Electronic Supplementary Material (ESI) for ChemComm.

Supporting information

General Methods

All reactions were carried out with magnetic stirring and in flame dried glassware. Standard syringe techniques were applied for transfer of dry solvents. All solvents before used were dried and distilled under standard methods. All other commercially available reagents were used as received. Proton (^{1}H NMR) and carbon (^{13}C NMR) nuclear magnetic resonance spectra were recorded at 400 MHz and 101 MHz, respectively. The chemical shifts are given in parts per million (ppm) on the delta (δ) scale. The solvent peak was used as a reference value, for ^{1}H NMR: $CDCl_3$ = 7.27 ppm, for ^{13}C NMR: $CDCl_3$ = 77.23. Infrared spectra were recorded on a FT-IR spectrometer with KBr discs. Analytical TLC was performed on precoated silica gel GF254 plates. Column chromatography was carried out on silica gel or alumina (200–300 mesh). HRMS were carried out on an Orbitrap analyzer.

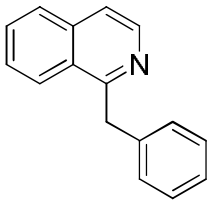
General procedure for the benzylation reaction of isoquinolines

In a 10 mL tube, **1a** (0.2 mmol, 1.0 equiv), **2a** (1.8 mmol, 9 equiv), $Y(OTf)_3$ (0.01 mmol, 0.05 equiv) and di-tert-butyl peroxide (0.6 mmol, 3.0 equiv) were added. Then the tube was sealed and the resulting solution was heated in a 120 °C oil bath with vigorous stirring for 24 h. Then the reaction mixture was cooled to 0 °C and treated with saturated aqueous $NaHCO_3$. The mixture was extracted with ethyl acetate (10 mL × 3), and the combined organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated under vacuum. The residue was purified by flash chromatography using ethyl acetate/petroleum ether (10:90) as eluent to afford **3a** (32.0 mg, 73% yield).

General procedure for the benzoylation reaction of isoquinolines

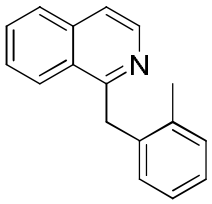
In a 10 mL tube, **1a** (0.2 mmol, 1.0 equiv), **2a** (1.8 mmol, 9 equiv), TFA (0.2 mmol, 1.0 equiv), MnO_2 (0.02 mmol, 10 mol %) and TBHP (5~6 M solution in decane, 1.0 mmol, 5.0 equiv) were added. Then the tube was sealed and the resulting solution was heated in a 120 °C oil bath with vigorous stirring for 24 h. Then the reaction mixture was cooled to 0 °C and treated with saturated aqueous $NaHCO_3$. The mixture was extracted with ethyl acetate (10 mL × 3), and the combined organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated under vacuum. The residue was purified by flash chromatography using ethyl acetate/petroleum ether (10:90) as eluent to afford **4a** (30.3 mg, 65% yield).

Analytical data for products



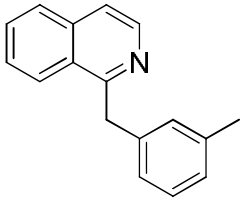
1-Benzylisoquinoline (3a)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, *J* = 5.7 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.60–7.51 (m, 2H), 7.33–7.24 (m, 4H), 7.18 (t, *J* = 6.9 Hz, 1H), 4.70 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.3, 142.2, 139.6, 136.8, 130.0, 128.8, 128.7, 127.5, 127.4, 126.4, 126.0, 120.0, 42.2. These data are consistent with reported literature values.[1]



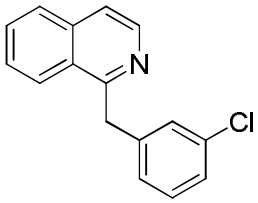
1-(2-Methylbenzyl)isoquinoline (3b)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3b** (35.0 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, *J* = 5.7 Hz, 1H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.72–7.64 (m, 1H), 7.59 (d, *J* = 5.7 Hz, 1H), 7.56–7.51 (m, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 1H), 4.66 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.2, 142.3, 138.0, 136.6, 136.4, 130.3, 130.1, 129.0, 127.7, 127.6, 127.4, 126.5, 126.2, 125.8, 119.9, 39.5, 20.2; IR ν_{max} 3045, 2920, 2851, 1586, 1529, 1387, 1036, 815, 787 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{17}H_{16}N$: 234.1277, found 234.1280.



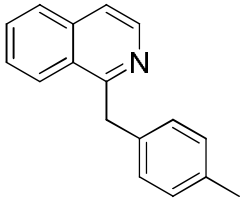
1-(3-Methylbenzyl)isoquinoline (3c)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3c** (37.3 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.53 (d, *J* = 5.7 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.69–7.62 (m, 1H), 7.60–7.50 (m, 2H), 7.21–7.07 (m, 3H), 7.00 (d, *J* = 7.3 Hz, 1H), 4.66 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.4, 142.2, 139.5, 138.3, 136.7, 130.0, 129.5, 128.6, 127.5, 127.4, 127.2, 126.0, 125.8, 120.0, 42.2, 21.6. These data are consistent with reported literature values.[2]



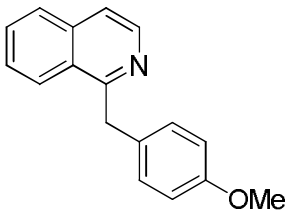
1-(3-Chlorobenzyl)isoquinoline (3d)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3d** (27.9 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.50 (d, *J* = 5.7 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.55 (dd, *J* = 17.4, 6.8 Hz, 2H), 7.29–7.25 (m, 1H), 7.18–7.11 (m, 3H), 4.63 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.4, 142.3, 141.6, 136.8, 134.5, 130.2, 129.9, 128.9, 127.6, 127.6, 127.3, 127.0, 126.7, 125.7, 120.2, 41.7; IR ν_{max} 3051, 2927, 2856, 1574, 1522, 1388, 1023, 828, 793 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{16}H_{13}{}^{35}ClN$: 254.0731, found 254.0733; $[M + H]^+$ calculated for $C_{16}H_{13}{}^{37}ClN$: 256.0702, found 256.0703.



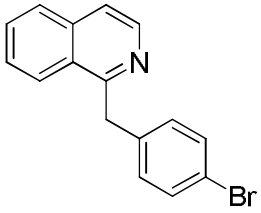
1-(4-Methylbenzyl)isoquinoline (3e)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3e** (33.6 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.51 (d, *J* = 5.7 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.67–7.61 (m, 1H), 7.58–7.51 (m, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 2H), 4.65 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.6, 142.2, 136.8, 136.6, 135.9, 130.0, 129.4, 128.7, 127.5, 127.4, 126.0, 119.9, 41.9, 21.2; IR ν_{max} 3050, 2920, 2856, 1561, 1513, 1384, 1020, 823, 797 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{17}H_{16}N$: 234.1277, found 234.1275.



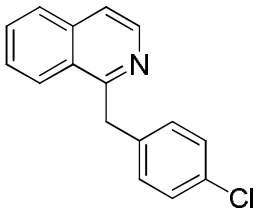
1-(4-Methoxybenzyl)isoquinoline (3f)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (20:80) as eluent to afford **3f** (30.4 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.50 (d, *J* = 5.7 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.60–7.51 (m, 2H), 7.21 (d, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 8.6 Hz, 2H), 4.62 (s, 2H), 3.75 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.7, 158.3, 142.2, 136.8, 131.8, 130.1, 129.8, 127.6, 127.4, 126.1, 120.0, 114.2, 55.4, 41.4. These data are consistent with reported literature values.[1]



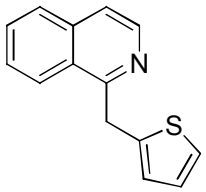
1-(4-Bromobenzyl)isoquinoline (3g)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3g** (41.7 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.50 (d, *J* = 5.7 Hz, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 8.3 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.60–7.51 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 4.62 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.7, 142.2, 138.6, 136.8, 131.8, 130.6, 130.2, 127.6, 127.5, 127.2, 125.7, 120.4, 120.2, 41.5; IR ν_{max} 3055, 2927, 2849, 1566, 1519, 1387, 1026, 819, 795 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{16}H_{13}{}^{79}BrN$: 298.0226, found 298.0228; $[M + H]^+$ calculated for $C_{16}H_{13}{}^{81}BrN$: 300.0205, found 300.0207.



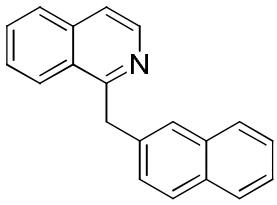
1-(4-Chlorobenzyl)isoquinoline (3h)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3h** (24.9 mg, 49% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.51 (d, *J* = 5.7 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.61–7.51 (m, 2H), 7.24–7.19 (m, 4H), 4.64 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.8, 142.3, 138.1, 136.8, 132.3, 130.2, 128.8, 127.7, 127.6, 127.3, 125.7, 120.2, 41.5; IR ν_{max} 3051, 2916, 2852, 1554, 1517, 1388, 1022, 826, 790 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{16}H_{13}{}^{35}ClN$: 254.0731, found 254.0732; $[M + H]^+$ calculated for $C_{16}H_{13}{}^{37}ClN$: 256.0702, found 256.0701.



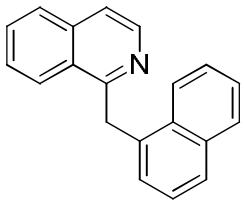
1-(Thiophen-2-ylmethyl)isoquinoline (3i)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3i** (15.8 mg, 35% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.51 (d, *J* = 5.7 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.62–7.54 (m, 2H), 7.13 (d, *J* = 4.9 Hz, 1H), 6.91–6.87 (m, 1H), 6.86–6.84 (m, 1H), 4.84 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.4, 142.3, 141.9, 136.8, 130.2, 127.6, 127.5, 127.0, 127.0, 125.7, 125.6, 124.3, 120.3, 36.6; IR ν_{max} 2920, 2851, 1586, 1559, 1499, 1387, 805, 757, 703 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{14}H_{12}NS$: 226.0685, found 226.0689.



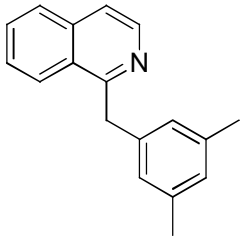
1-(Naphthalen-2-ylmethyl)isoquinoline (3j)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3j** (38.8 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.57 (d, *J* = 5.7 Hz, 1H), 8.22 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.80–7.71 (m, 4H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 6.0 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.49–7.38 (m, 3H), 4.87 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.2, 142.3, 137.3, 136.8, 133.8, 132.3, 130.0, 128.3, 127.8, 127.8, 127.6, 127.4, 127.3, 127.1, 126.1, 126.0, 125.6, 120.1, 42.5. These data are consistent with reported literature values.[3]



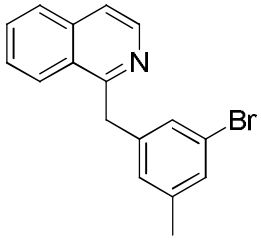
1-(Naphthalen-1-ylmethyl)isoquinoline (3k)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3k** (22.1 mg, 41% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, *J* = 5.7 Hz, 1H), 8.26 (d, *J* = 8.2 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.85 (dd, *J* = 15.6, 7.9 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.65–7.42 (m, 5H), 7.30–7.23 (m, 1H), 6.96 (d, *J* = 7.1 Hz, 1H), 5.12 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.2, 142.4, 136.6, 135.9, 134.0, 132.3, 130.1, 129.0, 127.8, 127.6, 127.4, 127.2, 126.7, 126.3, 125.9, 125.8, 125.7, 124.0, 120.0, 39.2; IR ν_{max} 3049, 2918, 1560, 1498, 1383, 1014, 822, 790, 774, 751 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{20}H_{16}N$: 270.1277, found 270.1275.



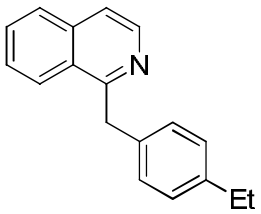
1-(3,5-Dimethylbenzyl)isoquinoline (3l)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3l** (34.6 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.54 (d, *J* = 5.7 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.70–7.61 (m, 1H), 7.60–7.51 (m, 2H), 6.94 (s, 2H), 6.83 (s, 1H), 4.62 (s, 2H), 2.26 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.6, 142.2, 139.5, 138.1, 136.8, 130.0, 128.2, 127.5, 127.3, 126.6, 126.1, 119.9, 42.1, 21.4; IR ν_{max} 3054, 2922, 1553, 1480, 1381, 1002, 836, 778 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{18}H_{18}N$: 248.1434, found 248.1431.



1-(3-Bromo-5-methylbenzyl)isoquinoline (3m)

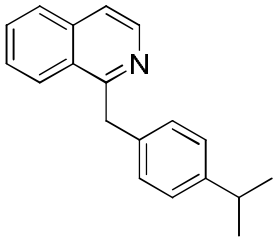
It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3m** (45.0 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.51 (d, *J* = 5.5 Hz, 1H), 8.11 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.68–7.61 (m, 1H), 7.60–7.51 (m, 2H), 7.25 (s, 1H), 7.15 (s, 1H), 7.02 (s, 1H), 4.60 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.5, 142.2, 141.6, 140.4, 136.8, 130.3, 130.1, 128.8, 128.3, 127.6, 127.6, 127.3, 125.7, 122.5, 120.2, 41.6, 21.3; IR ν_{max} 3048, 2927, 2864, 1550, 1506, 1372, 1029, 834, 786 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{17}H_{15}{}^{79}BrN$: 312.0382, found 312.0387; $[M + H]^+$ calculated for $C_{17}H_{15}{}^{81}BrN$: 314.0362, found 314.0364.



1-(4-Ethylbenzyl)isoquinoline (3n)

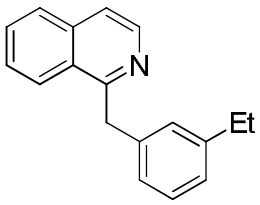
It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3n** (37.1 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, *J* = 5.5 Hz, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.59–7.49 (m, 2H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.11 (d, *J* = 7.5 Hz, 2H), 4.67 (s, 2H), 2.60 (q, *J* = 7.4 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.6, 142.3, 142.2, 136.8, 136.8, 130.0, 128.7, 128.2, 127.5, 127.4, 127.3, 126.1,

119.9, 41.8, 28.6, 15.7; IR ν_{max} 3042, 2909, 2840, 1573, 1525, 1377, 1033, 834, 780 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{18}H_{18}N$: 248.1434, found 248.1433.



1-(4-Isopropylbenzyl)isoquinoline (3o)

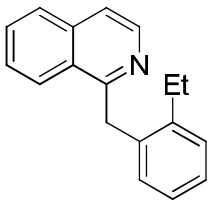
It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3o** (42.9 mg, 82% yield). ^1H NMR (400 MHz, $CDCl_3$) δ = 8.51 (d, *J* = 5.7 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.68–7.62 (m, 1H), 7.59–7.51 (m, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.66 (s, 2H), 2.85 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.21 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.6, 146.9, 142.2, 136.9, 136.8, 130.1, 128.7, 127.5, 127.5, 127.4, 126.8, 126.1, 119.9, 41.8, 33.8, 24.2; IR ν_{max} 3039, 2930, 2839, 1548, 1508, 1377, 1009, 837, 778 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{19}H_{20}N$: 262.1590, found 262.1591.



1-(3-Ethylbenzyl)isoquinoline (3p)

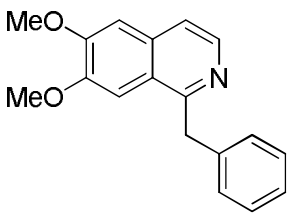
It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3p** (29.7 mg, 60% yield). ^1H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, *J* = 5.7 Hz, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.59–7.51 (m, 2H), 7.21–7.14 (m, 2H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.03 (d, *J* = 7.6 Hz,

1H), 4.67 (s, 2H), 2.59 (q, J = 7.6 Hz, 2H), 1.19 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.5, 144.7, 142.2, 139.6, 136.8, 130.1, 128.7, 128.5, 127.5, 127.5, 127.4, 126.1, 126.0, 120.0, 42.3, 29.0, 15.7; IR ν_{max} 3043, 2922, 2846, 1569, 1521, 1396, 1011, 826, 785 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{18}H_{18}N$: 248.1434, found 248.1436.



1-(2-Ethylbenzyl)isoquinoline (3q)

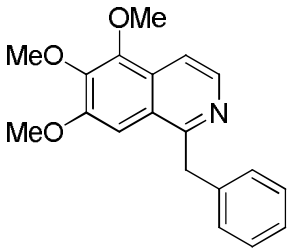
It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3q** (30.7 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, J = 5.7 Hz, 1H), 8.05 (d, J = 8.5 Hz, 1H), 7.85 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.5 Hz, 1H), 7.59 (d, J = 5.7 Hz, 1H), 7.55–7.50 (m, 1H), 7.28 (d, J = 6.7 Hz, 1H), 7.19 (t, J = 7.3 Hz, 1H), 7.03 (t, J = 7.4 Hz, 1H), 6.80 (d, J = 7.6 Hz, 1H), 4.72 (s, 2H), 2.84 (q, J = 7.5 Hz, 2H), 1.30 (t, J = 7.5 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.5, 142.3, 142.1, 137.3, 136.6, 130.0, 129.3, 128.5, 127.7, 127.6, 127.4, 126.7, 126.1, 125.9, 119.8, 39.0, 26.3, 14.8; IR ν_{max} 3058, 2914, 2860, 1557, 1518, 1374, 1039, 829, 782 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{18}H_{18}N$: 248.1434, found 248.1432.



1-Benzyl-6,7-dimethoxyisoquinoline (3r)

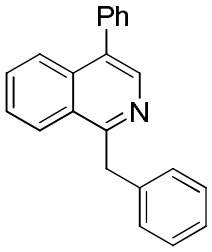
It was prepared following the general method for benzylation and purified by flash

chromatography on silica gel using ethyl acetate/petroleum ether (30:70) as eluent to afford **3r** (27.9 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.40 (d, *J* = 5.6 Hz, 1H), 7.45 (d, *J* = 5.6 Hz, 1H), 7.34–7.25 (m, 5H), 7.23–7.15 (m, 1H), 7.06 (s, 1H), 4.63 (s, 2H), 4.01 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 157.8, 152.5, 149.9, 141.2, 139.8, 133.6, 128.7, 126.4, 123.1, 118.9, 105.4, 104.4, 56.1, 56.0, 42.9; IR ν_{max} 3050, 2920, 2856, 1561, 1513, 1384, 1020, 823, 797 cm^{-1}; HRMS (EI) *m/z* [M + H]$^+$ calculated for $C_{18}H_{18}NO_2$: 280.1332, found 280.1336.



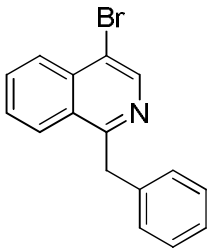
1-Benzyl-5,6,7-trimethoxyisoquinoline (3s)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (30:70) as eluent to afford **3s** (25.4 mg, 41% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.41 (d, *J* = 5.8 Hz, 1H), 7.77 (d, *J* = 5.8 Hz, 1H), 7.31–7.24 (m, 4H), 7.21–7.16 (m, 1H), 7.14 (s, 1H), 4.60 (s, 2H), 4.03 (s, 3H), 3.99 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 158.1, 153.5, 147.3, 143.8, 140.7, 139.8, 128.8, 128.8, 128.7, 126.5, 124.4, 114.0, 100.7, 61.7, 61.3, 56.0, 43.0; IR ν_{max} 3030, 2929, 2838, 1539, 1493, 1382, 1010, 805, 778 cm^{-1}; HRMS (EI) *m/z* [M + H]$^+$ calculated for $C_{19}H_{20}NO_3$: 310.1438, found 310.1436.



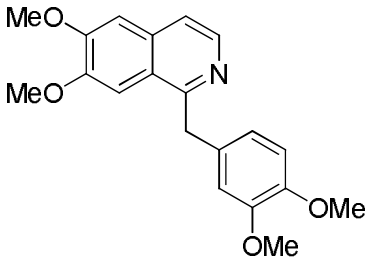
1-Benzyl-4-phenylisoquinoline (3t)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3t** (38.4 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.50 (s, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.65–7.56 (m, 2H), 7.56–7.52 (m, 4H), 7.51–7.46 (m, 1H), 7.37 (d, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 4.75 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.7, 142.0, 139.7, 137.5, 135.2, 132.6, 130.4, 130.1, 128.9, 128.7, 128.7, 128.0, 127.2, 127.0, 126.5, 126.2, 125.8, 42.4; IR ν_{max} 3028, 2927, 2848, 1507, 1490, 1384, 1257, 1028, 763, 754 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{22}H_{18}N$: 296.1434, found 296.1433.



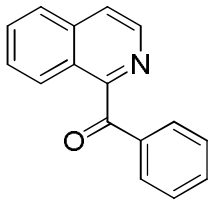
1-Benzyl-4-bromoisoquinoline (3u)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **3u** (25.0 mg, 42% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.71 (s, 1H), 8.18 (dd, *J* = 15.2, 8.5 Hz, 2H), 7.77 (t, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.30–7.26 (m, 4H), 7.24–7.17 (m, 1H), 4.66 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.0, 143.9, 139.1, 135.4, 131.3, 128.8, 128.8, 128.6, 128.4, 127.0, 126.7, 126.5, 118.7, 42.0. These data are consistent with reported literature values.[1]



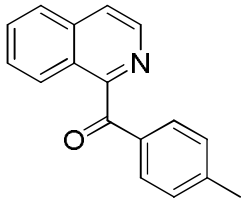
1-(3,4-Dimethoxybenzyl)-6,7-dimethoxyisoquinoline (3v)

It was prepared following the general method for benzylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (60:40) as eluent to afford **3v** (27.2 mg, 40% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.37 (d, *J* = 5.6 Hz, 1H), 7.43 (d, *J* = 5.7 Hz, 1H), 7.35 (s, 1H), 7.05 (s, 1H), 6.82 (d, *J* = 7.0 Hz, 2H), 6.76 (d, *J* = 8.6 Hz, 1H), 4.54 (s, 2H), 4.00 (s, 3H), 3.91 (s, 3H), 3.82 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 158.0, 152.7, 150.0, 149.3, 147.8, 141.2, 133.7, 132.5, 123.2, 120.7, 118.9, 112.2, 111.5, 105.5, 104.5, 56.2, 56.1, 56.2, 56.0, 42.4. These data are consistent with reported literature values.[5]



Isoquinolin-1-yl(phenyl)methanone (4a)

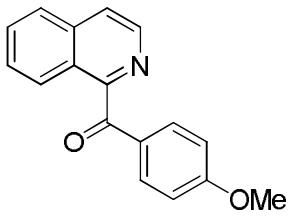
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.62 (d, *J* = 5.6 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 8.00–7.91 (m, 3H), 7.82 (d, *J* = 5.6 Hz, 1H), 7.79–7.72 (m, 1H), 7.66–7.59 (m, 2H), 7.49 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 194.9, 156.7, 141.4, 136.9, 136.9, 133.9, 131.0, 130.9, 128.7, 128.5, 127.3, 126.6, 126.4, 122.8. These data are consistent with reported literature values.[4]



Isoquinolin-1-yl(4-methylphenyl)methanone (4b)

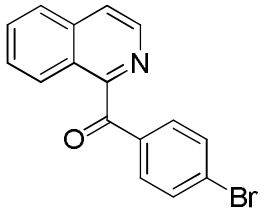
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4b** (29.7 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.61 (d, *J* = 5.6 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.81

(d, J = 5.6 Hz, 1H), 7.78–7.72 (m, 1H), 7.67–7.57 (m, 1H), 7.28 (d, J = 8.8 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 194.7, 157.1, 144.9, 141.4, 136.9, 134.3, 131.1, 130.9, 129.4, 128.4, 127.3, 126.6, 126.5, 122.6, 22.0. These data are consistent with reported literature values.[5]



Isoquinolin-1-yl(4-methoxyphenyl)methanone (4c)

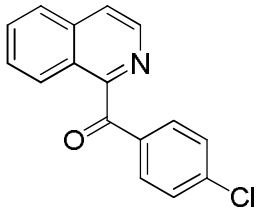
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (20:80) as eluent to afford **4c** (26.3 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.60 (d, J = 5.6 Hz, 1H), 8.18 (d, J = 8.5 Hz, 1H), 8.00–7.90 (m, 3H), 7.80 (d, J = 5.7 Hz, 1H), 7.74 (t, J = 7.6 Hz, 1H), 7.61 (t, J = 7.7 Hz, 1H), 6.96 (d, J = 8.9 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 193.6, 164.4, 157.3, 141.4, 136.9, 133.4, 130.9, 129.8, 128.3, 127.2, 126.6, 126.5, 122.4, 114.0, 55.8. These data are consistent with reported literature values.[5]



(4-Bromophenyl)(isoquinolin-1-yl)methanone (4d)

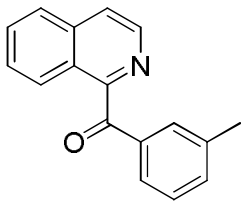
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4d** (30.6 mg, 49% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.60 (d, J=5.6 Hz, 1H), 8.27 (d, J = 8.5 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H), 7.87–7.81 (m, 3H), 7.79–7.74

(m, 1H), 7.68–7.60 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 193.8, 155.8, 141.3, 137.0, 135.7, 132.4, 132.0, 131.0, 129.2, 128.7, 127.4, 126.7, 126.3, 123.2. These data are consistent with reported literature values.[6]



(4-Chlorophenyl)(isoquinolin-1-yl)methanone (4e)

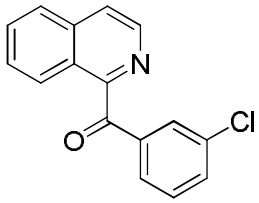
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4e** (21.4 mg, 40% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.61 (d, *J* = 5.6 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 7.97–7.89 (m, 3H), 7.83 (d, *J* = 5.6 Hz, 1H), 7.80–7.73 (m, 1H), 7.70–7.60 (m, 1H), 7.46 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 193.6, 155.9, 141.3, 140.4, 137.0, 135.3, 132.4, 131.0, 129.0, 128.7, 127.4, 126.7, 126.3, 123.2. These data are consistent with reported literature values.[7]



Isoquinolin-1-yl(3-methylphenyl)methanone (4f)

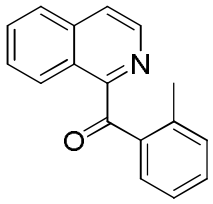
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4f** (31.7 mg, 64% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.62 (d, *J* = 5.6 Hz, 1H), 8.21 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 5.6 Hz, 1H), 7.78 (brs, 1H), 7.74 (dd, *J* = 7.2, 5.4 Hz, 2H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.2,

156.9, 141.4, 138.5, 136.9, 134.7, 131.2, 130.9, 128.6, 128.5, 128.3, 127.3, 126.6, 126.4, 122.7, 21.5. These data are consistent with reported literature values.[5]



(3-Chlorophenyl)(isoquinolin-1-yl)methanone (4g)

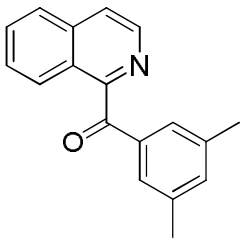
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4g** (20.3 mg, 38% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.62 (d, *J* = 5.6 Hz, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 7.95 (d, *J* = 9.2 Hz, 2H), 7.85 (d, *J* = 5.7 Hz, 2H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 193.4, 155.6, 141.3, 138.6, 137.0, 134.9, 133.6, 131.0, 130.9, 130.0, 129.1, 128.8, 127.4, 126.7, 126.2, 123.3. IR ν_{max} 3047, 2922, 1660, 1582, 1424, 1249, 1158, 830, 748 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{16}H_{10}{}^{35}ClNO$: 268.0524, found 268.0526; $[M + H]^+$ calculated for $C_{16}H_{10}{}^{37}ClNO$: 270.0494, found 270.0497.



Isoquinolin-1-yl(2-methylphenyl)methanone (4h)

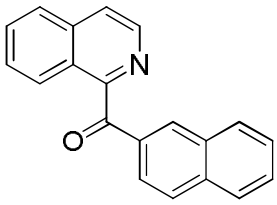
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4h** (29.7 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.57 (d, *J* = 5.5 Hz, 1H), 8.43 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.82–7.74 (m, 2H), 7.68 (t, *J* = 7.7 Hz, 1H), 7.48–7.38 (m, 2H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H),

2.55 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 197.9, 157.2, 141.6, 139.9, 137.5, 137.0, 132.3, 132.0, 132.0, 130.9, 128.8, 127.3, 126.6, 126.5, 125.7, 123.1, 21.5. These data are consistent with reported literature values.[5]



(3,5-Dimethylphenyl)(isoquinolin-1-yl)methanone (4i)

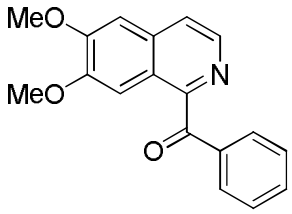
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4i** (26.7 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.61 (d, *J* = 5.6 Hz, 1H), 8.19 (d, *J* = 8.3 Hz, 1H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.81 (d, *J* = 5.6 Hz, 1H), 7.74 (dd, *J* = 8.0, 7.1 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.55 (s, 2H), 7.25 (s, 1H), 2.35 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.5, 157.2, 141.4, 138.4, 137.0, 136.9, 135.7, 130.9, 128.6, 128.4, 127.3, 126.5, 126.4, 122.5, 21.4; IR ν_{max} 3044, 2921, 1663, 1579, 1464, 1253, 1205, 825, 751 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{18}H_{16}NO$: 262.1226, found 262.1228.



Isoquinolin-1-yl(naphthalen-2-yl)methanone (4j)

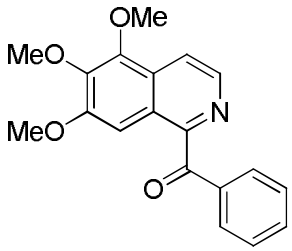
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (10:90) as eluent to afford **4j** (27.8 mg, 49% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.66 (d, *J* = 5.6 Hz, 1H), 8.36 (s, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 8.17 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.96 (d, *J* =

8.4 Hz, 2H), 7.82–7.74 (m, 3H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.66–7.58 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (101 MHz, CDCl3) δ = 195.0, 156.9, 141.5, 136.9, 136.1, 134.2, 133.9, 132.6, 130.9, 130.0, 129.0, 128.6, 128.5, 128.0, 127.3, 126.9, 126.7, 126.4, 125.5, 122.8. These data are consistent with reported literature values.[5]



(6,7-Dimethoxyisoquinolin-1-yl)(phenyl)methanone (4k)

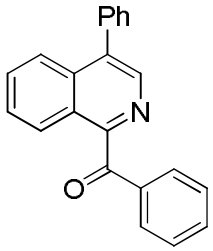
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (30:70) as eluent to afford **4k** (26.4 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.47 (d, *J* = 5.4 Hz, 1H), 7.96 (d, *J* = 7.1 Hz, 2H), 7.68–7.58 (m, 3H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.15 (s, 1H), 4.06 (s, 3H), 3.97 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.6, 153.4, 153.2, 151.5, 140.3, 137.4, 134.3, 133.6, 131.1, 128.5, 123.3, 121.8, 105.1, 104.3, 56.3, 56.3. These data are consistent with reported literature values.[4]



Phenyl(5,6,7-trimethoxyisoquinolin-1-yl)methanone (4l)

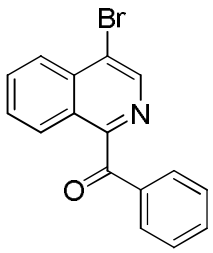
It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (30:70) as eluent to afford **4l** (35.6 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.50 (d, *J* = 5.6 Hz, 1H), 8.02 (d, *J* = 5.6 Hz, 1H), 7.96 (d, *J* = 7.4 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.49

(t, J = 7.7 Hz, 2H), 7.45 (s, 1H), 4.09 (s, 3H), 4.04 (s, 3H), 3.95 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.5, 155.0, 153.6, 147.0, 144.5, 139.8, 137.3, 133.7, 131.1, 129.5, 128.6, 124.2, 117.1, 100.5, 61.9, 61.5, 56.3; IR ν_{max} 3032, 2941, 2836, 1678, 1461, 1272, 1248, 1150, 965, 860, 765 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{19}H_{18}NO_4$: 324.1230, found 324.1234.



Phenyl(4-phenylisoquinolin-1-yl)methanone (4m)

It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (5:95) as eluent to afford **4m** (40.8 mg, 66% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.58 (s, 1H), 8.32 (d, J = 8.4 Hz, 1H), 8.03 (t, J = 8.0 Hz, 3H), 7.75–7.69 (m, 1H), 7.68–7.61 (m, 2H), 7.60–7.56 (m, 4H), 7.55–7.49 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.0, 155.9, 141.2, 136.9, 136.8, 135.5, 135.3, 133.9, 131.0, 131.0, 130.3, 128.9, 128.7, 128.5, 128.3, 126.5, 126.4, 125.6. IR ν_{max} 3051, 2924, 2852, 1674, 1450, 1263, 1241, 1146, 957, 862, 777 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{22}H_{16}NO$: 310.1226, found 310.1229.



(4-Bromoisoquinolin-1-yl)(phenyl)methanone (4n)

It was prepared following the general method for benzoylation and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (5:95) as eluent to afford **4n** (26.8 mg, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.81 (s, 1H), 8.30 (d, *J* = 8.5 Hz, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.88 (t, *J* = 7.7 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 194.2, 155.9, 143.1, 136.6, 135.7, 134.1, 132.2 130.9, 129.4, 128.7, 127.8, 126.9, 126.7, 122.0. IR ν_{max} 3035, 2922, 1685, 1578, 1443, 1231, 1193, 1141, 952, 836, 753 cm^{-1}; HRMS (EI) *m/z* $[M + H]^+$ calculated for $C_{16}H_{11}{}^{79}BrNO$: 312.0019, found 312.0017; $[M + H]^+$ calculated for $C_{16}H_{11}{}^{81}BrNO$: 313.9998, found 314.0001.

Mechanistic Studies

Procedure for determination of intermolecular KIE under the benzylation condition:

In a 10 mL tube, **1a** (0.2 mmol, 1.0 equiv), **2a** (0.9 mmol, 4.5 equiv), **D_8-2a** (0.9 mmol, 4.5 equiv), $Y(OTf)_3$ (0.01 mmol, 0.05 equiv) and di-tert-butyl peroxide (0.6 mmol, 3.0 equiv) were added. Then the tube was sealed and the resulting solution was heated in a 120 °C oil bath with vigorous stirring for 4 h. Then the reaction mixture was cooled to 0 °C and treated with saturated aqueous $NaHCO_3$. The mixture was extracted with ethyl acetate (10 mL × 3), and the combined organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated under vacuum. The residue was purified by flash chromatography using ethyl acetate/petroleum ether (10:90) as eluent to afford a mixture of non-deuterated and deuterated products. The product ratio of D_0 to D_7 was calculated by acquiring a ^{1}H NMR spectrum (400 MHz, $CDCl_3$) and comparing the intensities of the signals from benzyl-H to signals from hydrogen of N**C**H**C**H.

Procedure for determination of intermolecular KIE under the benzoylation condition:

In a 10 mL tube, **1a** (0.2 mmol, 1.0 equiv), **2a** (0.9 mmol, 4.5 equiv), **D_8-2a** (0.9 mmol, 4.5 equiv), TFA (0.2 mmol, 1.0 equiv), MnO_2 (0.02 mmol, 10 mol %) and TBHP (5~6 M solution in decane, 1.0 mmol, 5.0 equiv) were added. Then the tube was sealed and the resulting solution was heated in a 120 °C oil bath with vigorous stirring for 4 h. Then the reaction mixture was cooled to 0 °C and treated with saturated aqueous $NaHCO_3$. The mixture was extracted with ethyl acetate (10 mL × 3), and the combined organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated under vacuum. The residue was purified by flash chromatography using ethyl acetate/petroleum ether (10:90) as eluent to afford a mixture of non-deuterated and deuterated products. The product ratio of D_0 to D_5 was calculated by acquiring a ^{1}H NMR spectrum (400 MHz, $CDCl_3$) and comparing the intensities of the signals from hydrogen of the phenyl ring to signals from hydrogen of N**C**H**C**H.[5]

Reference

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2011, *50*, 7686.

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4) Shankar, R.; More, S. S.; Madhubabu, M. V.; Vembu, N.; Syam Kumar, U. K. *Synlett*, **2012**, *7*, 1013.

5) Matcha, K.; Antonchick, A. P. *Angew. Chem. Int. Ed*. **2013**, *52*, 2082.

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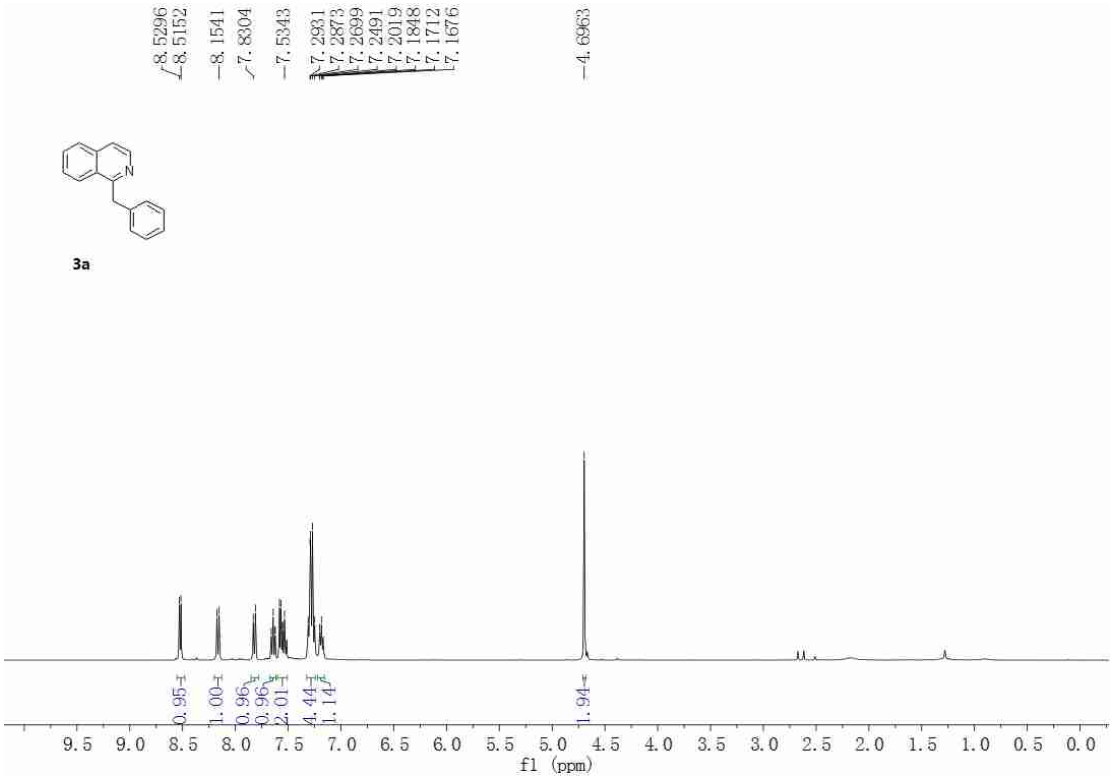
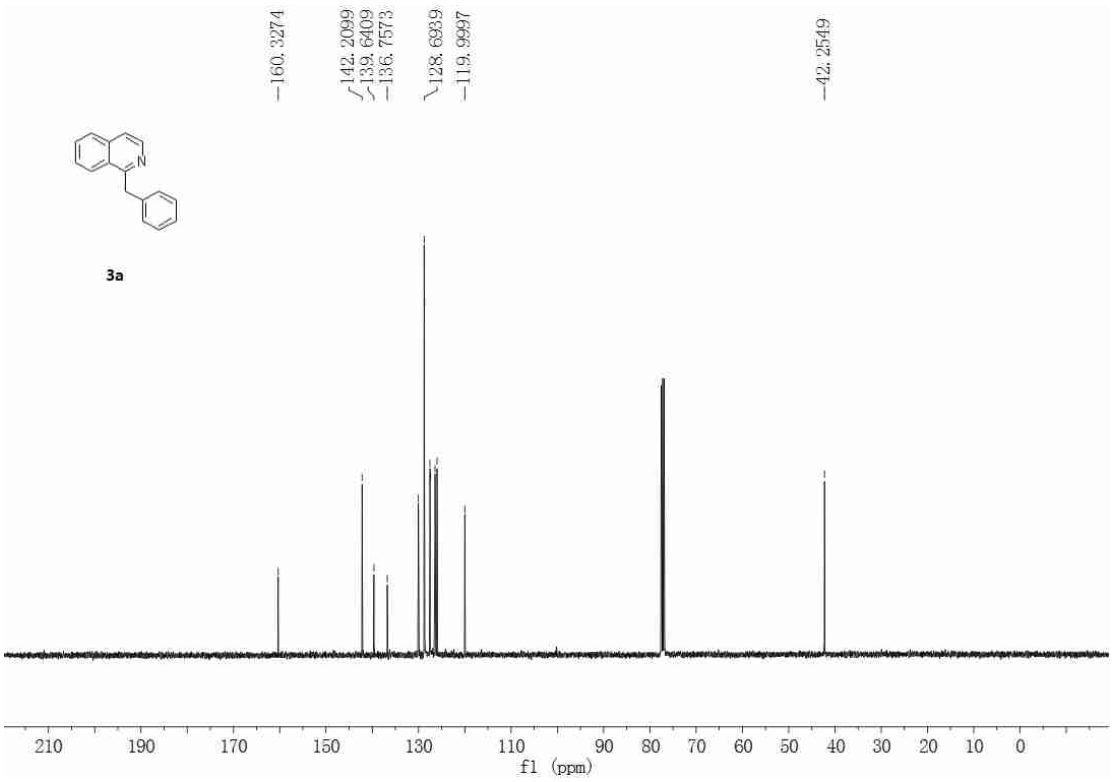
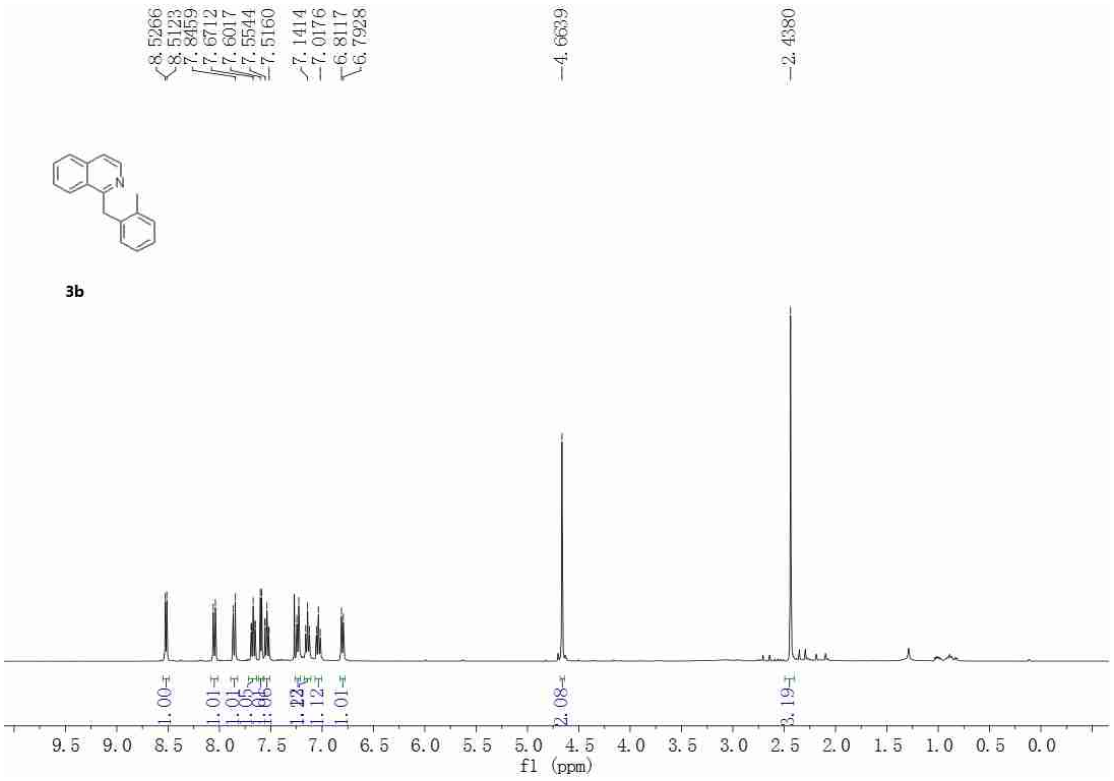
7) Reux, B.; Nevalainen, T.; Raitio, K. H.; Koskinen, Ari M. P. *Bioorg. Med. Chem.* **2009**, *17*, 4441.

^{1}H and ^{13}C NMR spectra



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1.23
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2.08
3.19
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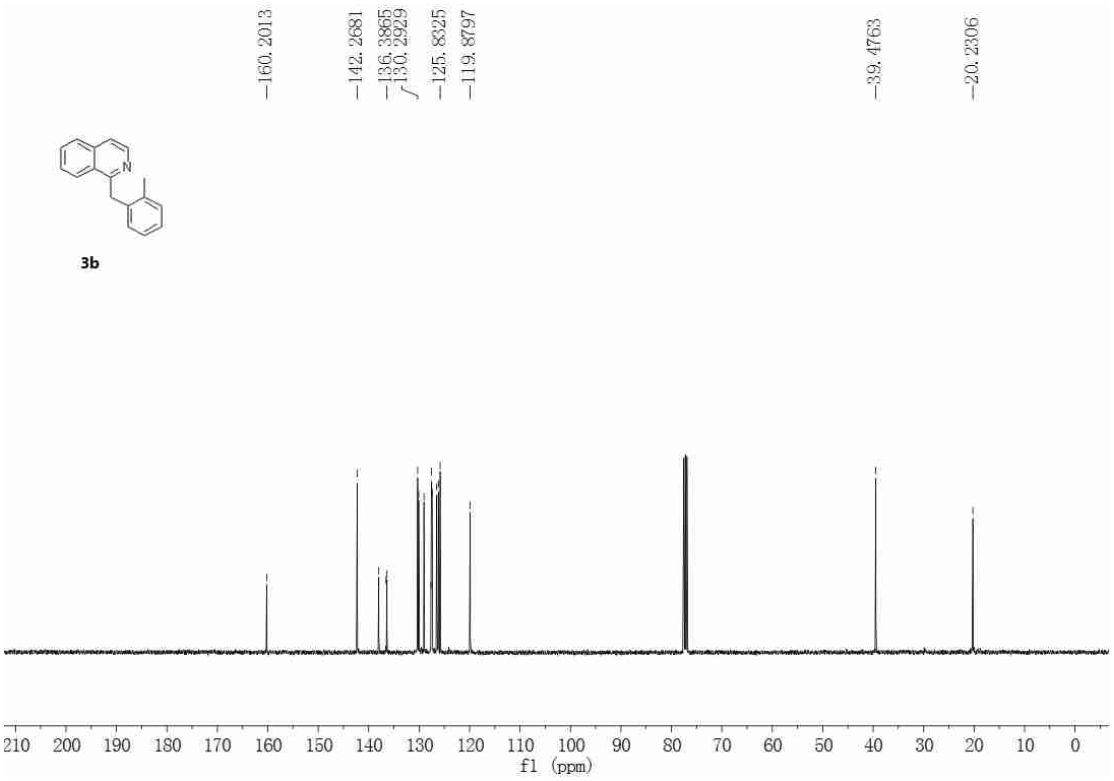
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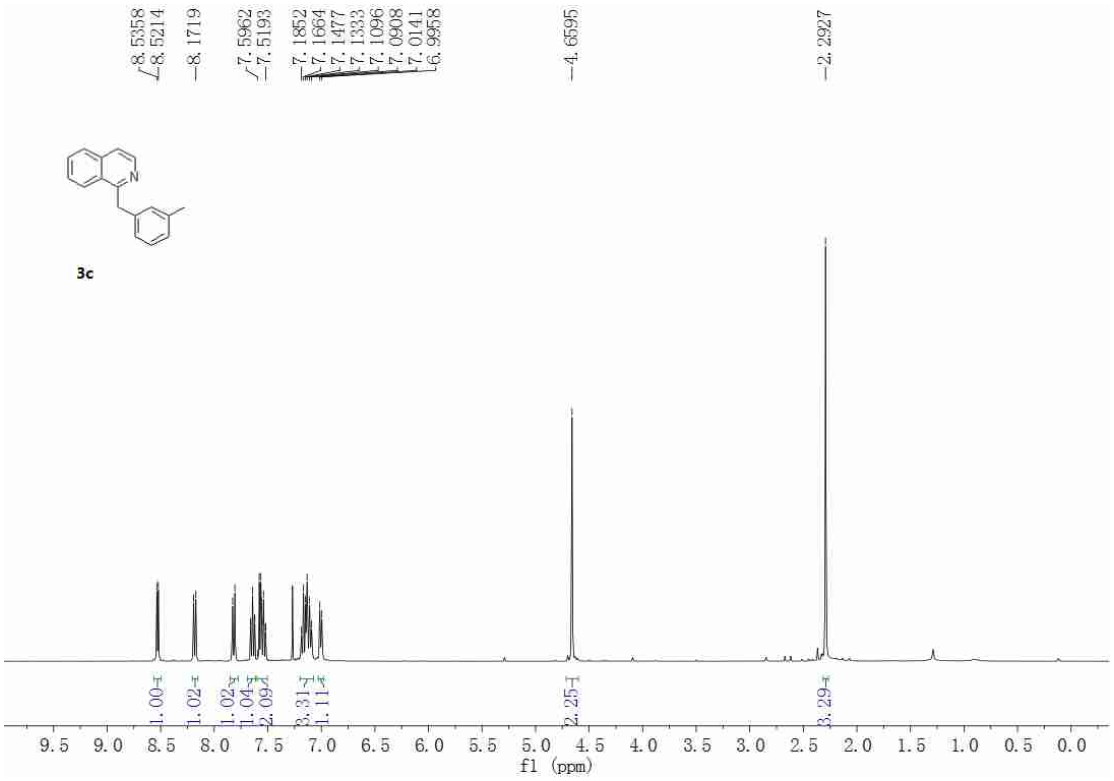
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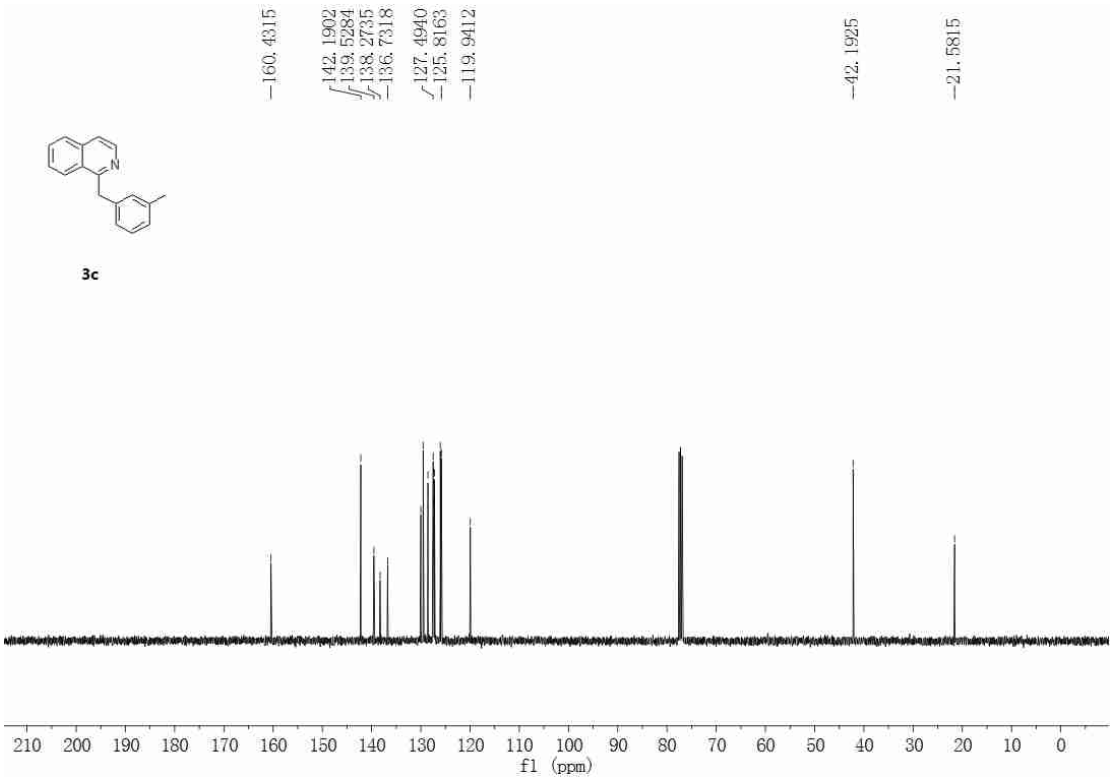
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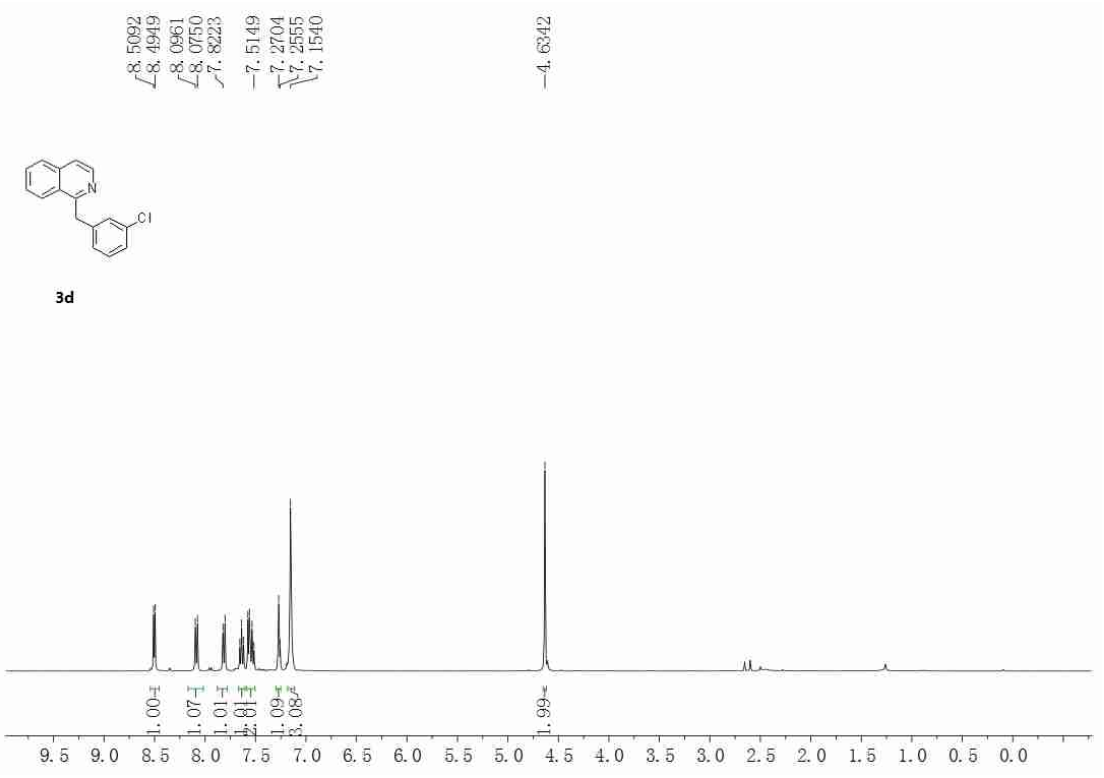
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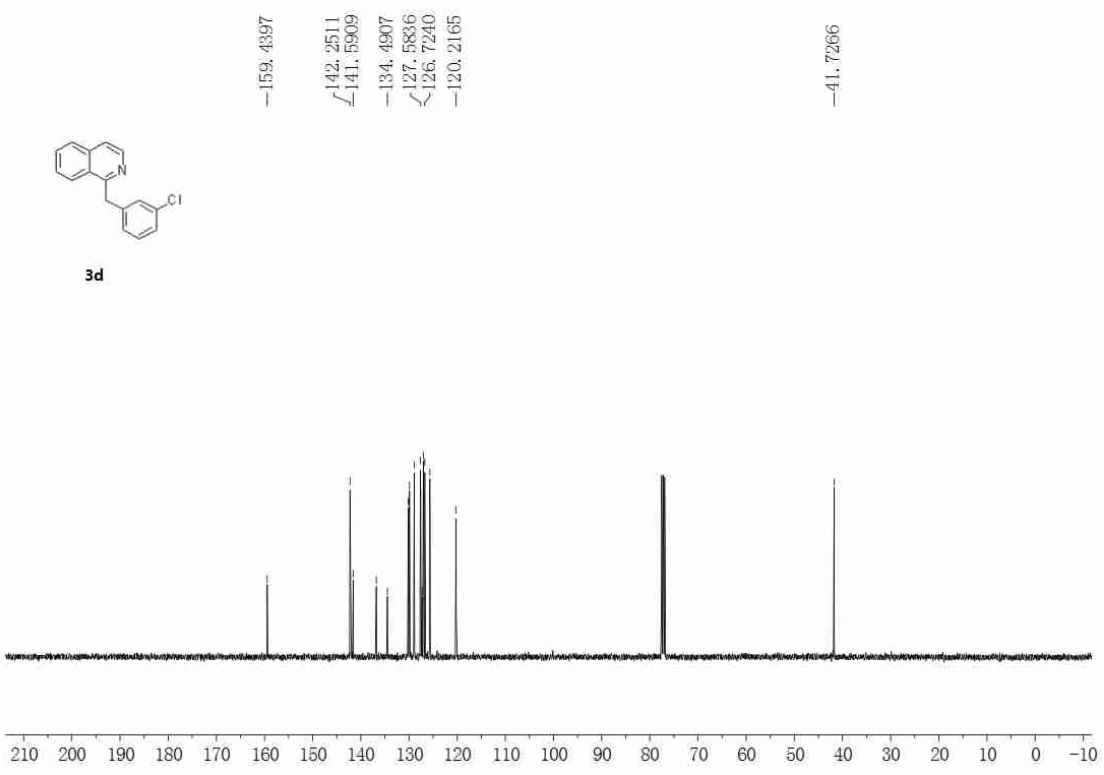
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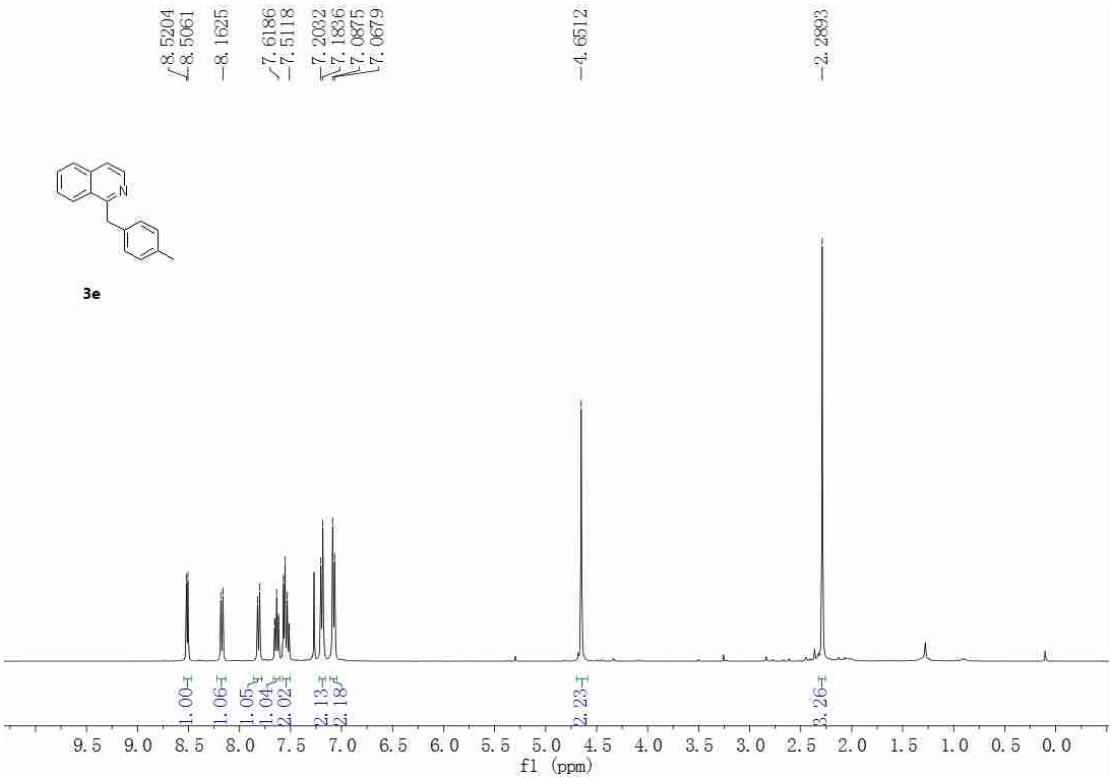
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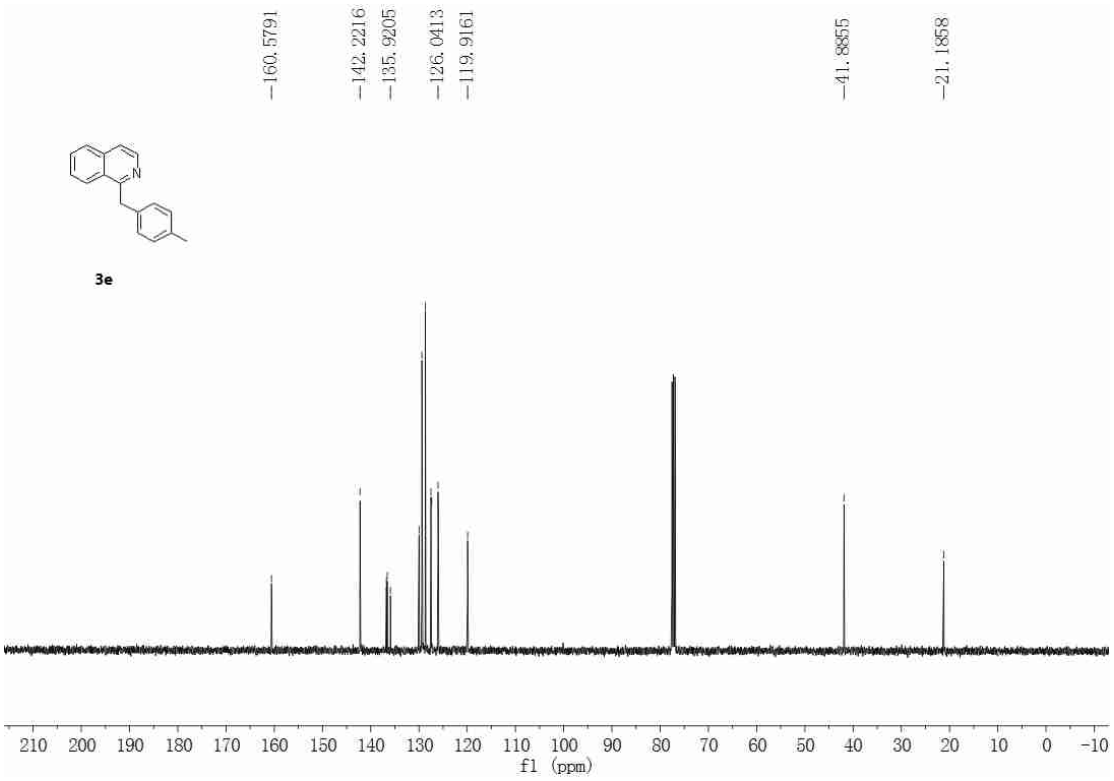
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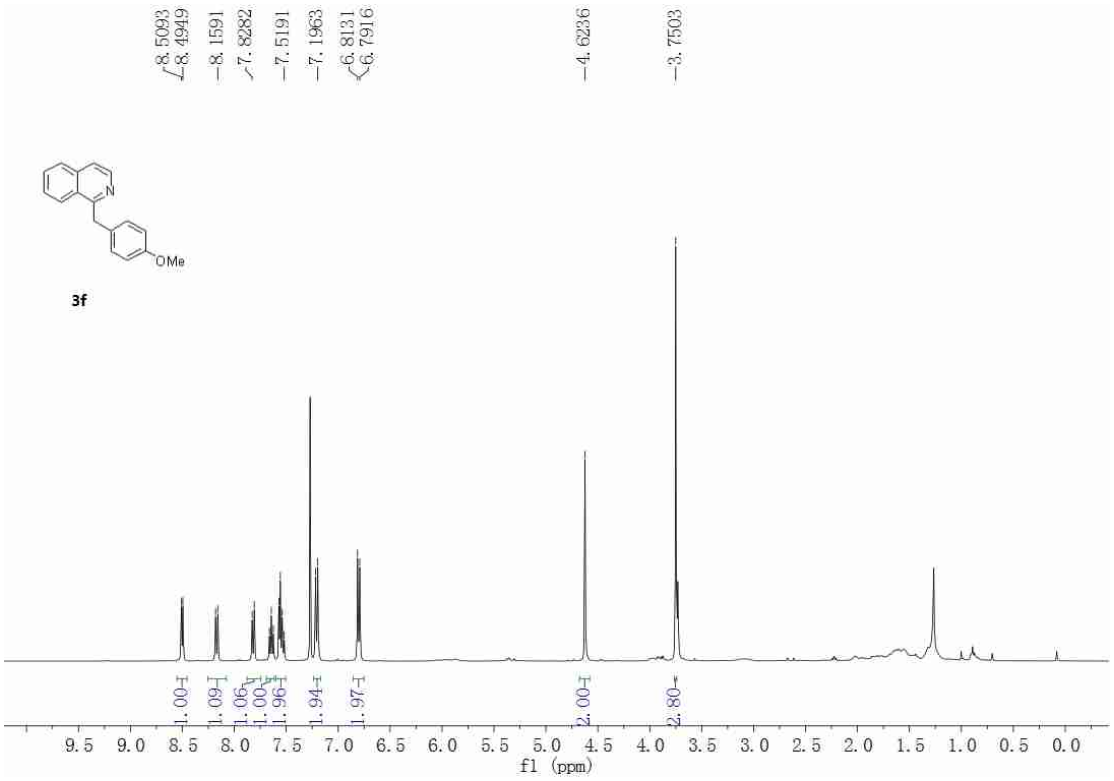
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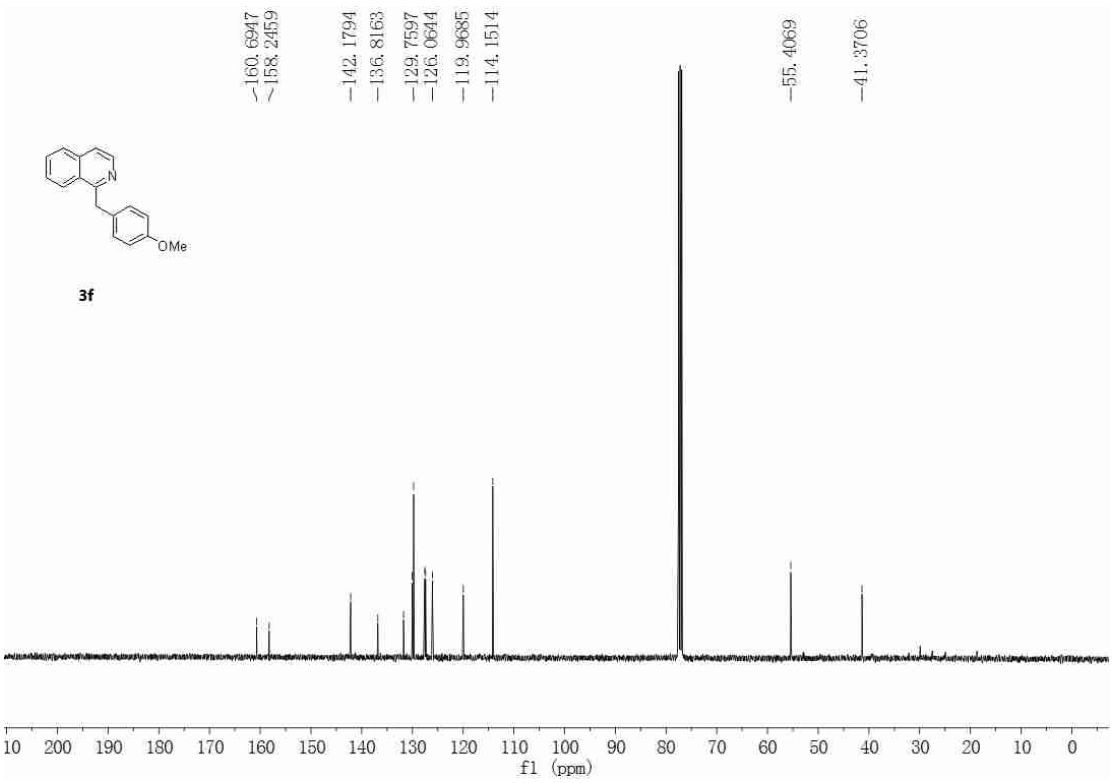
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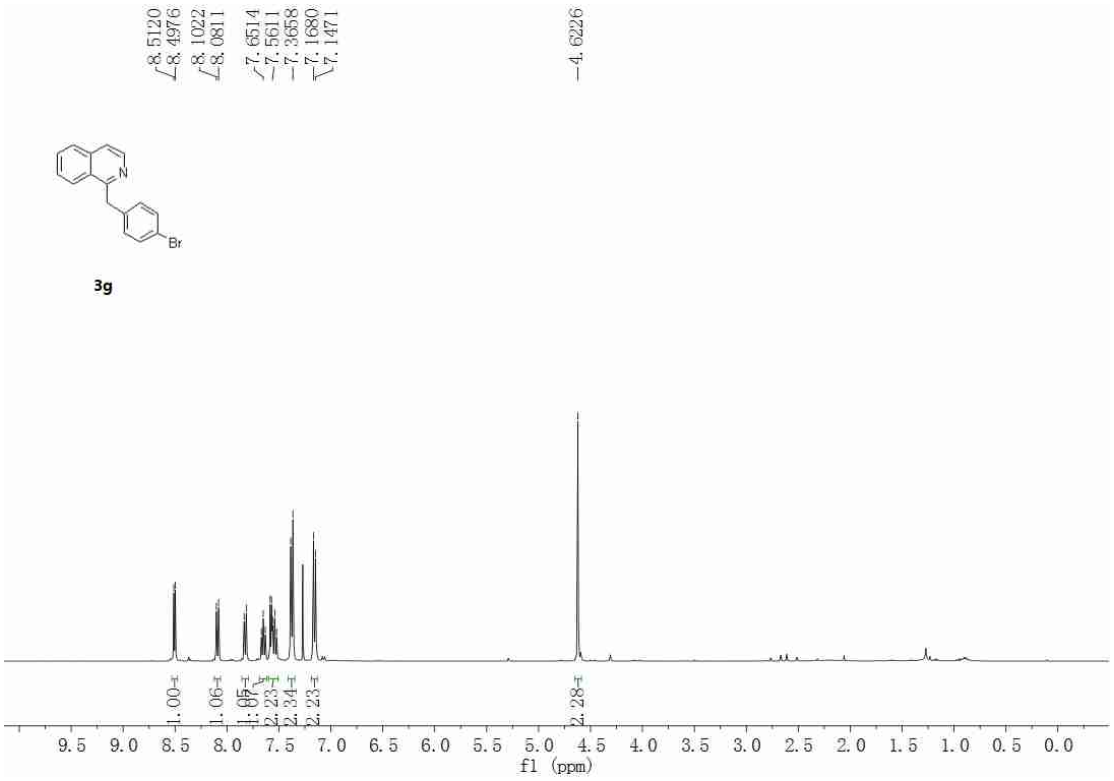
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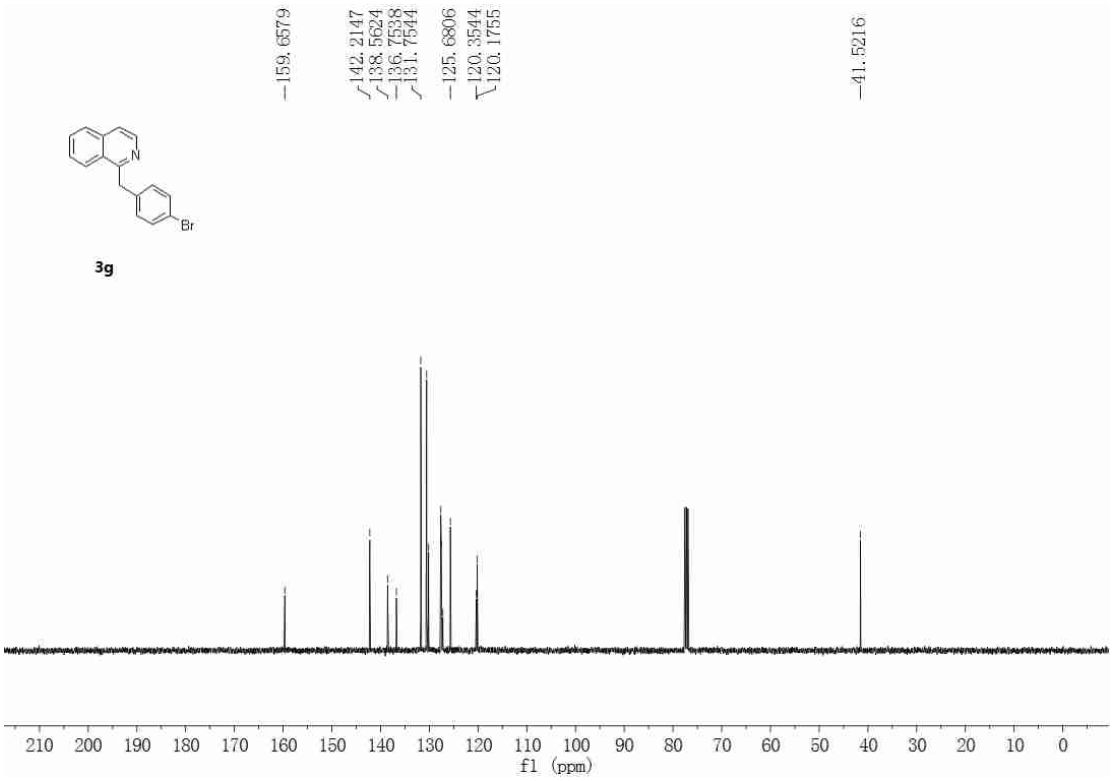
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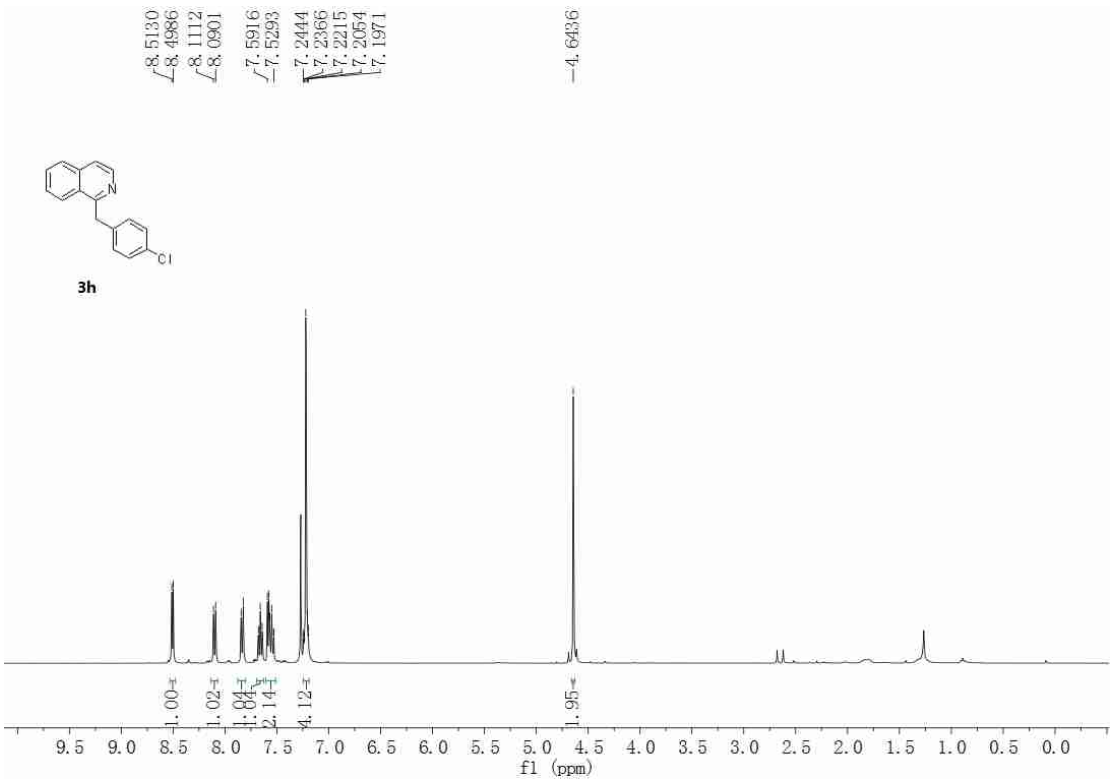
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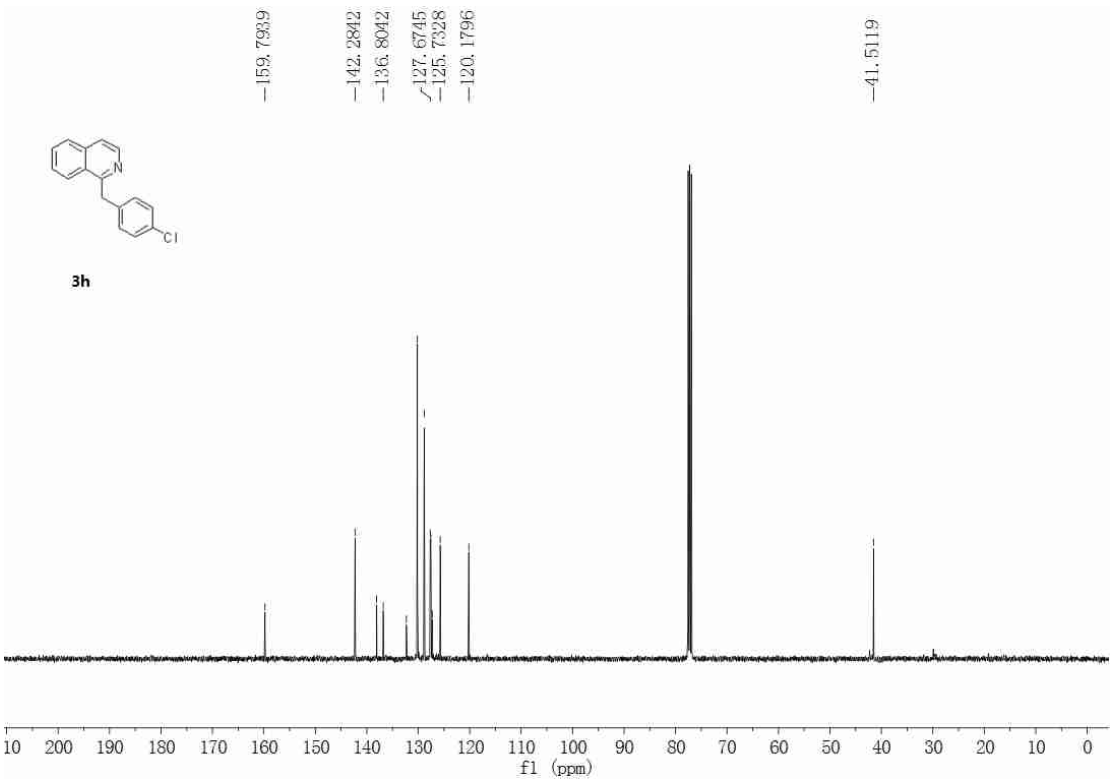
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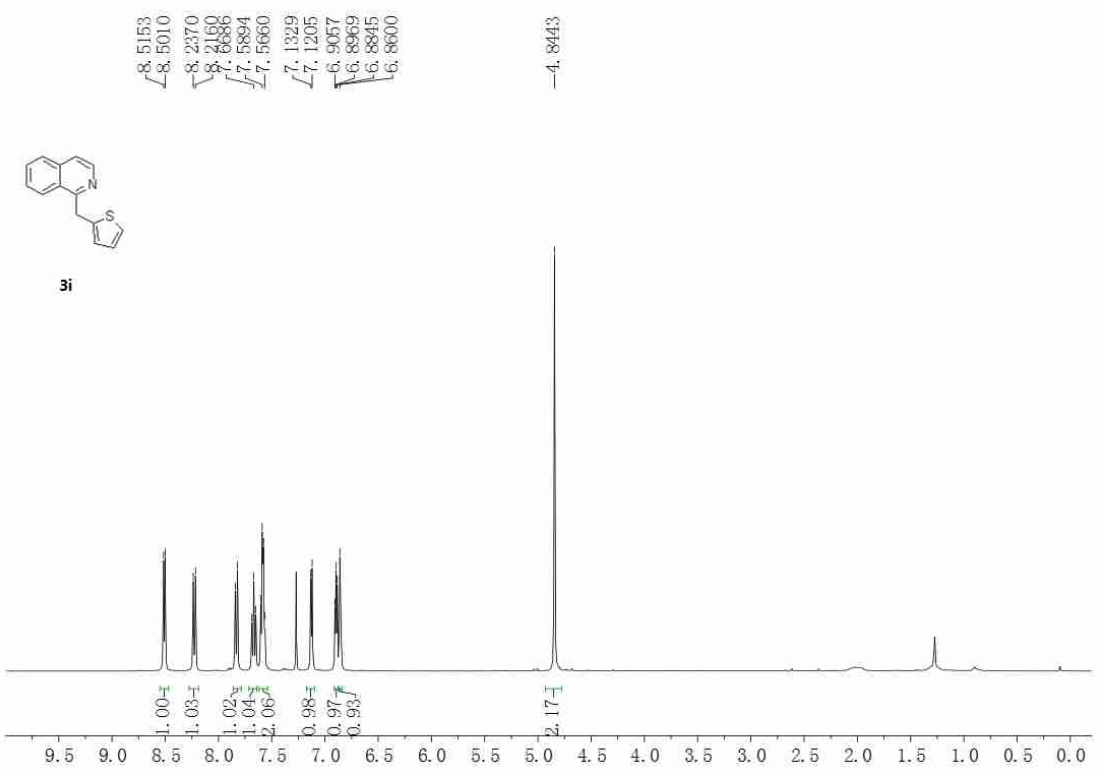
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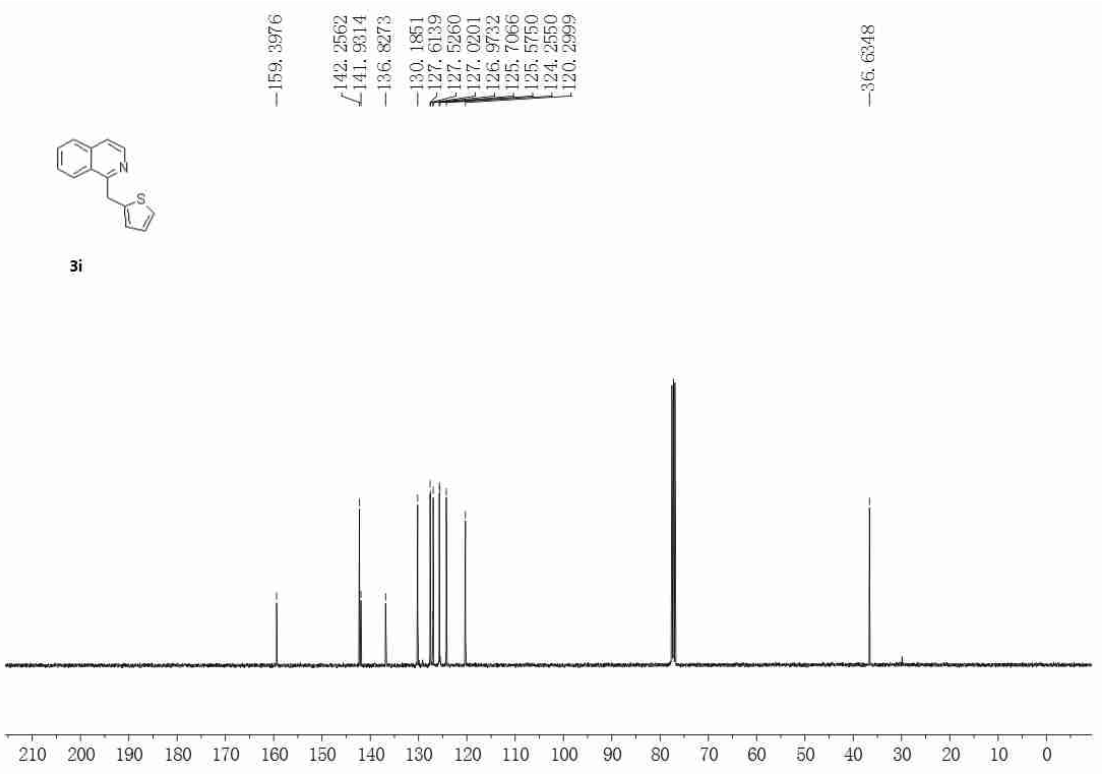
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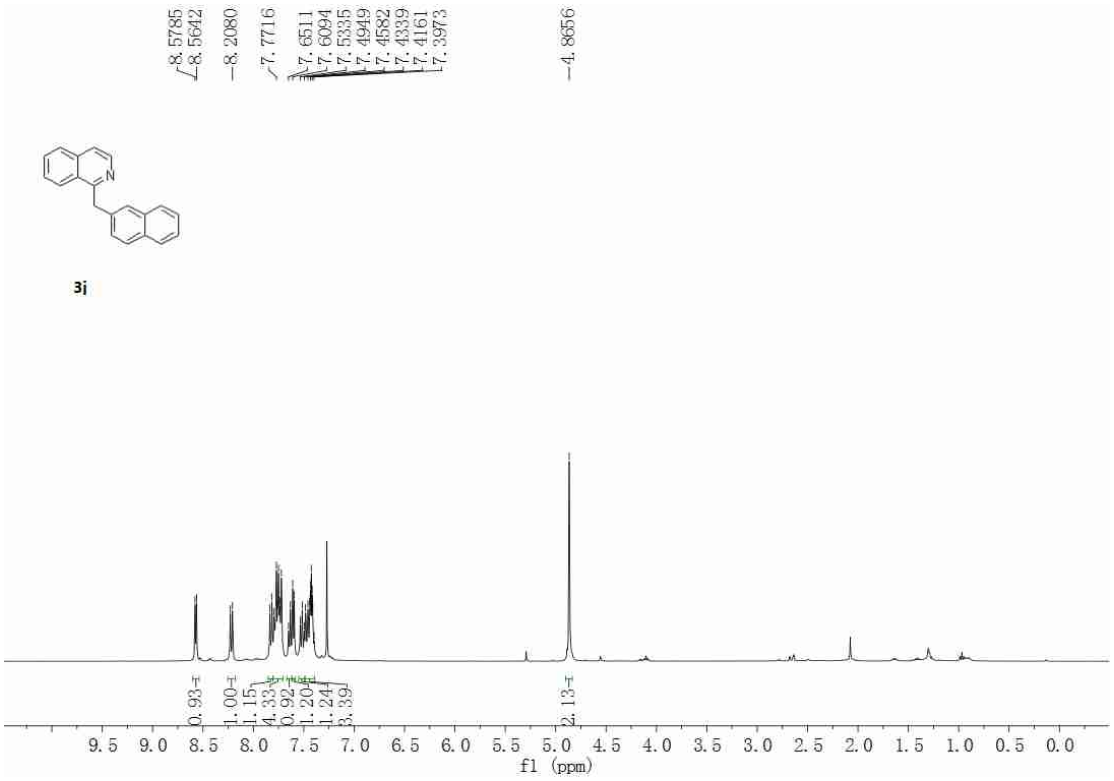
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7.3973
4.8656
3j
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1.00
1.15
4.33
0.92
1.20
1.24
3.39
2.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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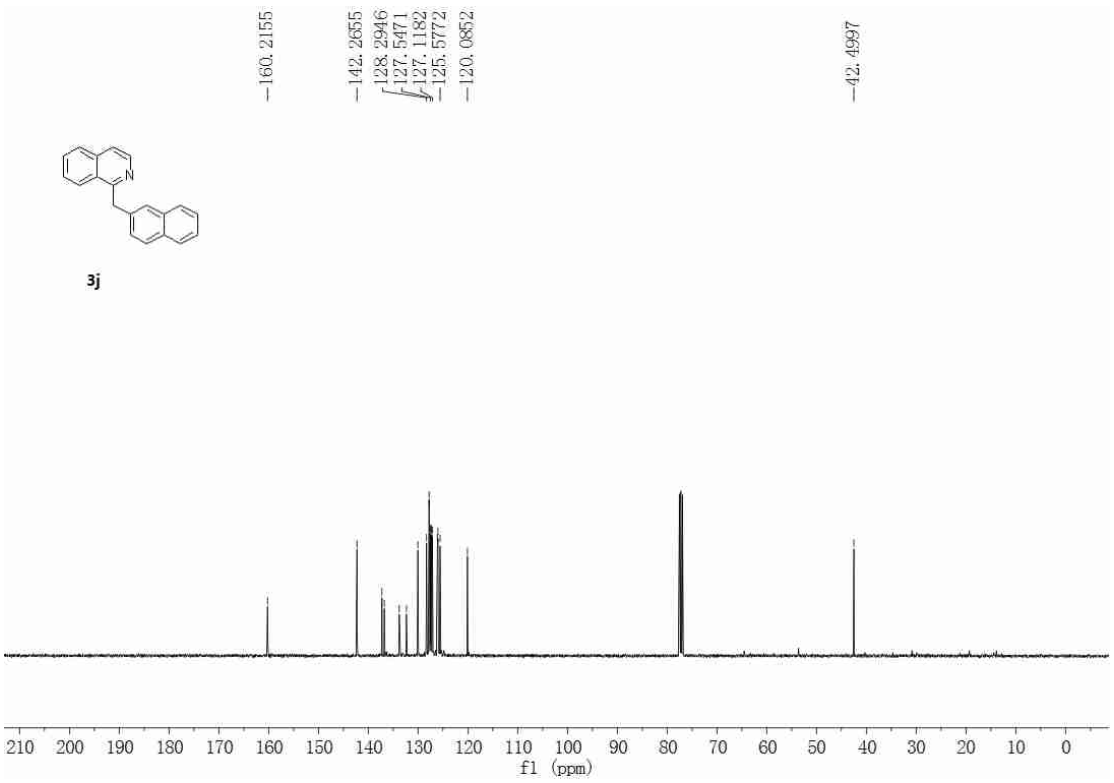
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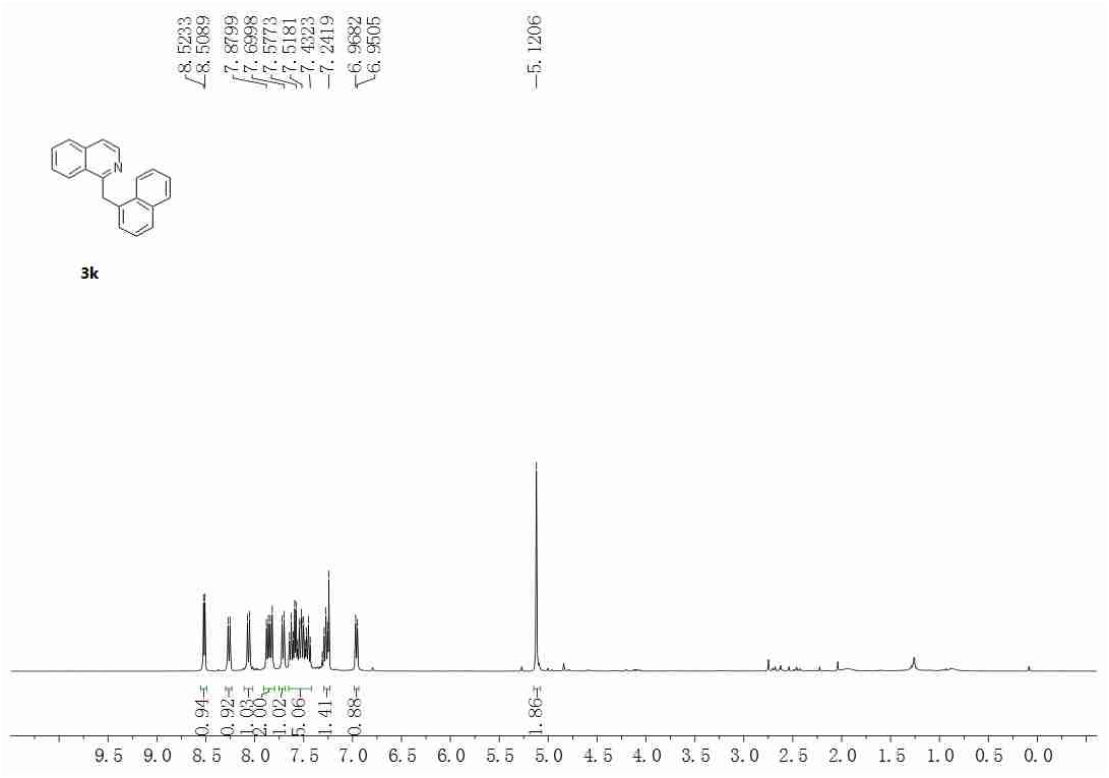
f1 (ppm)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5.1206
3k
0.94
0.92
1.03
2.00
1.02
5.06
1.41
0.88
1.86
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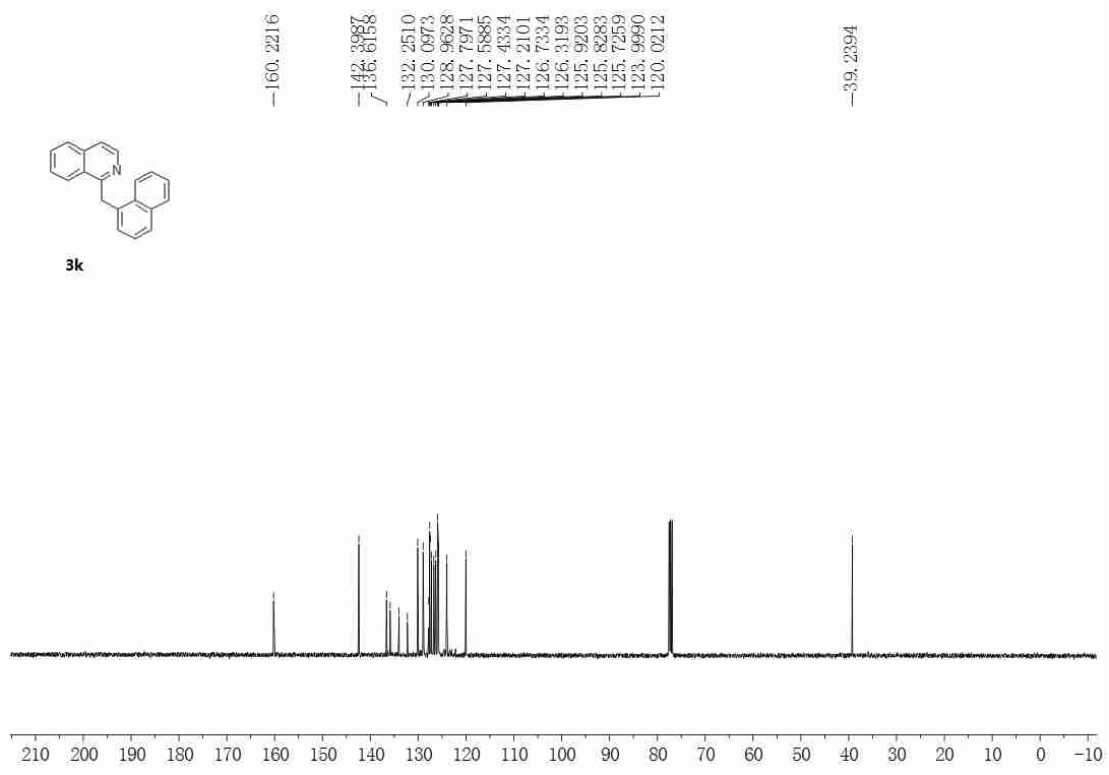
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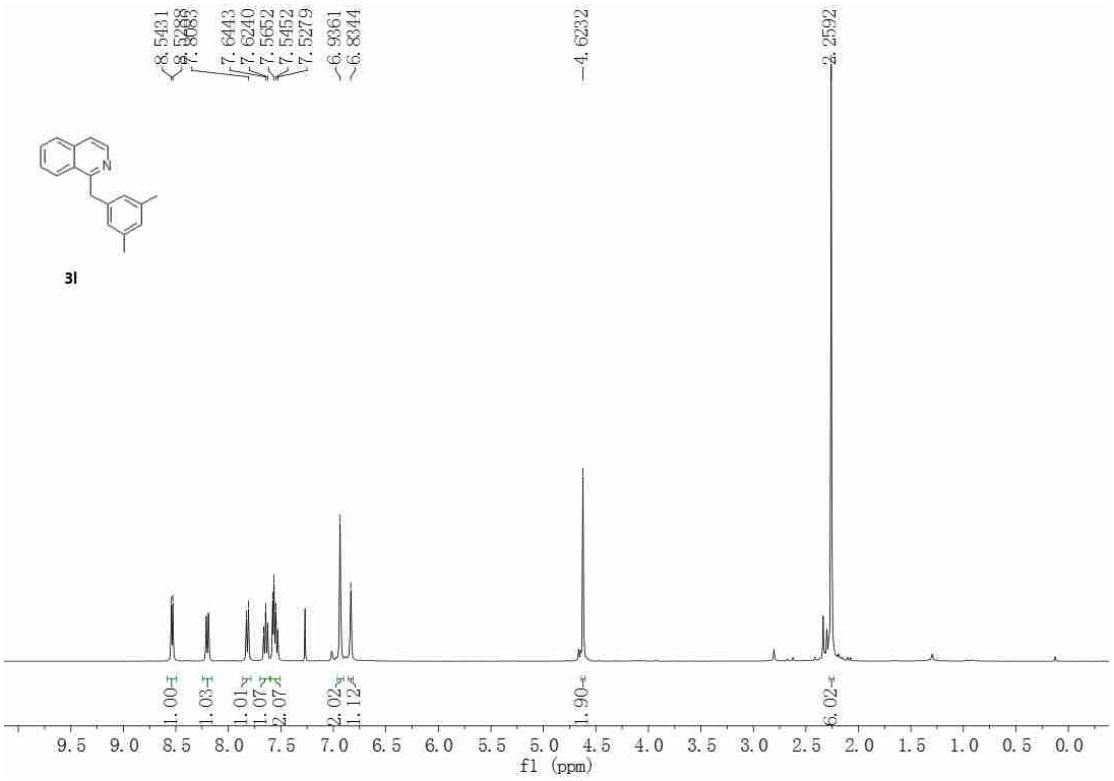
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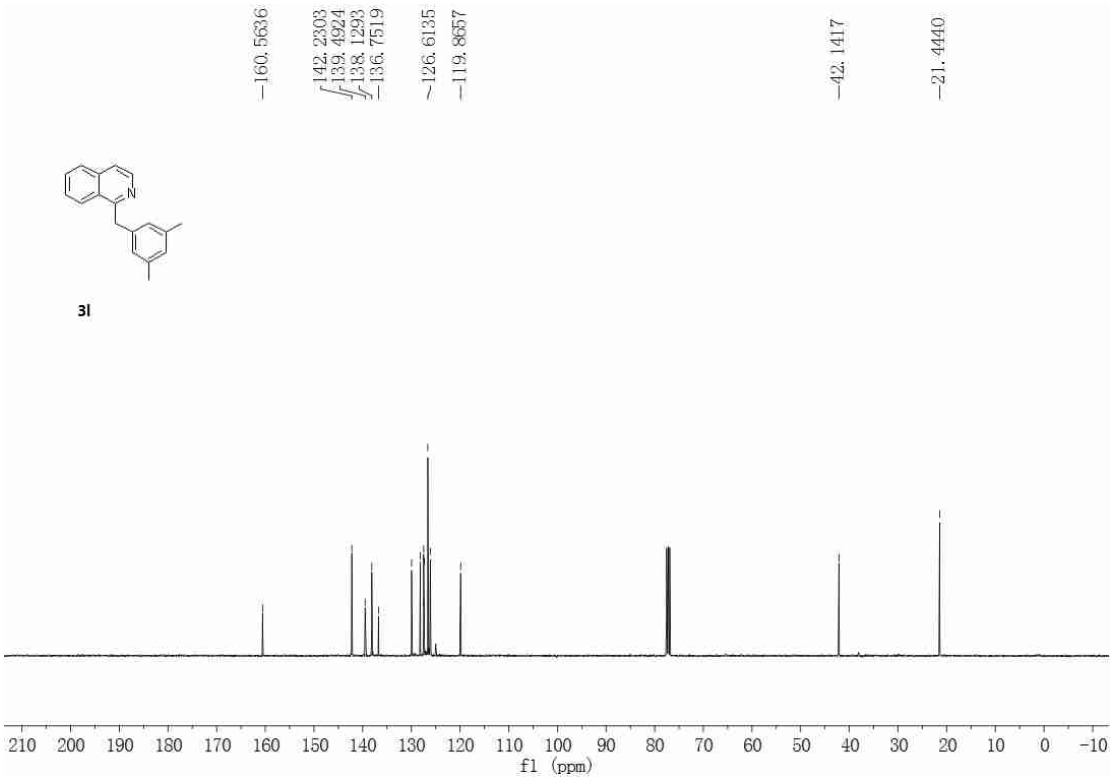
6.02
f1 (ppm)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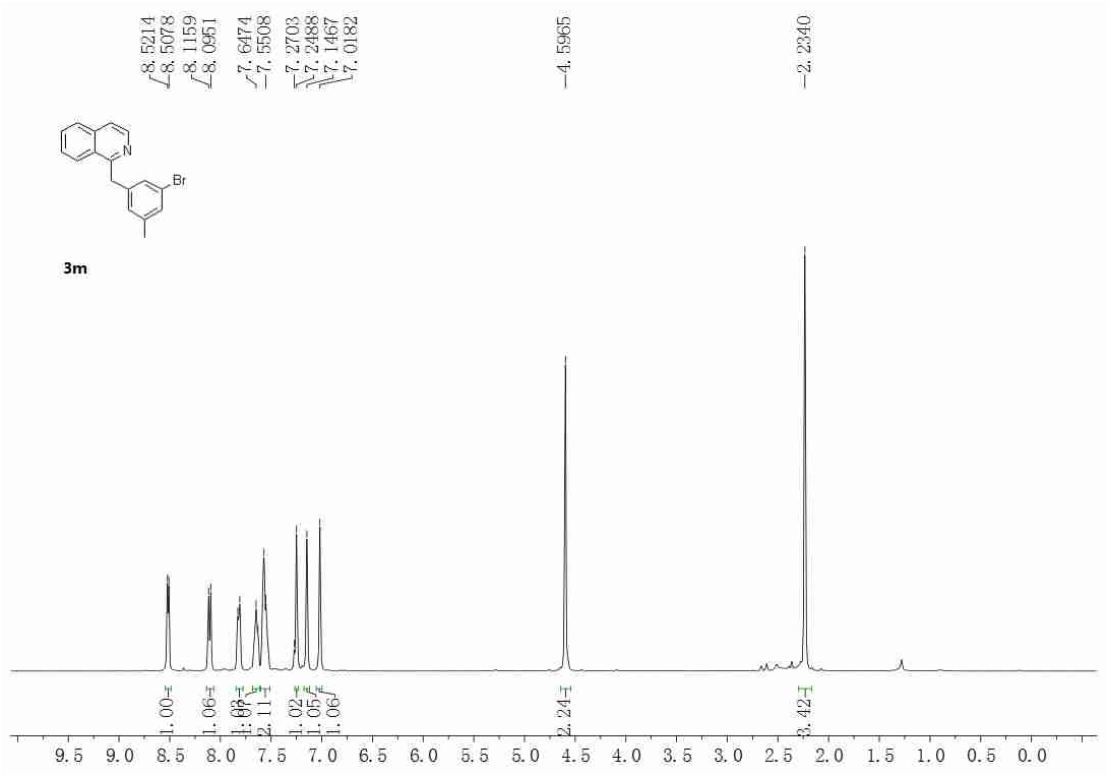
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Br
3m
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1.06
1.03
1.09
2.11
1.02
1.05
1.06
2.24
3.42
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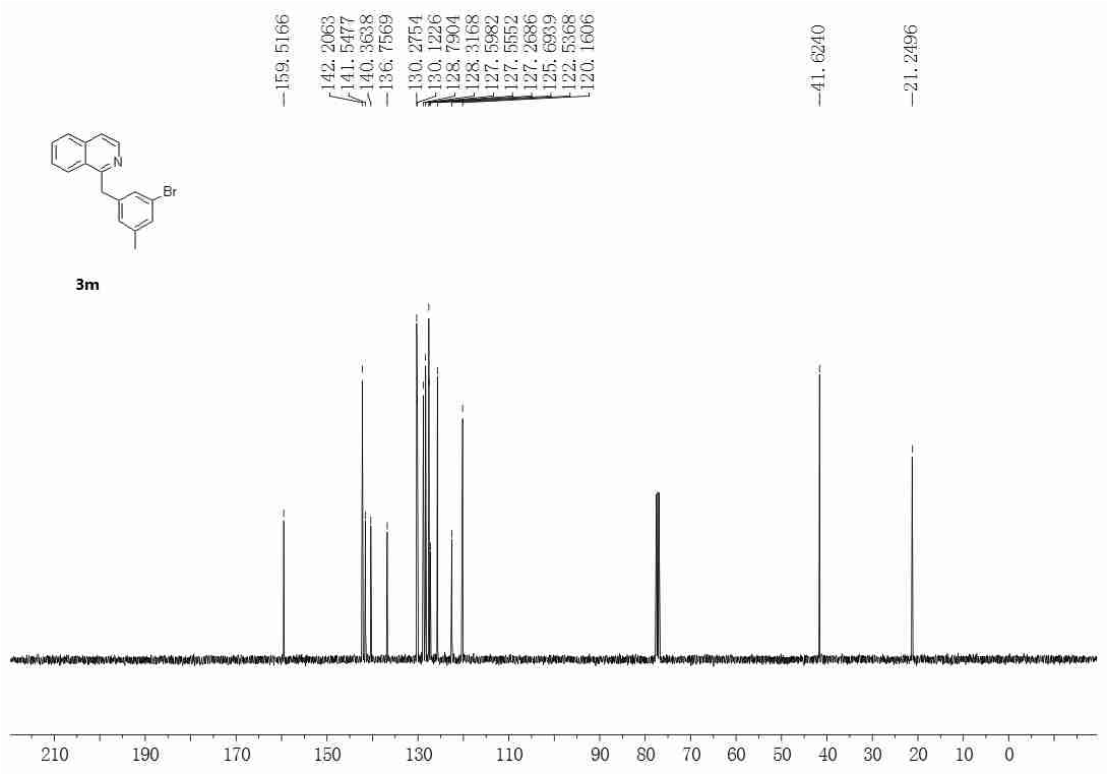
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Br
3m
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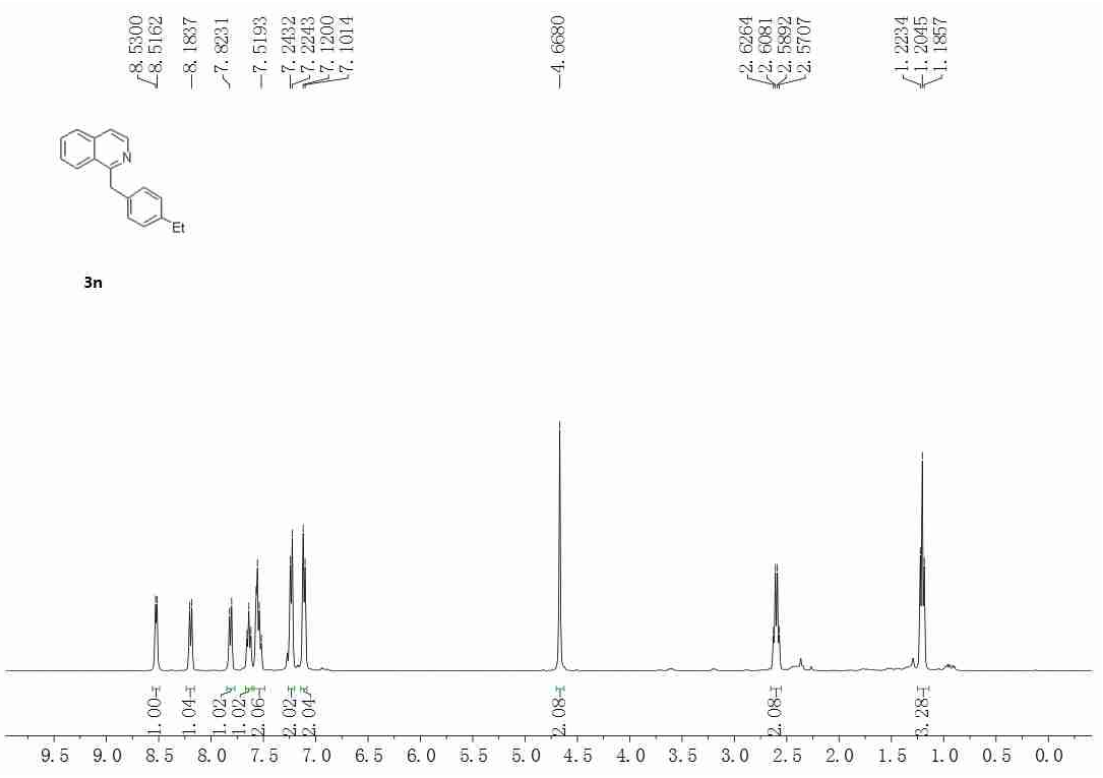
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2.6081
2.5892
2.5707
1.2234
1.2045
1.1857
N
Et
3n
1.00
1.04
1.02
1.02
2.06
2.02
2.04
2.08
2.08
3.28
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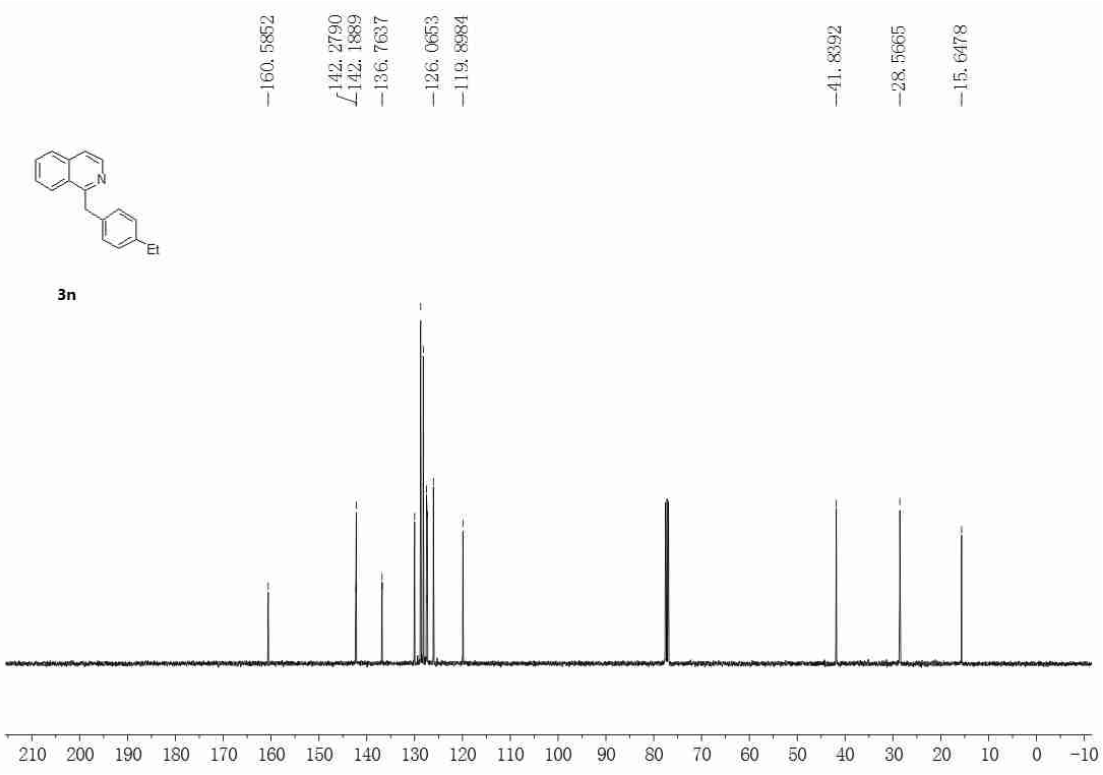
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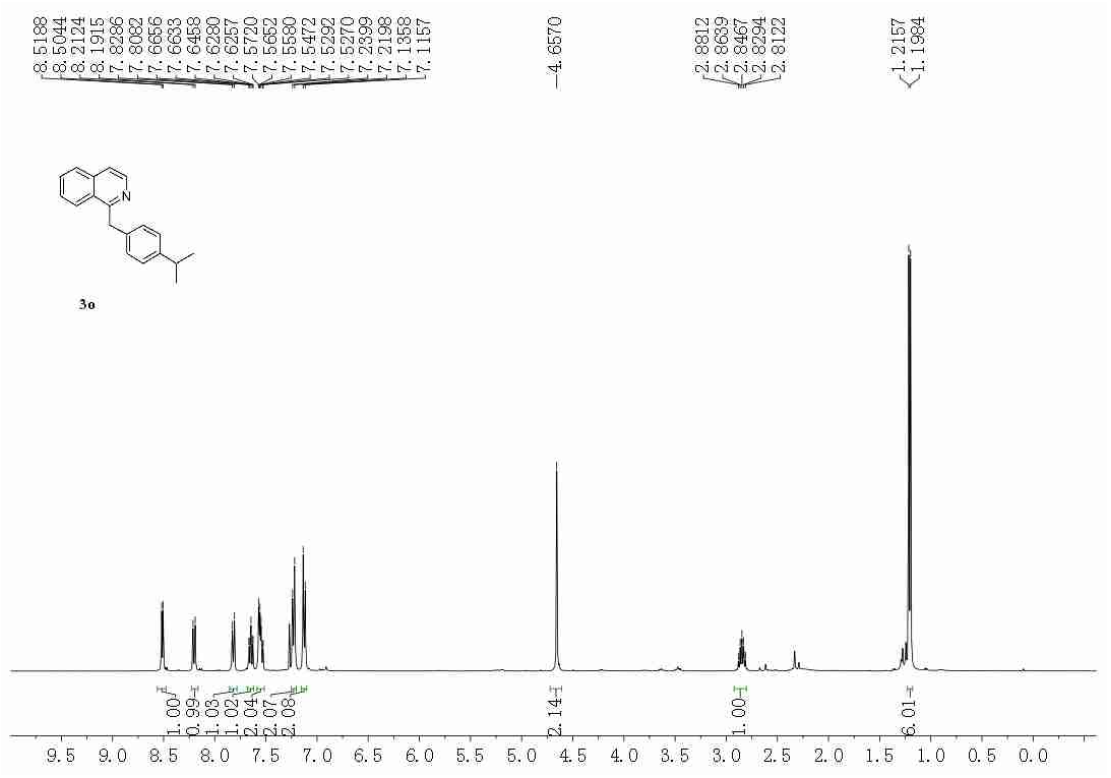
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1.02
2.04
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2.08
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1.00
6.01
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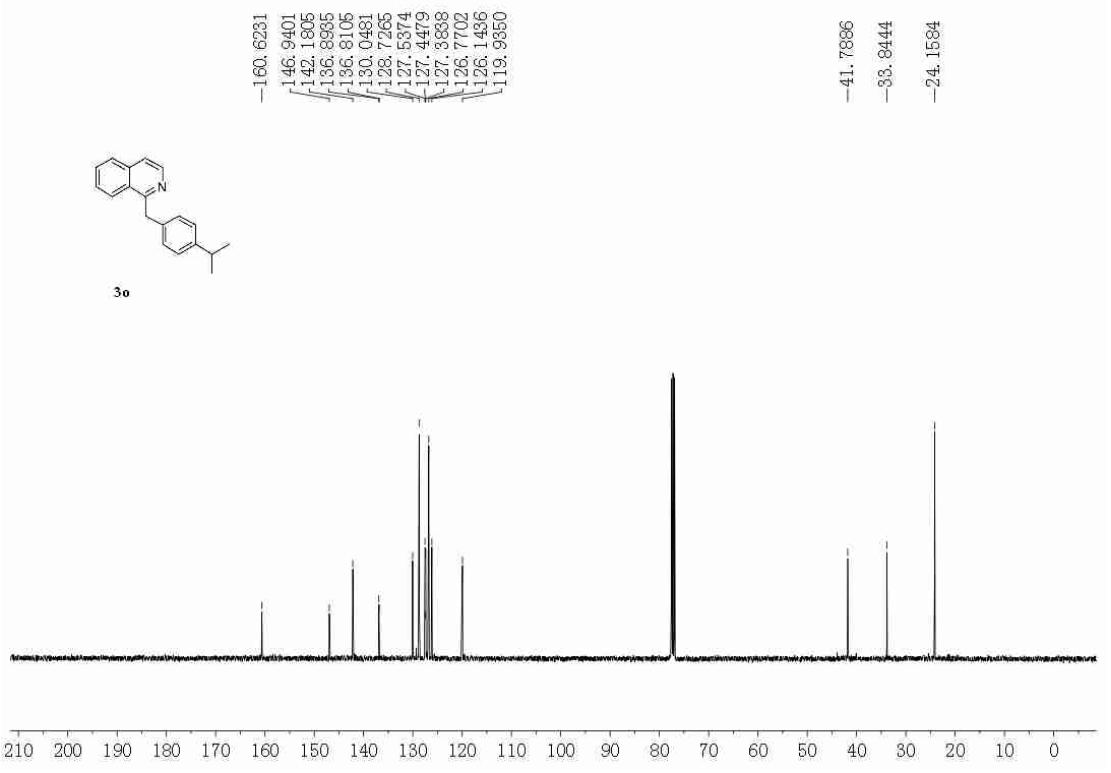
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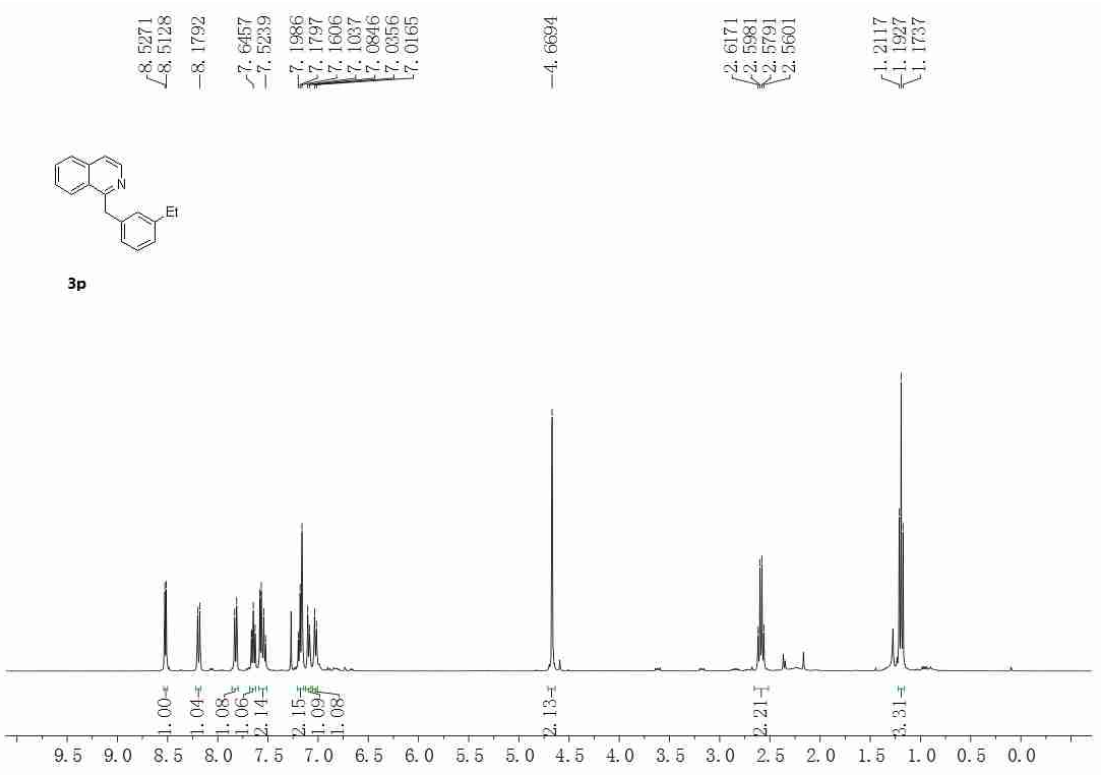
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1.08
1.06
2.14
2.15
1.09
1.08
2.13
2.21
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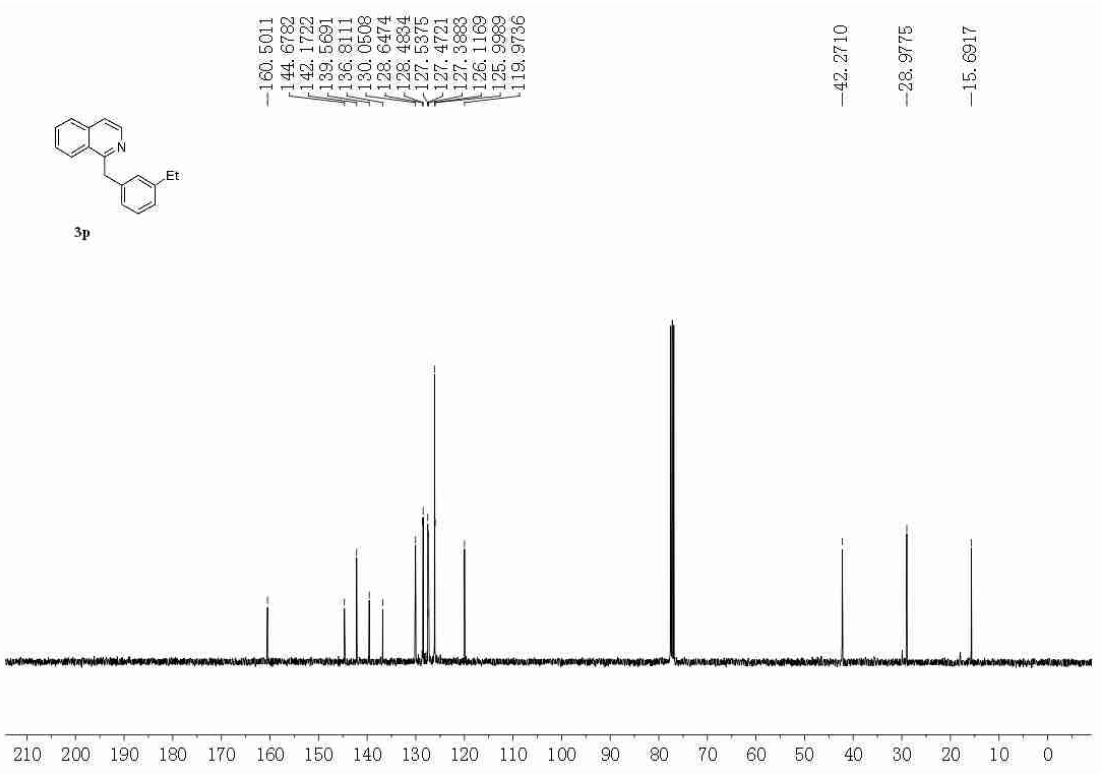
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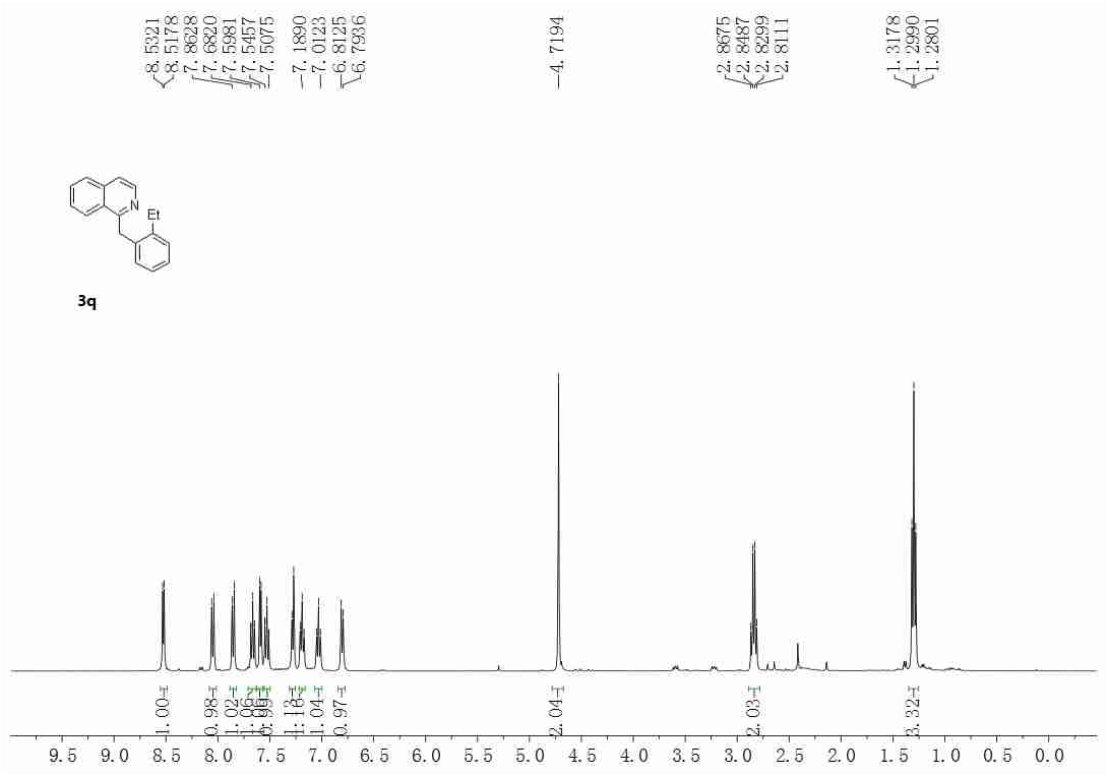
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1.02
1.06
1.13
1.04
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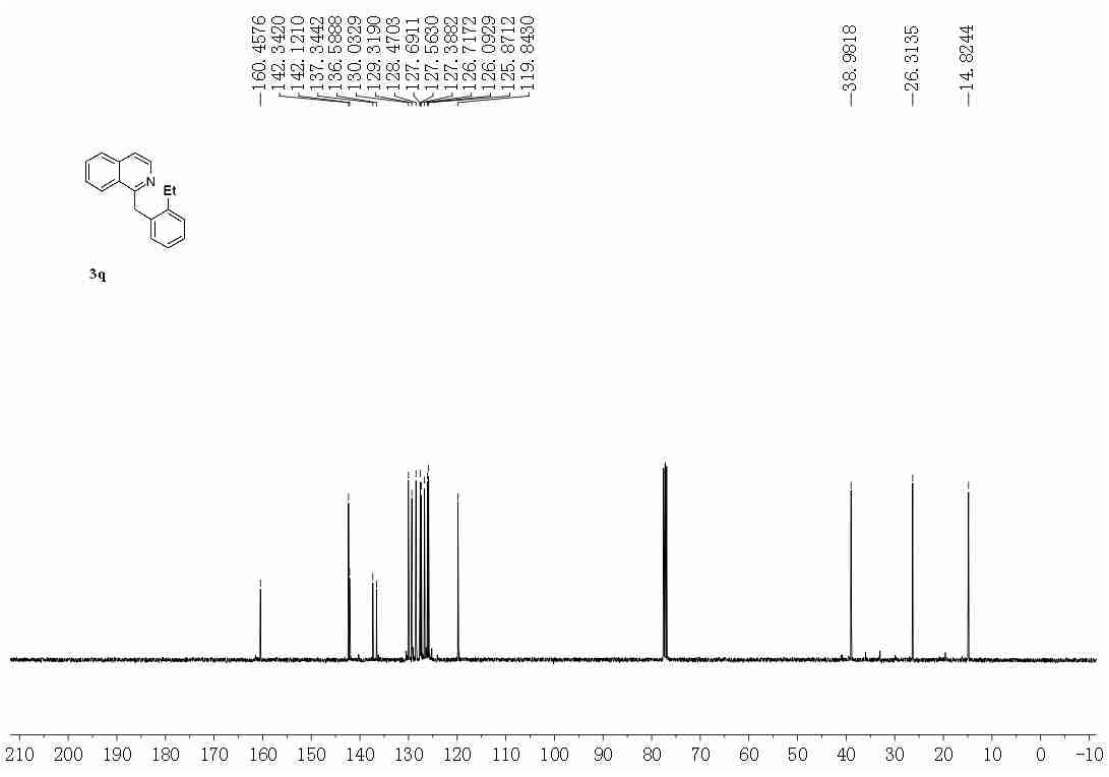
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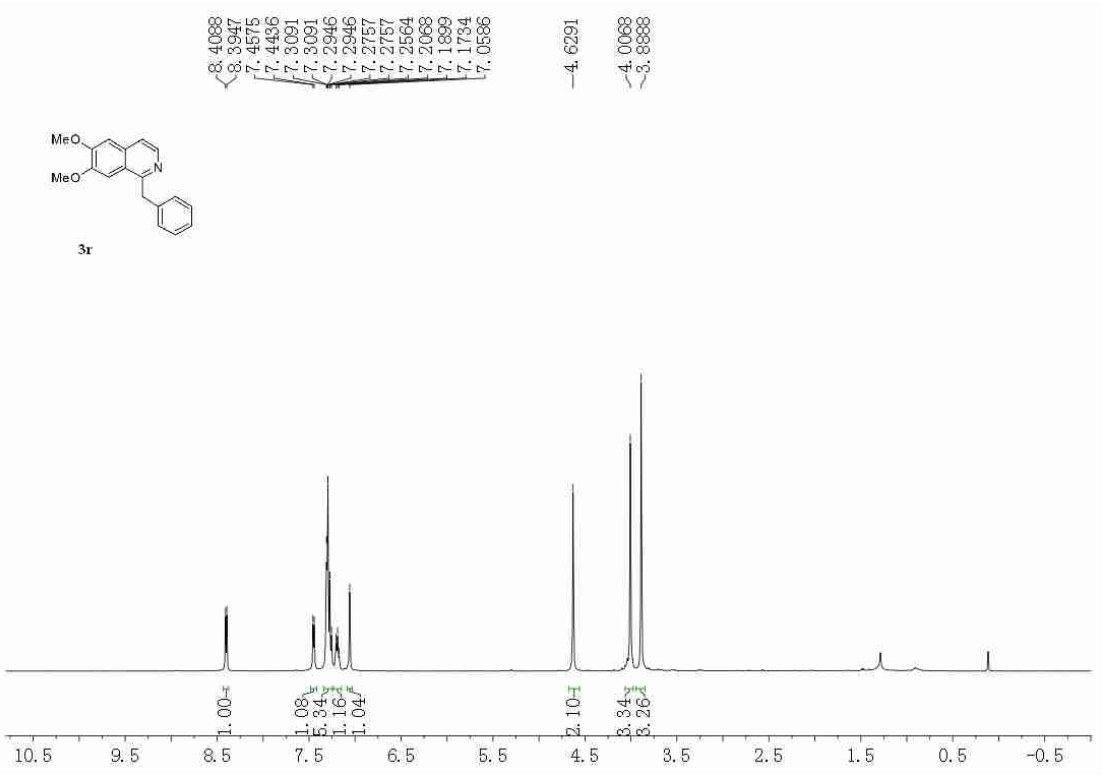
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MeO
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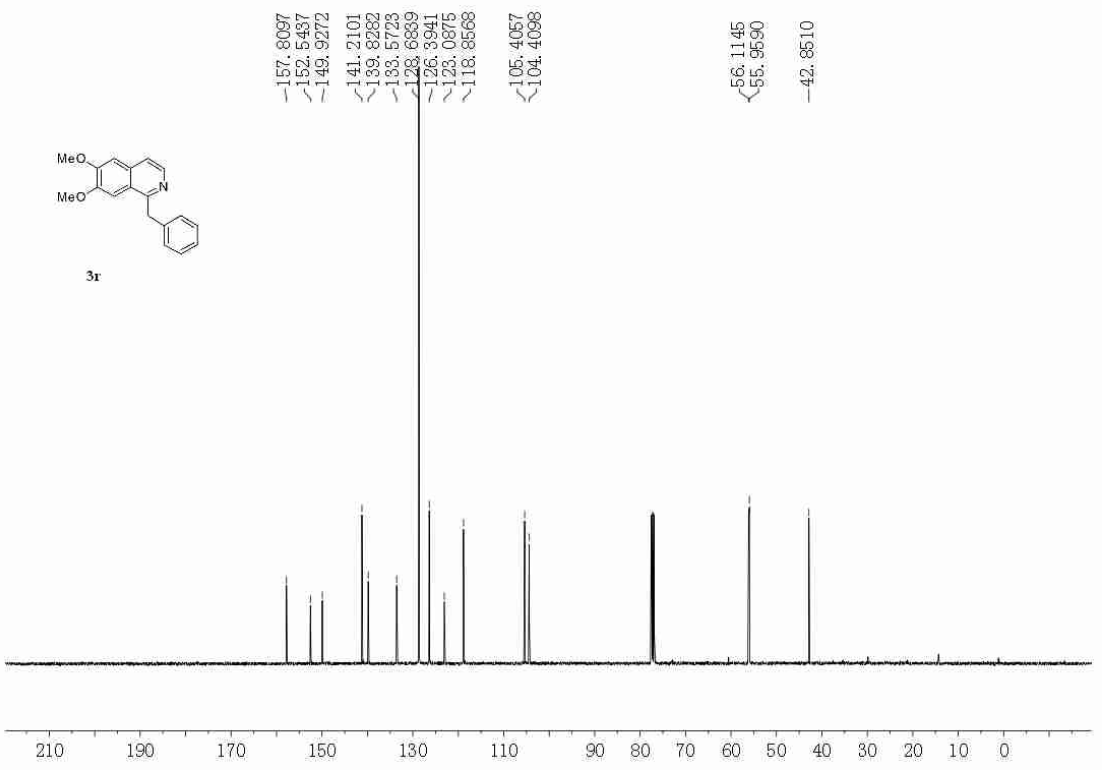
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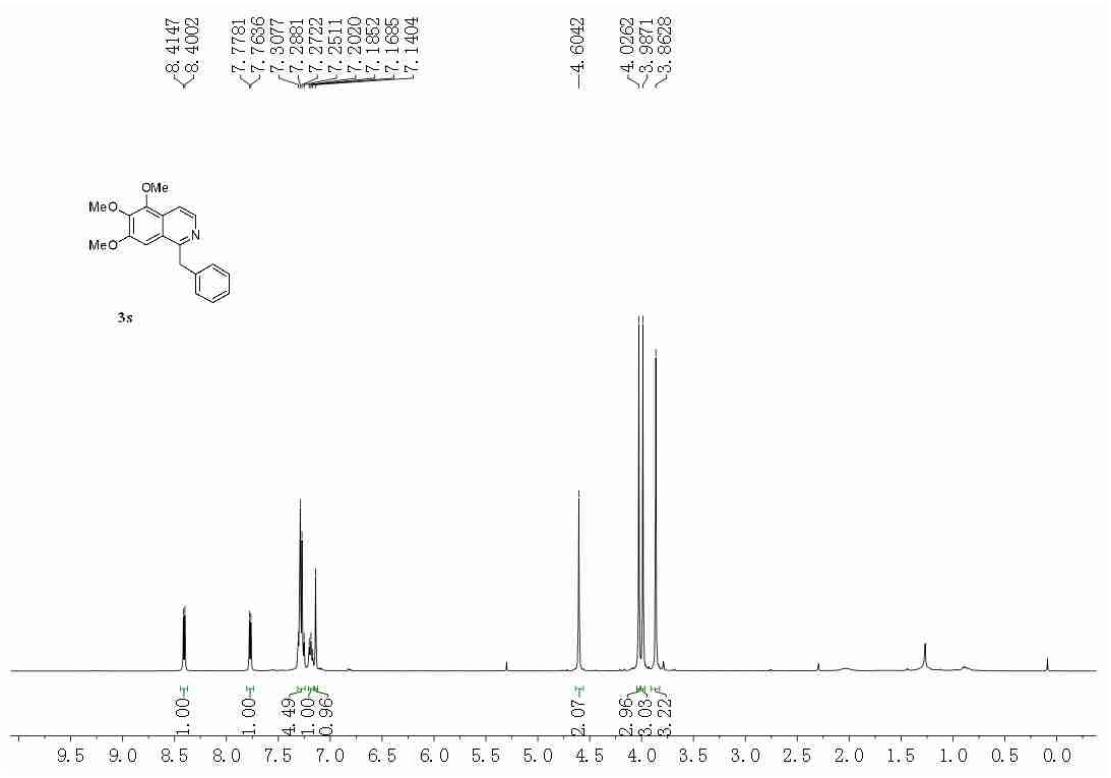
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MeO
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3.22
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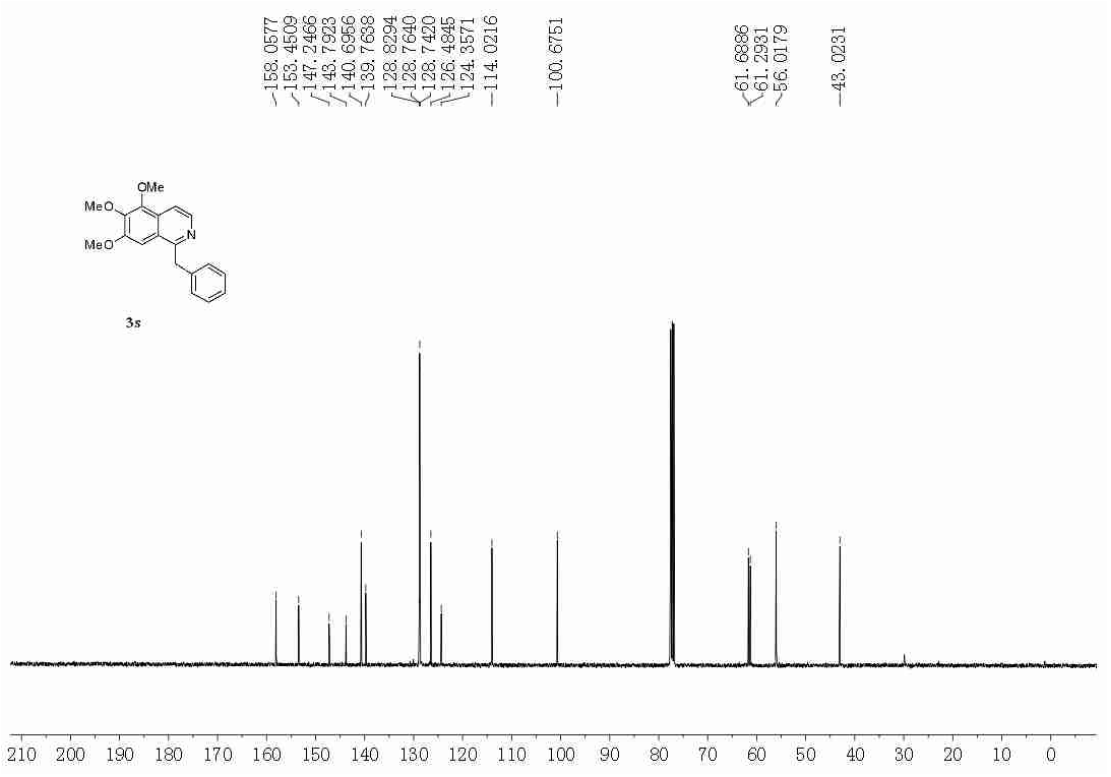
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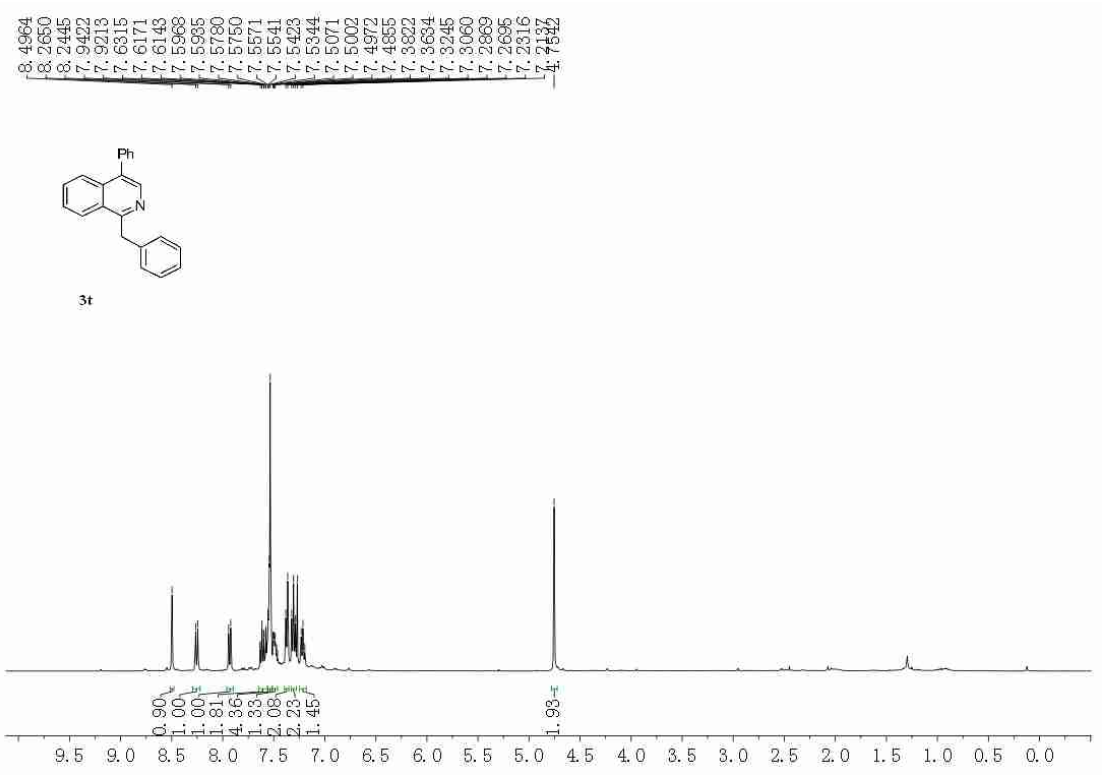
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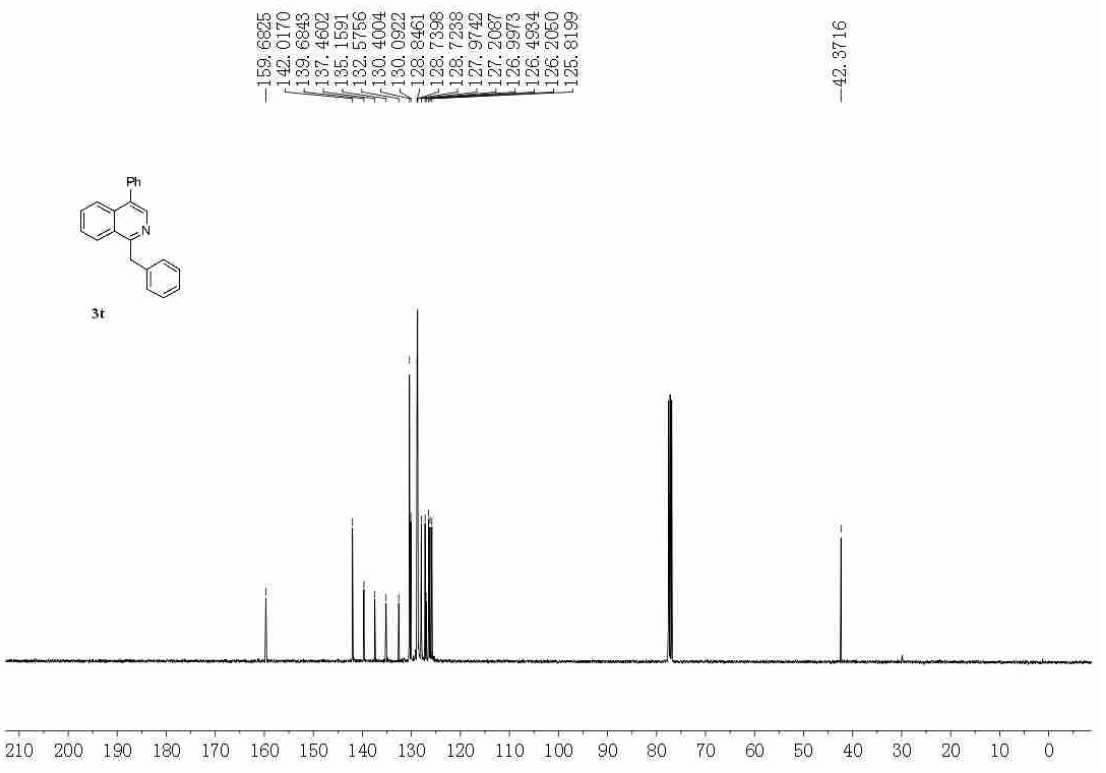
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Ph
N
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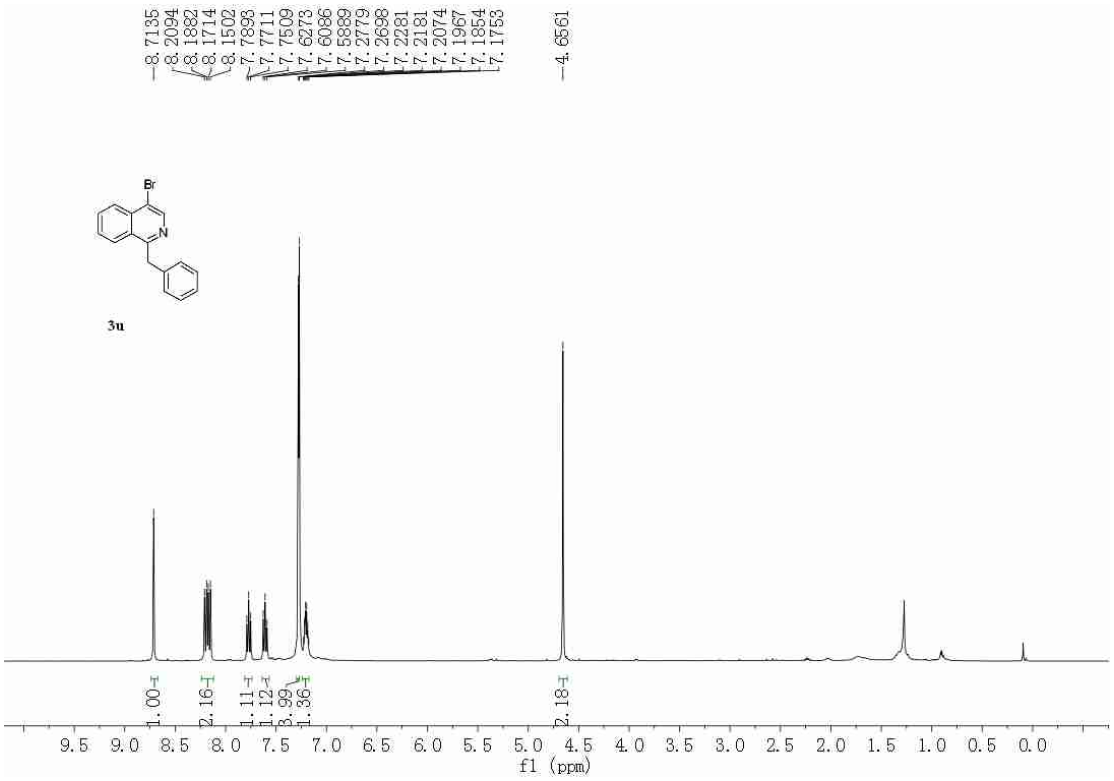
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1.11
1.12
3.99
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2.18
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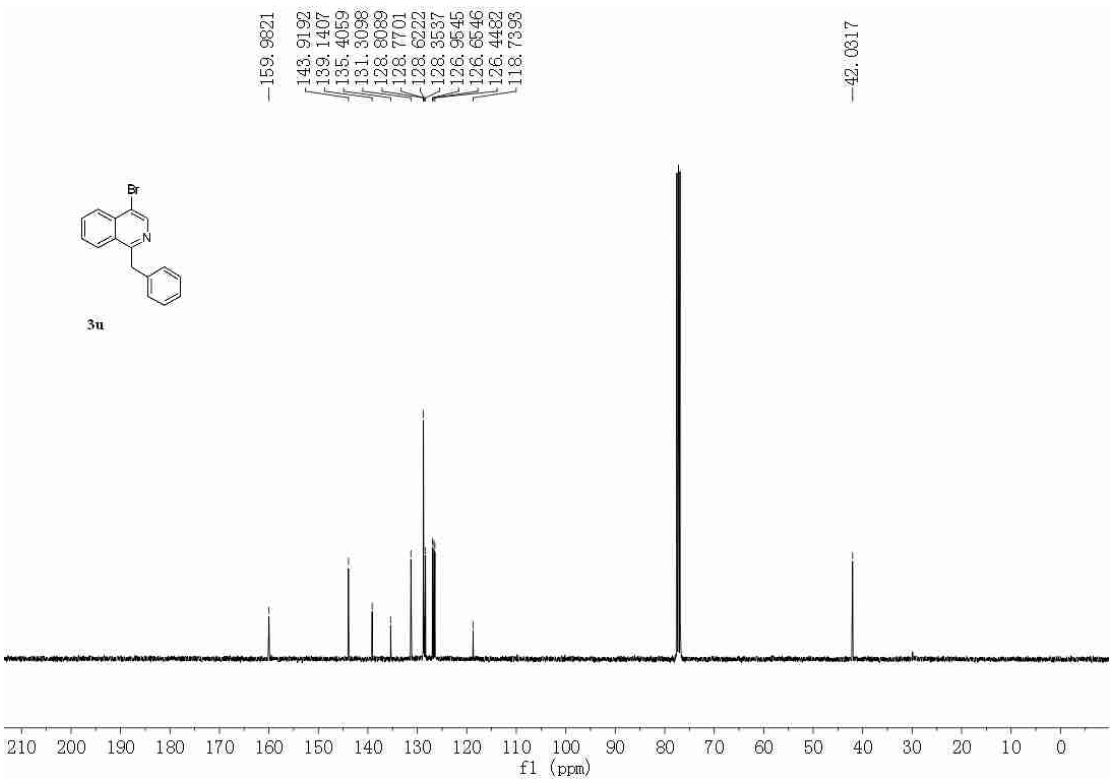
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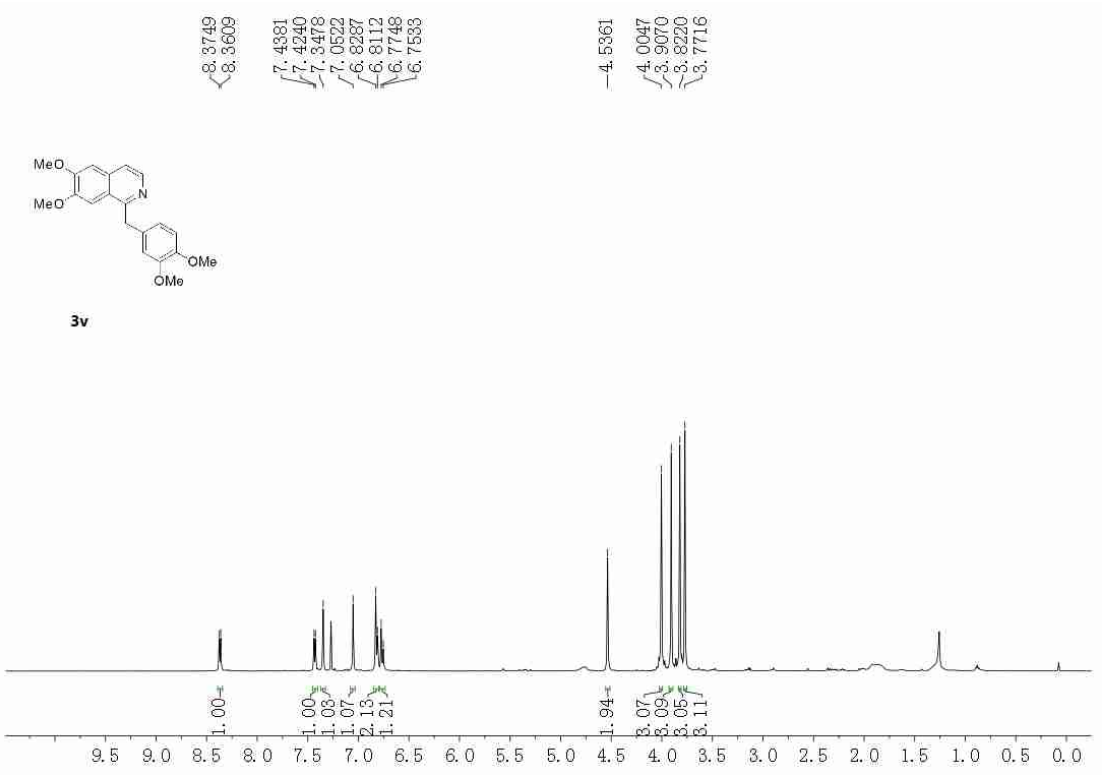
f1 (ppm)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MeO
N
OMe
OMe
3v
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1.00
1.03
1.07
2.13
1.21
1.94
3.07
3.09
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3.11
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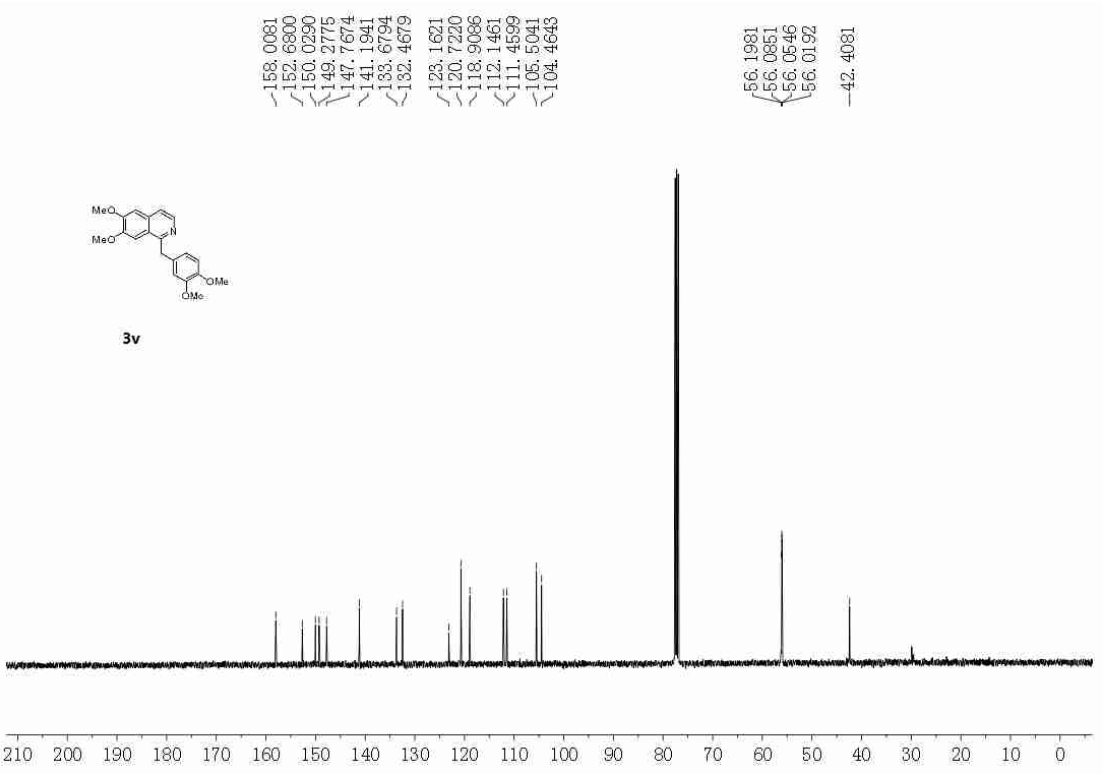
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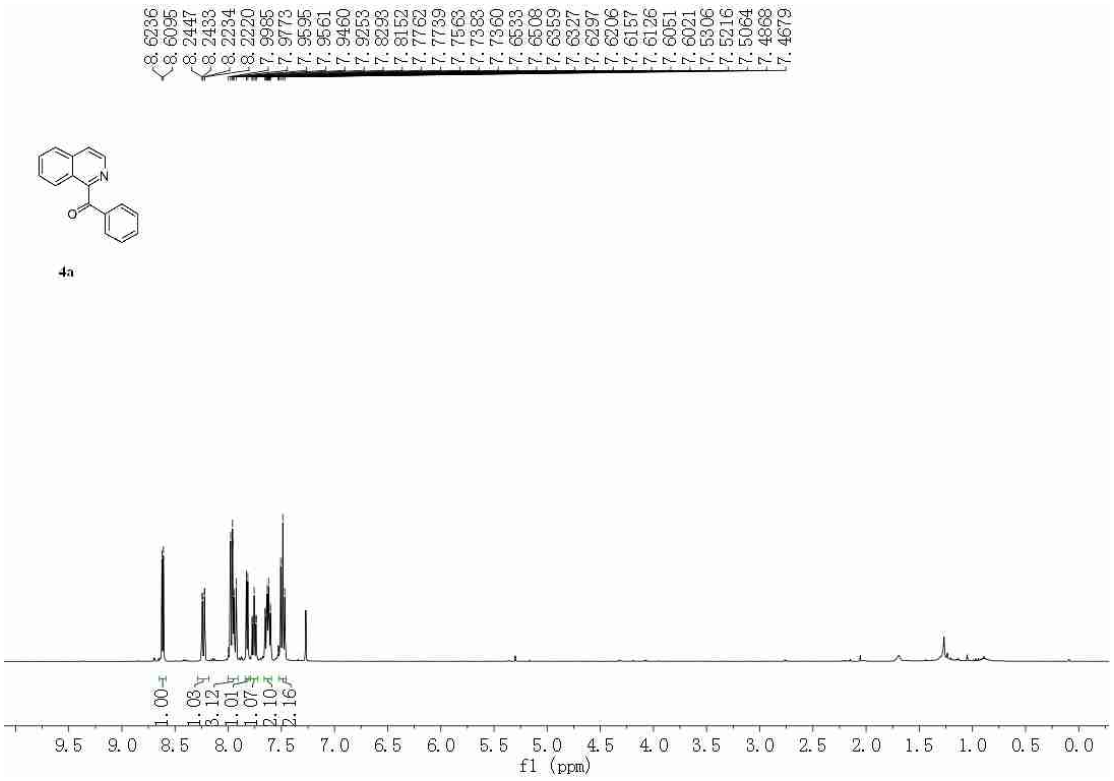
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7.7383
7.7360
7.6533
7.6508
7.6359
7.6327
7.6297
7.6206
7.6157
7.6126
7.6051
7.6021
7.5306
7.5216
7.5064
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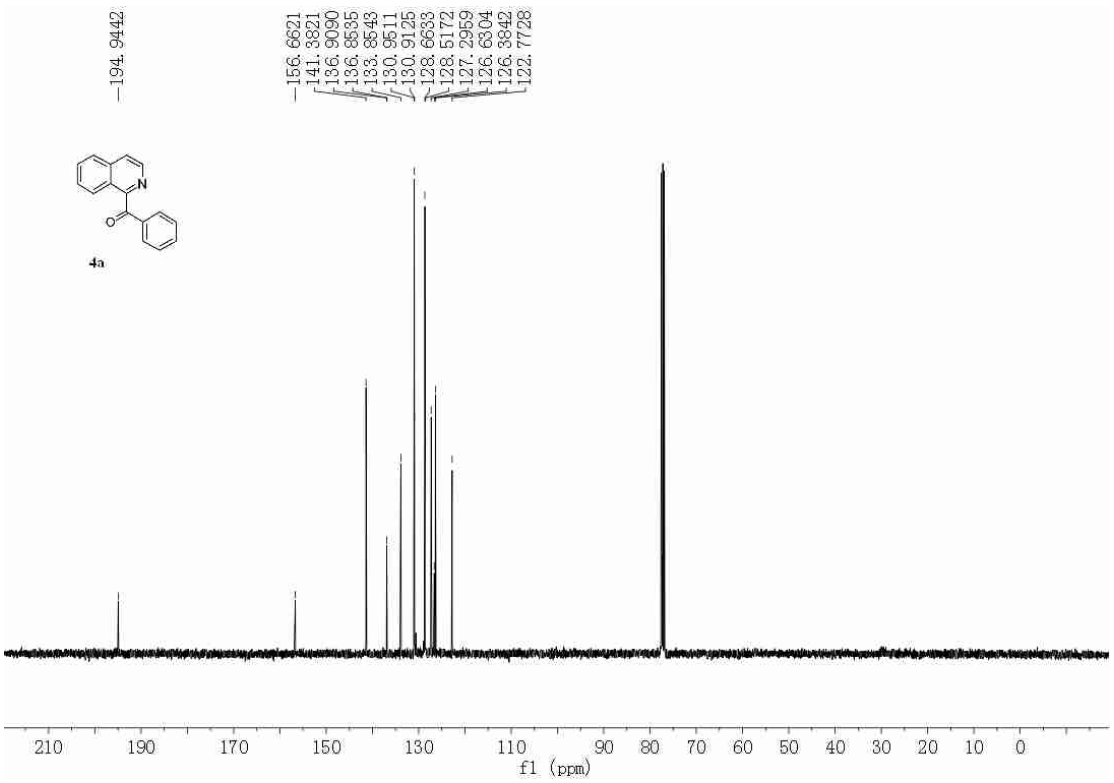
1.03
3.12
1.01
1.07
2.10
2.16
f1 (ppm)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133.8543
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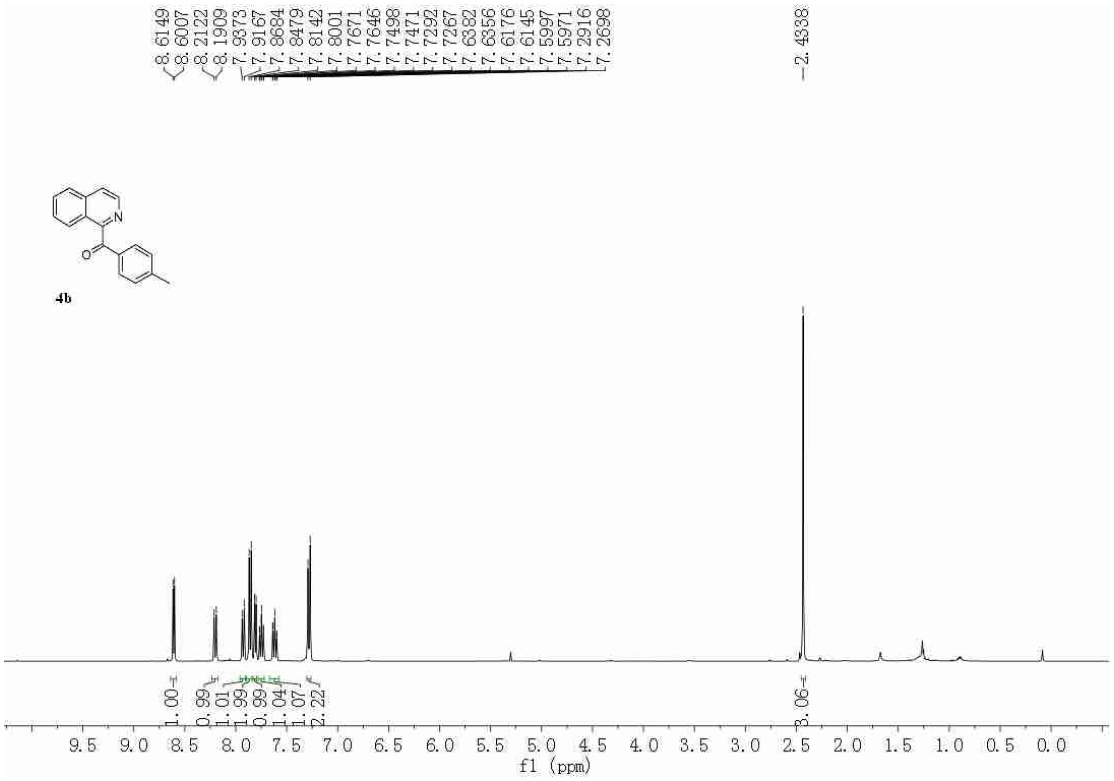
126.3942
122.7728
4a
f1 (ppm)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7.7646
7.7498
7.7471
7.7292
7.7267
7.6382
7.6356
7.6176
7.6145
7.5997
7.5971
7.2916
7.2698
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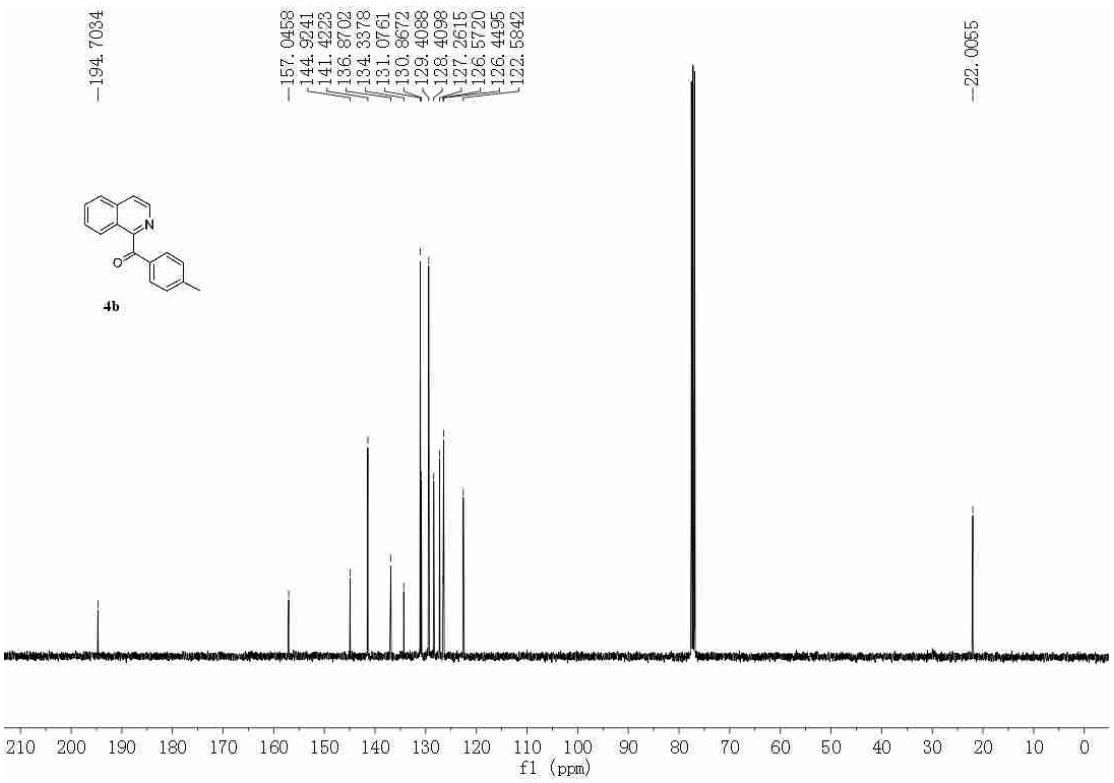
1.99
0.99
1.04
1.07
2.22
3.06
f1 (ppm)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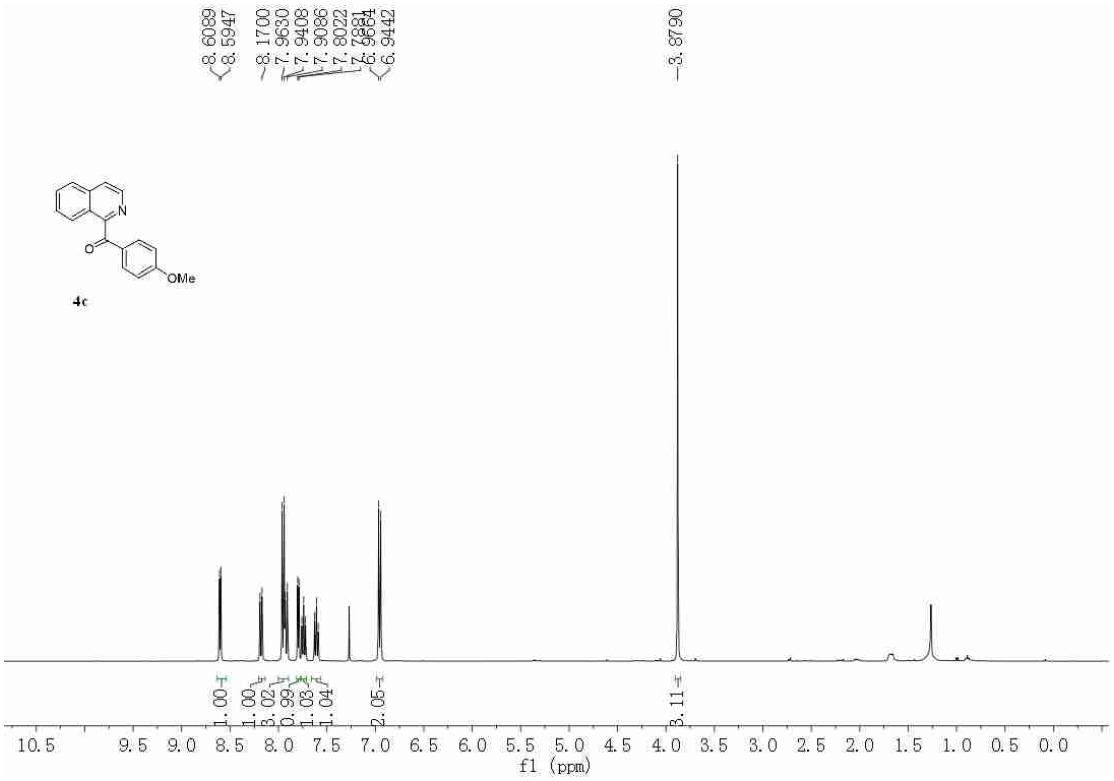
126.4495
122.5842
22.0055
4b
f1 (ppm)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7.8022
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OMe
4c
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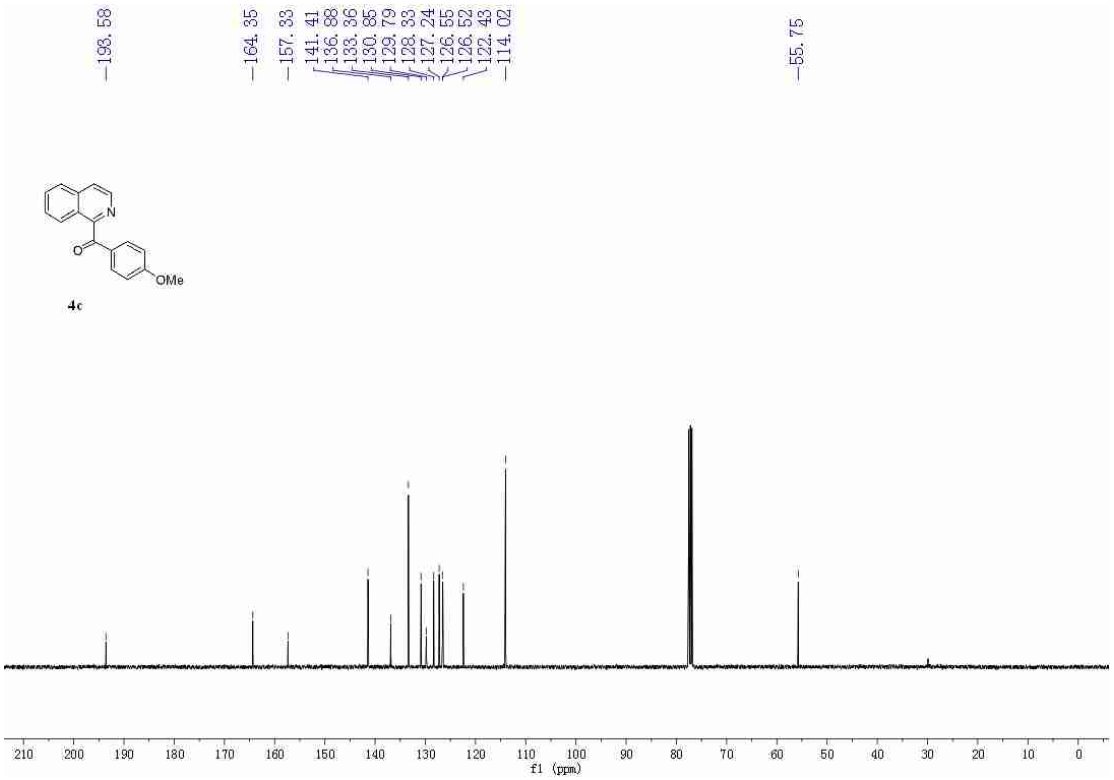
1.00
3.02
0.99
1.03
1.04
2.05
3.11
f1 (ppm)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133.36
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114.02
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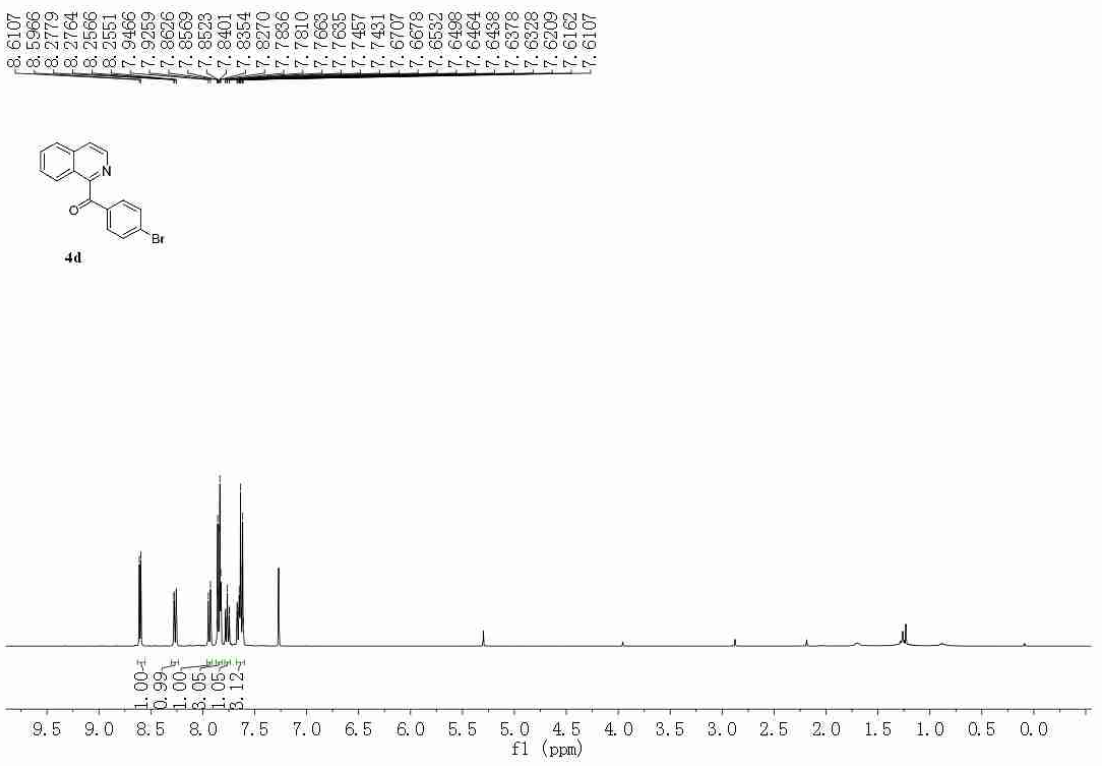
OMe
4c
f1 (ppm)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7.8523
7.8401
7.8354
7.8270
7.7836
7.7810
7.7663
7.7635
7.7457
7.7431
7.6707
7.6678
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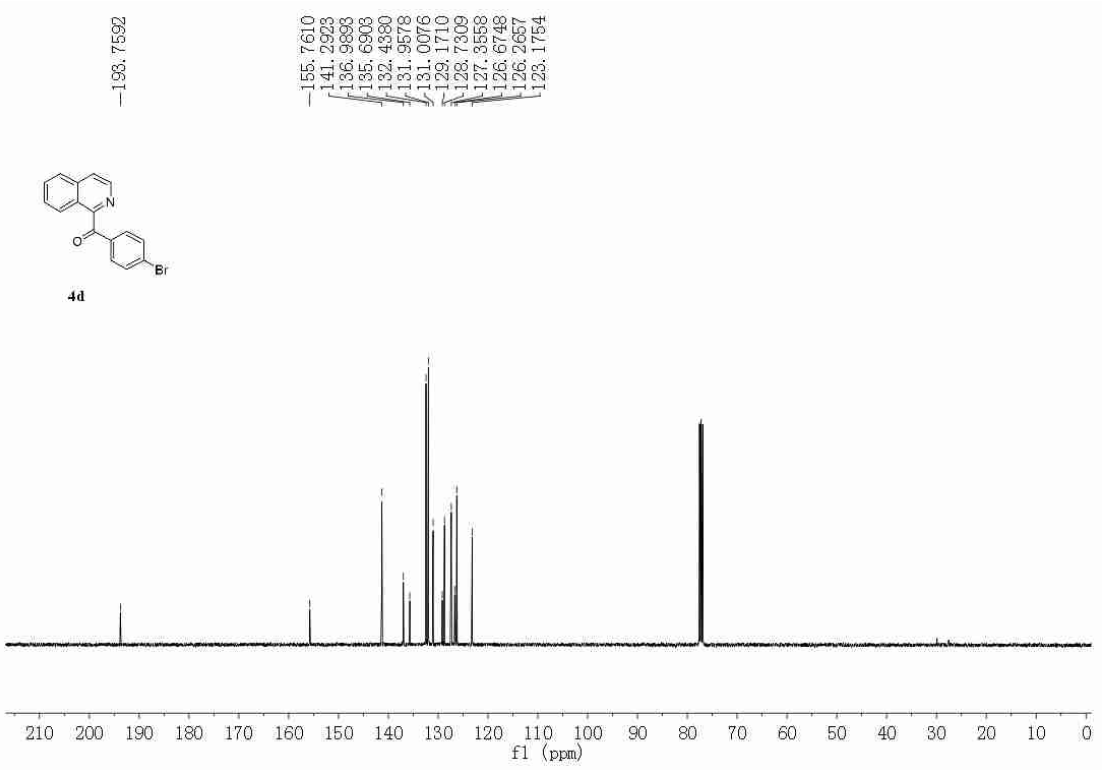
7.6464
7.6438
7.6378
7.6328
7.6209
7.6162
7.6107
N
O
Br
4d
1.00
0.99
1.00
3.05
1.05
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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N
O
Br
4d
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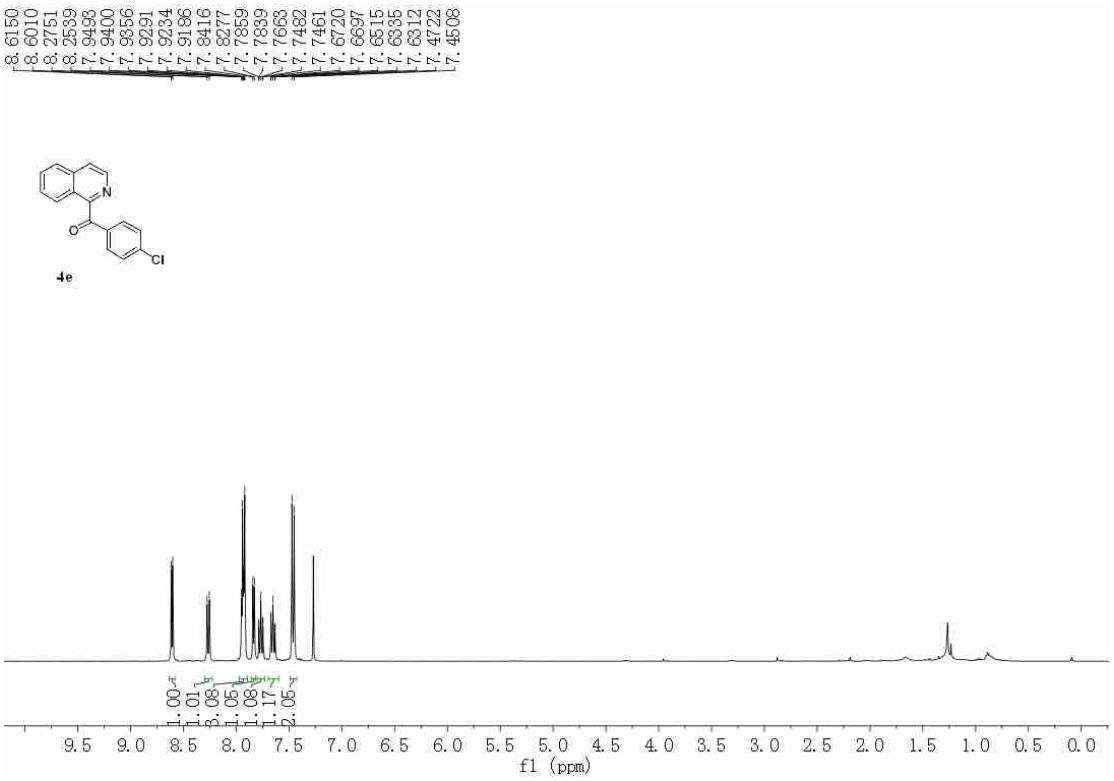
f1 (ppm)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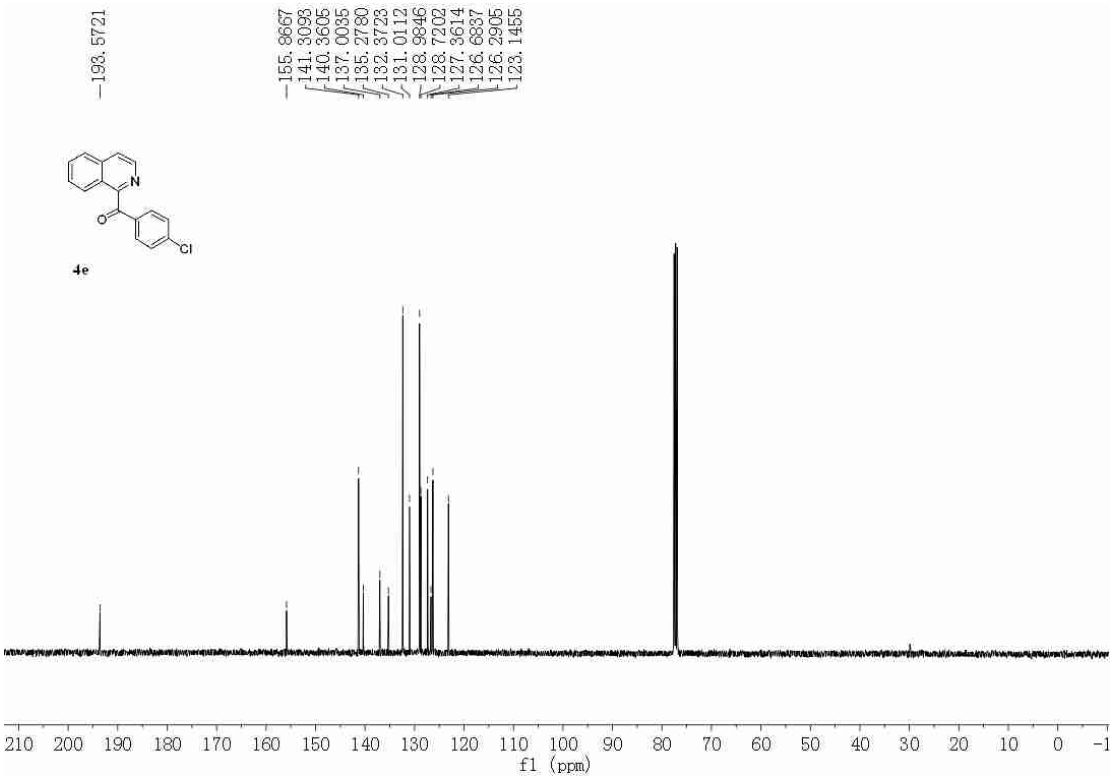
7.8416
7.8277
7.7859
7.7839
7.7663
7.7482
7.7461
7.6720
7.6697
7.6515
7.6335
7.6312
7.4722
7.4508
4e
1.00
1.01
3.08
1.05
1.08
1.17
2.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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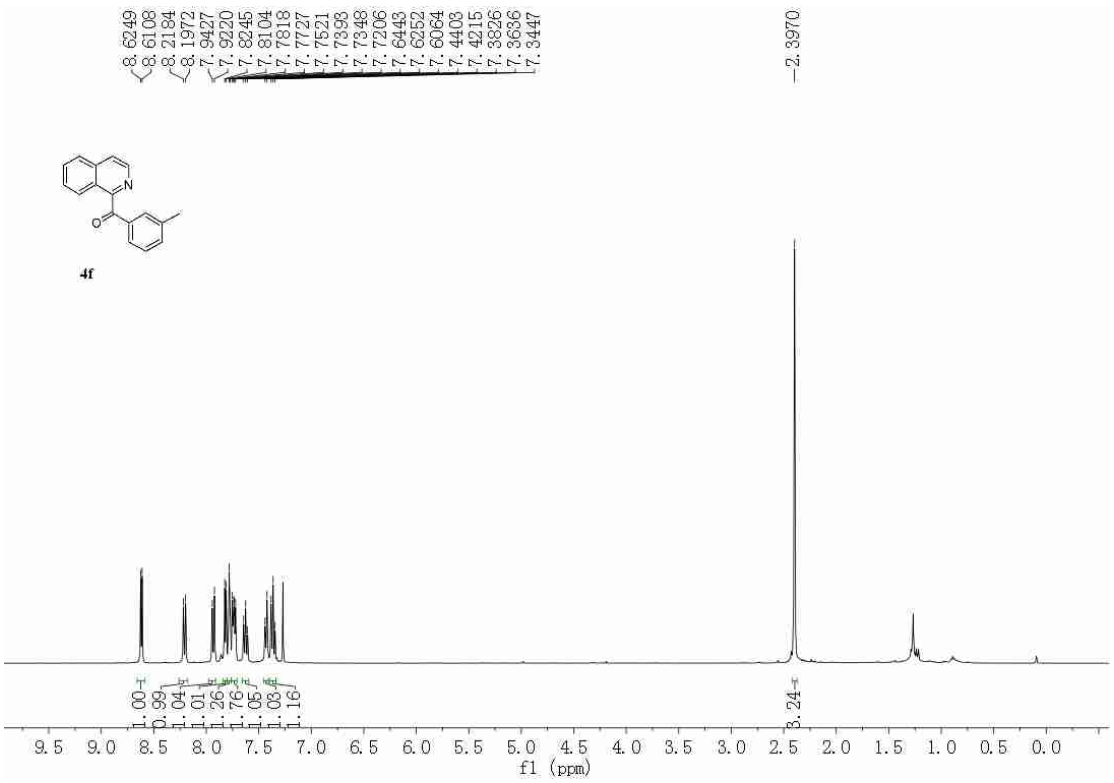
126.2905
123.1455
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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7.7393
7.7348
7.7206
7.6443
7.6252
7.6064
7.4403
7.4215
7.3826
7.3636
7.3447
2.3970
4f
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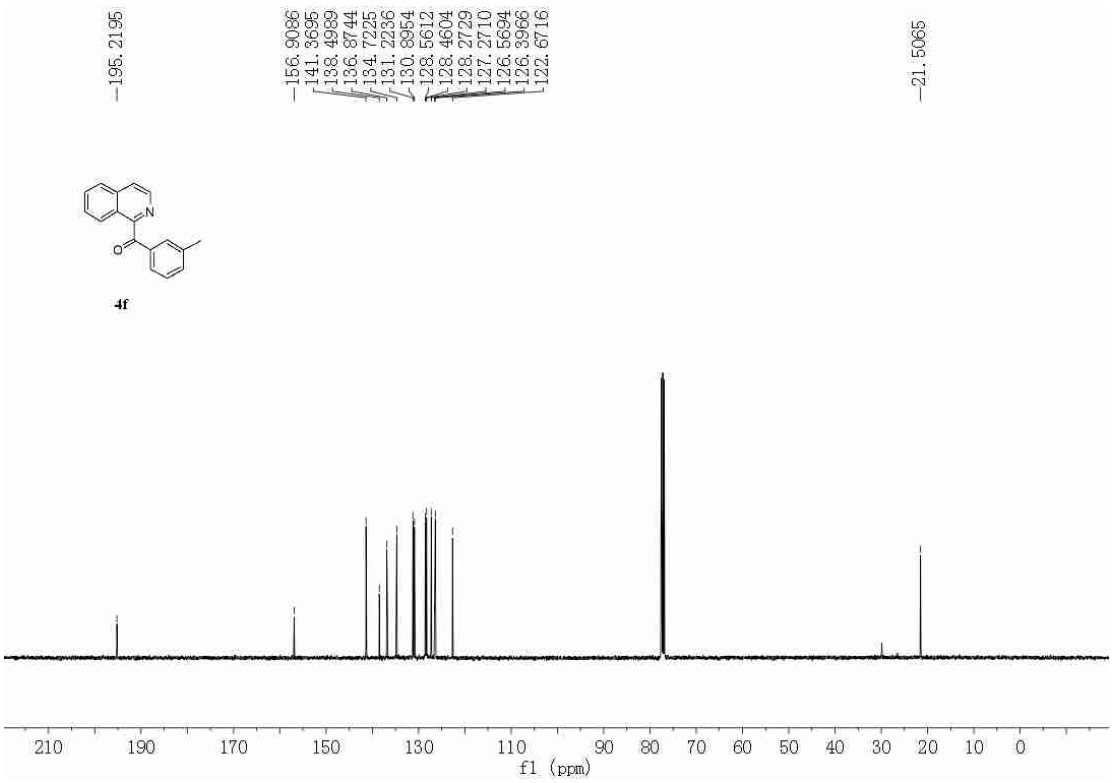
0.99
1.04
1.01
1.26
1.76
1.05
1.03
1.16
3.24
f1 (ppm)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130.8954
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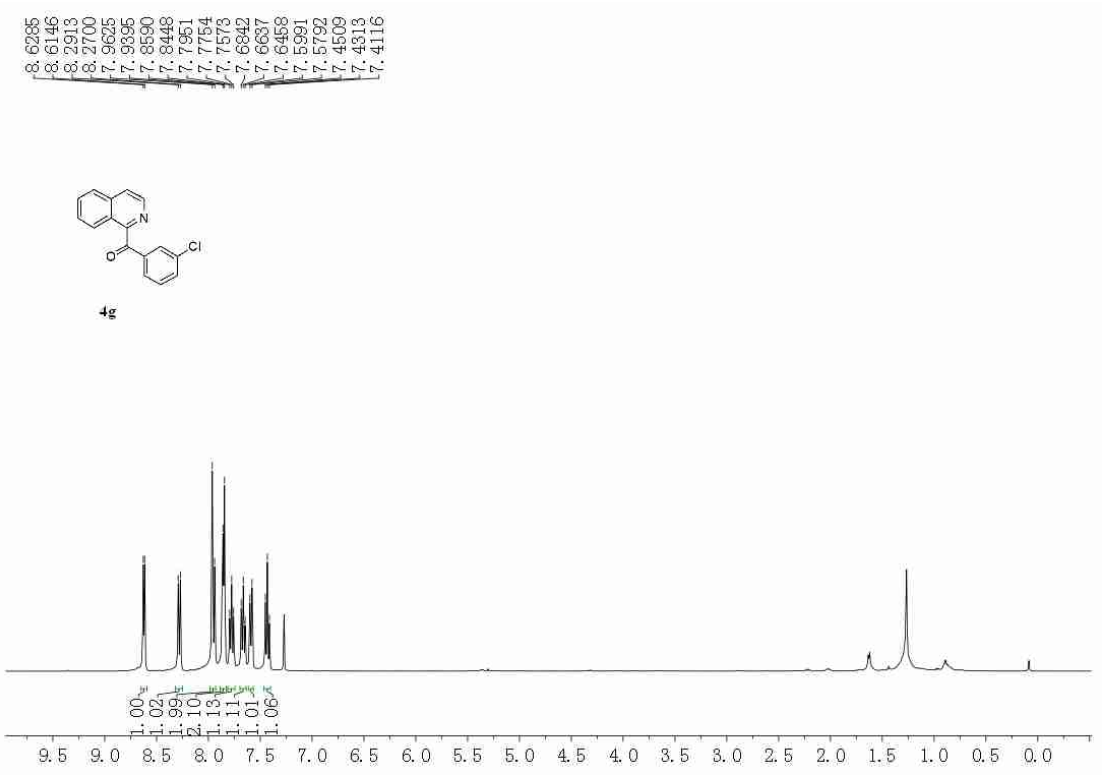
127.2710
126.5694
126.3966
122.6716
21.5065
4f
f1 (ppm)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7.5792
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4g
1.00
1.02
1.99
2.10
1.13
1.11
1.01
1.06
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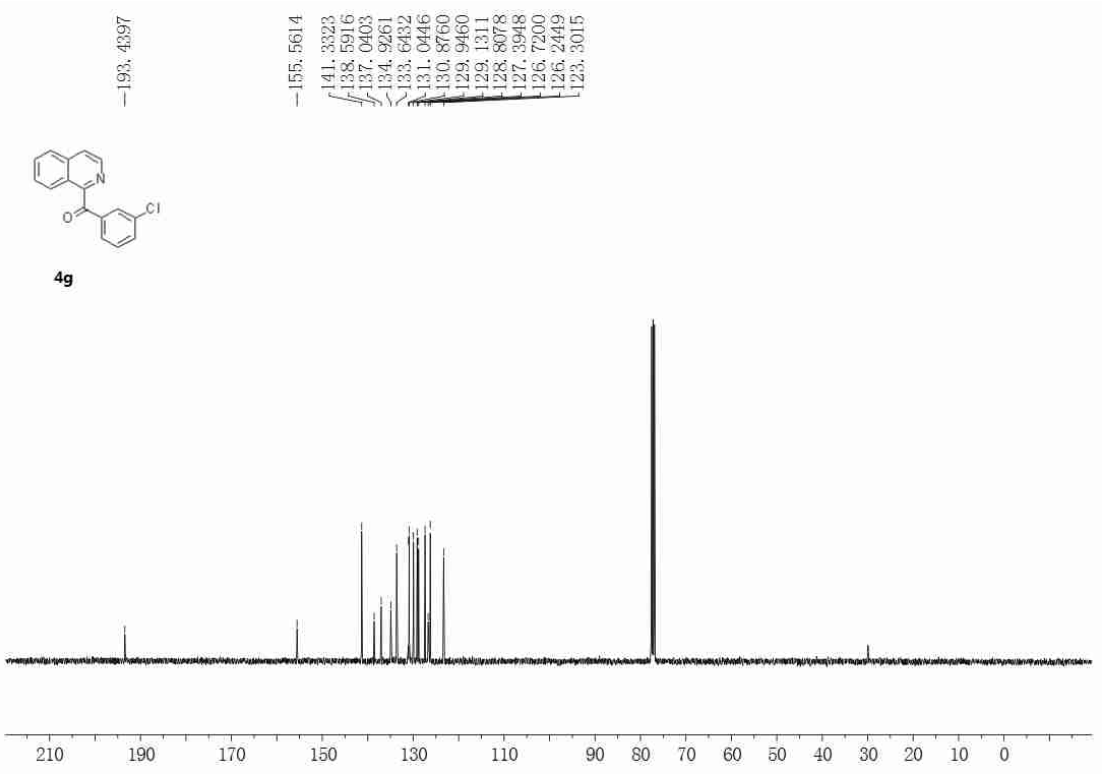
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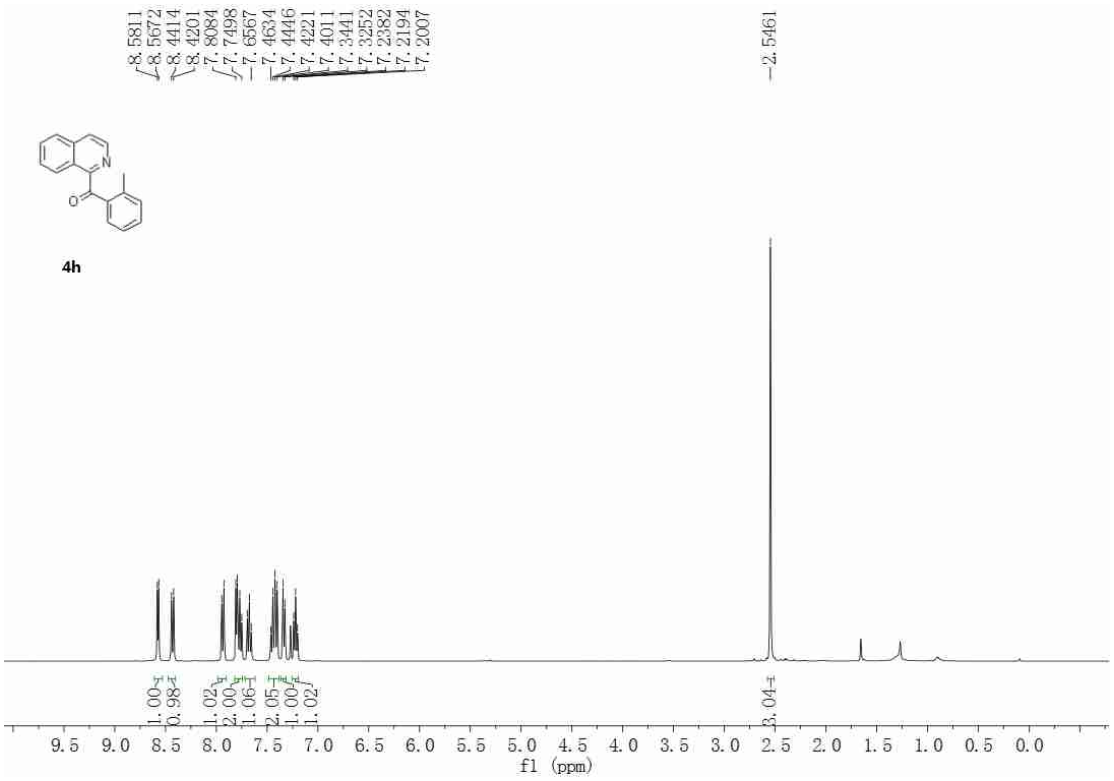
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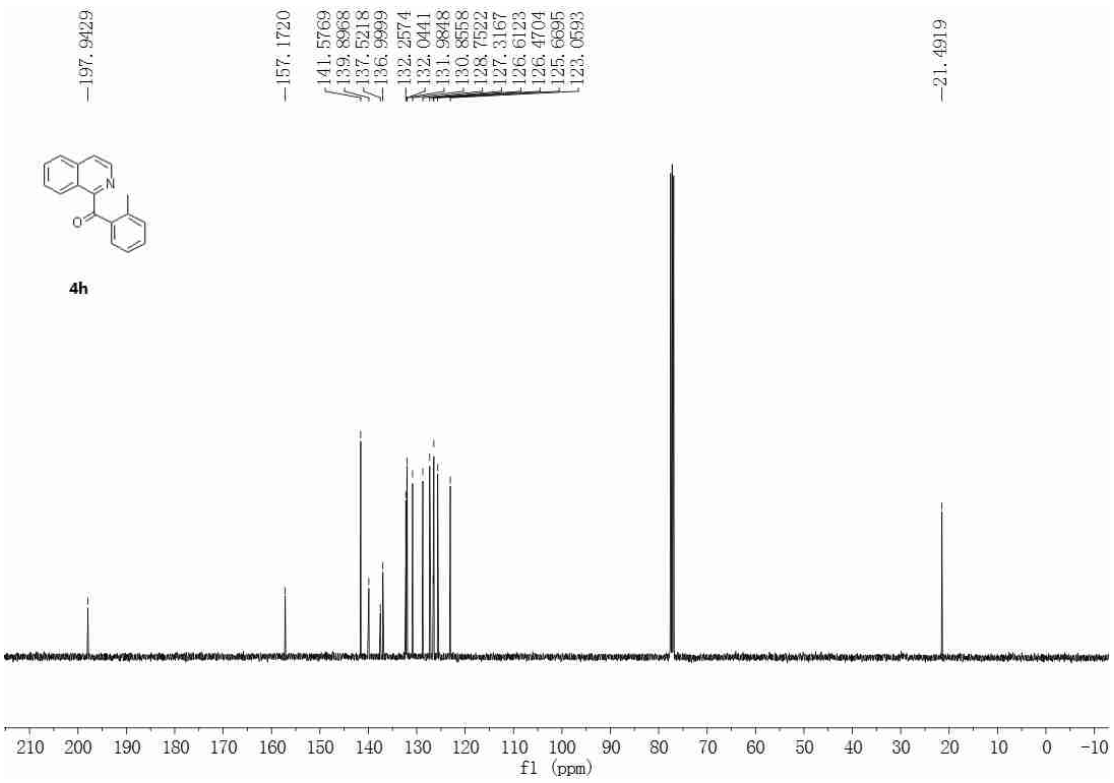
7.4011
7.3441
7.3252
7.2382
7.2194
7.2007
2.5461
4h
1.00
0.98
1.02
2.00
1.06
2.05
1.00
1.02
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.3167
126.6123
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4h
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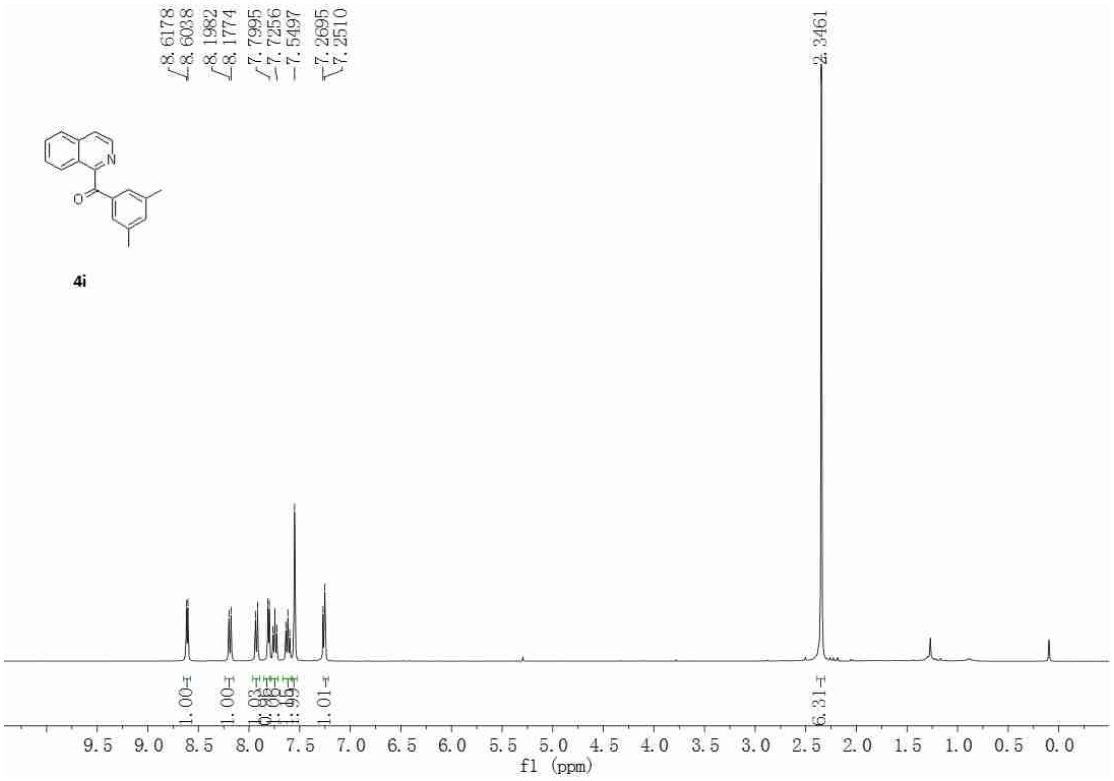
f1 (ppm)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0.86
1.99
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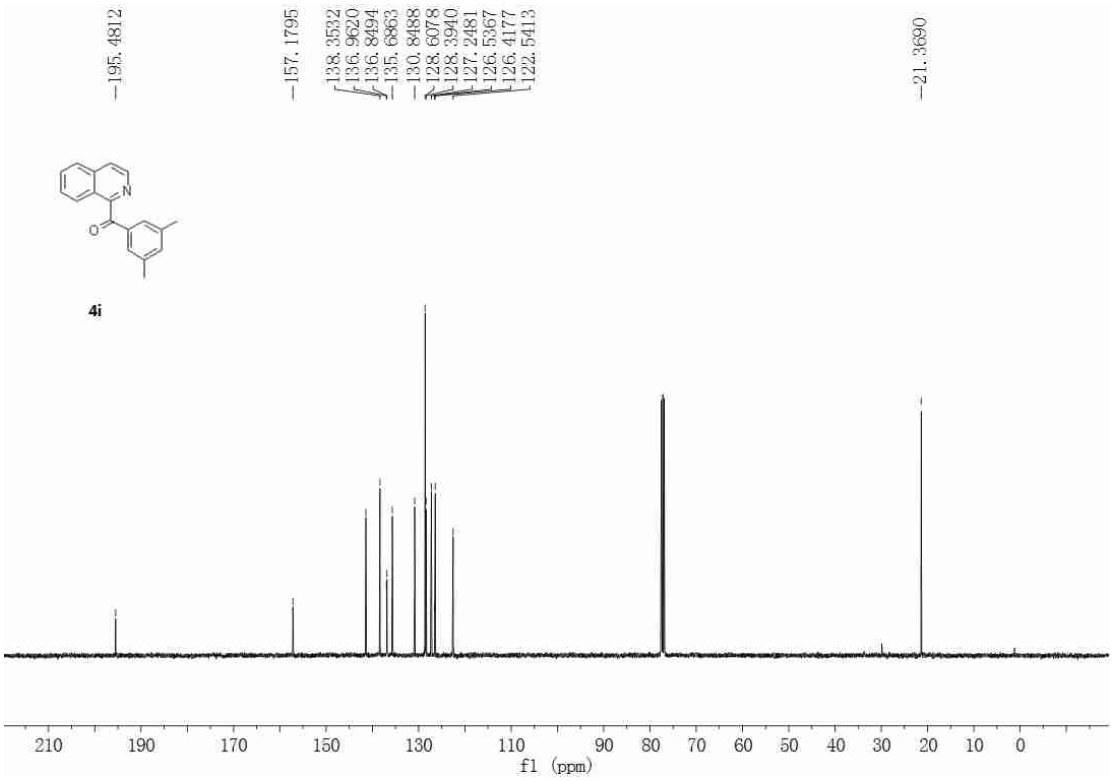
6.31
f1 (ppm)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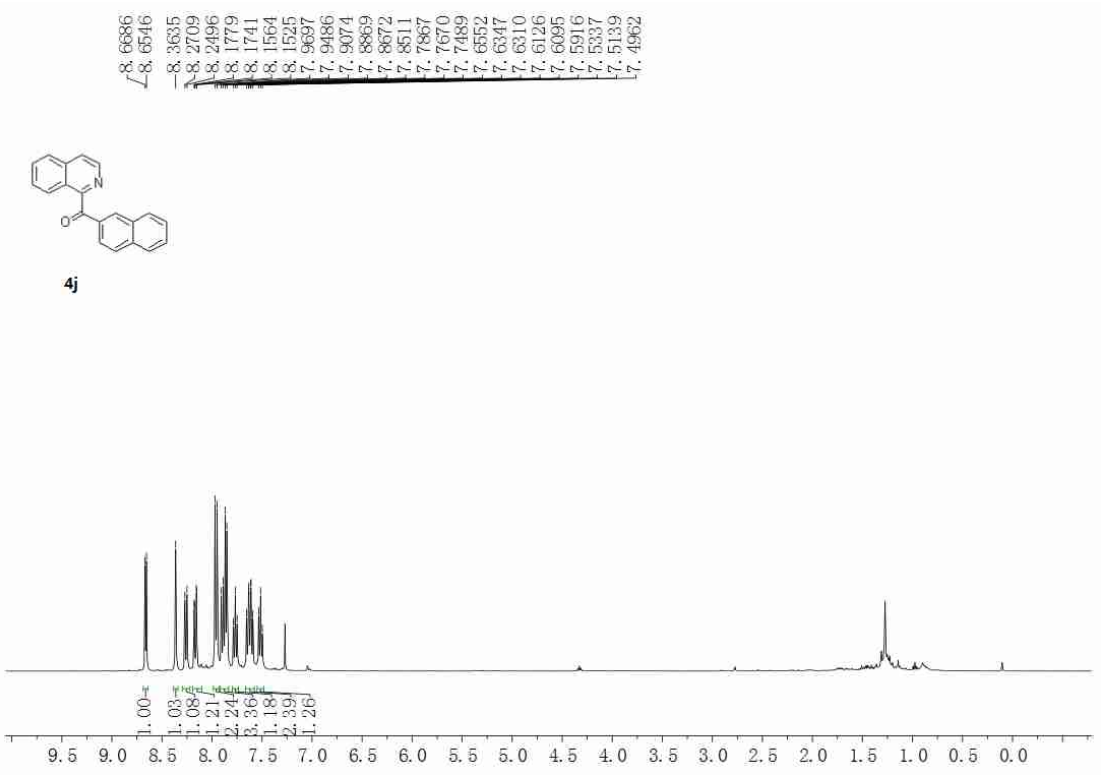
f1 (ppm)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7.6310
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7.6095
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7.5139
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4j
1.00
1.03
1.08
1.21
2.24
3.36
1.18
2.39
1.26
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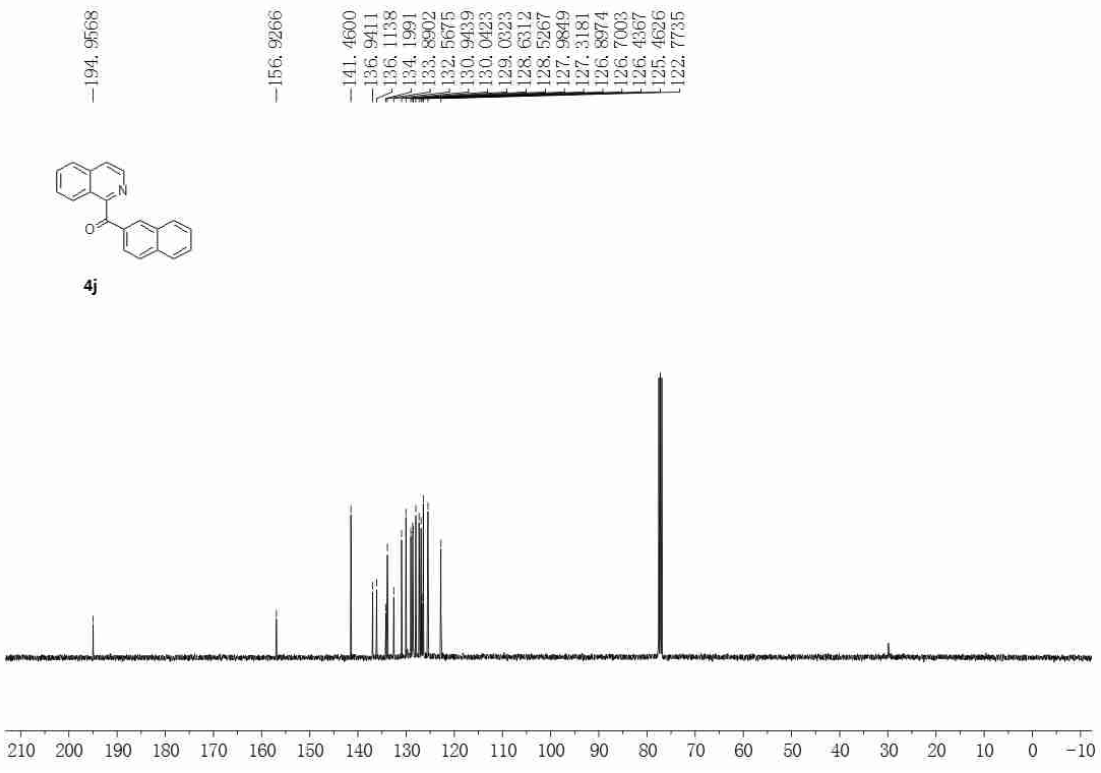
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127.3181
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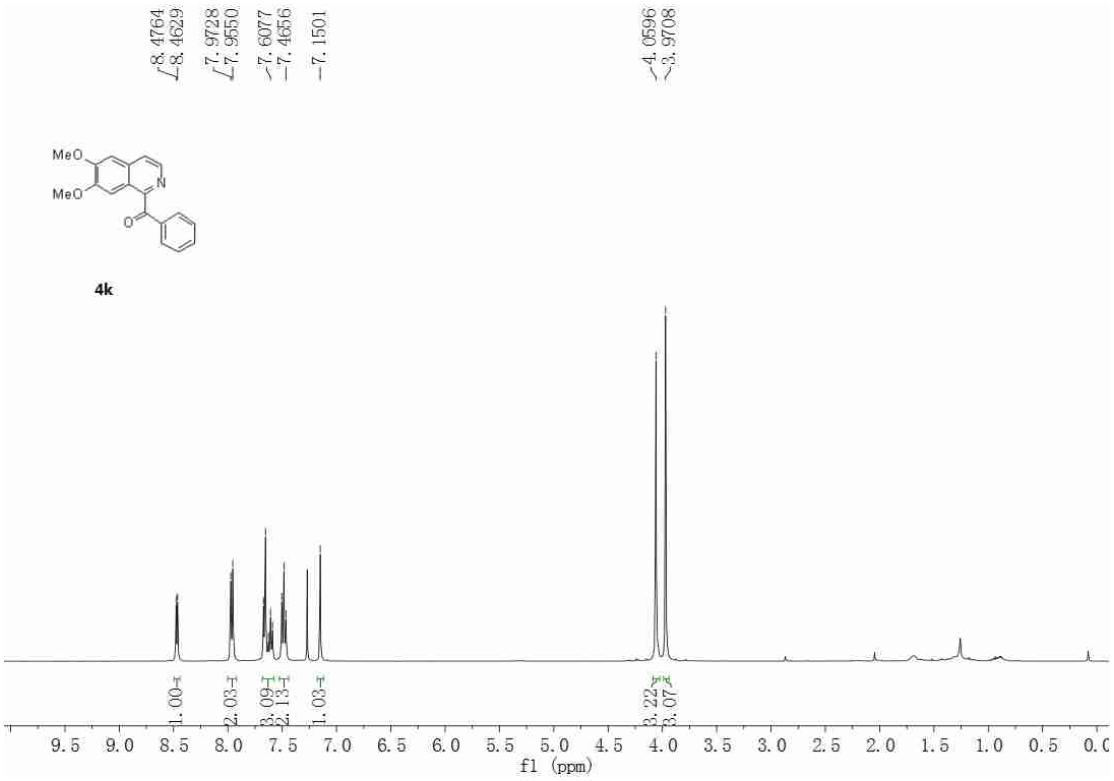
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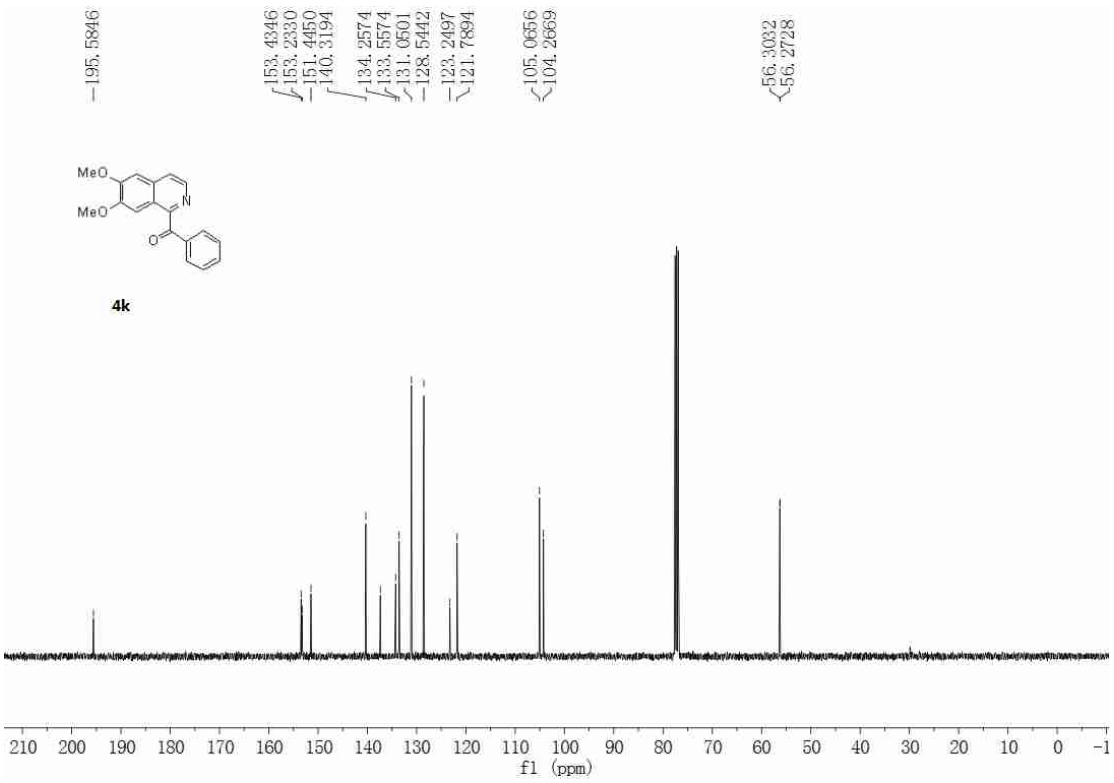
MeO
MeO
N
O
4k
1.00
2.03
3.09
2.13
1.03
3.22
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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104.2669
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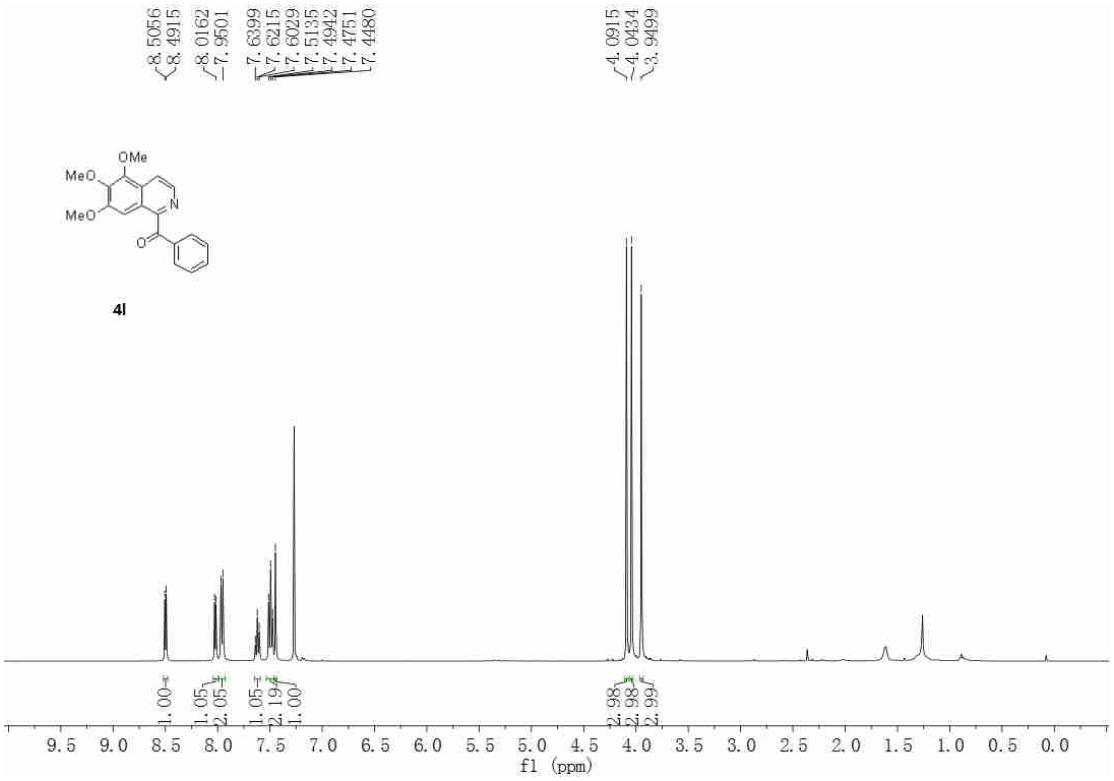
MeO
N
O
4k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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4.0915
4.0434
3.9499
OMe
MeO
MeO
N
O
4l
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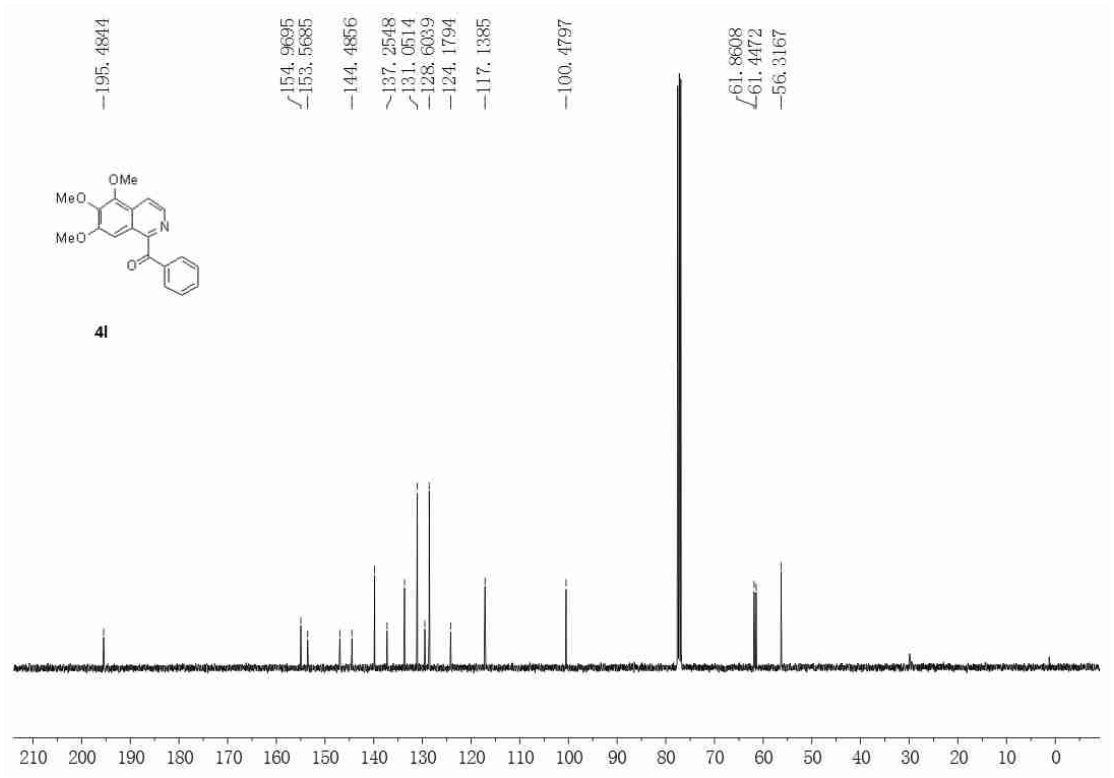
1.05
2.05
1.05
2.19
1.00
2.98
2.98
2.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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OMe
MeO
MeO
N
O
4l
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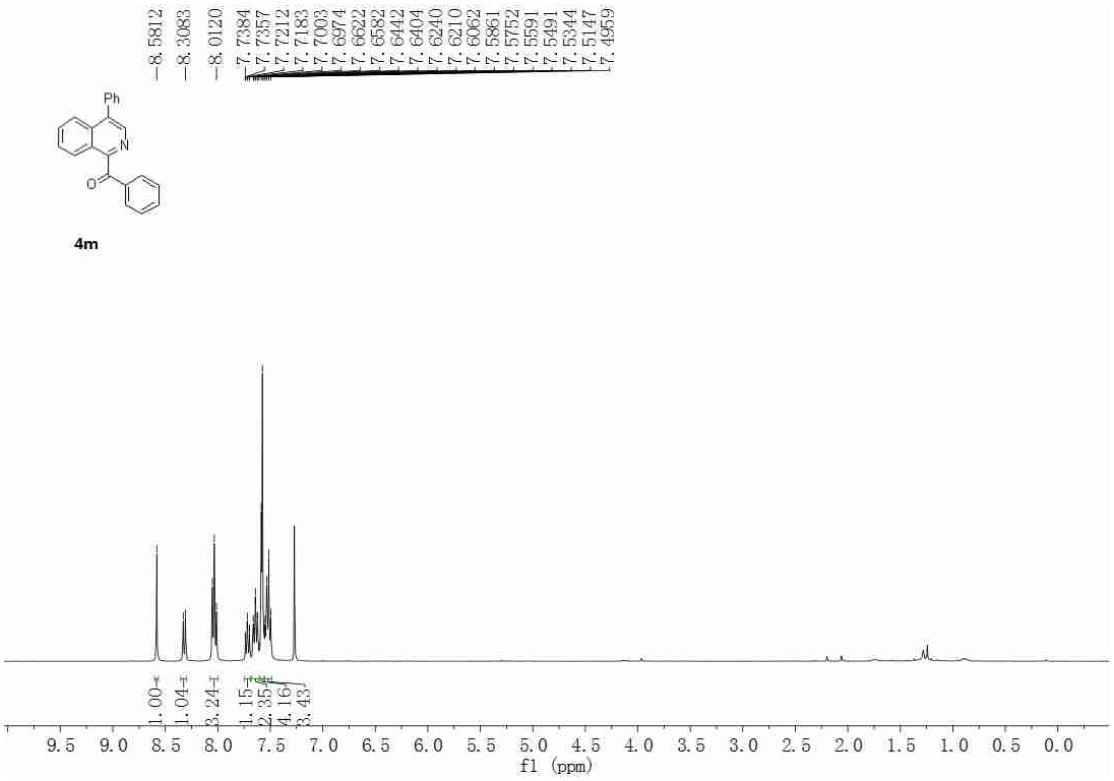
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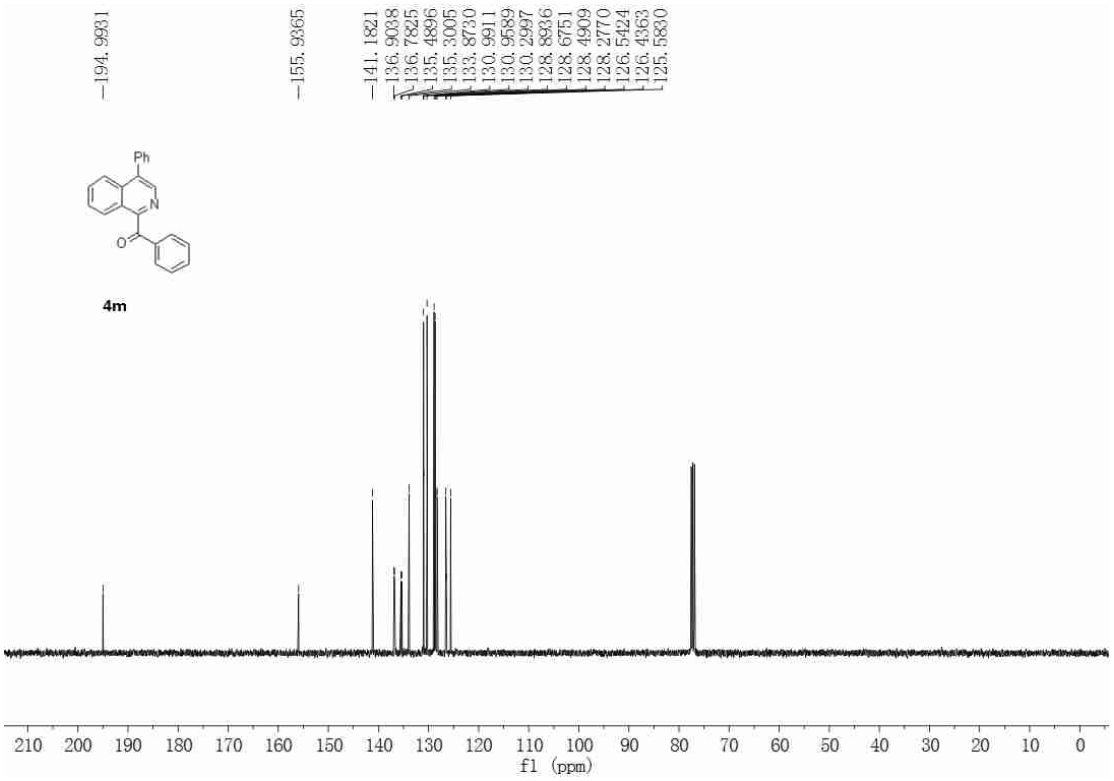
7.4959
Ph
N
O
4m
1.00
1.04
3.24
1.15
2.35
4.16
3.43
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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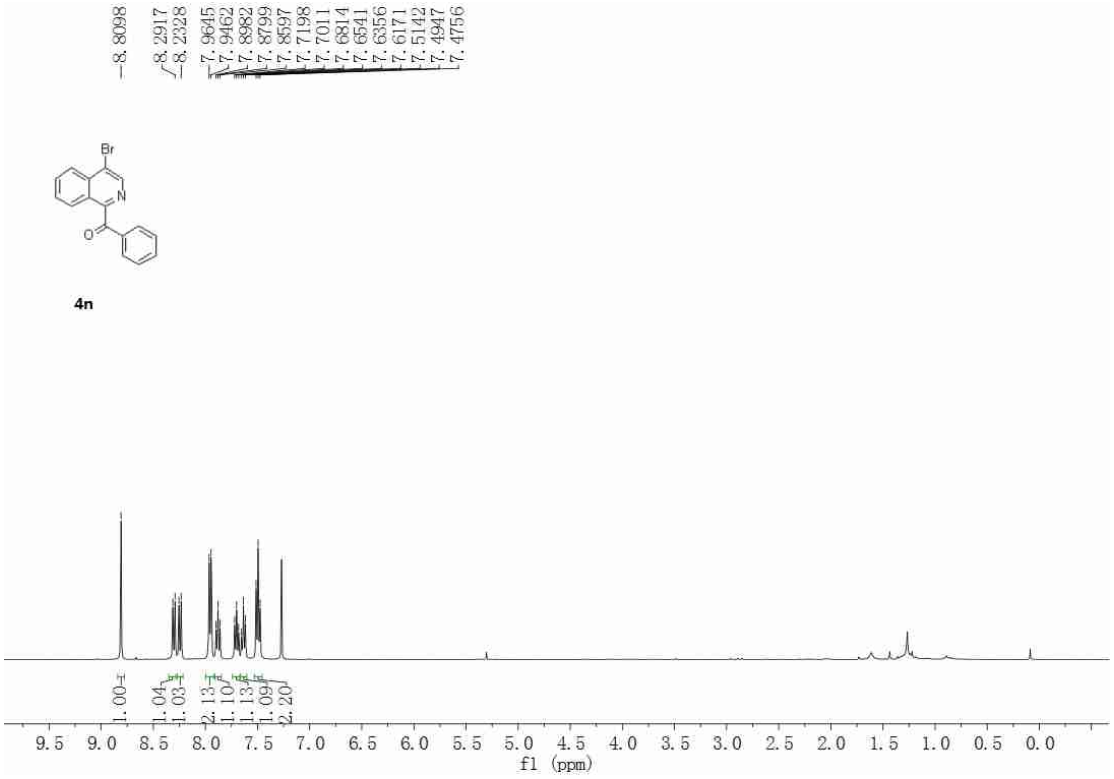
Ph
N
O
4m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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Br
N
O
4n
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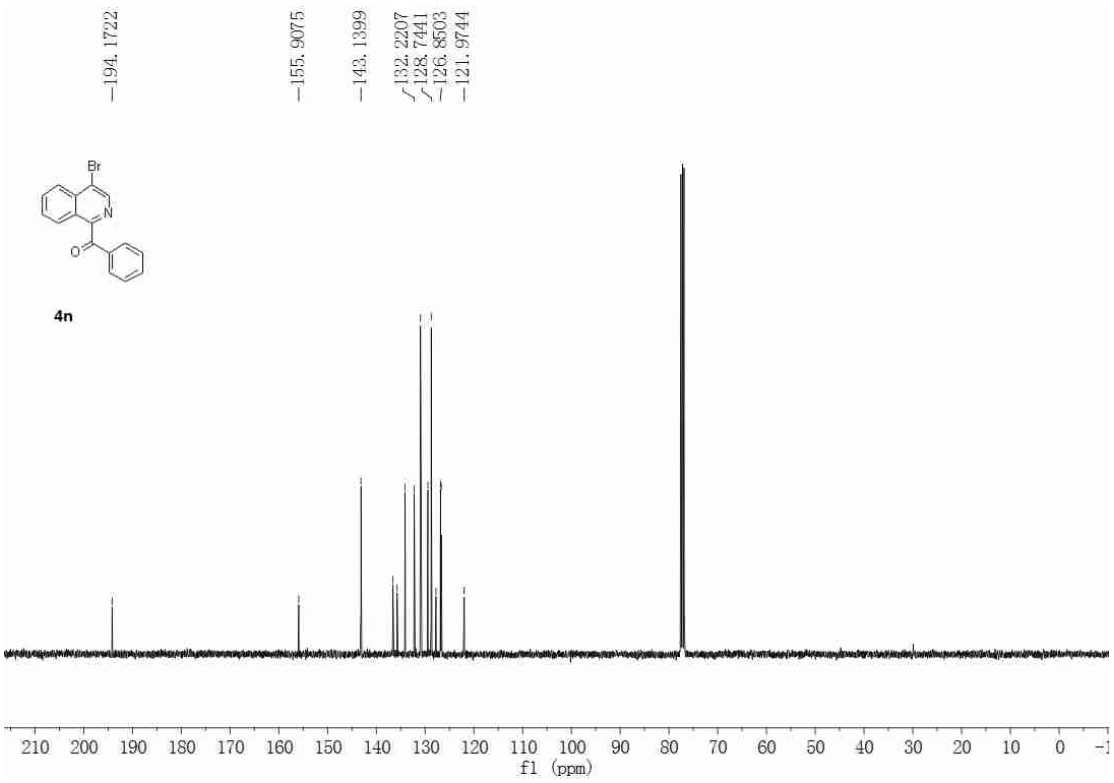
1.04
1.03
2.13
1.10
1.13
1.09
2.20
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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O
4n
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f1 (ppm)