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Supporting Information

Site-Selective Desaturation of C(sp^3)-C(sp^3) Bond via Photoinduced Ruthenium Catalysis

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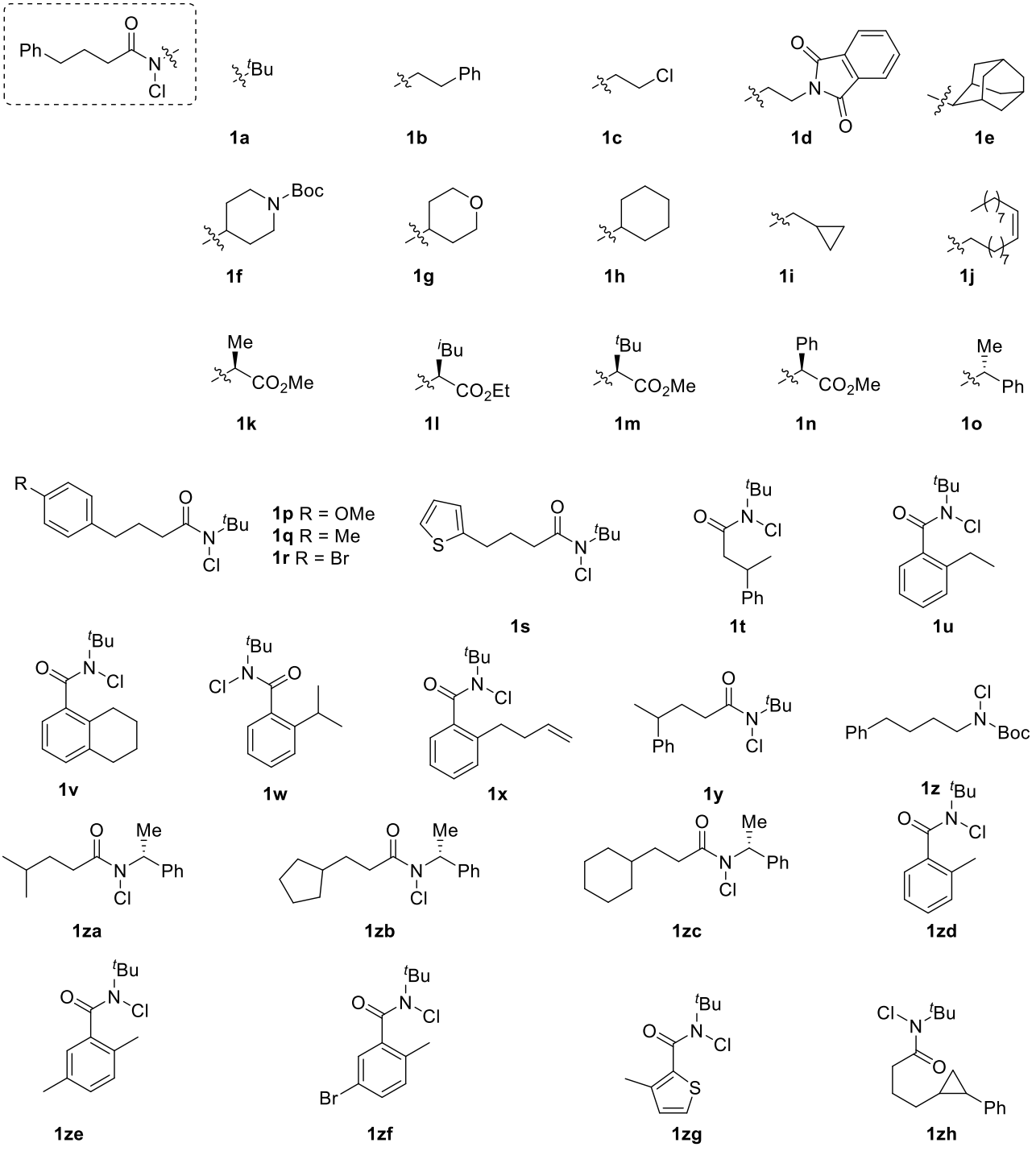
Contents

1. General Information

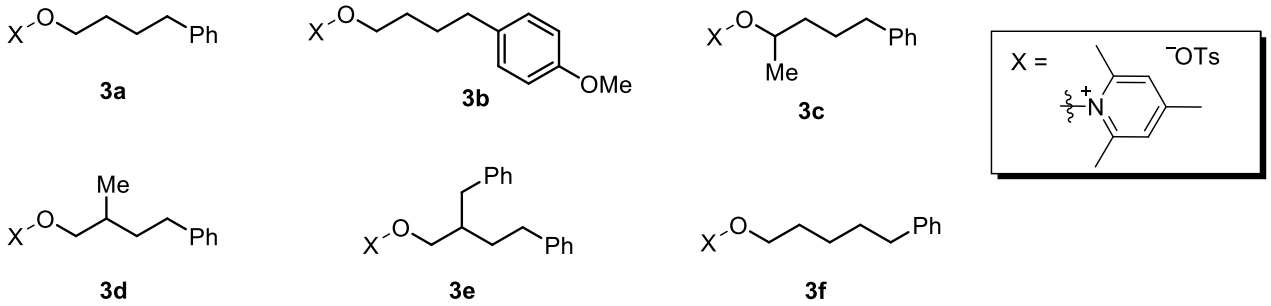
All the reactions were carried out under an atmosphere of nitrogen with magnetic stirring. Catalysis reactions were performed in a Schlenk tube (10 mL) unless indicated otherwise. Solvents were distilled under nitrogen from calcium hydride (CH_3CN, CH_2Cl_2, DMF and DMA), sodium/benzophenone (THF and toluene). All other reagents were commercially available and used without further purification. Flash column chromatography was performed with silica gel 60 M from Greagent (300–400 mesh, pH 6.5–7.0). ^1H NMR and proton-decoupled ^{13}C NMR were recorded on Agilent 400-MR DD2 (400 MHz) spectrometers at ambient temperature. NMR standards were used as follows: ^1H NMR spectroscopy: δ = 7.26 ppm ($CDCl_3$); $^{13}C\{^1H\}$ NMR spectroscopy: δ = 77.0 ppm ($CDCl_3$). IR spectra were recorded on a Bruker Tension-28 spectrometer. High-resolution mass spectra were recorded on a Bruker maXis instrument using ESI technique. X-ray data was collected with a Bruker Smart Apex II diffractometer with MoKα radiation.

2. Synthesis of Substrates

N-chlorocarboxamides **1**[1] were synthesized according to reported procedures without any modification.

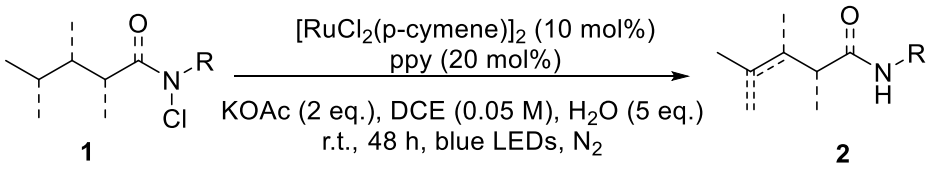


N-alkoxypyridinium salts **3**[2] were synthesized according to reported procedures without any modification.



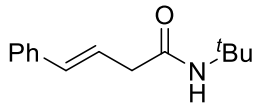
3. Ruthenium-Catalyzed Photoredox Reactions

3.1 General procedure for the synthesis of 2



A dried 10 mL Schlenk tube was charged with the catalyst $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), 2-phenylpyridine (20 mol%), *N*-chlorocarboxamides **1** (0.20 mmol, 1.0 eq.), KOAc (0.40 mmol, 2.0 eq.) and H_2O (5.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs (460 nm or 400 nm). The reaction was stirred at room temperature for 48 h under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:10 to 1:5) to afford products **2**. The ratio of E/Z of the product was determined by the crude ^{1}H NMR.

***(E)*-N-(*tert*-butyl)-4-phenylbut-3-enamide (2a)**



Colorless solid (32.2 mg, 0.138 mmol, yield: 74%, E/Z >20:1).

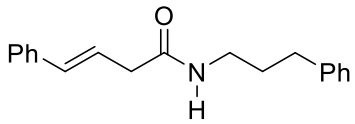
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.4 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.23 (d, *J* = 7.2 Hz, 1H), 6.50 (d, *J* = 15.9 Hz, 1H), 6.29 (dt, *J* = 15.8, 7.3 Hz, 1H), 5.42 (brs, 1H), 3.07 (d, *J* = 8.4 Hz, 2H), 1.35 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 169.9, 136.7, 134.1, 128.6, 127.6, 126.3, 123.0, 51.3, 41.9, 28.8.

IR (film): *ν* (cm^{-1}) 3310, 2972, 2926, 1668, 1640, 1546, 1452, 1389, 1252, 1177, 963 , 757, 691.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{19}NONa$ $[M+Na]^+$: 240.1359, found: 240.1364.

(*E*)-4-phenyl-N-(3-phenylpropyl)but-3-enamide (2b)



Colorless solid (36.8 mg, 0.142 mmol, yield: 71%, E/Z>20:1).

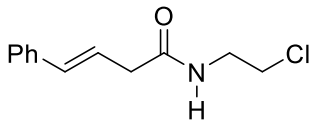
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.0 Hz, 2H), 7.32 (dd, *J* = 8.2, 6.7 Hz, 2H), 7.28–7.23 (m, 3H), 7.19–7.13 (m, 3H), 6.50 (d, *J* = 15.8 Hz, 1H), 6.30–6.19 (m, 1H), 5.62 (brs, 1H), 3.30 (q, *J* = 6.9 Hz, 2H), 3.11 (dd, *J* = 7.3, 1.1 Hz, 2H), 2.64 (t, *J* = 7.6 Hz, 2H), 1.84 (q, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 141.3, 136.5, 134.7, 128.6, 128.4, 128.3, 127.8, 126.3, 126.0, 122.4, 40.9, 39.4, 33.3, 31.1.

IR (film): *v* (cm^{-1}) 3310, 3029, 2969, 2923, 1634, 1546, 1493, 1358, 1248, 1181, 963, 748, 691.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{21}NONa$ $[M+Na]^+$: 302.1515, found: 302.1516.

(*E*)-N-(2-chloroethyl)-4-phenylbut-3-enamide (2c)



Yellow solid (23.3 mg, 0.104 mmol, yield: 52%, E/Z>20:1).

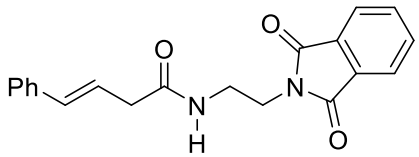
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.4 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.27–7.25 (m, 1H), 6.56 (d, *J* = 15.9 Hz, 1H), 6.28 (dt, *J* = 15.8, 7.3 Hz, 1H), 6.06 (brs, 1H), 3.73–3.55 (m, 4H), 3.18 (dd, *J* = 7.3, 1.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 136.5, 135.0, 128.6, 127.9, 126.3, 121.9, 43.9, 41.3, 40.7.

IR (film): *v* (cm^{-1}) 3310, 3055, 2921, 2621, 1740, 1644, 1544, 1450, 1407, 1358, 1218, 1175, 1150, 1087, 1026, 999, 916, 742, 691.

HRMS (ESI, *m*/*z*) calcd for $C_{12}H_{14}NONa$ $[M+Na-Cl]^+$: 206.1176, found: 206.1172.

(*E*)-N-(2-(1,3-dioxoisoindolin-2-yl)ethyl)-4-phenylbut-3-enamide (2d)



Colorless solid (28.0 mg, 0.084 mmol, yield: 42%, E/Z>20:1)

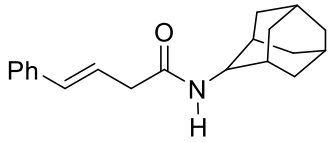
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 5.3, 3.2 Hz, 2H), 7.67 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.35 (d, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 2H), 7.23 (t, *J* = 3.2 Hz, 1H), 6.48 (d, *J* = 15.9 Hz, 1H), 6.20 (dd, *J* = 15.8, 7.4 Hz, 1H), 6.11 (brs, 1H), 3.86 (dd, *J* = 6.4, 4.4 Hz, 2H), 3.58–3.53 (m, 2H), 3.09 (d, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 168.5, 136.7, 134.5, 134.0, 132.0, 128.5, 127.6, 126.3, 123.3, 122.3, 40.7, 39.1, 37.5.

IR (film): *v* (cm^{-1}) 3547, 3306, 3036, 1740, 1699, 1644, 1577, 1450, 1383, 1281, 1209, 1187, 1105, 1065, 985, 912, 850, 763, 689.

HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{18}N_2O_3Na$ $[M+Na]^+$: 357.1022, found: 357.1025.

(*E*)-N-((1r,3r,5r,7r)-adamantan-2-yl)-4-phenylbut-3-enamide (2e)



Colorless solid (40.1 mg, 0.136mmol, yield: 68%, E/Z>20:1).

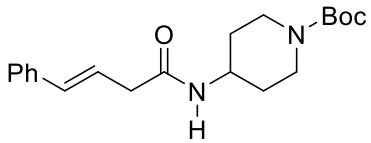
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.34 (m, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.25–7.20 (m, 1H), 6.49 (d, *J* = 15.9 Hz, 1H), 6.27 (dt, *J* = 15.8, 7.2 Hz, 1H), 5.27 (brs, 1H), 3.05 (dd, *J* = 7.2, 1.2 Hz, 2H), 2.05 (s, 3H), 1.98 (d, *J* = 2.6 Hz, 6H), 1.66 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 136.8, 134.1, 128.6, 127.6, 126.3, 123.1, 52.0, 42.0, 41.6, 36.3, 29.4.

IR (film): *v* (cm^{-1}) 3299, 2906, 2851, 1689, 1638, 1540, 1450, 1362, 1307, 1275, 1238, 1167, 1142, 965, 734, 693.

HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{25}NONa$ $[M+Na]^+$: 318.1828, found: 318.1829.

***tert*-butyl (*E*)-4-(4-phenylbut-3-enamido)piperidine-1-carboxylate (2f)**



Colorless solid (34.6mg, 0.101 mmol, yield: 50%, E/Z>20:1. **Note: trace of de-Cl-amide side product was retained which cannot be separated**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64–7.47 (m, 1H), 7.32–7.26 (m, 2H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.21–7.14 (m, 1H), 6.44 (d, *J* = 15.8 Hz, 1H), 6.23 (dt, *J* = 15.8, 7.2 Hz, 1H), 6.11 (d, *J* = 7.8 Hz,

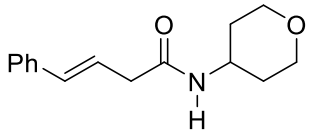
1H), 3.97–3.87 (m, 3H), 3.08 (dd, *J* = 7.2, 1.4 Hz, 2H) 2.78 (t, *J* = 11.8 Hz, 2H), 1.89–1.77 (m, 2H), 1.39 (s, 9H), 1.30–1.19 (ddd, *J*= 26.16, 12.32, 3.88, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 154.6, 136.6, 134.1, 132.1, 128.6, 127.7, 126.2, 122.6, 79.6, 46.8, 42.5, 40.8, 31.9, 28.4.

IR (film): *v* (cm^{-1}) 3267, 2932, 1687, 1640, 1546, 1475, 1424, 1364, 1311, 1275, 1236,1167, 1081, 969, 763, 698.

HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{25}NONa$ $[M+Na]^+$: 367.1992, found: 367.1995.

(*E*)-4-phenyl-N-(tetrahydro-2H-pyran-4-yl)but-3-enamide (2g)



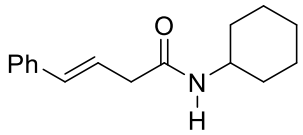
Yellow oil (32.7 mg, 0.135 mmol, yield: 67%, E/Z>20:1. **Note: trace of de-Cl-amide side product was retained which cannot be separated**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.8 Hz, 2H), 7.31 (dd, *J* = 7.5 Hz, 2H), 7.25 (dd, *J* = 4.2 Hz, 1H), 6.52 (d, *J* = 15.9 Hz, 1H), 6.27 (dt, *J* = 14.9, 7.3 Hz, 1H), 5.56 (brs, 1H), 4.05–3.87 (m, 3H), 3.45 (t, *J* = 12.0 Hz, 2H), 3.13 (d, *J* = 7.3 Hz, 2H), 1.91–1.83 (m, 2H), 1.43 (qd, *J* = 11.9, 4.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0, 136.5, 134.7, 128.6, 127.8, 126.3, 122.3, 66.7, 45.8, 40.9, 33.1.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{19}NO_2Na$ $[M+Na]^+$: 268.1308, found: 268.1307.

(*E*)-N-cyclohexyl-4-phenylbut-3-enamide (2h)



Colorless solid (33.8 mg, 0.140 mmol, yield: 70%, E/Z>20:1).

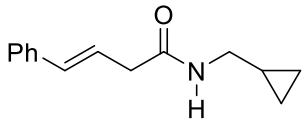
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.3 Hz, 2H), 7.31 (dd, *J* = 7.6 Hz, 2H), 7.23 (dd, *J* = 7.6 Hz, 1H), 6.51 (d, *J* = 15.9 Hz, 1H), 6.27 (dt, *J* = 15.6, 7.3 Hz, 1H), 5.48 (brs, 1H), 3.77 (ddt, *J* = 14.4, 6.3, 3.6 Hz, 1H), 3.11 (dd, *J* = 7.3, 1.3 Hz, 2H), 1.89 (dt, *J* = 12.6, 4.0 Hz, 2H), 1.73–1.53 (m, 3H), 1.33 (tt, *J* = 24.7, 10.9 Hz, 2H), 1.19–1.02 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 136.7, 134.5, 128.6, 127.7, 126.3, 122.6, 48.3, 41.1, 33.1, 25.5, 24.8.

IR (film): ν (cm^{-1}) 3547, 3306, 3036, 1740, 1699, 1644, 1577, 1450, 1383, 1281, 1209, 1187, 1105, 1065, 985, 912, 850, 763, 689.

HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{21}NONa$ $[M+Na]^+$: 266.1515, found: 266.1514.

(*E*)-N-(cyclopropylmethyl)-4-phenylbut-3-enamide (2i)



Yellow solid (19.9 mg, 0.082 mmol, yield: 41%, E/Z>20:1).

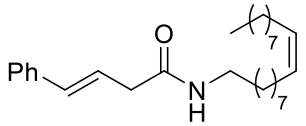
^1H NMR (400 MHz, $CDCl_3$) δ 7.40–7.36 (m, 2H), 7.34–7.29 (m, 2H), 7.26 (d, *J* = 1.6 Hz, 1H), 6.53 (d, *J* = 15.8 Hz, 1H), 6.30 (dt, *J* = 15.8, 7.3 Hz, 1H), 5.74 (brs, 1H), 3.17–3.09 (m, 4H), 0.93 (ddt, *J* = 12.4, 7.6, 3.7 Hz, 1H), 0.51–0.46 (m, 2H), 0.20–0.16 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 136.6, 134.6, 128.6, 127.8, 126.3, 122.5, 44.5, 40.9, 10.6, 3.4.

IR (film): ν (cm^{-1}) 3236, 3073, 3036, 1740, 1699, 1644, 1577, 1450, 1383, 1281, 1209, 1187, 1105, 1065, 985, 912, 850, 763, 689.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{17}NONa$ $[M+Na]^+$: 238.1202, found: 238.1201.

(*E*)-N-((*Z*)-octadec-9-en-1-yl)-4-phenylbut-3-enamide (2j)



Colorless solid (41.0 mg, 0.099 mmol, yield: 50%, E/Z>20:1).

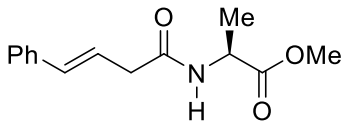
^1H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.50 (d, *J* = 15.9 Hz, 1H), 6.28 (dt, *J* = 15.3, 7.3 Hz, 1H), 5.85 (s, 1H), 5.50–5.21 (m, 2H), 3.24–3.18 (m, 2H), 3.13 (d, *J* = 7.2 Hz, 2H), 1.98 (ddt, *J* = 15.7, 12.1, 5.8 Hz, 4H), 1.45 (dt, *J* = 14.6, 7.3 Hz, 3H), 1.33–1.20 (m, 28H), 0.86 (q, *J* = 5.9 Hz, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6, 136.6, 134.5, 129.9, 129.8, 128.6, 127.7, 126.3, 122.6, 40.9, 39.7, 31.9, 29.76, 29.73, 29.69, 29.67, 29.65, 29.59, 29.53, 29.51, 29.43, 29.31, 29.26, 29.21, 27.2, 26.9, 22.7, 14.1.

IR (film): ν (cm^{-1}) 3250, 3069, 2919, 2851, 1628, 1560, 1466, 1422, 1248, 963, 753, 716, 689.

HRMS (ESI, *m*/*z*) calcd for $C_{28}H_{45}NONa$ $[M+Na]^+$: 434.3393, found: 434.3386.

ethyl (*E*)-(4-phenylbut-3-enoyl)-L-alaninate (2k)



Colorless solid (25.7 mg, 0.104 mmol, yield: 57%, E/Z>20:1).

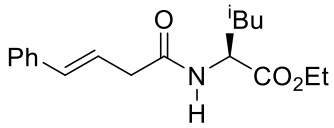
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.3 Hz, 2H), 7.28 (dd, *J* = 7.3 Hz, 2H), 7.24–7.17 (dd, 1H), 6.51 (d, *J* = 15.8 Hz, 1H), 6.38 (brs, 1H), 6.28 (dt, *J* = 15.4, 7.2 Hz, 1H), 4.59 (q, *J* = 7.1 Hz, 1H), 3.70 (s, 3H), 3.16 (d, *J* = 7.1 Hz, 2H), 1.38 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5, 170.3, 136.6, 134.5, 128.6, 127.7, 126.3, 122.1, 52.4, 48.1, 40.5, 18.3.

IR (film): *v* (cm^{-1}) 3547, 3306, 3255, 3036, 2957, 1740, 1644, 1577, 1497, 1434, 1383, 1209, 1081, 985, 912, 850, 763, 689.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{17}NO_3Na$ $[M+Na]^+$: 270.1101, found: 270.1099.

methyl (*E*)-(4-phenylbut-3-enoyl)-L-valinate (2l)



Yellow oil (37.0 mg, 0.122 mmol, yield: 61%, E/Z>20:1).

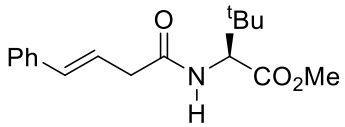
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.33 (m, 2H), 7.29 (td, *J* = 6.7, 6.2, 1.6 Hz, 2H), 7.24–7.19 (m, 1H), 6.54 (d, *J* = 15.9 Hz, 1H), 6.34–6.26 (td, *J*=15.88, 7.2 1H), 6.24 (brs, 1H), 4.59 (dd, *J* = 8.6, 4.9 Hz, 1H), 4.21–4.12 (m, 2H), 1.88 (dqd, *J* = 9.4, 4.8, 2.6 Hz, 1H), 1.46–1.39 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.19–1.11 (m, 1H), 0.90 (t, *J* = 7.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 170.4, 136.7, 134.5, 128.6, 127.7, 126.3, 122.2, 61.2, 56.4, 40.7, 38.0, 25.2, 15.4, 14.2, 11.6.

IR (film): *v* (cm^{-1}) 3301, 2961, 2901, 3 1736, 1642, 1540, 1454, 1371, 1244, 1191, 1095, 1024, 965, 736, 691.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{25}NO_3Na$ $[M+Na]^+$: 326.1727, found: 326.1728.

methyl (*S*,*E*)-3,3-dimethyl-2-(4-phenylbut-3-enamido)butanoate (2m)



Colorless solid (36.4 mg, 0.126 mmol, yield: 63%, E/Z>20:1).

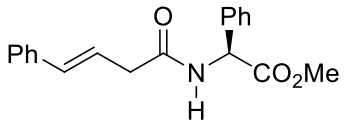
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.32 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.21 (td, *J* = 6.0, 4.9, 3.1 Hz, 1H), 6.54 (dt, *J* = 15.8, 1.5 Hz, 1H), 6.33–6.28 (m, 1H), 6.26 (brs, 1H), 4.48 (d, *J* = 9.4 Hz, 1H), 3.69 (s, 3H), 3.18 (dd, *J* = 7.2, 1.2 Hz, 2H), 0.94 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 170.4, 136.7, 134.6, 128.6, 127.7, 126.3, 122.2, 59.9, 51.8, 40.6, 34.7, 26.5.

IR (film): *v* (cm^{-1}) 3314, 2967, 1740, 1648, 1532, 1475, 1438, 1368, 1216, 1158, 981, 738, 693.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{23}NO_3Na$ $[M+Na]^+$: 312.1570, found: 312.1570.

(*S*,*E*)-methyl 2-phenyl-2-(4-phenylbut-3-enamido)acetate (2n)



Yellow solid (37.7 mg, 0.122 mmol, yield: 61%, E/Z>20:1).

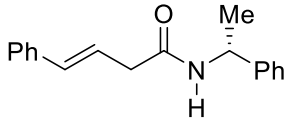
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.23 (m, 6H), 7.21–7.15 (m, 2H), 7.11–7.01 (m, 2H), 6.48 (d, *J* = 15.9 Hz, 1H), 6.25–6.15 (m, 1H), 6.12 (brs, 1H), 4.91–4.83 (m, 1H), 3.71 (s, 3H), 3.12 (d, *J* = 6.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 170.2, 136.5, 135.6, 134.8, 129.2, 128.5, 127.8, 127.1, 126.3, 125.7, 121.9, 53.0, 40.5, 37.7.

IR (film): *v* (cm^{-1}) 3301, 3034, 2950, 1740, 1646, 1536, 1499, 1440, 1366, 1273, 1175, 969.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{19}NO_3Na$ $[M+Na]^+$: 332.1257, found: 332.1255.

(*R*,*E*)-4-phenyl-N-(1-phenylethyl)but-3-enamide (2o)



Yellow solid (48.5 mg, 0.183 mmol, yield: 92%, E/Z>20:1).

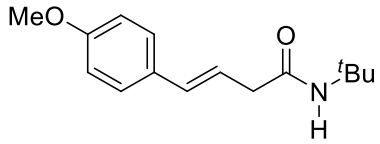
^{1}H NMR (400 MHz, $CDCl_3$) δ δ 7.38–7.16 (m, 10H), 6.51 (d, *J* = 15.9 Hz, 1H), 6.29 (dt, *J* = 15.8, 7.2 Hz, 1H), 5.96 (brs, 1H), 5.15 (p, *J* = 6.9 Hz, 1H), 3.15 (d, *J* = 7.3 Hz, 2H), 1.48 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.72, 143.04, 136.61, 134.51, 128.67, 128.60, 127.74, 127.37, 126.31, 126.13, 122.39, 48.79, 40.89, 21.75.

IR (film): *v* (cm^{-1}) 3296, 3032, 2918, 1634, 1540, 1491, 1444, 1428, 1160, 969.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{19}NONa$ $[M+Na]^+$: 288.1359, found: 288.1359.

(*E*)-N-(*tert*-butyl)-4-(4-methoxyphenyl)but-3-enamide (2p)



Yellow solid (19.8 mg, 0.080 mmol, yield: 40%, E/Z>20:1).

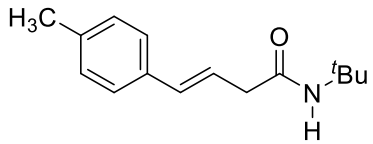
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 6.43 (dt, *J* = 15.7, 1.5 Hz, 1H), 6.11 (dt, *J* = 15.7, 7.3 Hz, 1H), 5.39 (brs, 1H), 3.79 (s, 3H), 3.03 (dd, *J* = 7.3, 1.2 Hz, 2H), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 159.2, 133.7, 129.6, 127.4, 120.7, 114.0, 55.3, 51.2, 41.9, 28.8.

IR (film): *v* (cm^{-1}) 3318, 2972, 1670, 1642, 1607, 1544, 1509, 1454, 1419, 1391, 1362, 1297, 1248, 1224, 1175, 1032, 963, 830, 808.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{21}NO_2Na$ $[M+Na]^+$: 270.1465, found: 270.1463.

(*E*)-N-(*tert*-butyl)-4-(*p*-tolyl)but-3-enamide (2q)



Yellow solid (25.2 mg, 0.121 mmol, yield: 55%, E/Z>20:1).

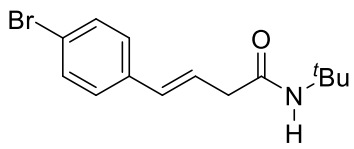
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.2 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.46 (d, *J* = 15.8 Hz, 1H), 6.21 (dt, *J* = 15.8, 7.3 Hz, 1H), 5.43 (brs, 1H), 3.05 (dd, *J* = 7.3, 1.2 Hz, 2H), 2.32 (s, 3H), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 137.5, 134.2, 129.3, 126.2, 125.3, 121.9, 51.3, 41.9, 28.8, 21.2.

IR (film): *v* (cm^{-1}) 3310, 2976, 2921, 1670, 1640, 1546, 1454, 1391, 1360, 1252, 1224, 1177, 965, 940, 799.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{21}NONa$ $[M+Na]^+$: 254.1515, found: 254.1514.

(*E*)-4-(4-bromophenyl)-N-(*tert*-butyl)but-3-enamide (2r)



Colorless solid (53.9 mg, 0.182 mmol, yield: 91%, E/Z>20:1).

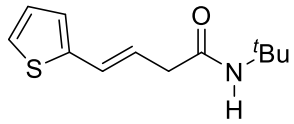
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dt, *J* = 9.1, 2.4 Hz, 2H), 7.22 (dd, *J* = 8.7, 2.2 Hz, 2H), 6.42 (d, *J* = 15.9 Hz, 1H), 6.28 (dt, *J* = 15.8, 7.1 Hz, 1H), 5.35 (brs, 1H), 3.04 (dd, *J* = 7.1, 1.2 Hz, 2H), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 135.7, 132.7, 131.7, 127.8, 123.9, 121.4, 51.4, 41.8, 28.8.

IR (film): *v* (cm^{-1}) 3310, 2979, 1670, 1638, 1544, 1481, 1454, 1393, 1360, 1222, 1175, 1069, 1005, 963, 940, 822.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{18}BrNONa$ $[M+Na]^+$: 318.0464, found: 318.0464.

(*E*)-N-(*tert*-butyl)-4-(thiophen-2-yl)but-3-enamide (2s)



Colorless solid (24.1 mg, 0.108 mmol, yield: 54%, E/Z>20:1).

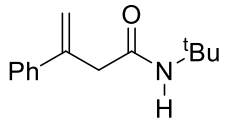
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16–7.09 (m, 1H), 6.94 (d, *J* = 4.7 Hz, 2H), 6.61 (d, *J* = 15.7 Hz, 1H), 6.09 (dt, *J* = 15.6, 7.3 Hz, 1H), 5.39 (brs, 1H), 3.02 (dd, *J* = 7.3, 1.3 Hz, 2H), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 141.8, 127.3, 127.2, 125.5, 124.2, 122.5, 51.3, 41.6, 28.8.

IR (film): *v* (cm^{-1}) 3318, 2972, 2928, 1640, 1609, 1544, 1454, 1419, 1391, 1360, 1322, 1297, 1250, 1222, 1175, 1034, 963, 810.

HRMS (ESI, *m*/*z*) calcd for $C_{12}H_{17}NOSNa$ $[M+Na]^+$: 246.0923, found: 246.0920.

N-(*tert*-butyl)-3-phenylbut-3-enamide (2t)



Colorless solid (30.4 mg, 0.140 mmol, yield: 70%).

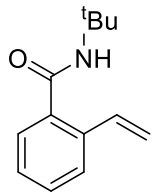
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45–7.41 (m, 2H), 7.36–7.31 (m, 2H), 7.31–7.27 (m, 1H), 5.60 (d, *J* = 1.1 Hz, 1H), 5.49 (brs, 1H), 5.24 (d, *J* = 1.0 Hz, 1H), 3.36 (s, 2H), 1.20 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 142.9, 139.2, 128.6, 128.1, 125.8, 116.5, 51.1, 45.3, 28.4.

IR (film): *v* (cm^{-1}) 3284, 2921, 1638, 1550, 1450, 1356, 1258, 1226, 897, 799, 777, 700, 602.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{19}NONa$ $[M+Na]^+$: 240.1359, found: 240.1354.

N-(*tert*-butyl)-2-vinylbenzamide (2u)



Yellow solid (17.1 mmg, 0.084 mmol, yield: 42%).

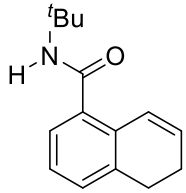
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 7.8 Hz, 1H), 7.42–7.31 (m, 2H), 7.27 (d, J = 8.5 Hz, 1H), 7.01 (dd, J = 17.5, 11.0 Hz, 1H), 5.70 (dd, J = 17.5, 1.0 Hz, 1H), 5.58 (brs, 1H), 5.34 (dd, J = 11.0, 1.0 Hz, 1H), 1.45 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 136.7, 135.4, 134.5, 129.7, 127.7, 127.2, 126.1, 116.5, 52.0, 28.8.

IR (film): ν (cm^{-1}) 3310, 2969, 2926, 1644, 1544, 1452, 1391, 1360, 1222, 895, 777, 700.

HRMS (ESI, m/z) calcd for $C_{13}H_{17}NONa$ $[M+Na]^+$: 226.1202, found: 226.1197.

N-(*tert*-butyl)-5,6-dihydronaphthalene-1-carboxamide (2v)



Colorless solid (25.7 mg, 0.125 mmol, yield: 56%).

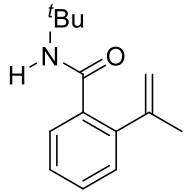
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (dd, J = 7.1, 1.6 Hz, 1H), 7.13–7.06 (m, 2H), 6.79 (d, J = 9.9 Hz, 1H), 6.12 (dt, J = 9.3, 4.5 Hz, 1H), 5.55 (brs, 1H), 2.77 (t, J = 8.2 Hz, 2H), 2.28 (tdd, J = 7.9, 4.5, 1.8 Hz, 2H), 1.45 (s, 9H).

13C NMR (101 MHz, CDCl3) δ 169.2, 136.6, 134.6, 131.1, 130.3, 128.8, 126.4, 124.9, 124.6, 51.8, 28.9, 27.9, 22.6.

IR (film): ν (cm^{-1}) 3310, 2923, 1640, 1521, 1452, 1389, 1358, 1307, 1287, 1220, 771.

HRMS (ESI, m/z) calcd for $C_{15}H_{19}NONa$ $[M+Na]^+$: 254.1515, found: 254.1512.

N-(*tert*-butyl)-2-(prop-1-en-2-yl)benzamide (2w)



Colorless solid (31.7 mg, 0.147 mmol, yield: 73%).

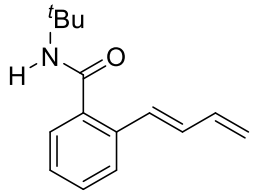
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.30 (dtd, *J* = 20.5, 7.4, 1.5 Hz, 2H), 7.16 (dd, *J* = 7.3, 1.5 Hz, 1H), 6.04 (brs, 1H), 5.21–5.18 (m, 1H), 5.07–5.03 (m, 1H), 2.07 (s, 3H), 1.39 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 146.7, 141.5, 135.1, 129.9, 128.8, 128.4, 127.4, 115.6, 51.6, 28.5, 24.5.

IR (film): *v* (cm^{-1}) 3259, 2965, 1628, 1540, 1479, 1450, 1362, 1322, 1222, 895, 761.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{19}NONa$ $[M+Na]^+$: 240.1359, found: 240.1356.

(*E*)-2-(buta-1,3-dien-1-yl)-N-(tert-butyl)benzamide (2x)



Yellow solid (18.4 mg, 0.080 mmol, yield: 40%, E/Z>20:1).

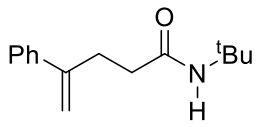
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.42–7.29 (m, 2H), 7.22 (d, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 15.7 Hz, 1H), 6.72 (dd, *J* = 15.6, 10.2 Hz, 1H), 6.50 (dt, *J* = 16.9, 10.1 Hz, 1H), 5.55 (s, 1H), 5.34 (d, *J* = 16.9 Hz, 1H), 5.19 (d, *J* = 10.0 Hz, 1H), 1.45 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 137.1, 136.8, 134.7, 132.0, 129.9, 129.6, 127.40, 127.35, 126.0, 118.5, 52.0, 28.8.

IR (film): *v* (cm^{-1}) 3247, 2967, 2921, 1632, 1597, 1536, 1473, 1391, 1360, 1320, 1260, 1222, 1005, 893.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{19}NONa$ $[M+Na]^+$: 252.1359, found: 252.1357.

N-(*tert*-butyl)-3-phenylbut-3-enamide (2y)



Colorless solid (28.2 mg, 0.130 mmol, yield: 65%).

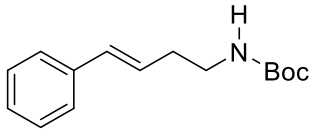
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43–7.37 (m, 2H), 7.32 (t, *J* = 7.3 Hz, 2H), 7.27 (d, *J* = 6.9 Hz, 1H), 5.28 (s, 1H), 5.14 (brs, 1H), 5.09 (s, 1H), 2.83 (t, *J* = 7.6 Hz, 2H), 2.25–2.15 (m, 2H), 1.29 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 147.2, 140.5, 128.4, 127.6, 126.2, 113.2, 51.1, 36.3, 31.3, 28.8.

IR (film): *v* (cm^{-1}) 3310, 2969, 1644, 1544, 1452, 1391, 1360, 1222, 895, 777, 700.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{21}NONa$ $[M+Na]^+$: 254.1515, found: 254.1512.

***tert*-butyl (*E*)-(4-phenylbut-3-en-1-yl)carbamate (2z)**



Colorless solid (25.2 mg, 0.102 mmol, yield: 51%, E/Z>20:1)

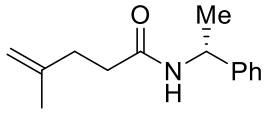
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.32 (m, 2H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.23–7.17 (m, 1H), 6.44 (d, *J* = 15.9 Hz, 1H), 6.14 (dt, *J* = 15.8, 7.1 Hz, 1H), 4.61 (brs, 1H), 3.26 (d, *J* = 6.1 Hz, 2H), 2.39 (q, *J* = 6.7 Hz, 2H), 1.43 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9, 137.2, 132.2, 128.5, 127.2, 127.0, 126.1, 79.2, 40.0, 33.6, 28.4.

IR (film): *v* (cm^{-1}) 3334, 2977, 2922, 1689, 1513, 1452, 1364, 1271, 1248, 1165, 963 .

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{21}NONa$ $[M+Na]^+$: 270.1465, found: 270.1472.

(*R*)-4-methyl-N-(1-phenylethyl)pent-4-enamide (2za)



Colorless solid (29.1 mg, 0.134 mmol, yield: 67%, t/l = 1:1)

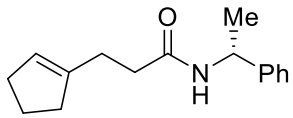
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47–7.16 (m, 5H), 6.00 (d, *J* = 7.9 Hz, 1H), 5.11 (t, *J* = 7.2 Hz, 1H), 4.73 (s, 1H), 4.67 (s, 1H), 2.31 (d, *J* = 3.0 Hz, 4H), 1.71 (s, 3H), 1.45 (dd, *J* = 7.0, 1.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 144.4, 143.2, 128.5, 127.2, 126.1, 110.43, 48.5, 34.7, 33.2, 22.4, 21.7.

IR (film): *v* (cm^{-1}) 3290, 2971, 2920, 1734, 1623, 1515, 1460, 1332, 1294, 1199, 1120, 963, 752 .

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{19}NONa$ $[M+Na]^+$: 240.1346, found: 240.1343.

(*R*)-3-(cyclopent-1-en-1-yl)-N-(1-phenylethyl)propanamide (2zb)



Colorless solid (29.7 mg, 0.122 mmol, yield: 61%)

Notice: The dechlorination by-product cannot be completely removed by column or recrystallization.

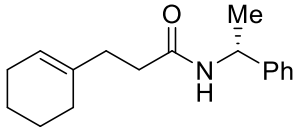
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.20 (m, 5H), 5.79 (br s, 1H), 5.37–5.30 (m, 1H), 5.12 (p, *J* = 7.0 Hz, 1H), 2.48–2.30 (m, 3H), 2.28–2.12 (m, 3H), 2.10–1.88 (m, 1H), 1.86–1.78 (m, 1H), 1.76–1.56 (m, 2H), 1.46 (d, *J* = 6.9 Hz,3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ171.6, 143.20, 143.18, 128.6, 127.3, 126.1, 124.4, 48.5, 35.0, 32.4, 27.0, 23.3, 23.1, 21.7.

IR (film): *v* (cm^{-1}) 3335, 2990, 2912, 2890, 1773, 1600, 1583, 1444, 1386, 1260, 1219, 1139, 973, 863, 721.

HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{21}NONa$ $[M+Na]^+$: 266.1521, found: 266.1520.

(*R*)-3-(cyclohex-1-en-1-yl)-N-(1-phenylethyl)propanamide (2zc)



Colorless solid (36.0 mg, 0.140 mmol, yield: 70%)

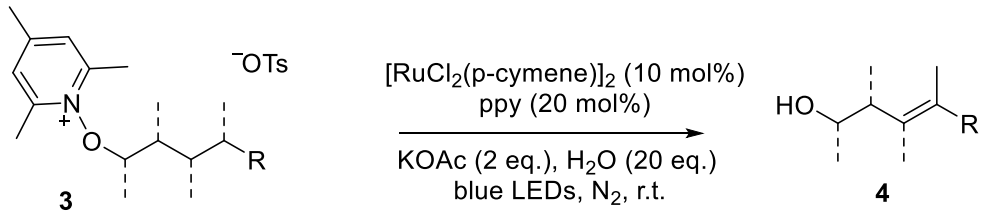
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.26 (m, 5H), 5.84 (br s, 1H), 5.46–5.41 (m, 1H), 5.13 (p, *J* = 7.0 Hz, 1H), 2.35–2.23 (m, 4H), 1.98–1.88 (m, 4H), 1.61–1.56 (m, 2H), 1.55–1.50 (m, 2H), 1.47 (d, *J* = 6.9 Hz,3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 143.3, 136.4, 128.6, 127.3, 126.2, 122.2, 48.6, 34.8, 33.7, 28.1, 25.2, 22.8, 22.4, 21.8.

IR (film): *v* (cm^{-1}) 3340, 2987, 2920, 2864, 1663, 1589, 1562, 1452, 1387, 1257, 1230, 1133, 963, 887, 705 .

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{23}NONa$ $[M+Na]^+$: 280.1658, found: 280.1656.

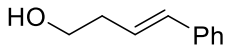
3.2 General procedure for the synthesis of 4



A dried 10 mL Schlenk tube was charged with the catalyst $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), 2-phenylpyridine (20 mol%), *N*-alkoxypyridinium salts **3** (0.20 mmol, 1.0 eq.), KOAc (0.40 mmol, 2.0 eq.) and H_2O (20.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned

approximately 8 cm from 20 W blue LEDs. The reaction was stirred at room temperature for the indicated time (monitored by TLC) under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:10 to 1:5) to afford products **4**. The ratio of E/Z of the product was determined by the crude ^{1}H NMR.

(*E*)-4-phenylbut-3-en-1-ol (4a)



Yellow oil (20.8 mg, 0.140 mmol, yield: 70%, E/Z = 9:1).

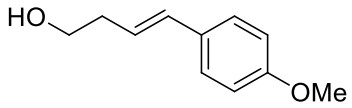
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dt, *J* = 19.6, 7.5 Hz, 4H), 7.22 (t, *J* = 7.3 Hz, 1H), 6.51 (d, *J* = 15.9 Hz, 1H), 6.21 (dt, *J* = 15.8, 7.1 Hz, 1H), 3.76 (t, *J* = 6.3 Hz, 2H), 2.50 (q, *J* = 6.7, 6.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 132.8, 128.5, 127.3, 126.3, 126.1, 62.0, 36.4.

IR (film): *v* (cm^{-1}) 3277, 2965, 2921, 1638, 1560, 1513, 1454, 1360, 1295, 1248, 1226, 1177, 1032, 824.

HRMS (ESI, *m*/*z*) calcd for $C_{10}H_{12}NONa$ $[M+Na]^+$: 171.0780, found: 171.0776.

(*E*)-4-(4-methoxyphenyl)but-3-en-1-ol (4b)



Colorless oil (28.2 mg, 0.158 mmol, yield: 79%, E/Z = 8:1).

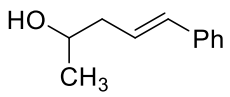
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 9.0 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 6.43 (d, *J* = 15.8 Hz, 1H), 6.04 (dt, *J* = 15.9, 7.2 Hz, 1H), 3.79 (s, 3H), 3.73 (t, *J* = 6.1 Hz, 2H), 2.45 (q, *J* = 6.7, 6.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 132.2, 130.0, 127.2, 124.0, 113.9, 62.0, 55.3, 36.4.

IR (film): *v* (cm^{-1}) 3239, 2957, 2931, 1603, 1507, 1458, 1289, 1240, 1171, 1114, 1030, 999, 965, 836 .

HRMS (ESI, *m*/*z*) calcd for $C_{11}H_{14}O_2Na$ $[M+Na]^+$: 201.0886, found: 201.0877.

(*E*)-5-phenylpent-4-en-2-ol (4c)



Yellow oil (24.0 mg, 0.148 mmol, yield:74%, E/Z>20:1).

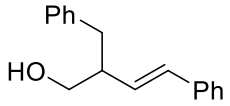
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.22 (q, *J* = 7.1 Hz, 1H), 6.48 (d, *J* = 15.8 Hz, 1H), 6.22 (dt, *J* = 15.6, 7.4 Hz, 1H), 3.93 (q, *J* = 6.0 Hz, 1H), 2.36 (ddt, *J* = 29.1, 14.1, 7.5 Hz, 2H), 1.25 (d, *J* = 6.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 133.1, 128.5, 127.2, 126.24, 126.15, 67.3, 42.9, 22.9.

IR (film): *v* (cm^{-1}) 3394, 3345, 3275, 2967, 2921, 2853, 1644, 1548, 1491, 1454, 1395, 1364, 1318, 1295, 1248, 1181, 1112, 1071, 1034, 1014, 965, 938.

HRMS (ESI, *m*/*z*) calcd for $C_{11}H_{14}ONa$ $[M+Na]^+$: 185.0937, found: 185.0930.

(*E*)-2-benzyl-4-phenylbut-3-en-1-ol (4d)



Colorless oil (20.0 mg, 0.084 mmol, yield: 42%, E/Z=9:1).

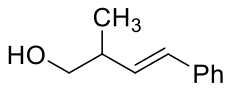
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (t, *J* = 5.9 Hz, 2H), 7.26 (dd, *J* = 17.6, 7.6 Hz, 4H), 7.19 (q, *J* = 7.3, 5.8 Hz, 4H), 6.43 (d, *J* = 16.0 Hz, 1H), 6.10 (dd, *J* = 15.9, 8.2 Hz, 1H), 3.68 (dd, *J* = 10.3, 4.4 Hz, 1H), 3.57 (dd, *J* = 10.6, 6.9 Hz, 1H), 2.86–2.68 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.5, 137.0, 132.4, 130.7, 129.2, 128.5, 128.3, 127.4, 126.2, 126.1, 65.2, 47.5, 37.8.

IR (film): ν (cm^{-1}) 3361, 2921, 2855, 1493, 1452, 1063, 1028, 965, 742, 693.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{18}ONa$ $[M+Na]^+$: 261.1250, found: 261.1246.

(*E*)-2-methyl-4-phenylbut-3-en-1-ol (4e)



Yellow oil (18.2 mg, 0.112 mmol, yield: 56%, E/Z=10:1).

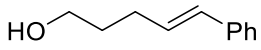
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 6.48 (d, *J* = 15.9 Hz, 1H), 6.09 (dd, *J* = 15.9, 7.9 Hz, 1H), 3.55 (ddd, *J* = 31.6, 10.5, 6.8 Hz, 2H), 2.55 (dq, *J* = 13.5, 6.5 Hz, 1H), 1.11 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 132.4, 131.0, 128.5, 127.3, 126.1, 67.4, 40.2, 16.5.

IR (film): ν (cm^{-1}) 3342, 2957, 2916, 2872, 2849, 1464, 1067, 1032, 987, 965.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{18}ONa$ $[M+Na]^+$: 185.0937, found: 185.0928.

(*E*)-5-phenylpent-4-en-1-ol (4f)



Colorless oil (11.04 mg, 0.068 mmol, yield: 34%, E/Z = 10:1).

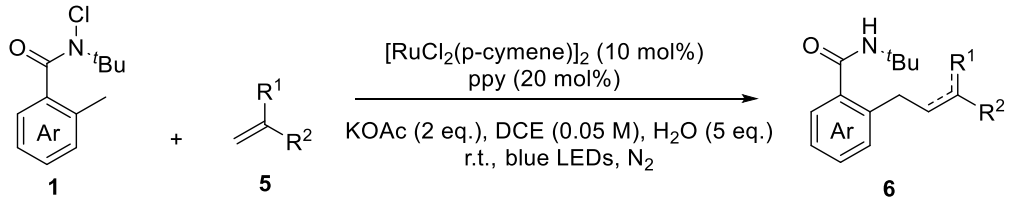
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.6 Hz, 2H), 7.19 (t, *J* = 6.6 Hz, 1H), 6.42 (d, *J* = 15.9 Hz, 1H), 6.22 (dt, *J* = 15.9, 6.9 Hz, 1H), 3.71 (t, *J* = 6.5 Hz, 2H), 2.31 (q, *J* = 7.4 Hz, 2H), 1.75 (p, *J* = 6.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6, 130.4, 130.0, 128.5, 126.9, 125.9, 62.4, 32.2, 29.3.

IR (film): ν (cm^{-1}) 3342, 2957, 2916, 2872, 2849, 1464, 1067, 1032, 987, 965.

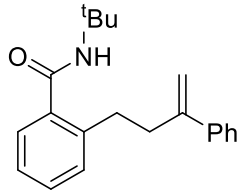
HRMS (ESI, *m*/*z*) calcd for $C_{11}H_{14}ONa$ $[M+Na]^+$: 185.0937, found: 185.0928.

3.3 General procedure for the synthesis of 6



A dried 10 mL Schlenk tube was charged with the catalyst $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), 2-phenylpyridine (20 mol%), *N*-chlorocarboxamides **1** (0.20 mmol, 1.0 eq.), olefins **5** (1.0 mmol, 5.0 eq.), KOAc (0.40 mmol, 2.0 eq.) and H_2O (5.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs. The reaction was stirred at room temperature for the indicated time (monitored by TLC) under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:15) to afford products **6**.

N-(*tert*-butyl)-2-(3-phenylbut-3-en-1-yl)benzamide (6a)



Colorless solid (33.0 mg, 0.09.0 mmol, yield: 45%).

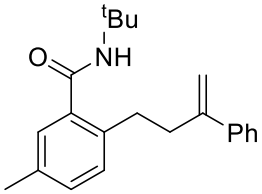
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.1 Hz, 2H), 7.34–7.24 (m, 5H), 7.23–7.14 (m, 3H), 5.52 (brs, 1H), 5.29 (s, 1H), 5.07 (s, 1H), 2.94–2.87 (m, 2H), 2.86–2.79 (m, 2H), 1.42 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 147.9, 140.9, 139.5, 137.8, 130.2, 129.4, 128.3, 127.4, 126.6, 126.2, 125.9, 112.7, 51.7, 37.2, 32.5, 28.8.

IR (film): ν (cm^{-1}) 3320, 2965, 2925, 1638, 1530, 1450, 1362, 1309, 1222, 883.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{26}NO$ $[M+H]^+$: 308.2009, found: 308.2003.

N-(*tert*-butyl)-5-methyl-2-(3-phenylbut-3-en-1-yl)benzamide (6b)



Colorless solid (24.5 mg, 0.076 mmol, yield: 38%).

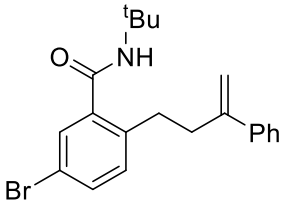
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50–7.42 (m, 2H), 7.34–7.29 (m, 2H), 7.25 (m, 1H), 7.11–7.04 (m, 3H), 5.51 (brs, 1H), 5.29 (s, 1H), 5.07 (s, 1H), 2.85 (d, *J* = 8.2 Hz, 2H), 2.81 (d, *J* = 7.9 Hz, 2H), 2.31 (s, 3H), 1.42 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 148.0, 140.9, 137.8, 136.4, 135.5, 130.1, 128.3, 127.2, 126.2, 112.6, 51.7, 37.4, 32.1, 28.8, 20.9.

IR (film): ν (cm^{-1}) 3326, 2963, 2923, 1636, 1532, 1493, 1450, 1391, 1360, 1313, 1222, 893.

HRMS (ESI, *m*/*z*) calcd for $C_{22}H_{27}NONa$ $[M+Na]^+$: 344.1985, found:344.1979.

5-bromo-N-(*tert*-butyl)-2-(3-phenylbut-3-en-1-yl)benzamide (6c)



Colorless solid (52.0 mg, 0.126 mmol, yield: 63%)

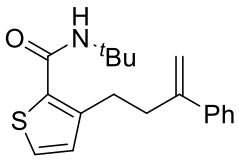
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (td, *J* = 7.7, 6.8, 3.2 Hz, 4H), 7.34–7.25 (m, 3H), 7.03–6.99 (m, 1H), 5.52 (br 1H), 5.28 (s, 1H), 5.04 (s, 1H), 2.82 (q, *J* = 3.5 Hz, 4H), 1.41 (s, 9H).

^{13}C NMR (101 MHz, CDCl3) δ 168.0, 147.5, 140.7, 139.5, 138.5, 132.3, 132.0, 129.4, 128.4, 127.5, 126.2, 119.4, 113.0, 52.0, 36.9, 32.0, 28.7.

IR (film): ν (cm^{-1}) 3238, 2957, 2928, 1630, 1534, 1477, 1450, 1391, 1360, 1313, 1222, 895, 828.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{24}BrNONa$ $[M+Na]^+$: 408.0933, found:408.0930.

N-(*tert*-butyl)-3-(3-phenylbut-3-en-1-yl)thiophene-2-carboxamide (6d)



Yellow solid (17.4 mg, 0.058 mmol, yield: 29%)

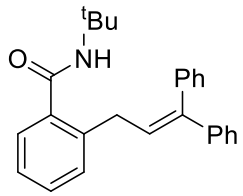
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.4 Hz, 2H), 7.35–7.25 (m, 3H), 7.18 (d, *J* = 5.0 Hz, 1H), 6.85 (d, *J* = 5.0 Hz, 1H), 5.60 (brs, 1H), 5.29 (s, 1H), 5.06 (s, 1H), 3.09–3.03 (m, 2H), 2.85–2.80 (m, 2H), 1.40 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 147.5, 144.4, 140.9, 132.3, 130.7, 128.3, 127.4, 126.1, 125.5, 112.9, 51.9, 36.0, 28.9, 28.3.

IR (film): ν (cm^{-1}) 3257, 2963, 2923, 1632, 1536, 1503, 1477, 1452, 1391, 1362, 1311, 1271, 1220, 895.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{23}NOSNa$ $[M+Na]^+$: 336.1393, found:336.1388.

N-(*tert*-butyl)-2-(3,3-diphenylallyl)benzamide (6e)



Colorless solid (33.4 mg, 0.090 mmol, yield: 45%).

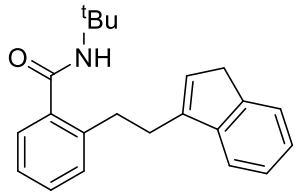
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.37 (m, 2H), 7.36–7.31 (m, 3H), 7.30–7.27 (m, 4H), 7.25–7.18 (m, 5H), 6.28 (t, *J* = 7.4 Hz, 1H), 5.54 (s, 1H), 3.63 (d, *J* = 7.4 Hz, 2H), 1.40 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 142.6, 142.4, 139.7, 138.7, 137.6, 129.9, 129.8, 129.7, 128.4, 128.3, 128.1, 127.9, 127.6, 127.3, 127.2, 127.0, 126.6, 126.0, 51.8, 29.7, 28.8.

IR (film): ν (cm^{-1}) 3391, 2391, 2965, 2921, 1630, 1538, 1511, 1475, 1452, 1422, 1391, 1362, 1303, 1216, 903.

HRMS (ESI, *m*/*z*) calcd for $C_{26}H_{27}NONa$ $[M+Na]^+$: 392.1985, found:392.1981.

2-(2-(1H-inden-3-yl)ethyl)-N-(tert-butyl)benzamide (6f)



Colorless solid (57.7 mg, 0.180 mmol, yield: 90%).

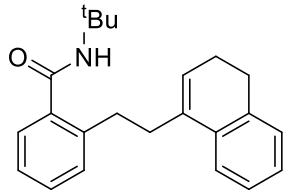
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49–7.41 (m, 2H), 7.30 (dd, *J* = 11.9, 4.3 Hz, 4H), 7.23–7.18 (m, 2H), 6.23 (s, 1H), 5.57 (s, 1H), 3.32 (s, 2H), 3.18–3.09 (m, 2H), 2.94–2.85 (m, 2H), 1.44 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 145.3, 144.4, 144.0, 139.9, 137.9, 130.2, 129.5, 128.2, 126.6, 126.04, 125.97, 124.5, 123.7, 119.2, 51.8, 37.7, 32.1, 30.0, 28.8.

IR (film): ν (cm^{-1}) 3391, 2391, 2965, 2921, 1630, 1538, 1511, 1475, 1452, 1422, 1391, 1362, 1303, 1216,

HRMS (ESI, *m*/*z*) calcd for $C_{22}H_{25}NONa$ $[M+Na]^+$: 342.1828, found:342.1824.

N-(*tert*-butyl)-2-(2-(3,4-dihydronaphthalen-1-yl)ethyl)benzamide (6g)



Colorless solid (54.6 mg, 0.164 mmol, yield: 82%)

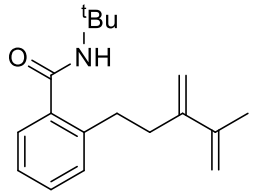
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 6.9 Hz, 2H), 7.23–7.16 (m, 3H), 7.13 (d, *J* = 4.1 Hz, 2H), 5.85 (t, *J* = 4.4 Hz, 1H), 5.58 (s, 1H), 2.98 (dd, *J* = 9.7, 6.5 Hz, 2H), 2.74 (dt, *J* = 16.0, 8.4 Hz, 4H), 2.25–2.18 (m, 2H), 1.45 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 140.0, 137.8, 136.7, 136.2, 134.7, 130.3, 129.4, 127.5, 126.6, 126.5, 125.9, 125.4, 122.9, 51.8, 35.1, 32.8, 28.8, 28.4, 23.1.

IR (film): ν (cm^{-1}) 3259, 2925, 1628, 1540, 1481, 1450, 1360, 1324, 1222, 775.

HRMS (ESI, *m*/*z*) calcd for $C_{23}H_{27}NONa$ $[M+Na]^+$: 356.1985, found:256.1979.

N-(*tert*-butyl)-2-(4-methyl-3-methylenepent-4-en-1-yl)benzamide (6h)



Colorless solid (13.1 mg, 0.048 mmol, yield: 24%)

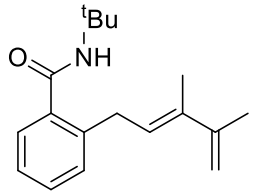
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.4 Hz, 2H), 7.18 (d, *J* = 6.6 Hz, 2H), 5.57 (brs, 1H), 5.19 (s, 1H), 5.08 (s, 1H), 5.00 (s, 1H), 4.97 (s, 1H), 2.92 (dd, *J* = 9.5, 6.8 Hz, 2H), 2.60–2.54 (m, 2H), 1.90 (s, 3H), 1.44 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 147.4, 142.3, 139.9, 137.8, 130.1, 129.4, 126.6, 125.9, 113.0, 112.5, 51.8, 35.8, 33.0, 28.8, 21.2.

IR (film): ν (cm^{-1}) 3279, 2963, 2921, 1634, 1599, 1542, 1450, 1391, 1362, 1320, 1222, 887.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{25}NONa$ $[M+Na]^+$: 294.1828, found:294.1823.

(*E*)-N-(*tert*-butyl)-2-(3,4-dimethylpenta-2,4-dien-1-yl)benzamide (6h')



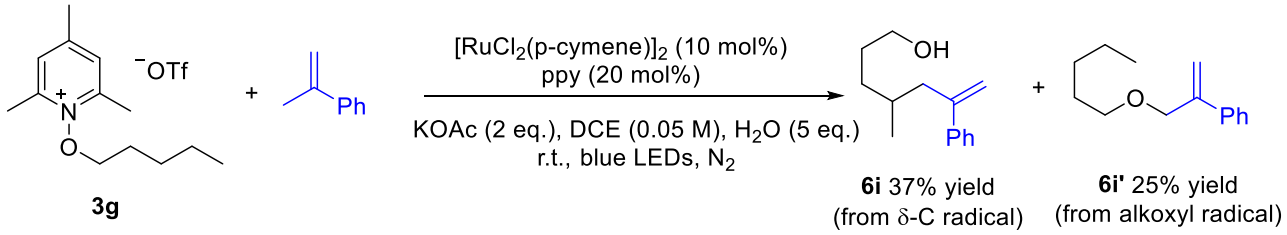
Colorless solid (12.8 mg, 0.040 mmol, yield: 20%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.27 (m, 2H), 7.22–7.16 (m, 2H), 5.69 (t, *J* = 7.0 Hz, 1H), 5.59 (s, 1H), 5.03 (s, 1H), 4.91 (s, 1H), 3.66 (d, *J* = 7.0 Hz, 2H), 1.89 (s, 3H), 1.87 (s, 3H), 1.42 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 147.4, 142.3, 139.9, 137.8, 133.0, 130.1, 129.4, 126.6, 125.9, 113.0, 112.5, 51.8, 35.8, 33.0, 28.8, 21.2.

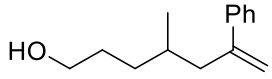
IR (film): ν (cm^{-1}) 3289, 2967, 1638, 1601, 1538, 1481, 1450, 1391, 1362, 1318, 1222, 881.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{25}NONa$ $[M+Na]^+$: 294.1828, found:294.1822.



A dried 10 mL Schlenk tube was charged with the catalyst $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), 2-phenylpyridine (20 mol%), *N*-alkoxypyridinium salt **3g** (0.20 mmol, 1.0 eq.), prop-1-en-2-ylbenzene (1.0 mmol, 5.0 eq.), KOAc (0.40 mmol, 2.0 eq.) and H_2O (5.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs. The reaction was stirred at room temperature for the indicated time (monitored by TLC) under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:10) to afford products **6i and 6i′**.

4-methyl-6-phenylhept-6-en-1-ol (6i)

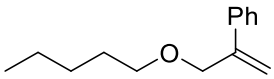


Colorless oil (15.1 mg, 0.074 mmol, yield: 37%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.26–7.21 (m, 1H), 5.25 (s, 1H), 5.02 (s, 1H), 3.57 (t, *J* = 6.6 Hz, 2H), 2.60 – 2.43 (m, 2H), 2.33 – 2.21 (m, 1H), 1.65–1.45 (m, 4H), 0.84 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 141.3, 128.2, 127.2, 126.3, 113.8, 63.3, 43.3, 32.6, 30.8, 30.1, 19.4.

(3-(pentyloxy)prop-1-en-2-yl)benzene (6i')



Colorless solid (10.2 mg, 0.050 mmol, yield: 25%)

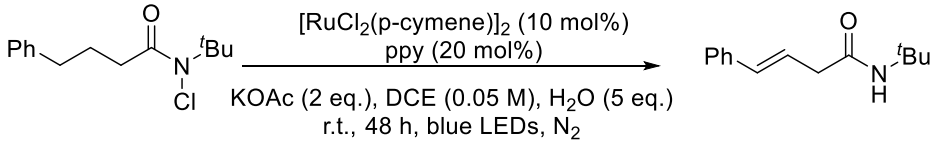
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50–7.43 (m, 2H), 7.35–7.22 (m, 3H), 5.50 (s, 1H), 5.33 (s, 1H), 4.34 (s, 2H), 3.47 (t, J = 6.6 Hz, 2H), 1.64–1.48 (m, 2H), 1.36–1.22 (m, 3H), 0.92–0.81 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 138.9, 128.3, 127.7, 126.1, 113.9, 72.7, 70.3, 29.4, 28.3, 22.5, 14.0.

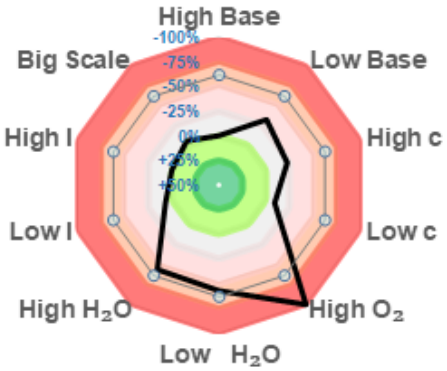
3.4 Sensitivity Assessment

The reaction-condition-based sensitivity assessment procedure was followed by a published paper[3] .

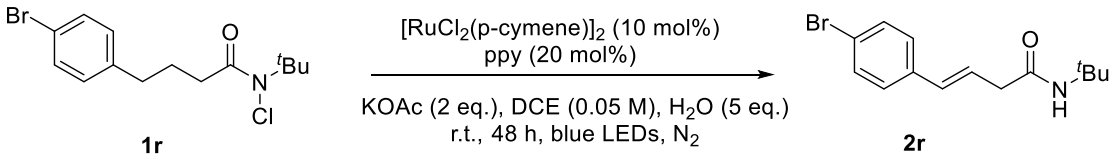
Table S1. Sensitivity Screen reaction set-up and results.



entry	modification	execution	yield(%)	deviation(%)
1	High Base	30 % base	75	0
‘’2	Low Base	10 % base	51	-32
3	High c	0.1 M	58	-22.7
4	Low c	0.025 M	68	-9.3
5	High O_2	air	0	-100
6	Low H_2O	no H_2O	32	-57.3
7	High H_2O	10 eq H_2O	33	-56
8	Low I	15 W Blue LEDs	70	-6.7
9	High I	53W Blue LEDs	75	0
10	large scale	1 mmol	71	-5.3



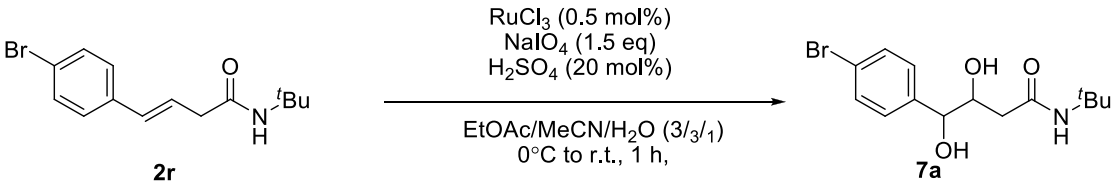
4. Scale-Up Reaction



A dried 120 mL Schlenk tube was charged with the catalyst $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), 2-phenylpyridine (20 mol%), *N*-chlorocarboxamides **1r** (5.0 mmol, 1.0 eq.), KOAc (10.0 mmol, 2.0 eq.) and H_2O (5.0 eq.). Then DCE (60 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs. The reaction was stirred at room temperature for 24 h under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:15 to 1:5) to afford products **2r** (1.211 g, 4.1 mmol, yield: 83%, E/Z>20:1).

5. Synthetic Transformations

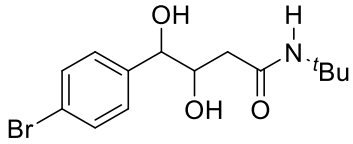
5.1 Dihydroxylation[4]



A dried 15 mL Schlenk tube was charged with $NaIO_4$ (64.2 mg, 0.3 mmol, 1.5 eq.) was dissloved in 0.15 mL H_2O. Then 1 M H_2SO_4 (40 μL, 0.04 mmol, 20 mol%) was added. The solution was cooled to °C. A 0.1 M aqueous solution of $RuCl_3$ (10 μL, 0.001 mmol, 5 mol%) was added and the mixture was stirred until the color turned bright yellow. Ethyl acetate (0.6 mL) was added and stirring was

continued for 5 min. Acetonitrile (0.6 mL) was added and stirring was continued for further 5 min. The **2r** (59 mg, 0.2 mmol, 1 eq) was added at 0 °C. Stirring at r.t. for 1 h, quenched with 1.5 mL $NaHCO_3$-solution, and 2 mL $Na_2S_2O_3$-solution and extracted with EtOAc (5 mL × 3). The organic layers were combined, dried over Na_2SO_4, filtered, concentrated, and purified by preparative TLC (Hexanes/ EtOAc=2:1) to afford **7a**.

4-(4-bromophenyl)-N-(*tert*-butyl)-3,4-dihydroxybutanamide (7a)



Yellow oil (33.0 mg, 0.100 mmol, yield: 50%, dr > 20:1).

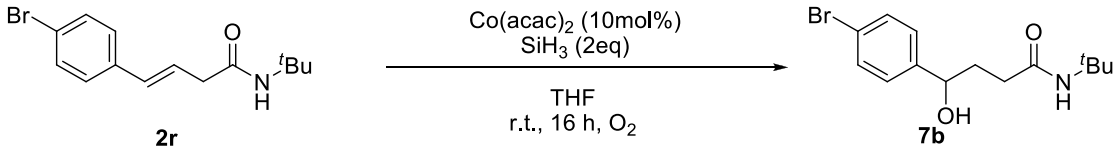
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 5.48 (brs, 1H), 4.59 (brs, 1H), 4.47 (d, *J* = 6.7 Hz, 1H), 3.96 (q, *J* = 6.1 Hz, 1H), 3.50 (brs, 1H), 2.13 (d, *J* = 5.8 Hz, 2H), 1.31 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 139.4, 131.6, 128.7, 122.0, 76.3, 72.9, 51.7, 38.7, 28.7.

IR (film): ν (cm^{-1}) 3340, 3267, 2921, 2851, 1652, 1628, 1544, 1489, 1473, 1456, 1434, 1393, 1364, 1318, 1222, 1191, 1069, 1040, 1010.

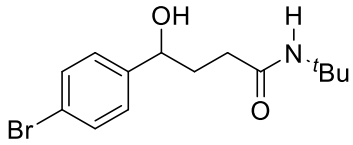
HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{20}NO_3BrNa$ $[M+Na]^+$: 352.0519, found: 352.0520.

5.2 Hydroxylation[5]



A dried 15 mL Schlenk tube was charged with the catalyst $Co(acac)_2$ (5.2 mg, 0.02 mmol, 10 mol%) and **2r** (59.0 mg, 0.2 mmol, 1 eq.). Then THF (1 mL) was addition. To this solution was added $PhSiH_3$ (50 μL, 0.4 mmol, 2 eq.). The vial was purged with O_2 and equipped with an O_2 balloon. The reaction was allowed to stir at room temperature for 16 h, quenched with water (2 mL), and extracted with EtOAc (5 mL × 3). The organic layers were combined, dried over Na_2SO_4, filtered, concentrated, and purified by preparative TLC (Hexanes/ EtOAc=2:1) to afford **7b**.

4-(4-bromophenyl)-N-(*tert*-butyl)-4-hydroxybutanamide (7b)



Yellow oil (35.2 mg, 0.112 mmol, yield: 56%).

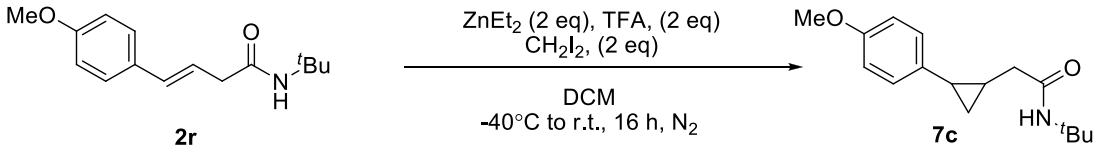
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 5.44 (brs, 1H), 4.71 (dd, *J* = 7.8, 3.8 Hz, 1H), 4.51 (brs, 1H), 2.23 (t, *J* = 6.5 Hz, 2H), 1.94 (td, *J* = 13.7, 6.7 Hz, 2H), 1.32 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.0, 143.8, 131.3, 127.5, 120.8, 72.9, 51.5, 34.2, 33.7, 28.7.

IR (film): ν (cm^{-1}) 3312, 2925, 1642, 1548, 1487, 1454, 1424, 1395, 1362, 1222, 1136, 1105, 1069, 1008.

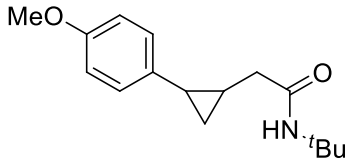
HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{20}NO_2BrNa$ $[M+Na]^+$: 336.057, found: 336.0566.

5.3 Cyclopropanation[6]



A dried 15 mL Schlenk tube was charged with a stir bar, DCM (0.5 mL) under nitrogen atmosphere was added and cooled to –40 ℃. $ZnEt_2$ (1.0 M, 0.4 mL, 0.4 mmol, 2 eq.) was added followed by a solution of TFA (0.33 mL, 0.4 mmol, 2.0 eq.) in DCM (0.5 mL). The reaction mixture was stirred at this temperature for 1 h followed by warming to –10 ℃. Next, CH_2I_2 (108 mg, 0.4 mmol, 2.0 eq.) was dropwise into the reaction mixture and the resulting solution was allowed to stir at –10 ℃ for another 1 h. A solution of **2p** (0.2 mmol, 1.0 eq.) in DCM (0.5 mL) was then added, the reaction mixture was allowed to warmed to room temperature and stirred for 16 h. The reaction was quenched by sat. NH_4Cl (3 mL) and extracted with DCM (5 mL × 3). The combined organic layers were washed with aq. $NaHCO_3$ (1.0 M, 20 mL) and brine (20 mL), dried over Na_2SO_4, filtered, concentrated, and purified by preparative TLC (Hexanes/ EtOAc=30:1 to 10:1) to afford **7c**.

N-(*tert*-butyl)-2-(2-(4-methoxyphenyl)cyclopropyl)acetamide (7c)



Colorless solid (48.1mg, 0.184mmol, yield: 92%, dr > 20:1).

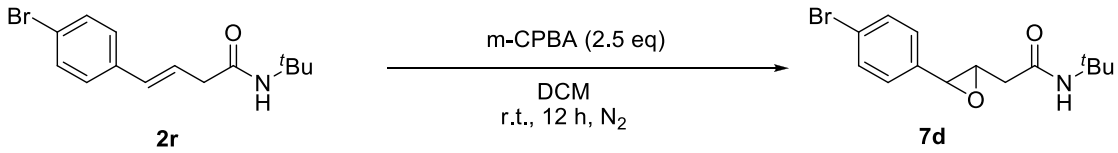
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 (d, *J* = 8.7 Hz, 2H), 6.79 (d, *J* = 8.6 Hz, 2H), 5.65 (brs, 1H), 3.75 (s, 3H), 2.28–2.13 (m, 2H), 1.67 (dd, *J* = 8.9, 4.6 Hz, 1H), 1.29 (s, 9H), 1.16–1.09 (m, 1H), 0.99–0.94 (m, 1H), 0.82 (dd, *J* = 8.8, 5.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.30, 157.84, 134.10, 126.80, 113.88, 55.27, 51.04, 42.12, 28.80, 22.39, 19.05, 15.05.

IR (film): ν (cm^{-1}) 3265, 2965, 1638, 1560, 1513, 1454, 1360, 1295, 1248, 1226, 1177, 1032.

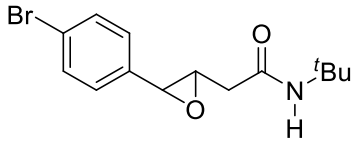
HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{23}NO_2Na$ $[M+Na]^+$: 284.1621, found: 284.1619.

5.4 Epoxidation[7]



A dried 15 mL Schlenk tube was charged with (*E*)-N-(tert-butyl)-4-(p-tolyl)but-3-enamide **2r** (59.0 mg, 0.2 mmol, 1.0 eq.), m-CPBA (86.1 mg, 0.5 mmol, 2.5 eq.) were dissolved in anhydrous DCM (2 mL) and the solution was stirred at room temperature for 12 h. Then saturated $Na_2S_2O_3$ aqueous solution was added. The mixture was extracted with DCM (5 mL × 3). The organic layer was washed by Na_2CO_3 aqueous solution then dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was recrystallization by petroleum ether / ethyl acetate (30:1) to afford **7d**.

2-(3-(4-bromophenyl)oxiran-2-yl)-N-(tert-butyl)acetamide (7d)



Yellow solid (45.0 mg, 0.144 mmol, yield: 72%, dr = 3:1).

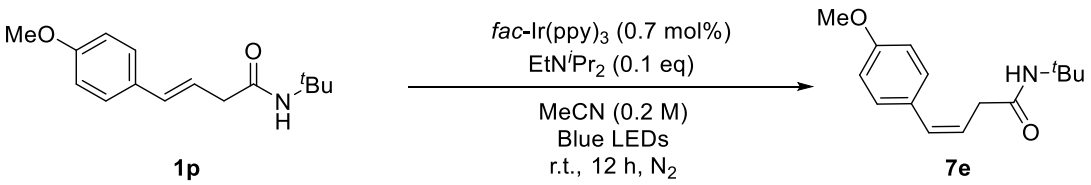
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 5.70 (brs, 1H), 3.67 (d, *J* = 1.8 Hz, 1H), 3.27–3.21 (m, 1H), 2.69 (dd, *J* = 15.2, 3.6 Hz, 1H), 2.36 (dd, *J* = 15.2, 7.0 Hz, 1H), 1.36 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 131.9, 131.4, 130.3, 126.9, 80.4, 51.1, 36.5, 34.5, 28.8, 26.8.

IR (film): ν (cm^{-1}) 3299, 2969, 1666, 1640, 1550, 1489, 1452, 1395, 1364, 1226, 1207, 1071, 1008, 889.

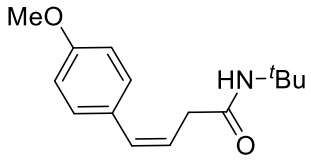
HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{18}NO_2BrNa$ $[M+Na]^+$: 334.0413, found: 334.0412.

5.5 Photosensitized alkene isomerization[8]



A dried 10 mL Schlenk tube was charged with **2p** (59 mg, 0.2 mmol, 1 eq.), N,N-diisopropylethylamine (4.0 μL, 0.02 mmol), $Ir(ppy)_3$ (1 mg, 0.0014 mmol, 0.7 mol%), then CH_3CN (1 mL) was added. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs. The reaction mixture was stirring at room temperature for 24h, removed solvent by vacuum to afford product **7e**.

(*Z*)-N-(*tert*-butyl)-4-(4-methoxyphenyl)but-3-enamide (7e)



Colorless solid (43.0 mg, 0.198 mmol, yield: 99%, E/Z = 1:8).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.3 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 11.4 Hz, 1H), 5.73 (dt, *J* = 11.7, 7.6 Hz, 1H), 5.53 (s, 1H), 3.78 (s, 3H), 3.13 (d, *J* = 7.1 Hz, 2H), 1.29 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 158.8, 132.4, 129.9, 129.0, 122.8, 113.8, 55.3, 51.2, 37.5, 28.7.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{21}NO_2Na$ $[M+Na]^+$: 270.1465, found: 270.1461.

6. Mechanistic Studies

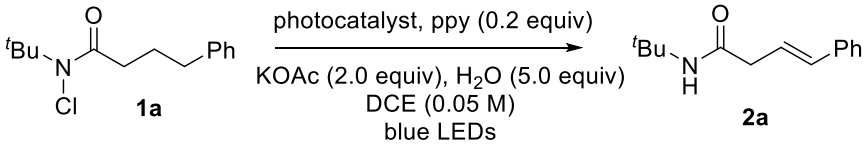
6.1 Photocatalyst investigation

1) Photocatalyst screening

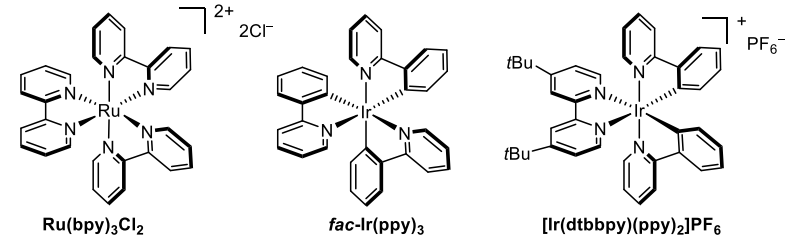
Performed in analogy to entry 13 of Table 1 with replacement of $[RuCl_2(p\text{-cymene})]_2$ to commonly used photocatalyst, such as $Ru(bpy)_3Cl_2$, *fac*-$Ir(ppy)_3$, $[Ir(dtbbpy)(ppy)_2]PF_6$ and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ or other fleshly synthezied Ru complexes, such as Ru(ppy)(*p*-cymene)Cl, Ru(ppy)(*p*-cymene)OAc, $Ru(ppy)(CH_3CN)_4PF_6$.

The results are listed as following: (a) the use of $Ru(bpy)_3Cl_2$, *fac*-$Ir(ppy)_3$, $[Ir(dtbbpy)(ppy)_2]PF_6$ or $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ in this reaction found that it was not capable of catalyzing the desaturation reaction and the desired product was not observed. (b) the use of Ru(ppy)(*p*-cymene)Cl or Ru(ppy)(*p*-cymene)OAc in this reaction found that it displayed the similar catalytic activity (65% or 74%, respectively), whereas $Ru(ppy)(CH_3CN)_4PF_6$ was less effective (17%).

Table S2[a]. Photocatalysts screening



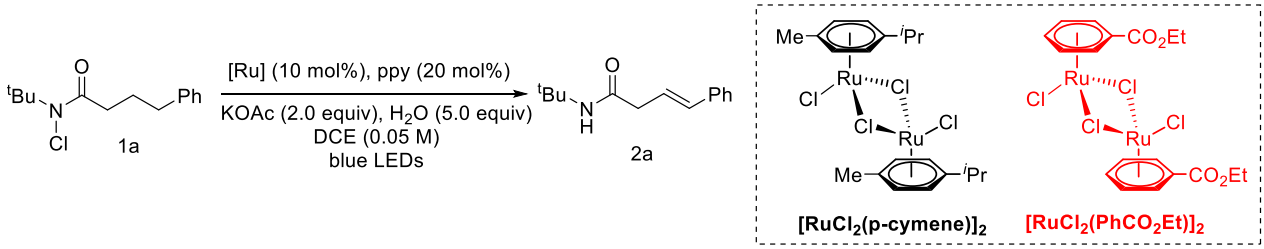
entry	photocatalyst	yield(%)[b]
1	$[RuCl_2(p\text{-cymene})]_2$ (5 mol%)	72
2	$Ru(bpy)_3Cl_2$ (5 mol%)	0
3	*fac*-$Ir(ppy)_3$ (5 mol%)	0
4	$[Ir(dtbbpy)(ppy)_2]PF_6$ (5 mol%)	0
5	$[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (5 mol%)	0
6	Ru(ppy)(*p*-cymene)Cl (10 mol%)	65
7	Ru(ppy)(*p*-cymene)OAc (10 mol%)	74
8	$Ru(ppy)(CH_3CN)_4PF_6$ (10 mol%)	17

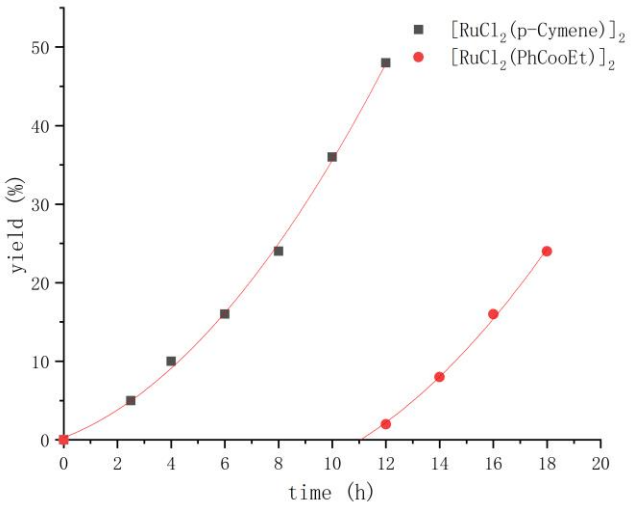


[a] Reaction conditions: N-chlorocarboxamide **1a** (0.2 mmol) with photocatalyst (5.0 or 10.0 mol%), ppy (0.2 equiv), KOAc (2.0 equiv) and H_2O (5.0 equiv) in DCE (4.0 mL) under light irradiation using 20 W blue LEDs at room temperature for 48 h under nitrogen atmosphere. [b] isolated yield.

2) Influence of *p*-cymene:

Performed in analogy to entry 13 of Table 1 with replacement of $[RuCl_2(p\text{-cymene})]_2$ to $[RuCl_2(PhCO_2Et)]_2$. It is easy to observe that *p*-cymene ligand is more efficient to deliver the target product.

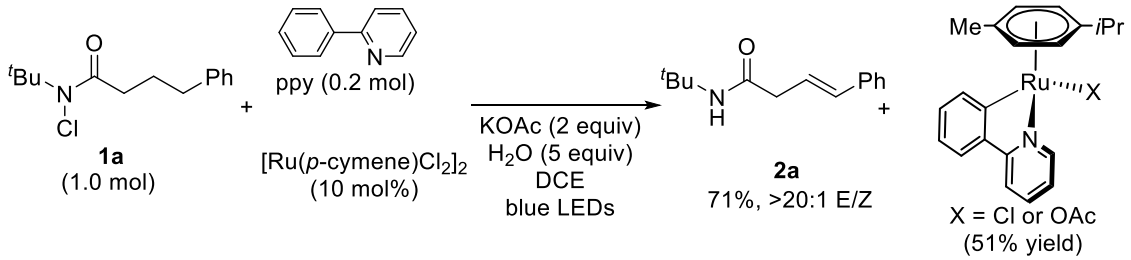




3) Isolation of intermediate ruthenium complex

Performed in analogy to entry 13 of Table 1 with 1.0 mmol scale. Product **2a** was isolated in 71%. Ru(ppy)(*p*-cymene)X (X = Cl or OAc) was isolated in 51%.

Note: Ru(ppy)(*p*-cymene)OAc was unstable on the column and could be easily transformed to Ru(ppy)(*p*-cymene)Cl. [9]



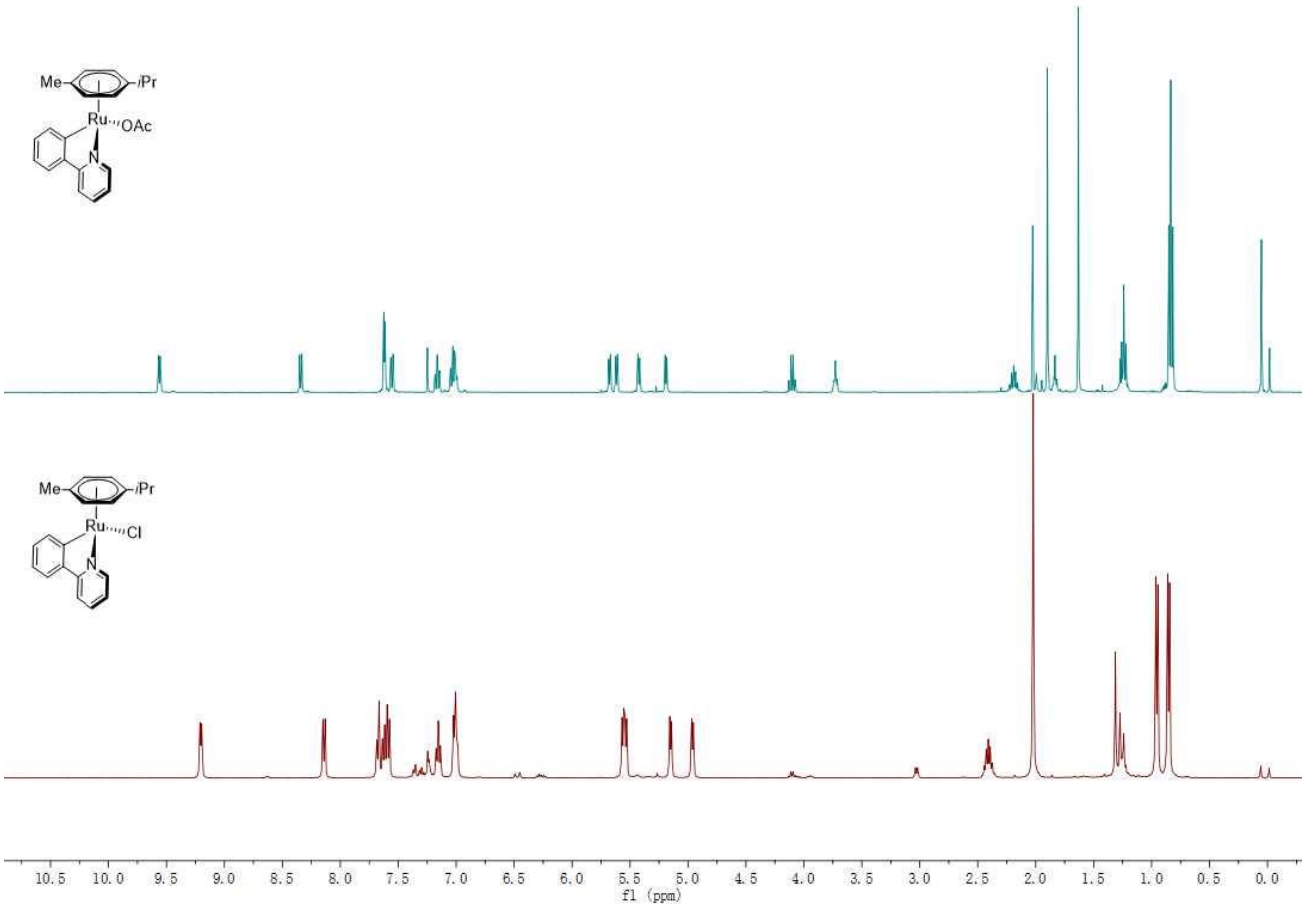
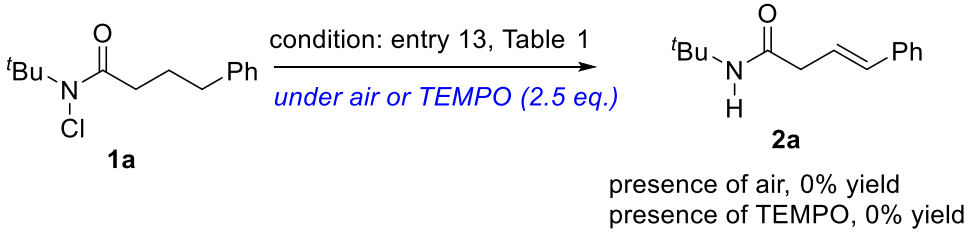


Figure 1S ^{1}H NMR spectra of Ru(ppy)(*p*-cymene)OAc or Ru(ppy)(*p*-cymene)Cl .

6.2 Control reactions

Control reaction a or b is shown that in the presence of air or TEMPO (2.5 eq.) results in the inhibition of product **2a**, which provides evidence for a radical pathway.

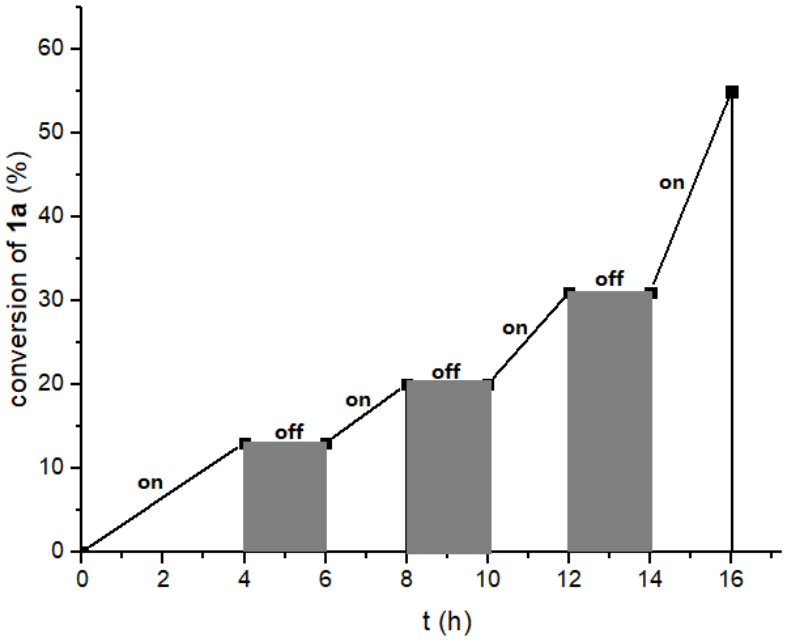


6.3 Off-on light effect

To elucidate the role of the visible light, we conducted an on/off light experiments. The conversion of **1a** was completely suppressed in the absence of light, being indicative of the photoinduced Ru-catalyzed desaturation not involving a radical chain process.

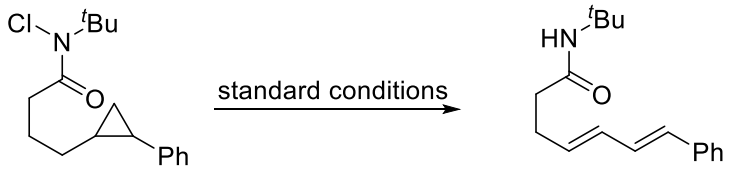
t (h)	conversion of **1a** (%)

4.0	13
6.0	13
8.0	20
10.0	20
12.0	31
14.0	31
16.0	55



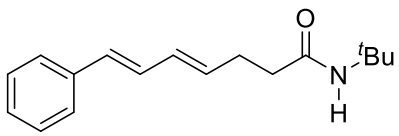
6.4 Radical clock reaction

Performed in analogy to entry 13 of Table 1 with replacement of **1a** to **1zh** afforded the ring-opened diene product **2zh**.



1zh **2zh** 47% yield

(4*E*,6*E*)-N-(*tert*-butyl)-7-phenylhepta-4,6-dienamide (2zh)



Yellow solid (24.0 mg, 0.093 mmol, yield: 47%, E/Z = 1:1)

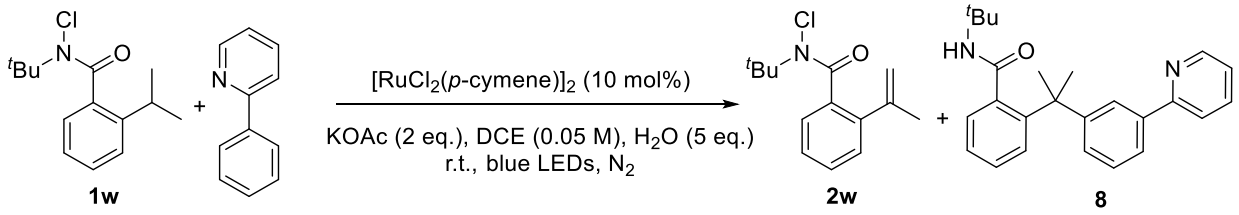
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28–7.24 (m, 5H), 6.68 (dd, *J* = 15.6, 10.4 Hz, 1H), 6.38 (d, *J* = 15.6 Hz, 1H), 6.21 (dd, *J* = 14.9, 10.5 Hz, 1H), 5.80 (dt, *J* = 14.7, 7.0 Hz, 1H), 5.25 (brs, 1H), 2.44 (q, *J* = 7.1 Hz, 2H), 2.19 (t, *J* = 7.3 Hz, 2H), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 135.9, 134.1, 132.7, 131.3, 129.5, 129.4, 128.7, 127.3, 51.2, 37.1, 28.8.

IR (film): ν (cm^{-1}) 3328, 2921, 1699, 1644, 1595, 1542, 1491, 1454, 1413, 1395, 1362, 1267, 1222, 1181, 1089, 1054, 1012, 983.

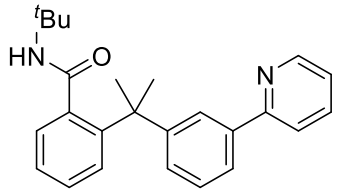
HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{23}NONa$ $[M+Na]^+$: 258.1852, found: 258.1844.

6.5 Isolation of radical addition product



A dried 10 mL Schlenk tube was charged with the catalyst $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), 2-phenylpyridine (62.1 mg, 0.40 mmol, 2.0 eq.), *N*-chlorocarboxamide **1w** (0.20 mmol, 1.0 eq.), KOAc (0.40 mmol, 2.0 eq.) and H_2O (5.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs. The reaction was stirred at room temperature for 48 h under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:2) to afford desaturation product **2w** (24% yield) and radical addition product **8** (8% yield).

N-(*tert*-butyl)-2-(2-(3-(pyridin-2-yl)phenyl)propan-2-yl)benzamide (8)



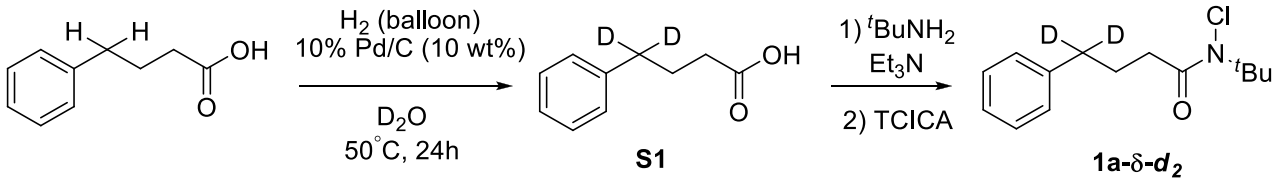
Colorless solid (6.0 mg, 0.016 mmol, yield: 8%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.3 Hz, 1H), 7.81–7.68 (m, 3H), 7.60 (dd, *J* = 21.0, 7.9 Hz, 2H), 7.36 (q, *J* = 8.0 Hz, 2H), 7.24–7.17 (m, 3H), 4.87 (brs, 1H), 1.82 (s, 6H), 0.98 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.77, 157.64, 151.82, 149.63, 145.68, 139.17, 136.70, 129.60, 128.83, 128.77, 127.46, 127.29, 126.22, 125.21, 124.52, 122.02, 120.67, 50.95, 44.21, 31.82, 28.06. HRMS (ESI, *m*/*z*) calcd for $C_{25}H_{28}N_2ONa$ $[M+Na]^+$: 395.2099, found: 395.2102.

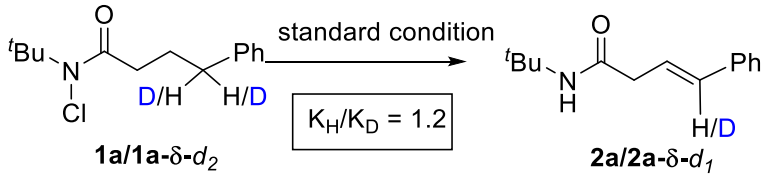
6.6 Deuterium labeling experiments

1) δ-deuterium labeling experiments



Synthesis of 1a-δ-d_2 acid:

The procedure was modified from a previously reported preparation. A 50 mL Schlenk flask was charged with 4-phenylbutanoic acid (1.500 g, 1.0 equiv) and 10 % Pd/C (0.300 g, 10 wt%) with 6 mL D_2O. The reaction flask was fitted with a balloon full of H_2 and purged with H_2 three times. The resulted black suspension was heated at 50 ℃. After 24 h, the reaction mixture was filtered through Celite to remove Pd/C and washed with diethyl ether. The aqueous phase was extracted three times with diethyl ether. The combined organic phases were washed with brine, dried over $NaSO_4$, filtered, and concentrated. The product was used without further purification. The deuterium content (93%) was determined by ^{1}H NMR integration of methyl groups to the benzylic hydrogens. The following **1a-δ-d_2** was synthesized according to reported procedures without any modification[1].



Reaction progress was monitored by ^{1}H NMR spectroscopy. Rate constants were determined by plotting the corresponding products (with CH_2Br_2 as internal standard) over time and extracting the slope after linear fitting of the data.

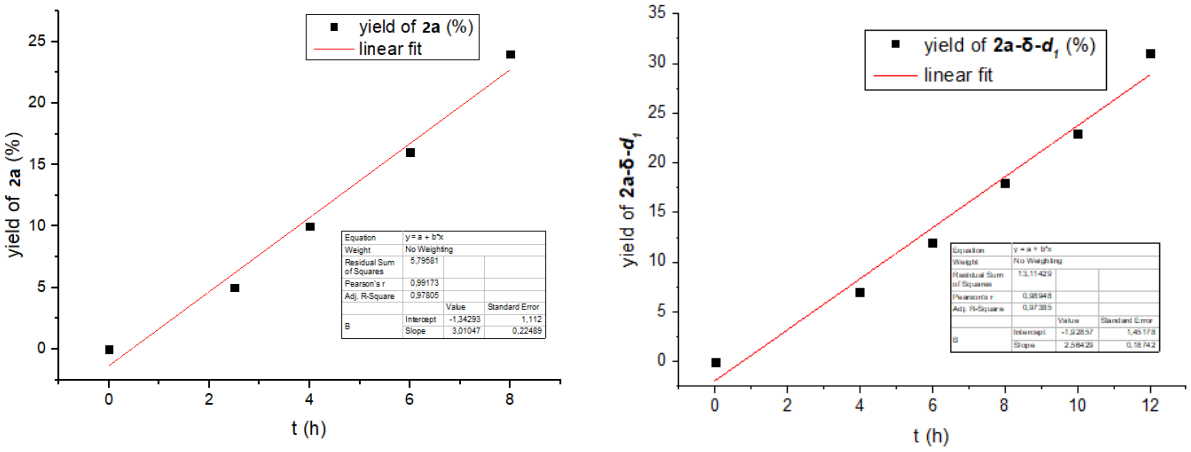
t (h)	**2a** (%)	**2a-δ-*d_1*** (%)

2.5	5	-
4.0	10	7
6.0	16	12
8.0	24	18
10.0	40	24
12.0	-	30

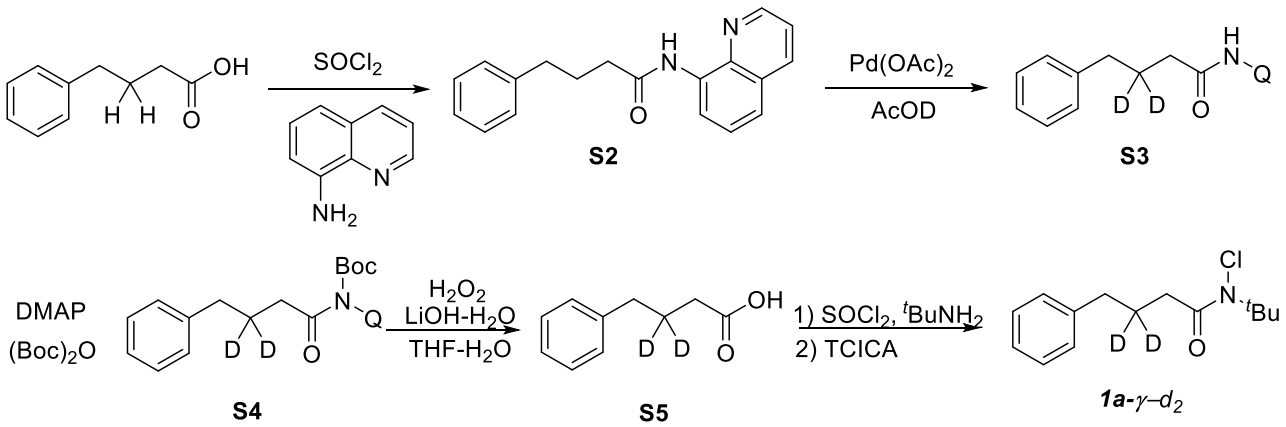
2a: y = 3.0104 (K_H)x – 1.3429, R^2 = 0.9780

2a-ö-*d*$_1$: y = 2.5642 (K_D)x – 1.0265, R^2 = 0.9738

K_H/K_D= 3.0104/2.5642 = 1.2



2) γ-deuterium labeling experiments



Synthesis of 1a-γ-d$_2$ acid:

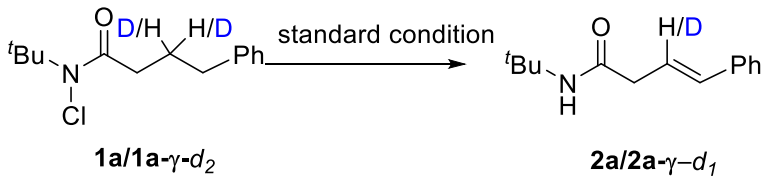
S2 was synthesized according to reported procedures without any modification[1]. The solution of **S2** (4.64 g, 16 mmol, 1 equiv) and $Pd(OAc)_2$ (358.9 mg, 1.6 mmol, 0.1 equiv) indeuterated acetic acid (16 mL) was heated at 90 ℃ for 24 hours. After completion the reaction wasfiltrated and

concentrated, then the product was purified on flash silica gel chromatography (PE :EtOAc = 20:1). This procedure was repeated twice, giving 3.25 g of deuterated substrate **S3** in 70% yield. [10]

A mixture of **S3** (3.25, 11.2 mmol, 1 equiv), Boc_2O (7.32 g, 33.6 mmol, 3 equiv) and DMAP (2.72 g, 22.4 mmol, 2 equiv) in anhydrous CH_3CN (40 mL) was stirred at room temperature for 8 hours. The resulting residue was concentrated in vacuo and then purified by silica gel flash chromatography to give the 3.83g product **S4** in 90 % yield.

S4 (3.83 g, 10.1 mmol, 1 equiv) was dissolved in THF/H_2O (30 mL, 3:1), LiOH•H_2O (820 mg, 20.2 mmol, 2 equiv) and 30% H_2O_2 (50.5 mmol, 5 equiv) were added at 0 ℃. The reaction was stirred at room temperature for overnight, Na_2SO_3 (0.1 mol, 10 equiv) was added. The reaction was diluted with EtOAc (40 mL), and acidified with 0.5 M aq. HCl, the mixture was extracted with EtOAc. The organic layer was concentrated in vacuo and the residue was purified by flash chromatography to give 1.37 g product **S5** in 90 % yield.[11]

The following **1a-γ-d2** were synthesized according to reported procedures without any modification[1].



1a/1a-γ-d_2 **2a/2a-γ–d_1**

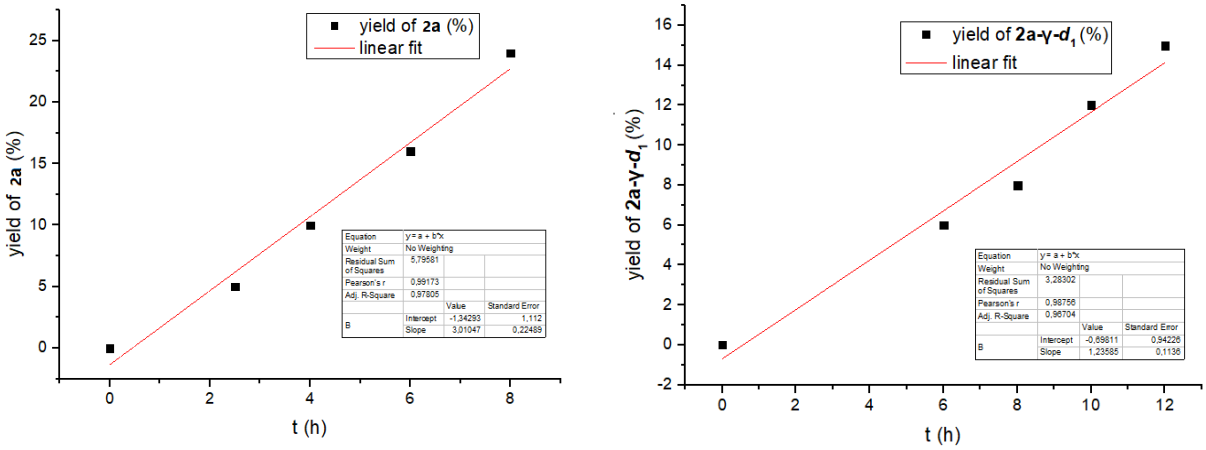
Reaction progress was monitored by ^{1}H NMR spectroscopy. Rate constants were determined by plotting the corresponding products (with CH_2Br_2 as internal standard) over time and extracting the slope after linear fitting of the data.

t (h)	**2a** (%)	**2a-γ-*d*$_1$** (%)
2.5	5	-
4.0	10	-
6.0	16	6
8.0	24	8
10.0	40	12
12.0	-	15

2a: y = 3.0104 (K_H)x – 1.3429, R^2 = 0.9780

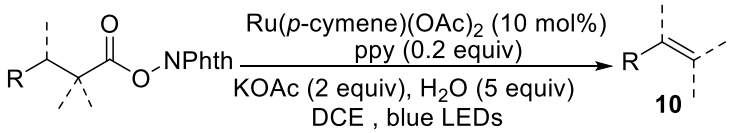
2a-γ-*d*$_1$: y = 1.2358 (K_D)x – 0.6981, R^2 = 0.9670

K_H/K_D= 3.0104/1.2358 = 2.4

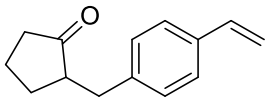


6.7 Evaluation of the role of Cl atom in the catalytic reaction

A dried 10 mL Schlenk tube was charged with the catalyst Ru(*p*-cymene)$(OAc)_2$ (10 mol%), 2-phenylpyridine (20 mol%), **9** (0.20 mmol, 1.0 eq.), KOAc (0.40 mmol, 2.0 eq.) and H_2O (5.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs. The reaction was stirred at room temperature for 48 h under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/ petroleum ether = 1:10 to 1:5) to afford products **10**.



2-(4-vinylbenzyl)cyclopentan-1-one (10a)



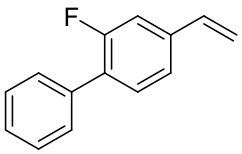
Colorless oil (23.2 mg, 0.116 mmol, yield: 58%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.68 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.70 (d, *J* = 17.6 Hz, 1H), 5.20 (d, *J* = 10.9 Hz, 1H), 3.12 (dd, *J* = 13.9, 4.1 Hz, 1H), 2.54 (dd, *J* = 13.8, 9.4 Hz, 1H), 2.33 (dd, *J* = 19.0, 8.3 Hz, 2H), 2.16–2.02 (m, 2H), 1.98–1.90 (m 1H), 1.81–1.67 (m, 1H), 1.54 (qd, *J* = 10.9, 6.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 220.2, 139.7, 136.5, 135.6, 129.1, 126.3, 113.2, 50.9, 38.2, 35.3, 29.1, 20.5.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{16}ONa$ $[M+Na]^+$: 223.1099, found: 223.1102.

2-fluoro-4-vinyl-1,1'-biphenyl (10b)



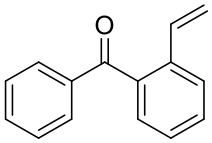
Yellow oil (26.0 mg, 0.180 mmol, yield: 45%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.51 (m, 2H), 7.49–7.31 (m, 4H), 7.26–7.18 (m, 2H), 6.71 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.80 (d, *J* = 17.6 Hz, 1H), 5.33 (d, *J* = 10.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 158.7, 138.9, 138.8, 135.57, 135.56, 135.51, 135.5, 130.73, 130.69, 128.92, 128.89, 128.5, 128.3, 128.2, 127.7, 122.4, 115.2, 113.5, 113.3.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{11}FNa$ $[M+Na]^+$: 221.0742, found: 221.0738.

phenyl(2-vinylphenyl)methanone (10c)



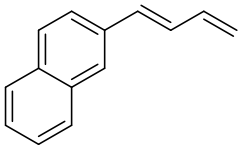
Colorless oil (28.2 mg, 0.136 mmol, yield: 68%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86–7.77 (m, 3H), 7.69–7.56 (m, 3H), 7.46 (dt, *J* = 20.1, 7.8 Hz, 3H), 6.75 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.81 (d, *J* = 17.6 Hz, 1H), 5.32 (d, *J* = 10.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 137.9, 137.8, 137.5, 136.0, 132.5, 130.1, 129.9, 129.4, 128.5, 128.3, 127.7, 115.3.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{12}ONa$ $[M+Na]^+$: 231.0786, found: 231.0780.

(*E*)-2-(buta-1,3-dien-1-yl)naphthalene (10d)



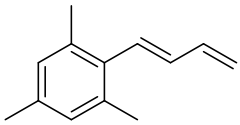
Colorless oil (29.9 mg, 0.166 mmol, yield: 83%, E/Z = 10:1)

1H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 7.9, 4.7 Hz, 3H), 7.76–7.72 (m, 1H), 7.63 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.50–7.39 (m, 2H), 6.92 (dd, *J* = 15.6, 10.4 Hz, 1H), 6.73 (d, *J* = 15.7 Hz, 1H), 6.57 (dt, *J* = 17.3, 10.2 Hz, 1H), 5.38 (d, *J* = 17.5 Hz, 1H), 5.21 (d, *J* = 10.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.23, 134.62, 133.63, 133.02, 132.96, 129.98, 128.22, 127.97, 127.66, 126.51, 126.29, 125.89, 123.45, 117.79.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{12}Na$ $[M+Na]^+$: 203.0837, found: 203.0833.

(*E*)-2-(buta-1,3-dien-1-yl)-1,3,5-trimethylbenzene (10e)



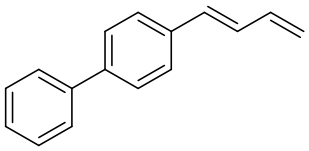
Yellow oil (24.2 mg, 0.14 mmol, yield: 70%, E/Z > 20:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 2H), 6.61–6.46 (m, 2H), 6.27 (dd, *J* = 16.0, 10.4 Hz, 1H), 5.24 (d, *J* = 16.9 Hz, 1H), 5.13 (d, *J* = 10.0 Hz, 1H), 2.29 (s, 6H), 2.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.7, 136.3, 136.0, 134.7, 133.5, 131.0, 128.7, 116.5, 21.0.

HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{16}Na$ $[M+Na]^+$: 195.1150, found: 195.1148.

(*E*)-4-(buta-1,3-dien-1-yl)-1,1'-biphenyl (10f)



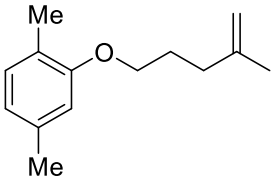
Colorless oil (25.5 mg, 0.124 mmol, yield: 62%, E/Z = 10:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63–7.54 (m, 4H), 7.49–7.42 (m, 4H), 7.33 (d, *J* = 7.3 Hz, 1H), 6.84 (dd, *J* = 15.6, 10.5 Hz, 1H), 6.61 (d, *J* = 16.1 Hz, 1H), 6.57–6.47 (m, 1H), 5.36 (d, *J* = 16.9 Hz, 1H), 5.20 (d, *J* = 10.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.6, 140.3, 137.2, 136.2, 132.4, 129.7, 128.8, 127.32, 127.28, 126.89, 126.86, 117.7.

HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{14}Na$ $[M+Na]^+$: 229.0993, found: 229.0991.

1,4-dimethyl-2-((4-methylpent-4-en-1-yl)oxy)benzene (10g)



Colorless oil (12.2 mg, 0.060 mmol, yield: 30%, t/l = 5:1)

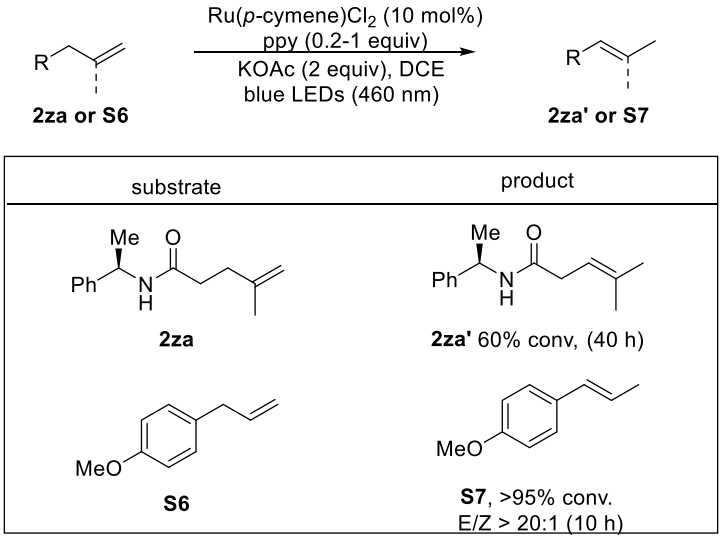
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, *J* = 7.4 Hz, 1H), 6.69–6.60 (m, 2H), 4.75 (s, 1H), 4.73 (s, 1H), 3.95 (t, *J* = 6.4 Hz, 2H), 2.31 (s, 3H), 2.25–2.15 (m, 5H), 1.95 (dt, *J* = 8.7, 6.5 Hz, 2H), 1.76 (s, 3H).

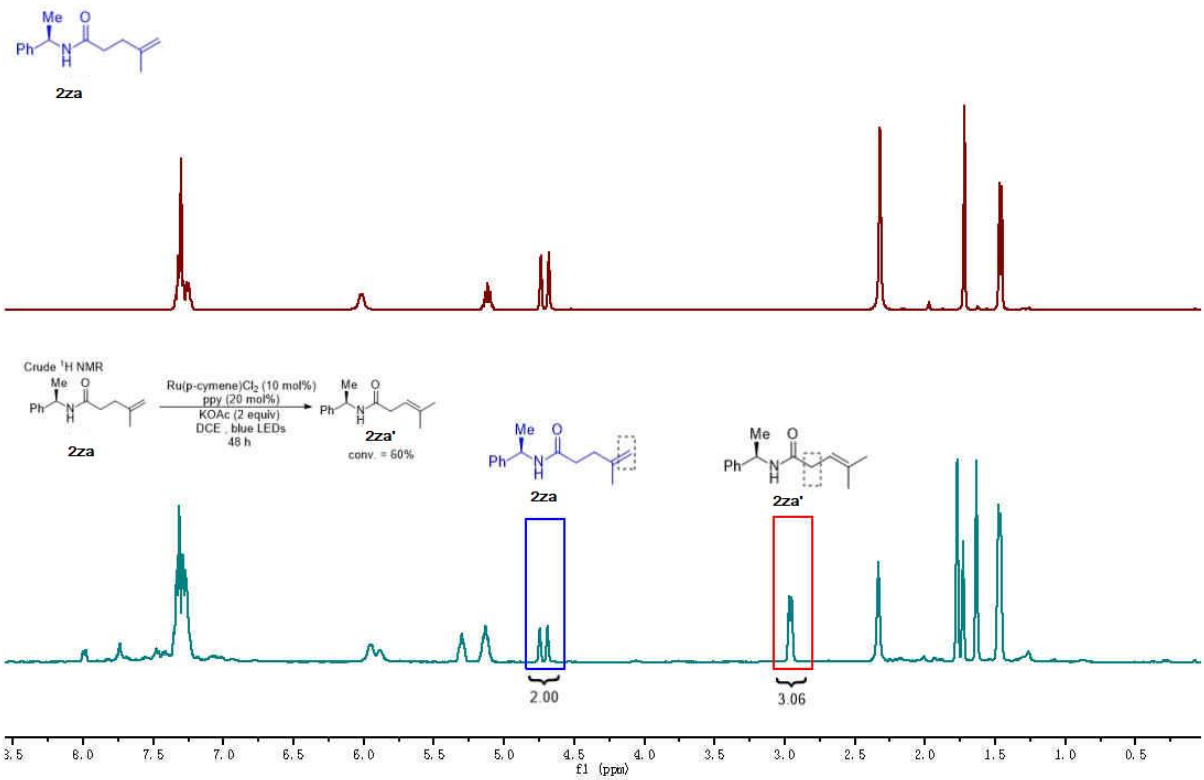
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 145.1, 136.4, 130.3, 123.6, 120.6, 112.0, 110.2, 67.2, 34.2, 27.4, 22.5, 21.4, 15.8.

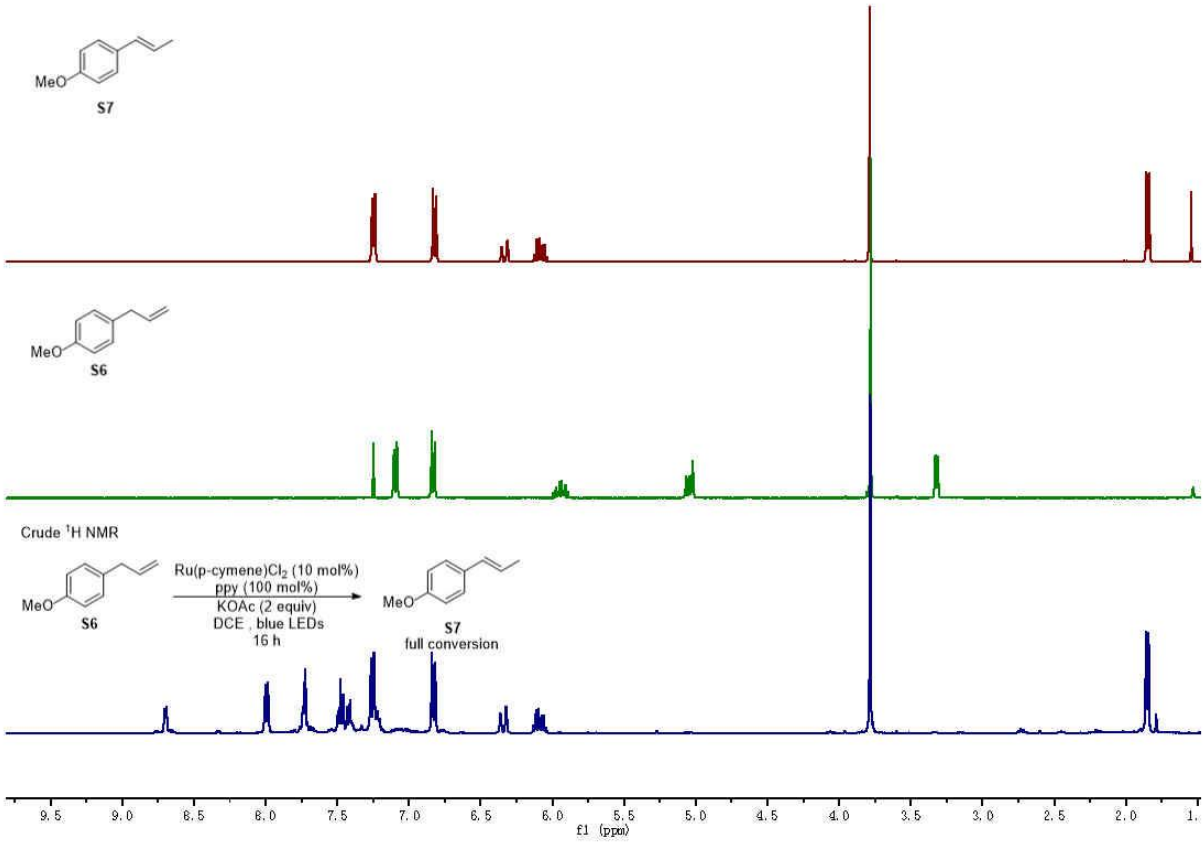
HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{20}ONa$ $[M+Na]^+$: 227.1412, found: 227.1416.

6.8 Olefins isomerization

A dried 10 mL Schlenk tube was charged with the catalyst Ru(*p*-cymene)Cl_2 (10 mol%), 2-phenylpyridine (20 or 100 mol%), **2za** or 4-allylanisole **S6** (0.20 mmol, 1.0 eq.) and KOAc (0.40 mmol, 2.0 eq.). Then DCE (4.0 mL) was added via syringe. The tube was purged with nitrogen. After the mixture was thoroughly degassed, the tube was sealed and positioned approximately 8 cm from 20 W blue LEDs (460 nm). The reaction was stirred at room temperature under nitrogen atmosphere. Afterwards, the solvent was removed under reduced pressure. The conversion was determined by crude ^{1}H NMR. Isomer **2za′:2za** = 1.5:1; isomer **S7:S6** > 20:1.

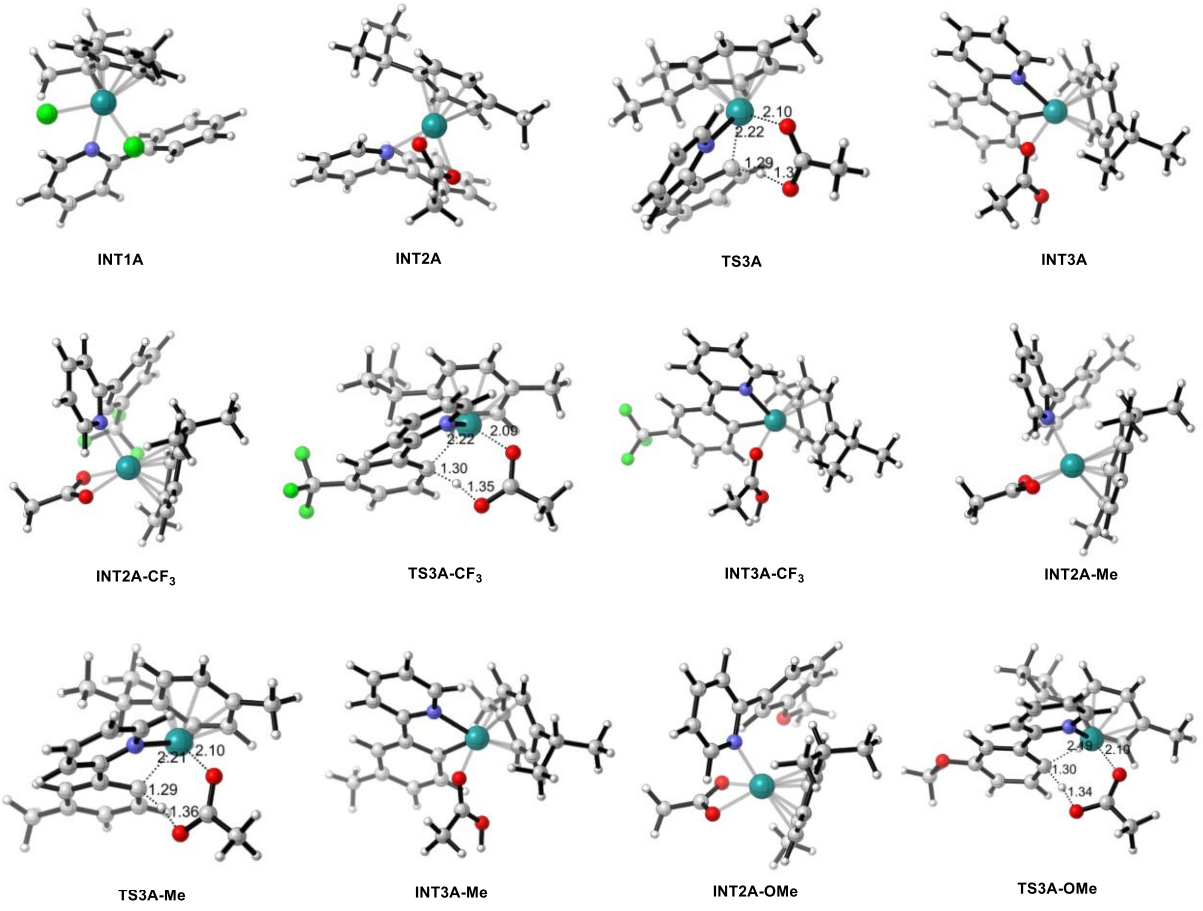


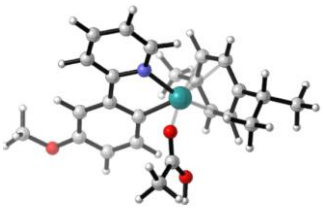

Me
O
Ph
N
H
2za
Crude ¹H NMR
Ru(p-cymene)Cl2 (10 mol%)
ppy (20 mol%)
KOAc (2 equiv)
DCE , blue LEDs
48 h
2za'
conv. = 60%
2.00
3.06
f1 (ppm)


MeO
S7
S6
Crude ¹H NMR
Ru(p-cymene)Cl2 (10 mol%)
ppy (100 mol%)
KOAc (2 equiv)
DCE , blue LEDs
16 h
S7
full conversion
f1 (ppm)

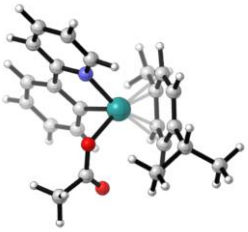
7. DFT Calculations

We performed density functional theory (DFT) calculations to well understand the mechanism of the visible-light-induced ruthenium catalyzed site-selective desaturation of C(sp^3)-C(sp^3) bond using the Gaussian 09 program package. [12] B3LYP-D3[13] level of theory with a mixed basis set of LANL2DZ[14] for Ru atom and 6-31G(d)[15] for all other atoms was employed to optimize all the structures in gas phase. Vibrational frequencies calculation was carried out at the same level to check that the optimized structure was either a local minimum or a transition state, and to obtain all the thermal corrections to free energies at 298.15 K and 1 atm pressure. Single-point solvation energies were then calculated with B3LYP-D3 method and a mixed basis set of SDD[16] for Ru and 6-311+G(d,p)[17] for all other atoms with continuum model SMD[18] (solvent = 1,2-dichloroethane). All energies are reported here in kcal/mol. The calculated optimized structures are visualized using CYLview.[19]

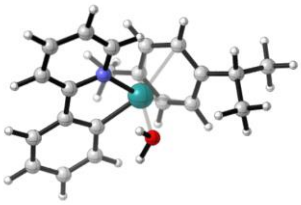




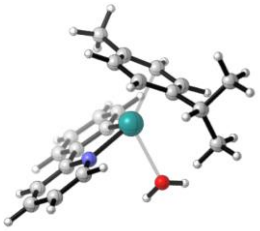
INT3A-OMe



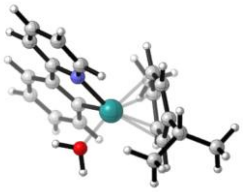
INT4A



INT5A

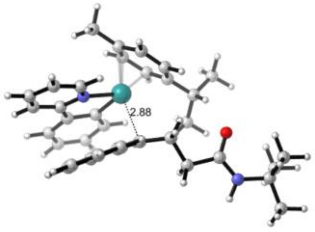


INT5A-excited

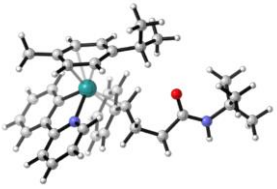


INT6A

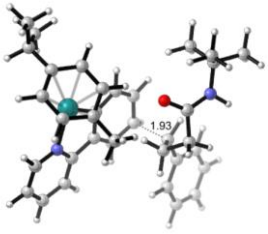
INT7A



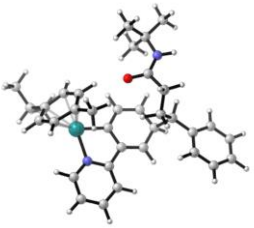
TS8A



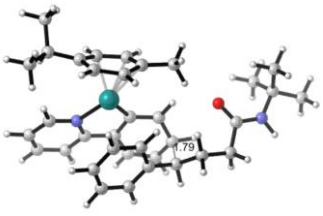
INT8A



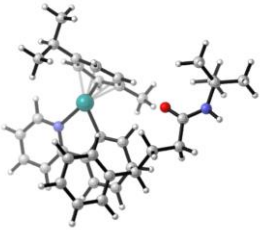
TS8B



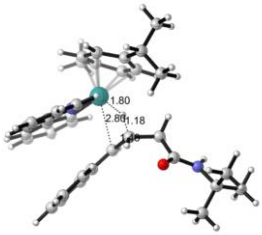
INT8B



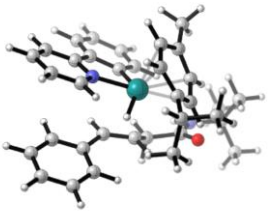
TS8C



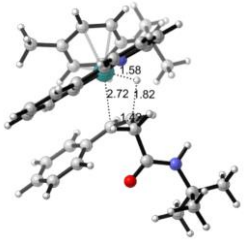
INT8C



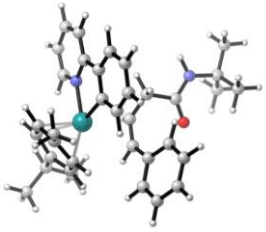
TS9A-E



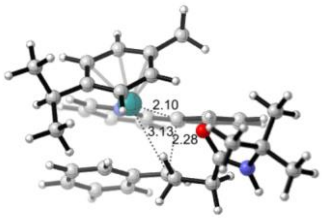
INT9A-E



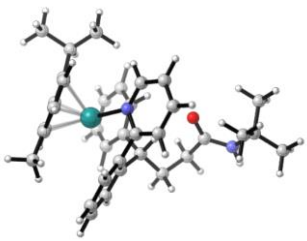
TS9A-Z



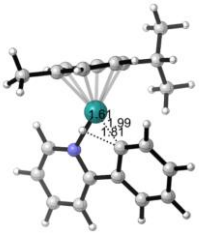
INT9A-Z



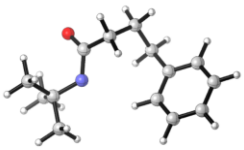
TS9B



INT9B

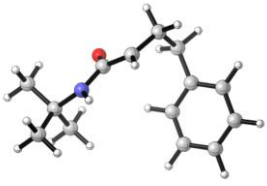


TS10A

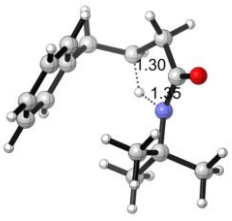


radical-A

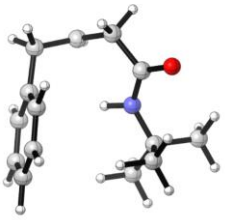
TSB



radical-B



TSC



radical-C

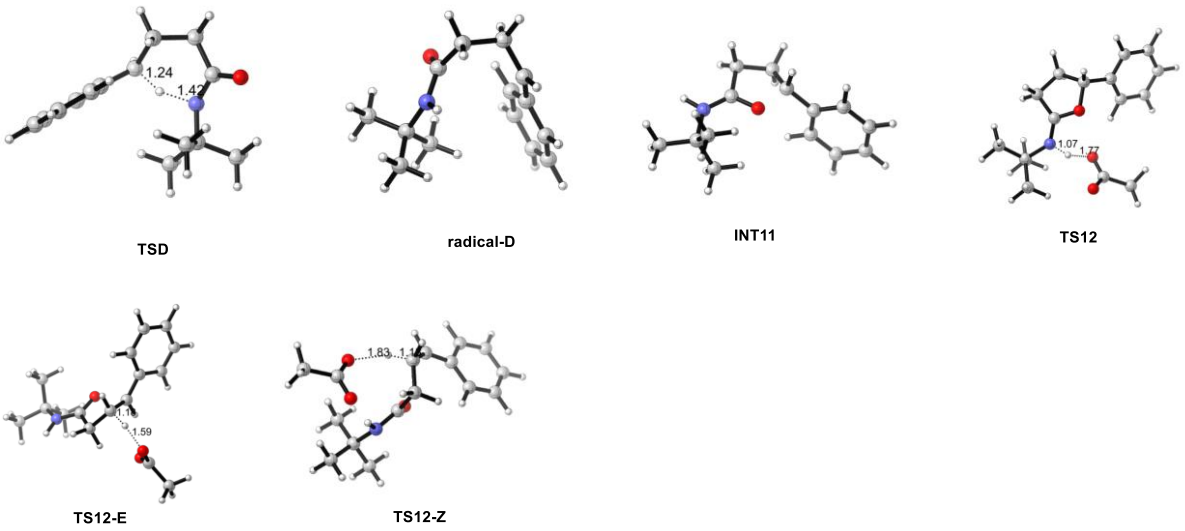


Figure S2. The calculated optimized structures of the key intermediates and transition states. Distances are in Å.

Table S3. The calculated energies of stationary points (in Hartree/Particle) E_{ele} (electronic energies in solvent), E_0 (sum of electronic and zero-point energies in solvent), E (sum of electronic and thermal energies in solvent), H (sum of electronic and thermal ethalpies in solvent) and G (sum of electronic and thermal free energies in solvent).

Structure	E_{ele}	E_0	E	H	G
$[RuCl_2(p\text{-cymene})]_2$	-2810.307752	-2809.869614	-2809.837863	-2809.836919	-2809.933112
2-Phenylpyridine	-479.496286	-479.326010	-479.317246	-479.316301	-479.360756
INT1A	-1884.659225	-1884.268294	-1884.242941	-1884.241997	-1884.323904
OAc^-	-228.6928319	-228.644530	-228.640094	-228.639149	-228.672001
INT2A	-1192.557417	-1192.115843	-1192.089230	-1192.088286	-1192.175058
Cl^-	-460.4013625	-460.401363	-460.399947	-460.399003	-460.416386
TS3A	-1192.532270	-1192.096227	-1192.070178	-1192.069233	-1192.152001
INT3A	-1192.547887	-1192.106812	-1192.080099	-1192.079155	-1192.163851
INT2A-CF_3	-1529.711616	-1529.264928	-1529.234933	-1529.233989	-1529.326091
TS3A-CF_3	-1529.683453	-1529.242511	-1529.212881	-1529.211937	-1529.303426
INT3A-CF_3	-1529.703610	-1529.257830	-1529.227386	-1529.226442	-1529.320995

INT2A-Me	-1231.888363	-1231.419402	-1231.390861	-1231.389917	-1231.480904
TS3A-Me	-1231.864279	-1231.400508	-1231.372643	-1231.371699	-1231.458934
INT3A-Me	-1231.878072	-1231.409519	-1231.380837	-1231.379893	-1231.469516
INT2A-OMe	-1307.119956	-1306.645474	-1306.616288	-1306.615344	-1306.707555
TS3A-OMe	-1307.096625	-1306.627972	-1306.599263	-1306.598319	-1306.686913
INT3A-OMe	-1307.108149	-1306.634473	-1306.605028	-1306.604084	-1306.695178
INT4A	-1192.095686	-1191.667607	-1191.641313	-1191.640368	-1191.724409
HOAc	-229.176566	-229.114536	-229.109974	-229.109030	-229.141776
H_2O	-76.466524	-76.445387	-76.442552	-76.441608	-76.463053
INT5A	-1039.835906	-1039.433455	-1039.409751	-1039.408807	-1039.486062
INT5A-excited	-1039.803239	-1039.403342	-1039.378231	-1039.377287	-1039.459719
1a	-1135.954269	-1135.636458	-1135.618815	-1135.617871	-1135.684541
INT6A	-1039.634749	-1039.232617	-1039.208624	-1039.207680	-1039.286211
radical-A	-675.711234	-675.397348	-675.380752	-675.379807	-675.444833
TSB	-675.656729	-675.348787	-675.332403	-675.331459	-675.394830
radical-B	-675.734659	-675.420731	-675.404021	-675.403077	-675.467174
TSC	-675.6886821	-675.379697	-675.363818	-675.362873	-675.423588
radical-C	-675.7295771	-675.416029	-675.399389	-675.398445	-675.461101
TSD	-675.700320	-675.390791	-675.375191	-675.374247	-675.434344
radical-D	-675.746437	-675.432028	-675.415627	-675.414683	-675.476832
INT7A	-1638.942960	-1638.247713	-1638.209122	-1638.208178	-1638.318141
TS8A	-1638.925965	-1638.231670	-1638.193081	-1638.192137	-1638.304320
INT8A	-1638.956470	-1638.259498	-1638.221165	-1638.220221	-1638.32955
TS8B	-1638.925134	-1638.229263	-1638.191172	-1638.190227	-1638.301419
INT8B	-1638.931888	-1638.234747	-1638.196553	-1638.195609	-1638.306847
TS8C	-1638.912146	-1638.215554	-1638.178353	-1638.177408	-1638.283395
INT8C	-1638.923482	-1638.226794	-1638.18855	-1638.187606	-1638.299144

TS9A-E	-1638.927766	-1638.234376	-1638.196417	-1638.195473	-1638.305182
INT9A-E	-1638.931632	-1638.238154	-1638.199661	-1638.198717	-1638.308377
TS9A-Z	-1638.920157	-1638.228564	-1638.190109	-1638.189165	-1638.299921
INT9A-Z	-1638.921620	-1638.228703	-1638.189826	-1638.188882	-1638.301148
TS9B	-1638.923424	-1638.228106	-1638.19016	-1638.189216	-1638.297713
INT9B	-1638.972749	-1638.273687	-1638.235818	-1638.234874	-1638.342028
TS10A	-963.729399	-963.3464399	-963.3249279	-963.3239829	-963.3981839
INT11	-675.609465	-675.2902569	-675.2748489	-675.2739049	-675.3333059
TS12	-904.317868	-903.9496864	-903.9291164	-903.9281724	-904.0004494
TS12-E	-904.298382	-903.9332006	-903.9120686	-903.9111246	-903.9856286
TS12-Z	-904.279883	-903.9140989	-903.8930279	-903.8920839	-903.9652009
E-**2a**	-675.156900	-674.8530921	-674.8366921	-674.8357471	-674.8991791
Z-**2a**	-675.1551796	-674.8509146	-674.8347466	-674.8338026	-674.8957636

Cartesian coordinates of the optimized structures

[RuCl$_2$(p-cymene)]$_2$

C	3.241026	-0.216186	1.920246	Cl	1.094397	-2.765889	-0.273035
C	3.735194	-1.322898	1.188661	Cl	0.446419	0.346775	-1.655764
C	3.973542	-1.127693	-0.217882	H	4.229765	-1.983256	-0.833692
C	3.744178	0.125964	-0.825195	H	2.559991	1.847850	1.888457
C	3.279228	1.263721	-0.068071	H	2.939384	-0.357693	2.953118
C	3.029319	1.064634	1.306302	C	3.911317	-2.679418	1.809321
C	-3.068991	-1.275398	0.568014	H	3.432942	-3.440419	1.185260
C	-3.807229	-0.089558	0.290493	H	4.978643	-2.916002	1.903050
C	-3.788766	0.374312	-1.068792	H	3.458365	-2.719017	2.803508
C	-3.060640	-0.303348	-2.073198	C	3.018213	2.572774	-0.785184
C	-2.338554	-1.513651	-1.776144	H	2.582184	2.307011	-1.756483
C	-2.368676	-1.998008	-0.448370	C	4.364573	3.284721	-1.032369
H	-4.230412	1.338869	-1.297400	H	4.834178	3.568050	-0.082540
H	-1.725868	-2.824994	-0.169446	H	5.068972	2.649467	-1.582504
Ru	1.894981	-0.510392	0.191296	H	4.203370	4.197709	-1.615779
Ru	-1.713042	0.160268	-0.375776	C	2.018176	3.484374	-0.067123
Cl	-0.147691	-0.120110	1.563305	H	1.807895	4.357834	-0.692947
Cl	-1.664264	2.545478	0.027946	H	1.068849	2.973585	0.118732
				H	2.421166	3.856770	0.883553

H	3.837279	0.217823	-1.902852	C	0.014119	-1.649034	0.888943
H	-2.944950	-1.596021	1.595801	C	-0.381382	-0.667690	1.865283
H	-2.979612	0.135532	-3.062172	C	-1.752199	-0.343131	1.953820
C	-1.518591	-2.193793	-2.834434	Ru	-1.118225	0.042548	-0.161187
H	-0.650230	-2.684944	-2.389432	Cl	-2.740607	1.895466	-0.271394
H	-2.134353	-2.943431	-3.348878	Cl	-1.234666	-0.058936	-2.593678
H	-1.161514	-1.471414	-3.572978	H	-0.558427	-2.833109	-0.815944
C	-4.529040	0.716931	1.352058	H	-2.094810	0.434596	2.624170
H	-4.474674	1.762462	1.024642	H	-3.718677	-0.568406	1.063885
C	-3.865608	0.639485	2.733219	C	-3.281887	-2.397891	-0.954748
H	-2.808080	0.913174	2.671965	H	-2.877459	-2.274488	-1.964201
H	-4.363682	1.333676	3.418401	H	-3.463889	-3.464252	-0.770145
H	-3.946758	-0.363087	3.171288	H	-4.235435	-1.865972	-0.906108
C	-6.009336	0.291305	1.406491	C	0.682063	-0.041078	2.747974
H	-6.557505	0.913362	2.122947	H	1.582009	0.049692	2.127807
H	-6.494745	0.391017	0.428548	C	1.010171	-0.994480	3.914095
H	-6.102556	-0.754400	1.725025	H	0.134798	-1.131784	4.559841
				H	1.321020	-1.980096	3.549506
2-Phenylpyridine				H	1.822699	-0.584874	4.524895
C	-0.724523	0.025670	-0.004936	C	0.318716	1.361053	3.251951
C	-1.467951	1.196796	-0.226575	H	1.178490	1.804864	3.765418
C	-2.862261	1.169879	-0.217842	H	0.032022	2.017493	2.424420
C	-3.540277	-0.028973	0.011354	H	-0.508965	1.332189	3.970235
C	-2.811352	-1.202408	0.222830	H	1.059329	-1.912893	0.796880
C	-1.418683	-1.176981	0.210817	C	1.920930	1.136678	-0.650856
C	0.762801	0.027910	-0.000972	C	0.297768	2.779590	-0.436925
C	2.701433	-1.199417	-0.236015	C	2.911615	2.125666	-0.743884
C	3.518744	-0.087122	-0.025050	C	1.235217	3.802552	-0.529108
C	2.897511	1.135823	0.226441	C	2.577340	3.472892	-0.679112
C	1.506792	1.195760	0.245200	H	3.939372	1.812839	-0.892194
H	-0.960244	2.133797	-0.435614	H	0.897921	4.832764	-0.484063
H	-3.418671	2.085720	-0.398981	H	3.343422	4.239113	-0.757752
H	-4.626798	-0.049787	0.019158	N	0.610689	1.466431	-0.479841
H	-3.330299	-2.141120	0.398504	H	-0.756328	2.999832	-0.324508
H	-0.845941	-2.084457	0.366934	C	2.373809	-0.277667	-0.743041
H	3.142251	-2.177739	-0.423699	C	1.884934	-1.147444	-1.727855
H	4.599999	-0.182354	-0.048605	C	3.362657	-0.732748	0.144413
H	3.486131	2.029645	0.415698	C	2.349898	-2.461409	-1.789544
H	1.006107	2.131062	0.470847	H	1.121441	-0.800681	-2.415505
N	1.367722	-1.155198	-0.227965	C	3.816778	-2.051569	0.086963
				H	3.756948	-0.056227	0.898560
INT1A				C	3.305385	-2.922096	-0.878704
C	-2.698410	-0.934583	1.053148	H	1.961767	-3.127013	-2.556019
C	-2.309941	-1.851459	0.052457	H	4.566593	-2.396322	0.793723
C	-0.913210	-2.195509	-0.013349	H	3.656630	-3.949282	-0.927101

$^{-}$OAc			
C	-1.354122	-0.059263	-0.000003
H	-1.749679	0.469498	-0.879839
H	-1.749274	0.466799	0.881647
H	-1.730818	-1.090441	-0.001403
C	0.221066	0.002068	-0.000171
O	0.812592	-1.106646	-0.000085
O	0.690921	1.168810	0.000165
Cl^{-}			
Cl	0.000000	0.000000	0.000000

INT2A

C	2.679770	-0.280890	-1.437649
C	1.873555	-1.418267	-1.652621
C	0.472329	-1.203013	-1.909559
C	-0.063429	0.094973	-1.956621
C	0.747918	1.256953	-1.715759
C	2.119452	1.040967	-1.450275
Ru	0.982148	-0.183694	0.027770
H	-0.195477	-2.053821	-1.993739
H	2.758676	1.875684	-1.187242
H	3.722462	-0.407767	-1.164924
C	2.414293	-2.816045	-1.543872
H	1.738600	-3.444637	-0.955883
H	2.507246	-3.258321	-2.543209
H	3.398993	-2.828301	-1.070033
C	0.093606	2.626347	-1.730562
H	-0.884150	2.506208	-1.243012
C	-0.152182	3.050867	-3.193786
H	0.797872	3.175761	-3.725575
H	-0.750469	2.310437	-3.736026
H	-0.686045	4.006203	-3.223439
C	0.875491	3.700837	-0.965436
H	0.289428	4.623921	-0.925410
H	1.090775	3.392380	0.063031
H	1.823155	3.941651	-1.460744
H	-1.132914	0.213791	-2.086851
C	-1.915580	0.465242	1.096589
C	-0.186860	1.735002	2.024933
C	-2.855307	1.264471	1.764113
C	-1.074333	2.553679	2.708768
C	-2.441797	2.319567	2.569152
H	-3.907145	1.024198	1.656800
H	-0.691681	3.353174	3.333736
H	-3.169806	2.935268	3.088476
N	-0.584366	0.722198	1.218740
H	0.882749	1.873336	2.115347
C	-2.393390	-0.661754	0.257114
C	-1.923768	-1.968889	0.454840
C	-3.367329	-0.420428	-0.726200
C	-2.404989	-3.010608	-0.339481
H	-1.188457	-2.167153	1.225802
C	-3.834256	-1.462344	-1.528165
H	-3.742160	0.589245	-0.874977
C	-3.350875	-2.760030	-1.337856
H	-2.047085	-4.022178	-0.169761
H	-4.577349	-1.262592	-2.294441
H	-3.721413	-3.573620	-1.954509
O	1.026768	-1.764816	1.494890
C	1.801728	-1.079189	2.241015
O	2.178542	0.053022	1.776664
C	2.217859	-1.547626	3.599710
H	1.528563	-1.134038	4.345899
H	2.174033	-2.637327	3.654365
H	3.223725	-1.188956	3.830467

TS3A

C	0.593204	-2.235286	-1.647000
C	1.093098	-2.841964	-0.473557
C	0.261173	-2.832434	0.695153
C	-1.021666	-2.249120	0.653326
C	-1.557178	-1.651298	-0.537328
C	-0.706454	-1.633474	-1.666079
Ru	0.450172	-0.662665	0.011129
H	0.640233	-3.241065	1.625842
H	-1.022957	-1.122508	-2.568295
H	1.216757	-2.186535	-2.533657
C	2.492468	-3.381578	-0.393469
H	2.482601	-4.414765	-0.029649
H	2.988630	-3.358834	-1.366810
H	3.077581	-2.774564	0.306130
C	-2.956669	-1.064093	-0.522860
H	-3.061953	-0.534763	0.432591
C	-3.992315	-2.207521	-0.556090
H	-3.920380	-2.771268	-1.493372
H	-3.849682	-2.909252	0.273152
H	-5.005806	-1.799899	-0.482527
C	-3.213295	-0.055704	-1.649495

H	-4.187944	0.419017	-1.502170
H	-2.454460	0.733105	-1.665539
H	-3.235172	-0.541661	-2.632136
H	-1.611507	-2.209801	1.563308
C	-0.103719	2.186296	-0.650852
C	1.624412	1.324992	-1.983871
C	-0.027130	3.411829	-1.321016
C	1.747478	2.521848	-2.679807
C	0.898336	3.579810	-2.346715
H	-0.669915	4.229737	-1.016049
H	2.494609	2.617659	-3.459814
H	0.968948	4.528893	-2.868865
N	0.710646	1.155664	-1.012287
H	2.260814	0.472348	-2.191006
C	-0.979940	1.895000	0.490692
C	-0.568659	0.811076	1.316430
C	-2.153705	2.600563	0.768355
C	-1.355847	0.499211	2.441567
H	0.676421	0.872957	1.640263
C	-2.926302	2.249396	1.877700
H	-2.485901	3.403940	0.117133
C	-2.524506	1.207192	2.721470
H	-1.024292	-0.283868	3.118455
H	-3.840010	2.796576	2.089664
H	-3.118906	0.958344	3.595805
O	1.912810	1.233626	2.105763
C	2.748532	0.493411	1.522300
O	2.432358	-0.365134	0.624296
C	4.206332	0.596537	1.901229
H	4.509620	1.647120	1.897503
H	4.331662	0.224405	2.923850
H	4.831676	0.016222	1.221560

HOAc

C	1.396954	-0.108697	0.000035
H	1.681840	-0.692736	-0.881341
H	1.682471	-0.689847	0.883132
H	1.916218	0.849867	-0.001633
C	-0.093488	0.126732	0.000367
O	-0.646820	1.202969	-0.000254
O	-0.775523	-1.048281	-0.000039
H	-1.722574	-0.812997	-0.000228

H_2O

O	0.000000	0.000000	0.119419
H	0.000000	0.762666	-0.477675
H	0.000000	-0.762666	-0.477675

INT3A

C	1.377341	-1.321599	-1.769733
C	0.651678	-0.329938	-2.510780
C	0.947408	1.028669	-2.220744
C	2.034477	1.403398	-1.355461
C	2.716525	0.439650	-0.615728
C	2.306709	-0.937775	-0.788112
Ru	0.302016	0.062198	-0.337036
H	0.375751	1.806614	-2.717659
H	2.765953	-1.706013	-0.177288
H	1.146688	-2.371416	-1.913247
C	-0.375477	-0.718420	-3.537749
H	-1.090979	0.091713	-3.704425
H	0.115882	-0.942067	-4.492506
H	-0.931322	-1.604551	-3.219855
C	3.831336	0.800449	0.347395
H	3.904697	1.895426	0.362928
C	5.173151	0.239014	-0.163546
H	5.160844	-0.857270	-0.183195
H	5.395614	0.593623	-1.175305
H	5.989288	0.552331	0.495747
C	3.539898	0.331649	1.784258
H	4.352403	0.639601	2.450421
H	2.603184	0.759251	2.155150
H	3.463144	-0.761029	1.839871
H	2.273793	2.454946	-1.228972
C	-2.402336	1.166863	0.219222
C	-0.756068	2.827084	0.425063
C	-3.389394	2.100031	0.567217
C	-1.691836	3.791684	0.771477
C	-3.036829	3.415774	0.839444
H	-4.425694	1.788595	0.625735
H	-1.372041	4.806179	0.981826
H	-3.799258	4.141223	1.106441
N	-1.097807	1.555269	0.147561
H	0.301235	3.058534	0.362371
C	-2.615960	-0.251398	-0.064584
C	-3.876662	-0.870010	-0.047326
C	-1.443731	-0.999275	-0.333546
C	-3.986451	-2.237095	-0.284421
H	-4.774876	-0.291731	0.150601
C	-1.575633	-2.377999	-0.538217

C	-2.833449	-2.991306	-0.521605
H	-4.961933	-2.713616	-0.277556
H	-0.695285	-2.991770	-0.704262
H	-2.913486	-4.061425	-0.695867
O	0.229989	-0.271667	1.816291
C	0.428303	-1.304999	2.445594
C	0.166518	-1.407776	3.922827
H	-0.192870	-0.450294	4.298871
H	-0.589618	-2.178483	4.115395
H	1.083286	-1.689658	4.454036
O	0.906240	-2.382607	1.813658
H	0.984586	-3.138148	2.422167

INT2A-CF$_3$

C	1.190067	-2.624414	-1.377475
C	-0.179830	-2.308982	-1.501645
C	-0.522286	-0.941977	-1.799798
C	0.472745	0.034910	-1.967831
C	1.869766	-0.277750	-1.827926
C	2.203520	-1.618037	-1.528687
Ru	0.767544	-0.950261	0.045317
H	-1.566608	-0.654998	-1.817295
H	3.234990	-1.890315	-1.338144
H	1.482914	-3.623714	-1.071735
C	-1.264604	-3.319290	-1.256434
H	-2.101150	-2.863098	-0.720929
H	-1.642688	-3.693930	-2.215814
H	-0.894148	-4.170559	-0.679507
C	2.890062	0.835341	-1.978619
H	2.459031	1.717203	-1.484059
C	3.059601	1.164351	-3.476912
H	3.479733	0.308120	-4.016570
H	2.104730	1.426002	-3.945839
H	3.741847	2.011586	-3.600610
C	4.242054	0.536590	-1.320197
H	4.880293	1.423956	-1.368895
H	4.128903	0.259059	-0.266897
H	4.773157	-0.271586	-1.835952
H	0.173998	1.065806	-2.121821
C	0.454089	2.036498	1.077833
C	2.316967	0.873551	1.870730
C	0.917668	3.202272	1.703374
C	2.822956	1.999277	2.506688
C	2.110753	3.193962	2.417480
H	0.314840	4.101241	1.639135
H	3.754050	1.928377	3.058256
H	2.468084	4.095866	2.904831
N	1.167672	0.879070	1.155831
H	2.832347	-0.076327	1.929296
C	-0.824056	2.079793	0.323692
C	-1.039680	3.097295	-0.620610
C	-1.830758	1.134051	0.551775
C	-2.229183	3.148131	-1.348839
H	-0.265367	3.838546	-0.799495
C	-3.009316	1.182773	-0.191431
H	-1.697929	0.358433	1.295270
C	-3.216344	2.182985	-1.144967
H	-2.383947	3.936653	-2.078599
H	-4.141701	2.209543	-1.710516
O	-0.585860	-1.481771	1.635398
C	0.376389	-1.949939	2.330729
O	1.531707	-1.930923	1.779822
C	0.174661	-2.456018	3.723758
H	0.260690	-1.616182	4.424006
H	-0.825163	-2.883836	3.826997
H	0.939629	-3.194337	3.973479
C	-4.014176	0.071930	-0.034509
F	-3.700484	-0.961535	-0.879939
F	-4.022774	-0.438075	1.208350
F	-5.260005	0.461191	-0.346878

TS3A-CF$_3$

C	2.505318	1.751827	1.358043
C	3.042428	2.024646	0.081602
C	2.128278	2.390844	-0.964557
C	0.749723	2.499456	-0.702900
C	0.194019	2.265588	0.603893
C	1.097166	1.863108	1.608833
Ru	1.395044	0.409710	-0.112319
H	2.501928	2.540419	-1.972094
H	0.723254	1.598063	2.591403
H	3.163122	1.421199	2.155428
C	4.499146	1.832688	-0.229190
H	4.926890	2.759086	-0.628544
H	5.065521	1.543653	0.659575
H	4.614135	1.047072	-0.983835
C	-1.294658	2.449941	0.831513
H	-1.797647	2.051627	-0.056700
C	-1.611991	3.958252	0.916923
H	-1.121153	4.411706	1.785652

H	-1.280748	4.494589	0.020766	C	2.622534	-1.557349	-0.783629
H	-2.691627	4.106684	1.020542	Ru	1.083082	0.077228	-0.331651
C	-1.840370	1.700773	2.054524	H	1.716693	1.654041	-2.747610
H	-2.933875	1.699926	2.020497	H	2.803442	-2.429169	-0.165997
H	-1.510086	0.657530	2.069196	H	1.025265	-2.522965	-1.869563
H	-1.535363	2.178070	2.993144	C	0.130029	-0.471396	-3.508003
H	0.074017	2.730612	-1.520322	H	-0.276553	0.530916	-3.669252
C	-0.175246	-1.861135	0.990261	H	0.500123	-0.849333	-4.468703
C	2.016306	-1.873466	1.823840	H	-0.684330	-1.119655	-3.173215
C	-0.496906	-2.974481	1.771906	C	4.666648	-0.426875	0.303145
C	1.755323	-2.983598	2.619114	H	5.098276	0.582115	0.310584
C	0.472646	-3.536206	2.598287	C	5.736129	-1.399624	-0.233711
H	-1.489347	-3.406320	1.707310	H	5.361530	-2.430048	-0.248479
H	2.543226	-3.402180	3.235400	H	6.042662	-1.135649	-1.251175
H	0.236167	-4.403612	3.206532	H	6.623270	-1.375609	0.407574
N	1.070850	-1.316236	1.047698	C	4.269855	-0.775994	1.748713
H	2.993765	-1.406116	1.791320	H	5.156572	-0.769224	2.390796
C	-1.075607	-1.204948	0.032854	H	3.548928	-0.054351	2.144944
C	-0.443755	-0.463536	-1.003035	H	3.824889	-1.776412	1.811540
C	-2.465152	-1.233086	0.146773	H	3.740665	1.637493	-1.285564
C	-1.260123	0.163141	-1.962166	C	-1.087082	2.037724	0.212812
H	0.545610	-1.089440	-1.564263	C	1.021378	3.055454	0.355452
C	-3.242344	-0.533826	-0.777887	C	-1.702018	3.254407	0.536177
H	-2.952794	-1.747441	0.968374	C	0.466002	4.286294	0.677506
C	-2.649284	0.138242	-1.851937	C	-0.925704	4.384144	0.764956
H	-0.797066	0.668688	-2.805034	H	-2.781931	3.308617	0.609475
H	-3.275303	0.641632	-2.581168	H	1.109273	5.141080	0.854288
O	1.343512	-1.964224	-2.219669	H	-1.397836	5.329779	1.013000
C	2.531267	-1.678031	-1.907389	N	0.269991	1.964323	0.119531
O	2.843217	-0.759511	-1.069872	H	2.093992	2.917834	0.278698
C	3.658423	-2.447356	-2.551299	C	-1.765370	0.763309	-0.025920
H	3.512902	-3.516548	-2.369505	C	-3.156833	0.603948	0.023399
H	3.619972	-2.294313	-3.634608	C	-0.914759	-0.337833	-0.288969
H	4.626262	-2.127487	-2.163561	C	-3.716395	-0.653039	-0.182980
C	-4.724674	-0.401958	-0.531505	H	-3.814694	1.445111	0.214112
F	-5.234368	-1.501510	0.055450	C	-1.504681	-1.596772	-0.466013
F	-4.953490	0.643143	0.303725	C	-2.890332	-1.756308	-0.421972
F	-5.406930	-0.170753	-1.665843	H	-0.883987	-2.471363	-0.633392
				H	-3.336334	-2.733604	-0.580676
INT3A-CF$_3$				O	0.936342	-0.155095	1.827117
C	1.602584	-1.612892	-1.748332	C	0.762648	-1.175024	2.486608
C	1.246803	-0.444277	-2.501142	C	0.522149	-1.138964	3.970259
C	1.993775	0.735027	-2.239859	H	0.552377	-0.108078	4.321903
C	3.154486	0.729423	-1.389629	H	-0.459487	-1.570793	4.200018
C	3.477321	-0.398602	-0.637780	H	1.284229	-1.727753	4.494259

O	0.796160	-2.366181	1.880911
H	0.612922	-3.084967	2.511264
C	-5.204926	-0.851233	-0.074370
F	-5.646289	-1.768384	-0.960522
F	-5.882145	0.296428	-0.290357
F	-5.548339	-1.293311	1.157833

INT2A-Me

C	-2.270007	-0.940187	1.990380
C	-1.317782	-1.950755	1.741357
C	0.063370	-1.553059	1.640160
C	0.443764	-0.210447	1.802266
C	-0.524854	0.826891	2.032274
C	-1.880829	0.436299	2.116455
Ru	-1.112501	-0.332310	0.167717
H	0.813905	-2.284273	1.359015
H	-2.657391	1.185707	2.214410
H	-3.326195	-1.189785	1.992743
C	-1.711146	-3.381291	1.503381
H	-1.175336	-3.788172	0.640454
H	-1.456842	-3.989395	2.380004
H	-2.784518	-3.475430	1.320376
C	-0.048702	2.263870	2.139781
H	0.737069	2.385306	1.381207
C	0.590879	2.481078	3.527295
H	-0.155269	2.361771	4.321047
H	1.403389	1.770555	3.715011
H	1.002011	3.493313	3.597281
C	-1.140199	3.304248	1.862342
H	-0.698434	4.305004	1.840205
H	-1.631496	3.129610	0.899367
H	-1.905278	3.305895	2.647064
H	1.483229	0.058755	1.656003
C	1.227904	0.998225	-1.479453
C	-0.847084	2.063957	-1.630085
C	1.817908	2.057954	-2.184221
C	-0.313768	3.135049	-2.332796
C	1.053046	3.137945	-2.609168
H	2.876845	2.001362	-2.409943
H	-0.963481	3.943053	-2.650886
H	1.510289	3.955813	-3.157670
N	-0.102454	1.021942	-1.190485
H	-1.904357	2.017021	-1.403562
C	2.072785	-0.146020	-1.056424
C	1.733753	-1.463438	-1.390504
C	3.255467	0.105149	-0.340207
C	2.564253	-2.509588	-0.984316
H	0.834016	-1.666708	-1.958742
C	4.088417	-0.936791	0.081159
H	3.518980	1.130802	-0.090305
C	3.720643	-2.251469	-0.247586
H	2.309503	-3.531262	-1.252188
H	4.356468	-3.075808	0.065865
O	-1.395185	-1.649400	-1.519207
C	-2.436715	-1.003965	-1.874004
O	-2.797882	-0.045071	-1.106251
C	-3.174483	-1.317024	-3.137582
H	-2.768044	-0.700612	-3.948693
H	-3.040727	-2.367727	-3.403536
H	-4.234553	-1.078208	-3.025411
C	5.360928	-0.661523	0.846356
H	6.239267	-0.814336	0.207032
H	5.397682	0.367477	1.217281
H	5.465736	-1.336559	1.702935

TS3A-Me

C	1.875206	1.858856	1.398146
C	2.445331	2.123171	0.135577
C	1.557064	2.426046	-0.952488
C	0.165467	2.483930	-0.745885
C	-0.429518	2.241714	0.540296
C	0.454335	1.898191	1.587018
Ru	0.859176	0.438535	-0.084610
H	1.962781	2.571443	-1.948132
H	0.055834	1.627745	2.558195
H	2.515842	1.578720	2.228106
C	3.918899	1.982581	-0.118691
H	4.319182	2.901830	-0.560368
H	4.467542	1.771232	0.802499
H	4.091424	1.159278	-0.820649
C	-1.933281	2.353534	0.707713
H	-2.379914	1.904232	-0.187659
C	-2.331590	3.843716	0.747331
H	-1.900061	4.339252	1.624705
H	-1.990082	4.378436	-0.145904
H	-3.420689	3.941323	0.804101
C	-2.475156	1.602943	1.930436
H	-3.569117	1.609515	1.910464
H	-2.145621	0.559312	1.938530
H	-2.165336	2.077796	2.868873

H	-0.486489	2.670294	-1.593296	H	-0.945948	0.117478	-3.682083
C	-0.710205	-1.872197	0.947056	H	0.031534	-1.178914	-4.396719
C	1.403528	-1.761007	1.959042	H	-1.083886	-1.535114	-3.059690
C	-1.042567	-2.979678	1.734394	C	4.124599	0.245981	0.243358
C	1.128561	-2.860500	2.763713	H	4.367897	1.315044	0.191860
C	-0.121978	-3.473032	2.654088	C	5.349265	-0.546899	-0.254339
H	-2.004505	-3.461493	1.601664	H	5.163489	-1.626816	-0.213457
H	1.880902	-3.225262	3.454166	H	5.602827	-0.285521	-1.286933
H	-0.369241	-4.334860	3.266087	H	6.218927	-0.333444	0.375917
N	0.502434	-1.268411	1.091632	C	3.800271	-0.087867	1.710316
H	2.358430	-1.249300	1.992226	H	4.660770	0.144000	2.346397
C	-1.554198	-1.290681	-0.104608	H	2.939313	0.488765	2.061893
C	-0.865936	-0.520241	-1.083850	H	3.573734	-1.153409	1.837805
C	-2.940026	-1.445834	-0.155560	H	2.811821	2.033679	-1.407621
C	-1.633590	0.046726	-2.120327	C	-1.959006	1.636512	0.175240
H	0.156561	-1.138885	-1.569234	C	-0.045359	2.989189	0.314732
C	-3.690480	-0.858290	-1.184069	C	-2.765962	2.746195	0.464739
H	-3.459836	-2.003415	0.619361	C	-0.796249	4.119802	0.605017
C	-3.015040	-0.116168	-2.169362	C	-2.186769	3.991149	0.674966
H	-1.128930	0.595080	-2.911724	H	-3.841117	2.625832	0.527070
H	-3.584843	0.328440	-2.981533	H	-0.302506	5.070945	0.770120
O	1.040213	-1.999220	-2.144139	H	-2.809604	4.852539	0.896348
C	2.189174	-1.656207	-1.755606	N	-0.606320	1.786131	0.094370
O	2.404704	-0.707893	-0.922063	H	1.036354	3.026230	0.251749
C	3.392833	-2.379189	-2.311109	C	-2.417299	0.263961	-0.032528
H	4.294182	-2.130661	-1.749089	C	-3.766840	-0.122532	0.010454
H	3.213079	-3.457274	-2.292387	C	-1.394510	-0.688434	-0.247479
H	3.525168	-2.086835	-3.358733	C	-4.139706	-1.457995	-0.146633
C	-5.184718	-1.045267	-1.253097	H	-4.545151	0.620264	0.167124
H	-5.683079	-0.151064	-1.641248	C	-1.773646	-2.031027	-0.365962
H	-5.436429	-1.874566	-1.926945	C	-3.119079	-2.406041	-0.321464
H	-5.609572	-1.278780	-0.272000	H	-1.019386	-2.803430	-0.486873
				H	-3.384351	-3.456189	-0.427599
INT3A-Me				O	0.431570	-0.148816	1.842475
C	1.298354	-1.570905	-1.690074	C	0.444636	-1.167294	2.524602
C	0.723047	-0.519625	-2.479498	C	0.178415	-1.145471	4.004653
C	1.245798	0.786455	-2.283501	H	0.016577	-0.119090	4.332882
C	2.403175	1.029153	-1.463242	H	-0.714613	-1.741072	4.229989
C	2.941699	0.012777	-0.677103	H	1.023575	-1.577567	4.553143
C	2.308174	-1.286245	-0.754551	O	0.712011	-2.345063	1.949916
Ru	0.508098	0.052642	-0.329502	H	0.657970	-3.069728	2.597249
H	0.794660	1.616941	-2.818072	C	-5.591314	-1.875762	-0.144770
H	2.653432	-2.082024	-0.104535	H	-6.235882	-1.094583	0.270390
H	0.896122	-2.575283	-1.760922	H	-5.941839	-2.084996	-1.163547
C	-0.385125	-0.794187	-3.457919	H	-5.744823	-2.788015	0.442417

INT2A-OMe

C	-1.449647	-1.901907	2.050135
C	-0.201905	-2.419666	1.633845
C	0.867972	-1.475033	1.460547
C	0.695358	-0.106245	1.743337
C	-0.577623	0.411128	2.158008
C	-1.645052	-0.504221	2.306467
Ru	-0.847742	-0.780935	0.222558
H	1.806358	-1.811425	1.028879
H	-2.638552	-0.152071	2.555975
H	-2.309574	-2.563664	2.090105
C	-0.006422	-3.870389	1.289016
H	0.569941	-3.970385	0.364060
H	0.543150	-4.378948	2.090211
H	-0.964797	-4.379603	1.157059
C	-0.715362	1.904696	2.383751
H	-0.099308	2.389069	1.614884
C	-0.113405	2.254997	3.761592
H	-0.684321	1.780441	4.567774
H	0.928643	1.927223	3.842546
H	-0.141864	3.338237	3.917754
C	-2.149073	2.431282	2.251158
H	-2.146822	3.523570	2.317020
H	-2.596021	2.150750	1.291838
H	-2.793814	2.061449	3.056678
H	1.514146	0.579572	1.563739
C	0.005102	1.819167	-1.394907
C	-2.277041	1.326255	-1.393868
C	-0.250968	2.990105	-2.122403
C	-2.586599	2.476629	-2.106185
C	-1.549899	3.329869	-2.481117
H	0.588661	3.613017	-2.409688
H	-3.620348	2.687544	-2.357392
H	-1.747540	4.235235	-3.046831
N	-1.014812	0.993239	-1.032557
H	-3.051777	0.630131	-1.100272
C	1.397860	1.515659	-0.982196
C	2.125335	2.501887	-0.290600
C	1.979138	0.274251	-1.241218
C	3.409088	2.213697	0.166264
H	1.676826	3.470531	-0.091637
C	3.263027	-0.016298	-0.756886
H	1.449260	-0.492601	-1.793648
C	3.984101	0.957546	-0.050394
H	3.971636	2.967983	0.708505
H	4.979722	0.753520	0.325086
O	-0.398005	-1.834700	-1.596923
C	-1.638841	-1.976639	-1.856499
O	-2.455994	-1.530568	-0.978274
C	-2.115654	-2.589988	-3.135329
H	-2.252183	-1.796628	-3.880352
H	-1.373411	-3.294695	-3.516319
H	-3.077416	-3.084838	-2.982312
O	3.698280	-1.282644	-0.993927
C	5.044399	-1.617343	-0.656971
H	5.211736	-1.564205	0.426696
H	5.187583	-2.644084	-0.995321
H	5.756847	-0.960011	-1.170023

TS3A-OMe

C	2.308711	1.832717	1.161952
C	2.718706	2.033437	-0.170892
C	1.709069	2.340958	-1.146527
C	0.358578	2.466188	-0.767002
C	-0.074223	2.279903	0.590844
C	0.925065	1.926738	1.525907
Ru	1.042830	0.412425	-0.139495
H	1.989527	2.442515	-2.189707
H	0.644917	1.696828	2.547738
H	3.040261	1.553919	1.913436
C	4.140217	1.822110	-0.608350
H	4.506327	2.696005	-1.158197
H	4.801219	1.644844	0.243758
H	4.190689	0.951509	-1.271912
C	-1.539390	2.456943	0.944768
H	-2.113712	1.998792	0.129588
C	-1.876900	3.962085	0.982420
H	-1.318738	4.466394	1.779725
H	-1.634077	4.455832	0.034923
H	-2.945469	4.104782	1.174533
C	-1.946922	1.767639	2.252720
H	-3.033152	1.819772	2.373744
H	-1.659352	0.711633	2.258054
H	-1.499908	2.258238	3.125430
H	-0.388756	2.661854	-1.529280
C	-0.474781	-1.816682	1.125379
C	1.738562	-1.755669	1.895455
C	-0.753897	-2.896755	1.968280
C	1.519879	-2.830034	2.750294

C	0.247192	-3.403668	2.792010
H	-1.740022	-3.346784	1.953627
H	2.332150	-3.205756	3.362612
H	0.042553	-4.245104	3.446604
N	0.763877	-1.251214	1.119283
H	2.706619	-1.274738	1.814437
C	-1.411058	-1.222623	0.160368
C	-0.800217	-0.494185	-0.908198
C	-2.788390	-1.332301	0.271784
C	-1.666096	0.082187	-1.859931
H	0.093181	-1.208109	-1.519310
C	-3.620638	-0.728923	-0.691935
H	-3.266899	-1.853789	1.094472
C	-3.051186	-0.024963	-1.770180
H	-1.237712	0.598321	-2.715682
H	-3.677617	0.419466	-2.534549
O	0.872009	-2.094531	-2.158847
C	2.071095	-1.783989	-1.914827
O	2.416154	-0.826674	-1.140915
C	3.171006	-2.576812	-2.579920
H	4.153288	-2.260752	-2.226548
H	3.020444	-3.641791	-2.379931
H	3.103432	-2.437146	-3.663908
O	-4.940565	-0.889266	-0.489221
C	-5.866375	-0.326449	-1.422886
H	-5.726109	-0.753908	-2.422625
H	-6.855606	-0.589318	-1.048267
H	-5.767966	0.764935	-1.467286

INT3A-OMe

C	1.454474	-1.595982	-1.688748
C	0.923620	-0.522450	-2.479349
C	1.496172	0.762460	-2.280108
C	2.657135	0.959642	-1.453060
C	3.151137	-0.077308	-0.664367
C	2.469171	-1.351269	-0.747257
Ru	0.720916	0.056100	-0.332238
H	1.079713	1.610026	-2.815998
H	2.781365	-2.160538	-0.097339
H	1.014134	-2.584066	-1.762782
C	-0.190862	-0.751731	-3.462255
H	-0.725011	0.179021	-3.672743
H	0.215110	-1.134592	-4.406486
H	-0.911302	-1.477616	-3.075359
C	4.337618	0.108702	0.262143
H	4.625797	1.166516	0.209544
C	5.530537	-0.736168	-0.227021
H	5.300123	-1.807339	-0.182736
H	5.799043	-0.489682	-1.259516
H	6.405657	-0.556316	0.406154
C	3.991574	-0.207778	1.727993
H	4.859341	-0.016330	2.367667
H	3.157387	0.409216	2.075495
H	3.713695	-1.261139	1.855211
H	3.103900	1.947624	-1.393801
C	-1.692203	1.724264	0.167254
C	0.266803	3.009545	0.310988
C	-2.459749	2.860375	0.461256
C	-0.444403	4.165093	0.604329
C	-1.838245	4.084307	0.674646
H	-3.538355	2.777966	0.525839
H	0.082083	5.098042	0.771952
H	-2.431012	4.965847	0.899266
N	-0.334871	1.827452	0.086463
H	1.349270	3.009340	0.249791
C	-2.198003	0.368600	-0.043089
C	-3.567483	0.043741	-0.002062
C	-1.209171	-0.614534	-0.256465
C	-3.964644	-1.284478	-0.162114
H	-4.308313	0.818819	0.151944
C	-1.636467	-1.945486	-0.380627
C	-2.987038	-2.279533	-0.339368
H	-0.910109	-2.743072	-0.505717
H	-3.318210	-3.308118	-0.447766
O	0.625709	-0.140473	1.841507
C	0.587052	-1.158621	2.523123
C	0.312967	-1.125143	4.001607
H	0.201961	-0.092272	4.330616
H	-0.610941	-1.674464	4.220040
H	1.131162	-1.600951	4.554750
O	0.802599	-2.347645	1.949835
H	0.708035	-3.069350	2.595841
O	-5.251780	-1.722054	-0.152964
C	-6.294387	-0.766264	-0.008825
H	-6.279305	-0.030122	-0.823849
H	-7.226084	-1.331997	-0.050905
H	-6.231200	-0.243527	0.955349

INT4A

C	1.341656	-1.513747	-1.573647

C	0.620397	-0.632568	-2.448314	C	0.655490	-1.171389	2.373052
C	0.918156	0.749145	-2.352741	O	1.110723	-2.190994	1.849630
C	1.994489	1.235961	-1.529587	C	0.469278	-1.075014	3.886130
C	2.679382	0.381966	-0.667821	H	0.974411	-0.183181	4.272868
C	2.277059	-1.007358	-0.655996	H	-0.596717	-0.970488	4.117063
Ru	0.271104	0.029789	-0.321669	H	0.864204	-1.968776	4.373634
H	0.352852	1.454763	-2.954834				
H	2.695115	-1.682944	0.077793	**INT5A**			
H	1.097307	-2.569954	-1.556042	C	-1.414255	-1.979287	0.744535
C	-0.419194	-1.166585	-3.396794	C	-0.746558	-1.301072	1.818501
H	-1.091975	-0.370112	-3.729327	C	-1.087382	0.062793	2.021323
H	0.055021	-1.607476	-4.282950	C	-2.152219	0.699033	1.294935
H	-1.023311	-1.938064	-2.908789	C	-2.779601	0.047143	0.233042
C	3.784094	0.877310	0.246220	C	-2.332090	-1.293996	-0.070855
H	3.835424	1.968751	0.128411	Ru	-0.347890	-0.145727	-0.054168
C	5.138446	0.288797	-0.195488	H	-0.559772	0.625174	2.785772
H	5.137459	-0.803298	-0.097317	H	-2.751827	-1.807705	-0.928901
H	5.361669	0.534629	-1.239985	H	-1.152278	-3.006748	0.516252
H	5.947866	0.680423	0.431199	C	0.262983	-2.005801	2.681531
C	3.503804	0.574789	1.729103	H	0.945829	-1.292623	3.151643
H	4.302367	0.994180	2.352226	H	-0.249723	-2.561637	3.476009
H	2.543799	0.994054	2.041553	H	0.856370	-2.712701	2.095424
H	3.459126	-0.503458	1.915450	C	-3.888298	0.704889	-0.564999
H	2.224169	2.298106	-1.534684	H	-3.873456	1.773693	-0.314087
C	-2.427768	1.164650	0.142829	C	-5.249000	0.129067	-0.119501
C	-0.791310	2.842955	0.193455	H	-5.309406	-0.943897	-0.337265
C	-3.420728	2.124956	0.393128	H	-5.412871	0.268192	0.954235
C	-1.731357	3.834593	0.439563	H	-6.062088	0.626918	-0.657946
C	-3.076086	3.462202	0.535412	C	-3.701260	0.572303	-2.085949
H	-4.454992	1.812784	0.482991	H	-4.465008	1.161359	-2.603469
H	-1.414591	4.865328	0.557151	H	-2.714272	0.920971	-2.403821
H	-3.843093	4.206947	0.728205	H	-3.814466	-0.465952	-2.418501
N	-1.124709	1.551297	0.032080	H	-2.422915	1.722106	1.538345
H	0.267454	3.065799	0.118756	C	2.331797	1.155134	-0.007071
C	-2.630284	-0.274498	0.013779	C	0.621238	2.740933	0.290536
C	-3.886170	-0.900341	0.097446	C	3.293115	2.167085	0.125051
C	-1.443929	-1.033735	-0.147080	C	1.531657	3.779232	0.425911
C	-3.976290	-2.286948	0.047173	C	2.895616	3.480023	0.346389
H	-4.792862	-0.310465	0.209568	H	4.345754	1.919575	0.054711
C	-1.556573	-2.431876	-0.137556	H	1.178856	4.790963	0.591796
C	-2.806214	-3.050453	-0.054384	H	3.638766	4.264228	0.453234
H	-4.946066	-2.773096	0.108303	N	1.004263	1.463547	0.087620
H	-0.658026	-3.039860	-0.151285	H	-0.448376	2.910173	0.346906
H	-2.870057	-4.136484	-0.056601	C	2.593379	-0.259136	-0.273403
O	0.291748	-0.077101	1.762647	C	3.877251	-0.793108	-0.465580

C	1.441237	-1.081635	-0.369525	H	3.713810	4.141758	1.182723
C	4.032788	-2.142805	-0.772493	N	1.102244	1.450055	0.261341
H	4.758602	-0.163274	-0.383312	H	-0.361526	2.865479	0.618718
C	1.622333	-2.428475	-0.709539	C	2.697842	-0.225197	-0.218761
C	2.905065	-2.956820	-0.905092	C	3.980889	-0.763445	-0.392792
H	5.026248	-2.555265	-0.918125	C	1.544446	-1.014146	-0.490514
H	0.763993	-3.085662	-0.820880	C	4.133955	-2.072314	-0.845174
H	3.021851	-4.007105	-1.158710	H	4.864333	-0.167677	-0.181935
O	-0.244794	0.192426	-2.258287	C	1.724083	-2.327167	-0.951555
H	0.270109	1.004098	-2.416137	C	3.007638	-2.850655	-1.132525
H	0.319006	-0.530127	-2.593293	H	5.129235	-2.485023	-0.978071
				H	0.864799	-2.951824	-1.179117
INT5A-excited				H	3.130154	-3.868086	-1.493579
C	-1.493816	-2.069741	0.232062	O	-0.294753	1.263093	-2.307156
C	-1.051795	-1.850542	1.572782	H	0.634189	1.473873	-2.500172
C	-1.493484	-0.685701	2.216748	H	-0.634706	0.828133	-3.106599
C	-2.358584	0.219836	1.564593				
C	-2.876694	-0.029808	0.279505	**INT6A**			
C	-2.405878	-1.187178	-0.394286	C	-1.430272	-2.219789	0.276983
Ru	-0.235605	-0.128309	-0.206104	C	-0.690981	-1.863962	1.442284
H	-1.147072	-0.465316	3.221543	C	-0.879488	-0.544132	1.932630
H	-2.795309	-1.437895	-1.375665	C	-1.940660	0.288902	1.447426
H	-1.210839	-2.988797	-0.271329	C	-2.749002	-0.104691	0.370845
C	-0.157500	-2.854955	2.247597	C	-2.382190	-1.334006	-0.275025
H	0.259914	-2.460340	3.177664	Ru	-0.280166	-0.191368	-0.247840
H	-0.722540	-3.764059	2.487498	H	-0.275497	-0.196027	2.765095
H	0.670336	-3.141063	1.590503	H	-2.915388	-1.639482	-1.170341
C	-3.929420	0.878000	-0.331801	H	-1.267898	-3.186207	-0.189943
H	-3.966645	1.788180	0.281100	C	0.253519	-2.816479	2.111179
C	-5.310576	0.194112	-0.245472	H	1.091819	-2.292873	2.577647
H	-5.330687	-0.722384	-0.847176	H	-0.294597	-3.343071	2.903900
H	-5.562690	-0.072161	0.786335	H	0.642269	-3.567014	1.420227
H	-6.088201	0.864290	-0.626288	C	-3.890424	0.744355	-0.143026
C	-3.607800	1.297970	-1.776006	H	-3.907884	1.662138	0.457569
H	-4.376821	1.985347	-2.142808	C	-5.229132	0.002626	0.072694
H	-2.637194	1.799193	-1.841956	H	-5.275476	-0.917356	-0.521434
H	-3.598262	0.434251	-2.452206	H	-5.385023	-0.256125	1.124514
H	-2.672247	1.117204	2.091077	H	-6.055005	0.646075	-0.244863
C	2.432877	1.143089	0.215651	C	-3.697554	1.140276	-1.620466
C	0.709425	2.690160	0.613389	H	-4.506679	1.808531	-1.928515
C	3.388513	2.111996	0.550959	H	-2.746760	1.661492	-1.781596
C	1.612389	3.688623	0.949555	H	-3.733681	0.265557	-2.280868
C	2.978519	3.387169	0.920795	H	-2.103373	1.251480	1.923374
H	4.442978	1.863187	0.520670	C	2.218889	1.327643	0.194412
H	1.253745	4.673566	1.226986	C	0.319052	2.715546	0.351451

C	3.048597	2.411345	0.501920
C	1.100628	3.822811	0.651018
C	2.488546	3.663218	0.736503
H	4.122046	2.270731	0.554994
H	0.629333	4.785945	0.812835
H	3.124767	4.508952	0.977859
N	0.863068	1.498497	0.139686
H	-0.759578	2.785479	0.266225
C	2.635390	-0.031056	-0.130595
C	3.959910	-0.455940	-0.274301
C	1.568270	-0.940635	-0.387534
C	4.227436	-1.768363	-0.672008
H	4.785710	0.225105	-0.094096
C	1.853442	-2.258452	-0.781644
C	3.178853	-2.661824	-0.941653
H	5.256373	-2.097594	-0.777378
H	1.053227	-2.964377	-0.980573
H	3.400512	-3.673892	-1.266674
O	-0.287587	0.566044	-2.277122
H	0.554523	0.952038	-2.581122
H	-0.624182	0.008501	-3.001272

1a

C	-3.468855	-0.733116	0.119374
C	-3.118702	-1.238447	1.528601
H	-2.095615	-1.624129	1.577010
H	-3.212189	-0.424276	2.254462
H	-3.799724	-2.044390	1.824639
C	-4.937335	-0.257631	0.092552
H	-5.161526	0.449920	0.891691
H	-5.180224	0.209995	-0.866395
H	-5.584745	-1.129849	0.227586
C	-3.364877	-1.856258	-0.937542
H	-3.427177	-1.440368	-1.948054
H	-2.458025	-2.452584	-0.855077
H	-4.207440	-2.540711	-0.799066
N	-2.560738	0.419615	-0.251610
Cl	-3.097980	1.990485	0.332770
C	-1.178235	0.428648	-0.492158
O	-0.542172	1.468735	-0.474149
C	-0.482371	-0.890891	-0.849629
H	-0.730434	-1.664464	-0.116273
H	-0.868939	-1.235070	-1.815224
C	1.039389	-0.720138	-0.925701
H	1.468752	-1.614953	-1.394028
H	1.275107	0.129713	-1.572563
C	1.696580	-0.505611	0.451813
H	1.200294	0.335567	0.946765
H	1.531579	-1.395790	1.074501
C	3.176766	-0.222613	0.330653
C	3.615252	1.060671	-0.028023
C	4.133204	-1.227050	0.521255
C	4.973824	1.331935	-0.190322
H	2.878316	1.846655	-0.179324
C	5.495019	-0.960034	0.360729
H	3.807889	-2.227156	0.801155
C	5.919458	0.321071	0.003873
H	5.295763	2.333321	-0.464856
H	6.223298	-1.751964	0.516933
H	6.978527	0.531893	-0.119376

radical-A

C	2.847652	-0.864171	0.030038
C	3.568295	-0.538089	1.366434
H	3.818945	0.523722	1.405018
H	2.927235	-0.783659	2.218860
H	4.484329	-1.137307	1.430305
C	2.490384	-2.362239	-0.010923
H	1.850201	-2.629357	0.835992
H	1.958762	-2.609742	-0.936206
H	3.403499	-2.965965	0.033566
C	3.740745	-0.487029	-1.166446
H	3.224913	-0.696556	-2.110909
H	4.005324	0.572578	-1.137736
H	4.663375	-1.077238	-1.146862
N	1.581727	-0.139220	0.058316
C	1.459593	1.172385	-0.337612
O	2.283847	2.021184	0.011490
C	0.178647	1.534035	-1.064251
H	0.463720	2.167271	-1.912466
H	-0.308068	0.631932	-1.450026
C	-0.782104	2.315236	-0.144449
H	-0.240497	3.176188	0.264777
H	-1.608211	2.704653	-0.752228
C	-1.360717	1.473076	1.013905
H	-0.537357	1.065459	1.612203
H	-1.927947	2.142955	1.672603
C	-2.258894	0.349877	0.538466
C	-3.586489	0.613600	0.171617
C	-1.779511	-0.961700	0.413534

C	-4.414706	-0.402137	-0.307132	H	-4.021311	-2.699271	-0.604568
H	-3.974137	1.626188	0.267550				
C	-2.605622	-1.981142	-0.065939	**radical-B**			
H	-0.748254	-1.173426	0.682218	C	-2.989136	-0.592564	0.090541
C	-3.925642	-1.705550	-0.427549	C	-2.394748	-1.361846	-1.105873
H	-5.442465	-0.178135	-0.581695	H	-1.948598	-0.664565	-1.818530
H	-2.216476	-2.992456	-0.155303	H	-1.620947	-2.060490	-0.765630
H	-4.569536	-2.498954	-0.797955	H	-3.177168	-1.935237	-1.616376
				C	-3.592975	-1.579916	1.100840
TSB				H	-2.841293	-2.298573	1.452707
C	2.392586	-1.056380	-0.109441	H	-4.004950	-1.051554	1.968954
C	3.115273	-1.099637	1.255455	H	-4.403271	-2.147362	0.632518
H	3.629624	-0.153456	1.441164	C	-4.070772	0.394330	-0.385502
H	2.397057	-1.271373	2.063933	H	-4.500569	0.929761	0.468377
H	3.847460	-1.916314	1.257934	H	-3.641150	1.123218	-1.074928
C	1.617031	-2.358794	-0.348205	H	-4.874913	-0.149448	-0.894885
H	0.890176	-2.530535	0.451933	N	-1.922103	0.140583	0.803046
H	1.071488	-2.318571	-1.297744	C	-1.090358	1.074484	0.228843
H	2.307784	-3.208411	-0.383026	O	-1.261150	1.515353	-0.918831
C	3.402236	-0.804251	-1.243597	C	0.028214	1.508799	1.061469
H	2.890364	-0.765826	-2.212313	H	0.145781	1.095123	2.060527
H	3.925281	0.144298	-1.086333	C	1.076626	2.417652	0.511811
H	4.146288	-1.607950	-1.283004	H	0.611438	3.354968	0.174542
N	1.405991	0.034122	-0.033133	H	1.793950	2.665359	1.301987
C	1.669193	1.383542	-0.050634	C	1.837073	1.812089	-0.709129
O	2.593509	2.017005	0.429628	H	1.139155	1.781135	-1.548982
C	0.480571	1.801184	-0.899613	H	2.654557	2.494504	-0.973049
H	0.773245	2.140923	-1.896967	C	2.372845	0.426283	-0.427852
H	0.411977	0.406425	-0.873449	C	1.627886	-0.706980	-0.786678
C	-0.703377	2.514024	-0.288336	C	3.586340	0.240894	0.247440
H	-0.342682	3.495721	0.060328	C	2.081144	-1.989768	-0.473972
H	-1.454055	2.712009	-1.062457	H	0.687529	-0.574964	-1.315356
C	-1.364203	1.779301	0.899664	C	4.044030	-1.040241	0.561627
H	-0.600811	1.539188	1.648425	H	4.178149	1.110204	0.527972
H	-2.064431	2.476537	1.377682	C	3.290627	-2.160970	0.203538
C	-2.106126	0.521080	0.493645	H	1.491446	-2.855849	-0.764850
C	-3.268621	0.606287	-0.286579	H	4.990404	-1.164046	1.082198
C	-1.653093	-0.747612	0.875652	H	3.646980	-3.158985	0.444973
C	-3.954502	-0.542346	-0.681855	H	-1.623390	-0.253588	1.684544
H	-3.642951	1.584453	-0.582718				
C	-2.336226	-1.900917	0.482968	**TSC**			
H	-0.748090	-0.827920	1.469776	C	-1.934788	-1.037554	0.243960
C	-3.488377	-1.802884	-0.298710	C	-1.099401	-1.776389	-0.817656
H	-4.854820	-0.454072	-1.284582	H	-1.282232	-1.349476	-1.806837
H	-1.965792	-2.876327	0.788391	H	-0.032417	-1.694021	-0.593542

H	-1.369502	-2.839043	-0.836640	H	-3.900948	-0.125733	0.061867
C	-1.652556	-1.616186	1.641906	H	-3.935058	-1.805165	0.653747
H	-0.585451	-1.544737	1.878813	N	-1.214498	0.247966	0.391497
H	-2.219811	-1.077091	2.408834	C	-1.516353	1.377124	-0.299274
H	-1.941507	-2.672084	1.673555	O	-2.483643	1.501668	-1.043466
C	-3.440968	-1.147806	-0.077781	C	-0.562750	2.589069	-0.082239
H	-4.034966	-0.619104	0.675293	H	-0.227960	2.873179	-1.088027
H	-3.644149	-0.707028	-1.057165	H	-1.232990	3.392999	0.252282
H	-3.744942	-2.201456	-0.088099	C	0.594080	2.444278	0.844132
N	-1.587104	0.383204	0.302024	H	0.399766	2.379485	1.912840
C	-1.447717	1.240226	-0.741400	C	1.983051	2.142867	0.354054
O	-1.914499	1.075792	-1.862610	H	2.192249	2.727999	-0.552276
C	-0.648664	2.480116	-0.272627	H	2.720687	2.440841	1.109325
H	0.120207	2.684983	-1.023469	C	2.157069	0.660192	0.036506
H	-1.320190	3.344669	-0.246951	C	1.894125	0.167129	-1.248726
C	-0.088369	2.120191	1.090706	C	2.512352	-0.248688	1.043649
H	-0.507591	2.696831	1.918953	C	1.989070	-1.197919	-1.523619
C	1.411764	1.869299	1.226651	H	1.610119	0.858369	-2.038633
H	1.945168	2.758502	0.855228	C	2.609608	-1.615054	0.772282
H	1.660443	1.781755	2.290498	H	2.720582	0.120108	2.045854
C	1.914372	0.637808	0.496752	C	2.346734	-2.094675	-0.513568
C	2.224243	0.668789	-0.869178	H	1.784978	-1.561025	-2.527330
C	2.062229	-0.574221	1.185494	H	2.893627	-2.303826	1.563611
C	2.654023	-0.482287	-1.532547	H	2.422000	-3.157228	-0.727078
H	2.138427	1.602353	-1.419303	H	-0.314267	0.226430	0.852849
C	2.501909	-1.725242	0.529930				
H	1.835659	-0.613164	2.248885	**TSD**			
C	2.795902	-1.683341	-0.835013	C	1.752149	-1.385519	-0.096000
H	2.883400	-0.437790	-2.593715	C	1.369986	-1.462185	1.393919
H	2.613236	-2.653339	1.084324	H	2.061820	-0.870477	1.998522
H	3.134456	-2.578185	-1.349778	H	0.350949	-1.087818	1.546492
H	-0.734399	0.988254	1.152638	H	1.402536	-2.501027	1.741825
				C	0.752746	-2.193408	-0.942688
radical-C				H	-0.271709	-1.831473	-0.799959
C	-1.938376	-1.038343	0.276511	H	1.001094	-2.117772	-2.006750
C	-1.863799	-1.557674	-1.171421	H	0.781740	-3.249075	-0.651651
H	-2.331106	-0.842392	-1.852128	C	3.179478	-1.936060	-0.320063
H	-0.819280	-1.698886	-1.468916	H	3.455822	-1.858853	-1.376824
H	-2.383476	-2.519230	-1.256420	H	3.899918	-1.372100	0.274260
C	-1.234258	-2.021111	1.224172	H	3.209996	-2.992696	-0.027114
H	-0.186653	-2.165742	0.936315	N	1.721243	-0.001324	-0.606410
H	-1.265598	-1.659162	2.259263	C	2.317332	1.050927	0.046167
H	-1.734112	-2.994650	1.190519	O	3.304362	0.941385	0.774962
C	-3.402424	-0.848726	0.710238	C	1.675302	2.407128	-0.261184
H	-3.450708	-0.486271	1.743395	H	2.197360	3.161553	0.331821

H	1.824784	2.641269	-1.323629
C	0.166410	2.375861	0.058112
H	0.041788	2.184791	1.129711
H	-0.291849	3.353493	-0.140955
C	-1.760929	0.633041	-0.297518
C	-2.671047	0.117114	-1.241807
C	-2.043290	0.430098	1.067791
C	-3.818970	-0.562654	-0.842165
H	-2.468049	0.256500	-2.301129
C	-3.191727	-0.249787	1.468448
H	-1.358735	0.801948	1.823791
C	-4.085778	-0.749335	0.517225
H	-4.507141	-0.945977	-1.590757
H	-3.388934	-0.392186	2.527571
H	-4.979900	-1.279972	0.832234
C	-0.518757	1.287627	-0.767521
H	-0.570630	1.560577	-1.827957
H	0.388114	0.440394	-0.810620

radical-D

C	2.180334	-1.090056	-0.225048
C	0.952518	-1.817990	0.349760
H	0.635737	-1.346437	1.280972
H	0.112687	-1.781690	-0.351993
H	1.197476	-2.868087	0.548617
C	2.603463	-1.739071	-1.551424
H	1.781670	-1.724151	-2.278984
H	3.468030	-1.223774	-1.988008
H	2.881510	-2.784340	-1.384474
C	3.349656	-1.126241	0.774711
H	4.225390	-0.613105	0.361173
H	3.064461	-0.635106	1.707071
H	3.626149	-2.165023	0.989254
N	1.839320	0.317626	-0.538459
C	1.399273	1.248029	0.352094
O	1.300546	1.051285	1.562755
C	0.990080	2.590837	-0.252576
H	1.531480	3.372756	0.292065
H	1.264599	2.669262	-1.312123
C	-0.536637	2.811788	-0.081689
H	-0.761652	2.770840	0.988443
H	-0.773932	3.828473	-0.421856
C	-1.347178	1.818166	-0.855928
H	-1.448136	2.003106	-1.925062
C	-1.912151	0.621087	-0.354299
C	-2.600718	-0.261141	-1.241428
C	-1.831093	0.230289	1.015830
C	-3.165172	-1.444424	-0.791321
H	-2.678618	0.011340	-2.291793
C	-2.405340	-0.954151	1.454149
H	-1.271748	0.840869	1.715081
C	-3.076116	-1.802246	0.562457
H	-3.680718	-2.096370	-1.492116
H	-2.319998	-1.230707	2.501890
H	-3.518897	-2.729649	0.914476
H	1.779371	0.558873	-1.517190

INT7A

C	-0.541523	-0.078840	-2.937131
C	0.456969	-1.030443	-2.613279
C	0.080922	-2.135696	-1.794068
C	-1.216828	-2.229716	-1.280891
C	-2.241164	-1.276011	-1.608028
C	-1.875292	-0.218090	-2.470081
Ru	-0.504743	-0.027775	-0.530541
H	0.828389	-2.868169	-1.505437
H	-2.604330	0.538255	-2.736414
H	-0.287052	0.763964	-3.571888
C	1.853111	-0.916401	-3.152031
H	2.574674	-1.368450	-2.467996
H	1.914970	-1.453219	-4.107779
H	2.132035	0.123944	-3.336048
C	-3.652443	-1.489725	-1.096611
H	-3.558002	-1.883885	-0.075393
C	-4.331902	-2.575900	-1.962928
H	-4.443620	-2.233978	-2.997775
H	-3.761821	-3.511144	-1.970215
H	-5.329258	-2.790807	-1.567733
C	-4.497568	-0.210458	-1.043209
H	-5.447641	-0.422658	-0.545000
H	-3.995098	0.591489	-0.492855
H	-4.739905	0.157557	-2.046582
H	-1.465489	-3.055010	-0.620249
C	-2.171042	0.955637	1.701702
C	-1.585569	-1.311025	1.976013
C	-2.928165	0.909118	2.879304
C	-2.329561	-1.408653	3.141598
C	-3.011051	-0.275045	3.601573
H	-3.455917	1.794907	3.212994
H	-2.370355	-2.350876	3.676931

H	-3.602148	-0.319979	4.510908	H	1.290927	-5.461968	0.292034
N	-1.505505	-0.160137	1.273690	H	4.313914	-2.638216	-0.913644
H	-1.022269	-2.148200	1.585298	H	3.173162	-4.831972	-1.216876
C	-1.999829	2.099216	0.820534	H	3.295922	2.512574	1.657870
C	-2.505027	3.385744	1.063148				
C	-1.247444	1.842815	-0.352171	**TS8A**			
C	-2.271050	4.405606	0.144171	C	-1.715309	-3.031196	-0.843964
H	-3.074543	3.596358	1.963241	C	-1.954300	-2.225934	-1.999774
C	-1.026896	2.872042	-1.271971	C	-0.826631	-1.601596	-2.635187
C	-1.531715	4.150460	-1.018474	C	0.438706	-1.689516	-2.061487
H	-2.665778	5.399572	0.328600	C	0.675274	-2.447095	-0.857903
H	-0.454858	2.699644	-2.177286	C	-0.409444	-3.150070	-0.293536
H	-1.352345	4.949755	-1.731700	Ru	-1.165754	-0.961494	-0.322043
C	3.579920	2.400748	-0.459574	H	-0.979805	-1.018196	-3.537675
C	2.557779	2.893506	-1.495212	H	-0.260510	-3.760270	0.589627
H	1.872040	2.095106	-1.784199	H	-2.548783	-3.539436	-0.369587
H	1.972873	3.730758	-1.101502	C	-3.330855	-2.135683	-2.596312
H	3.091515	3.236649	-2.386802	H	-3.466983	-2.958534	-3.309490
C	4.581032	3.518169	-0.131539	H	-4.105557	-2.223389	-1.829961
H	4.070619	4.418774	0.227950	H	-3.476949	-1.197703	-3.137459
H	5.308868	3.195712	0.622696	C	2.077222	-2.581441	-0.296913
H	5.140105	3.786958	-1.031712	H	2.714929	-1.843617	-0.790438
C	4.313438	1.142902	-0.951287	C	2.625260	-3.983907	-0.645536
H	5.062651	0.815764	-0.222576	H	2.048947	-4.772638	-0.148163
H	3.610345	0.325476	-1.125680	H	2.601503	-4.169510	-1.724285
H	4.831165	1.363588	-1.889989	H	3.665067	-4.061208	-0.313189
N	2.887538	2.082570	0.835141	C	2.153564	-2.312932	1.214457
C	1.866525	1.267495	1.058867	H	3.200226	-2.317995	1.531733
O	1.345282	0.624118	0.086332	H	1.726849	-1.335903	1.472714
C	1.462425	1.040365	2.491689	H	1.628549	-3.076607	1.799603
H	1.726890	1.916354	3.093055	H	1.274103	-1.168242	-2.519142
H	0.381148	0.915247	2.545427	C	-3.676646	0.457712	0.409357
C	2.181424	-0.222563	3.086130	C	-2.921060	1.152715	-1.701908
H	3.249452	-0.164784	2.845448	C	-4.832486	1.232784	0.259636
H	2.107555	-0.128166	4.175002	C	-4.040095	1.952621	-1.895434
C	1.590210	-1.535792	2.679505	C	-5.020785	1.979080	-0.899380
H	0.785677	-1.905376	3.310210	H	-5.579260	1.242064	1.045187
C	2.005359	-2.367533	1.611063	H	-4.143255	2.524913	-2.810647
C	1.365000	-3.628572	1.406225	H	-5.919266	2.575243	-1.025536
C	3.069885	-2.030642	0.723647	N	-2.745071	0.414821	-0.589035
C	1.773638	-4.494782	0.400889	H	-2.134054	1.092187	-2.444801
H	0.579367	-3.935842	2.093779	C	-3.299560	-0.318308	1.589588
C	3.474546	-2.904513	-0.276446	C	-3.994635	-0.298886	2.804299
H	3.596311	-1.091089	0.847943	C	-2.100603	-1.070371	1.456145
C	2.833896	-4.142170	-0.450248	C	-3.507403	-1.022977	3.895255

H	-4.907839	0.278137	2.915860	C	-2.423494	2.611738	-0.282429
C	-1.636888	-1.803392	2.560800	C	-1.730523	2.591778	0.951886
C	-2.325929	-1.762434	3.777444	C	-0.306141	2.598667	1.013153
H	-4.050207	-1.011546	4.835092	C	0.486228	2.633194	-0.158218
H	-0.728678	-2.393580	2.488420	C	-0.213450	2.479974	-1.389816
H	-1.949394	-2.320300	4.629897	Ru	-1.094644	0.610221	-0.052894
C	0.426501	1.385034	0.191669	H	-2.297993	2.598675	1.877882
H	0.192819	0.698990	1.017563	H	0.346151	2.417548	-2.315634
C	-0.409407	2.510412	0.067553	H	-2.109927	2.396812	-2.420985
C	-1.477167	2.681126	1.003855	C	-3.915385	2.754707	-0.348164
C	-0.209612	3.510703	-0.934417	H	-4.395226	2.367093	0.554238
C	-2.291953	3.796352	0.947026	H	-4.165429	3.820266	-0.431672
H	-1.634918	1.923408	1.765334	H	-4.330902	2.237275	-1.215327
C	-1.044476	4.609426	-0.995262	C	1.986054	2.827524	-0.070314
H	0.594112	3.406318	-1.654696	H	2.363368	2.145991	0.700064
C	-2.084457	4.755174	-0.057111	C	2.257562	4.282310	0.391693
H	-3.090323	3.928913	1.669384	H	1.898083	5.005848	-0.348287
H	-0.896421	5.366549	-1.758505	H	1.781770	4.506629	1.352152
H	-2.730763	5.626778	-0.108608	H	3.335722	4.424661	0.509621
C	1.749903	1.193733	-0.430521	C	2.742212	2.525500	-1.369652
H	1.904613	0.152117	-0.718328	H	3.814934	2.604505	-1.180855
H	1.904017	1.811283	-1.317642	H	2.565182	1.506780	-1.730701
C	2.860849	1.482961	0.612949	H	2.489968	3.237474	-2.164580
H	2.962796	2.557592	0.796476	H	0.177628	2.632182	1.984483
H	2.622206	1.008433	1.573896	C	-2.903536	-1.015398	1.686401
C	4.178051	0.840762	0.099115	C	-1.093739	-0.162855	2.912458
O	4.127539	-0.123992	-0.667052	C	-3.430984	-1.582360	2.854643
N	5.303515	1.388187	0.581771	C	-1.583156	-0.684862	4.099262
H	5.216330	2.182665	1.202199	C	-2.770553	-1.423513	4.065889
C	6.693915	0.882230	0.337980	H	-4.365879	-2.128170	2.808634
C	6.809654	-0.558446	0.861705	H	-1.042695	-0.515643	5.023935
H	6.582057	-0.602872	1.932589	H	-3.179234	-1.855276	4.974060
H	6.129003	-1.223401	0.324007	N	-1.717582	-0.340083	1.727182
H	7.831804	-0.921500	0.716060	H	-0.174472	0.405060	2.890346
C	7.006061	0.952779	-1.164974	C	-3.527203	-1.036428	0.370241
H	6.917507	1.980973	-1.531609	C	-4.726880	-1.700344	0.068589
H	8.032142	0.614546	-1.341390	C	-2.839129	-0.330897	-0.635639
H	6.328640	0.313014	-1.735164	C	-5.242574	-1.656445	-1.224724
C	7.626423	1.814497	1.124063	H	-5.260753	-2.252536	0.835849
H	7.546718	2.849551	0.770836	C	-3.356587	-0.298700	-1.930671
H	7.407943	1.787212	2.198622	C	-4.559224	-0.957280	-2.221748
H	8.663771	1.496640	0.988723	H	-6.173998	-2.164046	-1.453753
				H	-2.839705	0.224197	-2.727268
INT8A				H	-4.960295	-0.916424	-3.230641
C	-1.624070	2.468665	-1.453782	C	0.781399	-0.554191	0.068433

H	1.498412	0.146095	-0.346003	H	-1.135222	2.013236	0.745661
C	0.024104	-1.286793	-0.925750	H	-2.787543	2.372800	-1.098912
C	0.059003	-0.843555	-2.286391	H	-3.883667	-0.748368	2.656212
C	-0.694407	-2.492129	-0.627855	C	-0.716824	-2.917747	-0.117679
C	-0.613742	-1.540069	-3.282446	C	-2.792288	-3.384206	0.875611
H	0.679006	0.010387	-2.538804	C	-0.329685	-4.248669	0.037035
C	-1.343337	-3.184395	-1.625243	C	-2.461766	-4.722505	1.051017
H	-0.730807	-2.847156	0.395469	C	-1.206208	-5.159694	0.625628
C	-1.317383	-2.700813	-2.950493	H	0.643721	-4.577028	-0.309119
H	-0.574590	-1.200244	-4.312335	H	-3.173676	-5.399138	1.510375
H	-1.884434	-4.096432	-1.396111	H	-0.913745	-6.197953	0.747100
H	-1.838526	-3.252434	-3.727676	N	-1.945475	-2.502078	0.306025
C	1.340678	-1.200320	1.310792	H	-3.753022	-2.992478	1.189029
H	1.611446	-0.418157	2.025117	C	0.083968	-1.846665	-0.736122
H	0.629556	-1.873471	1.793634	C	1.378137	-1.999786	-1.184245
C	2.633647	-1.979788	0.977140	C	-0.594249	-0.582623	-0.862809
H	2.928079	-2.561157	1.859615	H	1.904300	-2.946327	-1.102633
H	2.450790	-2.704000	0.172682	C	0.077617	0.486630	-1.501608
C	3.784748	-1.037721	0.577553	H	-0.427913	1.434432	-1.643837
O	3.594986	0.182788	0.483734	C	3.271720	-0.352705	-0.237702
N	4.961807	-1.643048	0.342368	H	3.496591	0.640443	-0.627736
H	5.006418	-2.645827	0.473471	C	4.444754	-1.241023	-0.331731
C	6.233613	-0.972292	-0.065235	C	5.562597	-0.809480	-1.075494
C	6.030408	-0.275736	-1.421284	C	4.488808	-2.507973	0.285160
H	5.735286	-0.999832	-2.188921	C	6.701451	-1.603421	-1.172749
H	5.260928	0.496451	-1.347607	H	5.539647	0.161272	-1.565741
H	6.966027	0.195044	-1.739554	C	5.624743	-3.303499	0.181612
C	6.656768	0.036026	1.015782	H	3.636033	-2.870425	0.852187
H	6.796164	-0.465517	1.979395	C	6.733981	-2.852980	-0.545585
H	7.606492	0.502112	0.733964	H	7.561671	-1.251806	-1.733561
H	5.904873	0.819751	1.132861	H	5.653266	-4.273606	0.668015
C	7.282995	-2.085523	-0.194224	H	7.619613	-3.476140	-0.623503
H	7.437832	-2.599957	0.761677	C	2.476895	-0.278044	1.057574
H	6.990585	-2.823595	-0.950984	H	1.402549	-0.225684	0.866830
H	8.241521	-1.657156	-0.499863	H	2.656748	-1.164656	1.668584
				C	2.843019	0.997543	1.847163
TS8B				H	2.460091	0.898918	2.869185
C	-3.033296	1.711150	-0.276945	H	3.929129	1.122561	1.918295
C	-4.245025	0.963828	-0.309101	C	2.141820	2.201735	1.212261
C	-4.581351	0.143566	0.821350	O	0.918493	2.151035	1.014746
C	-3.658994	-0.055941	1.849572	N	2.924673	3.238283	0.856776
C	-2.359425	0.570242	1.812036	H	3.897381	3.197338	1.132595
C	-2.103311	1.521028	0.767329	C	2.467772	4.521897	0.247076
Ru	-2.461470	-0.505123	-0.098328	C	1.812087	4.228240	-1.113766
H	-5.525199	-0.392494	0.823321	H	2.521418	3.726439	-1.783073

H	0.931061	3.594616	-0.985949	C	-0.917552	-5.239932	0.498444
H	1.504384	5.164933	-1.588837	H	0.940608	-4.516294	-0.316835
C	1.483192	5.228954	1.193370	H	-2.909428	-5.624083	1.270616
H	1.957165	5.437294	2.158157	H	-0.570709	-6.263369	0.600837
H	1.168679	6.182129	0.756310	N	-1.797042	-2.619975	0.229016
H	0.597295	4.613092	1.364434	H	-3.614293	-3.244301	1.004119
C	3.726806	5.378428	0.051399	C	0.237782	-1.809286	-0.678186
H	4.214554	5.593680	1.009565	C	1.561125	-1.848133	-1.023601
H	4.448650	4.882651	-0.608852	C	-0.530878	-0.592176	-0.827341
H	3.458576	6.335293	-0.404872	H	2.154766	-2.751127	-0.915615
C	1.371658	0.340669	-1.944526	C	0.085604	0.536065	-1.429496
H	1.878603	1.170869	-2.428976	H	-0.493389	1.434212	-1.607773
C	2.111191	-0.871251	-1.695488	C	3.368483	-0.182126	-0.265019
H	2.916576	-1.092545	-2.390348	H	3.673969	0.806073	-0.624036
C	-1.351810	0.345285	2.903805	C	4.567445	-1.093817	-0.326621
H	-1.626860	0.944925	3.781210	C	5.680011	-0.702692	-1.089124
H	-1.324937	-0.704428	3.211123	C	4.602842	-2.337372	0.326851
H	-0.360328	0.662939	2.572872	C	6.805576	-1.520465	-1.182312
C	-5.215976	1.075781	-1.466952	H	5.671007	0.255950	-1.603843
C	-4.531549	1.135436	-2.841988	C	5.725919	-3.158024	0.232076
C	-6.117884	2.310030	-1.229551	H	3.759278	-2.665605	0.929618
H	-5.851850	0.181752	-1.441855	C	6.830258	-2.751830	-0.522972
H	-3.852187	0.288294	-2.996625	H	7.662852	-1.195372	-1.763728
H	-5.291038	1.103386	-3.628407	H	5.743955	-4.111296	0.751777
H	-3.964523	2.062756	-2.978822	H	7.705270	-3.390475	-0.594113
H	-6.641950	2.253229	-0.269949	C	2.692110	-0.035132	1.119268
H	-5.528817	3.233797	-1.246530	H	1.607850	-0.155071	1.050356
H	-6.868312	2.370296	-2.023788	H	3.055564	-0.817665	1.788408
				C	2.953024	1.338530	1.759832
INT8B				H	2.705447	1.287636	2.826901
C	-3.096725	1.557859	-0.205262	H	4.013253	1.607460	1.690536
C	-4.271949	0.753436	-0.245270	C	2.035160	2.397944	1.147311
C	-4.546090	-0.123293	0.857779	O	0.817946	2.169607	1.055492
C	-3.595919	-0.314486	1.862800	N	2.624492	3.528199	0.711923
C	-2.330278	0.378670	1.829458	H	3.613607	3.630289	0.899692
C	-2.143263	1.381316	0.818029	C	1.934991	4.734917	0.169068
Ru	-2.403848	-0.644187	-0.117364	C	1.190359	4.358228	-1.123778
H	-5.463737	-0.703112	0.857700	H	1.888716	3.959887	-1.869385
H	-1.203675	1.927889	0.803859	H	0.420250	3.610570	-0.918472
H	-2.902663	2.266196	-1.002493	H	0.712498	5.245741	-1.550274
H	-3.772280	-1.044950	2.647635	C	0.964016	5.298101	1.220242
C	-0.526402	-2.949142	-0.141064	H	1.501838	5.575742	2.132572
C	-2.618106	-3.568853	0.726321	H	0.472394	6.194792	0.829368
C	-0.067587	-4.259349	-0.012083	H	0.198743	4.561752	1.476871
C	-2.216983	-4.890965	0.872123	C	3.036317	5.759220	-0.140919

H	3.585855	6.038163	0.765980	H	-5.370267	1.412946	1.255511
H	3.748146	5.370301	-0.878882	H	-5.429381	3.167570	1.483096
H	2.593004	6.670664	-0.551386	H	-2.455006	2.187333	-2.145029
C	1.414705	0.514640	-1.747482	C	-2.168812	-1.928983	-1.381313
H	1.887065	1.402376	-2.160759	C	-4.097702	-0.916675	-0.546497
C	2.270189	-0.641190	-1.458373	C	-2.927079	-2.956742	-1.949151
H	2.945845	-0.850037	-2.295351	C	-4.908337	-1.911290	-1.093962
C	-1.296527	0.173480	2.900151	C	-4.314642	-2.944486	-1.817012
H	-1.590905	0.732855	3.797785	H	-2.438594	-3.756664	-2.493190
H	-1.212621	-0.881590	3.177181	H	-5.982464	-1.864019	-0.950562
H	-0.327067	0.552417	2.568002	H	-4.916995	-3.729458	-2.262820
C	-5.255881	0.861055	-1.392509	N	-2.764988	-0.907193	-0.697101
C	-4.578987	0.800247	-2.773185	H	-4.522388	-0.108682	0.032806
C	-6.079768	2.158218	-1.221921	C	-0.712622	-1.834043	-1.394257
H	-5.941875	0.008828	-1.313648	C	0.134612	-2.909026	-1.809389
H	-3.975559	-0.108659	-2.892066	C	-0.194952	-0.623475	-0.863672
H	-5.344105	0.795342	-3.554916	C	1.448991	-2.877447	-1.450166
H	-3.934597	1.667547	-2.953186	H	-0.275293	-3.777664	-2.313375
H	-6.588375	2.193077	-0.253168	C	1.178311	-0.523448	-0.739405
H	-5.440838	3.044273	-1.308735	H	2.095057	-3.732994	-1.625096
H	-6.840227	2.210814	-2.007080	H	1.674298	0.382300	-0.418949
				C	1.928315	-2.154089	1.006770
TS8C				H	2.296124	-3.181935	0.954867
C	-1.194785	2.416034	1.494947	C	0.506822	-2.134843	1.499188
C	-0.225058	2.534442	0.468158	C	-0.293434	-3.270857	1.375041
C	-0.716804	2.401515	-0.863391	C	-0.093510	-0.959575	2.025833
C	-2.113855	2.283516	-1.118907	C	-1.652405	-3.266208	1.745757
C	-3.089127	2.437906	-0.065316	H	0.140598	-4.185749	0.981425
C	-2.604573	2.448106	1.247746	C	-1.451176	-0.941155	2.382042
Ru	-1.499741	0.578867	0.133207	H	0.513846	-0.086317	2.232436
H	-0.019576	2.380298	-1.695580	C	-2.234962	-2.109775	2.234588
H	-3.284642	2.471067	2.090316	H	-2.234133	-4.178099	1.654823
H	-0.852562	2.393618	2.526707	H	-1.856966	-0.090738	2.920766
C	1.230585	2.790909	0.774903	H	-3.277579	-2.101648	2.536880
H	1.843838	1.886379	0.822065	C	2.908172	-1.304465	1.825804
H	1.671356	3.425585	0.000351	H	2.562597	-0.271695	1.896810
H	1.330735	3.311842	1.731244	H	2.853033	-1.731494	2.835526
C	-4.552664	2.579935	-0.430493	C	4.373597	-1.281439	1.370598
H	-4.764629	1.837324	-1.212806	H	5.021819	-1.229147	2.253184
C	-4.758996	3.979852	-1.061188	H	4.650778	-2.211404	0.855026
H	-4.544320	4.768748	-0.332411	C	4.685914	-0.076302	0.462260
H	-4.117231	4.134096	-1.934525	O	3.778680	0.680126	0.079781
H	-5.799318	4.086919	-1.382632	N	5.977364	0.068982	0.125509
C	-5.523168	2.368773	0.738959	H	6.637707	-0.590862	0.517567
H	-6.553143	2.390031	0.372215	C	6.551124	1.140235	-0.745164

C	5.923690	1.049586	-2.146376	C	5.532555	1.090712	-1.700831
H	6.113337	0.067310	-2.593321	H	4.210901	2.738380	-2.118996
H	4.844922	1.217023	-2.099359	H	6.550953	-0.744360	-1.165820
H	6.365378	1.809936	-2.798297	H	6.427977	1.621947	-2.007186
C	6.289538	2.516343	-0.110669	N	3.225727	-0.270270	-0.918355
H	6.737968	2.574693	0.886772	H	4.437231	-1.882924	-0.482020
H	6.736656	3.299289	-0.731703	C	1.774031	1.552057	-1.379147
H	5.217261	2.707716	-0.026897	C	1.459202	2.856436	-1.852198
C	8.060136	0.867776	-0.820943	C	0.778019	0.654735	-0.883567
H	8.525013	0.916864	0.171057	C	0.168517	3.302187	-1.795013
H	8.267502	-0.115469	-1.260267	H	2.232156	3.501533	-2.255120
H	8.541345	1.621465	-1.450301	C	-0.521475	1.111755	-0.850008
C	1.987676	-1.723196	-0.729579	H	-0.078612	4.303932	-2.135736
H	3.052907	-1.554427	-0.876955	H	-1.336828	0.476667	-0.510000
				C	-1.600770	3.273504	0.034282
INT8C				H	-2.025944	4.163738	-0.442431
C	-0.554445	-2.206277	0.126667	C	-0.546804	3.708914	1.031817
C	-0.131088	-2.366661	-1.225079	C	-0.204249	5.064663	1.128023
C	1.180719	-2.910679	-1.442305	C	0.101904	2.787631	1.867972
C	1.954836	-3.460691	-0.364581	C	0.762184	5.493190	2.039895
C	1.555868	-3.278339	0.961001	H	-0.706584	5.794963	0.497406
C	0.323964	-2.553251	1.174834	C	1.068872	3.213744	2.779175
Ru	1.437924	-1.151704	-0.197988	H	-0.156505	1.732520	1.822605
H	1.553085	-2.989837	-2.459528	C	1.403656	4.567900	2.865310
H	0.035271	-2.306938	2.192268	H	1.005113	6.549102	2.110909
H	-1.505131	-1.725691	0.336599	H	1.550887	2.492480	3.433461
C	-1.015077	-1.977120	-2.374129	H	2.151181	4.900403	3.579202
H	-0.434177	-1.568268	-3.206001	C	-2.741300	2.465598	0.686163
H	-1.530787	-2.875116	-2.738489	H	-2.326188	1.600126	1.207753
H	-1.777786	-1.259595	-2.063552	H	-3.145273	3.121687	1.464942
C	2.396681	-3.742290	2.133909	C	-3.891704	1.997823	-0.237741
H	3.302221	-4.202966	1.719298	H	-4.815016	2.533395	0.003745
C	1.637581	-4.816544	2.938731	H	-3.684416	2.237877	-1.290227
H	0.728964	-4.405807	3.394396	C	-4.104485	0.478005	-0.184969
H	1.352073	-5.665049	2.308901	O	-3.123555	-0.291642	-0.168164
H	2.273285	-5.191594	3.746673	N	-5.377050	0.058533	-0.192937
C	2.830422	-2.567002	3.030485	H	-6.098511	0.767910	-0.182850
H	3.478308	-2.931200	3.833507	C	-5.852901	-1.358298	-0.196608
H	3.388788	-1.812726	2.461811	C	-5.320306	-2.080198	-1.445602
H	1.971154	-2.077070	3.502545	H	-5.640833	-1.566028	-2.357992
H	2.902184	-3.943694	-0.585651	H	-4.228854	-2.127771	-1.432161
C	3.140191	1.020236	-1.374054	H	-5.713138	-3.101575	-1.474624
C	4.425177	-0.864669	-0.852424	C	-5.387073	-2.059052	1.090501
C	4.283942	1.716120	-1.767660	H	-5.771160	-1.540737	1.975296
C	5.604880	-0.218435	-1.235332	H	-5.762707	-3.087233	1.107612

H	-4.296031	-2.085638	1.145823	C	-3.915748	-2.177735	-0.316830
C	-7.386593	-1.291818	-0.239216	C	-2.282246	-0.481899	-0.955957
H	-7.787265	-0.769648	0.637816	C	-4.164637	-2.445465	-1.660242
H	-7.738650	-0.784404	-1.145157	H	-4.459621	-2.726894	0.445794
H	-7.801906	-2.303297	-0.241272	C	-2.513527	-0.781885	-2.297698
C	-0.902892	2.476877	-1.223933	C	-3.455290	-1.757457	-2.649445
H	-1.742624	2.418177	-1.938152	H	-4.902057	-3.192054	-1.936841
				H	-1.970148	-0.263200	-3.082616
TS9A-E				H	-3.636038	-1.975149	-3.698530
C	-0.992358	2.613463	-2.032190	C	0.474110	-1.218242	-0.816389
C	-2.361854	2.466599	-1.707451	H	0.417815	-1.072175	-1.893095
C	-2.707880	2.557864	-0.323439	C	0.006346	-2.463300	-0.329547
C	-1.774288	3.051216	0.640657	C	-0.589447	-3.367645	-1.254102
C	-0.437638	3.342267	0.298292	C	0.131066	-2.858284	1.033177
C	-0.053383	2.989566	-1.033614	C	-1.044409	-4.606993	-0.835948
Ru	-1.064031	1.044909	-0.244841	H	-0.692324	-3.071529	-2.292730
H	-3.727067	2.348184	-0.014653	C	-0.328673	-4.096896	1.441997
H	0.989249	3.074450	-1.321301	H	0.599654	-2.197732	1.753891
H	-0.656360	2.461173	-3.052517	C	-0.915582	-4.971926	0.511117
C	-3.412966	2.218414	-2.744221	H	-1.492855	-5.293107	-1.546664
H	-4.172073	1.516853	-2.390910	H	-0.221696	-4.402035	2.477862
H	-3.911201	3.174695	-2.953972	H	-1.263307	-5.947393	0.838992
H	-2.991931	1.848690	-3.681303	C	1.235803	-0.231800	-0.060389
C	0.507833	3.979982	1.297832	H	1.568491	-0.609522	0.913603
H	0.041643	3.878184	2.286419	H	0.602240	0.677690	0.341297
C	0.613258	5.489400	0.977327	C	2.464899	0.348590	-0.781046
H	1.076119	5.649487	-0.003421	H	2.411586	0.199711	-1.864964
H	-0.368911	5.972655	0.976725	H	2.549412	1.423188	-0.601849
H	1.235322	5.984313	1.729245	C	3.723731	-0.311885	-0.153931
C	1.898386	3.331026	1.360119	O	3.652212	-0.761774	0.991202
H	2.487415	3.800569	2.153166	N	4.824914	-0.298472	-0.922049
H	1.845249	2.258155	1.579162	H	4.753268	0.103386	-1.847873
H	2.456365	3.472971	0.427533	C	6.182516	-0.782186	-0.512216
H	-2.105912	3.178652	1.667240	C	6.666353	0.023496	0.704379
C	-2.558439	-0.918918	1.413480	H	6.710892	1.092798	0.469392
C	-1.065933	0.360565	2.711251	H	6.002390	-0.125408	1.559043
C	-3.011138	-1.566043	2.571166	H	7.671855	-0.304448	0.986153
C	-1.469643	-0.261207	3.882530	C	6.112678	-2.283465	-0.189192
C	-2.471419	-1.236584	3.807992	H	5.764764	-2.851605	-1.058962
H	-3.776852	-2.328791	2.493203	H	7.109644	-2.647336	0.078959
H	-1.016231	0.018734	4.826818	H	5.439027	-2.469783	0.650223
H	-2.821315	-1.734563	4.706901	C	7.101521	-0.536605	-1.716886
N	-1.599447	0.046333	1.510901	H	6.762953	-1.094294	-2.598595
H	-0.302506	1.131048	2.712268	H	7.154378	0.529675	-1.969004
C	-2.967895	-1.204948	0.042594	H	8.115402	-0.871553	-1.481717

INT9A-E

C	-1.765391	-0.648090	-1.619403
C	-1.203027	0.230675	-2.582815
C	0.128197	-0.047953	-2.982547
C	0.761818	-1.272770	-2.624245
C	0.105119	-2.258830	-1.839364
C	-1.129761	-1.863149	-1.254296
Ru	0.368953	-0.126743	-0.655888
H	0.661896	0.657106	-3.612844
H	-1.636011	-2.489203	-0.530250
H	-2.731555	-0.429146	-1.182669
C	-1.943610	1.418974	-3.111385
H	-1.286907	2.285727	-3.225093
H	-2.341376	1.167786	-4.103938
H	-2.786068	1.691709	-2.473068
C	0.684468	-3.642836	-1.652264
H	1.711574	-3.624554	-2.037910
C	-0.139827	-4.618901	-2.527658
H	-1.173747	-4.686179	-2.170701
H	-0.155004	-4.311731	-3.578351
H	0.302609	-5.617834	-2.472769
C	0.726432	-4.104333	-0.188449
H	1.138761	-5.115889	-0.133603
H	1.363894	-3.445349	0.410272
H	-0.271073	-4.133882	0.263678
H	1.762896	-1.468253	-2.996964
C	2.377063	2.090375	-0.598227
C	3.415266	-0.001198	-0.865565
C	3.624335	2.723408	-0.680513
C	4.671257	0.578140	-0.956427
C	4.776294	1.969297	-0.866230
H	3.683070	3.802480	-0.600502
H	5.543810	-0.051817	-1.087685
H	5.744055	2.456249	-0.933557
N	2.293044	0.733041	-0.701408
H	3.289089	-1.075832	-0.907482
C	1.092431	2.746519	-0.393185
C	0.917067	4.134816	-0.265661
C	-0.023021	1.890455	-0.310270
C	-0.355993	4.661741	-0.065333
H	1.767981	4.806309	-0.325029
C	-1.295735	2.422434	-0.111169
C	-1.459957	3.808423	0.008866
H	-0.488159	5.734644	0.029664
H	-2.168907	1.781688	-0.053184
H	-2.455197	4.218576	0.155918
C	0.897410	0.151647	1.947455
H	0.852899	1.234552	2.050111
C	2.182107	-0.437503	2.283778
C	3.291783	0.420321	2.429423
C	2.352889	-1.821108	2.511341
C	4.542115	-0.089088	2.768376
H	3.165653	1.488435	2.272436
C	3.602223	-2.326661	2.848029
H	1.500165	-2.490404	2.462934
C	4.700410	-1.463041	2.972195
H	5.388005	0.580925	2.885644
H	3.723177	-3.388391	3.039124
H	5.672029	-1.862013	3.247628
C	-0.320232	-0.487335	1.693694
H	-0.355484	-1.573066	1.674342
H	1.284642	-1.195476	0.049771
C	-1.601662	0.152113	2.168178
H	-1.670755	-0.100112	3.239556
H	-1.553941	1.242563	2.118587
C	-2.869984	-0.413448	1.520458
O	-2.875148	-1.545836	1.030848
N	-3.935224	0.418861	1.539756
H	-3.832977	1.274917	2.071703
C	-5.341093	0.056142	1.172792
C	-5.394701	-0.345343	-0.310211
H	-5.009483	0.464275	-0.943887
H	-4.818939	-1.256767	-0.487146
H	-6.431109	-0.534682	-0.605672
C	-5.832179	-1.091951	2.069509
H	-5.802745	-0.799634	3.124548
H	-6.867020	-1.343147	1.816372
H	-5.216450	-1.984363	1.932833
C	-6.178850	1.321168	1.406104
H	-6.150423	1.630754	2.458003
H	-5.828415	2.153134	0.783028
H	-7.223930	1.127288	1.150126

TS9A-Z

C	2.806613	0.810567	-1.621510
C	3.567964	0.868170	-0.421886
C	3.743341	-0.358832	0.267282
C	3.396019	-1.607114	-0.335328
C	2.814517	-1.678568	-1.621742

C	2.439354	-0.431871	-2.200695	C	-0.521436	3.971542	-2.782308
Ru	1.447730	-0.347502	-0.057503	H	0.273517	2.064391	-3.349814
H	4.210212	-0.359554	1.247670	C	-1.983660	3.976297	-0.841551
H	1.907161	-0.425326	-3.145780	H	-2.338507	2.098070	0.109764
H	2.536015	1.730151	-2.130151	C	-1.347278	4.661536	-1.880872
C	4.122215	2.150704	0.117402	H	-0.049436	4.500156	-3.604484
H	4.073340	2.182992	1.208730	H	-2.646997	4.507564	-0.166516
H	5.178834	2.219640	-0.174436	H	-1.508912	5.728098	-2.006771
H	3.605282	3.023300	-0.285654	C	-1.058454	-0.542376	-0.598343
C	2.587132	-2.998563	-2.328377	H	-1.174953	-1.501829	-1.105869
H	2.786921	-3.795130	-1.600722	H	0.452958	-1.539614	-0.371288
C	3.619464	-3.127348	-3.473405	C	-1.857252	-0.450880	0.672906
H	3.453251	-2.363679	-4.242065	H	-1.678276	-1.355612	1.263815
H	4.646229	-3.029929	-3.106952	H	-1.577350	0.408714	1.277613
H	3.519868	-4.108365	-3.947026	C	-3.379198	-0.314369	0.371738
C	1.151446	-3.175480	-2.848886	O	-3.930745	0.765645	0.549034
H	1.053412	-4.149710	-3.336039	N	-3.970240	-1.426265	-0.117105
H	0.422696	-3.133317	-2.030789	H	-3.449977	-2.293073	-0.077704
H	0.885742	-2.415844	-3.592988	C	-5.417299	-1.545869	-0.482715
H	3.610300	-2.522298	0.208384	C	-6.288725	-1.298176	0.759655
C	0.769382	-0.427658	2.854079	H	-6.055189	-2.021023	1.549256
C	1.082429	-2.589856	1.982363	H	-6.134774	-0.288479	1.146975
C	0.532064	-0.972033	4.124052	H	-7.345498	-1.411022	0.497353
C	0.852497	-3.175954	3.216439	C	-5.739725	-0.536103	-1.595866
C	0.574604	-2.347087	4.310127	H	-5.107630	-0.712671	-2.473683
H	0.313323	-0.312942	4.955803	H	-6.784956	-0.647890	-1.900480
H	0.889321	-4.255167	3.315180	H	-5.588410	0.488608	-1.250064
H	0.390150	-2.772540	5.291528	C	-5.607275	-2.980824	-0.993983
N	1.048880	-1.249788	1.803756	H	-4.979370	-3.179056	-1.871238
H	1.295540	-3.188261	1.104634	H	-5.373751	-3.717790	-0.214933
C	0.738976	0.983389	2.500295	H	-6.649162	-3.133611	-1.288016
C	0.485695	2.024363	3.406783				
C	0.972210	1.273205	1.138221	**INT9A-Z**			
C	0.487014	3.346606	2.967712	C	-2.739642	-1.671833	0.539161
H	0.290677	1.810105	4.452888	C	-3.266089	-0.667905	1.400356
C	0.981001	2.598978	0.711022	C	-3.675639	0.539273	0.781824
C	0.738585	3.632669	1.625354	C	-3.747251	0.658633	-0.636475
H	0.295775	4.150061	3.671613	C	-3.415927	-0.420822	-1.497291
H	1.166772	2.853284	-0.326065	C	-2.833055	-1.557550	-0.869894
H	0.743941	4.661507	1.278202	Ru	-1.521748	0.268563	-0.116654
C	-0.696009	0.483415	-1.504126	H	-3.971880	1.383055	1.397589
H	-0.278209	0.089672	-2.428315	H	-2.480694	-2.379107	-1.481138
C	-0.952211	1.897622	-1.562580	H	-2.298633	-2.569573	0.960491
C	-0.338869	2.606198	-2.631803	C	-3.343741	-0.847986	2.884602
C	-1.789216	2.609483	-0.669502	H	-3.126225	0.083334	3.413855

H	-4.366563	-1.152269	3.144667	H	1.542558	-5.716025	2.094303
H	-2.662310	-1.623465	3.238536	C	0.784297	-0.102935	-0.973454
C	-3.661842	-0.353759	-2.989042	H	0.651566	0.330724	-1.962489
H	-3.818028	0.701703	-3.245260	H	-1.161549	0.651623	-1.598564
C	-4.973225	-1.118442	-3.293346	C	1.918801	0.558607	-0.240439
H	-4.870310	-2.183582	-3.056175	H	1.818276	1.646631	-0.305626
H	-5.819432	-0.718048	-2.725997	H	1.954531	0.302166	0.819051
H	-5.206556	-1.031027	-4.358507	C	3.238326	0.066758	-0.904739
C	-2.495205	-0.887639	-3.834159	O	3.259438	-1.036881	-1.447586
H	-2.716201	-0.746136	-4.895679	N	4.286494	0.901698	-0.783526
H	-1.561079	-0.358585	-3.610500	H	4.139762	1.783832	-0.311304
H	-2.333154	-1.961092	-3.683674	C	5.680791	0.616782	-1.248790
H	-4.100358	1.592372	-1.063583	C	6.212454	-0.634994	-0.531717
C	-0.476293	2.786347	1.105848	H	6.211561	-0.489384	0.554607
C	-1.409144	3.190332	-1.013903	H	5.603846	-1.509025	-0.774781
C	-0.234495	4.157462	1.263833	H	7.241999	-0.831508	-0.847191
C	-1.187951	4.554341	-0.906486	C	5.680086	0.422565	-2.773686
C	-0.591848	5.047399	0.259132	H	5.294643	1.315795	-3.277600
H	0.229844	4.516952	2.174559	H	6.703055	0.249145	-3.122689
H	-1.475206	5.210495	-1.720549	H	5.067394	-0.436312	-3.056513
H	-0.407120	6.110418	0.377723	C	6.515364	1.847090	-0.866600
N	-1.068347	2.324167	-0.032764	H	6.140601	2.752504	-1.359497
H	-1.864963	2.763666	-1.898923	H	6.517502	2.007596	0.218678
C	-0.138256	1.738658	2.058976	H	7.552227	1.702863	-1.182109
C	0.506852	1.955024	3.287090				
C	-0.459328	0.427047	1.658839	**TS9B**			
C	0.830684	0.874425	4.104687	C	0.759515	1.369833	-1.637794
H	0.762589	2.960484	3.606786	C	-0.191806	0.862381	-2.581155
C	-0.133756	-0.649868	2.478884	C	-1.527003	1.356656	-2.480491
C	0.511935	-0.424507	3.701629	C	-1.875314	2.421907	-1.588938
H	1.329510	1.044692	5.053323	C	-0.939221	2.922115	-0.672678
H	-0.362984	-1.667390	2.187196	C	0.367409	2.308604	-0.667729
H	0.763335	-1.270017	4.335522	Ru	-1.028912	0.472534	-0.542601
C	0.427330	-1.462228	-0.941141	H	-2.287768	0.944866	-3.137475
H	-0.183031	-1.761271	-1.790824	H	1.099802	2.604243	0.075002
C	0.776755	-2.565241	-0.076231	H	1.772269	0.984088	-1.605137
C	0.047347	-3.769074	-0.248567	C	0.190457	-0.134823	-3.636484
C	1.816667	-2.548049	0.883713	H	-0.655697	-0.772308	-3.908099
C	0.305366	-4.887879	0.532233	H	0.512479	0.400724	-4.538293
H	-0.714481	-3.826248	-1.022656	H	1.017431	-0.769216	-3.309789
C	2.081284	-3.672968	1.654828	C	-1.307791	4.091095	0.225292
H	2.443192	-1.677222	0.995249	H	-2.336572	3.919536	0.570267
C	1.323884	-4.839114	1.492358	C	-1.308398	5.376239	-0.639547
H	-0.261021	-5.801529	0.382097	H	-0.305804	5.581212	-1.031053
H	2.894944	-3.651717	2.372917	H	-1.997285	5.296154	-1.486188

H	-1.615333	6.231644	-0.029957	C	3.776384	-0.442422	0.860959
C	-0.403888	4.283248	1.450547	O	3.297558	0.350816	0.031697
H	-0.789882	5.103406	2.062612	N	5.086056	-0.669126	1.023607
H	-0.353077	3.395160	2.088906	H	5.360682	-1.317803	1.750717
H	0.617189	4.554447	1.160634	C	6.199339	-0.042773	0.242842
H	-2.886494	2.817608	-1.599980	C	6.040896	-0.395746	-1.245009
C	-2.633368	-2.053413	-0.483868	H	6.047848	-1.481908	-1.388817
C	-4.002699	-0.159023	-0.313508	H	5.108732	0.010619	-1.644626
C	-3.756717	-2.884648	-0.388380	H	6.874630	0.027468	-1.813870
C	-5.152794	-0.936939	-0.221542	C	6.180888	1.479558	0.457200
C	-5.025517	-2.326565	-0.264388	H	6.293602	1.723118	1.519056
H	-3.635952	-3.961556	-0.408194	H	7.012683	1.937482	-0.087465
H	-6.120872	-0.457751	-0.124666	H	5.246788	1.912989	0.092204
H	-5.900765	-2.965149	-0.198337	C	7.498816	-0.644079	0.796807
N	-2.776959	-0.695759	-0.447391	H	7.623281	-0.413537	1.861653
H	-4.047208	0.922667	-0.278182	H	7.524868	-1.732340	0.663984
C	-1.249498	-2.502749	-0.628227	H	8.356389	-0.223771	0.264460
C	-0.897809	-3.817651	-0.930535				
C	-0.245027	-1.476275	-0.521612	**INT9B**			
C	0.441821	-4.153850	-1.169253	C	-3.642540	0.580668	0.846569
H	-1.655652	-4.588800	-1.029051	C	-3.552685	1.436032	-0.298085
C	1.090913	-1.850813	-0.812877	C	-3.257202	0.844438	-1.558527
C	1.429390	-3.168025	-1.131282	C	-3.105860	-0.565636	-1.681473
H	0.701942	-5.180501	-1.408076	C	-3.246891	-1.431469	-0.560288
H	1.869141	-1.098522	-0.770154	C	-3.486342	-0.809641	0.711411
H	2.462451	-3.421862	-1.351216	Ru	-1.645177	0.146550	-0.165837
C	0.220486	-1.320959	1.704359	H	-3.119122	1.478381	-2.428336
H	0.274881	-2.405552	1.761634	H	-3.478016	-1.429915	1.601050
C	-1.046499	-0.730432	2.100748	H	-3.779836	1.016728	1.830388
C	-2.124220	-1.564169	2.475474	C	-3.745410	2.912949	-0.158532
C	-1.219417	0.679470	2.151095	H	-3.360972	3.280907	0.795548
C	-3.324175	-1.011073	2.905249	H	-3.270789	3.466689	-0.970286
H	-2.000697	-2.642302	2.441837	H	-4.823742	3.121378	-0.188457
C	-2.439714	1.223048	2.562262	C	-3.252241	-2.939892	-0.685637
H	-0.373463	1.336355	1.987351	H	-3.072725	-3.345854	0.315417
C	-3.490479	0.381908	2.936205	C	-2.187526	-3.511684	-1.628840
H	-4.136866	-1.659786	3.216067	H	-2.318225	-3.169669	-2.661792
H	-2.554290	2.300965	2.619139	H	-1.179321	-3.250852	-1.291808
H	-4.430921	0.805982	3.274654	H	-2.261116	-4.602923	-1.645841
C	1.490357	-0.553635	1.921288	C	-4.677348	-3.358239	-1.123348
H	1.504825	0.332136	1.276350	H	-4.746924	-4.450162	-1.142304
H	1.411255	-0.168059	2.949331	H	-5.442251	-2.982050	-0.436074
C	2.831117	-1.282440	1.746915	H	-4.903853	-2.985988	-2.128850
H	3.286015	-1.497459	2.719010	H	-2.836012	-0.980116	-2.646864
H	2.694815	-2.249888	1.249424	C	0.588820	1.364463	-1.552572

C	0.366221	-0.799138	-2.406098	H	4.691089	-2.444052	-0.931085
C	1.611603	1.651250	-2.451093	H	6.357882	-2.322031	-1.539344
C	1.395984	-0.584045	-3.316268	C	5.287824	0.236563	-1.376163
C	2.023457	0.661406	-3.345720	H	5.331644	1.287043	-1.066281
H	2.087851	2.625426	-2.426658	H	5.929446	0.112893	-2.254864
H	1.696691	-1.384630	-3.982838	H	4.259823	-0.010156	-1.651435
H	2.829964	0.856771	-4.045098	C	7.207955	-0.307856	0.163053
N	-0.027930	0.158356	-1.548543	H	7.271318	0.739873	0.480843
H	-0.154960	-1.745831	-2.350425	H	7.570175	-0.946231	0.977655
C	0.095918	2.307631	-0.513377	H	7.882939	-0.441398	-0.686923
C	-0.337333	3.593543	-0.885922				
C	0.134696	1.928722	0.864473	**TS10A**			
C	-0.748385	4.503772	0.079446	C	1.791315	2.066169	-0.217412
H	-0.332717	3.870825	-1.936220	C	1.672010	1.958176	1.199693
C	-0.318140	2.871609	1.815699	C	2.028708	0.692386	1.790575
C	-0.750652	4.134702	1.435234	C	2.474353	-0.393506	1.010495
H	-1.060242	5.501952	-0.212628	C	2.483733	-0.303658	-0.403234
H	-0.254118	2.632183	2.871944	C	2.130724	0.960123	-0.998078
H	-1.057602	4.852041	2.190533	Ru	0.314690	0.255978	0.367034
C	0.862867	0.652052	1.283692	H	1.956983	0.585062	2.869212
H	1.373231	0.269842	0.404396	H	2.121049	1.046858	-2.079728
C	-0.105860	-0.450921	1.712058	H	1.549378	3.008207	-0.699778
C	-0.059452	-1.706279	1.052714	C	1.289002	3.122085	2.065314
C	-0.857586	-0.355752	2.918022	H	0.655516	2.810625	2.900589
C	-0.712898	-2.828635	1.602944	H	2.200033	3.565244	2.490147
H	0.636876	-1.831900	0.230722	H	0.773121	3.900530	1.497893
C	-1.483695	-1.467142	3.455199	C	2.844472	-1.482891	-1.277231
H	-0.897325	0.588757	3.449976	H	3.007156	-2.341500	-0.615650
C	-1.403912	-2.715040	2.800052	C	4.173078	-1.179207	-2.012009
H	-0.621289	-3.792279	1.111749	H	4.059122	-0.360400	-2.731188
H	-2.014466	-1.387073	4.399401	H	4.976258	-0.921672	-1.314584
H	-1.866314	-3.589259	3.249269	H	4.479490	-2.070760	-2.567945
C	1.999073	0.874604	2.309376	C	1.718656	-1.844949	-2.267327
H	2.570011	1.759039	2.000221	H	2.029934	-2.704001	-2.868818
H	1.598878	1.085746	3.307645	H	0.795329	-2.118594	-1.742950
C	2.946648	-0.345650	2.396072	H	1.500093	-1.024899	-2.960958
H	3.692724	-0.154853	3.174438	H	2.752188	-1.325657	1.491110
H	2.382037	-1.232772	2.705811	C	-2.508560	0.202232	-0.372011
C	3.599136	-0.672089	1.047280	C	-1.664194	2.356411	-0.760987
O	2.905116	-1.062139	0.090810	C	-3.753921	0.575142	-0.869682
N	4.927826	-0.470291	0.965304	C	-2.887527	2.789268	-1.265580
H	5.412197	-0.188543	1.807256	C	-3.946724	1.883808	-1.323252
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C	-2.153194	-1.125329	0.160642
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C	-2.909586	-2.282212	-0.029719
C	-0.545716	-2.437417	1.506159
H	-0.452431	0.241538	1.787528
C	-2.501218	-3.490222	0.550377
H	-3.818779	-2.256594	-0.621695
C	-1.323460	-3.572243	1.315201
H	0.345921	-2.478829	2.122894
H	-3.119013	-4.374278	0.423223
H	-1.033705	-4.515462	1.767479

INT11

C	3.000229	0.825810	0.093348
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C	4.475350	0.871094	-0.326089
H	5.069840	0.124875	0.214009
H	4.591794	0.712289	-1.404665
H	4.886891	1.855799	-0.090228
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H	1.120909	1.829894	-0.417211
H	2.560808	2.856202	-0.479048
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C	1.331357	-1.076162	-0.104551
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C	0.909587	-2.472746	-0.476545
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H	1.228805	-3.152240	0.325140
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H	-0.950331	-2.024252	-1.522936
H	-1.148560	-3.238700	-0.251963
C	-0.908910	-1.198096	0.483997
H	-0.932380	-1.574955	1.510101
C	-2.067756	-0.293489	0.214375
C	-3.077795	-0.157225	1.173380
C	-2.157348	0.414241	-0.994005
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H	-3.009383	-0.696060	2.115320
C	-3.247751	1.245190	-1.237891
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H	-3.310297	1.796124	-2.171402
H	-5.115318	2.009184	-0.476632
H	3.205669	-1.178092	-0.703287

TS12

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H	-4.089063	-0.258582	2.203978
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H	-3.701169	1.402755	-0.454548
H	-4.270281	0.117787	-1.524211
H	-5.117873	0.405805	0.011842
C	-3.760781	-2.031289	0.014304
H	-3.698245	-2.307508	-1.044243
H	-3.248624	-2.791947	0.609302
H	-4.816062	-2.053287	0.304012
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C	-0.852772	-1.206931	-0.397310
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H	-0.911204	-3.340414	-0.576884
C	0.898607	-2.550055	0.397652
H	1.118078	-2.125872	1.382131
H	1.371682	-3.532173	0.330394
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C	2.362625	0.510435	0.357469
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C	3.468301	1.256950	0.770480
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H	0.820900	3.871725	-0.307909	H	-4.005951	-4.085736	0.708023
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TS12-E

C	3.879650	0.275739	0.217328
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H	5.303626	-1.382919	0.171771
H	5.390080	-0.311114	-1.250782
H	6.043753	0.219348	0.307651
C	3.801892	1.731203	-0.274912
H	3.950127	1.779822	-1.359423
H	2.830517	2.168332	-0.033548
H	4.583895	2.327784	0.207473
N	2.841050	-0.537008	-0.472077
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C	0.599792	-1.365624	-1.076733
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H	0.414384	-2.177221	-0.353823
C	-0.726771	-0.641994	-1.292354
H	-0.765374	-0.062688	-2.218773
C	-1.013957	0.109560	-0.091887
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C	-1.728270	1.369547	-0.014648
C	-2.358740	1.712014	1.197846
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C	-3.068475	2.903606	1.316363
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C	-2.515517	3.454408	-0.980365
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C	-3.147181	3.775595	0.226998
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H	-2.574111	4.137881	-1.822581
H	-3.697907	4.707978	0.317761
H	3.158093	-1.349556	-0.984104
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C	-2.098583	-3.223903	0.158515

TS12-Z

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H	-4.172682	1.083514	-0.239368
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C	-2.204737	1.366478	1.700308
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H	0.804096	-2.683827	-0.885543
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H	1.762664	-1.964014	1.325558
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C	4.003638	-0.902752	1.119376
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C	3.797338	-1.103273	1.154178	C	0.822436	1.464729	0.766691
H	4.665083	-0.479381	1.392342	H	0.336006	0.527142	1.023421
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C	1.073540	1.006049	1.187325	C	-2.250638	0.475016	1.063507
H	1.333355	0.035426	1.610858	C	-2.825764	0.147784	-1.256065
H	1.163030	1.752660	1.988535	C	-3.073658	-0.594723	1.417043
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H	-0.621164	1.906040	0.130163	C	-3.646508	-0.922451	-0.904499
C	-1.189608	-0.024966	0.802060	H	-2.730840	0.436903	-2.300145
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C	-2.573432	-0.109092	0.310898	H	-3.180732	-0.867307	2.463784
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C	-3.204611	0.929496	-0.400536	H	-4.410127	-2.135736	0.710544
C	-4.624933	-1.416920	0.109083				
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H	-2.665269	1.849217	-0.606655				
C	-5.234861	-0.378011	-0.595113				
H	-5.171610	-2.334139	0.312186				
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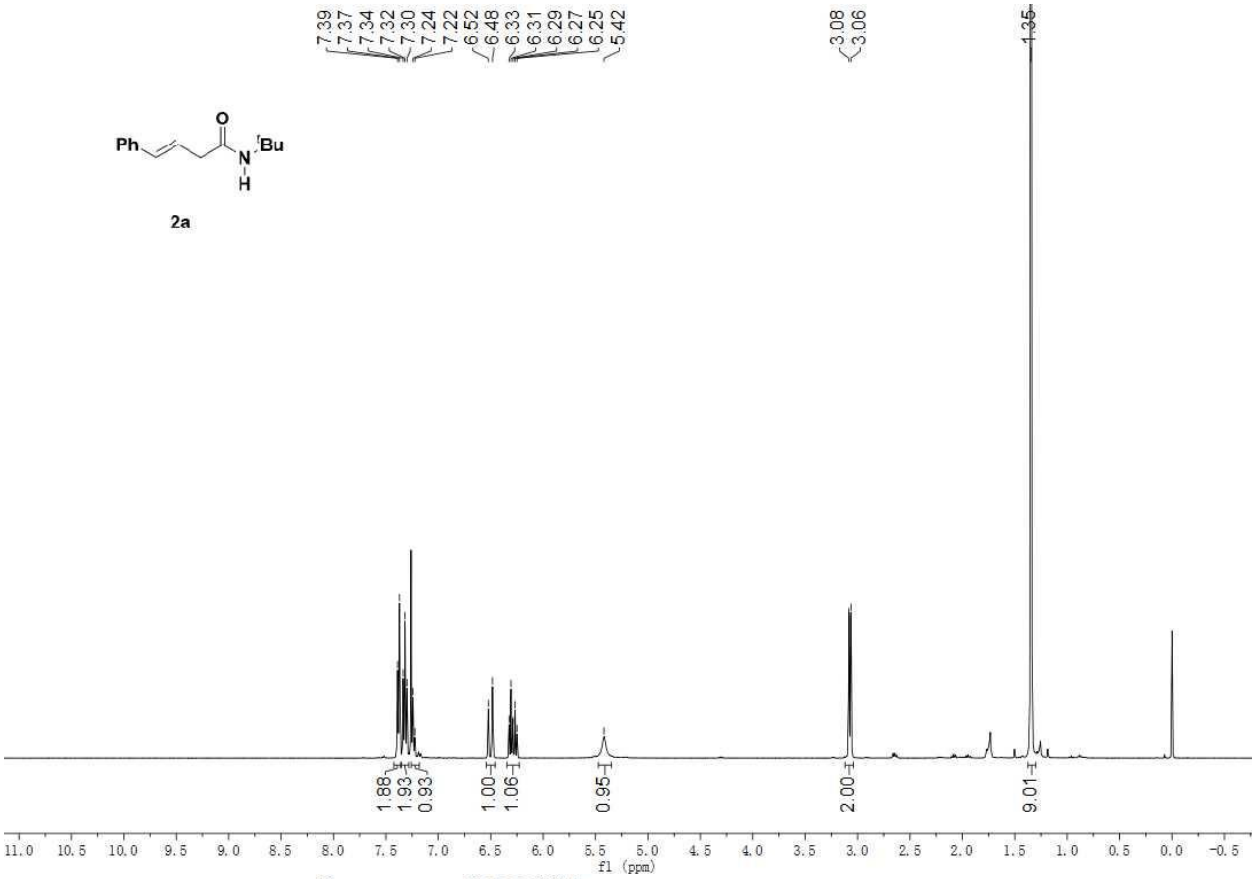
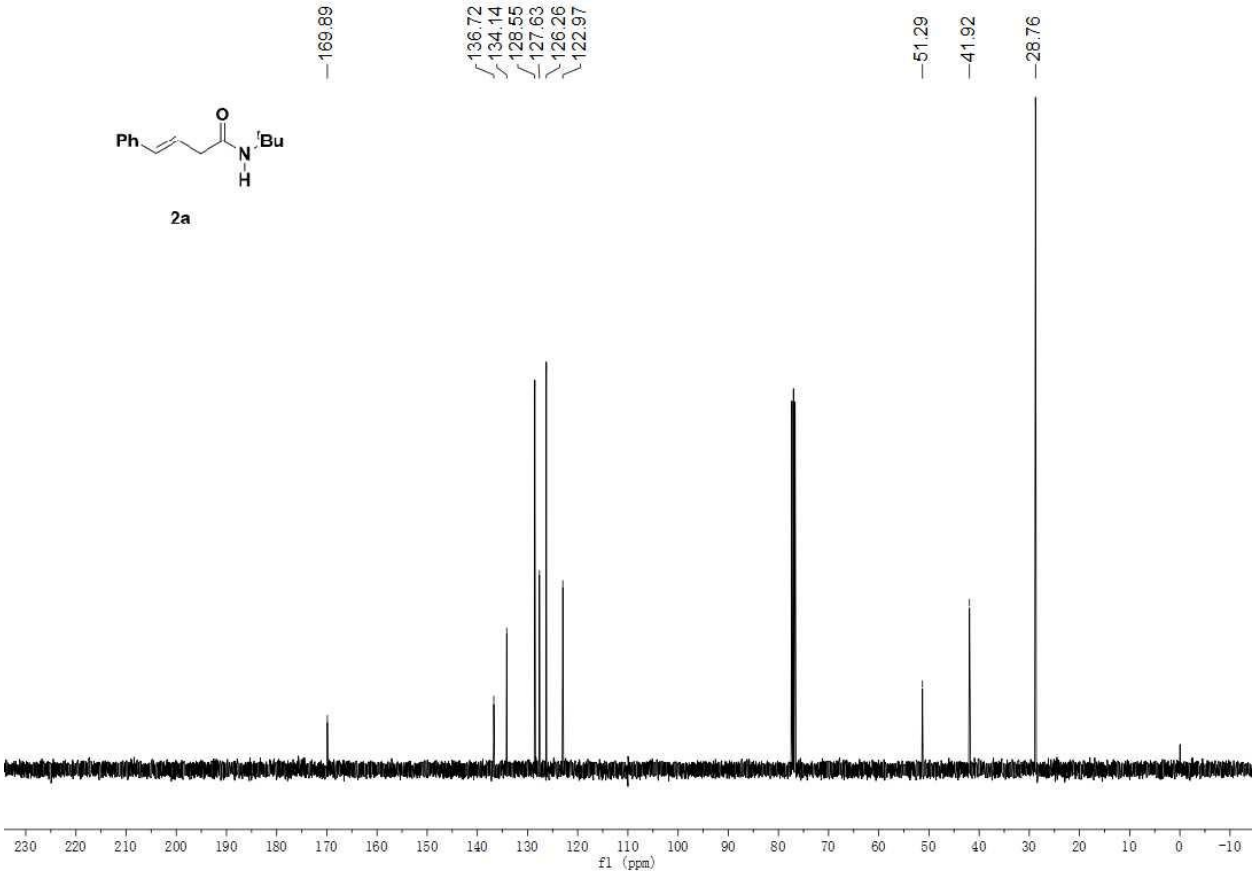
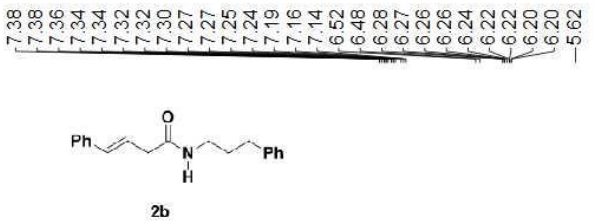
***Z*-2a**

8. NMR Spectra



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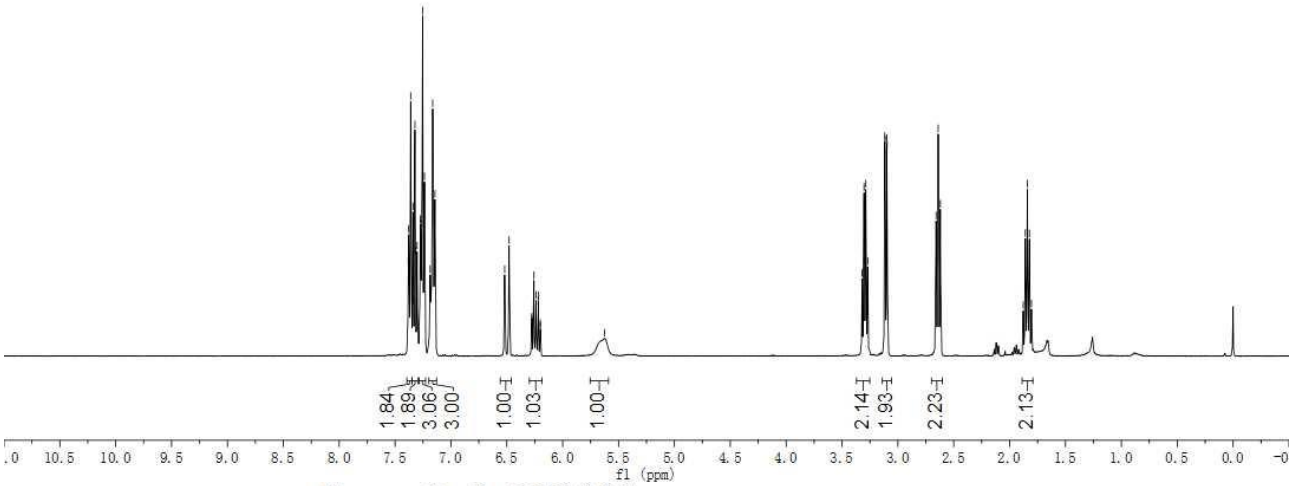
N
H
Ph

2b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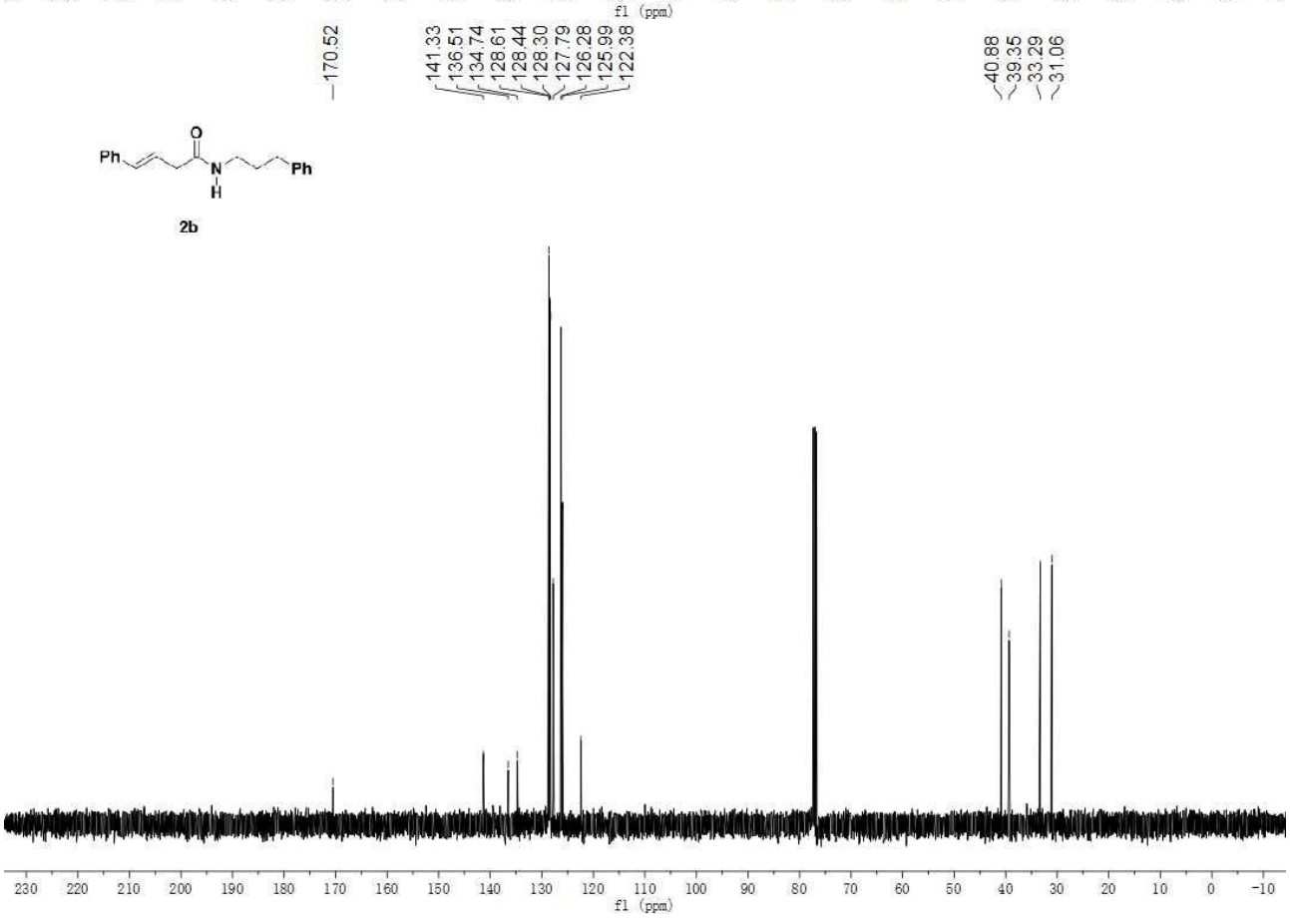
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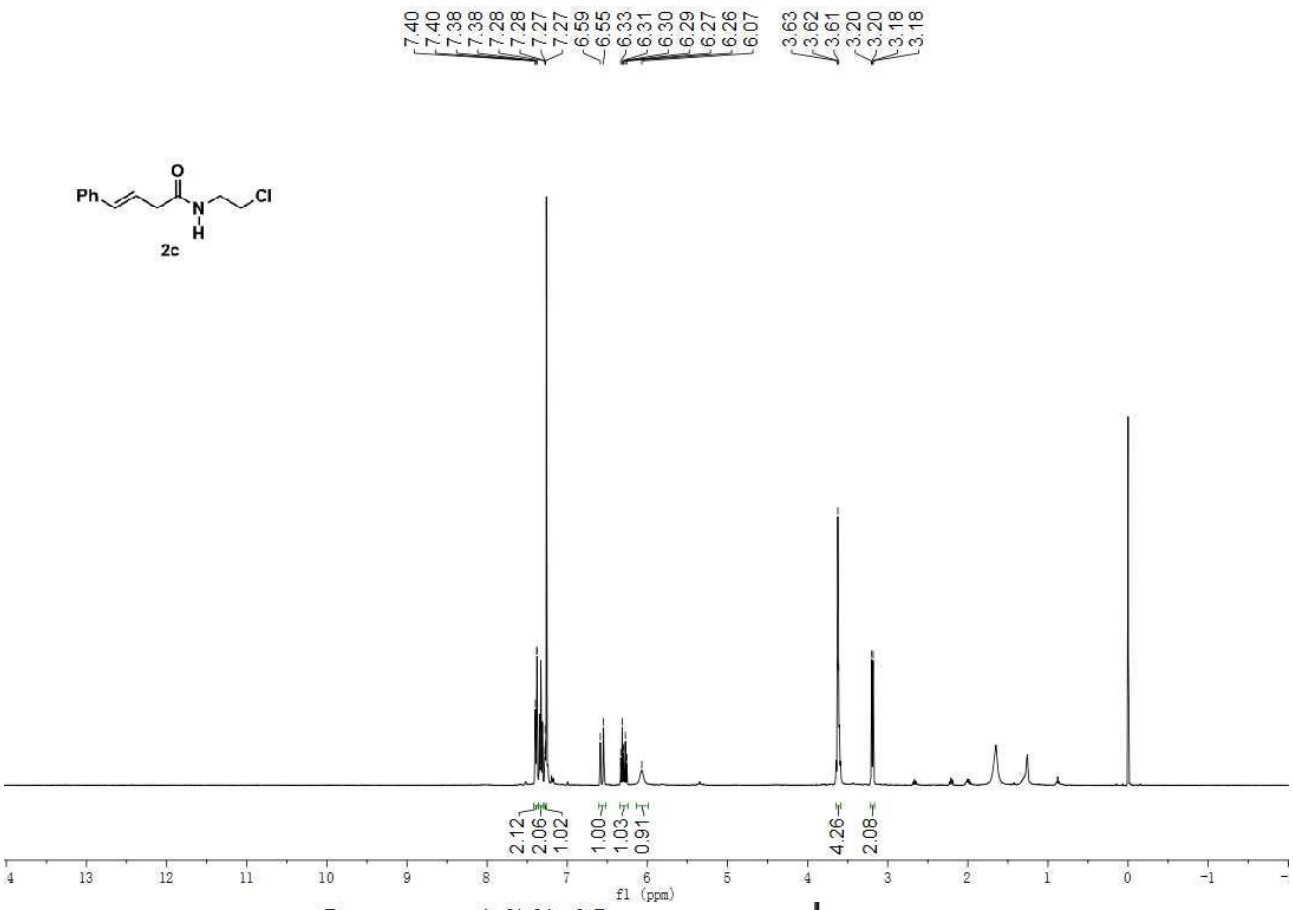
Ph
O
N
H
Ph
f1 (ppm)

2b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3.18
Ph
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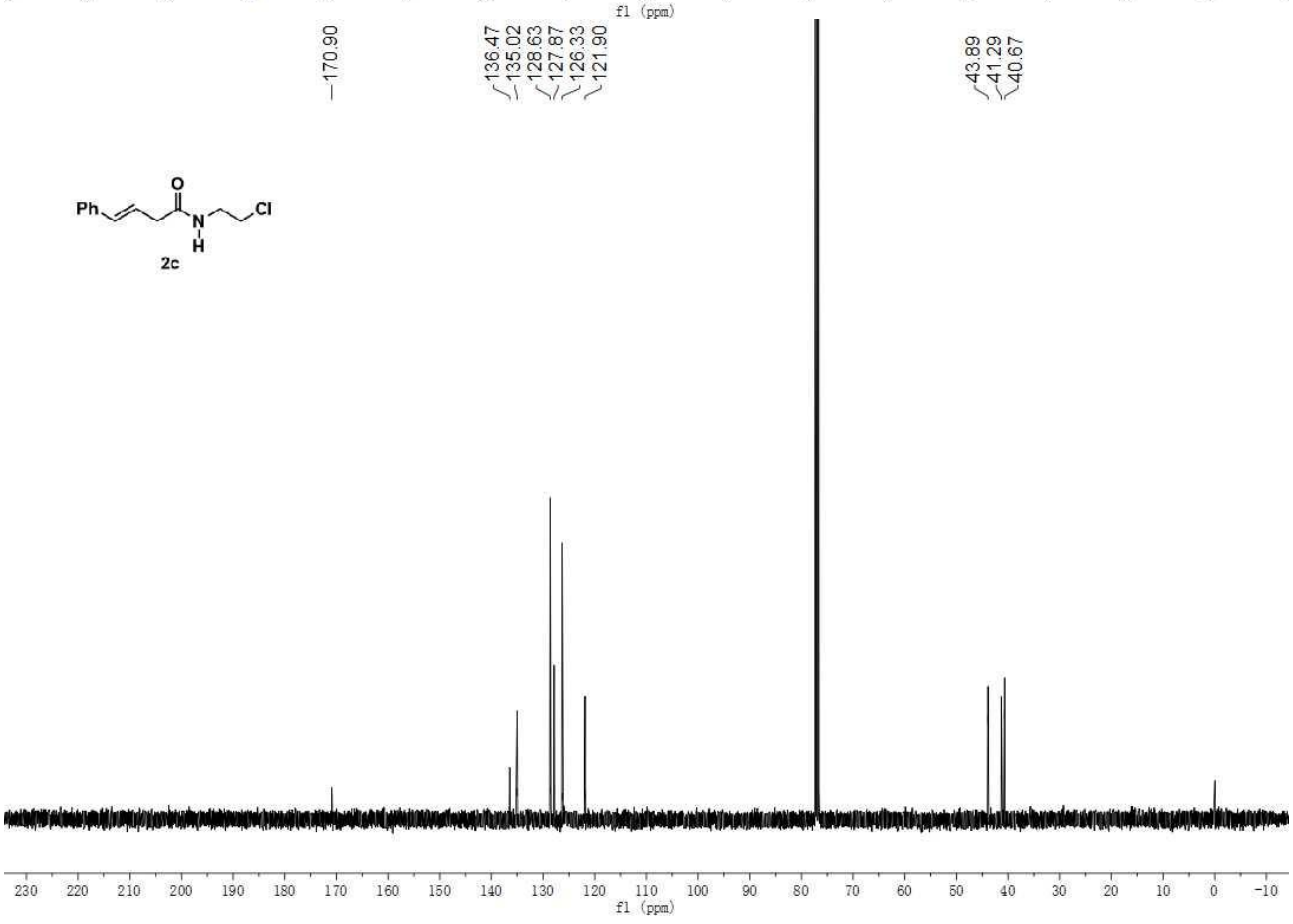
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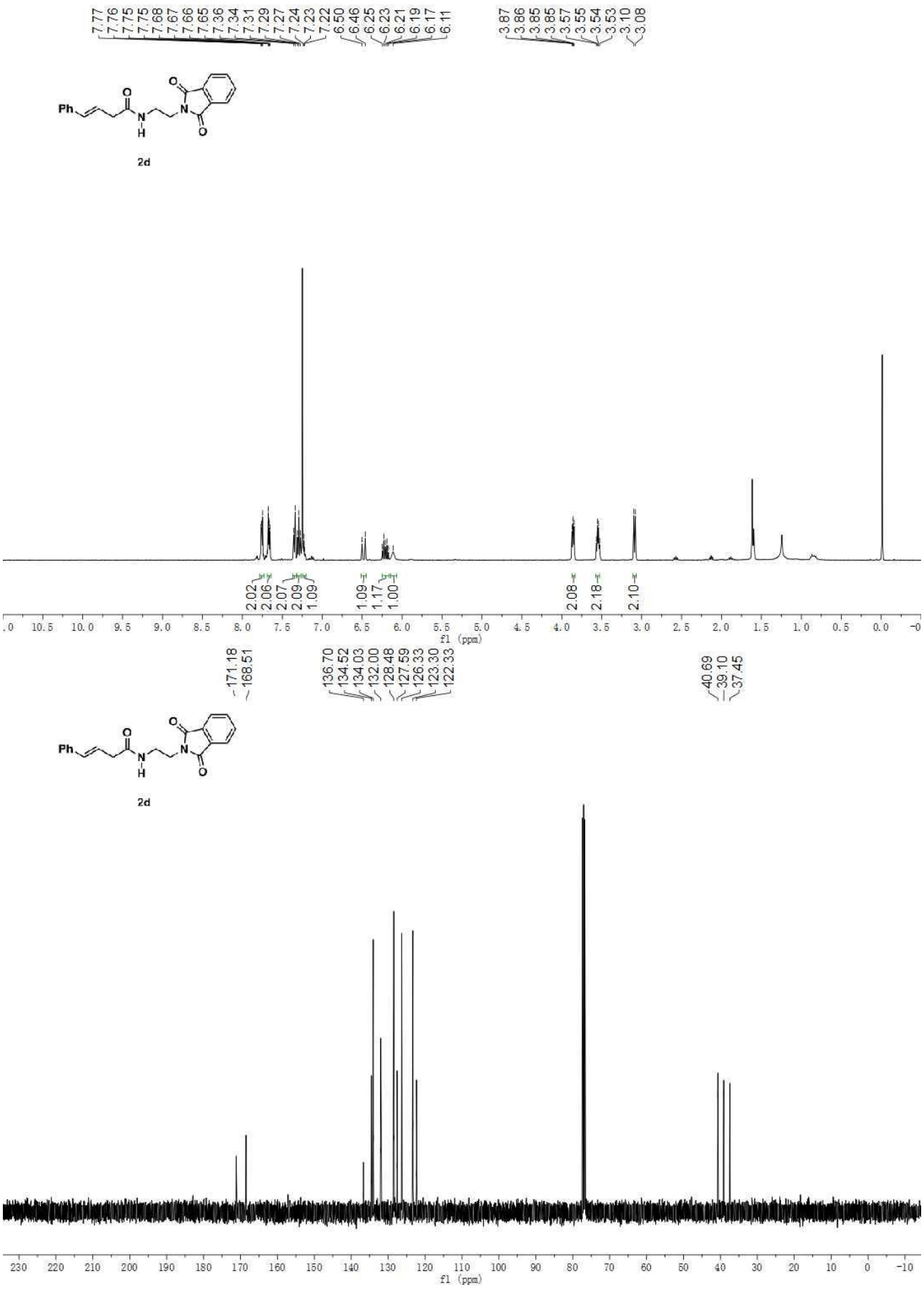
Cl
2c
f1 (ppm)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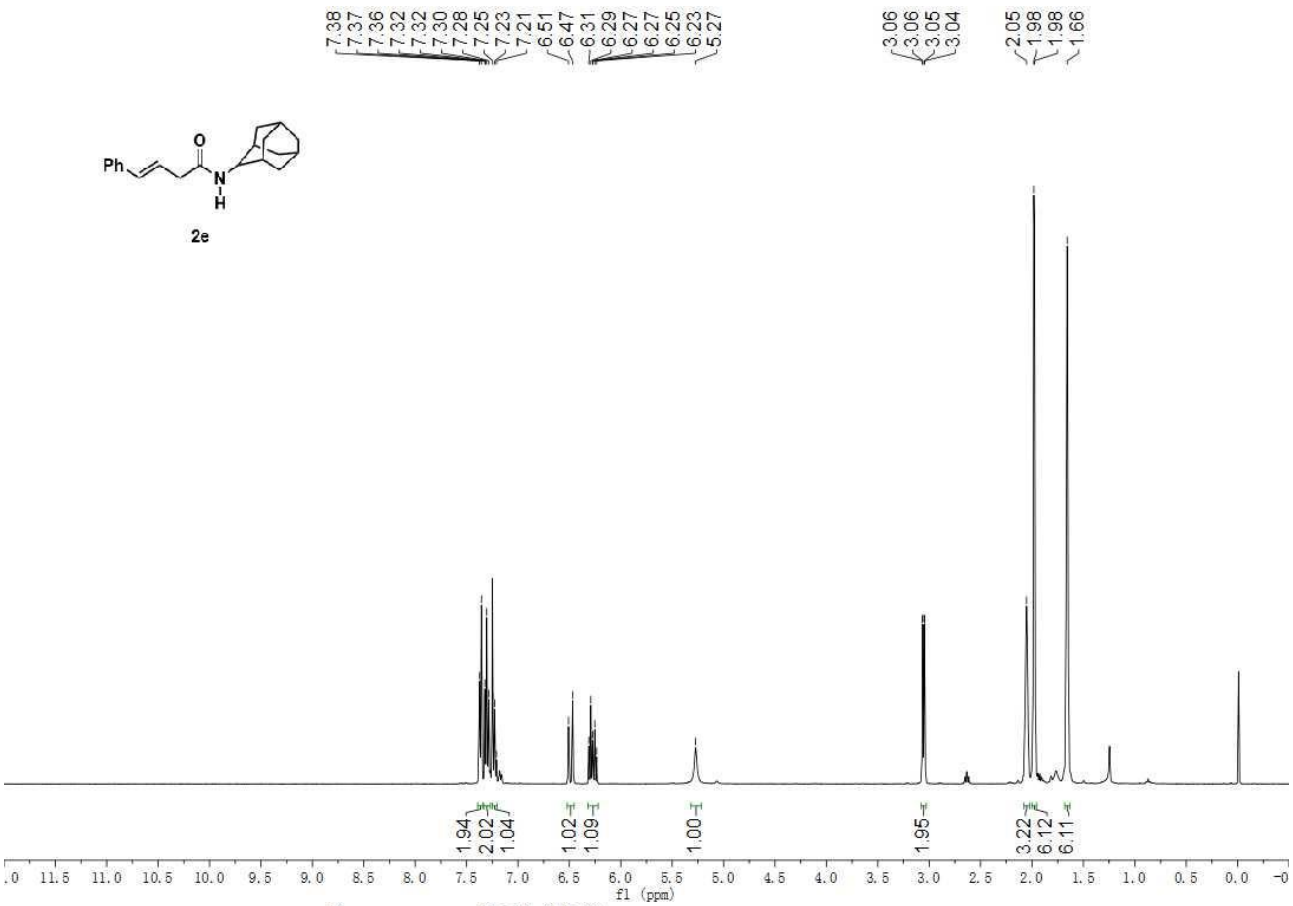
f1 (ppm)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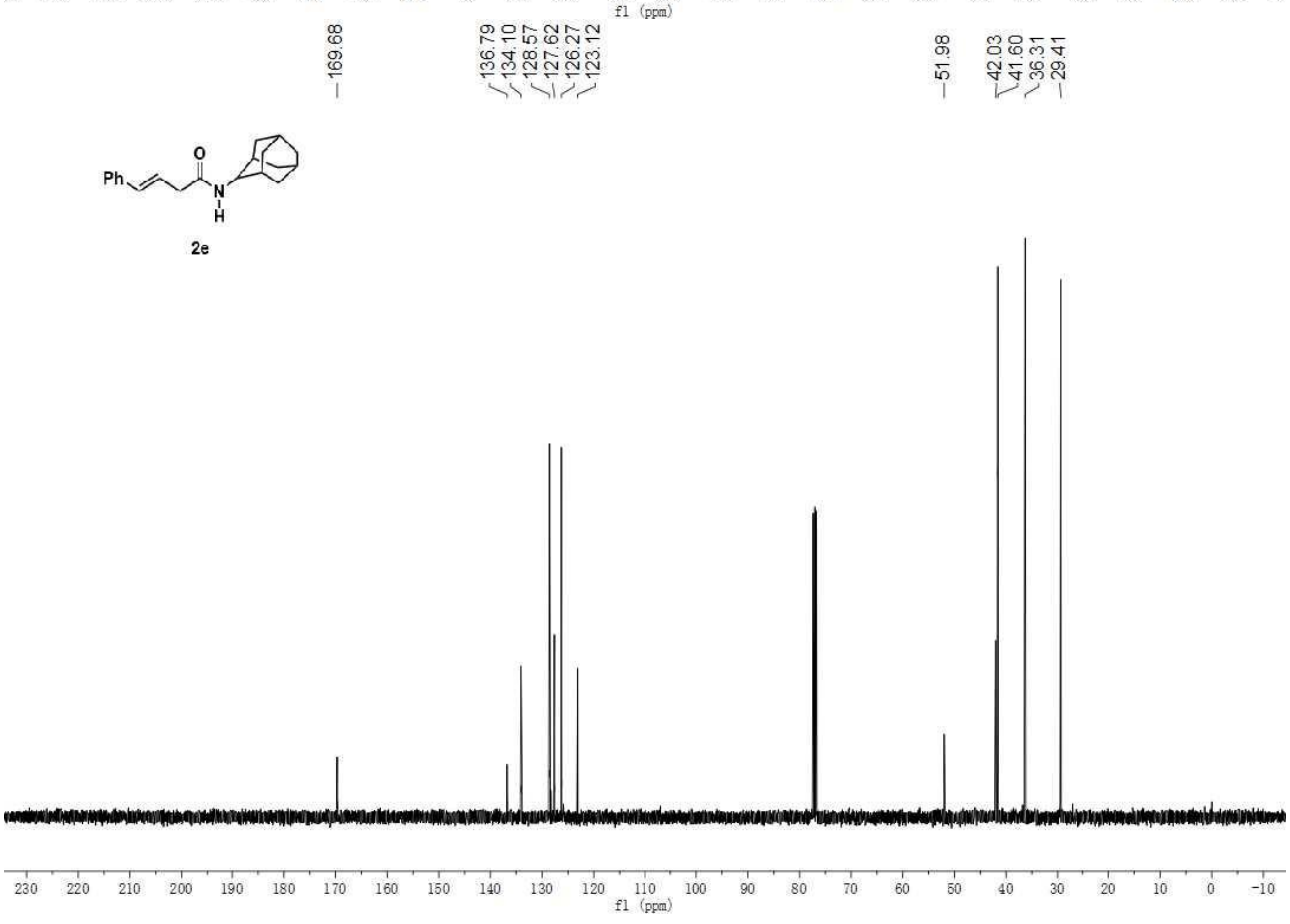
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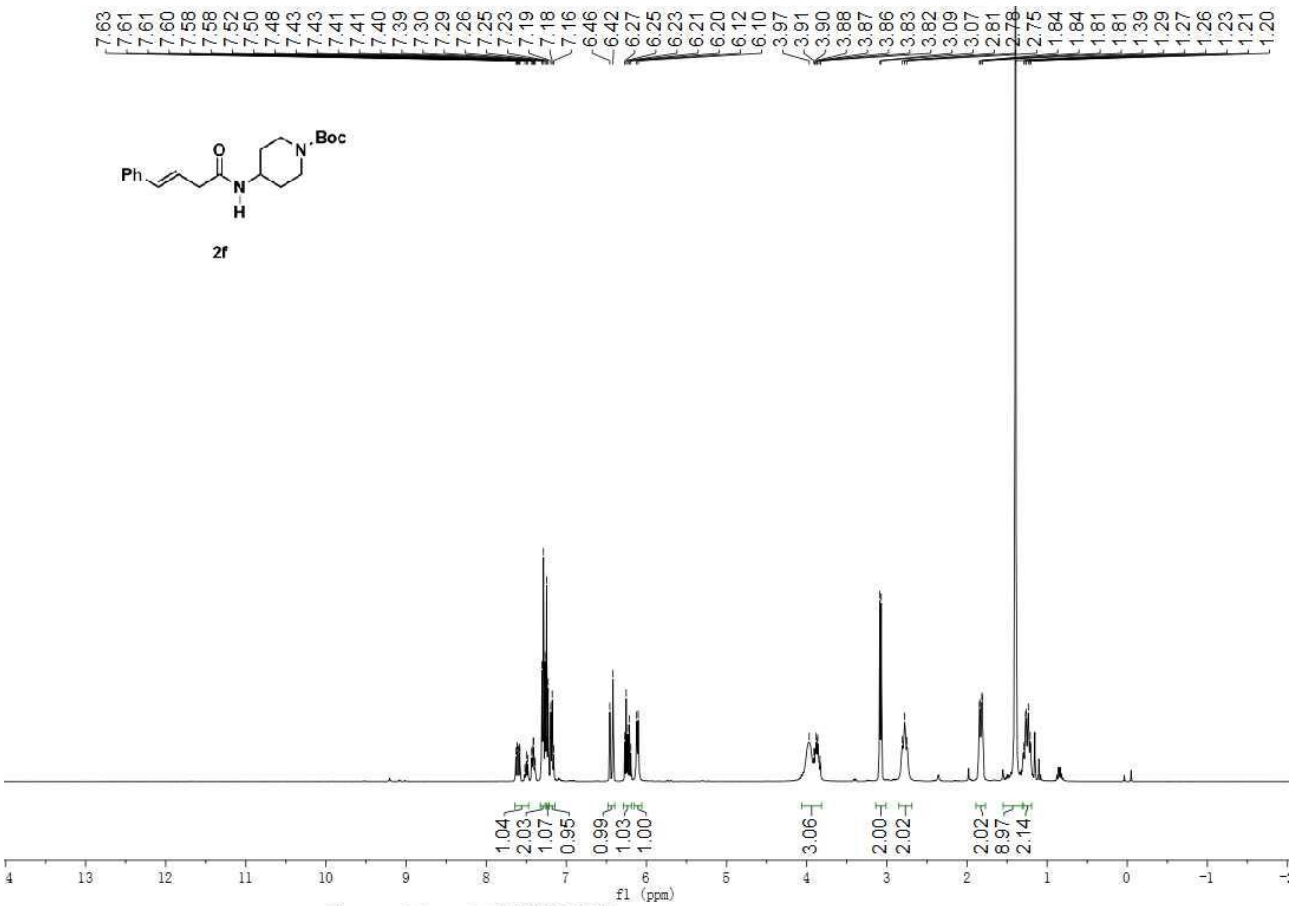
f1 (ppm)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Ph
O
N
H
N
Boc
2f
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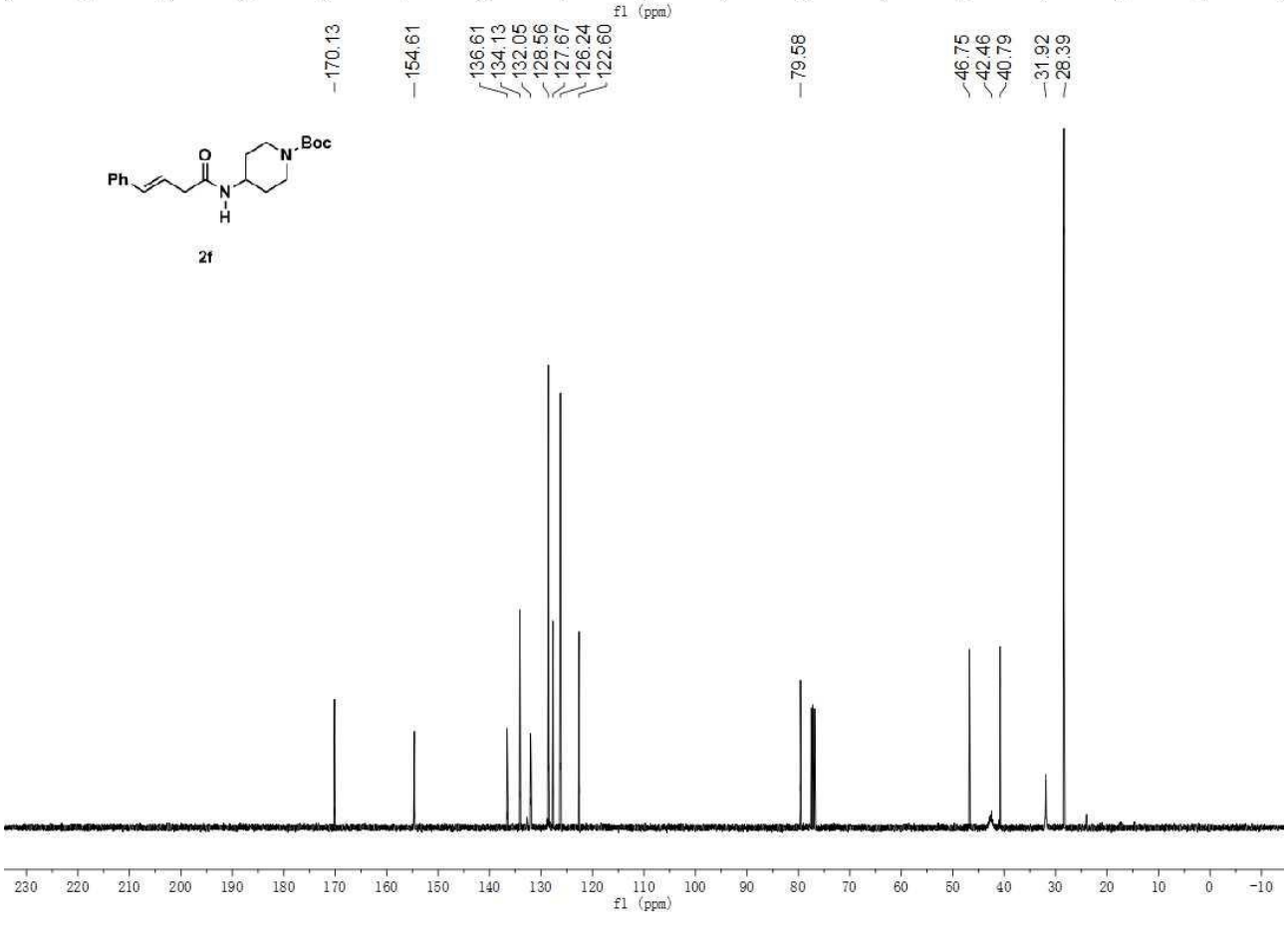
f1 (ppm)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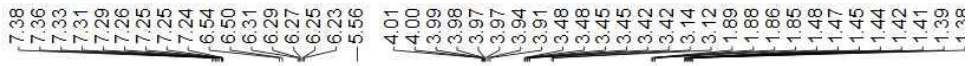
Ph
O
N
H
N
Boc
2f
f1 (ppm)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6.29
6.27
6.25
6.23
5.56
4.01
4.00
3.99
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3.97
3.97
3.94
3.91
3.48
3.48
3.45
3.45
3.42
3.42
3.14
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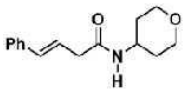
1.39


Ph
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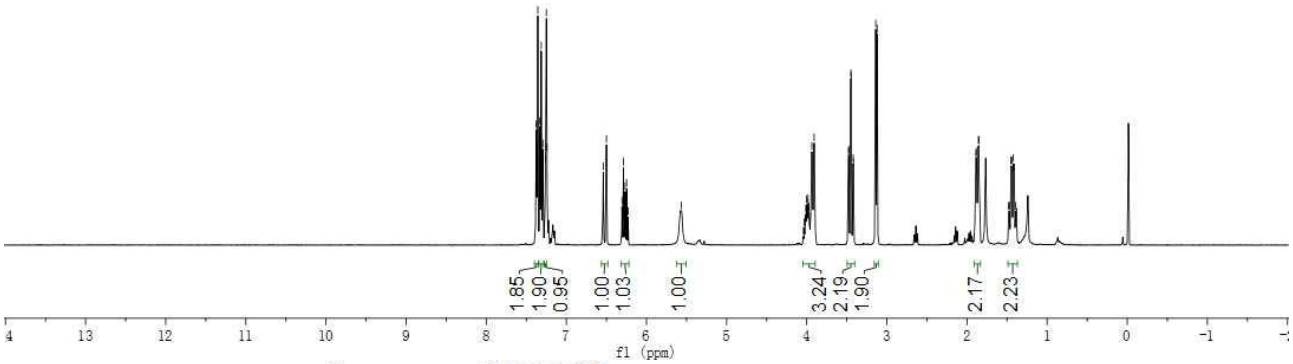
N
H
O

2g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1.00
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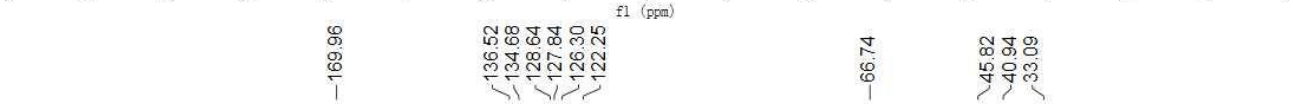
2.19
1.90
2.17
2.23
f1 (ppm)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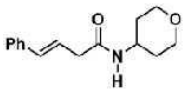
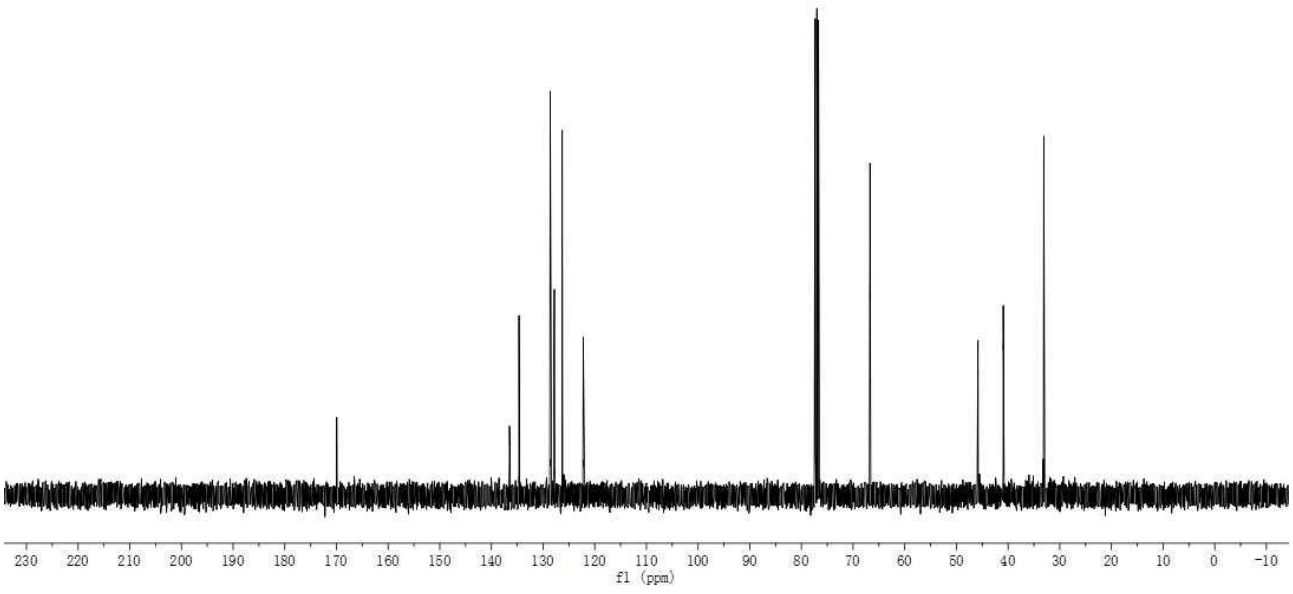
45.82
40.94
33.09


Ph
O
N
H
O

2g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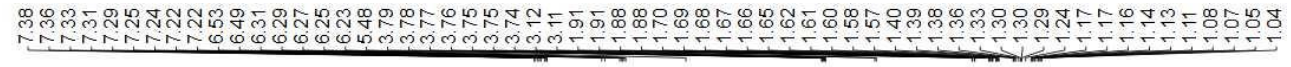
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6.29
6.27
6.25
6.23
5.48
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3.78
3.77
3.76
3.75
3.75
3.74
3.12
3.11
1.91
1.91
1.88
1.88
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1.67
1.66
1.65
1.62
1.61
1.60
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1.39
1.38
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1.30
1.30
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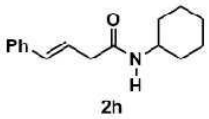
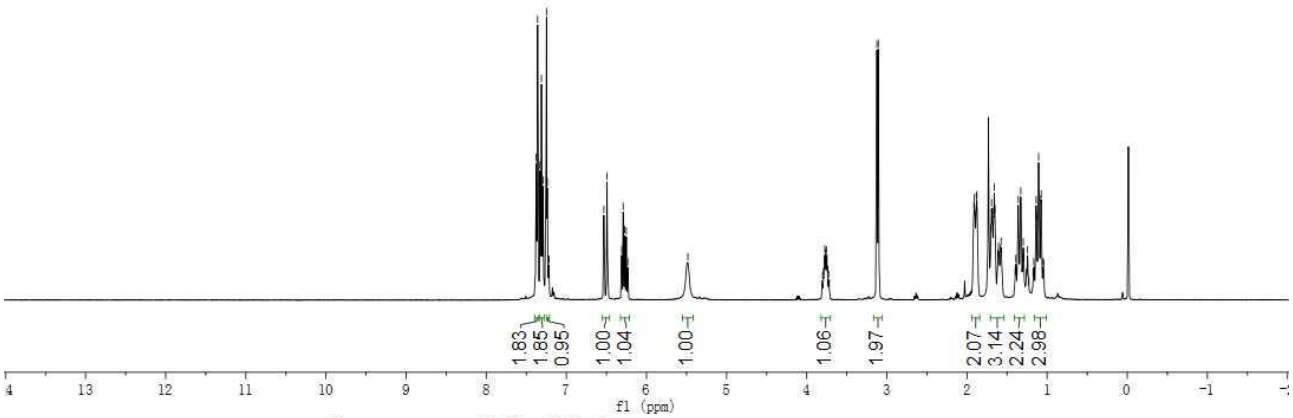
1.05
1.04


Ph
O
N
H

2h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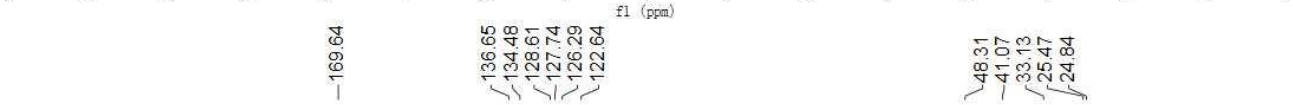
1.97
2.07
3.14
2.24
2.98
f1 (ppm)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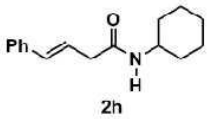
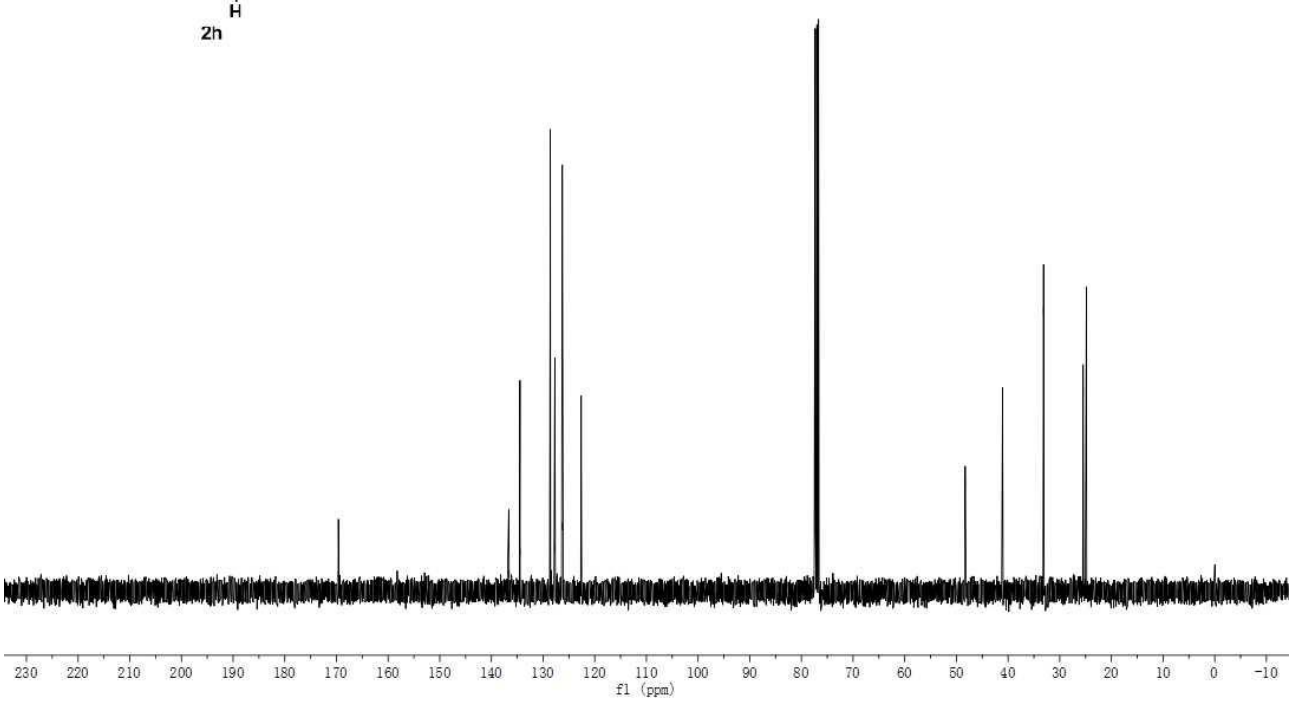
41.07
33.13
25.47
24.84


Ph
O
N
H

2h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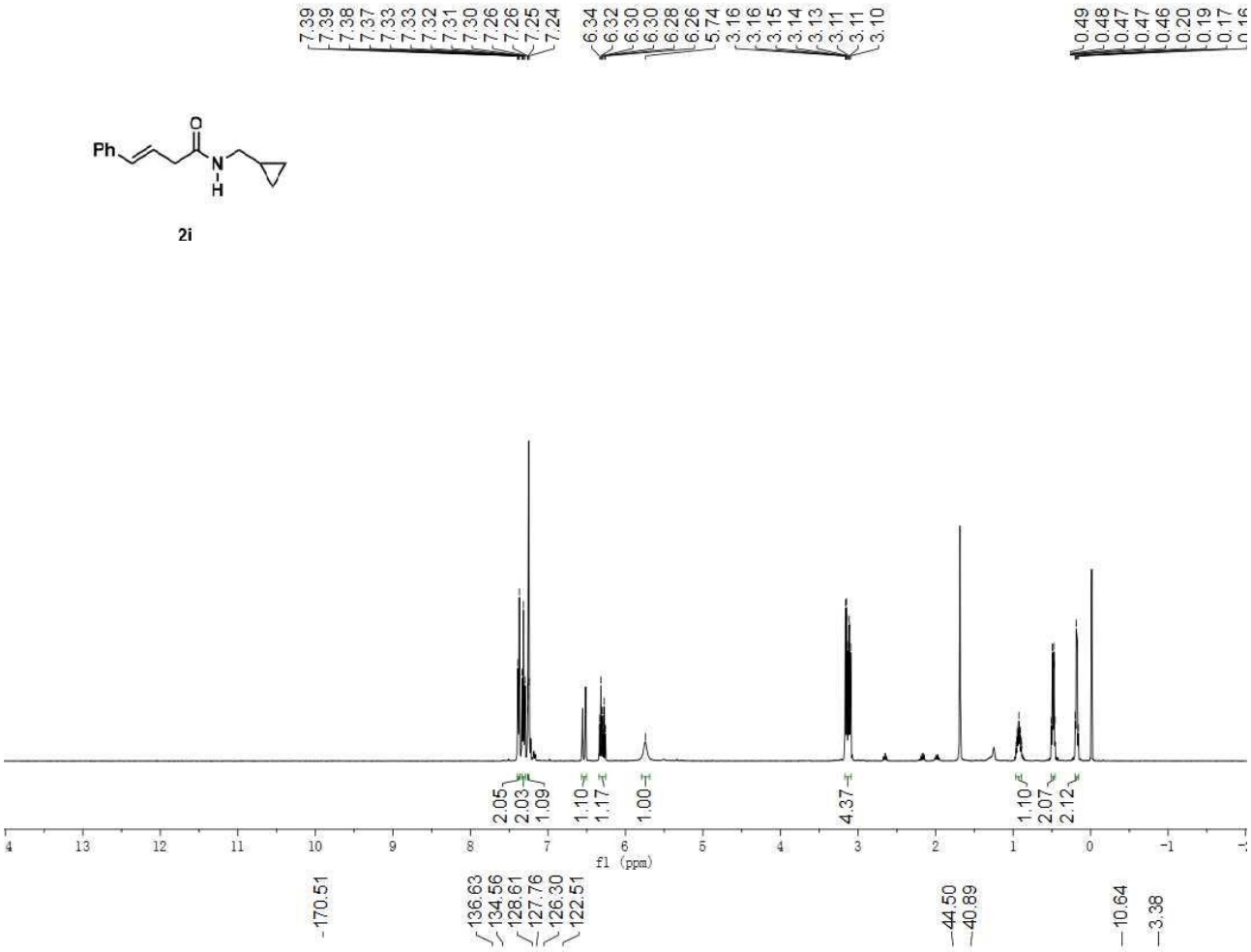
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7.24
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6.26
5.74
3.16
3.15
3.14
3.13
3.11
3.11
3.10
0.49
0.48
0.47
0.47
0.46
0.20
0.19
0.17
Ph
O
N
H
2i
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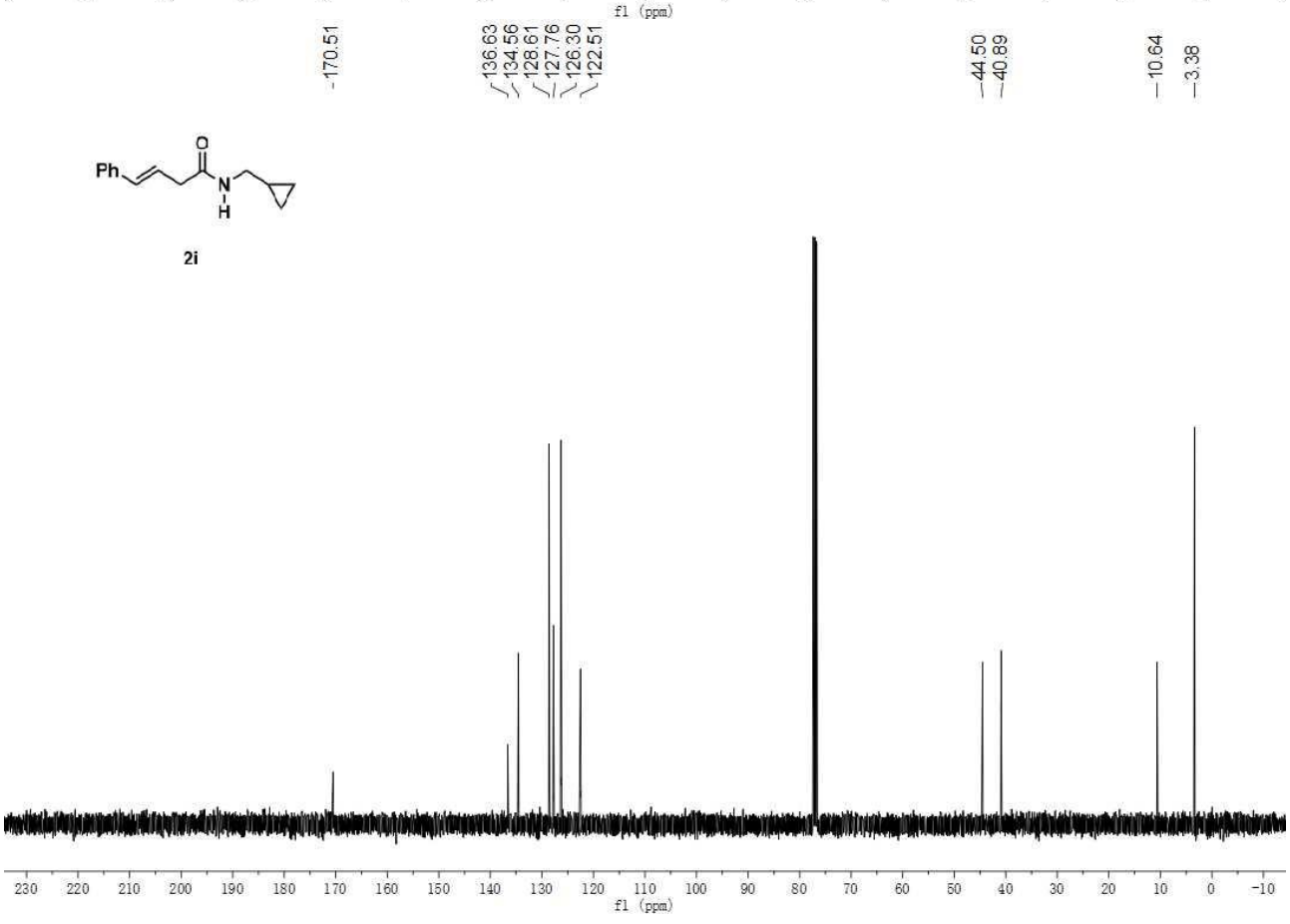
1.09
1.10
1.17
1.00
4.37
1.10
2.07
2.12
f1 (ppm)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Ph
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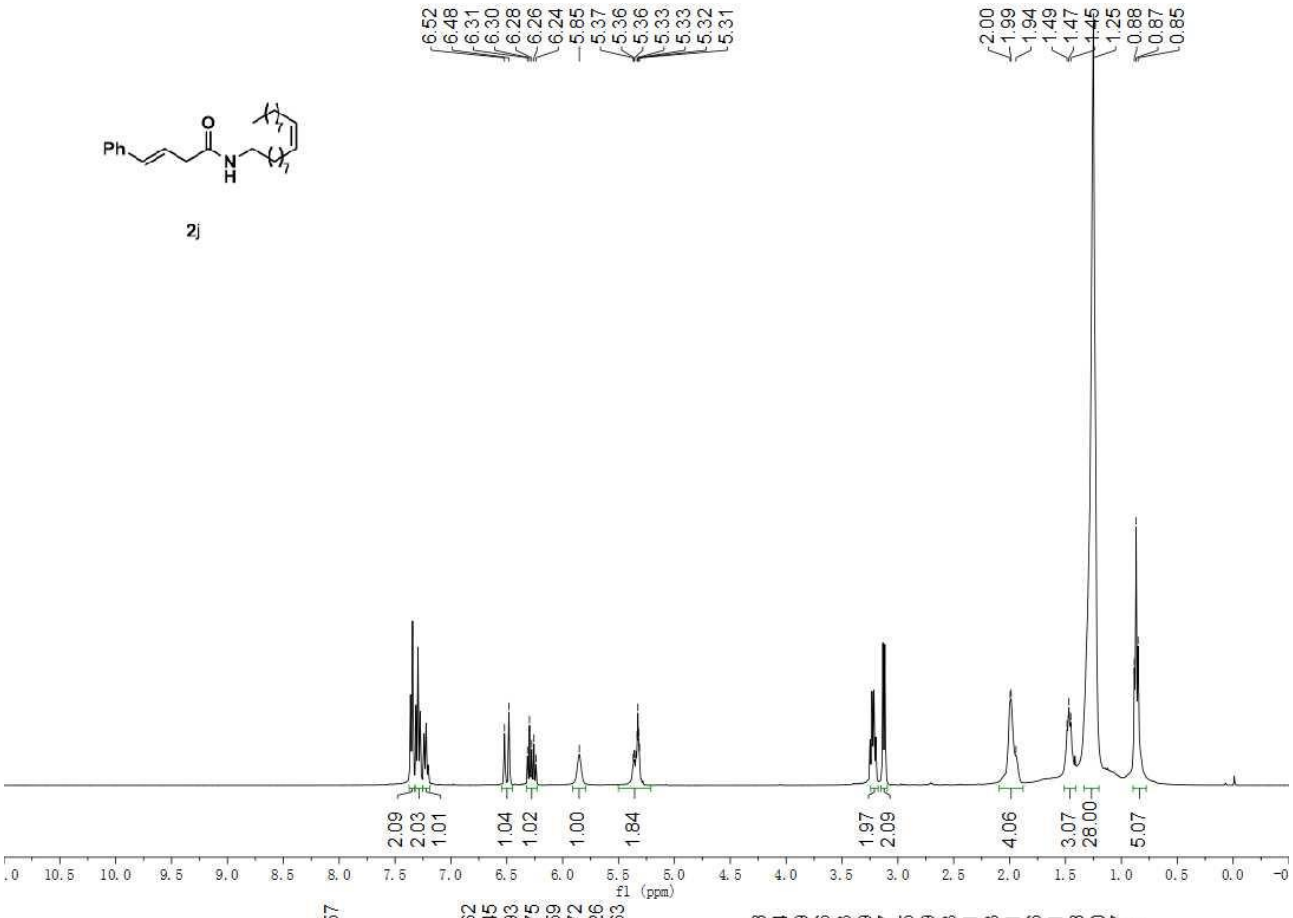
N
H
2i
f1 (ppm)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5.32
5.31
2.00
1.99
1.94
1.49
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1.45
1.25
0.88
0.87
0.85
Ph
O
N
H
2j
2.09
2.03
1.01
1.04
1.02
1.00
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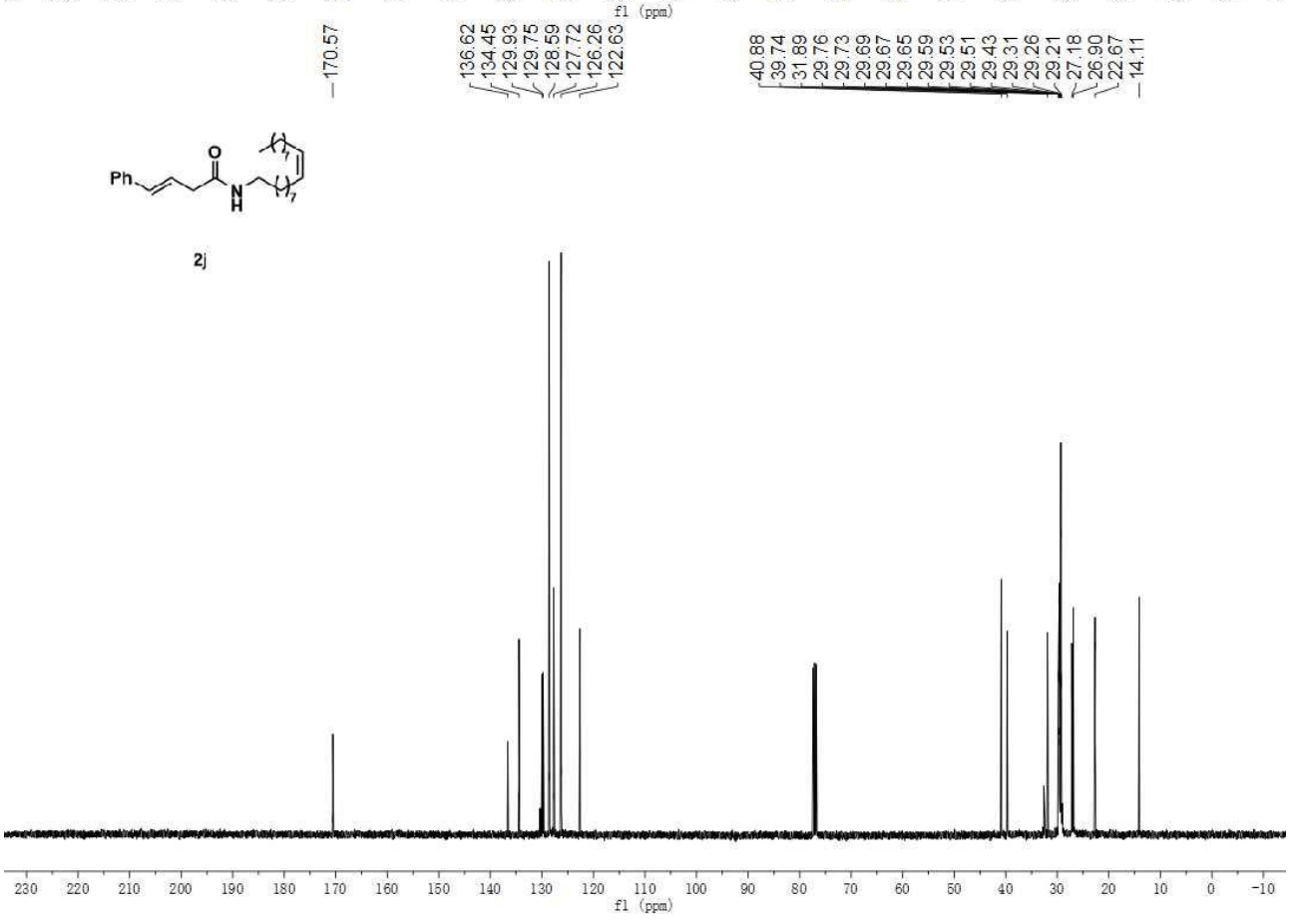
1.97
2.09
4.06
3.07
28.00
5.07
f1 (ppm)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29.69
29.67
29.65
29.59
29.53
29.51
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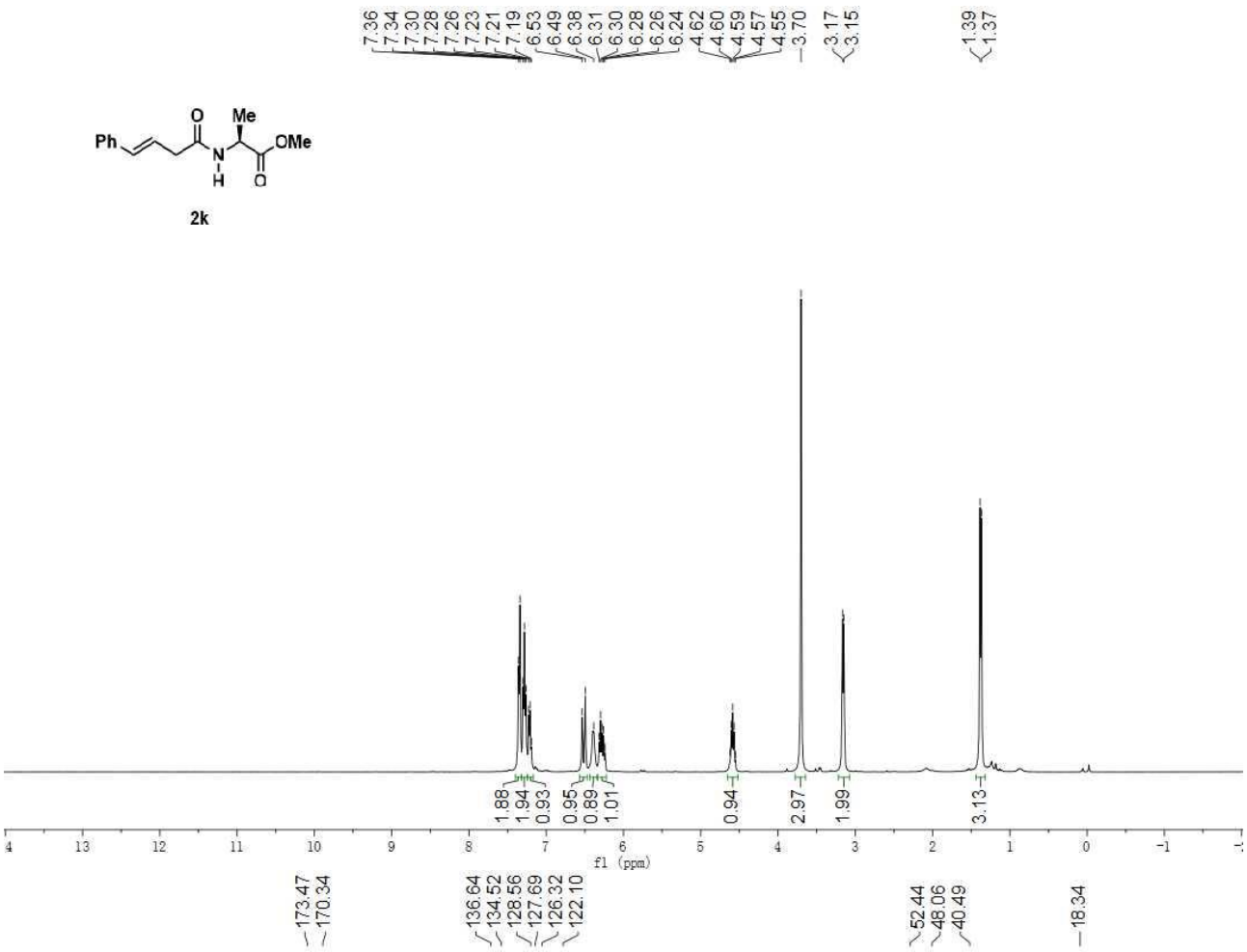
29.21
27.18
26.90
22.67
14.11
Ph
O
N
H
2j
f1 (ppm)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6.28
6.26
6.24
4.62
4.60
4.59
4.57
4.55
3.70
3.17
3.15
1.39
1.37
Ph
O
Me
N
H
OMe
O
2k
1.88
1.94
0.93
0.95
0.89
1.01
0.94
2.97
1.99
3.13
f1 (ppm)
173.47
170.34
136.64
134.52
128.56
127.69
126.32
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48.06
40.49
18.34
Ph
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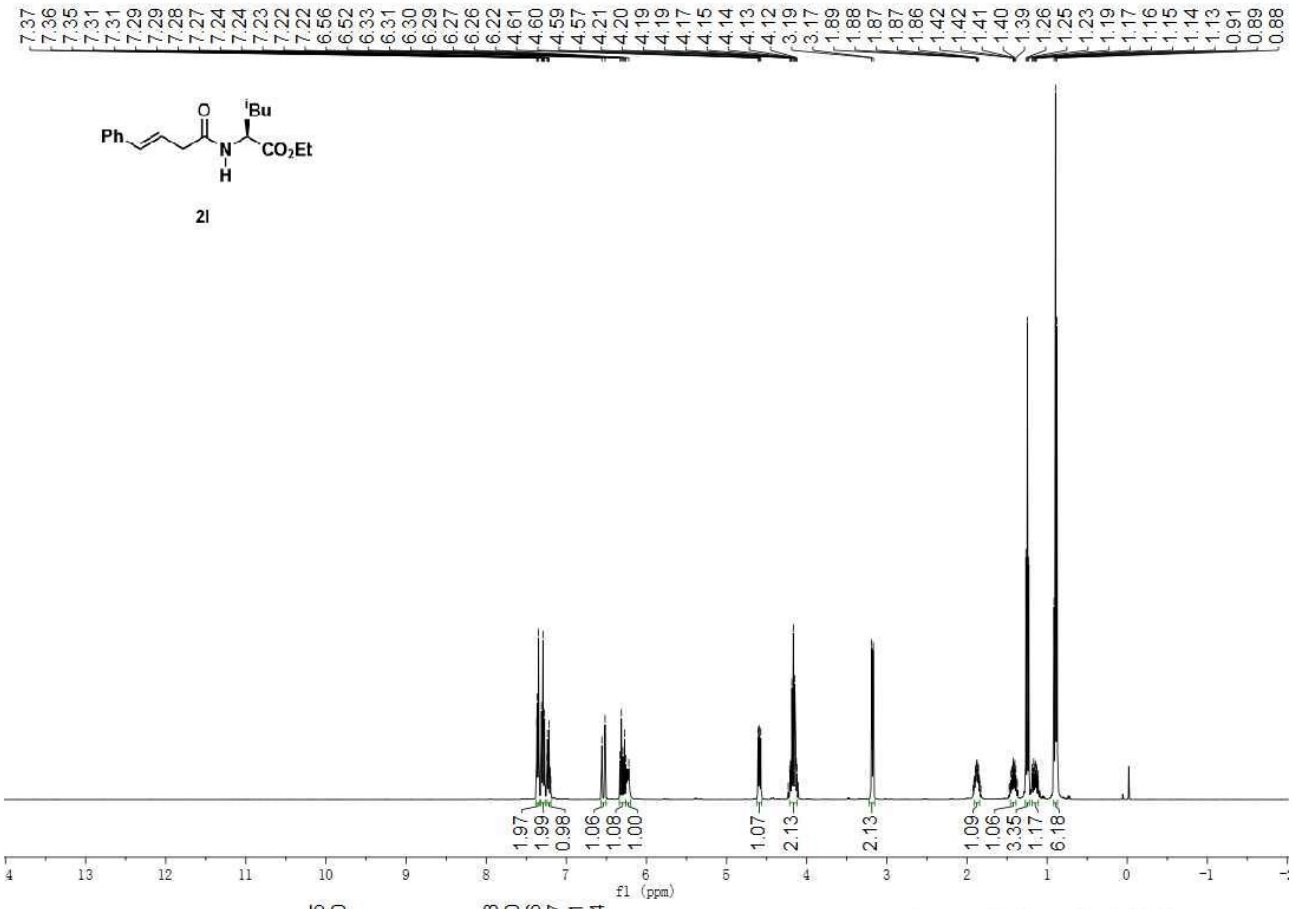
Me
N
H
OMe
O
2k
f1 (ppm)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4.19
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4.15
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4.12
3.19
3.17
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1.87
1.87
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1.42
1.41
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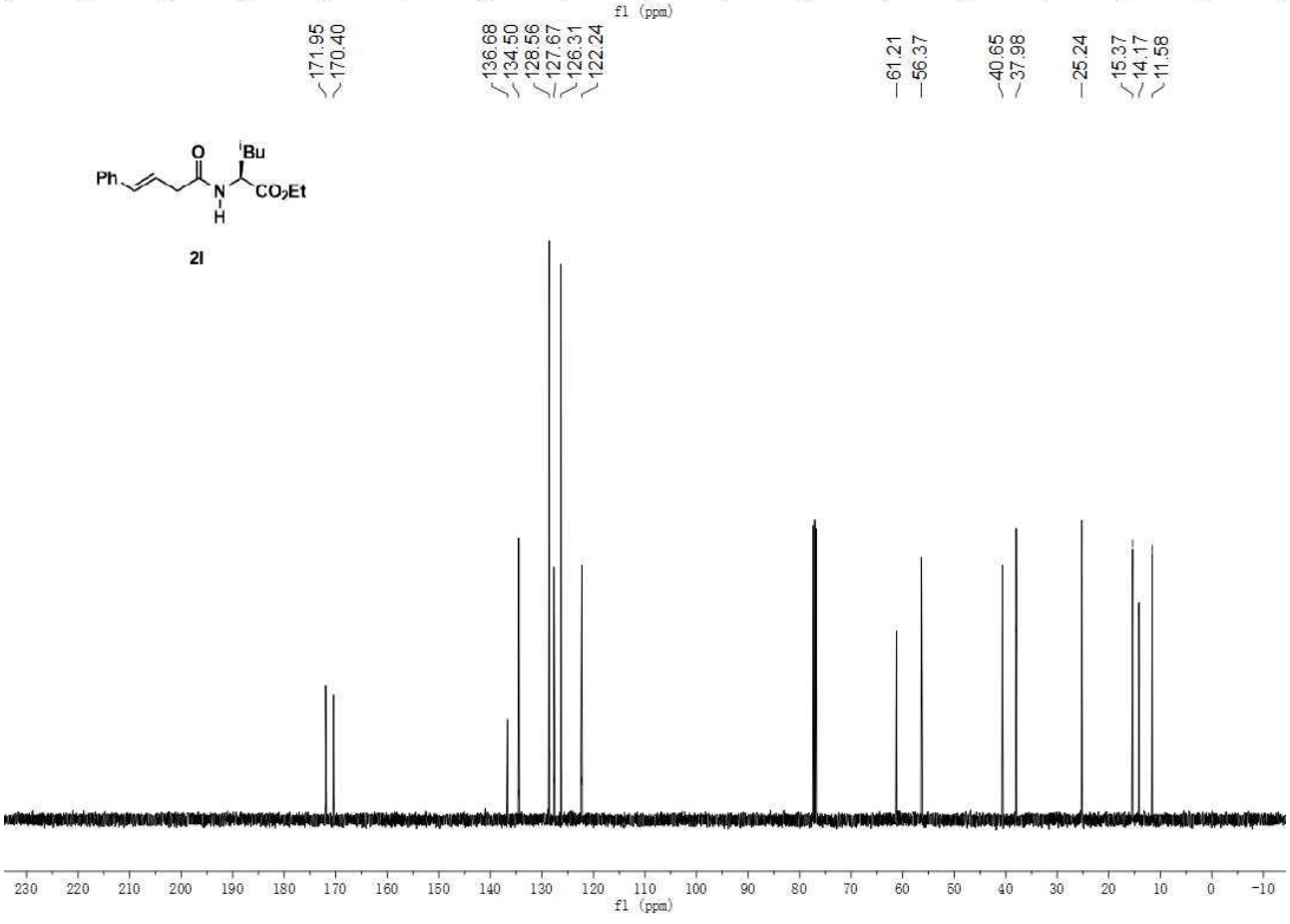
1.26
1.25
1.23
1.19
1.17
1.16
1.15
1.14
1.13
0.91
0.89
0.88
Ph
O
N
H
iBu
CO2Et
2l
1.97
1.99
0.98
1.06
1.08
1.00
1.07
2.13
2.13
1.09
1.06
3.35
1.17
6.18
f1 (ppm)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122.24
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15.37
14.17
11.58
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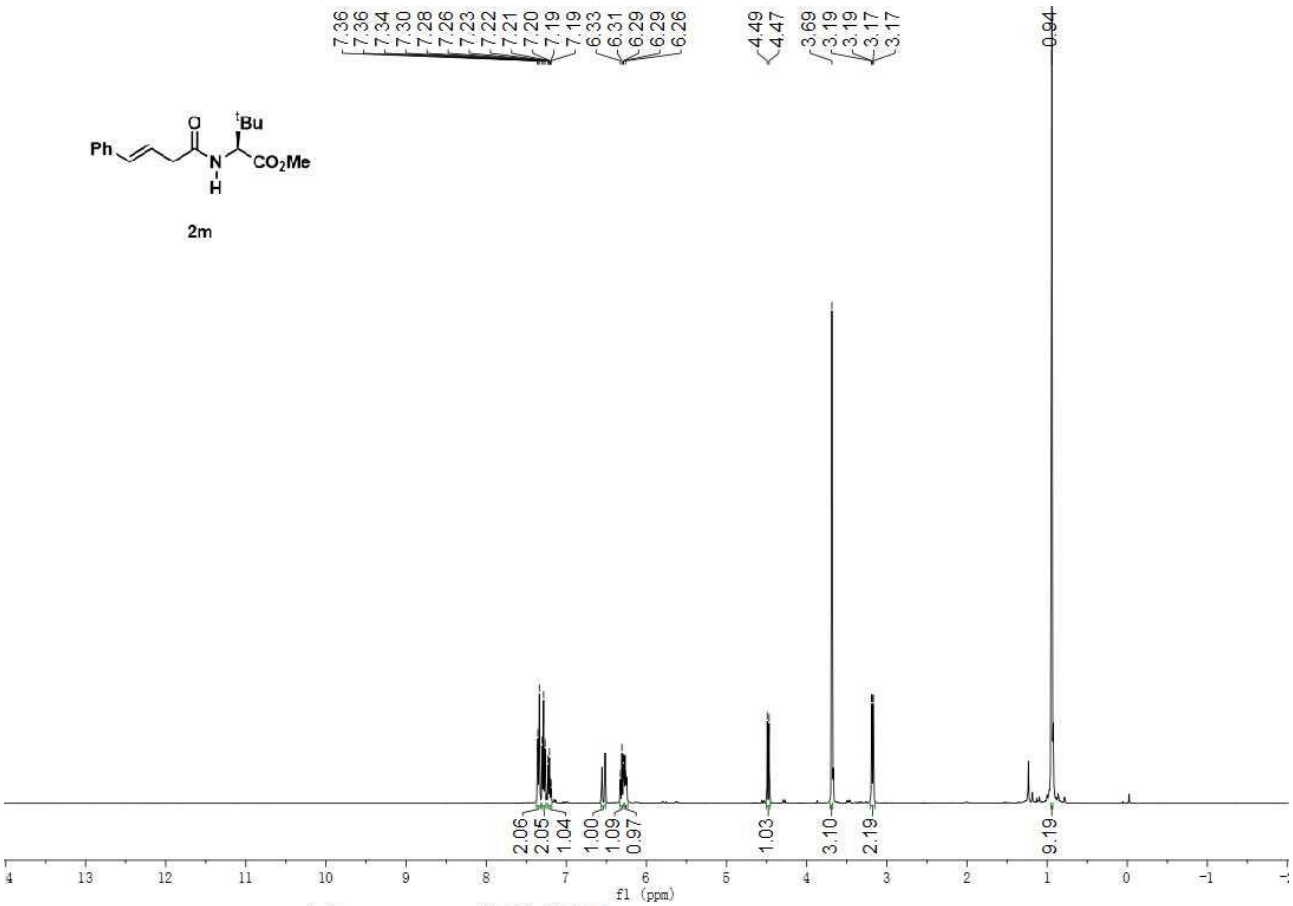
N
H
iBu
CO2Et
2l
f1 (ppm)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7.19
6.33
6.31
6.29
6.29
6.26
4.49
4.47
3.69
3.19
3.19
3.17
3.17
0.94
Ph
O
N
H
tBu
CO2Me
2m
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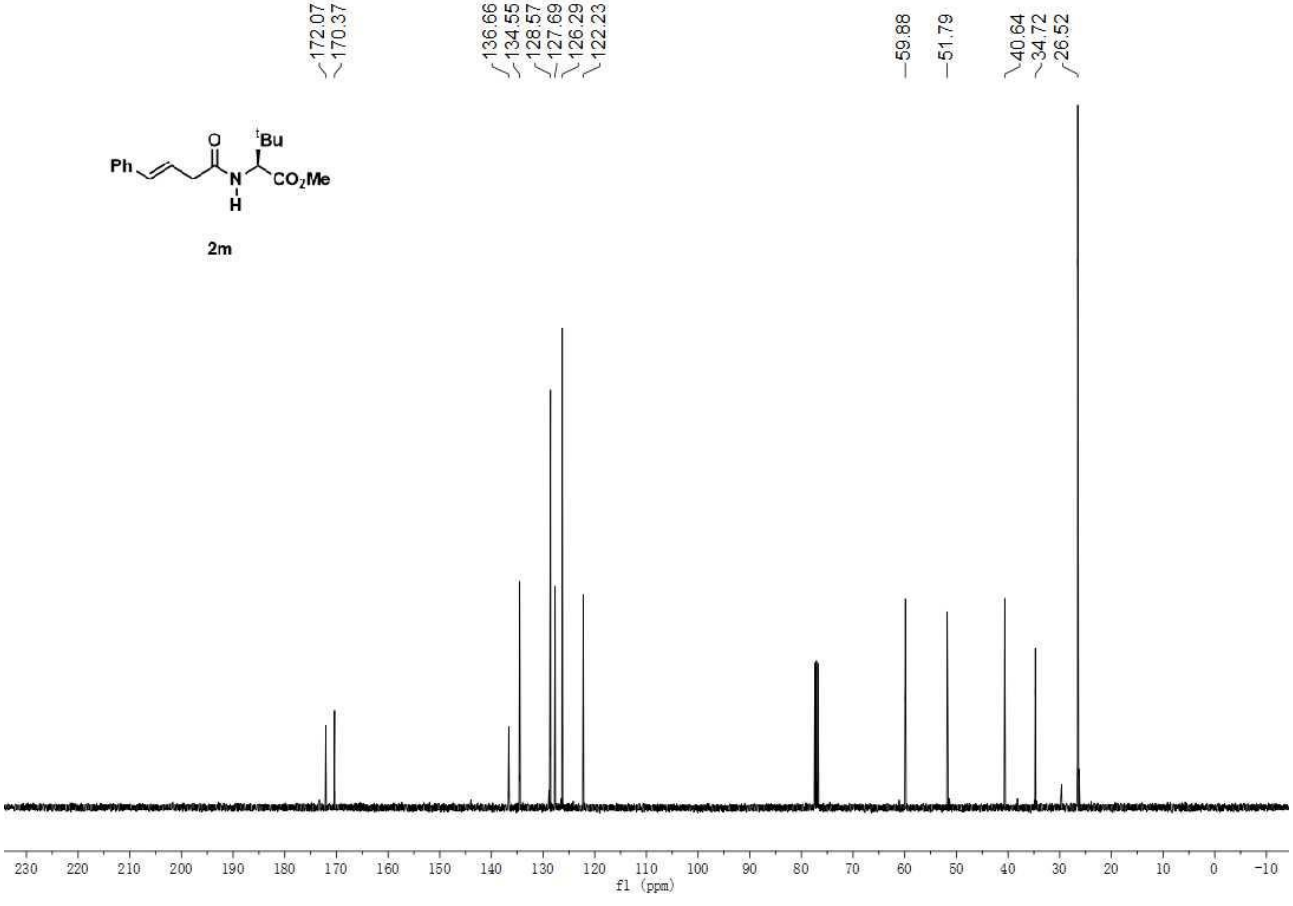
2.05
1.04
1.00
1.09
0.97
1.03
3.10
2.19
9.19
f1 (ppm)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26.52
Ph
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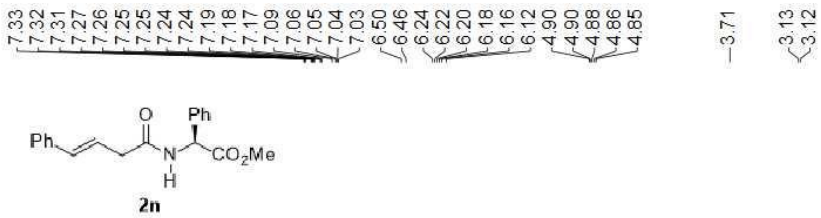
N
H
tBu
CO2Me
2m
f1 (ppm)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7.09
7.06
7.05
7.04
7.03
6.50
6.46
6.24
6.22
6.20
6.18
6.16
6.12
4.90
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4.85
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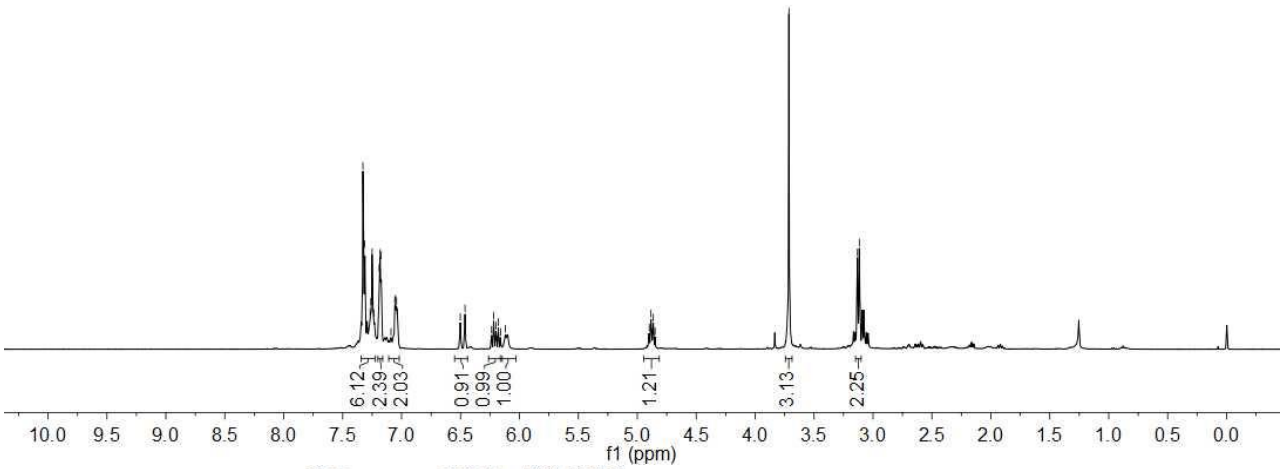
3.12
Ph
O
Ph
N
H
CO2Me
2n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2.03
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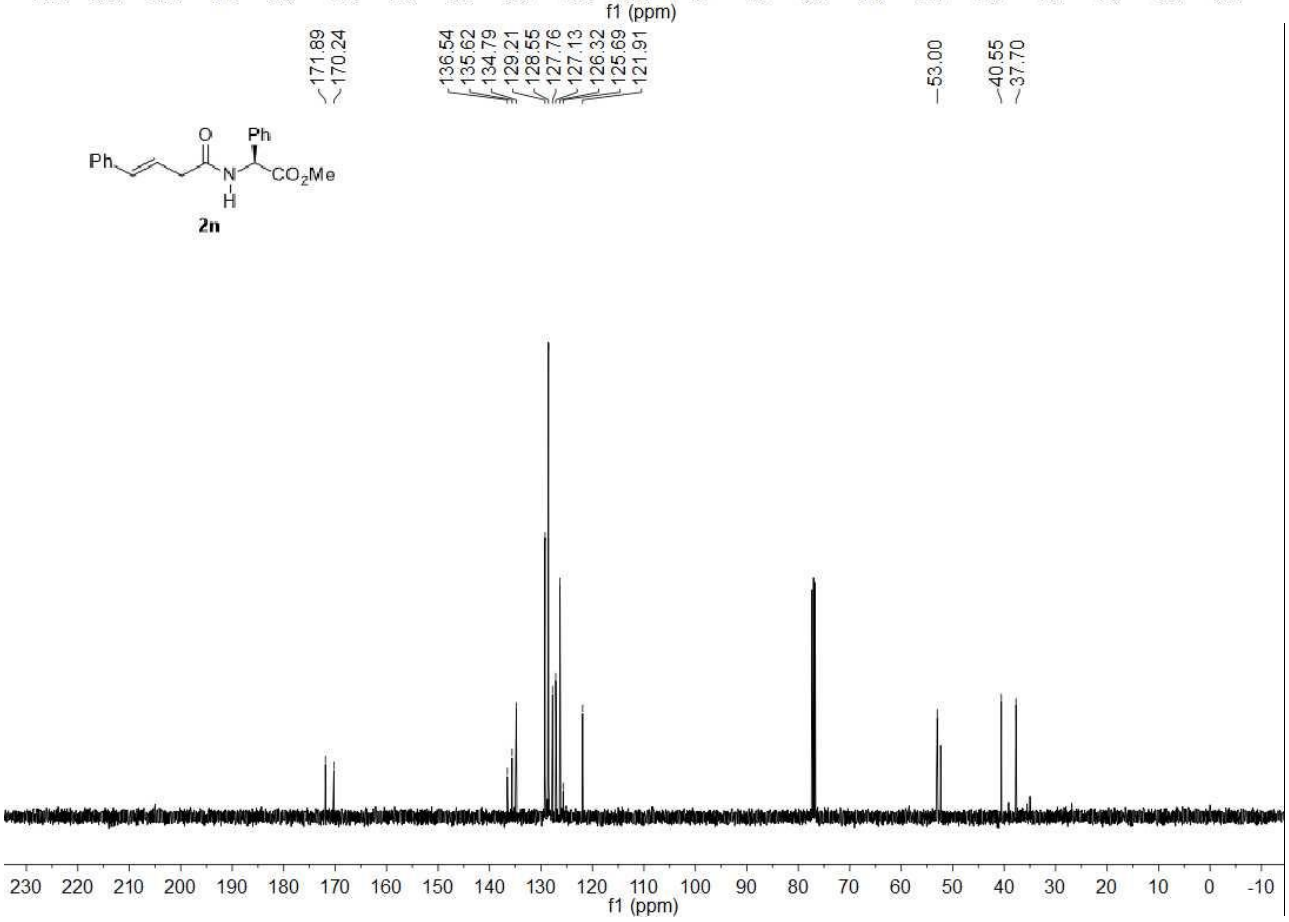
0.99
1.00
1.21
3.13
2.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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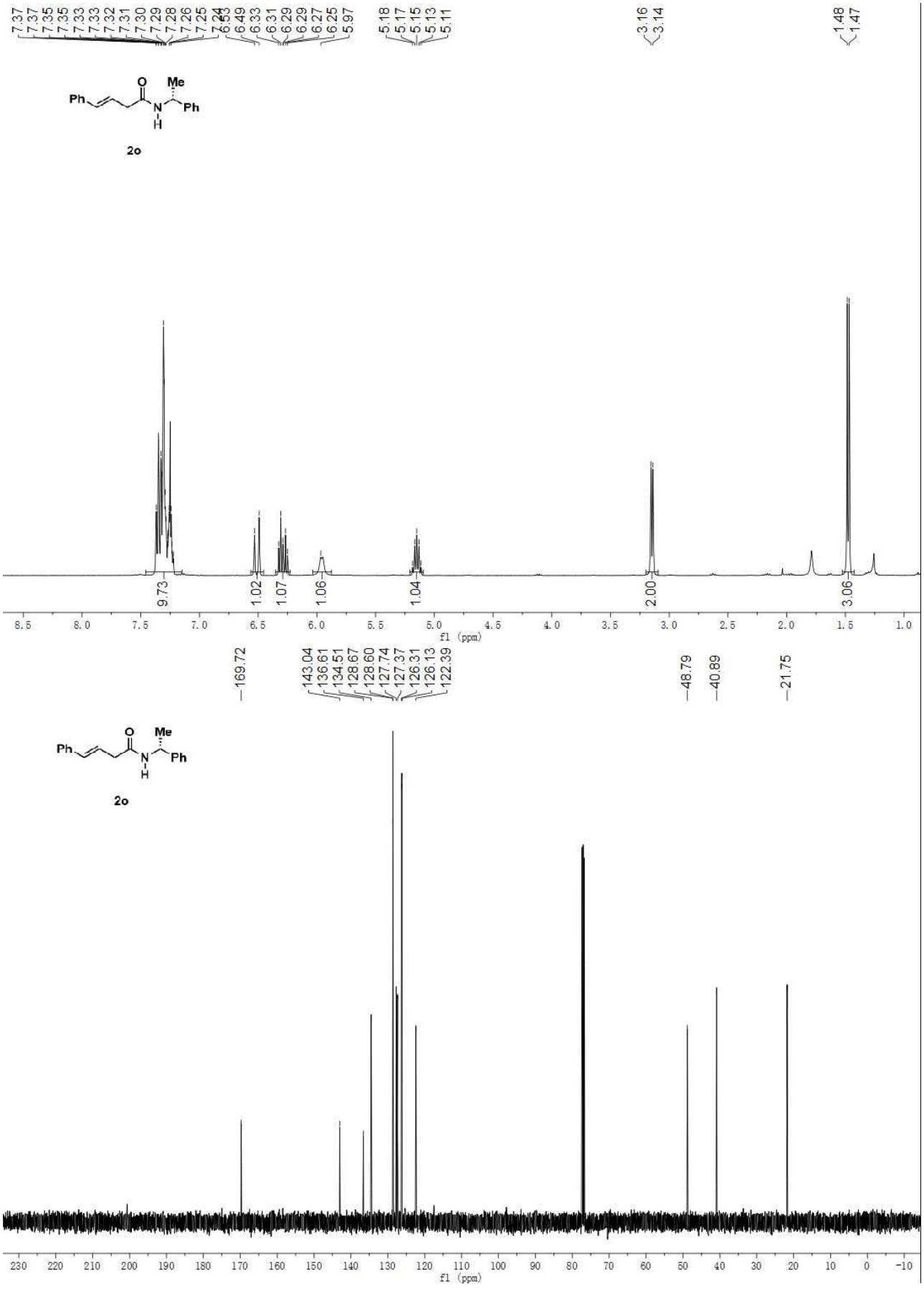
126.32
125.69
121.91
53.00
40.55
37.70
Ph
O
Ph
N
H
CO2Me
2n
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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Ph
O
Me
N
H
Ph
2o
9.73
1.02
1.07
1.06
1.04
2.00
3.06
f1 (ppm)
169.72
143.04
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127.37
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122.39
48.79
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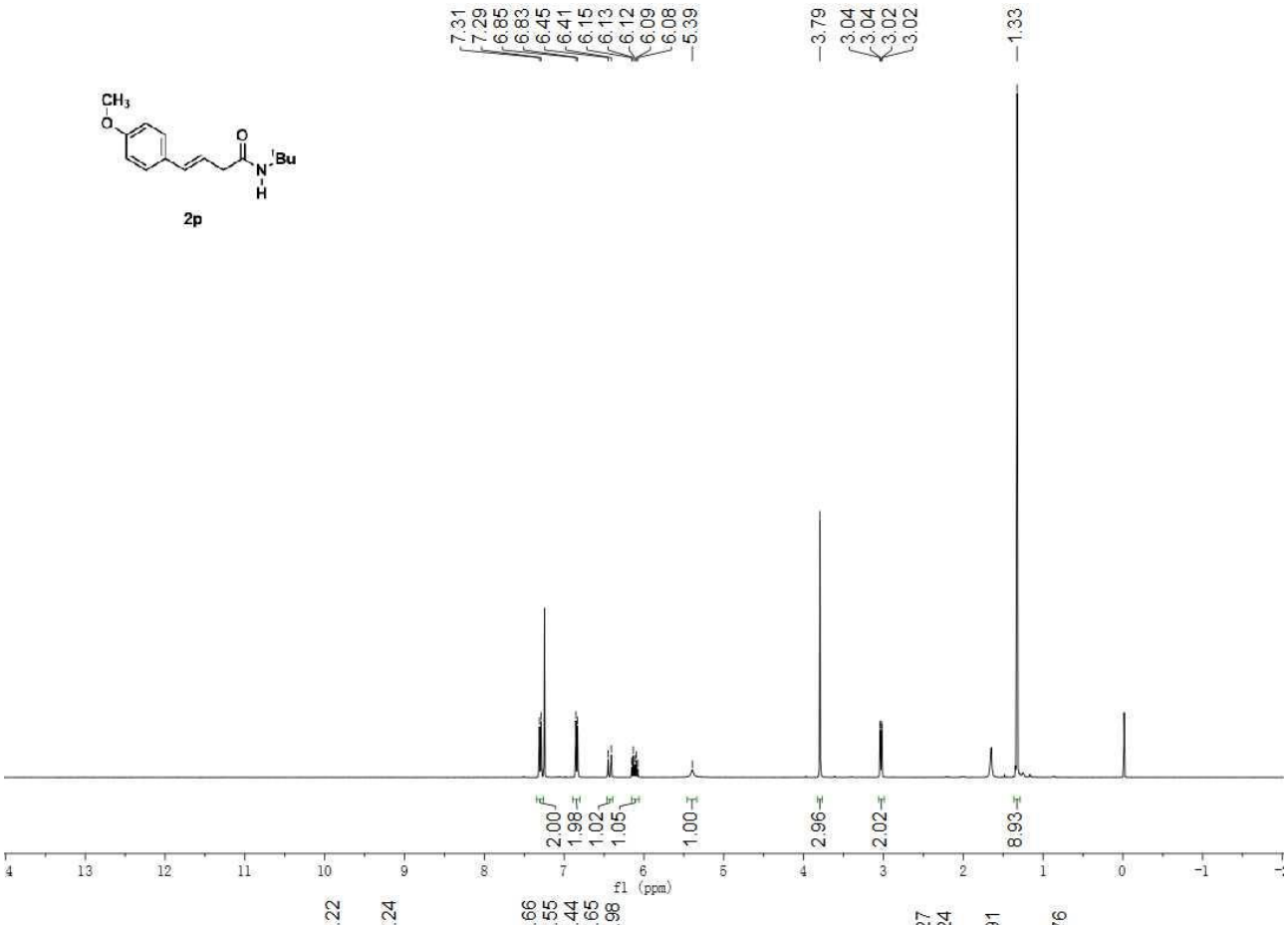
21.75
f1 (ppm)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6.12
6.09
6.08
5.39
3.79
3.04
3.04
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3.02
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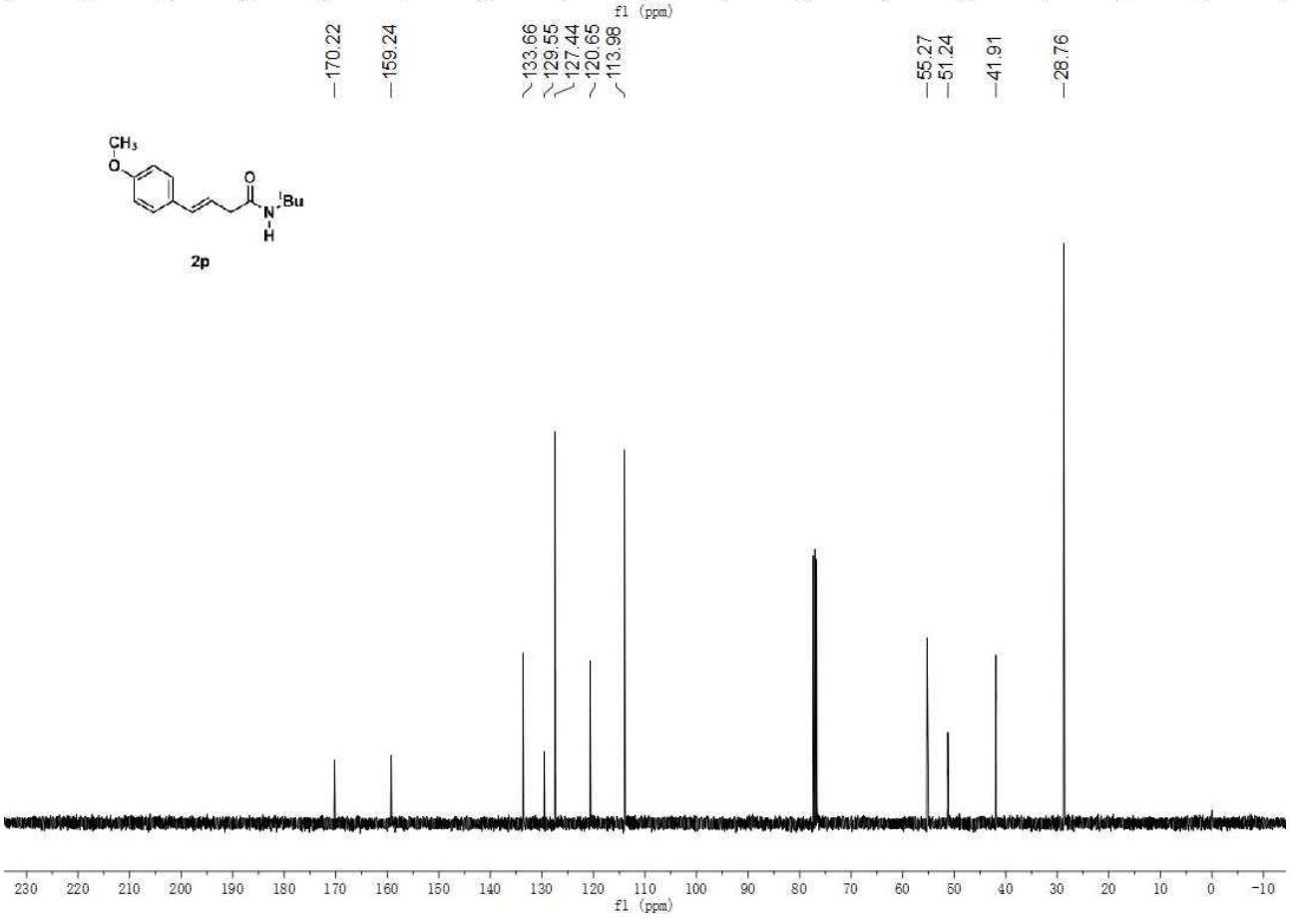
1.02
1.05
1.00
2.96
2.02
8.93
f1 (ppm)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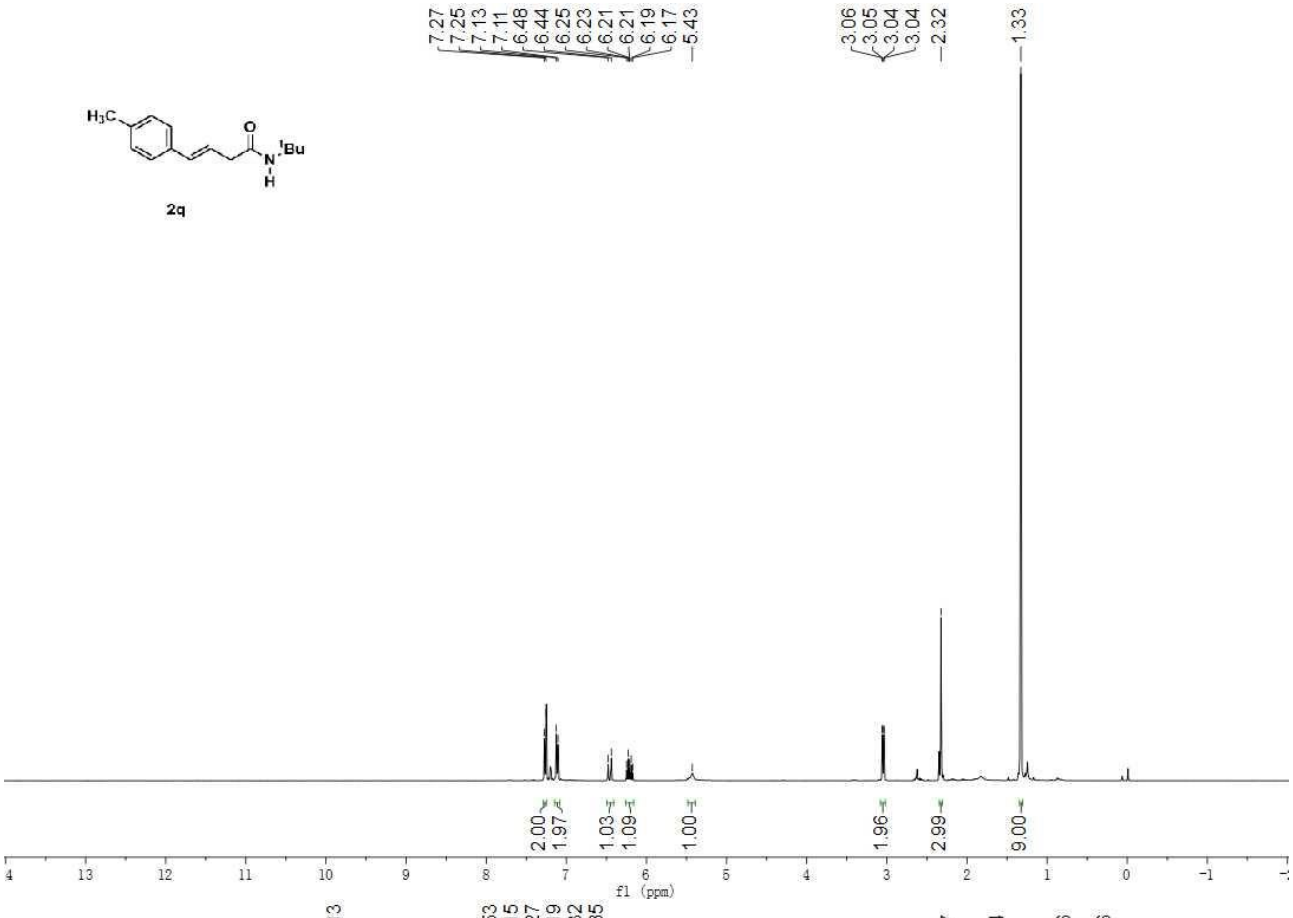
28.76
f1 (ppm)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6.17
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3.04
3.04
2.32
1.33
2.00
1.97
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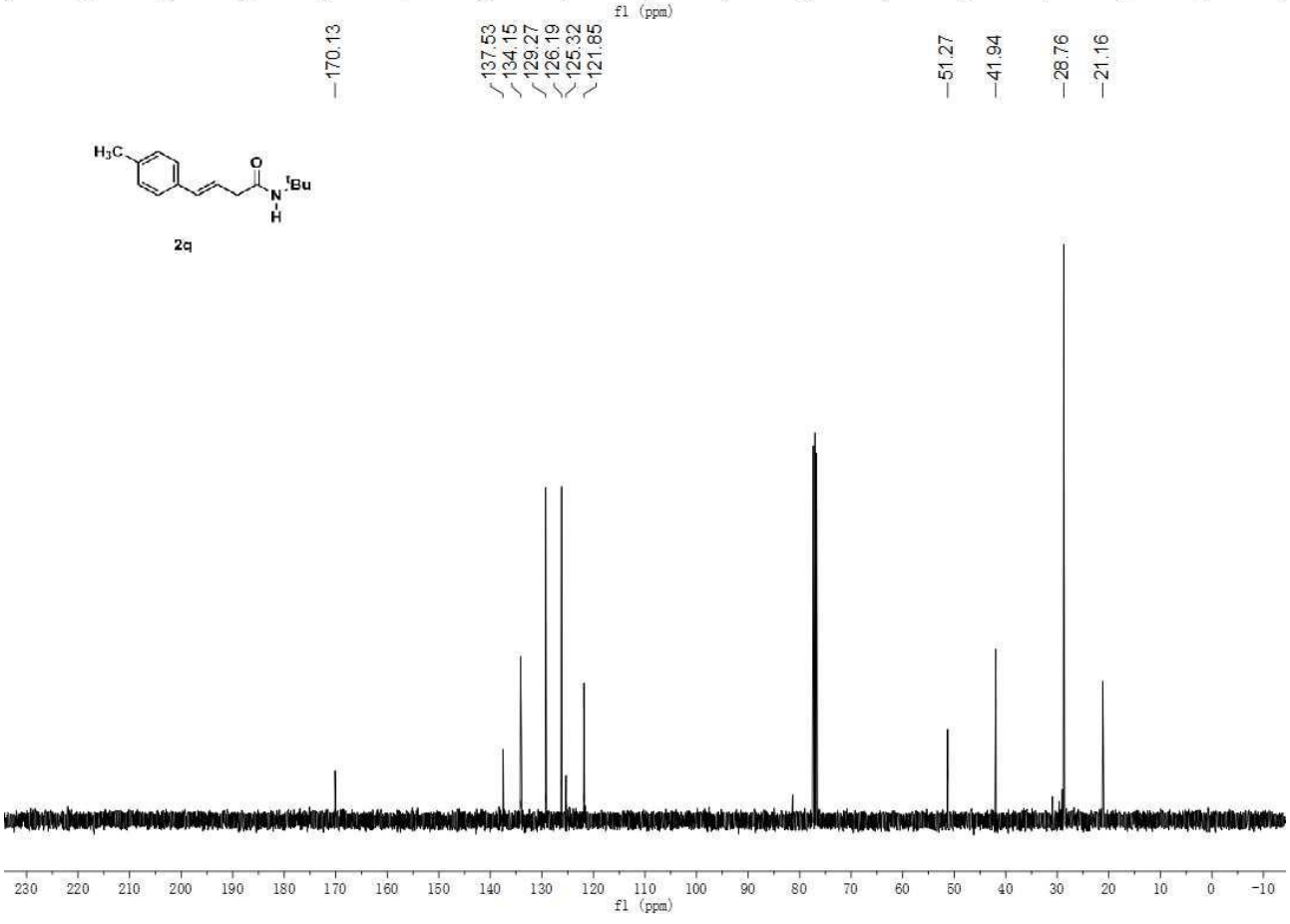
1.09
1.00
1.96
2.99
9.00
f1 (ppm)

H3C
O
N
tBu
H

2q


170.13
137.53
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129.27
126.19
125.32
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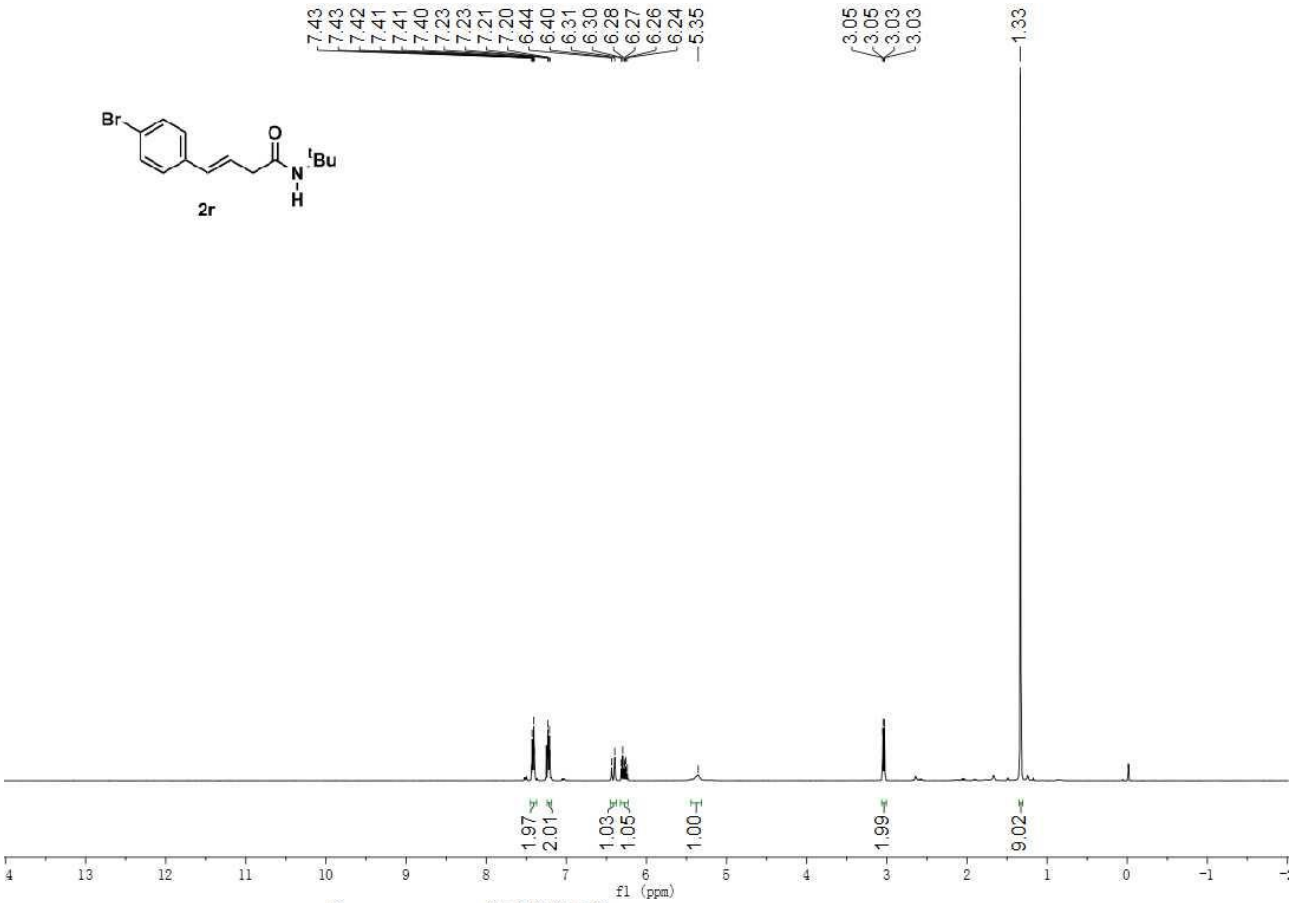
51.27
41.94
28.76
21.16
f1 (ppm)

H3C
O
N
tBu
H

2q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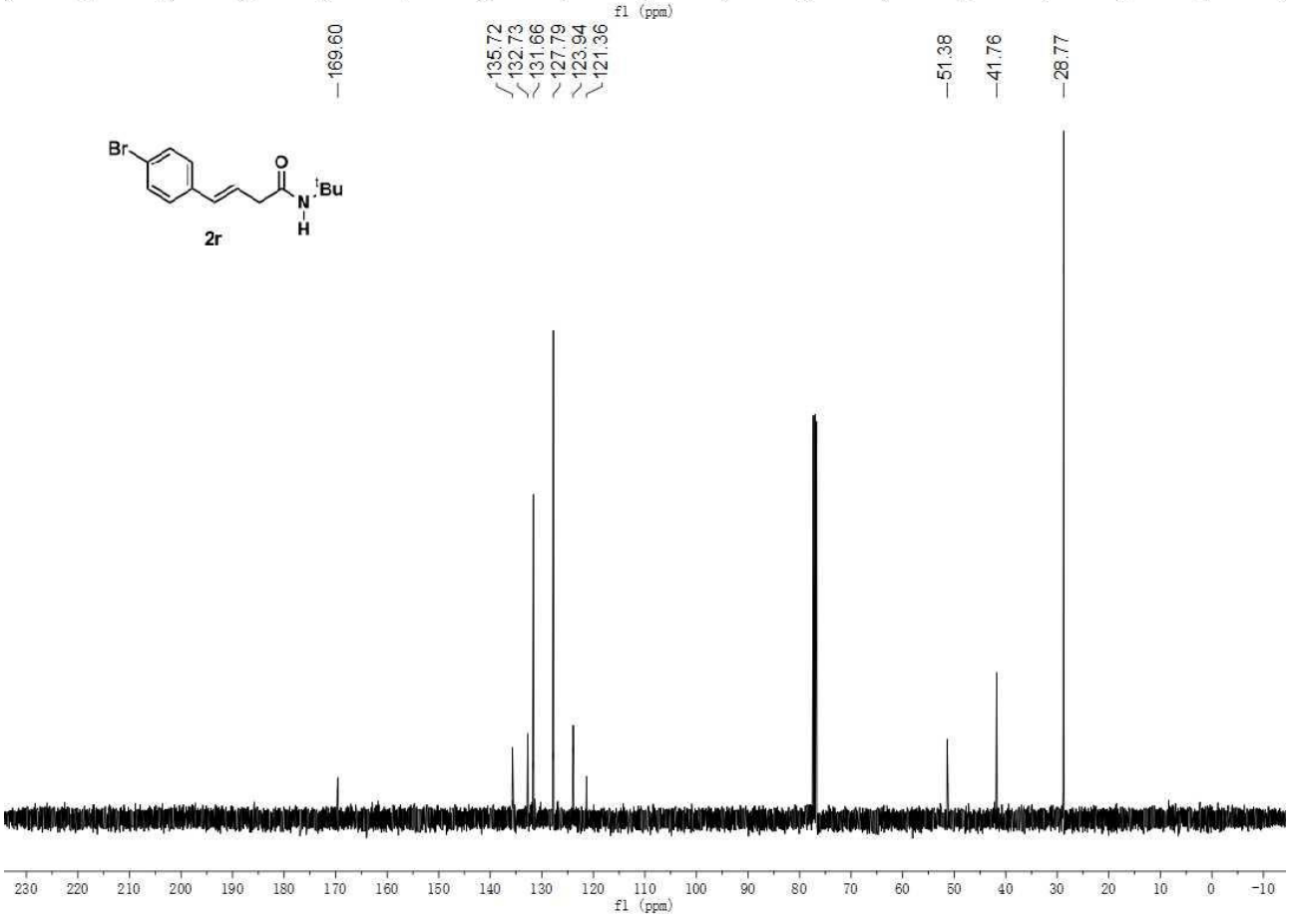
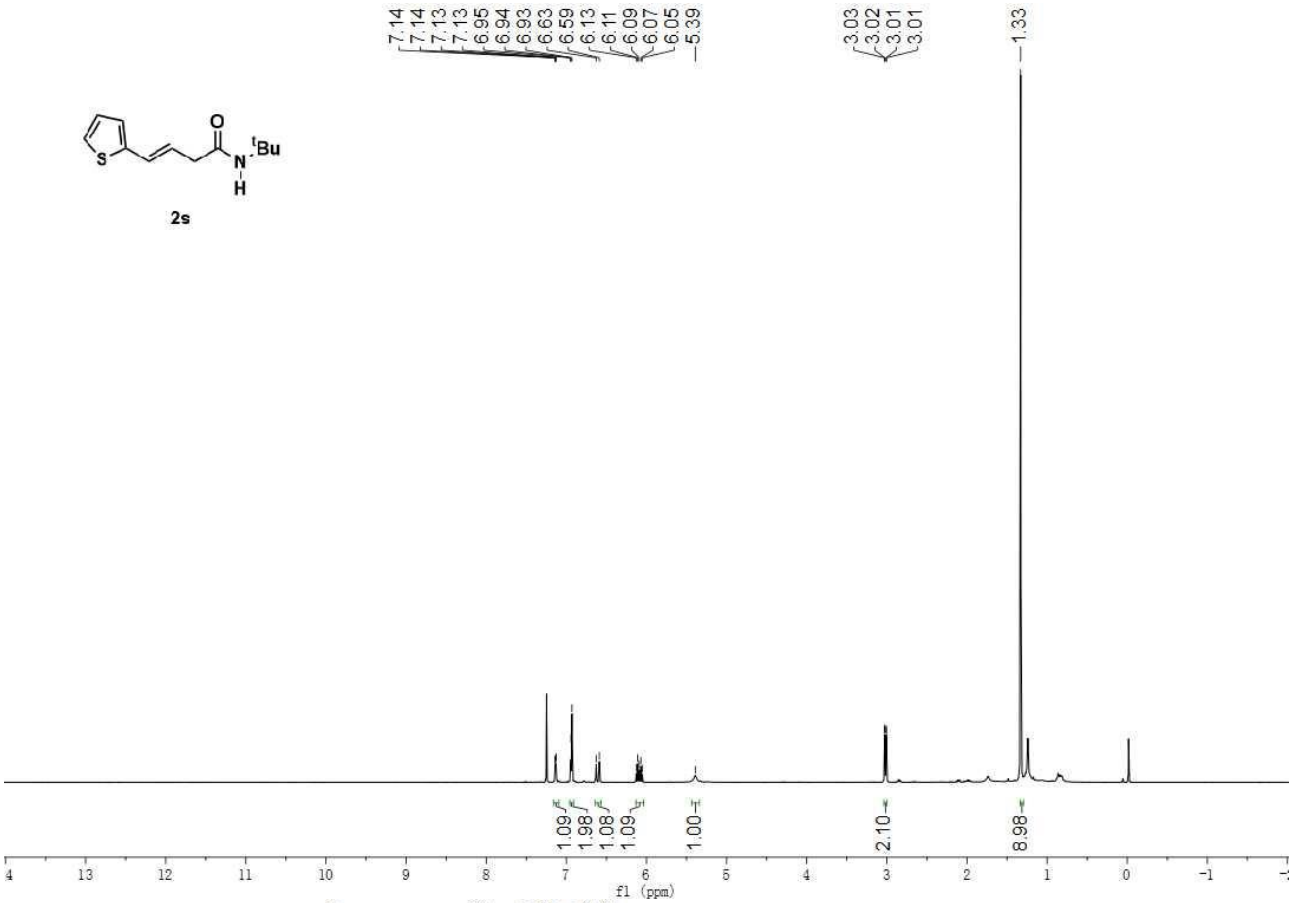
7.42
7.41
7.41
7.40
7.23
7.23
7.21
7.20
6.44
6.40
6.31
6.30
6.28
6.27
6.26
6.24
5.35
3.05
3.05
3.03
3.03
1.33
Br
O
N
H
tBu
2r
1.97
2.01
1.03
1.05
1.00
1.99
9.02
f1 (ppm)


169.60
135.72
132.73
131.66
127.79
123.94
121.36
51.38
41.76
28.77
Br
O
N
H
tBu
2r
f1 (ppm)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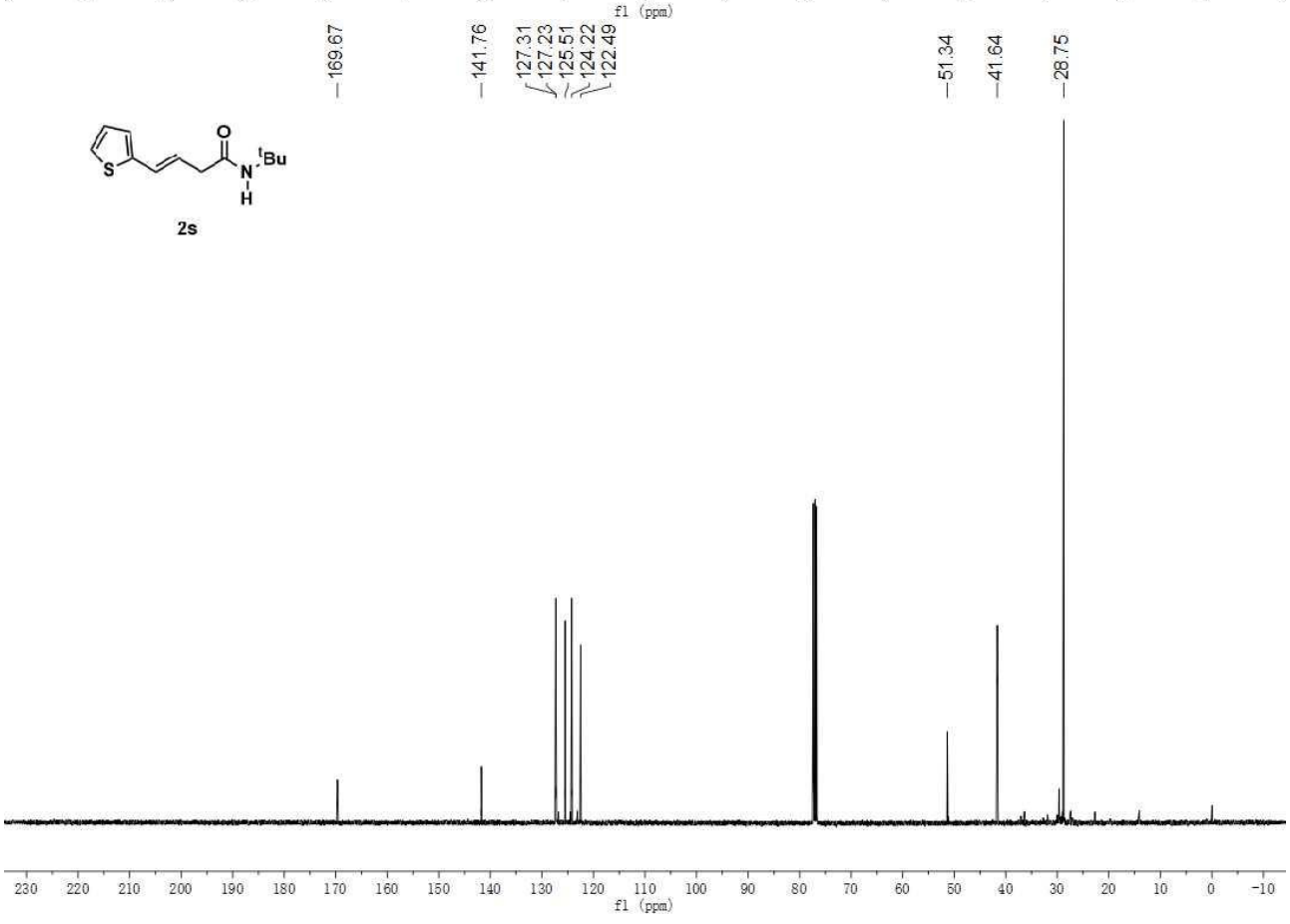
6.93
6.63
6.59
6.13
6.11
6.09
6.07
6.05
5.39
3.03
3.02
3.01
3.01
1.33
1.09
1.98
1.08
1.09
1.00
2.10
8.98
f1 (ppm)

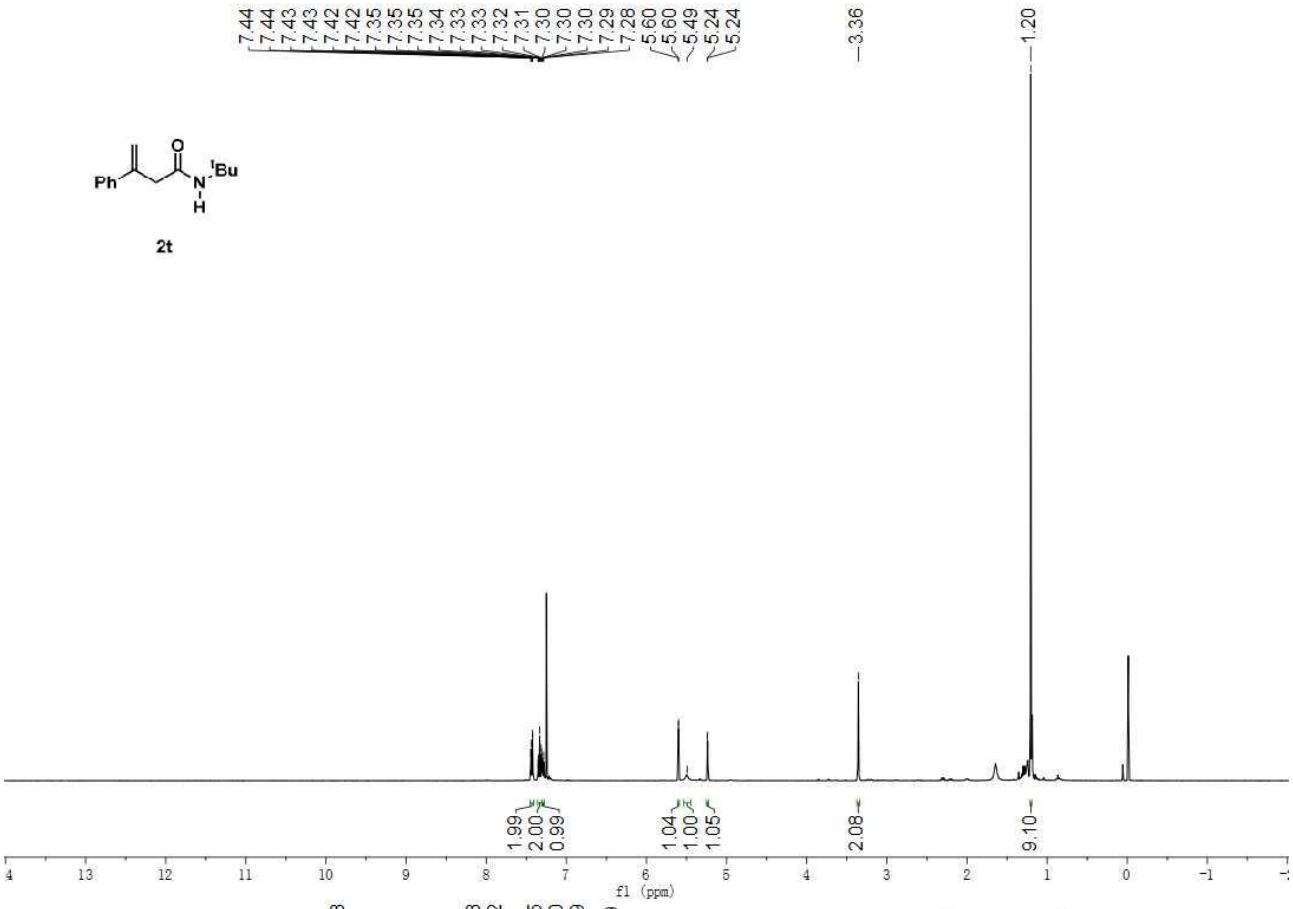
O
N
H
tBu

2s


169.67
141.76
127.31
127.23
125.51
124.22
122.49
51.34
41.64
28.75
f1 (ppm)

O
N
H
tBu

2s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7.35
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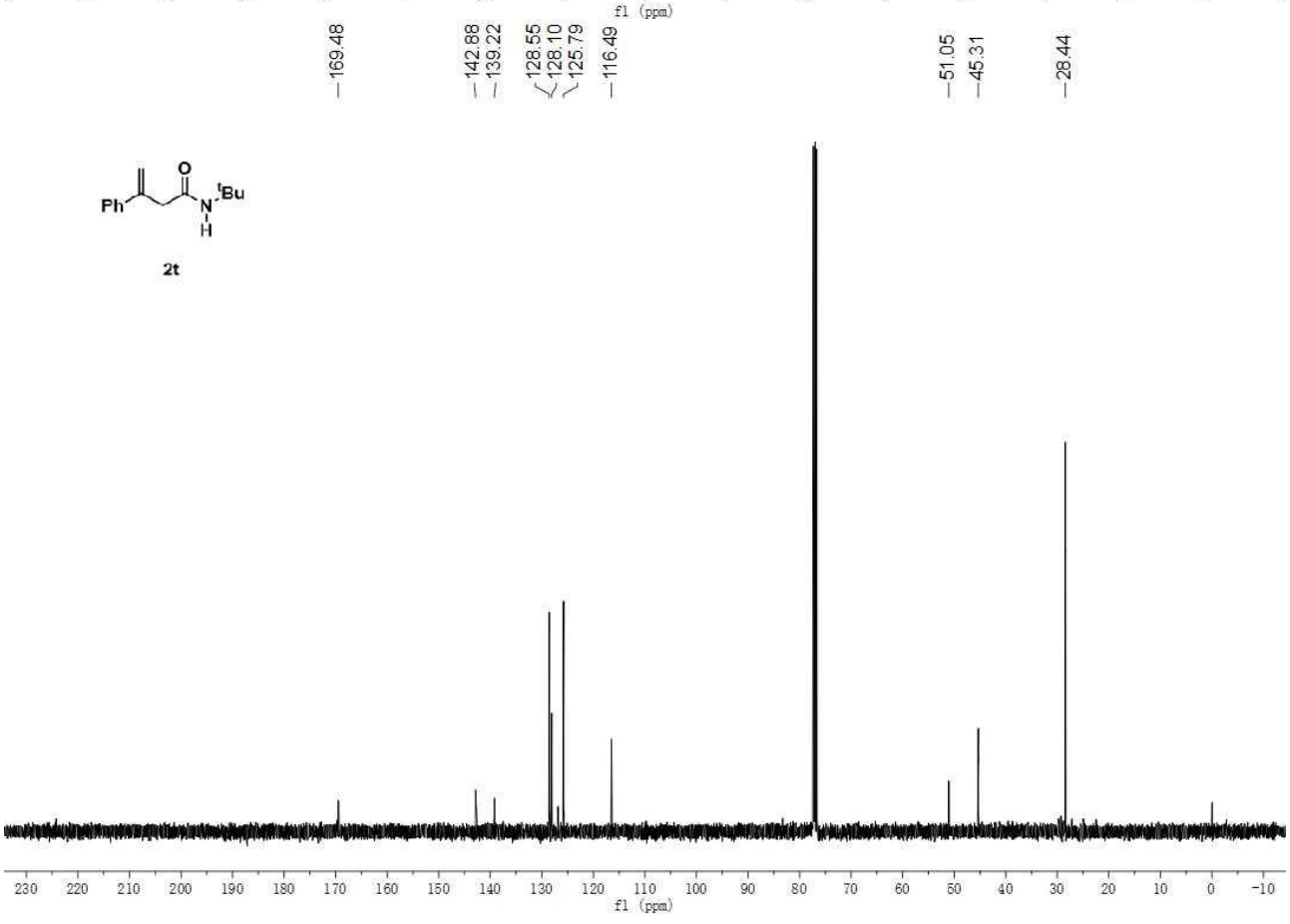
7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.30
7.29
7.28
5.60
5.60
5.49
5.24
5.24
3.36
1.20
Ph
O
N
H
tBu
2t
1.99
2.00
0.99
1.04
1.00
1.05
2.08
9.10
f1 (ppm)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142.88
139.22
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128.10
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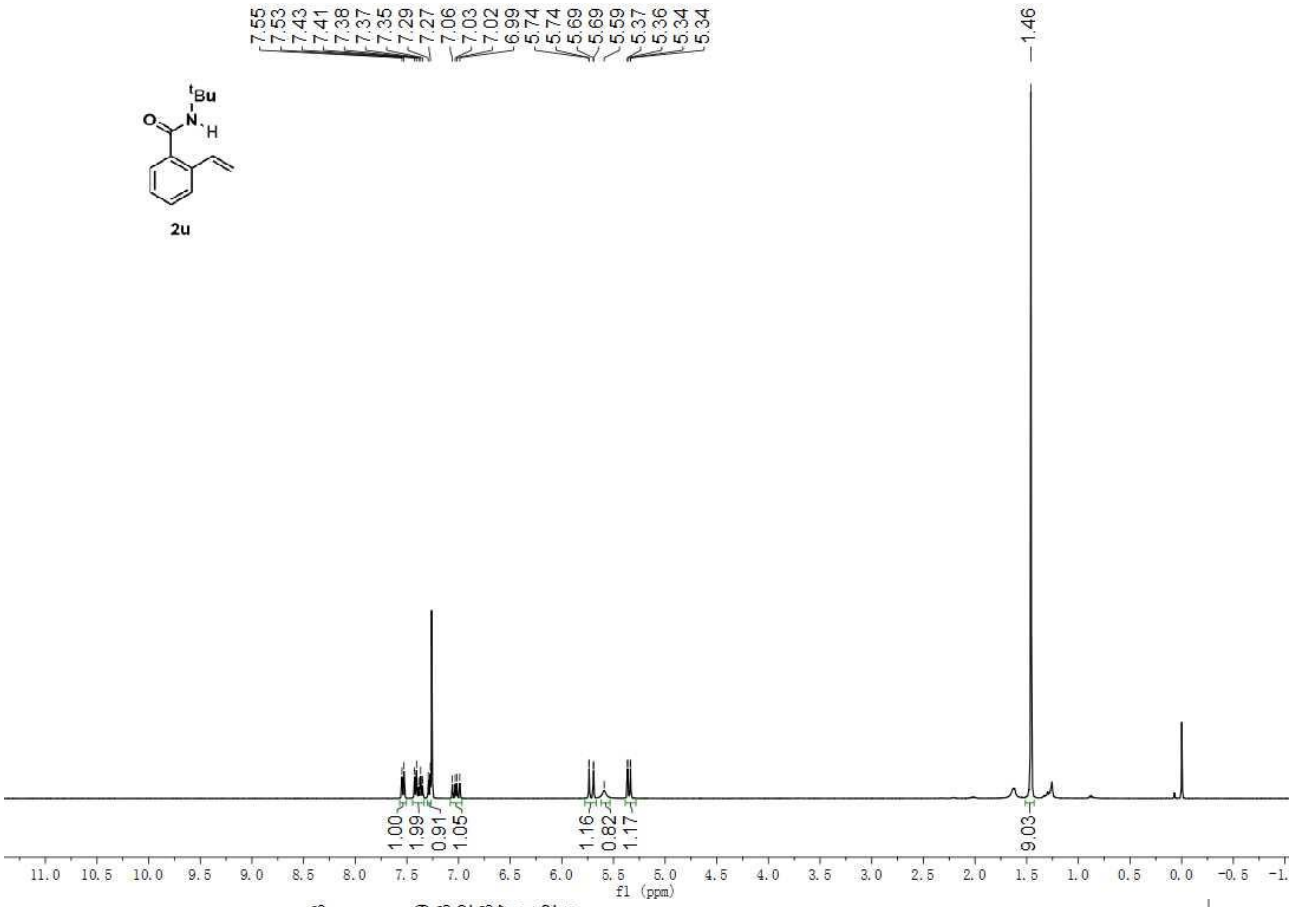
116.49
51.05
45.31
28.44
Ph
O
N
H
tBu
2t
f1 (ppm)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7.53
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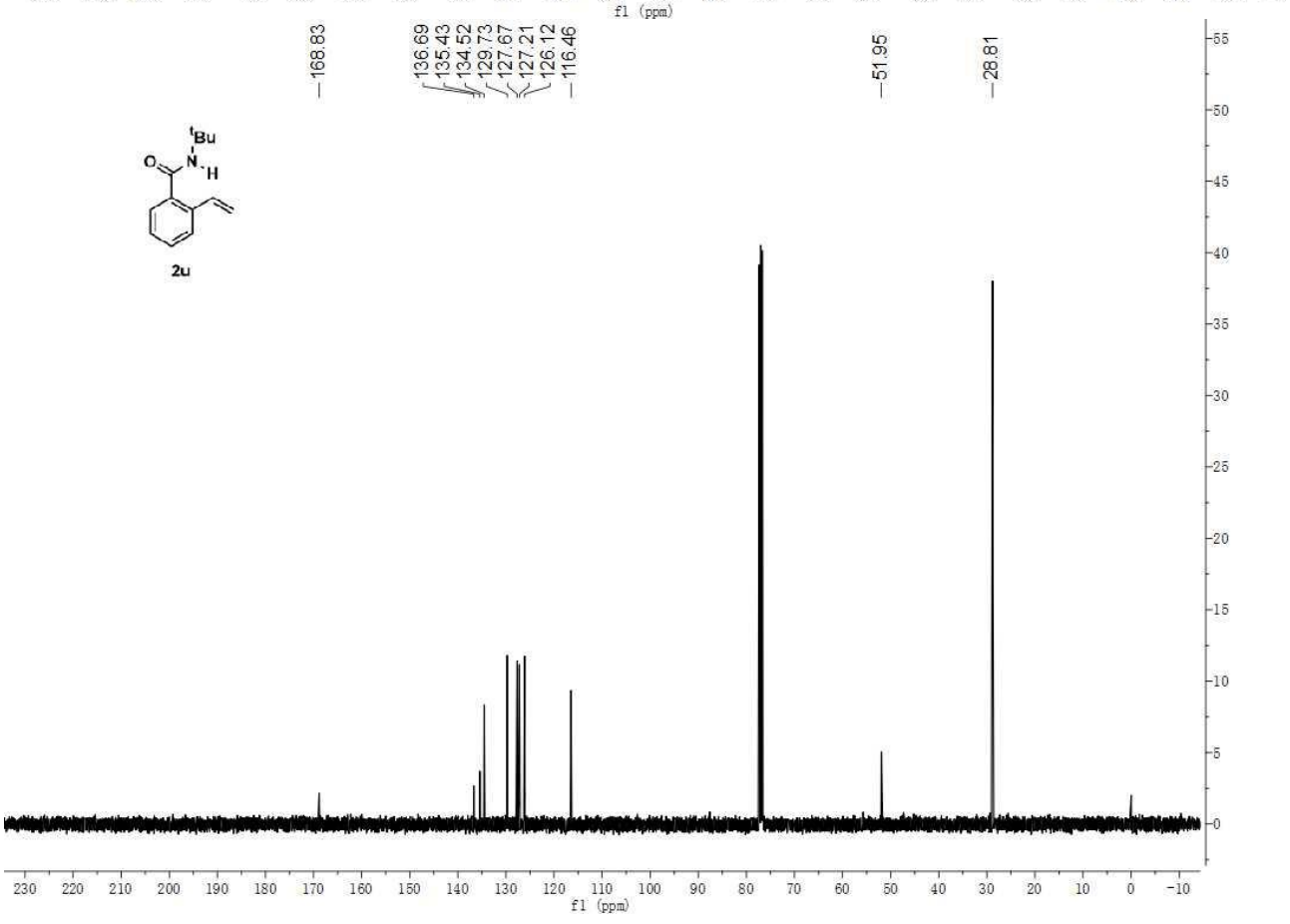
7.29
7.27
7.06
7.03
7.02
6.99
5.74
5.74
5.69
5.69
5.59
5.37
5.36
5.34
5.34
1.46
tBu
N
H
O
2u
1.00
1.99
0.91
1.05
1.16
0.82
1.17
9.03
f1 (ppm)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136.69
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134.52
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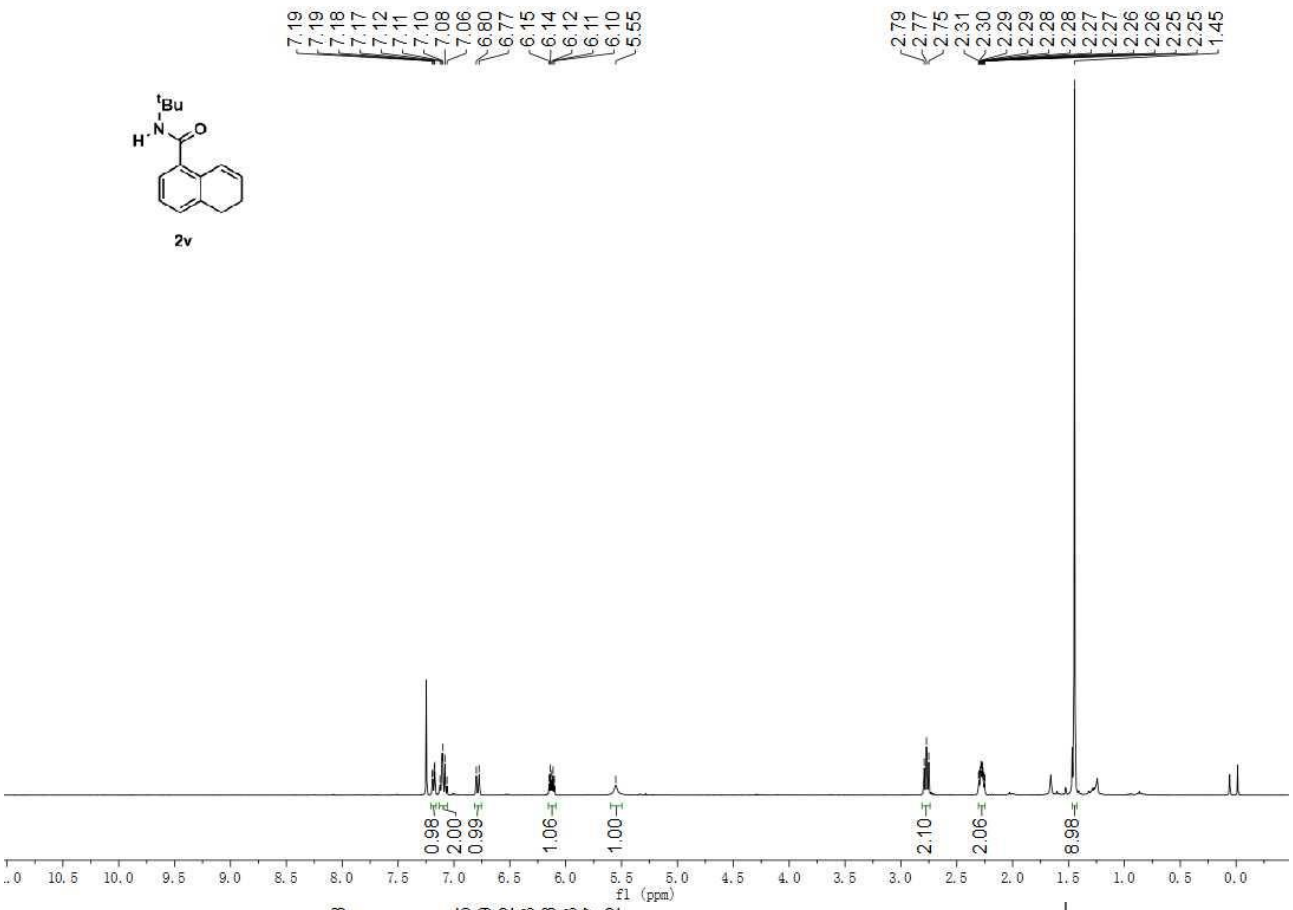
127.21
126.12
116.46
51.95
28.81
tBu
N
H
O
2u
f1 (ppm)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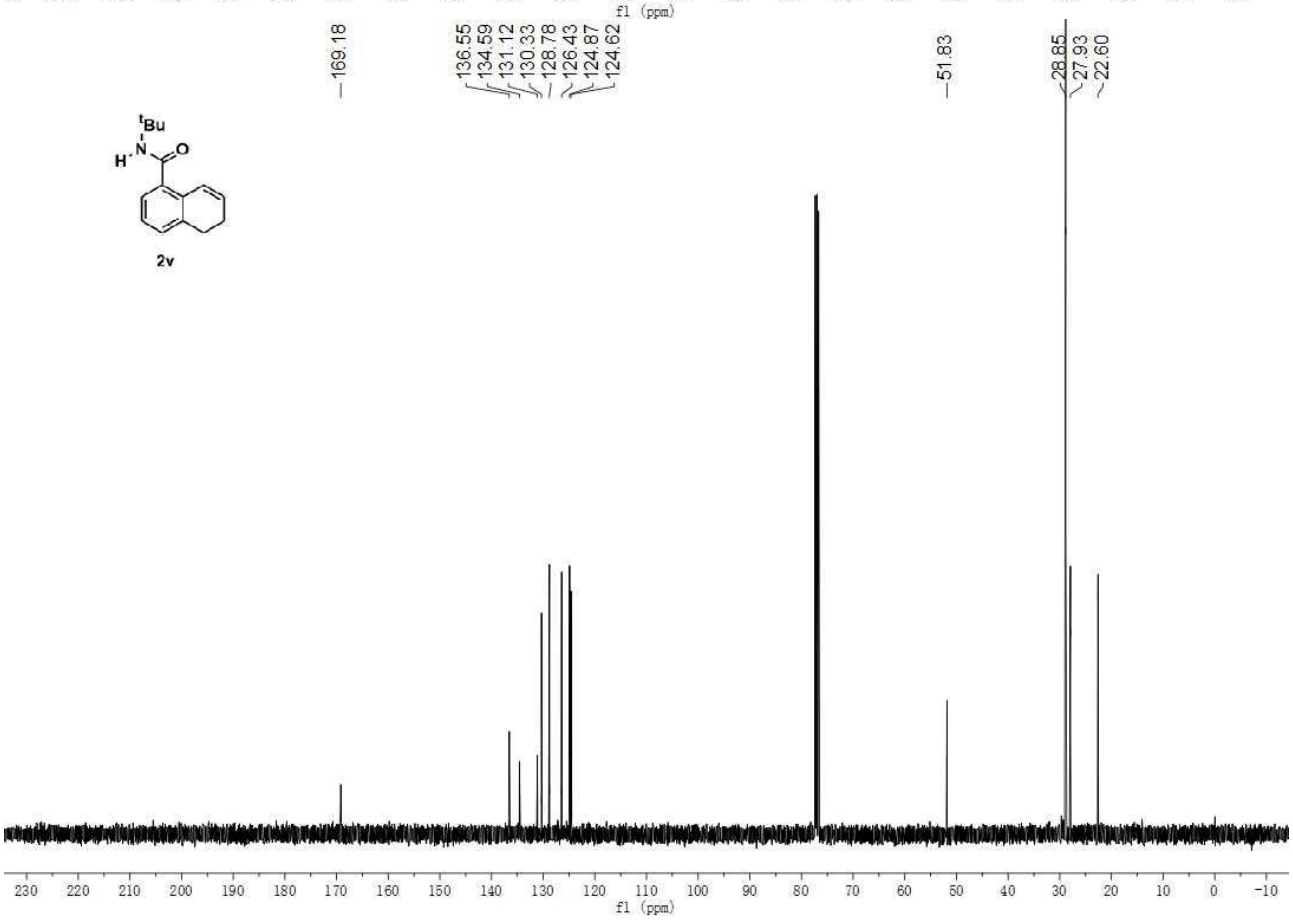
7.19
7.18
7.17
7.12
7.11
7.10
7.08
7.06
6.80
6.77
6.15
6.14
6.12
6.11
6.10
5.55
2.79
2.77
2.75
2.31
2.30
2.29
2.29
2.28
2.28
2.27
2.27
2.26
2.26
2.25
2.25
1.45
0.98
2.00
0.99
1.06
1.00
2.10
2.06
8.98
f1 (ppm)

2v


169.18
136.55
134.59
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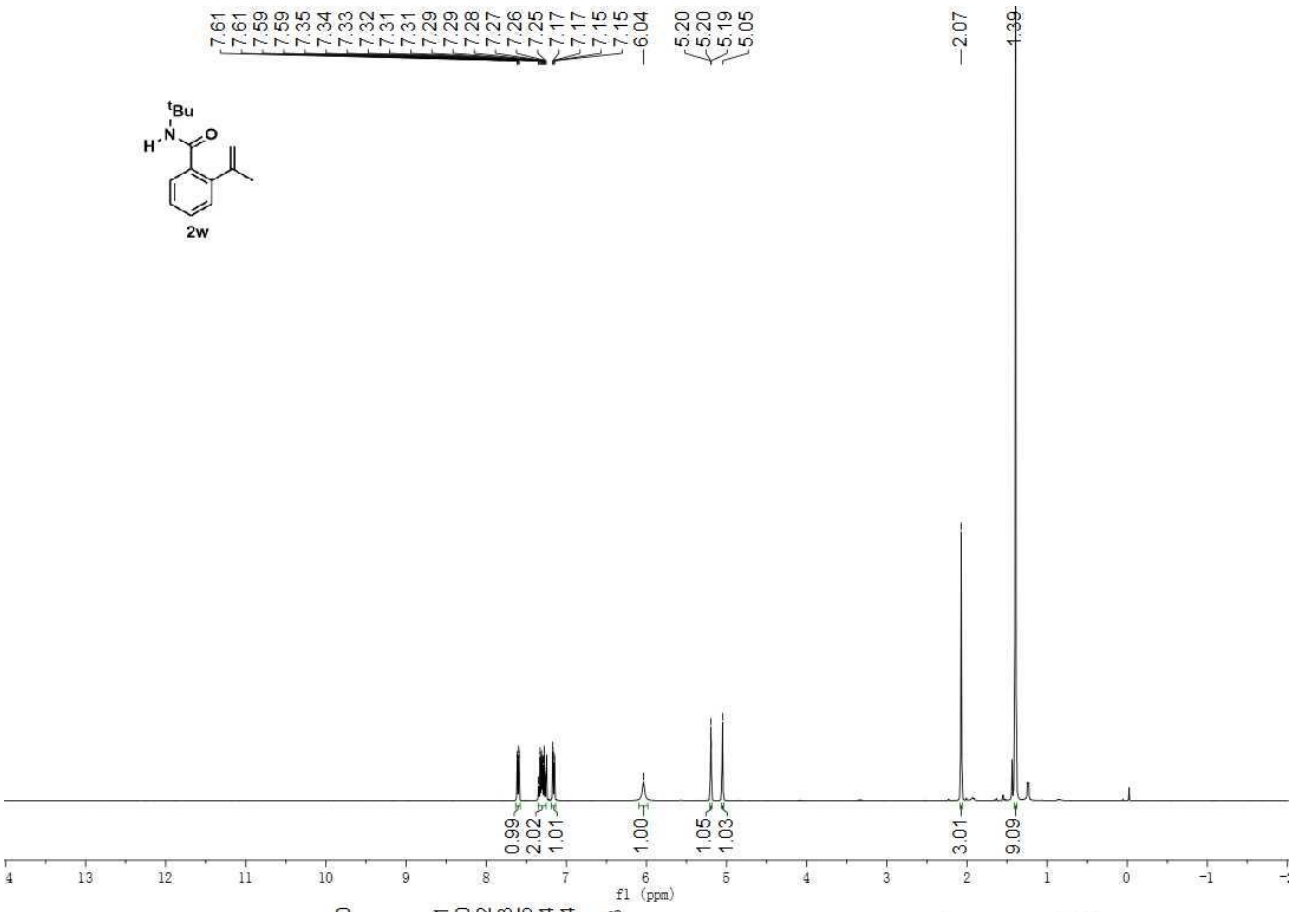
130.33
128.78
126.43
124.87
124.62
51.83
28.85
27.93
22.60
f1 (ppm)

2v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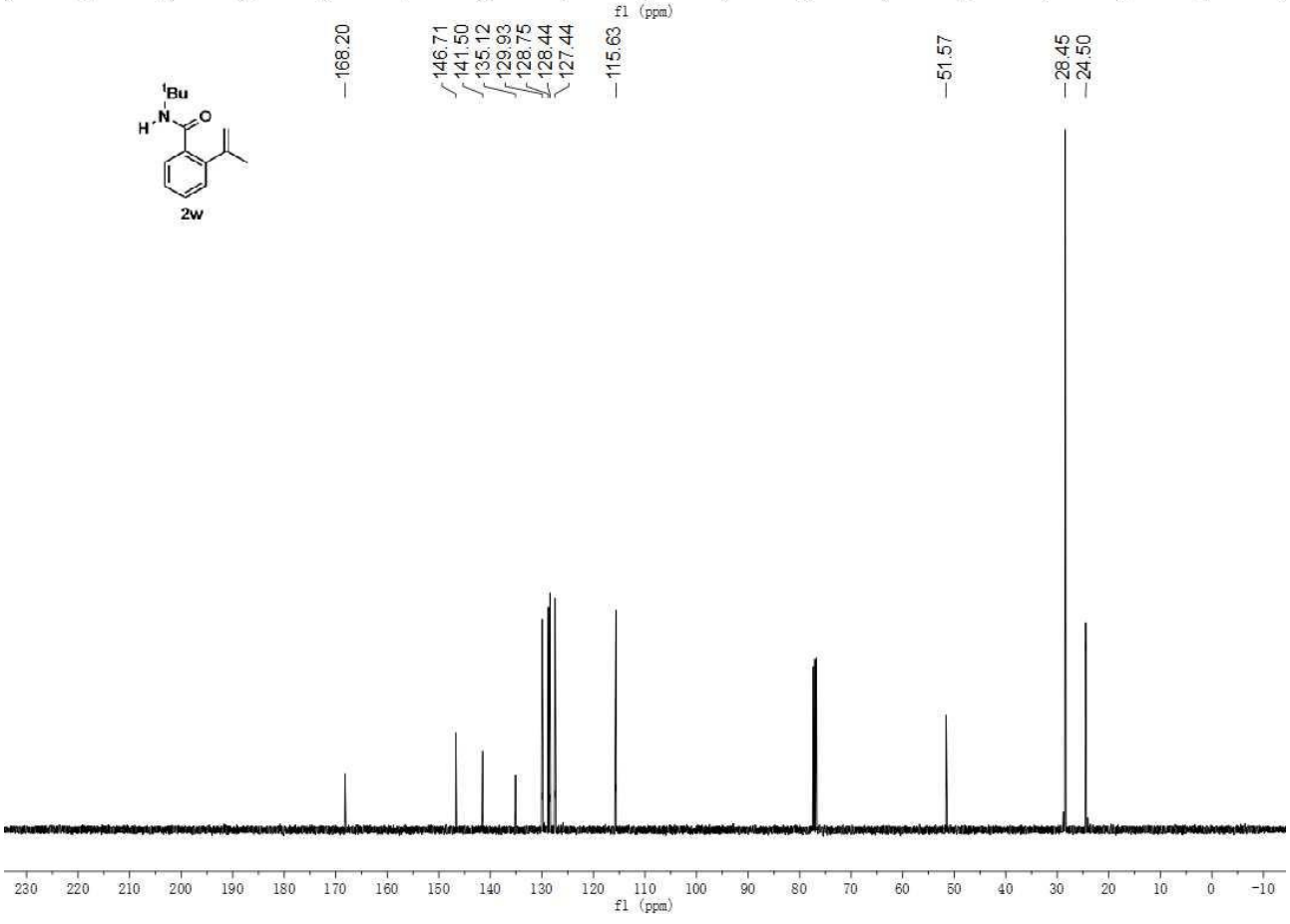
7.61
7.59
7.59
7.35
7.34
7.33
7.32
7.31
7.31
7.29
7.29
7.28
7.27
7.26
7.25
7.17
7.17
7.15
7.15
6.04
5.20
5.20
5.19
5.05
2.07
1.39
tBu
H
N
O
2w
0.99
2.02
1.01
1.00
1.05
1.03
3.01
9.09
f1 (ppm)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141.50
135.12
129.93
128.75
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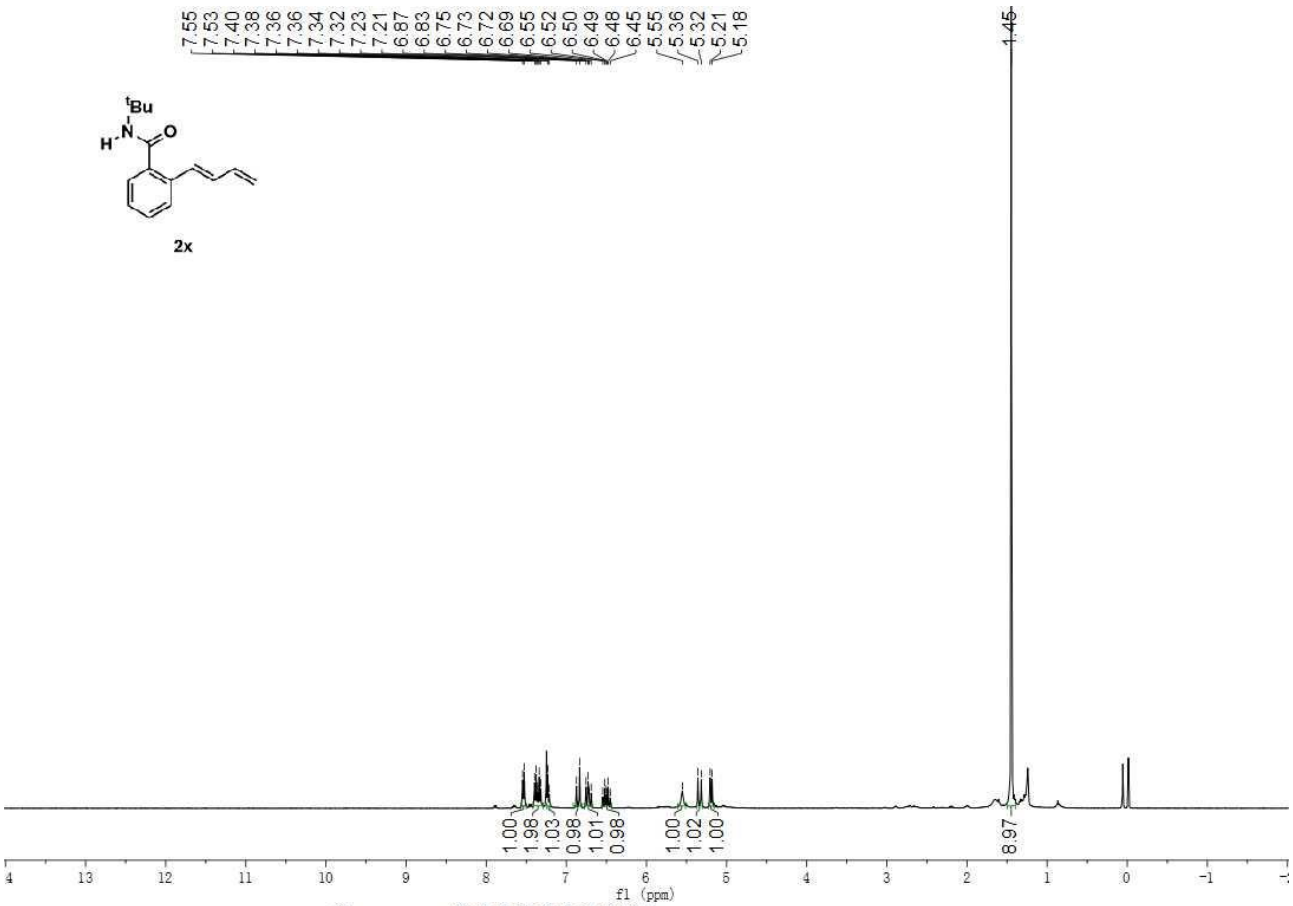
127.44
115.63
51.57
28.45
24.50
tBu
H
N
O
2w
f1 (ppm)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7.53
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7.36
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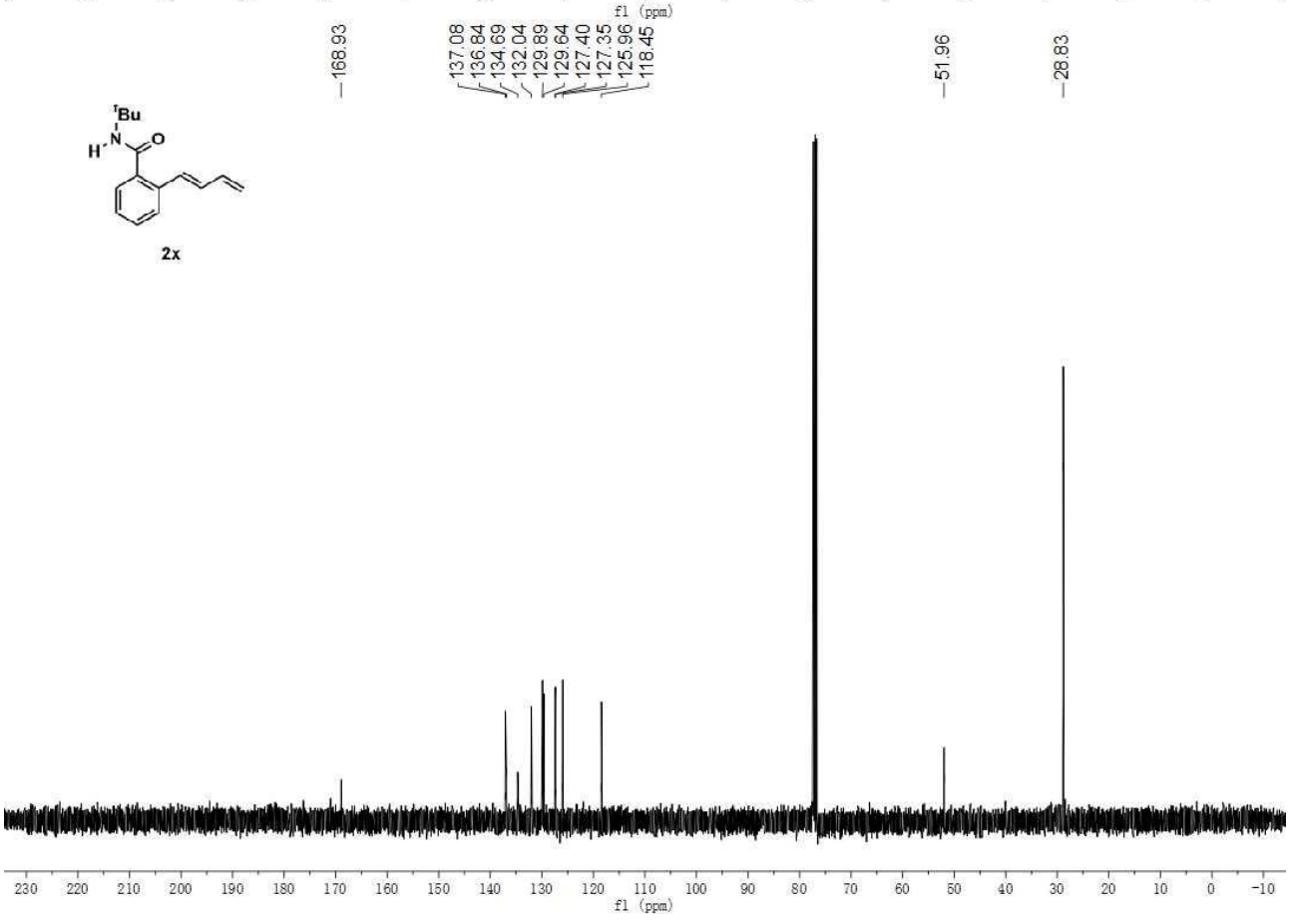
7.32
7.23
7.21
6.87
6.83
6.75
6.73
6.72
6.69
6.55
6.52
6.50
6.49
6.48
6.45
5.55
5.36
5.32
5.21
5.18
1.45
tBu
H
N
O
2x
1.00
1.98
1.03
0.98
1.01
0.98
1.00
1.02
1.00
8.97
f1 (ppm)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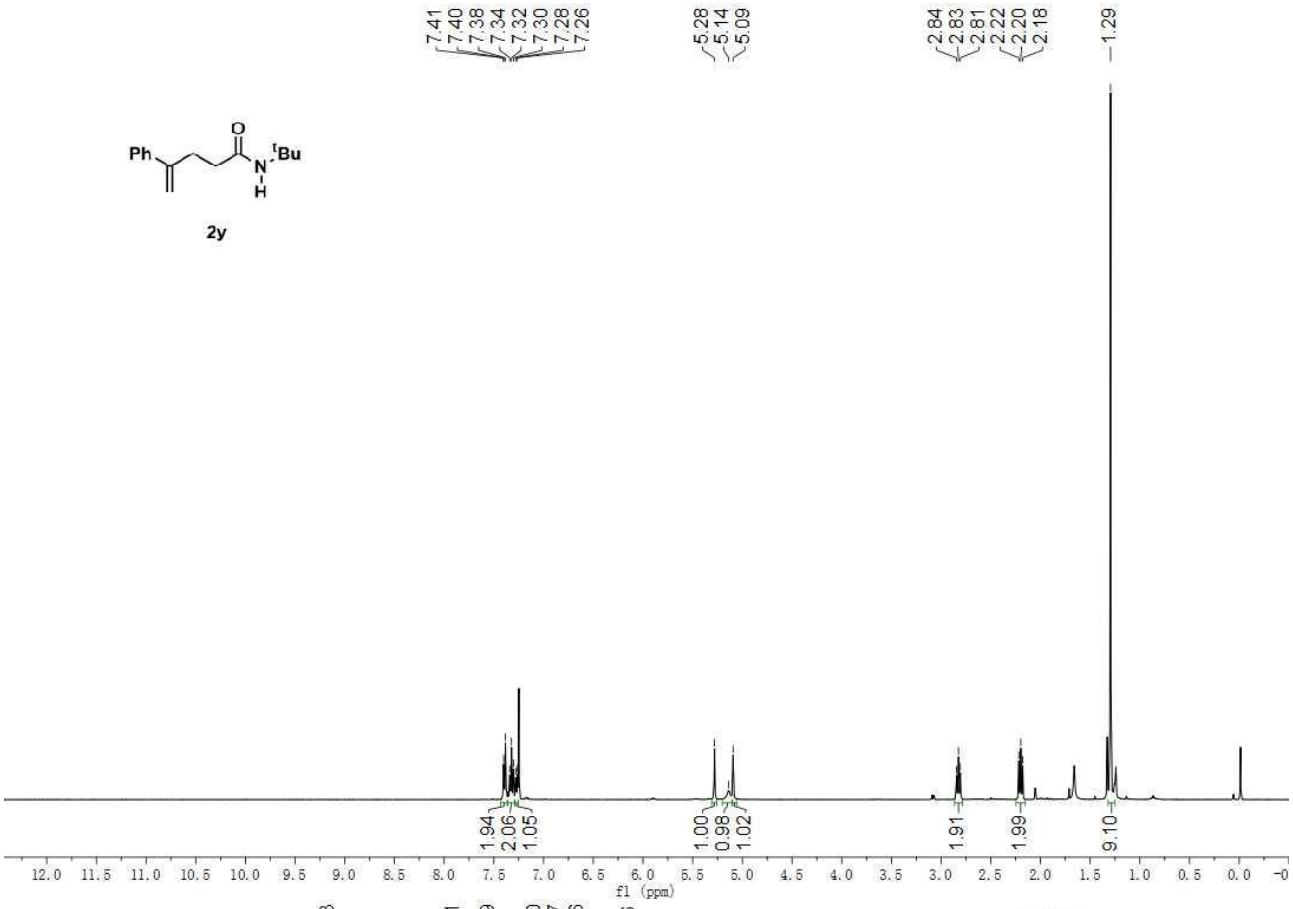
134.69
132.04
129.89
129.64
127.40
127.35
125.96
118.45
51.96
28.83
tBu
H
N
O
2x
f1 (ppm)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7.40
7.38
7.34
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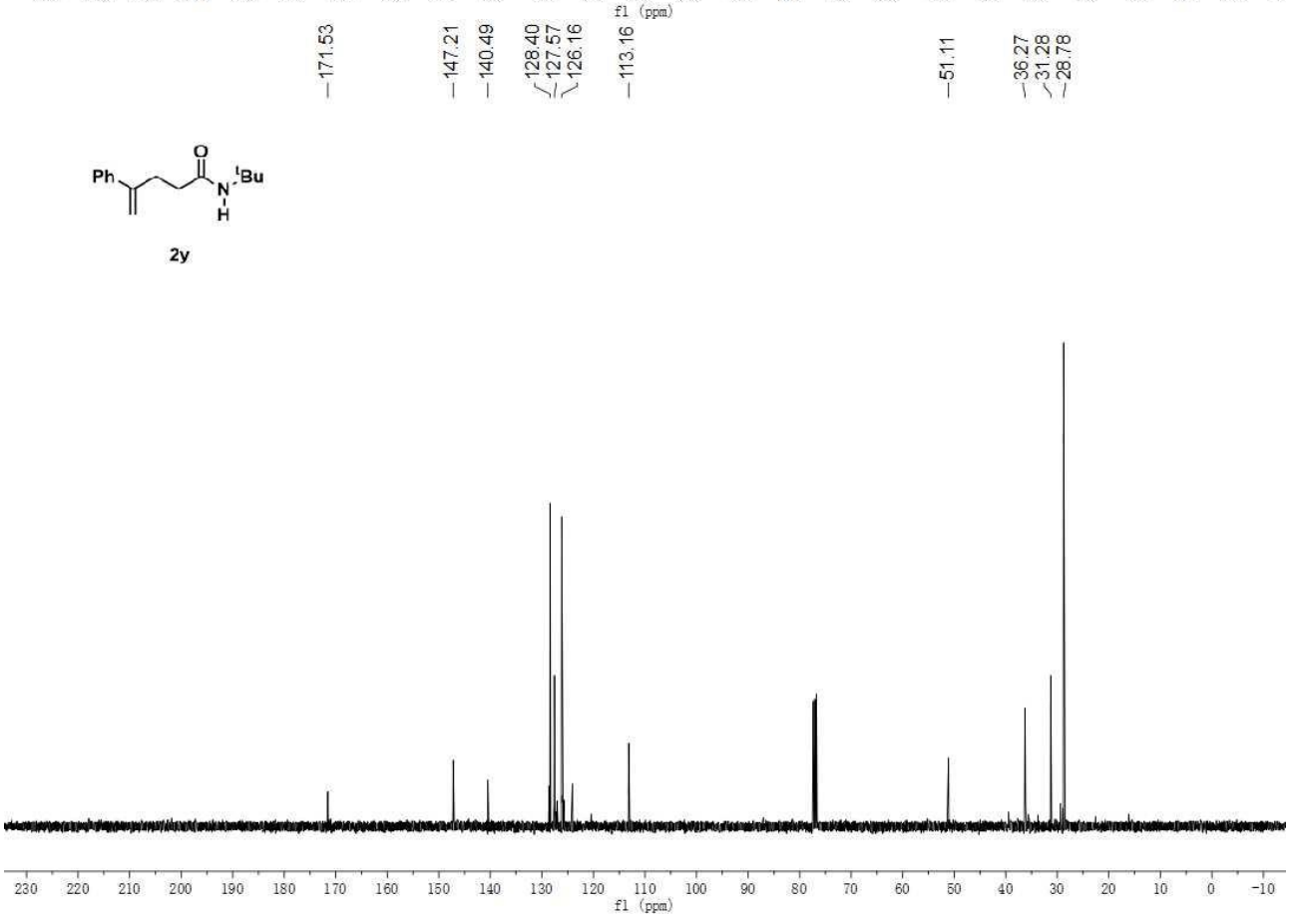
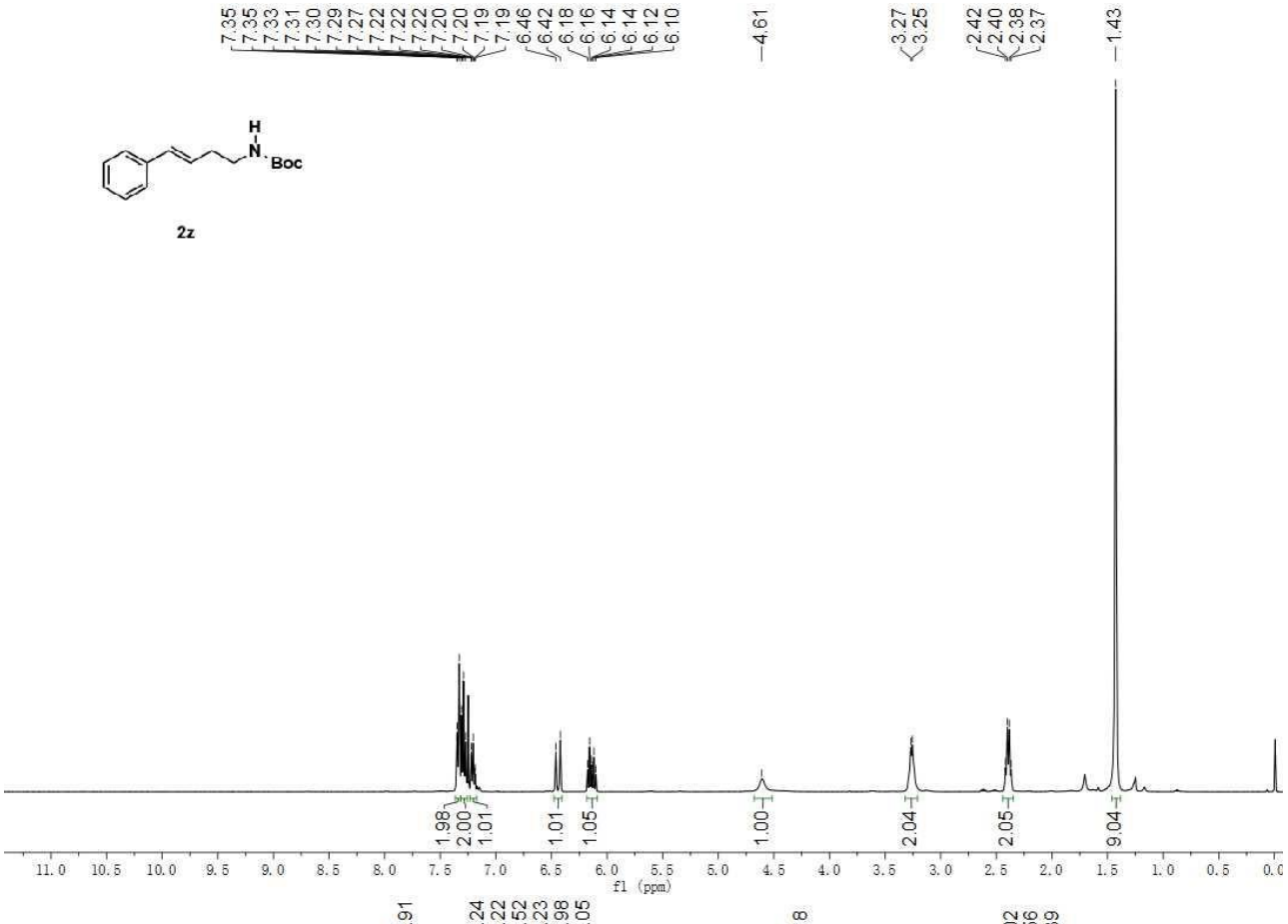
7.30
7.28
7.26
5.28
5.14
5.09
2.84
2.83
2.81
2.22
2.20
2.18
1.29
Ph
O
N
H
tBu
1.94
2.06
1.05
1.00
0.98
1.02
1.91
1.99
9.10
f1 (ppm)

2y


171.53
147.21
140.49
128.40
127.57
126.16
113.16
51.11
36.27
31.28
28.78
Ph
O
N
H
tBu
f1 (ppm)

2y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7.29
7.27
7.22
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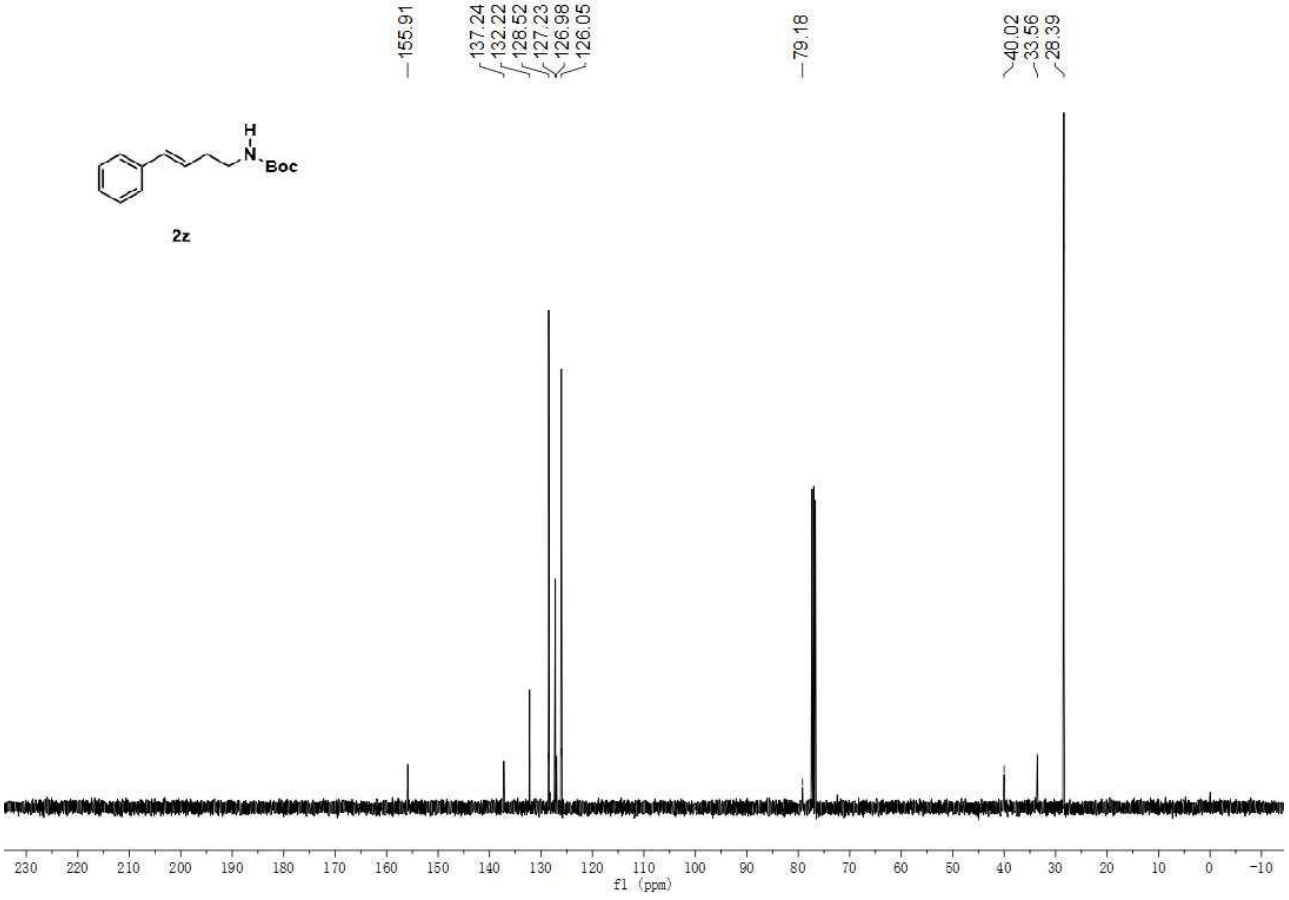
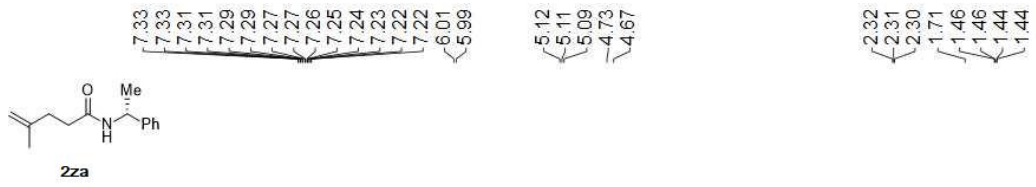
7.22
7.20
7.20
7.19
7.19
6.46
6.42
6.18
6.16
6.14
6.14
6.12
6.10
4.61
3.27
3.25
2.42
2.40
2.38
2.37
1.43
H
N
Boc
2z
1.98
2.00
1.01
1.01
1.05
1.00
2.04
2.05
9.04
f1 (ppm)


155.91
137.24
132.22
128.52
127.23
126.98
126.05
79.18
40.02
33.56
28.39
H
N
Boc
2z
f1 (ppm)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7.29
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7.27
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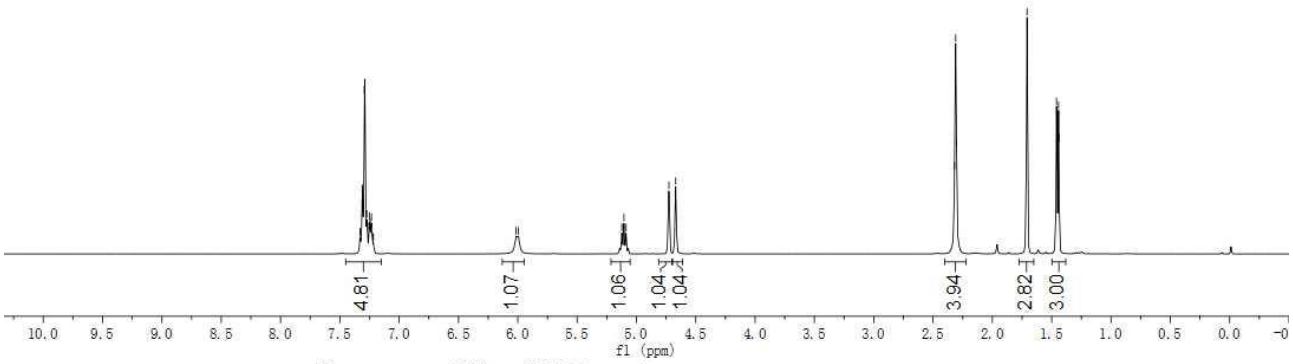
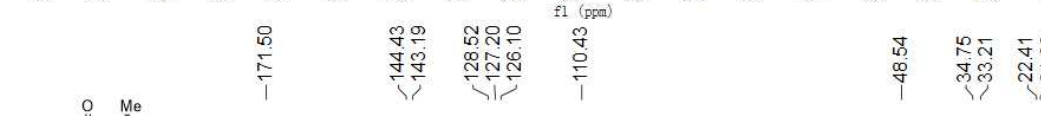
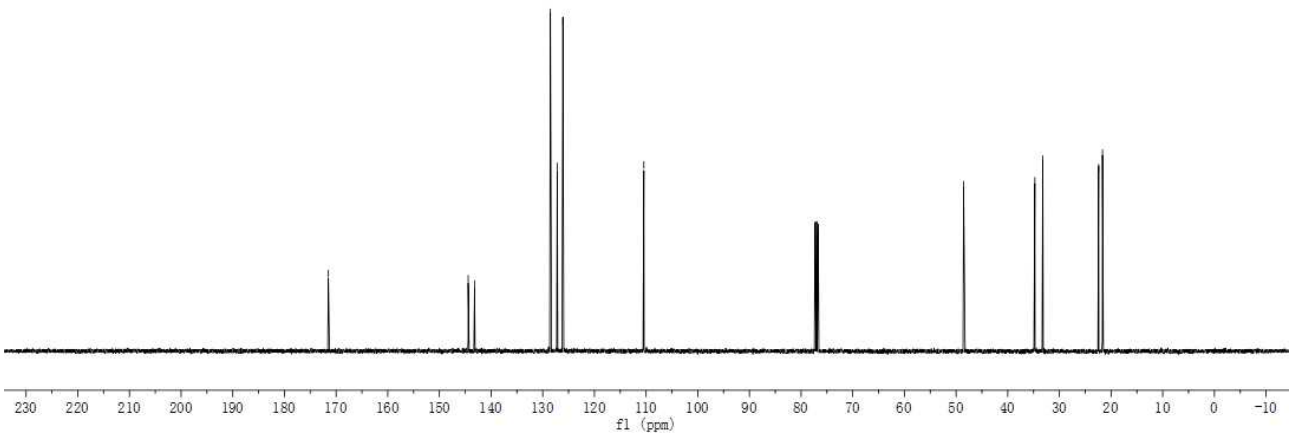
7.25
7.24
7.23
7.22
7.22
6.01
5.99
5.12
5.11
5.09
4.73
4.67
2.32
2.31
2.30
1.71
1.46
1.46
1.44
1.44
1.44
O
Me
N
H
Ph

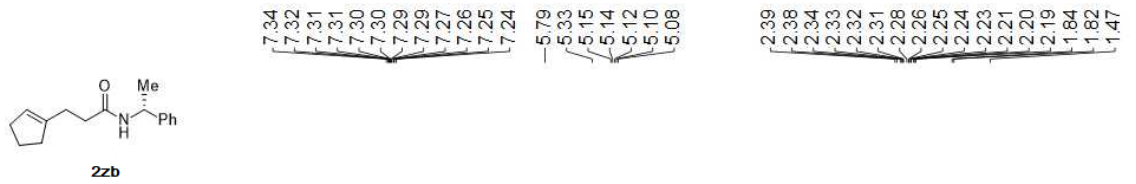
2za


4.81
1.07
1.06
1.04
1.04
3.94
2.82
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


171.50
144.43
143.19
128.52
127.20
126.10
110.43
48.54
34.75
33.21
22.41
21.66
O
Me
N
H
Ph

2za


230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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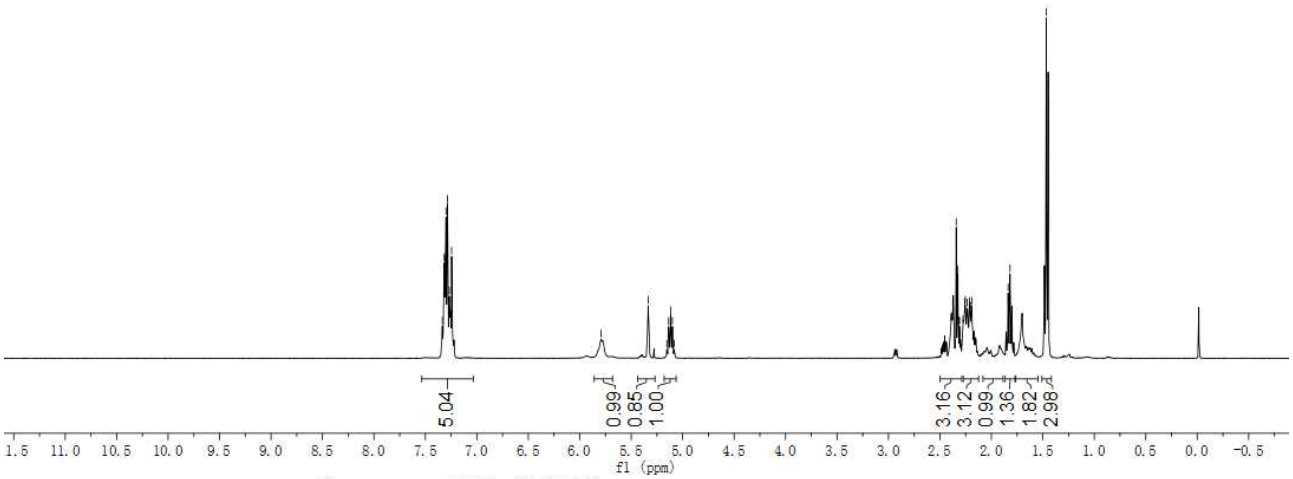
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.27
7.26
7.25
7.24
5.79
5.33
5.15
5.14
5.12
5.10
5.08
2.39
2.38
2.34
2.33
2.32
2.31
2.28
2.26
2.25
2.24
2.23
2.21
2.20
2.19
1.84
1.82
1.47

O
Me
N
H
Ph

2zb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1.00
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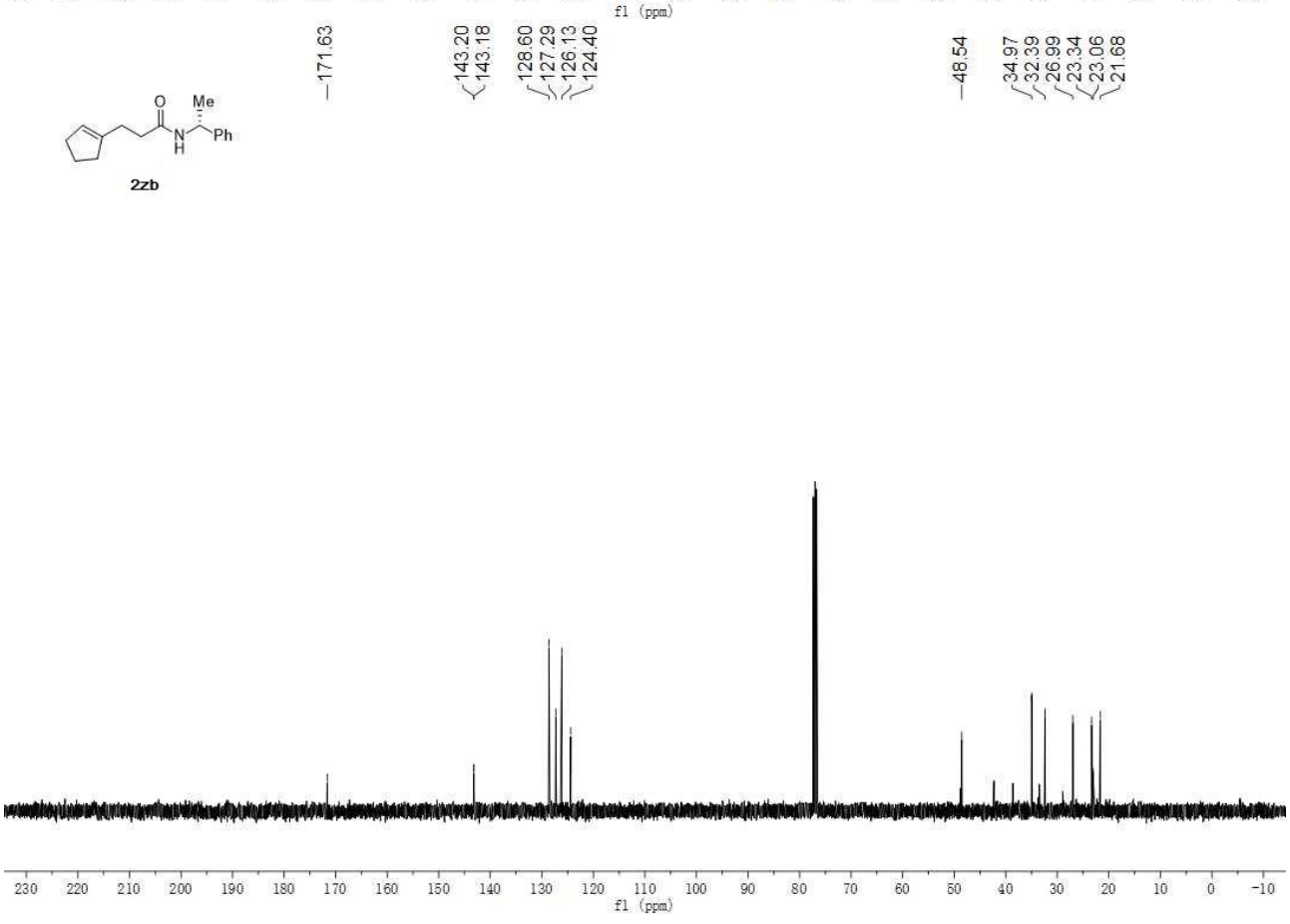
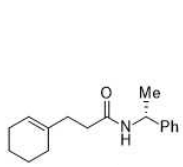
3.12
0.99
1.36
1.82
2.98
f1 (ppm)

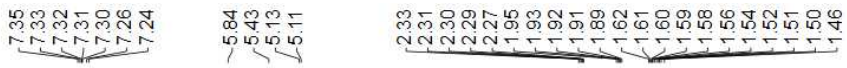

171.63
143.20
143.18
128.60
127.29
126.13
124.40
48.54
34.97
32.39
26.99
23.34
23.06
21.68
f1 (ppm)

O
Me
N
H
Ph

2zb


Me
O
N
H
Ph

2zc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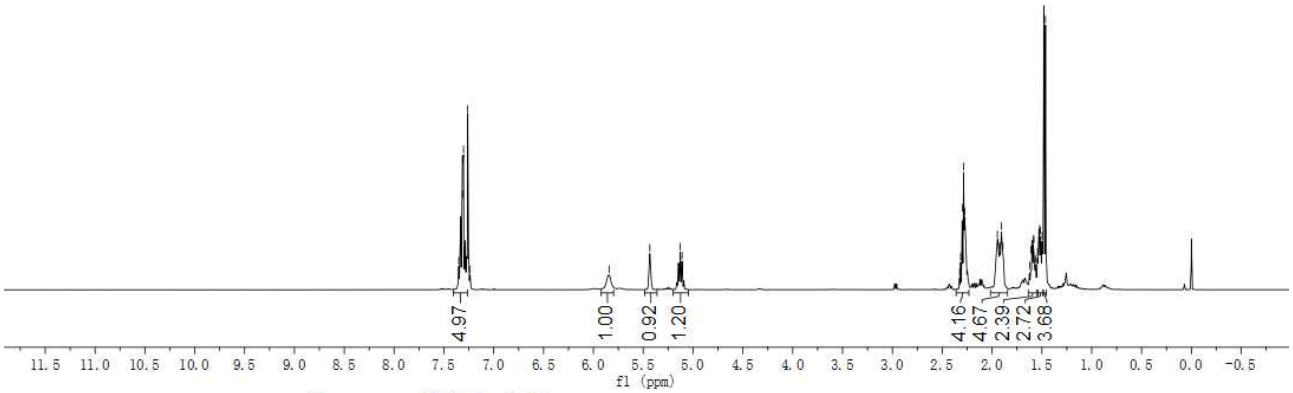
7.30
7.26
7.24
5.84
5.43
5.13
5.11
2.33
2.31
2.30
2.29
2.27
1.95
1.93
1.92
1.91
1.89
1.62
1.61
1.60
1.59
1.58
1.56
1.54
1.52
1.51
1.50
1.46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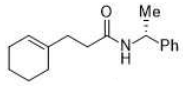
4.16
4.67
2.39
2.72
3.68
f1 (ppm)


Me
O
N
H
Ph

2zc


171.86
143.25
136.36
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127.31
126.17
122.24
48.58
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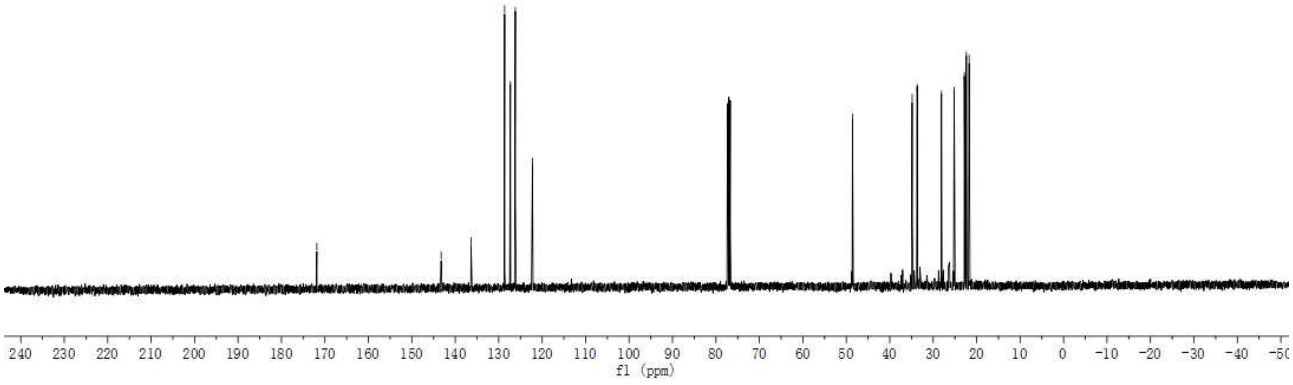
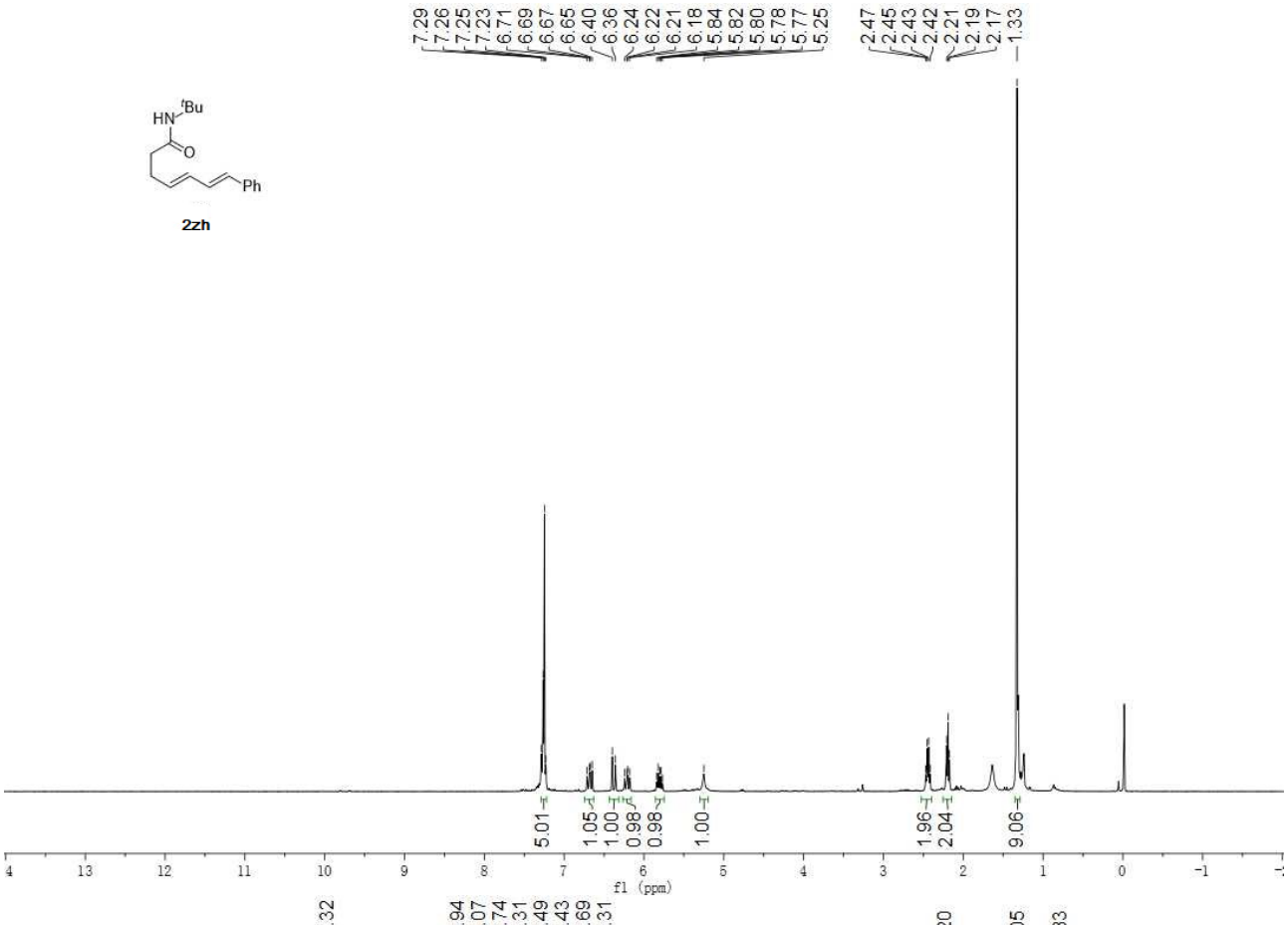
33.69
28.11
25.18
22.84
22.38
21.75


f1 (ppm)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7.23
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6.69
6.67
6.65
6.40
6.36
6.24
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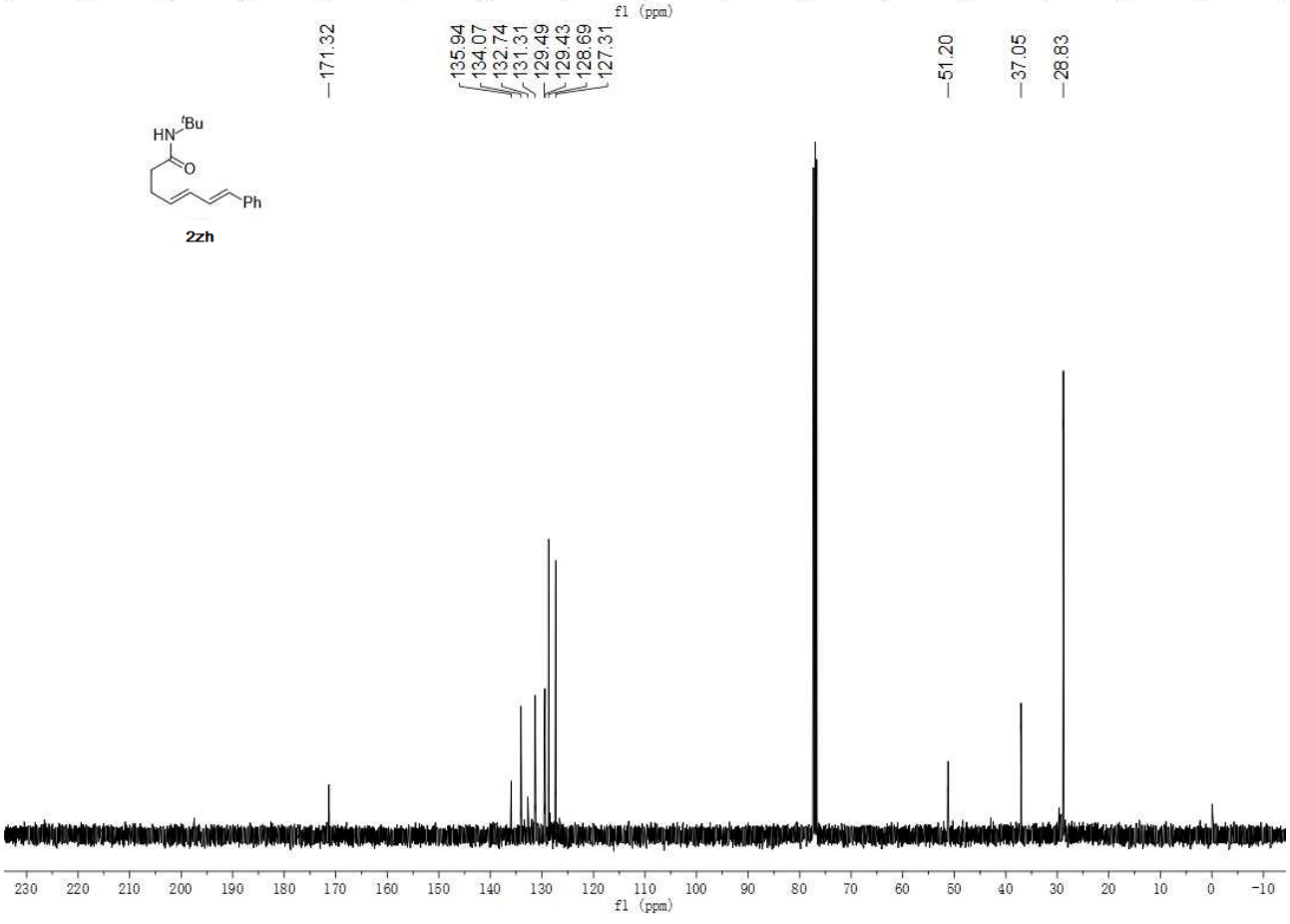
6.21
6.18
5.84
5.82
5.80
5.78
5.77
5.25
2.47
2.45
2.43
2.42
2.21
2.19
2.17
1.33
HN
tBu
O
Ph
2zh
5.01
1.05
1.00
0.98
0.98
1.00
1.96
2.04
9.06
f1 (ppm)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134.07
132.74
131.31
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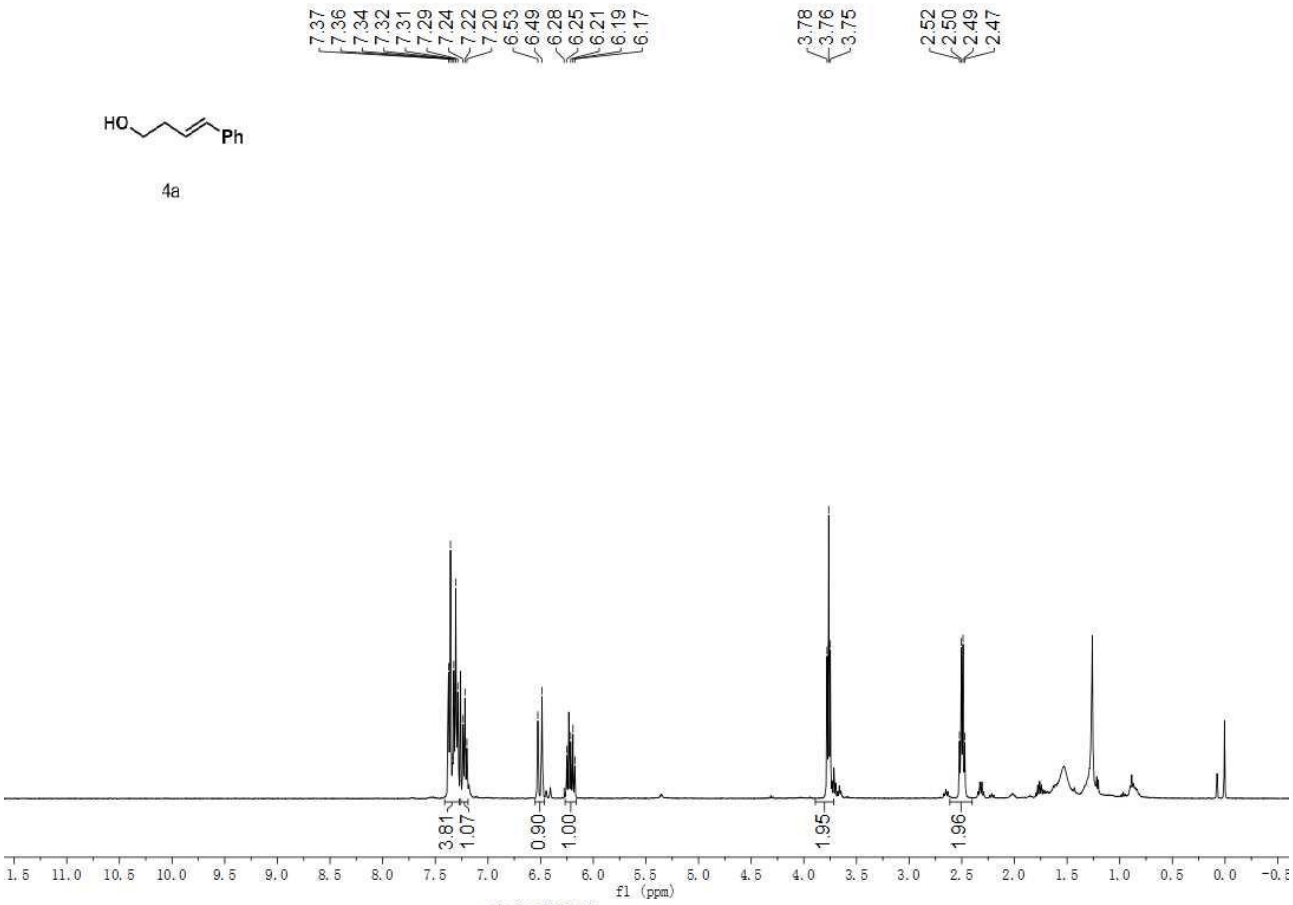
128.69
127.31
51.20
37.05
28.83
HN
tBu
O
Ph
2zh
f1 (ppm)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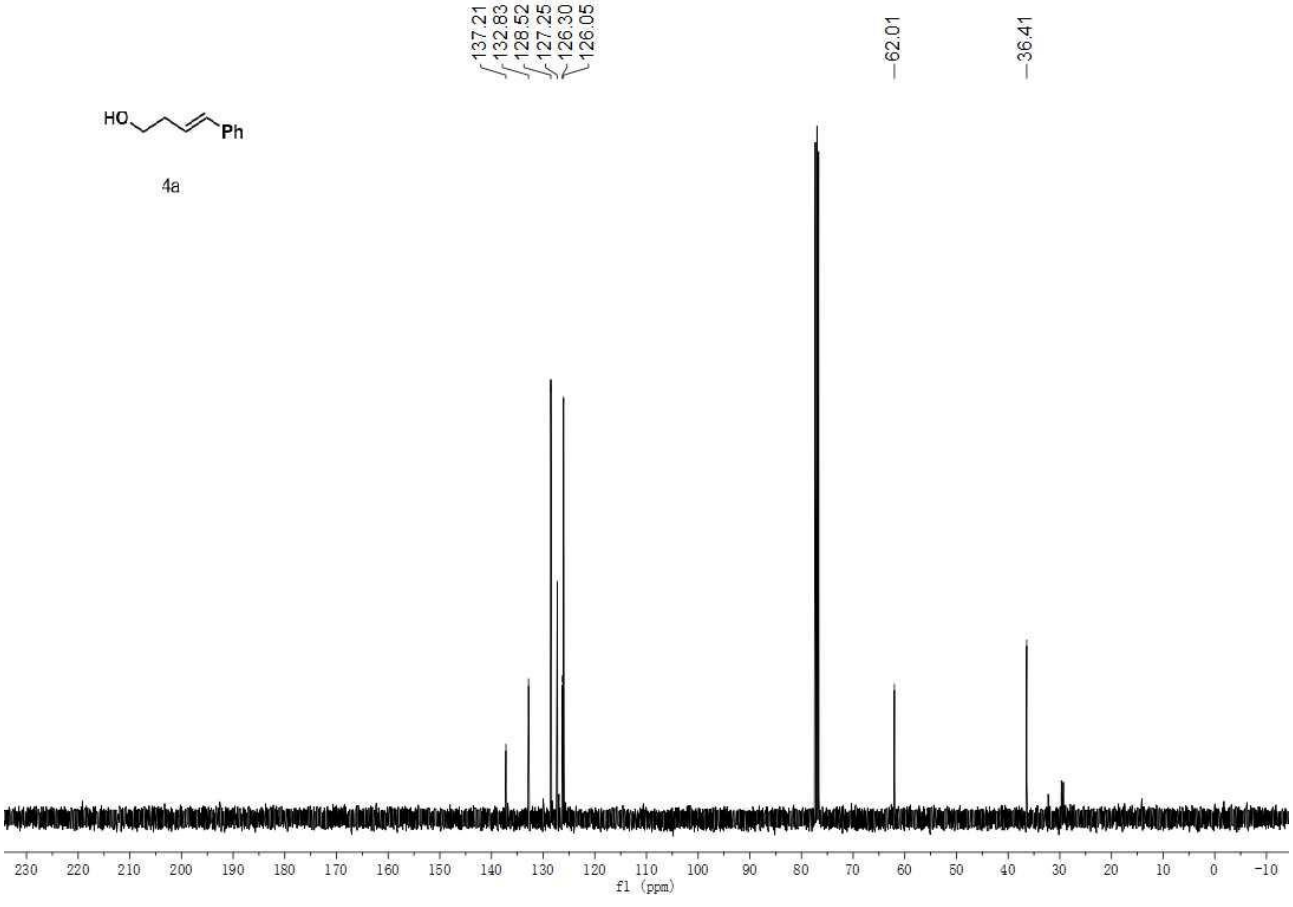
6.21
6.19
6.17
3.78
3.76
3.75
2.52
2.50
2.49
2.47
HO
Ph
4a
3.81
1.07
0.90
1.00
1.95
1.96
f1 (ppm)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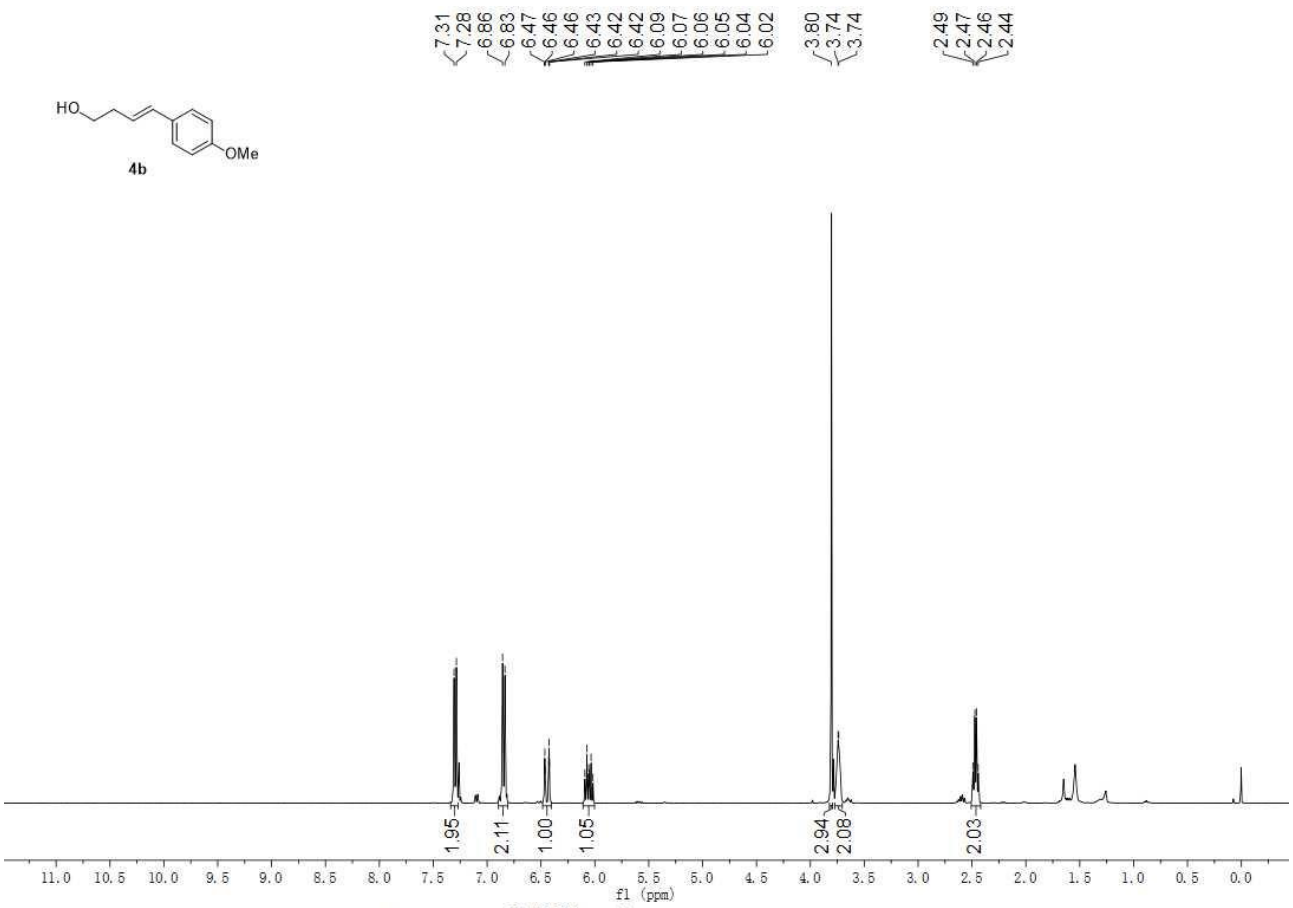
126.05
62.01
36.41
HO
Ph
4a
f1 (ppm)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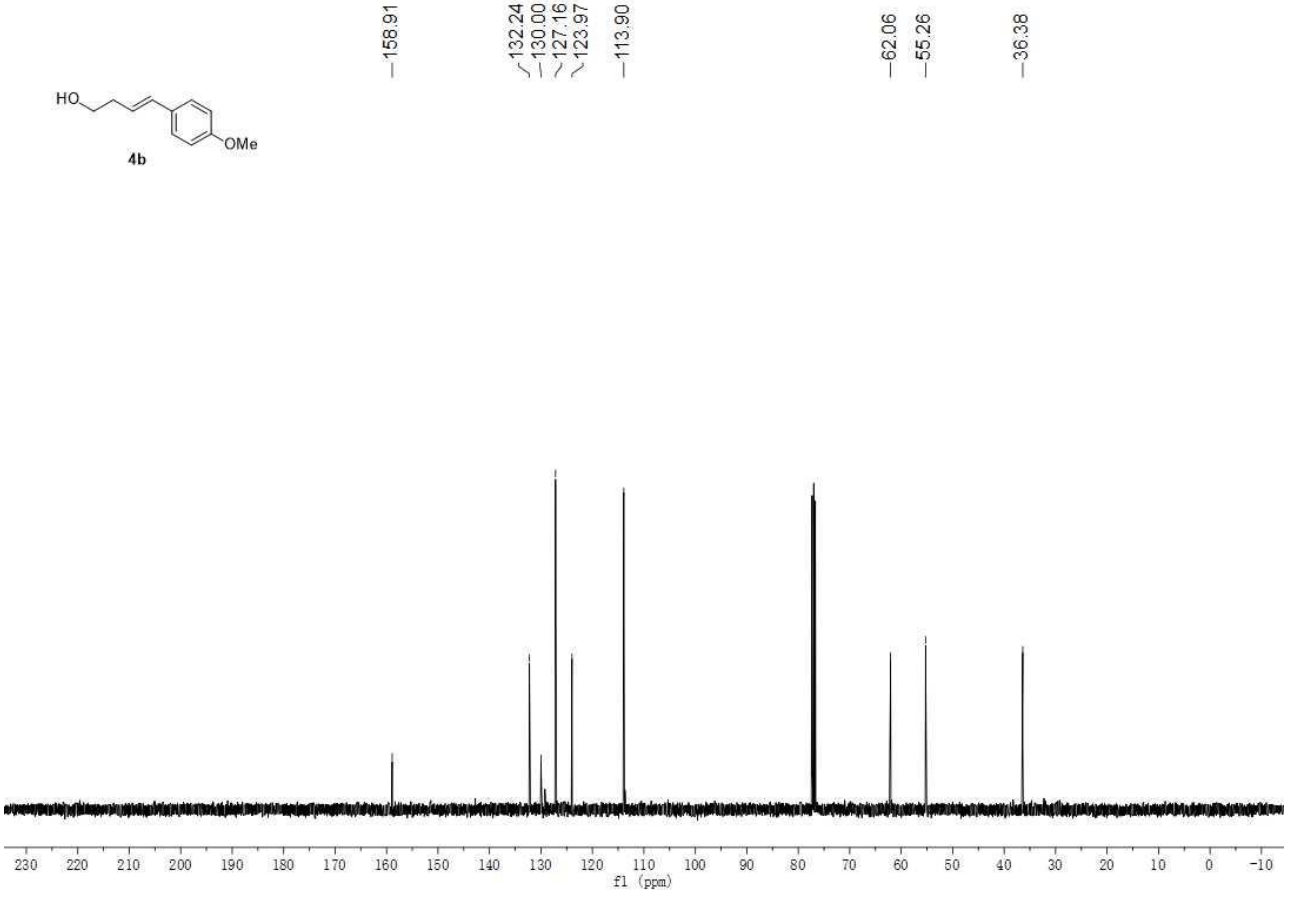
6.46
6.43
6.42
6.42
6.09
6.07
6.06
6.05
6.04
6.02
3.80
3.74
3.74
2.49
2.47
2.46
2.44
HO
OMe
4b
1.95
2.11
1.00
1.05
2.94
2.08
2.03
f1 (ppm)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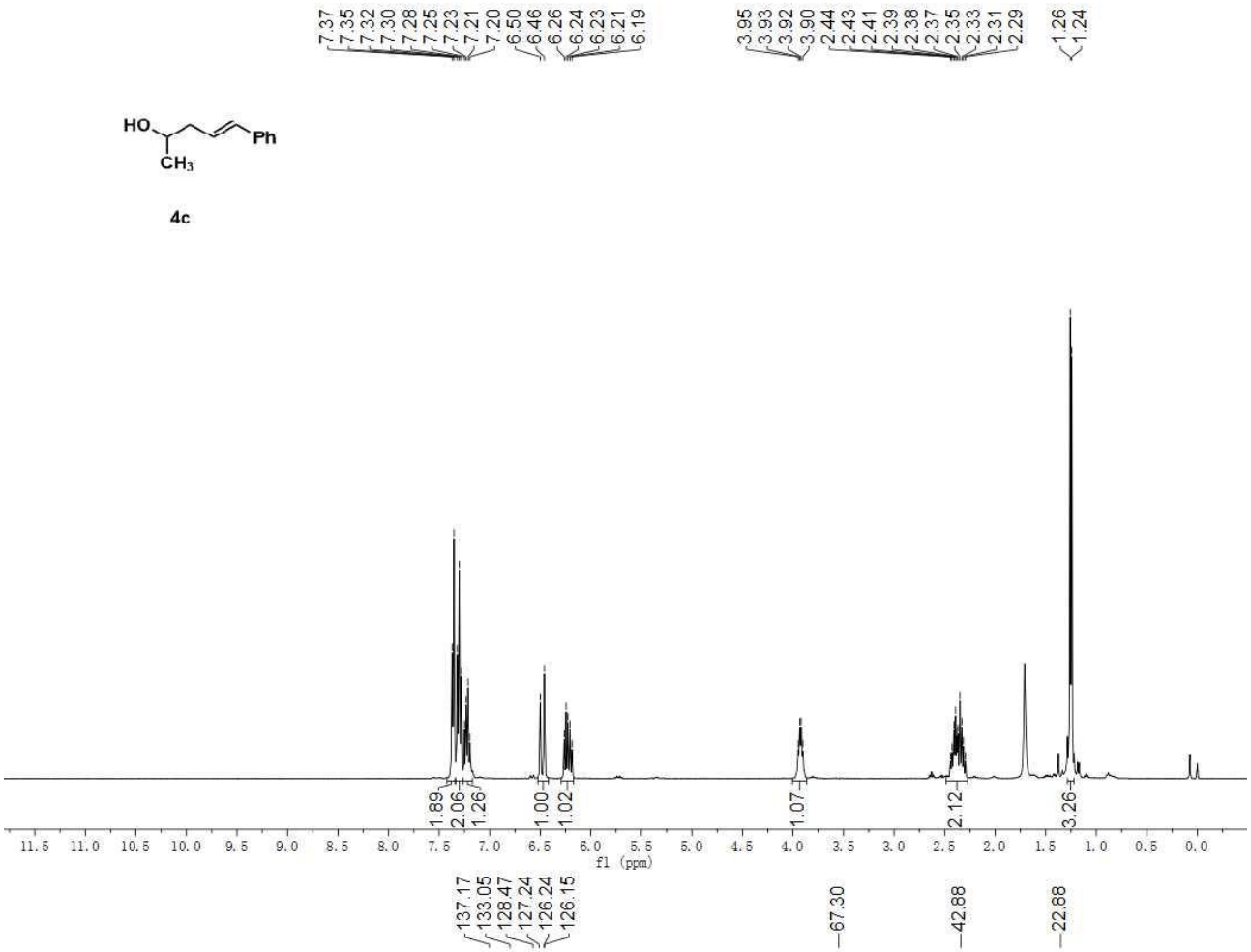
62.06
55.26
36.38
HO
OMe
4b
f1 (ppm)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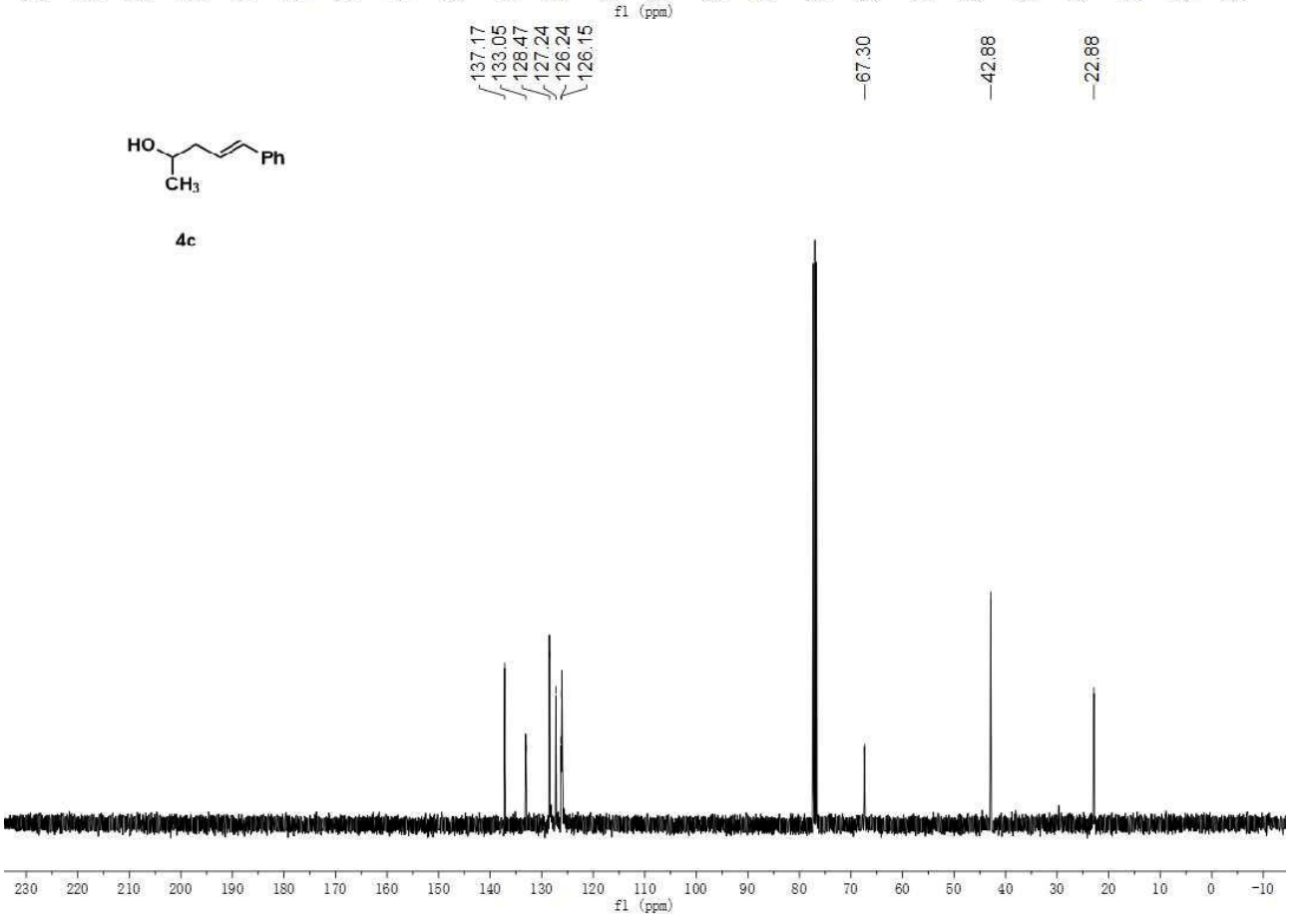
6.26
6.24
6.23
6.21
6.19
3.95
3.93
3.92
3.90
2.44
2.43
2.41
2.39
2.38
2.37
2.35
2.33
2.31
2.29
1.26
1.24
HO
Ph
CH3
4c
1.89
2.06
1.26
1.00
1.02
1.07
2.12
3.26
f1 (ppm)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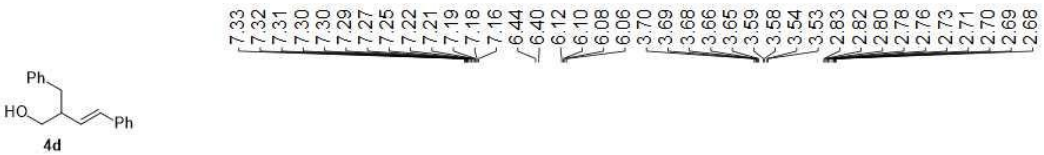
22.88
HO
Ph
CH3
4c
f1 (ppm)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7.19
7.18
7.16
6.44
6.40
6.12
6.10
6.08
6.06
3.70
3.69
3.68
3.66
3.65
3.59
3.58
3.54
3.53
2.83
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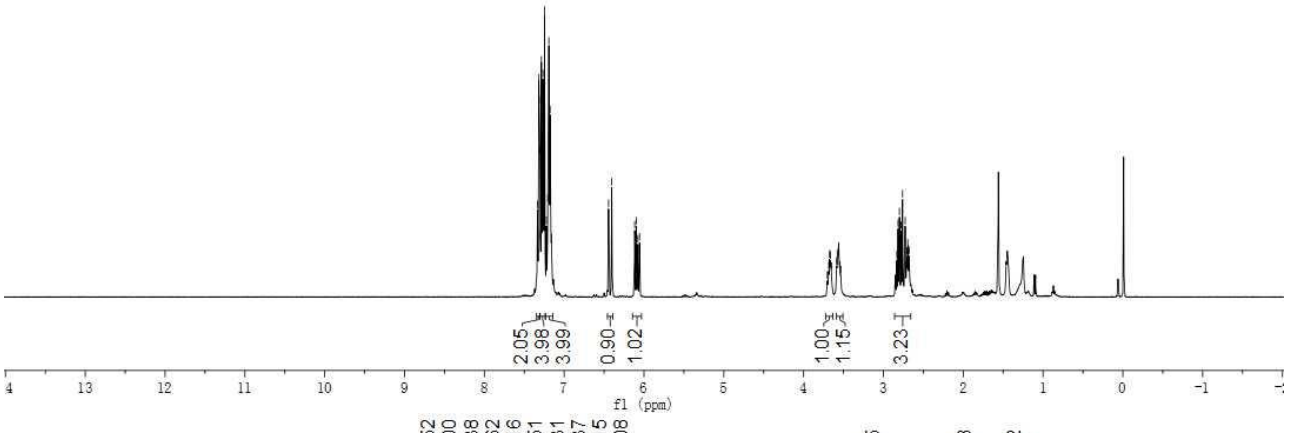
2.76
2.73
2.71
2.70
2.69
2.68

Ph
HO
Ph

4d


2.05
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3.99
0.90
1.02
1.00
1.15
3.23
f1 (ppm)


139.52
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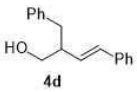
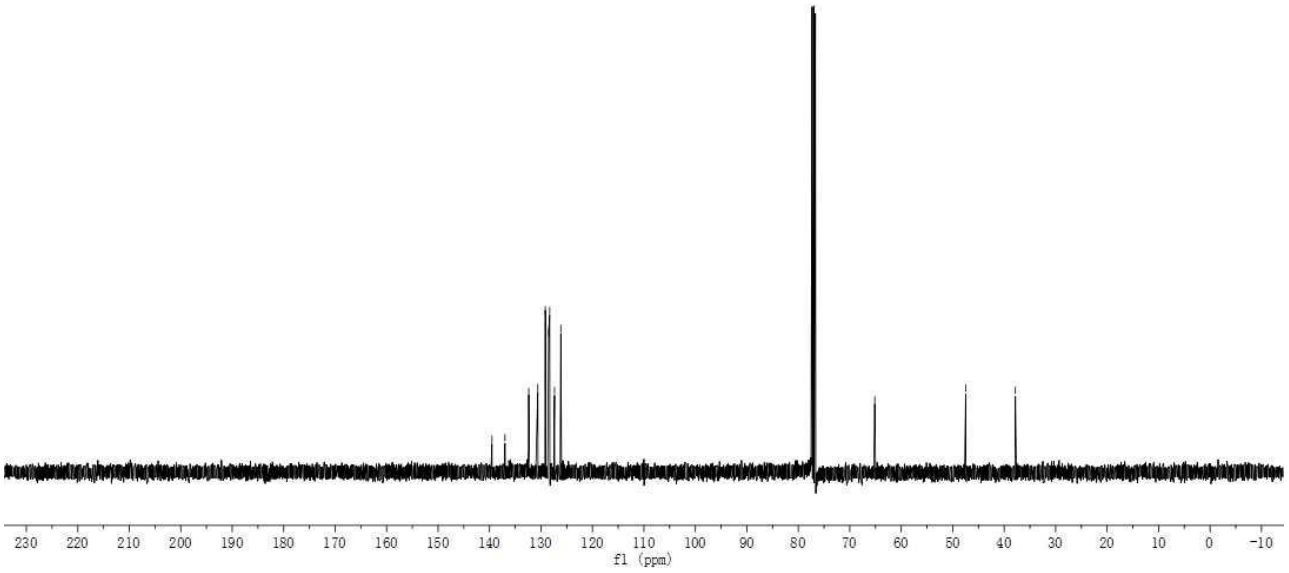
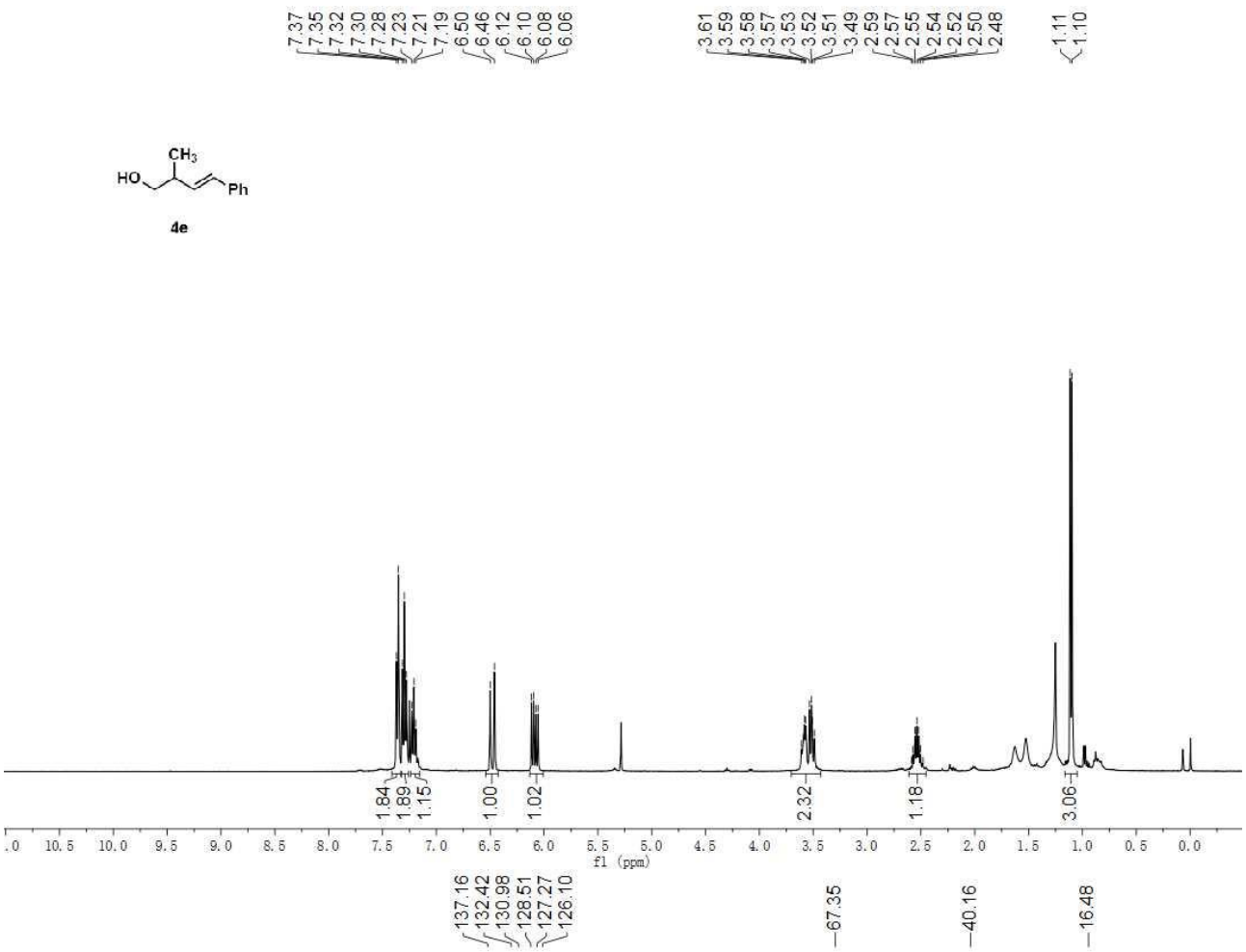
129.16
128.51
128.31
127.37
126.15
126.08
65.15
47.48
37.82


Ph
HO
Ph

4d


f1 (ppm)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6.46
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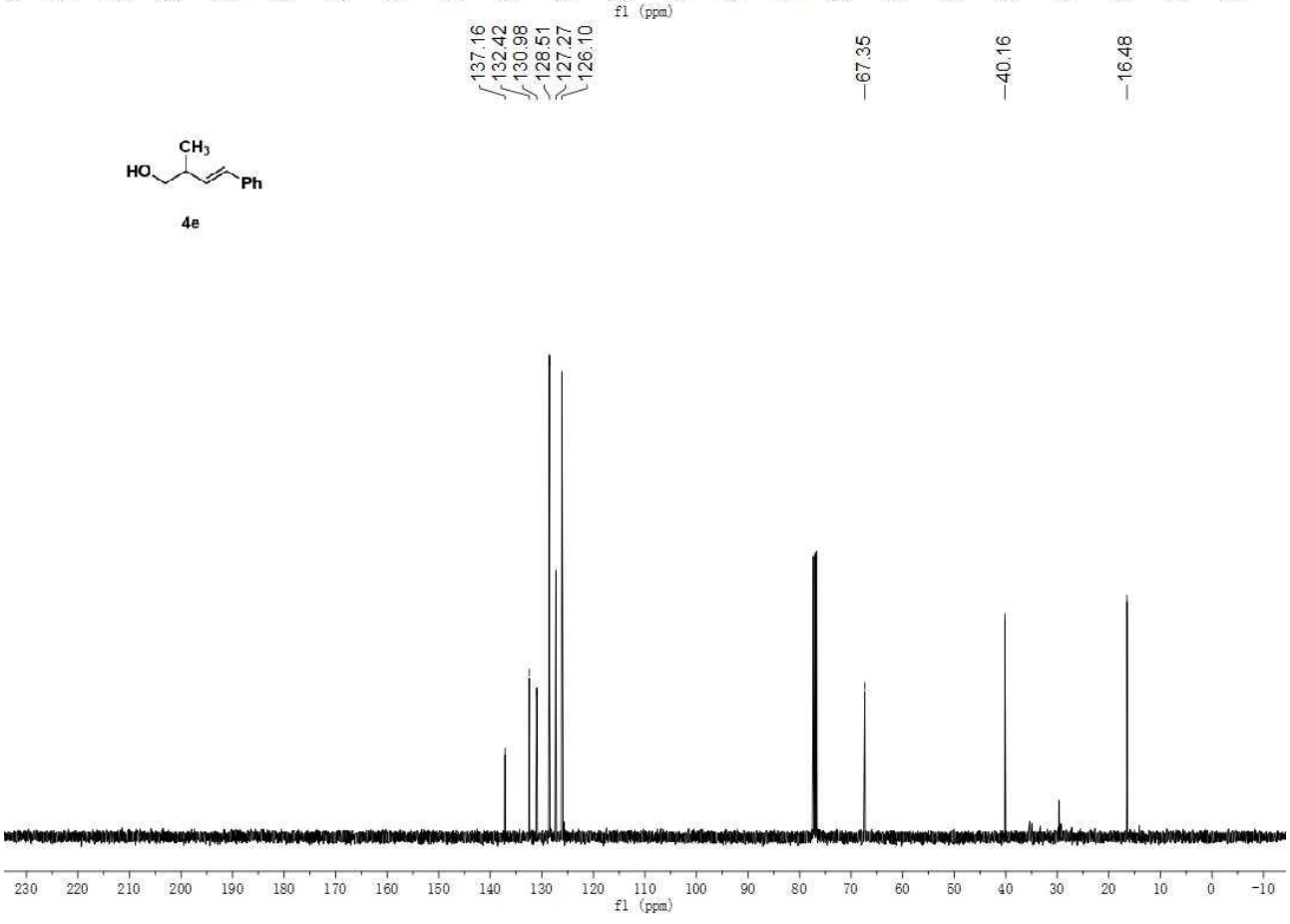
6.10
6.08
6.06
3.61
3.59
3.58
3.57
3.53
3.52
3.51
3.49
2.59
2.57
2.55
2.54
2.52
2.50
2.48
1.11
1.10
CH3
HO
Ph
4e
1.84
1.89
1.15
1.00
1.02
2.32
1.18
3.06
f1 (ppm)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126.10
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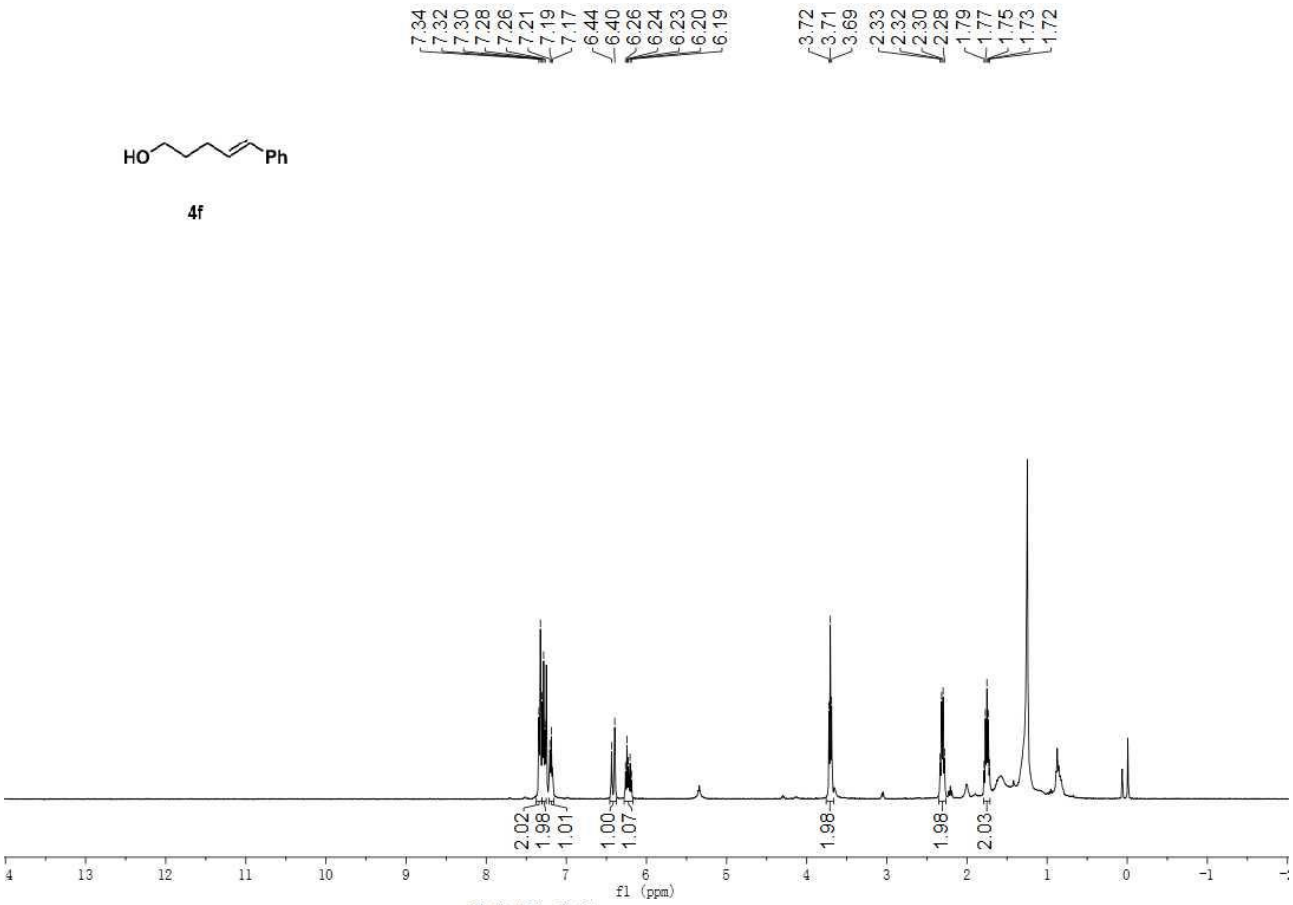
16.48
CH3
HO
Ph
4e
f1 (ppm)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7.28
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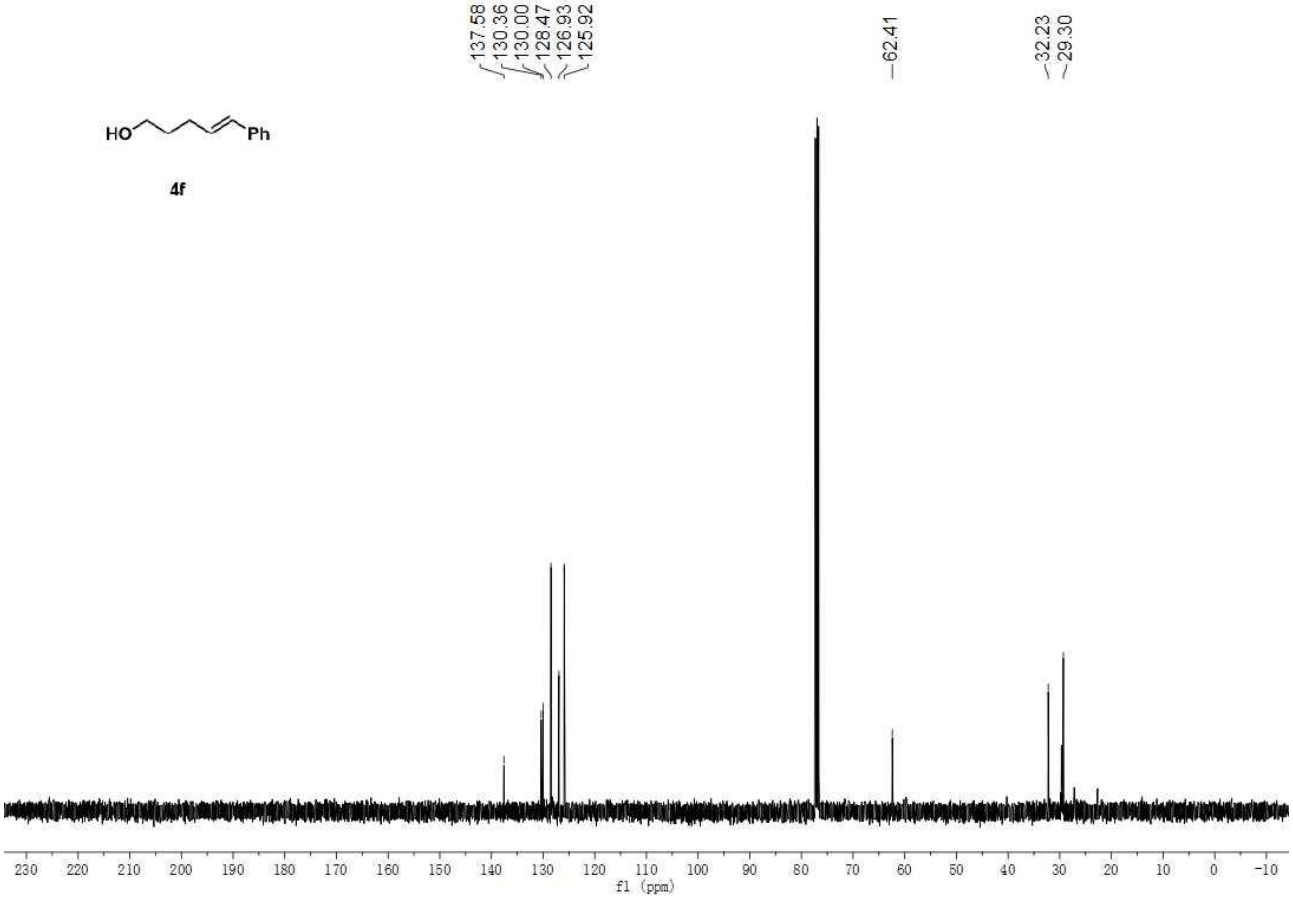
7.21
7.19
7.17
6.44
6.40
6.26
6.24
6.23
6.20
6.19
3.72
3.71
3.69
2.33
2.32
2.30
2.28
1.79
1.77
1.75
1.73
1.72
HO
Ph
4f
2.02
1.98
1.01
1.00
1.07
1.98
1.98
2.03
f1 (ppm)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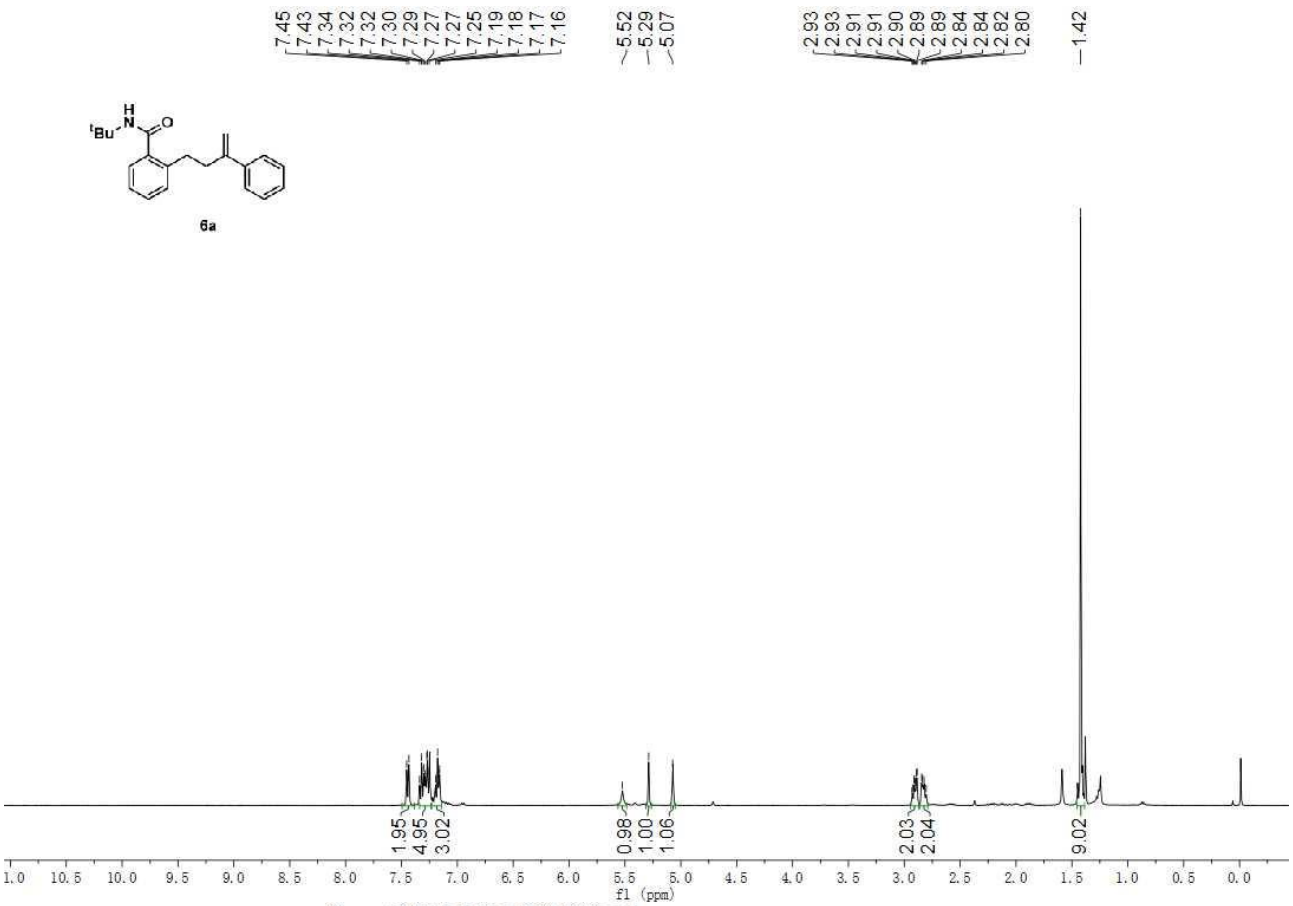
29.30
HO
Ph
4f
f1 (ppm)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7.30
7.29
7.27
7.27
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7.19
7.18
7.17
7.16
5.52
5.29
5.07
2.93
2.93
2.91
2.91
2.90
2.89
2.89
2.84
2.84
2.82
2.80
1.42
6a
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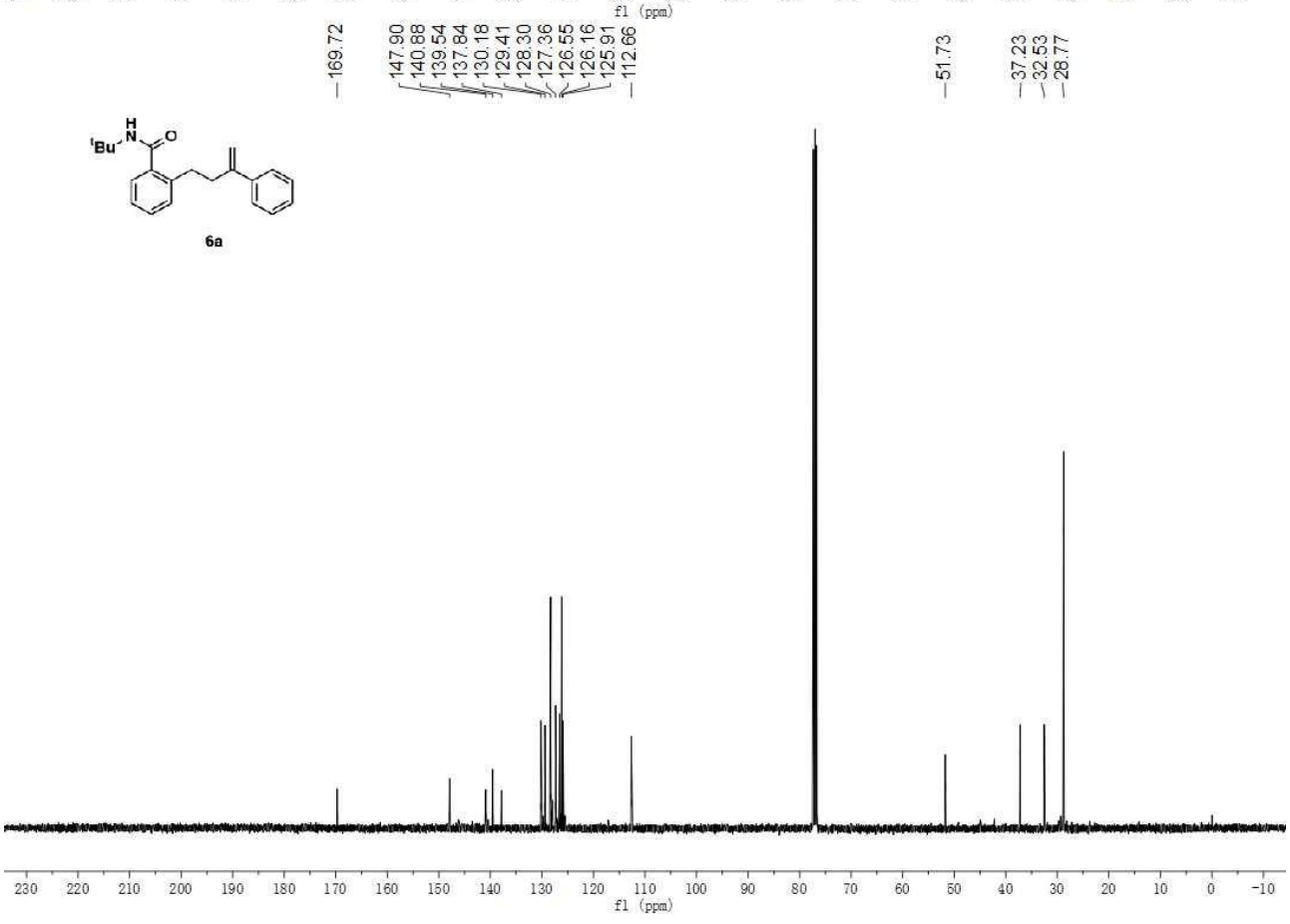
4.95
3.02
0.98
1.00
1.06
2.03
2.04
9.02
f1 (ppm)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126.16
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112.66
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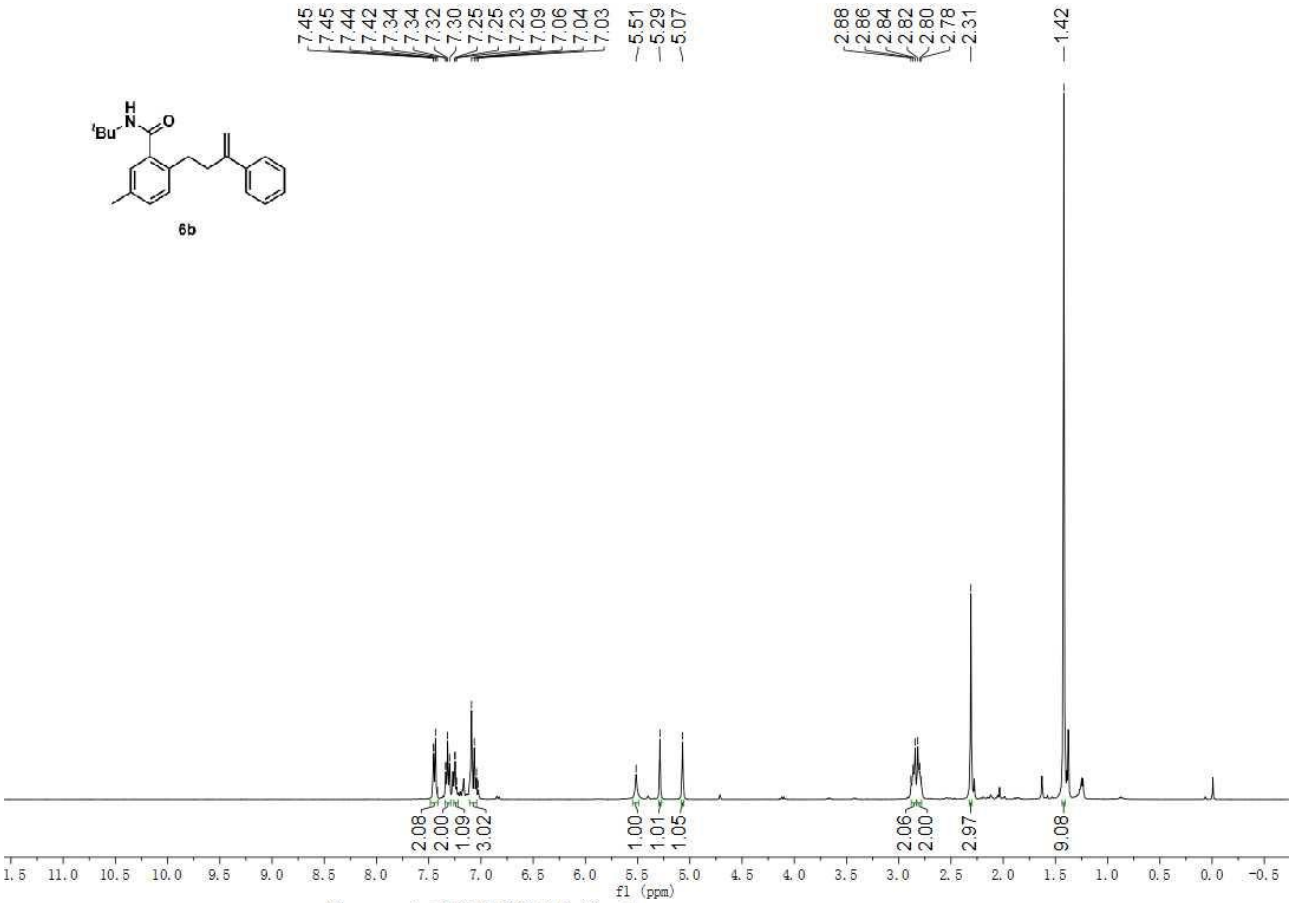
37.23
32.53
28.77
6a
f1 (ppm)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7.32
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7.25
7.23
7.09
7.06
7.04
7.03
5.51
5.29
5.07
2.88
2.86
2.84
2.82
2.80
2.78
2.31
1.42
2.08
2.00
1.09
3.02
1.00
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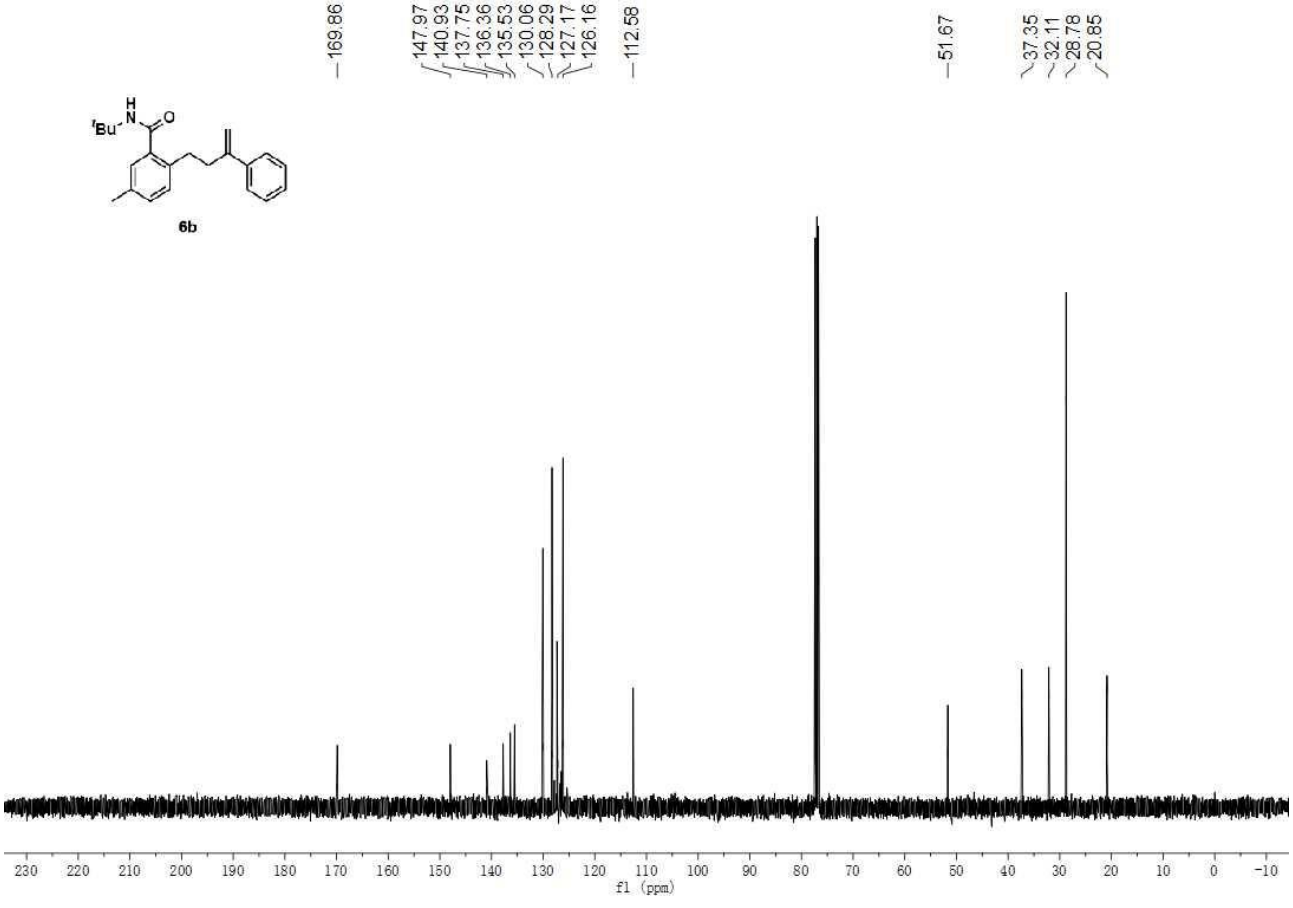
2.00
2.97
9.08
f1 (ppm)

6b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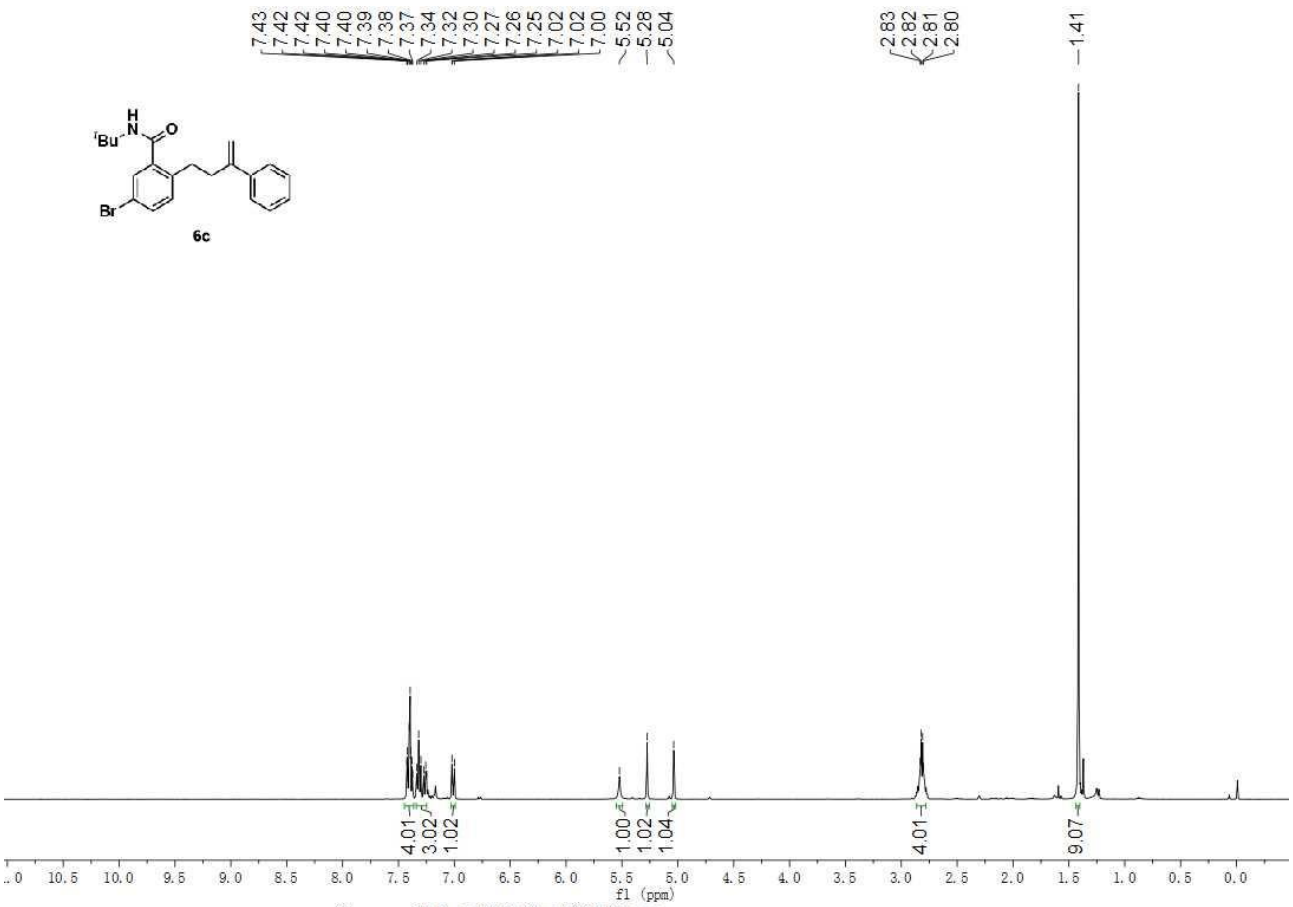
126.16
112.58
51.67
37.35
32.11
28.78
20.85
f1 (ppm)

6b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7.42
7.42
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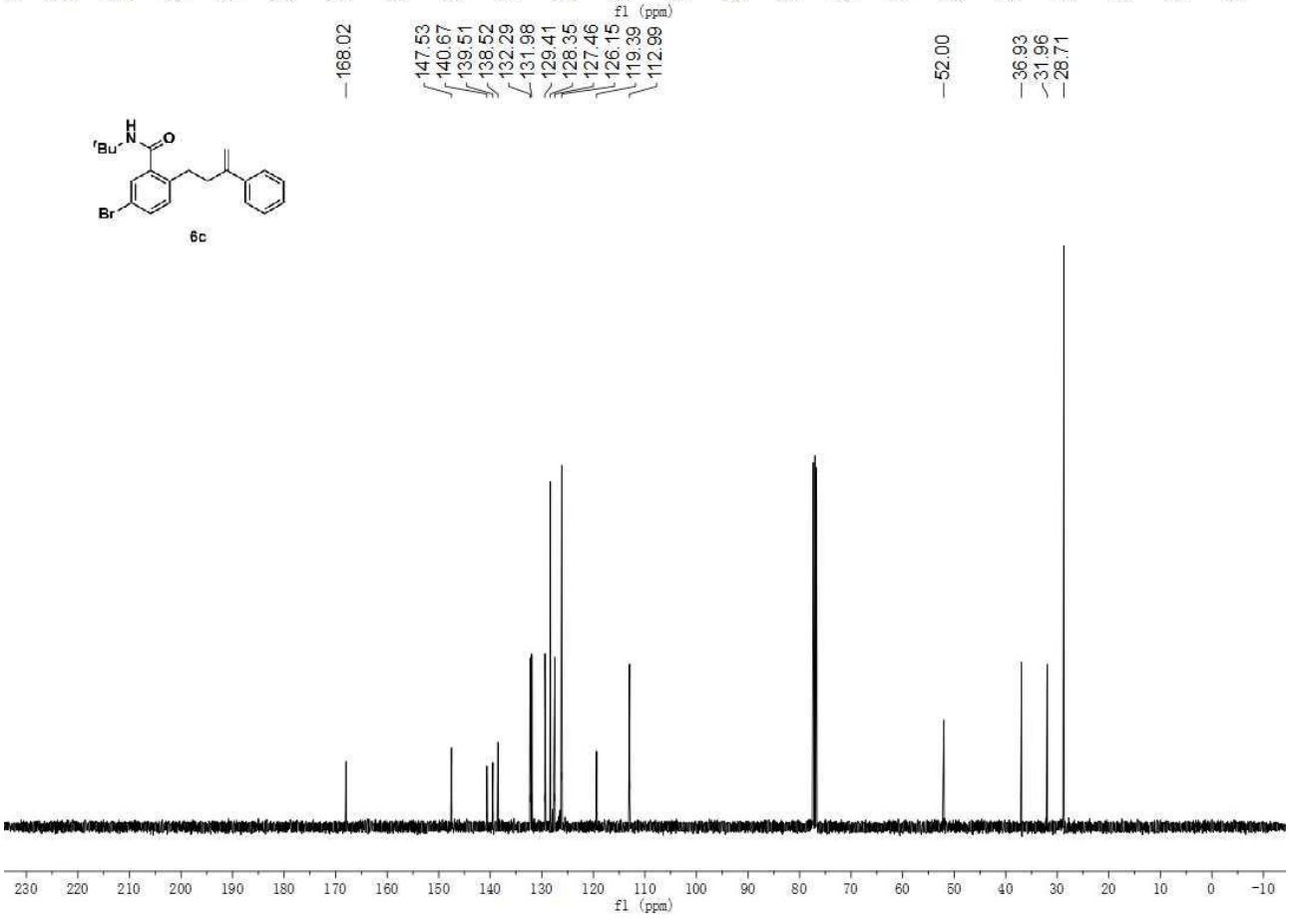
7.39
7.38
7.37
7.34
7.32
7.30
7.27
7.26
7.25
7.02
7.02
7.00
5.52
5.28
5.04
2.83
2.82
2.81
2.80
1.41
4.01
3.02
1.02
1.00
1.02
1.04
4.01
9.07
f1 (ppm)

tBu
H
N
O
Br

6c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129.41
128.35
127.46
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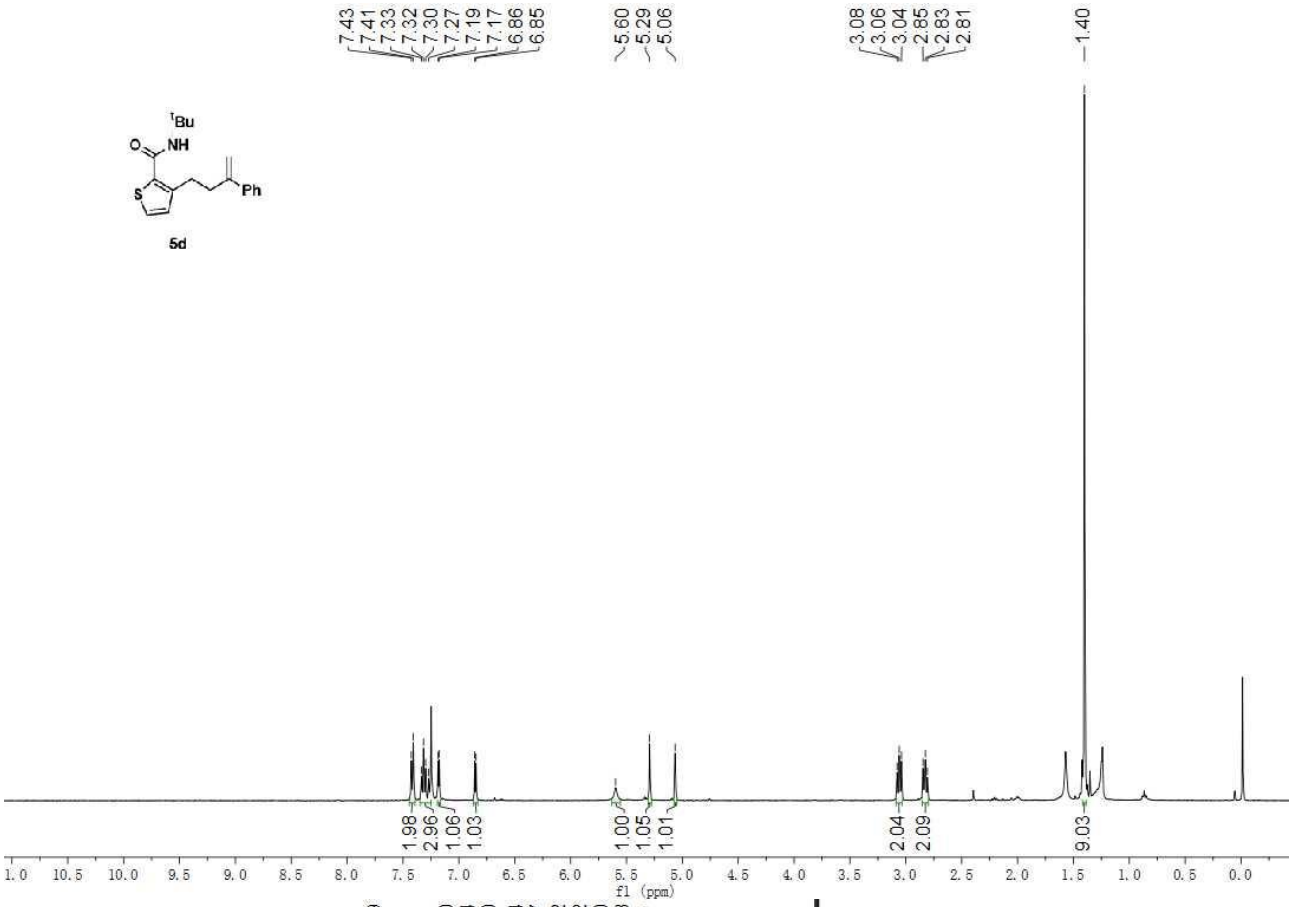
119.39
112.99
52.00
36.93
31.96
28.71
f1 (ppm)

tBu
H
N
O
Br

6c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7.17
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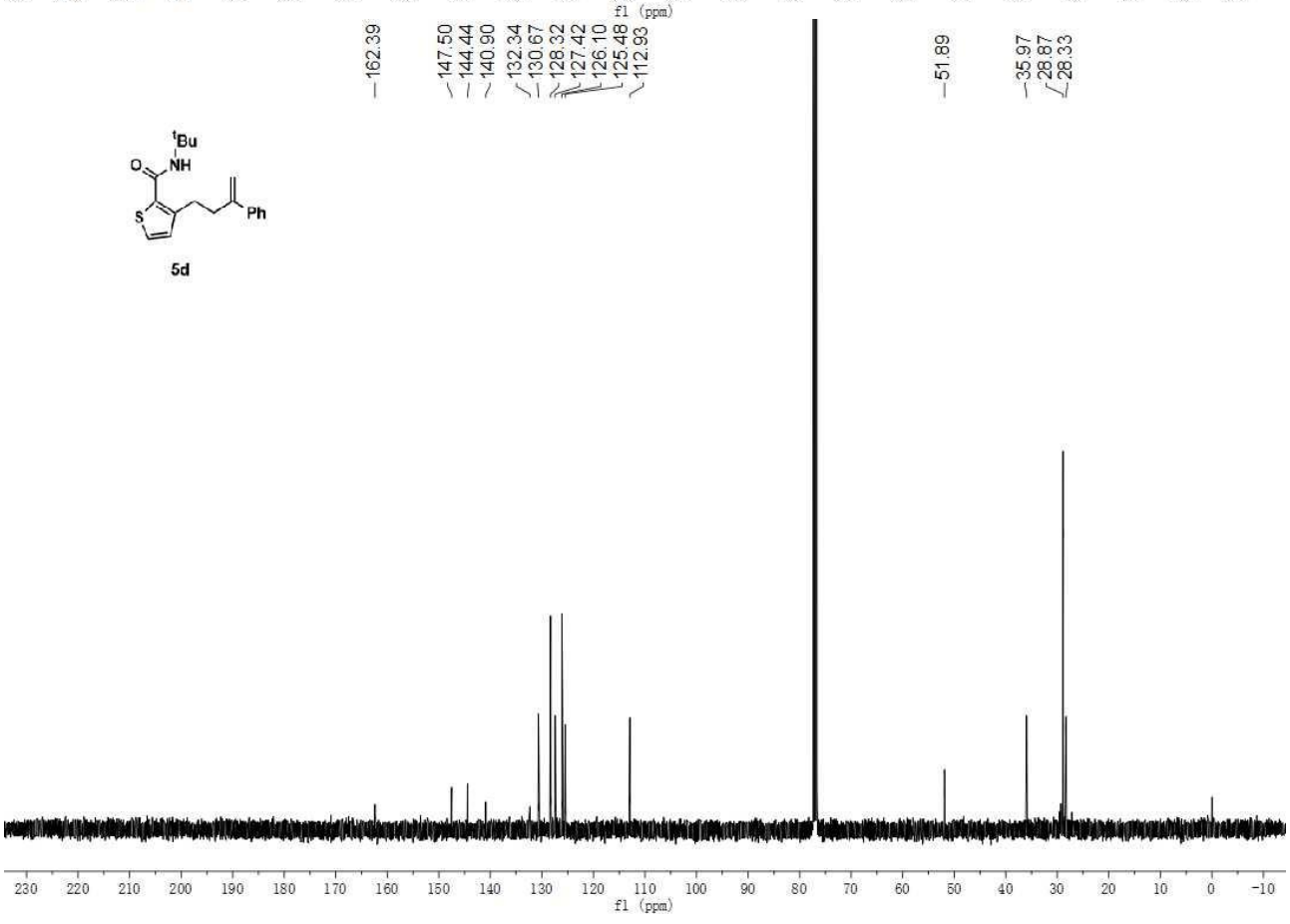
6.85
5.60
5.29
5.06
3.08
3.06
3.04
2.85
2.83
2.81
1.40
tBu
NH
O
S
Ph
5d
1.98
2.96
1.06
1.03
1.00
1.05
1.01
2.04
2.09
9.03
f1 (ppm)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51.89
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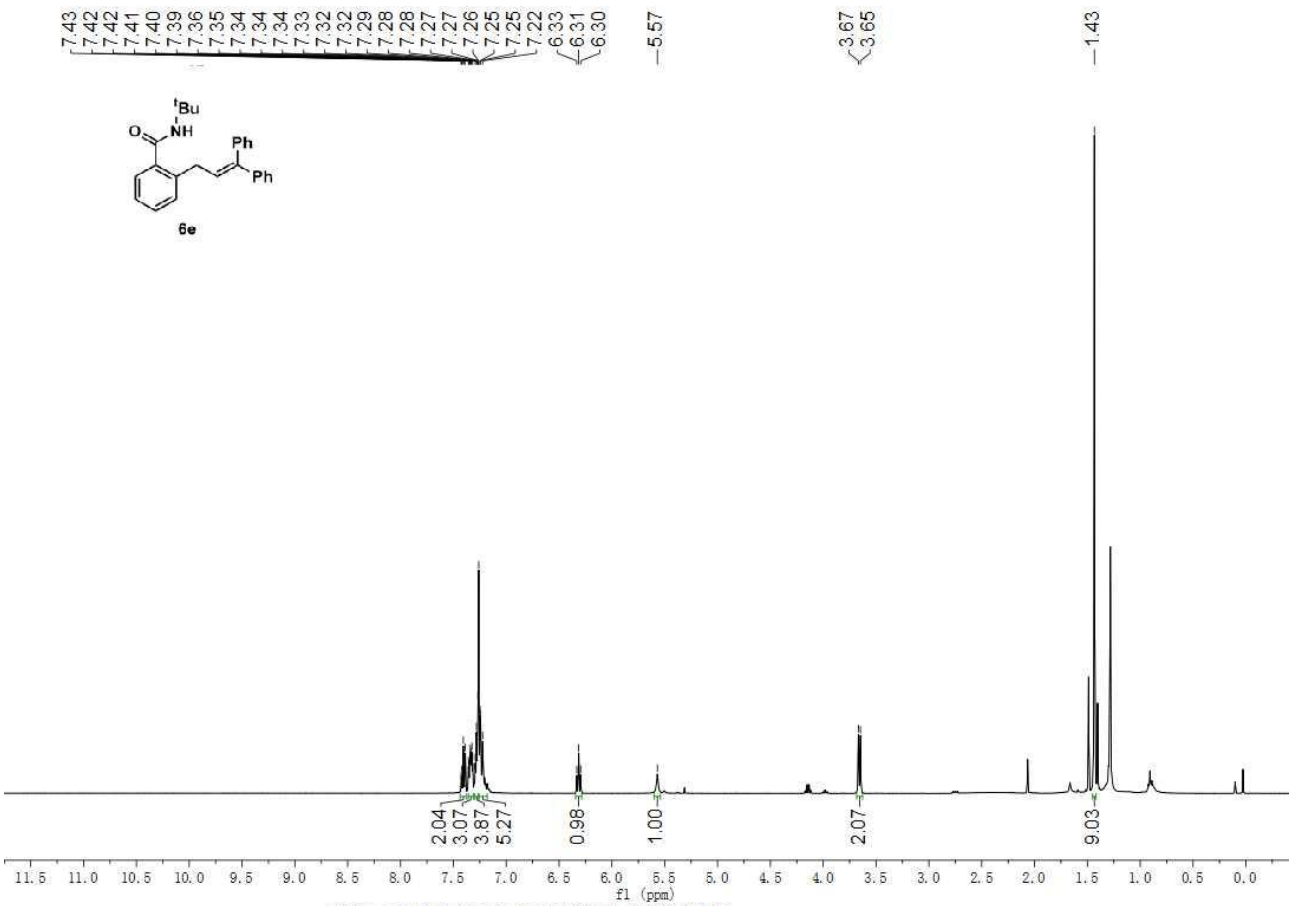
tBu
NH
O
S
Ph
5d
f1 (ppm)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7.25
7.22
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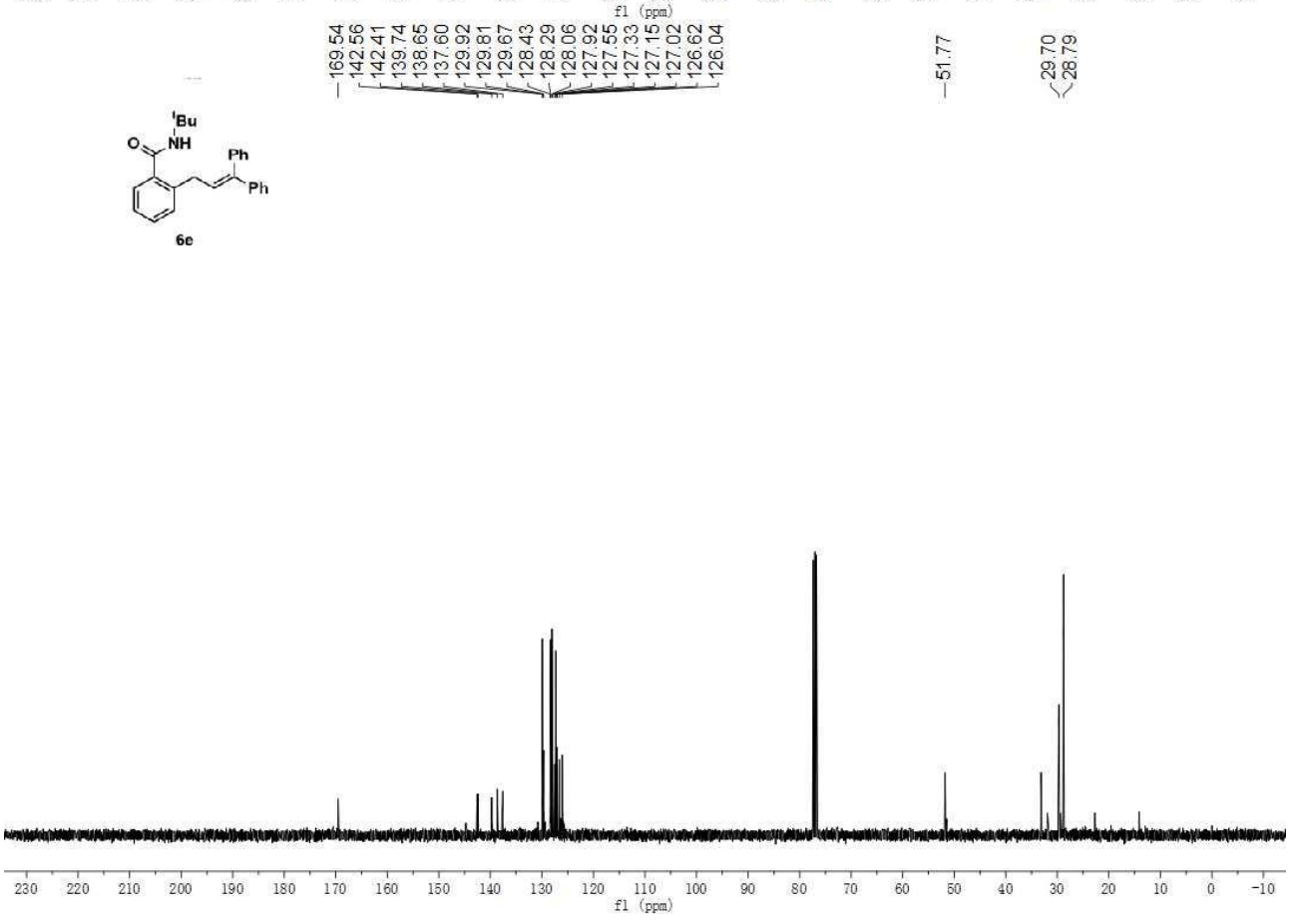
6.31
6.30
5.57
3.67
3.65
1.43
tBu
NH
O
Ph
Ph
6e
2.04
3.07
3.87
5.27
0.98
1.00
2.07
9.03
f1 (ppm)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128.43
128.29
128.06
127.92
127.55
127.33
127.15
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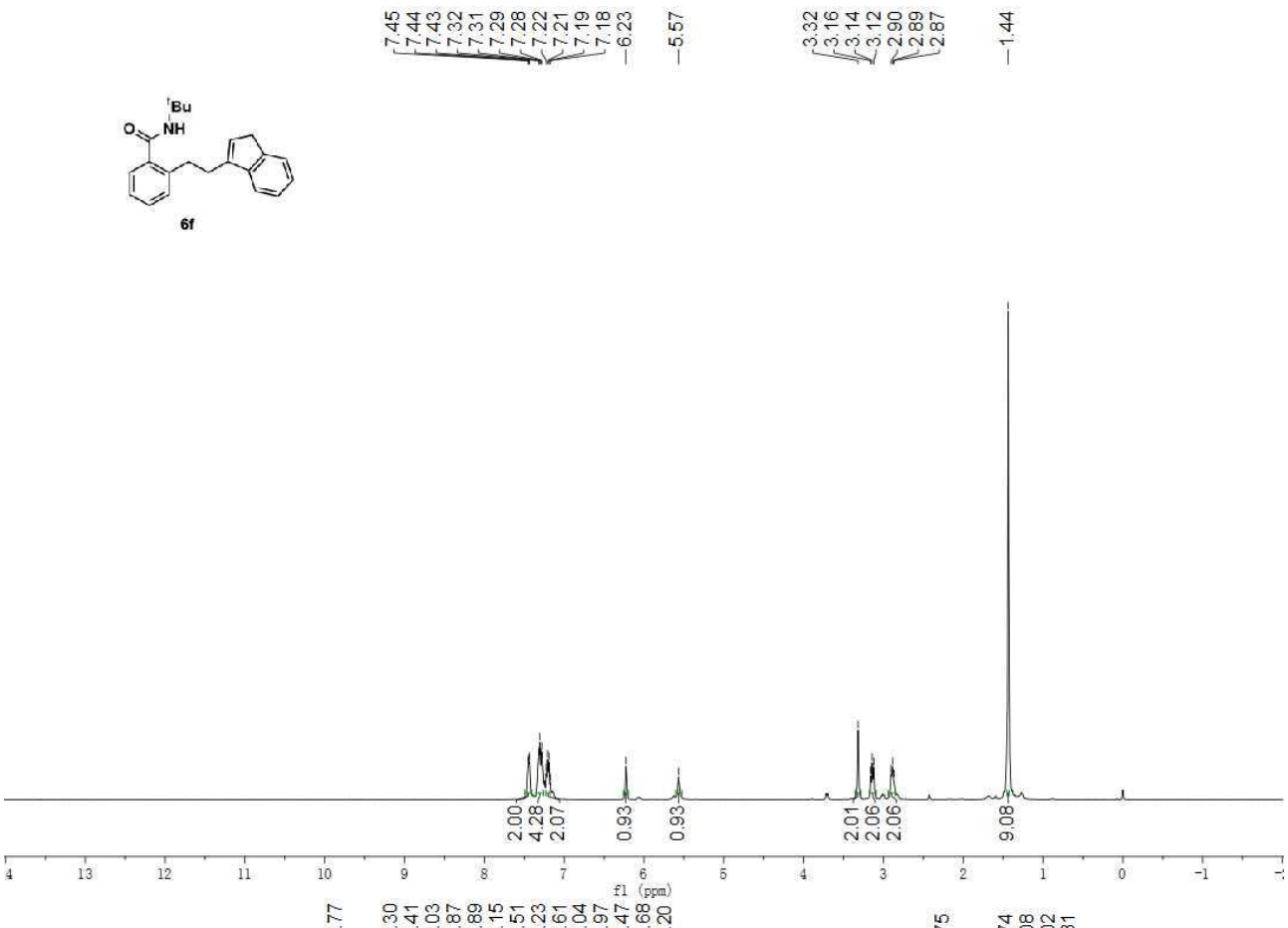
126.04
51.77
29.70
28.79
tBu
NH
O
Ph
Ph
6e
f1 (ppm)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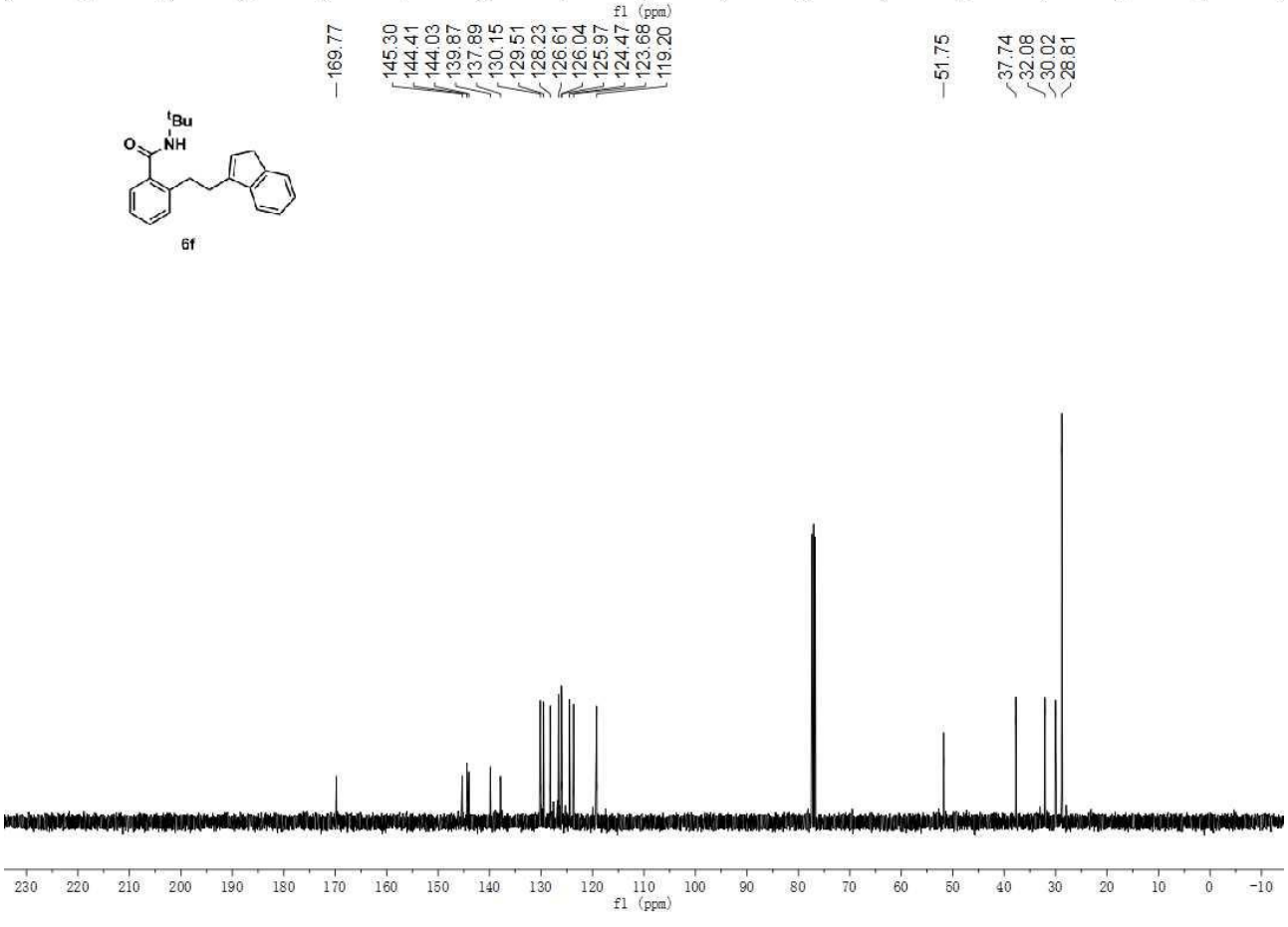
7.22
7.21
7.19
7.18
6.23
5.57
3.32
3.16
3.14
3.12
2.90
2.89
2.87
1.44
tBu
NH
O
6f
2.00
4.28
2.07
0.93
0.93
2.01
2.06
2.06
9.08
f1 (ppm)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126.61
126.04
125.97
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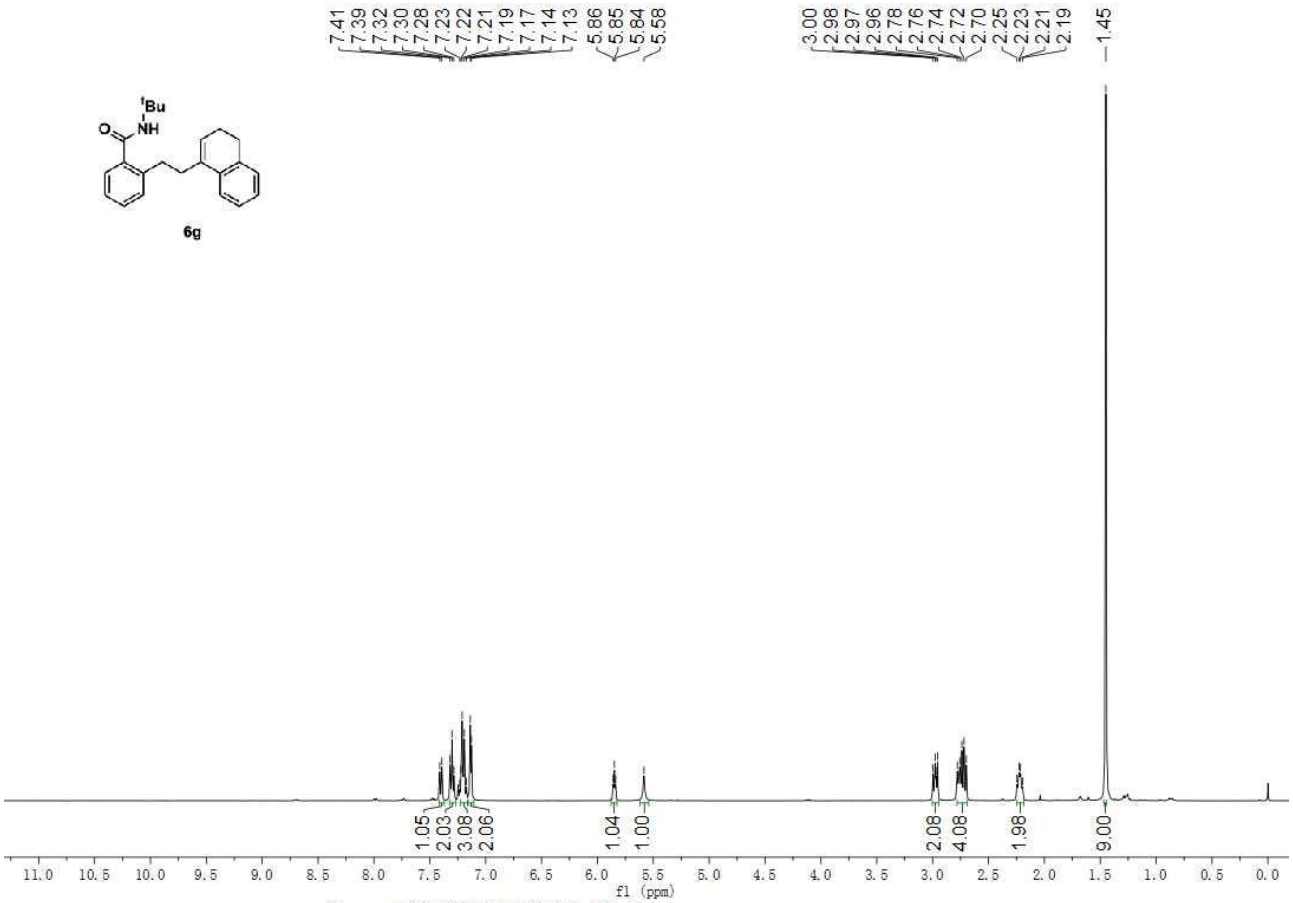
32.08
30.02
28.81
tBu
NH
O
6f
f1 (ppm)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7.17
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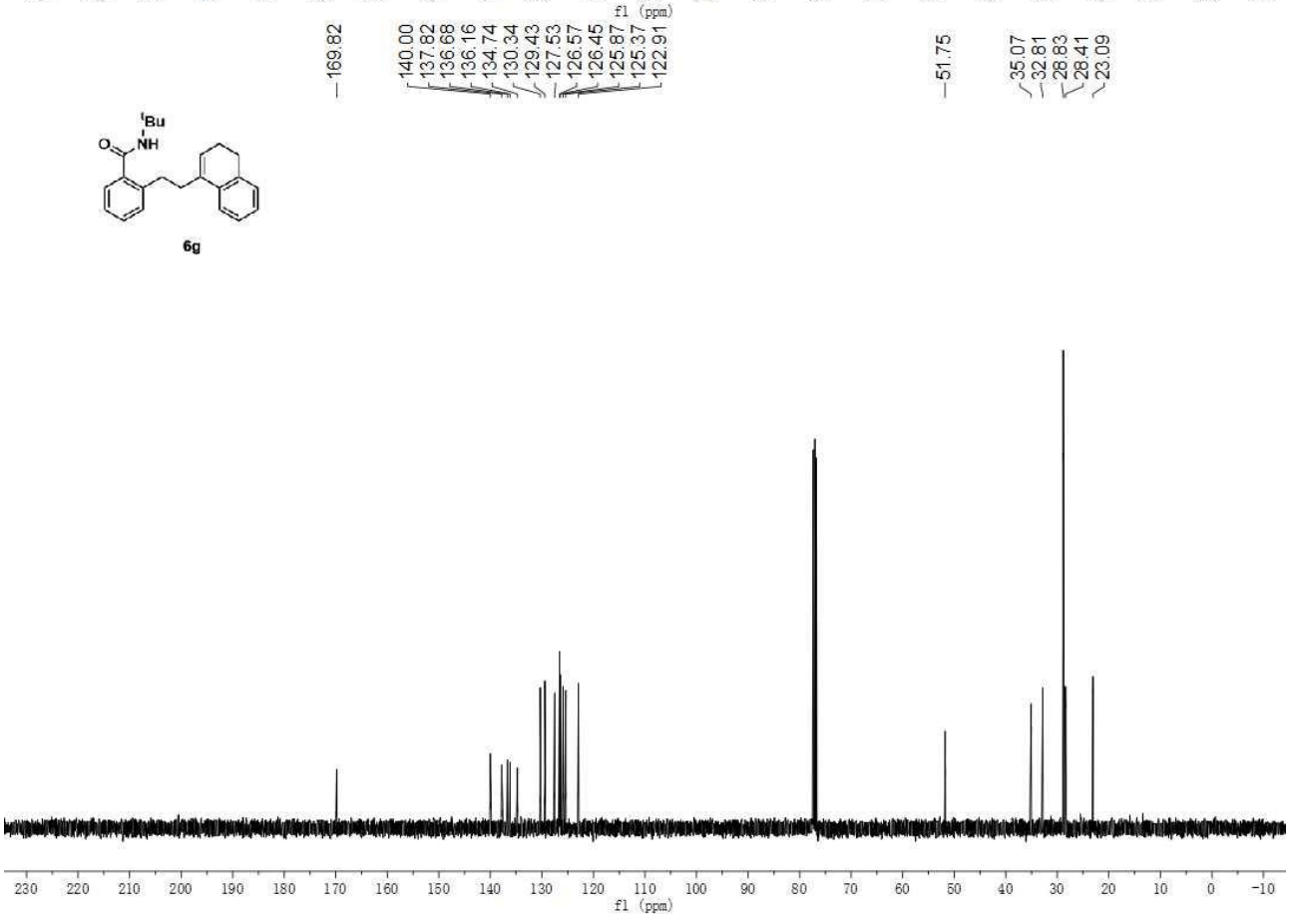
2.97
2.96
2.78
2.76
2.74
2.72
2.70
2.25
2.23
2.21
2.19
1.45
tBu
NH
O
6g
1.05
2.03
3.08
2.06
1.04
1.00
2.08
4.08
1.98
9.00
f1 (ppm)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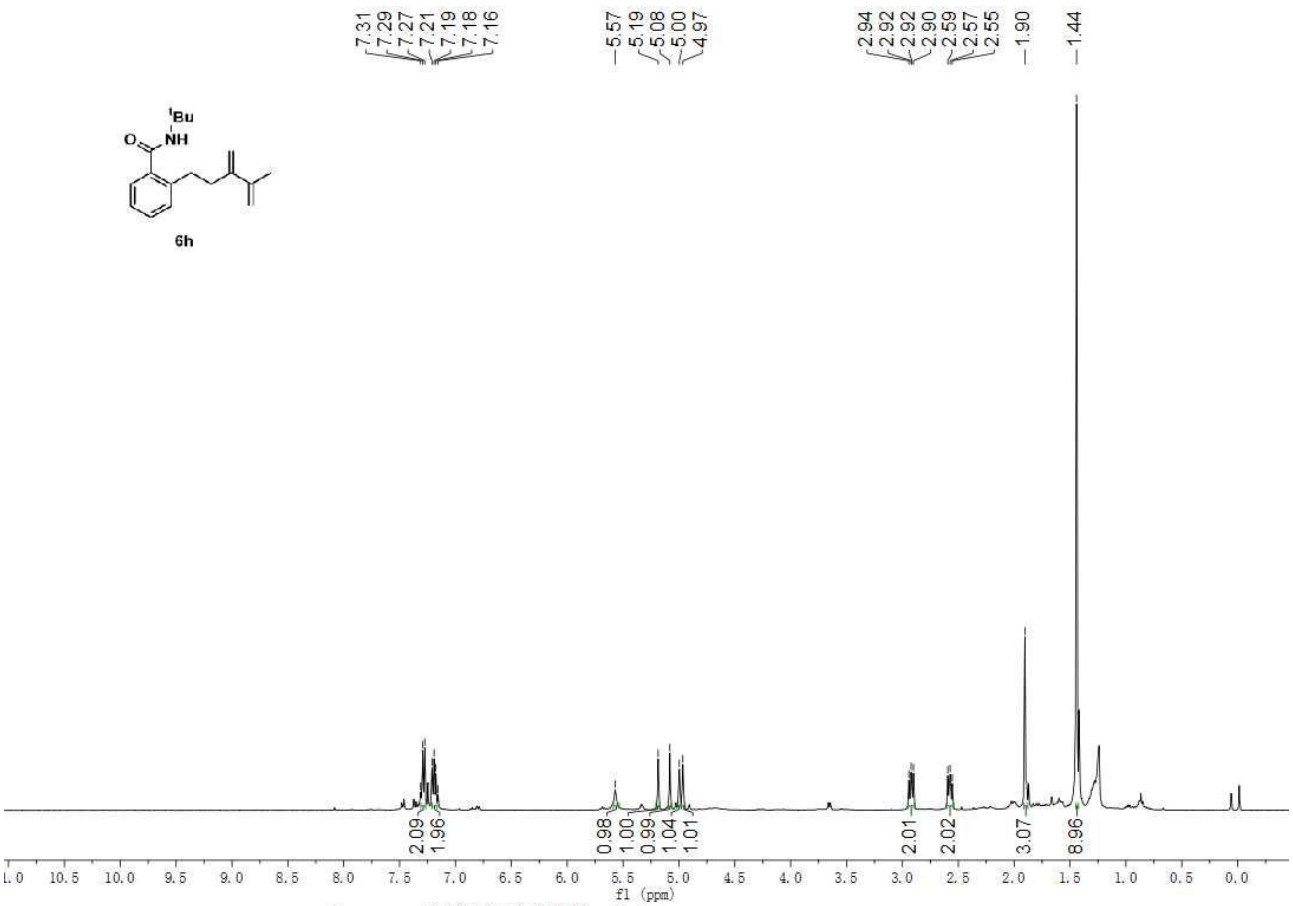
35.07
32.81
28.83
28.41
23.09
tBu
NH
O
6g
f1 (ppm)


7.31
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7.19
7.18
7.16
5.57
5.19
5.08
5.00
4.97
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2.92
2.90
2.59
2.57
2.55
1.90
1.44
tBu
NH
O
6h
2.09
1.96
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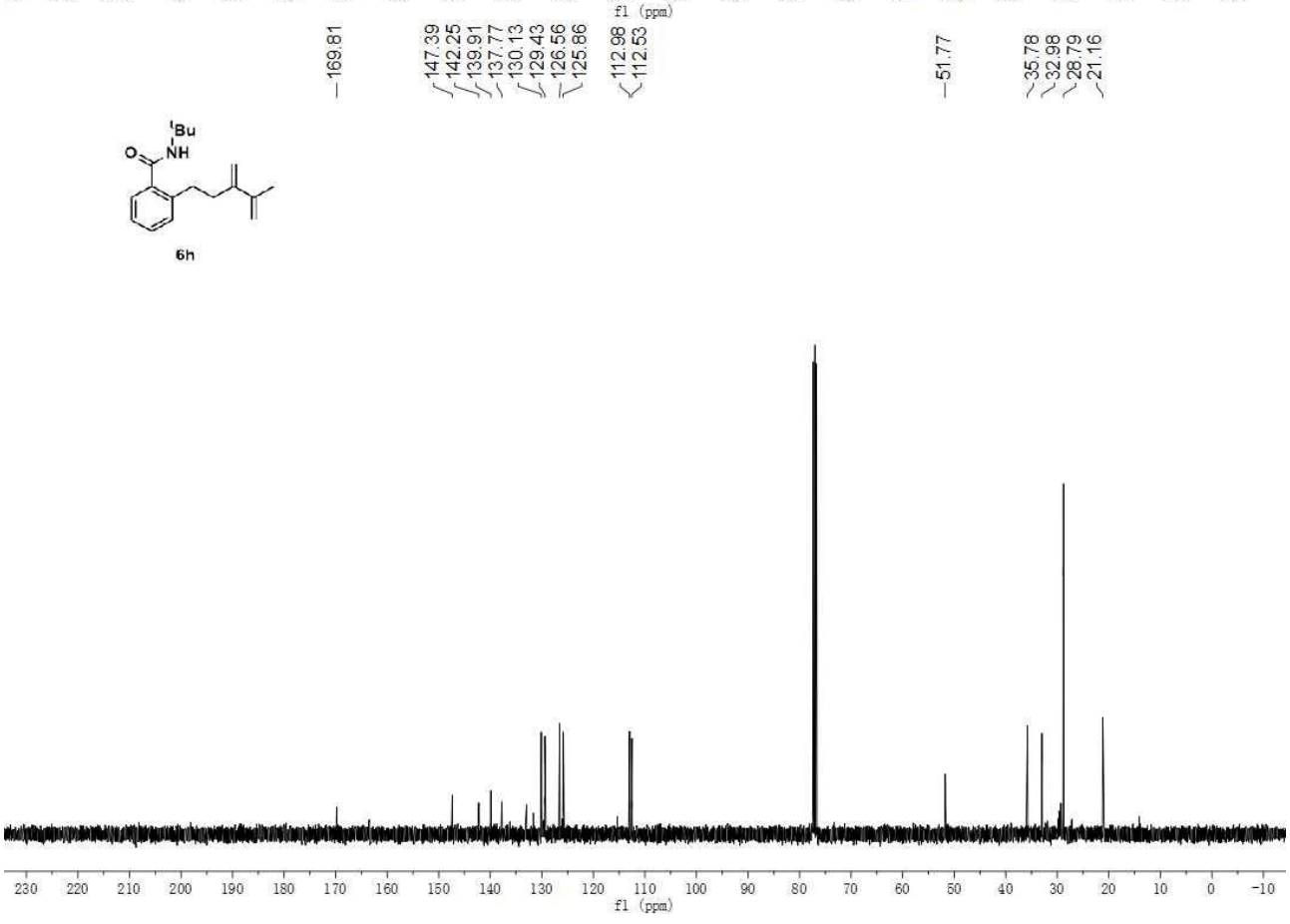
1.00
0.99
1.04
1.01
2.01
2.02
3.07
8.96
f1 (ppm)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126.56
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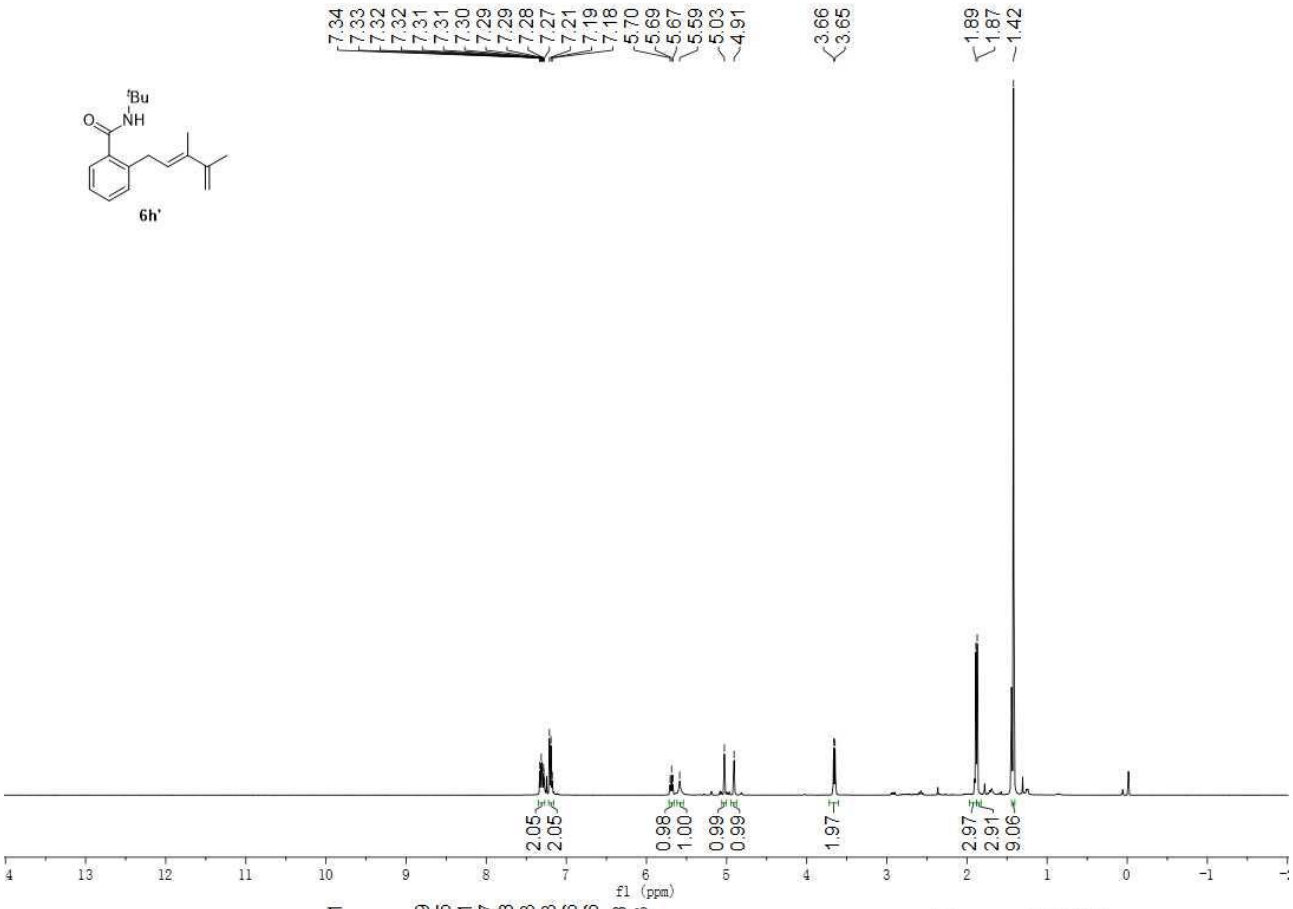
32.98
28.79
21.16
tBu
NH
O
6h
f1 (ppm)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7.30
7.29
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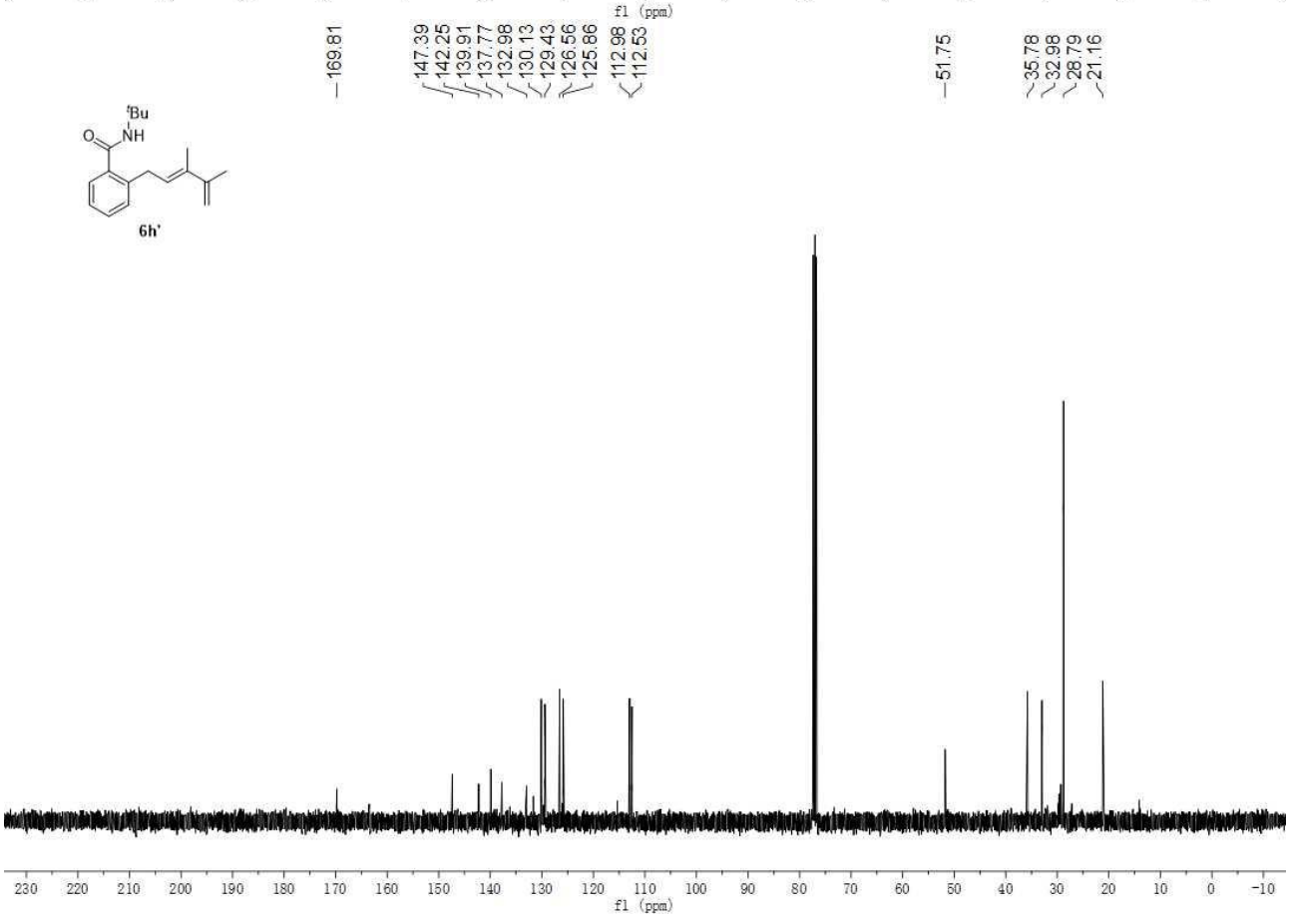
7.28
7.27
7.21
7.19
7.18
5.70
5.69
5.67
5.59
5.03
4.91
3.66
3.65
1.89
1.87
1.42
tBu
NH
O
6h'
2.05
2.05
0.98
1.00
0.99
0.99
1.97
2.97
2.91
9.06
f1 (ppm)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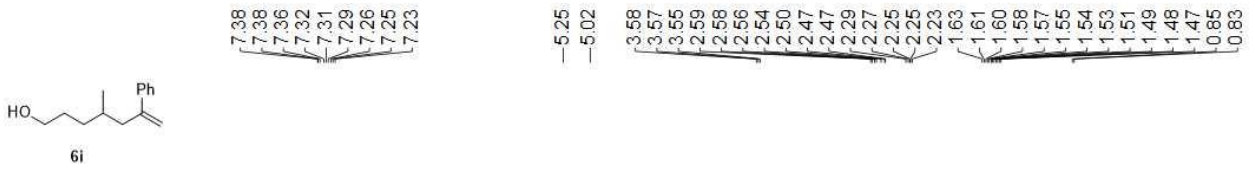
32.98
28.79
21.16
tBu
NH
O
6h'
f1 (ppm)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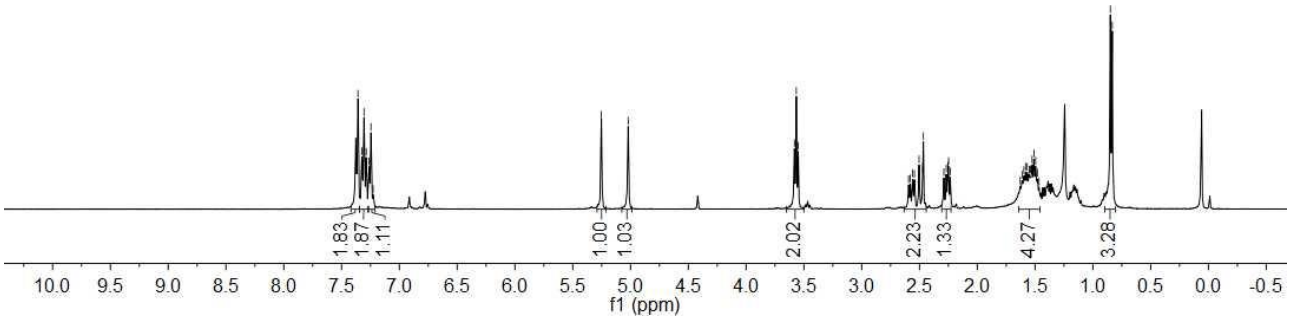
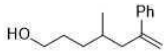
7.38
7.36
7.32
7.31
7.29
7.26
7.25
7.23
5.25
5.02
3.58
3.57
3.55
2.59
2.58
2.56
2.54
2.50
2.47
2.29
2.27
2.25
2.25
2.23
1.63
1.61
1.60
1.58
1.57
1.55
1.54
1.53
1.51
1.49
1.48
1.47
0.85
0.83

HO
Ph

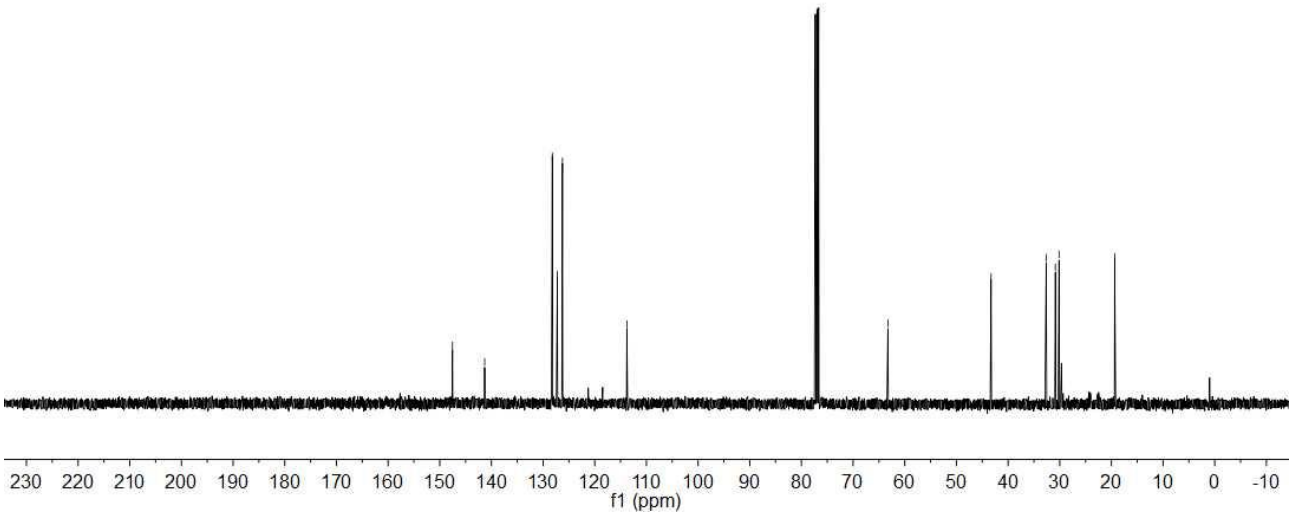
6i

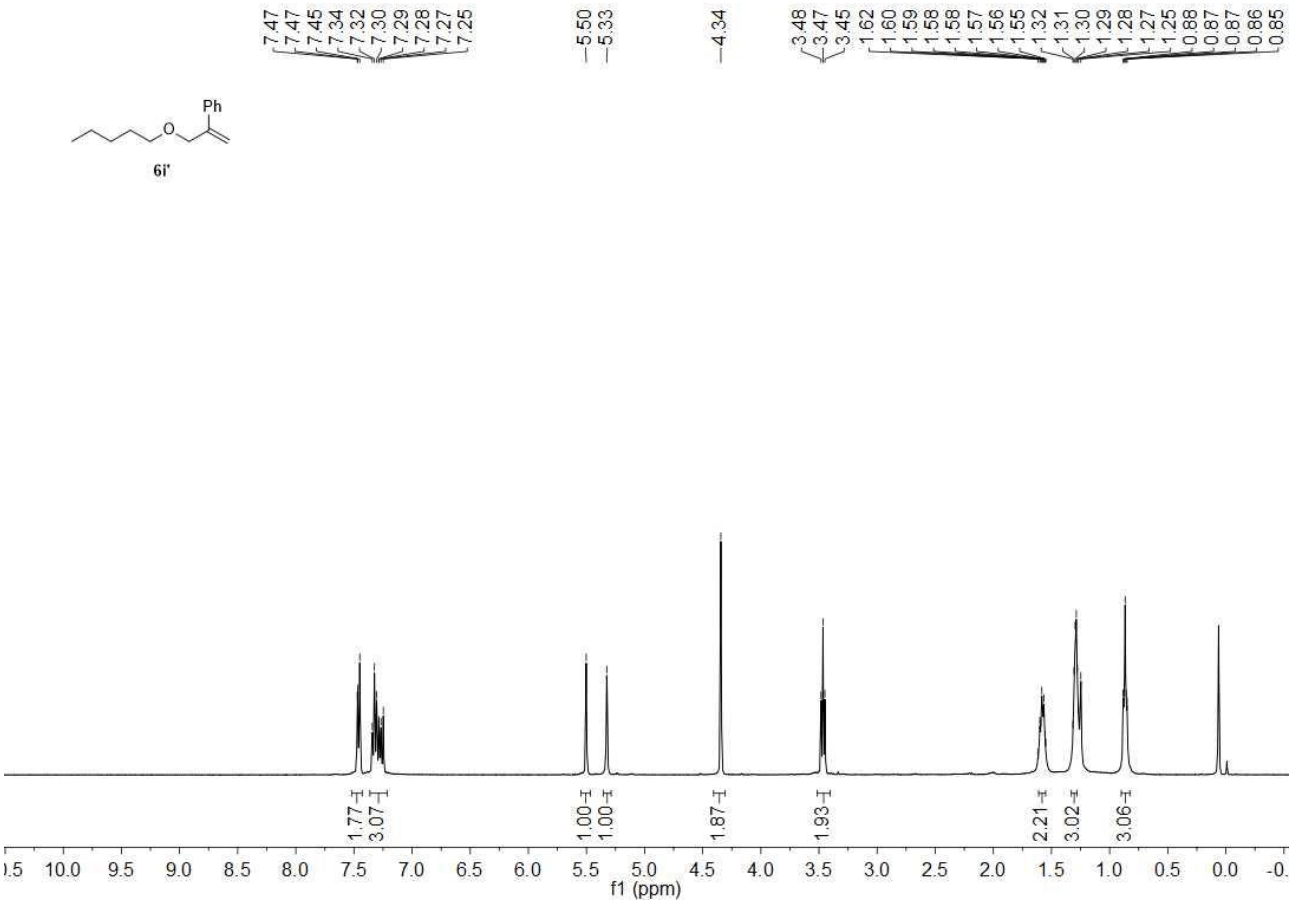

1.83
1.87
1.11
1.00
1.03
2.02
2.23
1.33
4.27
3.28
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


147.53
141.31
128.21
127.24
126.25
113.78
63.26
43.29
32.62
30.84
30.14
19.37


HO
Ph

6i


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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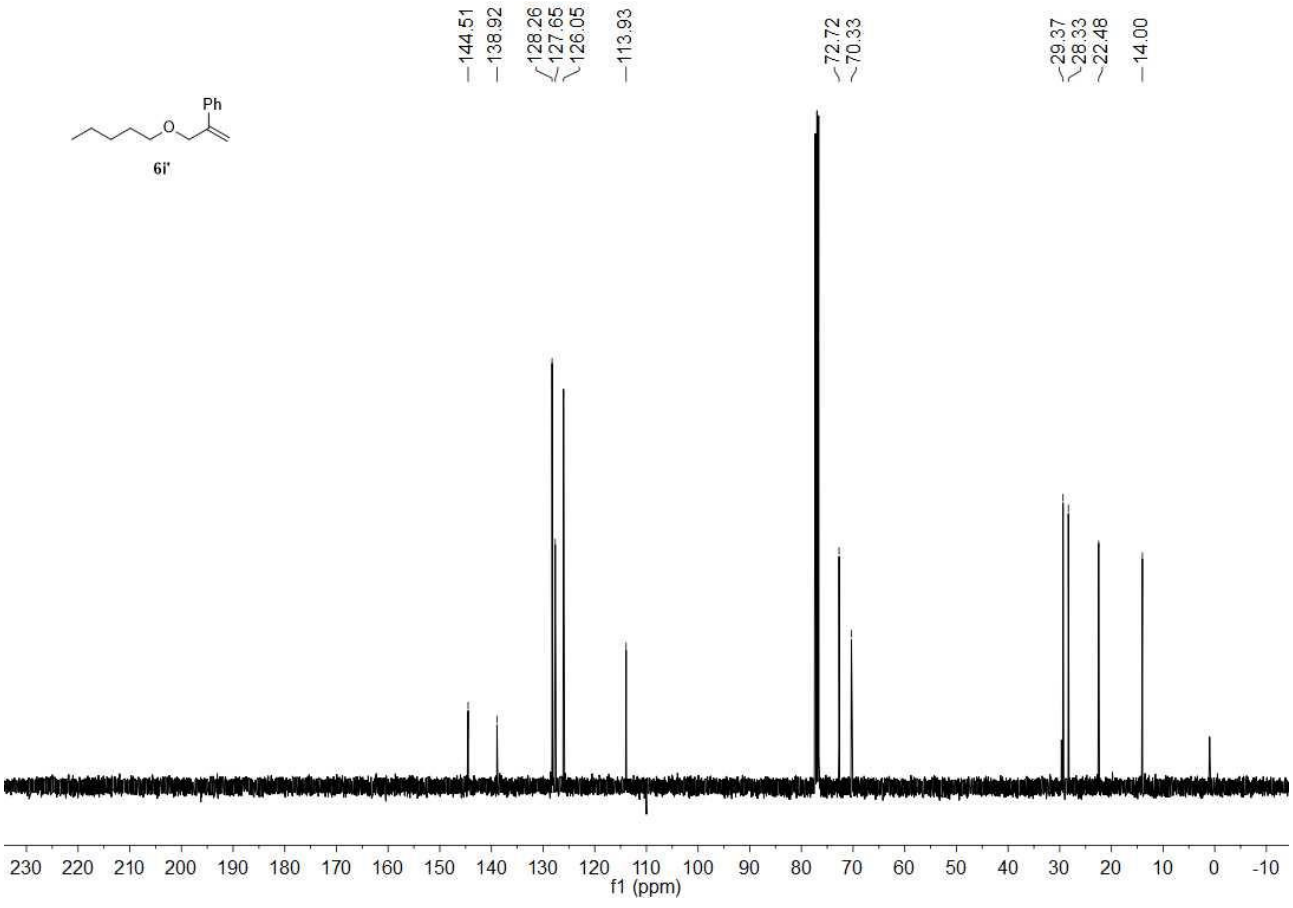
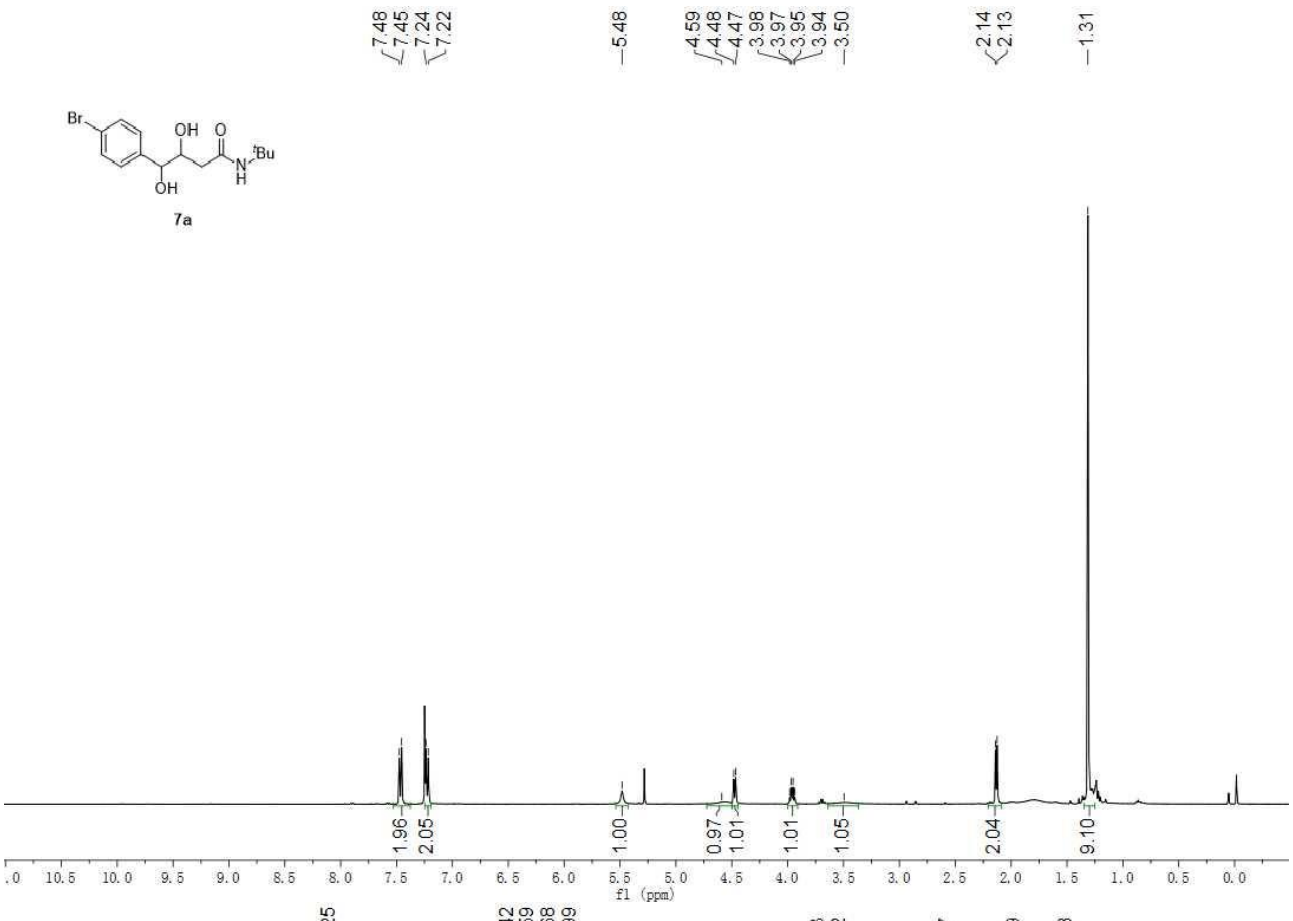
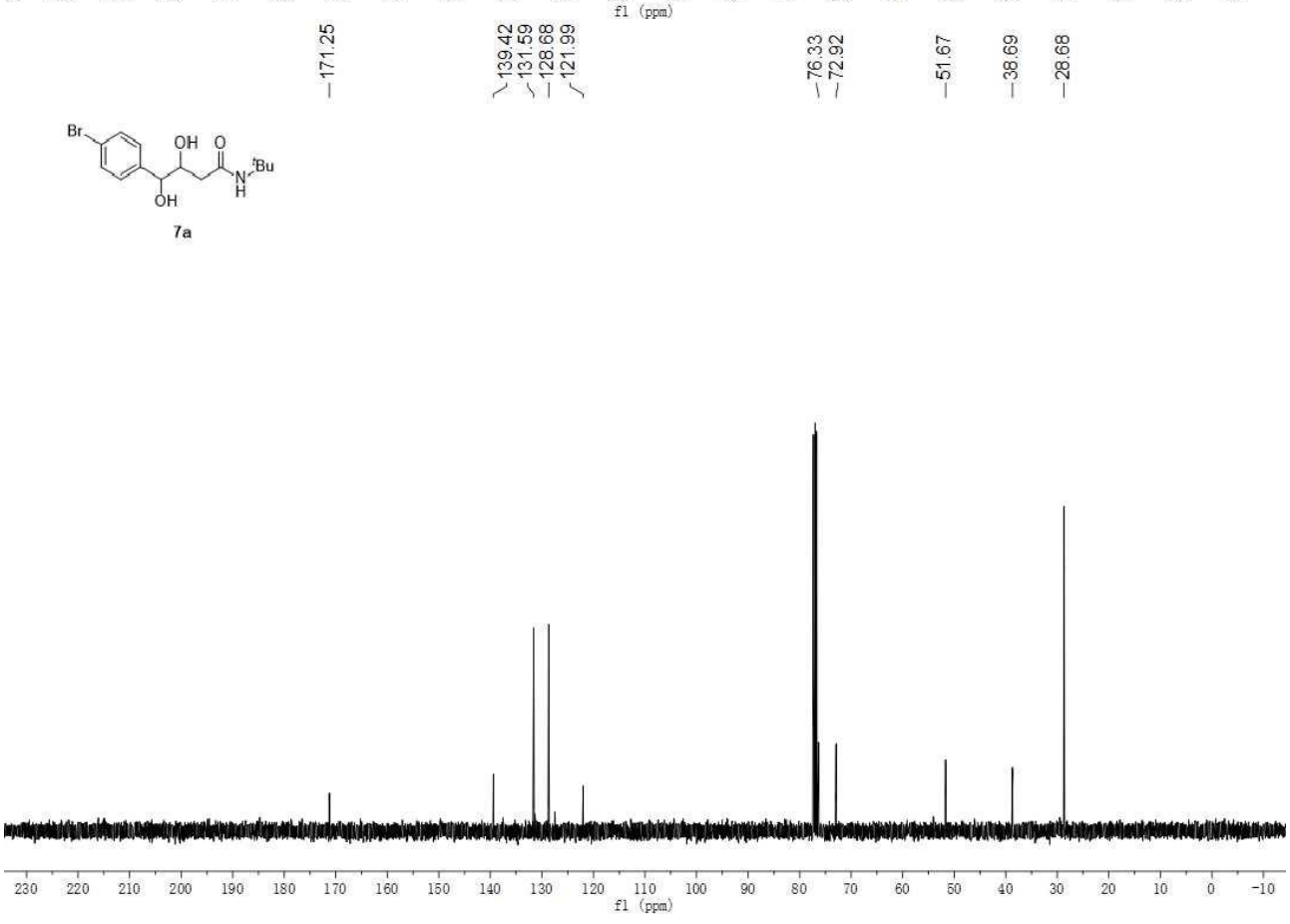
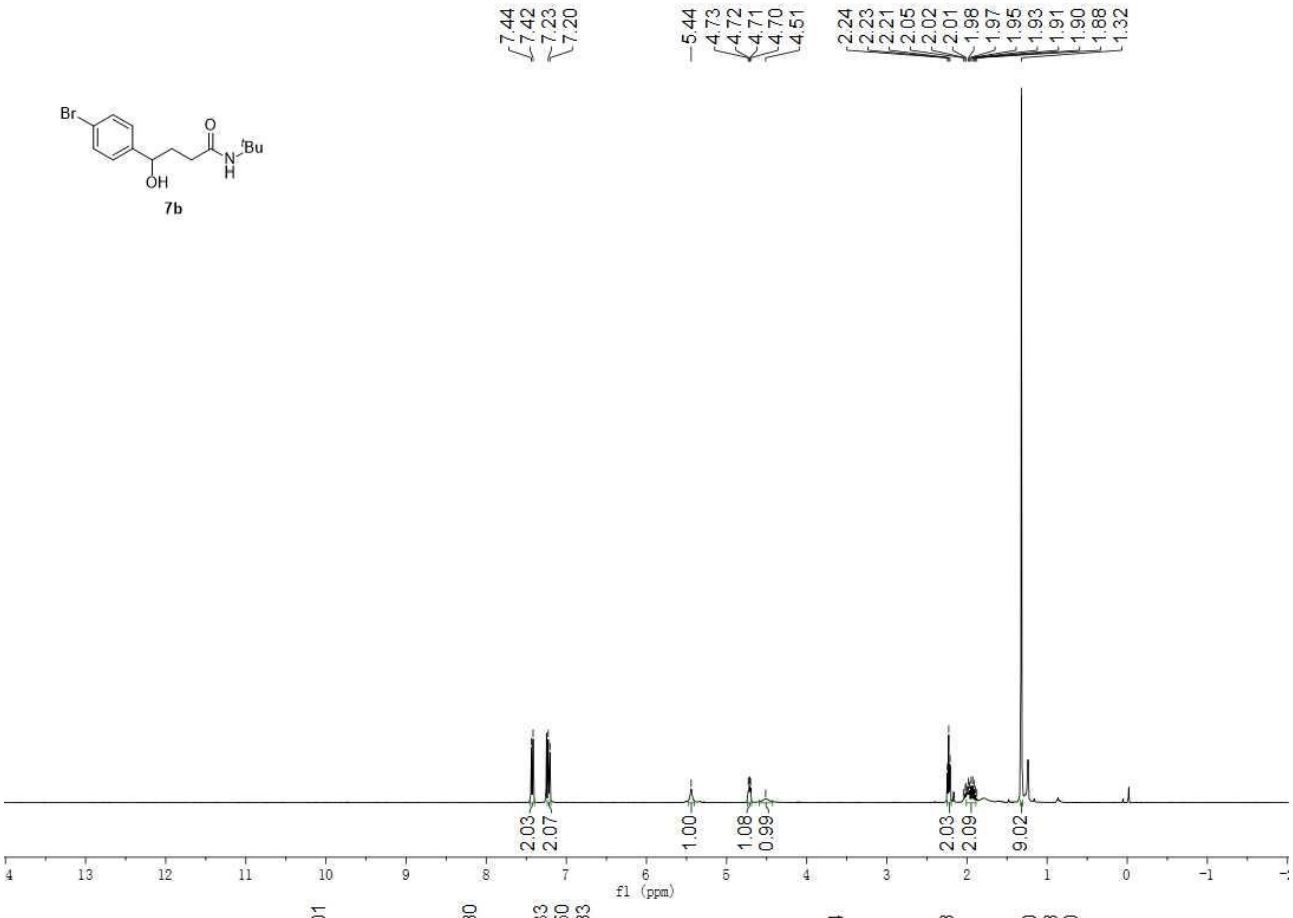
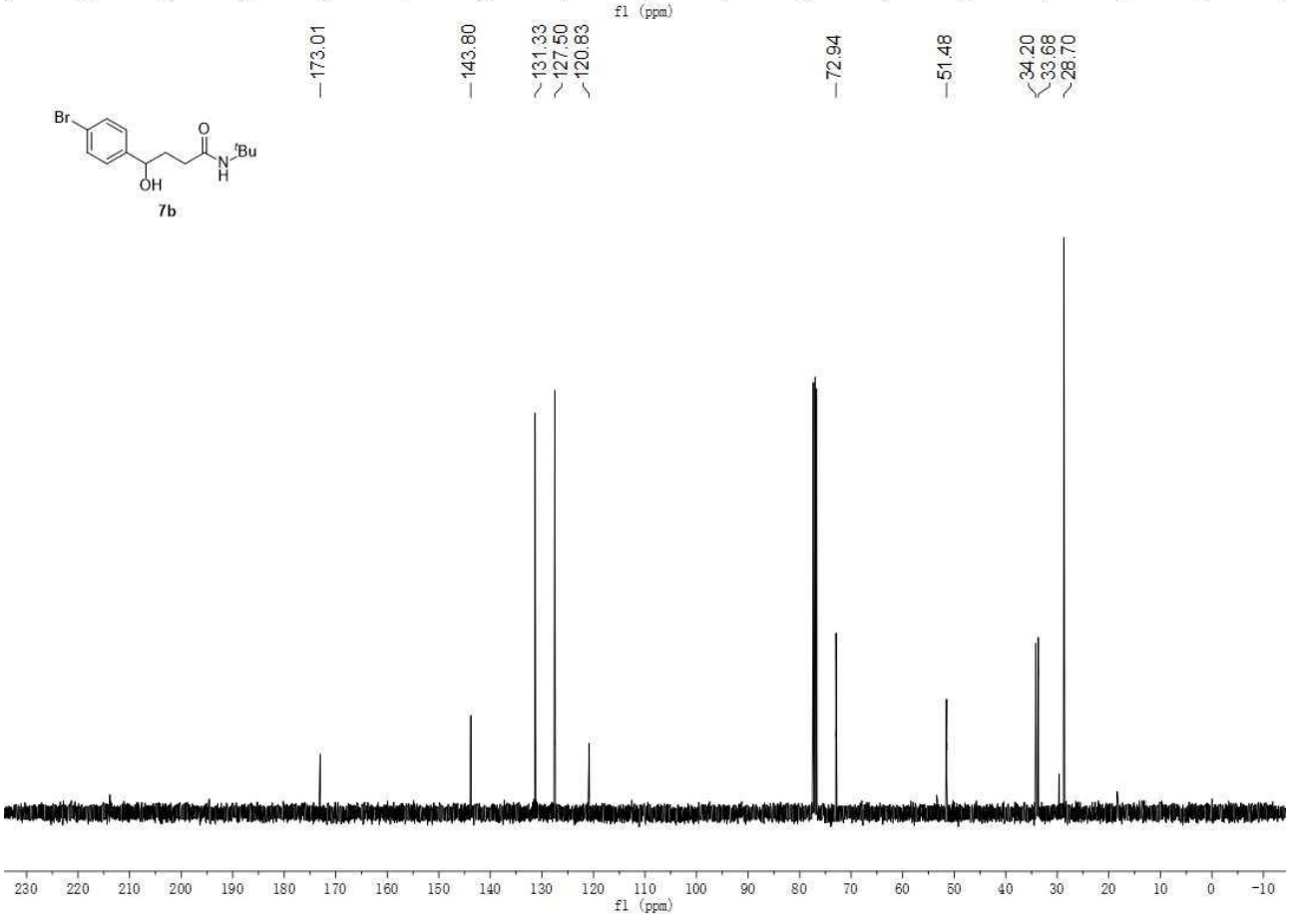
7.47
7.45
7.34
7.32
7.30
7.29
7.28
7.27
7.25
5.50
5.33
4.34
3.48
3.47
3.45
1.62
1.60
1.59
1.58
1.58
1.57
1.56
1.55
1.32
1.31
1.30
1.29
1.28
1.27
1.25
0.88
0.87
0.87
0.86
0.85
Ph
O
6i'
1.77
3.07
1.00
1.00
1.87
1.93
2.21
3.02
3.06
f1 (ppm)

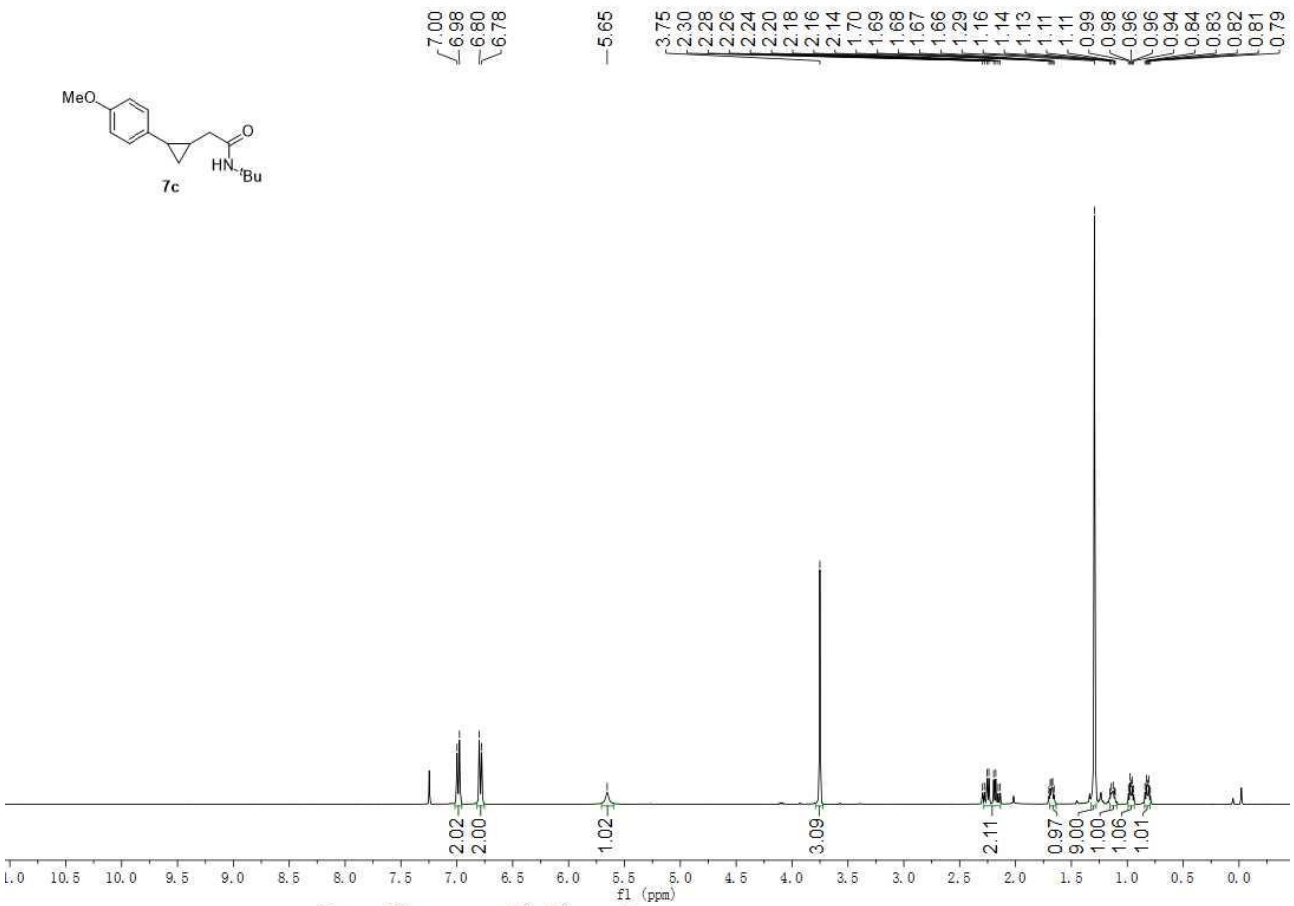

144.51
138.92
128.26
127.65
126.05
113.93
72.72
70.33
29.37
28.33
22.48
14.00
Ph
O
6i'
f1 (ppm)

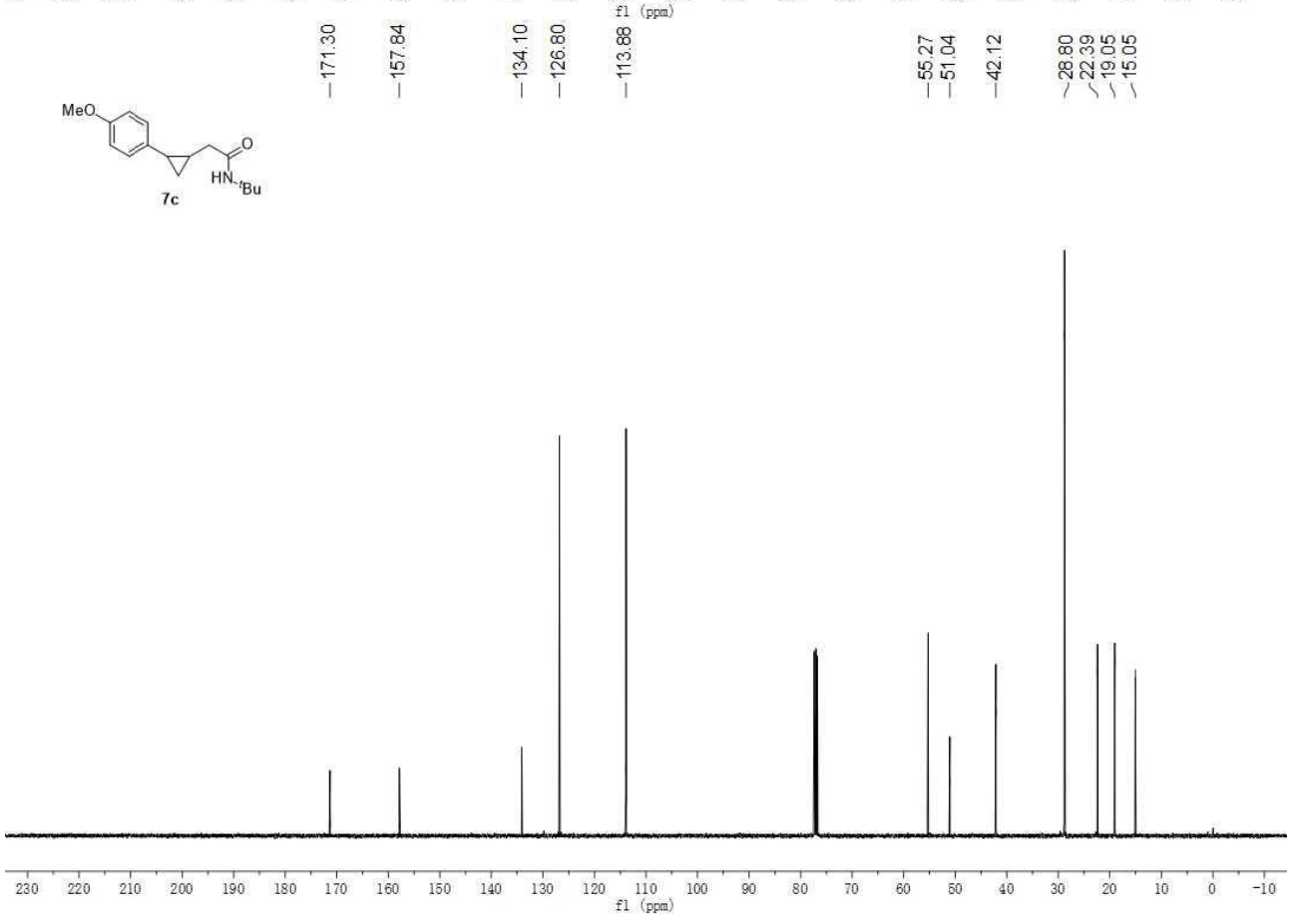

7.48
7.45
7.24
7.22
5.48
4.59
4.48
4.47
3.98
3.97
3.95
3.94
3.50
2.14
2.13
1.31
Br
OH
O
tBu
N
H
OH
7a
1.96
2.05
1.00
0.97
1.01
1.01
1.05
2.04
9.10
f1 (ppm)


171.25
139.42
131.59
128.68
121.99
76.33
72.92
51.67
38.69
28.68
Br
OH
O
tBu
N
H
OH
7a
f1 (ppm)


7.44
7.42
7.23
7.20
5.44
4.73
4.72
4.71
4.70
4.51
2.24
2.23
2.21
2.05
2.02
2.01
1.98
1.97
1.95
1.93
1.91
1.90
1.88
1.32
Br
O
N
H
tBu
OH
7b
2.03
2.07
1.00
1.08
0.99
2.03
2.09
9.02
f1 (ppm)


173.01
143.80
131.33
127.50
120.83
72.94
51.48
34.20
33.68
28.70
Br
O
N
H
tBu
OH
7b
f1 (ppm)


7.00
6.98
6.80
6.78
5.65
3.75
2.30
2.28
2.26
2.24
2.20
2.18
2.16
2.14
1.70
1.69
1.68
1.67
1.66
1.29
1.16
1.14
1.13
1.11
1.11
0.99
0.98
0.96
0.96
0.94
0.84
0.83
0.82
0.81
0.79
MeO
O
HN
tBu
7c
2.02
2.00
1.02
3.09
2.11
0.97
9.00
1.00
1.06
1.01
f1 (ppm)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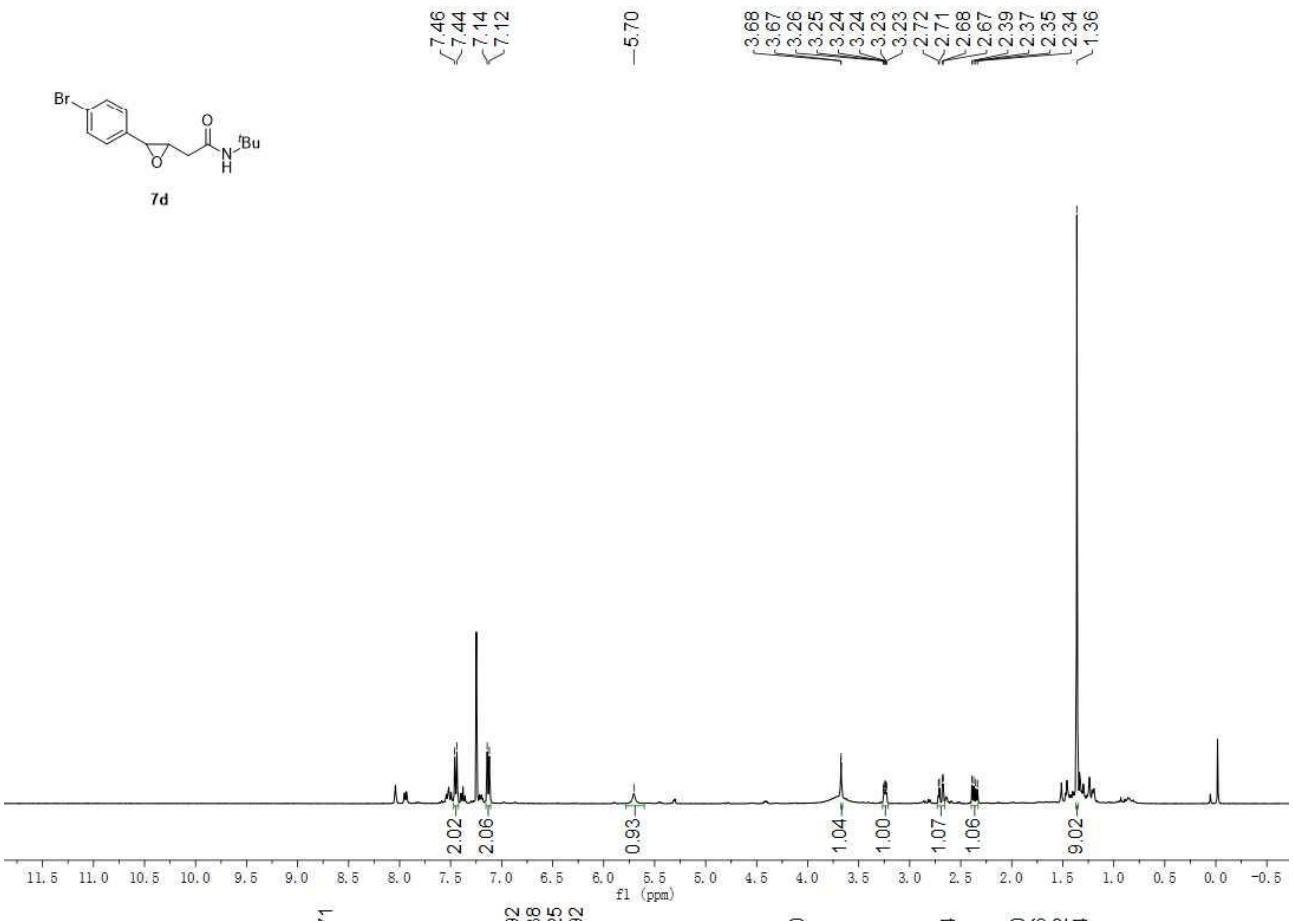
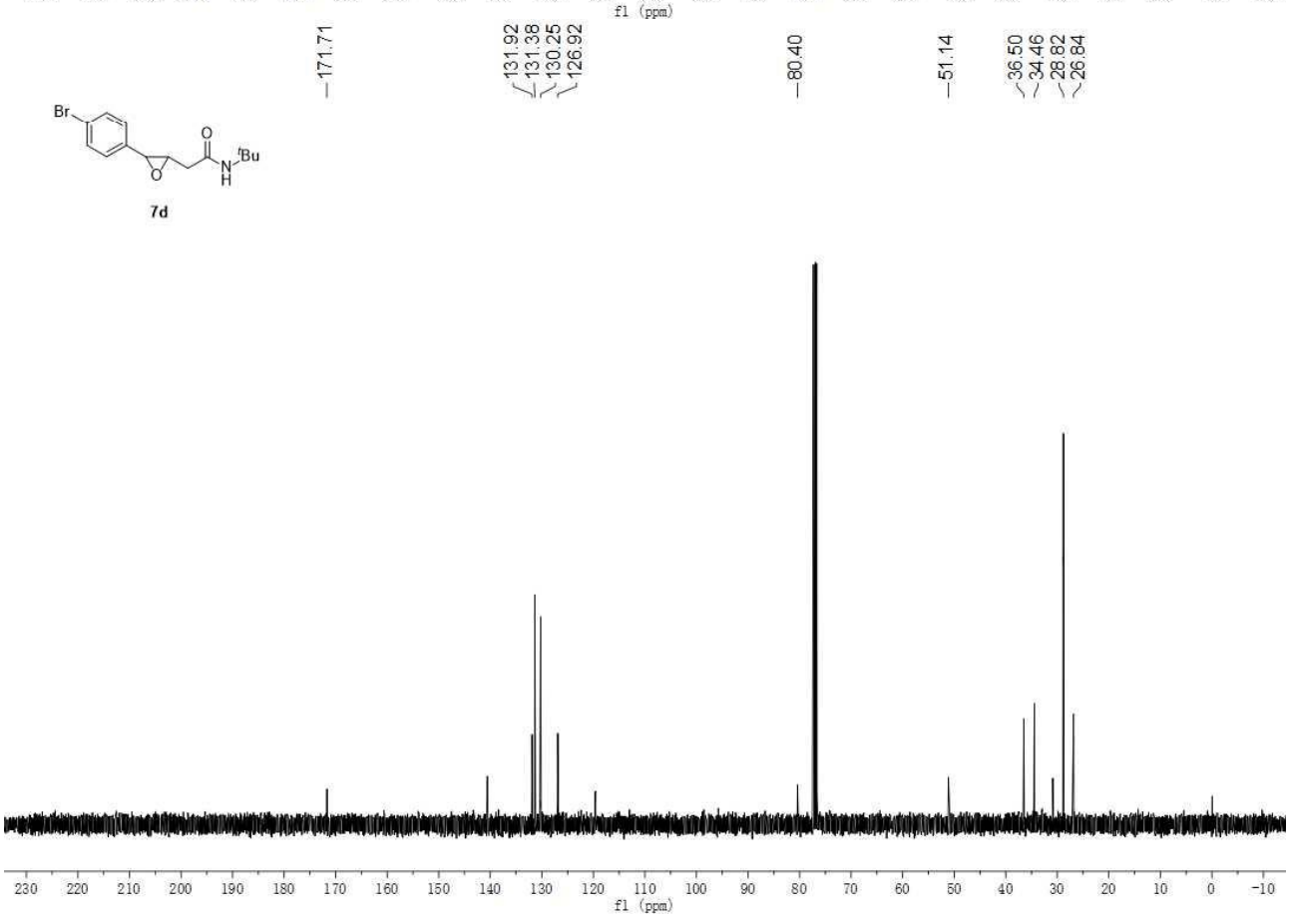
157.84
134.10
126.80
113.88
55.27
51.04
42.12
28.80
22.39
19.05
15.05
MeO
O
HN
tBu
7c
f1 (ppm)


7.46
7.44
7.14
7.12
5.70
3.68
3.67
3.26
3.25
3.24
3.24
3.23
3.23
2.72
2.71
2.68
2.67
2.39
2.37
2.35
2.34
1.36
Br
O
N
H
tBu
O
7d
2.02
2.06
0.93
1.04
1.00
1.07
1.06
9.02
f1 (ppm)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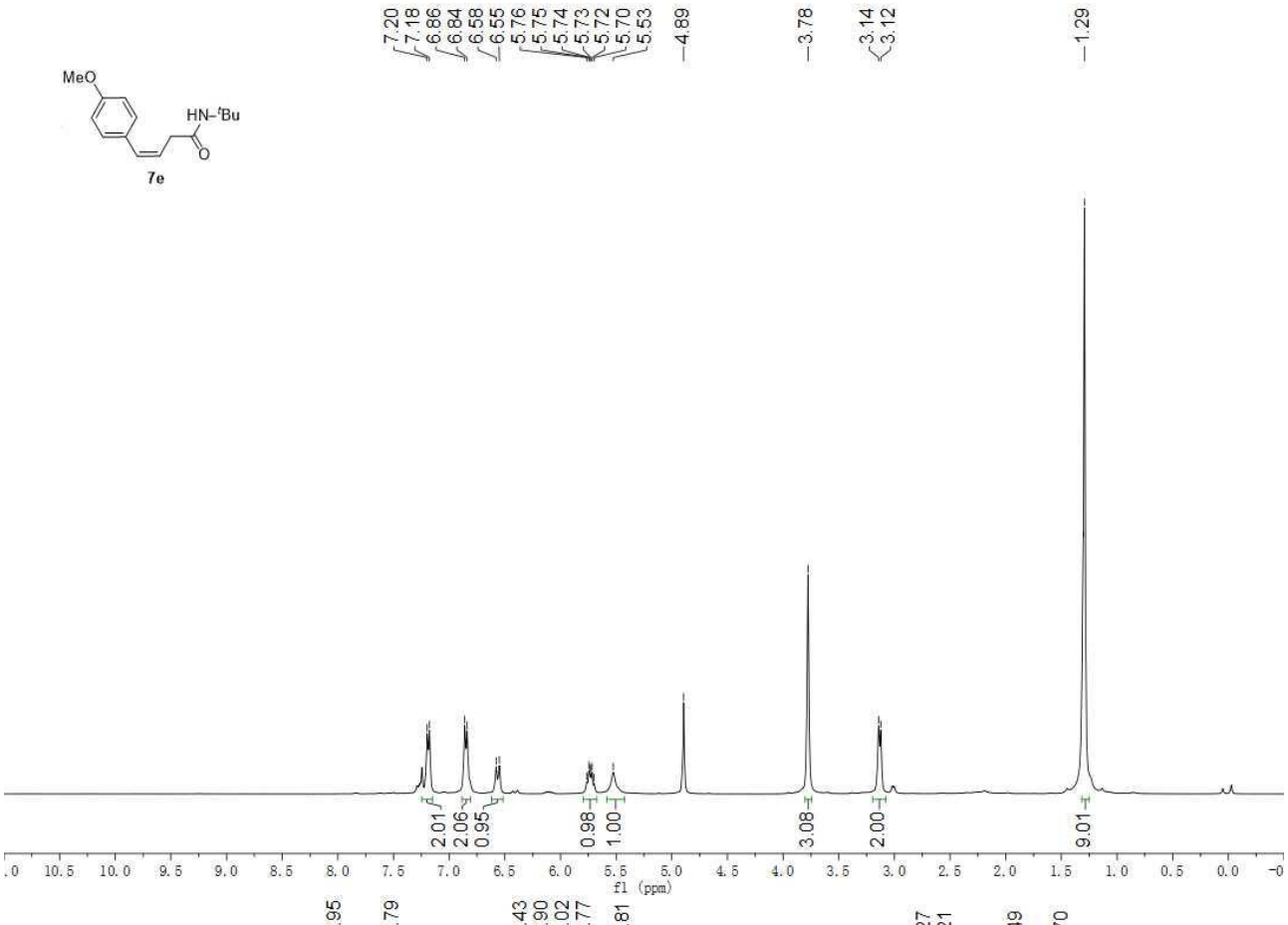
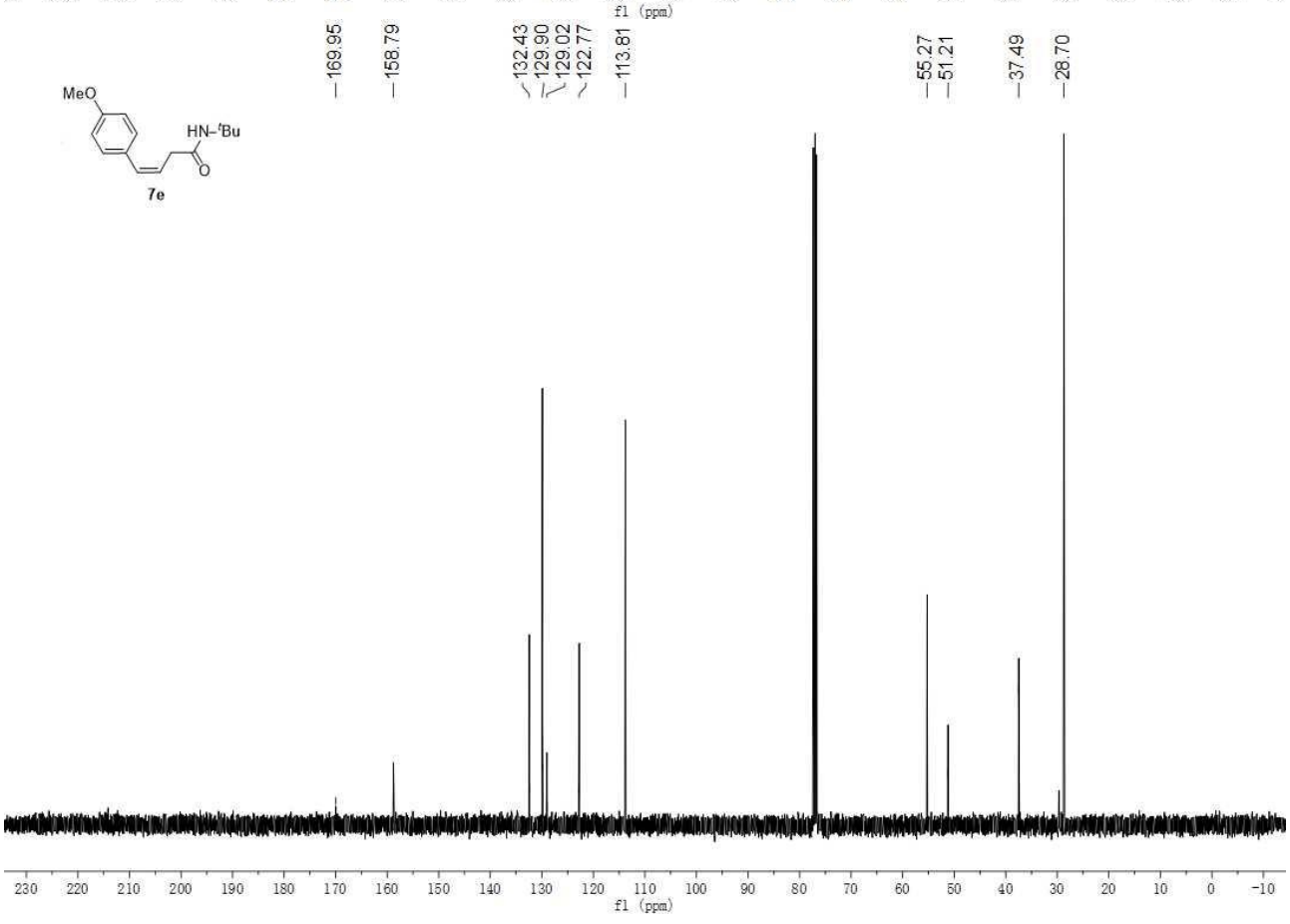
131.92
131.38
130.25
126.92
80.40
51.14
36.50
34.46
28.82
26.84
Br
O
N
H
tBu
O
7d
f1 (ppm)


7.20
7.18
6.86
6.84
6.58
6.55
5.76
5.75
5.74
5.73
5.72
5.70
5.53
4.89
3.78
3.14
3.12
1.29
MeO
HN-tBu
O
7e
2.01
2.06
0.95
0.98
1.00
3.08
2.00
9.01
f1 (ppm)


169.95
158.79
132.43
129.90
129.02
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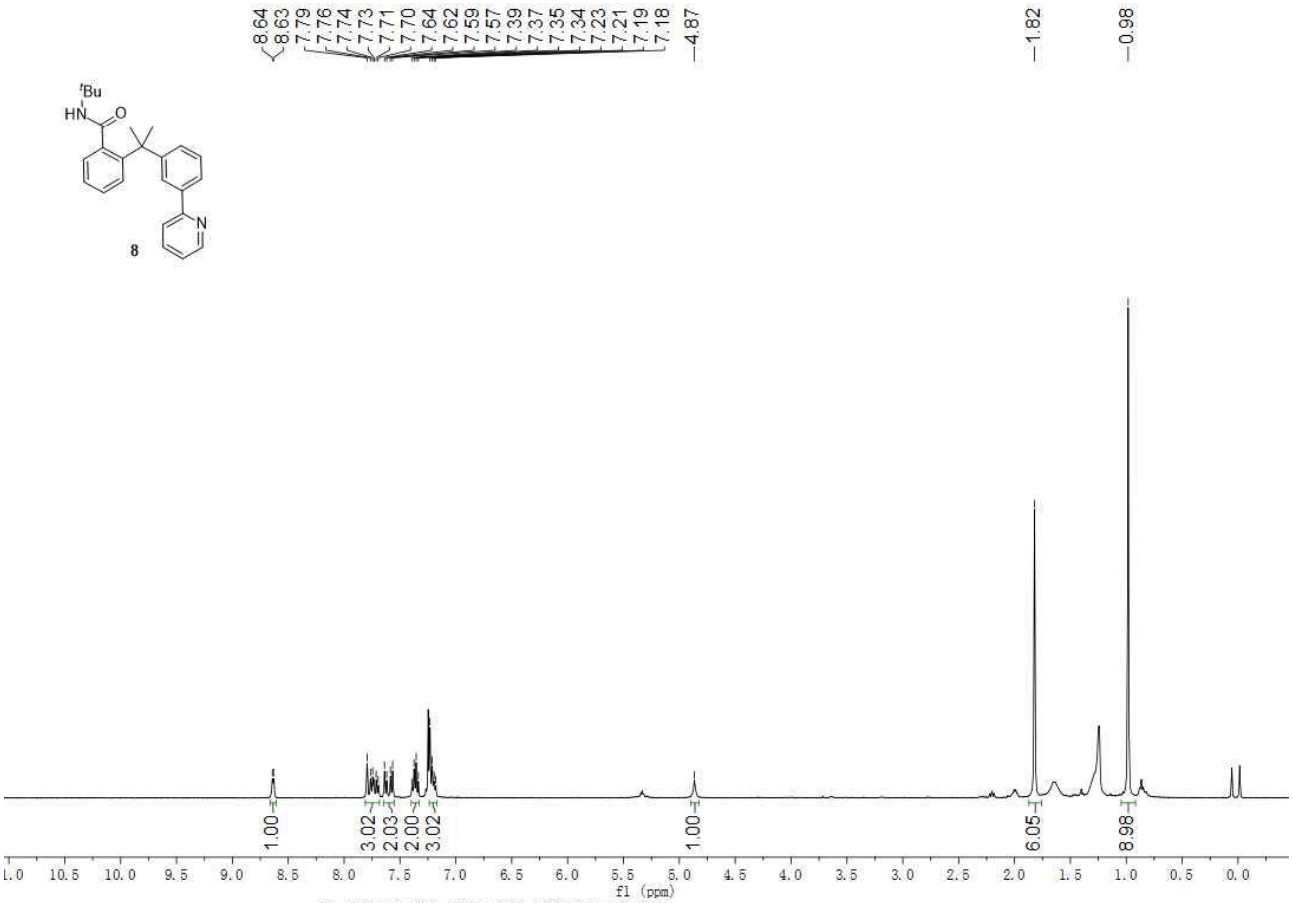
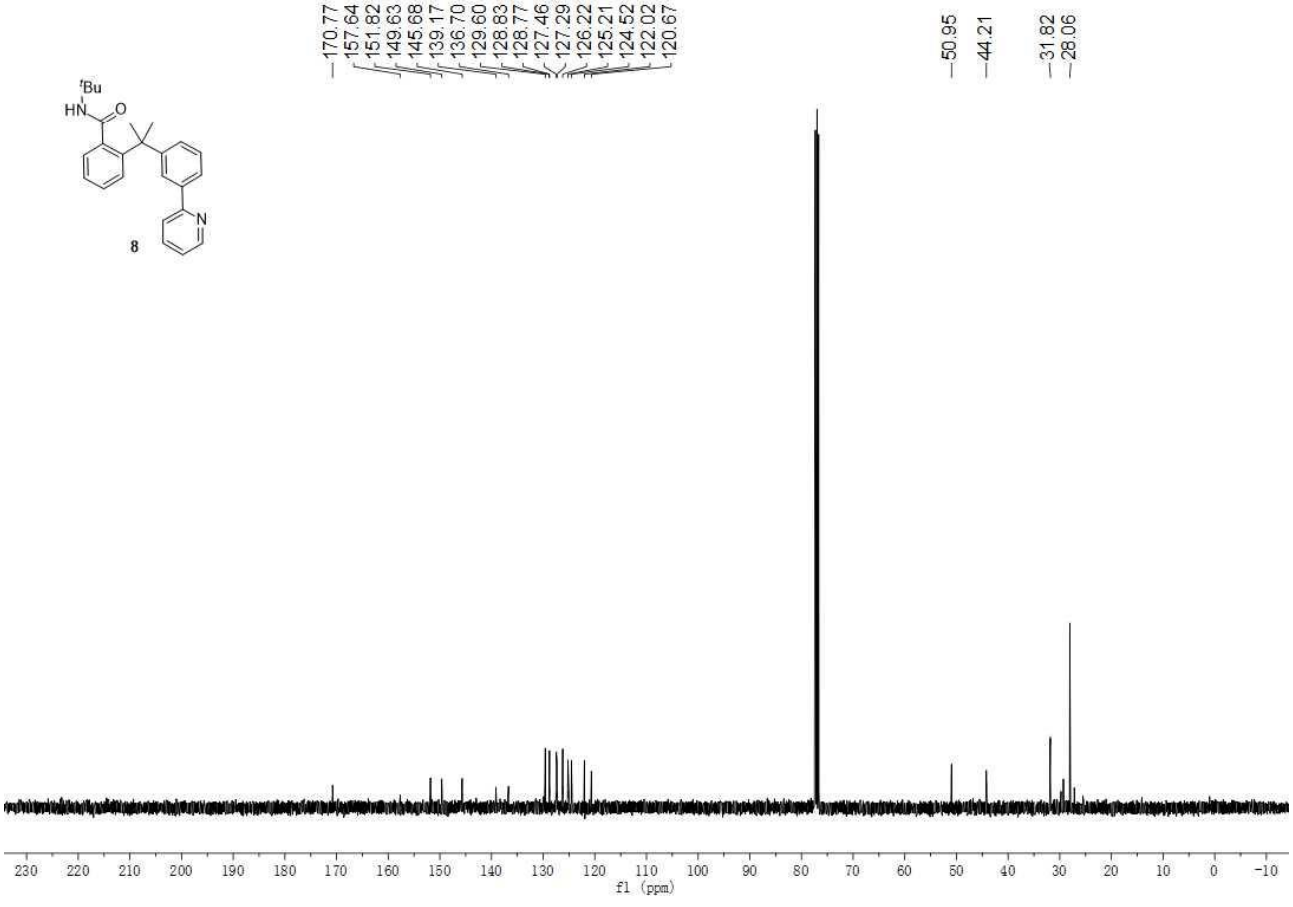
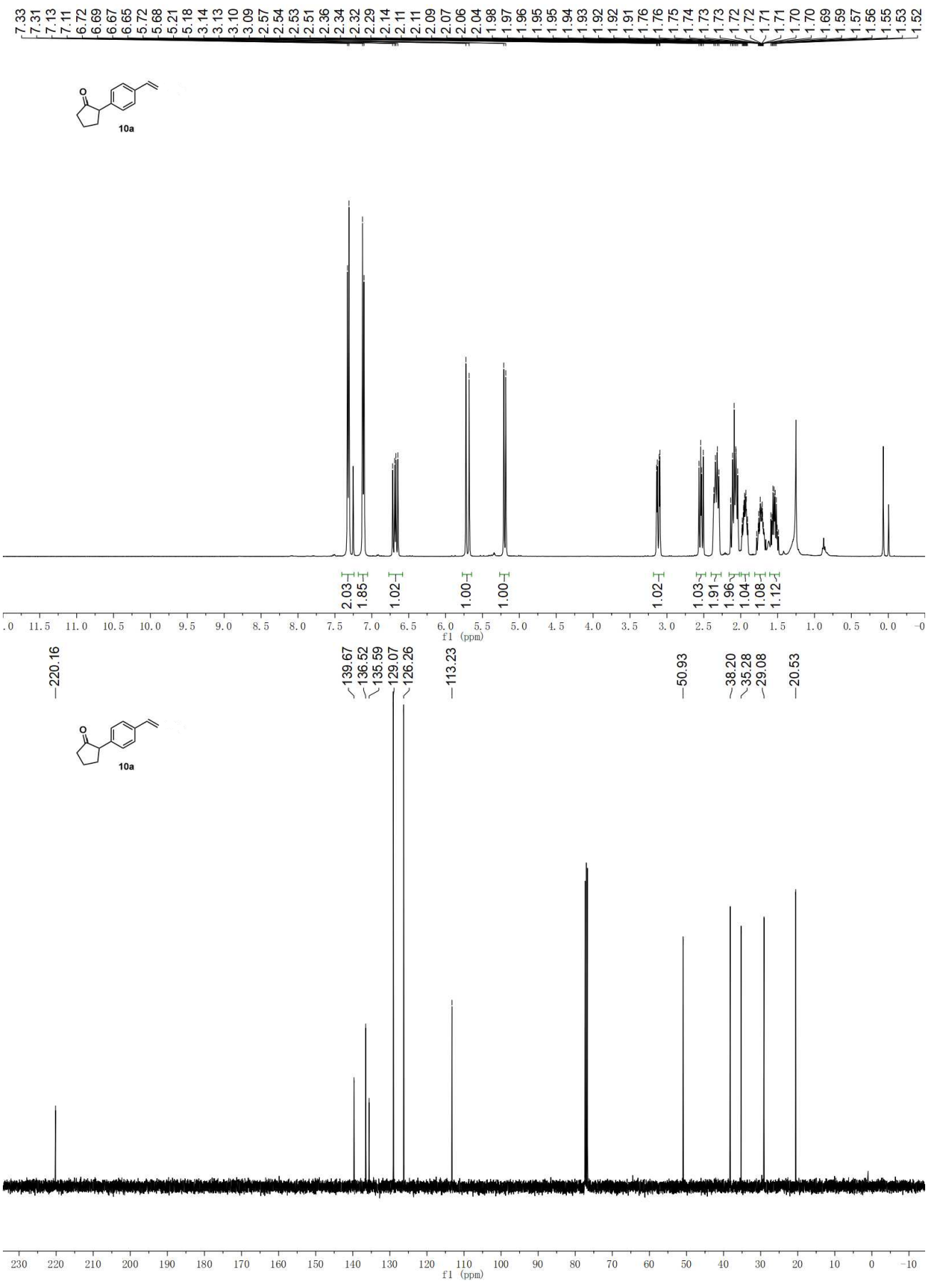
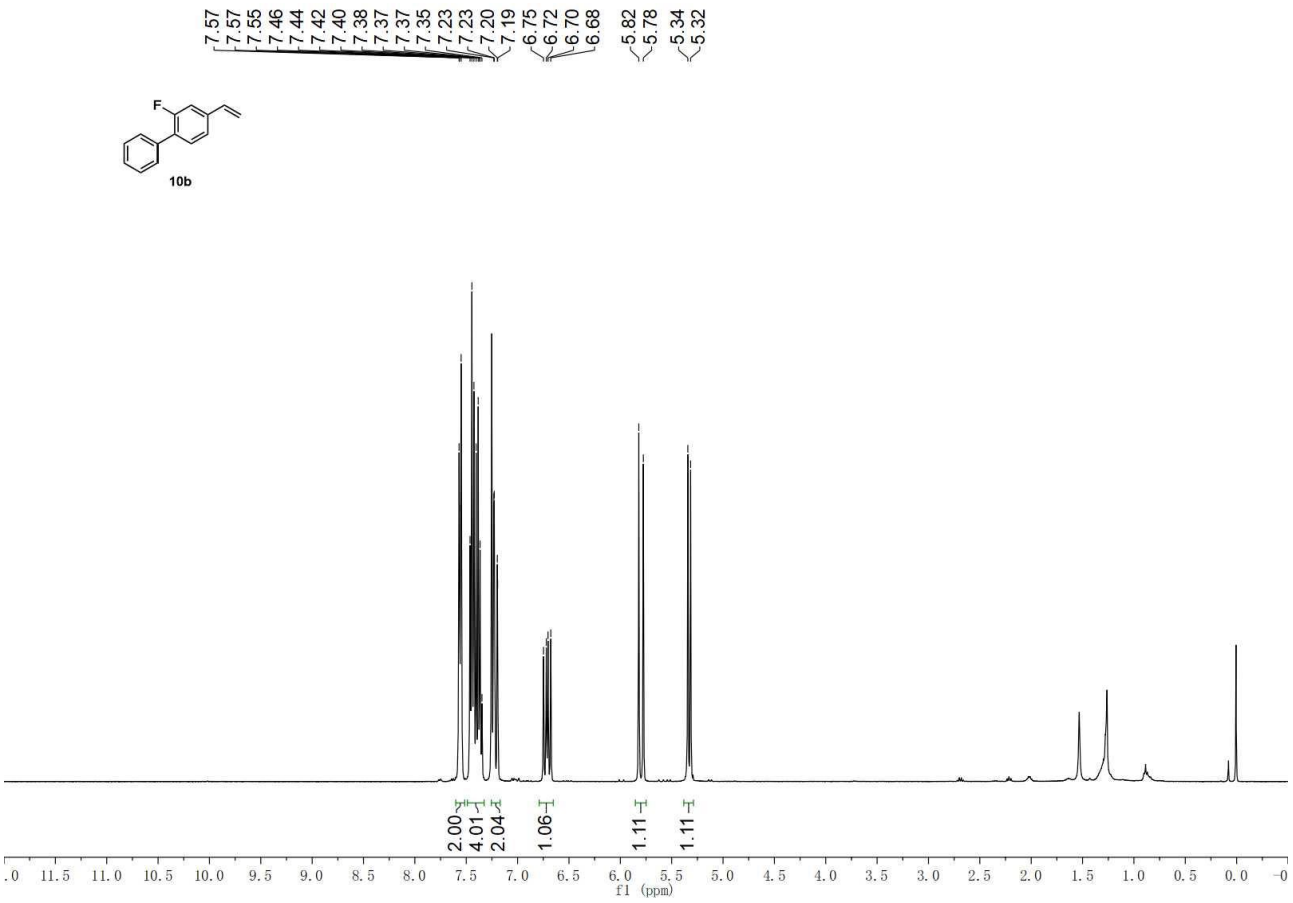
113.81
55.27
51.21
37.49
28.70
MeO
HN-tBu
O
7e
f1 (ppm)


8.64
8.63
7.79
7.76
7.74
7.73
7.71
7.70
7.64
7.62
7.59
7.57
7.39
7.37
7.35
7.34
7.23
7.21
7.19
7.18
4.87
1.82
0.98
tBu
HN
O
N
8
1.00
3.02
2.03
2.00
3.02
1.00
6.05
8.98
f1 (ppm)


170.77
157.64
151.82
149.63
145.68
139.17
136.70
129.60
128.83
128.77
127.46
127.29
126.22
125.21
124.52
122.02
120.67
50.95
44.21
31.82
28.06
tBu
HN
O
N
8
f1 (ppm)


7.33 7.31 7.13 7.11 6.72 6.69 6.67 6.65 5.72 5.68 5.21 5.18 3.14 3.13 3.10 3.09 2.57 2.54 2.53 2.51 2.36 2.34 2.32 2.29 2.14 2.11 2.11 2.09 2.07 2.06 2.04 1.98 1.97 1.96 1.95 1.95 1.94 1.93 1.92 1.92 1.91 1.76 1.75 1.74 1.73 1.73 1.72 1.72 1.71 1.71 1.70 1.70 1.69 1.59 1.57 1.56 1.55 1.53 1.52
10a
2.03 1.85 1.02 1.00 1.00 1.02 1.03 1.91 1.96 1.04 1.08 1.12
f1 (ppm)
220.16 139.67 136.52 135.59 129.07 126.26 113.23 50.93 38.20 35.28 29.08 20.53
10a
f1 (ppm)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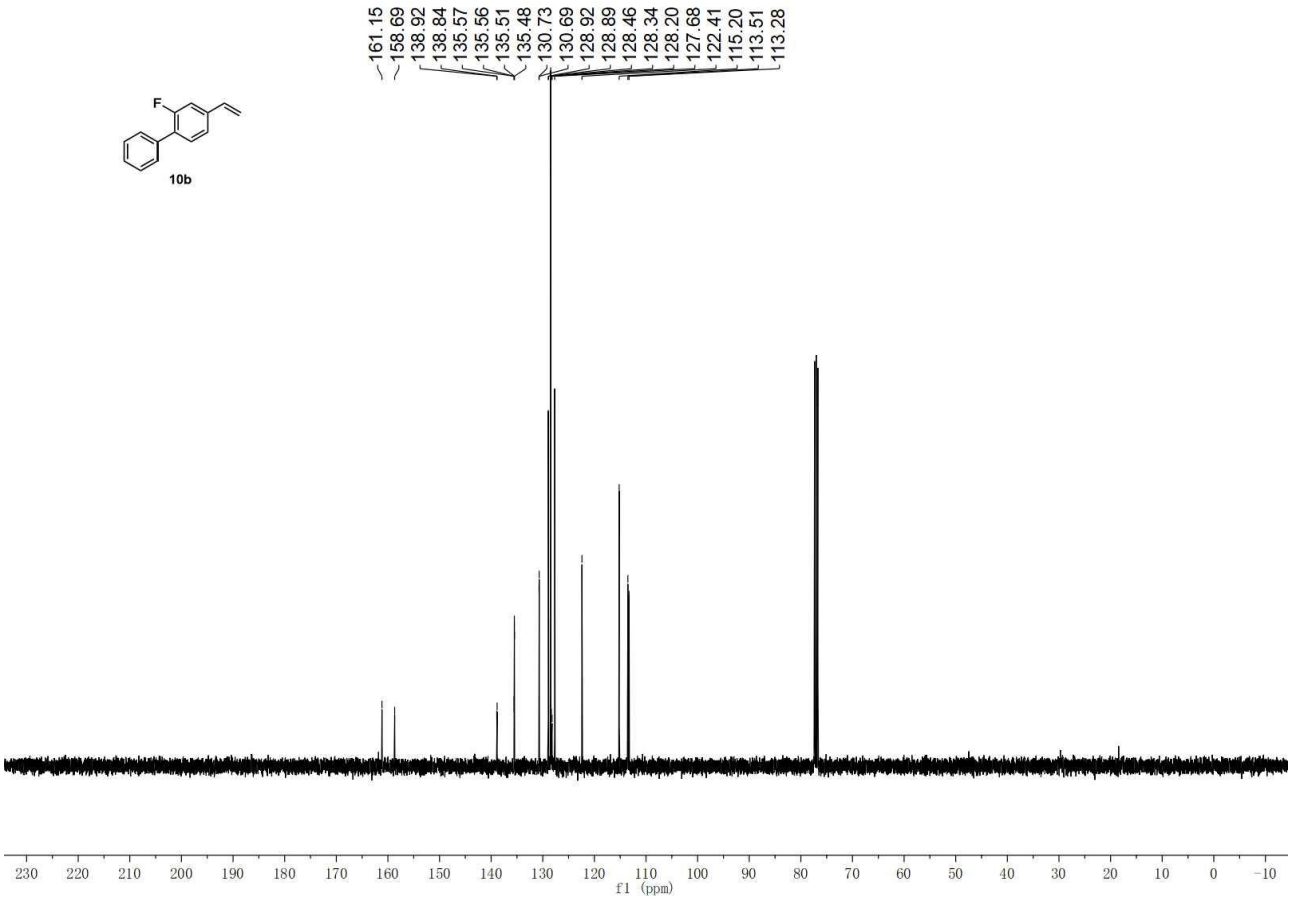
7.57
7.55
7.46
7.44
7.42
7.40
7.38
7.37
7.37
7.35
7.23
7.23
7.20
7.19
6.75
6.72
6.70
6.68
5.82
5.78
5.34
5.32
F
10b
2.00
4.01
2.04
1.06
1.11
1.11
f1 (ppm)


161.15
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138.84
135.57
135.56
135.51
135.48
130.73
130.69
128.92
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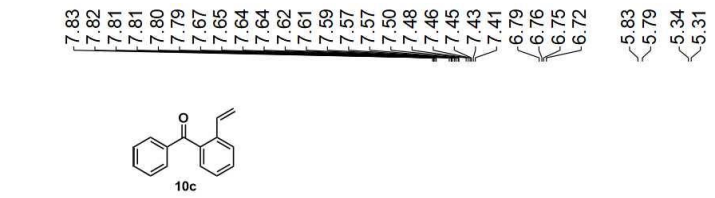
128.34
128.20
127.68
122.41
115.20
113.51
113.28
F
10b
f1 (ppm)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7.81
7.80
7.79
7.67
7.65
7.64
7.64
7.62
7.61
7.59
7.57
7.57
7.50
7.48
7.46
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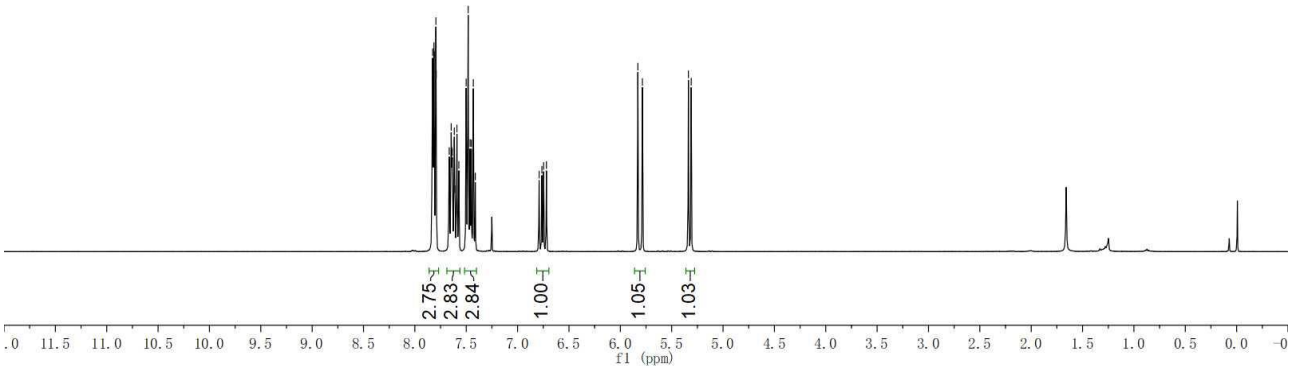
6.79
6.76
6.75
6.72
5.83
5.79
5.34
5.31
O
10c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2.84
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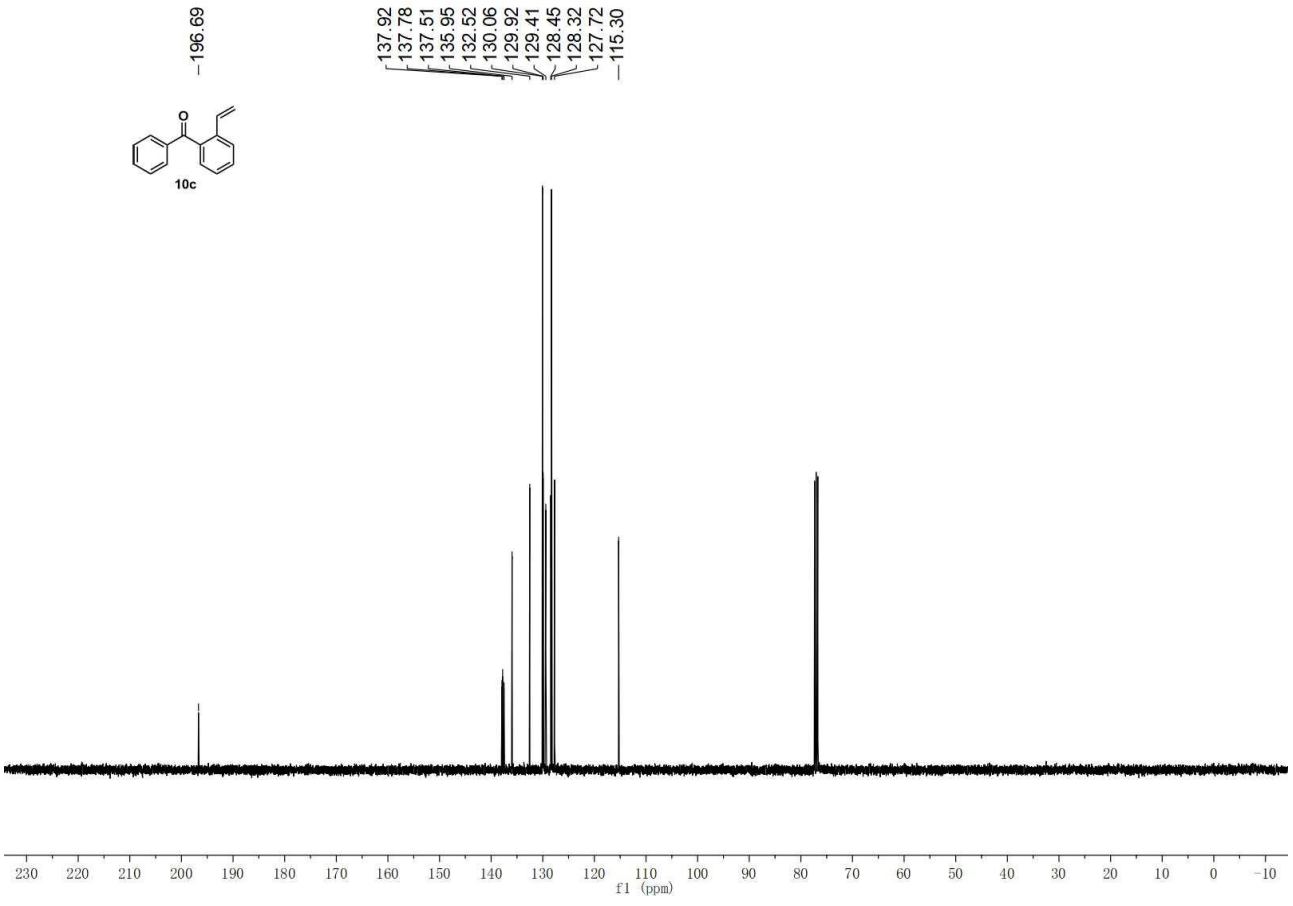
1.03
f1 (ppm)


196.69
137.92
137.78
137.51
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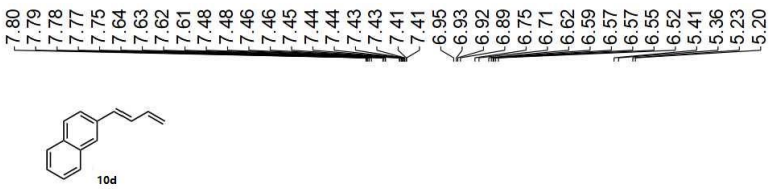
132.52
130.06
129.92
129.41
128.45
128.32
127.72
115.30
O
10c
f1 (ppm)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7.62
7.61
7.48
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7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.41
7.41
6.95
6.93
6.92
6.89
6.75
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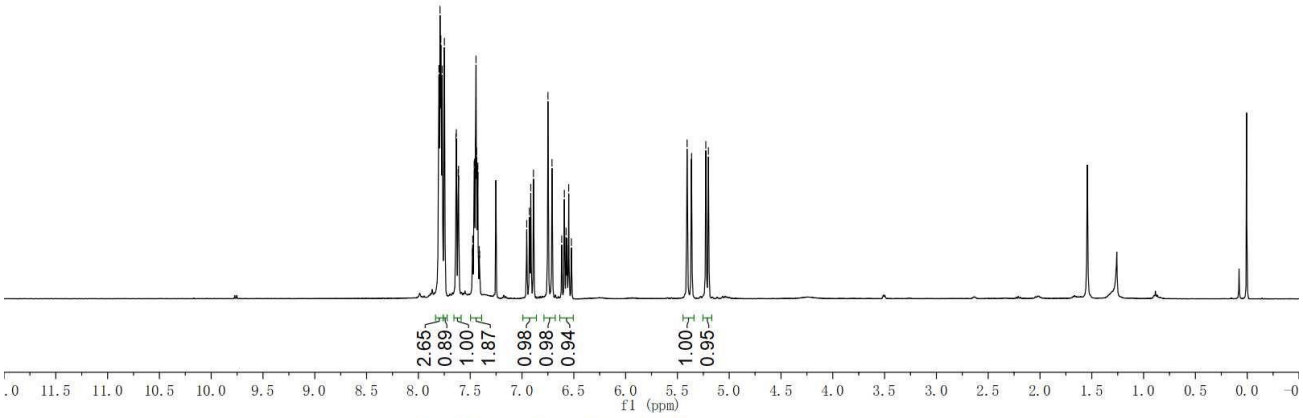
5.41
5.36
5.23
5.20

10d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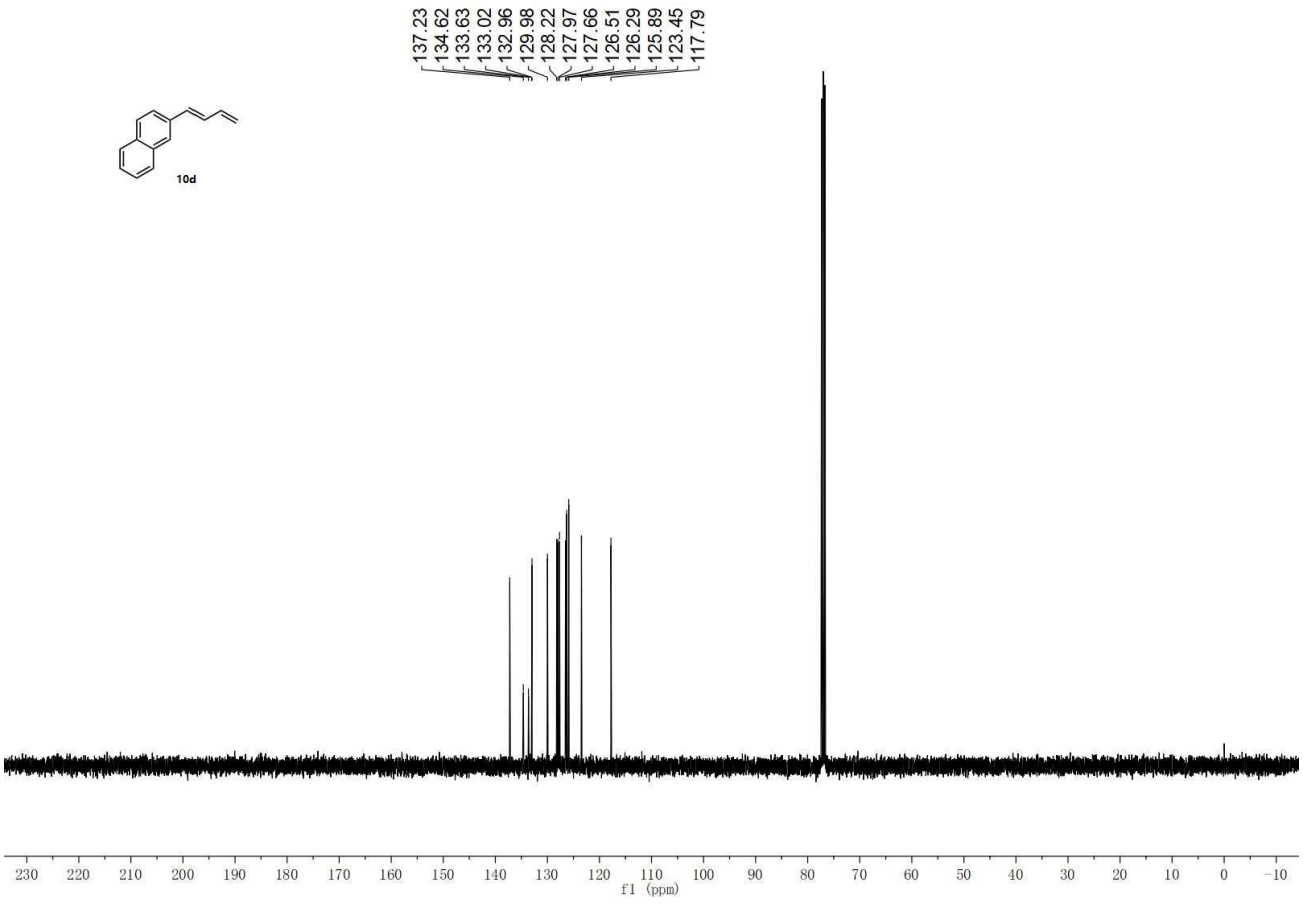
0.98
0.94
1.00
0.95
f1 (ppm)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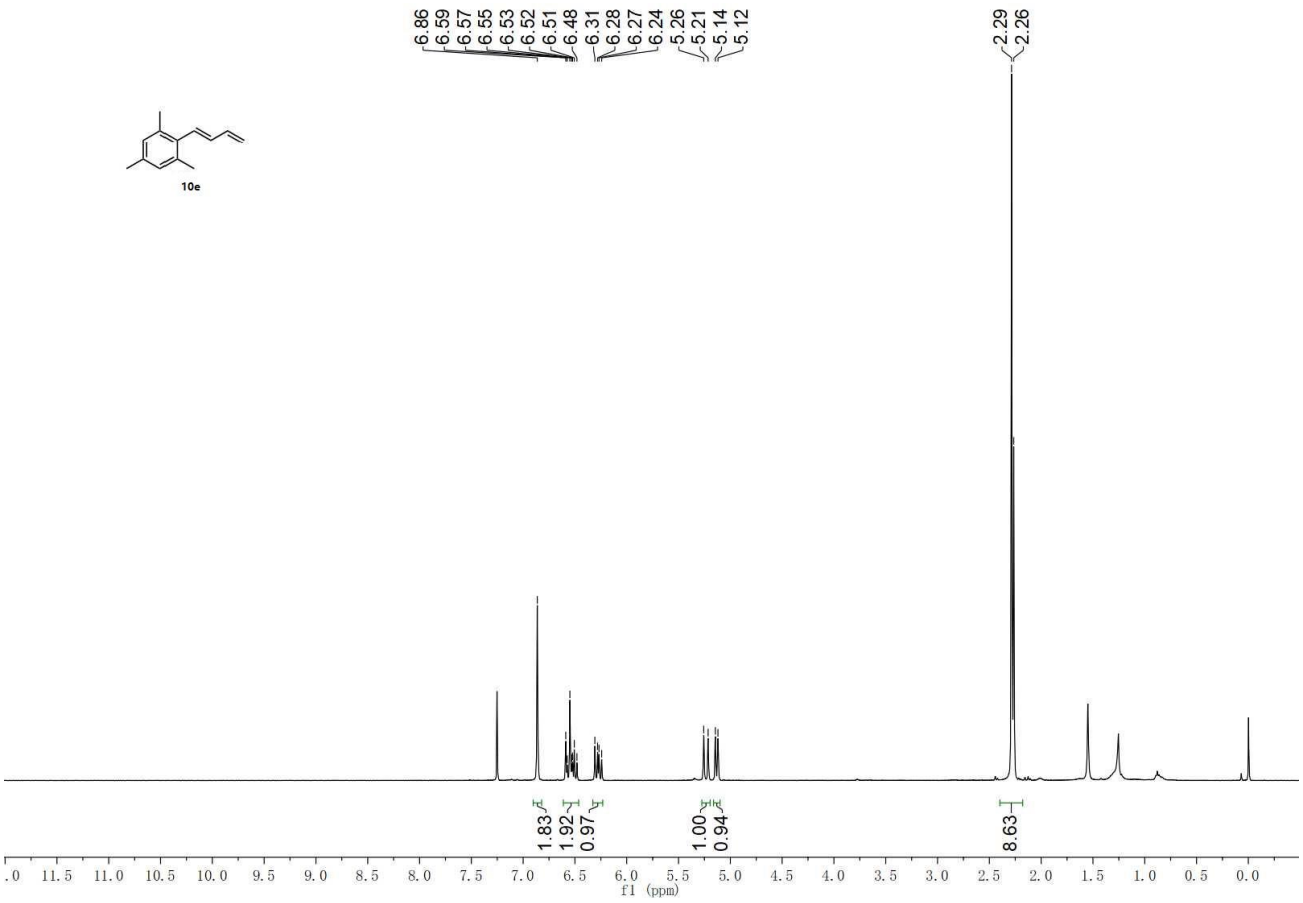
134.62
133.63
133.02
132.96
129.98
128.22
127.97
127.66
126.51
126.29
125.89
123.45
117.79
10d
f1 (ppm)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6.57
6.55
6.53
6.52
6.51
6.48
6.31
6.28
6.27
6.24
5.26
5.21
5.14
5.12
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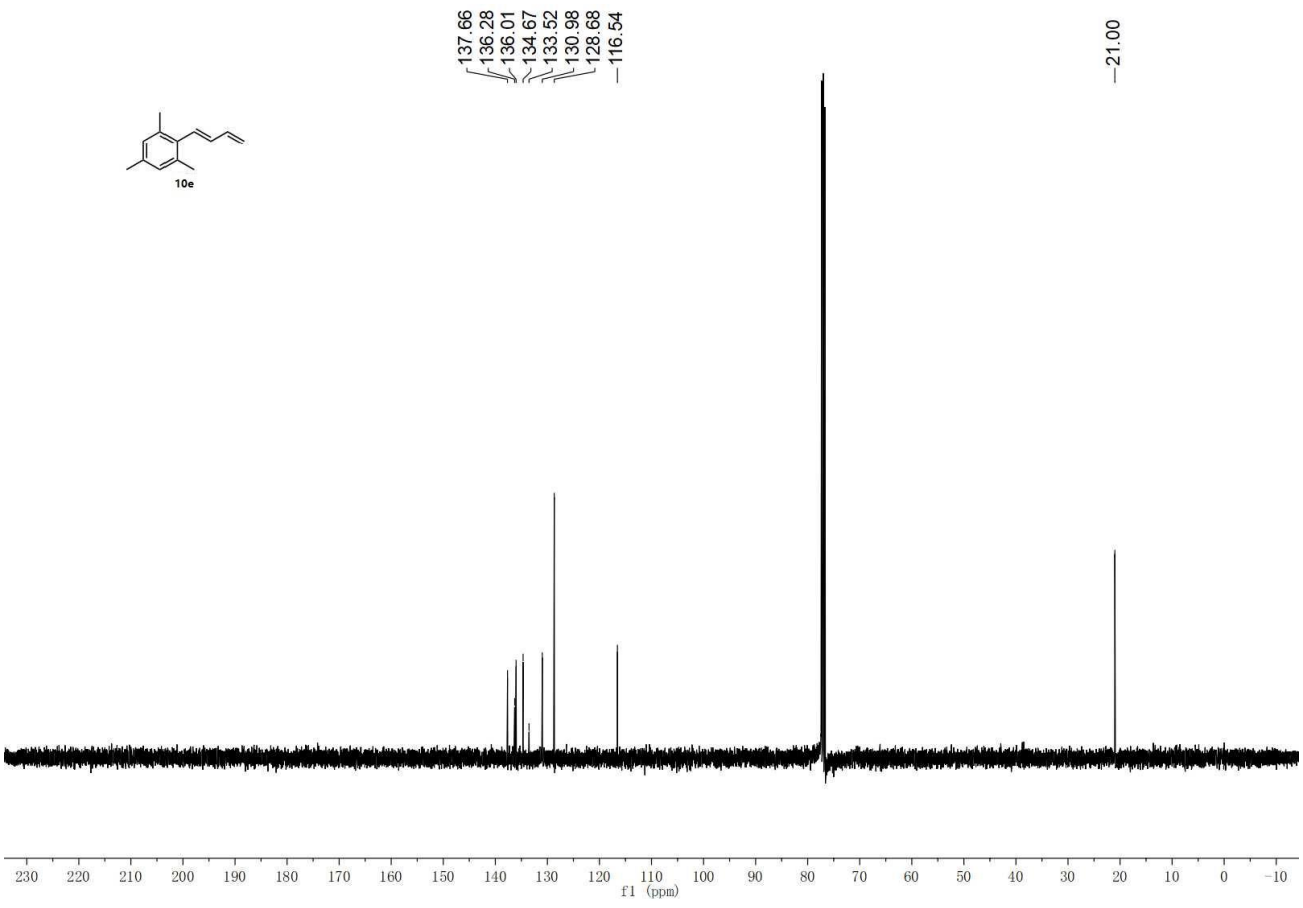
2.26
10e
1.83
1.92
0.97
1.00
0.94
8.63
f1 (ppm)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136.01
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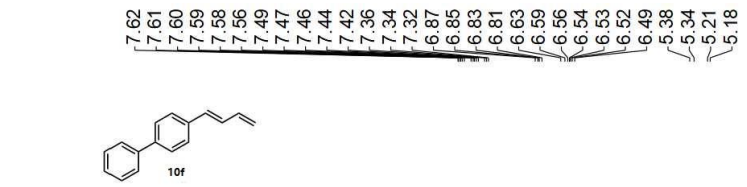
130.98
128.68
116.54
21.00
10e
f1 (ppm)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7.59
7.58
7.56
7.49
7.47
7.46
7.44
7.42
7.36
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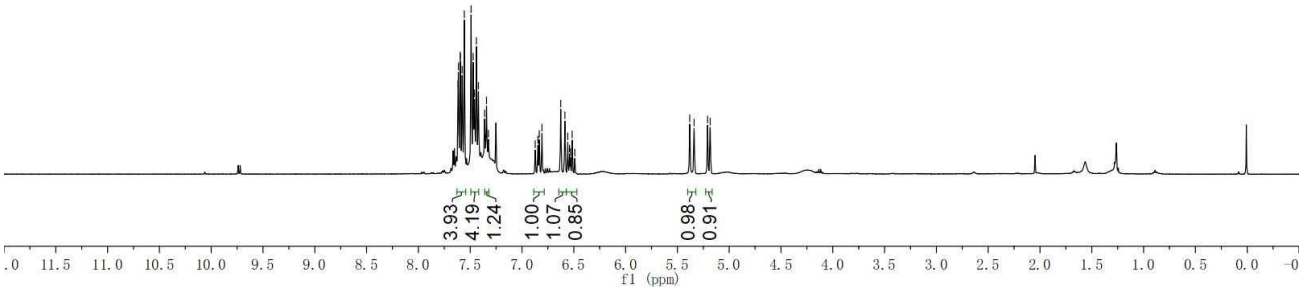
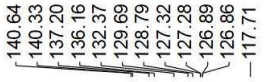
7.32
6.87
6.85
6.83
6.81
6.63
6.59
6.56
6.54
6.53
6.52
6.49
5.38
5.34
5.21
5.18

10f


3.93
4.19
1.24
1.00
1.07
0.85
0.98
0.91
f1 (ppm)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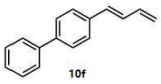
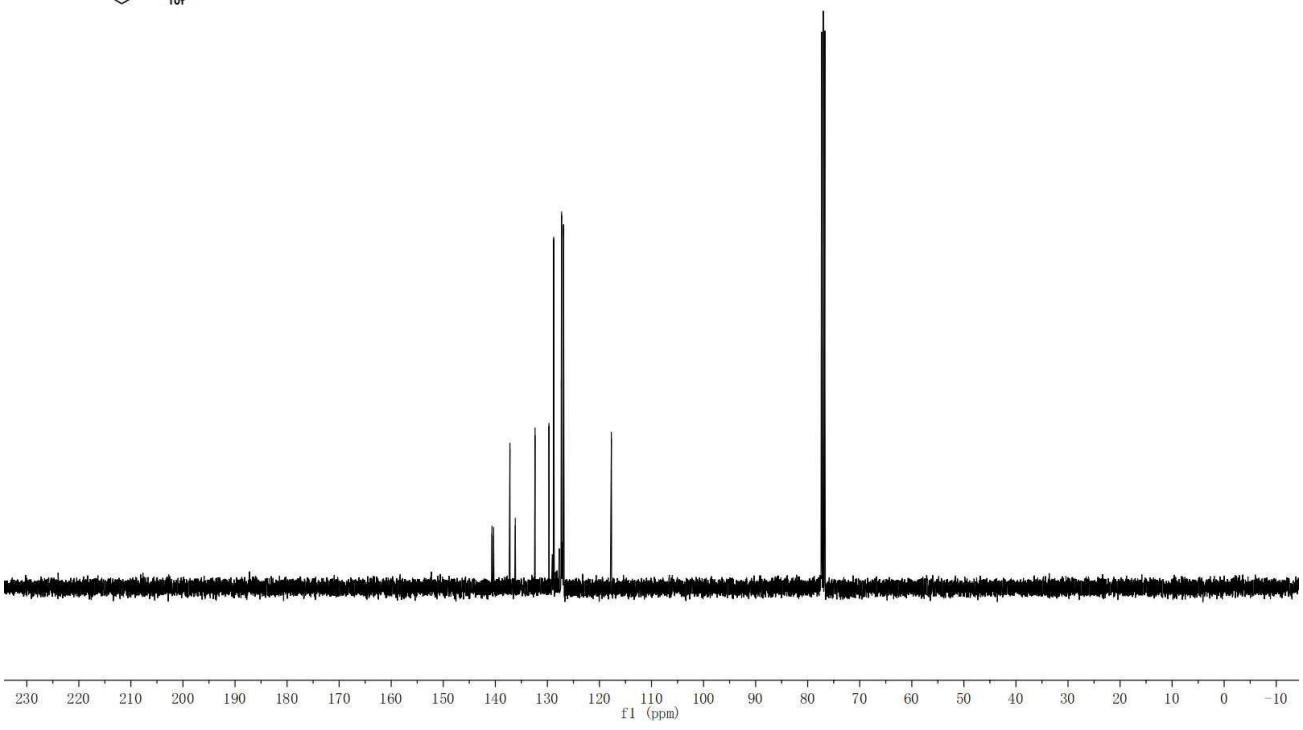
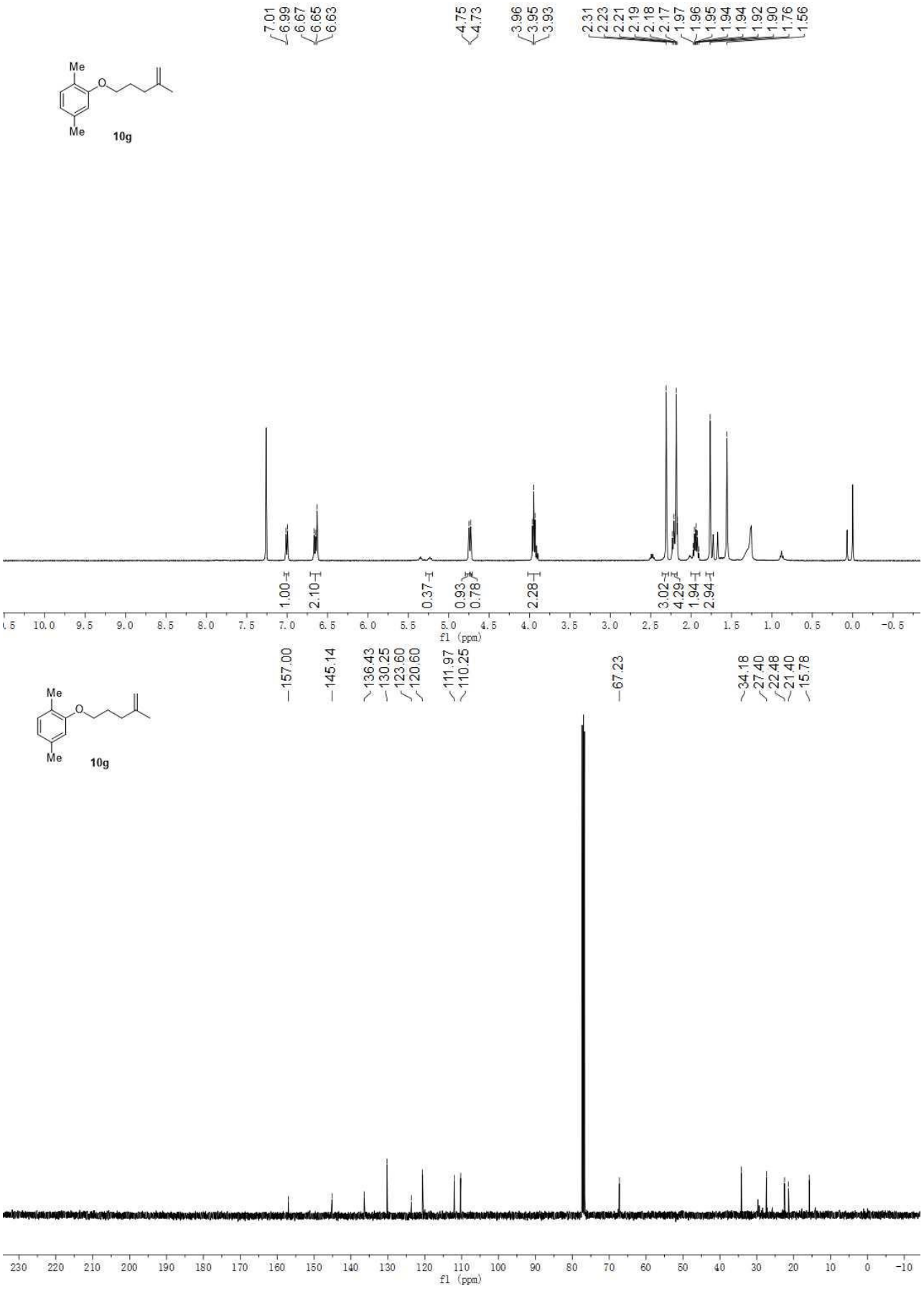
132.37
129.69
128.79
127.32
127.28
126.89
126.86
117.71


10f


f1 (ppm)


7.01
6.99
6.67
6.65
6.63
4.75
4.73
3.96
3.95
3.93
2.31
2.23
2.21
2.19
2.18
2.17
1.97
1.96
1.95
1.94
1.94
1.92
1.90
1.76
1.56
Me
O
Me
10g
1.00
2.10
0.37
0.93
0.78
2.28
3.02
4.29
1.94
2.94
f1 (ppm)
157.00
145.14
136.43
130.25
123.60
120.60
111.97
110.25
67.23
34.18
27.40
22.48
21.40
15.78
Me
O
Me
10g
f1 (ppm)

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