

Supporting Information

Cascade Reaction of 2-Halo-4-alkenyloxazoles with Arynes: A Switchable Divergent Synthesis of 2-Arylnaphtho[2,1-*d*]oxazoles, *N*-Acylnaphthylamines, and α -Halonaphthalenes

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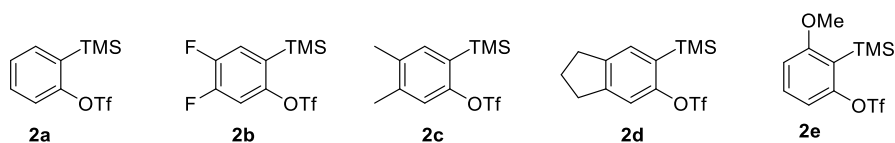
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1. General Information

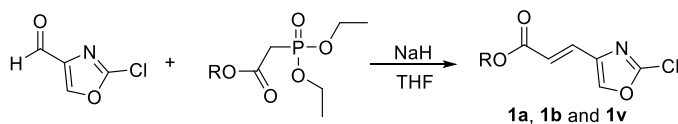
^1H NMR and ^{13}C NMR spectra were recorded on Bruker 400 spectrometer and Bruker 600 spectrometer, and the chemical shifts were referenced to tetramethylsilane ($\delta = 0.00$ ppm) for ^1H NMR, central CDCl_3 resonance ($\delta = 77.0$ ppm) and central $\text{DMSO}-d_6$ resonance ($\delta = 39.5$ ppm) for ^{13}C NMR. IR spectra were recorded on Niolet Magna-I 550 spectrometer. High resolution mass spectra (HRMS) was recorded on a Q-TOF (AB SCIEX X500R with ESI source, and Agilent 7250 with EI source), which combines quadrupole precursor ion selection and a high-resolution accurate-mass (HR/AM) Time of Flight mass analyzer to deliver mass accuracy. Melting points were taken on SGW X-4 digital melting-point apparatus without correction.

Anhydrous solvents were distilled from CaH_2 (CH_2Cl_2 and CH_3CN) or sodium-benzophenone (toluene, Et_2O and THF) under N_2 atmosphere. Other reagents were commercially available and were used directly without further purification. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 10-40 μm . Silica gel column chromatography was performed using silica gel (300-400 mesh). All reactions were carried out using anhydrous solvents, with heating reactions conducted in an oil bath. Aryne precursors **2a-2e** are known compounds and were prepared according to a literature procedure.^[1] The analytical data matched the previously published values.^[2]



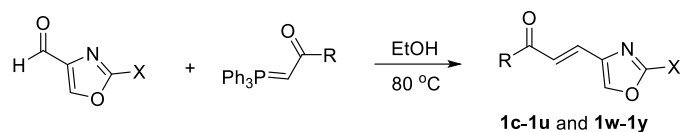
2. Synthetic Procedures and Compound Characterisation

General Procedure A: Synthesis of 2-Halo-4-alkenyloxazoles.

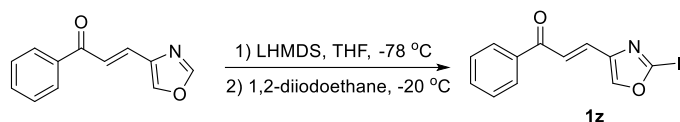


Method A:^[3] To a suspension of NaH (1.1 equiv, 60 wt.%) in THF (0.5 M) at 0°C was added dropwise phosphonate (1.1 equiv). The reaction mixture was stirred at room temperature for 30 min. A solution of aldehyde (1.0 equiv) in THF (1.0 M) was added dropwise at room temperature. The reaction mixture was stirred at room temperature for 1 h, quenched with 2 N HCl , extracted with EtOAc , and the organic layer

dried (Na₂SO₄), filtered and concentrated. Purified by silica gel column chromatography (petroleum ether/ethyl acetate) to give compounds **1a**, **1b** and **1v**.

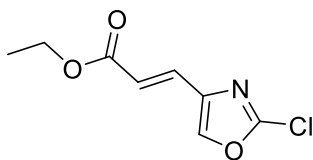


Method B:^[3] To a solution of oxazole-4-carbaldehyde (1.0 equiv) in anhydrous EtOH (0.25 M) was added phosphorus ylide (1.5 equiv) in one portion, and the reaction mixture was stirred at 80 °C and monitored by TLC. The mixture was then concentrated under reduced pressure, and the residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compounds **1c-1u** and **1w-1y**.



Method C:^[4] LHMDS (4.7 mL, 4.7 mmol, 1.5 equiv, 1 M in THF,) was added dropwise to a stirred solution of 4-alkenyloxazole^[5] (617.5 mg, 3.1 mmol, 1.0 equiv) in THF (0.5 M) at -78 °C. After stirring at the same temperature for 1 h a solution of 1,2-diiodoethane (1.05 g, 3.72 mmol, 1.2 equiv) in THF (0.5 M) was added dropwise to the mixture over 10 min at -78 °C. The resulting mixture was allowed to warm to -20 °C over 5 h. The resulting mixture was poured into water, the aqueous phase was extracted with Et₂O and the combined organic extracts were dried over MgSO₄, filtered and concentrated under reduced pressure. The crude residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **1z** (201 mg, 20%).

ethyl (*E*)-3-(2-chlorooxazol-4-yl)acrylate (**1a**)



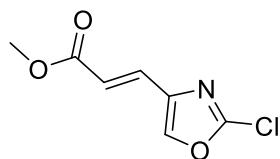
Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), White solid, 639 mg, 79% yield, m.p. 80.0-80.3 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.77 (s, 1H), 7.40 (d, *J* = 15.6 Hz, 1H), 6.62 (d, *J* = 15.6 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 166.4, 148.3, 140.4, 139.0, 130.6, 121.7, 60.6, 14.2.

IR (ATR, cm⁻¹): ν 3156, 2980, 1704, 1536, 1295, 1160, 971, 781.

HRMS (ESI, m/z): Calculated for $[C_8H_8ClNO_3+H]^+$, 202.0265; found, 202.0260.

methyl (*E*)-3-(2-chlorooxazol-4-yl)acrylate (1b)



Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), White solid, 505 mg, 67% yield, m.p. 102.9-103.5 °C.

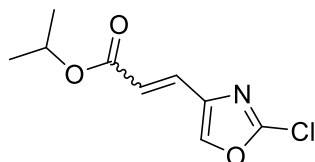
^1H NMR (400 MHz, $CDCl_3$): δ 7.77 (s, 1H), 7.41 (d, J = 15.2 Hz, 1H), 6.63 (d, J = 15.2 Hz, 1H), 3.80 (s, 3H).

$^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, ppm): δ 166.8, 148.4, 140.5, 139.0, 130.9, 121.1, 51.8.

IR (ATR, cm^{-1}): ν 3136, 3070, 3000, 2953, 1703, 1651, 1538, 1304, 977, 780.

HRMS (ESI, m/z): Calculated for $[C_7H_6ClNO_3+H]^+$, 188.0109; found, 188.0106.

***tert*-butyl (*Z*)-3-(2-chlorooxazol-4-yl)acrylate and *tert*-butyl (*E*)-3-(2-chlorooxazol-4-yl)acrylate (1c)**



Prepared according to General Procedure A (4.9 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), White oil, 844 mg, 80% yield.

(*Z*)- ^1H NMR (400 MHz, $CDCl_3$): δ 8.86 (s, 0.8H), 6.75 (d, J = 12.8 Hz, 0.8H), 5.97 (d, J = 12.8 Hz, 0.8H), 5.15-5.03 (m, 0.8H), 1.29 (d, J = 6.4 Hz, 4.8H).

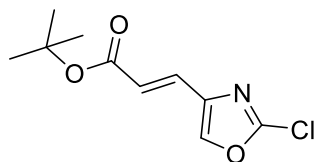
(*E*)- ^1H NMR (400 MHz, $CDCl_3$): δ 7.76 (s, 1H), 7.38 (d, J = 15.6 Hz, 1H), 6.60 (d, J = 15.6 Hz, 1H), 5.15-5.03 (m, 1H), 1.29 (d, J = 6.4 Hz, 6H),

$^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, ppm): δ 165.9, 165.4, 148.3, 146.2, 144.6, 140.3, 139.1, 137.2, 132.3, 130.3, 122.2, 120.2, 68.0, 67.9, 21.8, 21.8.

IR (ATR, cm^{-1}): ν 3146, 2982, 2942, 1710, 1649, 1527, 1311, 993, 827.

HRMS (ESI, m/z): Calculated for $[C_9H_{10}ClNO_3+H]^+$, 216.0422; found, 216.0417.

***tert*-butyl (*E*)-3-(2-chlorooxazol-4-yl)acrylate (1d)**



Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), White solid, 500 mg, 55% yield, m.p. 56.8-57.9 °C.

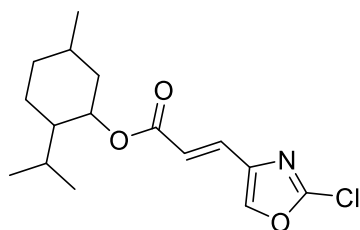
¹H NMR (400 MHz, CDCl₃): δ 7.67 (s, 1H), 7.22 (d, J = 15.6 Hz, 1H), 6.48 (d, J = 15.6 Hz, 1H), 1.43 (s, 9H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 165.6, 148.2, 140.1, 139.2, 129.6, 123.6, 80.7, 28.1.

IR (ATR, cm⁻¹): ν 3159, 3006, 2986, 2938, 1698, 1652, 1559, 1313, 980, 782.

HRMS (ESI, m/z): Calculated for [C₁₀H₁₂ClNO₃+H]⁺, 230.0578; found, 230.0578.

(±)-2-isopropyl-5-methylcyclohexyl (*E*)-3-(2-chlorooxazol-4-yl)acrylate (1e)



Prepared according to General Procedure A (8.7 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), White oil, 967 mg, 53% yield, m.p. 115.4-117.1 °C.

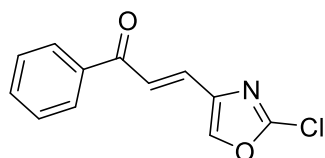
¹H NMR (400 MHz, CDCl₃): δ 7.75 (s, 1H), 7.38 (d, J = 15.2 Hz, 1H), 6.62 (d, J = 15.2 Hz, 1H), 4.78 (td, J_1 = 10.8 Hz, J_2 = 4.4 Hz, 1H), 2.08-2.01 (m, 1H), 1.94-1.83 (m, 1H), 1.73-1.66 (m, 3H), 1.57-1.38 (m, 2H), 1.14-0.97 (m, 2H), 0.90 (t, J = 7.6 Hz, 6H), 0.77 (d, J = 6.8 Hz, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 166.0, 148.3, 140.3, 139.1, 130.4, 122.2, 74.6, 47.1, 40.9, 34.2, 31.4, 26.3, 23.5, 22.0, 20.7, 16.4.

IR (ATR, cm⁻¹): ν 3136, 3095, 2943, 2869, 1705, 1652, 1532, 1313, 1173, 973.

HRMS (ESI, m/z): Calculated for [C₁₆H₂₂ClNO₃+H]⁺, 312.1361; found, 312.1363.

(*E*)-3-(2-chlorooxazol-4-yl)-1-phenylprop-2-en-1-one (1f)



Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), Yellow solid, 631 mg, 68% yield, m.p. 125.0-125.4 °C.

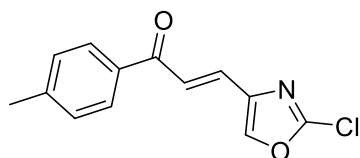
¹H NMR (400 MHz, CDCl₃): δ 8.06 (d, *J* = 7.2 Hz, 2H), 7.84 (s, 1H), 7.80 (d, *J* = 15.2 Hz, 1H), 7.63-7.46 (m, 4H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.5, 148.5, 141.4, 139.7, 137.5, 133.2, 130.2, 128.7, 128.6, 124.6.

IR (ATR, cm⁻¹): ν 3144, 3083, 1668, 1614, 1554, 1305, 1203, 980, 767.

HRMS (EI, *m/z*): Calculated for [C₁₂H₈ClNO₂+H]⁺, 234.0316; found, 234.0311.

(*E*)-3-(2-chlorooxazol-4-yl)-1-(*p*-tolyl)prop-2-en-1-one (1g)



Prepared according to General Procedure A (6.0 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 724 mg, 73% yield, m.p. 130.2-130.4 °C.

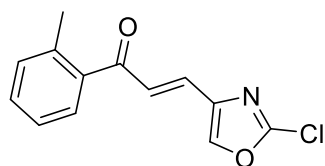
¹H NMR (400 MHz, CDCl₃): δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.83 (s, 1H), 7.79 (d, *J* = 15.2 Hz, 1H), 7.54 (d, *J* = 15.2 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 188.9, 148.4, 144.1, 141.3, 139.7, 135.0, 129.8, 129.3, 128.7, 124.6, 21.6.

IR (ATR, cm⁻¹): ν 3143, 3032, 1663, 1602, 1551, 1327, 1244, 980, 731.

HRMS (ESI, *m/z*): Calculated for [C₁₃H₁₀ClNO₂+H]⁺, 248.0473; found, 248.0470.

(*E*)-3-(2-chlorooxazol-4-yl)-1-(*p*-tolyl)prop-2-en-1-one (1h)



Prepared according to General Procedure A (3.5 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 412 mg, 48% yield, m.p. 101.3-101.6 °C.

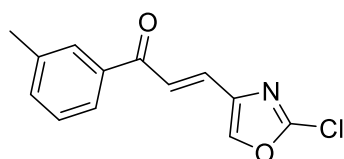
¹H NMR (400 MHz, CDCl₃): δ 7.80 (s, 1H), 7.58 (dd, $J_1 = 8.4$ Hz, $J_2 = 1.6$ Hz, 1H), 7.46-7.34 (m, 2H), 7.34-7.24 (m, 3H), 2.47 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 194.6, 148.4, 141.2, 139.4, 138.2, 137.7, 131.5, 131.0, 130.6, 128.7, 128.5, 125.5, 20.5.

IR (ATR, cm⁻¹): ν 3159, 3013, 1670, 1601, 1569, 1381, 1263, 995, 748.

HRMS (ESI, m/z): Calculated for [C₁₃H₁₀ClNO₂+H]⁺, 248.0473; found, 248.0472.

(E)-3-(2-chlorooxazol-4-yl)-1-(m-tolyl)prop-2-en-1-one (1i)



Prepared according to General Procedure A (3.0 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 454 mg, 61% yield, m.p. 119.4-119.9 °C.

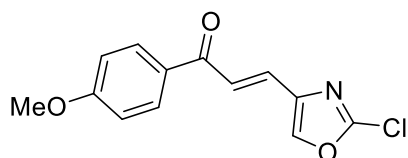
¹H NMR (400 MHz, CDCl₃): δ 7.89-7.82 (m, 3H), 7.78 (d, $J = 15.2$ Hz, 1H), 7.55 (d, $J = 15.2$ Hz, 1H), 7.42-7.34 (m, 2H), 2.44 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.5, 148.4, 141.4, 139.6, 138.5, 137.5, 134.0, 130.0, 129.1, 128.5, 125.8, 124.6, 21.3.

IR (ATR, cm⁻¹): ν 3147, 3038, 1662, 1613, 1592, 1303, 1089, 778.

HRMS (EI, m/z): Calculated for [C₁₃H₁₀ClNO₂+H]⁺, 248.0473; found, 248.0470.

(E)-3-(2-chlorooxazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (1j)



Prepared according to General Procedure A (6.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), Yellow solid, 823 mg, 78% yield, m.p. 146.0-146.9 °C.

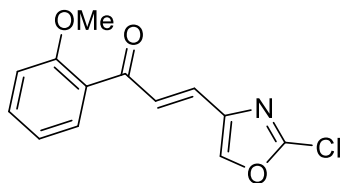
¹H NMR (400 MHz, CDCl₃): δ 8.07 (d, $J = 8.8$ Hz, 2H), 7.84-7.75 (m, 2H), 7.54 (d, $J = 15.2$ Hz, 1H), 6.97 (d, $J = 8.8$ Hz, 2H), 3.89 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 187.8, 163.8, 148.4, 141.1, 139.8, 131.0, 130.6, 129.5, 124.6, 113.9, 55.5.

IR (ATR, cm⁻¹): ν 3148, 3021, 2972, 2840, 1658, 1595, 1238, 969, 789.

HRMS (ESI, m/z): Calculated for [C₁₃H₁₀ClNO₃+H]⁺, 264.0422; found, 264.0424.

(E)-3-(2-chlorooxazol-4-yl)-1-(2-methoxyphenyl)prop-2-en-1-one (1k)



Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), Yellow solid, 670 mg, 64% yield, m.p. 116.0-116.9 °C.

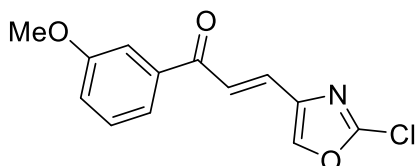
¹H NMR (400 MHz, CDCl₃): δ 7.80 (s, 1H), 7.64 (d, J =8.0 Hz 1H), 7.59 (d, J =15.6 Hz, 1H), 7.47 (t, J =8.0 Hz, 1H), 7.39 (d, J =15.6 Hz, 1H), 7.06-6.95 (m, 2H), 3.90 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 191.8, 158.4, 148.2, 141.0, 139.8, 133.3, 130.5, 129.6, 128.7, 128.3, 120.6, 111.5, 55.7.

IR (ATR, cm⁻¹): ν 3155, 2965, 2842, 1661, 1597, 1318, 967, 749.

HRMS (ESI, m/z): Calculated for [C₁₃H₁₀ClNO₃+Na]⁺, 286.0241; found, 286.0236.

(E)-3-(2-chlorooxazol-4-yl)-1-(3-methoxyphenyl)prop-2-en-1-one (1l)



Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (18/1 petroleum ether/ethyl acetate), White solid, 642 mg, 61% yield, m.p. 117.9-118.0 °C.

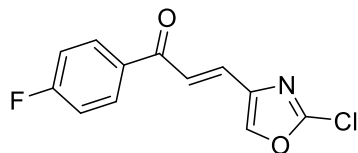
¹H NMR (400 MHz, CDCl₃): δ 7.84 (s, 1H), 7.76 (d, J =15.2 Hz, 1H), 7.64 (d, J =7.6 Hz, 1H), 7.59-7.51 (m, 2H), 7.40 (t, J =8.0 Hz, 1H), 7.14 (dd, J_1 =8.0 Hz, J_2 =2.4 Hz, 1H), 3.88 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.2, 159.9, 148.4, 141.4, 139.6, 138.9, 130.2, 129.6, 124.6, 121.3, 119.8, 112.7, 55.4.

IR (ATR, cm⁻¹): ν 3149, 3040, 3017, 2836, 1663, 1585, 1299, 1085, 795.

HRMS (ESI, m/z): Calculated for [C₁₃H₁₀ClNO₃+H]⁺, 264.0422; found, 264.0417.

(E)-3-(2-chlorooxazol-4-yl)-1-(4-fluorophenyl)prop-2-en-1-one (1m)



Prepared according to General Procedure A (6.0 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 750 mg, 75% yield, m.p. 148.4-148.9 °C.

¹H NMR (400 MHz, CDCl₃): δ 8.09 (t, J = 6.8 Hz, 2H), 7.85 (s, 1H), 7.76 (d, J = 15.2 Hz, 1H), 7.56 (d, J = 15.2 Hz, 1H), 7.17 (t, J = 8.0 Hz, 2H).

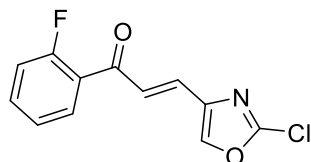
¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 187.8, 165.8 (d, J_{C-F} = 253.7 Hz), 148.5, 141.5, 139.5, 133.9 (d, J_{C-F} = 2.9 Hz), 131.2 (d, J_{C-F} = 9.4 Hz), 130.39, 124.08, 115.8 (d, J_{C-F} = 21.7 Hz).

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -104.8.

IR (ATR, cm⁻¹): ν 3151, 1671, 1621, 1597, 1529, 1304, 1236, 1086, 968, 835.

HRMS (ESI, m/z): Calculated for [C₁₂H₇ClFNO₂+H]⁺, 252.0222; found, 252.0231.

(E)-3-(2-chlorooxazol-4-yl)-1-(2-fluorophenyl)prop-2-en-1-one (1n)



Prepared according to General Procedure A (3.3 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 540 mg, 65% yield, m.p. 133.7-134.1 °C.

¹H NMR (400 MHz, CDCl₃): δ 7.87-7.78 (m, 2H), 7.64-7.45 (m, 3H), 7.25 (t, J = 7.6 Hz, 1H), 7.21-7.11 (t, J = 9.6 Hz, 1H).

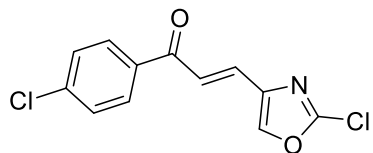
¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 188.3 (d, J_{C-F} = 3.0 Hz), 161.4 (d, J_{C-F} = 253.1 Hz), 148.4, 141.5, 139.5, 134.3 (d, J_{C-F} = 9.0 Hz), 130.9 (d, J_{C-F} = 9.0 Hz), 130.2, 128.0 (d, J_{C-F} = 6.8 Hz), 126.6 (d, J_{C-F} = 12.6 Hz), 124.5 (d, J_{C-F} = 3.5 Hz), 116.6 (d, J_{C-F} = 22.8 Hz).

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -110.2.

IR (ATR, cm⁻¹): ν 2988, 1665, 1604, 1551, 1320, 1266, 977, 747.

HRMS (ESI, m/z): Calculated for [C₁₂H₇ClFNO₂+H]⁺, 252.0222; found, 252.0220.

(E)-3-(2-chlorooxazol-4-yl)-1-(4-chlorophenyl)prop-2-en-1-one (1o)



Prepared according to General Procedure A (6.0 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 894 mg, 84% yield, m.p. 146.1-146.7 °C.

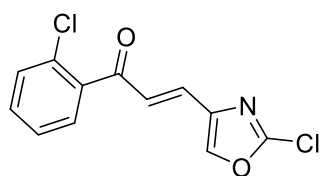
¹H NMR (400 MHz, CDCl₃): δ 7.99 (d, J = 8.4 Hz, 2H), 7.85 (s, 1H), 7.73 (d, J = 15.2 Hz, 1H), 7.56 (d, J = 15.2 Hz, 1H), 7.47 (d, J = 8.4 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 188.1, 148.5, 141.6, 139.6, 139.5, 135.8, 130.6, 130.0, 129.0, 124.0.

IR (ATR, cm⁻¹): ν 3150, 1666, 1571, 1303, 1241, 1084, 1009, 965, 775.

HRMS (ESI, m/z): Calculated for [C₁₂H₇Cl₂NO₂+H]⁺, 267.9927; found, 267.9925.

(E)-3-(2-chlorooxazol-4-yl)-1-(2-chlorophenyl)prop-2-en-1-one (1p)



Prepared according to General Procedure A (3.0 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 412 mg, 51% yield, m.p. 117.8-117.6 °C.

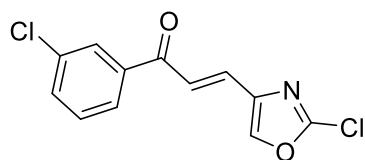
¹H NMR (400 MHz, CDCl₃): δ 7.83 (s, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.46-7.39 (m, 2H), 7.38-7.32 (m, 2H), 7.28 (d, J = 15.6 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.6, 148.6, 141.6, 139.2, 138.6, 131.8, 131.5, 131.2, 130.4, 129.4, 128.5, 126.9.

IR (ATR, cm⁻¹): ν 3135, 3059, 1676, 1616, 1530, 1306, 1082, 743.

HRMS (ESI, m/z): Calculated for [C₁₂H₇Cl₂NO₂+H]⁺, 267.9927; found, 267.9922.

(E)-3-(2-chlorooxazol-4-yl)-1-(3-chlorophenyl)prop-2-en-1-one (1q)



Prepared according to General Procedure A (3.0 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 492 mg, 61% yield, m.p. 115.5-116.2 °C.

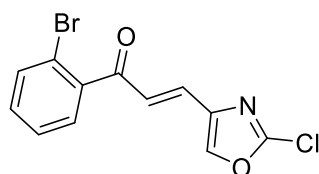
¹H NMR (400 MHz, CDCl₃): δ 8.03 (s, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.87 (s, 1H), 7.73 (d, J = 15.2 Hz, 1H), 7.62-7.54 (m, 2H), 7.45 (t, J = 7.6 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 188.1, 148.6, 141.7, 139.4, 139.0, 135.0, 133.1, 130.9, 130.0, 128.6, 126.6, 123.9.

IR (ATR, cm⁻¹): ν 3131, 3098, 1662, 1537, 1303, 1080, 959, 725.

HRMS (ESI, m/z): Calculated for [C₁₂H₇Cl₂NO₂+H]⁺, 267.9927; found, 267.9926.

(E)-1-(2-bromophenyl)-3-(2-chlorooxazol-4-yl)prop-2-en-1-one (1r)



Prepared according to General Procedure A (5.3 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 862 mg, 79% yield, m.p. 118.0-119.2°C.

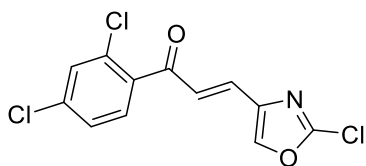
¹H NMR (400 MHz, CDCl₃): δ 7.81 (s, 1H), 7.64 (d, J = 7.6 Hz, 1H), 7.46-7.37 (m, 2H), 7.36-7.28 (m, 2H), 7.24 (d, J = 15.6 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 193.5, 148.6, 141.5, 140.6, 139.2, 133.5, 131.7, 131.5, 129.2, 128.4, 127.4, 119.5.

IR (ATR, cm⁻¹): ν 3150, 3058, 1675, 1616, 1532, 1321, 1259, 976, 739.

HRMS (ESI, m/z): Calculated for [C₁₂H₇⁷⁹BrClNO₂+H]⁺, 311.9421; found, 311.9414.

(E)-3-(2-chlorooxazol-4-yl)-1-(2,4-dichlorophenyl)prop-2-en-1-one (1s)



Prepared according to General Procedure A (3.0 mmol scale) and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 712 mg, 79% yield, m.p. 113.1-114.3 °C.

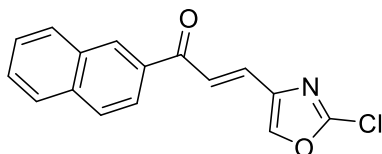
¹H NMR (400 MHz, CDCl₃): δ 7.85 (s, 1H), 7.48-7.45 (m, 2H), 7.37-7.31 (m, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 191.2, 148.6, 141.7, 139.1, 137.4, 136.9, 132.6, 131.3, 130.5, 130.3, 128.0, 127.3.

IR (ATR, cm⁻¹): ν 3150, 3041, 1676, 1618, 1552, 1311, 983, 791.

HRMS (ESI, *m/z*): Calculated for [C₁₂H₆Cl₃NO₂+H]⁺, 301.9537; found, 301.9534.

(E)-3-(2-chlorooxazol-4-yl)-1-(naphthalen-2-yl)prop-2-en-1-one (1t)



Prepared according to General Procedure A (6.0 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 425 mg, 38% yield, m.p. 146.0-146.9 °C.

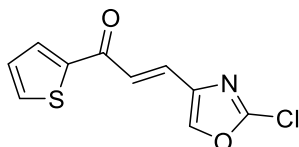
¹H NMR (400 MHz, CDCl₃): δ 8.60 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 8.02-7.83 (m, 5H), 7.65-7.53 (m, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.1, 148.5, 141.5, 139.7, 135.6, 134.8, 132.5, 130.4, 130.1, 129.6, 128.6, 128.6, 127.8, 126.8, 124.5, 124.2.

IR (ATR, cm⁻¹): ν 3136, 1661, 1627, 1528, 1320, 1206, 1087, 966, 749.

HRMS (ESI, *m/z*): Calculated for [C₁₆H₁₀ClNO₂+H]⁺, 284.0473; found, 284.0470.

(E)-3-(2-chlorooxazol-4-yl)-1-(thiophen-2-yl)prop-2-en-1-one (1u)



Prepared according to General Procedure A (3.0 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 260 mg, 54% yield, m.p. 86.4-88.2 °C.

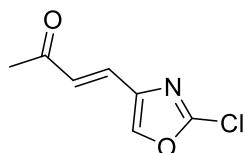
¹H NMR (400 MHz, CDCl₃): δ 7.93-7.87 (m, 1H), 7.84 (s, 1H), 7.71 (d, *J* = 4.4 Hz, 1H), 7.64 (d, *J* = 15.2 Hz, 1H), 7.56 (d, *J* = 15.2 Hz, 1H), 7.19 (t, *J* = 4.4 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 181.5, 148.5, 145.2, 141.5, 139.5, 134.5, 132.5, 129.6, 128.4, 124.5.

IR (ATR, cm⁻¹): ν 3147, 3106, 1652, 1601, 1527, 1411, 1060, 840.

HRMS (ESI, *m/z*): Calculated for [C₁₀H₆ClNO₂S+H]⁺, 239.9881; found, 239.9874.

(*E*)-4-(2-chlorooxazol-4-yl)but-3-en-2-one (1v)



Prepared according to General Procedure A (4.0 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 470 mg, 68% yield, m.p. 110.1-110.2 °C.

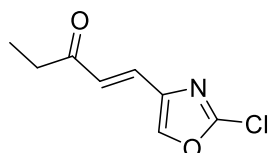
¹H NMR (400 MHz, CDCl₃): δ 7.81 (s, 1H), 7.28 (d, *J* = 15.6 Hz, 1H), 6.93 (d, *J* = 15.6 Hz, 1H), 2.34 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 197.4, 148.5, 141.1, 139.1, 129.0, 128.7, 28.7.

IR (ATR, cm⁻¹): ν 3130, 3083, 3028, 1671, 1635, 1536, 1153, 946, 793.

HRMS (ESI, *m/z*): Calculated for [C₇H₆ClNO₂+H]⁺, 172.0160; found, 172.0156.

(*E*)-1-(2-chlorooxazol-4-yl)pent-1-en-3-one (1w)



Prepared according to General Procedure A (5.3 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 472 mg, 73% yield, m.p. 117.0-117.5 °C.

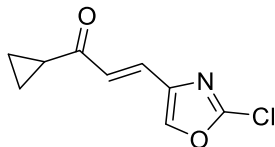
¹H NMR (400 MHz, CDCl₃): δ 7.80 (s, 1H), 7.31 (d, *J* = 15.6 Hz, 1H), 6.96 (d, *J* = 15.6 Hz, 1H), 2.64 (q, *J* = 7.2 Hz, 2H), 1.15 (t, *J* = 7.2 Hz, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 200.2, 148.4, 141.1, 139.2, 128.0, 127.8, 35.4, 7.9.

IR (ATR, cm⁻¹): ν 3161, 2986, 1692, 1623, 1534, 1223, 1090, 791.

HRMS (ESI, m/z): Calculated for [C₈H₈ClNO₂+H]⁺, 186.0316; found, 186.0311.

(*E*)-3-(2-chlorooxazol-4-yl)-1-cyclopropylprop-2-en-1-one (1x)



Prepared according to General Procedure A (6.0 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 509 mg, 64% yield, m.p. 83.3-84.2 °C.

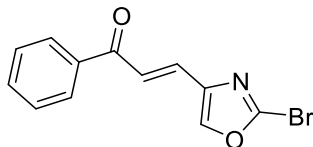
¹H NMR (400 MHz, CDCl₃): δ 7.80 (s, 1H), 7.31 (d, J = 15.6 Hz, 1H), 7.08 (d, J = 15.6 Hz, 1H), 2.20-2.09 (m, 1H), 1.18-1.13 (m, 2H), 1.02-0.96 (dt, J_1 = 11.2 Hz, J_2 = 3.2 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 199.5, 148.3, 141.1, 139.3, 128.2, 127.5, 20.8, 11.6.

IR (ATR, cm⁻¹): ν 3149, 2988, 1675, 1618, 1534, 1378, 1081, 981, 780.

HRMS (ESI, m/z): Calculated for [C₉H₈ClNO₂+H]⁺, 198.0316; found, 198.0310.

(*E*)-3-(2-bromooxazol-4-yl)-1-phenylprop-2-en-1-one (1y)



Prepared according to General Procedure A (4.1 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 412 mg, 36% yield, m.p. 140.8-142.1 °C.

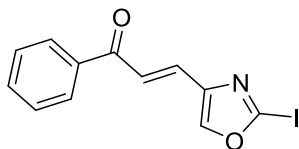
¹H NMR (400 MHz, CDCl₃): δ 8.09-8.00 (m, 2H), 7.90 (s, 1H), 7.81 (d, J = 15.2 Hz, 1H), 7.64-7.53 (m, 2H), 7.50 (t, J = 8.0 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.5, 143.0, 140.4, 137.5, 135.2, 133.2, 130.1, 128.7, 128.6, 124.5.

IR (ATR, cm⁻¹): ν 3164, 1665, 1606, 1548, 1324, 1299, 980, 769.

HRMS (ESI, m/z): Calculated for [C₁₂H₈⁷⁹BrNO₂+H]⁺, 277.9811; found, 277.9807.

(E)-3-(2-iodooxazol-4-yl)-1-phenylprop-2-en-1-one (1z)



Prepared according to General Procedure A (3.1 mmol scale) and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 201 mg, 20% yield, m.p. 153.0-154.2 °C.

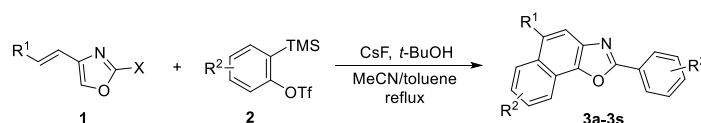
¹H NMR (400 MHz, CDCl₃): δ 8.06 (d, J = 6.8 Hz, 2H), 7.94 (s, 1H), 7.82 (d, J = 15.2 Hz, 1H), 7.61-7.54 (m, 2H), 7.50 (t, J = 7.6 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.5, 145.2, 141.0, 137.5, 133.1, 130.0, 128.6, 128.6, 124.3, 103.0.

IR (ATR, cm⁻¹): ν 3138, 1666, 1610, 1551, 1331, 1297, 966, 769.

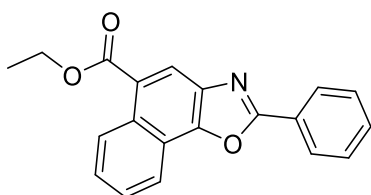
HRMS (ESI, m/z): Calculated for [C₁₂H₈INO₂+H]⁺, 325.9672; found, 325.9666.

General Procedure B : Synthesis of 2-Arylnaphtho[2,1-*d*]oxazoles.



Under a nitrogen atmosphere, 2-halo-4-alkenyloxazole **1** (0.2 mmol, 1.0 equiv), CsF (1.2 mmol, 6.0 equiv) and *t*-BuOH (0.3 mmol, 1.5 equiv) were placed in a 25 mL Schlenk tube equipped with a stir bar. Then 1.0 mL of MeCN and 1.0 mL of toluene were added. Then the aryne precursor **2** (0.6 mmol, 3.0 equiv) was dissolved in 1.0 mL of toluene. The resulting solution was added dropwise in six portions over a period of 3 h. When the reaction was complete as monitored by TLC, the reaction mixture was filtered through a short column of silica gel and eluted with CH₂Cl₂. The filtrate was concentrated under reduced pressure to afford a residue, which was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compounds **3a-3s**.

ethyl 2-phenylnaphtho[2,1-*d*]oxazole-5-carboxylate (3a)



Prepared according to General Procedure B and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 32.0 mg, 62% yield, m.p. 129.4-130.1 °C.

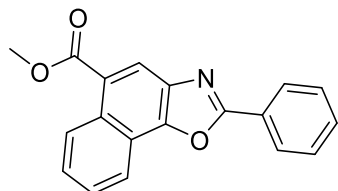
¹H NMR (400 MHz, CDCl₃): δ 8.57 (s, 1H), 8.05 (d, J = 8.4 Hz, 2H), 7.74 (t, J = 8.4 Hz 1H), 7.65 (t, J = 8.4 Hz 1H), 7.29 (t, J = 7.2 Hz, 2H), 7.07 (t, J = 7.2 Hz, 1H), 6.87 (d, J = 7.6 Hz, 2H), 4.52 (q, J = 7.2 Hz, 2H), 1.49 (t, J = 7.2 Hz, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 164.1, 158.5, 157.2, 134.8, 130.3, 129.9, 129.9, 129.7, 129.6, 129.2, 127.7, 123.6, 123.0, 115.6, 114.1, 102.9, 62.4, 14.1.

IR (ATR, cm⁻¹): ν 3070, 2983, 2227, 1716, 1589, 1488, 1221, 1031, 762.

HRMS (ESI, m/z): Calculated for [C₂₀H₁₅NO₃+H]⁺, 318.1125; found, 318.1120.

methyl 2-phenylnaphtho[2,1-*d*]oxazole-5-carboxylate (3b)



Prepared according to General Procedure B and Purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 37.0 mg, 61% yield, m.p. 123.4-126.0 °C.

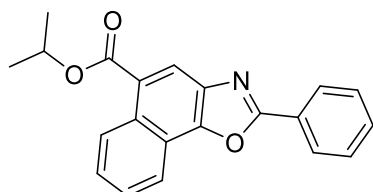
¹H NMR (400 MHz, CDCl₃): δ 8.58 (s, 1H), 8.05 (d, J = 8.4 Hz, 2H), 7.74 (t, J = 8.0 Hz, 1H), 7.66 (t, J = 8.0 Hz, 1H), 7.29 (t, J = 7.6 Hz, 2H), 7.07 (t, J = 7.2 Hz, 1H), 6.87 (d, J = 8.4 Hz, 2H), 4.05 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 164.6, 158.5, 157.3, 134.8, 130.3, 130.0, 129.9, 129.9, 129.6, 129.2, 127.4, 123.6, 123.1, 115.6, 114.1, 102.8, 52.9.

IR (ATR, cm⁻¹): ν 3076, 2954, 2232, 1722, 1589, 1486, 1202, 1030, 749.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₃NO₃+H]⁺, 304.0968; found, 304.0965.

isopropyl 2-phenylnaphtho[2,1-*d*]oxazole-5-carboxylate (3c)



Prepared according to General Procedure B and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 42.7 mg, 65% yield, m.p. 98.8-102.4 °C.

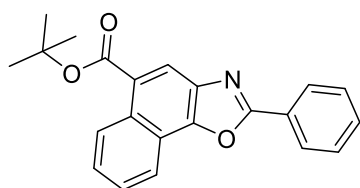
¹H NMR (400 MHz, CDCl₃): δ 8.55 (s, 1H), 8.04 (dd, $J_1 = 8.0$ Hz, $J_2 = 3.2$ Hz, 2H), 7.73 (td, $J_1 = 6.8$ Hz, $J_2 = 1.2$ Hz, 1H), 7.65 (td, $J_1 = 6.8$ Hz, $J_2 = 1.2$ Hz, 1H), 7.33-7.21 (m, 2H), 7.07 (t, $J = 7.6$ Hz, 1H), 6.87 (d, $J = 8.0$ Hz, 2H), 5.45-5.30 (m, 1H), 1.47 (d, $J = 6.4$ Hz, 6H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 163.6, 158.5, 157.1, 134.8, 130.2, 129.9, 129.8, 129.6, 129.6, 129.1, 128.1, 123.5, 123.0, 115.6, 114.1, 102.9, 70.4, 21.8.

IR (ATR, cm⁻¹): ν 3082, 2983, 2231, 1713, 1589, 1488, 1291, 1025, 749.

HRMS (ESI, m/z): Calculated for [C₂₁H₁₇NO₃+H]⁺, 332.1281; found, 332.1277.

***tert*-butyl 2-phenylnaphtho[2,1-*d*]oxazole-5-carboxylate (3d)**



Prepared according to General Procedure B and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 45.5 mg, 66% yield, m.p. 95.2-96.9 °C.

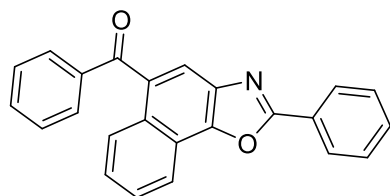
¹H NMR (400 MHz, CDCl₃): δ 8.51 (s, 1H), 8.03 (dd, $J_1 = 8.4$ Hz, $J_2 = 3.6$ Hz, 2H), 7.74-7.68 (m, 1H), 7.66-7.60 (m, 1H), 7.31-7.24 (m, 2H), 7.07 (t, $J = 7.6$ Hz, 1H), 6.87 (d, $J = 8.4$ Hz, 2H), 1.69 (s, 9H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 163.3, 158.6, 157.1, 134.8, 130.2, 129.9, 129.7, 129.6, 129.5, 129.3, 129.0, 123.6, 123.0, 115.6, 114.4, 103.0, 83.8, 28.1.

IR (ATR, cm⁻¹): ν 3078, 2980, 2231, 1708, 1588, 1486, 1299, 1042, 751.

HRMS (ESI, m/z): Calculated for [C₂₂H₁₉NO₃+H]⁺, 346.1438; found, 346.1435.

phenyl(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3e)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 39.1 mg, 56% yield, m.p. 173.6-175.3 °C.

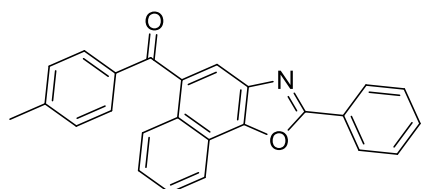
¹H NMR (400 MHz, CDCl₃): δ 8.10 (d, $J = 8.4$ Hz, 1H), 8.01 (s, 1H), 7.97 (d, $J = 8.4$ Hz, 1H), 7.91 (d, $J = 8.4$ Hz, 2H), 7.74 (t, $J = 7.6$ Hz, 1H), 7.74-7.62 (m, 2H), 7.54 (t, $J = 8.0$ Hz, 2H), 7.31 (t, $J = 8.0$ Hz, 2H), 7.09 (t, $J = 7.6$ Hz, 1H), 6.93 (d, $J = 7.6$ Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl₃, 100 MHz, ppm): δ 193.1, 158.5, 157.2, 136.3, 136.0, 134.7, 133.7, 130.5, 130.4, 130.0, 129.7, 129.4, 128.7, 128.6, 128.4, 123.7, 123.2, 115.8, 113.9, 102.6.

IR (ATR, cm⁻¹): ν 3060, 2227, 1652, 1593, 1486, 1292, 1200, 748.

HRMS (ESI, m/z): Calculated for [C₂₄H₁₅NO₂+H]⁺, 350.1176; found, 350.1174.

(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)(*p*-tolyl)methanone (3f)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 44.2 mg, 61% yield, m.p. 155.3-156.4 °C.

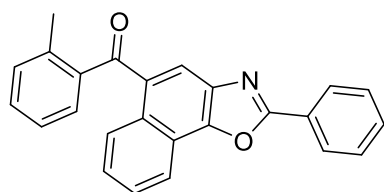
^1H NMR (400 MHz, CDCl₃): δ 8.01 (d, J = 8.4 Hz, 1H), 7.92 (s, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 8.4 Hz, 2H), 7.68-7.62 (m, 1H), 7.60-7.53 (m, 1H), 7.28-7.16 (m, 4H), 7.01 (t, J = 7.6 Hz, 1H), 6.85 (d, J = 8.4 Hz, 2H), 2.39 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl₃, 100 MHz, ppm): δ 192.8, 158.5, 157.1, 144.8, 136.5, 134.7, 133.7, 130.6, 130.4, 129.9, 129.5, 129.4, 129.3, 128.5, 128.0, 123.6, 123.2, 115.8, 114.0, 102.7, 21.8.

IR (ATR, cm⁻¹): ν 3052, 2227, 1651, 1487, 1223, 1203, 751.

HRMS (ESI, m/z): Calculated for [C₂₅H₁₇NO₂+H]⁺, 364.1332; found, 364.1336.

(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)(*o*-tolyl)methanone (3g)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), Yellow solid, 50.1 mg, 69% yield, m.p. 151.4-152.1 °C.

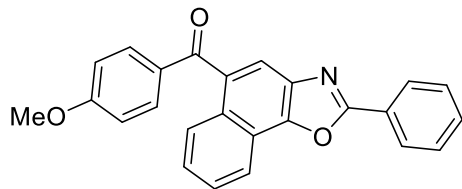
^1H NMR (400 MHz, CDCl₃): δ 8.08 (d, J = 7.6 Hz, 1H), 7.95-7.88 (m, 2H), 7.73-7.68 (m, 1H), 7.67-7.62 (m, 1H), 7.49 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.43 (t, J = 7.6 Hz, 1H), 7.37 (d, J = 7.6 Hz, 1H), 7.34-7.26 (m, 3H), 7.08 (t, J = 7.6 Hz, 1H), 6.92 (d, J = 7.6 Hz, 2H), 2.51 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl₃, 100 MHz, ppm): δ 195.0, 158.4, 157.5, 138.9, 136.8, 136.5, 134.6, 131.7, 131.7, 130.4, 130.2, 130.0, 129.9, 129.9, 129.6, 128.9, 125.4, 123.7, 123.1, 115.7, 114.0, 102.3, 20.5.

IR (ATR, cm^{-1}): ν 3063, 2227, 1662, 1591, 1485, 1299, 1196, 744.

HRMS (ESI, m/z): Calculated for $[\text{C}_{25}\text{H}_{17}\text{NO}_2+\text{H}]^+$, 364.1332; found, 364.1330.

(4-methoxyphenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3h)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 43.9 mg, 58% yield, m.p. 136.3-137.2 °C.

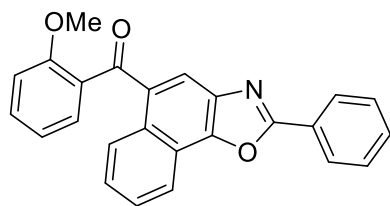
^1H NMR (400 MHz, CDCl_3): δ 8.09 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.4 Hz, 2H), 7.91 (d, J = 8.8 Hz, 2H), 7.73 (t, J = 8.0 Hz, 1H), 7.64 (t, J = 8.0 Hz, 1H), 7.31 (t, J = 8.0 Hz, 2H), 7.08 (t, J = 7.6 Hz, 1H), 7.00 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 8.0 Hz, 2H), 3.91 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz, ppm): δ 191.8, 164.2, 158.5, 156.9, 136.8, 134.8, 132.9, 130.3, 129.9, 129.3, 129.2, 129.1, 128.3, 127.5, 127.4, 123.6, 123.2, 115.8, 114.0, 102.7, 55.6.

IR (ATR, cm^{-1}): ν 3070, 2227, 1650, 1596, 1486, 1264, 1205, 748.

HRMS (ESI, m/z): Calculated for $[\text{C}_{25}\text{H}_{17}\text{NO}_3+\text{H}]^+$, 380.1281; found, 380.1277.

(2-methoxyphenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3i)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 53.7 mg, 71% yield, m.p. 137.2-138.6 °C.

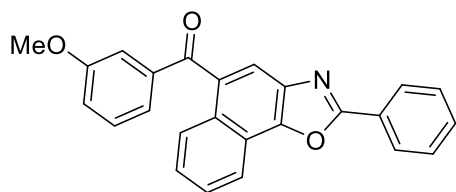
^1H NMR (400 MHz, CDCl_3): δ 8.05 (d, J = 8.4 Hz, 1H), 8.02 (s, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.73-7.52 (m, 4H), 7.29 (t, J = 7.6 Hz, 2H), 7.14-7.03 (m, 2H), 6.99 (d, J = 8.4 Hz, 1H), 6.90 (d, J = 8.4 Hz, 2H), 3.66 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz, ppm): δ 193.1, 158.6, 158.5, 156.8, 137.5, 135.0, 134.0, 131.0, 130.0, 129.9, 129.5, 129.5, 128.7, 128.5, 127.3, 123.5, 123.0, 121.0, 115.7, 114.0, 111.7, 102.1, 55.7.

IR (ATR, cm^{-1}): ν 3033, 2227, 1673, 1598, 1487, 1251, 1211, 748.

HRMS (ESI, m/z): Calculated for $[\text{C}_{25}\text{H}_{17}\text{NO}_3+\text{H}]^+$, 380.1281; found, 380.1282.

(3-methoxyphenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3j)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 40.9 mg, 54% yield, m.p. 133.6-135.7 °C.

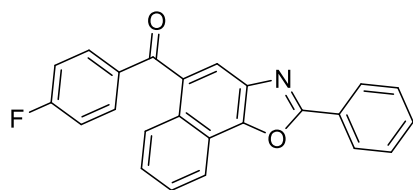
¹H NMR (400 MHz, CDCl₃): δ 8.10 (d, J = 8.8 Hz, 1H), 8.02 (s, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.73 (t, J = 8.0 Hz, 1H), 7.66 (t, J = 8.0 Hz, 1H), 7.49 (s, 1H), 7.43-7.39 (m, 2H), 7.31 (t, J = 7.2, 2H), 7.23-7.18 (m, 1H), 7.10 (t, J = 8.4 Hz, 1H), 6.93 (d, J = 7.6 Hz, 2H), 3.88 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.9, 159.9, 158.5, 157.2, 137.6, 136.2, 134.7, 130.4, 130.0, 129.6, 129.6, 129.4, 128.6, 128.2, 123.7, 123.4, 123.2, 120.3, 115.8, 114.4, 113.9, 102.6, 55.5.

IR (ATR, cm⁻¹): ν 3041, 2226, 1651, 1591, 1483, 1296, 1209, 746.

HRMS (ESI, m/z): Calculated for [C₂₅H₁₇NO₃+H]⁺, 380.1281; found, 380.1283.

(4-fluorophenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3k)



Prepared according to General Procedure B and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 33.8 mg, 46% yield, m.p. 150.3-151.7 °C.

¹H NMR (400 MHz, CDCl₃): δ 8.10 (d, J = 8.4 Hz, 1H), 8.01-7.92 (m, 4H), 7.78-7.72 (m, 1H), 7.71-7.65 (m, 1H), 7.36-7.27 (m, 2H), 7.25-7.18 (m, 2H), 7.10 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 8.0 Hz, 2H).

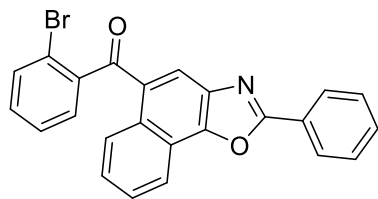
¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 191.7, 166.2 (d, J_{C-F} = 255.1 Hz), 158.5, 157.3, 136.0, 134.7, 133.2 (d, J_{C-F} = 9.5 Hz), 132.7 (d, J_{C-F} = 2.8 Hz), 130.6, 130.0, 129.7, 129.4, 128.6, 128.0, 123.7, 123.3, 116.0 (d, J_{C-F} = 21.9 Hz), 115.8, 113.9, 102.5.

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -103.4.

IR (ATR, cm⁻¹): ν 3063, 2233, 1654, 1597, 1486, 1297, 1201, 751.

HRMS (ESI, m/z): Calculated for [C₂₄H₁₄FN₂O₂+H]⁺, 368.1081; found, 368.1076.

(2-bromophenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3l)



Prepared according to General Procedure B and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 35.1 mg, 41% yield, m.p. 152.1-152.9 °C.

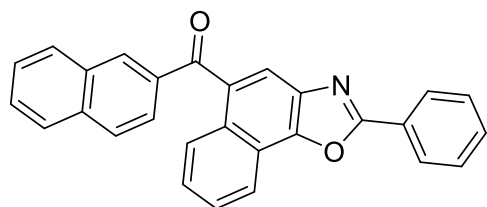
¹H NMR (400 MHz, CDCl₃): δ 8.08 (d, J = 7.2 Hz, 1H), 7.96-7.90 (m, 2H), 7.80-7.62 (m, 3H), 7.55 (dd, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 7.50 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.45 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.34-7.28 (m, 2H), 7.09 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 7.6 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 193.0, 158.4, 157.8, 139.4, 134.7, 134.6, 133.6, 132.4, 130.7, 130.4, 130.3, 130.3, 130.0, 129.8, 129.3, 127.6, 123.8, 123.2, 120.4, 115.7, 113.8, 102.0.

IR (ATR, cm⁻¹): ν 3151, 2921, 2227, 1673, 1618, 1486, 1296, 1198, 748.

HRMS (ESI, m/z): Calculated for [C₂₄H₁₄⁷⁹BrNO₂+H]⁺, 428.0281 ; found, 428.0279.

naphthalen-2-yl(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3m)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 47.1 mg, 59% yield, m.p. 183.6-183.9 °C.

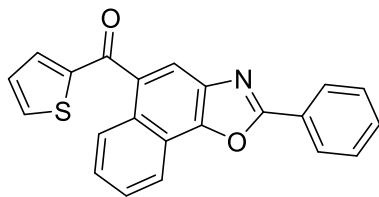
¹H NMR (400 MHz, CDCl₃): δ 8.33 (s, 1H), 8.13 (d, J = 8.4 Hz, 1H), 8.10-8.03 (m, 2H), 8.03-7.84 (m, 4H), 7.77-7.72 (m, 1H), 7.71-7.64 (m, 2H), 7.61-7.55 (m, 1H), 7.35-7.28 (m, 2H), 7.14-7.06 (m, 1H), 7.00-6.93 (m, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 193.1, 158.5, 157.3, 136.4, 135.9, 134.8, 133.7, 132.9, 132.2, 130.4, 130.0, 129.7, 129.6, 129.4, 129.0, 128.8, 128.6, 128.3, 127.9, 127.1, 125.4, 123.7, 123.2, 115.8, 114.0, 102.8.

IR (ATR, cm⁻¹): ν 3058, 2959, 2227, 1651, 1622, 1486, 1293, 1202, 749.

HRMS (ESI, m/z): Calculated for [C₂₈H₁₇NO₂+H]⁺, 400.1332; found, 400.1331.

(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)(thiophen-2-yl)methanone (3n)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 45.4 mg, 64% yield, m.p. 147.9-150.7 °C.

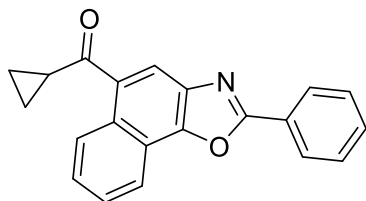
¹H NMR (400 MHz, CDCl₃): δ 8.17 (s, 1H), 8.10 (d, J = 8.4 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 5.2 Hz, 1H), 7.76 (t, J = 7.2 Hz, 1H), 7.71-7.63 (m, 2H), 7.32 (t, J = 8.4 Hz, 2H), 7.22 (t, J = 4.4 Hz, 1H), 7.09 (t, J = 7.2 Hz, 1H), 6.93 (d, J = 8.0 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 184.7, 158.5, 157.2, 142.9, 136.3, 136.0, 135.8, 134.8, 130.5, 130.0, 129.6, 129.3, 128.6, 128.3, 127.3, 123.7, 123.2, 115.8, 113.8, 102.3.

IR (ATR, cm⁻¹): ν 3065, 2949, 2228, 1629, 1514, 1411, 1200, 789.

HRMS (ESI, m/z): Calculated for [C₂₂H₁₃NO₂S+H]⁺, 356.0740; found, 356.0732.

cyclopropyl(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (3p)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 28.8 mg, 46% yield, m.p. 118.8-120.0 °C.

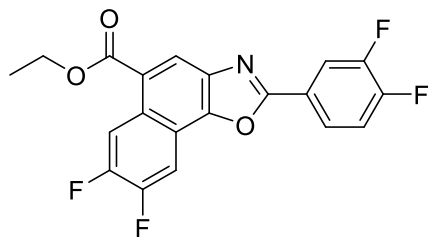
¹H NMR (400 MHz, CDCl₃): δ 8.40 (s, 1H), 8.06 (d, J = 9.2 Hz, 2H), 7.75 (t, J = 8.2 Hz, 1H), 7.65 (t, J = 8.2 Hz, 1H), 7.29 (t, J = 8.8 Hz, 2H), 7.08 (t, J = 7.6 Hz, 1H), 6.88 (d, J = 8.0 Hz, 2H), 2.81-2.70 (m, 1H), 1.43 (dt, J_1 = 7.6 Hz, J_2 = 4.0 Hz, 2H), 1.23-1.18 (m, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 198.8, 159.9, 158.5, 157.4, 136.7, 135.0, 130.3, 129.9, 129.8, 129.5, 128.9, 127.5, 123.7, 123.1, 115.7, 114.5, 19.3, 13.1.

IR (ATR, cm⁻¹): ν 3024, 2920, 2225, 1668, 1598, 1486, 1286, 1166, 753.

HRMS (ESI, m/z): Calculated for [C₂₁H₁₅NO₂+H]⁺, 314.1176; found, 314.1171.

ethyl 2-(3,4-difluorophenyl)-7,8-difluoronaphtho[2,1-*d*]oxazole-5-carboxylate (3q)



Prepared according to General Procedure B and purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 57.6 mg, 74% yield, m.p. 151.0-152.0 °C.

¹H NMR (400 MHz, CDCl₃): δ 8.53 (s, 1H), 7.87-7.72 (m, 2H), 7.12 (q, J = 9.2 Hz, 1H), 6.76-6.69 (m, 1H), 6.61-6.54 (m, 1H), 4.52 (q, J = 7.2 Hz, 2H), 1.48 (t, J = 7.2 Hz, 3H).

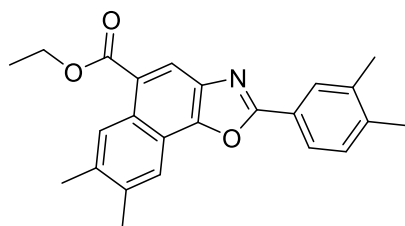
¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 163.4, 154.8 (dd, J_{C-F1} = 213.5 Hz, J_{C-F2} = 3.5 Hz), 154.7 (dd, J_{C-F1} = 213.5 Hz, J_{C-F2} = 3.5 Hz), 153.0 (dd, J_{C-F1} = 193.8 Hz, J_{C-F2} = 3.0 Hz), 152.9 (dd, J_{C-F1} = 193.8 Hz, J_{C-F2} = 3.0 Hz), 151.4, 132.2 (d, J_{C-F} = 8.3 Hz), 129.0 (dd, J_{C-F1} = 4.8 Hz, J_{C-F2} = 1.6 Hz), 128.7 (d, J_{C-F} = 2.0 Hz), 126.4 (d, J_{C-F} = 7.6 Hz), 118.0 (dd, J_{C-F1} = 19.0 Hz, J_{C-F2} = 1.4 Hz), 116.1 (dd, J_{C-F1} = 17.6 Hz, J_{C-F2} = 1.5 Hz), 113.3, 111.1 (dd, J_{C-F1} = 6.2 Hz, J_{C-F2} = 3.9 Hz), 110.2 (dd, J_{C-F1} = 19.3 Hz, J_{C-F2} = 1.1 Hz), 105.8, 105.6, 103.5 (d, J_{C-F} = 3.1 Hz), 62.8, 14.1.

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -127.34 (d, J = 20.3 Hz), -127.93 (d, J = 20.3 Hz), -133.08 (d, J = 21.4 Hz), -143.68 (d, J = 21.8 Hz).

IR (ATR, cm⁻¹): ν 3055, 2995, 2231, 1709, 1637, 1511, 1228, 782.

HRMS (ESI, m/z): Calculated for [C₂₀H₁₁F₄NO₃+H]⁺, 390.0748; found, 390.0745.

ethyl 2-(3,4-dimethylphenyl)-7,8-dimethylnaphtho[2,1-*d*]oxazole-5-carboxylate (3r)



Prepared according to General Procedure B and Purified by silica gel column chromatography (12/1 petroleum ether/ethyl acetate), White solid, 64.2 mg, 86% yield, m.p. 159.6-160.3 °C.

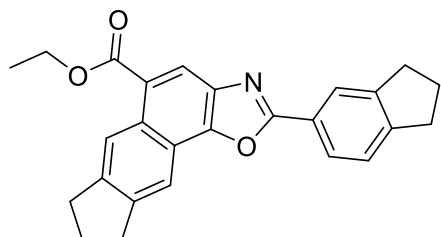
¹H NMR (400 MHz, CDCl₃): δ 8.43 (s, 1H), 7.78 (d, J = 6.8 Hz, 2H), 7.00 (d, J = 8.4 Hz, 1H), 6.69 (d, J = 2.8 Hz, 1H), 6.53 (dd, J_1 = 8.4 Hz, J_2 = 2.8 Hz, 1H), 4.49 (q, J = 7.2 Hz, 2H), 2.47 (s, 3H), 2.39 (s, 3H), 2.18 (s, 6H), 1.47 (t, J = 7.2 Hz, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz, ppm): δ 164.4, 156.9, 156.8, 140.9, 140.6, 138.3, 133.7, 130.9, 130.5, 129.1, 128.6, 128.2, 126.7, 122.9, 116.7, 114.6, 112.4, 101.8, 62.1, 20.6, 20.4, 20.0, 18.9, 14.1.

IR (ATR, cm^{-1}): ν 3675, 2972, 2314, 1720, 1496, 1373, 1064, 773.

HRMS (ESI, m/z): Calculated for $[\text{C}_{24}\text{H}_{23}\text{NO}_3+\text{H}]^+$, 374.1751; found, 374.1743.

ethyl 2-(2,3-dihydro-1H-inden-5-yl)-8,9-dihydro-7H-cyclopenta[6,7]naphtho [2,1-*d*]oxazole-5-carboxylate (3s)



Prepared according to General Procedure B and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 63.9 mg, 81% yield, m.p. 182.1-182.4 °C.

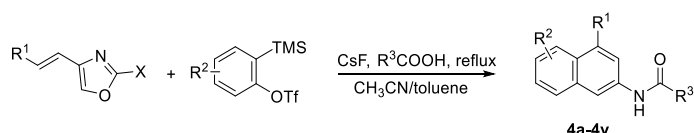
^1H NMR (400 MHz, CDCl_3): δ 8.45 (s, 1H), 7.86 (s, 1H), 7.82 (s, 1H), 7.09 (d, J = 8.0 Hz, 1H), 6.69 (d, J = 2.4 Hz, 1H), 6.64 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 4.50 (q, J = 7.2 Hz, 2H), 3.11 (t, J = 7.2 Hz, 2H), 3.02 (td, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 2H), 2.82 (q, J = 7.6 Hz, 4H), 2.19-2.11 (m, 2H), 2.09-2.00 (m, 2H), 1.47 (t, J = 7.2 Hz, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 125 MHz, ppm): δ 164.5, 157.6, 157.2, 148.7, 148.5, 146.1, 138.4, 134.5, 129.1, 128.9, 126.6, 125.0, 124.0, 117.9, 114.6, 113.3, 111.5, 101.9, 62.1, 33.1, 32.9, 32.7, 32.0, 25.7, 25.7, 14.1.

IR (ATR, cm^{-1}): ν 2948, 2229, 1722, 1660, 1594, 1264, 1185, 731.

HRMS (ESI, m/z): Calculated for $[\text{C}_{26}\text{H}_{23}\text{NO}_3+\text{NH}_4]^+$, 415.2016; found, 415.2017.

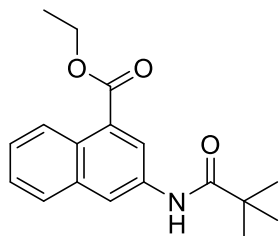
General Procedure C : Synthesis of *N*-Acyl naphthylamines.



Under a nitrogen atmosphere, 2-halo-4-alkenyloxazole **1** (0.2 mmol, 1.0 equiv), CsF (1.2 mmol, 6.0 equiv) and acid (0.3 mmol, 1.5 equiv) were placed in a 25 mL Schlenk tube equipped with a stir bar. Then 1.0 mL of MeCN and 1.0 mL of toluene were added. The reaction mixture was stirred at reflux for 10 min. Then the aryne precursor **2** (0.6 mmol, 3.0 equiv) was dissolved in 1.0 mL of toluene. The resulting solution was added dropwise in six portions over a period of 3 h. When the reaction was complete as

monitored by TLC, the reaction mixture was filtered through a short column of silica gel and eluted with CH_2Cl_2 . The filtrate was concentrated under reduced pressure to afford a residue, which was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compounds **4a-4v**.

ethyl 3-pivalamido-1-naphthoate (**4a**)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 46.0 mg, 73% yield, m.p. 181.2-183.0 °C.

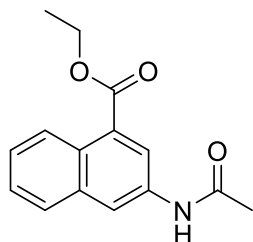
^1H NMR (400 MHz, DMSO- d_6): δ 9.64 (s, 1H), 8.69-8.63 (m, 1H), 8.60 (s, 1H), 8.39 (s, 1H), 7.95-7.88 (m, 1H), 7.66-7.40 (m, 2H), 4.43 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H), 1.28 (s, 9H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl₃, 100 MHz, ppm): δ 177.0, 167.1, 134.6, 134.2, 128.4, 128.4, 128.2, 126.8, 126.7, 125.5, 123.8, 121.8, 61.3, 39.7, 27.6, 14.4.

IR (ATR, cm^{-1}): ν 3277, 2976, 1708, 1656, 1544, 1204, 1149, 794.

HRMS (ESI, m/z): Calculated for $[\text{C}_{18}\text{H}_{21}\text{NO}_3+\text{H}]^+$, 300.1594; found, 300.1584.

ethyl 3-acetamido-1-naphthoate (**4b**)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 21.5 mg, 42% yield, m.p. 168.4-168.9 °C.

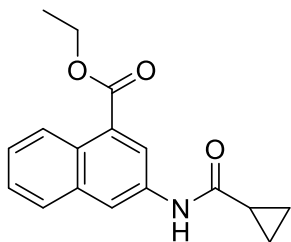
^1H NMR (400 MHz, DMSO- d_6): δ 10.41 (s, 1H), 8.75-8.68 (m, 1H), 8.60 (s, 1H), 8.29 (d, J = 2.0 Hz, 1H), 8.00-7.92 (m, 1H), 7.63-7.53 (m, 2H), 4.47 (q, J = 7.2 Hz, 2H), 2.17 (s, 3H), 1.44 (t, J = 7.2 Hz, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (DMSO- d_6 , 100 MHz, ppm): δ 168.9, 166.4, 135.8, 134.1, 128.2, 127.4, 127.0, 126.8, 126.2, 124.9, 123.6, 119.9, 61.0, 24.0, 14.2.

IR (ATR, cm^{-1}): ν 3352, 2921, 1686, 1541, 1250, 1197, 753.

HRMS (ESI, m/z): Calculated for $[\text{C}_{15}\text{H}_{15}\text{NO}_3+\text{H}]^+$, 258.1125; found, 258.1123.

ethyl 3-(cyclopropanecarboxamido)-1-naphthoate (4c)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 32.2 mg, 57% yield, m.p. 116.4-118.6 °C.

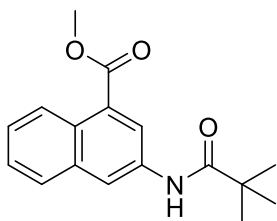
¹H NMR (400 MHz, DMSO-*d*₆): δ 10.62 (s, 1H), 8.70-8.62 (m, 1H), 8.55 (d, *J* = 2.0 Hz, 1H), 8.29 (d, *J* = 2.0 Hz, 1H), 7.93-7.86 (m, 1H), 7.56-7.49 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 1.90-1.80 (m, 1H), 1.40 (t, *J* = 7.2 Hz, 3H), 0.89-0.82 (m, 4H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 172.2, 166.4, 135.8, 134.1, 128.2, 127.4, 127.0, 126.8, 126.2, 124.9, 123.5, 119.9, 61.0, 14.6, 14.2, 7.5.

IR (ATR, cm⁻¹): ν 3365, 2922, 1712, 1661, 1557, 1239, 1149, 761.

HRMS (ESI, *m/z*): Calculated for [C₁₇H₁₇NO₃+H]⁺, 284.1281; found, 284.1277.

methyl 3-pivalamido-1-naphthoate (4d).



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 42.6 mg, 75% yield, m.p. 162.2-163.1 °C.

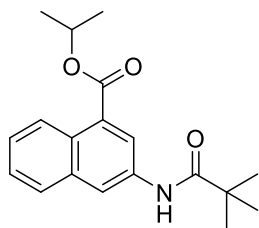
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.65 (s, 1H), 8.72-8.65 (m, 1H), 8.59 (s, 1H), 8.44 (s, 1H), 7.96-7.86 (m, 1H), 7.57-7.50 (m, 2H), 3.95 (s, 3H), 1.27 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 177.0, 166.9, 135.9, 134.0, 128.2, 127.2, 126.7, 126.7, 126.3, 124.9, 124.9, 121.5, 52.2, 39.3, 27.1.

IR (ATR, cm⁻¹): ν 3281, 2977, 1714, 1659, 1544, 1206, 1149, 794.

HRMS (ESI, *m/z*): Calculated for [C₁₇H₁₉NO₃+H]⁺, 286.1438; found, 286.1438.

isopropyl 3-pivalamido-1-naphthoate (4e)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 45.2 mg, 72% yield, m.p. 98.8-102.4 °C.

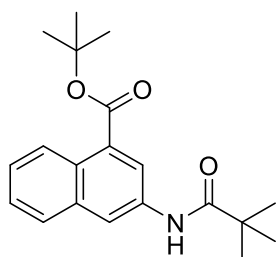
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.62 (s, 1H), 8.67-8.54 (m, 2H), 8.32 (s, 1H), 7.93-7.87 (m, 1H), 7.56-7.48 (m, 2H), 5.34-5.21 (m, 1H), 1.39 (d, *J* = 6.4 Hz, 6H), 1.27 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 177.1, 166.2, 135.9, 134.0, 128.2, 127.8, 127.1, 126.7, 126.2, 124.9, 124.3, 121.2, 68.5, 39.3, 27.2, 21.7.

IR (ATR, cm⁻¹): ν 3277, 2974, 1708, 1655, 1581, 1223, 1151, 793.

HRMS (ESI, *m/z*): Calculated for [C₁₉H₂₃NO₃+H]⁺, 314.1751; found, 314.1748.

***tert*-butyl 3-pivalamido-1-naphthoate (4f)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 36.4 mg, 71% yield, m.p. 197.6-199.1 °C.

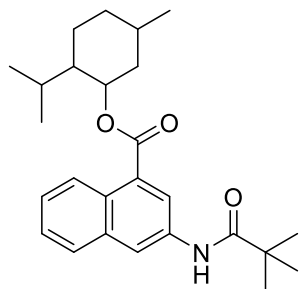
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.60 (s, 1H), 8.56 (s, 1H), 8.55-8.46 (m, 1H), 8.24 (s, 1H), 7.92-7.85 (m, 1H), 7.55-7.48 (m, 2H), 1.63 (s, 9H), 1.27 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 177.1, 166.4, 135.9, 134.0, 129.4, 128.2, 126.9, 126.6, 126.1, 124.9, 123.9, 120.7, 81.6, 39.3, 27.9, 27.2.

IR (ATR, cm⁻¹): ν 3278, 2972, 1709, 1656, 1541, 1209, 1145, 769.

HRMS (ESI, *m/z*): Calculated for [C₂₀H₂₅NO₃+H]⁺, 328.1907; found, 328.1906.

(±)-2-isopropyl-5-methylcyclohexyl 3-pivalamido-1-naphthoate (4g)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 64.7 mg, 79% yield, m.p. 58.5-60.1 °C.

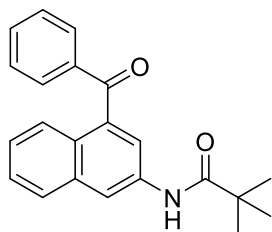
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.64 (s, 1H), 8.62 (d, J = 2.4 Hz, 1H), 8.60-8.56 (m, 1H), 8.35 (d, J = 2.4 Hz, 1H), 7.97-7.89 (m, 1H), 7.58-7.50 (m, 2H), 5.03 (td, J_1 = 10.8 Hz, J_2 = 4.4 Hz, 1H), 2.15-2.08 (m, 1H), 1.97-1.86 (m, 1H), 1.71 (s, 1H), 1.68 (s, 1H), 1.60-1.50 (m, 2H), 1.29 (s, 9H), 1.26-1.08 (m, 2H), 0.97-0.86 (m, 7H), 0.81 (d, J = 6.8 Hz, 3H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 177.0, 166.3, 135.9, 134.0, 128.2, 127.8, 127.0, 126.6, 126.2, 124.8, 124.1, 121.2, 74.3, 46.6, 40.6, 39.3, 33.7, 31.0, 27.2, 26.0, 23.0, 21.9, 20.5, 16.2.

IR (ATR, cm⁻¹): ν 3342, 2955, 1707, 1659, 1537, 1264, 1148, 1012, 793.

HRMS (ESI, *m/z*): Calculated for [C₂₆H₃₅NO₃+H]⁺, 410.2690; found, 410.2694.

***N*-(4-benzoylnaphthalen-2-yl)pivalamide (4h)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 50.0 mg, 76% yield, m.p. 165.9-167.2 °C.

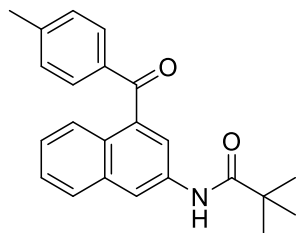
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.57 (s, 1H), 8.59 (s, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 2.4 Hz, 1H), 7.87-7.78 (m, 3H), 7.73 (t, J = 7.6 Hz, 1H), 7.62-7.50 (m, 3H), 7.47-7.39 (m, 1H), 1.25 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 196.8, 177.0, 137.6, 136.1, 135.8, 133.9, 133.7, 129.9, 128.9, 128.1, 126.9, 125.8, 124.8, 122.1, 122.1, 119.1, 39.3, 27.1.

IR (ATR, cm⁻¹): ν 3258, 2966, 1655, 1533, 1222, 1057, 776.

HRMS (ESI, *m/z*): Calculated for [C₂₂H₂₁NO₂+H]⁺, 332.1645; found, 332.1638.

***N*-(4-benzoylnaphthalen-2-yl)pivalamide (4i)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 42.1 mg, 61% yield, m.p. 113.1-113.9 °C.

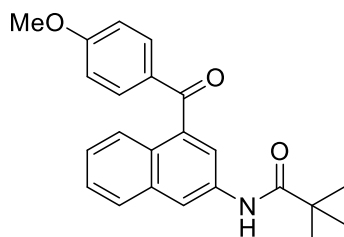
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.55 (s, 1H), 8.56 (s, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 2.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 6.8 Hz, 1H), 7.45-7.33 (m, 3H), 2.40 (s, 3H), 1.24 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 196.3, 177.0, 144.3, 136.4, 135.8, 135.0, 133.8, 130.1, 129.4, 128.1, 126.9, 126.8, 125.7, 124.8, 121.9, 118.8, 39.3, 27.1, 21.2.

IR (ATR, cm⁻¹): ν 3303, 2961, 1647, 1533, 1221, 1178, 787.

HRMS (ESI, *m/z*): Calculated for [C₂₃H₂₃NO₂+H]⁺, 346.1802; found, 346.1805.

***N*-(4-(4-methoxybenzoyl)naphthalen-2-yl)pivalamide (4j)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 56.8 mg, 79% yield, m.p. 64.1-65.2 °C.

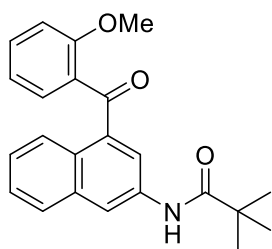
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.54 (s, 1H), 8.53 (s, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 2.4 Hz, 1H), 7.80-7.71 (m, 3H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.8, 2H), 3.86 (s, 3H), 1.25 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 195.2, 177.0, 163.7, 136.8, 135.8, 133.8, 132.4, 132.3, 130.2, 128.0, 126.8, 125.6, 124.8, 121.2, 118.5, 114.7, 55.6, 39.3, 27.1.

IR (ATR, cm⁻¹): ν 3348, 2920, 1651, 1595, 1250, 1192, 788.

HRMS (ESI, *m/z*): Calculated for [C₂₃H₂₃NO₃+H]⁺, 362.1751; found, 362.1749.

***N*-(4-(2-methoxybenzoyl)naphthalen-2-yl)pivalamide (4k)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 53.2 mg, 74% yield, m.p. 132.9-137.4 °C.

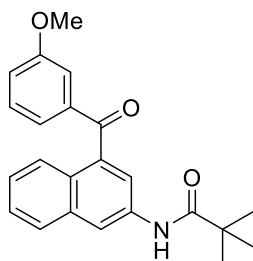
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.52 (s, 1H), 8.58 (s, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.85 (s, 1H), 7.63-7.57 (m, 1H), 7.56-7.45 (m, 3H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.11 (t, *J* = 8.4 Hz, 1H), 3.55 (s, 3H), 1.23 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 196.8, 176.9, 157.9, 137.0, 135.8, 133.9, 133.4, 130.2, 129.3, 128.0, 126.6, 126.6, 126.0, 124.9, 123.5, 120.6, 120.1, 112.8, 55.7, 39.2, 27.1.

IR (ATR, cm⁻¹): ν 3257, 2930, 1652, 1599, 1238, 1192, 754.

HRMS (ESI, *m/z*): Calculated for [C₂₃H₂₃NO₃+H]⁺, 362.1751; found, 362.1746.

***N*-(4-(3-methoxybenzoyl)naphthalen-2-yl)pivalamide (4l)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 54.9 mg, 76% yield, m.p. 132.6-134.9 °C.

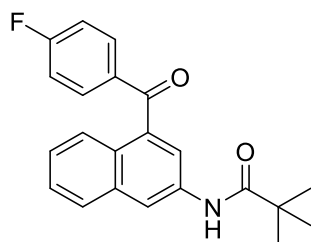
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.57 (s, 1H), 8.58 (s, 1H), 7.99-7.90 (m, 2H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.51-7.40 (m, 3H), 7.30 (dd, *J*₁ = 8.0 Hz, *J*₂ = 2.0 Hz, 2H), 3.83 (s, 3H), 1.26 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 196.4, 177.0, 159.4, 138.9, 136.0, 135.7, 133.8, 130.0, 128.0, 126.9, 126.8, 125.8, 124.8, 122.8, 122.2, 119.7, 119.2, 113.9, 55.3, 39.2, 27.1.

IR (ATR, cm⁻¹): ν 3410, 2963, 1678, 1593, 1238, 1186, 762.

HRMS (ESI, *m/z*): Calculated for [C₂₃H₂₃NO₃+H]⁺, 362.1751; found, 362.1746.

***N*-(4-(4-fluorobenzoyl)naphthalen-2-yl)pivalamide (4m)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 64.2 mg, 82% yield, m.p. 108.9-110.6 °C.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.58 (s, 1H), 8.59 (s, 1H), 7.96-7.82 (m, 5H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.42 (q, *J* = 8.8 Hz, 3H), 1.25 (s, 9H).

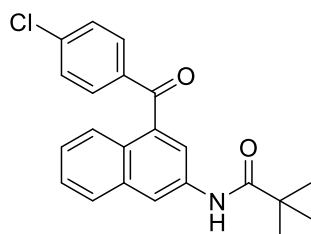
¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 195.3, 177.0, 165.3 (d, *J*_{C-F} = 251.3 Hz), 135.8, 135.8, 134.2 (d, *J*_{C-F} = 2.8 Hz), 133.9, 133.0 (d, *J*_{C-F} = 9.6 Hz), 128.1, 126.9, 126.8, 125.8, 124.7, 122.1, 119.1, 116.0 (d, *J*_{C-F} = 21.9 Hz), 39.3, 27.1.

¹⁹F{¹H} NMR (376 MHz, DMSO-*d*₆): δ -105.0.

IR (ATR, cm⁻¹): ν 3290, 2965, 1655, 1533, 1225, 1151, 750.

HRMS (ESI, *m/z*): Calculated for [C₂₂H₂₀FO₂+H]⁺, 350.1551; found, 350.1550.

***N*-(4-(4-chlorobenzoyl)naphthalen-2-yl)pivalamide (4n)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 56.8 mg, 78% yield, m.p. 90.4-92.3 °C.

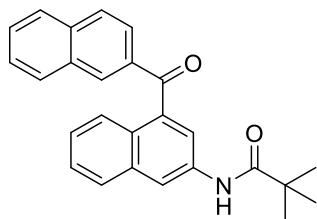
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.58 (s, 1H), 8.62 (s, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.92 (s, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 1.26 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 195.6, 177.0, 138.7, 136.3, 135.8, 135.5, 133.9, 131.8, 129.0, 128.1, 126.9, 126.8, 125.9, 124.7, 122.5, 119.4, 39.3, 27.1.

IR (ATR, cm⁻¹): ν 3314, 2955, 1654, 1537, 1222, 1190, 782.

HRMS (ESI, *m/z*): Calculated for [C₂₂H₂₀ClNO₂+H]⁺, 366.1255; found, 366.1256.

***N*-(4-(2-naphthoyl)naphthalen-2-yl)pivalamide (4o)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 65.8 mg, 86% yield, m.p. 157.6-158.4 °C.

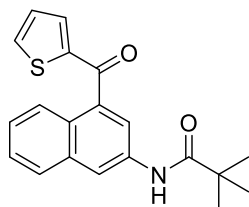
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.50 (s, 1H), 8.58 (s, 1H), 8.25 (s, 1H), 8.07-7.95 (m, 3H), 7.94-7.86 (m, 3H), 7.83 (dd, $J_1 = 8.4$ Hz, $J_2 = 1.2$ Hz, 1H), 7.65-7.60 (m, 1H), 7.55-7.44 (m, 2H), 7.38-7.32 (m, 1H), 1.17 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 196.9, 177.1, 136.3, 135.9, 135.3, 135.1, 134.0, 132.3, 132.0, 129.8, 129.1, 128.6, 128.1, 127.7, 127.1, 127.0, 126.9, 125.8, 124.9, 124.8, 122.4, 119.2, 39.3, 27.1.

IR (ATR, cm⁻¹): ν 3342, 3056, 2964, 1652, 1535, 1496, 1180, 747.

HRMS (ESI, *m/z*): Calculated for [C₂₆H₂₃NO₂+H]⁺, 382.1802; found, 382.1802.

***N*-(4-(thiophene-2-carbonyl)naphthalen-2-yl)pivalamide (4p)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), Yellow solid, 62.1 mg, 92% yield, m.p. 113.5-115.1 °C.

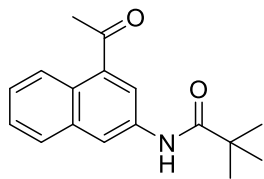
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.65 (s, 1H), 8.60 (s, 1H), 8.23 (d, $J = 4.0$ Hz, 1H), 8.15 (s, 1H), 7.98 (d, $J = 9.6$ Hz, 2H), 7.65 (s, 1H), 7.59 (t, $J = 8.0$ Hz, 1H), 7.50 (t, $J = 8.0$ Hz, 1H), 7.36-7.31 (m, 1H), 1.31 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 188.3, 177.1, 144.2, 136.7, 136.4, 135.8, 135.6, 133.9, 129.0, 128.0, 126.9, 126.5, 125.8, 124.6, 122.0, 119.2, 39.3, 27.1.

IR (ATR, cm⁻¹): ν 3272, 2967, 2309, 1656, 1407, 1223, 1058, 752.

HRMS (ESI, *m/z*): Calculated for [C₂₀H₁₉NO₂S+H]⁺, 338.1209; found, 338.1205.

***N*-(4-acetylnaphthalen-2-yl)pivalamide (4q)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 46.8 mg, 87% yield, m.p. 134.4-136.1 °C.

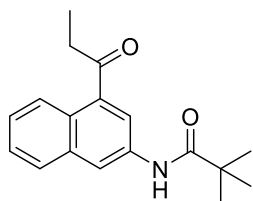
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.59 (s, 1H), 8.60-8.54 (m, 2H), 8.37 (d, *J* = 2.0 Hz, 1H), 7.94-7.86 (m, 1H), 7.57-7.46 (m, 2H), 2.72 (s, 3H), 1.30 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 201.1, 177.0, 135.8, 134.9, 134.1, 128.1, 126.7, 126.4, 126.2, 125.3, 124.2, 120.8, 39.3, 29.8, 27.2.

IR (ATR, cm⁻¹): ν 3308, 2964, 1682, 1646, 1600, 1497, 1234, 876.

HRMS (ESI, *m/z*): Calculated for [C₁₇H₁₉NO₂+H]⁺, 270.1489; found, 270.1490.

***N*-(4-propionynaphthalen-2-yl)pivalamide (4r)**



Prepared according to General Procedure C and purified by silica gel column chromatography (4/1 petroleum ether/ethyl acetate), Brown solid, 45.9 mg, 81% yield, m.p. 132.4-132.6 °C.

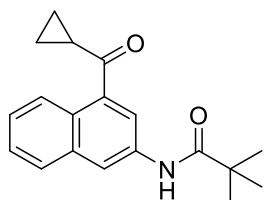
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.55 (s, 1H), 8.52 (s, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.29 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.55-7.45 (m, 2H), 3.09 (q, *J* = 7.2 Hz, 2H), 1.29 (s, 9H), 1.17 (t, *J* = 7.2 Hz, 3H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 204.3, 177.0, 135.9, 135.7, 134.0, 128.0, 126.7, 126.2, 126.1, 125.1, 122.8, 120.2, 39.3, 34.6, 27.2, 8.5.

IR (ATR, cm⁻¹): ν 3290, 2972, 1688, 1533, 1364, 1225, 756.

HRMS (ESI, *m/z*): Calculated for [C₁₈H₂₁NO₂+H]⁺, 284.1645; found, 284.1649.

***N*-(4-(cyclopropanecarbonyl)naphthalen-2-yl)pivalamide (4s)**



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 45.2 mg, 76% yield, m.p. 145.2-147.3 °C.

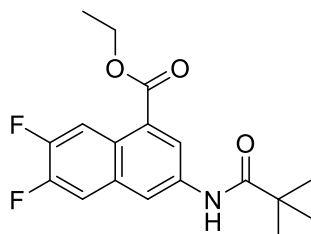
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.61 (s, 1H), 8.53 (s, 1H), 8.33 (d, J = 2.0 Hz, 1H), 8.26 (d, J = 8.0 Hz, 1H), 7.90 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.56-7.46 (m, 2H), 2.70-2.62 (m, 1H), 1.29 (s, 9H), 1.26-1.12 (m, 4H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 203.5, 177.0, 137.2, 136.0, 133.9, 128.0, 126.8, 126.1, 125.8, 124.9, 122.4, 119.9, 39.3, 27.2, 21.0, 12.2.

IR (ATR, cm⁻¹): ν 3354, 2966, 1654, 1537, 1354, 1225, 748.

HRMS (ESI, *m/z*): Calculated for [C₁₉H₂₁NO₂+H]⁺, 296.1645; found, 296.1647.

ethyl 6,7-difluoro-3-pivalamido-1-naphthoate (4t)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 59.6 mg, 89% yield, m.p. 143.8-145.1 °C.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.70 (s, 1H), 8.72-8.62 (m, 2H), 8.47 (d, J = 2.0 Hz, 1H), 8.05 (dd, J_1 = 11.6 Hz, J_2 = 8.4 Hz, 1H), 4.44 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H), 1.28 (s, 9H).

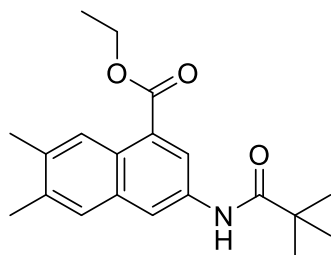
¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 177.1, 166.0, 149.1 (dd, J_{C-F1} = 255.1 Hz, J_{C-F2} = 7.8 Hz), 149.0 (dd, J_{C-F1} = 255.1 Hz, J_{C-F2} = 7.8 Hz), 136.6 (d, J_{C-F} = 2.3 Hz), 131.6 (d, J_{C-F} = 8.0 Hz), 126.2 (dd, J_{C-F1} = 5.5 Hz, J_{C-F2} = 1.5 Hz), 125.3, 124.0 (dd, J_{C-F1} = 8.6 Hz, J_{C-F2} = 0.9 Hz), 121.0, 114.3 (d, J_{C-F} = 16.4 Hz), 111.8 (d, J_{C-F} = 19.4 Hz), 61.3, 39.3, 27.1, 14.2.

¹⁹F{¹H} NMR (376 MHz, DMSO-*d*₆): δ -136.88 (d, J = 22.6 Hz), -137.19 (d, J = 22.6 Hz).

IR (ATR, cm⁻¹): ν 3287, 2919, 1711, 1655, 1509, 1264, 1123, 812.

HRMS (ESI, *m/z*): Calculated for [C₁₈H₁₉F₂NO₃+H]⁺, 336.1406; found, 336.1406.

ethyl 6,7-dimethyl-3-pivalamido-1-naphthoate (4u)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 60.3 mg, 92% yield, m.p. 137.3-137.6 °C.

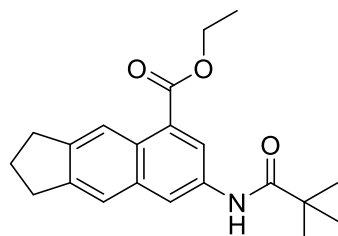
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.55 (s, 1H), 8.44 (s, 2H), 8.28 (d, *J* = 2.0 Hz, 1H), 7.64 (s, 1H), 4.42 (q, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 2.38 (s, 3H), 1.40 (t, *J* = 7.2 Hz, 3H), 1.27 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 176.9, 166.7, 136.1, 135.8, 135.1, 132.9, 127.5, 126.2, 126.1, 124.4, 123.8, 120.8, 60.8, 39.3, 27.2, 20.3, 19.6, 14.3.

IR (ATR, cm⁻¹): ν 3300, 2972, 1711, 1654, 1529, 1210, 894.

HRMS (ESI, *m/z*): Calculated for [C₂₀H₂₅NO₃+H]⁺, 328.1907; found, 328.1907.

ethyl 7-pivalamido-2,3-dihydro-1H-cyclopenta[*b*]naphthalene-5-carboxylate (4v)



Prepared according to General Procedure C and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 59.0 mg, 87% yield, m.p. 176.0-177.0 °C.

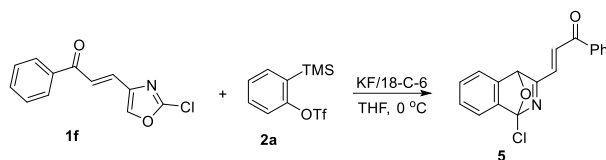
¹H NMR (400 MHz, DMSO-*d*₆): δ 9.55 (s, 1H), 8.49 (s, 1H), 8.46 (d, *J* = 2.4 Hz 1H), 8.29 (d, *J* = 2.4 Hz, 1H), 7.69 (s, 1H), 4.42 (q, *J* = 7.2 Hz, 2H), 3.05-2.96 (m, 4H), 2.13-2.03 (m, 2H), 1.40 (t, *J* = 7.2 Hz, 3H), 1.28 (s, 9H).

¹³C{¹H} NMR (DMSO-*d*₆, 125 MHz, ppm): δ 176.8, 166.9, 143.7, 143.6, 135.0, 133.4, 126.6, 126.6, 123.5, 122.3, 121.4, 119.2, 60.8, 39.4, 32.3, 31.9, 27.1, 25.6, 14.3.

IR (ATR, cm⁻¹): ν 3290, 2962, 1709, 1654, 1583, 1208, 892.

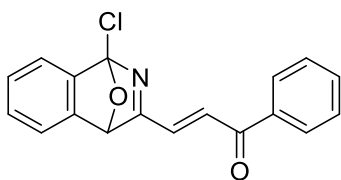
HRMS (ESI, *m/z*): Calculated for [C₂₁H₂₅NO₃+H]⁺, 340.1907; found, 340.1905.

Procedure D: Synthesis of Epoxyisoquinoline.



Under a nitrogen atmosphere, (*E*)-3-(2-chlorooxazol-4-yl)-1-phenylprop-2-en-1-one **1f** (46.7 mg, 0.2 mmol, 1.0 equiv), KF (43.5 mg, 0.75 mmol, 3.75 equiv), and 18-crown-6 (0.198 g, 0.75 mmol, 3.75 equiv) were placed in a 25 mL Schlenk tube equipped with a stir bar. Then 2.0 mL of THF and benzyne precursor **2a** (0.149 g, 0.5 mmol, 2.5 equiv) were added. The reaction mixture was stirred at 0 °C. After the reaction was complete as monitored by TLC, the mixture was concentrated directly, and the residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **5** (28.6 mg, 46%).

(*E*)-3-(1-chloro-1,4-dihydro-1,4-epoxyisoquinolin-3-yl)-1-phenylprop-2-en-1-one (**5**)



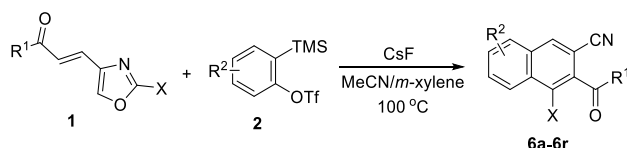
Prepared according to Procedure D and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White solid, 28.6 mg, 46% yield.

This sample is sensitive to both air and acid. Furthermore, it becomes highly unstable in high concentrations in deuterated solvents, which precludes the acquisition of ^{13}C NMR spectral data requiring prolonged signal accumulation.

^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, J = 7.2 Hz, 2H), 7.64 (t, J = 7.2 Hz, 1H), 7.57 (d, J = 8.8 Hz, 1H), 7.55-7.50 (m, 3H), 7.46-7.39 (m, 2H), 7.23 (t, J = 6.8 Hz, 1H), 7.17 (t, J = 7.2 Hz, 1H), 6.10 (s, 1H).

HRMS (ESI, m/z): Calculated for $[\text{C}_{18}\text{H}_{12}\text{ClNO}_2+\text{H}]^+$, 310.0629; found, 310.0626.

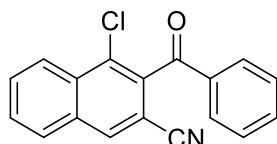
General Procedure E: Synthesis of α -Halonaphthalenes.



Under a nitrogen atmosphere, 2-halo-4-alkenyloxazole **1** (0.2 mmol, 1.0 equiv), CsF (0.9 mmol, 4.5 equiv) were placed in a 25 mL Schlenk tube equipped with a stir bar. Then 1.0 mL of MeCN and 1.0 mL of *m*-xylene were added. The reaction mixture was stirred at 100 °C for 10 min. Then the aryne precursor **2**

(0.6 mmol, 3.0 equiv) was dissolved in 1.0 mL of *m*-xylene. The resulting solution was added dropwise in six portions over a period of 3 h. When the reaction was complete as monitored by TLC, the reaction mixture was filtered through a short column of silica gel and eluted with CH₂Cl₂. The filtrate was concentrated under reduced pressure to afford a residue, which was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compounds **6a-6r**.

3-benzoyl-4-chloro-2-naphthonitrile (**6a**)



Prepared according to General Procedure E and Purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 44.9 mg, 77% yield, m.p. 200.8-202.1 °C.

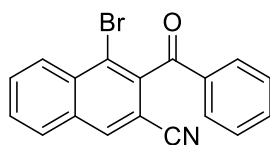
¹H NMR (400 MHz, CDCl₃): δ 8.39 (d, J = 8.4 Hz, 1H), 8.30 (s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.90-7.83 (m, 3H), 7.77 (t, J = 7.2 Hz, 1H), 7.66 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 8.0 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.6, 136.1, 135.4, 134.6, 134.3, 132.8, 132.1, 131.1, 130.2, 130.0, 129.3, 129.0, 129.0, 125.0, 116.2, 108.0.

IR (ATR, cm⁻¹): ν 2968, 2227, 1683, 1595, 1452, 1275, 896, 766.

HRMS (ESI, m/z): Calculated for [C₁₈H₁₀ClNO+H]⁺, 292.0524; found, 292.0517.

3-benzoyl-4-bromo-2-naphthonitrile (**6b**)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 51.1 mg, 76% yield, m.p. 170.7-171.4 °C.

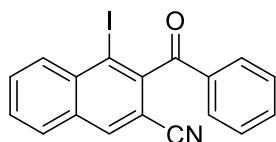
¹H NMR (400 MHz, CDCl₃): δ 8.40-8.31 (m, 2H), 7.98 (d, J = 8.0 Hz, 1H), 7.91-7.81 (m, 3H), 7.76 (t, J = 7.6 Hz, 1H), 7.64 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 8.0 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 193.3, 138.8, 135.0, 134.9, 134.6, 133.3, 132.6, 131.4, 130.1, 129.2, 129.1, 129.1, 127.6, 121.0, 116.1, 108.1.

IR (ATR, cm⁻¹): ν 2948, 2225, 1655, 1594, 1451, 1273, 891, 746.

HRMS (ESI, m/z): Calculated for [C₁₈H₁₀⁷⁹BrNO+NH₄]⁺, 353.0284; found, 353.0280.

3-benzoyl-4-iodo-2-naphthonitrile (6c)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 55.9 mg, 73% yield, m.p. 175.9-177.4 °C.

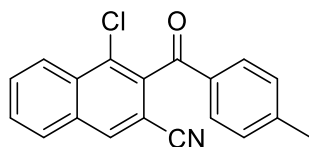
¹H NMR (400 MHz, CDCl₃): δ 8.35 (s, 1H), 8.28 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 8.4 Hz, 1H), 7.88-7.80 (m, 3H), 7.74 (t, J = 7.6 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 195.1, 143.8, 135.9, 135.6, 134.6, 134.3, 132.8, 131.8, 131.8, 130.3, 129.2, 129.2, 129.1, 116.1, 107.7, 98.8.

IR (ATR, cm⁻¹): ν 2944, 2222, 1652, 1593, 1450, 1269, 897, 756.

HRMS (ESI, m/z): Calculated for [C₁₈H₁₀INO+H]⁺, 383.9880; found, 383.9875.

4-chloro-3-(4-methylbenzoyl)-2-naphthonitrile (6d)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 42.6 mg, 70% yield, m.p. 218.9-219.4 °C.

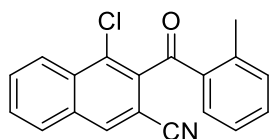
¹H NMR (400 MHz, CDCl₃): δ 8.38 (d, J = 8.4 Hz, 1H), 8.29 (s, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.85 (t, J = 6.8 Hz, 1H), 7.79-7.71 (m, 3H), 7.29 (d, J = 8.0 Hz, 2H), 2.44 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.1, 145.9, 136.4, 134.2, 133.0, 132.8, 132.1, 131.0, 130.2, 130.1, 129.8, 129.2, 129.0, 125.0, 116.2, 108.1, 21.9.

IR (ATR, cm⁻¹): ν 2948, 2229, 1660, 1601, 1449, 1274, 897, 771.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₂ClNO+H]⁺, 306.0680; found, 306.0681.

4-chloro-3-(2-methylbenzoyl)-2-naphthonitrile (6e)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 42.1 mg, 69% yield, m.p. 161.9-163.9 °C.

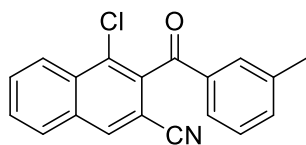
¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, J = 8.4 Hz, 1H), 8.28 (s, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.84 (t, J = 7.6 Hz, 1H), 7.75 (t, J = 7.6 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 7.6 Hz, 1H), 7.18 (t, J = 8.0 Hz, 1H), 2.78 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 194.2, 141.4, 137.5, 134.8, 134.2, 133.3, 132.7, 132.6, 132.3, 132.1, 131.0, 130.1, 129.2, 128.9, 125.9, 125.0, 116.3, 108.1, 21.9.

IR (ATR, cm⁻¹): ν 2948, 2228, 1659, 1601, 1458, 1287, 897, 747.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₂ClNO+H]⁺, 306.0680; found, 306.0676.

4-chloro-3-(3-methylbenzoyl)-2-naphthonitrile (6f)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 44.6 mg, 73% yield, m.p. 191.3-193.4 °C.

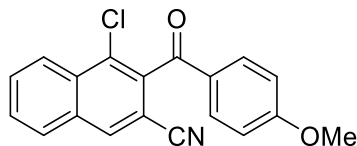
¹H NMR (400 MHz, CDCl₃): δ 8.39 (d, J = 8.4 Hz, 1H), 8.30 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.86 (t, J = 8.4 Hz, 1H), 7.77 (t, J = 6.8 Hz, 1H), 7.72 (s, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.47 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 2.40 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.7, 139.0, 136.4, 135.6, 135.4, 134.2, 132.8, 132.1, 131.1, 130.2, 130.1, 129.2, 129.0, 128.9, 127.5, 125.0, 116.2, 108.1, 21.3.

IR (ATR, cm⁻¹): ν 2953, 2225, 1669, 1599, 1447, 1271, 854, 767.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₂ClNO+H]⁺, 306.0680; found, 306.0681.

4-chloro-3-(4-methoxybenzoyl)-2-naphthonitrile (6g)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 47.6 mg, 74% yield, m.p. 196.5-197.9 °C.

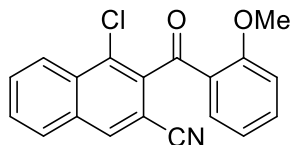
¹H NMR (400 MHz, CDCl₃): δ 8.39 (d, J = 8.8 Hz, 1H), 8.29 (s, 1H), 8.00 (d, J = 8.0 Hz, 1H), 7.87-7.80 (m, 3H), 7.76 (t, J = 7.2 Hz, 1H), 6.96 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 190.9, 164.8, 136.5, 134.2, 132.8, 132.5, 132.1, 131.0, 130.0, 129.1, 129.0, 128.5, 125.0, 116.3, 114.4, 108.2, 55.6.

IR (ATR, cm⁻¹): ν 2972, 2226, 1651, 1592, 1463, 1285, 895, 752.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₂ClNO₂+H]⁺, 322.0629; found, 322.0623.

4-chloro-3-(2-methoxybenzoyl)-2-naphthonitrile (6h)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 43.1 mg, 67% yield, m.p. 163.4-165.8 °C.

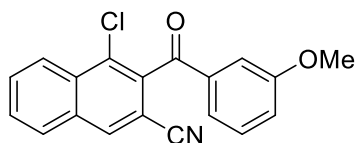
¹H NMR (400 MHz, CDCl₃): δ 8.35 (d, J = 7.2 Hz, 1H), 8.25 (s, 1H), 7.97 (td, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 2H), 7.82-7.77 (m, 1H), 7.74-7.68 (m, 1H), 7.63-7.53 (m, 1H), 7.11 (td, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H), 6.94 (d, J = 8.4 Hz, 1H), 3.53 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 191.4, 159.9, 139.6, 135.9, 133.8, 132.4, 132.1, 131.9, 130.6, 128.8, 128.7, 128.6, 125.9, 125.0, 121.2, 116.6, 112.1, 108.0, 55.8.

IR (ATR, cm⁻¹): ν 2946, 2230, 1648, 1593, 1462, 1294, 898, 756.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₂ClNO₂+H]⁺, 322.0629; found, 322.0626.

4-chloro-3-(3-methoxybenzoyl)-2-naphthonitrile (6i)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 51.8 mg, 81% yield, m.p. 184.2-186.1 °C.

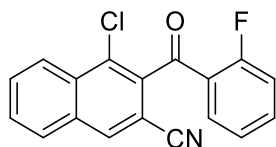
¹H NMR (400 MHz, CDCl₃): δ 8.38 (d, J = 8.8 Hz, 1H), 8.29 (s, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.92-7.80 (m, 1H), 7.79-7.73 (m, 1H), 7.52 (t, J = 2.8 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.29-7.25 (m, 1H), 7.20 (ddd, J_1 = 8.0 Hz, J_2 = 2.8 Hz, J_3 = 1.2 Hz, 1H), 3.88 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.4, 160.2, 136.7, 136.2, 134.2, 132.8, 132.1, 131.1, 130.0, 129.3, 129.0, 125.0, 123.3, 121.4, 118.5, 116.1, 113.3, 108.0, 55.5.

IR (ATR, cm⁻¹): ν 2953, 2228, 1667, 1592, 1454, 1273, 897, 749.

HRMS (ESI, m/z): Calculated for [C₁₉H₁₂ClNO₂+H]⁺, 322.0629; found, 322.0624.

4-chloro-3-(2-fluorobenzoyl)-2-naphthonitrile (6j)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 48.6 mg, 79% yield, m.p. 194.2-195.9 °C.

¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, J = 8.8 Hz, 1H), 8.29 (s, 1H), 8.03 (td, J_1 = 7.7 Hz, 1.6 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.85-7.80 (m, 1H), 7.77-7.72 (m, 1H), 7.67-7.59 (m, 1H), 7.34 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.14-7.07 (m, 1H).

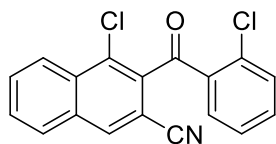
¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 189.1, 162.3 (d, J_{C-F} = 257.4 Hz), 137.7, 136.5 (d, J_{C-F} = 9.3 Hz), 134.3, 132.8, 132.0, 131.6, 130.9, 129.2, 128.9, 125.0, 124.9 (d, J_{C-F} = 3.7 Hz), 124.6 (d, J_{C-F} = 9.2 Hz), 118.2, 116.9 (d, J_{C-F} = 22.1 Hz), 116.3, 107.4 (d, J_{C-F} = 1.7 Hz).

¹⁹F{¹H} NMR (376 MHz, CDCl₃): δ -110.30.

IR (ATR, cm⁻¹): ν 3070, 2917, 2226, 1684, 1454, 1287, 899, 749.

HRMS (ESI, m/z): Calculated for [C₁₈H₉ClFNO+H]⁺, 310.0429; found, 310.0429.

4-chloro-3-(2-chlorobenzoyl)-2-naphthonitrile (6k)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 52.8 mg, 81% yield, m.p. 130.1.6-131.7 °C.

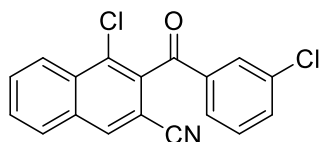
¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, J = 8.4 Hz, 1H), 8.30 (s, 1H), 7.98 (d, J = 8.8 Hz, 1H), 7.87-7.60 (m, 3H), 7.53 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.47 (d, J = 6.8 Hz, 1H), 7.40 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 125 MHz, ppm): δ 191.6, 136.7, 135.8, 134.7, 134.0, 133.8, 133.0, 132.3, 132.0, 131.3, 131.0, 130.7, 129.5, 128.9, 127.2, 125.2, 116.4, 108.5.

IR (ATR, cm⁻¹): ν 3067, 2233, 1672, 1585, 1459, 1266, 854, 770.

HRMS (ESI, m/z): Calculated for [C₁₈H₉Cl₂NO+H]⁺, 326.0134; found, 326.0135.

4-chloro-3-(3-chlorobenzoyl)-2-naphthonitrile (6l)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 50.7 mg, 78% yield, m.p. 156.2-157.4 °C.

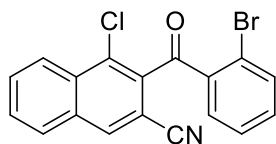
¹H NMR (400 MHz, CDCl₃): δ 8.39 (d, J = 8.0 Hz, 1H), 8.31 (s, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.90-7.83 (m, 2H), 7.81-7.76 (m, 1H), 7.71 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.62 (ddd, J_1 = 8.0 Hz, J_2 = 2.4 Hz, J_3 = 1.2 Hz, 1H), 7.44 (t, J = 8.0 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 125 MHz, ppm): δ 191.4, 137.0, 135.5, 135.4, 134.6, 134.4, 133.0, 132.0, 131.3, 130.4, 130.3, 129.7, 129.5, 129.1, 128.1, 125.1, 116.0, 107.9.

IR (ATR, cm⁻¹): ν 3072, 2923, 2227, 1676, 1446, 1254, 898, 747.

HRMS (ESI, m/z): Calculated for [C₁₈H₉Cl₂NO+H]⁺, 326.0134; found, 326.0135.

3-(2-bromobenzoyl)-4-chloro-2-naphthonitrile (6m)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 60.7 mg, 82% yield, m.p. 135.6-137.2 °C.

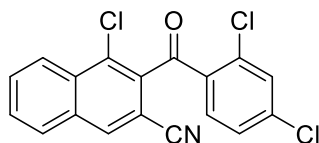
¹H NMR (400 MHz, CDCl₃): δ 8.37 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.30 (s, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.86-7.80 (m, 1H), 7.79-7.73 (m, 1H), 7.72-7.66 (m, 2H), 7.46-7.39 (m, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 192.2, 137.7, 136.1, 134.8, 134.8, 133.9, 133.1, 132.6, 132.1, 131.2, 131.1, 129.7, 129.0, 127.7, 125.3, 121.9, 116.4, 108.9.

IR (ATR, cm⁻¹): ν 3065, 2948, 2233, 1673, 1429, 1260, 898, 755.

HRMS (ESI, m/z): Calculated for [C₁₈H₉BrClNO+H]⁺, 369.9629; found, 369.9633.

4-chloro-3-(2,4-dichlorobenzoyl)-2-naphthonitrile (6n)



Prepared according to General Procedure E and Purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 48.3 mg, 67% yield, m.p. 184.1-185.0 °C.

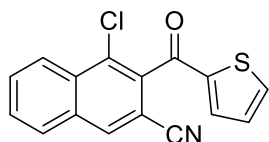
¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, J = 8.4 Hz, 1H), 8.30 (s, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.87-7.81 (m, 1H), 7.81-7.68 (m, 2H), 7.49 (d, J = 2.0 Hz, 1H), 7.39 (dd, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 1H).

¹³C{¹H} NMR (CDCl₃, 125 MHz, ppm): δ 190.5, 140.0, 136.3, 134.8, 134.7, 134.2, 133.2, 133.1, 132.0, 131.2, 131.1, 130.7, 129.7, 129.0, 127.8, 125.3, 116.2, 108.

IR (ATR, cm⁻¹): ν 3070, 2949, 2228, 1667, 1472, 1281, 898, 753.

HRMS (ESI, m/z): Calculated for [C₁₈H₈Cl₃NO+H]⁺, 359.9744; found, 359.9745.

4-chloro-3-(thiophene-2-carbonyl)-2-naphthonitrile (6o)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 40.5 mg, 68% yield, m.p. 177.4-178.1 °C.

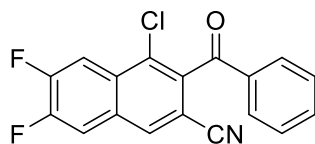
¹H NMR (400 MHz, CDCl₃): δ 8.41 (d, J = 8.4 Hz, 1H), 8.30 (s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.89-7.83 (m, 2H), 7.78 (t, J = 7.6 Hz, 1H), 7.43 (s, 1H), 7.17-7.13 (m, 1H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 184.4, 142.7, 136.9, 136.1, 136.0, 134.2, 132.9, 132.1, 131.1, 130.3, 129.4, 129.0, 128.7, 125.2, 116.1, 108.0.

IR (ATR, cm⁻¹): ν 3094, 2919, 2225, 1641, 1408, 1286, 895, 747.

HRMS (ESI, m/z): Calculated for [C₁₆H₈ClNOS+H]⁺, 298.0088; found, 298.0082.

3-benzoyl-4-chloro-6,7-difluoro-2-naphthonitrile (6p)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), Yellow solid, 55.3 mg, 84% yield, m.p. 162.3-163.9 °C.

¹H NMR (400 MHz, CDCl₃): δ 8.21 (s, 1H), 8.18-8.10 (m, 1H), 7.87-7.74 (m, 3H), 7.68 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 193.3, 153.2 (dd, J_{C-F1} = 257.4 Hz, J_{C-F2} = 15.4 Hz), 151.9 (dd, J_{C-F1} = 256.9 Hz, J_{C-F2} = 15.9 Hz), 136.7 (d, J_{C-F} = 2.2 Hz), 135.1, 134.9, 132.9 (dd, J_{C-F1} = 5.2 Hz,

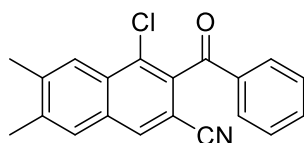
$J_{\text{C-F2}} = 2.2$ Hz), 129.9, 129.8 (d, $J_{\text{C-F}} = 1.2$ Hz), 129.4 (dd, $J_{\text{C-F1}} = 5.4$ Hz, $J_{\text{C-F2}} = 2.0$ Hz), 129.1, 128.5, 115.6, 115.3 (dd, $J_{\text{C-F1}} = 17.6$ Hz, $J_{\text{C-F2}} = 1.8$ Hz), 112.4 (dd, $J_{\text{C-F1}} = 20.0$ Hz, $J_{\text{C-F2}} = 1.5$ Hz), 108.9 (d, $J_{\text{C-F}} = 3.0$ Hz).

$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3): δ -126.44 (d, $J = 20.7$ Hz), -130.53 (d, $J = 20.7$ Hz).

IR (ATR, cm^{-1}): ν 3084, 2229, 1681, 1595, 1448, 1251, 877, 744.

HRMS (ESI, m/z): Calculated for $[\text{C}_{18}\text{H}_8\text{ClF}_2\text{NO}+\text{NH}_4]^+$, 345.0601; found, 345.0600.

3-benzoyl-4-chloro-6,7-dimethyl-2-naphthonitrile (6q)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 52.1 mg, 82% yield, m.p. 236.3-236.8 °C.

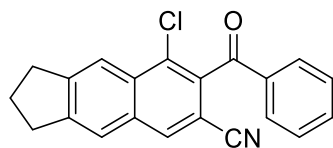
^1H NMR (400 MHz, CDCl_3): δ 8.16 (s, 1H), 8.10 (s, 1H), 7.85 (d, $J = 8.0$ Hz, 2H), 7.73 (s, 1H), 7.64 (t, $J = 7.2$ Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 2.54 (s, 3H), 2.51 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 125 MHz, ppm): δ 192.9, 142.1, 139.8, 135.6, 135.3, 134.5, 133.2, 131.7, 130.8, 130.0, 129.1, 129.0, 128.4, 124.5, 116.5, 106.9, 20.8, 20.1.

IR (ATR, cm^{-1}): ν 2944, 2226, 1671, 1594, 1451, 1267, 878, 736.

HRMS (ESI, m/z): Calculated for $[\text{C}_{20}\text{H}_{14}\text{ClNO}+\text{H}]^+$, 320.0837; found, 320.0832.

7-benzoyl-8-chloro-2,3-dihydro-1H-cyclopenta[b]naphthalene-6-carbonitrile (6r)



Prepared according to General Procedure E and purified by silica gel column chromatography (20/1 petroleum ether/ethyl acetate), White solid, 56.9 mg, 86% yield, m.p. 196.1-198.3 °C.

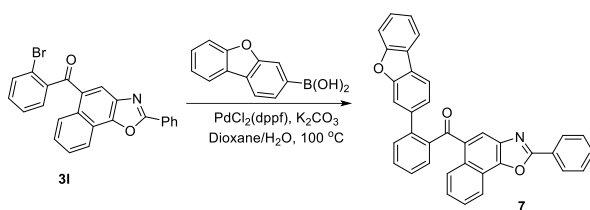
^1H NMR (400 MHz, CDCl_3): δ 8.18 (s, 2H), 7.85 (d, $J = 8.0$ Hz, 2H), 7.78 (s, 1H), 7.65 (t, $J = 7.6$ Hz, 1H), 7.50 (t, $J = 8.0$ Hz, 2H), 3.16 (q, $J = 8.0$ Hz, 4H), 2.27-2.17 (m, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 125 MHz, ppm): δ 193.0, 150.1, 147.5, 135.6, 135.2, 134.5, 133.7, 132.5, 131.6, 130.0, 129.5, 129.0, 123.3, 119.4, 116.6, 106.7, 33.2, 32.5, 25.8.

IR (ATR, cm^{-1}): ν 2954, 2226, 1670, 1595, 1449, 1263, 870, 745.

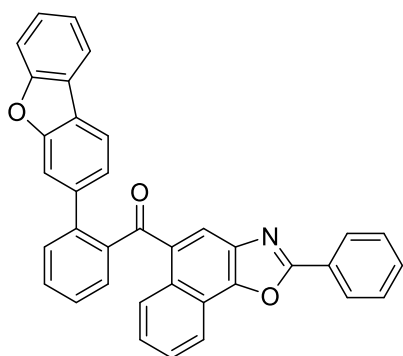
HRMS (ESI, m/z): Calculated for $[\text{C}_{21}\text{H}_{14}\text{ClNO}+\text{H}]^+$, 332.0837; found, 332.0839.

Procedure F: Synthesis of (2-(Dibenzo[*b,d*]furan-3-yl)phenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone.



To a 25 mL sealed tube was charged with **31** (42.8 mg, 0.1 mmol, 1.0 equiv), dibenzo[*b,d*]furan-3-ylboronic acid (31.8mg, 0.15 mmol, 1.5 equiv), PdCl₂(dppf) (7.2 mg, 0.01 mmol, 10 mol %), K₂CO₃ (69.1 mg, 0.5 mmol, 5.0 equiv) and dioxane-H₂O (4:1, 1.0 mL). The mixture was reacted at 100 °C overnight under nitrogen atmosphere. After completion of the reaction, the mixture was diluted with ethyl acetate and H₂O. The organic layer was separated and the aqueous layer was back-extracted with ethyl acetate. The combined organic layers were washed with brine, dried with Na₂SO₄, and then concentrated under reduced pressure. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **7** (38.1 mg, 74%).

(2-(dibenzo[*b,d*]furan-3-yl)phenyl)(2-phenylnaphtho[2,1-*d*]oxazol-5-yl)methanone (7**)**



Prepared according to Procedure F and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), Yellow solid, 38.1 mg, 74% yield, m.p. 159.3-160.9 °C.

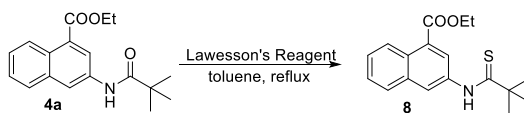
¹H NMR (400 MHz, CDCl₃): δ 7.88-7.83 (m, 2H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.77-7.68 (m, 3H), 7.66-7.59 (m, 2H), 7.58-7.51 (m, 2H), 7.50-7.39 (m, 4H), 7.32 (m, 2H), 6.85 (t, *J* = 7.2 Hz, 1H), 6.78 (t, *J* = 8.4 Hz, 2H), 6.34 (d, *J* = 8.0 Hz, 2H).

¹³C{¹H} NMR (CDCl₃, 125 MHz, ppm): δ 196.1, 158.3, 156.8, 156.5, 156.1, 141.5, 139.5, 138.2, 136.6, 134.1, 131.8, 130.3, 130.1, 130.0, 129.7, 129.5, 129.2, 128.5, 128.2, 127.9, 127.5, 124.4, 123.6, 123.4, 123.4, 122.9, 122.7, 121.0, 120.8, 115.2, 113.8, 111.8, 111.4, 102.3.

IR (ATR, cm⁻¹): ν 2920, 2229, 1659, 1589, 1485, 1295, 886, 751.

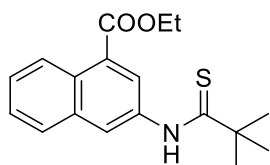
HRMS (ESI, *m/z*): Calculated for [C₃₆H₂₁NO₃+H]⁺, 516.1594; found, 516.1591.

Procedure G: Synthesis of Ethyl 3-(2,2-dimethylpropanethioamido)-1-naphthoate.



Under a nitrogen atmosphere, the mixture of compound **4a** (29.9 mg, 0.1 mmol, 1.0 equiv) and Lawesson's Reagent (24.7, 0.06 mmol, 0.6 equiv) and toluene (1.0 mL). The mixture was heated at reflux as it stirred for 4 h. After completion of the reaction, the mixture was diluted with ethyl acetate and H₂O. The organic layer was separated and the aqueous layer was back-extracted with ethyl acetate. The combined organic layers were washed with brine, dried with Na₂SO₄, and then concentrated under reduced pressure. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **8** (58.1 mg, 92%).

ethyl 3-(2,2-dimethylpropanethioamido)-1-naphthoate (**8**)



Prepared according to Procedure G and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), Yellow solid, 58.1 mg, 92% yield, m.p. 130.1-132.6 °C.

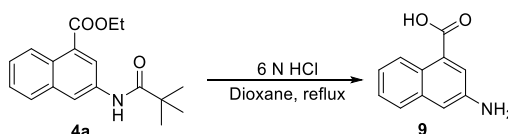
¹H NMR (400 MHz, DMSO-*d*₆): δ 11.02 (s, 1H), 8.74 (d, J = 9.2 Hz, 1H), 8.28 (s, 1H), 8.21 (d, J = 2.0 Hz, 1H), 8.04 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.71-7.57 (m, 2H), 4.43 (q, J = 7.2 Hz, 2H), 1.43 (s, 9H), 1.38 (t, J = 7.2 Hz, 3H).

¹³C{¹H} NMR (DMSO-*d*₆, 100 MHz, ppm): δ 214.0, 166.4, 136.7, 133.6, 129.1, 128.8, 128.7, 128.6, 127.8, 127.0, 126.8, 125.1, 61.1, 44.5, 29.9, 14.2.

IR (ATR, cm⁻¹): ν 3331, 2970, 1683, 1600, 1494, 1194, 748.

HRMS (ESI, m/z): Calculated for [C₁₈H₂₁NO₂S+H]⁺, 316.1366; found, 316.1361.

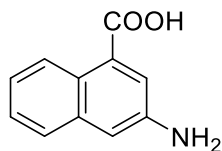
Procedure H: Synthesis of 3-Amino-1-naphthoic acid.



A mixture of compound **4a** (29.9 mg, 0.1 mmol, 1.0 eq) and HCl (6 N solution, 0.5 mL) and dioxane (0.5 mL) was heated at reflux as it stirred for 12 h. Upon complete conversion, quenched with K₂CO₃ (aq),

extracted with EtOAc, and the organic layer was dried over Na₂SO₄ and concentrated to afford compound **9** (18.1 mg, 97%).

3-amino-1-naphthoic acid (**9**)

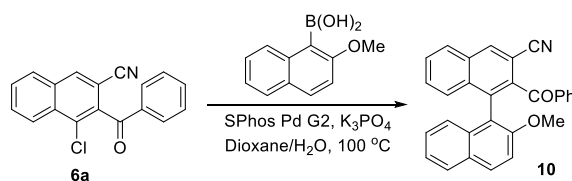


Prepared according to Procedure H, Yellow solid, 18.1 mg, 97% yield.

¹H NMR (400 MHz, DMSO-*d*₆): δ 8.57 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 2.4 Hz, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.36-7.29 (m, 1H), 7.22-7.17 (m, 1H), 7.03 (d, *J* = 2.4 Hz, 1H).

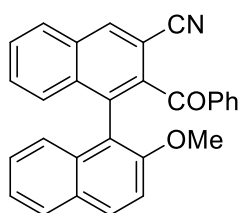
The product is a commercially available compound, and the data are in accordance with the literature.^[6]

Procedure I: Synthesis of 2-Benzoyl-2'-methoxy-[1,1'-binaphthalene]-3-carbonitrile.



To a 25 mL sealed tube was charged with **6a** (29.2 mg, 0.1 mmol, 1.0 equiv), (2-methoxynaphthalen-1-yl)boronic acid (40.4 mg, 0.2 mmol, 2.0 equiv), SPhos Pd G2 (2.6 mg, 0.003 mmol, 3 mol %), K₃PO₄ (63.7 mg, 0.3 mmol, 3.0 equiv) and dioxane-H₂O (4:1, 1.0 mL). The mixture was reacted at 100 °C overnight under nitrogen atmosphere. After completion of the reaction, the mixture was diluted with ethyl acetate and H₂O. The organic layer was separated and the aqueous layer was back-extracted with ethyl acetate. The combined organic layers were washed with brine, dried with Na₂SO₄, and then concentrated under reduced pressure. The residue was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **10** (26.1 mg, 63%).

2-benzoyl-2'-methoxy-[1,1'-binaphthalene]-3-carbonitrile (**10**)



Prepared according to Procedure I and purified by silica gel column chromatography (10/1 petroleum ether/ethyl acetate), White solid, 26.1 mg, 63% yield, m.p. 204.1-206.3 °C.

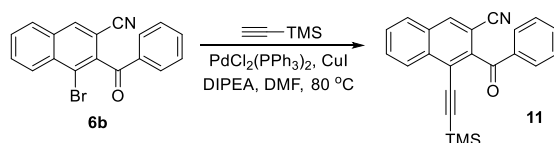
¹H NMR (400 MHz, CDCl₃): δ 8.47 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.79 (dd, *J*₁ = 9.2 Hz, *J*₂ = 2.8 Hz, 1H), 7.72 (d, *J* = 6.8 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.51-7.44 (m, 3H), 7.37-7.27 (m, 4H), 7.16 (t, *J* = 8.8 Hz, 2H), 7.09-6.99 (m, 2H), 3.56 (s, 3H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 195.0, 154.2, 138.4, 136.5, 135.1, 134.9, 134.3, 133.5, 133.0, 132.5, 131.0, 129.9, 129.1, 128.7, 128.4, 128.4, 127.8, 127.7, 127.0, 126.9, 125.1, 123.7, 117.5, 117.3, 111.9, 108.1, 55.5.

IR (ATR, cm⁻¹): ν 2929, 2230, 1660, 1593, 1453, 1278, 895, 755.

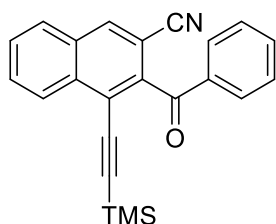
HRMS (ESI, *m/z*): Calculated for [C₂₉H₁₉NO₂+H]⁺, 414.1489; found, 414.1489.

Procedure J: Synthesis of 3-benzoyl-4-((trimethylsilyl)ethynyl)-2-naphthonitrile.



To a 25 mL sealed tube was charged with **6b** (33.6 mg, 0.1 mmol, 1.0 equiv), trimethylsilylacetylene (49.1 mg, 0.5 mmol, 5.0 equiv), PdCl₂(PPh₃)₂ (14.2 mg, 0.02 mmol, 20 mol %), CuI (4.8 mg, 0.02 mmol, 20 mol%), TEA (70.0 μL, 0.5 mmol, 5.0 equiv) and dry DMF (1.0 mL). The mixture was reacted at 80 °C overnight under nitrogen atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature. The reaction mixture was dilution with water and extracted with CH₂Cl₂. The organic layer was then dried and concentrated under vacuum to obtain crude product, which was further purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **11** (19.3 mg, 55%).

3-benzoyl-4-((trimethylsilyl)ethynyl)-2-naphthonitrile (**11**)



Prepared according to Procedure J and purified by silica gel column chromatography (15/1 petroleum ether/ethyl acetate), White oil, 19.3 mg, 55% yield, m.p. 124.7-126.2 °C.

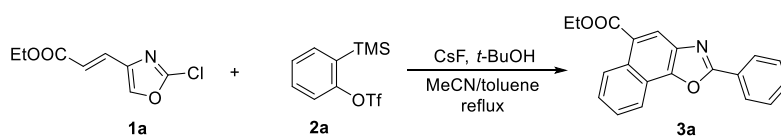
¹H NMR (400 MHz, CDCl₃): δ 8.41 (d, J = 7.2 Hz, 1H), 8.33 (s, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.91-7.87 (m, 2H), 7.83-7.78 (m, 1H), 7.74-7.69 (m, 1H), 7.67-7.59 (m, 1H), 7.48 (t, J = 8.0 Hz, 2H), -0.01 (s, 9H).

¹³C{¹H} NMR (CDCl₃, 100 MHz, ppm): δ 194.3, 141.1, 136.2, 135.4, 134.0, 133.8, 132.0, 130.7, 130.2, 129.0, 128.8, 128.7, 127.0, 120.7, 116.8, 109.2, 107.9, 98.4, -0.7.

IR (ATR, cm⁻¹): ν 3068, 2959, 2226, 1677, 1448, 1263, 843, 756.

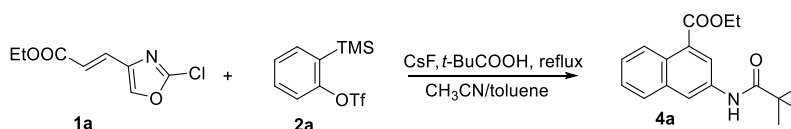
HRMS (ESI, m/z): Calculated for [C₂₉H₁₉NOSi+NH₄]⁺, 371.1574; found, 371.1569.

Procedure K: Large-Scale Synthesis of 3a.



Under a nitrogen atmosphere, **1a** (201.6 mg, 1.0 mmol, 1.0 equiv), CsF (0.91 g, 6.0 mmol, 6.0 equiv) and *t*-BuOH (0.15 mL, 1.5 mmol, 1.5 equiv) were placed in a 100 mL Schlenk tube equipped with a stir bar. Then 5.0 mL of MeCN and 5.0 mL of toluene were added. The reaction mixture was stirred at reflux for 10 min. Then the benzyne precursor **2a** (0.89 g, 3.0 mmol, 3.0 equiv) was dissolved in 5.0 mL of toluene. The resulting solution was added dropwise in six portions over a period of 3 h. When the reaction was complete as monitored by TLC, the reaction mixture was filtered through a short column of silica gel and eluted with CH₂Cl₂. The filtrate was concentrated under reduced pressure to afford a residue, which was purified by silica gel chromatography (15/1 petroleum ether/ethyl acetate) to give compound **3a** (187.4 mg, 59%).

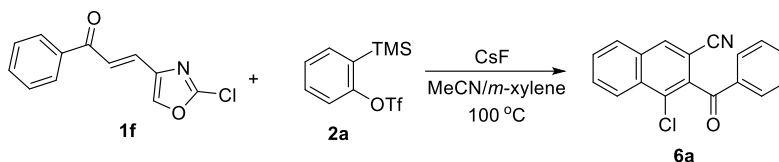
Procedure L : Large-Scale Synthesis of 4a.



Under a nitrogen atmosphere, **1a** (201.6 mg, 1.0 mmol, 1.0 equiv), CsF (0.91 g, 6.0 mmol, 6.0 equiv) and acid (0.15 g, 1.5 mmol, 1.5 equiv) were placed in a 100 mL Schlenk tube equipped with a stir bar. Then 5.0 mL of MeCN and 5.0 mL of toluene were added. The reaction mixture was stirred at reflux for 10 min. Then the benzyne precursor **2a** (0.89 g, 3.0 mmol, 3.0 equiv) was dissolved in 5.0 mL of toluene. The resulting solution was added dropwise in six portions over a period of 3 h. When the reaction was complete as monitored by TLC, the reaction mixture was filtered through a short column of silica gel and eluted with CH₂Cl₂. The filtrate was concentrated under reduced pressure to afford a residue, which was

purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **4a** (212.1 mg, 71%)

Procedure M : Large-Scale Synthesis of **6a**.



Under a nitrogen atmosphere, **1f** (233.5 mg, 1.0 mmol, 1.0 equiv), CsF (0.68 g, 4.5 mmol, 4.5 equiv) were placed in a 100 mL Schlenk tube equipped with a stir bar. Then 5.0 mL of MeCN and 5.0 mL of *m*-xylene were added. The reaction mixture was stirred at 100 °C for 10 min. Then the benzyne precursor **2a** (0.89 g, 3.0 mmol, 3.0 equiv) was dissolved in 5.0 mL of *m*-xylene. The resulting solution was added dropwise in six portions over a period of 3 h. When the reaction was complete as monitored by TLC, the reaction mixture was filtered through a short column of silica gel and eluted with CH₂Cl₂. The filtrate was concentrated under reduced pressure to afford a residue, which was purified by silica gel chromatography (petroleum ether/ethyl acetate) to give compound **6a** (213.4 mg, 73%).

3. Biological Experiments

Cell cytotoxicity assay

Cell cytotoxicity was assessed using the CCK-8 assay. H1299 and U2OS cells were seeded in 96-well plates at a density of 7,000 cells per well in DMEM supplemented with 10% FBS. After 24 hours of incubation, cells were treated with test compounds **3** and **4** at concentrations of 100 μM, 50 μM, 25 μM, 5 μM and 0 μM for 48 hours. Following treatment, 10 μL of CCK-8 solution was added to each well, and the plates were incubated for 2 hours at 37 °C. Absorbance was measured at 450 nm using an ELx800 microplate reader (Biotek, USA). The half-maximal inhibitory concentration (IC₅₀) values were determined using curve fitting in GraphPad Prism 5.

The dose-response curves and IC₅₀ values of compounds **3q**, **4p**, and **4t** against U2OS and H1299 cell lines are shown in Figure S1. Compound **4p** exhibited the higher potency against U2OS cells (IC₅₀ = 3.52 μM), compared to **3q** (6.86 μM) and **4t** (8.95 μM). Against H1299 cells, **4p** and **4t** showed similar activity (16.83 and 16.36 μM, respectively), while **3q** was less potent (IC₅₀ = 20.15 μM).

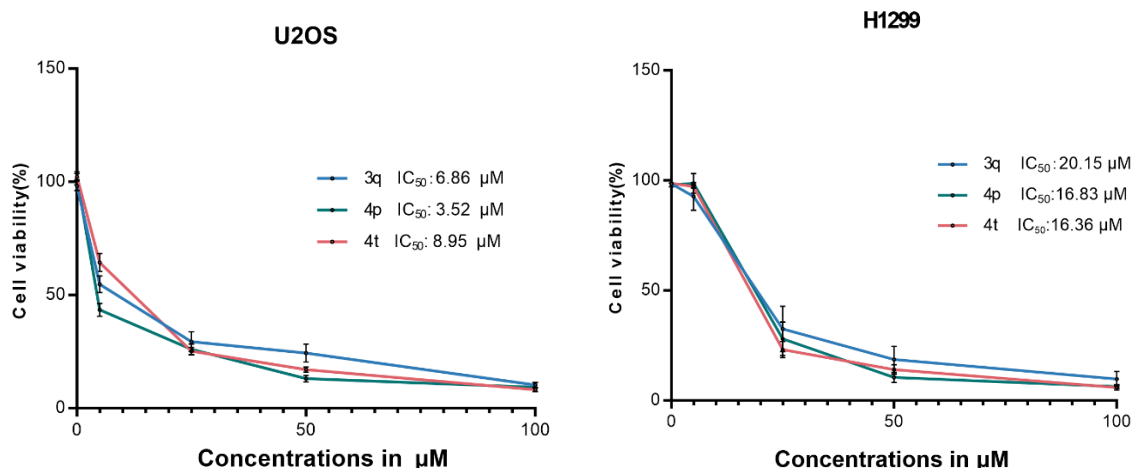


Figure S1. Determination of IC₅₀ values (μM) using CCK-8 assay.

4. DFT Calculations

Density functional theory (DFT) calculations were carried out for the reaction pathway in the construction of compound **6a** using the Gaussian 16 program (version A.03). The relative energies are all calculated at the level of B3LYP-D3(BJ)/def2TZVP.

DFT calculations reveal that the overall reaction pathway is initially governed by kinetic control, as reflected by the low energy barrier of the first Diels-Alder step (1.5 kcal/mol, **TS₁**) to form intermediate **i** (compound **5**). Subsequently, the rate-determining retro-Diels-Alder step (25.0 kcal/mol, **TS₂**) requires the absorption of external energy to undergo ring-opening to form intermediates **ii** and **iii**. The final Diels-Alder step (18.4 kcal/mol, **TS₃**) leads to the formation of the thermodynamically stable epoxy intermediate **iv**.

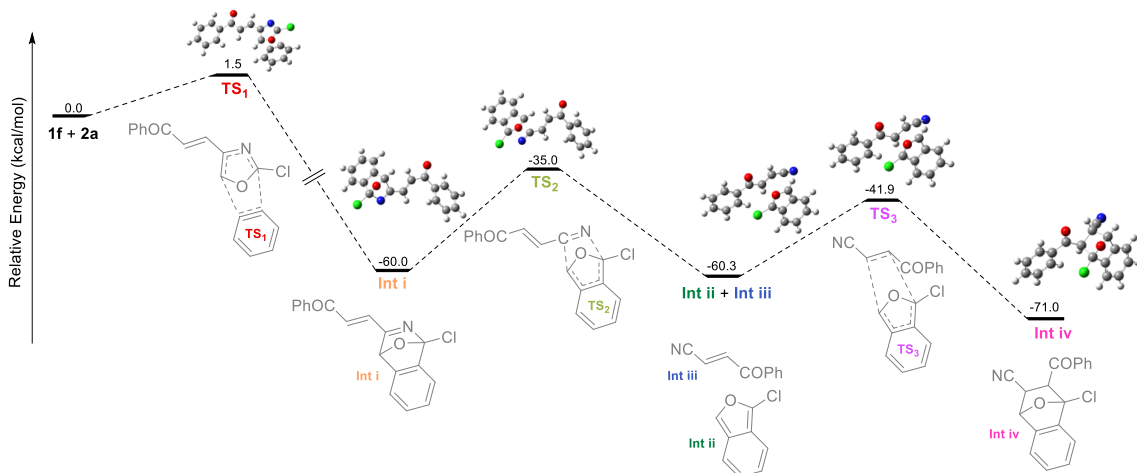


Figure S2. Reactive energy profile obtained from B3LYP-D3(BJ)/def2TZVP calculations for the cascade reaction of Diels-Alder/retro-Diels-Alder/Diels-Alder (energy in kcal mol⁻¹).

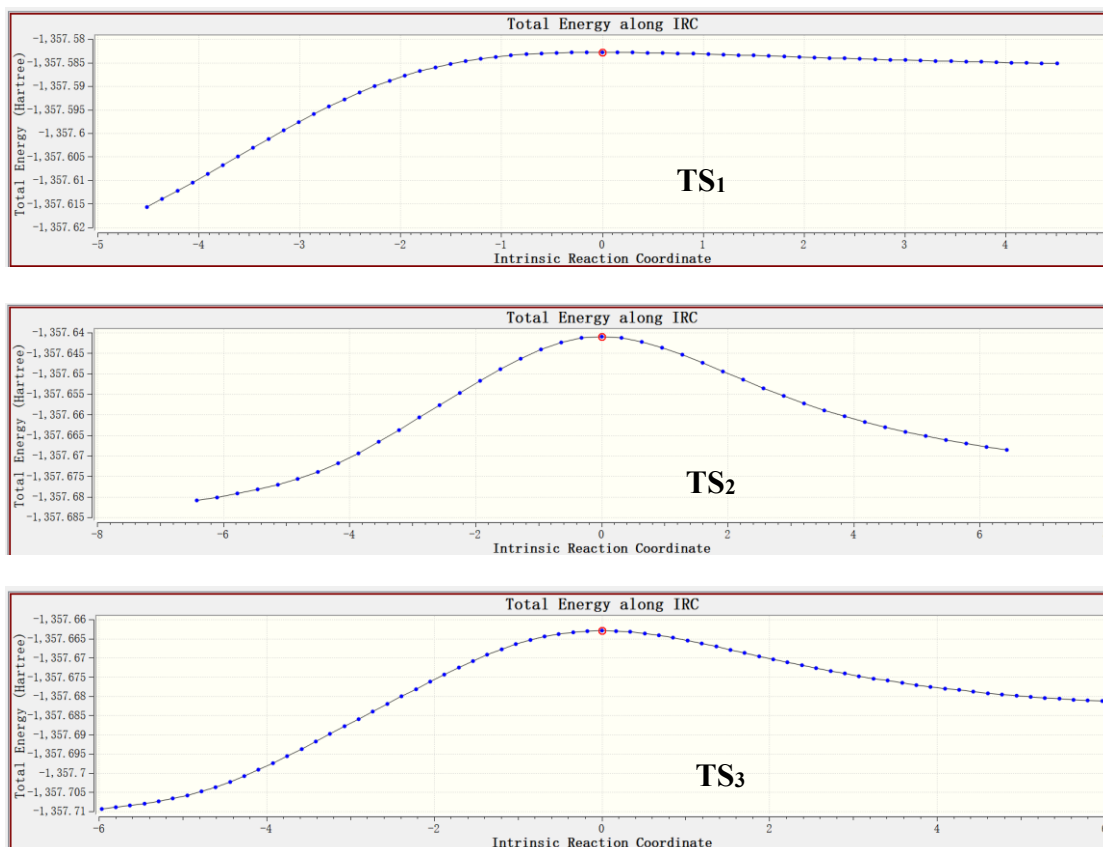


Figure S3. The intrinsic coordinate (IRC) paths.

Table S1. Cartesian coordinates for all stationary points (calculated at the B3LYP-D3(BJ)/def2TZVP level of theory)

1f and 2a			
C	-2.05947800	1.60704200	0.29188800
C	-1.32535800	2.77315200	0.43440300
C	-1.96937800	3.84588700	-0.22404000
C	-3.18680900	3.68322300	-0.91454500
C	-3.85050300	2.43768700	-0.99601200
C	-3.14621700	1.44821700	-0.32257500
N	-2.12922800	-1.76032300	-0.53159500
C	-0.99651200	-1.31956500	0.13957000
C	0.29967000	-1.28692600	-0.51286000
C	1.44834300	-0.80536400	0.00622100

C	2.70526800	-0.84755900	-0.79068000
Cl	-4.72710700	-2.05252300	0.13750000
C	3.97191200	-0.28944600	-0.19805100
O	2.71643600	-1.33149400	-1.91283100
C	5.14144400	-0.38344400	-0.97524500
C	6.35536800	0.10616500	-0.49866700
C	6.42221100	0.70227700	0.76667500
C	5.26844700	0.80479000	1.54836600
C	4.05123300	0.31211300	1.07032700
H	-0.38053000	2.89992200	0.96701100
H	-1.50258300	4.83521600	-0.19742900
H	-3.63371400	4.55122700	-1.40881100
H	-4.79345600	2.31674400	-1.53379300
H	0.32695000	-1.69206500	-1.52860100
H	1.46635900	-0.38225400	1.01196700
H	5.06341900	-0.85151000	-1.95812100
H	7.25557400	0.02456100	-1.11314800
H	7.37385300	1.08685600	1.14271900
H	5.31519000	1.27010700	2.53613000
H	3.16637100	0.40575600	1.70111200
C	-3.08587700	-1.63157800	0.32326800
C	-1.37559000	-0.94495900	1.41105200
H	-0.85487600	-0.57446000	2.28834800
O	-2.70716700	-1.17558900	1.53770700
TS₁			
C	-2.02469968	1.41062411	0.31852218
C	-1.30891568	2.58447211	0.49591918
C	-1.93713568	3.67773111	-0.13918482
C	-3.14094468	3.52925411	-0.85299682
C	-3.78965368	2.28111511	-0.97167382

C	-3.11162068	1.24976511	-0.32896982
N	-2.13708368	-1.68447789	-0.54471882
C	-1.02730968	-1.18629389	0.08499218
C	0.27776232	-1.21273089	-0.54421282
C	1.42456032	-0.72426889	-0.02639182
C	2.69753932	-0.83130589	-0.79434482
Cl	-4.71792768	-2.04396689	0.15287718
C	3.96538032	-0.28163289	-0.19957482
O	2.71432532	-1.35902889	-1.89616682
C	5.13598732	-0.38268689	-0.97457182
C	6.35125132	0.10125811	-0.49595882
C	6.41897832	0.69553011	0.77026318
C	5.26505732	0.80135611	1.55129018
C	4.04585932	0.31676611	1.07034018
H	-0.37647368	2.70077911	1.05373318
H	-1.47290968	4.66617611	-0.07323282
H	-3.58427568	4.40669011	-1.33375982
H	-4.72480868	2.17698511	-1.52840482
H	0.31666532	-1.68086589	-1.53191982
H	1.42938932	-0.24525289	0.95404418
H	5.05786432	-0.85070389	-1.95744382
H	7.25183332	0.01658811	-1.10939382
H	7.37177932	1.07564811	1.14782518
H	5.31320432	1.26309511	2.54060618
H	3.16158832	0.41063211	1.70193018
C	-3.11516568	-1.48301089	0.29149518
C	-1.43438768	-0.64617589	1.30885818
H	-0.89849668	-0.28510589	2.18157518
O	-2.73915068	-0.98519489	1.48695118
Int 1			

C	-2.33632800	1.03646800	0.49724100
C	-2.29602900	2.41221600	0.35204400
C	-3.20574100	2.99631700	-0.55054700
C	-4.11260500	2.21302400	-1.26943900
C	-4.12599300	0.81047000	-1.13829100
C	-3.21816100	0.24973300	-0.25908900
N	-1.44054000	-1.37070200	-0.62568400
C	-0.65298800	-0.64444900	0.08864500
C	0.76570500	-0.35539100	-0.12511100
C	1.40881100	0.53247200	0.67034000
C	2.80490500	1.07675600	0.61558000
Cl	-3.98299400	-2.44749000	-0.14792200
C	3.95794600	0.27491600	0.10086500
O	2.97293900	2.21400000	1.02876700
C	5.08432700	0.97182300	-0.37605800
C	6.20084600	0.27613900	-0.83467500
C	6.22014700	-1.12393300	-0.79048200
C	5.12054200	-1.82299300	-0.28513800
C	3.98906200	-1.12857100	0.15146400
H	-1.58852300	3.03176800	0.90899600
H	-3.20585500	4.08072300	-0.68562900
H	-4.81464200	2.69562100	-1.95391000
H	-4.81420900	0.19049300	-1.71700100
H	1.26279600	-0.87083900	-0.95176600
H	0.83994300	1.06167400	1.43992600
H	5.05723000	2.06317600	-0.38079600
H	7.06374700	0.82319000	-1.22260000
H	7.09845800	-1.67006600	-1.14416100
H	5.14239900	-2.91412900	-0.23074100
H	3.13959900	-1.68108200	0.55730800

C	-2.77664900	-1.17930400	0.07205100
C	-1.48158800	0.00420500	1.23319100
H	-0.98269800	0.28585000	2.16432300
O	-2.41241200	-1.06222600	1.43084100
TS₂			
C	-2.37475612	0.98980682	0.54709614
C	-2.26273512	2.37559282	0.33169214
C	-3.13012012	2.96614982	-0.57806886
C	-4.08264412	2.20315582	-1.29987686
C	-4.18803112	0.83236382	-1.12049686
C	-3.33470512	0.23077882	-0.17776486
N	-1.18360712	-1.37668118	-0.91776086
C	-0.48562812	-0.70523818	-0.19670786
C	0.91468588	-0.30528718	-0.13854386
C	1.45273088	0.58682482	0.71473414
C	2.84659288	1.11803182	0.67021814
Cl	-4.11669512	-2.46909518	-0.06777386
C	3.98287788	0.29432682	0.13719814
O	3.03612788	2.25837382	1.06364214
C	5.10180788	0.98050382	-0.36921886
C	6.20678788	0.27788182	-0.84567286
C	6.21994088	-1.12176518	-0.80003786
C	5.12492988	-1.81283818	-0.27428086
C	4.00884288	-1.11047718	0.18889514
H	-1.52174812	2.97371582	0.86723514
H	-3.07968412	4.04500282	-0.74504986
H	-4.74335612	2.70947182	-2.00757986
H	-4.91094012	0.23493282	-1.67965686
H	1.53629588	-0.77372018	-0.90739786
H	0.82969488	1.11371782	1.44159914

H	5.08024588	2.07199582	-0.37748086
H	7.06525088	0.82019682	-1.24990486
H	7.08870388	-1.67335118	-1.16860986
H	5.13987188	-2.90417018	-0.21983286
H	3.16952588	-1.65970518	0.61857914
C	-3.12246612	-1.11711318	0.24508914
C	-1.60661112	0.01758682	1.29037914
H	-1.03932312	0.20136482	2.20214714
O	-2.37695912	-1.13299718	1.34819014
Int 2 and Int 3			
N	2.84803500	2.63057600	-1.91843200
C	1.89732000	2.45878800	-1.27196400
C	0.73173100	2.27501700	-0.47154200
C	-0.21421800	1.34676100	-0.72936100
C	-1.45215600	1.31698700	0.10742200
C	-2.61313600	0.48860700	-0.35111600
O	-1.52885200	2.00663700	1.11191100
C	-3.84521800	0.69188500	0.29706300
C	-4.98278000	-0.00079600	-0.10971600
C	-4.90348300	-0.91926800	-1.16396900
C	-3.68048200	-1.14568400	-1.80156800
C	-2.54135000	-0.44400600	-1.40093200
C	2.80275200	-0.11908400	0.53429400
C	3.97993800	-0.17842700	-0.27281300
C	4.12829900	-1.23988000	-1.13001100
C	3.13492400	-2.27245600	-1.23800500
C	1.97956700	-2.24084200	-0.49721700
C	1.79357300	-1.15223600	0.40394600
C	0.79651300	-0.79646900	1.29987500
C	2.32954400	0.75973100	1.49401200

O	1.13298000	0.32177400	1.96035000
Cl	-0.63737000	-1.60359400	1.76266500
H	0.57574300	2.96072200	0.36862100
H	-0.10159300	0.67455500	-1.57949500
H	-3.88139000	1.41355100	1.11508200
H	-5.93749100	0.17441400	0.39248700
H	-5.79630000	-1.46108300	-1.48669100
H	-3.61337900	-1.86906300	-2.61781300
H	-1.59809400	-0.64000100	-1.91223800
H	4.73505400	0.60717900	-0.21097300
H	5.02152200	-1.30644800	-1.75574200
H	3.31078600	-3.09797400	-1.93211000
H	1.22348800	-3.02469500	-0.57932400
H	2.72220600	1.66193700	1.95323400
TS₃			
N	2.74526645	2.64652894	-1.92548648
C	1.92793845	2.35468294	-1.15277748
C	0.95292945	1.98210794	-0.16859748
C	-0.06635655	1.05494594	-0.47412148
C	-1.38467055	1.24023694	0.17148352
C	-2.57223555	0.46765594	-0.33505148
O	-1.51125955	2.02067294	1.10791052
C	-3.80763655	0.69909094	0.29650352
C	-4.95579855	0.02638694	-0.11672648
C	-4.88822655	-0.89208006	-1.17128548
C	-3.66667555	-1.13182306	-1.80688748
C	-2.51575455	-0.45689706	-1.39226748
C	2.73213145	-0.05343606	0.42439852
C	3.93020445	-0.13951006	-0.31049648
C	4.12993345	-1.26509206	-1.09686048

C	3.15363645	-2.29022206	-1.18694548
C	1.95411745	-2.20664506	-0.49722748
C	1.74872945	-1.07600306	0.31712752
C	0.66045845	-0.62498906	1.12407452
C	2.14005145	0.95999094	1.25037152
O	1.06537445	0.40480194	1.88699552
Cl	-0.62474755	-1.58536906	1.73079752
H	0.65622745	2.78042294	0.52069752
H	0.01929445	0.45653494	-1.37904948
H	-3.83415755	1.41970794	1.11578152
H	-5.90930955	0.21693594	0.38251352
H	-5.78798955	-1.41992806	-1.49810648
H	-3.60892355	-1.84716306	-2.63114548
H	-1.57452055	-0.66249306	-1.90393948
H	4.67745445	0.65444494	-0.26458848
H	5.05848445	-1.36667006	-1.66340748
H	3.35661345	-3.16218406	-1.81337348
H	1.19717345	-2.99056306	-0.56673648
H	2.63712445	1.75646394	1.80205352
Int 4			
N	2.60737200	2.65404200	-1.90890600
C	1.87430700	2.28095700	-1.09037500
C	1.10645300	1.80566400	0.06074400
C	0.01656500	0.69766800	-0.15153500
C	-1.38414100	1.18005200	0.23422600
C	-2.57473800	0.46457600	-0.32490600
O	-1.51074000	2.07867500	1.04298700
C	-3.81524400	0.70975900	0.29252300
C	-4.95971200	0.03427600	-0.12270600
C	-4.88564400	-0.88712100	-1.17447100

C	-3.66395900	-1.12240900	-1.81137600
C	-2.51295600	-0.45428900	-1.38759200
C	2.74159300	-0.03667500	0.36417700
C	3.95011600	-0.15772400	-0.30961000
C	4.15843000	-1.31541200	-1.07412200
C	3.17908500	-2.31363000	-1.15857400
C	1.94970300	-2.17700400	-0.49575200
C	1.75579800	-1.02581300	0.25604300
C	0.54595300	-0.39636400	0.91270400
C	2.06058300	1.10018300	1.10314200
O	1.10434200	0.42768900	1.91299100
Cl	-0.61385500	-1.52555000	1.65000200
H	0.61922000	2.65711100	0.55947000
H	0.04289900	0.27297100	-1.15953300
H	-3.84764200	1.42745500	1.11410000
H	-5.91427500	0.22102100	0.37543400
H	-5.78254300	-1.42096900	-1.49905400
H	-3.60485200	-1.83406300	-2.63839400
H	-1.56982800	-0.66240900	-1.89490600
H	4.70792200	0.62765900	-0.26915800
H	5.10004600	-1.43989700	-1.61425400
H	3.37413500	-3.20831400	-1.75503100
H	1.17365900	-2.94223900	-0.57238700
H	2.67387900	1.78693500	1.69684400

5. Mechanistic Studies

LC-MS tracking of key intermediates

LC-MS monitoring was employed to track the key intermediates during the formation of products **3** and **4** at 2 h, 4 h, and 6 h of the reaction, respectively (FigureS4).

a) For the construction of product **3**, the naphthoxazole intermediate **A** was detected at 2 h (1.73 min, found 277.9) alongside two starting materials, whereas no product was observed at this time point. As the reaction progressed to 4 h and 6 h, the product **3** gradually formed, accompanied by a progressive decrease in the signal intensity of intermediate **A** (see Figure S4-a).

b) For the construction of product **4**, both naphthoxazole intermediate **A** (1.73 min, found 277.7) and isocyanate intermediate **C** (1.73 min, found 241.8) were detected alongside two starting materials at 2 h, at which time product **4** was also observed. As the reaction progressed to 4 h and 6 h, the signals of intermediates **A** and **C** remained detectable, and the yield of product **4** continued to increase (see Figure 4S-b).

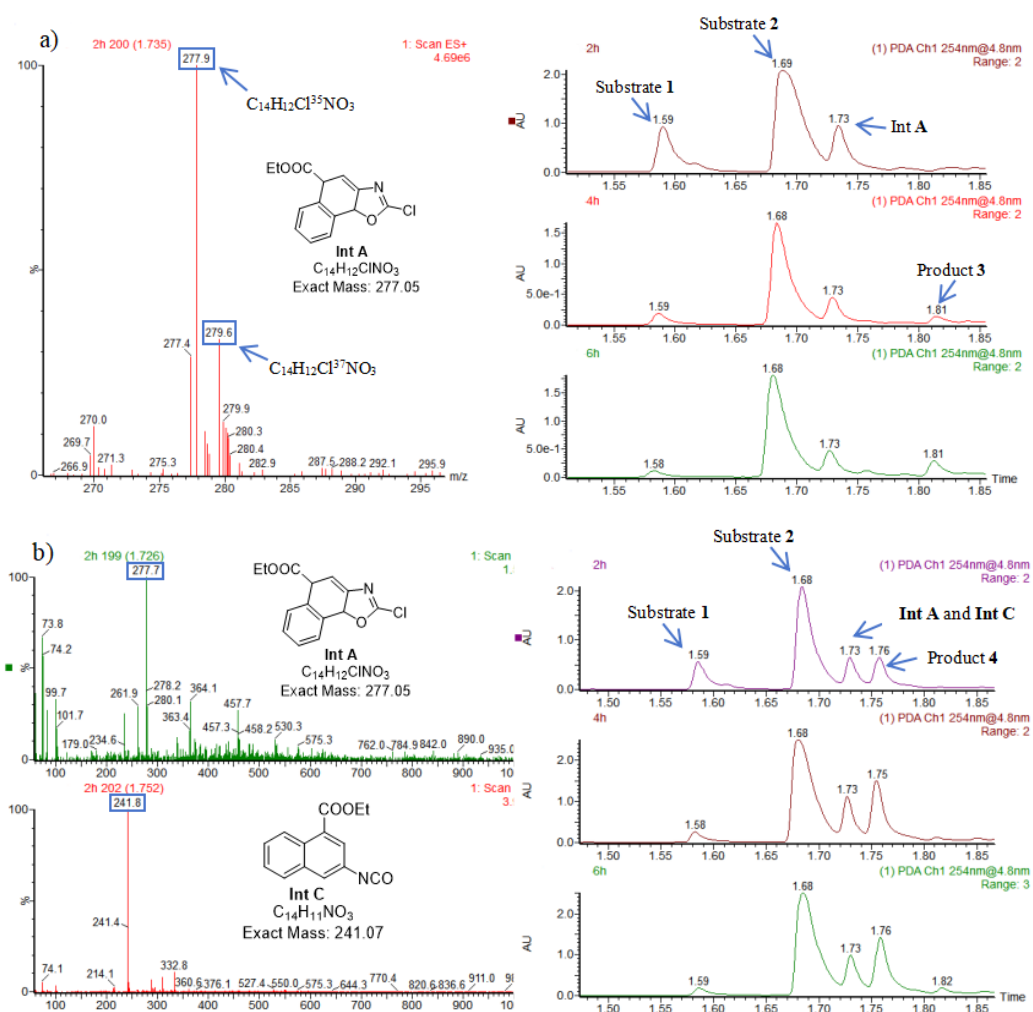


Figure S4. LC-MS analysis of key intermediates.

Plausible Mechanism

Based on literature precedence^[7-10], along with LC-MS monitoring and DFT calculation results, plausible reaction mechanisms for the formation of compounds **3**, **4** and **6** are proposed in Figure S4.

2-arylnaphtho[2,1-*d*]oxazoles: Alkenyl oxazole **1** undergoes a Diels-Alder reaction with benzyne (generated from arylalkyne precursor **2a**) to form intermediate **i**. Subsequently, intermediate **i** undergoes deprotonation under the action of a base to generate anion **ii**. Due to the electron-withdrawing effect of the chlorine atom at the 2-position, this anion can be resonance-stabilized, leading to intermediate **iii**. This intermediate then reacts with a second molecule of benzyne to afford intermediate **iv**, which finally undergoes dechlorinative aromatization to give product **3** (Figure S5-a).

***N*-acylnaphthylamine:**^[7,8] Alkenyloxazole **1** reacts with benzyne to form Diels-Alder reaction intermediate **i**. After protonation of the oxazole nitrogen atom, intermediate **ii** is obtained. Subsequently, under acid-promoted conditions, this anion induces the ring-opening of the oxazole via resonance, accompanied by the departure of a chloride ion, thereby generating isocyanate intermediate **iii**. Next, the pivaloyloxy anion nucleophilically attacks intermediate **iii** to afford intermediate **iv**. Finally, the intramolecular aminolysis of intermediate **iv** yields intermediate **v**, which undergoes decarboxylation to afford product **4** (Figure S5-b).

α -halonaphthalene:^[9,10] Alkenyloxazole **1** with benzyne undergo a cyclic diene Diels-Alder reaction to furnish epoxyisoquinoline intermediate **i**, introducing a halogen with electron-withdrawing ability may trigger a retro-Diels-Alder reaction under appropriate conditions. This process generates isobenzofuran **ii** and alkenyl cyanide **iii**, which subsequently undergo a Diels-Alder cycloaddition to afford epoxy intermediate **iv**. This intermediate then undergoes dehydration and aromatization to finally give product **6** (Figure S5-c).

Table S2. Crystal data, data collection and structure refinement for **6h**.

$C_{19}H_{12}ClNO_2$	$F(000) = 1328$
$M_r = 321.75$	$D_x = 1.363 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$a = 10.0487 (3) \text{ \AA}$	Cell parameters from 9682 reflections
$b = 26.8804 (9) \text{ \AA}$	$q = 3.3\text{--}73.4^\circ$
$c = 11.6116 (4) \text{ \AA}$	$m = 2.23 \text{ mm}^{-1}$
$\beta = 90.177 (2)^\circ$	$T = 298 \text{ K}$
$V = 3136.43 (18) \text{ \AA}^3$	Block, colourless
$Z = 8$	$0.1 \times 0.03 \times 0.02 \text{ mm}$
Bruker D8 Venture PHOTON III diffractometer	6334 independent reflections
Radiation source: microfocus sealed X-ray tube, Incoatec Ims Diamond II	4961 reflections with $I > 2\sigma(I)$
Mirror optics monochromator	$R_{\text{int}} = 0.052$
Detector resolution: $7.9 \text{ pixels mm}^{-1}$	$q_{\text{max}} = 74.9^\circ$, $q_{\text{min}} = 3.3^\circ$
ϕ and ω scans	$h = -12\text{--}12$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction.	$k = -33\text{--}33$
$wR2(\text{int})$ was 0.1082 before and 0.0592 after correction. The Ratio of minimum to maximum transmission is 0.8408. The $1/2$ correction factor is Not present.	
$T_{\text{min}} = 0.634$, $T_{\text{max}} = 0.754$	$l = -14\text{--}11$
41616 measured reflections	

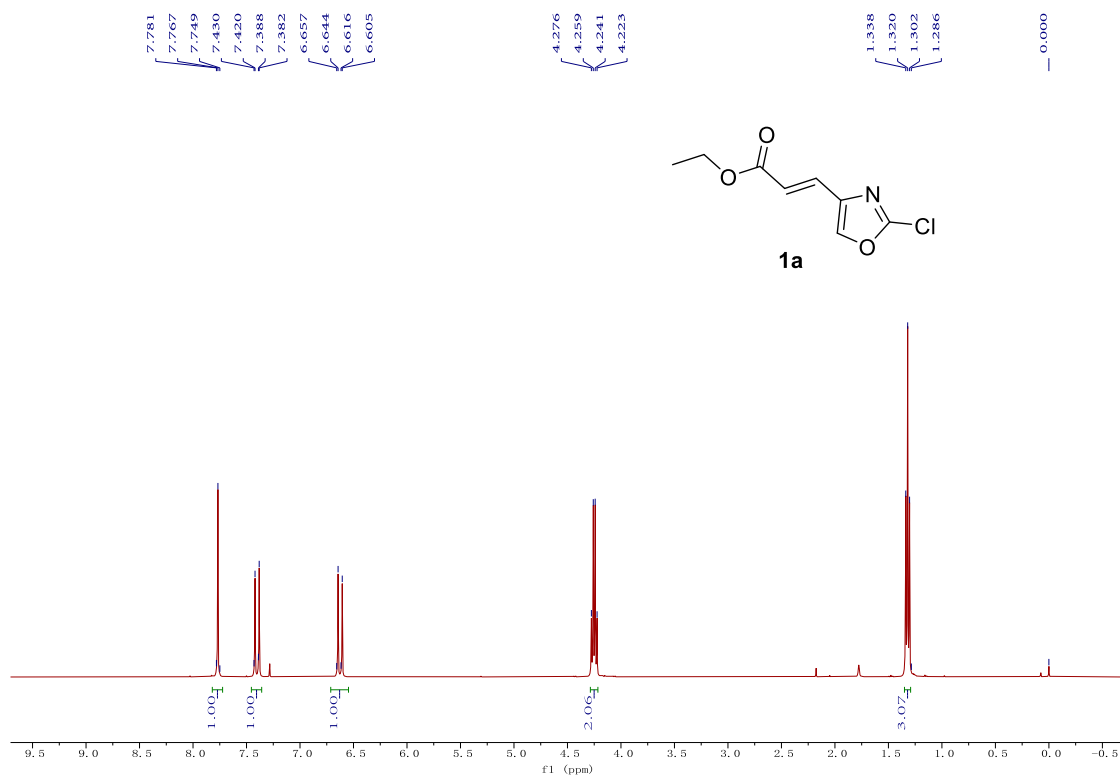
Refinement on F^2	0 restraints
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2s(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.117$	$w = 1/[s^2(F_o^2) + (0.0571P)^2 +$ $0.6089P]$
	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(D/s)_{\max} = 0.001$
6334 reflections	$D\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$
417 parameters	$D\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$

7. References

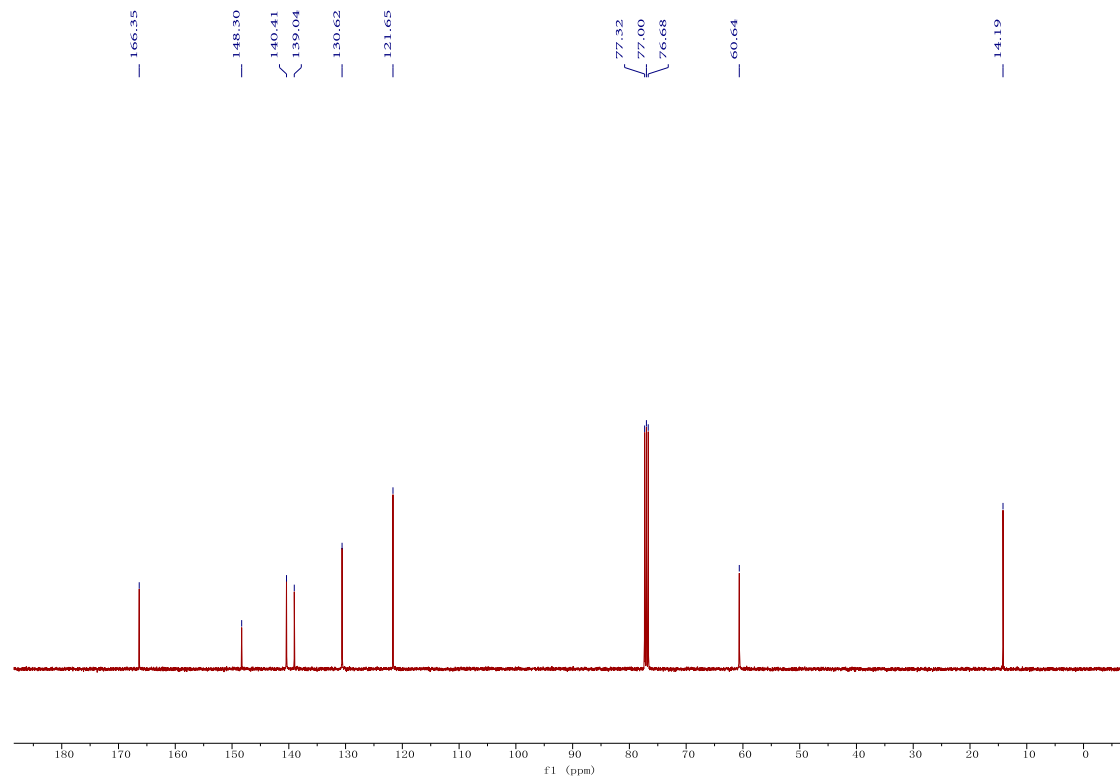
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8. NMR Spectra

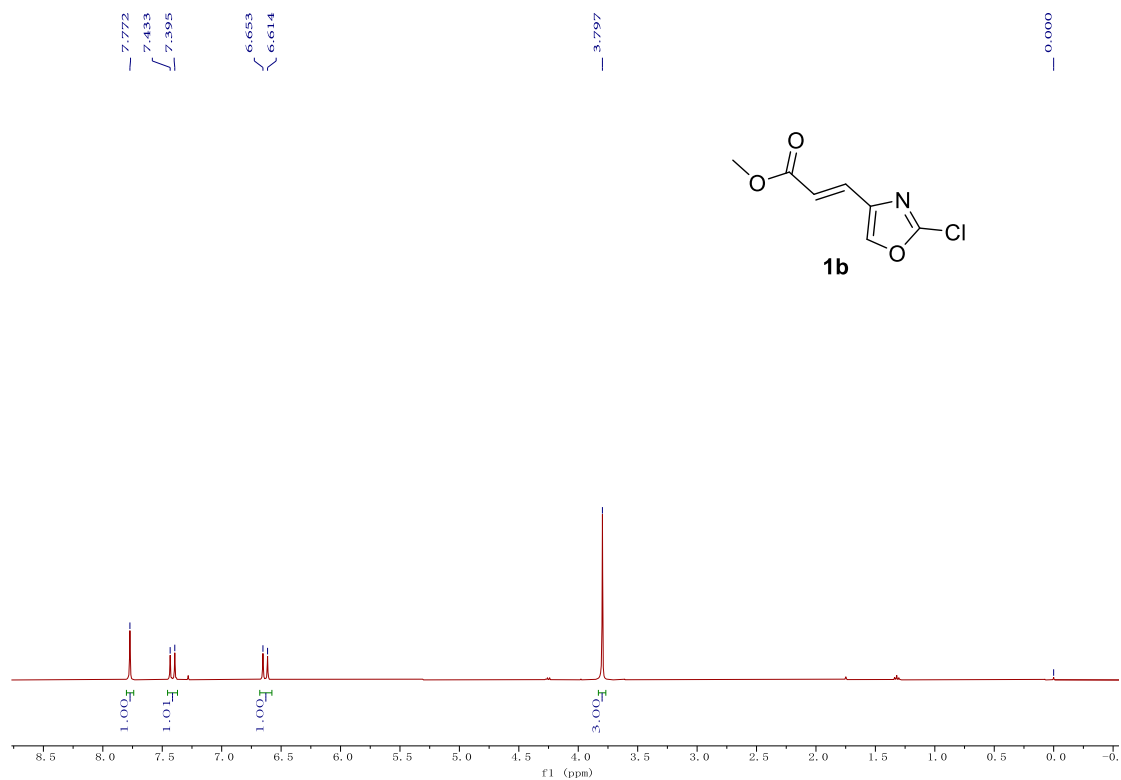
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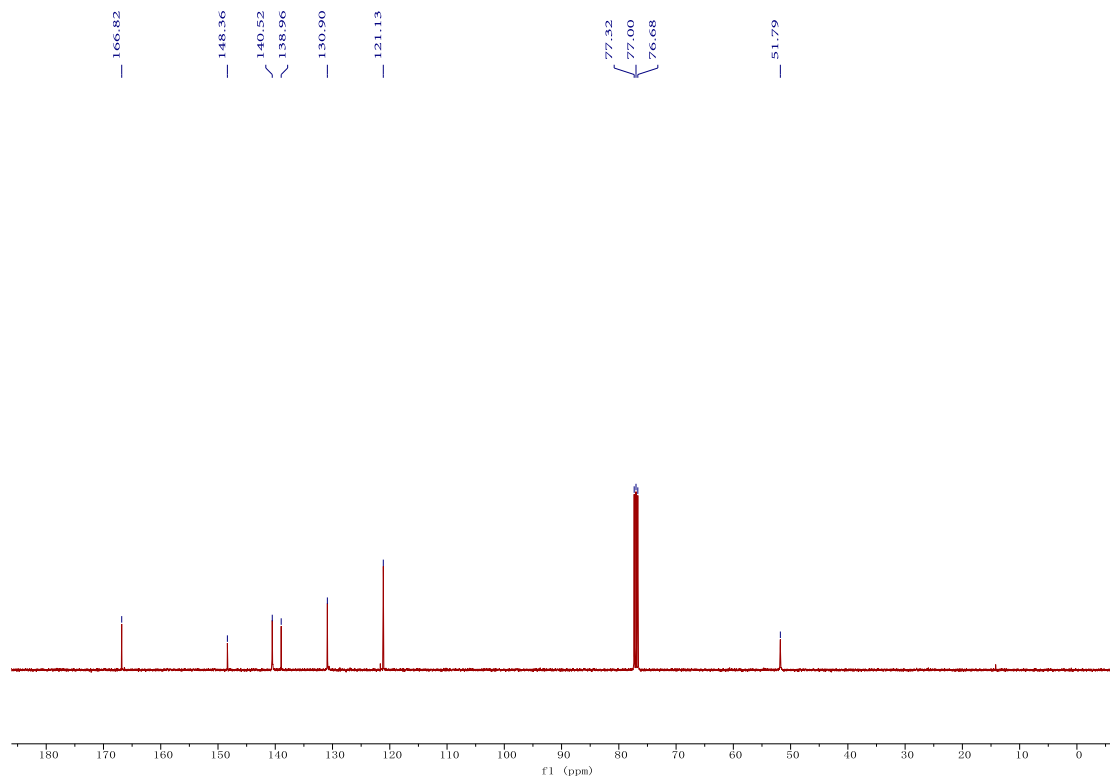
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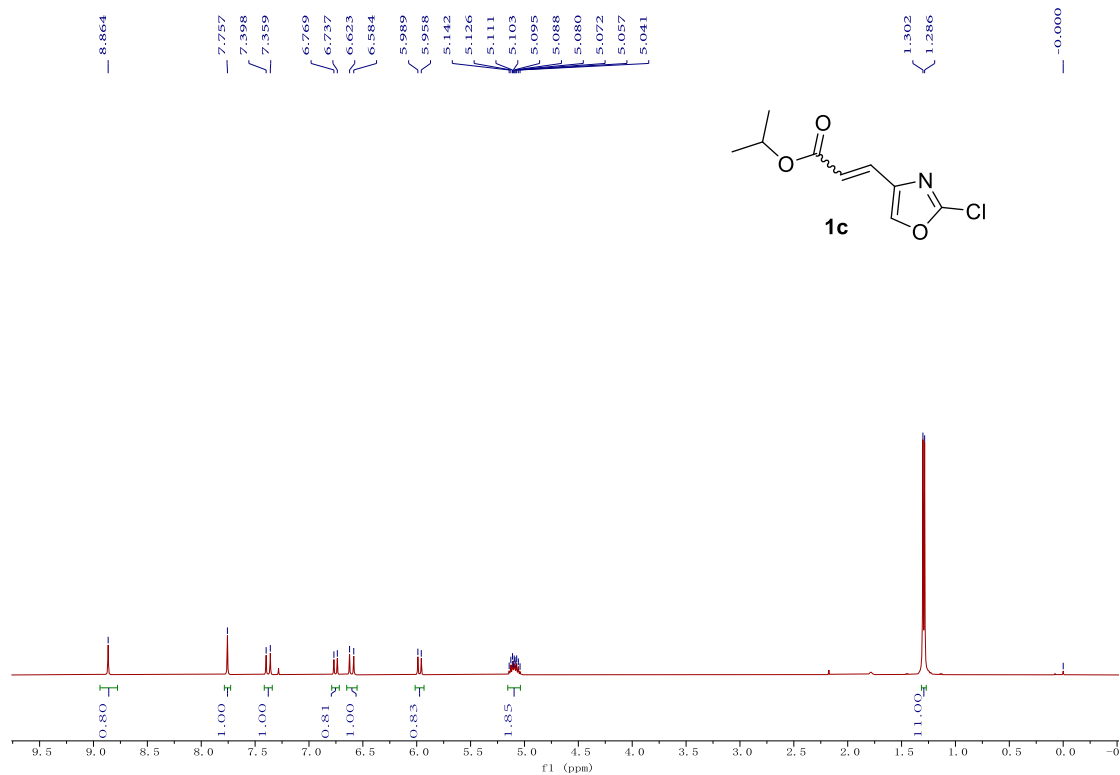
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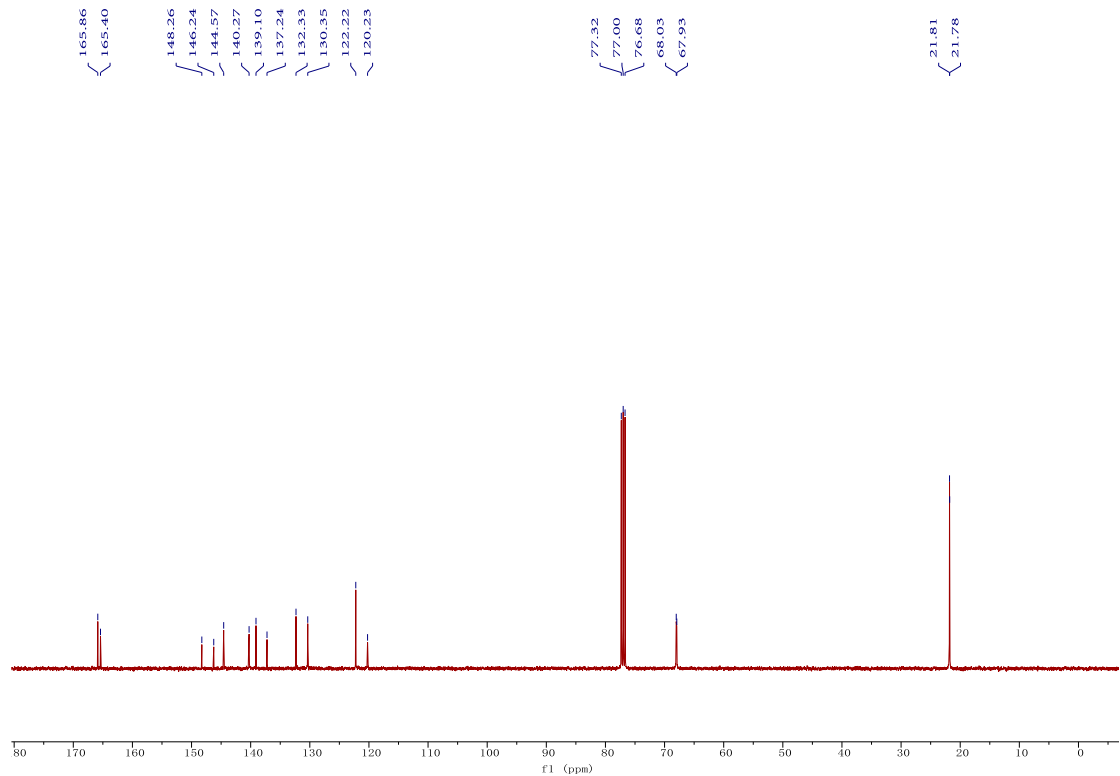
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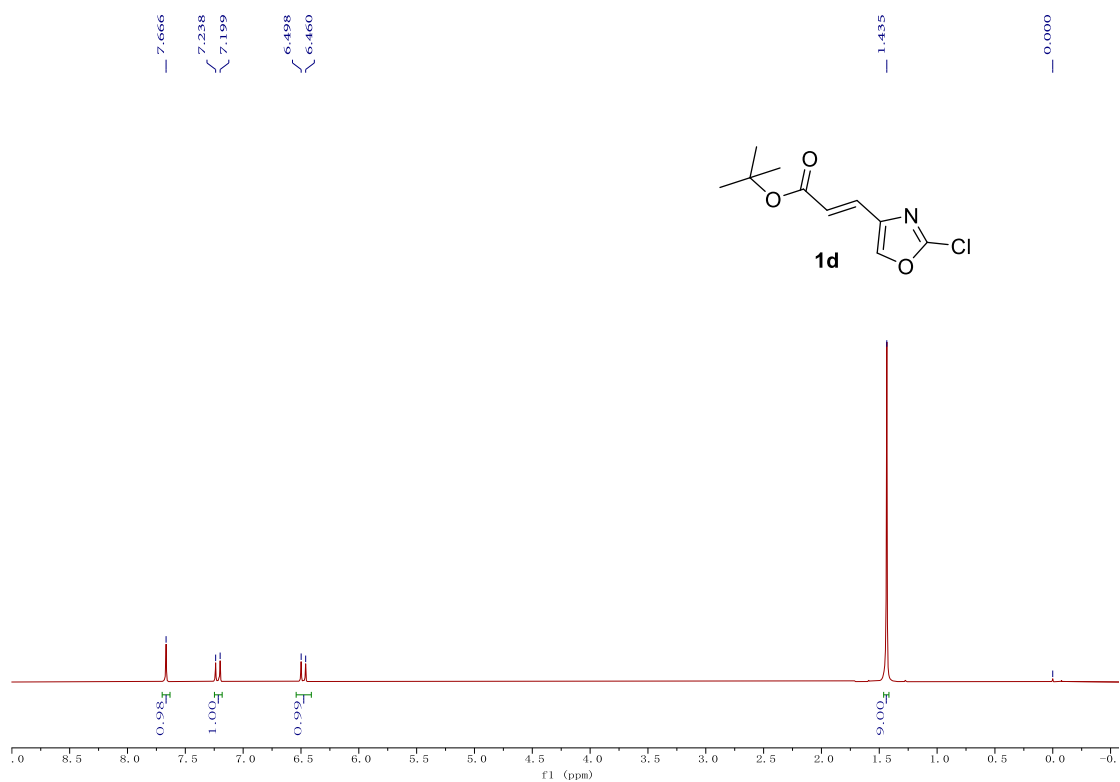
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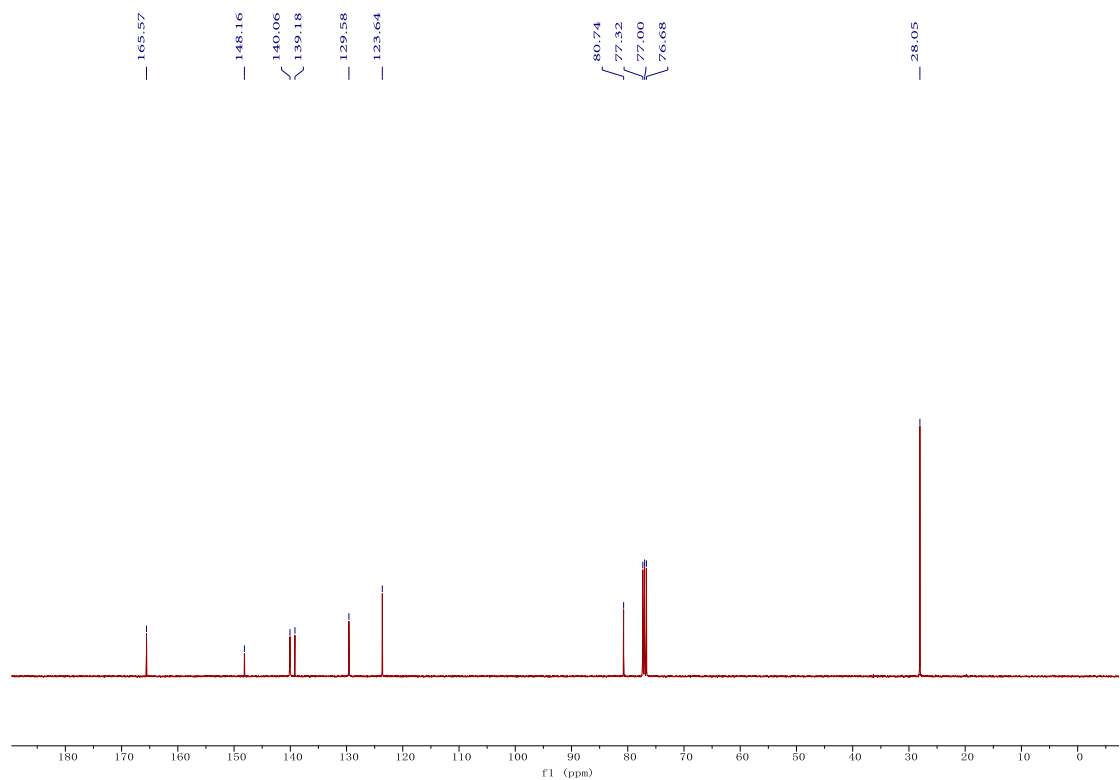
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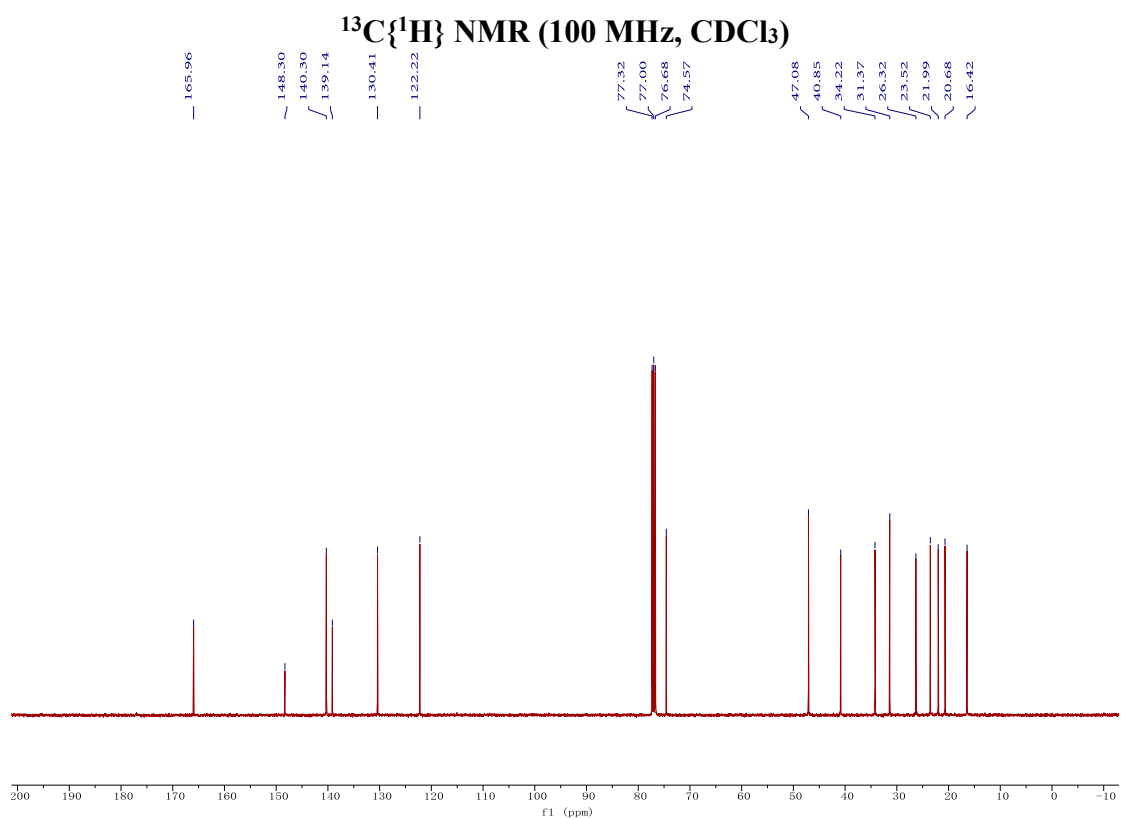
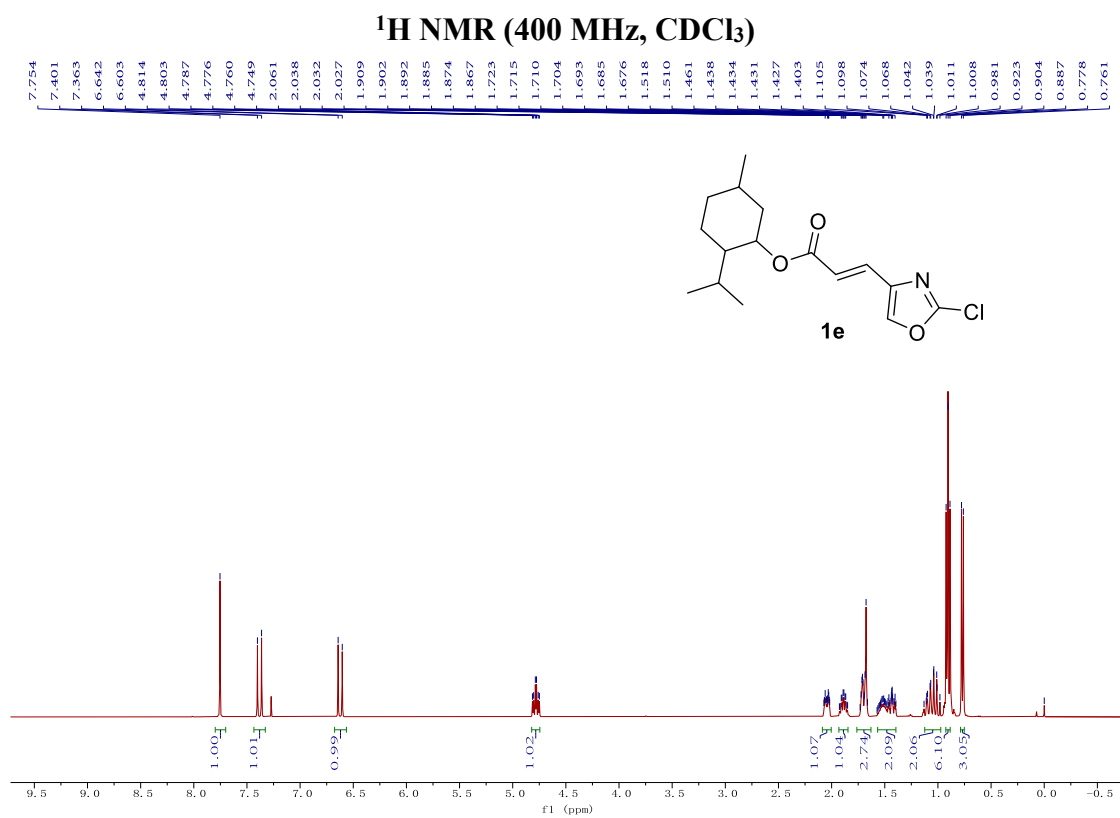


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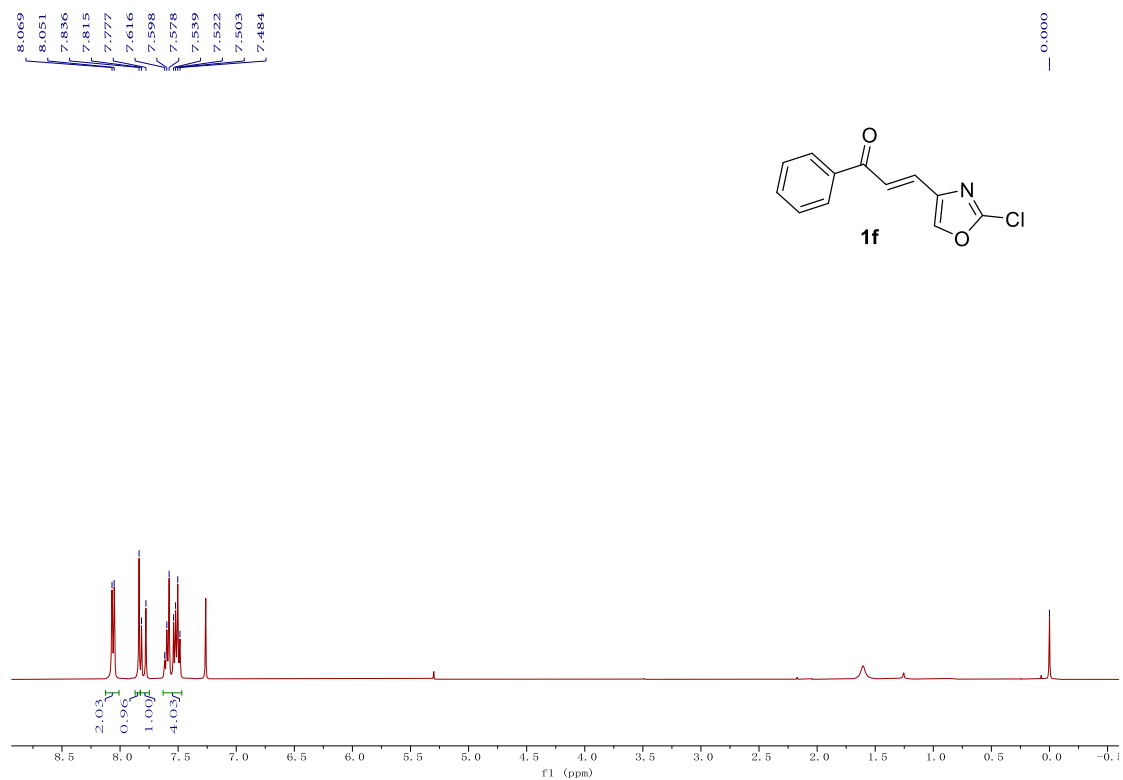


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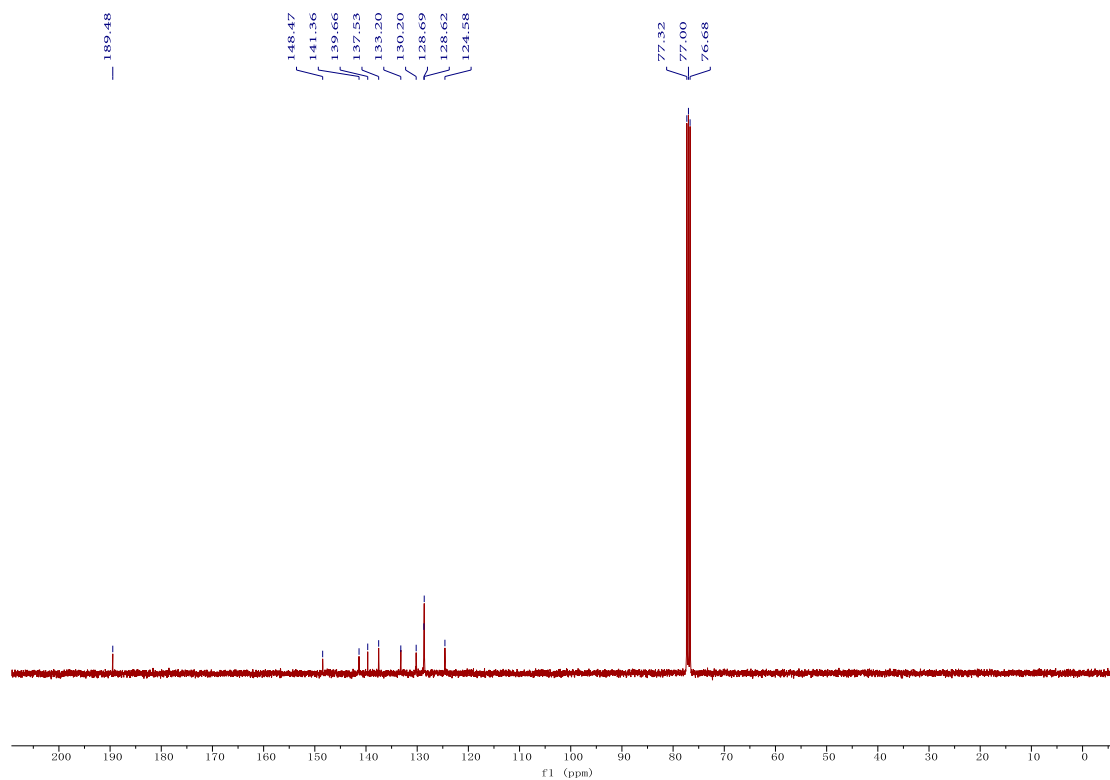




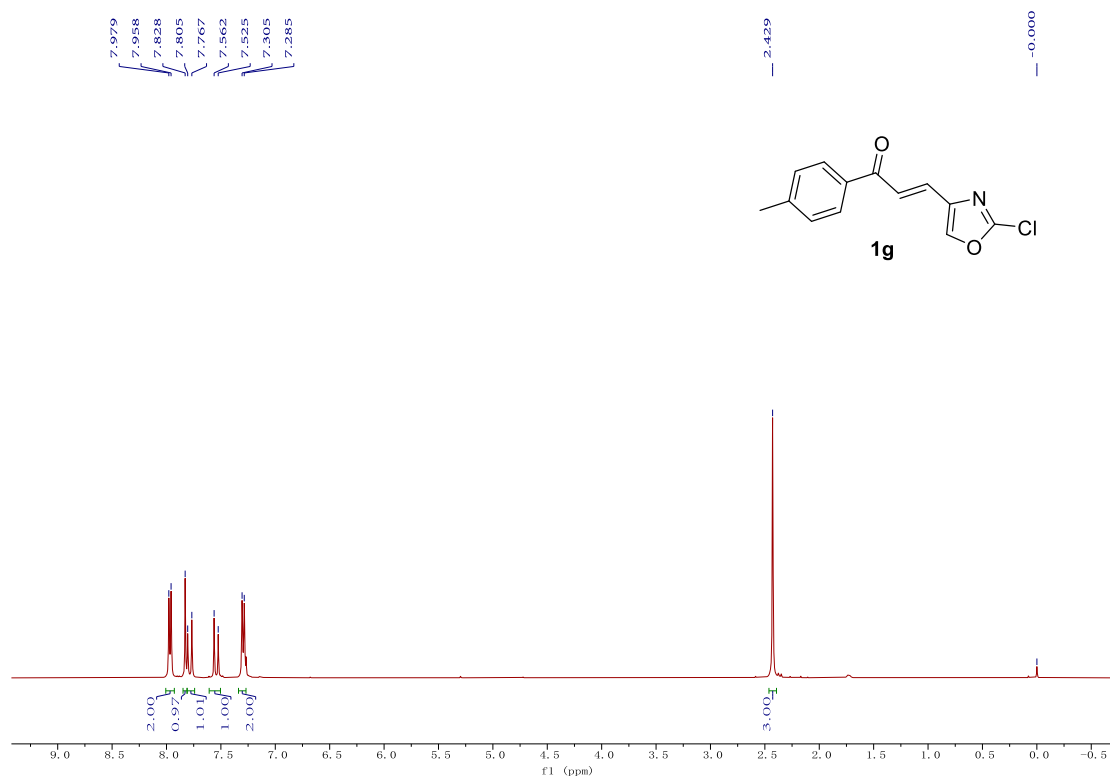
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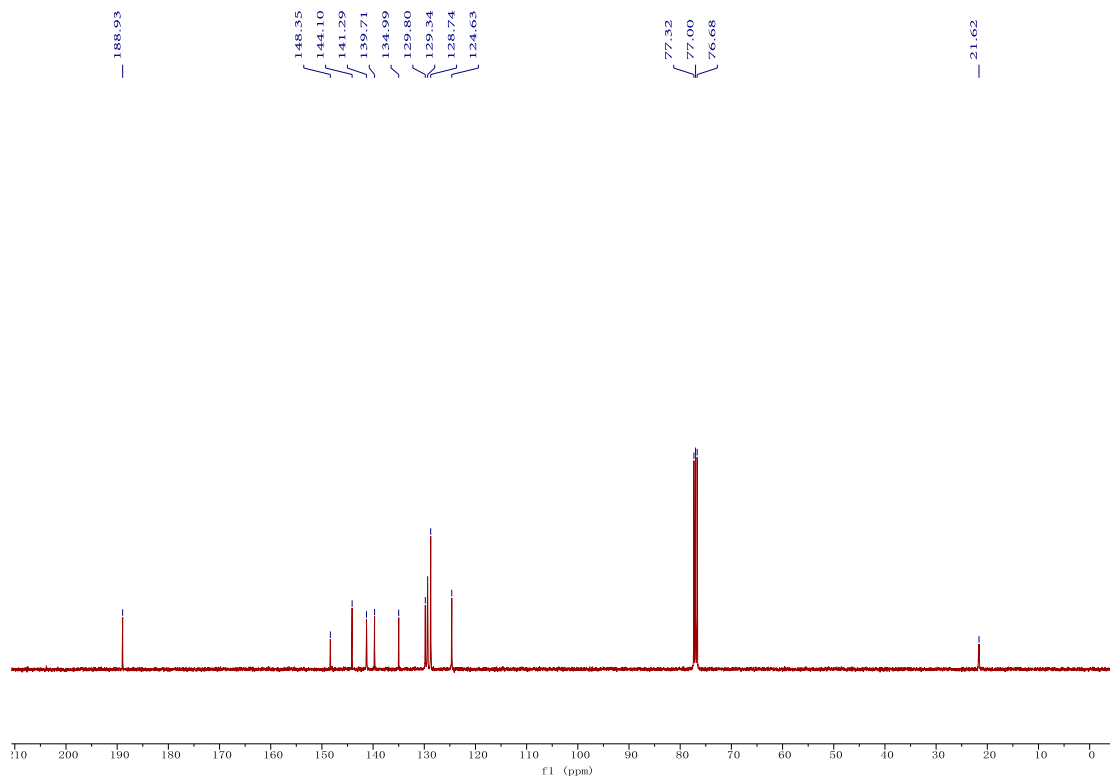
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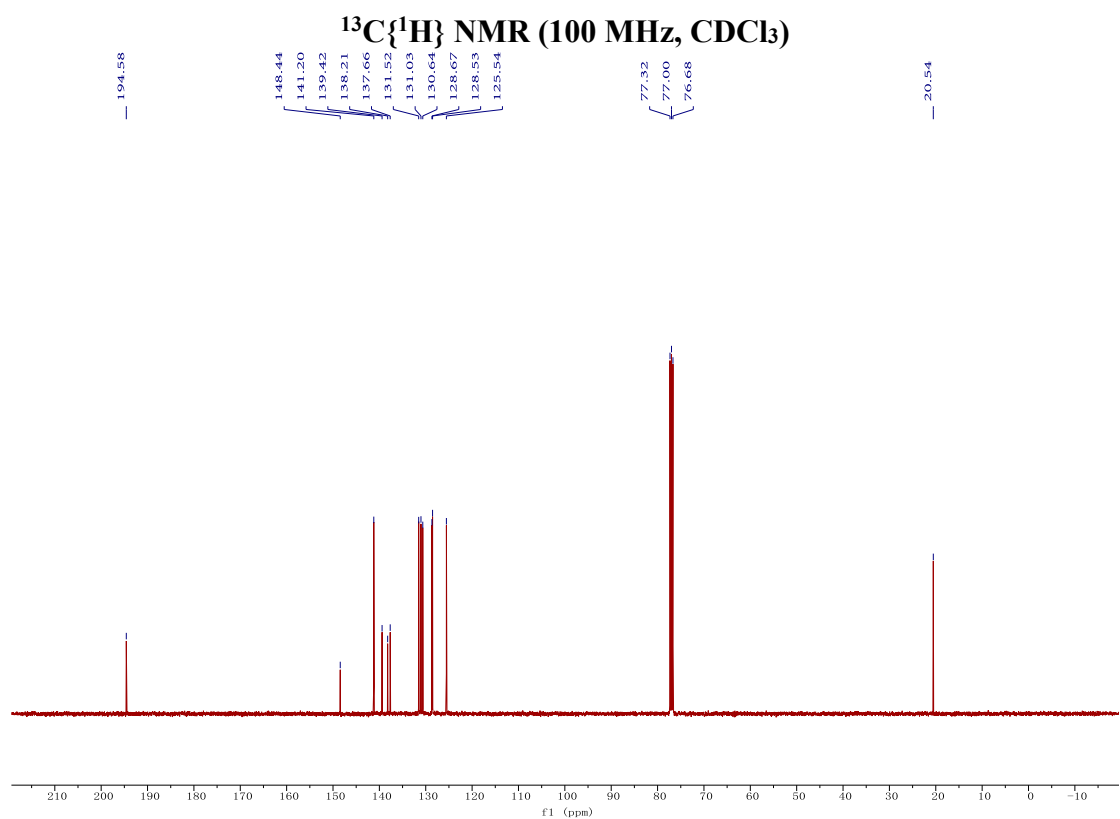
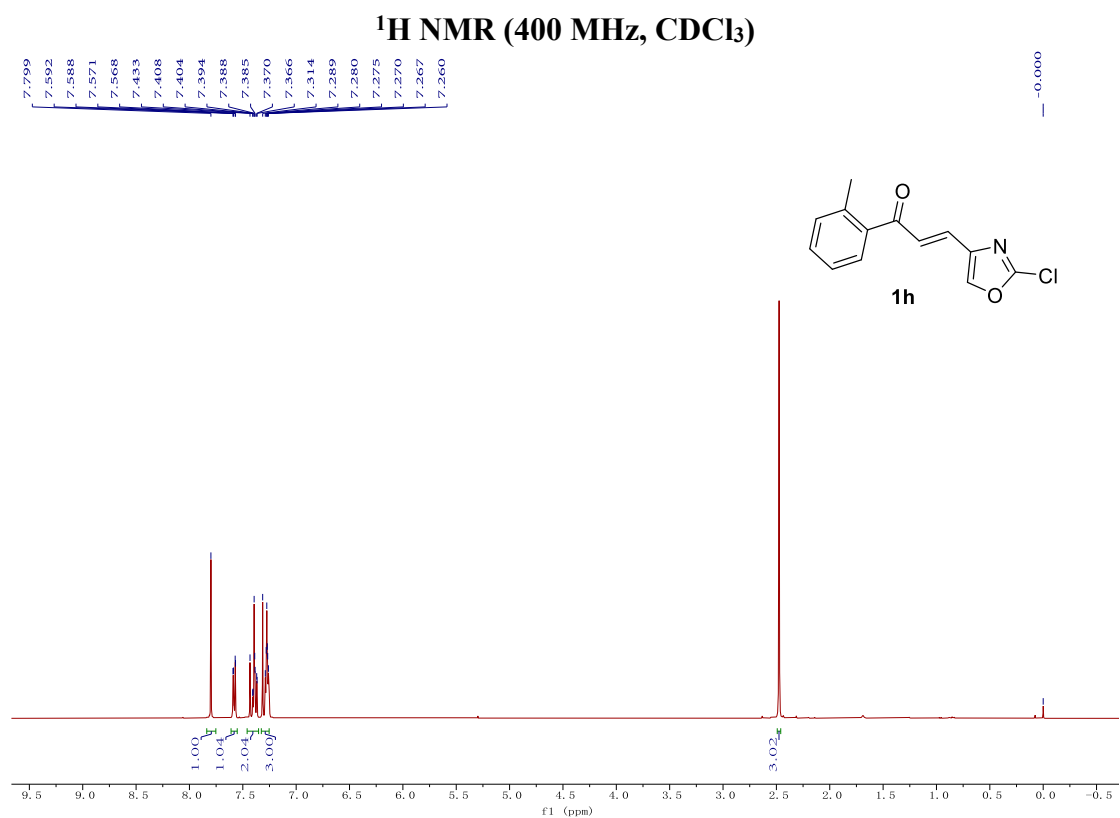


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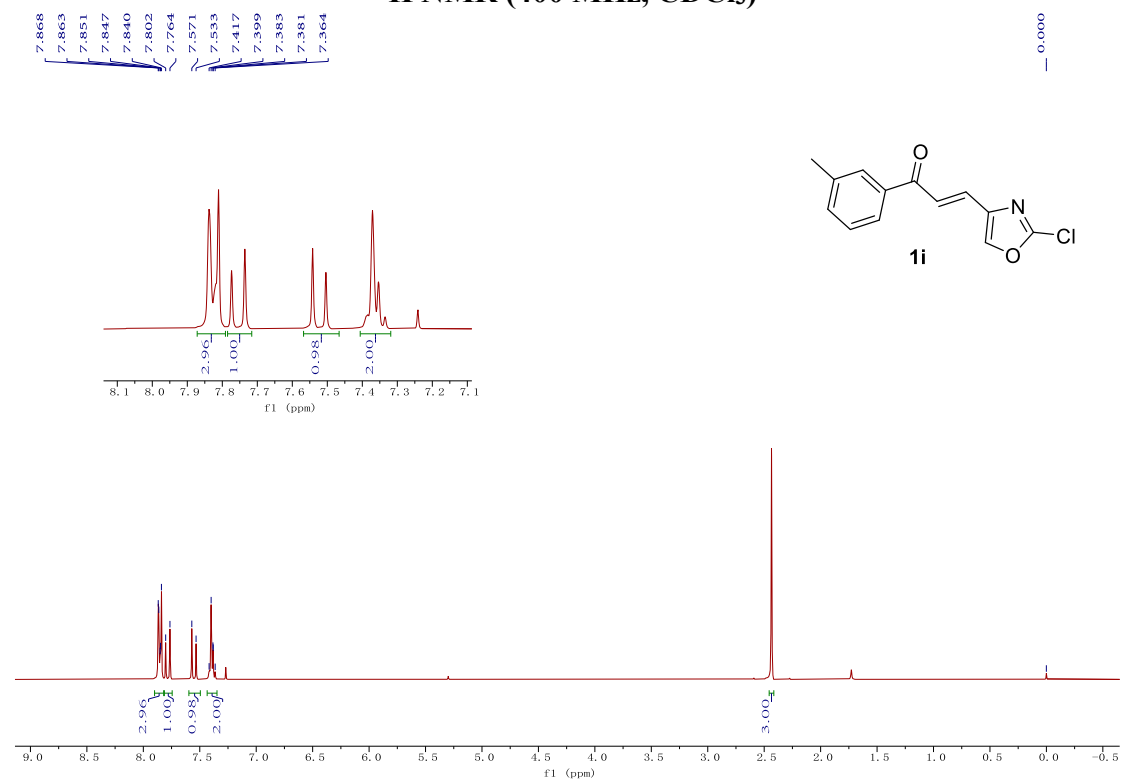


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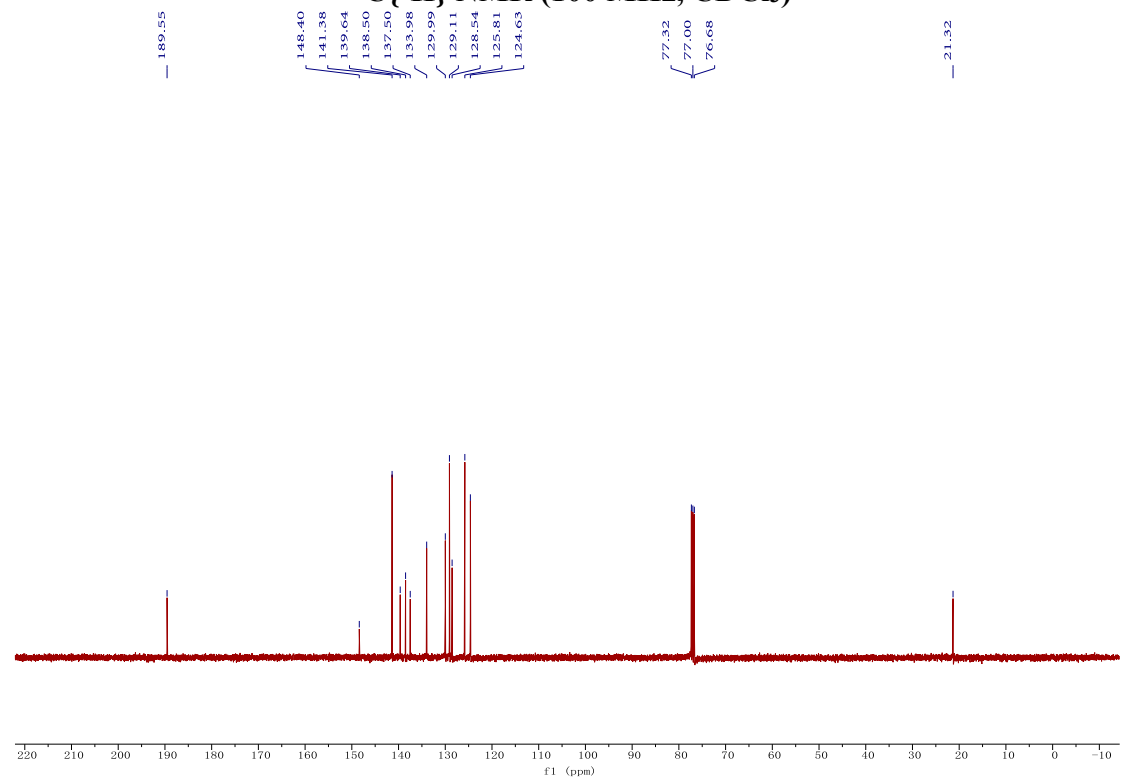




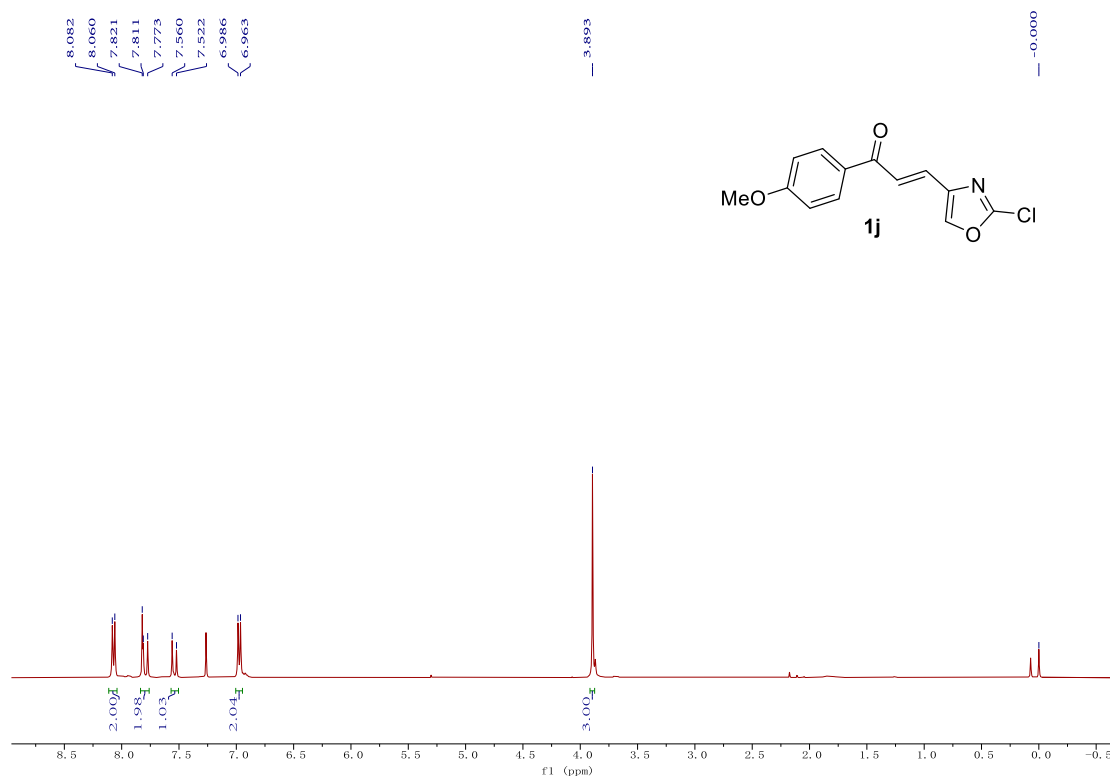
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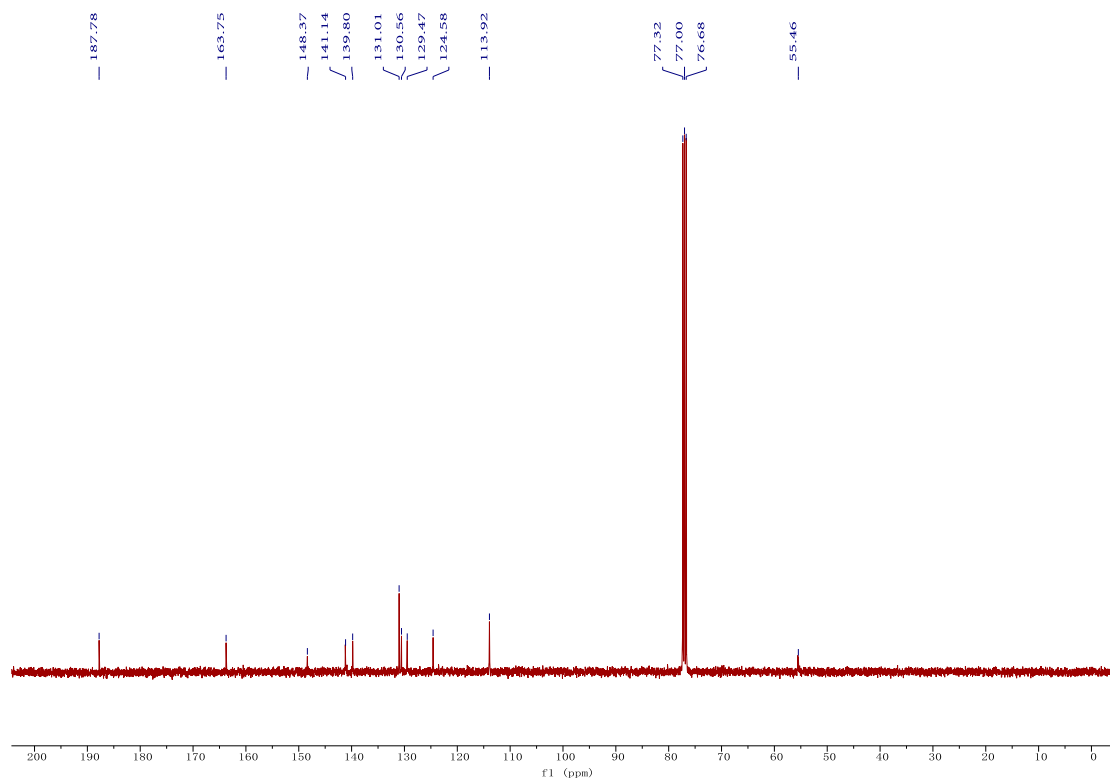
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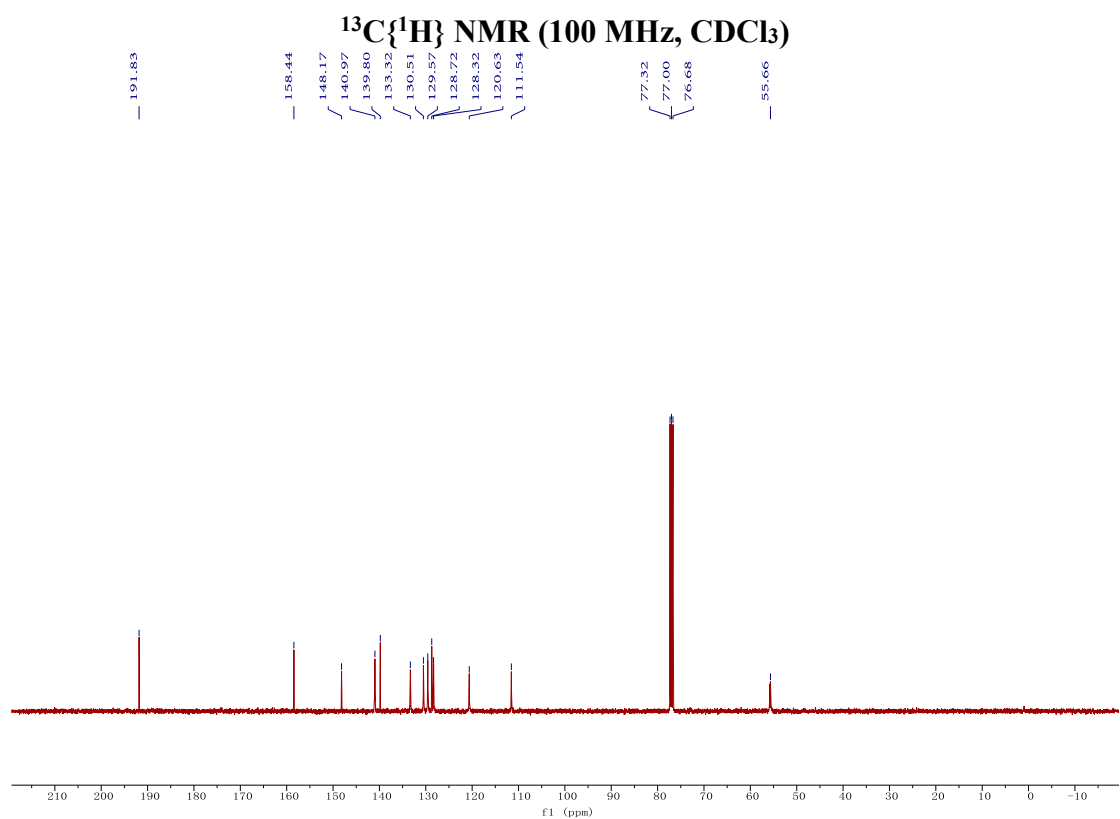
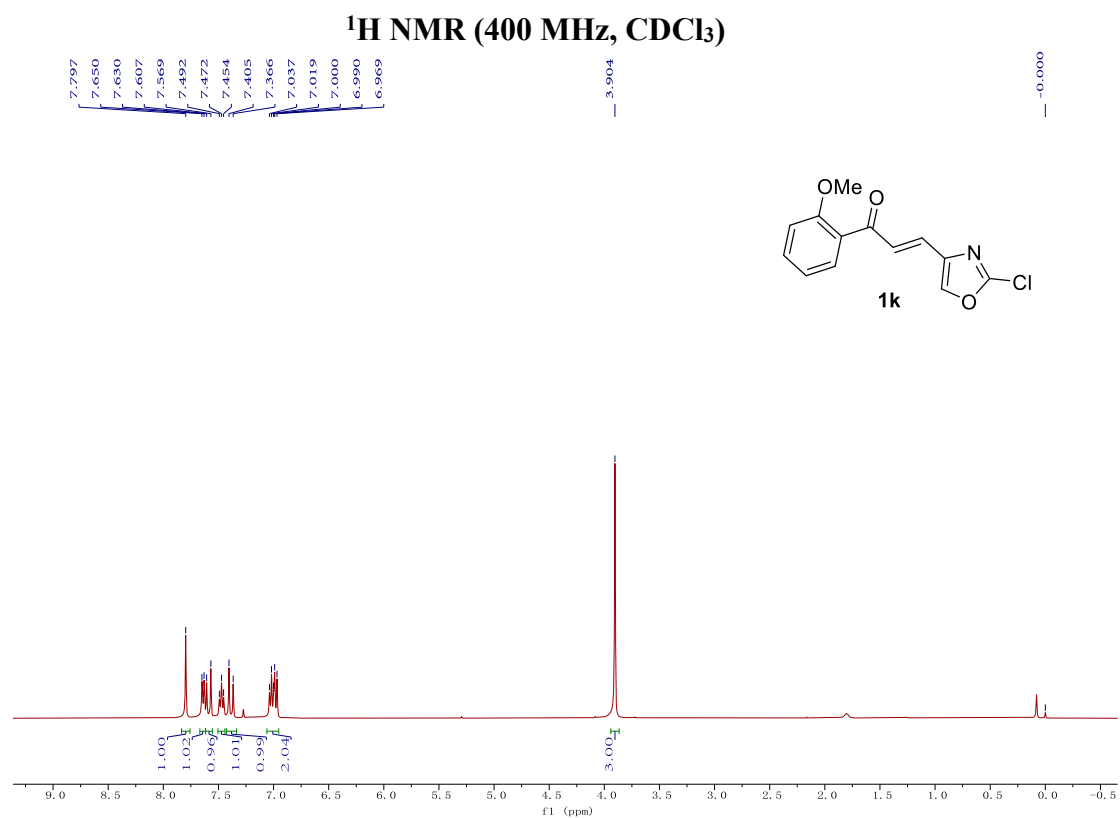


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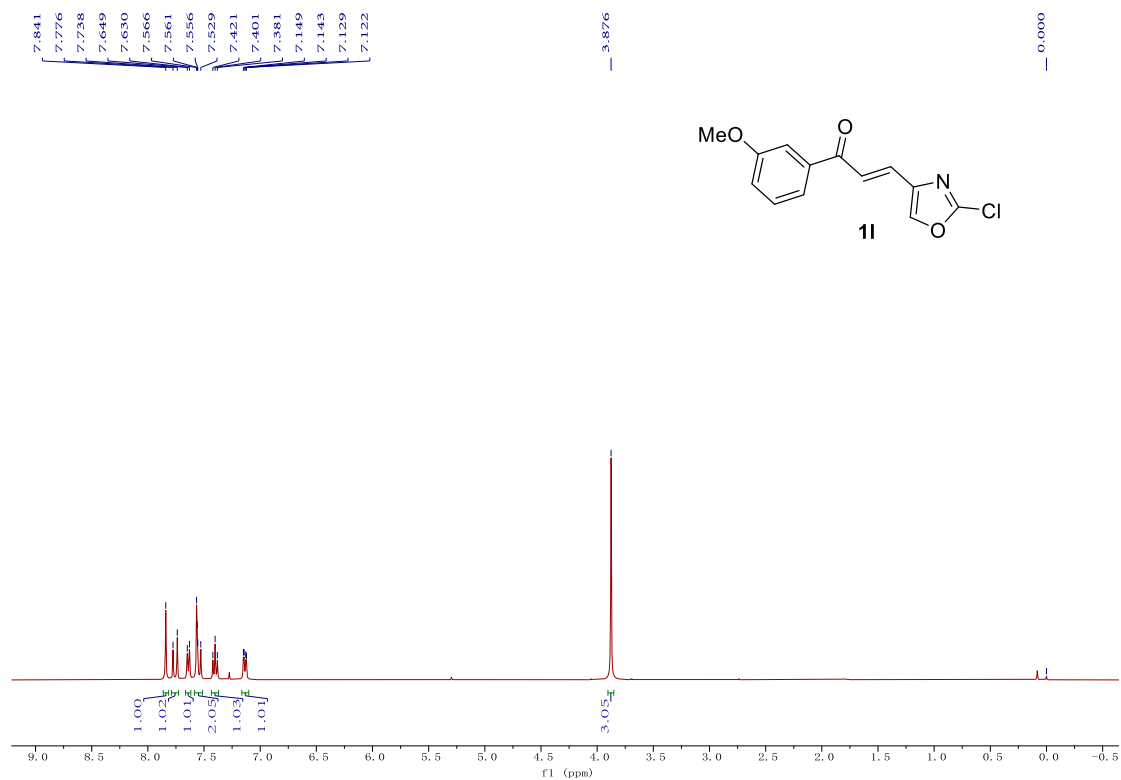


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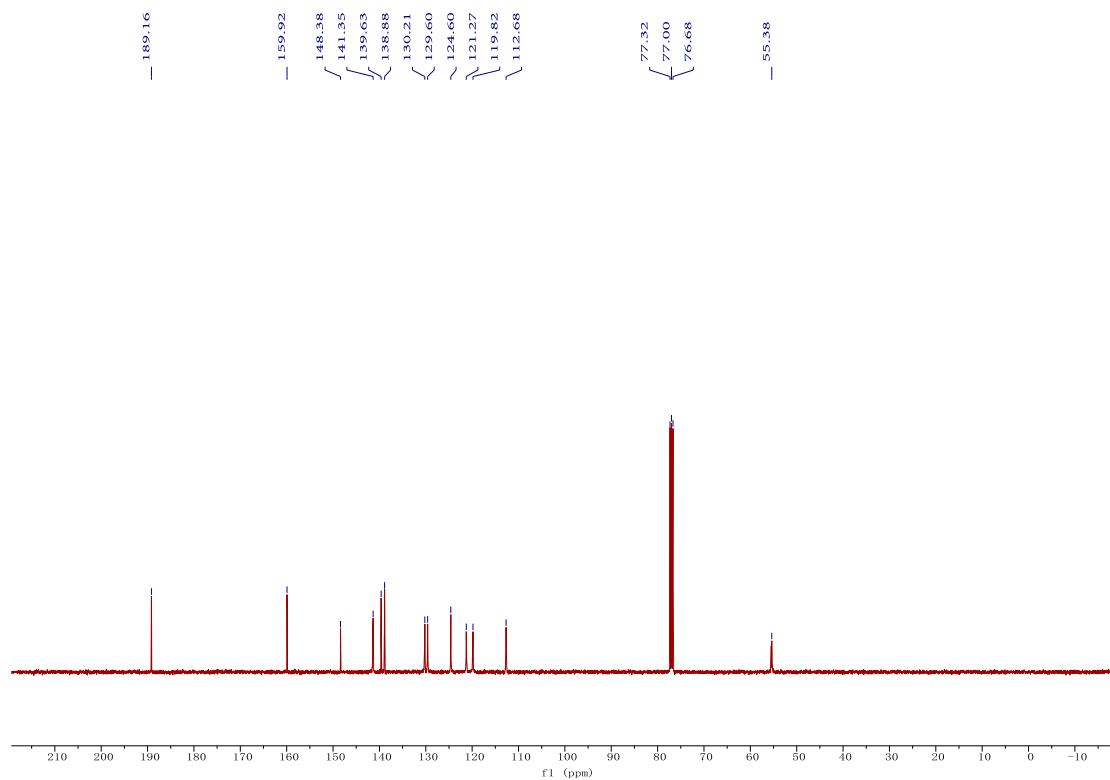




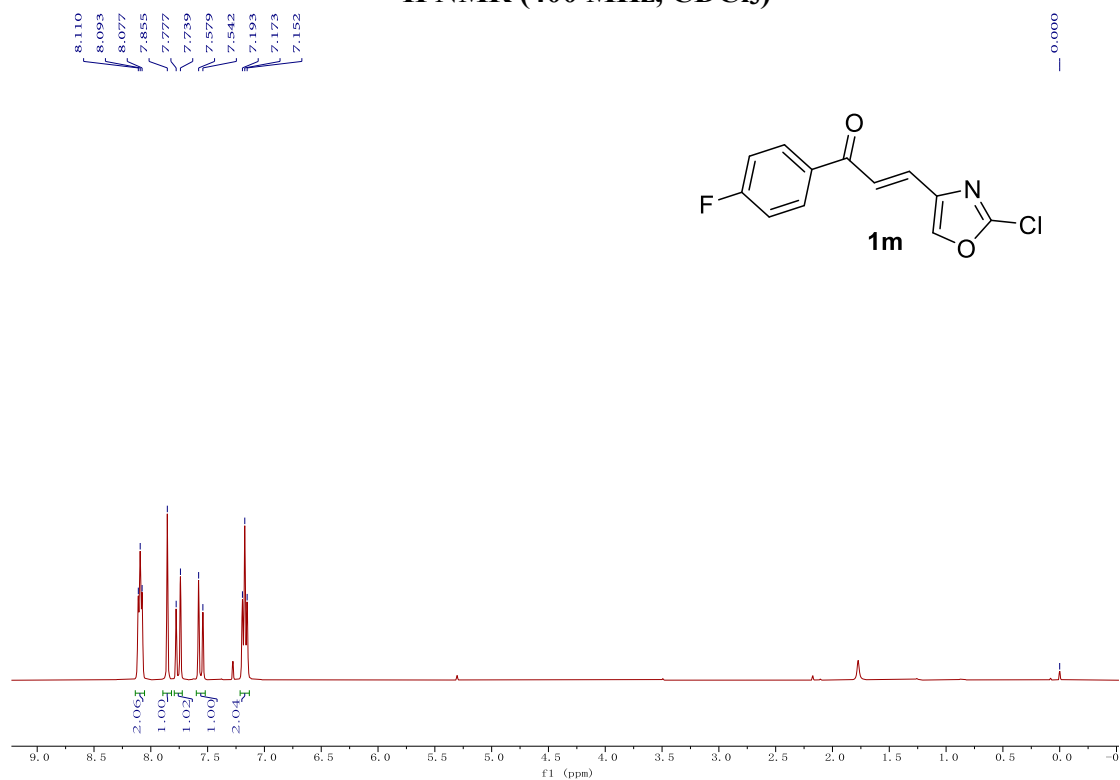
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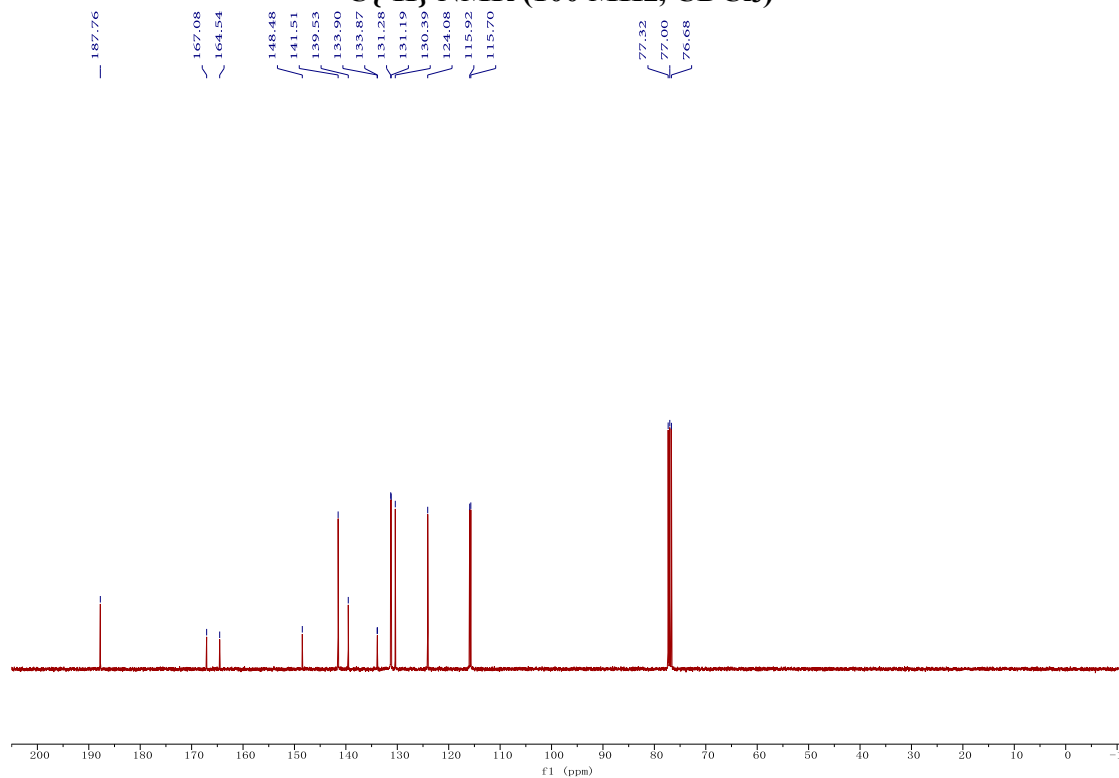
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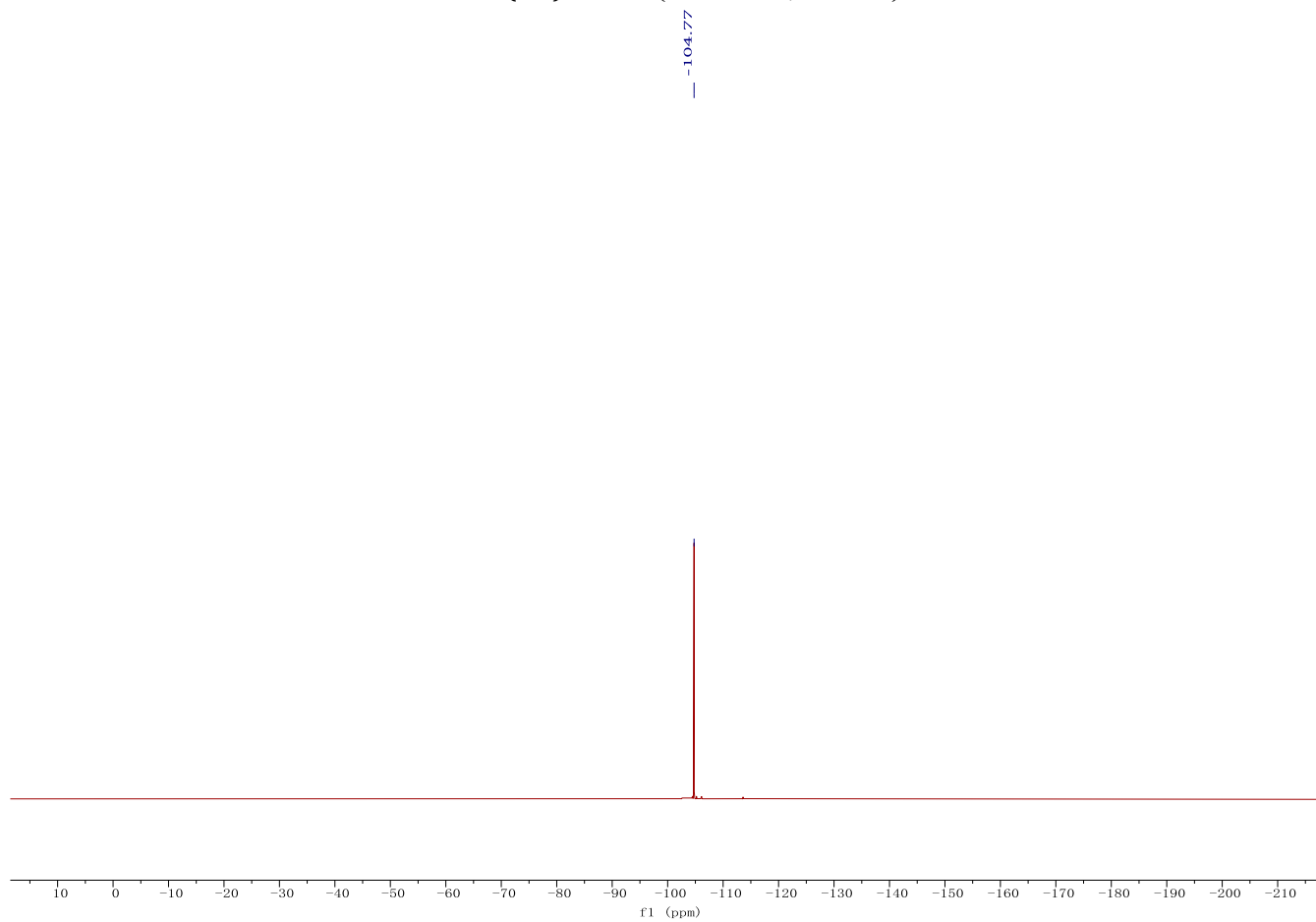
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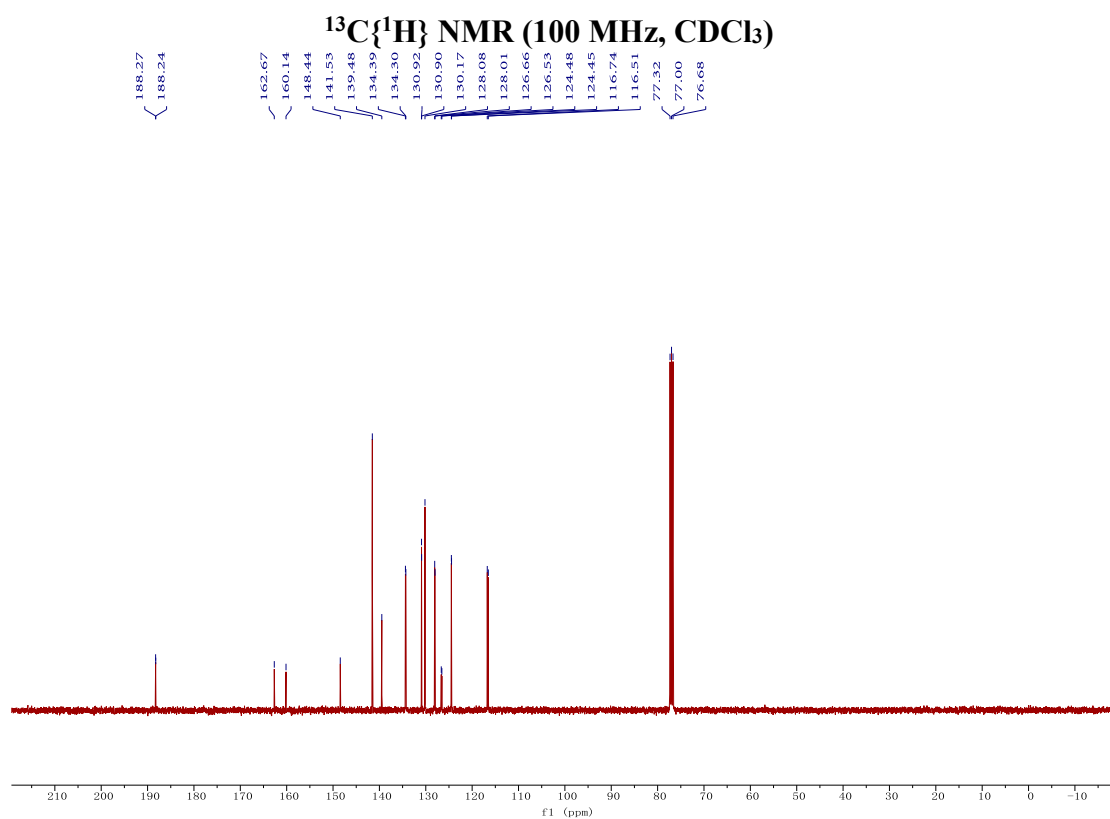
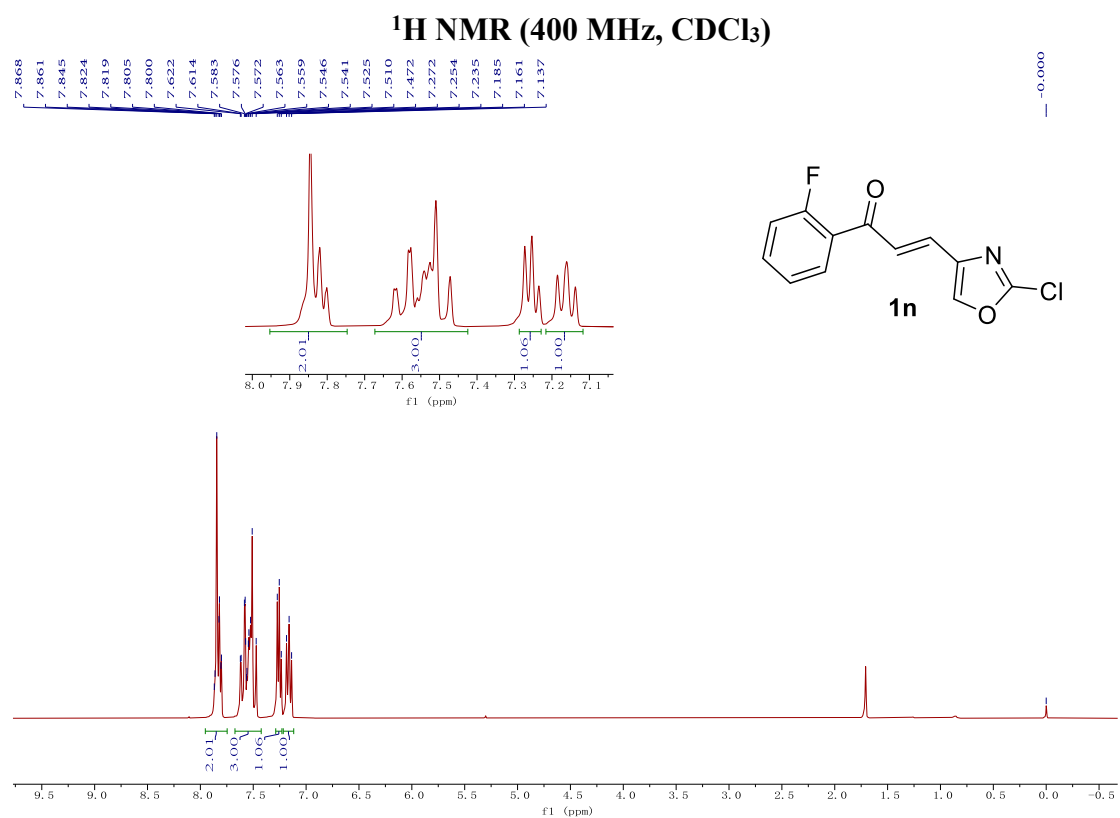


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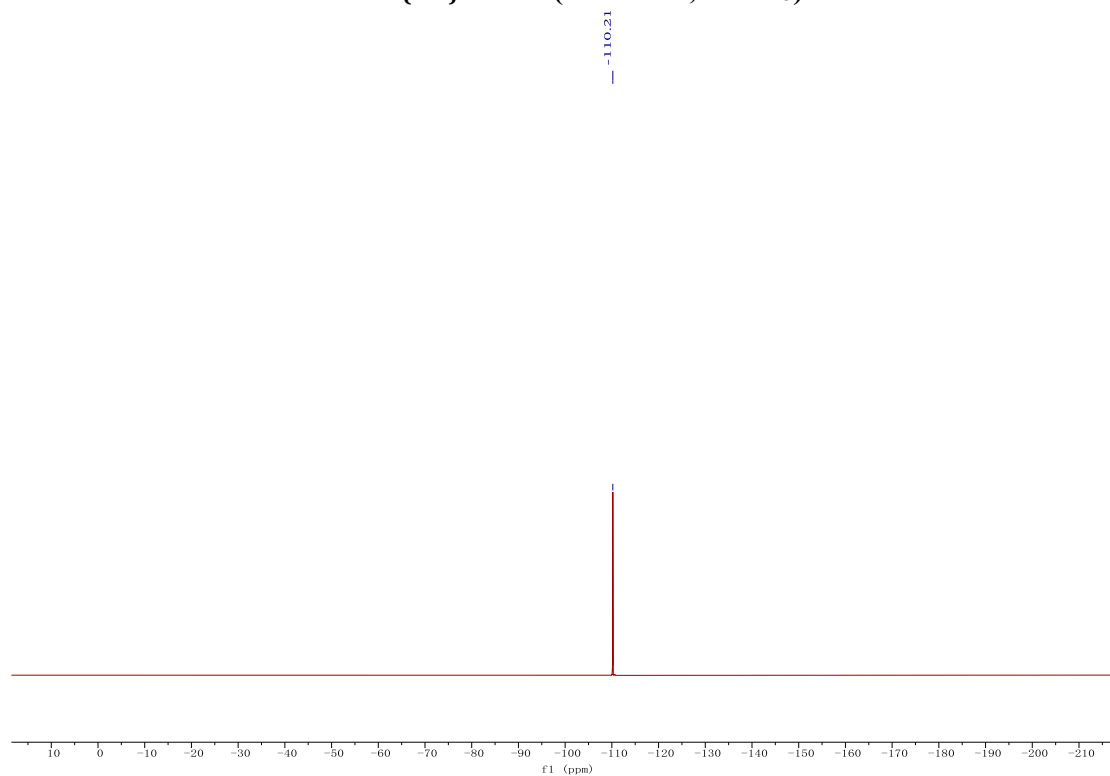


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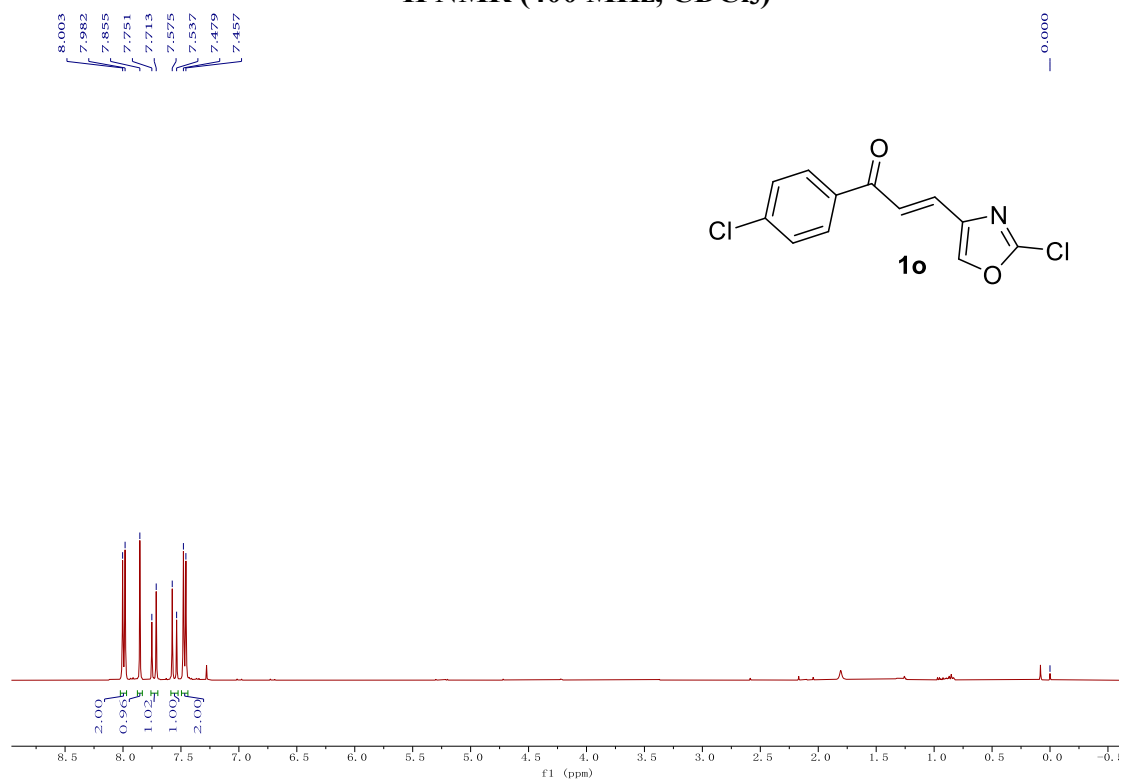




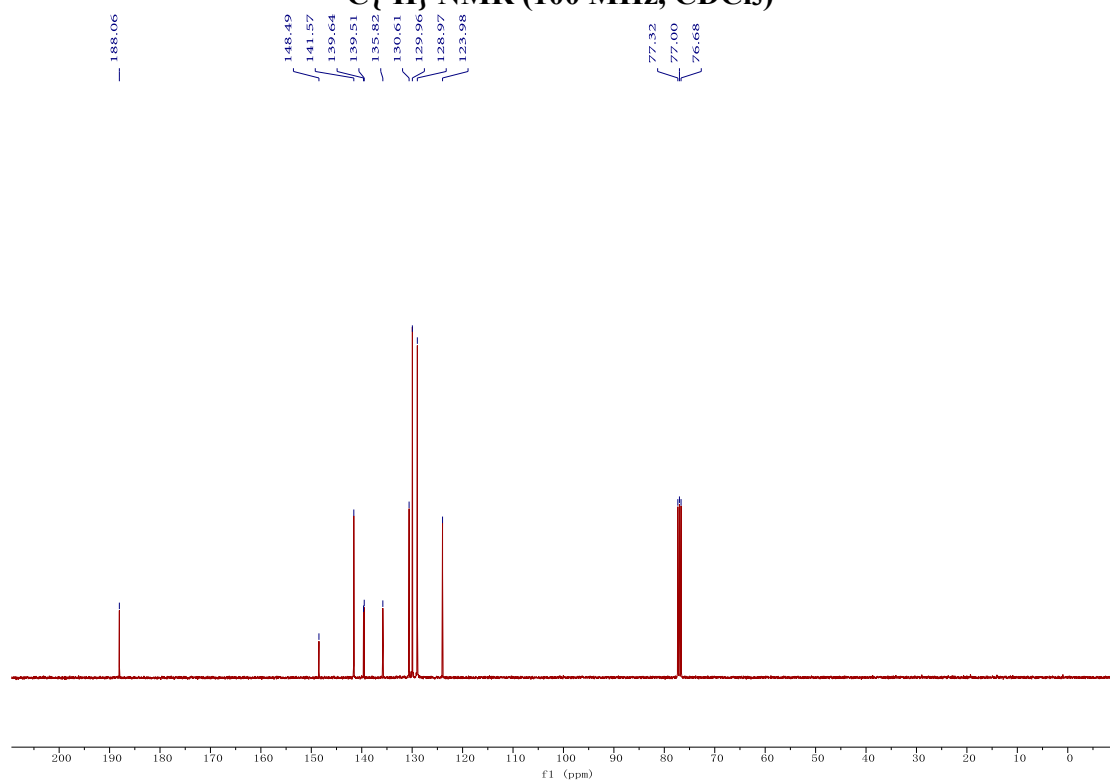
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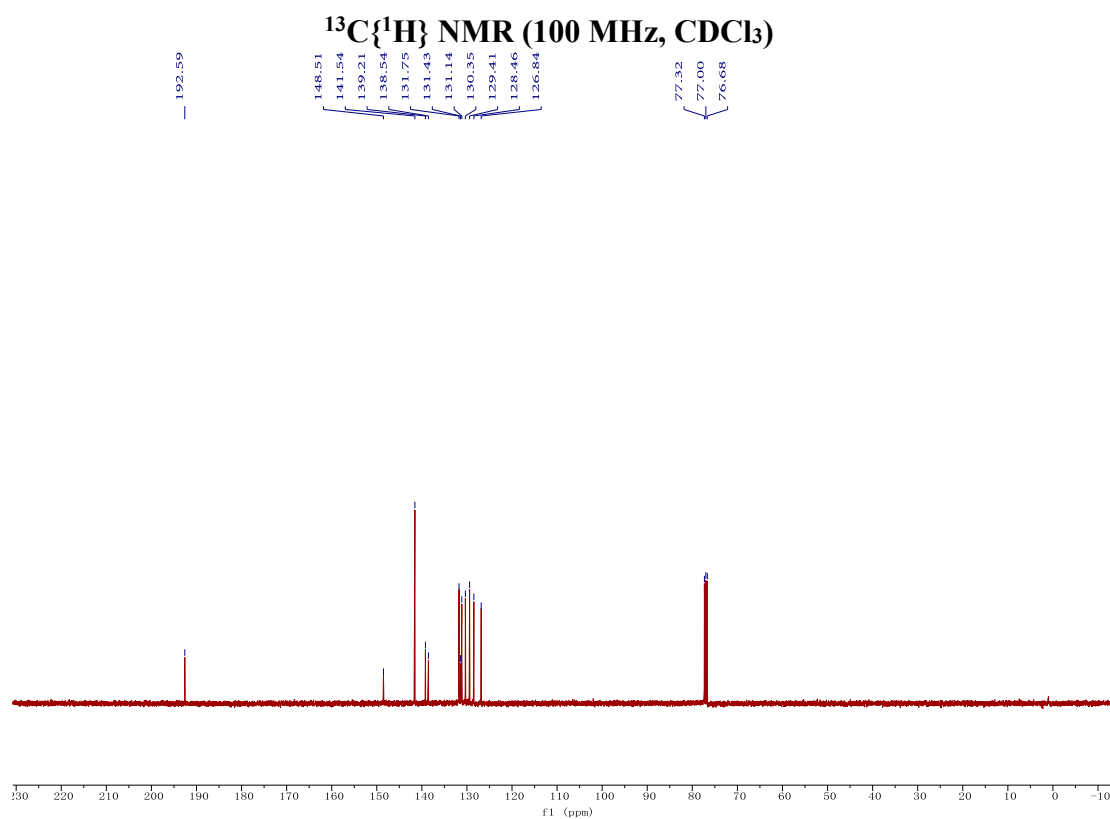
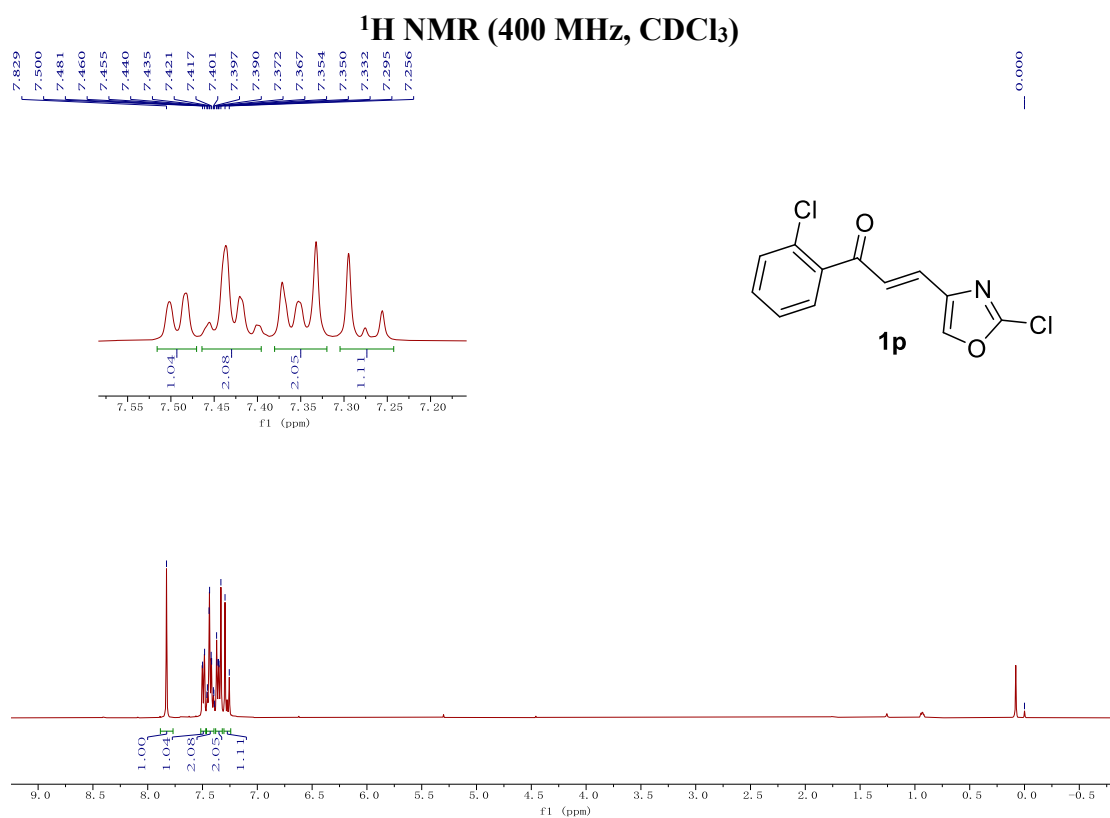


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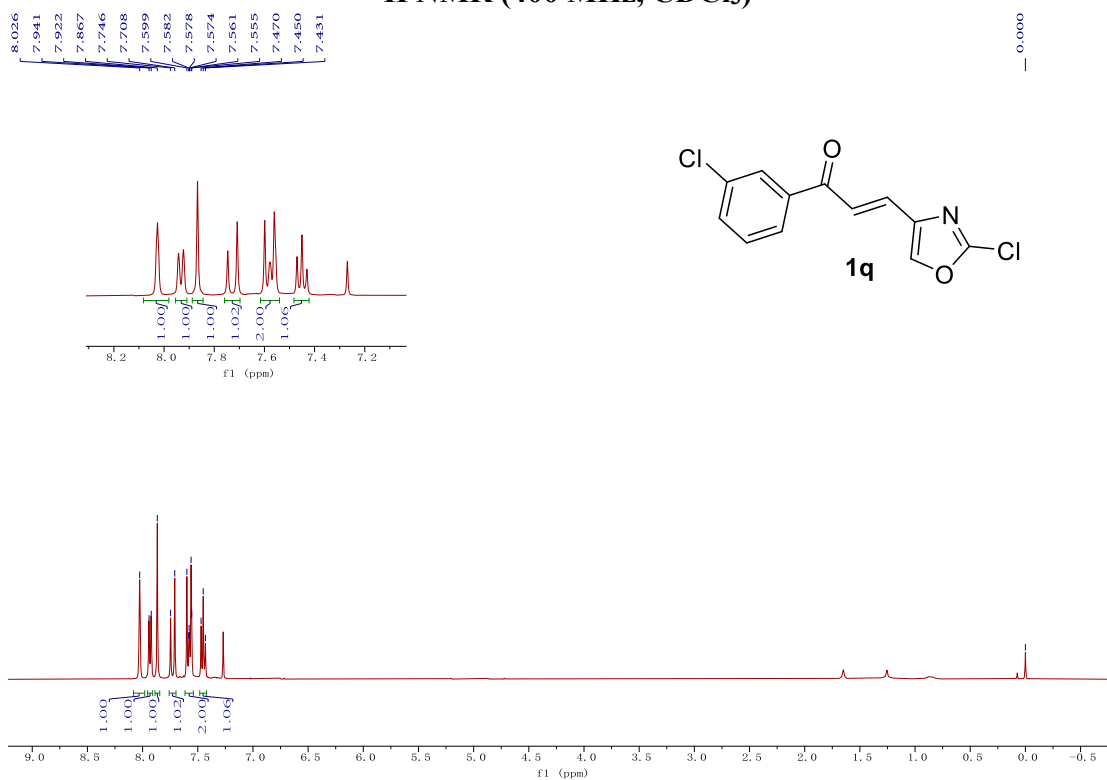


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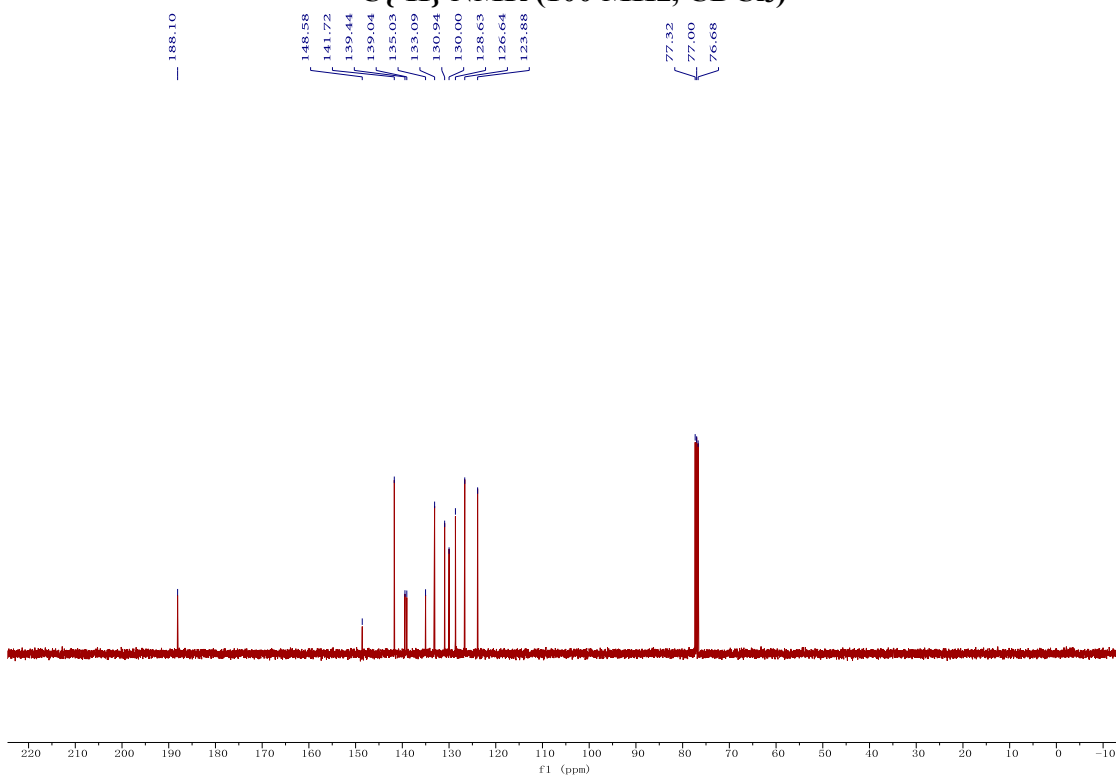




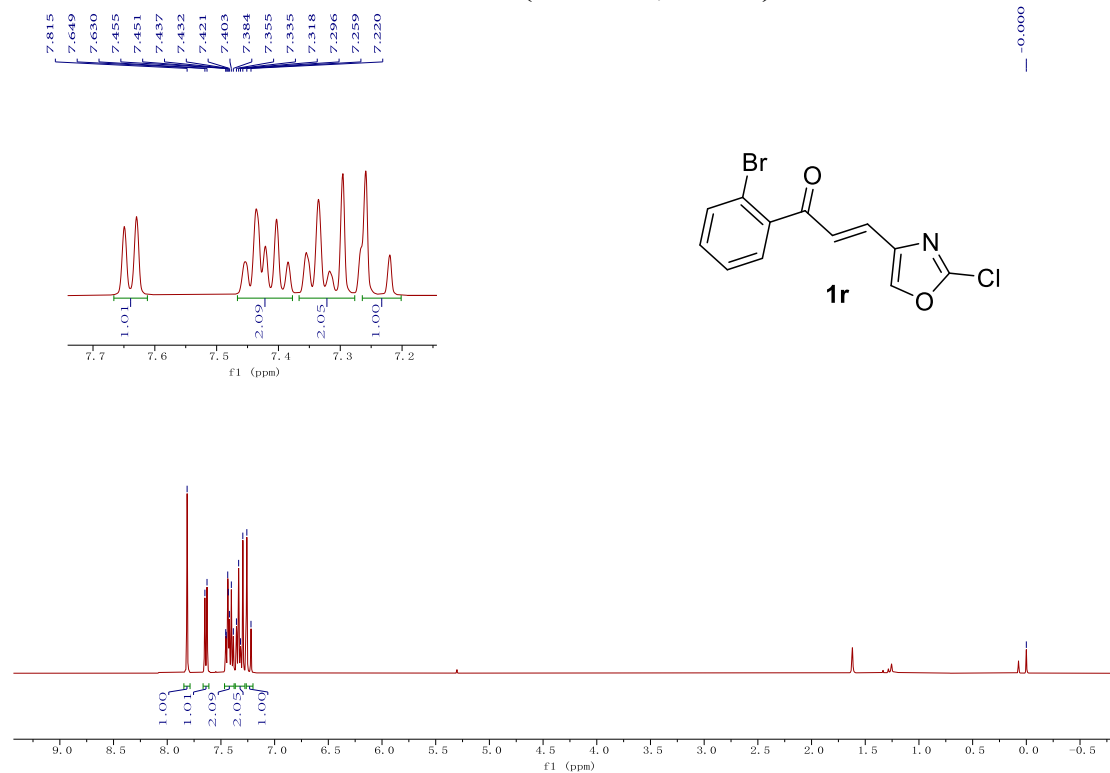
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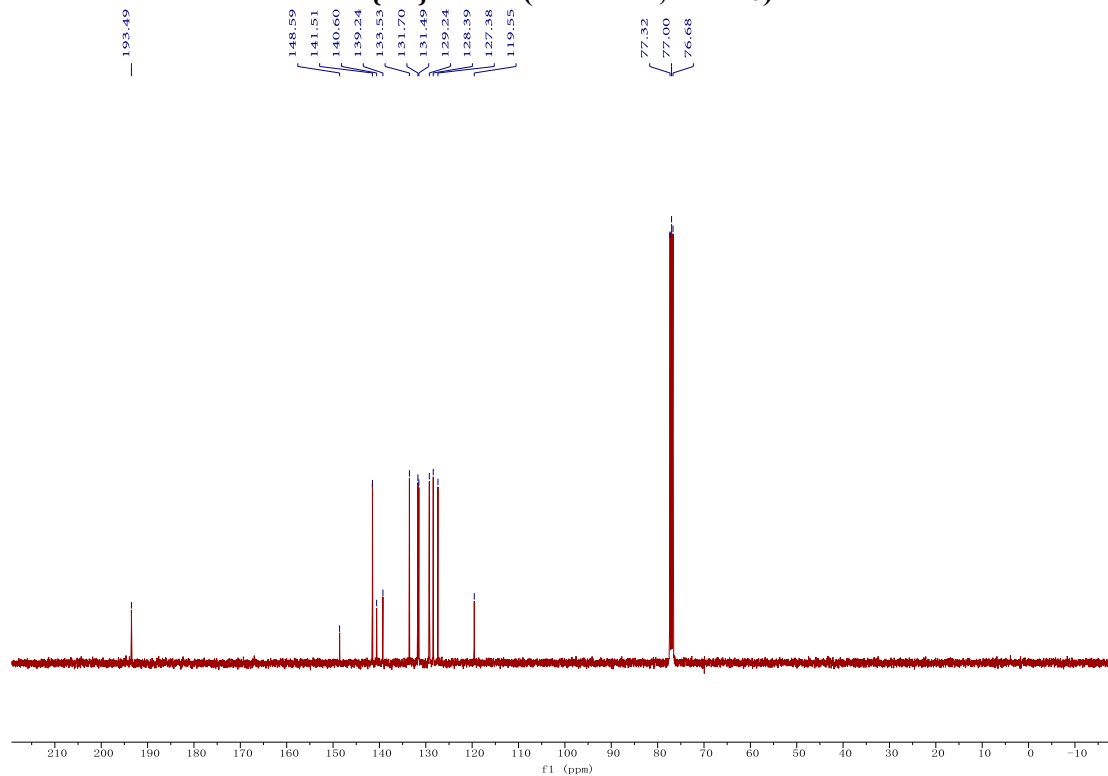
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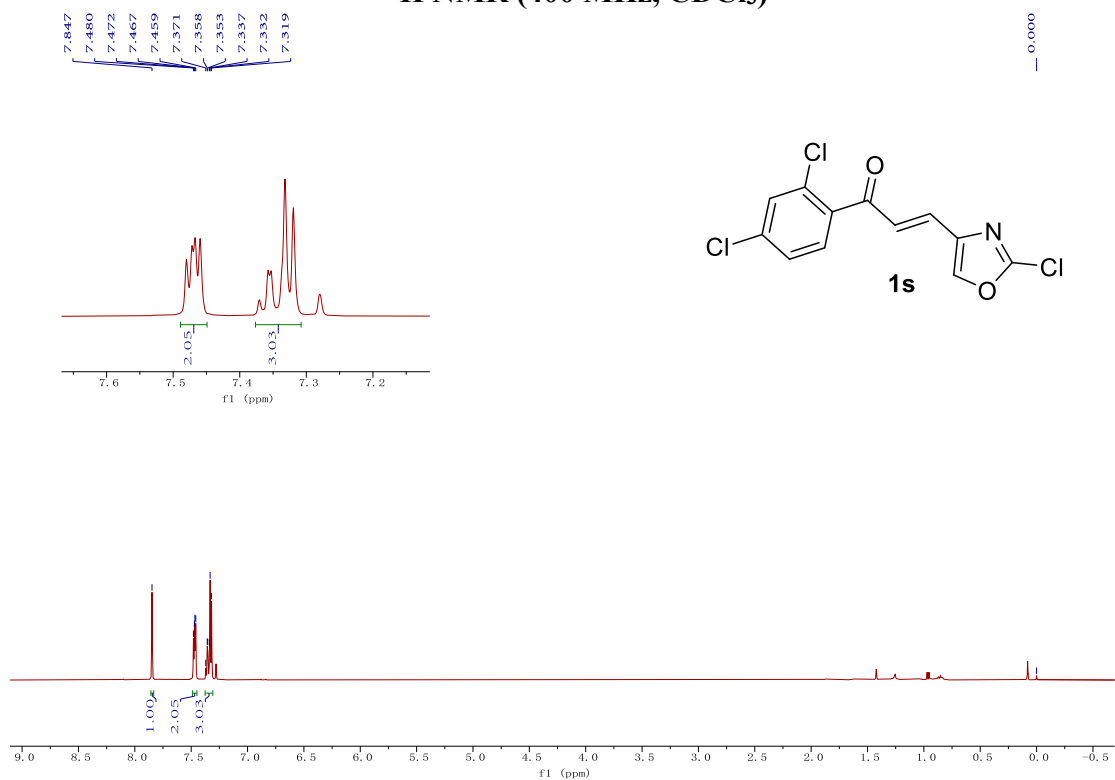
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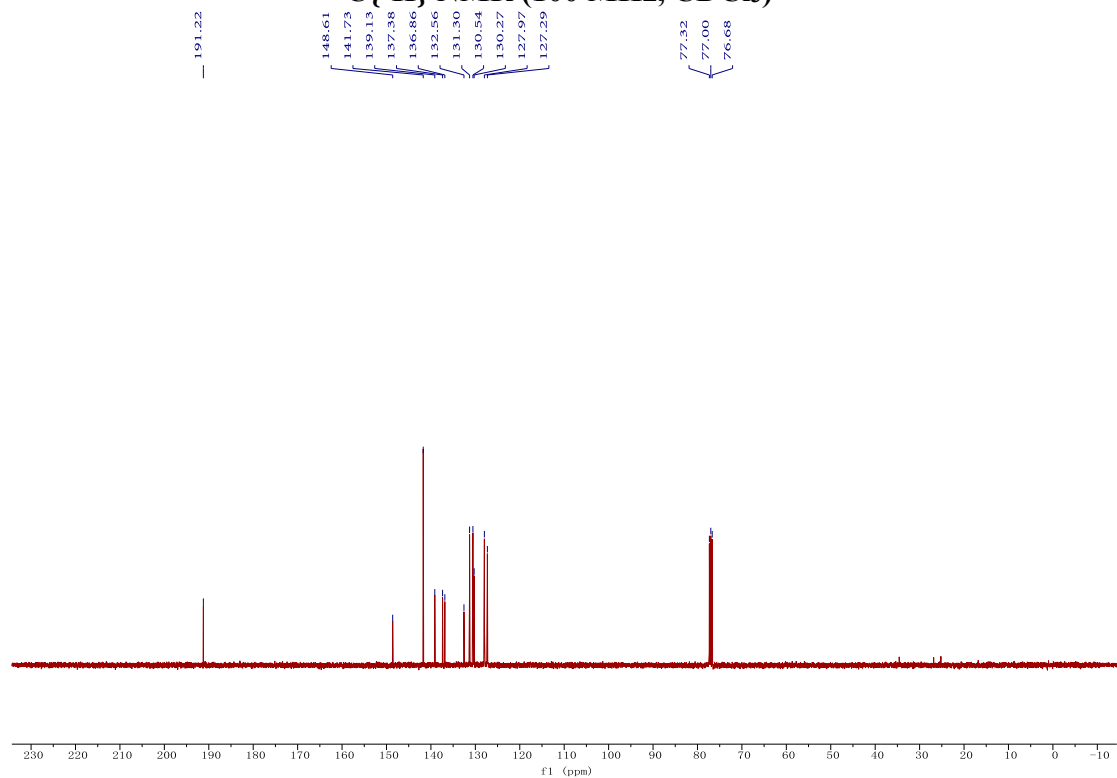
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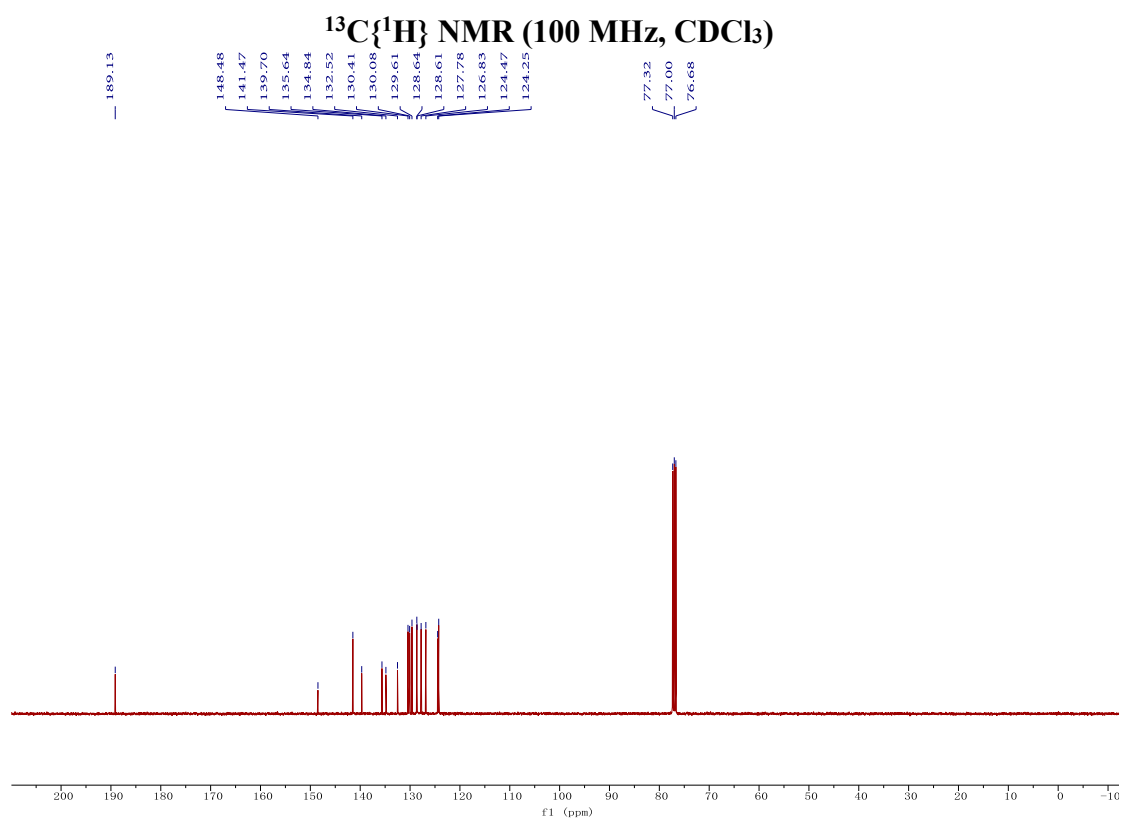
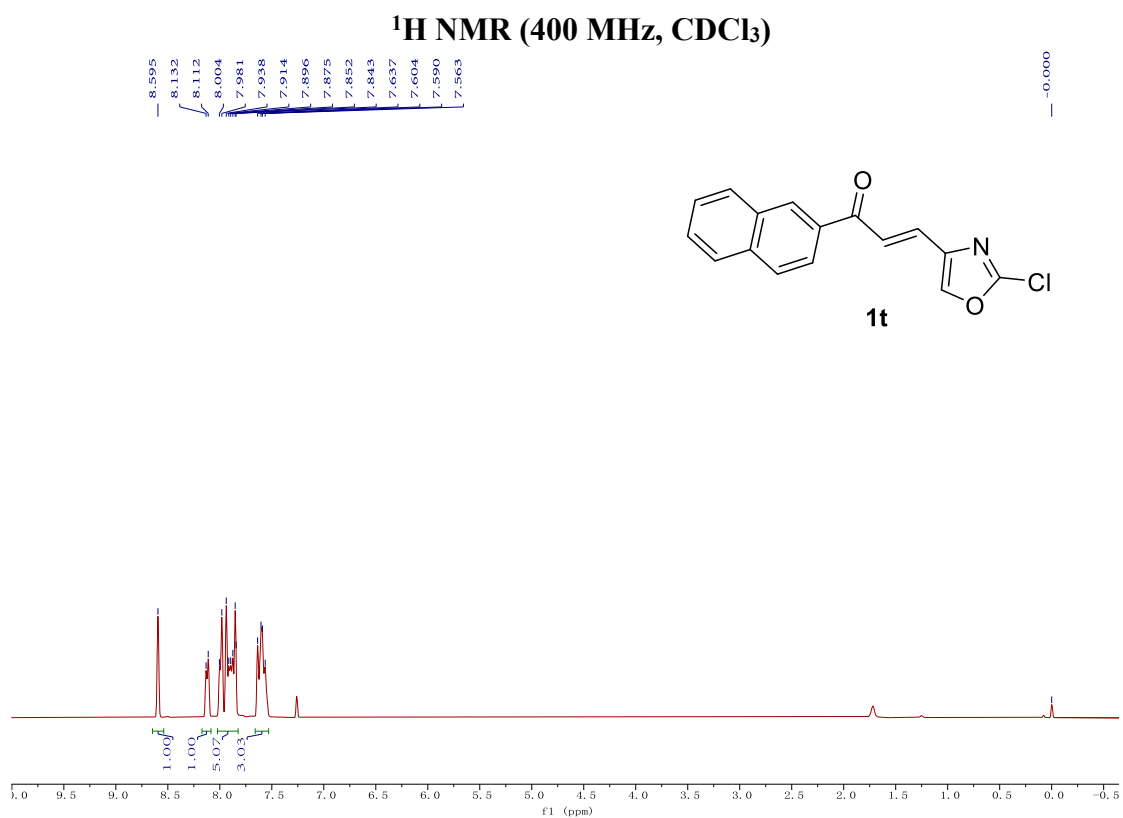


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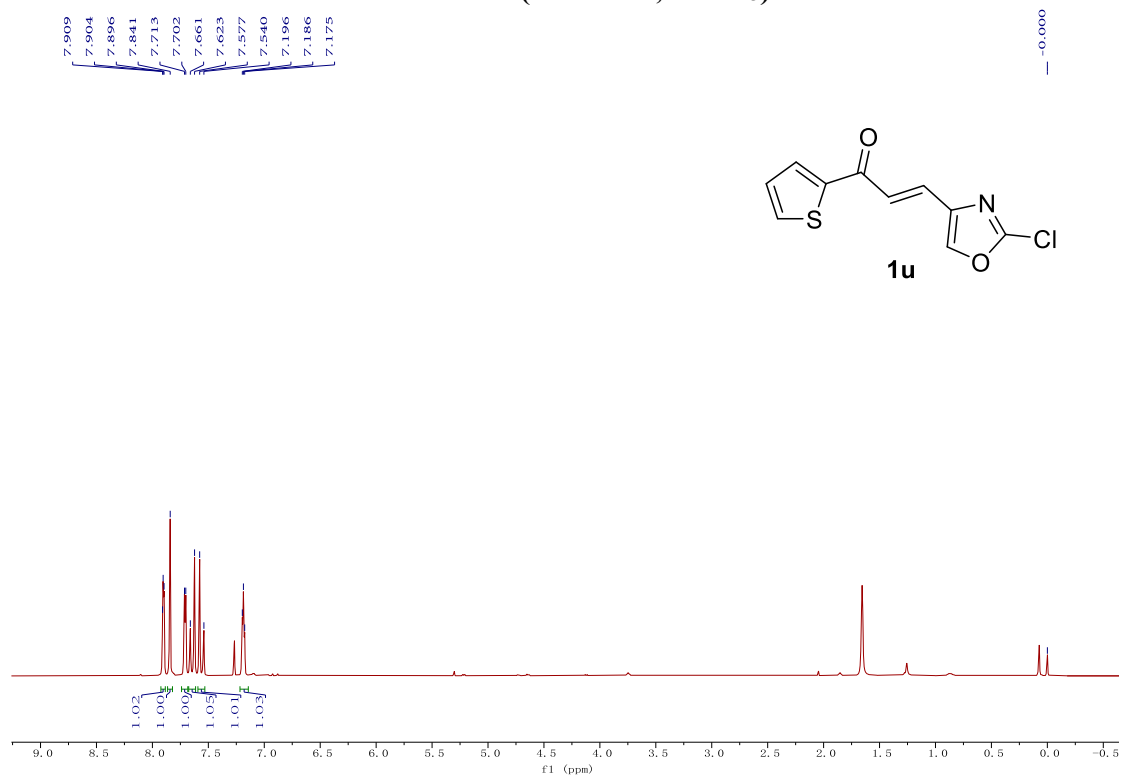


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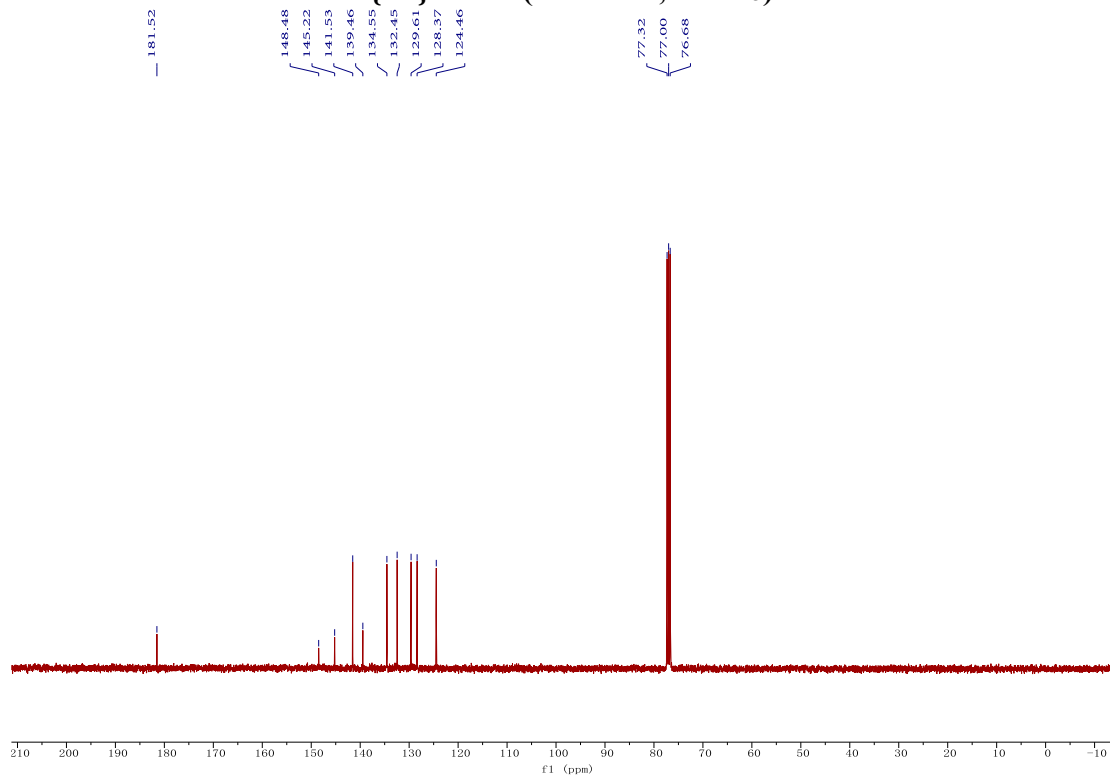




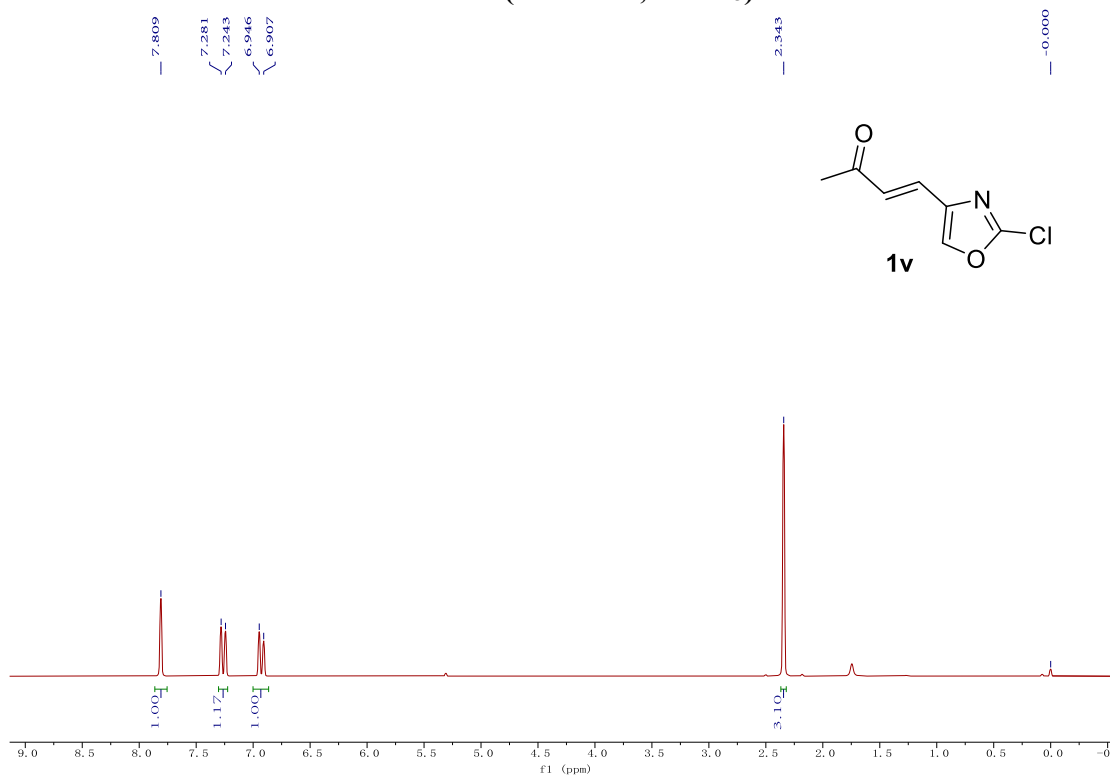
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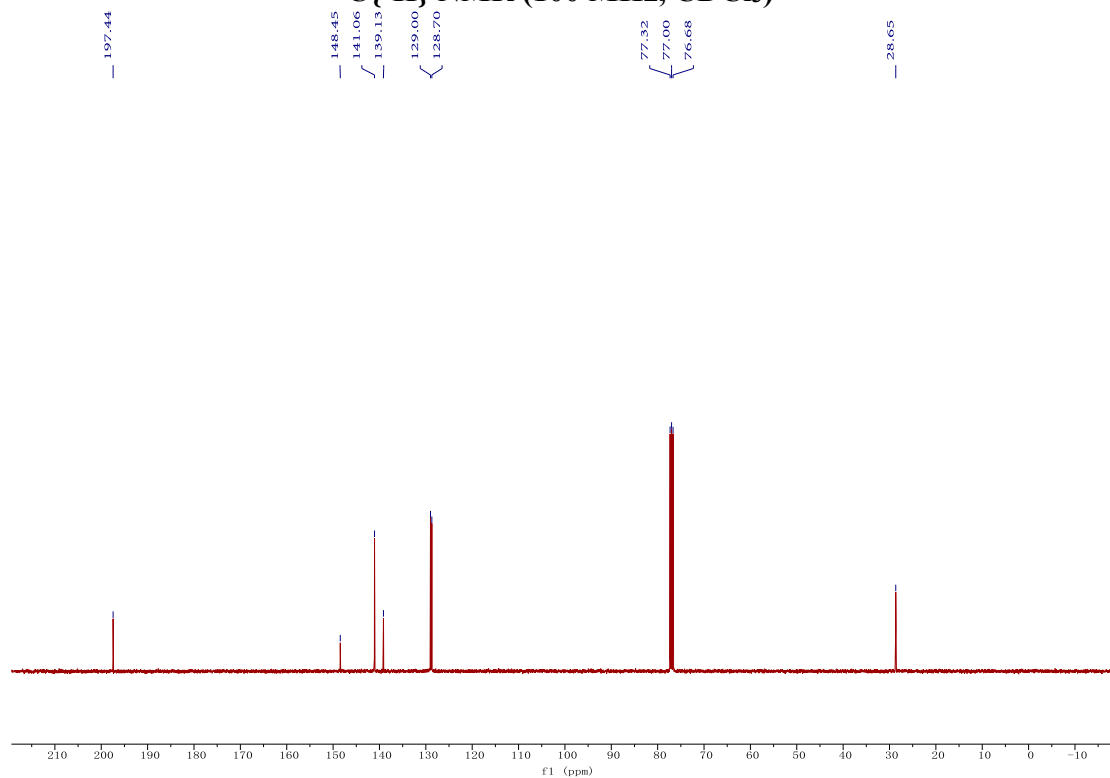
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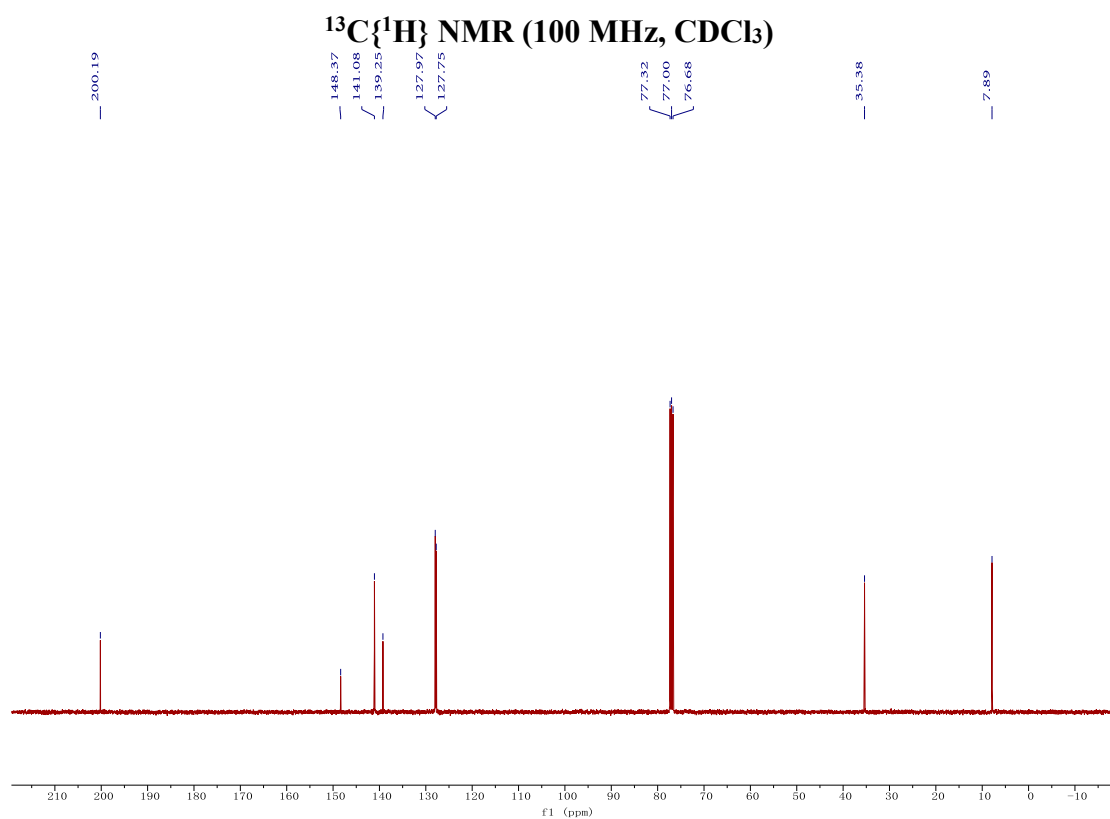
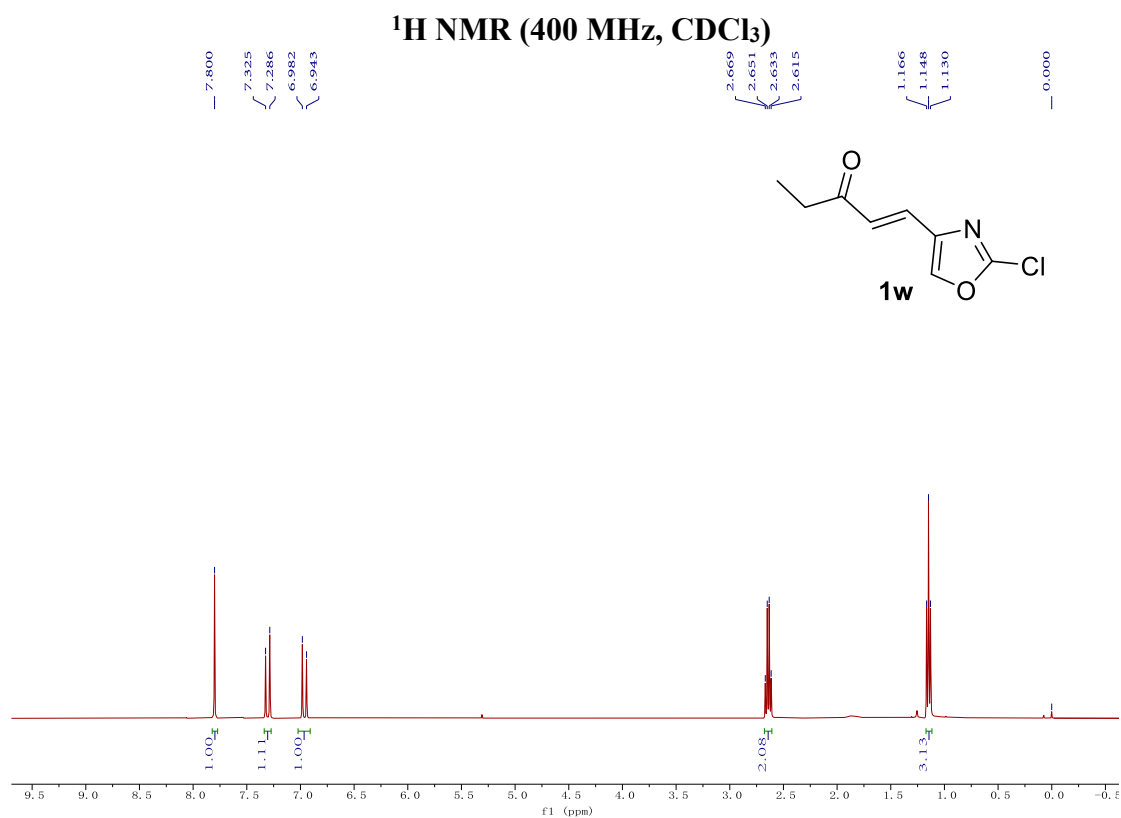


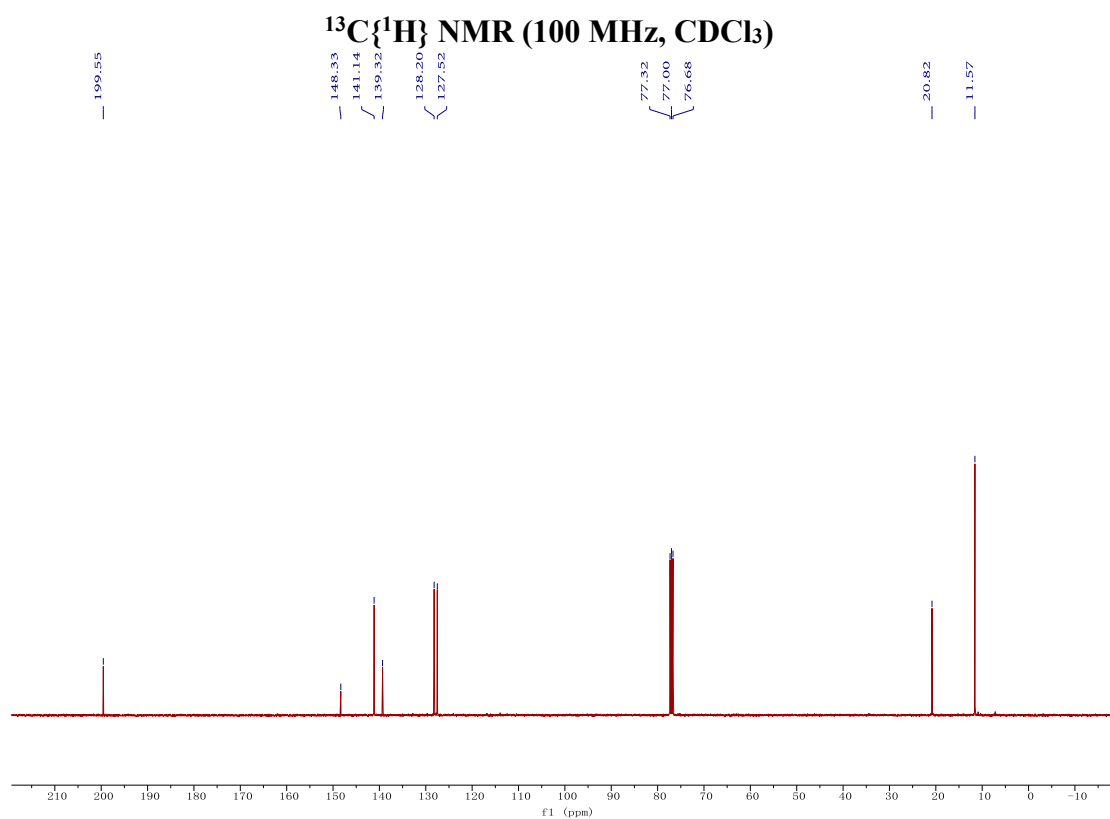
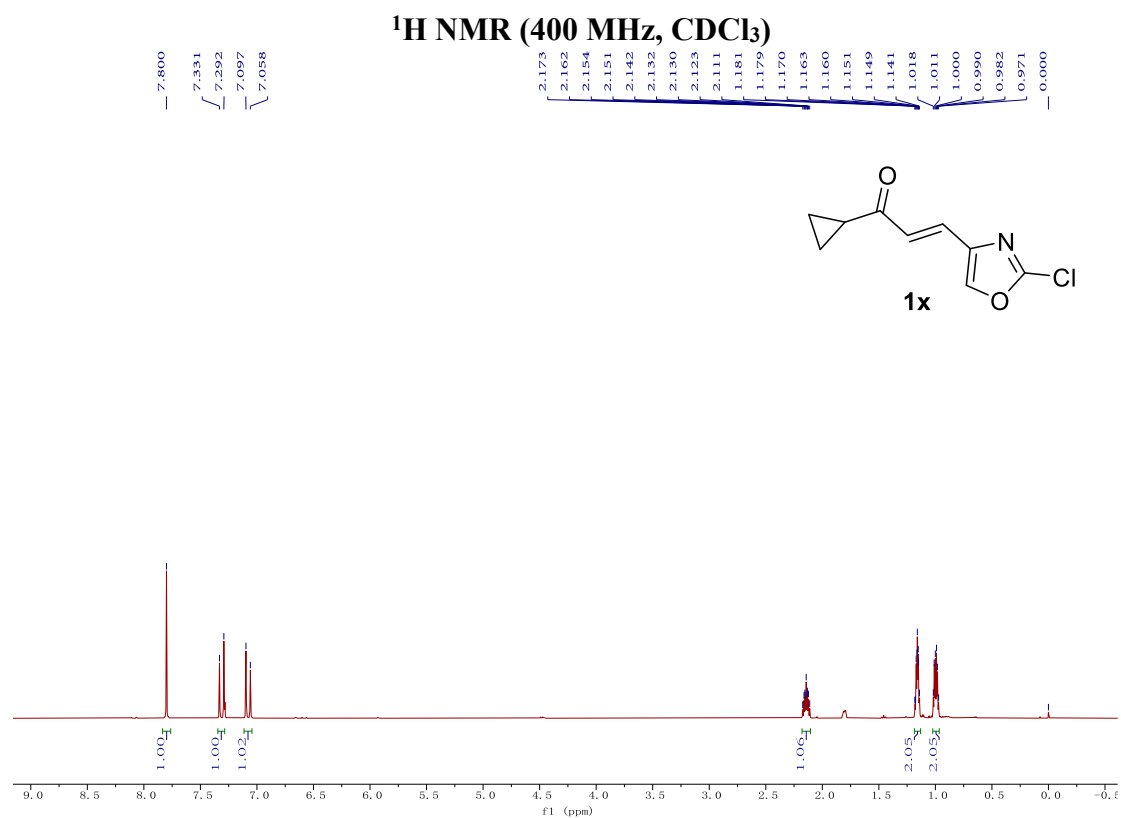
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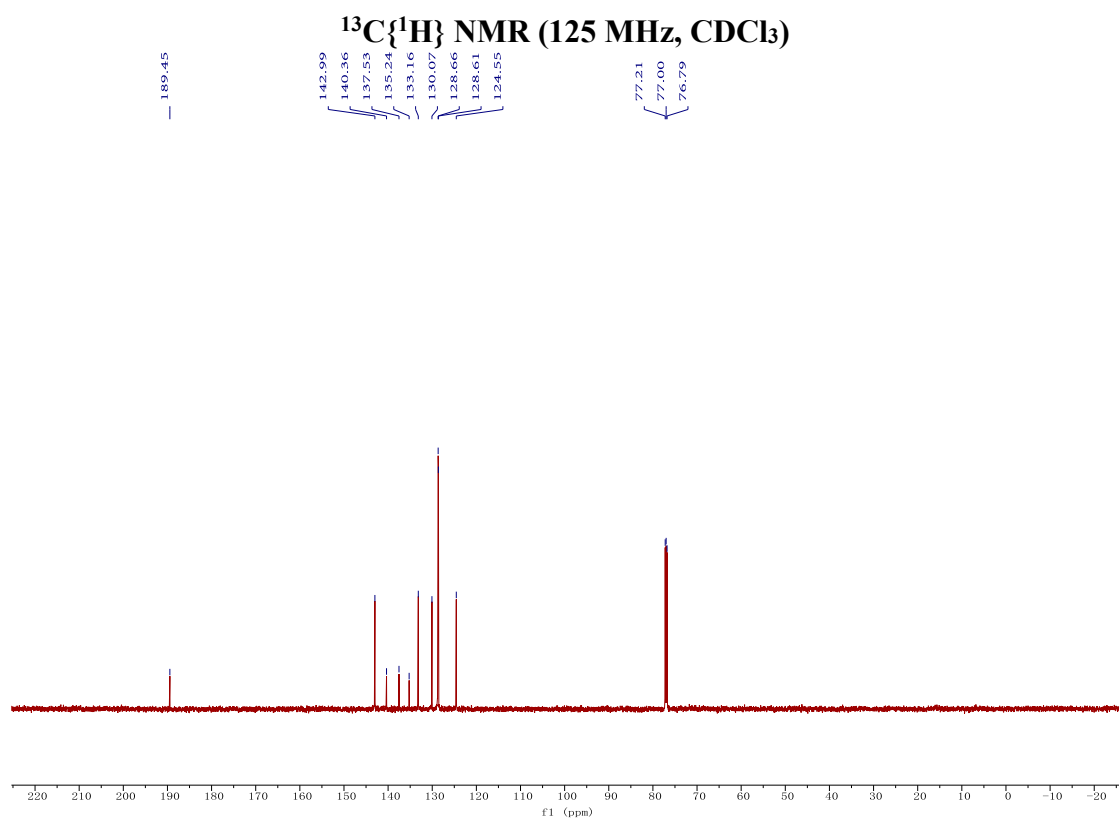
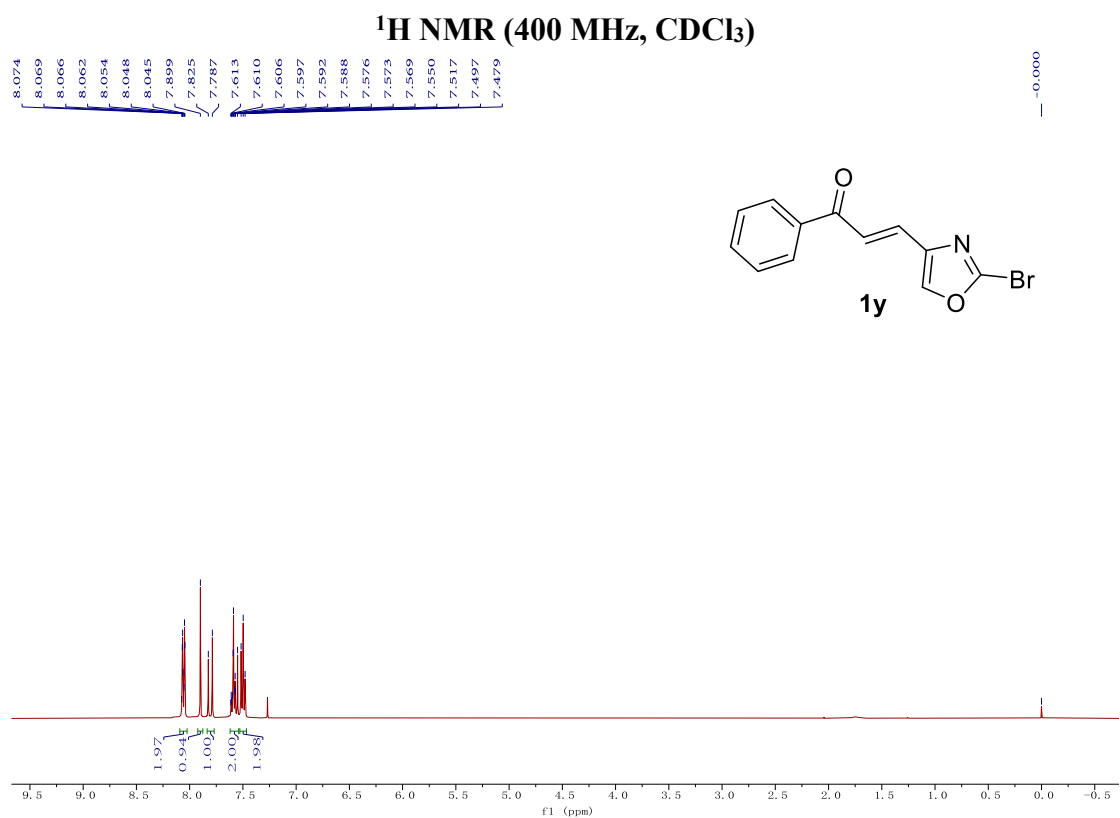


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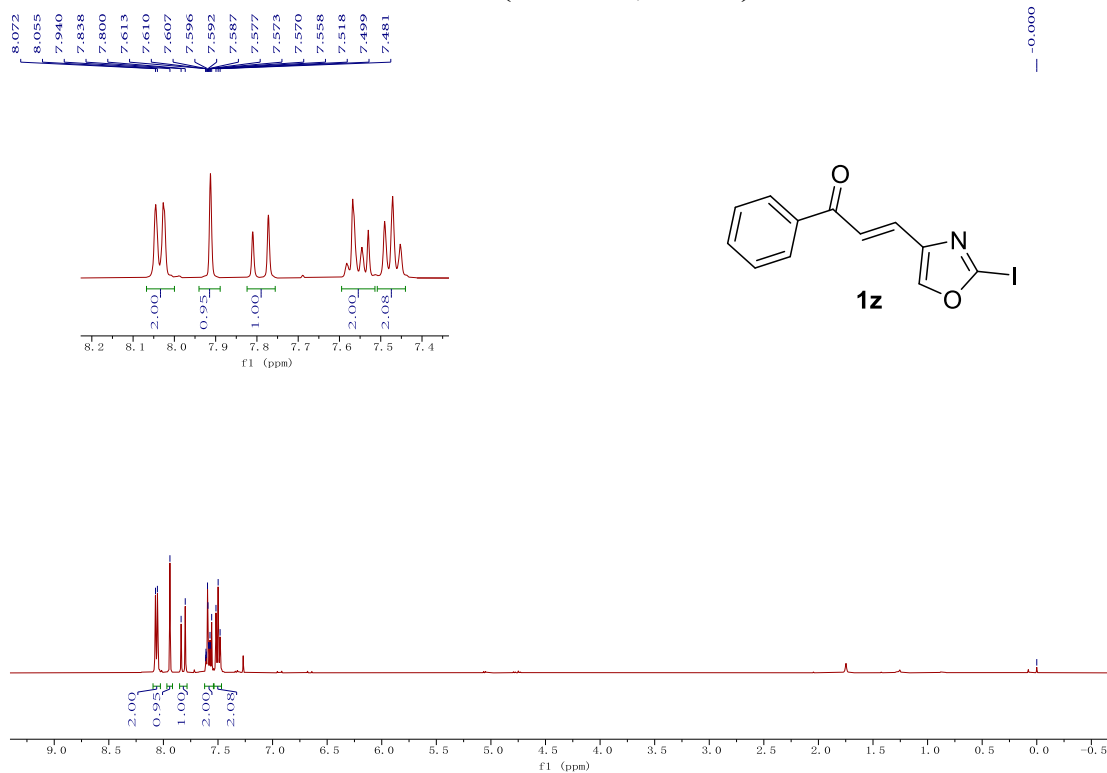




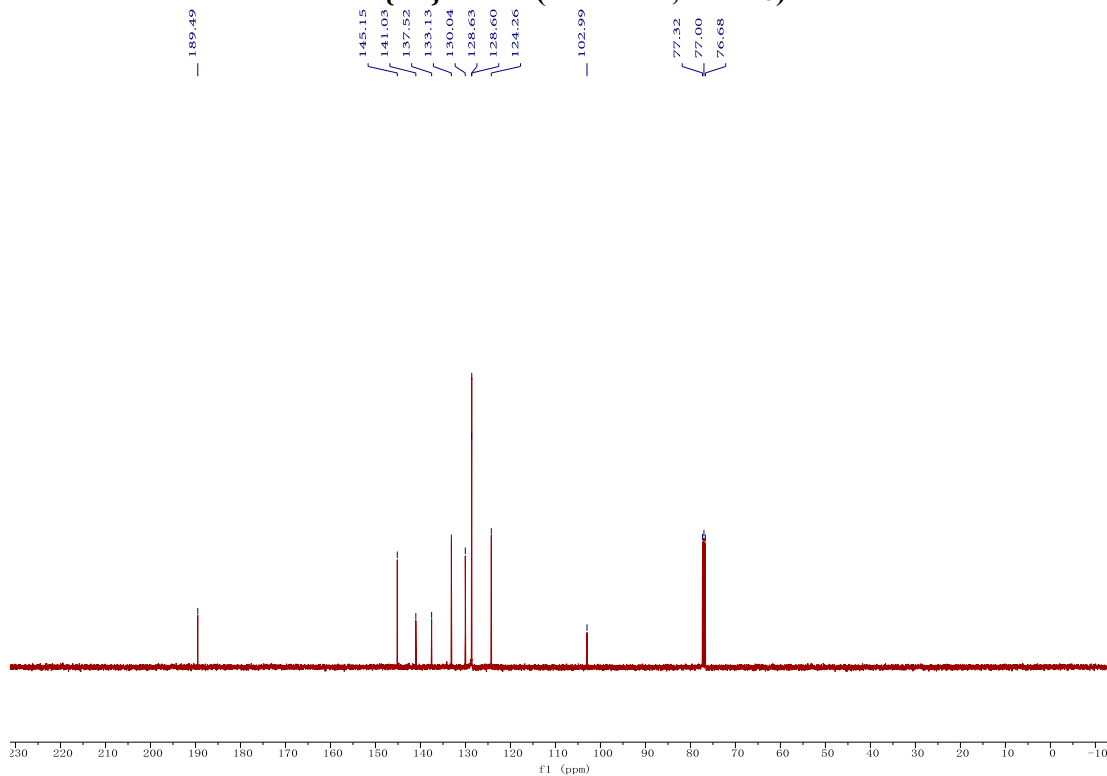




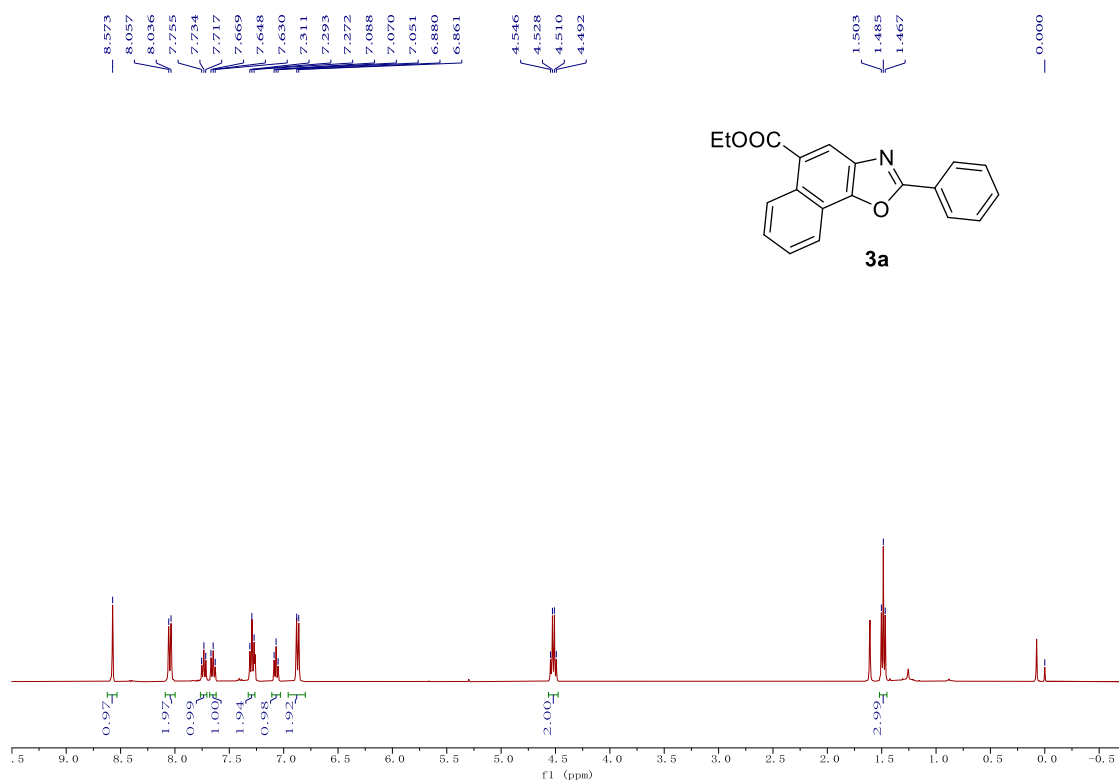
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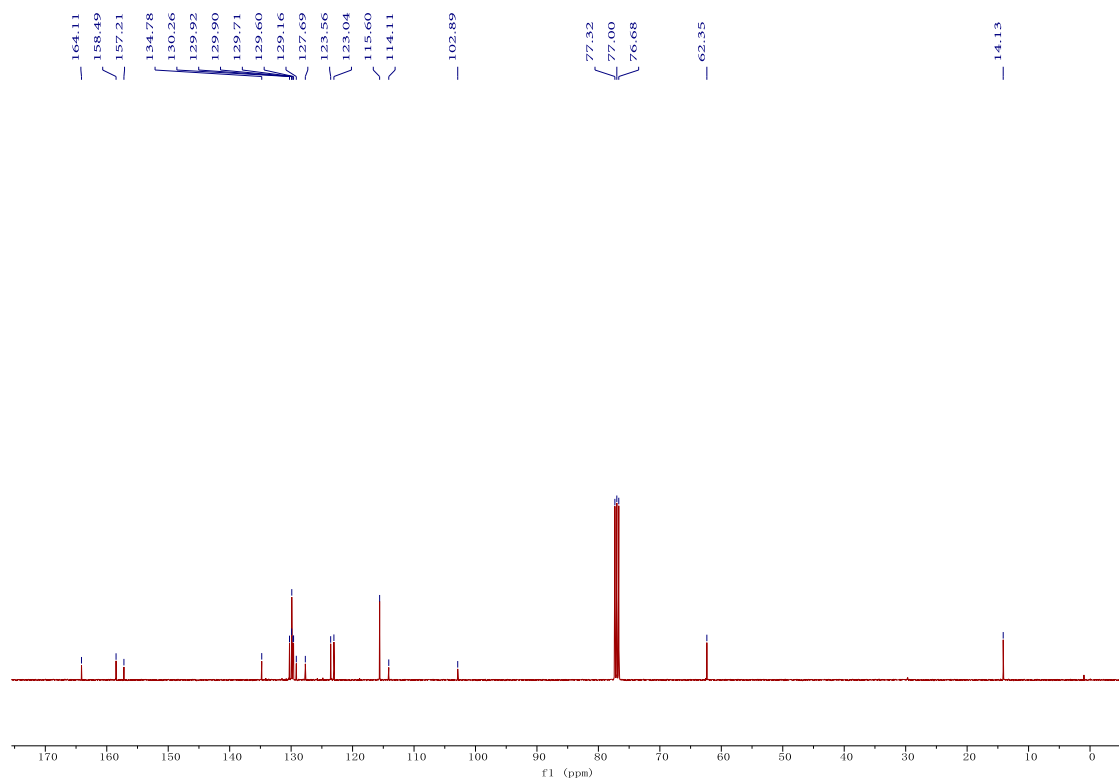
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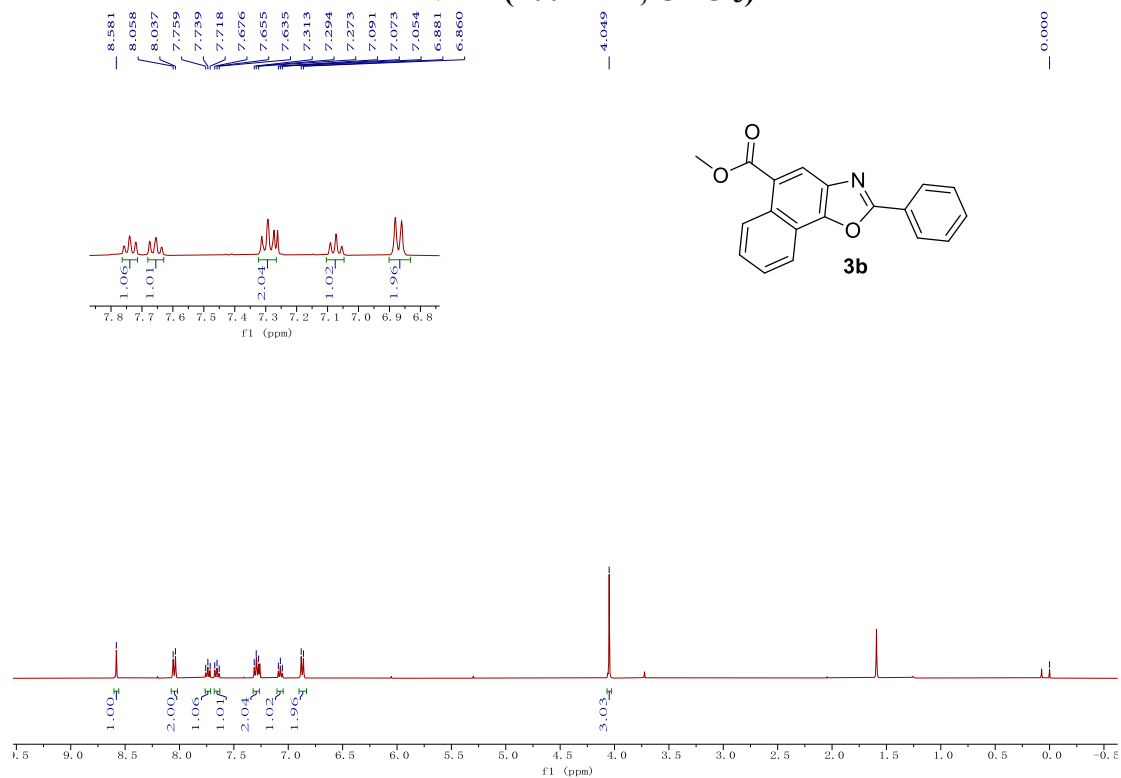
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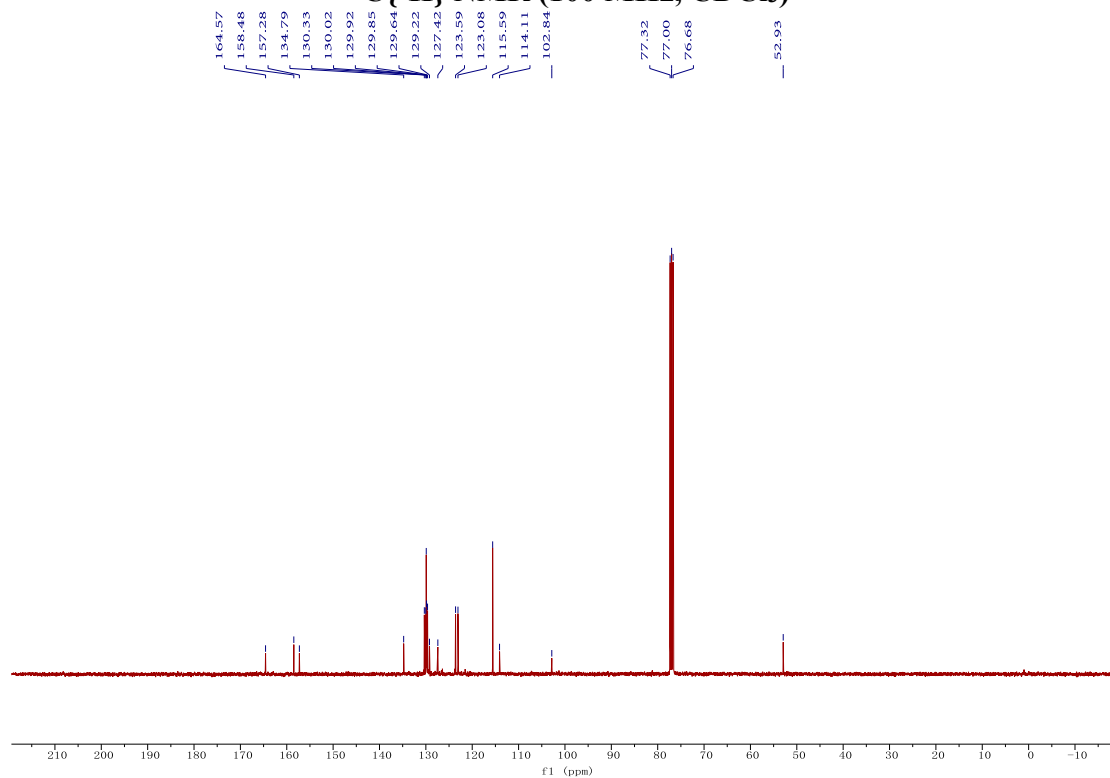
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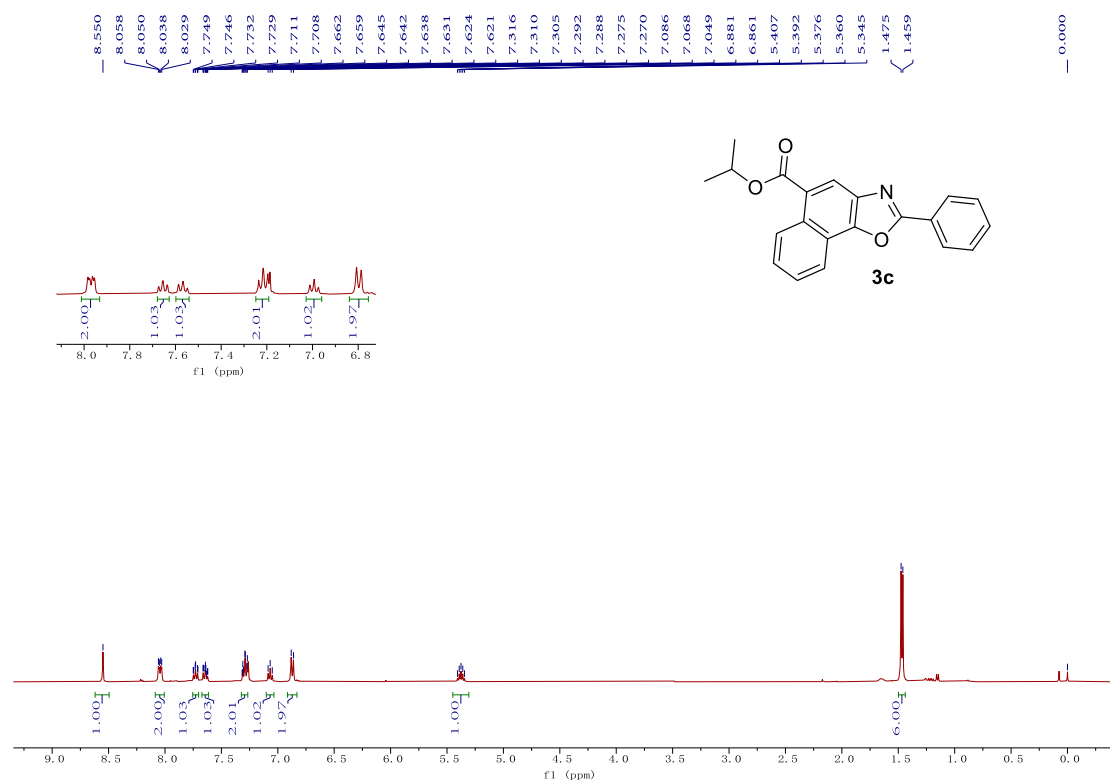
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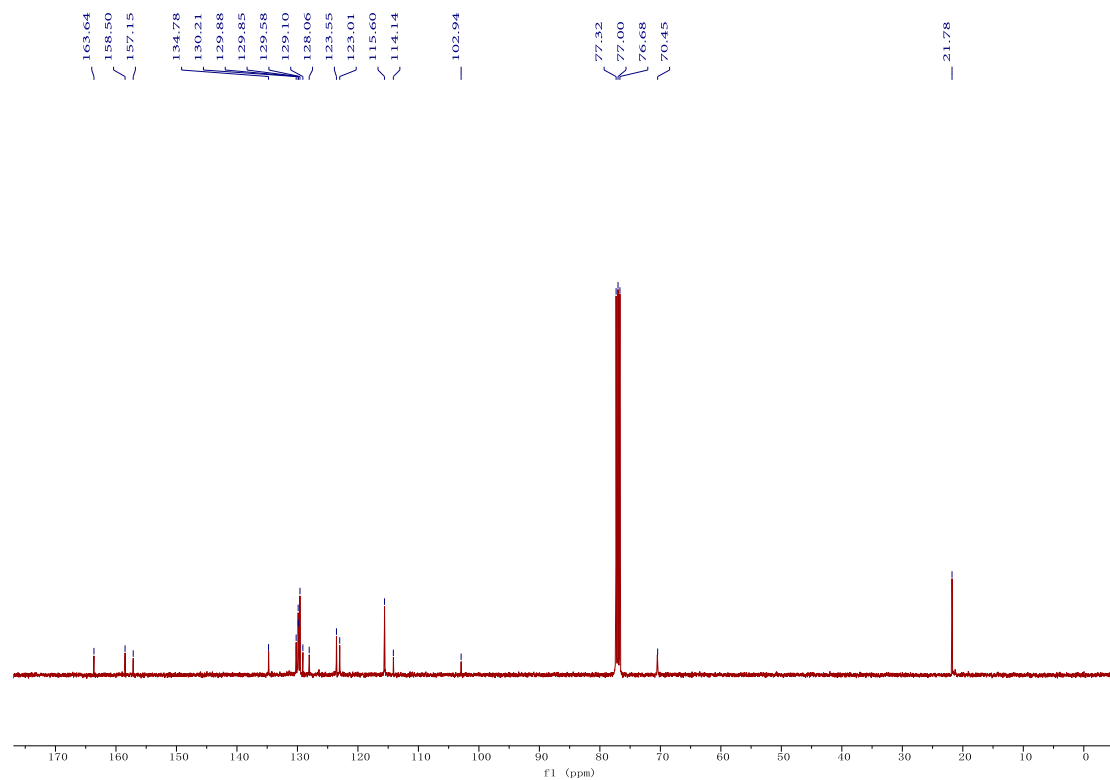
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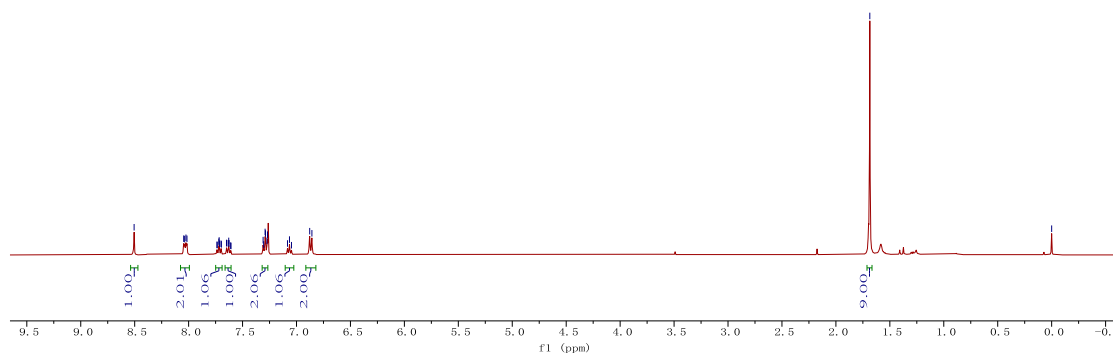
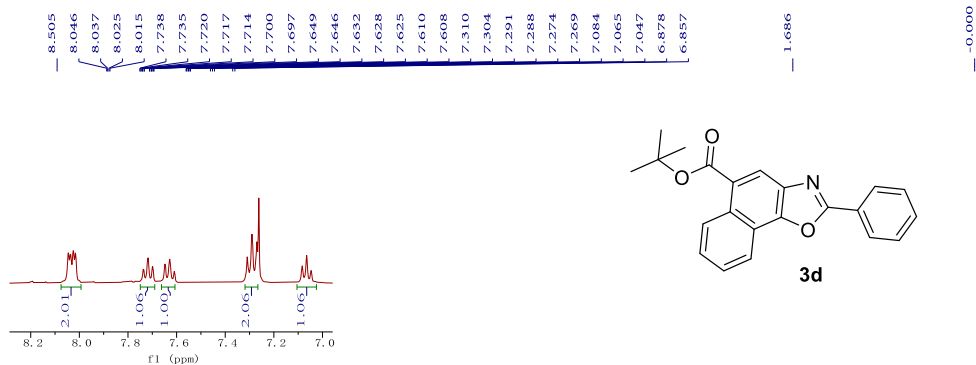
^1H NMR (400 MHz, CDCl_3)



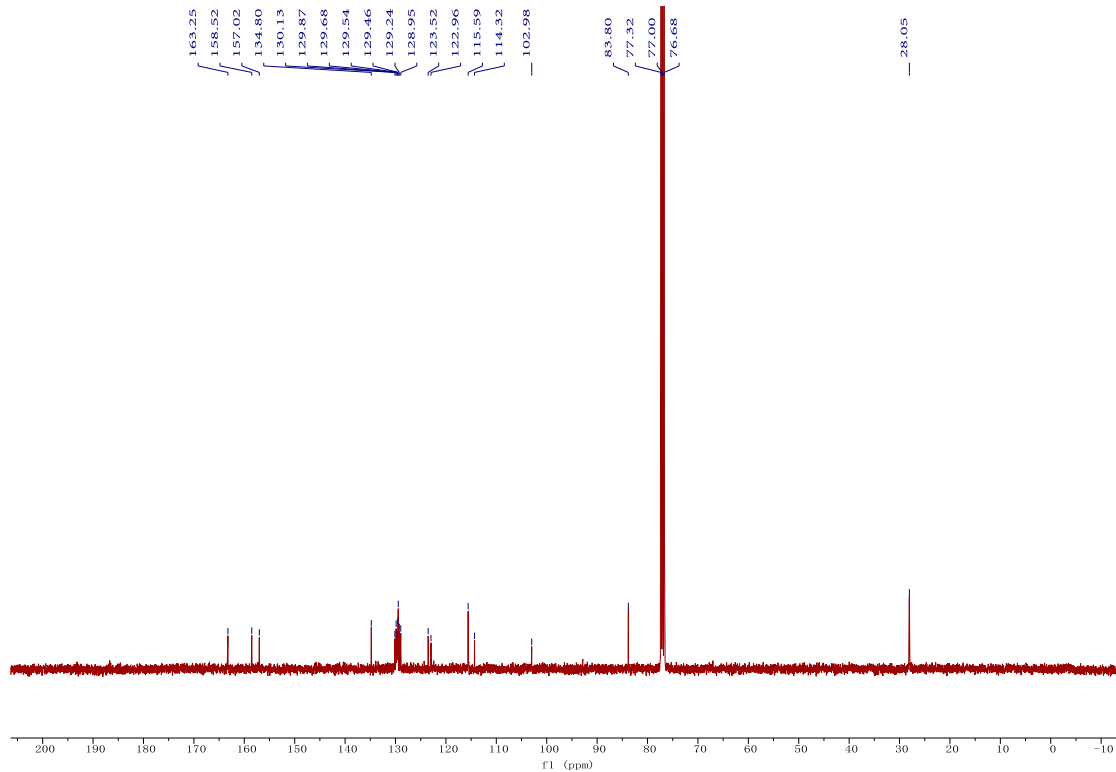
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



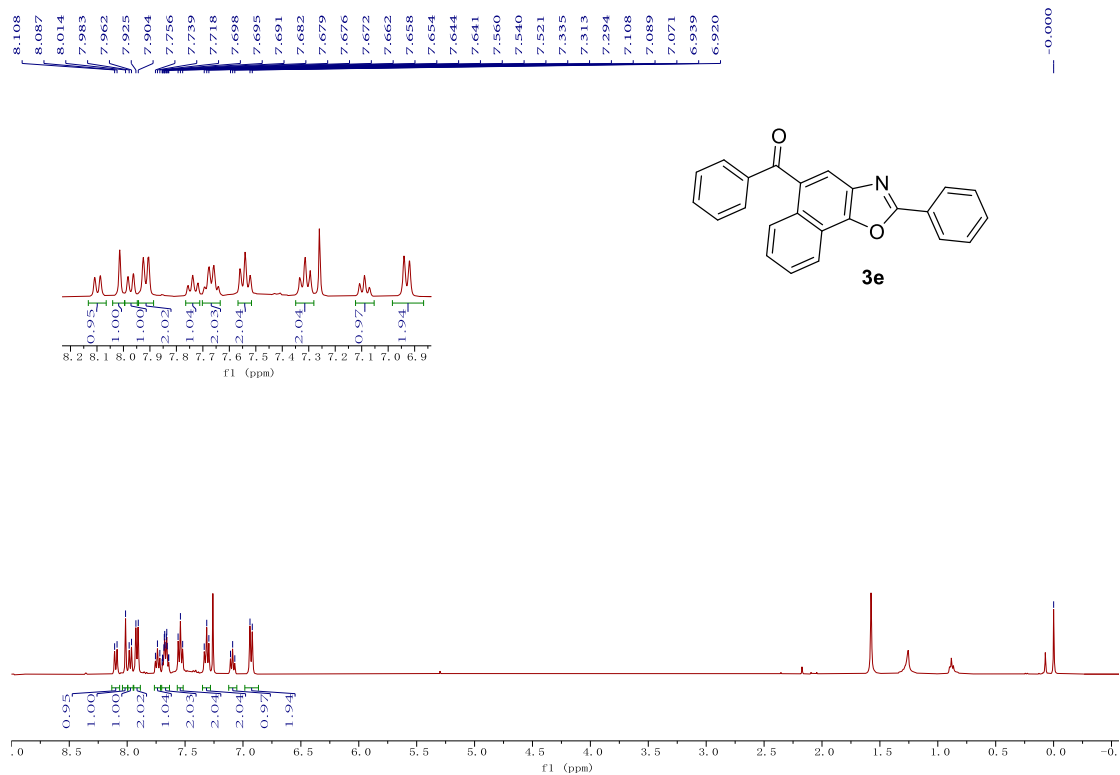
¹H NMR (400 MHz, CDCl₃)



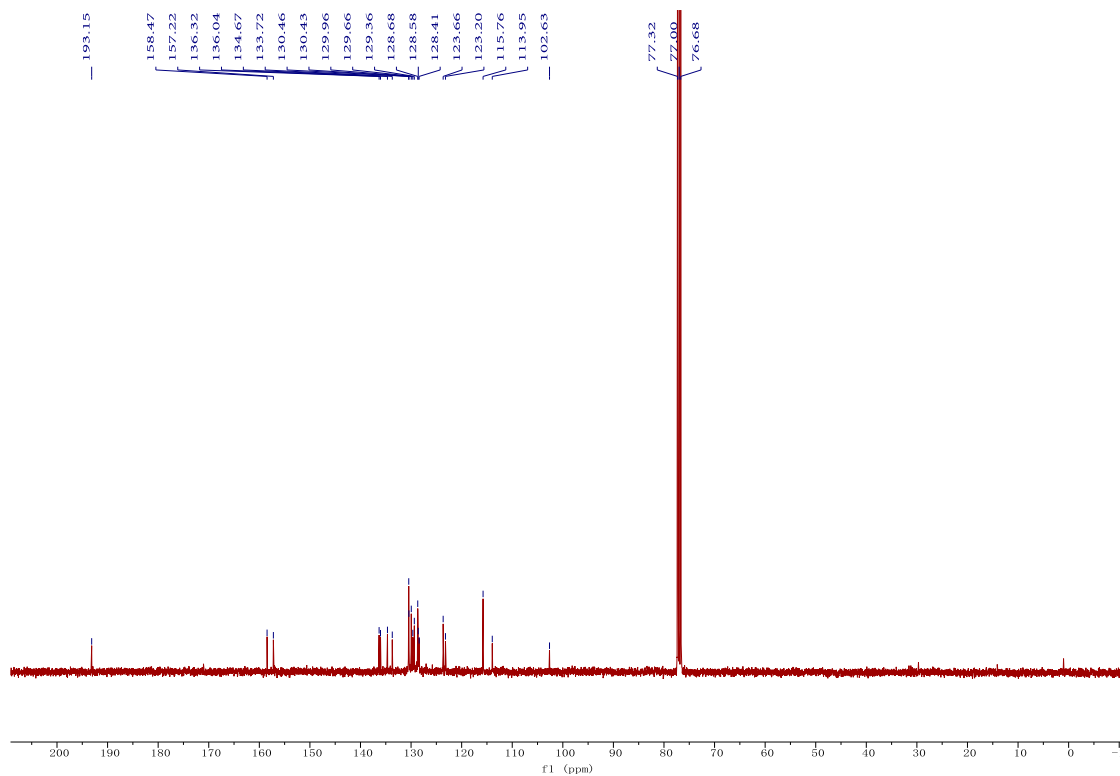
¹³C{¹H} NMR (100 MHz, CDCl₃)



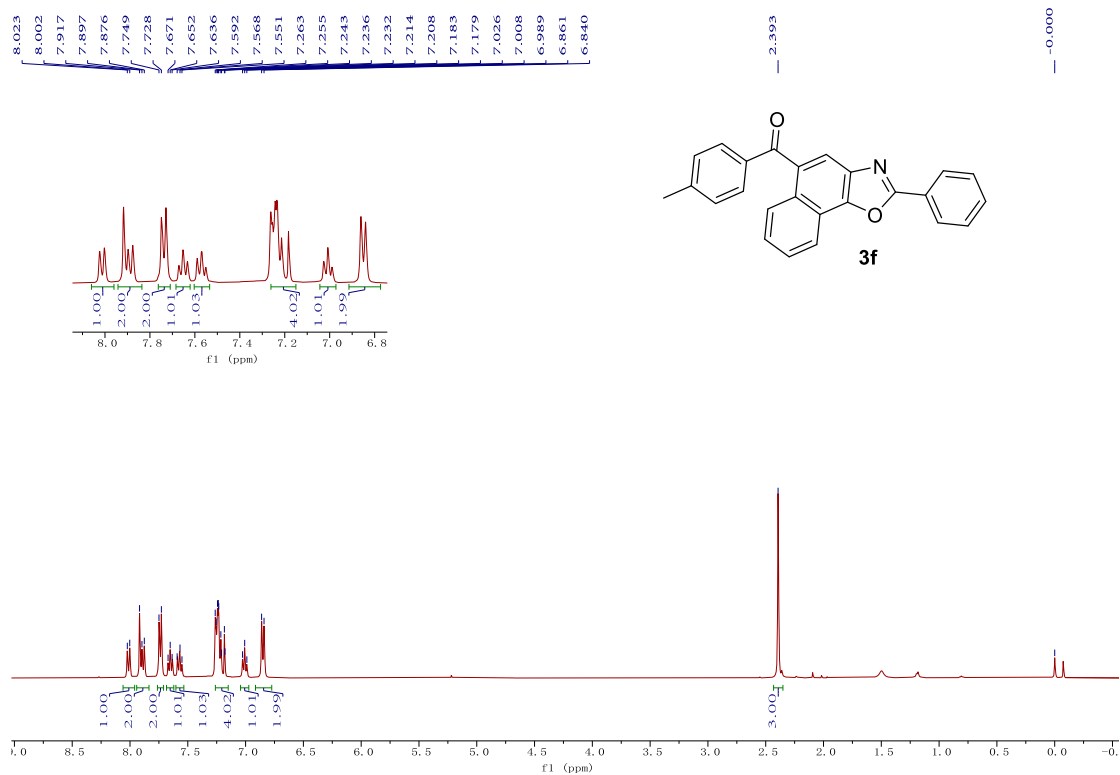
^1H NMR (400 MHz, CDCl_3)



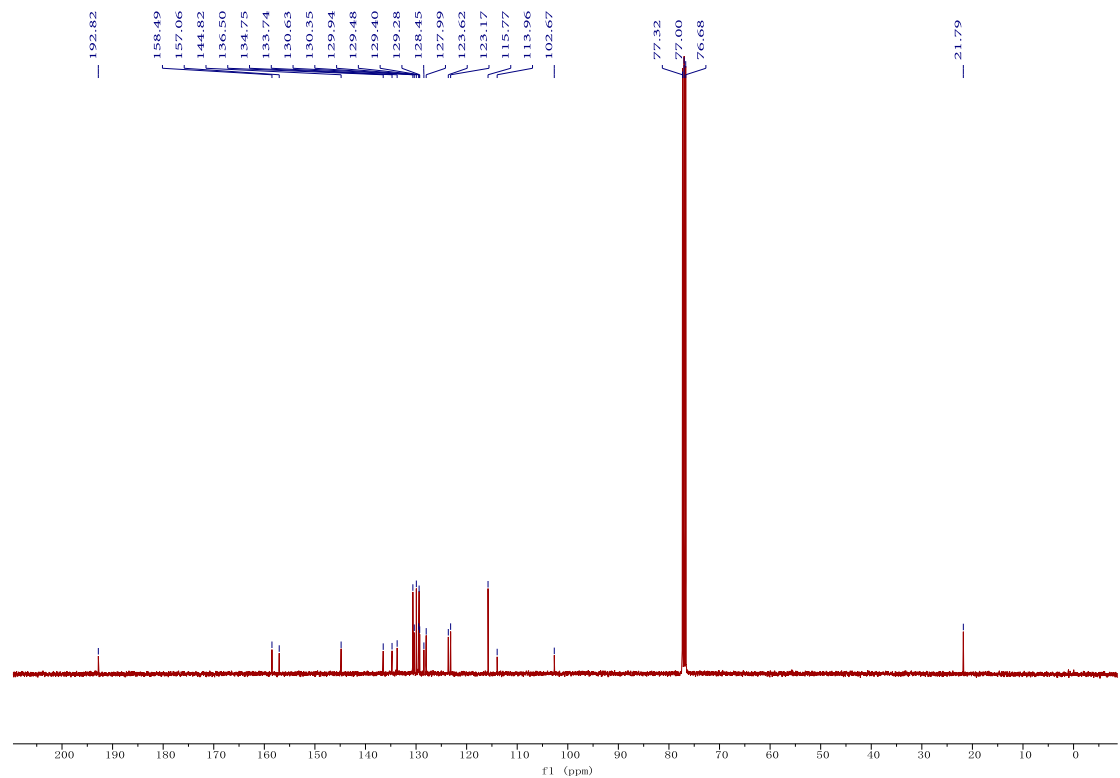
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

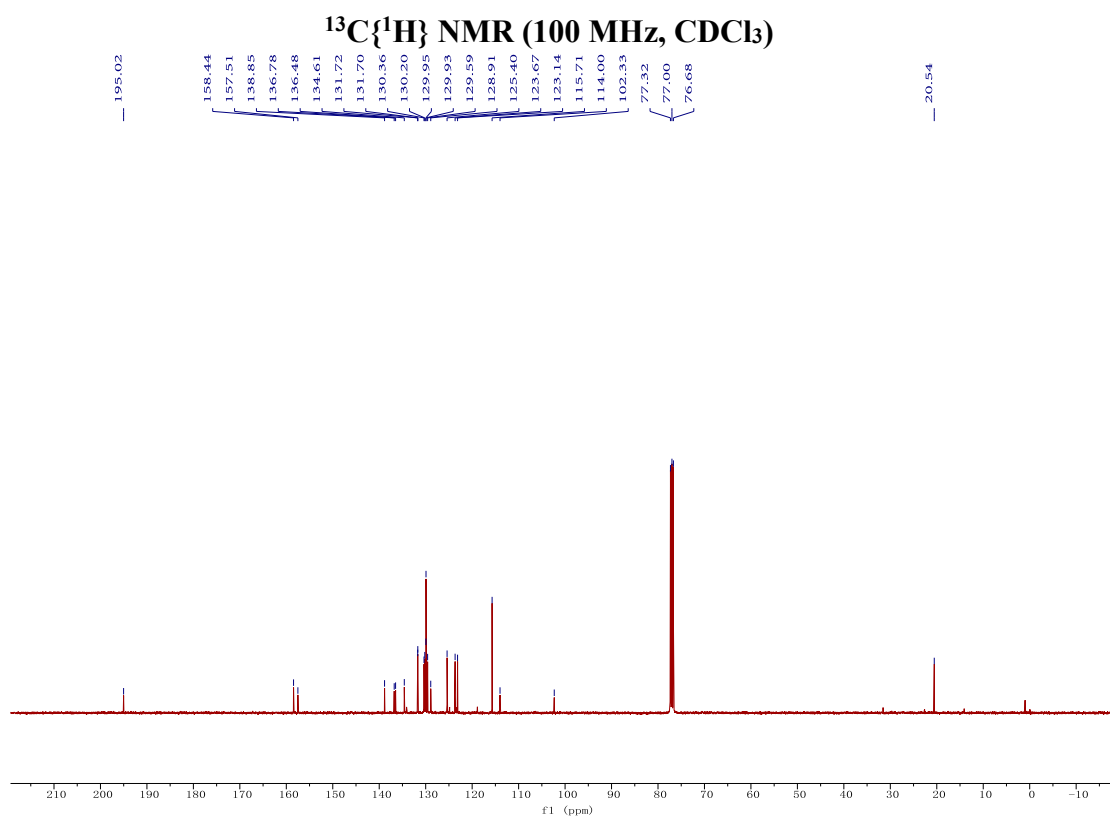
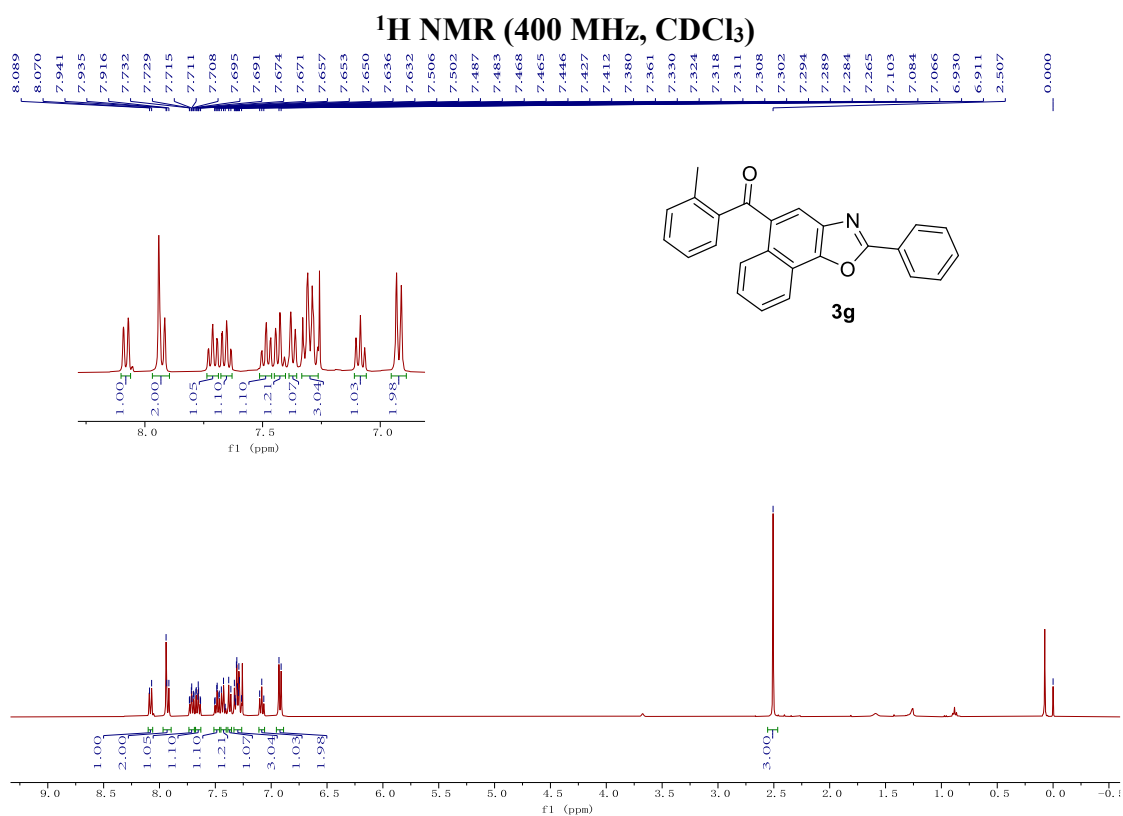


¹H NMR (400 MHz, CDCl₃)

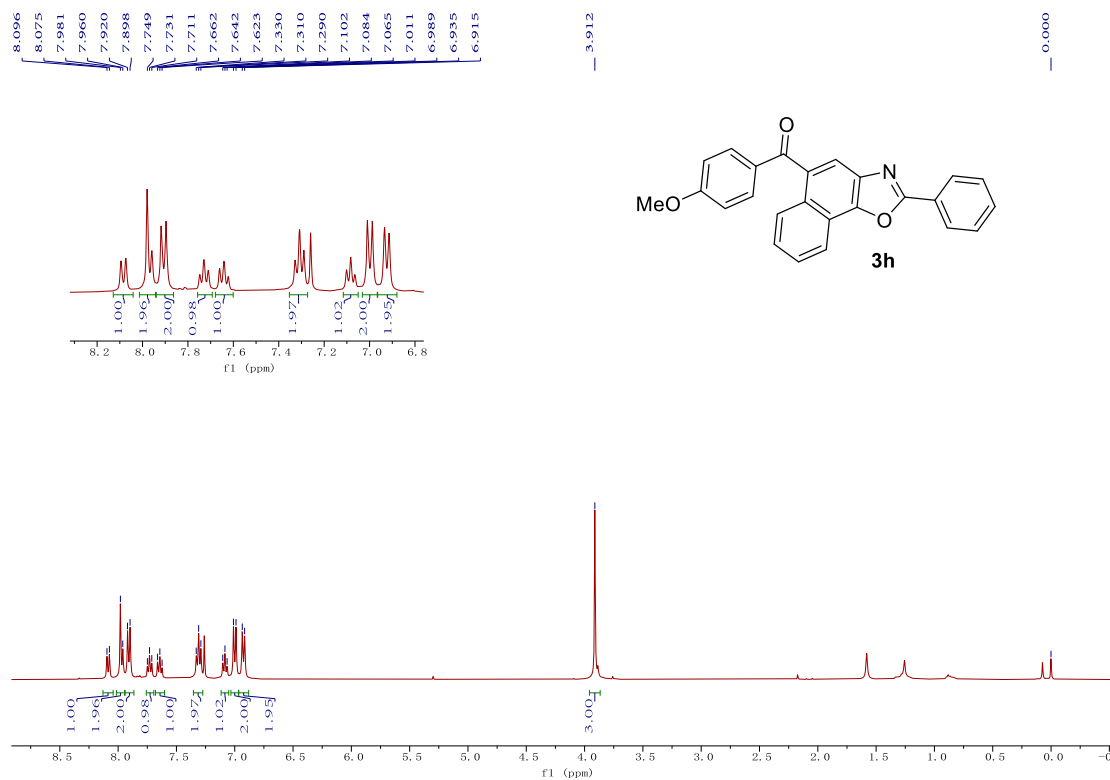


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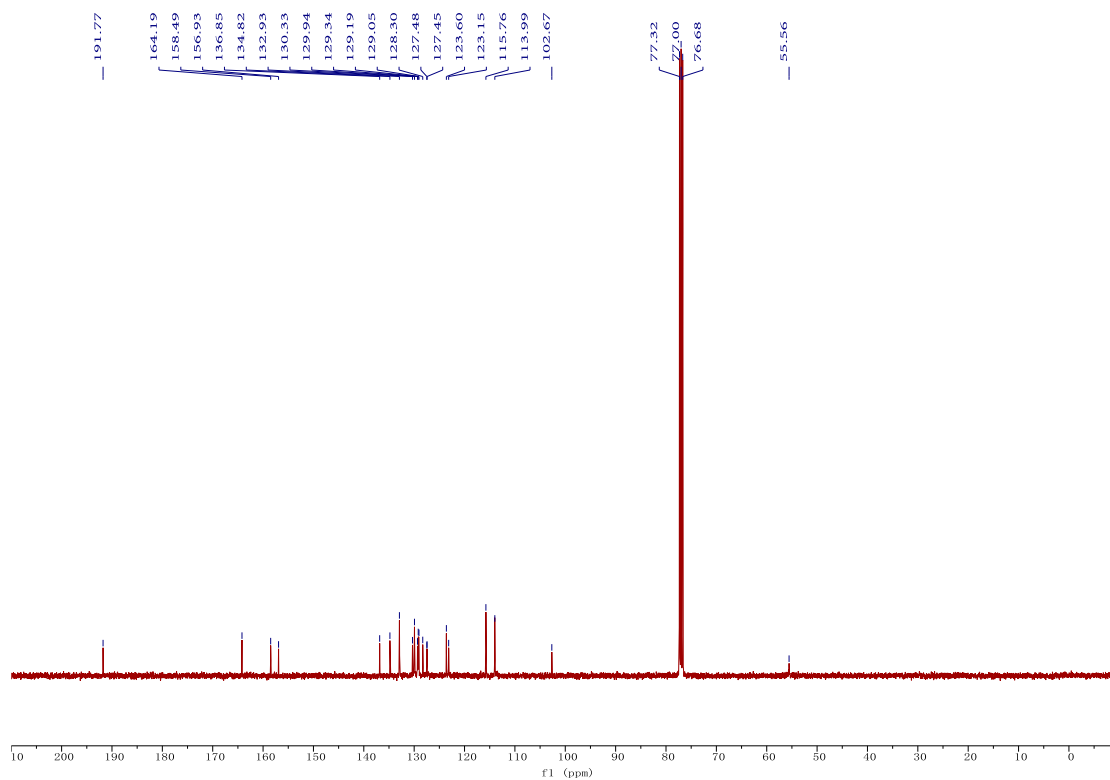




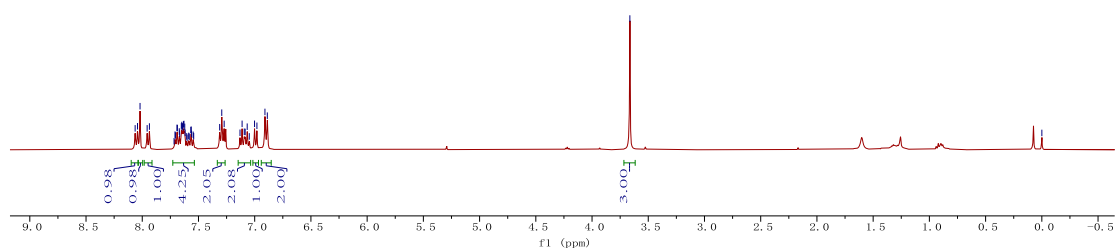
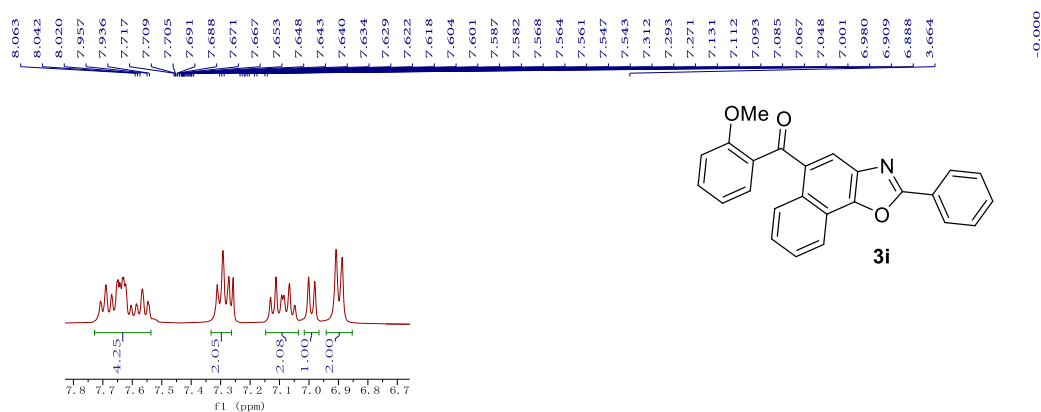
^1H NMR (400 MHz, CDCl_3)



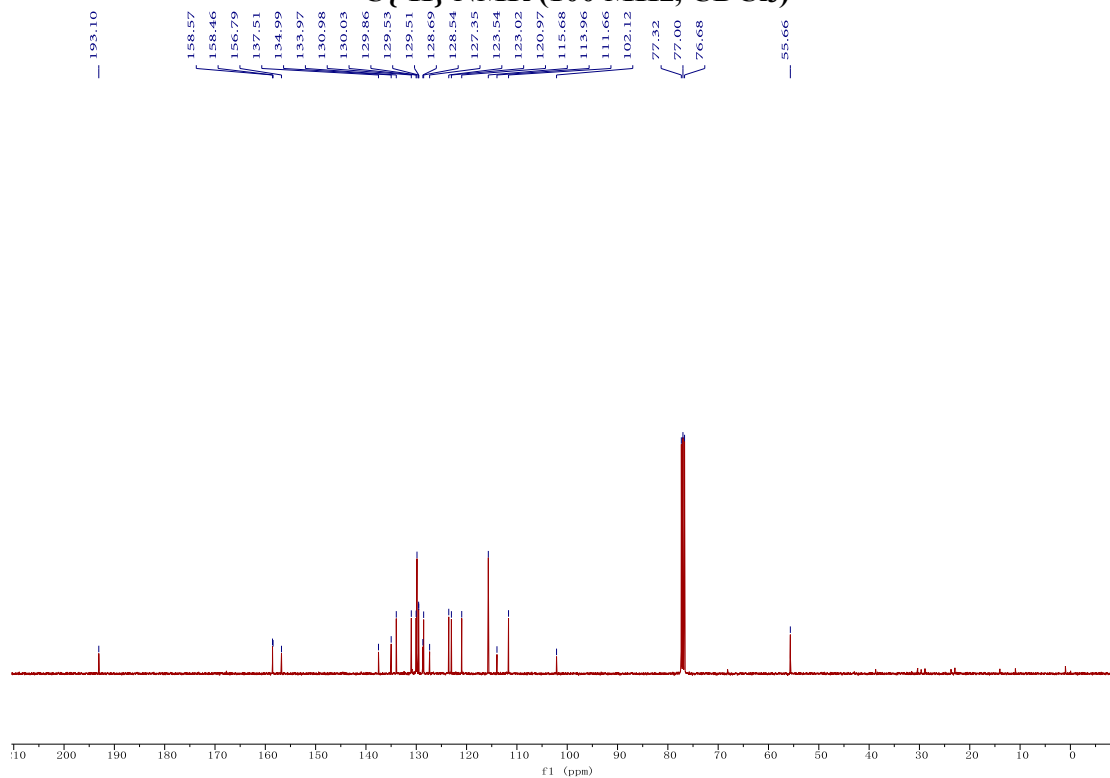
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

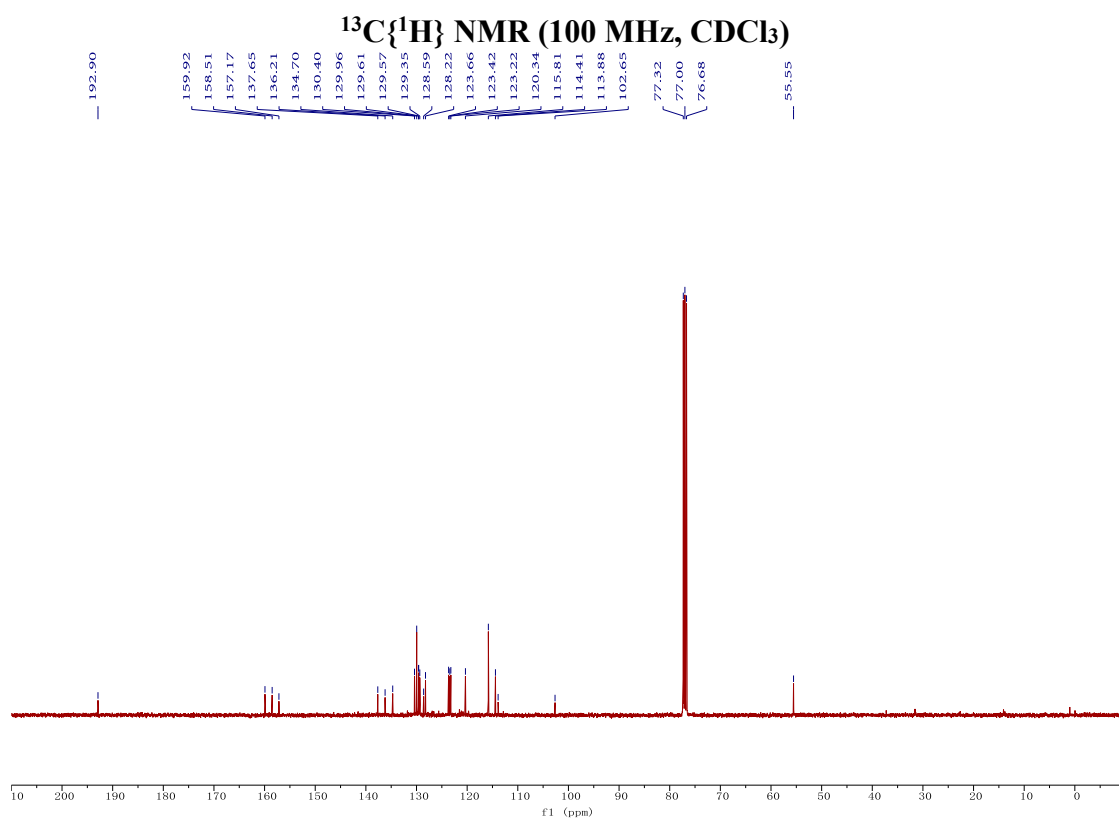
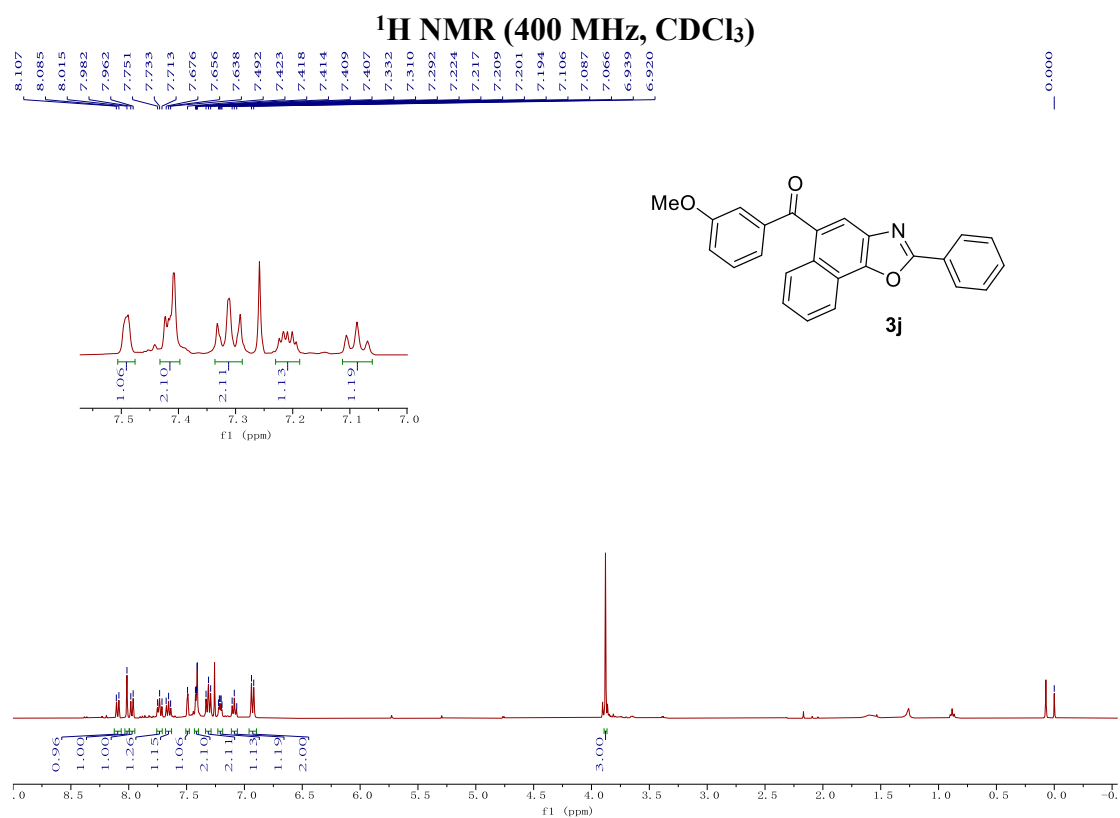


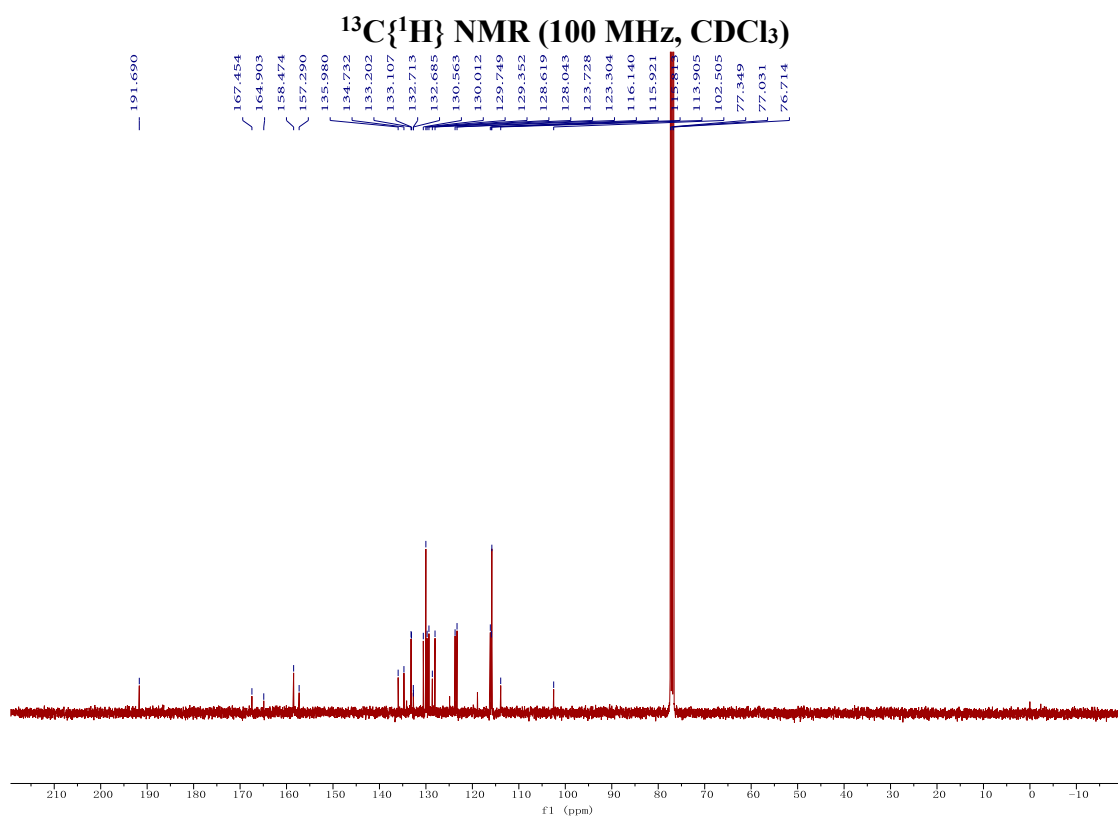
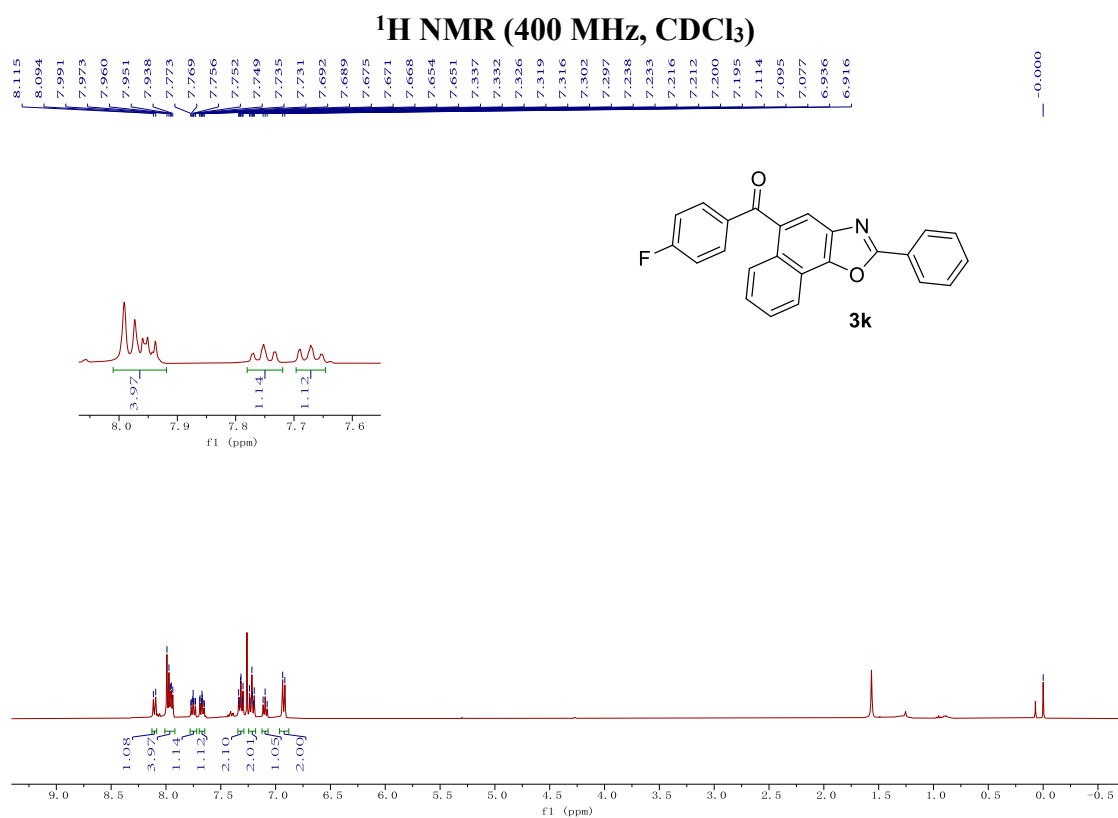
^1H NMR (400 MHz, CDCl_3)



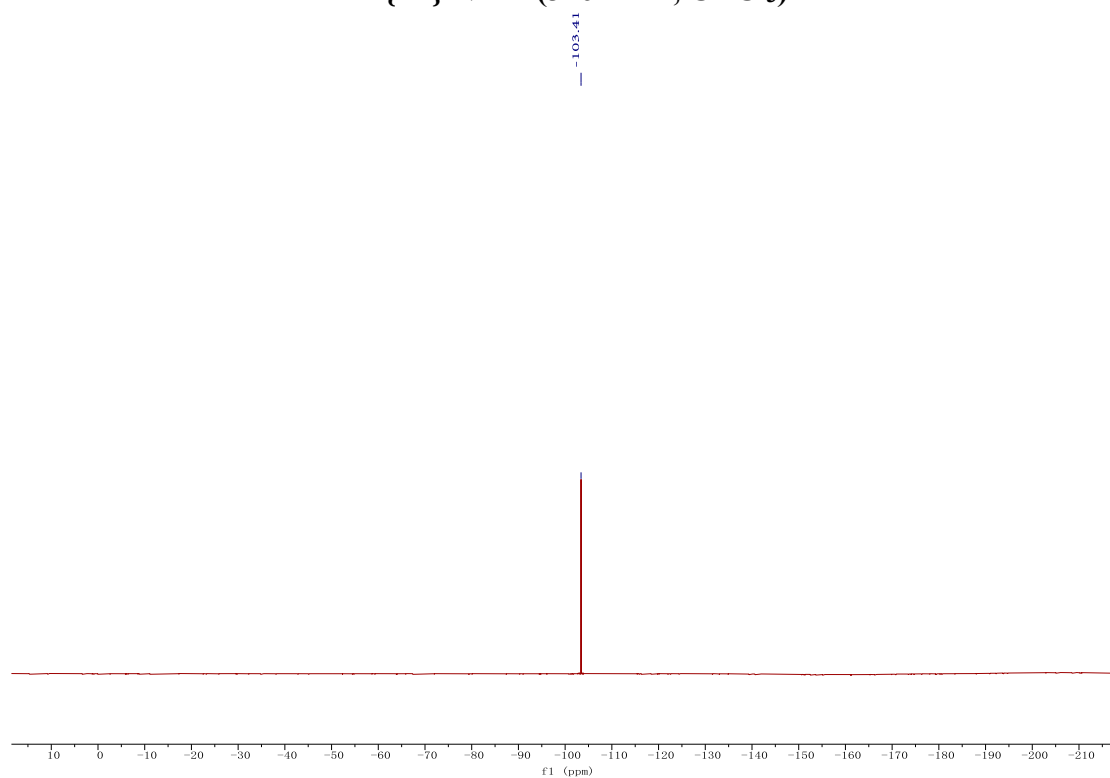
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

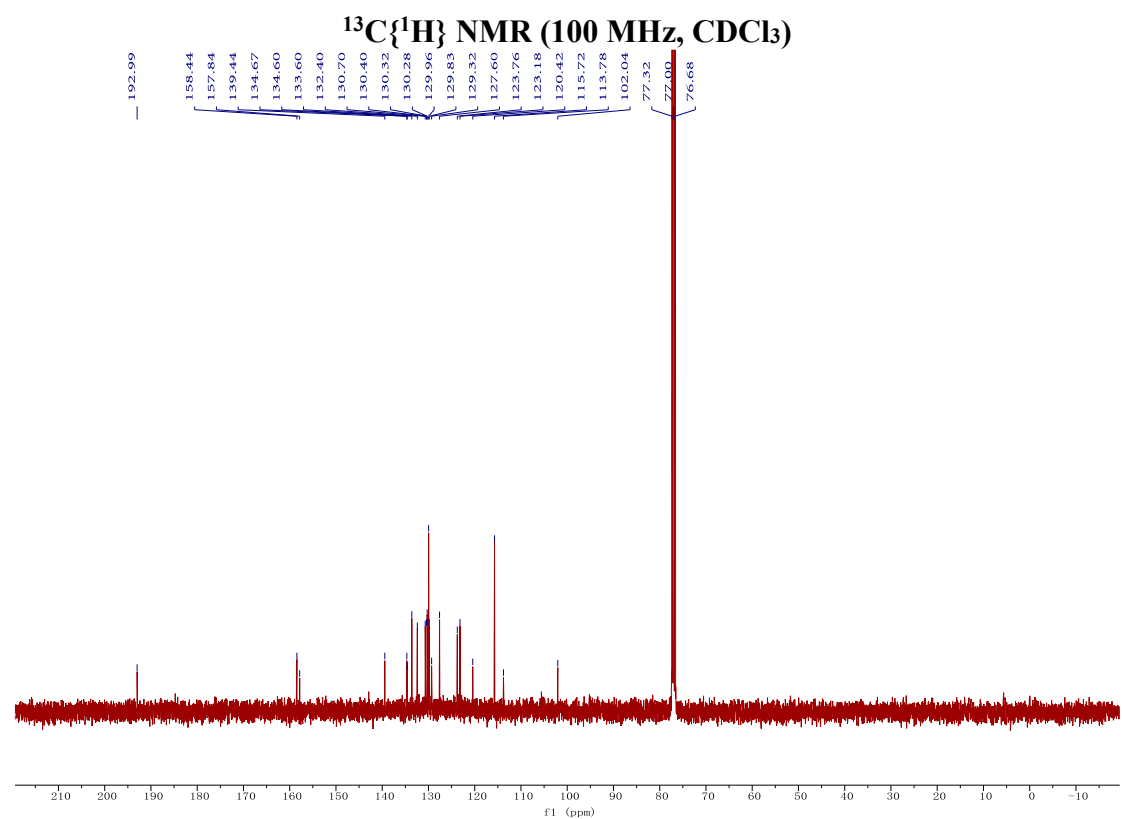
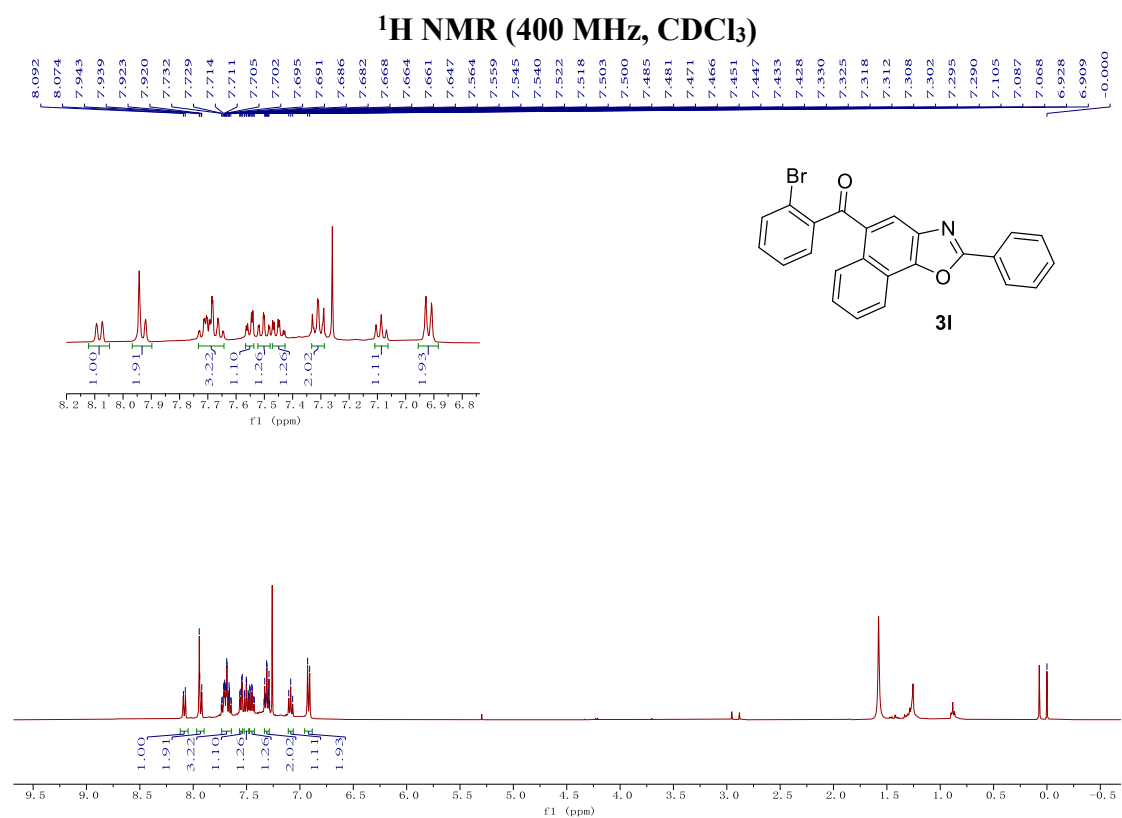




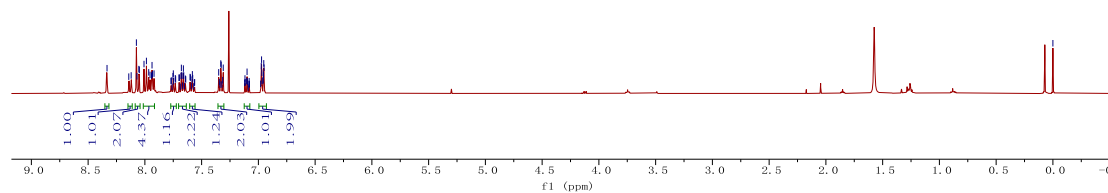
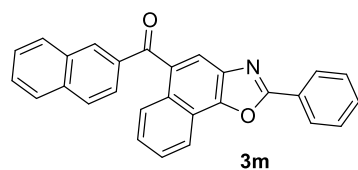


$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3)

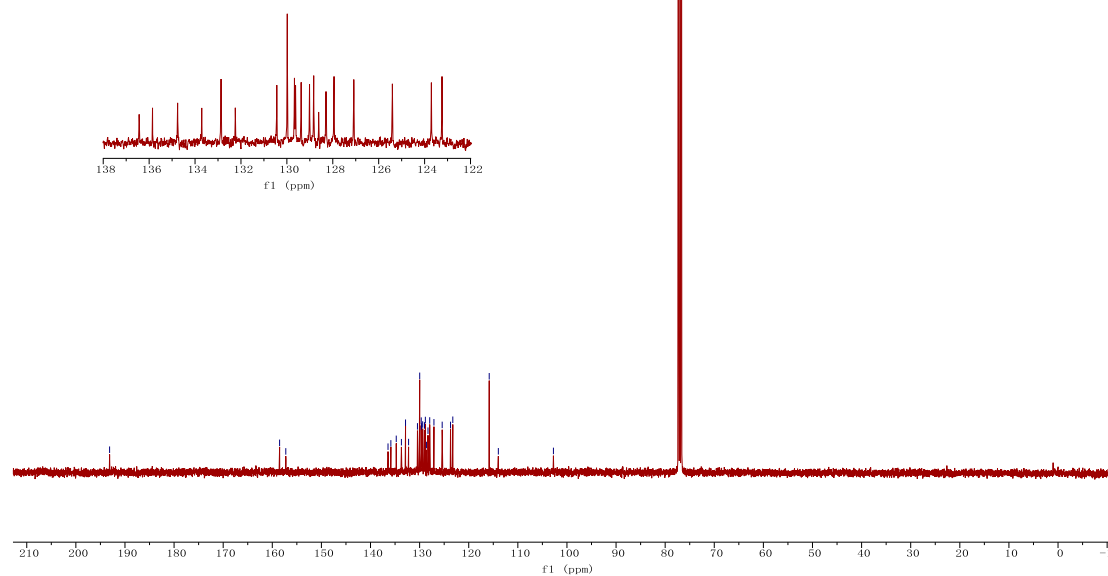




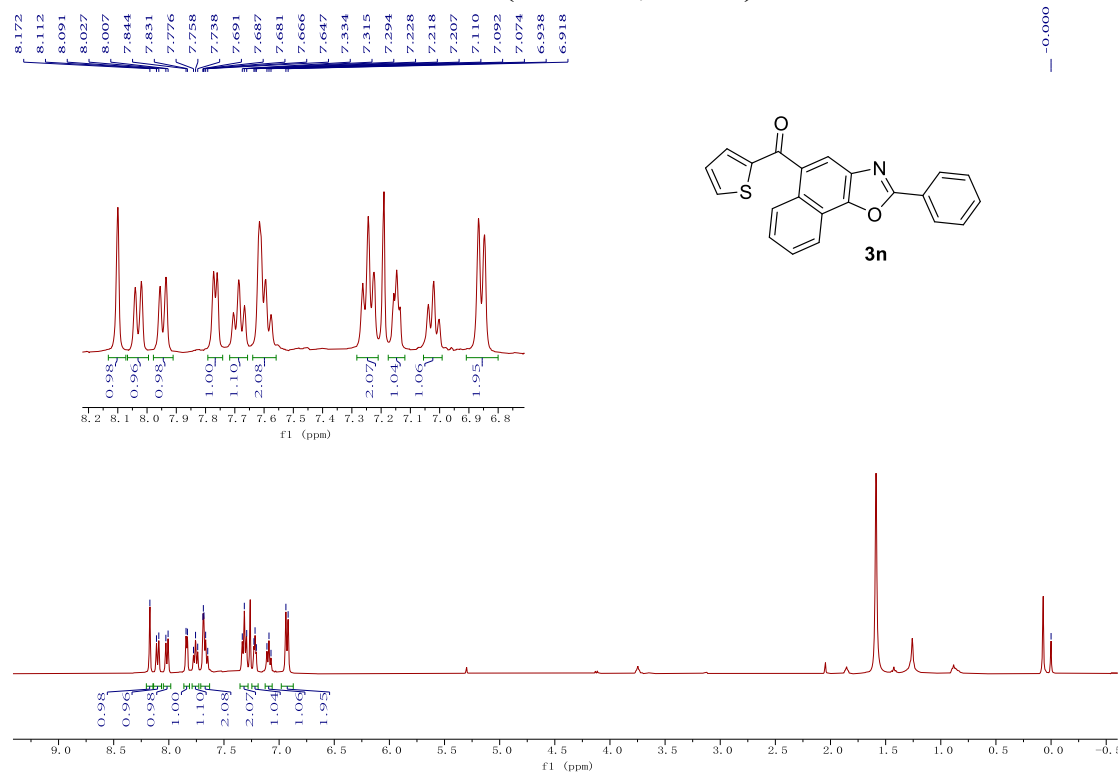
8.333	8.121	8.070	8.008	7.986	7.966	7.955	7.942	7.933	7.929	7.900	7.696	7.682	7.679	7.675	7.666	7.661	7.643	7.640	7.602	7.599	7.585	7.582	7.578	7.550	7.331	7.328	7.314	7.309	7.118	7.100	6.975	6.972	6.970	6.958	6.955	6.953	6.950
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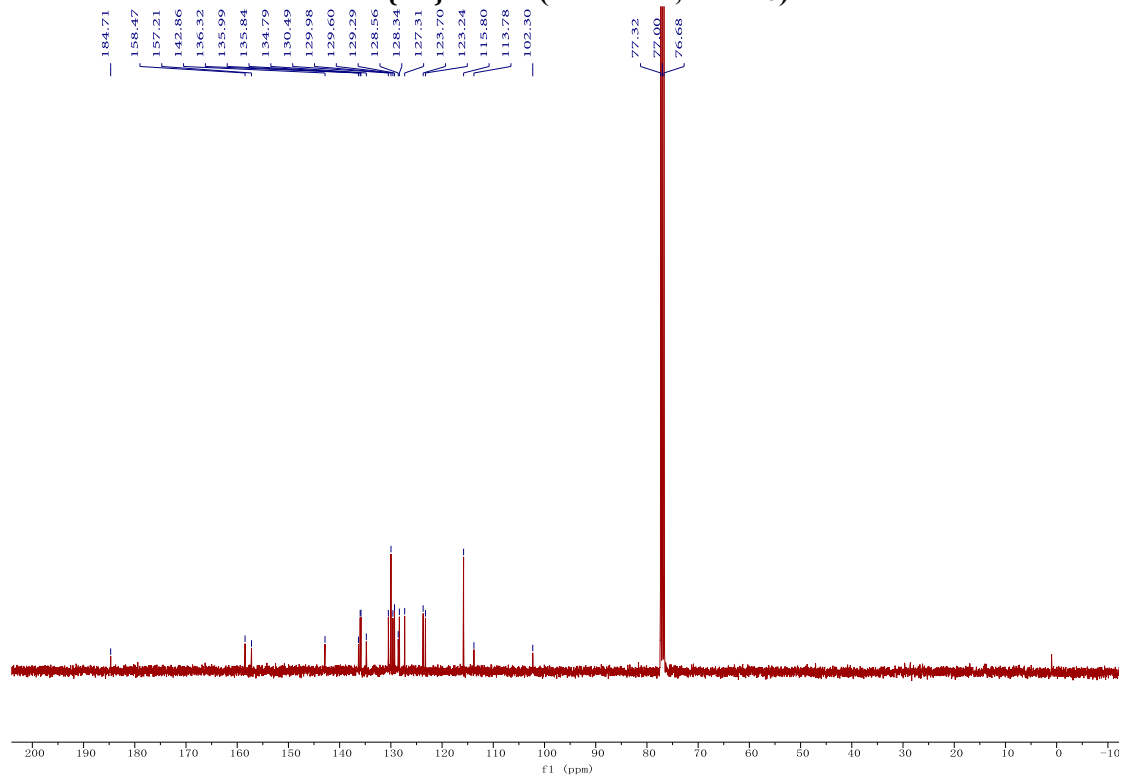
193.15



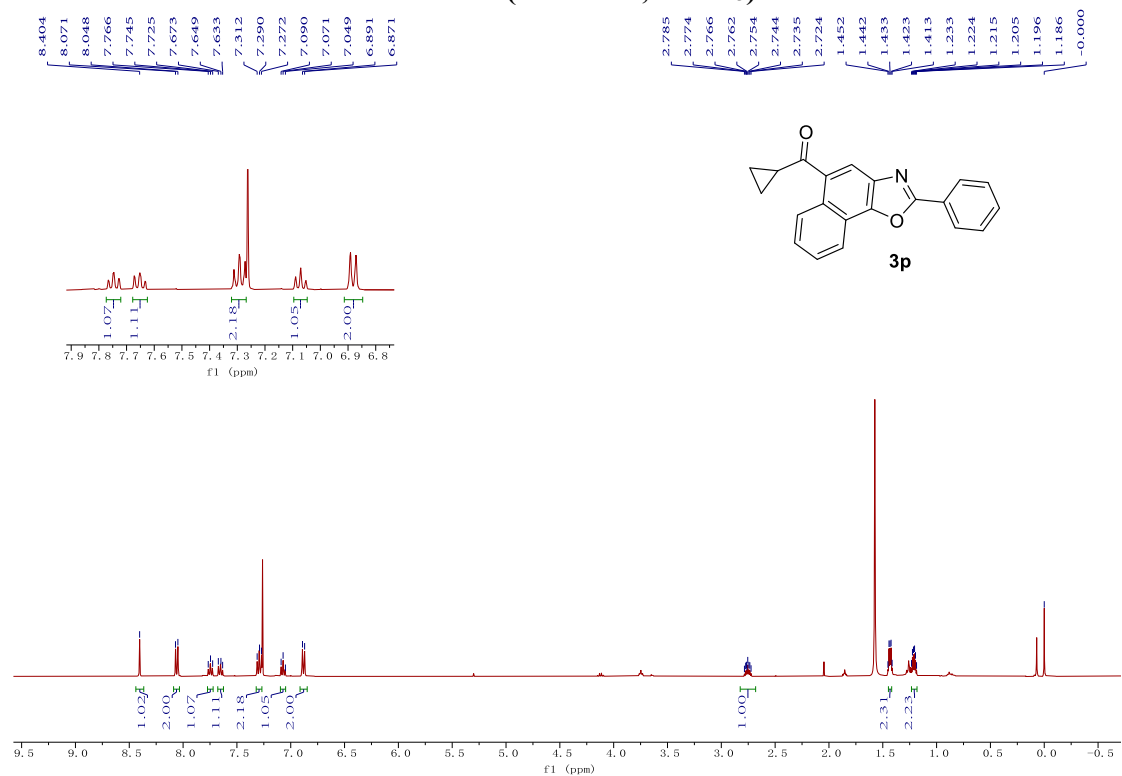
^1H NMR (400 MHz, CDCl_3)



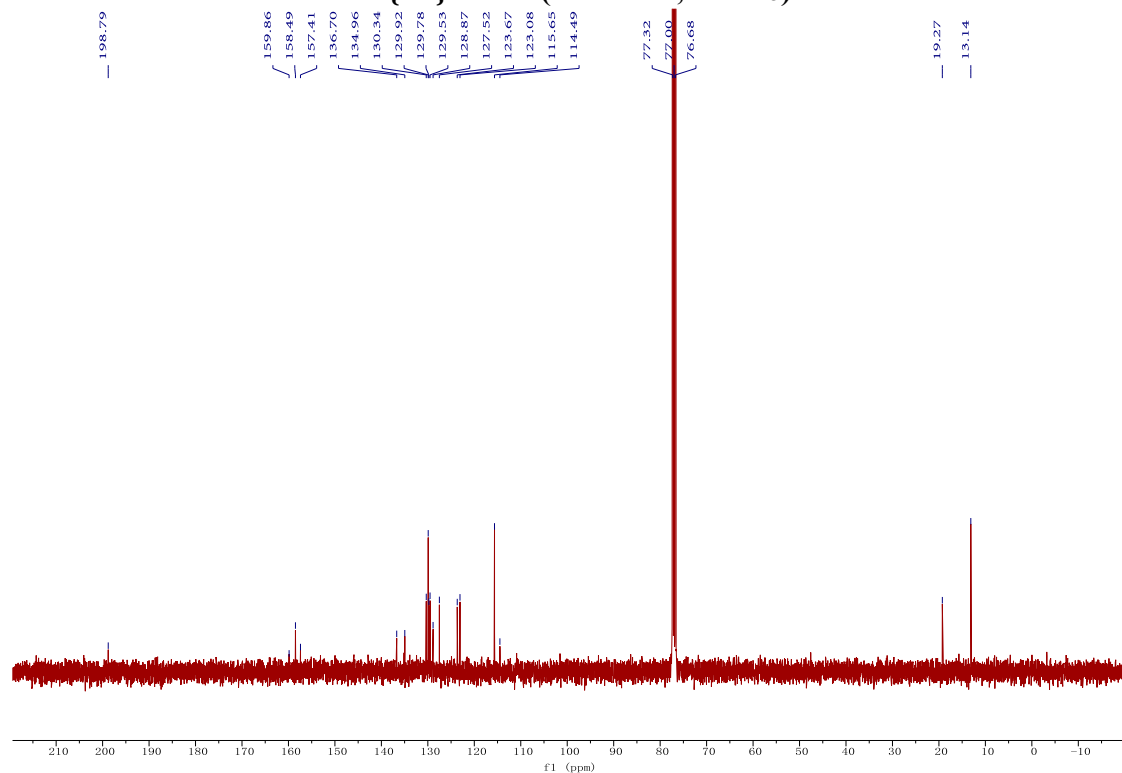
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

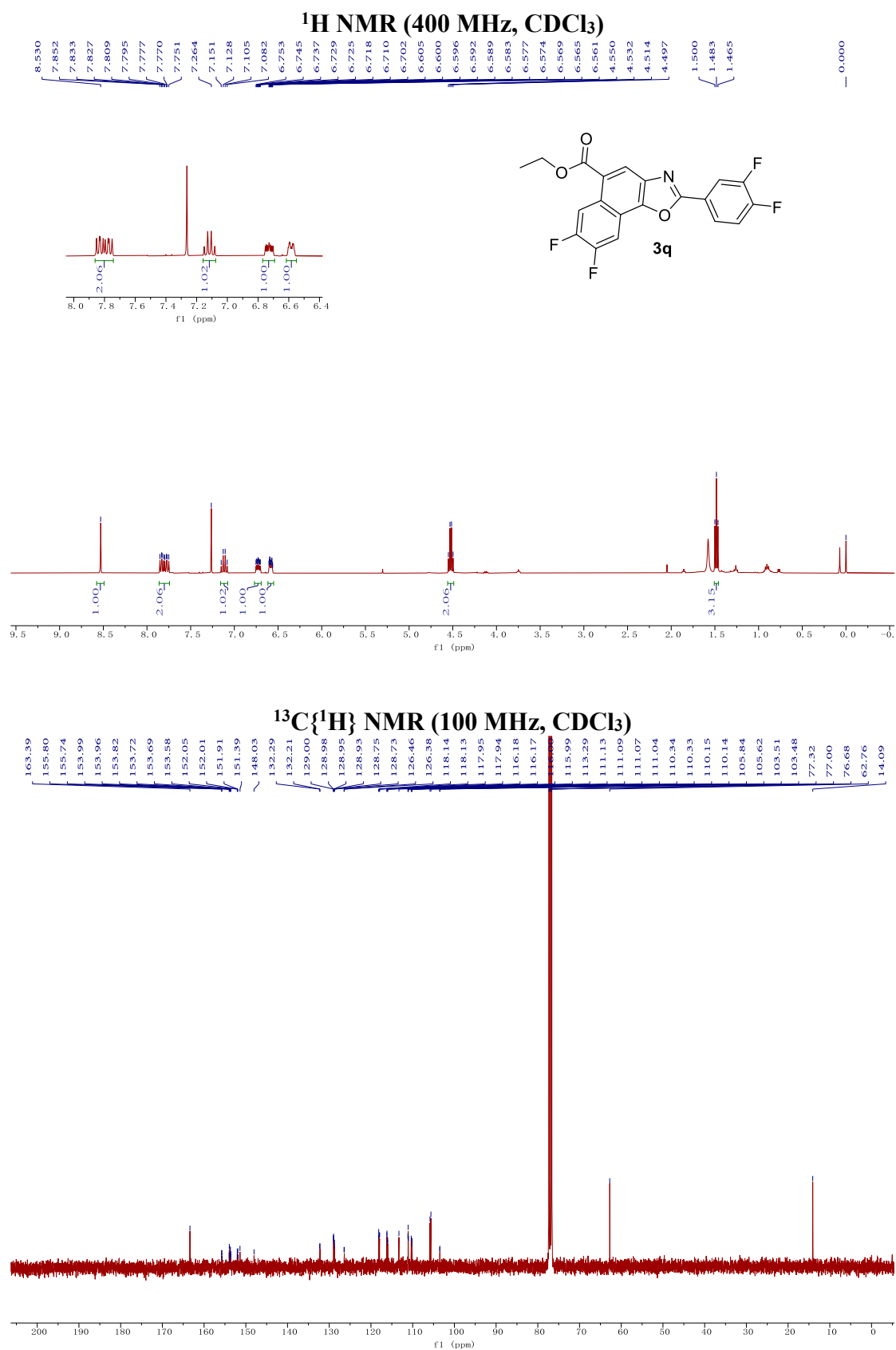


^1H NMR (400 MHz, CDCl_3)

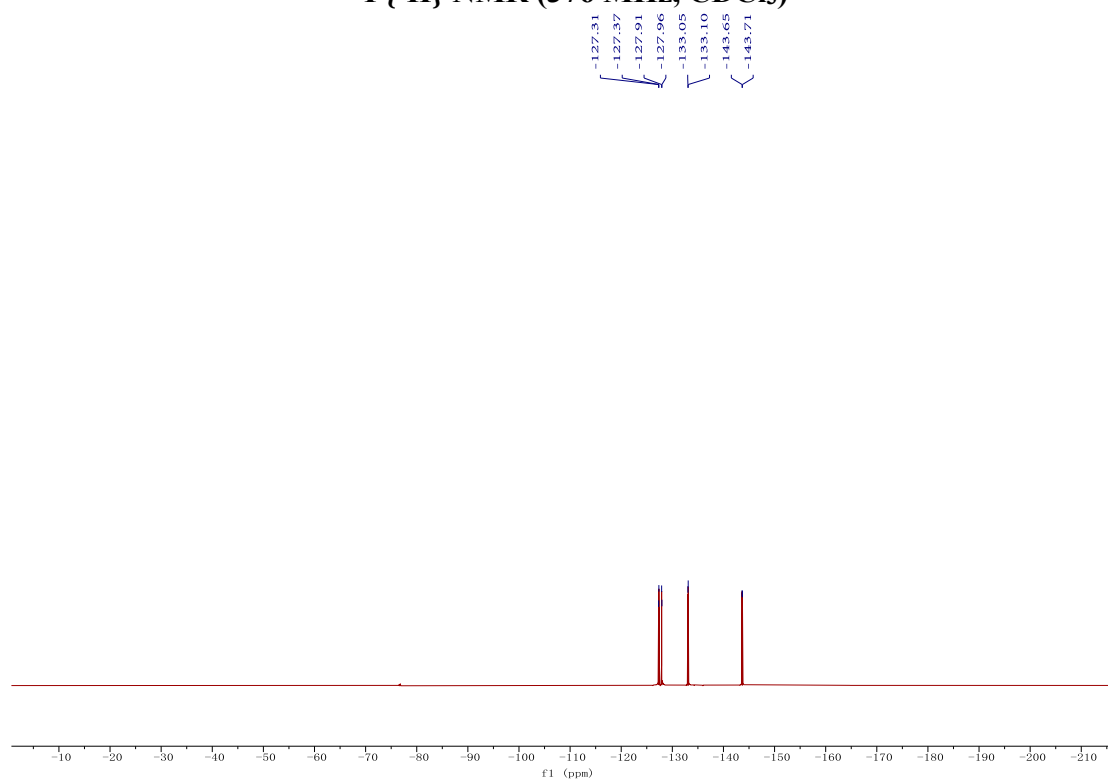


$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

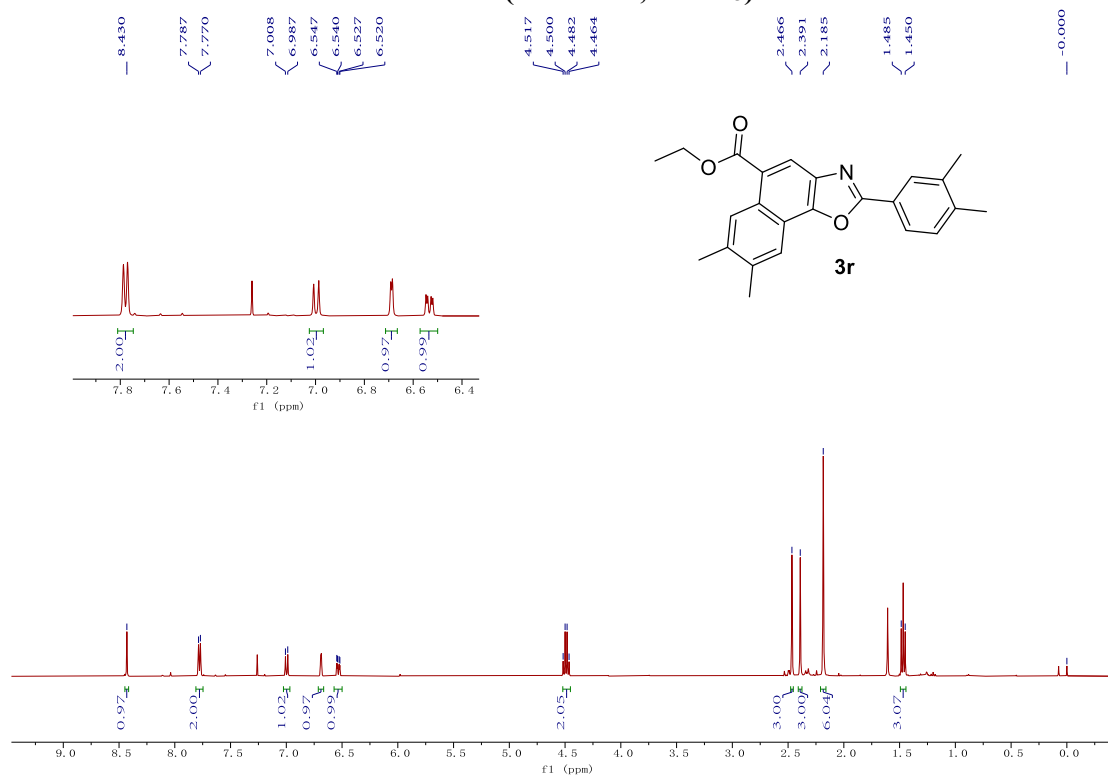




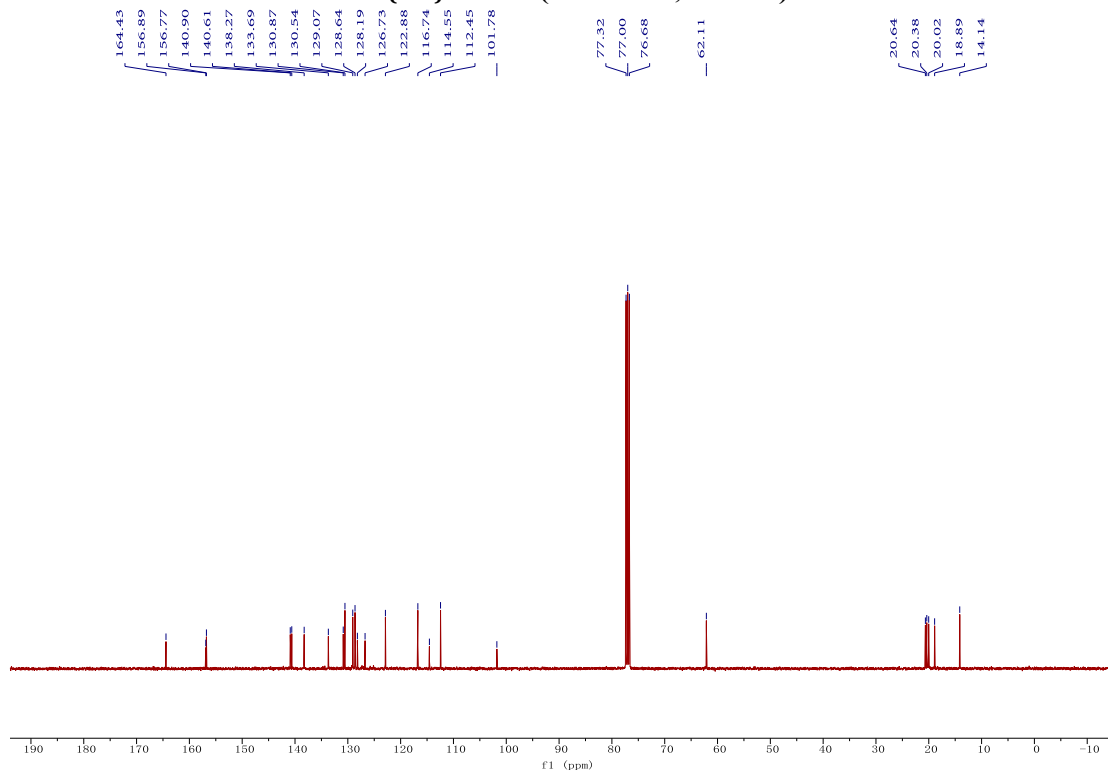
$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3)

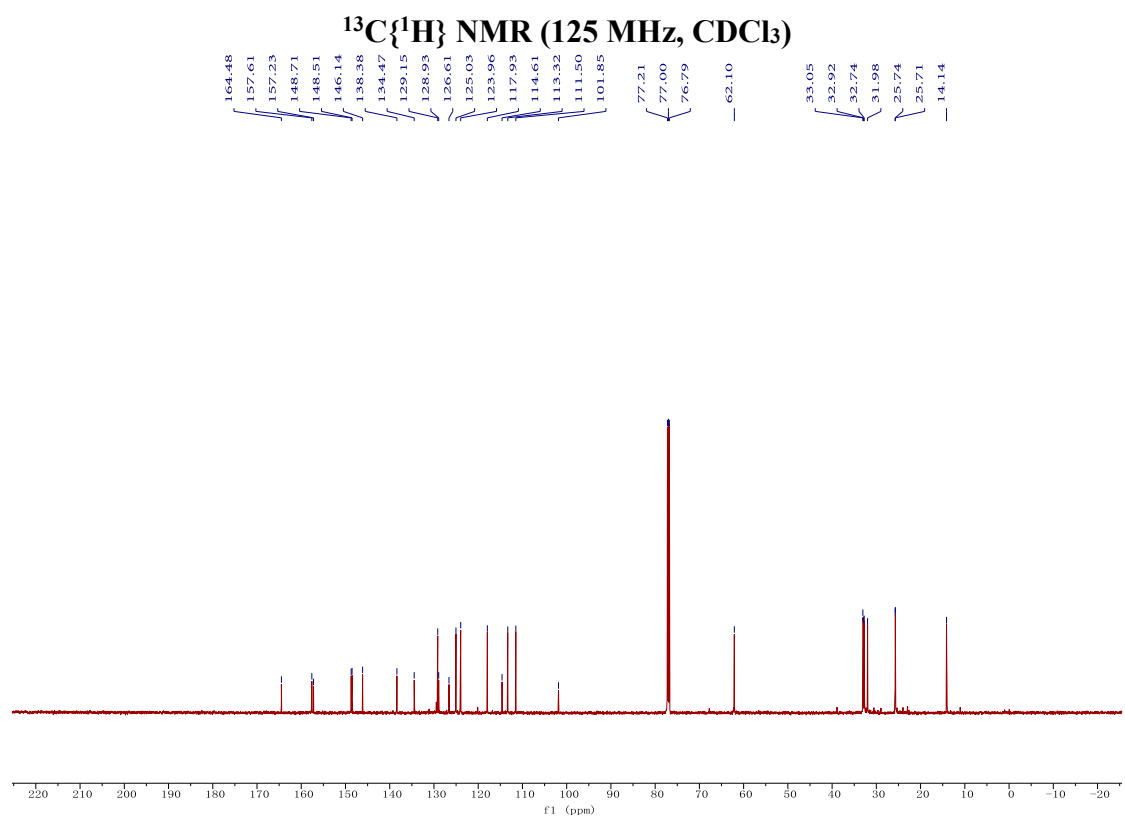
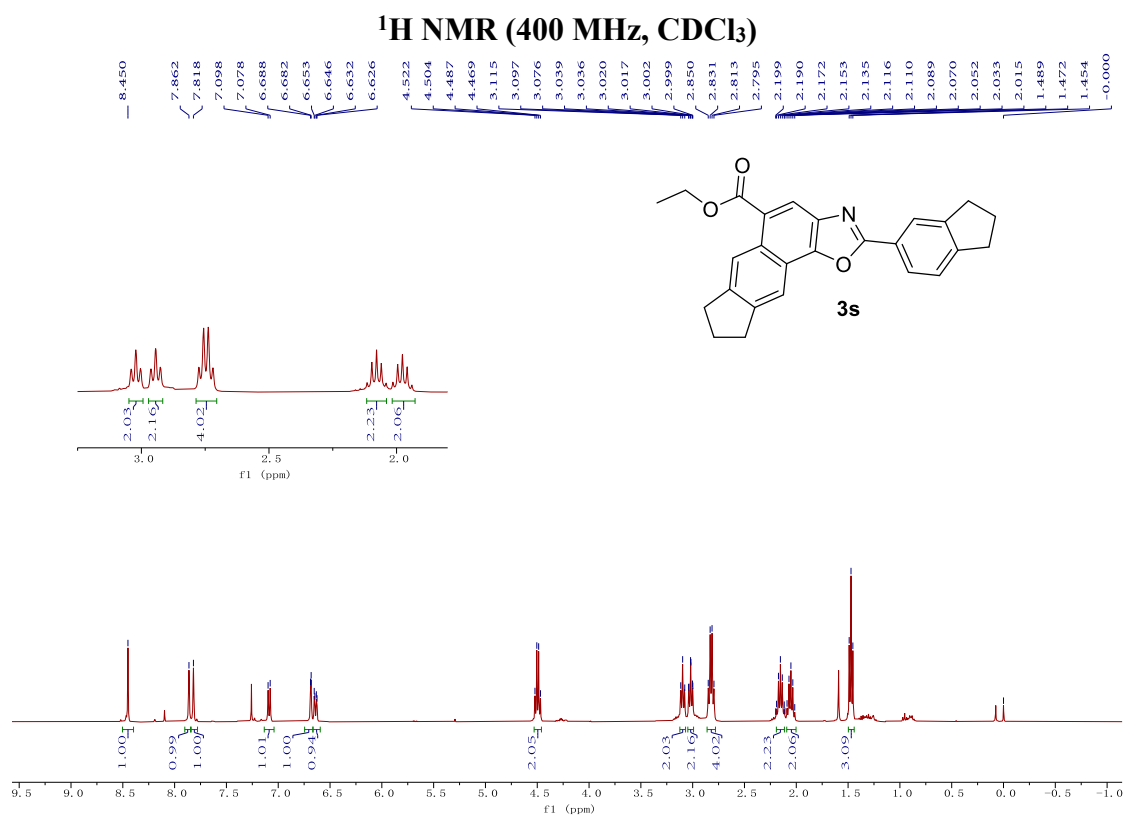


^1H NMR (400 MHz, CDCl_3)

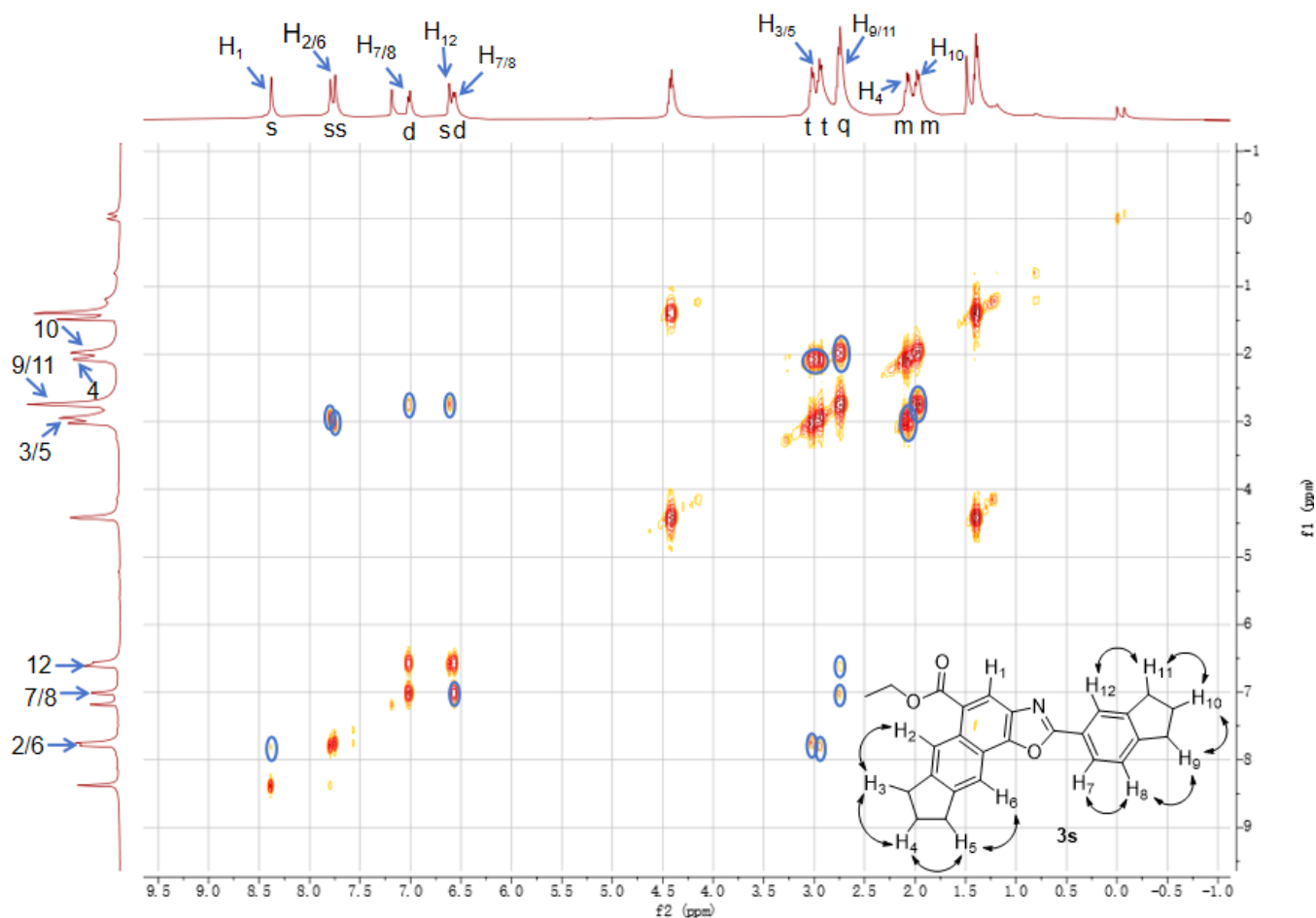


$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



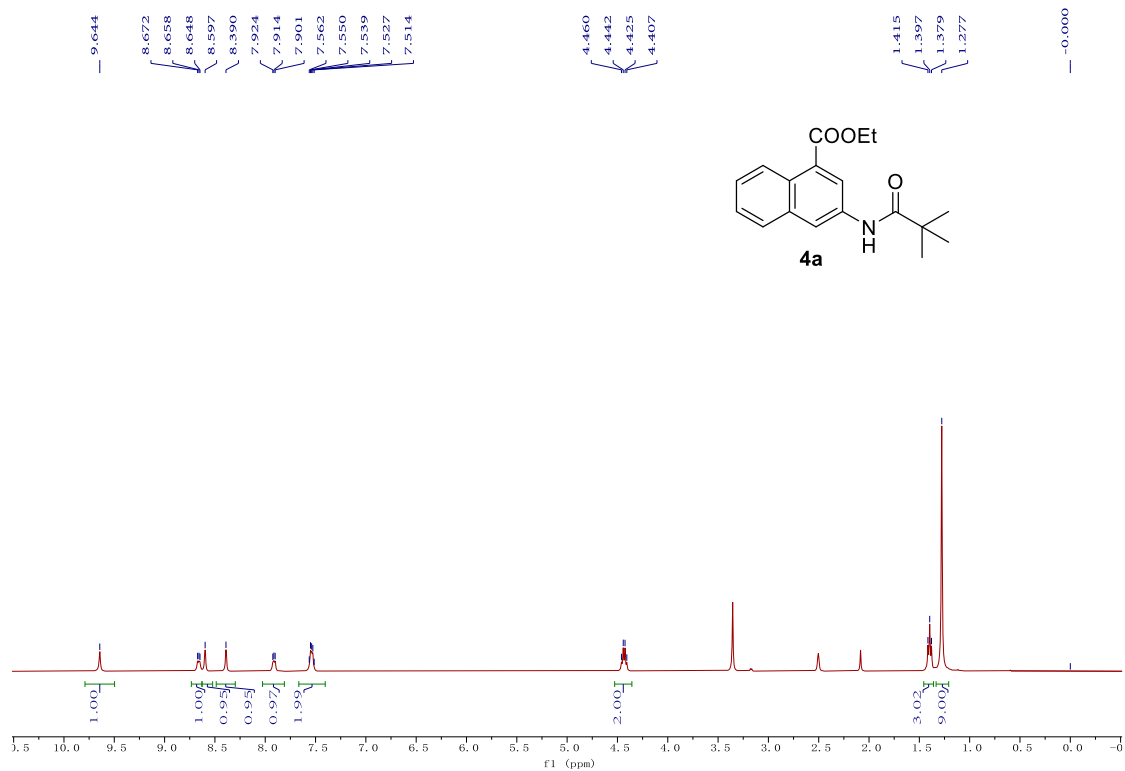


2D ^1H - ^1H COSY

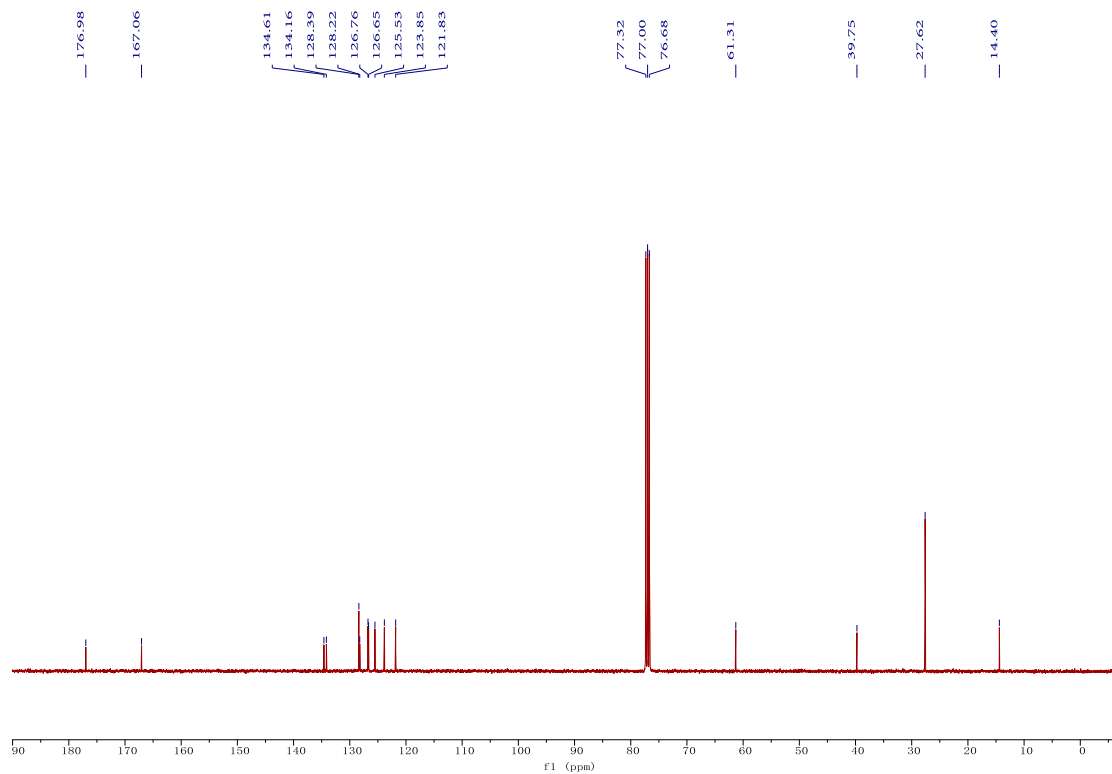


The hydrogen atoms were assigned based on the fine splitting patterns observed in the 1D NMR spectrum, and the assignments were subsequently verified by the 2D ^1H - ^1H COSY spectrum of **3s**. The coupling correlations indicate that **H₁** exhibits weak coupling with **H_{2/6}** due to their presence in a large π -conjugated system. **H_{2/6}** are coupled with **H_{3/5}** on the indene ring, and **H_{3/5}** show strong coupling with **H₄**. These coupling patterns confirm the presence of the left naphthoxazole framework. In addition, **H_{7/8}** are coupled with **H_{9/11}**, and **H_{9/11}** are further coupled with **H₁₀** and **H₁₂**, thereby essentially establishing the structure of the right indene ring framework.

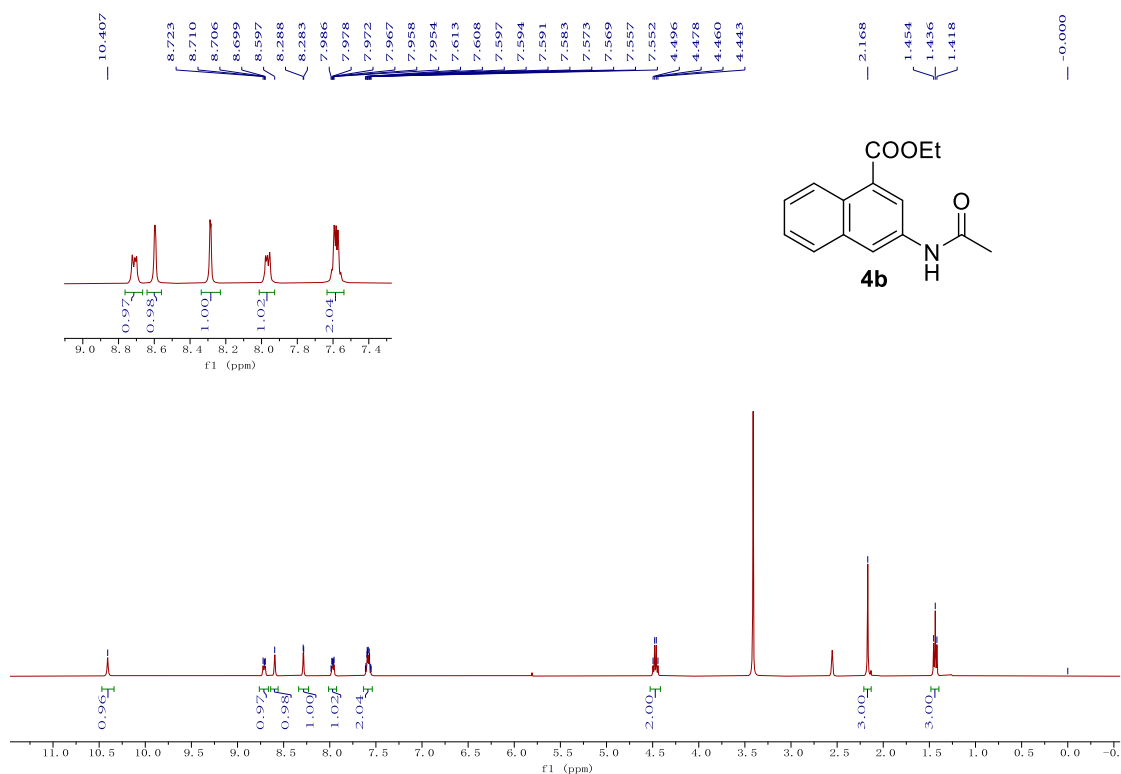
^1H NMR (400 MHz, $\text{DMSO}-d_6$)



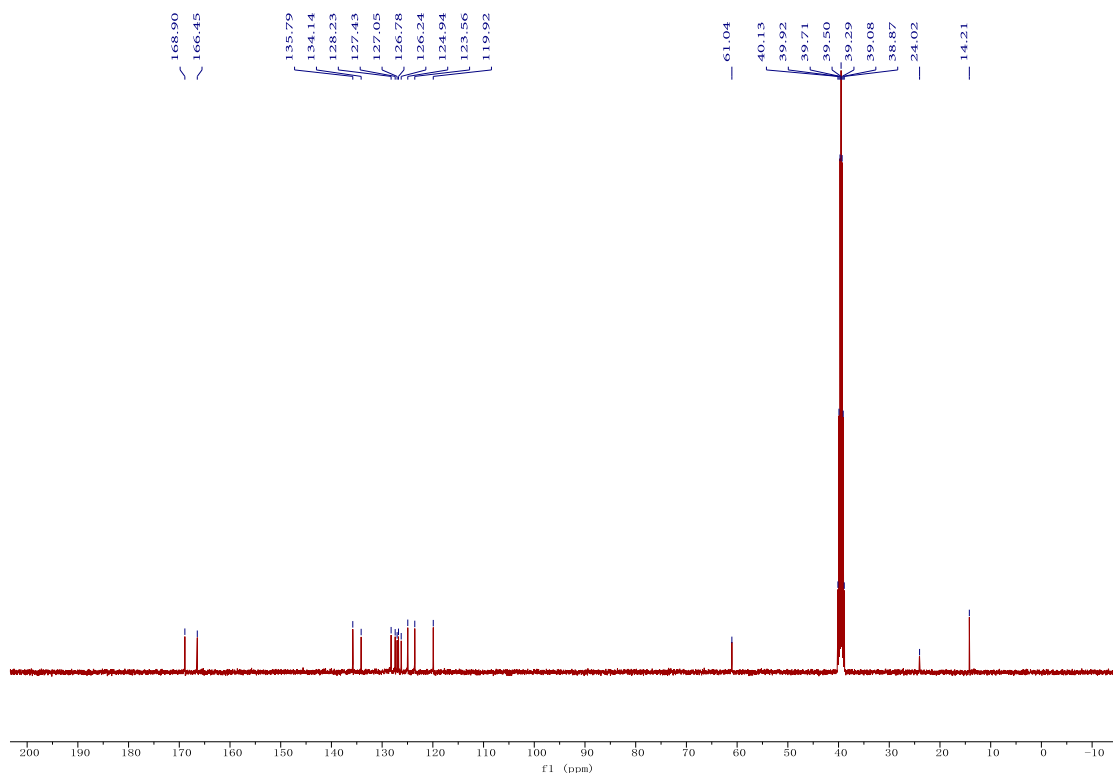
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

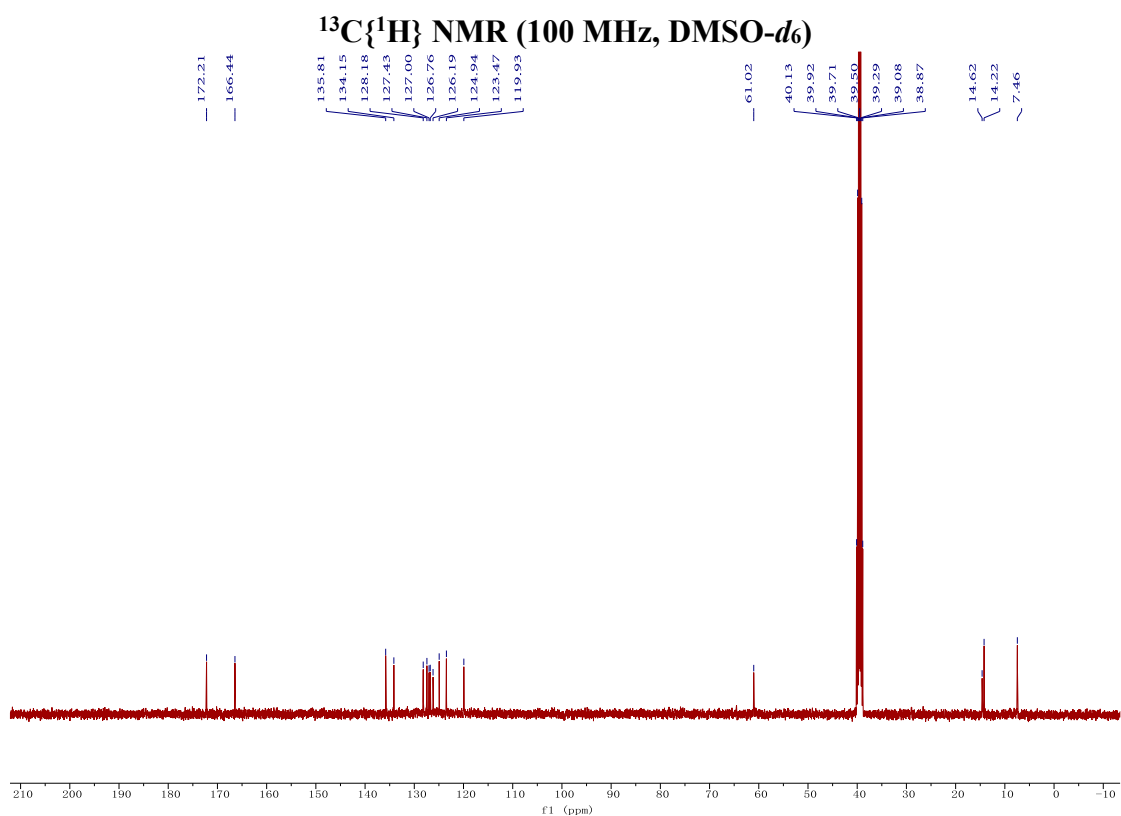
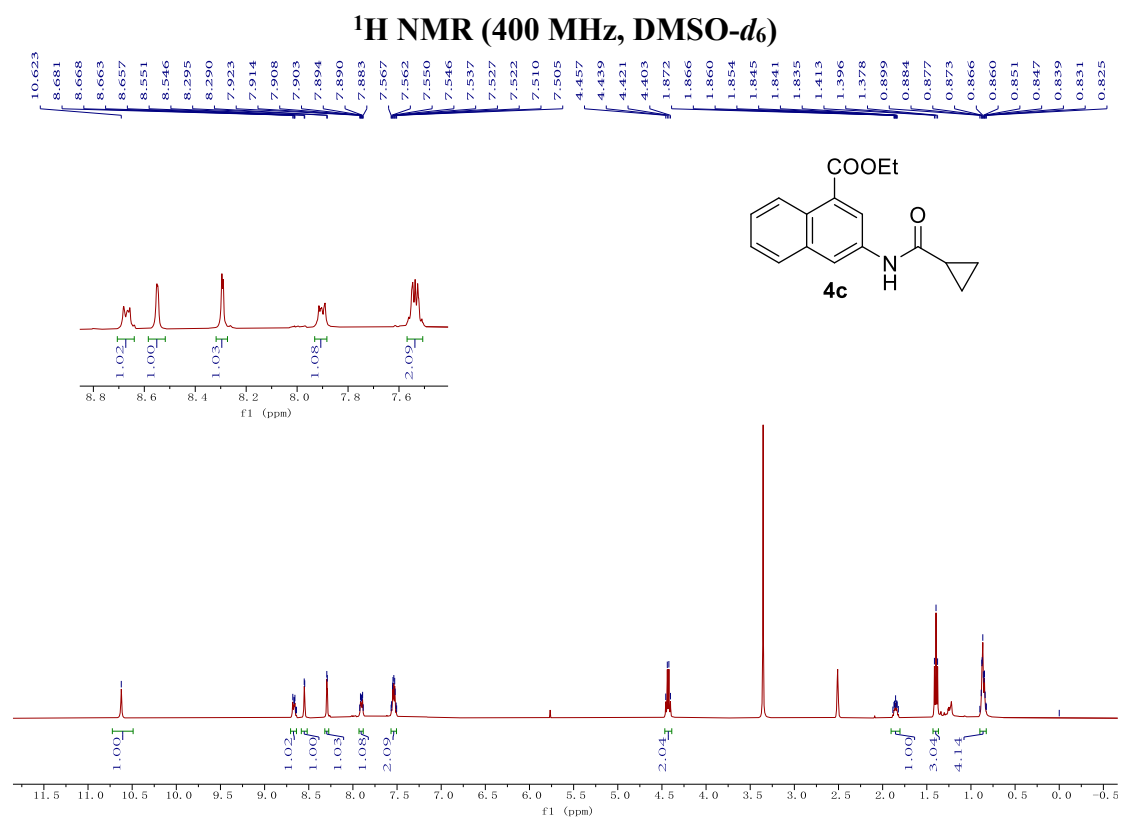


¹H NMR (400 MHz, DMSO-*d*₆)

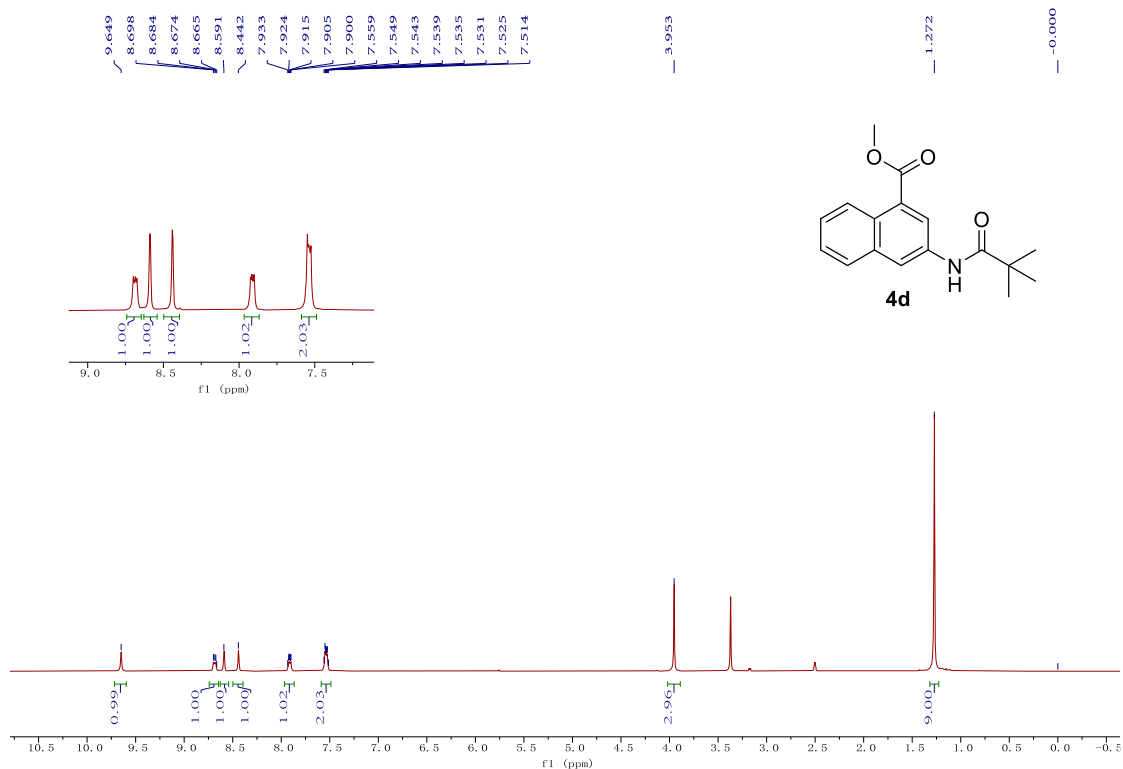


¹³C{¹H} NMR (100 MHz, DMSO-*d*₆)

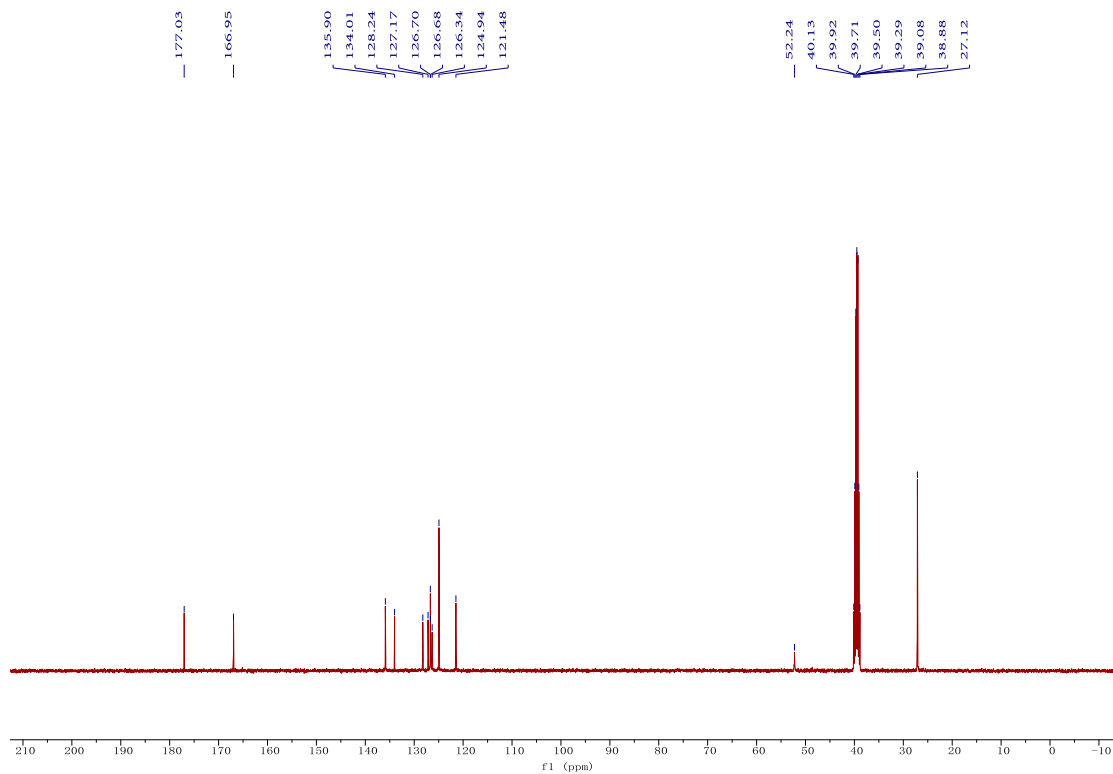




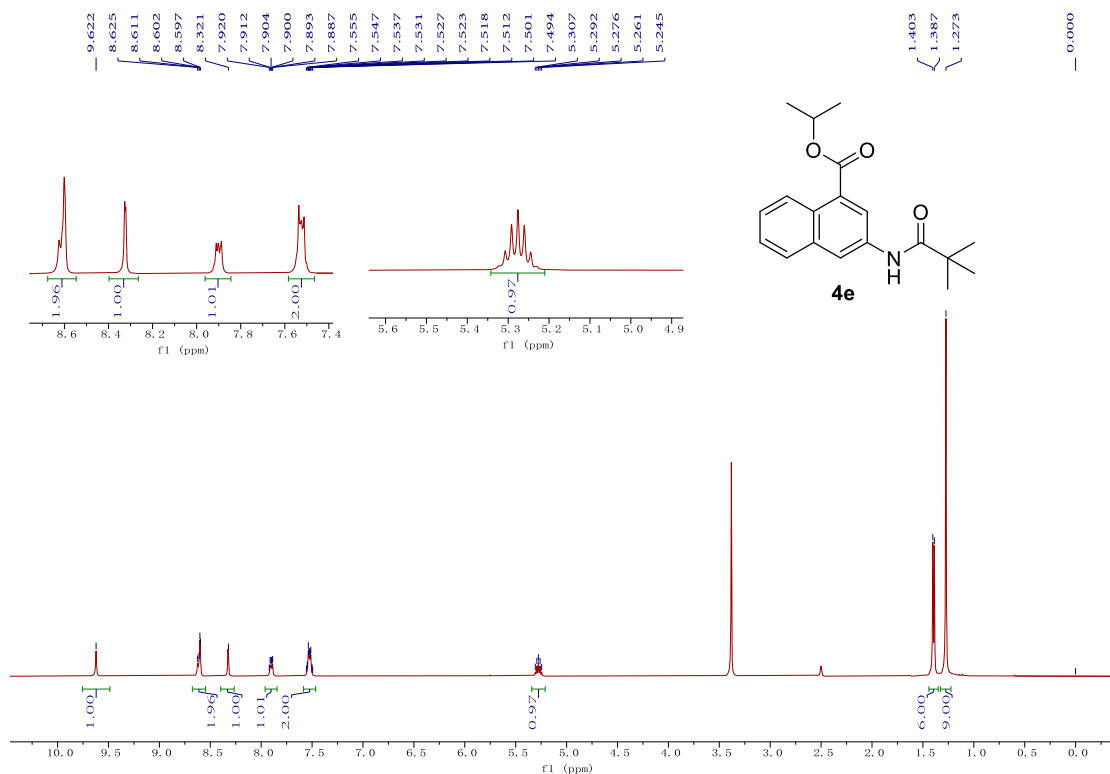
¹H NMR (400 MHz, DMSO-*d*₆)



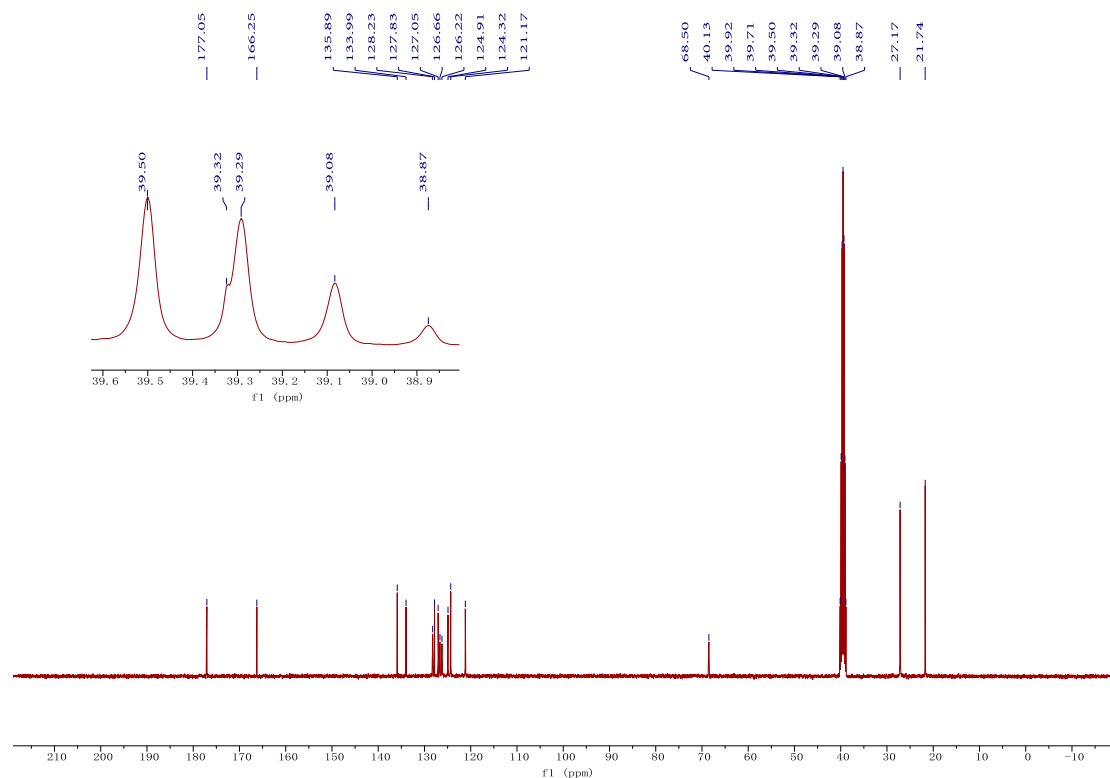
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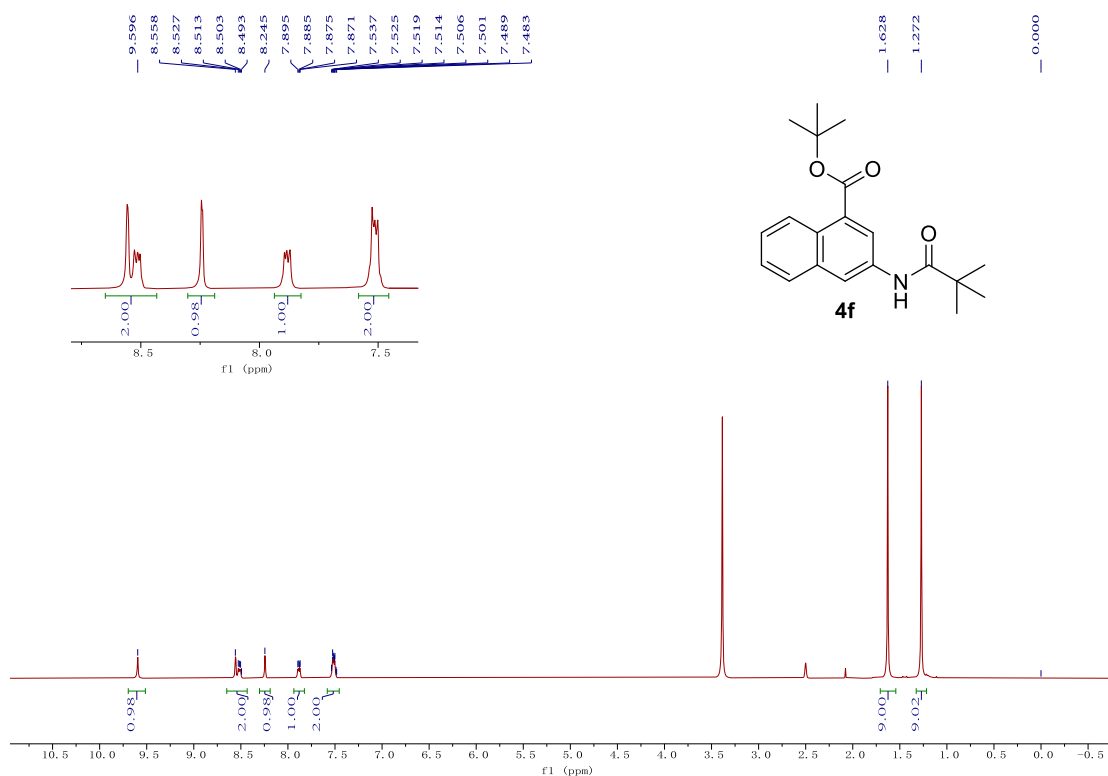
¹H NMR (400 MHz, DMSO-d₆)



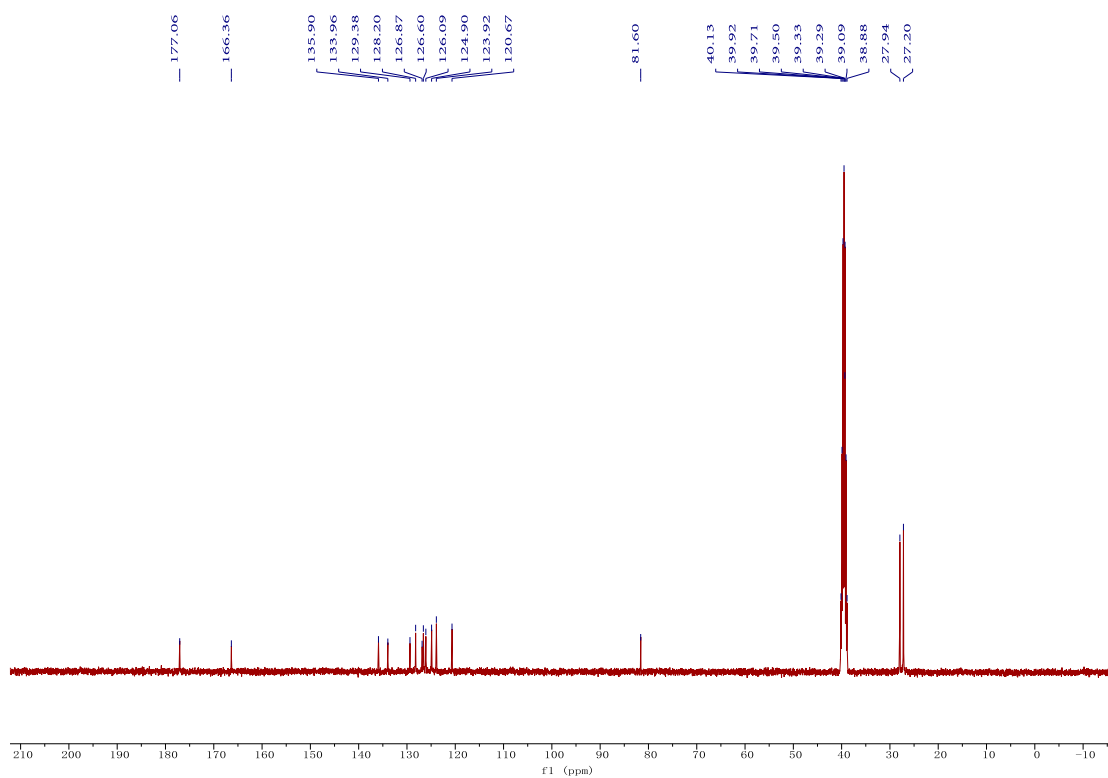
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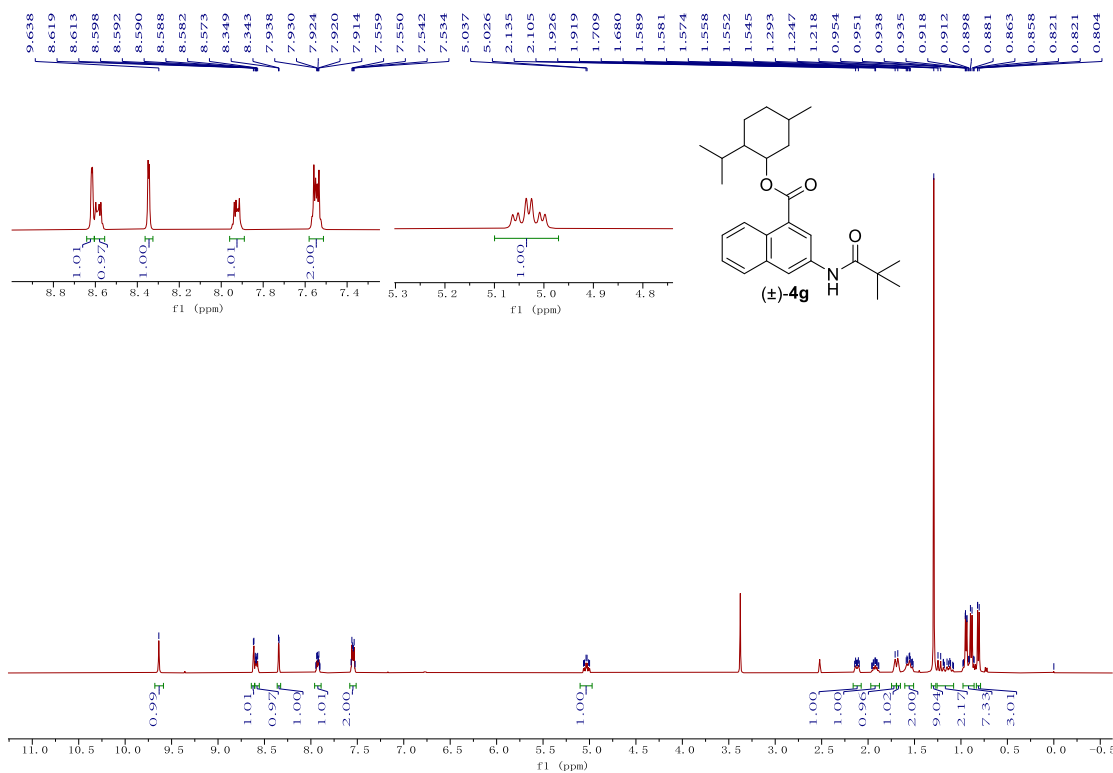
^1H NMR (400 MHz, DMSO- d_6)



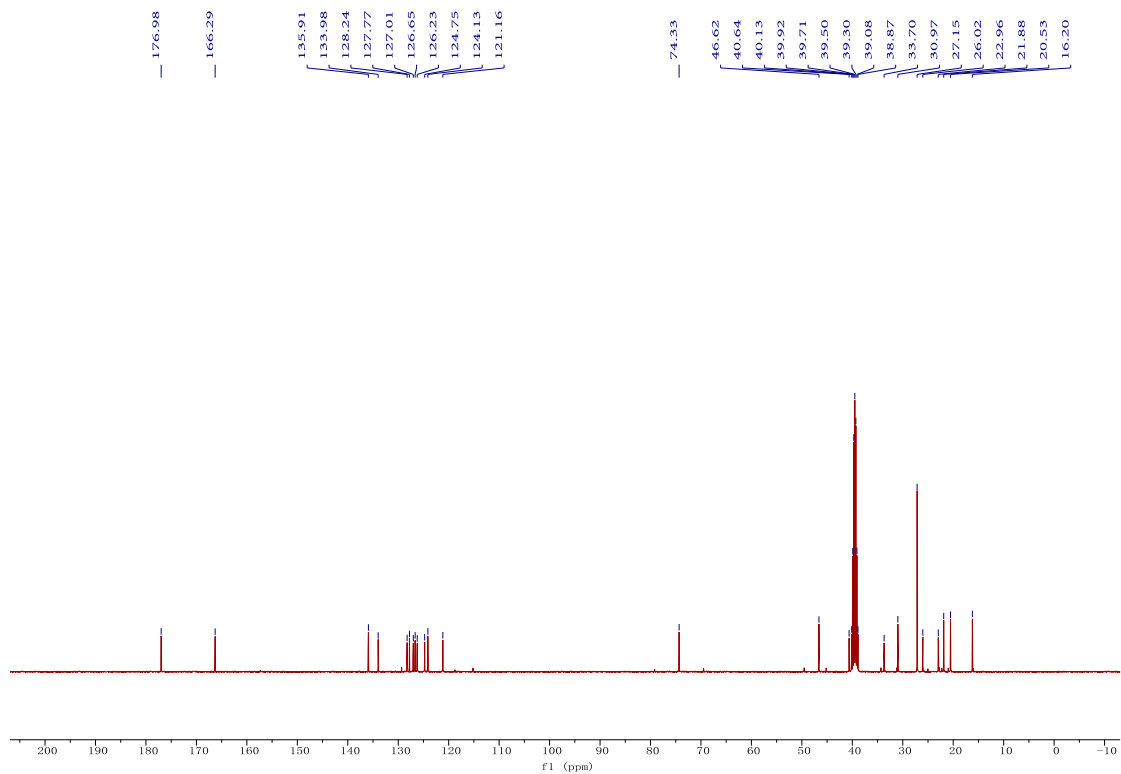
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6)



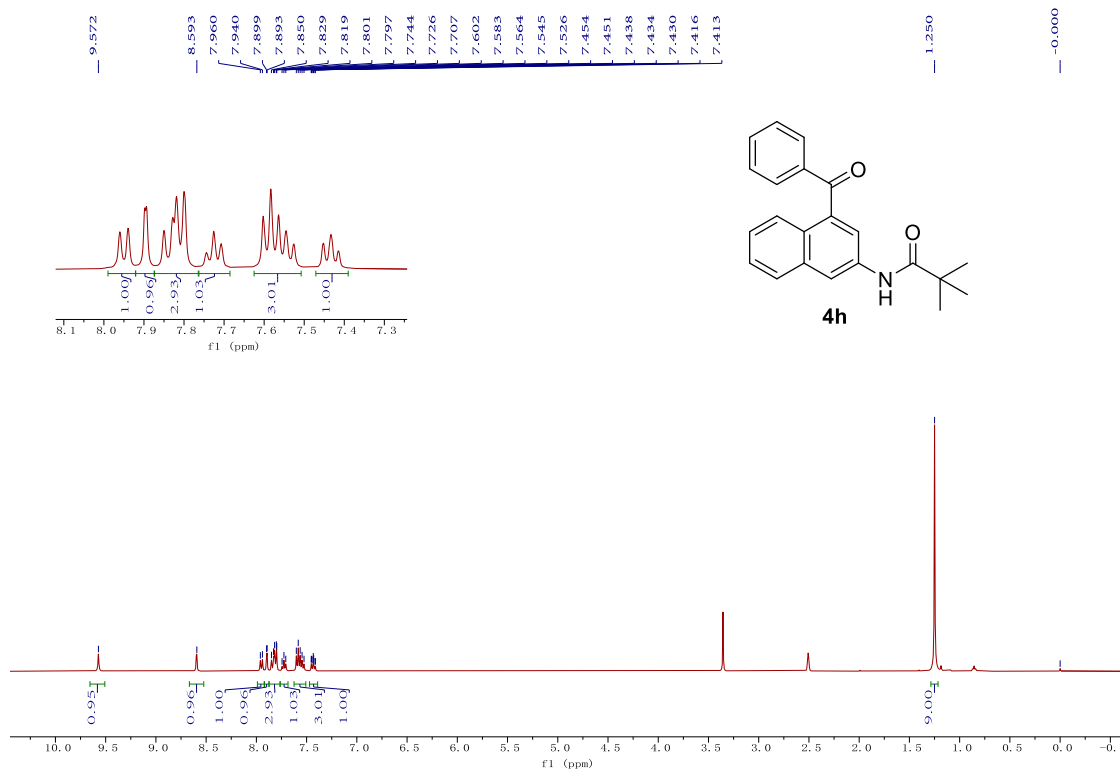
¹H NMR (400 MHz, DMSO-*d*₆)



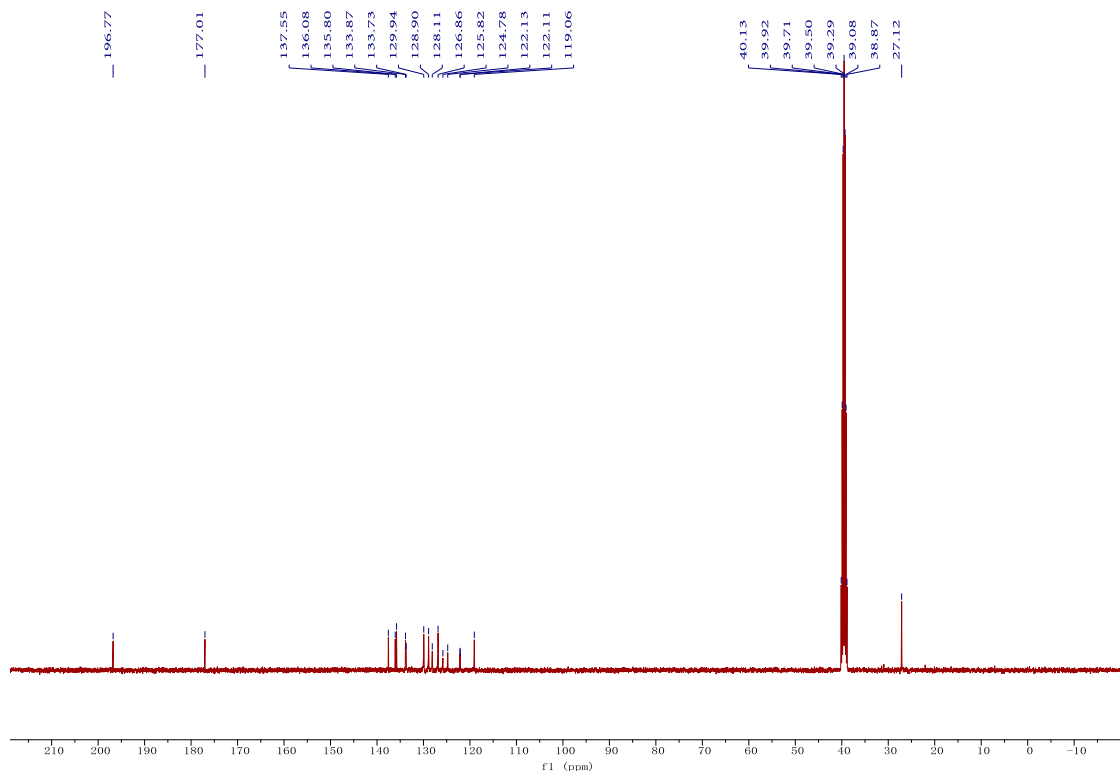
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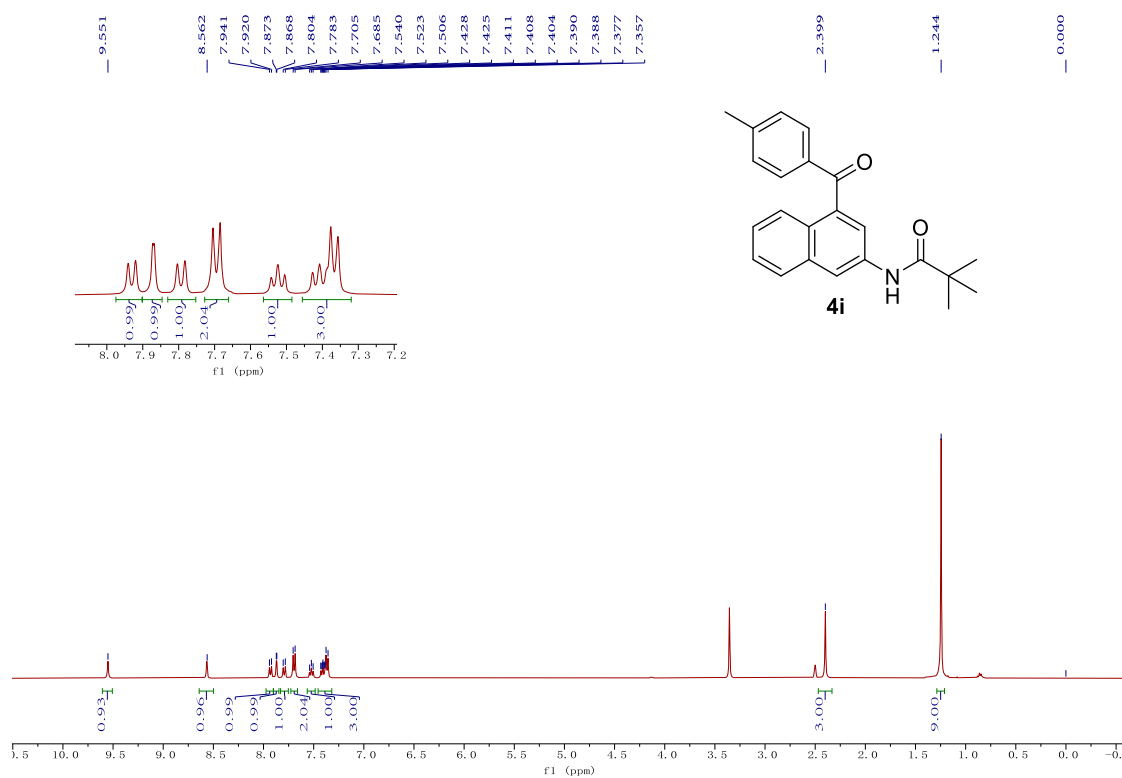
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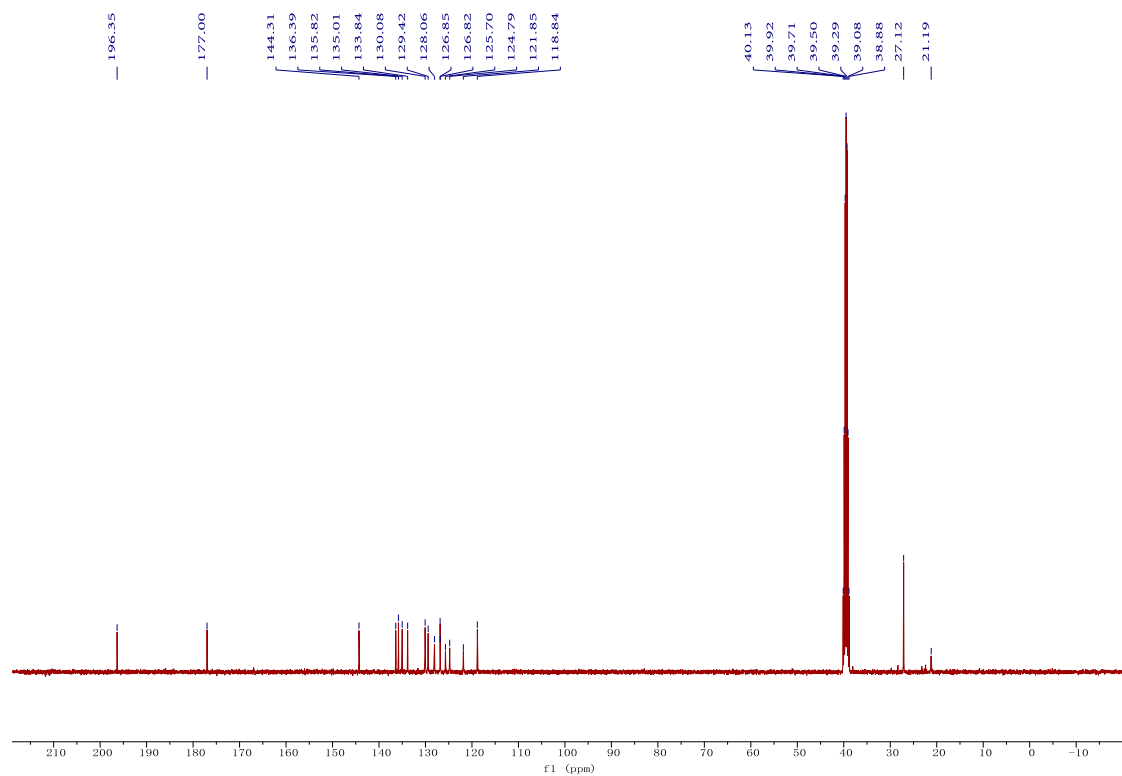
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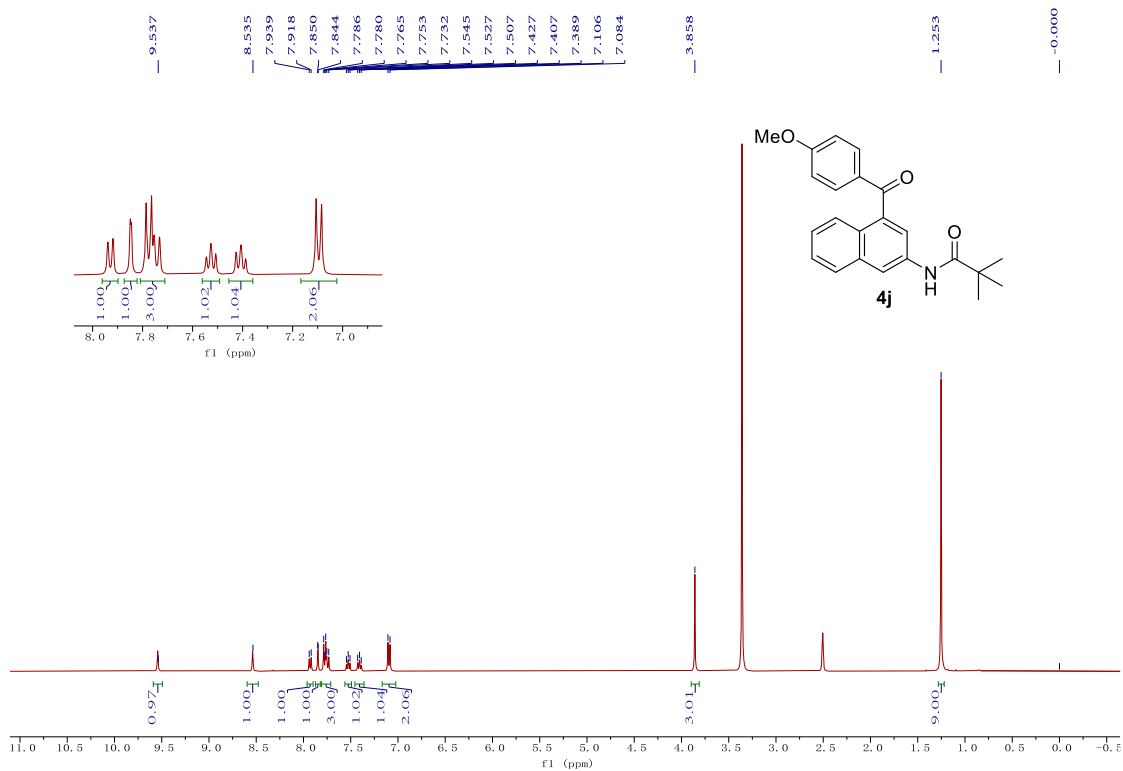
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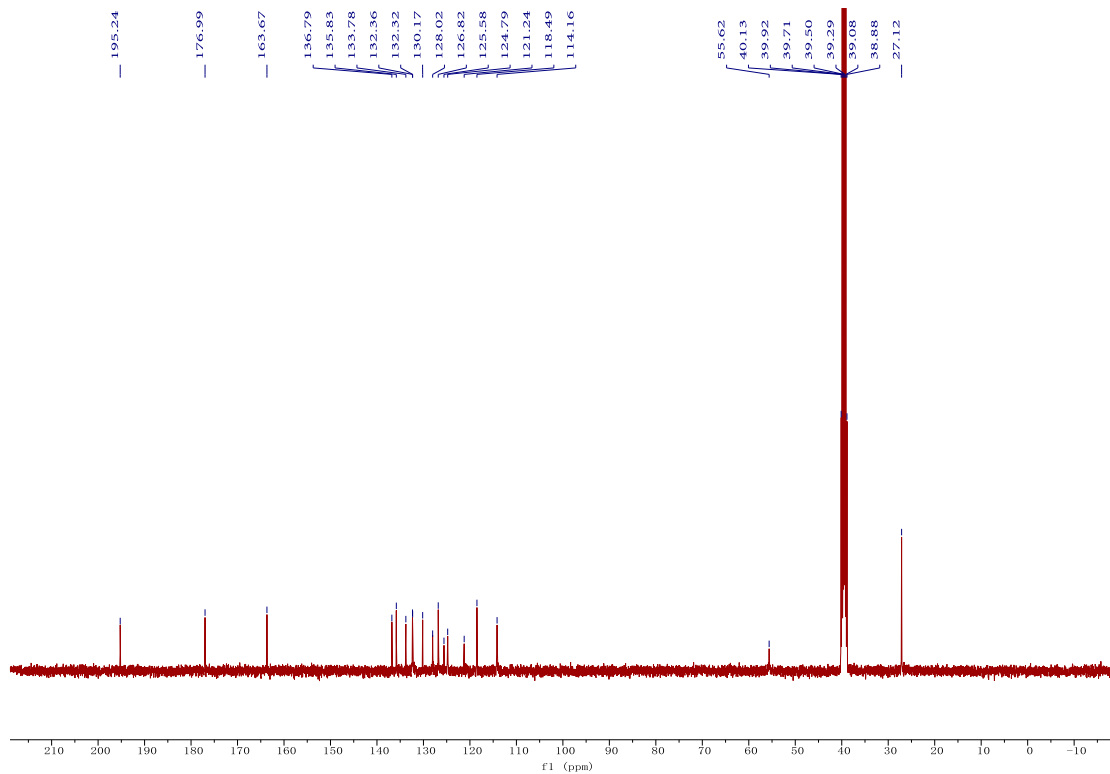
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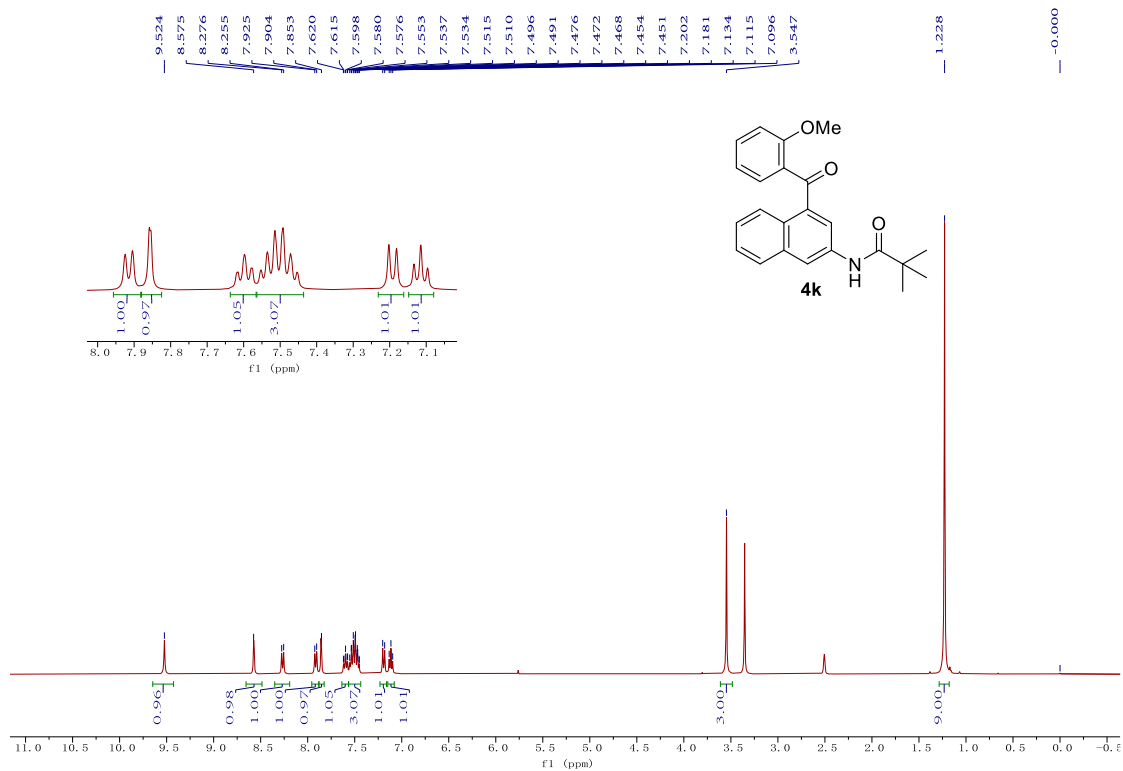
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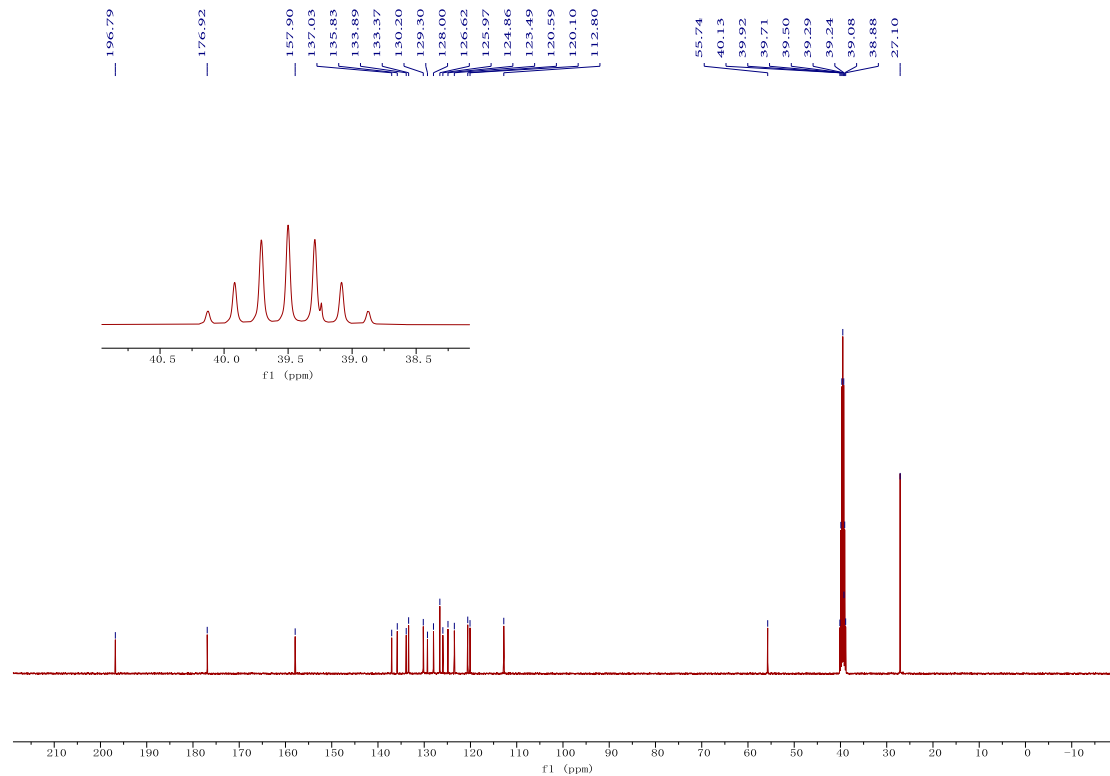
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆)



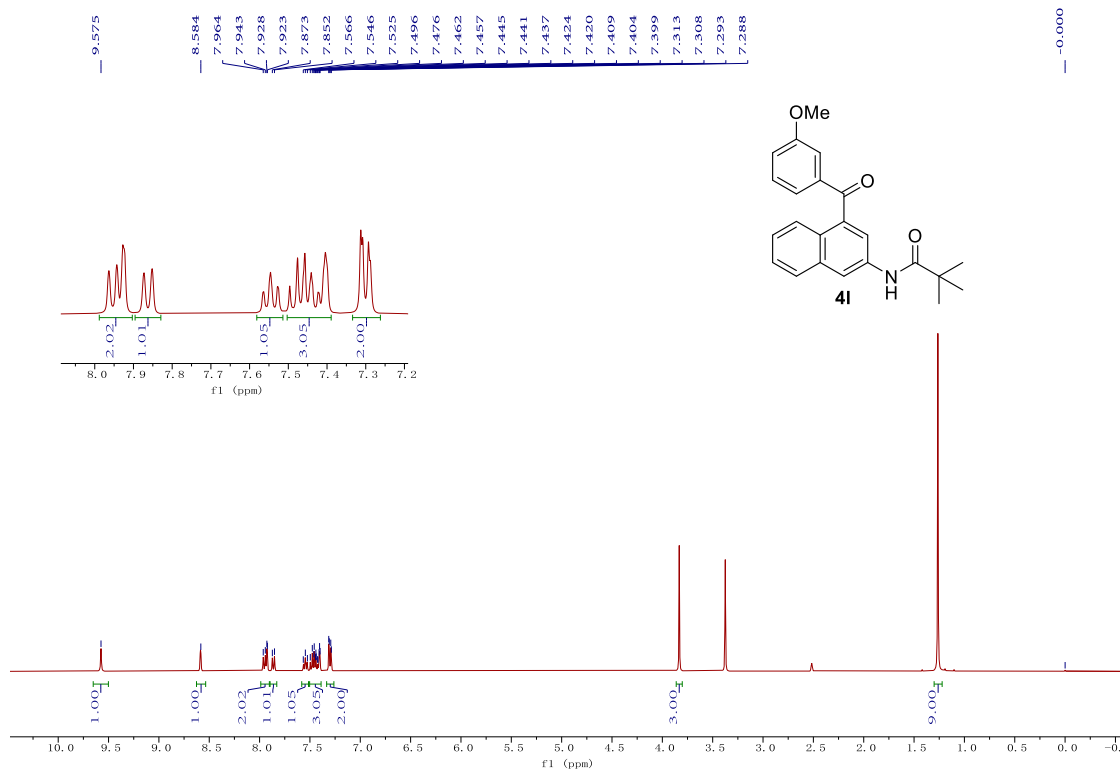
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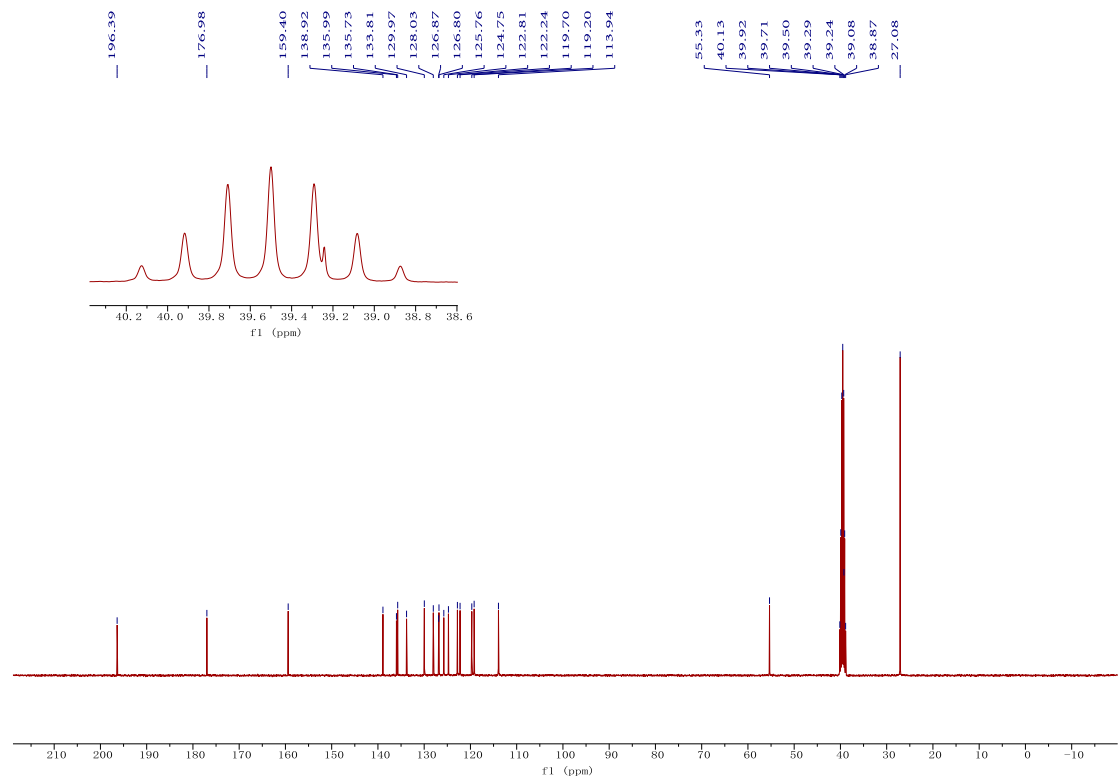
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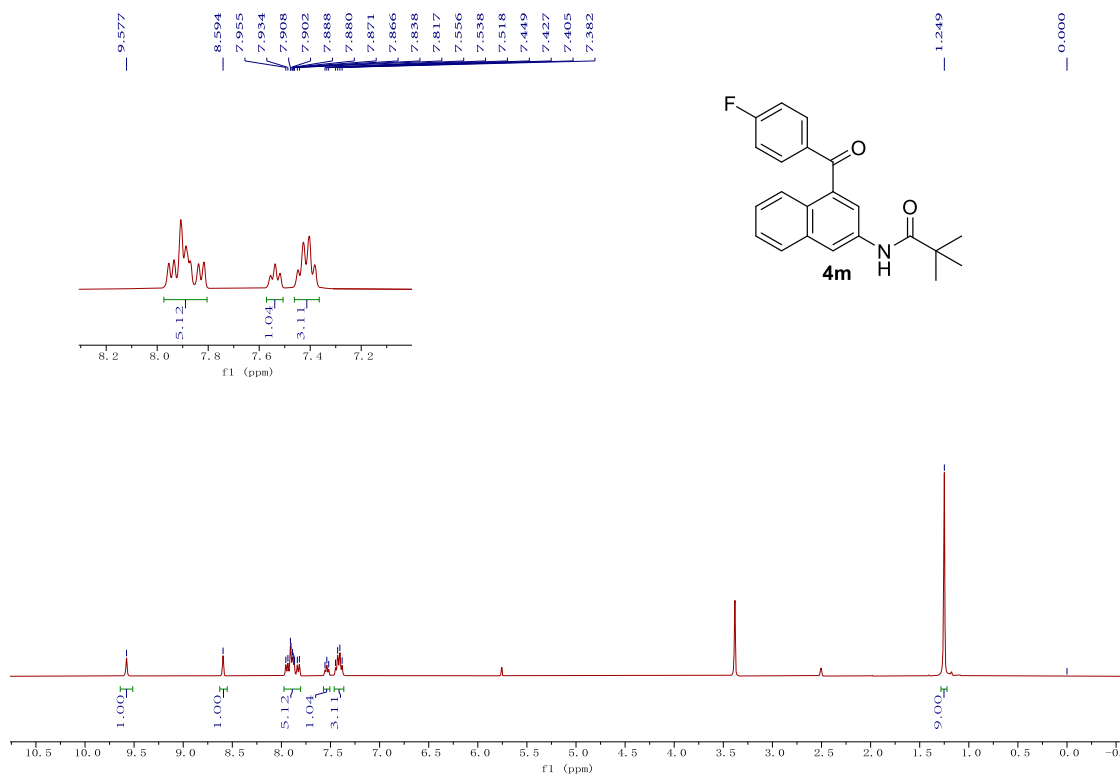
¹H NMR (400 MHz, DMSO-*d*₆)



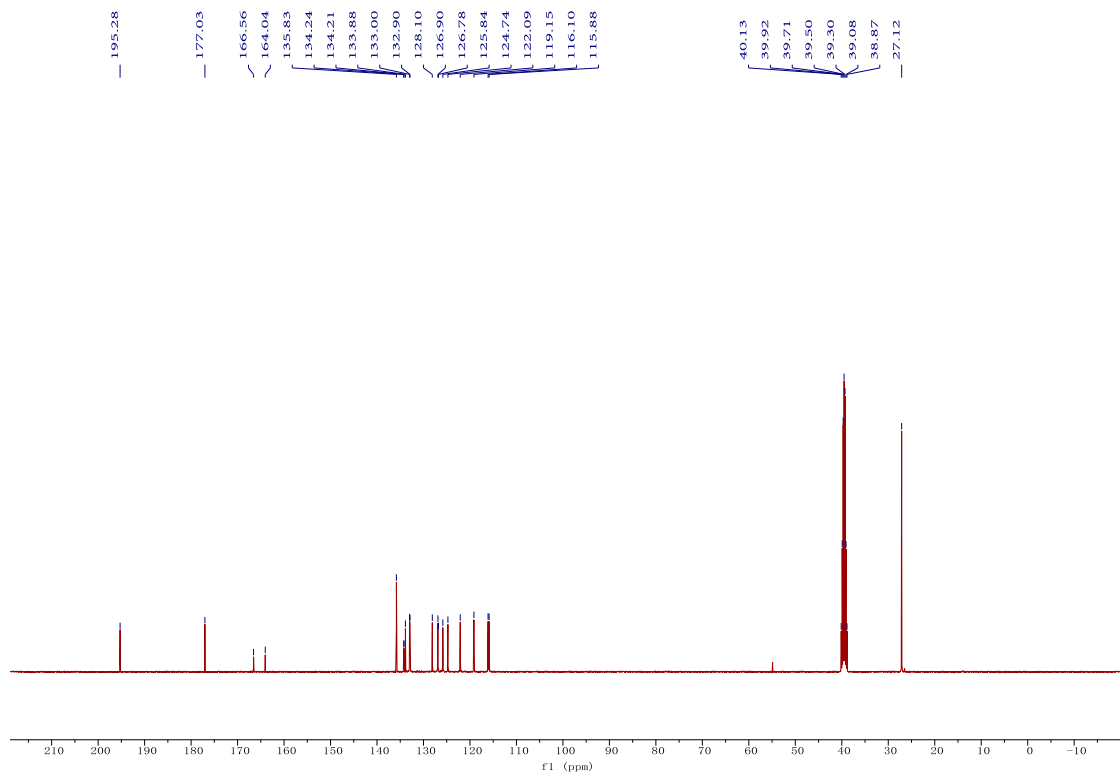
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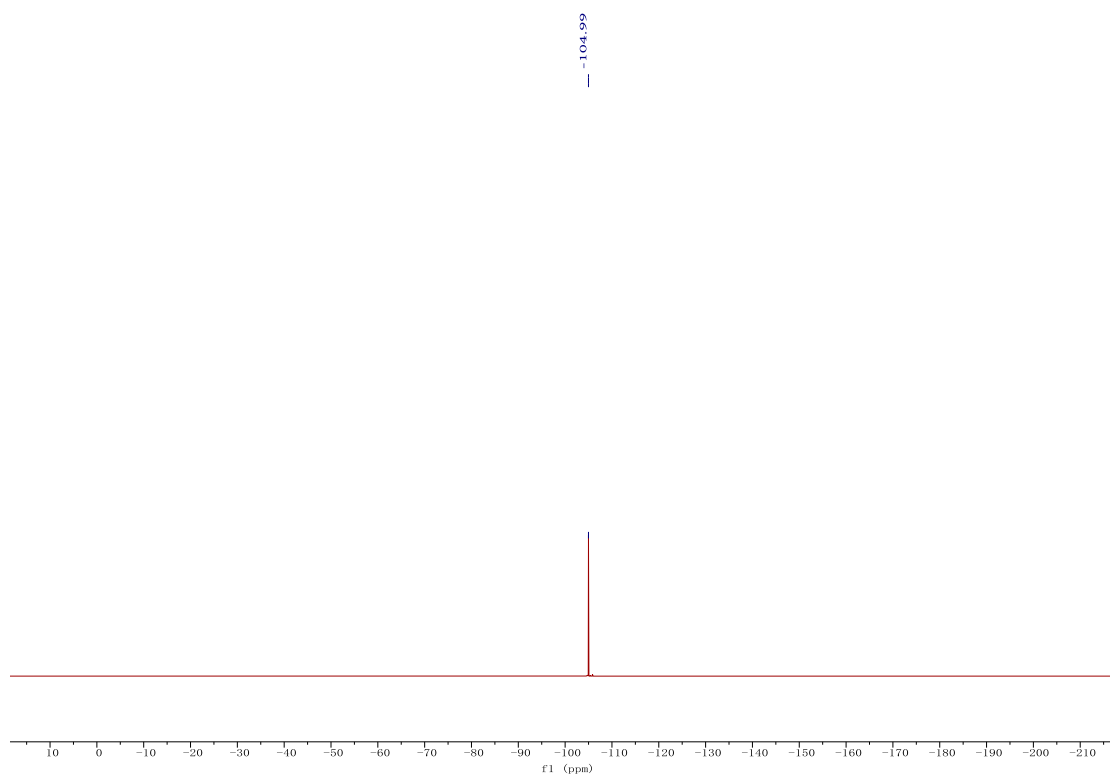
¹H NMR (400 MHz, DMSO-*d*₆)



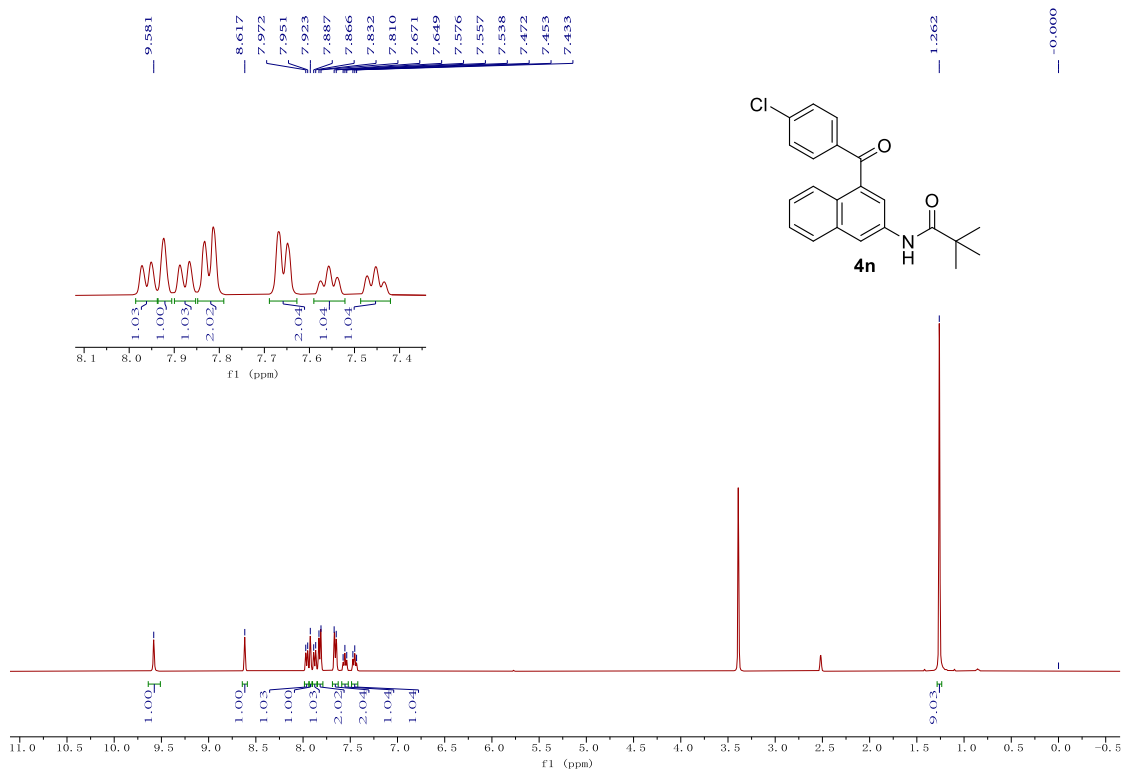
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆)



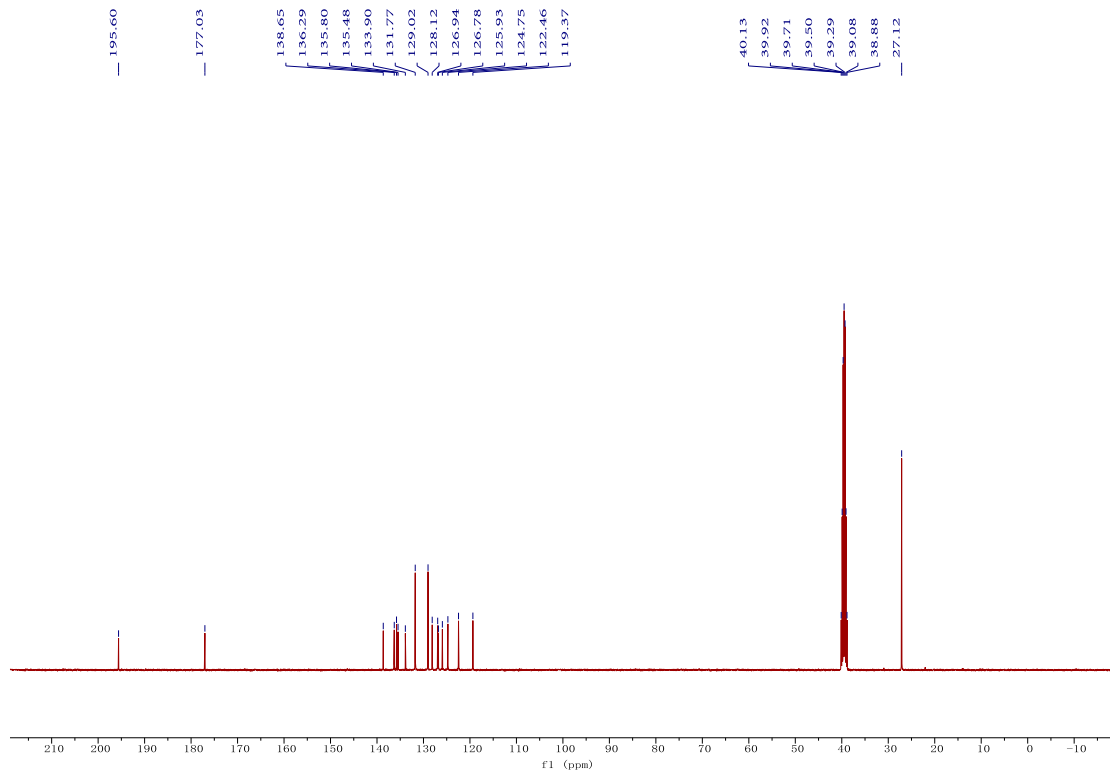
$^{19}\text{F}\{^1\text{H}\}$ (376 MHz, DMSO- d_6)

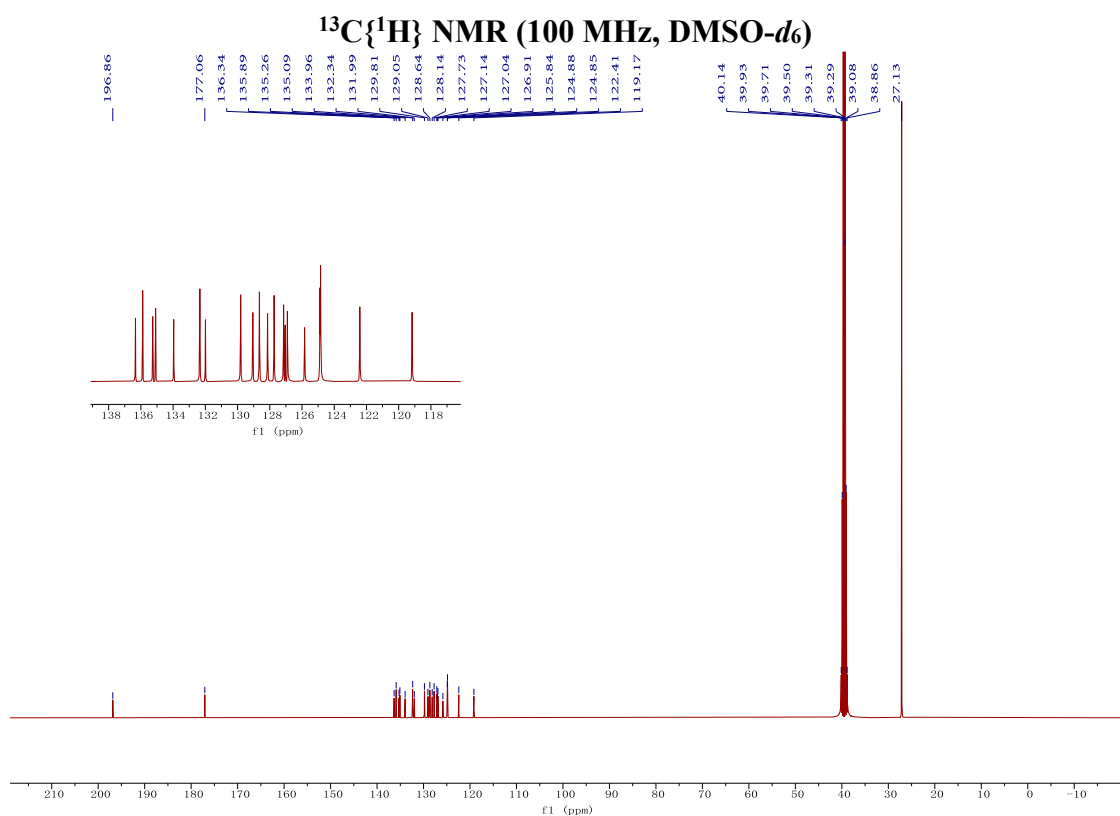
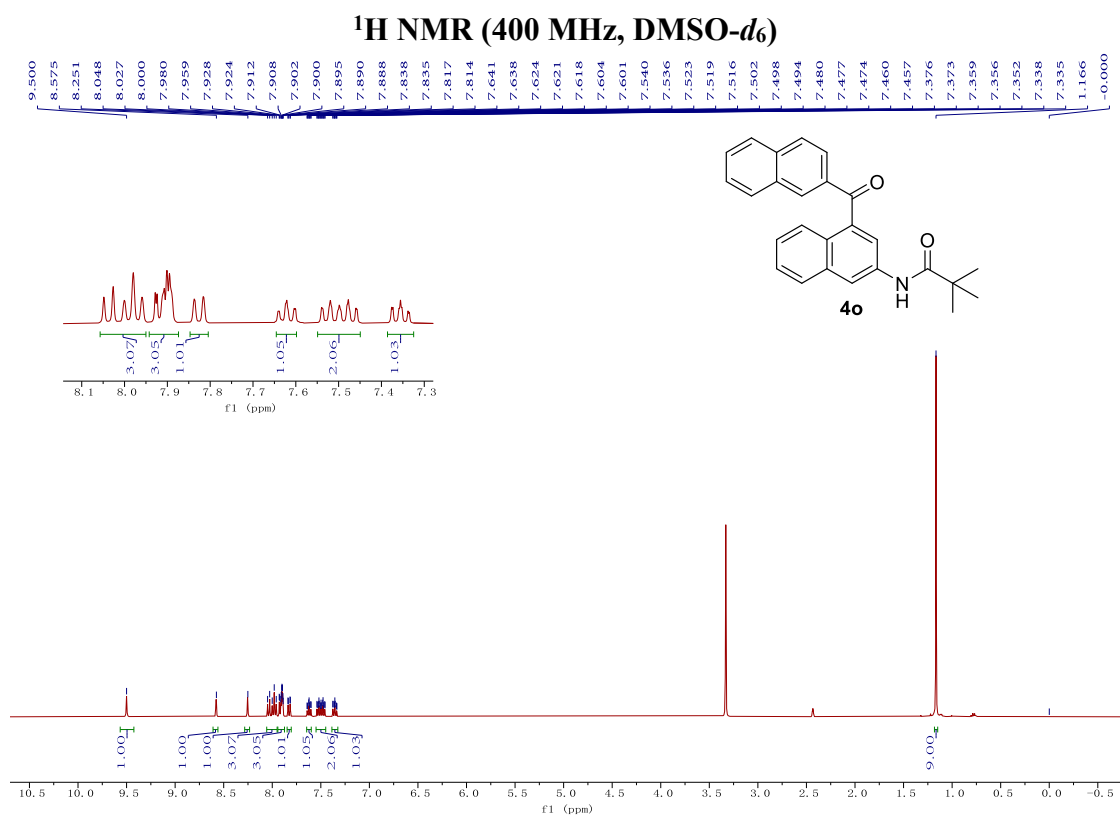


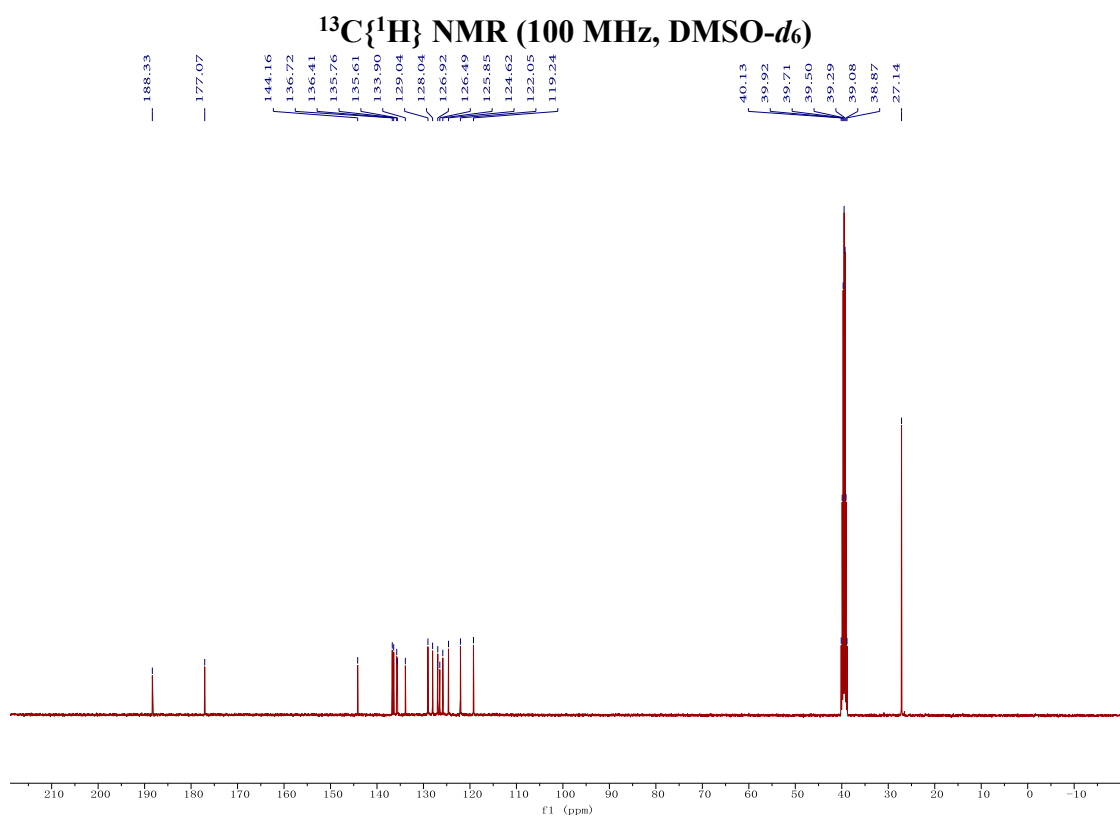
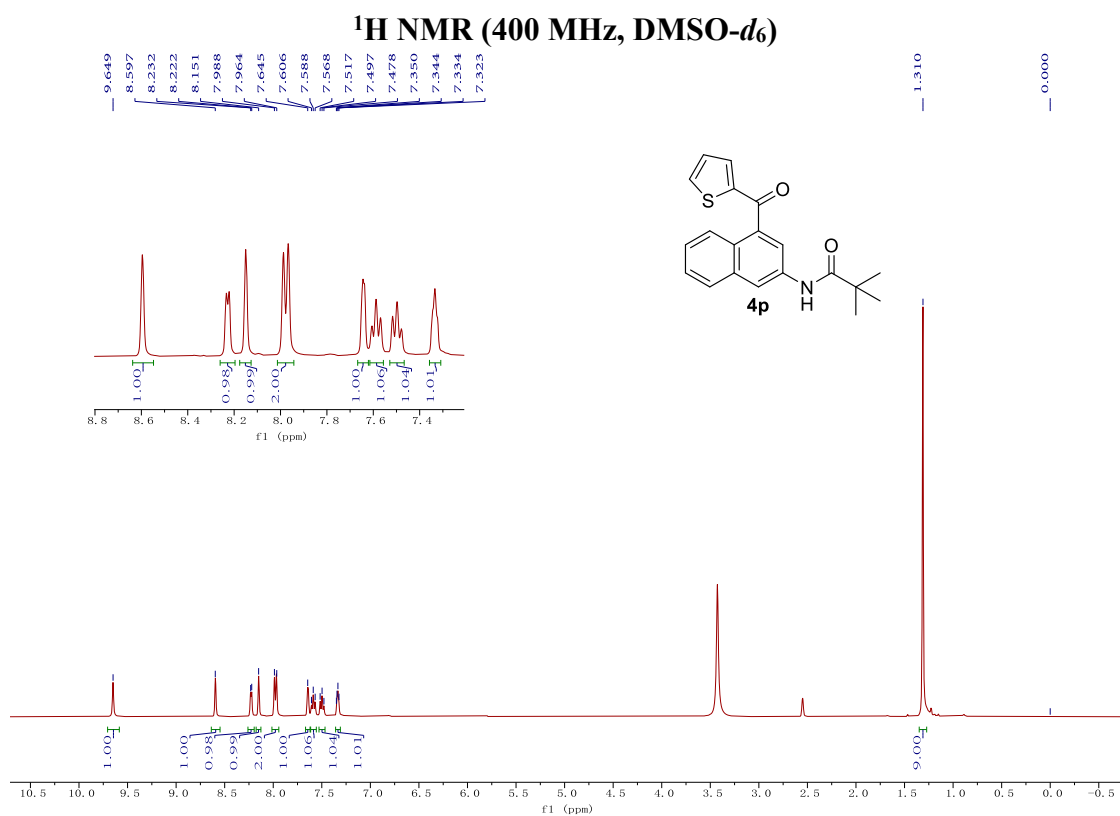
¹H NMR (400 MHz, DMSO-*d*₆)



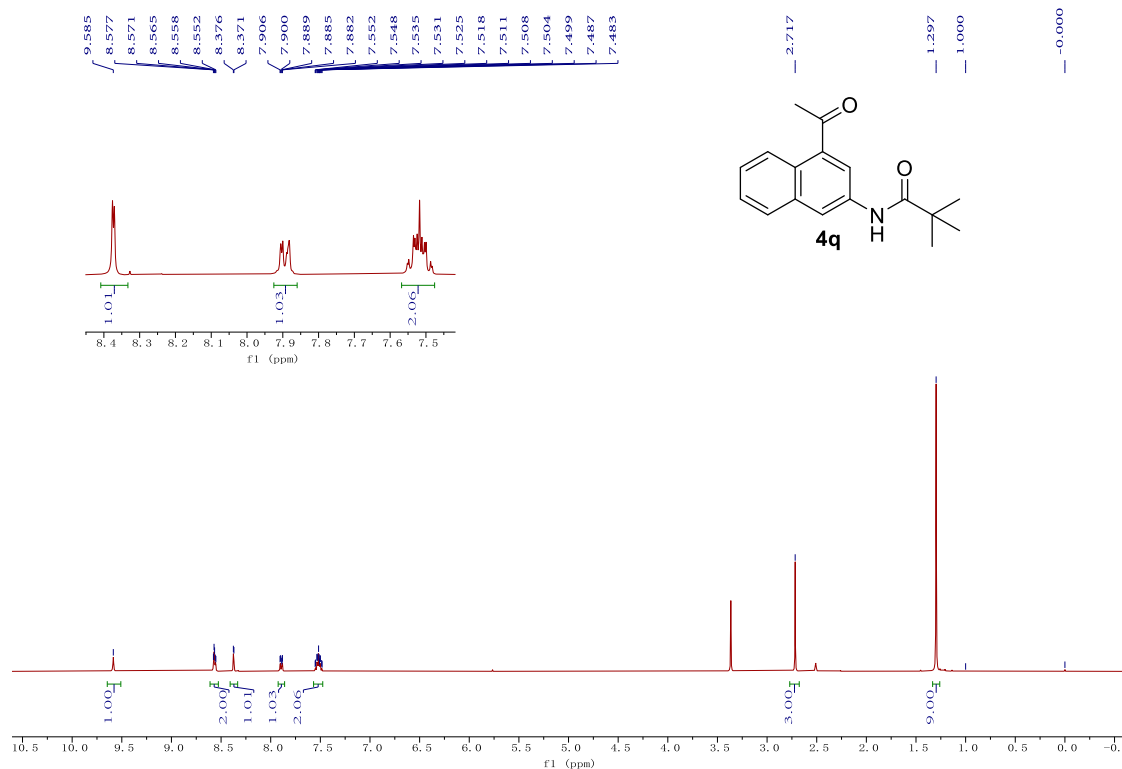
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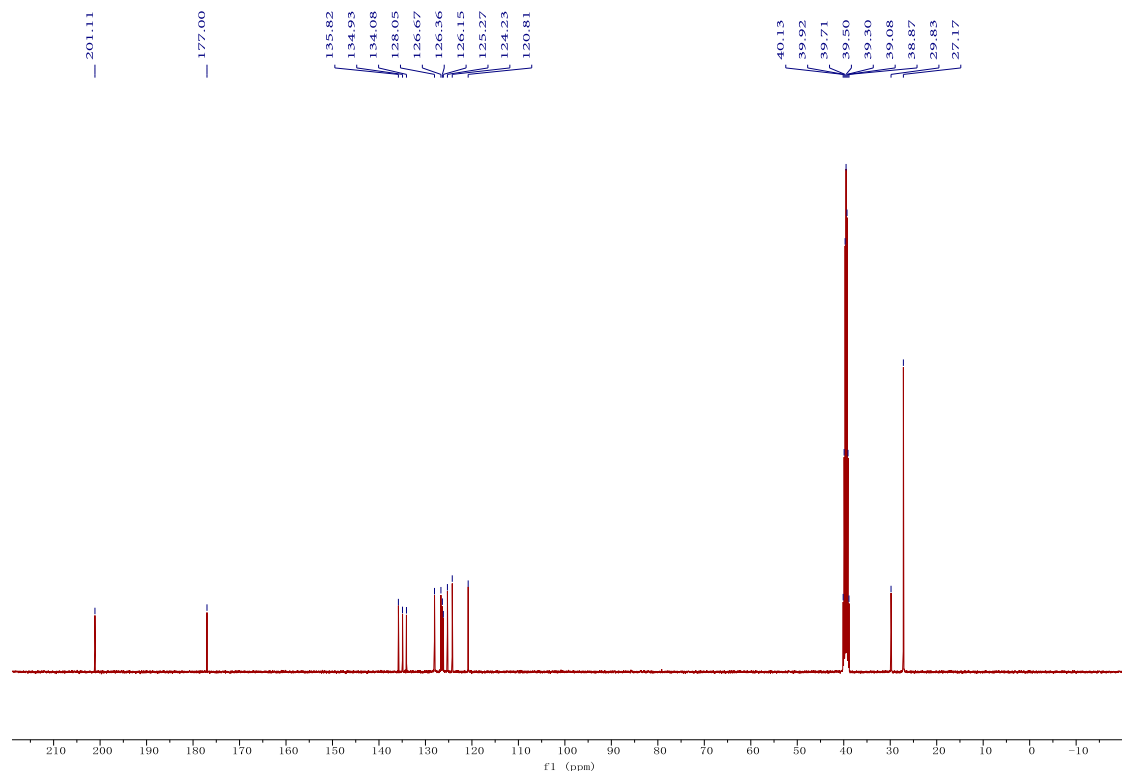


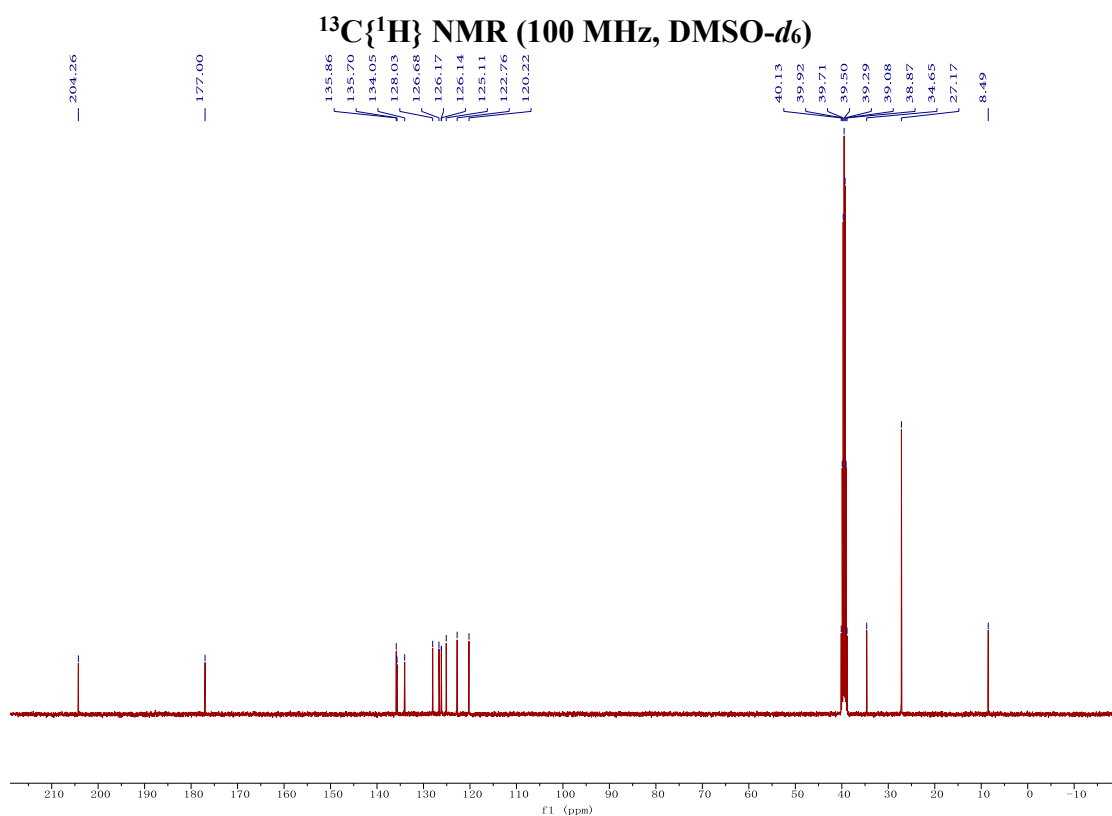
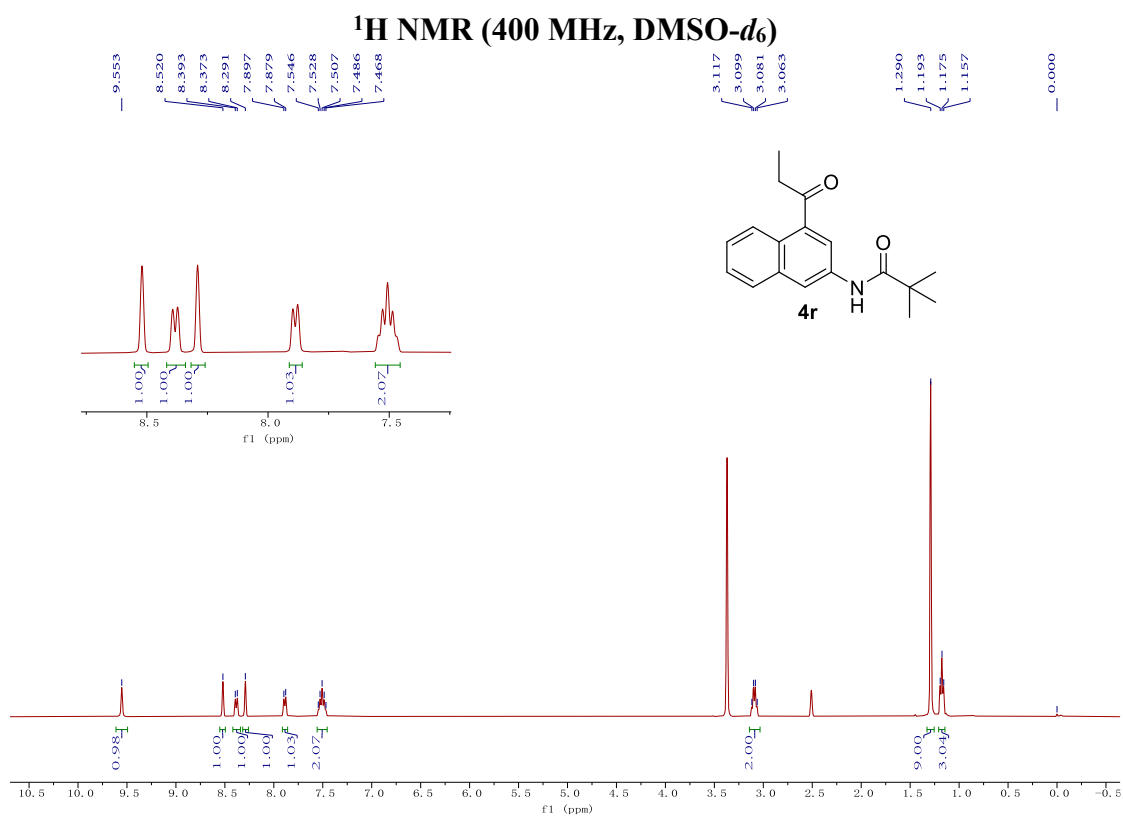


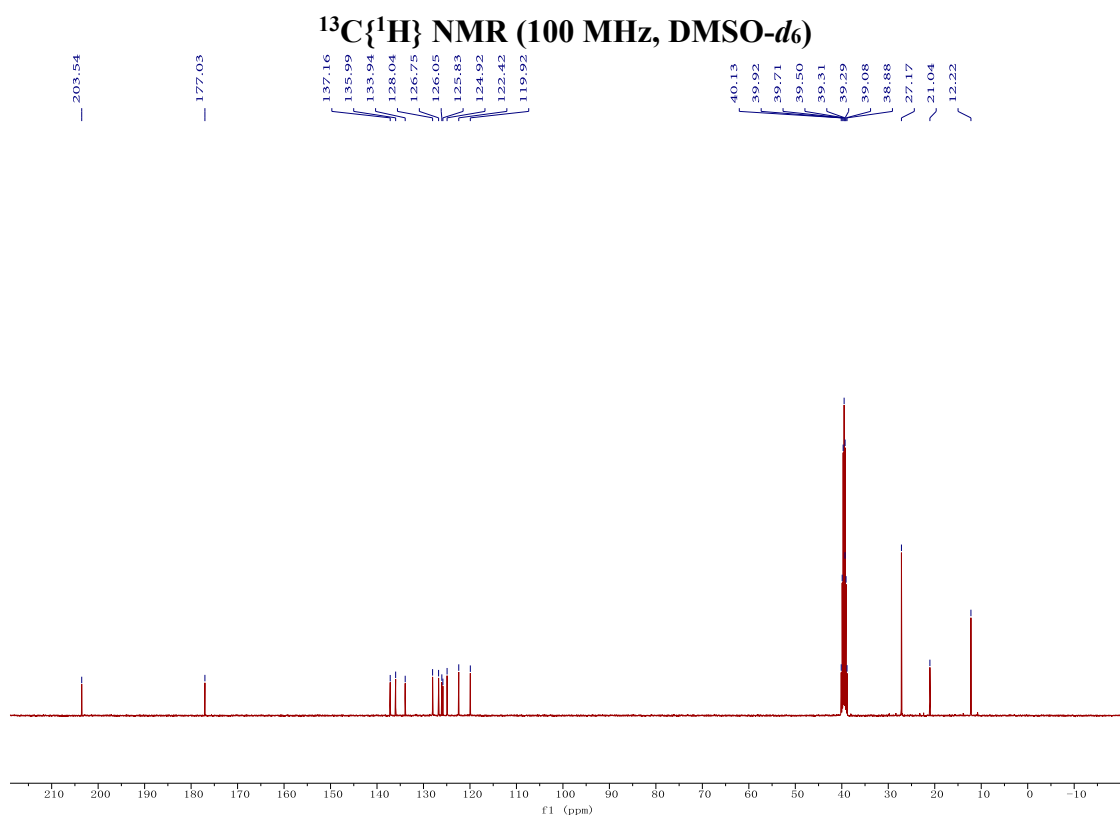
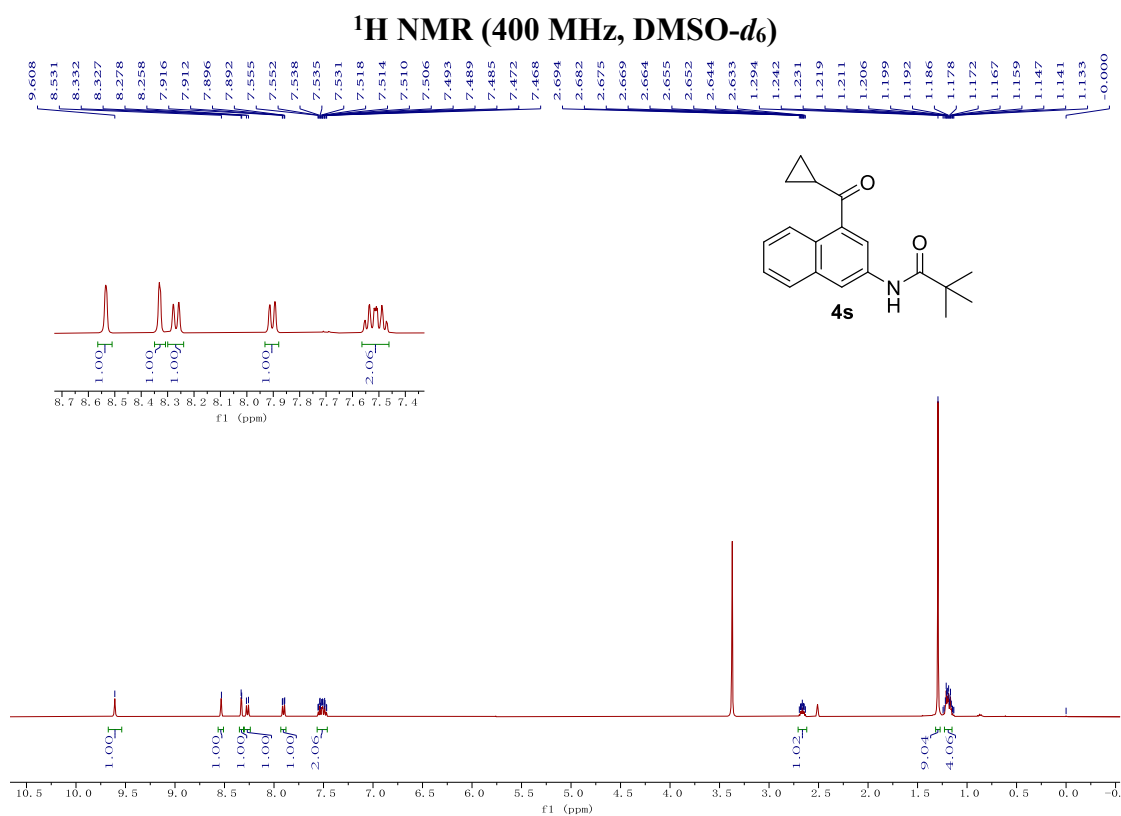
¹H NMR (400 MHz, DMSO-d₆)



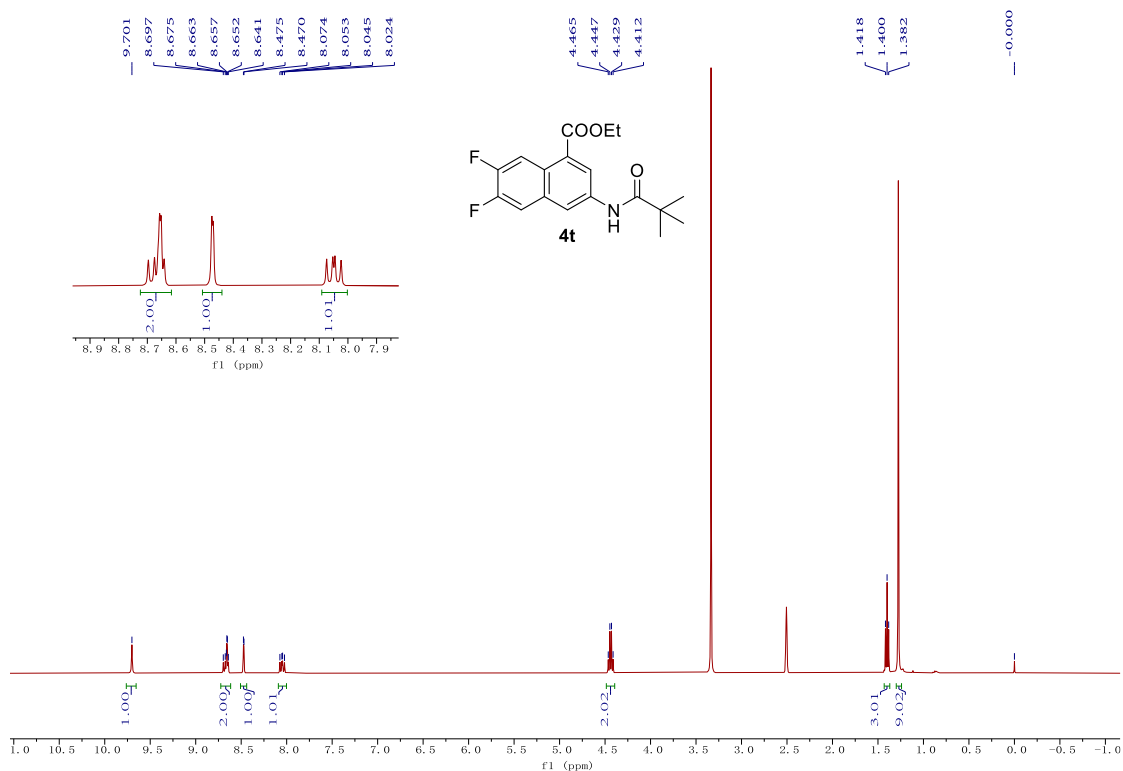
¹³C{¹H} NMR (100 MHz, DMSO-d₆)



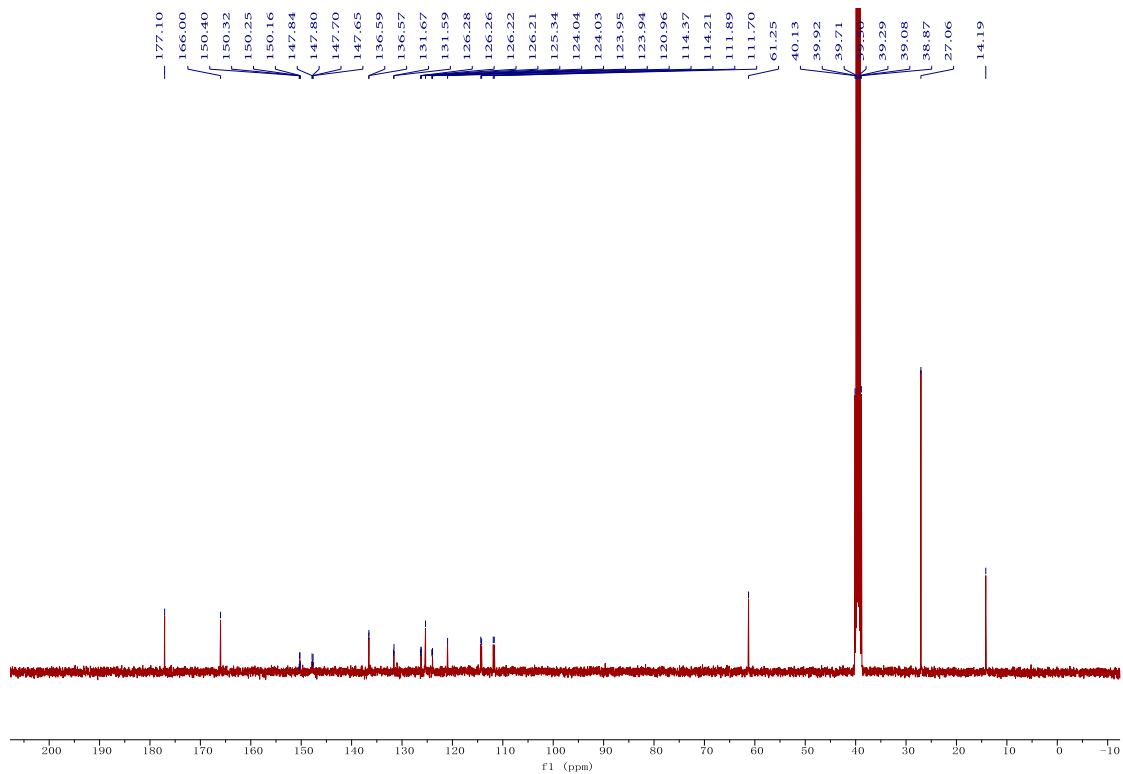




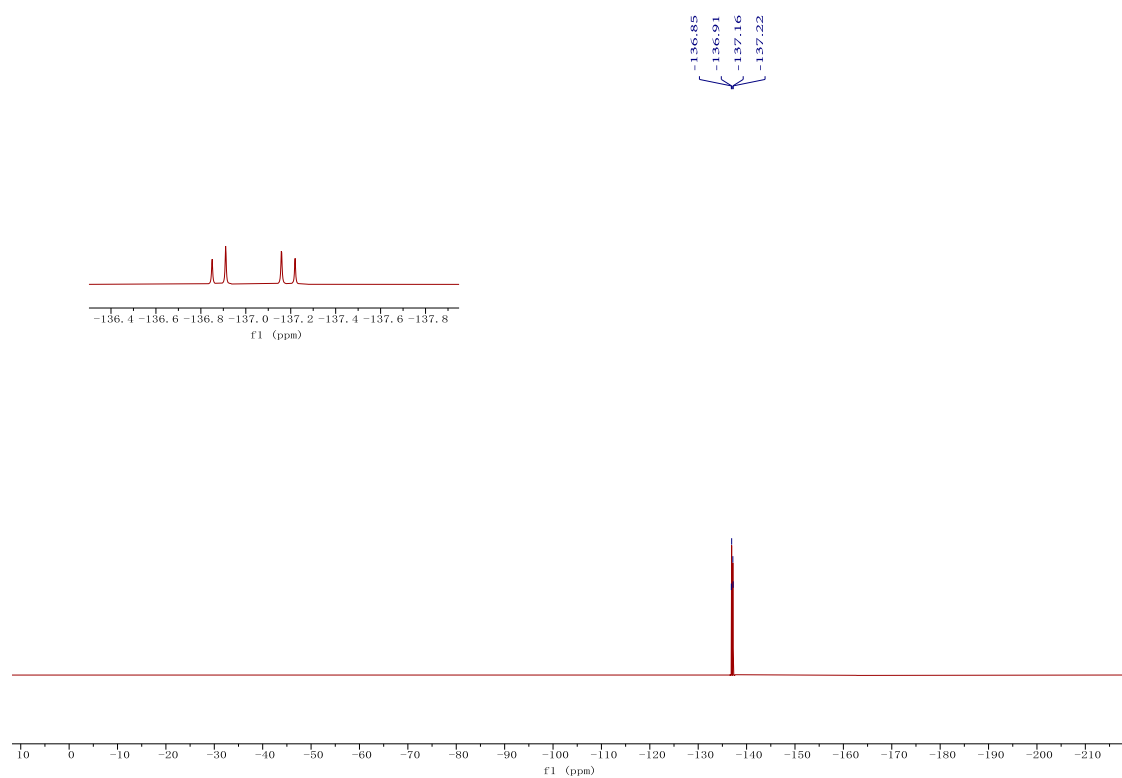
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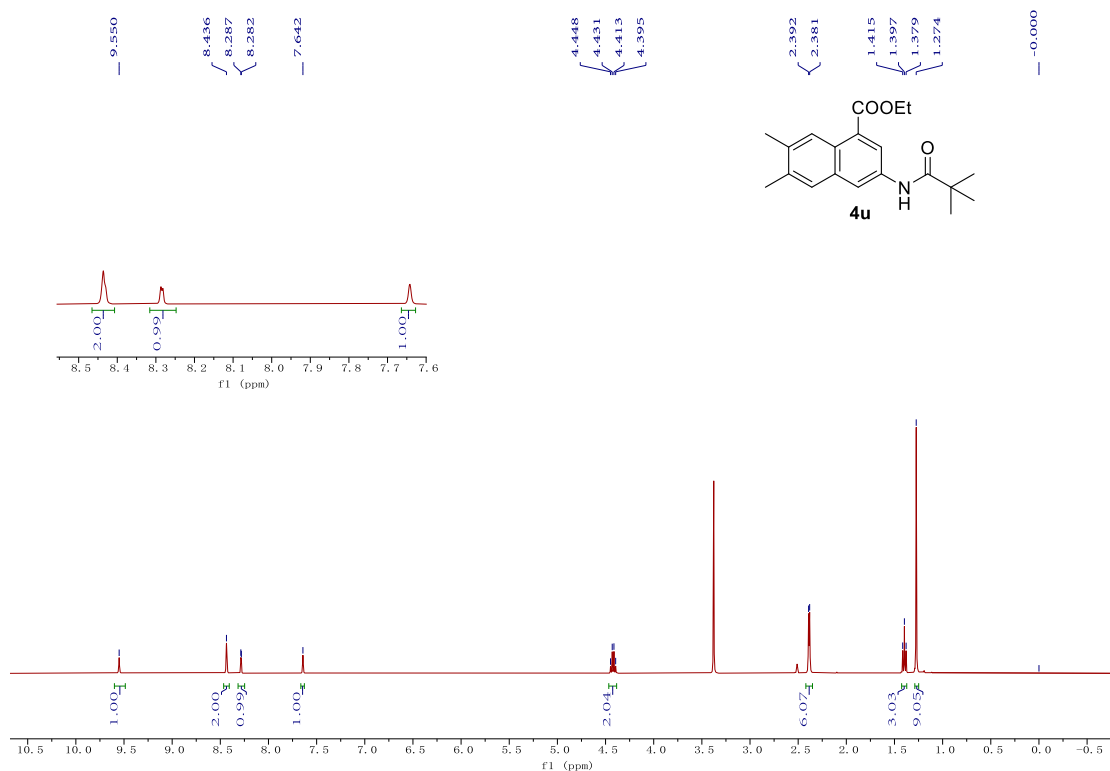
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆)



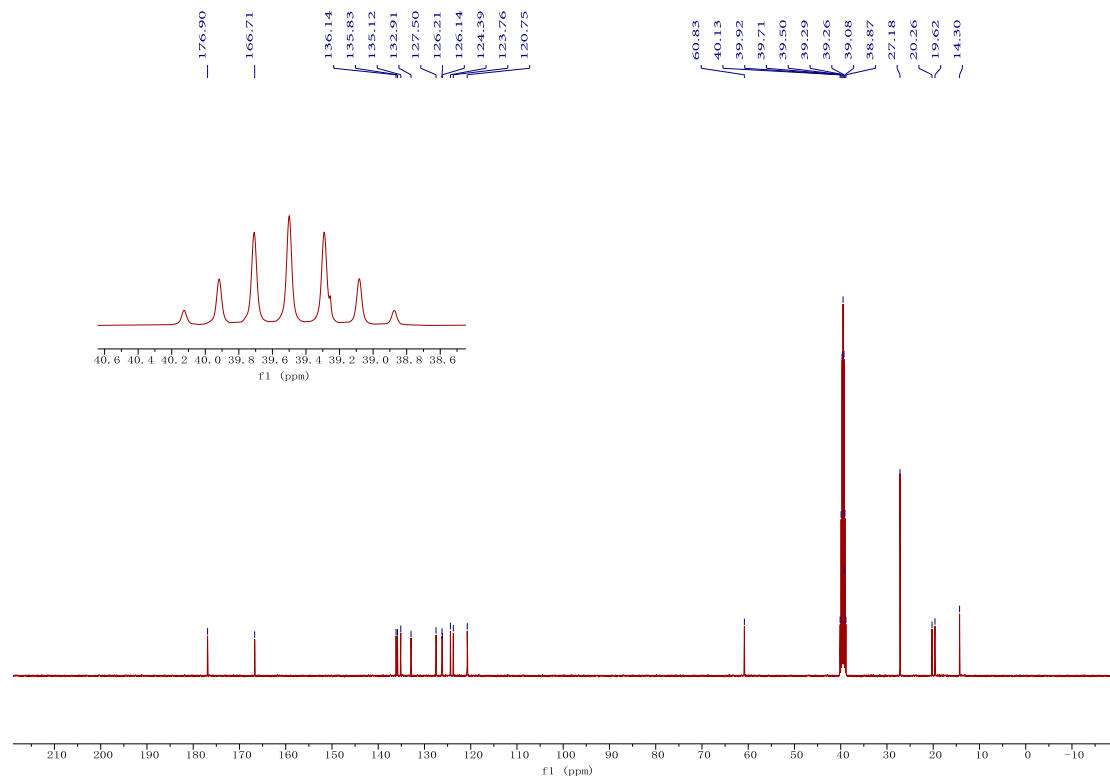
$^{19}\text{F}\{^1\text{H}\}$ (376 MHz, DMSO- d_6)



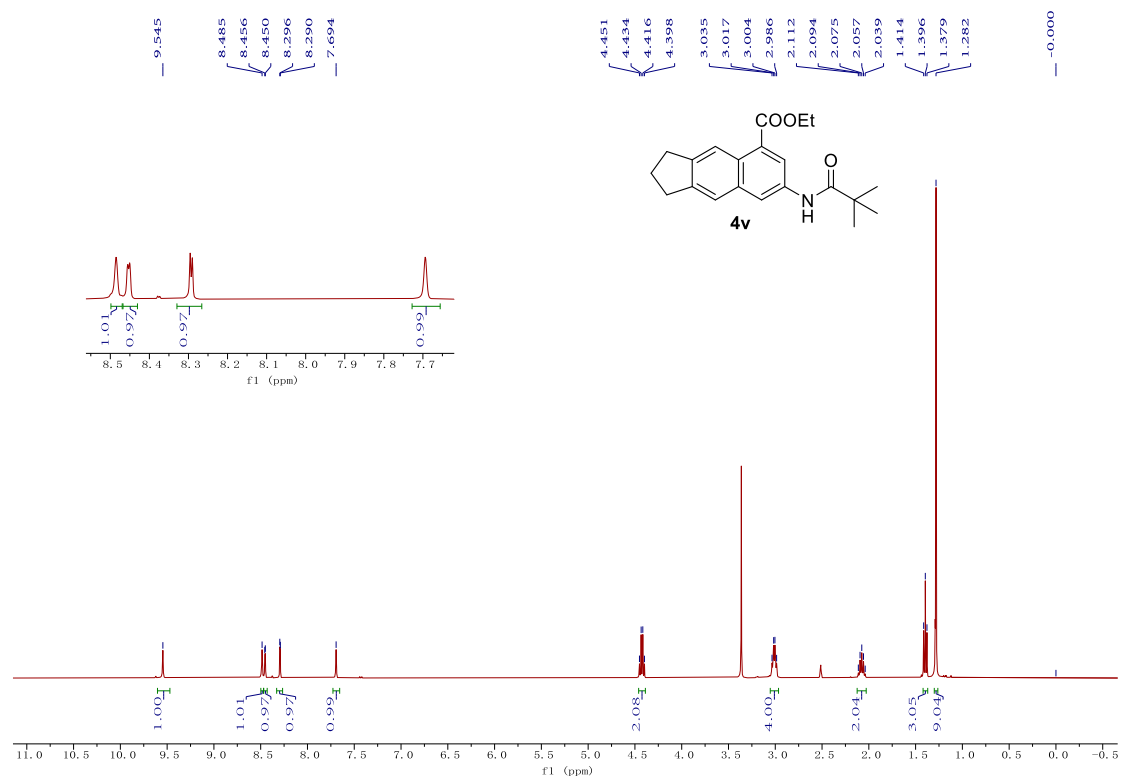
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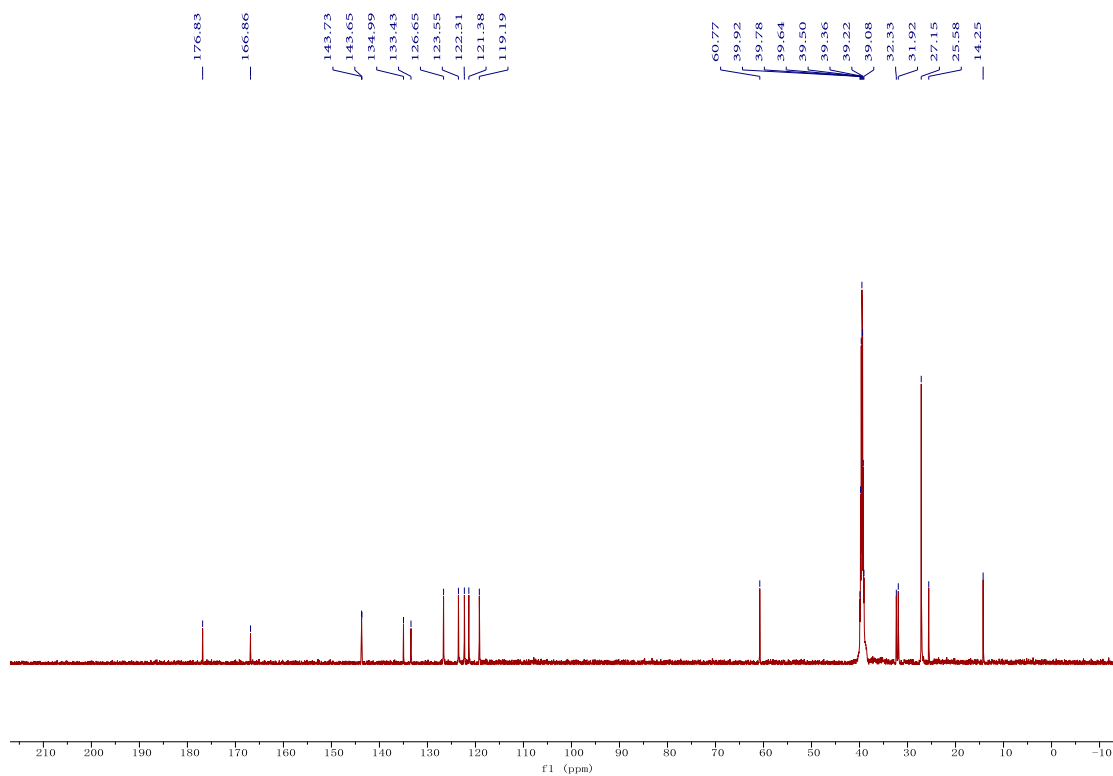
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆)



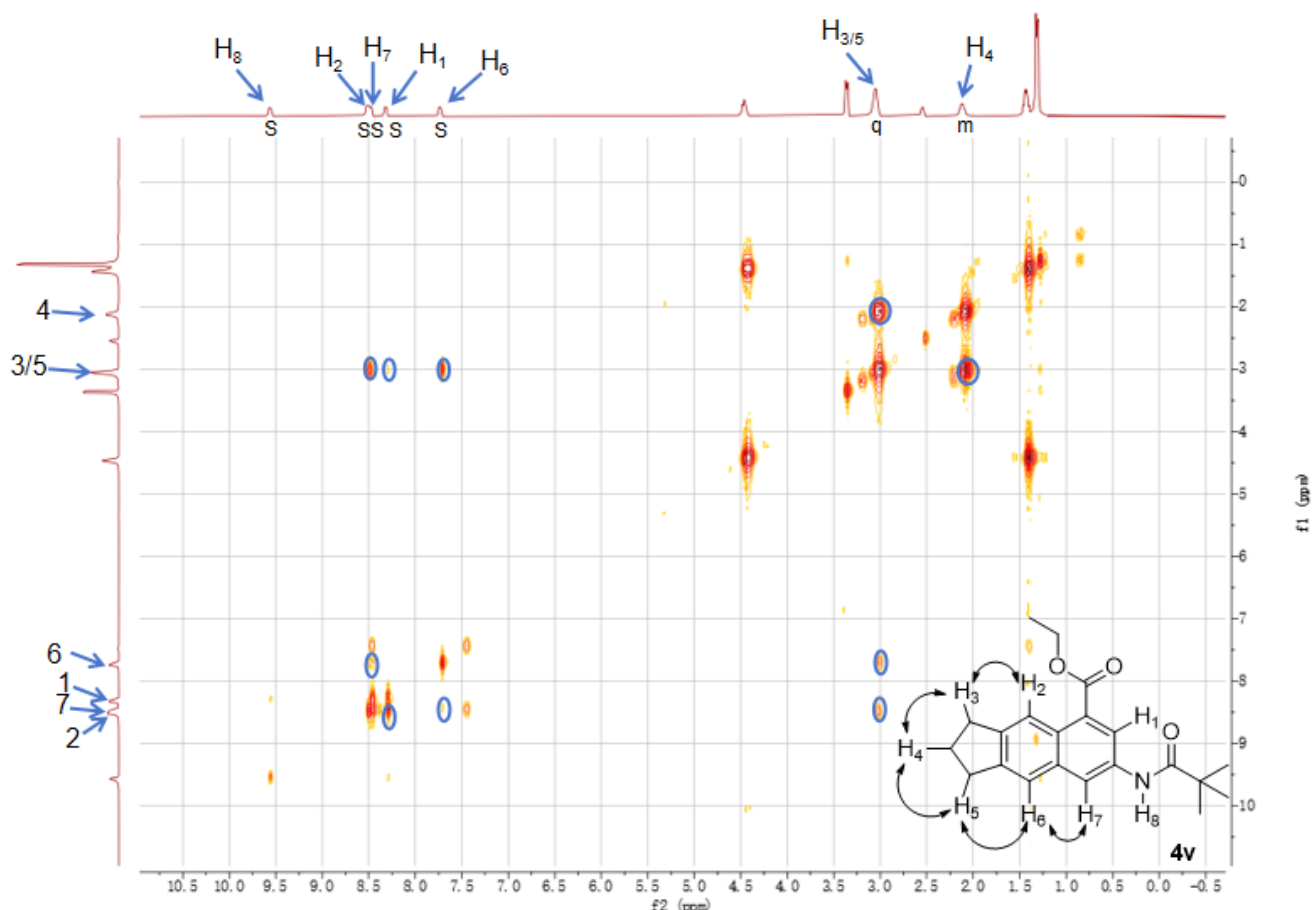
¹H NMR (400 MHz, DMSO-*d*₆)



¹³C{¹H} NMR (125 MHz, DMSO-*d*₆)



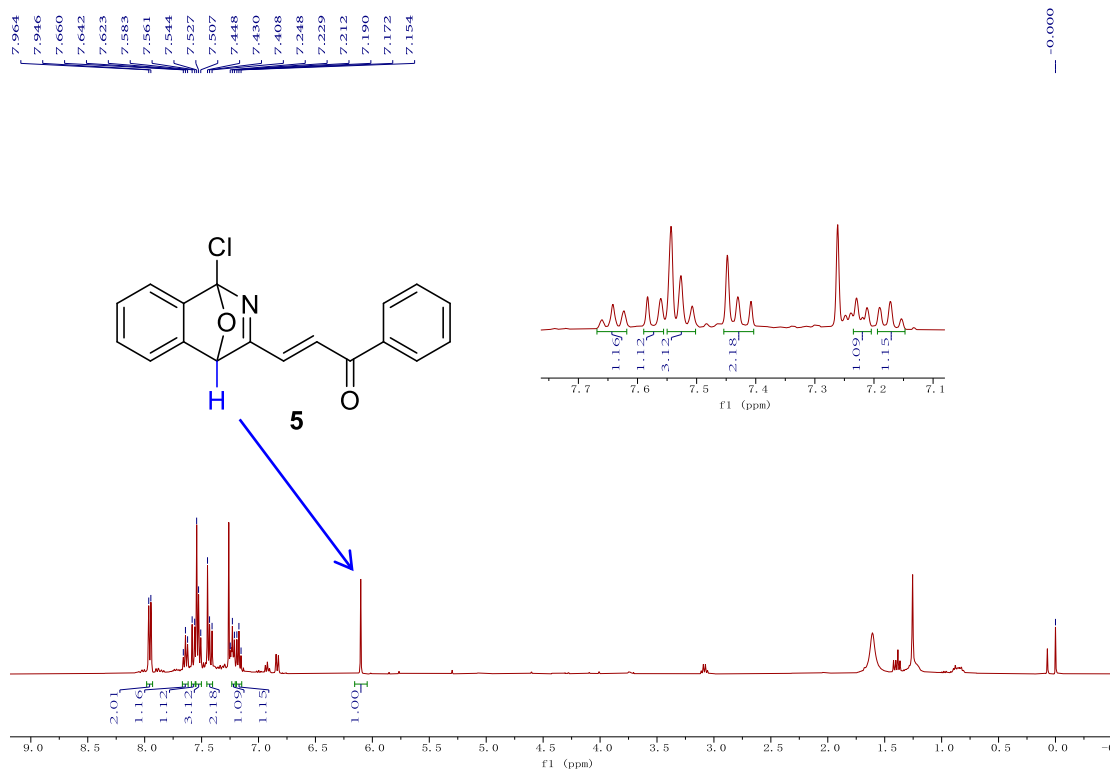
2D ^1H - ^1H COSY



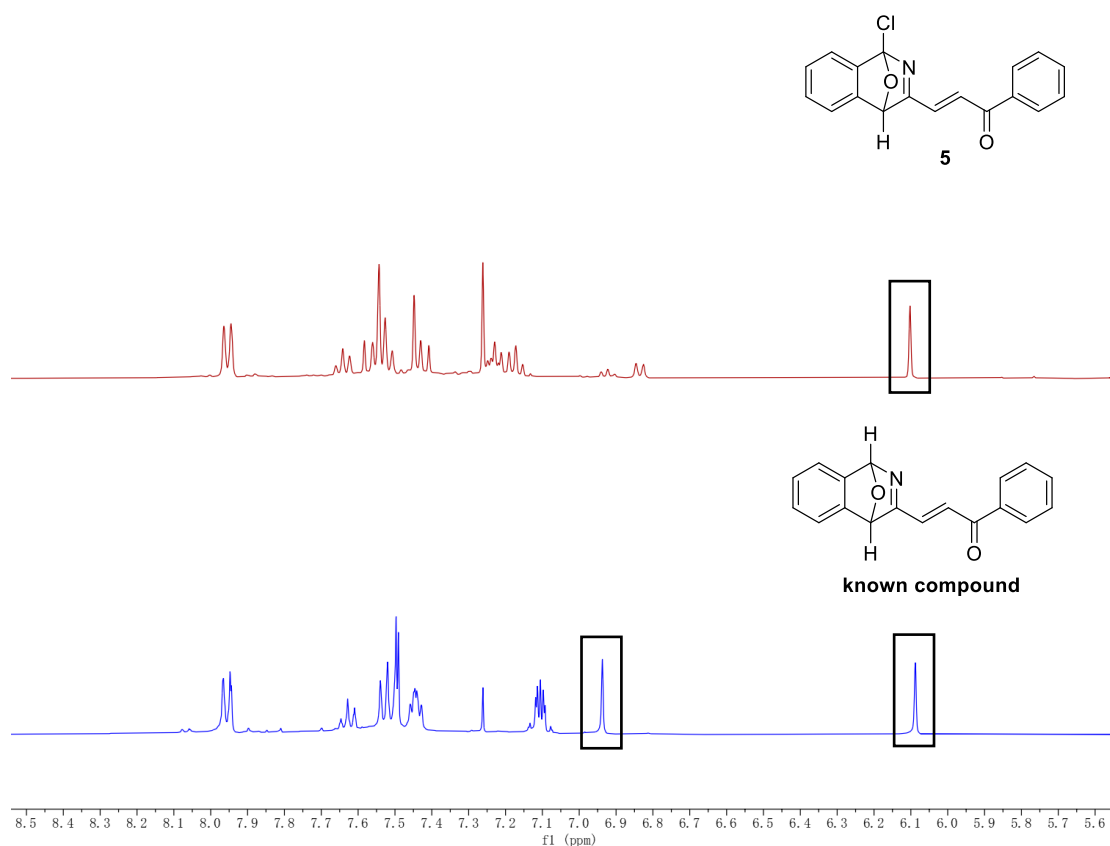
The hydrogen atoms were assigned based on the fine splitting patterns observed in the 1D NMR spectrum, and the assignments were subsequently verified by the 2D ^1H - ^1H COSY spectrum of **4v**

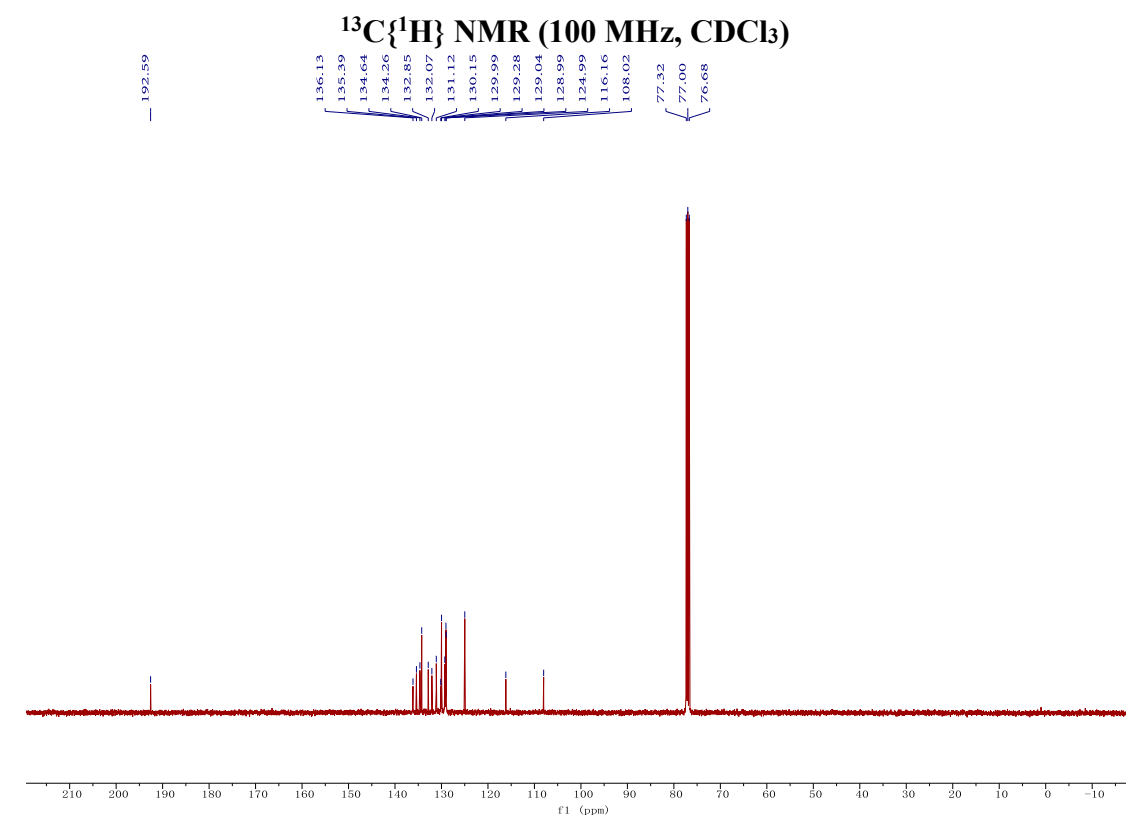
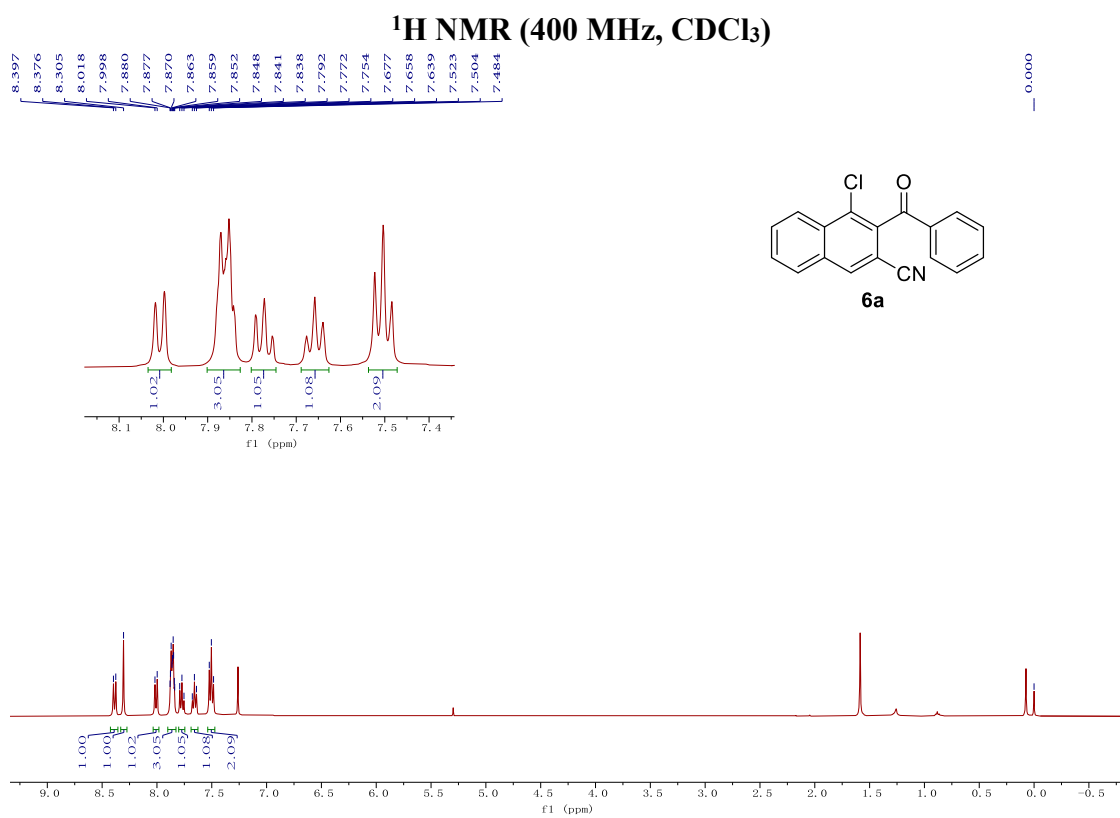
The coupling correlations indicate that there is strong coupling between **H**_{3/5} and **H**₄, suggesting that **H**_{3/5} and **H**₄ are all hydrogen atoms on the five-membered ring. In addition, **H**_{3/5} also show coupling with **H**₂ and **H**₆ in the aromatic region, which allows preliminary confirmation of the indene ring framework. Further analysis of the coupling patterns in the aromatic region reveals varying degrees of coupling among **H**₁, **H**₂, **H**₆, and **H**₇, suggesting that these hydrogen atoms are likely located within the same aromatic ring system.

^1H NMR (400 MHz, CDCl_3)

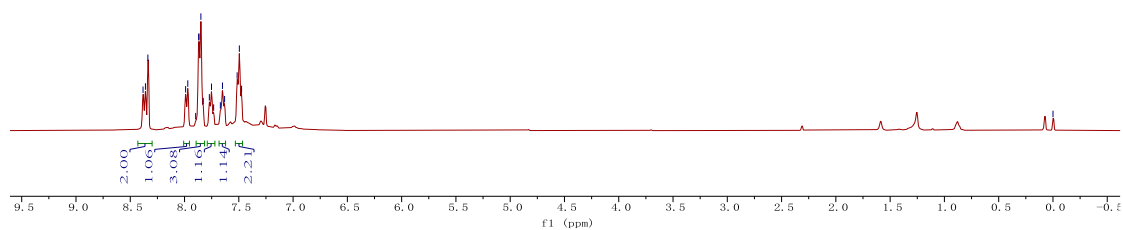
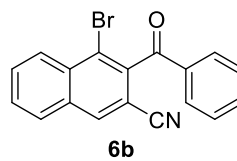
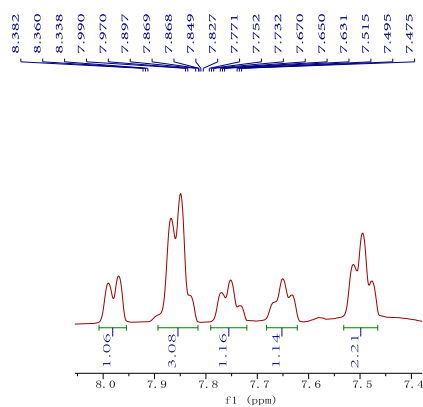


Compound **5** was highly sensitive, allowing only for the acquisition of ^1H NMR data. Therefore, a stacked spectral comparison was performed between compound **5** and the known compound (*E*)-3-(1,4-dihydro-1,4-epoxyisoquinolin-3-yl)-1-phenylprop-2-en-1-one (previously reported by our group).

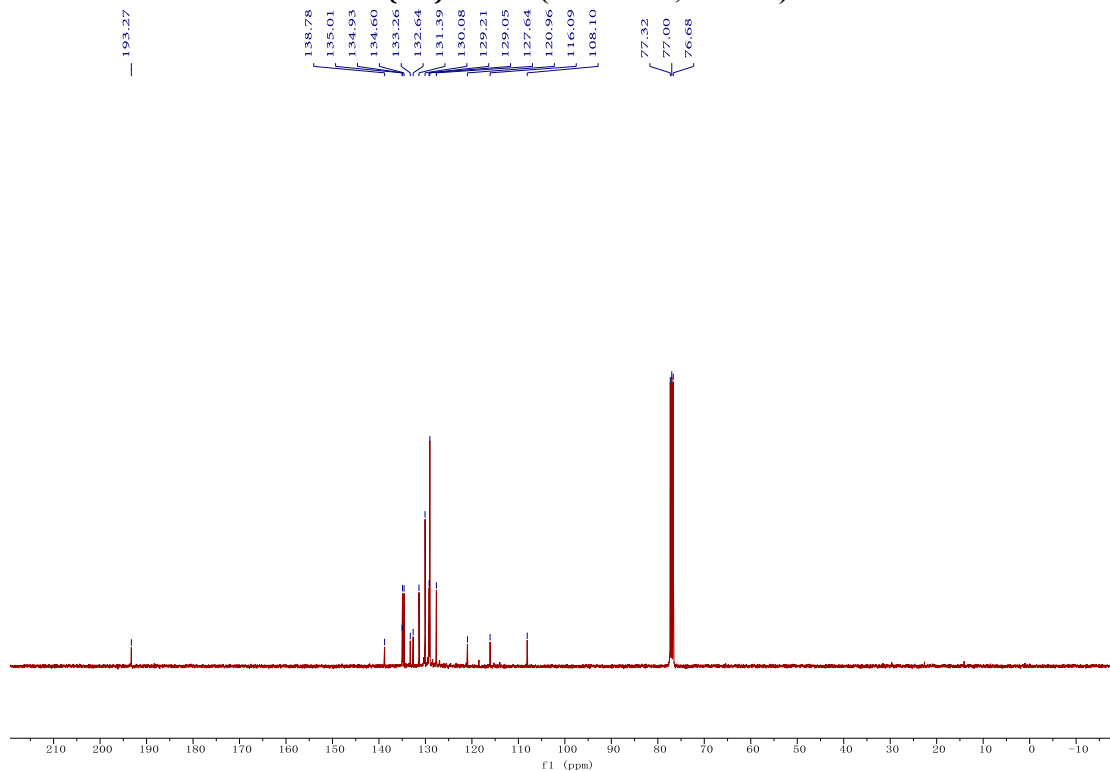


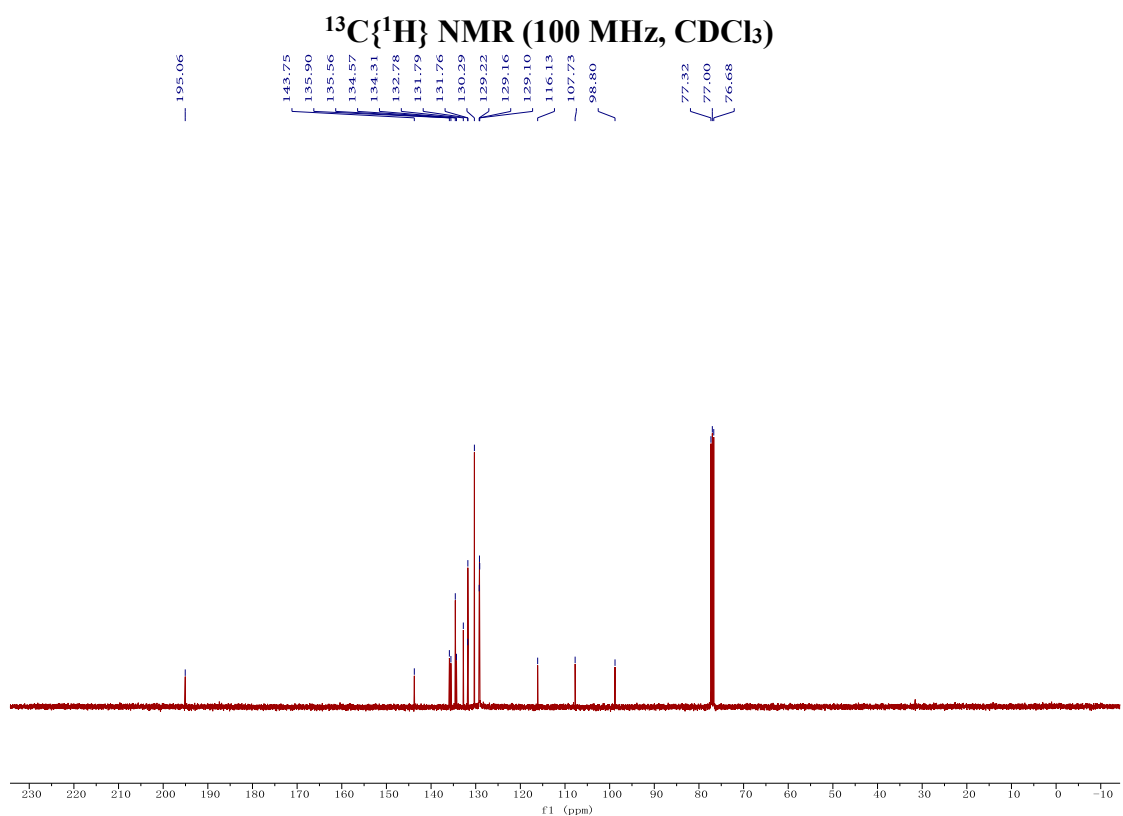
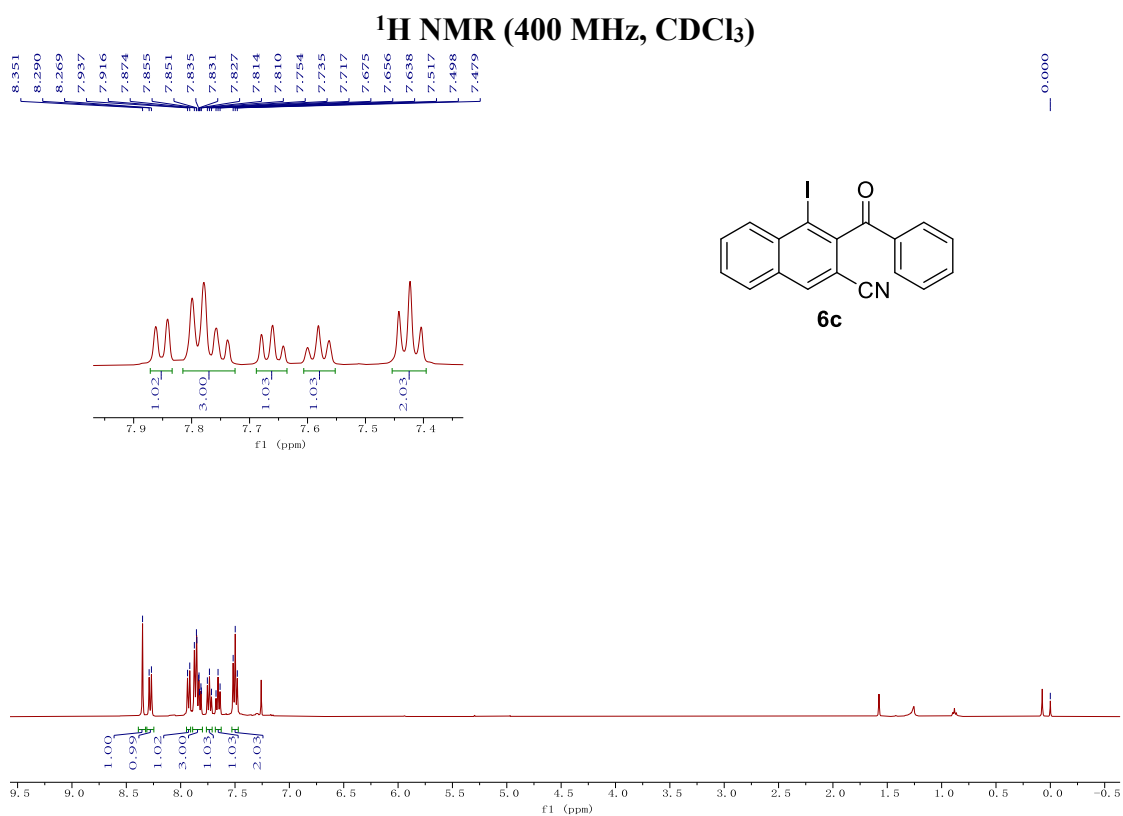


^1H NMR (400 MHz, CDCl_3)

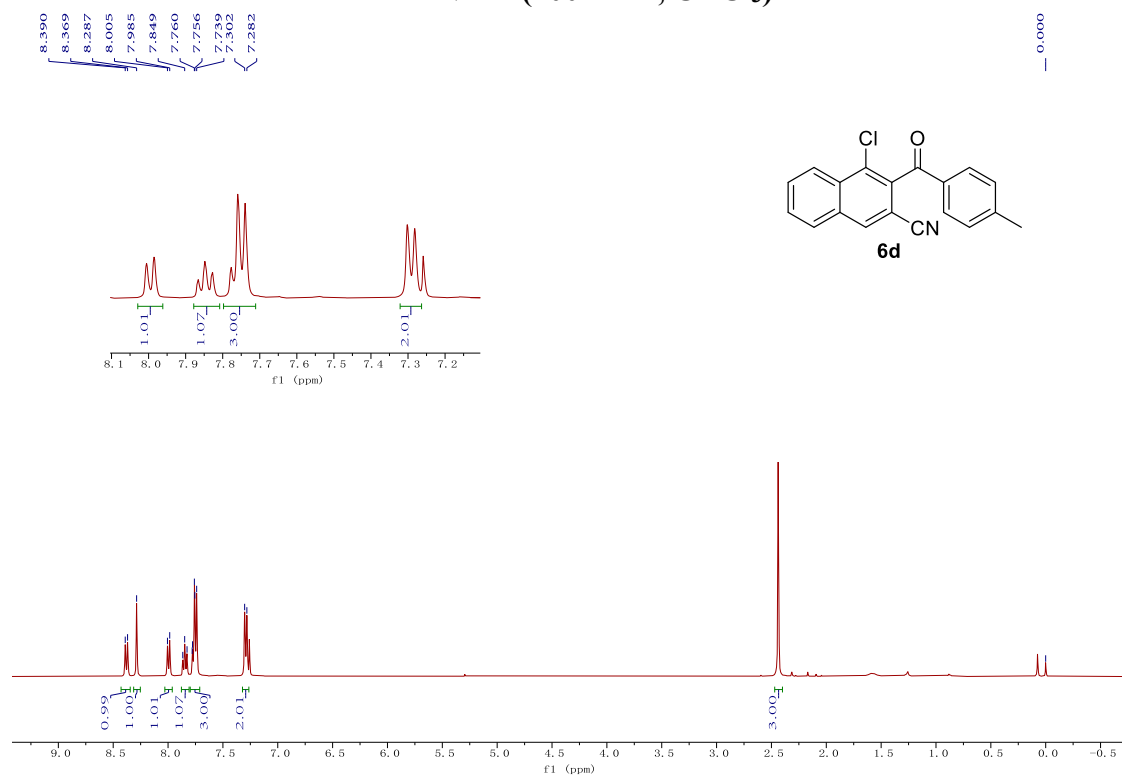


$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

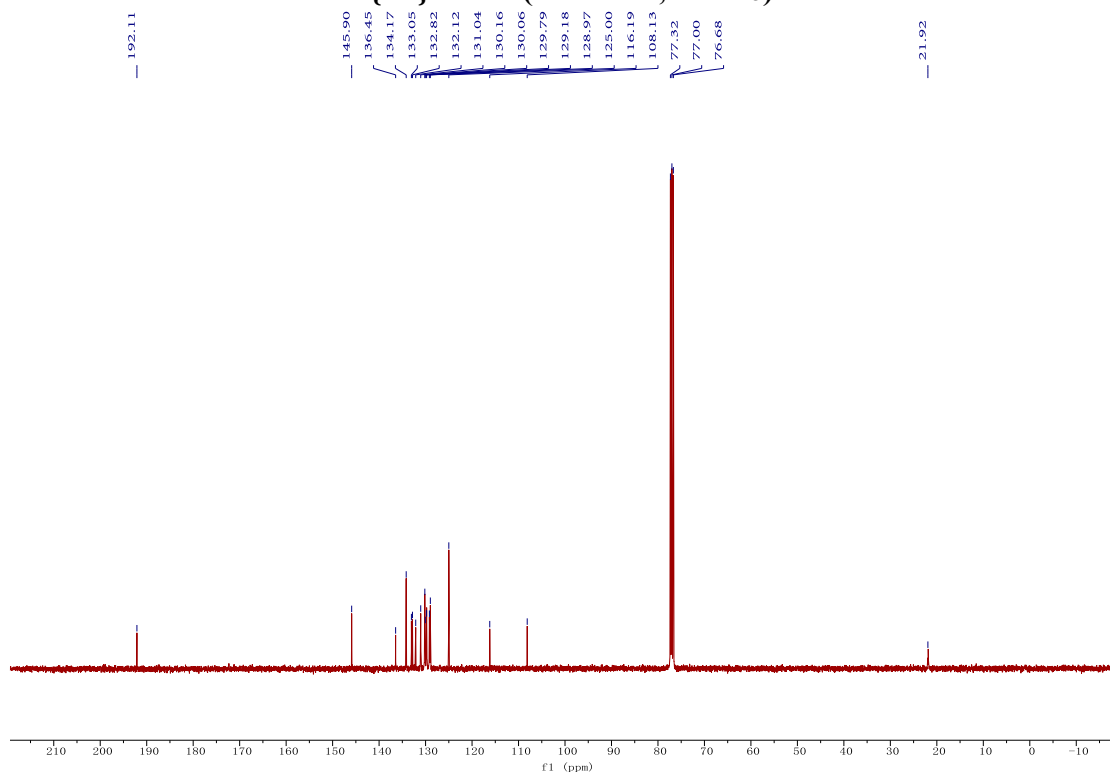


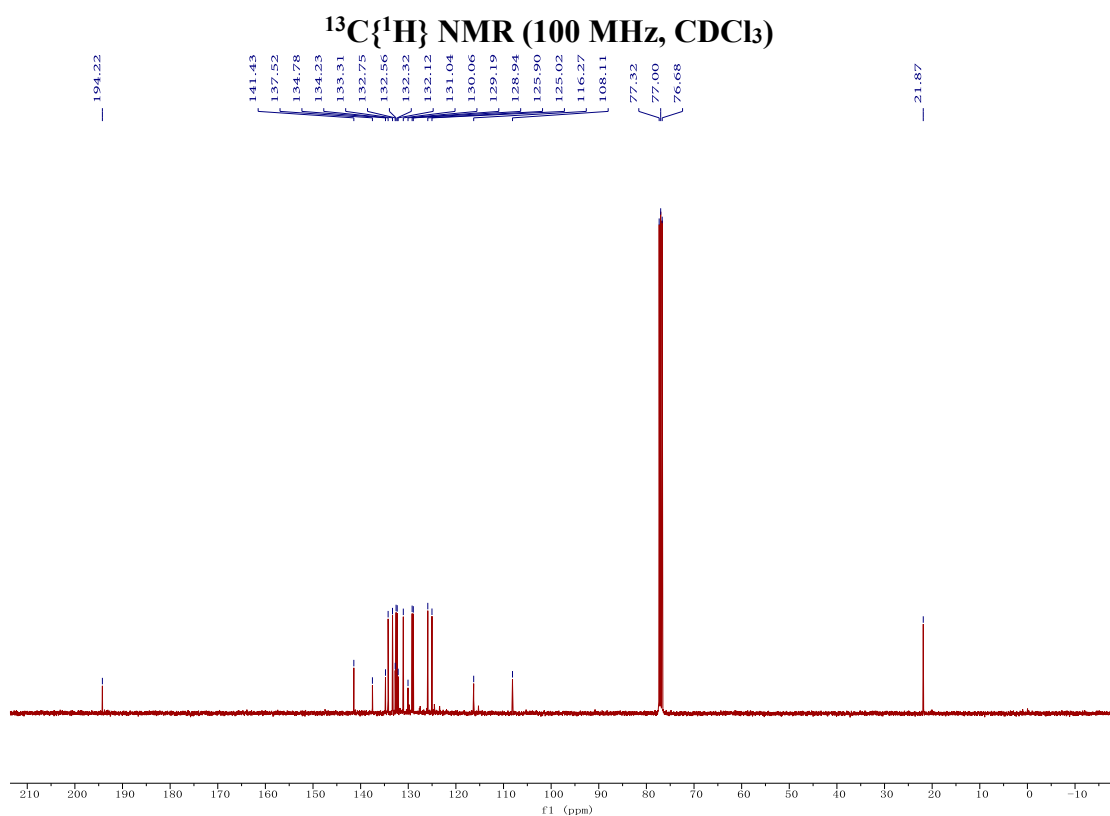
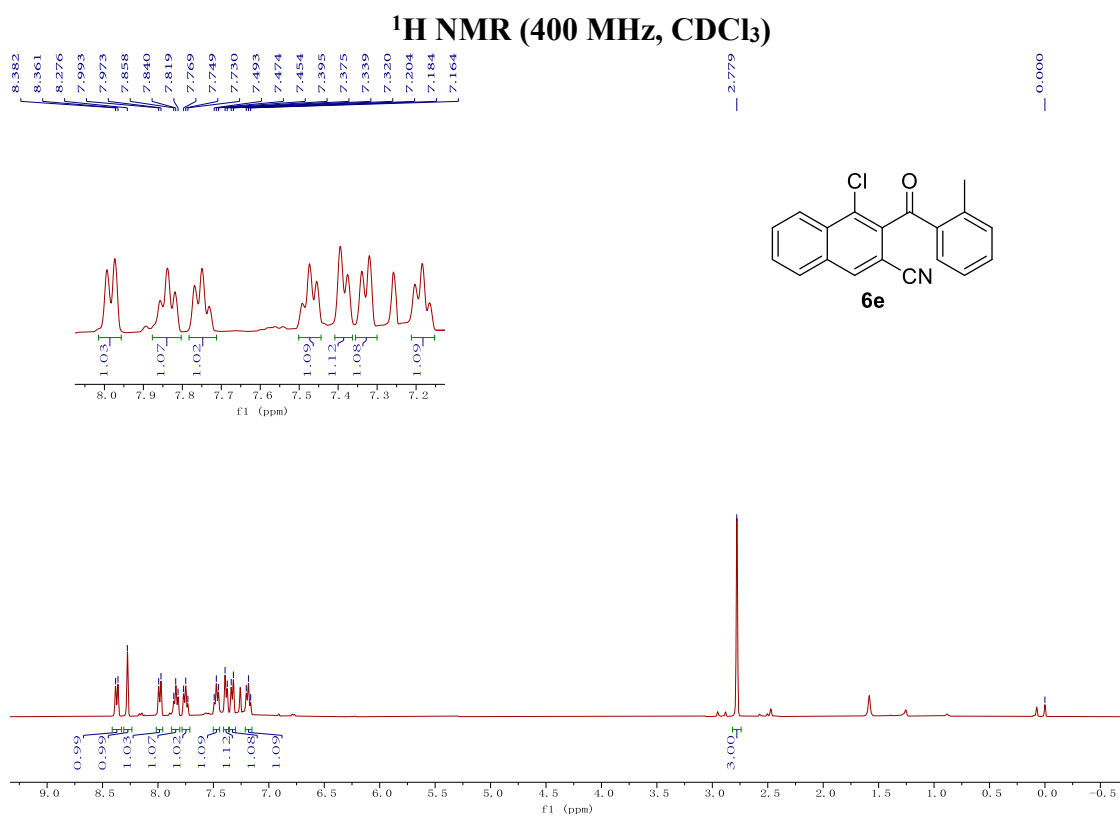


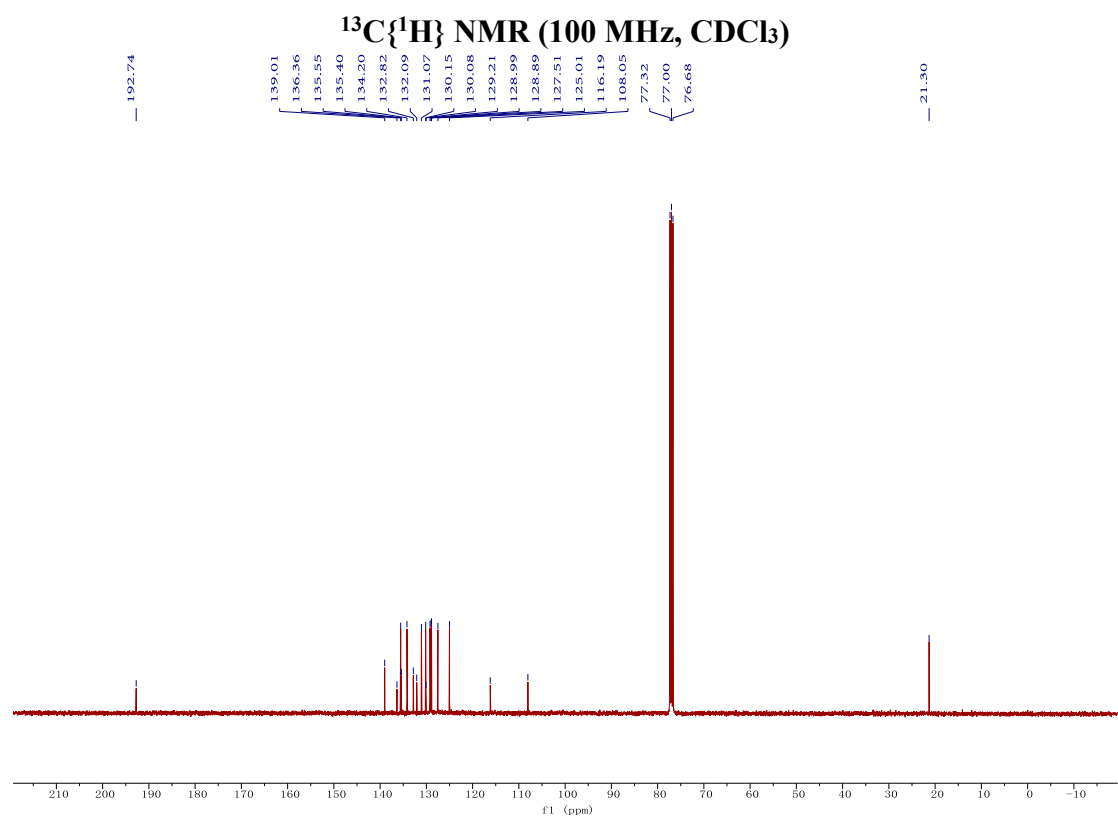
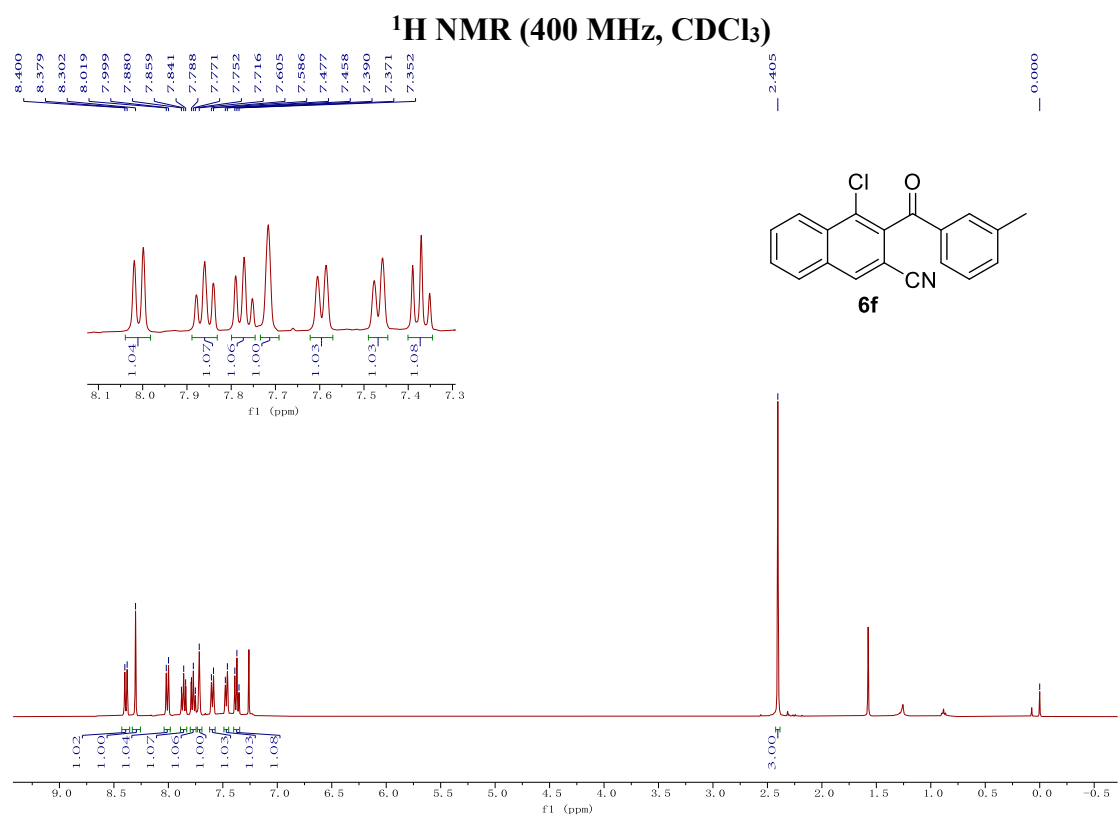
^1H NMR (400 MHz, CDCl_3)



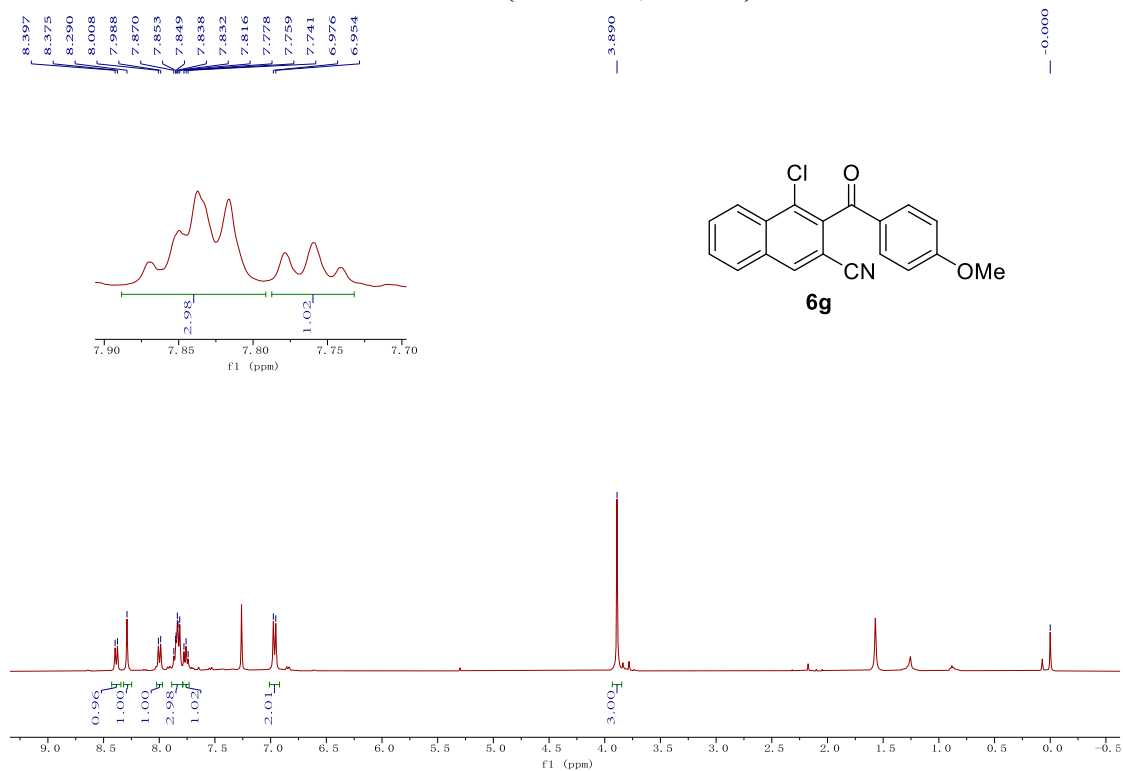
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



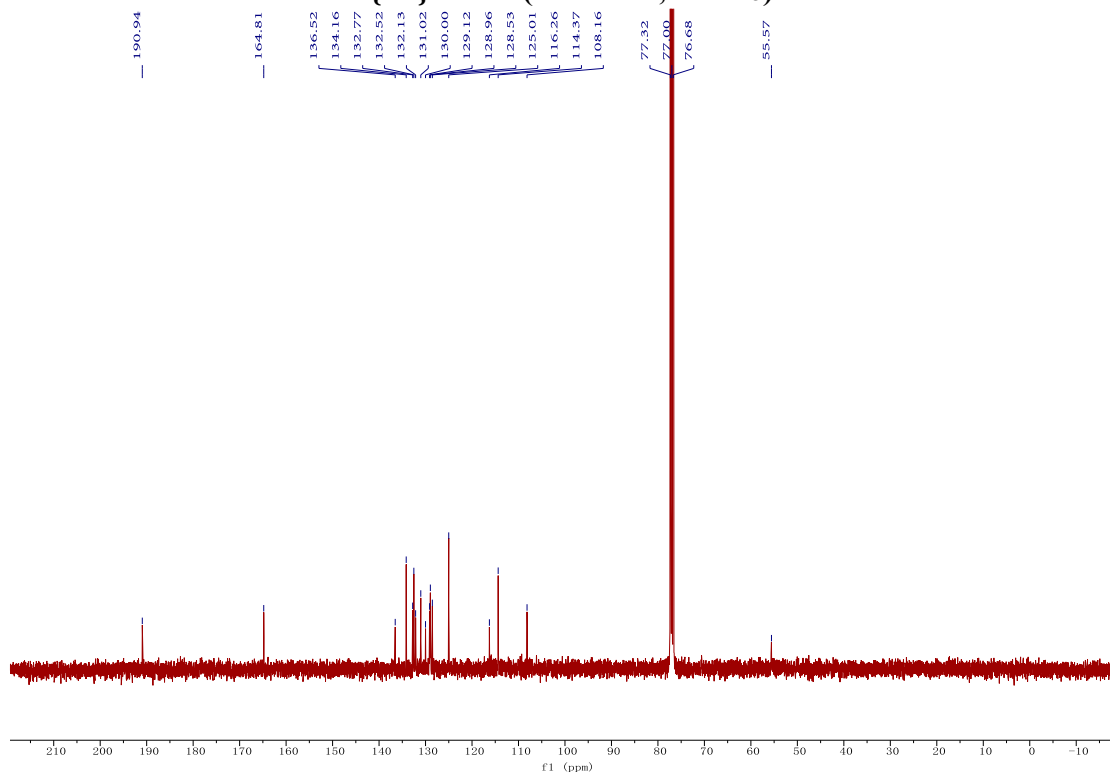


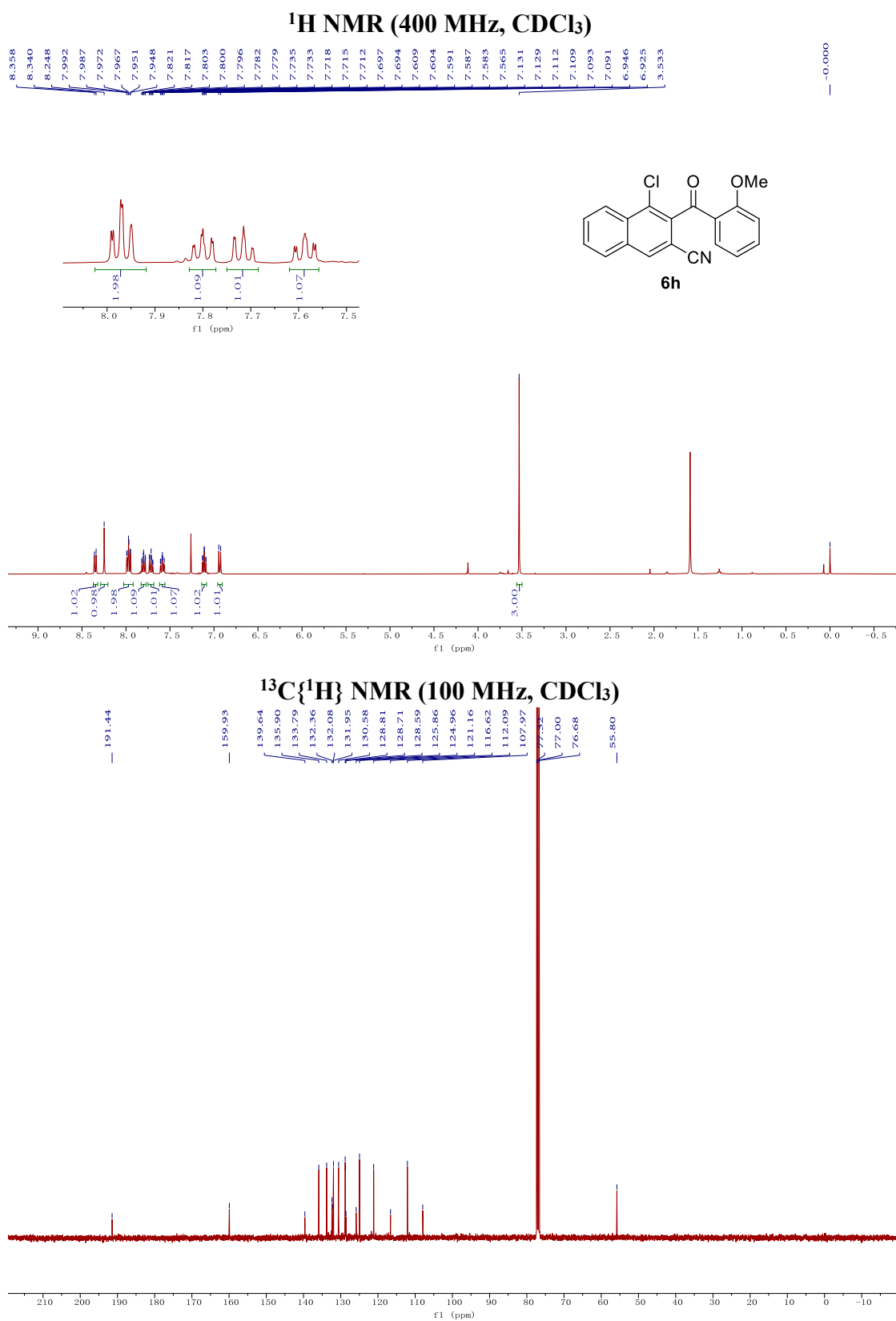


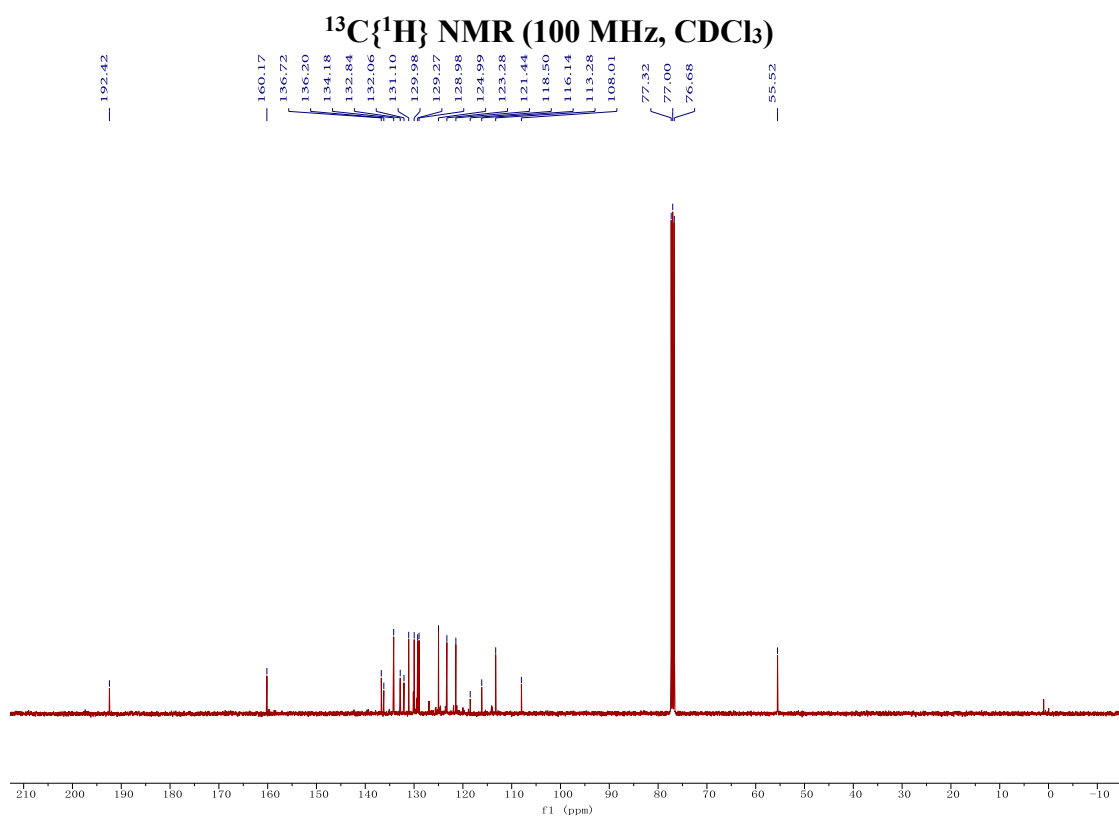
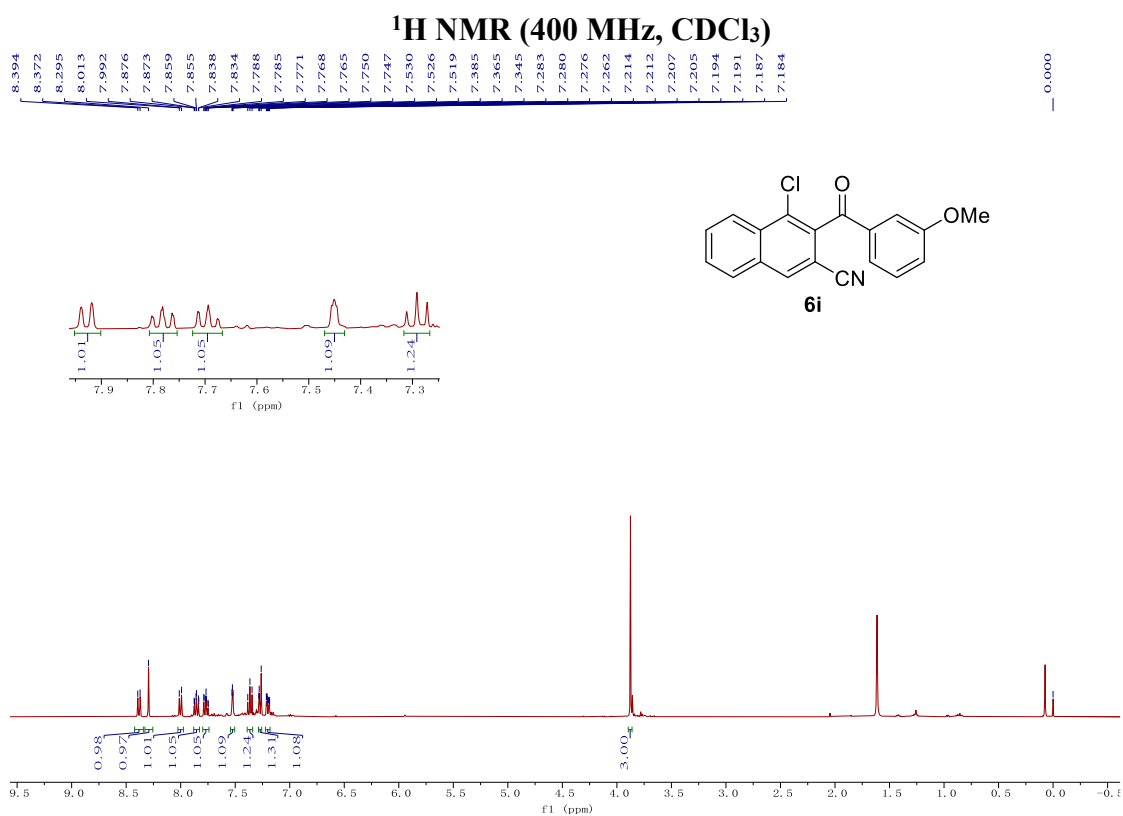
^1H NMR (400 MHz, CDCl_3)

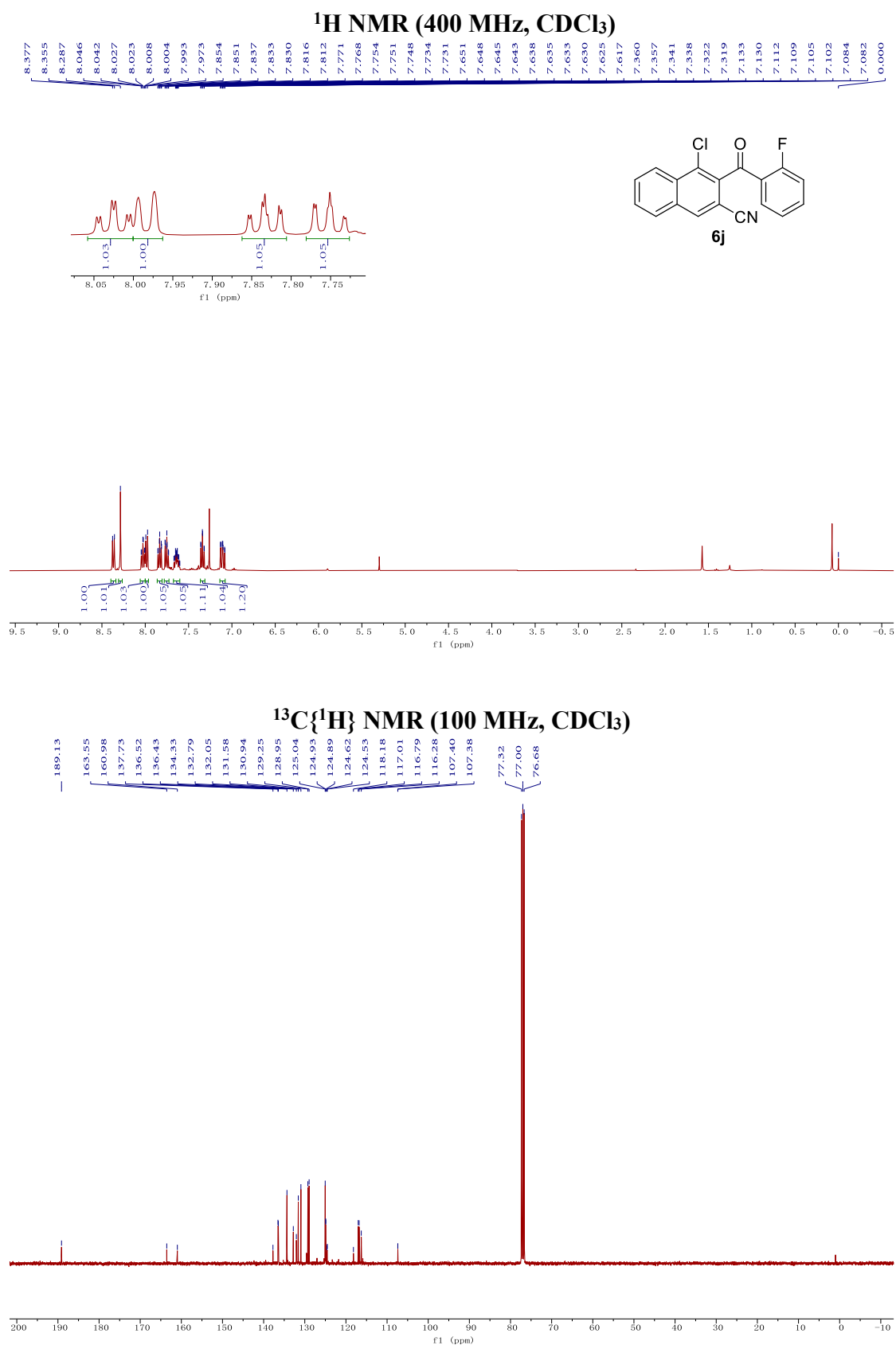


$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

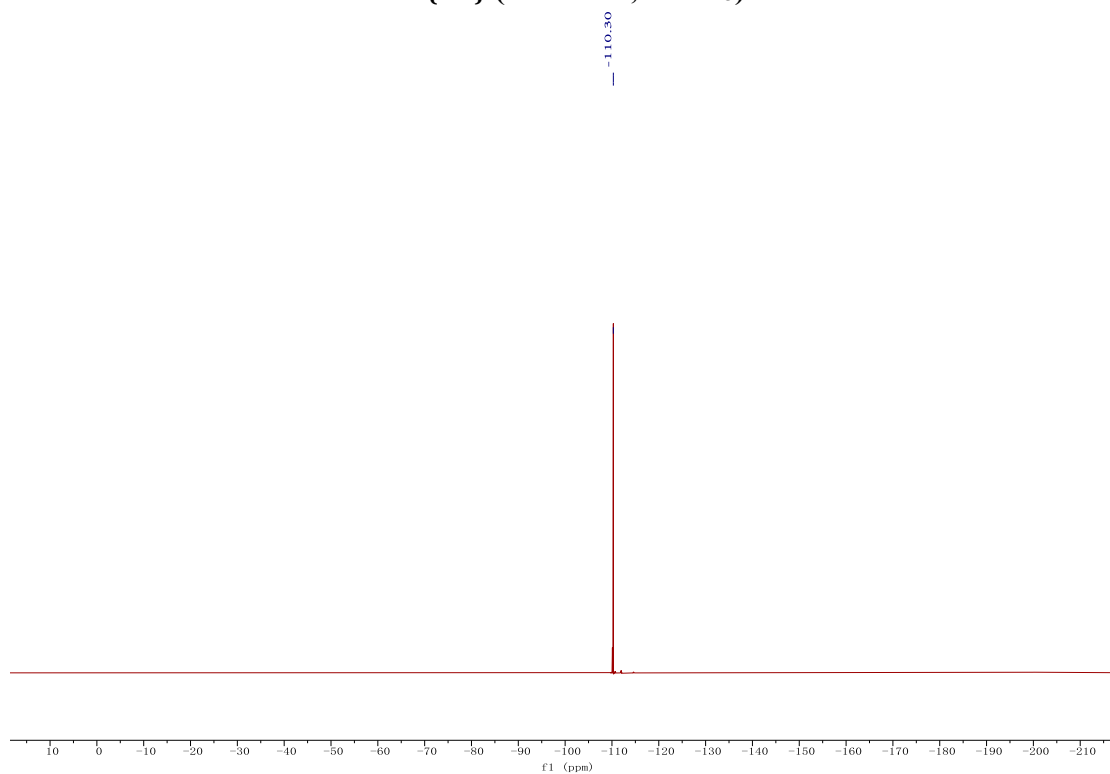


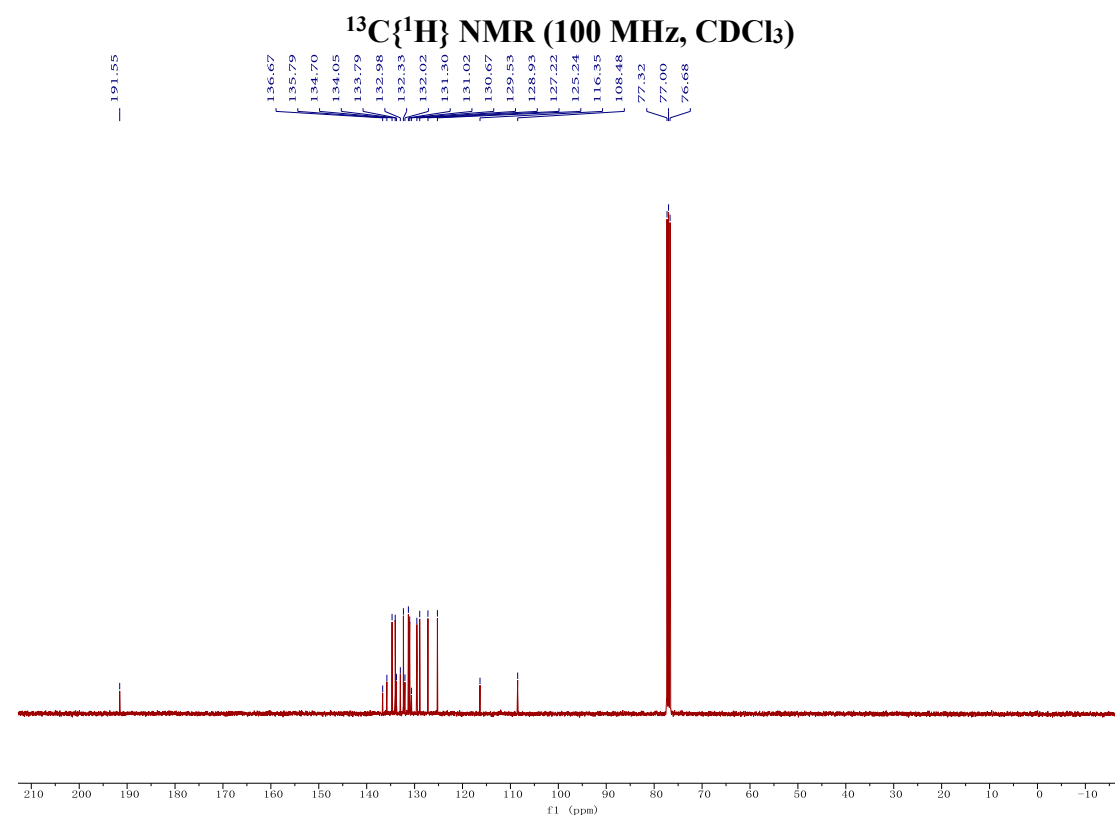
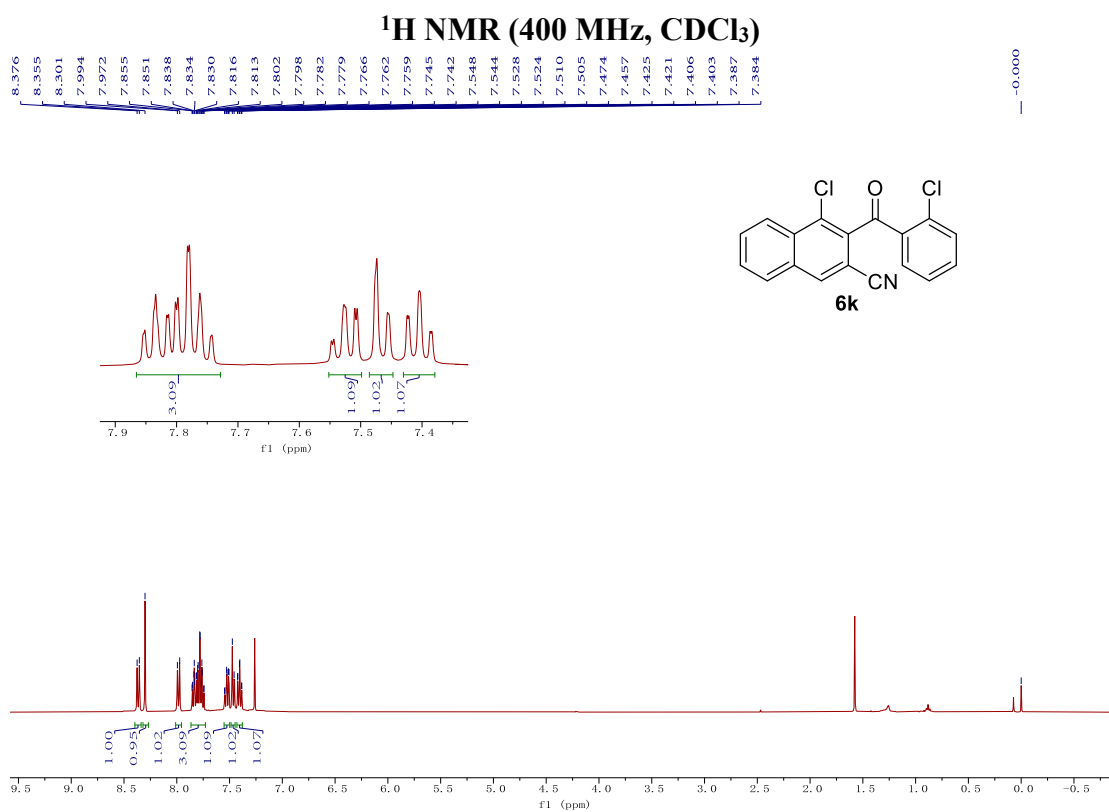


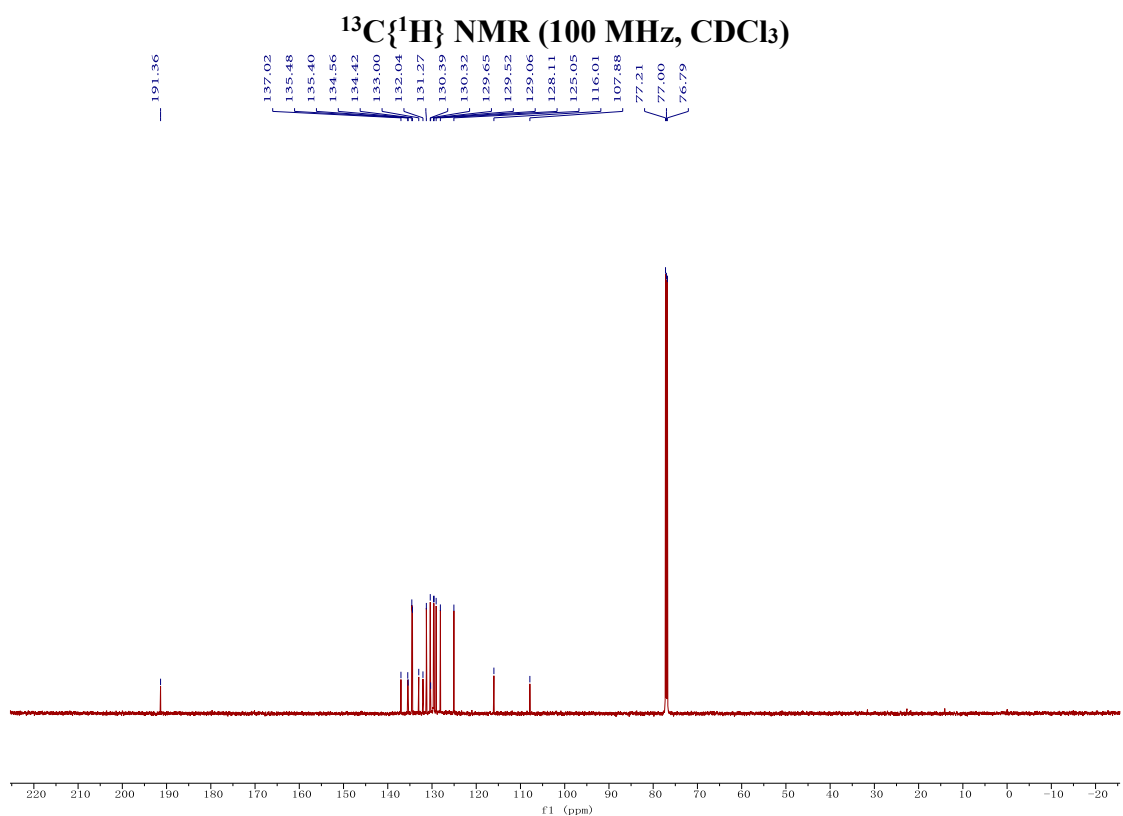
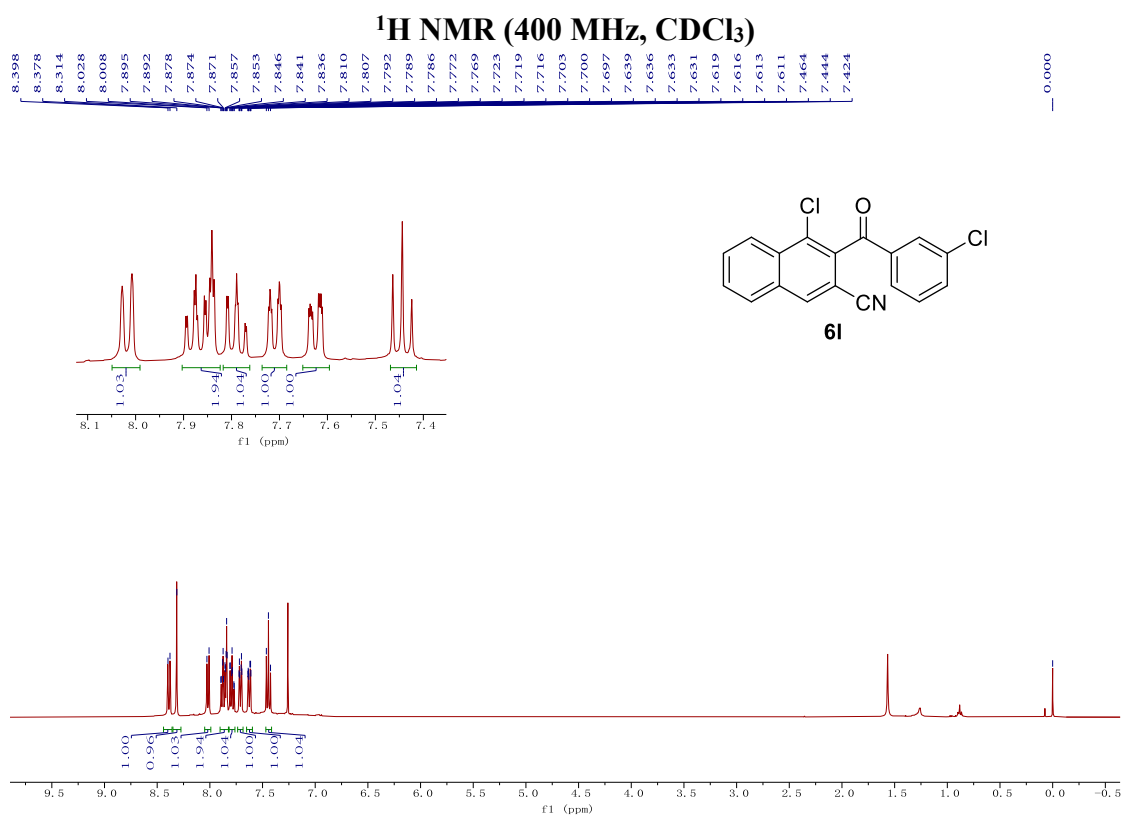


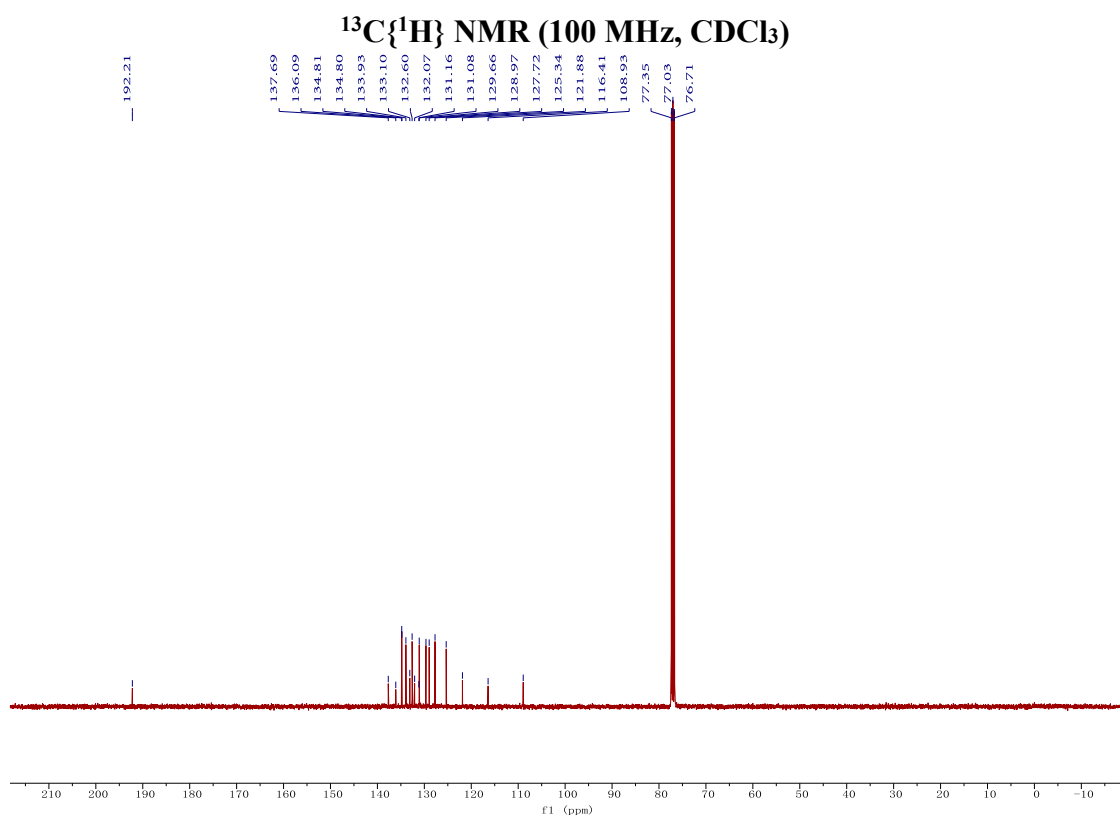
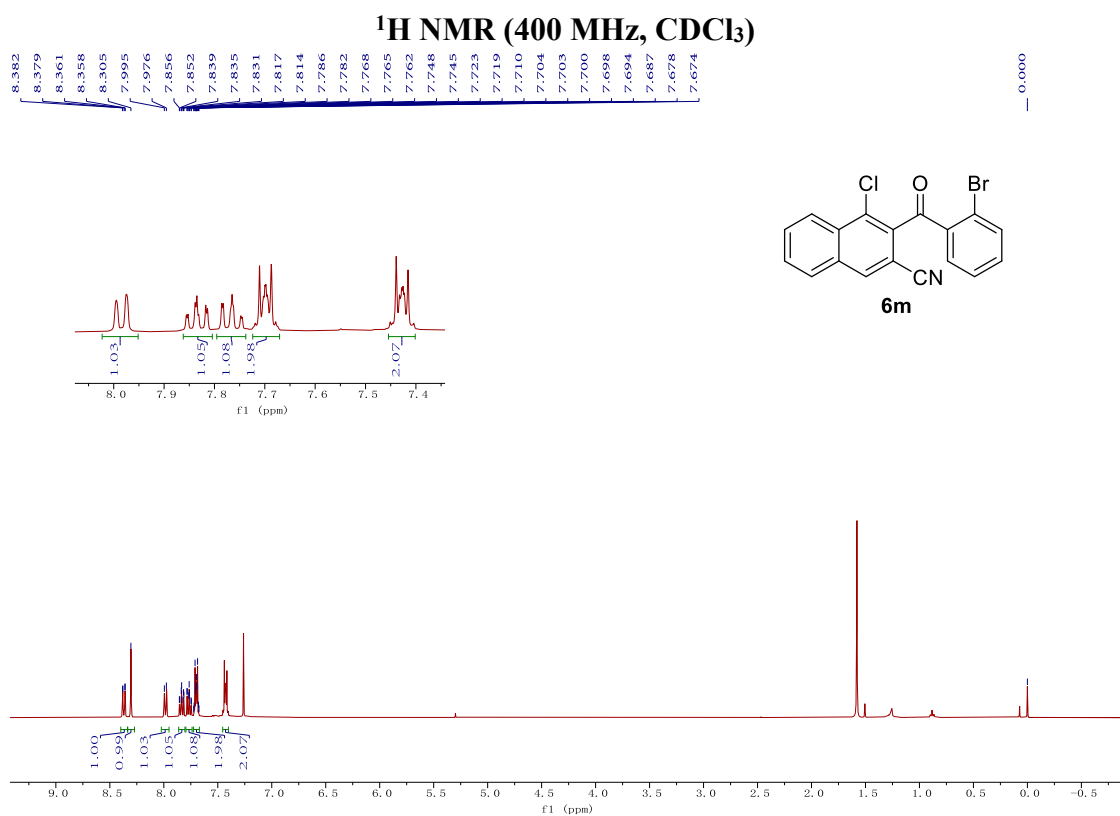


$^{19}\text{F}\{^1\text{H}\}$ (376 MHz, CDCl_3)

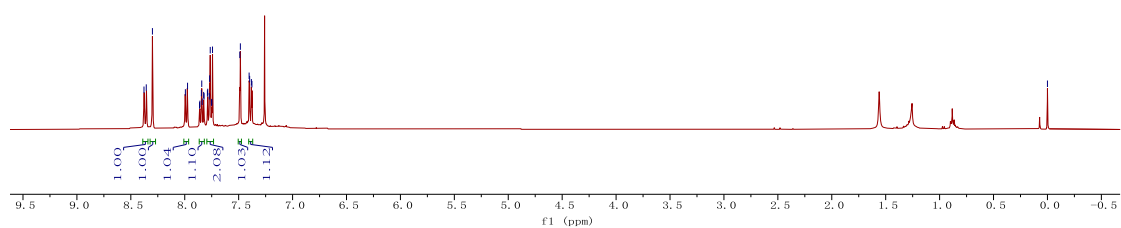
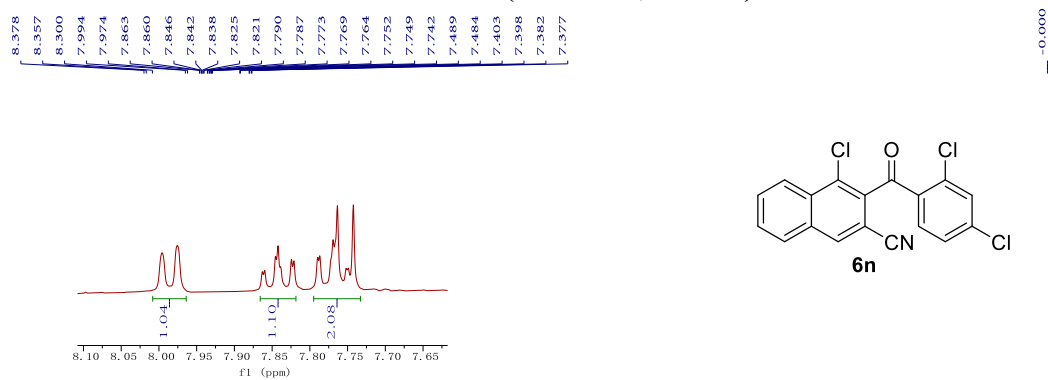




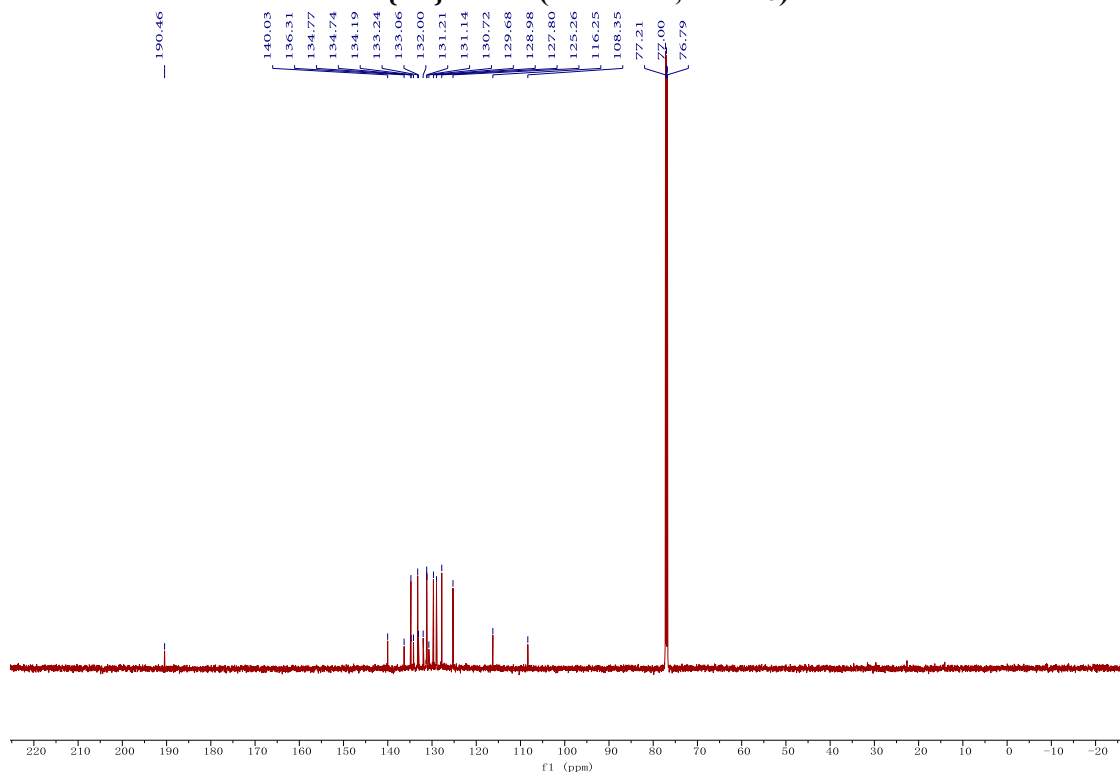




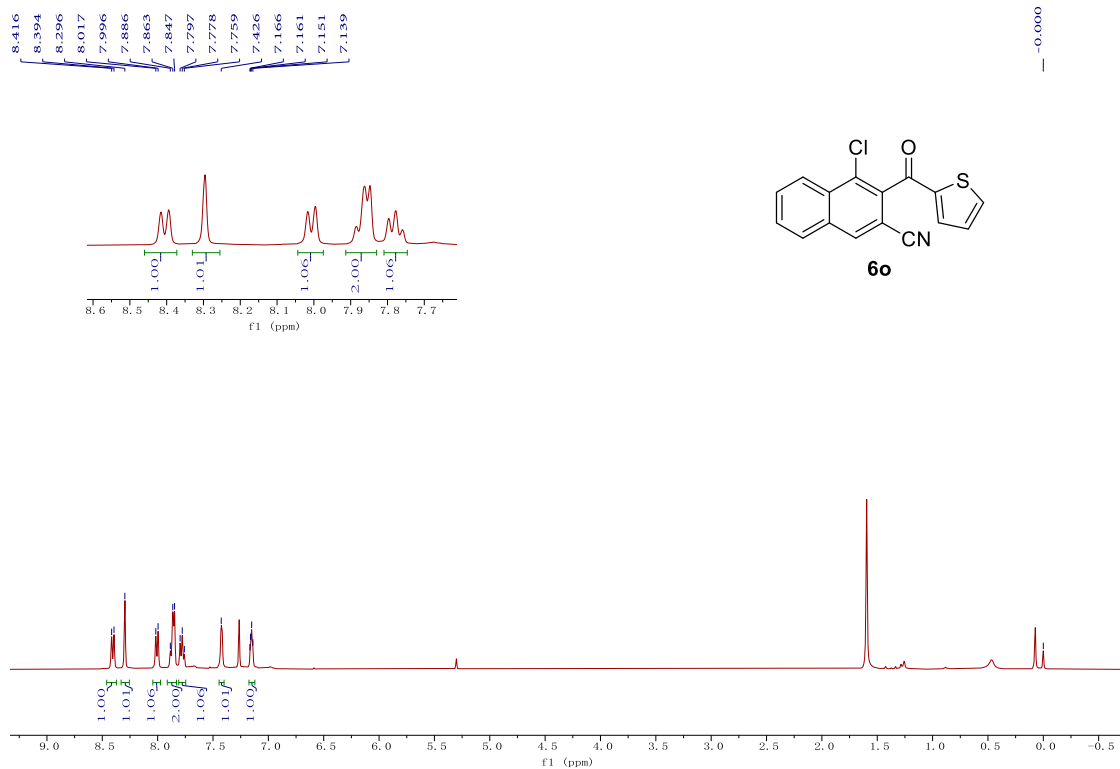
^1H NMR (400 MHz, CDCl_3)



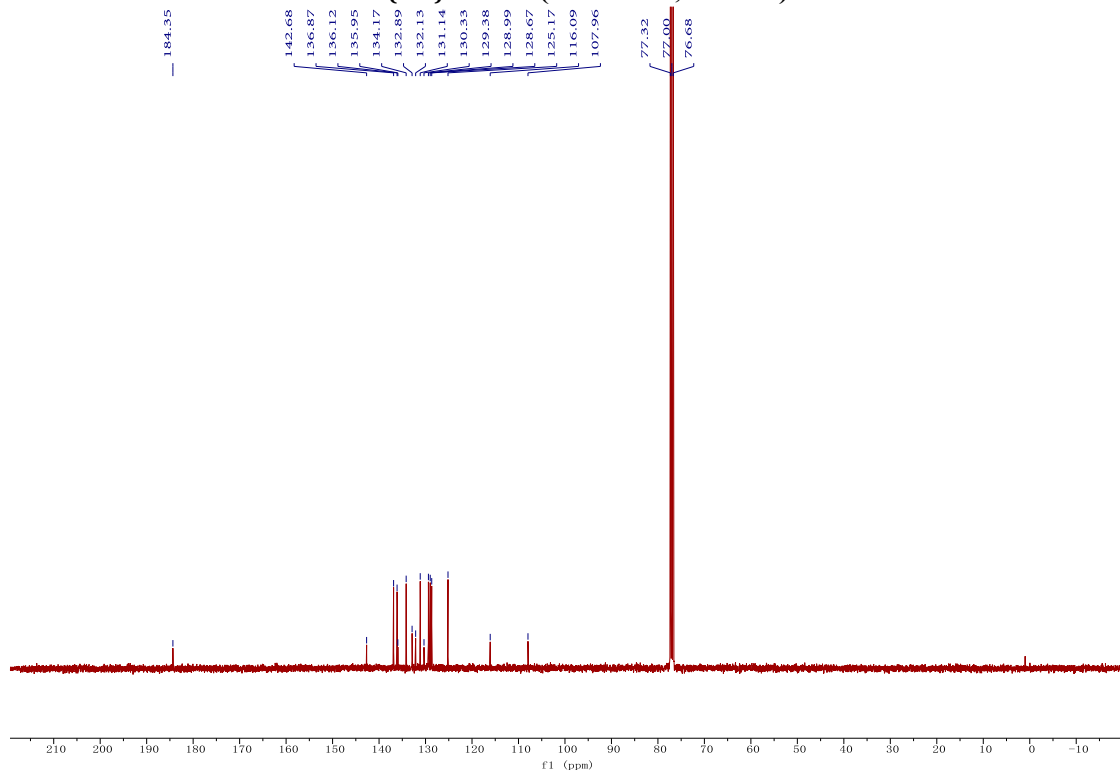
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



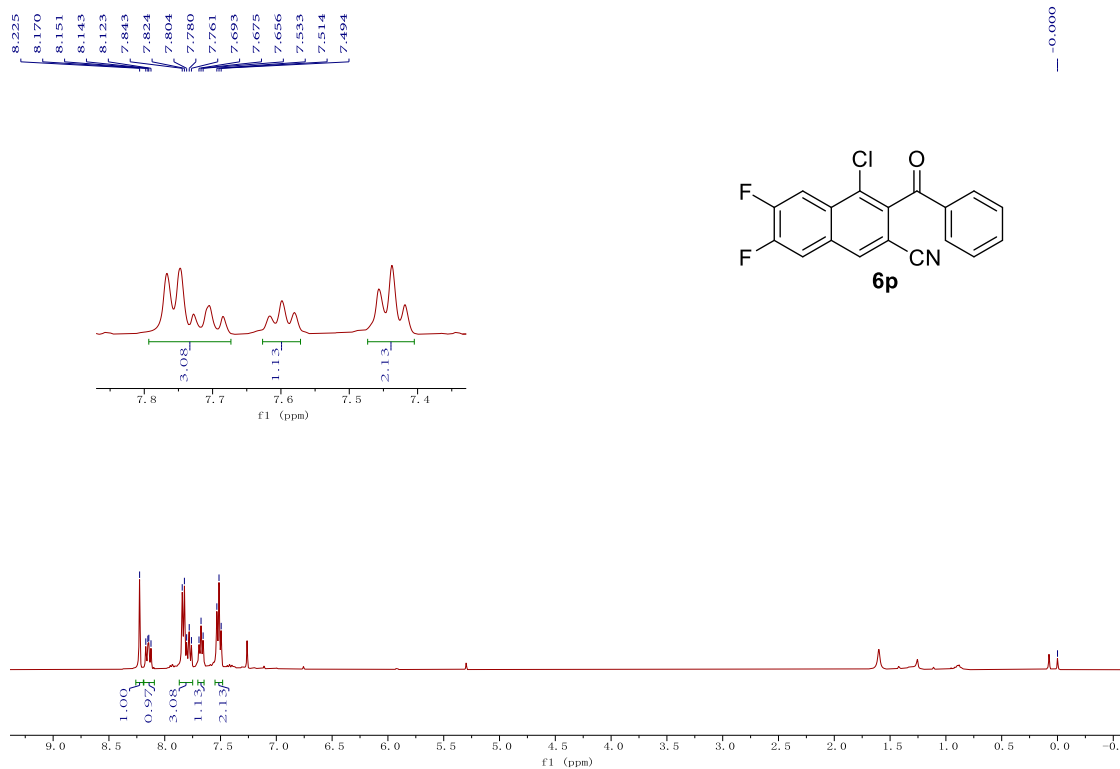
^1H NMR (400 MHz, CDCl_3)



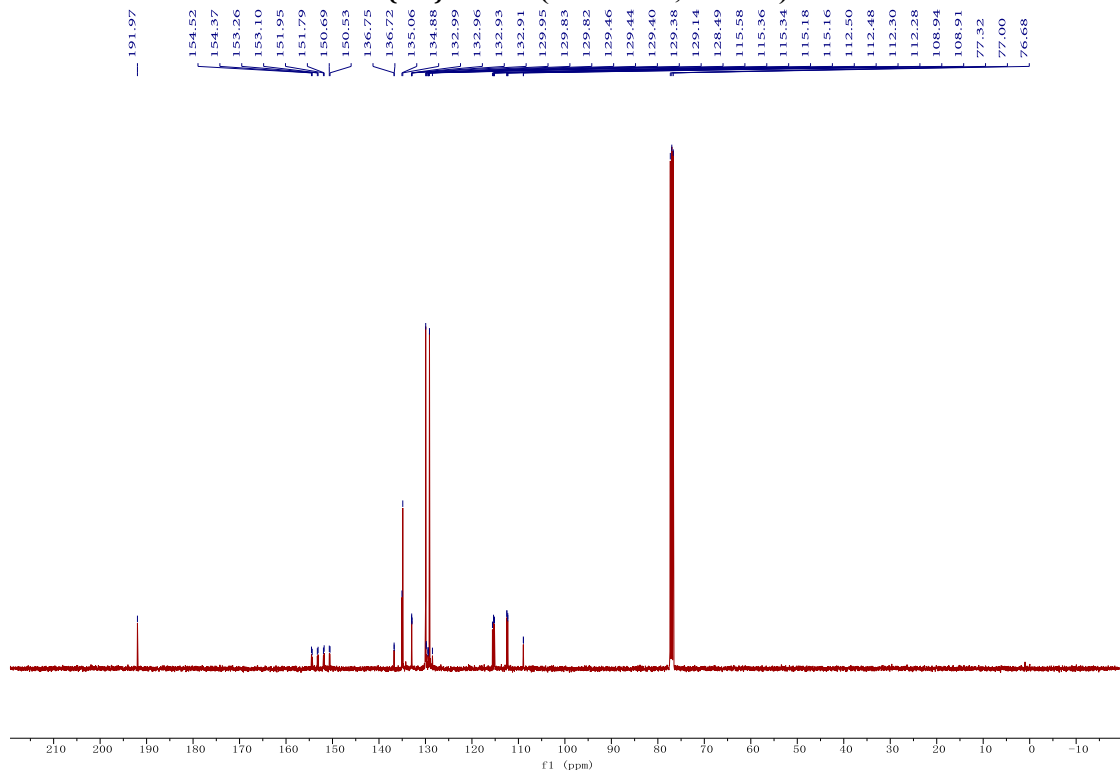
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



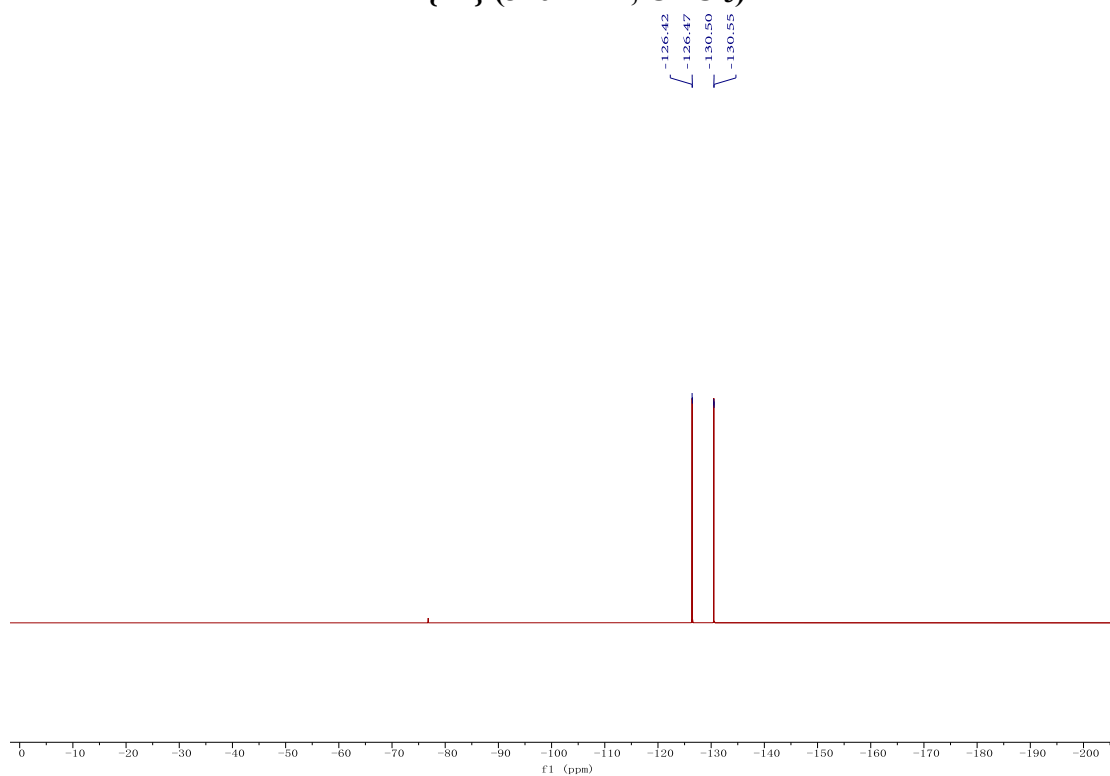
^1H NMR (400 MHz, CDCl_3)



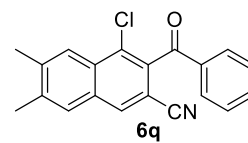
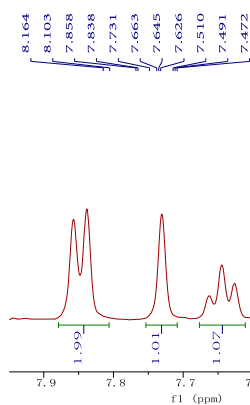
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



$^{19}\text{F}\{^1\text{H}\}$ (376 MHz, CDCl_3)

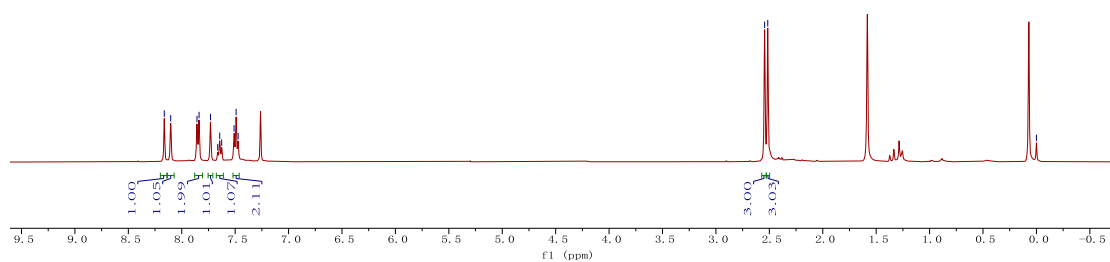


^1H NMR (400 MHz, CDCl_3)

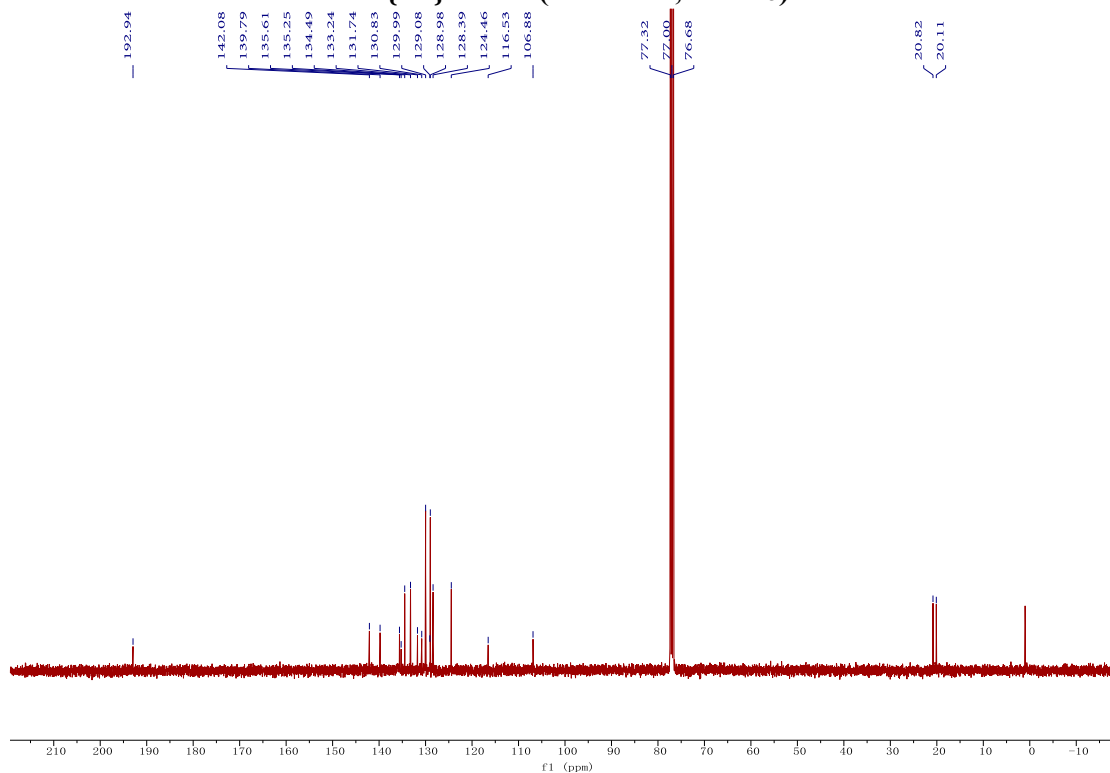


2.544
2.515

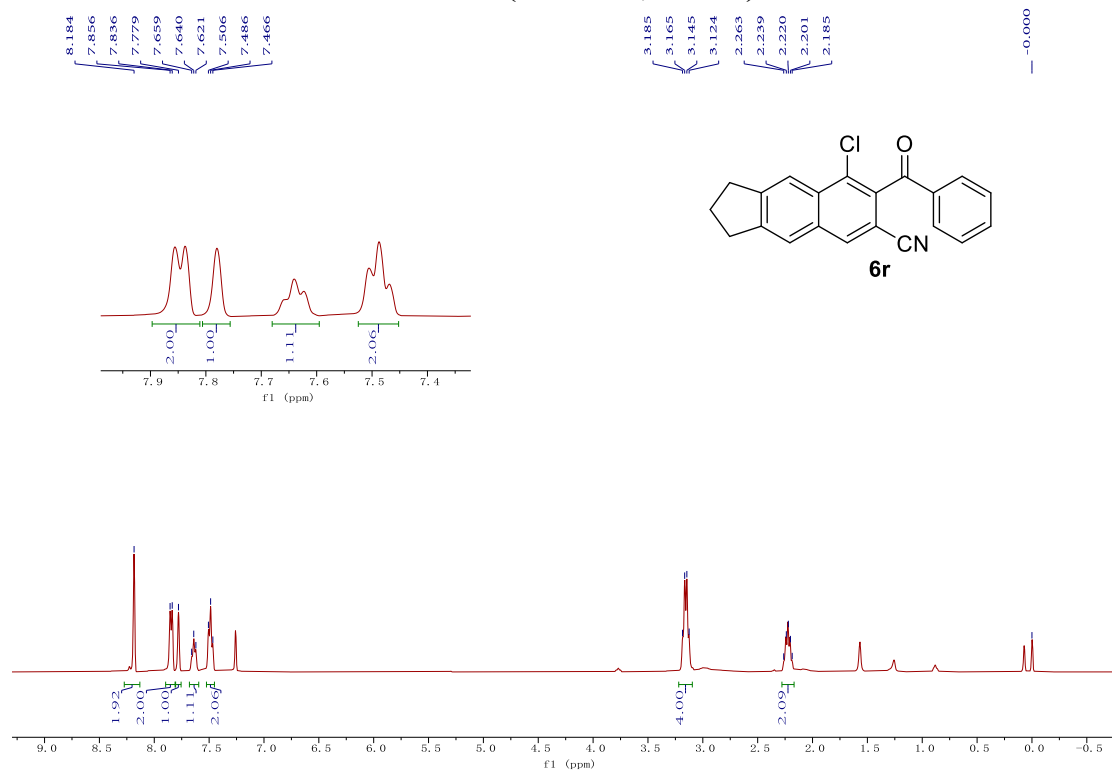
0.000



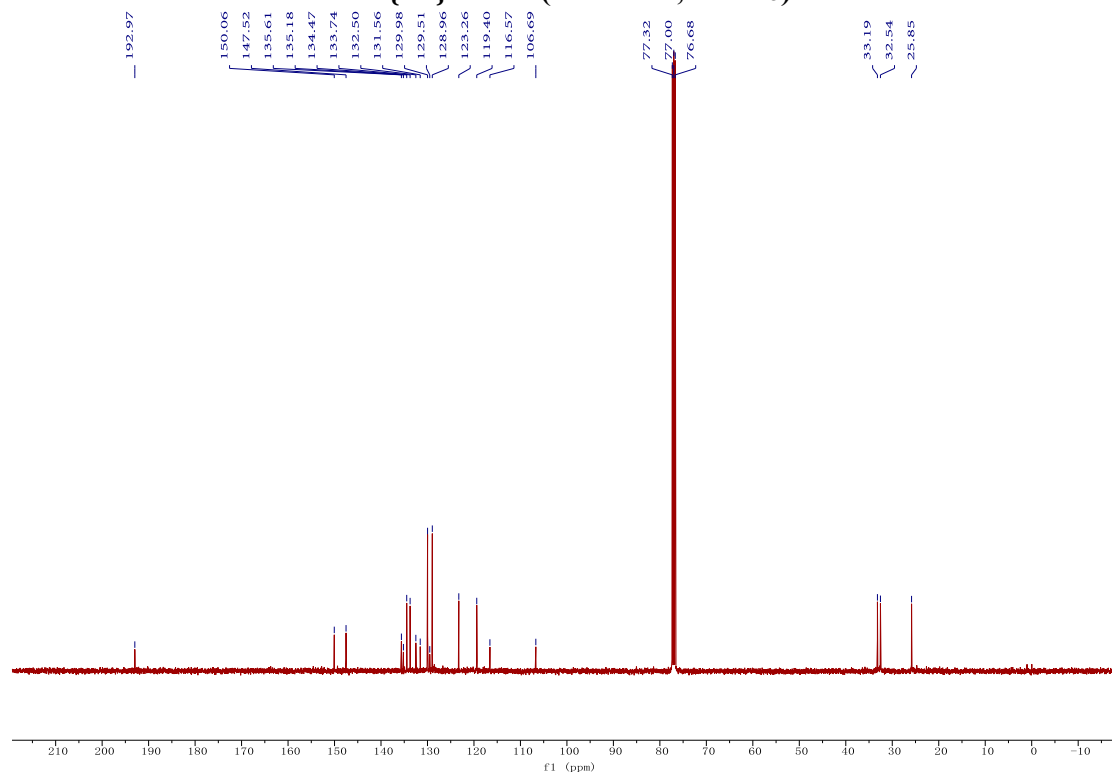
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



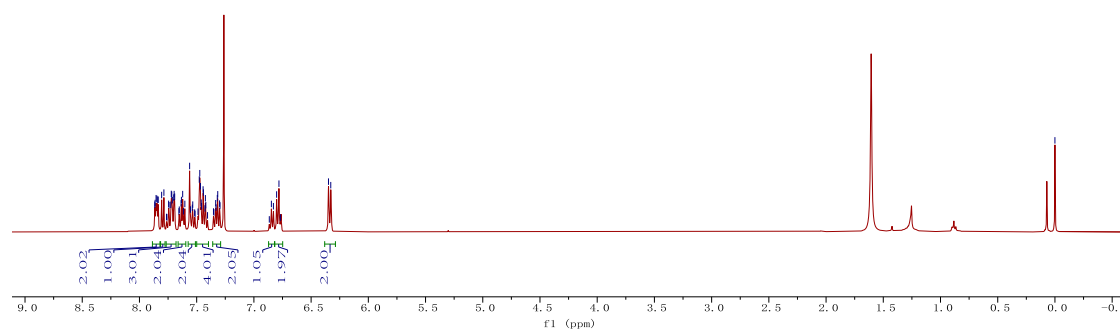
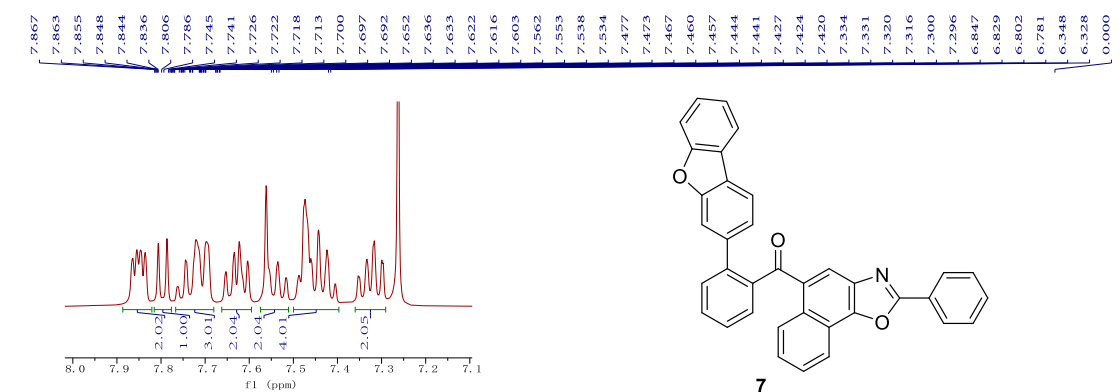
^1H NMR (400 MHz, CDCl_3)



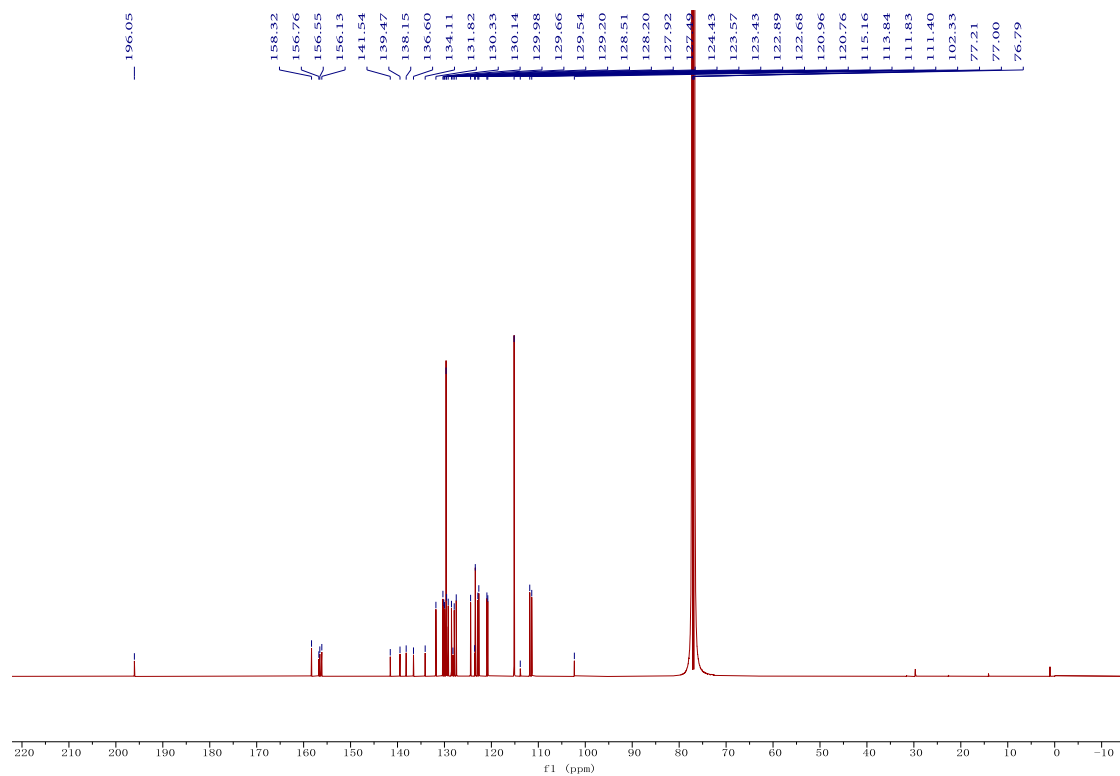
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



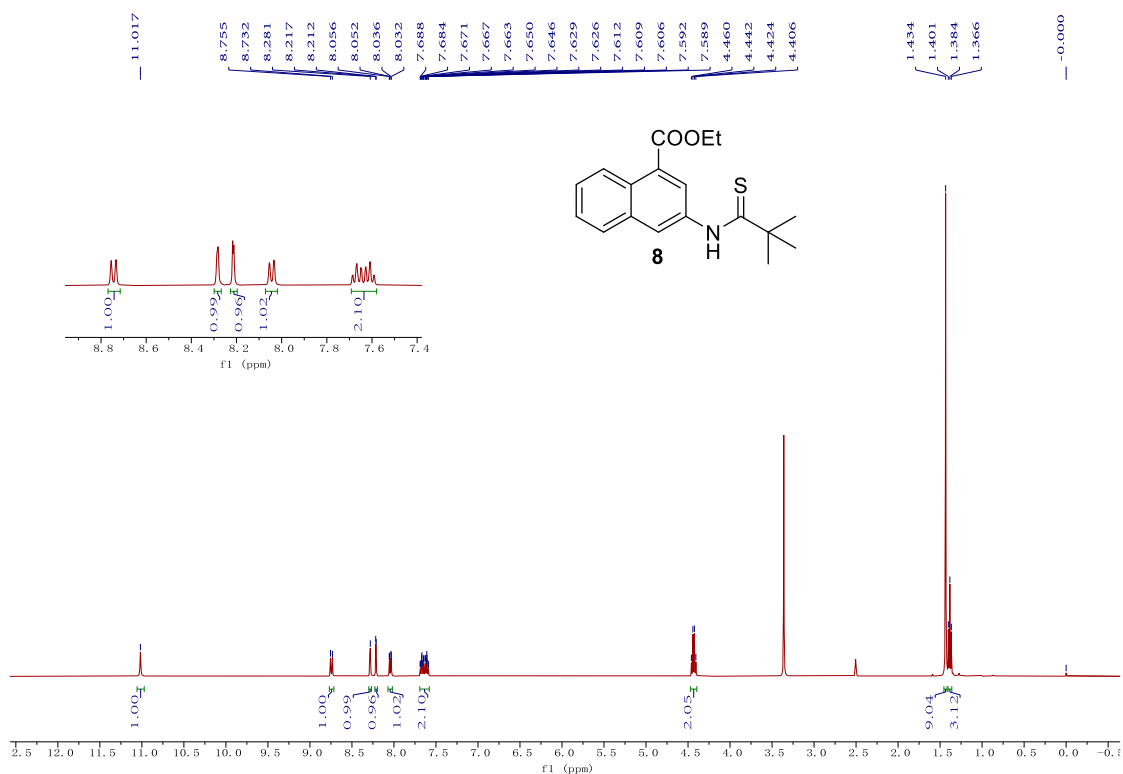
^1H NMR (400 MHz, CDCl_3)



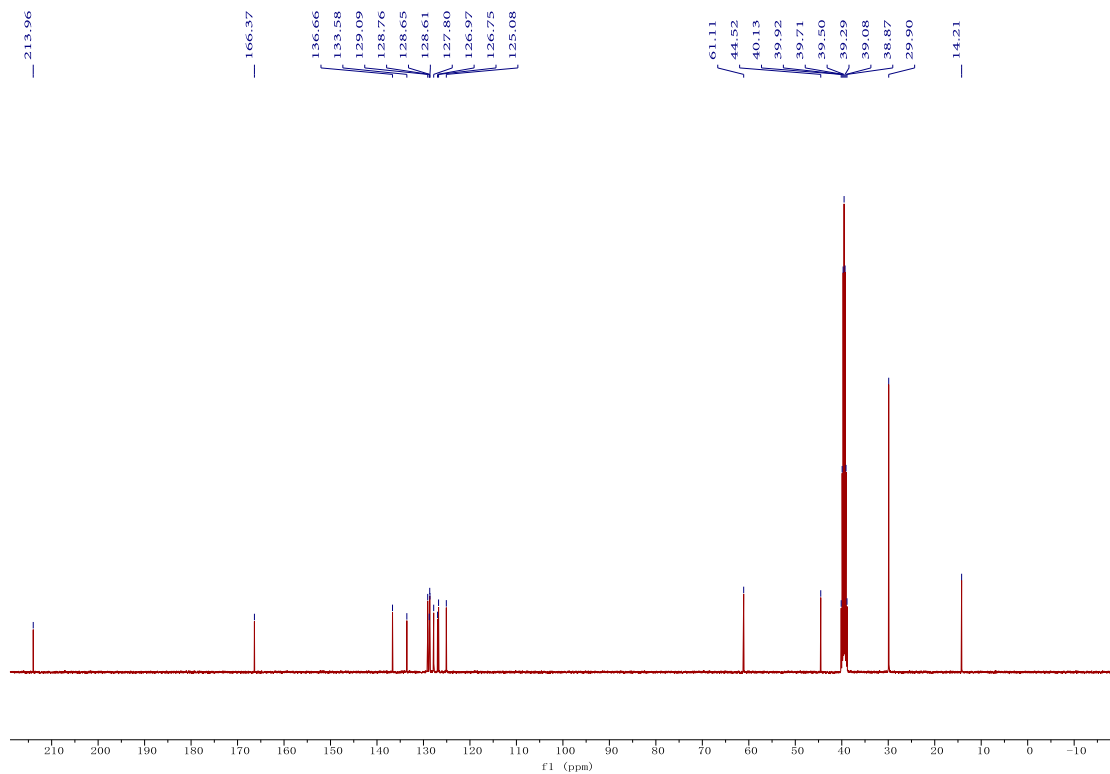
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



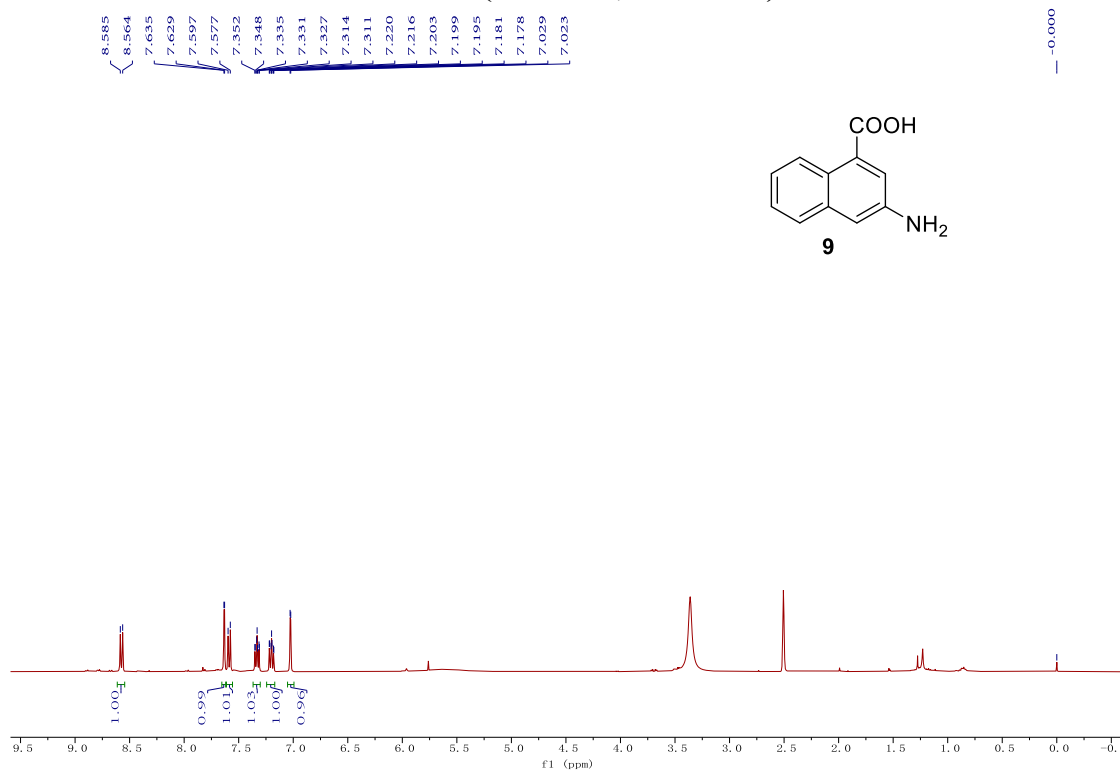
¹H NMR (400 MHz, DMSO-*d*₆)



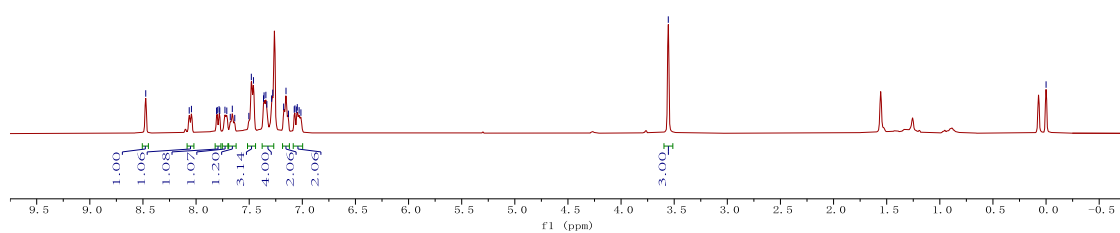
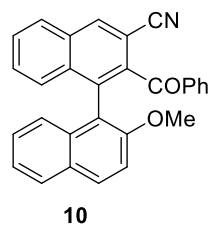
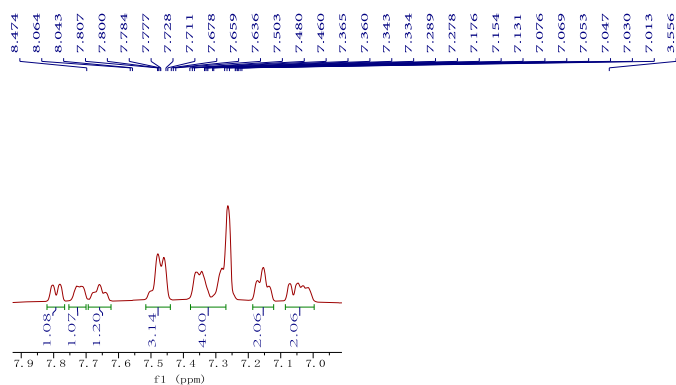
¹³C{¹H} NMR (100 MHz, DMSO-*d*₆)



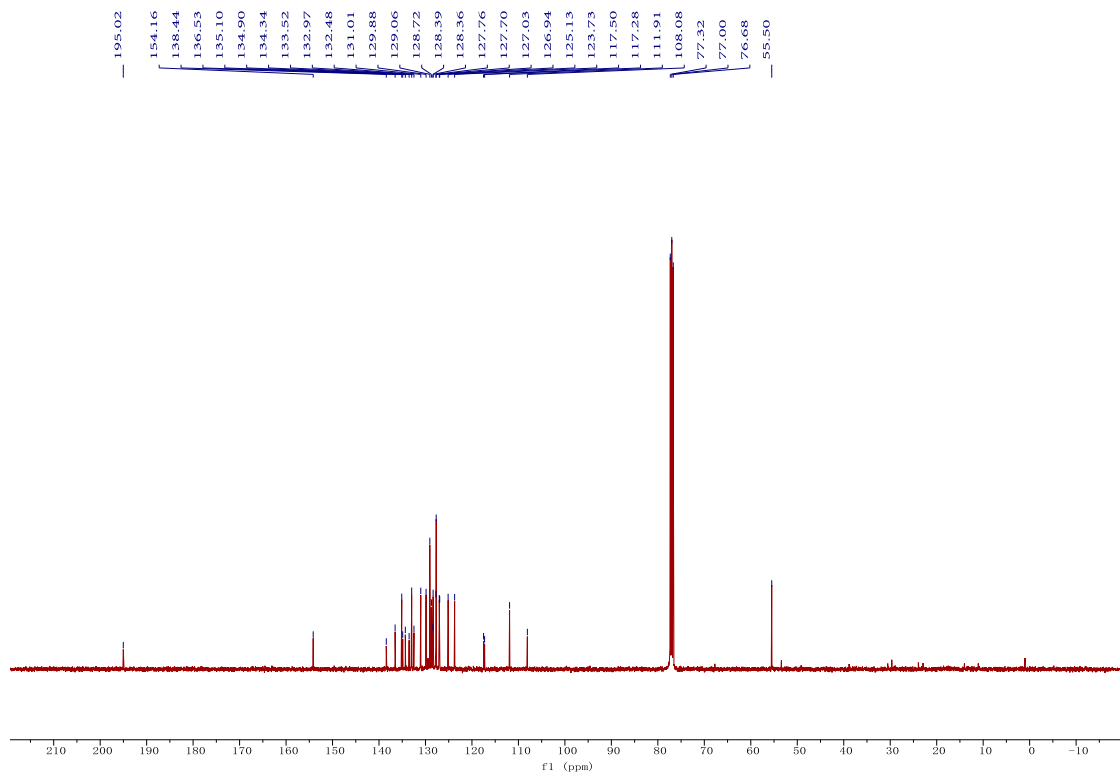
¹H NMR (400 MHz, DMSO-*d*₆)



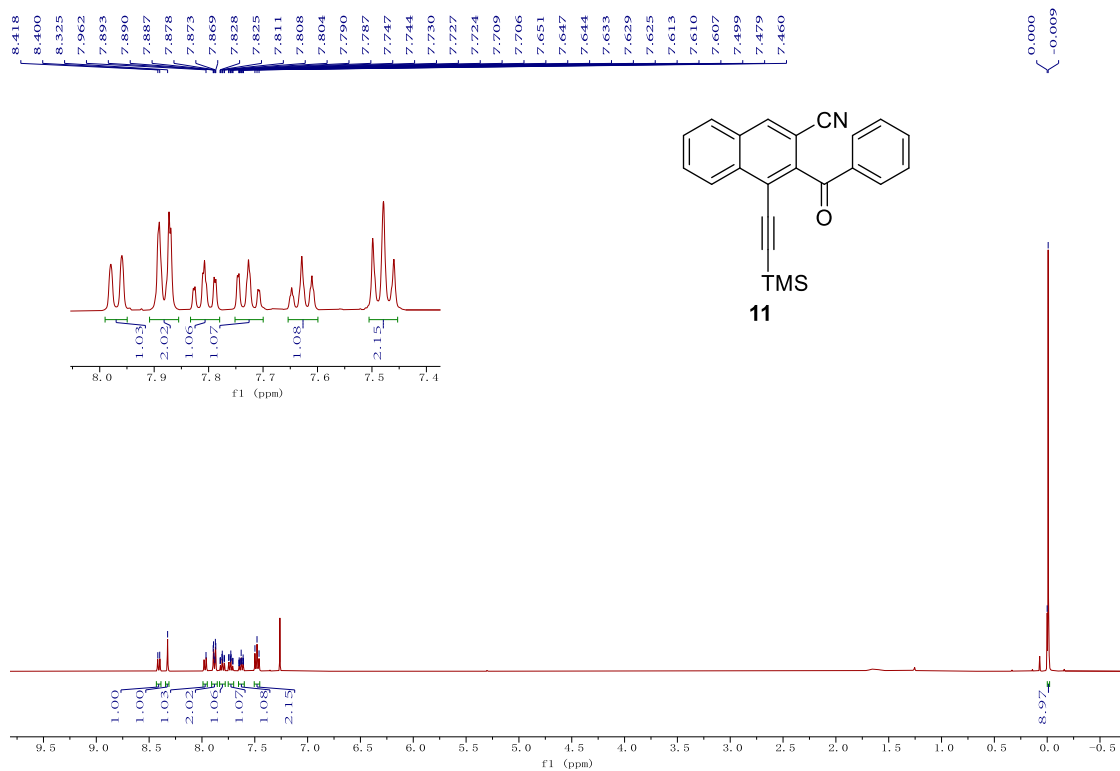
^1H NMR (400 MHz, CDCl_3)



$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3)



$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

