12646600	-0.17358500
H	-3.66127000	-3.35381100	-0.99172000
H	-3.15360800	-3.87083900	0.60964200
C	-1.54359900	-3.32908200	-0.73066400
H	-1.47039500	-2.87250600	-1.72302900
H	-1.35270000	-4.40039900	-0.85908800
P	-0.16386200	-2.57868000	0.26846800
C	1.32513200	-3.37658500	-0.46810700
C	2.38168300	-3.82854000	0.33752200

C	1.44333600	-3.48771400	-1.86395500
C	3.52564700	-4.38415700	-0.23963900
H	2.30898600	-3.76052900	1.41827300
C	2.58310300	-4.05257800	-2.43676200
H	0.64718900	-3.13345100	-2.51223900
C	3.62877600	-4.50057500	-1.62619800
H	4.33327800	-4.73064200	0.39939600
H	2.65245400	-4.14376300	-3.51759000
H	4.51662400	-4.93916600	-2.07328900
C	-0.34074200	-3.36434900	1.92155900
C	-0.37045100	-2.57587500	3.08079600
C	-0.47394100	-4.76034300	2.03727400
C	-0.53355900	-3.17416000	4.33388900
H	-0.24727400	-1.49961000	3.02041700
C	-0.64160400	-5.35141800	3.28803800
H	-0.43498400	-5.38937300	1.15183500
C	-0.67313500	-4.55748300	4.43913400
H	-0.54150300	-2.54927300	5.22210200
H	-0.74440700	-6.43050200	3.36550800
H	-0.80061200	-5.02064100	5.41394500
C	-3.04004300	-0.55491100	-2.22464900
C	-2.06629100	-0.50196600	-3.23323600
C	-4.36709600	-0.86517100	-2.56724300
C	-2.41734200	-0.76908200	-4.55953200
H	-1.04743700	-0.22174200	-2.98307100
C	-4.71235900	-1.13031300	-3.89236800
H	-5.13787700	-0.88777500	-1.80108600
C	-3.73525800	-1.08601500	-4.89073200
H	-1.65841600	-0.71460900	-5.33563900
H	-5.74240900	-1.36736000	-4.14564900
H	-4.00464500	-1.29001600	-5.92382700
C	-3.63146400	1.10075000	0.10687800
C	-4.03149000	1.16275200	1.45177100
C	-4.04183000	2.11472800	-0.77258000
C	-4.84686900	2.20138100	1.90140800
H	-3.70620100	0.40646500	2.16025800
C	-4.85913000	3.15050900	-0.31784800
H	-3.70837000	2.10452500	-1.80361000
C	-5.26849600	3.19462100	1.01612300
H	-5.14744100	2.23410700	2.94506400
H	-5.17178000	3.92689900	-1.01107500
H	-5.90550500	4.00270600	1.36597600
Pd	-0.17962500	-0.27725300	0.19672200
40-ts			
S	0.21820400	1.94329500	-1.41115200
O	0.58921900	0.67270100 _{S161}	-2.07287200

O	-1.07178300	2.56518700	-1.75252500
C	1.50762500	3.14162200	-1.87592100
C	2.50716800	2.75912000	-2.77152300
C	3.45470100	3.72330300	-3.11600400
H	2.52949300	1.75313000	-3.17142800
C	2.31721600	5.25760600	-1.66234400
C	3.36256000	4.99530100	-2.55101800
H	4.25259000	3.48192300	-3.81284800
H	2.21257100	6.23537500	-1.19717800
H	4.08313900	5.77133200	-2.79011400
N	1.39337600	4.34892200	-1.33180300
C	-1.30445300	4.26807100	2.31769000
C	-1.12190900	3.25647400	1.37827300
C	0.15484600	2.72570400	1.14614700
C	1.25504300	3.22501200	1.88419300
C	1.04882000	4.24201900	2.82957200
C	-0.22051700	4.76055000	3.05373400
H	-2.30288000	4.66576100	2.48010100
H	-1.96027600	2.87223000	0.81180100
C	2.65619000	2.77369100	1.63826900
H	1.91436400	4.61605800	3.36725400
H	-0.36897100	5.54301200	3.79278100
C	1.79104600	0.47113900	1.07576600
H	2.01055800	-0.51294600	0.68741100
O	3.61305500	3.45749300	1.98812500
C	2.85087300	1.45722700	0.93247600
C	4.04599300	1.26384500	0.30819600
H	4.76561500	2.06540500	0.47106100
N	0.34548800	1.66853500	0.20931300
H	1.29899100	0.45490600	2.04478200
C	4.53532600	0.13483300	-0.48248600
C	3.70815600	-0.69238000	-1.27085900
C	5.92181300	-0.12302200	-0.47387000
C	4.25023200	-1.76321400	-1.98060200
H	2.65097400	-0.46803400	-1.37125500
C	6.45787600	-1.19836900	-1.17748700
H	6.57450800	0.52187500	0.10960700
C	5.62140900	-2.02841400	-1.92863900
H	3.59517100	-2.38954900	-2.58017100
H	7.52779100	-1.38619500	-1.14441600
H	6.03737100	-2.86578800	-2.48256600
P	-0.27979000	-2.62305200	1.04566300
C	-1.78444500	-3.49972700	1.73102500
H	-1.91216800	-3.17909900	2.77151500
H	-1.58858500	-4.57827400	1.75460500
C	-3.08750000	-3.22744200	0.95149200

H	-3.80826500	-3.99859800	1.25304800
H	-2.92631000	-3.37850400	-0.12355600
C	-3.74869900	-1.85466800	1.20925900
H	-3.63069100	-1.59358400	2.26837500
H	-4.82639200	-1.92918000	1.02202100
P	-3.04532200	-0.43468300	0.20816800
C	-4.21050700	0.94384500	0.62489000
C	-4.25178200	2.05770800	-0.23633700
C	-4.98099200	0.97951300	1.79828100
C	-5.05243200	3.15921800	0.06174200
H	-3.64192000	2.06856500	-1.13571400
C	-5.77907700	2.08758300	2.09675900
H	-4.97293300	0.14279800	2.48978500
C	-5.82093000	3.17937200	1.22985200
H	-5.07176800	4.00596600	-0.61946900
H	-6.37170300	2.09108500	3.00836300
H	-6.44400700	4.03924300	1.46136300
C	-3.60921000	-0.86395300	-1.50570400
C	-4.93331900	-1.24009700	-1.78913900
C	-2.68818600	-0.78735200	-2.56012300
C	-5.32115500	-1.54938900	-3.09195800
H	-5.67301600	-1.27886200	-0.99354200
C	-3.07966500	-1.09163400	-3.86745600
H	-1.66931300	-0.46990500	-2.35992100
C	-4.39251800	-1.47785900	-4.13482400
H	-6.34884400	-1.83972200	-3.29566500
H	-2.35545600	-1.01921400	-4.67463300
H	-4.69666300	-1.71526400	-5.15110900
C	1.03025100	-3.02825000	2.28432500
C	0.78793900	-2.86920800	3.66181200
C	2.34134500	-3.33094500	1.87334500
C	1.80926300	-3.04490200	4.59484000
H	-0.20425700	-2.60208600	4.01538400
C	3.36412500	-3.49966100	2.80915100
H	2.56509600	-3.44699700	0.81713600
C	3.10246800	-3.36438600	4.17303300
H	1.59400000	-2.92960100	5.65410800
H	4.36756800	-3.73879300	2.46667100
H	3.89830600	-3.49845800	4.90052600
C	0.16234400	-3.69912900	-0.39524800
C	0.33721700	-5.08833100	-0.27287800
C	0.32566500	-3.10653000	-1.65631200
C	0.66008300	-5.86522700	-1.38506600
H	0.23673900	-5.56684300	0.69797800
C	0.64585200	-3.88640100	-2.77211100
H	0.20148900	-2.03174300	-1.75871600

C	0.81233200	-5.26508800	-2.63861000
H	0.79350900	-6.93832200	-1.27446800
H	0.75954000	-3.41312600	-3.74397000
H	1.06018600	-5.87218400	-3.50549200
Pd	-0.64383900	-0.41527800	0.53829400
NEt₃			
N	0.14736200	-0.00814800	0.32939400
C	-0.25368900	-1.12415100	-0.53026600
C	-1.22584900	-2.09627000	0.14278600
H	0.65515700	-1.67755700	-0.78889500
H	-0.68173700	-0.77954200	-1.49222700
H	-1.38006100	-2.97396200	-0.49526200
H	-0.82422700	-2.43221100	1.10488300
H	-2.20879500	-1.64754700	0.32222300
C	-0.94521500	0.89231000	0.71074300
C	-1.61992200	1.69902100	-0.41499400
H	-0.54077200	1.58990700	1.45552900
H	-1.70605900	0.30248100	1.23443900
H	-2.40038900	2.34605600	0.00296300
H	-0.90225900	2.34017900	-0.93964700
H	-2.09449700	1.04920900	-1.15891300
C	1.32809900	0.69868900	-0.17674700
C	2.63502400	-0.05654500	0.08597000
H	1.37897700	1.66465500	0.34002400
H	1.24762800	0.93082800	-1.25641100
H	3.49144900	0.53768800	-0.25444500
H	2.75013500	-0.25564800	1.15650100
H	2.67322900	-1.01582800	-0.44147300
Et₃NHI			
N	1.36436600	0.18365000	-0.02975100
C	1.84712000	-0.20843000	1.34223100
C	1.50947400	-1.64802800	1.71754700
H	1.34890600	0.47237500	2.03407700
H	2.92348100	-0.01231800	1.38592500
H	1.74645800	-1.79201800	2.77660600
H	0.44182700	-1.84476200	1.57788300
H	2.08769300	-2.38136300	1.14736400
C	1.76801000	-0.76013700	-1.13430300
C	3.27048500	-0.89287400	-1.35363000
H	1.26192800	-0.39100500	-2.03010800
H	1.31148200	-1.72173400	-0.89425000
H	3.43845200	-1.60184200	-2.17075500
H	3.73880700	0.05329000	-1.64161000
H	3.78789100	-1.28267000	-0.47101200
C	1.66668700	1.62070200	-0.37367000
C	1.02555800	2.62709700	0.57778300

H	1.27254500	1.76487800	-1.38323100
H	2.75446800	1.73339700	-0.40744800
H	1.15690400	3.62864900	0.15538400
H	-0.04748000	2.43725200	0.67849100
H	1.48795000	2.62644400	1.56911800
H	0.28527600	0.10507000	-0.00718400
I	-1.98247500	-0.14168200	-0.12767400
CO			
C	0.00000000	0.00000000	-0.65013800
O	0.00000000	0.00000000	0.48760300