Supporting Information

A designed bi-functional sugar-based surfactant: micellar catalysis for C-X coupling reaction in water

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Experiment

General

Nuclear magnetic resonance (NMR) spectra were measured at 400 MHz (^{1}H) or at 100 MHz (^{13}C) on a Bruker Avance DRX-400 spectrometer. Melting points were determined on an X4-Data microscopic melting point apparatus and were uncorrected. All reactions were monitored by analytical thin-layer chromatography (TLC) from Merck with detection by UV. The products were purified by column chromatography through silica gel (300-400 mesh). All reagents and solvents were general reagent grade unless otherwise stated.

The synthesis of *N*-alkyl Glucosamine (AGA12, AGA14, AGA16)

A mixture of glucose (50 mmol) and N-alkylamine (50 mmol) in CH_3OH (100 mL) were stirred for 24 hours at room temperature. Then the final mixture was suction filtered to remove solvent CH_3OH, washed the filter cake three times with cyclohexane, once with water, twice with ethanol, recrystallized twice with ethanol, and dried in vacuum to give solid powder. The yields of AGA12, AGA14, AGA16 are respectively 85%, 76%, 56%.

The synthesis of *N*-alkyl lactosamine (ALA12, ALA14, ALA16)

Lactose monohydrate (18 mmol, 6.486 g) was dissolved in 60 mL of ultrapure water, and N-alkylamine (30 mmol) was dissolved in 100 mL of isopropanol. the two solutions were mixed and

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mechanical stirred at room temperature for 24 hours, then transfer to a 60 °C water bath for 30 minutes. The final mixture was suction filtered to remove solvent and the filter cake were rinsed three times with ethanol, recrystallized with ethanol and dried in vacuum to give white solid powder. The yields of ALA12, ALA14, ALA16 are respectively 73%, 81%, 67%.

Surface Tension Measurements

The surface tension (γ) was measured at 40.0 ± 0.1 °C by the pendant method using an OCA 40 optical contact angle instrument (Dataphysics, Germany). The solution is equipped with ultra-pure water.

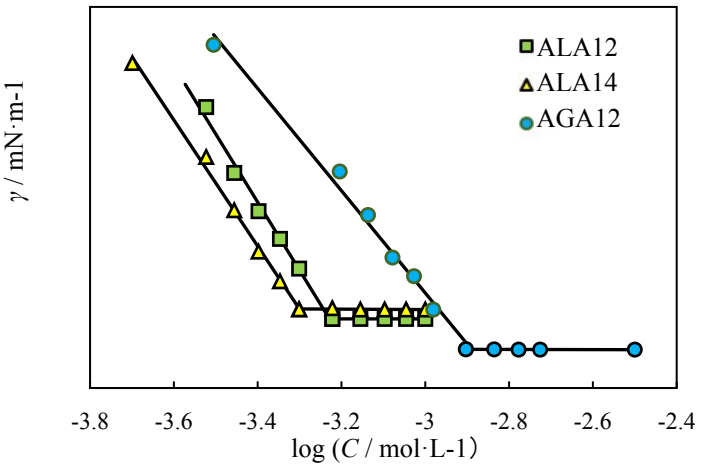


Figure S1. Surface tension (γ) of sugar-based surfactants aqueous solution as a function of surfactant molality at 40°C

Table S1. CMC of three characteristic surfactants at 40°C

Surfactant	CMC (mol·L^{-1})
G12	0.00115
L12	0.0006
L14	0.0005

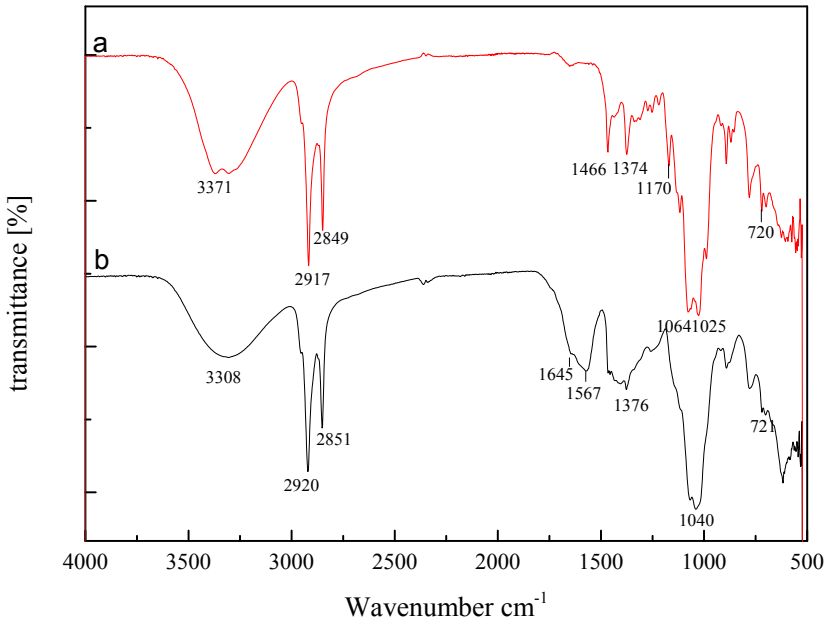


Figure S2. FTIR spectra of ALA14 (a), ALA14@CuI (b)

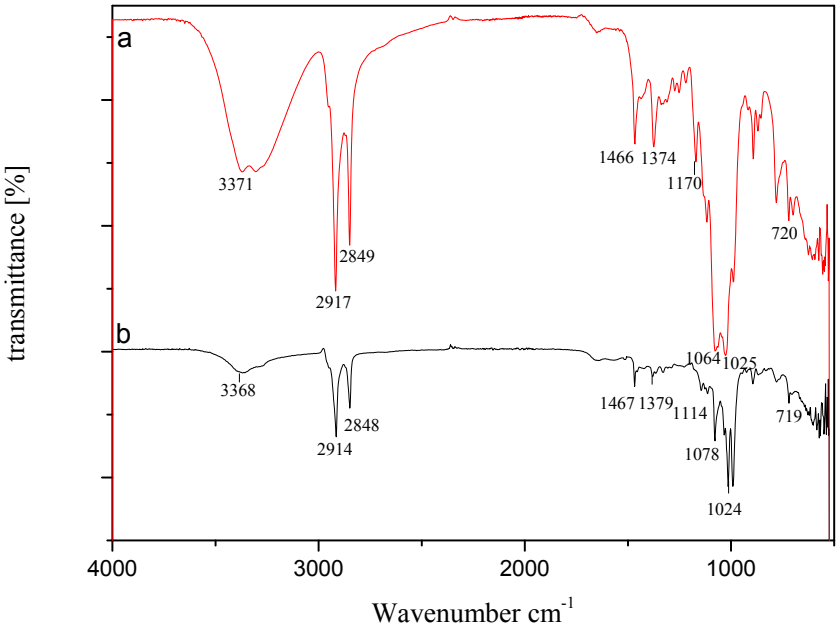


Figure S3. FTIR spectra of ALA14 (a), ALA14 precipitated after reaction (b)

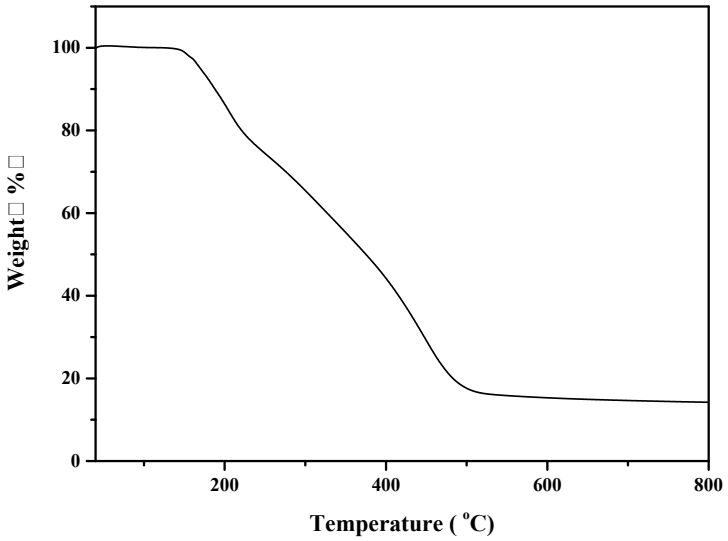


Figure S4. TG analysis of ALA14

DLS Measurements

Dynamic light scattering (DLS) was used to study the size of aggregates of surfactant ALA14 aqueous solution before and after solubilization of iodobenzene at 80℃, The size and distribution of aggregates were measured by the ALV / DLS / SLS-5022F laser light scattering system under the condition of He-Ne laser (λ=632.8 nm) 90°. A 0.22μm hydrophilic polyfluoroethylene (PVDF) film filter should be used to remove possible dust before the solution is determined. The autocorrelation function is analyzed by CONTIN software, and the corresponding data are obtained.

General procedure of Ullmann-type C-X coupling of aryl halides and nucleophiles in water

Added CuI (0.1 mmol, 19 mg), aryl halide (1.0 mmol), nucleophile (1.2 mmol) to a stirred solution of ALA14 (0.1 mol) and H_2O (10 ml). When the nucleophile is imidazole, Cs_2CO_3 (2 mmol, 651 mg) is needed. subsequently the mixture was heated to 100 °C under air and stirred for 12 h. When the reaction was finished, the mixture was cooled and partitioned by adding the ethyl acetate (20 ml) and water (20 ml). Then, the organic phase was separated and the aqueous phase was extracted with ethyl acetate (20 ml) twice. The combined organic phases were washed with saturated brine, dried over Na_2SO_4, and concentrated in vacuo. Then the crude product was purified by column chromatography through silica gel, eluting with ethyl acetate/petroleum ether solvent mixture, to give the pure product.

Experiment Details of Surfactant Recycling

Once the reaction was finished, ALA14 was precipitated after natural cooling. The reaction mixture was extracted with ethyl acetate to remove the product. After removal of the organic phase, the substrate and CuI were re-added to the obtained aqueous solution containing ALA14 for the next catalytic cycle.

The spectral data of the products

***N*-dodecyl Glucosamine AGA12.** white solid. m.p. 105.9 °C -106.5 °C. ^{1}H NMR (400 MHz, MeOD) δ 3.91 – 3.80 (m, 2H), 3.67 (dd, J = 11.6, 5.6 Hz, 1H), 3.38 (d, J = 8.4 Hz, 1H), 3.29 (dd, J = 8.8, 5.6 Hz, 1H), 3.27 – 3.21 (m, 1H), 3.08 (t, J = 8.8 Hz, 1H), 2.97 – 2.88 (m, 1H), 2.69 – 2.61 (m, 1H), 1.52 (m, 2H), 1.33 (d, J = 10.4 Hz, 18H), 0.92 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 91.29, 78.03 (d, J = 15.3 Hz), 74.01, 71.07, 61.91, 46.03, 31.76, 30.48, 29.51 (d, J = 5.5 Hz), 29.18, 27.32, 22.56, 14.42. HRMS (ESI) calcd for $C_{18}H_{38}NO_5$ $[M+H]^+$ 348.2750, found 348.2747.

***N*-tetradecyl Glucosamine AGA14.**[1] light yellow solid. m.p. 108.0 °C -108.3 °C. ^{1}H NMR (400 MHz, MeOD) δ 3.88 – 3.82 (m, 2H), 3.67 (dd, *J* = 8.0, 3.6 Hz, 1H), 3.39 – 3.34 (m, 1H), 3.31 – 3.27 (m, 1H), 3.24 (m, 1H), 3.08 (t, *J* = 6.0 Hz, 1H), 2.93 (m, 1H), 2.65 (m, 1H), 1.57 – 1.48 (m, 2H), 1.37 – 1.28 (m, 22H), 0.92 (t, *J* = 4.6 Hz, 3H). ^{13}C NMR (100 MHz, MeOD) δ 90.45, 77.57, 73.57, 70.47, 61.56, 45.83, 31.67, 29.66, 29.36 (d, *J* = 3.5 Hz), 29.07, 27.01, 22.33, 13.02. HRMS (ESI) calcd for $C_{20}H_{42}NO_5$ $[M+H]^+$ 376.3063, found 376.3049.

***N*-hexadecyl Glucosamine AGA16.** brown solid. m.p. 110.2 °C -110.4 °C. ^{1}H NMR (400 MHz, DMSO) δ 4.90 – 4.66 (m, 2H), 4.45 (d, *J* = 3.6 Hz, 1H), 4.39 – 4.26 (m, 1H), 3.70 – 2.97 (m, 7H), 2.86 (td, *J* = 8.4, 2.8 Hz, 1H), 2.78 (dt, *J* = 11.6, 6.8 Hz, 1H), 1.37(m, 2H), 1.24 (s, 26H), 0.86 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 91.29, 78.02 (d, *J* = 14.8 Hz), 74.01, 71.06, 61.90, 46.04, 31.77, 30.49, 29.50 (d, *J* = 4.3 Hz), 29.18, 27.34, 22.56, 14.40. HRMS (ESI) calcd for $C_{22}H_{46}NO_5$ $[M+H]^+$ 404.3376, found 404.3370.

***N*-dodecyl lactosamine ALA12.** white solid. m.p. 131.6 °C - 131.8 °C. ^{1}H NMR (400 MHz, MeOD) δ 4.38 (d, J = 3.2 Hz, 1H), 3.89 – 3.77 (m, 5H), 3.72 (dd, J = 7.6, 3.2 Hz, 1H), 3.62 – 3.48 (m, 5H), 3.40 – 3.35 (m, 1H), 3.15 (t, J = 6.0 Hz, 1H), 2.91 (m, 1H), 2.65 (m, 1H), 1.58 – 1.46 (m,

2H), 1.33 (d, J = 12.8 Hz, 18H), 0.92 (t, J = 4.8 Hz, 3H). ^{13}C NMR (100 MHz, MeOD) δ 103.72, 90.37, 79.57, 76.10, 75.87, 75.69, 73.45, 73.25, 71.19, 68.91, 61.10, 60.75, 31.67, 29.65, 29.31 (d, *J* = 7.0 Hz), 29.07, 27.00, 22.33, 13.02. HRMS (ESI) calcd for $C_{24}H_{48}NO_{10}$ $[M+H]^+$ 510.3278, found 510.3281.

***N*-tetradecyl lactosamine ALA14.** light yellow solid. m.p. 109.5 °C – 110.4 °C. ^{1}H NMR (400 MHz, DMSO) δ 5.12 (s, 1H), 4.80 (s, 1H), 4.64 (s, 2H), 4.49 (d, *J* = 29.6 Hz, 2H), 4.19 (dd, *J* = 12.4, 7.6 Hz, 1H), 3.76 – 3.15 (m, 14H), 2.93 (t, *J* = 8.4 Hz, 1H), 2.77 (dt, *J* = 11.2, 7.2 Hz, 1H), 1.37 (d, *J* = 6.4 Hz, 2H), 1.24 (s, 22H), 0.86 (t, *J* = 6.4 Hz, 3H).^{13}C NMR (100 MHz, MeOD) δ 103.72, 90.38, 79.58, 76.10, 75.87, 75.69, 73.45, 73.25, 71.19, 68.91, 61.10, 60.75, 40.92, 31.67, 29.21 (d, *J* = 11.0 Hz), 29.07, 27.01, 26.57, 22.33, 13.02. HRMS (ESI) calcd for $C_{26}H_{52}NO_{10}$ $[M+H]^+$ 538.3591, found 538.3589.

***N*-hexadecyl lactosamine ALA16.** buff solid. m.p. 125.6 °C – 126.5 °C. ^{1}H NMR (400 MHz, DMSO) δ 5.12 (s, 1H), 4.80 (s, 1H), 4.64 (s, 2H), 4.49 (d, J = 25.6 Hz, 2H), 4.19 (dd, J = 12.4, 7.6 Hz, 1H), 3.76 – 3.15 (m, 14H), 2.93 (t, J = 8.4 Hz, 1H), 2.77 (dt, J = 11.2, 7.2 Hz, 1H), 1.37 (m, 2H), 1.24 (s, 22H), 0.86 (t, J = 6.4 Hz, 3H).^{13}C NMR (100 MHz, MeOD) δ 103.71, 90.37, 79.56, 76.10, 75.86, 75.68, 73.44, 73.24, 71.18, 68.91, 61.09, 60.74, 40.66, 31.67, 29.37, 29.06, 27.00, 26.48, 22.33, 13.02. HRMS (ESI) calcd for $C_{28}H_{56}NO_{10}$ $[M+H]^+$ 566.3904, found 566.3912.

Diphenyl sulphone 3a.[2, 3] White solid, m.p.: 123-124 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.6 Hz, 4H), 7.58 (t, J = 7.4 Hz, 2H), 7.52 (t, J = 7.6 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 133.2, 129.3, 127.7.

4-Methoxyphenyl phenyl sulfone 3b.[2, 3] White solid, m.p.: 91-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, J = 14.3, 7.6 Hz, 4H), 7.44 (dd, J = 14.8, 7.0 Hz, 3H), 6.89 (d, J = 7.7 Hz, 2H), 3.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 141.4, 132.1, 131.8, 128.9, 128.2, 126.3, 113.5, 54.6.

Phenyltolyl sulfone 3c.[2, 3] White solid, m.p.: 125-126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 7.3 Hz, 2H), 7.76 (d, J = 8.2 Hz, 2H), 7.47 (d, J = 7.1 Hz, 1H), 7.43 (d, J = 7.6 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 140.9, 137.6, 131.9, 128.9, 128.2, 126.7, 126.5, 20.6.

4-Chlorophenyl phenyl sulfone 3d.[2, 3] White solid, m.p.: 93-95 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 7.5 Hz, 2H), 7.89 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 7.2 Hz, 1H), 7.55 – 7.44 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 140.1, 139.9, 133.5, 129.6, 129.4, 129.1, 127.6.

4-Acetylphenyl phenyl sulfone 3e.[3] White solid, m.p.: 130-131 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.03 (m, 4H), 8.01 – 7.94 (m, 2H), 7.62 (dd, J = 8.3, 6.5 Hz, 1H), 7.55 (t, J = 7.6 Hz, 2H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 145.4, 140.8, 140.4, 133.7, 129.5, 129.1, 127.9, 127.8, 26.9.

4-Nitrophenyl phenyl sulfone 3f.[2, 3] Yellow solid, m.p.: 141-143 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 8.8 Hz, 2H), 8.14 (d, J = 8.8 Hz, 2H), 7.98 (d, J = 7.7 Hz, 2H), 7.65 (t, J = 7.4 Hz, 1H), 7.57 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 147.4, 140.0, 134.2, 129.7, 128.9, 128.0, 124.5.

1-methoxy-2-(phenylsulfonyl)benzene 3g.[2, 3] White solid, m.p.: 74-76 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (dd, J = 7.9, 1.1 Hz, 1H), 7.93 – 7.86 (m, 2H), 7.59 (ddd, J = 6.7, 3.9, 1.2 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.42 (t, J = 7.4 Hz, 1H), 7.26 (d, J = 7.5 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 138.9, 138.0, 133.6, 132.9, 132.7, 129.5, 129.0, 127.7, 126.5, 20.2.

3-Nitro-(phenylsulfonyl)benzene 3h.[3] Yellow solid, m.p.: 78-80 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.35 (d, J = 8.2 Hz, 1H), 8.22 (d, J = 7.7 Hz, 1H), 7.93 (d, J = 7.5 Hz, 2H), 7.67 (t, J = 8.0 Hz, 1H), 7.58 (t, J = 7.4 Hz, 1H), 7.49 (dd, J = 15.3, 8.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 142.9, 139.1, 133.1, 132.1, 129.7, 128.7, 126.9, 126.7, 121.9.

1-(Phenylsulfonyl)-4-(trifluoromethyl)benzene 3i.[2, 3] White solid, m.p.: 91-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.2 Hz, 2H), 8.04 – 7.94 (m, 2H), 7.79 (d, J = 8.3 Hz, 2H), 7.69 – 7.60 (m, 1H), 7.56 (dd, J = 10.5, 4.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 140.6, 134.6 (J = 160 Hz), 129.6, 128.2, 127.9, 126.5 (J = 8.5 Hz), 124.5, 121.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.21.

1-Phenyl-1*H*-imidazole 5a.[4-8] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.49 (t, J = 7.7 Hz, 2H), 7.42 – 7.35 (m, 3H), 7.29 (s, 1H), 7.21 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.4, 135.6, 130.4, 129.8, 127.5, 121.5, 118.2. MS (EI): *m/z* = 144 $[M]^+$.

1-(4-Methoxyphenyl)-1*H*-imidazole 5b.[5, 7, 8] Pale yellow solid, m.p.: 60-61 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.30 (d, J = 8.9 Hz, 2H), 7.20 (d, J = 6.7 Hz, 2H), 6.99 (d, J = 8.9 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 135.8, 130.7, 129.9, 123.3, 118.8, 114.9, 55.6. MS (EI): m/z = 174 $[M]^+$.

1-(p-tolyl)-*1H*-imidazole 5c.[5, 6, 8] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.24 (d, J = 7.9 Hz, 5H), 7.17 (s, 1H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 135.6, 135.0,

130.4, 130.2, 121.4, 118.4, 20.9.

1-(4-Ethoxyphenyl)-*1H*-imidazole 5d.[6] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.30 – 7.20 (m, 2H), 7.16 (d, J = 9.1 Hz, 2H), 7.00 – 6.84 (m, 2H), 4.03 (qd, J = 6.9, 2.6 Hz, 2H), 1.41 (td, J = 7.0, 2.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.3, 135.9, 130.6, 130.0, 123.2, 118.8, 115.4, 63.9, 14.8.

1-(4-Chlorophenyl)-1*H*-imidazole 5e.[6, 7] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.52 – 7.42 (m, 2H), 7.35 (d, J = 8.7 Hz, 2H), 7.27 (s, 1H), 7.21 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 135.5, 133.2, 130.7, 130.0, 122.7, 118.2. MS (EI): *m/z* = 178 $[M]^+$.

1-(4-Fluorophenyl)-1*H*-imidazole 5f.[5, 7] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 15.0 Hz, 1H), 7.42 – 7.32 (m, 2H), 7.26 – 7.11 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 160.5, 134.8 (*J* = 194.4 Hz), 130.4, 123.5 (J = 8.5 Hz), 118.6, 116.8 (J = 23.0 Hz). MS (EI): m/z = 162 $[M]^+$.^{19}F NMR (376 MHz, $CDCl_3$) δ -58.08.

1-(4-(Trifluoromethoxy)phenyl)-1*H*-imidazole 5g.[7] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.44 (d, J = 8.9 Hz, 2H), 7.35 (d, J = 8.6 Hz, 2H), 7.27 (s, 1H), 7.22 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1 (J = 1 Hz), 135.7 (J = 27 Hz), 130.8, 122.9, 122.6, 121.7, 119.1, 118.3. MS (EI): m/z = 228 [M]+. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.85.

1-(4-(1H-Imidazol-1-yl)phenyl)ethanone 5h.[6] White solid. m.p.: 112-114 ^{o}C. ^{1}H NMR (400 MHz, CDCl3) δ 8.11 (dd, J = 8.9, 2.2 Hz, 2H), 7.99 (s, 1H), 7.53 – 7.50 (m, 2H), 7.38 (s, 1H), 7.27 (s, 1H), 2.66 (s, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 196.5, 140.7, 135.9, 135.4, 131.1, 130.3, 120.8, 117.8, 26.6.

1-(4-Nitrophenyl)-1*H*-imidazole 5i.[5, 8, 9] Yellow solid. m.p.: 208-209 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 8.9 Hz, 2H), 8.01 (s, 1H), 7.60 (d, J = 8.9 Hz, 2H), 7.41 (s, 1H), 7.29 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 146.3, 142.0, 135.4, 131.8, 125.8, 121.1, 117.7. MS (EI): *m/z* = 189 $[M]^+$.

1-(2-methoxyphenyl)-*1H*-imidazole 5j.[8] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.35 – 7.28 (m, 1H), 7.24 (d, J = 7.7 Hz, 1H), 7.15 (d, J = 15.4 Hz, 2H), 7.01 (dd, J = 13.4, 7.7 Hz, 2H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 137.8, 128.9, 128.7, 126.5, 125.5, 121.0, 120.3, 112.4, 55.8.

1-(4-Methoxyphenyl)pyrrolidine 5l.[7, 10] Yellow solid. m.p.: 45-46 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (d, J = 8.9 Hz, 2H), 6.45 (d, J = 8.9 Hz, 2H), 3.67 (s, 3H), 3.14 (t, J = 6.4 Hz, 4H),

1.99 – 1.79 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 142.2, 114.0, 111.6, 54.9, 47.2, 24.4. MS (EI): *m/z* = 177 $[M]^+$.

***N*-butyl-4-methoxyaniline 5m**.[10] Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.81 – 6.76 (m, 2H), 6.61 – 6.57 (m, 2H), 3.75 (s, 3H), 3.08 – 3.05 (m, 2H), 1.60 (dt, J = 20.0, 7.3 Hz, 2H), 1.43 (dt, J = 14.9, 7.4 Hz, 2H), 0.96 (t, J = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.0, 142.8, 114.9, 114.1, 55.9, 44.8, 31.8, 20.3, 13.9.

N-(4-methoxyphenyl)-2-pyrrolidinone 5n.[11] White solid. m.p.: 111-112 ^{o}C. 1H NMR (400 MHz, CDCl3) δ 7.50 (d, J = 9.0 Hz, 2H), 6.91 (d, J = 9.0 Hz, 2H), 3.98 – 3.63 (m, 5H), 2.60 (t, J = 8.1 Hz, 2H), 2.24 – 2.09 (m, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 173.9, 156.6, 132.7, 121.8, 114.1, 55.5, 49.2, 32.5, 18.0. MS (EI): *m/z* = 191 $[M]^+$.

1-(4-methoxyphenyl)-4-methyl-1*H*-imidazole 5o.[8] White solid, m.p.: 79-80 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.19 (d, J = 8.4 Hz, 2H), 6.94 – 6.80 (m, 3H), 3.76 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 138.7, 135.5, 130.4, 123.0, 115.7, 114.9, 55.6, 13.7.MS (EI): *m/z* = 188 $[M]^+$.

1-(4-Methoxyphenyl)-1*H*-benz[d]imidazole 5p.[7, 8] Yellow solid, m.p.: 96-97 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.87 – 7.73 (m, 1H), 7.43 – 7.36 (m, 1H), 7.33 (d, J = 8.8 Hz, 2H), 7.24 (p, J = 7.2 Hz, 2H), 7.00 (d, J = 8.8 Hz, 2H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 143.8, 142.6, 134.3, 129.2, 125.8, 123.6, 122.6, 120.5, 115.1, 110.4, 55.7. MS (EI): *m/z* = 224 $[M]^+$.

1-(4-methoxyphenyl)-5-nitro-1*H*-indole 5q. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 2.4 Hz, 1H), 8.10 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.43 (m, 3H), 7.40 – 7.38 (m, 1H), 7.12 – 7.06 (m, 2H), 6.84 (dd, *J* = 3.6, 0.8 Hz, 1H), 3.92 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.14, 142.05, 139.18, 131.66, 131.47, 128.12, 126.26, 118.27, 117.80, 115.04, 110.39, 105.13, 55.67.

1-(4-methoxyphenyl)-1H-indole-5-carbonitrile 5r. [9] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 1.6, 0.8 Hz, 1H), 7.49 – 7.46 (m, 1H), 7.44 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.40 (m, 2H), 7.39 – 7.37 (m, 1H), 7.10 – 7.06 (m, 2H), 6.75 (dd, *J* = 3.2, 0.8 Hz, 1H), 3.91 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 159.01, 137.95, 131.54, 130.76, 128.59, 126.61, 126.26, 125.07, 120.68, 111.29, 103.61, 103.18, 55.66.

4-chloro-1-(4-methoxyphenyl)-1H-indole 5s.[12] ^{1}H NMR (400 MHz, CDCl3) δ 7.43 – 7.38 (m, 2H), 7.35 (m, 2H), 7.20 (dd, J = 7.6, 0.8 Hz, 1H), 7.15 (t, J = 7.8 Hz, 1H), 7.09 – 7.04 (m, 2H), 6.80 (d, J = 3.2 Hz, 1H), 3.91 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ158.62, 137.15, 132.39,

128.92, 127.67, 126.21, 126.16, 122.72, 119.81, 114.82, 109.09, 101.43, 55.63.

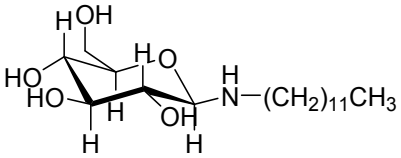
5-bromo-1-(4-methoxyphenyl)-1H-indole 5t.[12] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 1.2 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.34 – 7.27 (m, 3H), 7.10 – 7.02 (m, 2H), 6.62 (dd, *J* = 3.2, 0.4 Hz, 1H), 3.91 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 158.54, 135.09, 132.31, 130.64, 129.49, 125.99, 124.99, 123.47, 114.86, 111.91, 102.39, 55.65.

1-(4-methoxyphenyl)-1H-indole 5u.[9, 13] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.70 (m, 1H), 7.51 – 7.48 (m, 1H), 7.47 – 7.42 (m, 2H), 7.32 (d, *J* = 3.2 Hz, 1H), 7.22 (m, 2H), 7.09 – 7.04 (m, 2H), 6.69 (dd, *J* = 3.2, 0.8 Hz, 1H), 3.91 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.30, 136.39, 132.90, 128.99, 128.28, 126.01, 122.16, 121.02, 120.09, 114.76, 110.37, 102.91, 55.58.

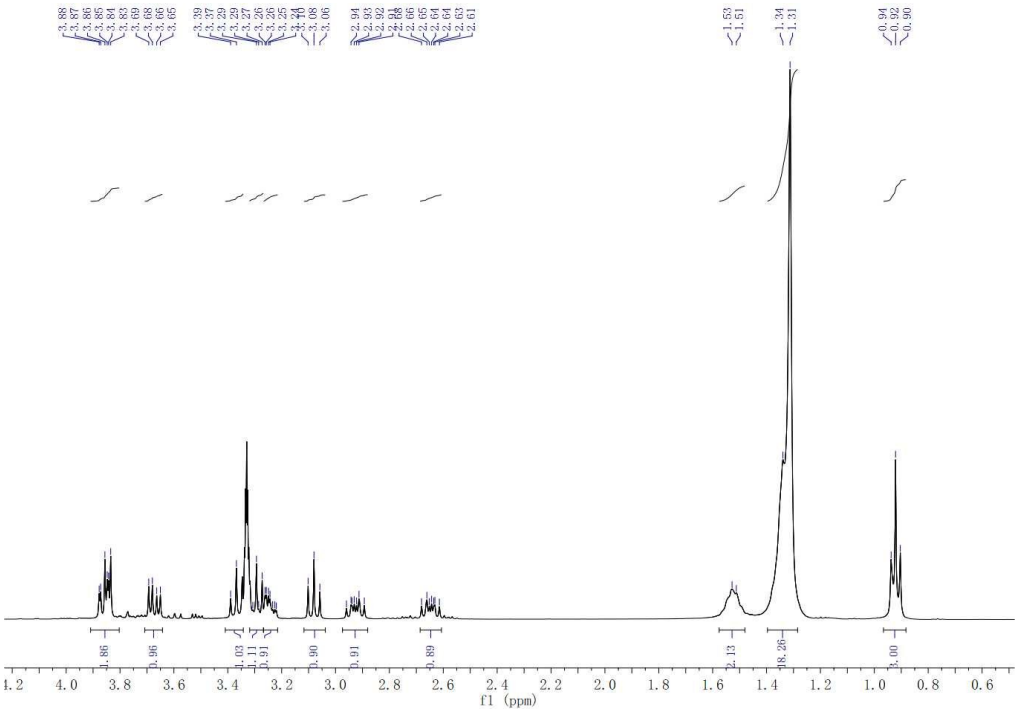
1-(4-methoxyphenyl)-3-methyl-1H-indole 5v.[9] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.63 (m, 1H), 7.50 – 7.45 (m, 1H), 7.44 – 7.38 (m, 2H), 7.26 – 7.16 (m, 2H), 7.10 (d, *J* = 0.8 Hz, 1H), 7.07 – 7.02 (m, 2H), 3.90 (s, 3H), 2.42 (d, *J* = 0.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.90, 136.42, 133.08, 129.35, 125.88, 125.67, 122.14, 119.46, 119.09, 114.70, 112.12, 110.22, 55.60, 9.59.

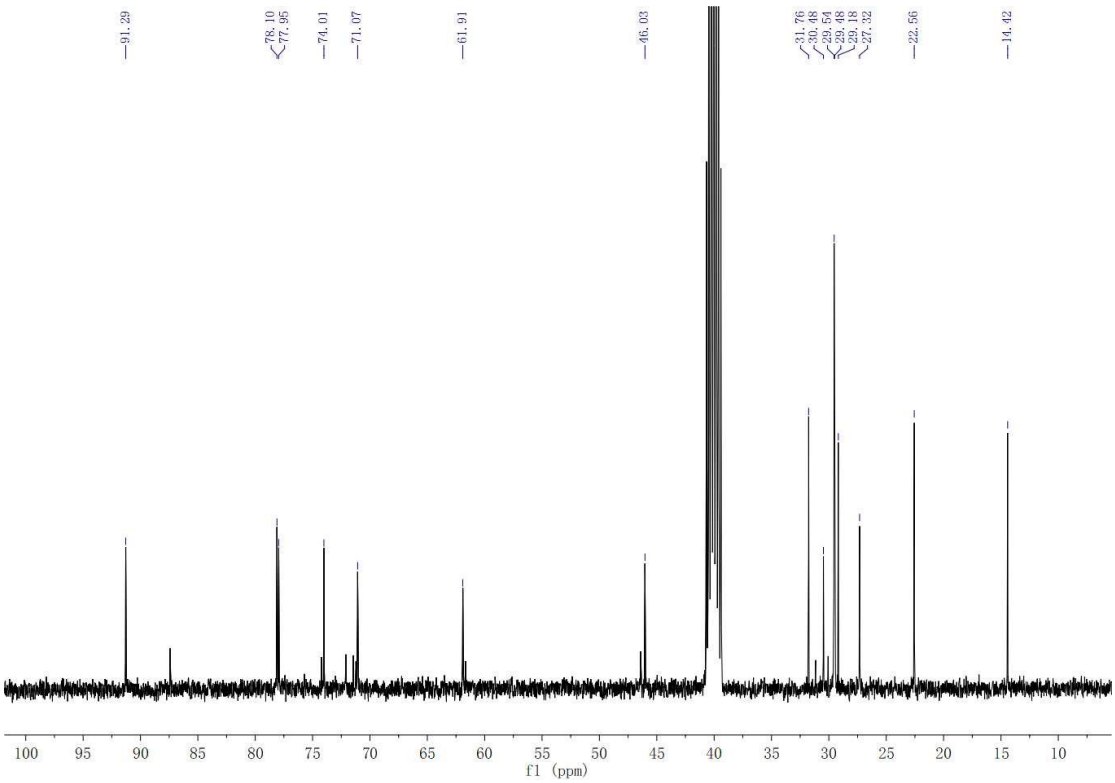
1-(4-methoxyphenyl)-4-methyl-1H-indole 5w. [7, 10] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.41 (m, 2H), 7.34 – 7.30 (m, 2H), 7.152 (t, *J* = 7.2 Hz, 1H), 7.08 – 7.04 (m, 2H), 7.00 (d, *J* = 6.8 Hz, 1H), 6.71 (dd, *J* = 3.2, 0.8 Hz, 1H), 3.91 (s, 3H), 2.64 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.23, 136.07, 133.04, 130.49, 127.70, 126.01, 122.31, 120.26, 114.71, 108.03, 101.35, 55.61, 18.77.

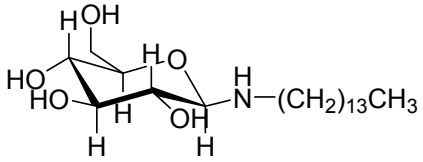
NMR spectra of products



AGA12



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H
OH
H
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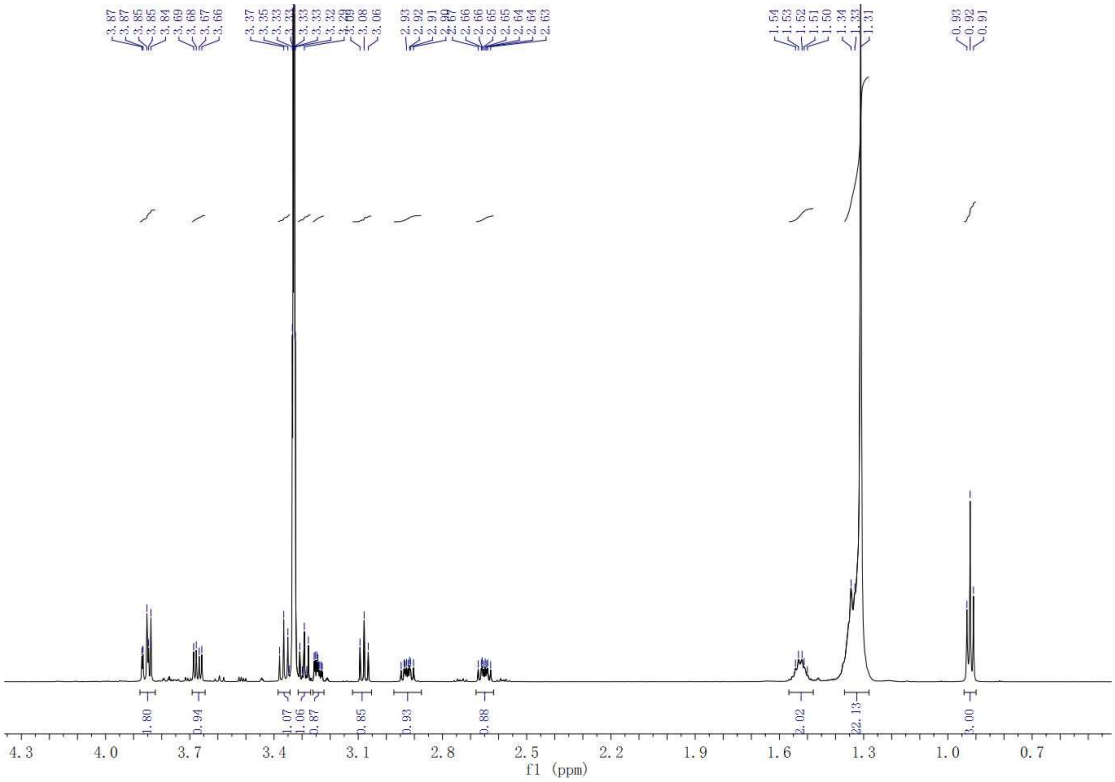
AGA14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2.92
2.91
2.66
2.65
2.64
2.63
1.54
1.53
1.52
1.51
1.50
1.34
1.31
0.93
0.92
0.91
1.80
0.94
1.07
1.06
2.87
0.85
0.93
0.88
2.02
22.13
3.00
4.3
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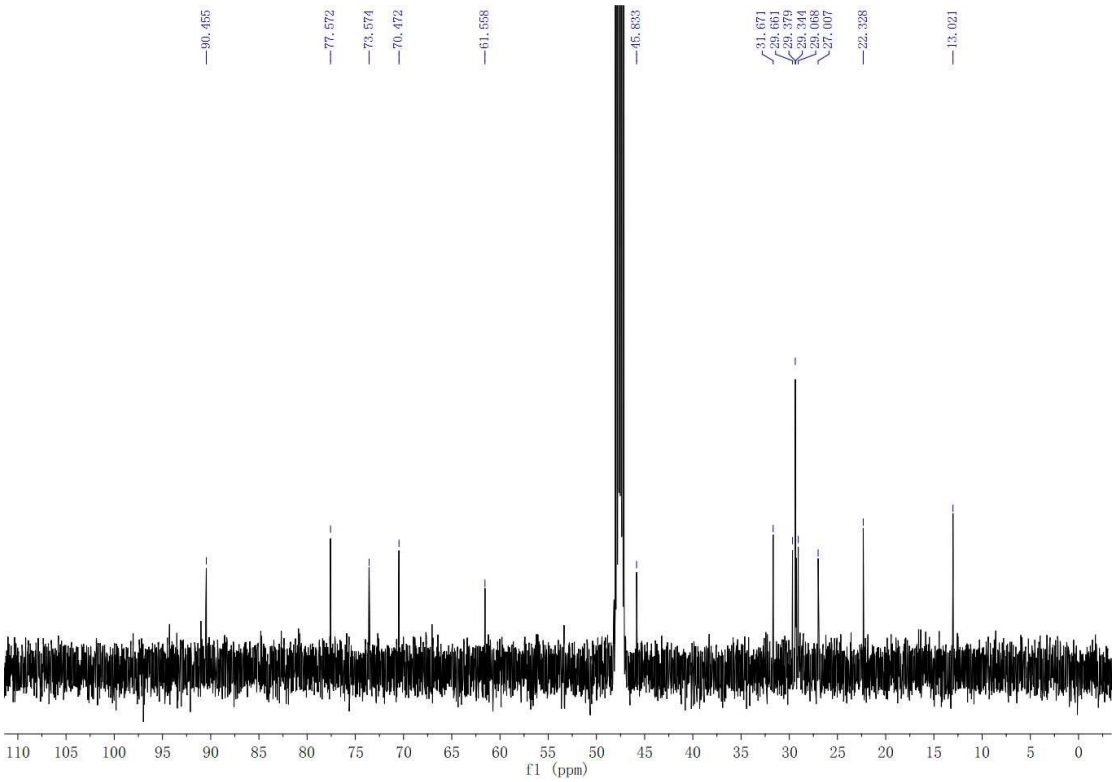
f1 (ppm)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29.344
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13.021
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105
100
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90
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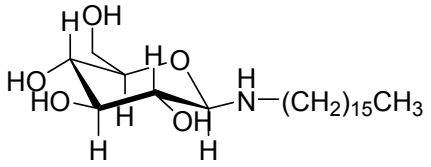
f1 (ppm)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OH
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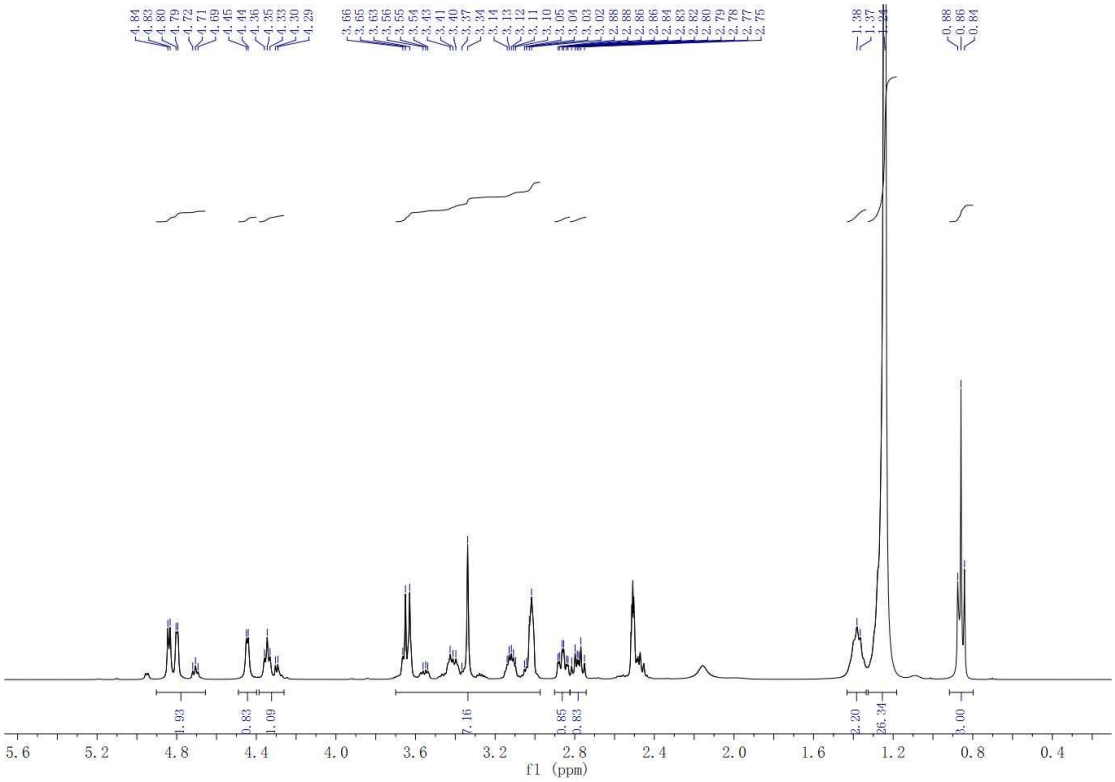
N—(CH2)15CH3

AGA16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3.63
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3.54
3.43
3.41
3.40
3.37
3.34
3.14
3.13
3.12
3.11
3.10
3.05
3.04
3.03
3.02
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2.86
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2.79
2.78
2.77
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1.37
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5.2
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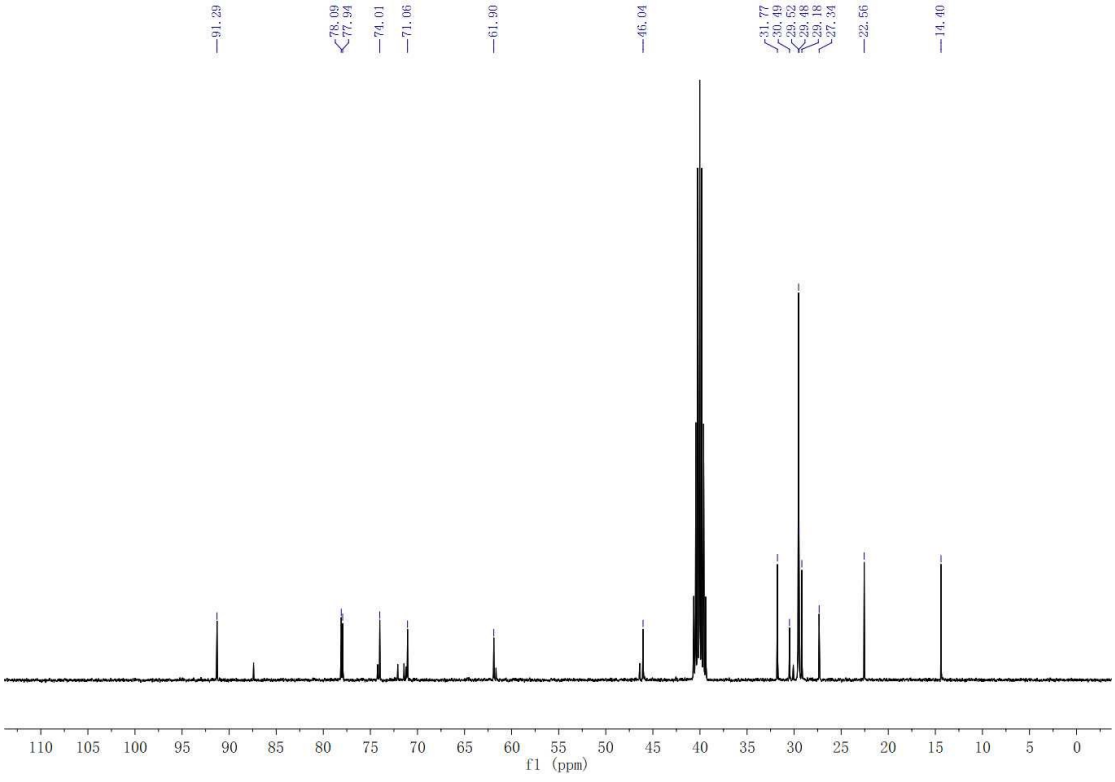
f1 (ppm)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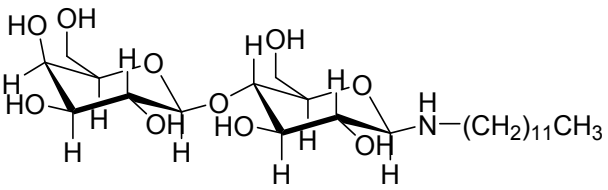
f1 (ppm)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OH
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H
OH
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H
O
H
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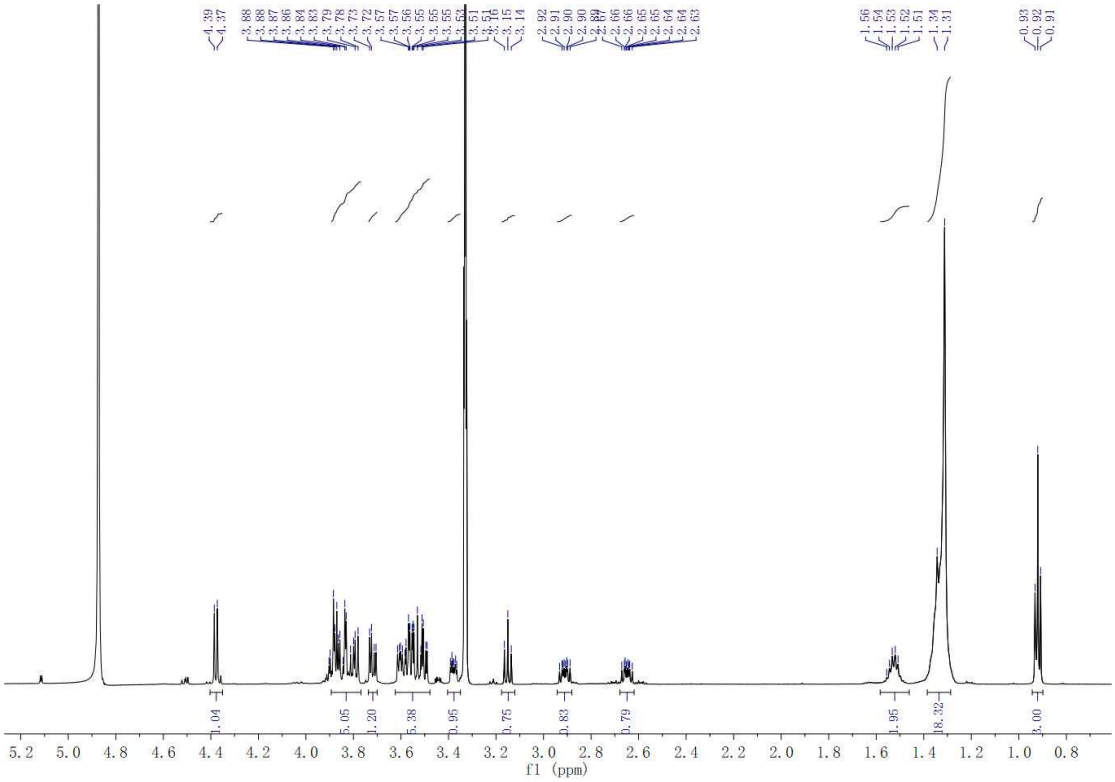
H
H

ALA12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3.55
3.53
3.51
3.16
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2.91
2.90
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2.65
2.64
2.63
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1.51
1.34
1.31
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0.92
0.91
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5.05
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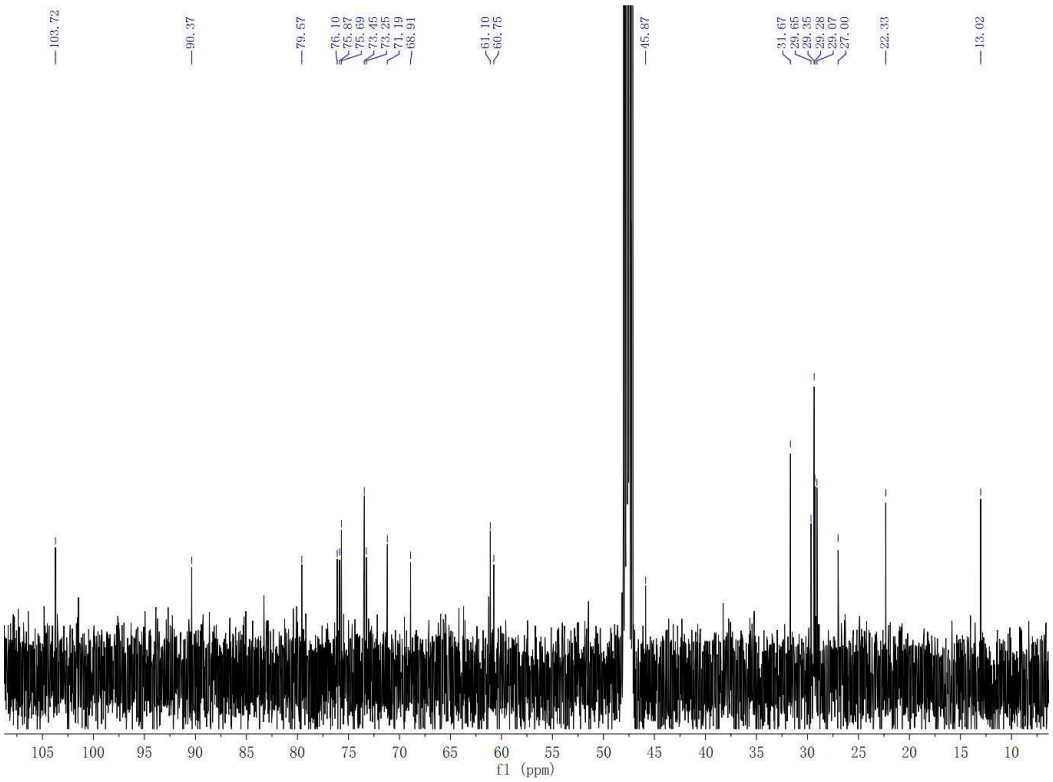
f1 (ppm)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73.25
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29.28
29.07
27.00
22.33
13.02
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100
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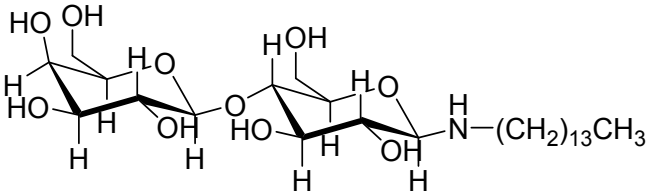
f1 (ppm)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HO
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OH
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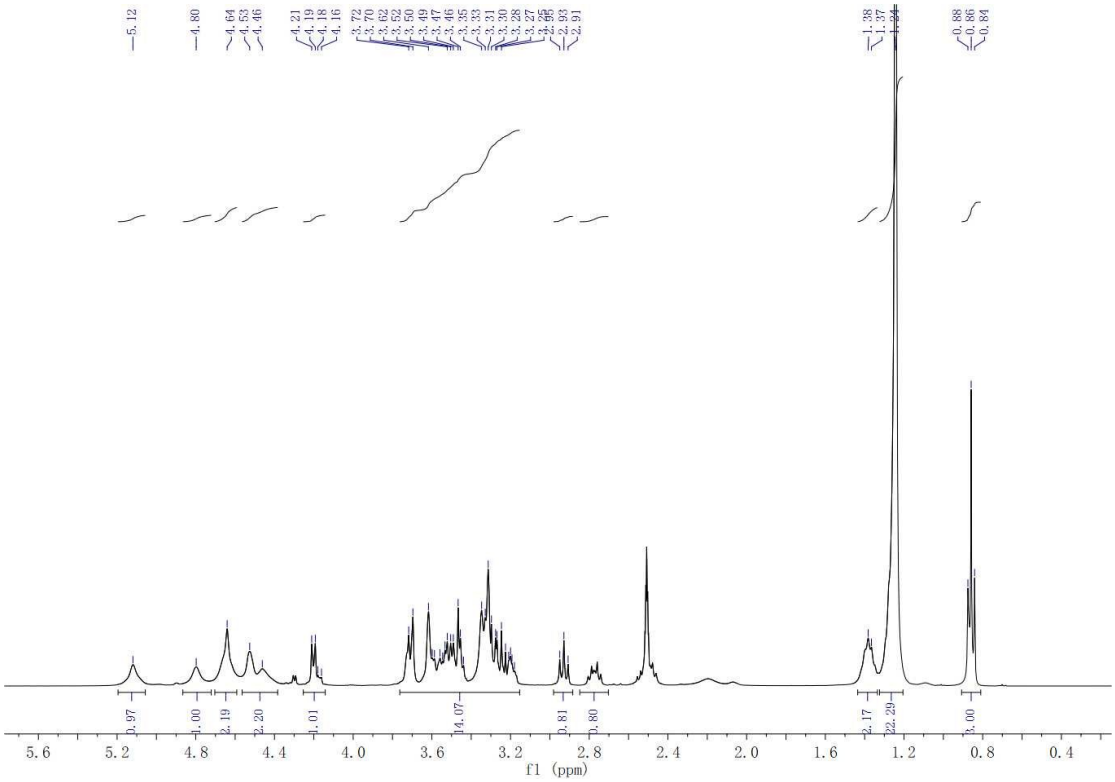
O
H
N—(CH2)13CH3

ALA14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1.37
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0.84
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1.01
14.07
1.81
0.80
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2.0
1.6
1.2
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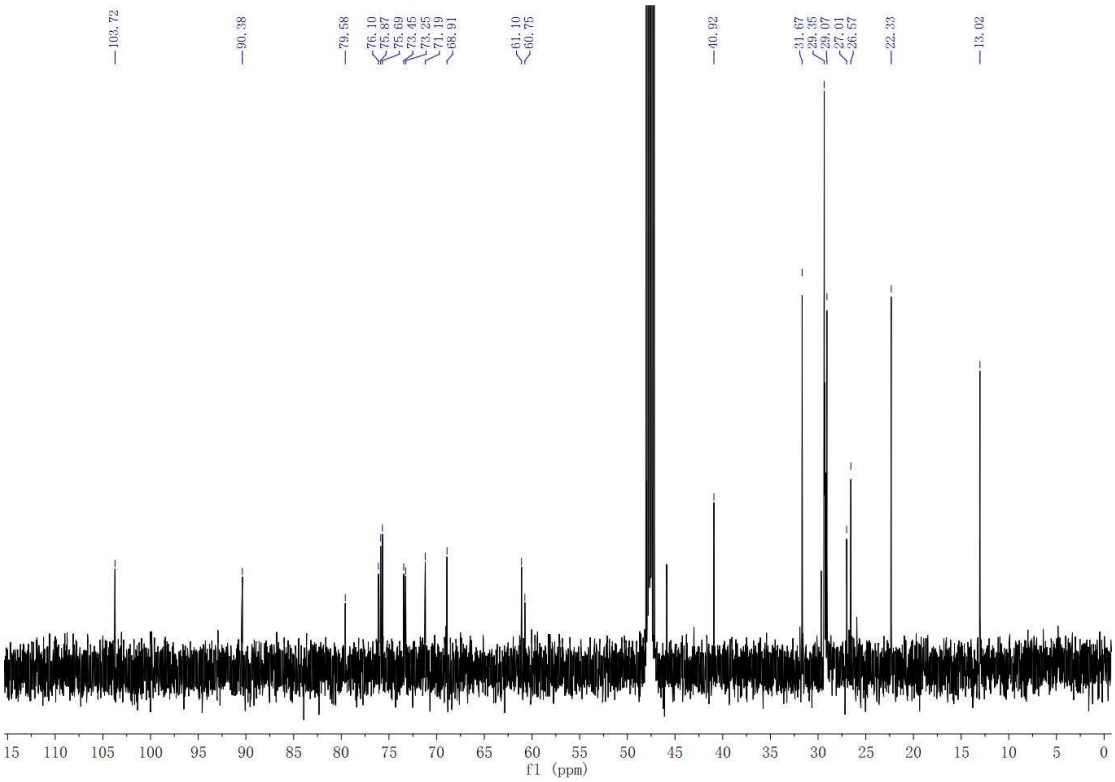
0.4
f1 (ppm)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13.02
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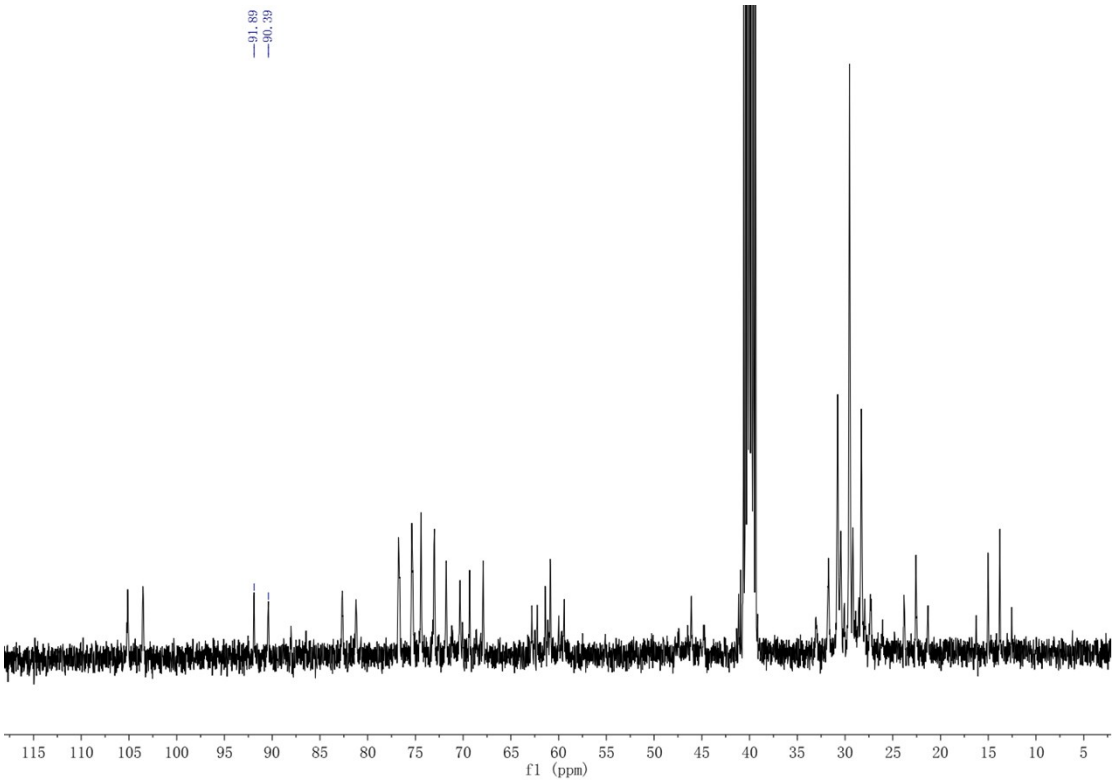
f1 (ppm)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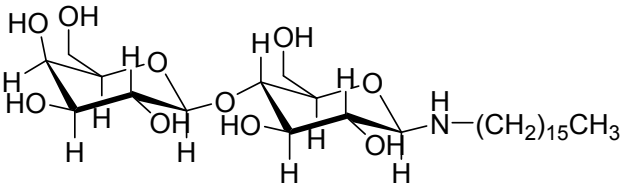
f1 (ppm)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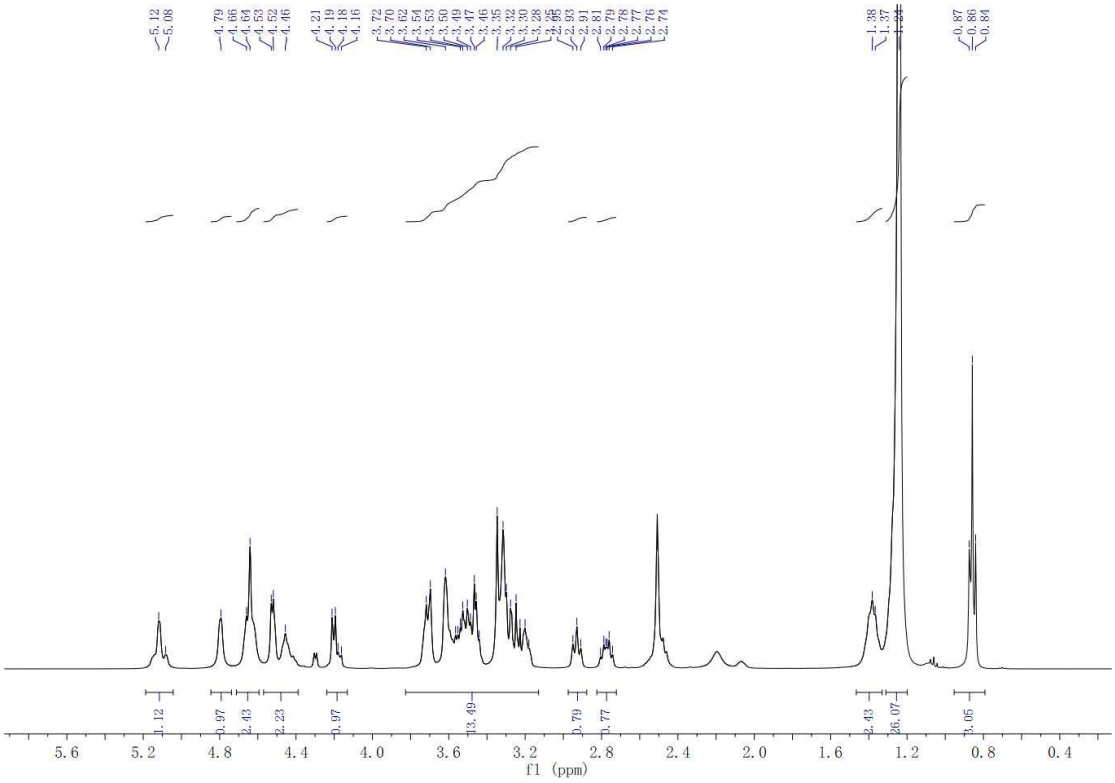
(CH2)15CH3

ALA16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3.62
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3.53
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3.35
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2.91
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0.97
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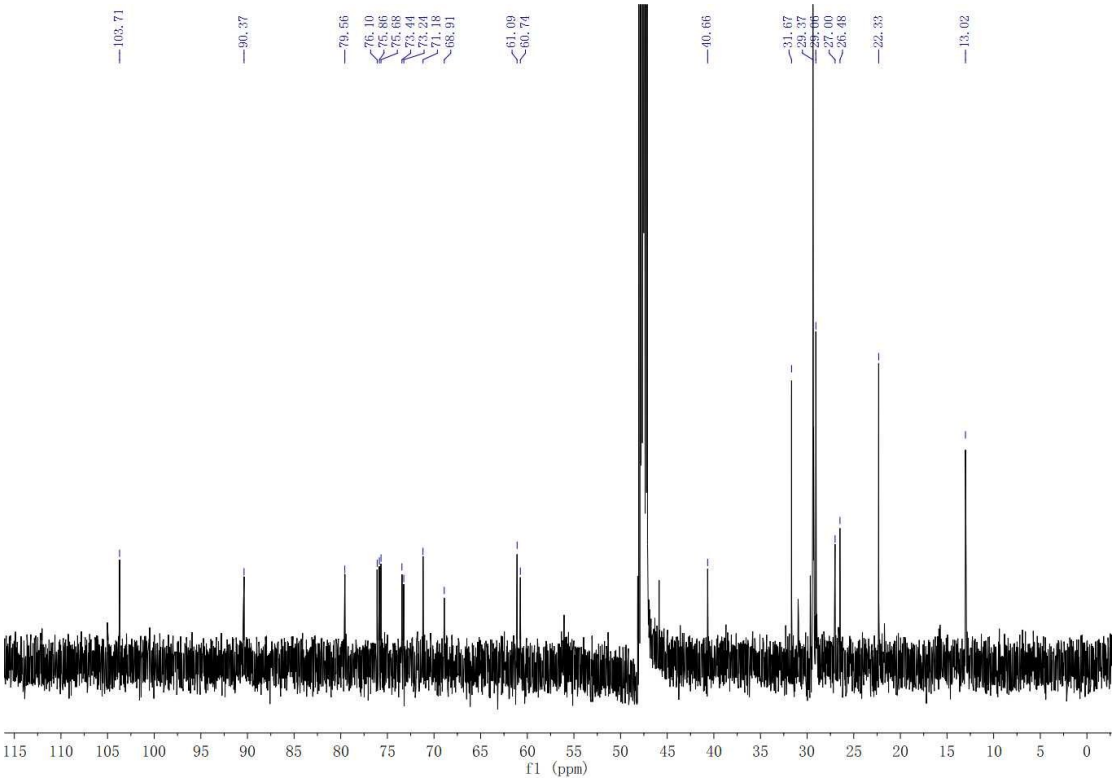
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13.02
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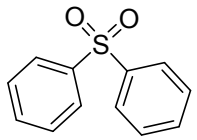

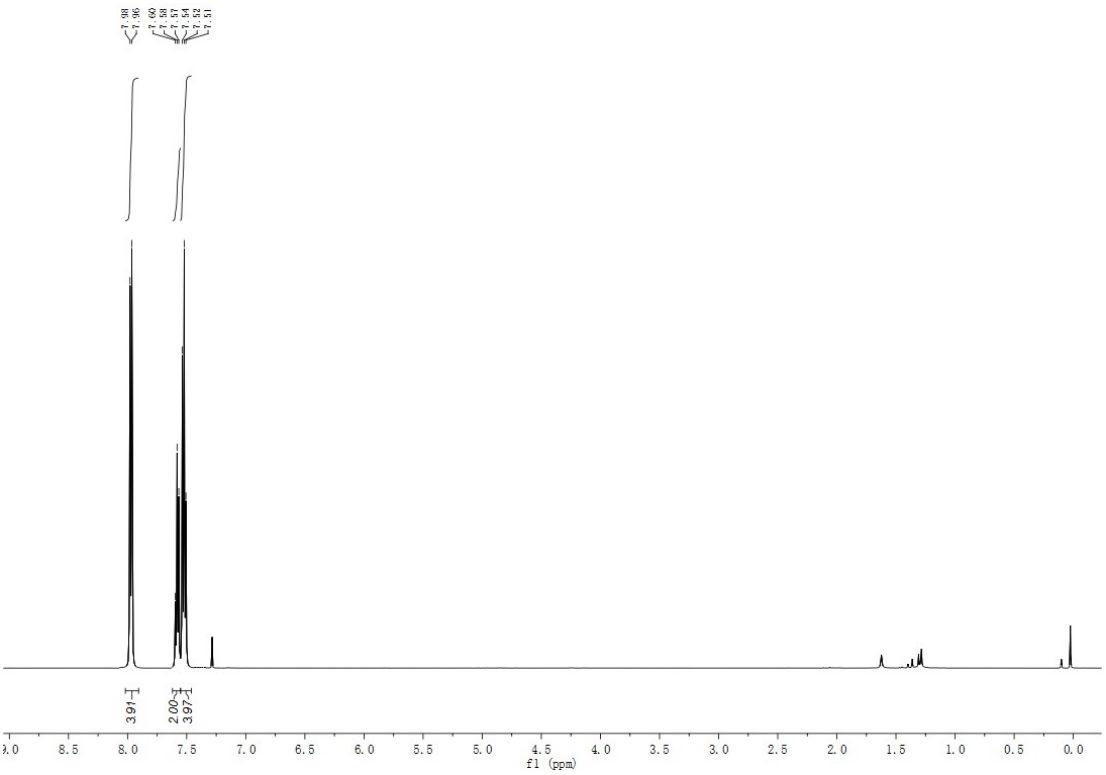
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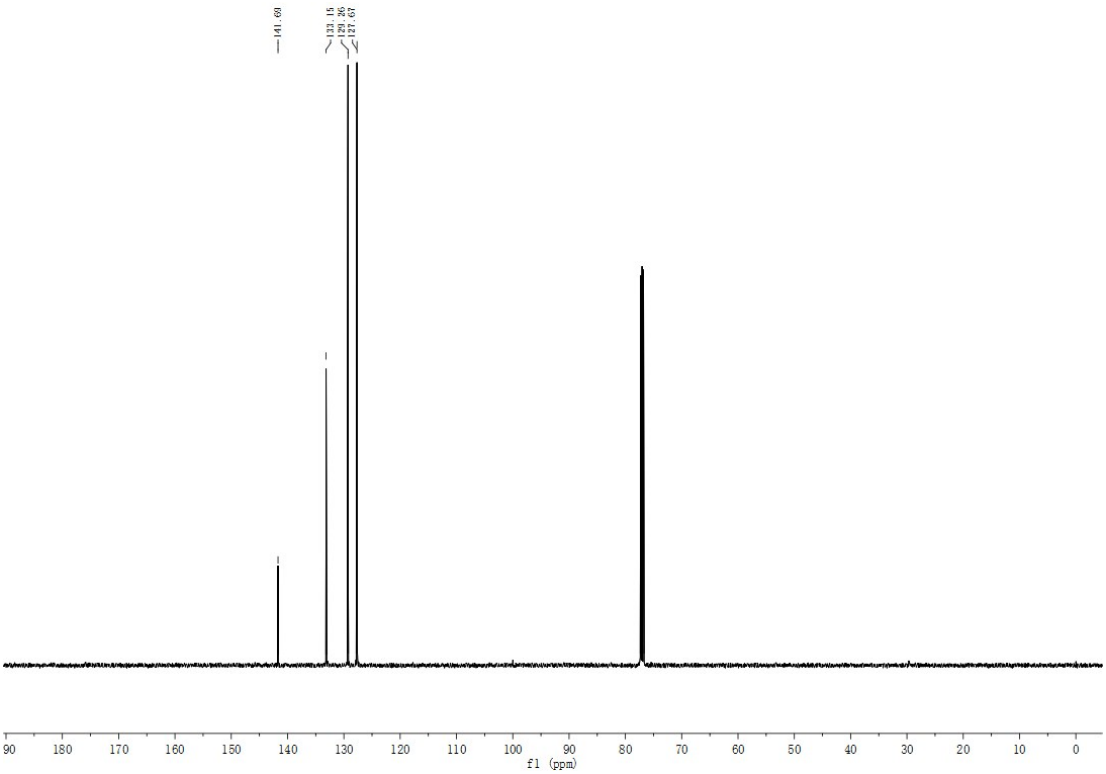
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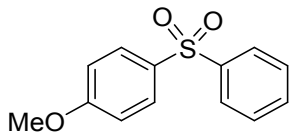
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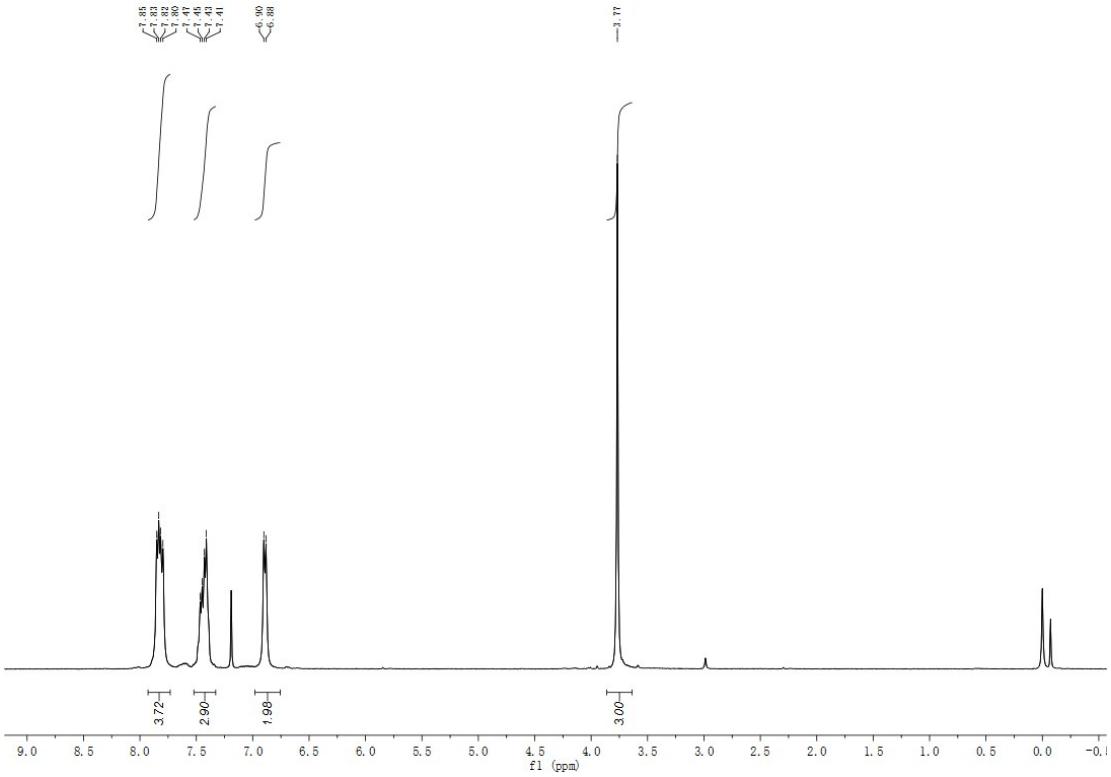
O
S
MeO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1.98
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8.5
8.0
7.5
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4.0
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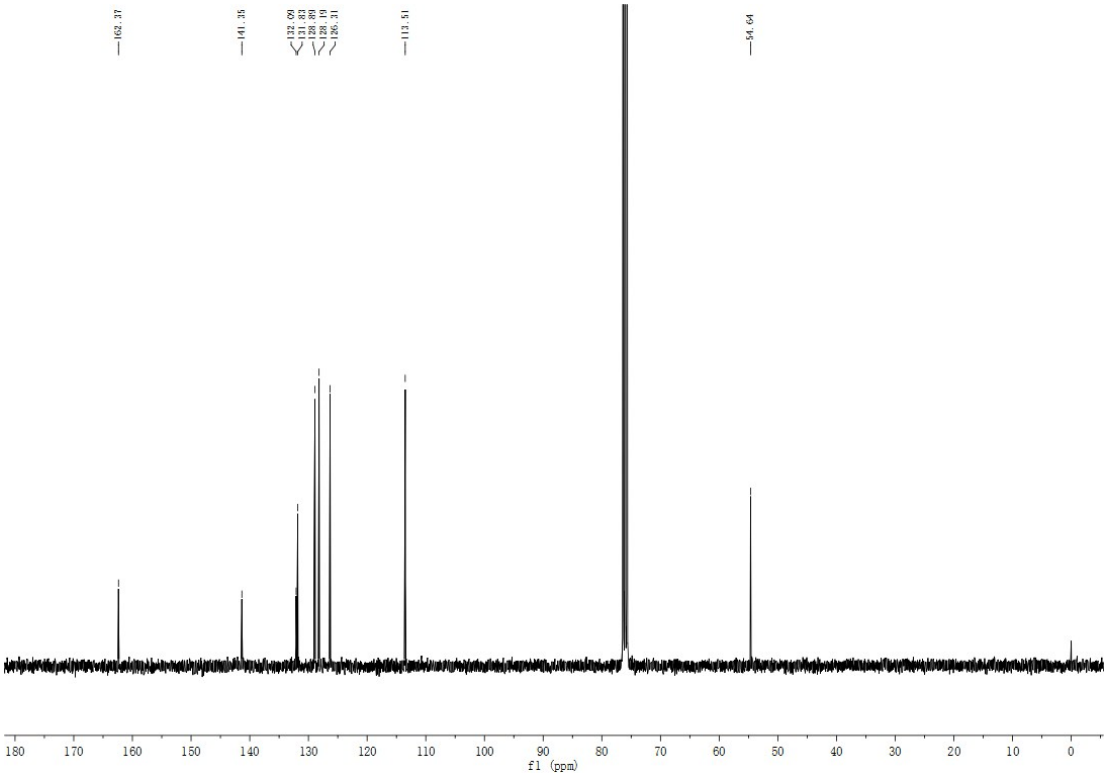
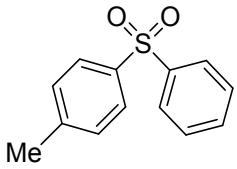
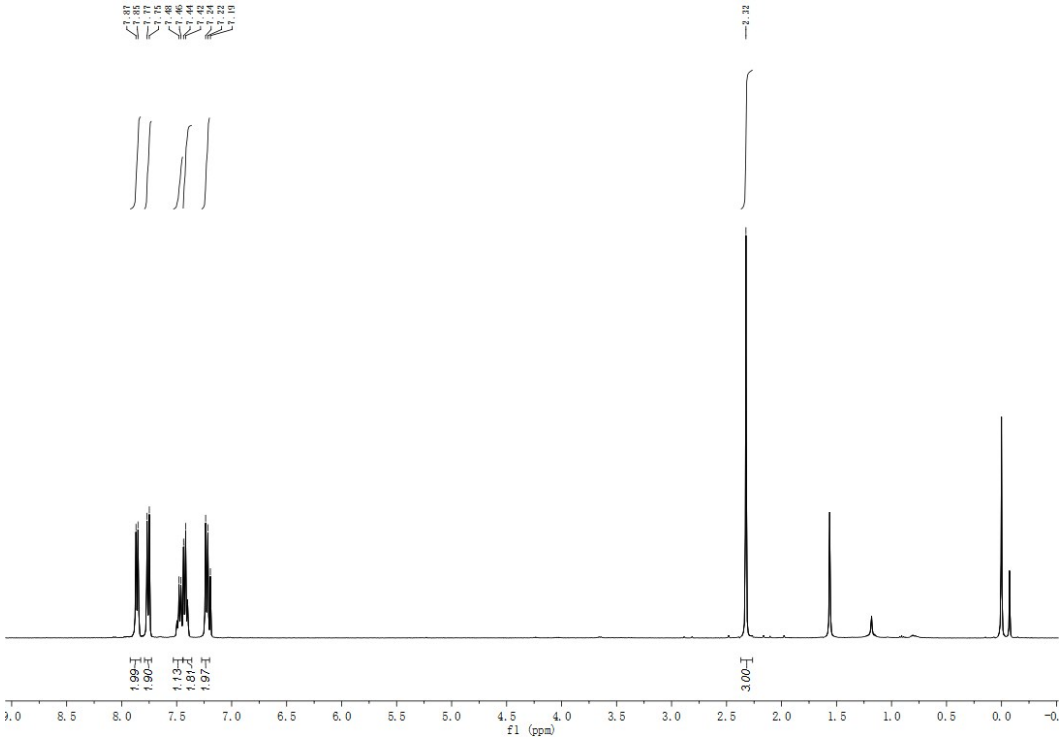
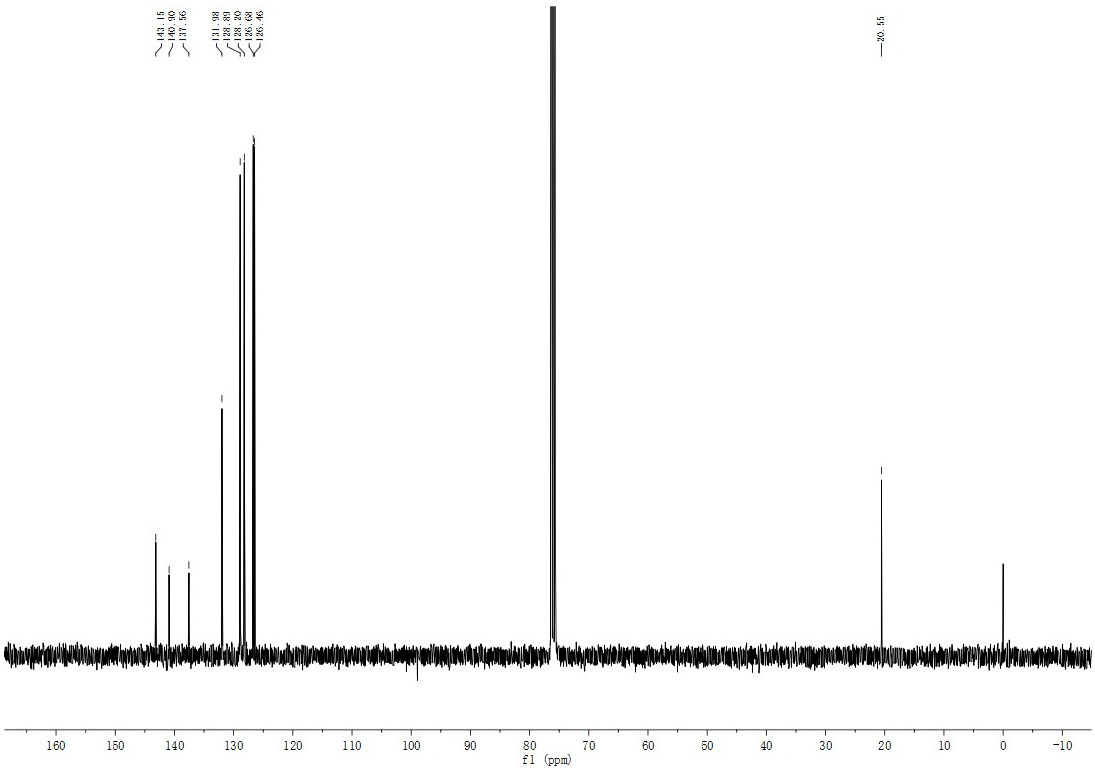
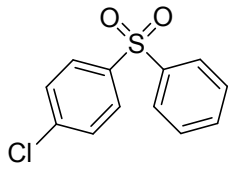
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


162.37
141.35
132.09
131.83
128.89
128.10
126.31
113.51
54.64
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

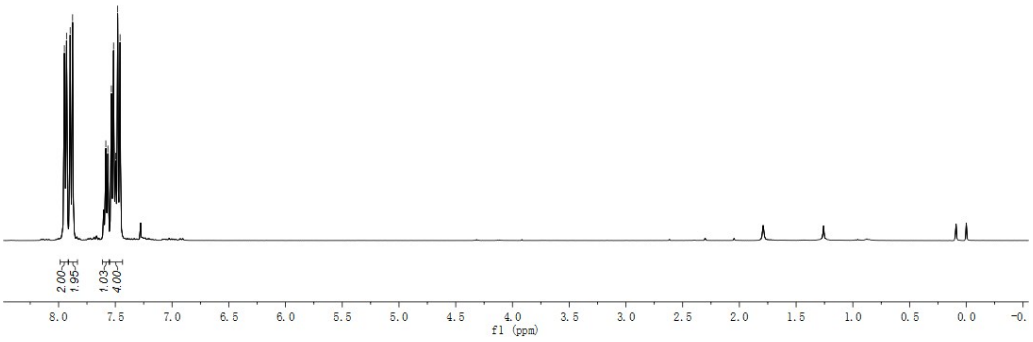

O
O
S
Me

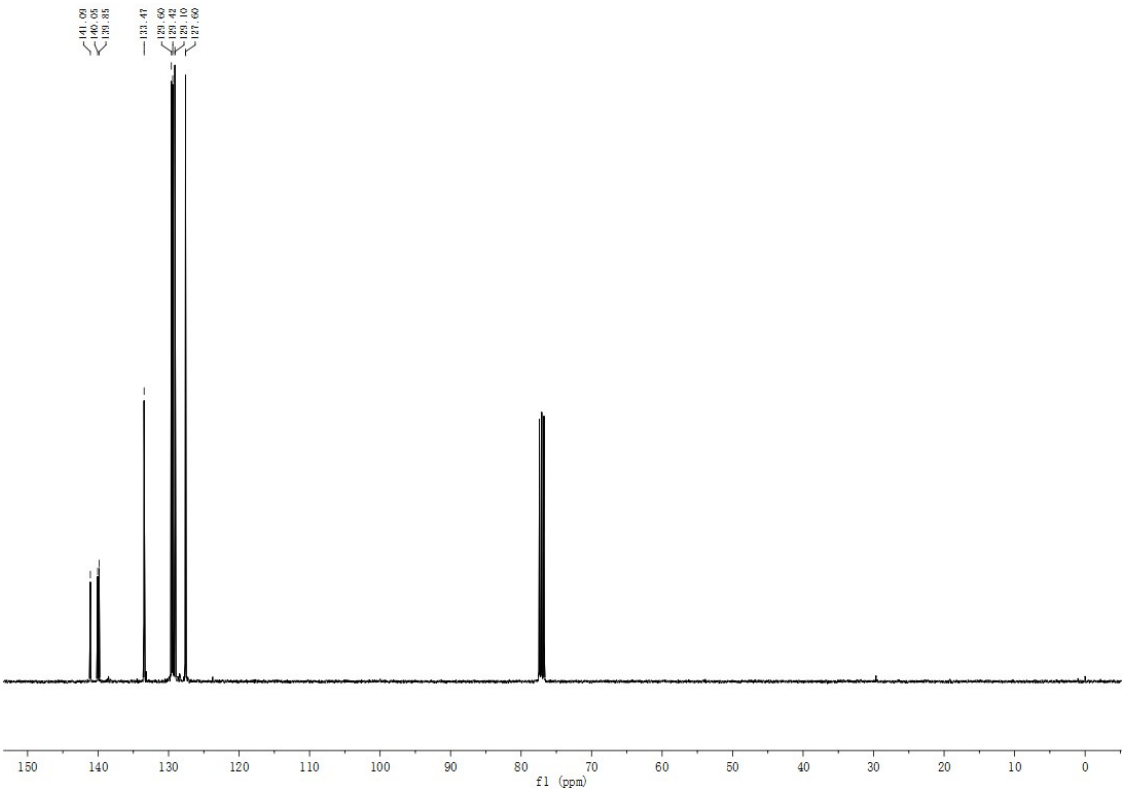

7.87
7.85
7.77
7.75
7.48
7.46
7.44
7.43
7.24
7.22
7.19
2.32
1.99
1.90
1.13
1.81
1.97
3.00
f1 (ppm)

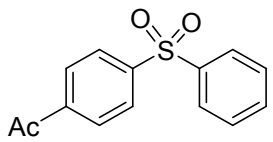

143.15
140.90
137.96
131.98
129.99
129.29
126.68
125.46
20.55
f1 (ppm)

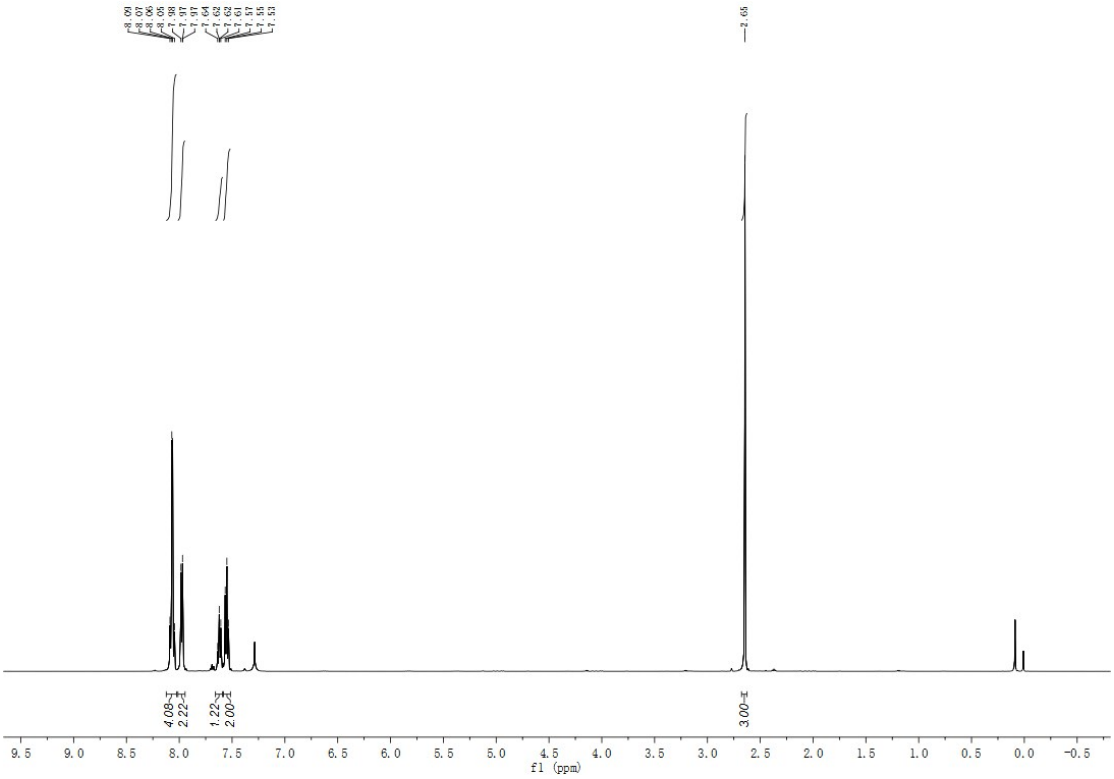

O
O
S
Cl

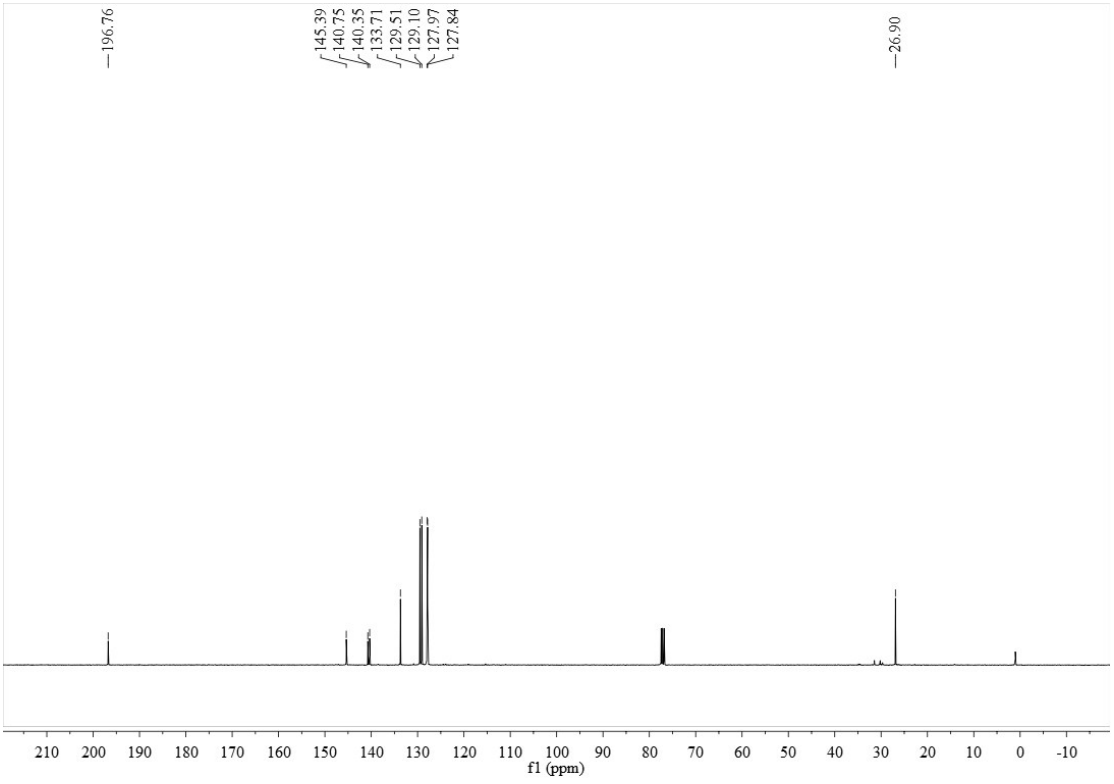

7.95
7.93
7.90
7.88
7.58
7.57
7.53
7.52
7.50
7.48
7.46

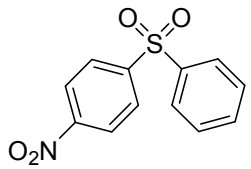

2.00
1.95
1.03
4.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

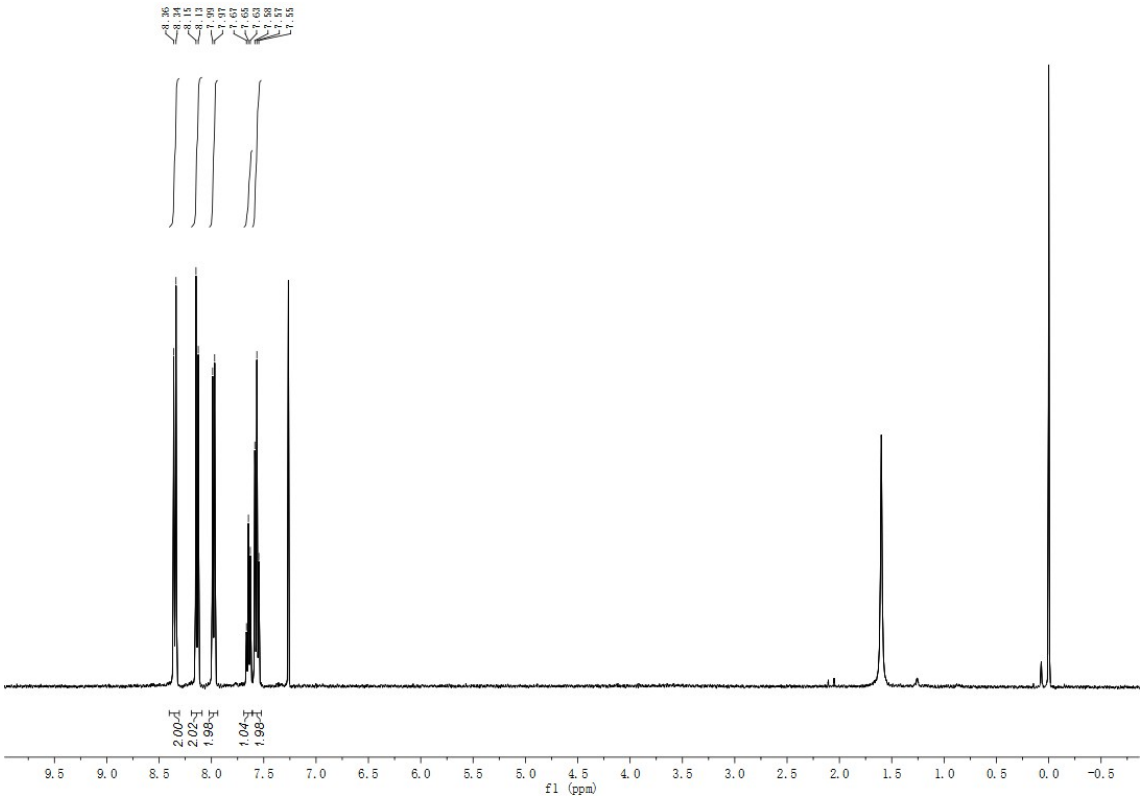

141.09
140.05
139.85
133.47
129.60
129.42
129.10
127.60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

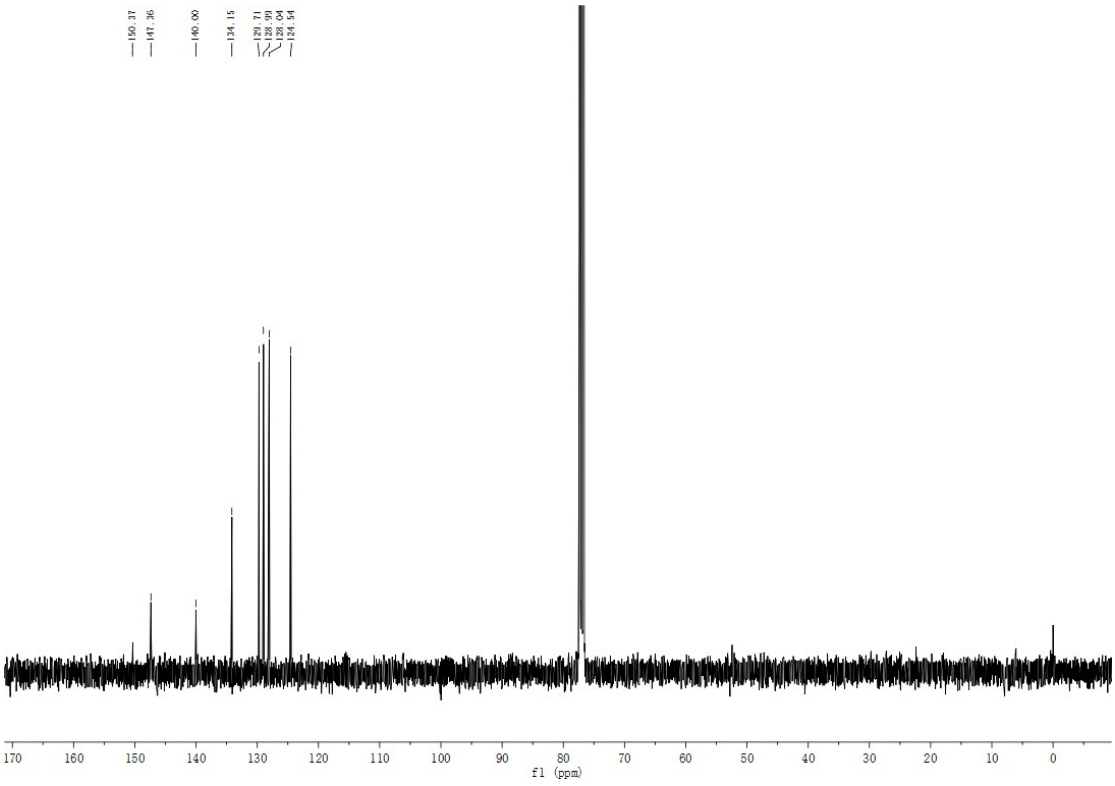

O
O
S
Ac

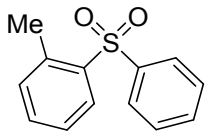

8.09
8.07
8.06
8.05
7.98
7.97
7.97
7.64
7.62
7.62
7.61
7.57
7.55
7.53
2.65
4.08
2.22
1.22
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

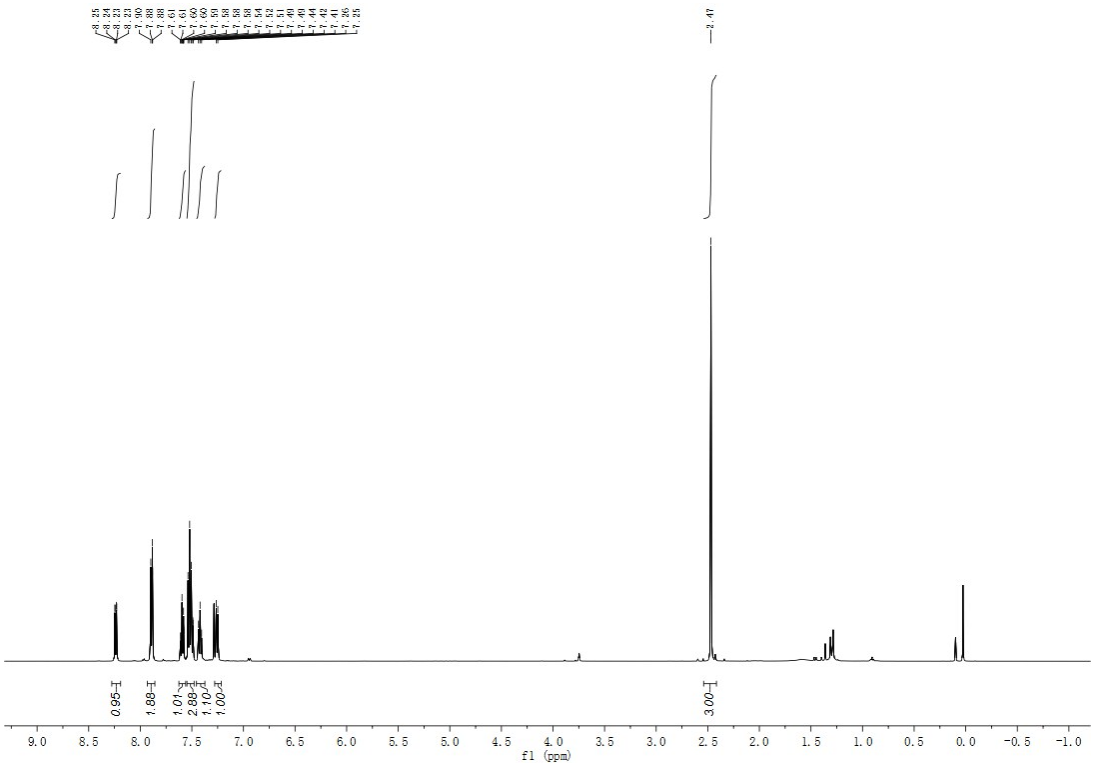

196.76
145.39
140.75
140.35
133.71
129.51
129.10
127.97
127.84
26.90
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

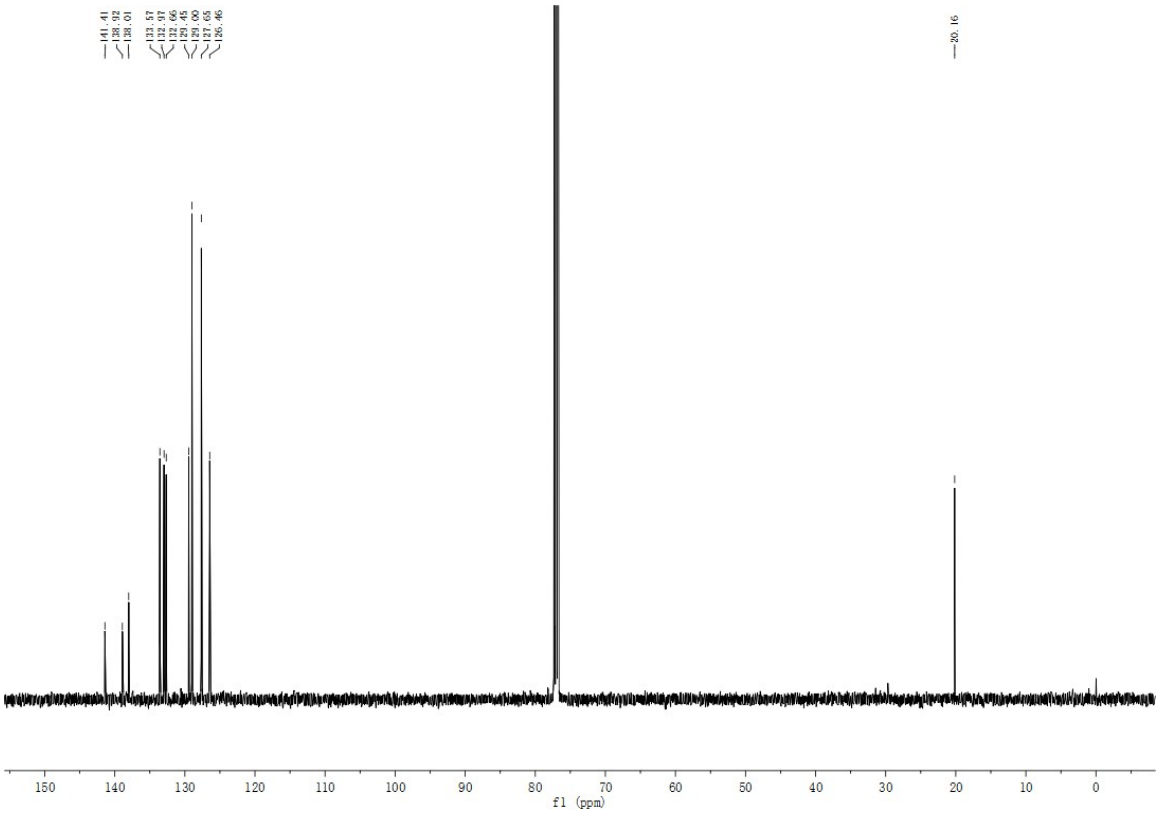

O
O
S
O2N

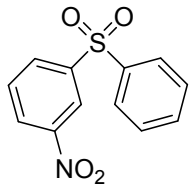

8.36
8.34
8.15
8.13
7.99
7.97
7.67
7.65
7.63
7.61
7.57
7.55
2.00
2.02
1.98
1.04
1.98
f1 (ppm)

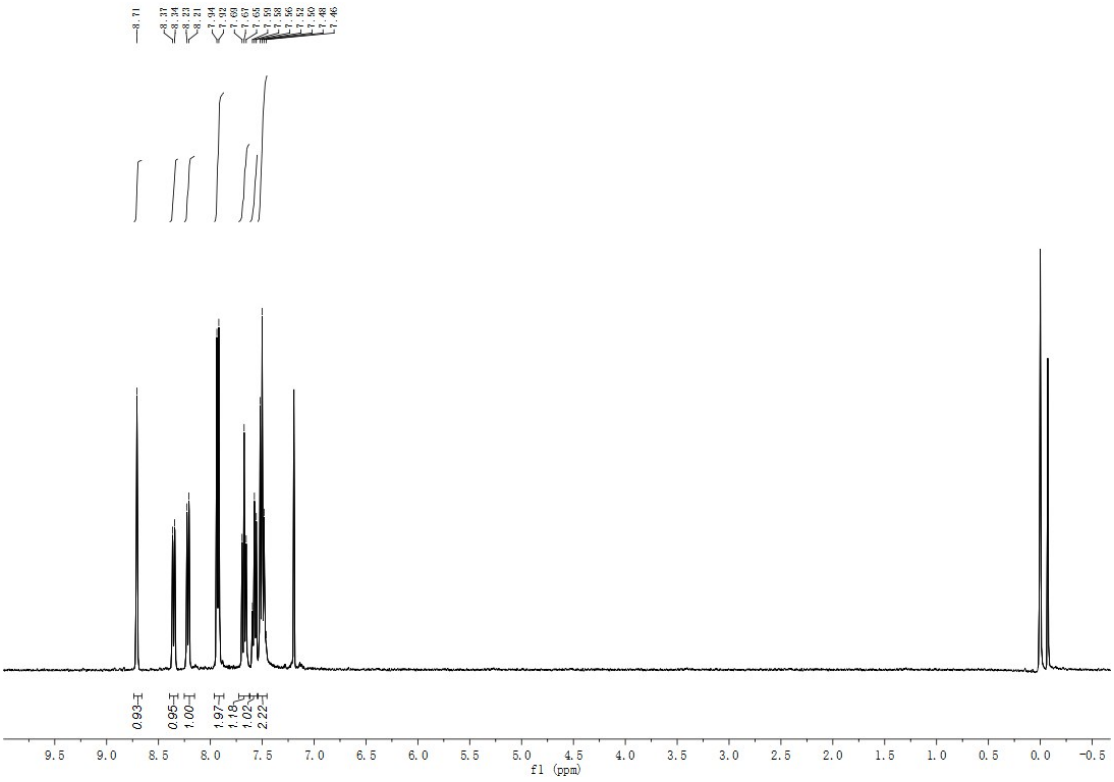

150.37
147.36
140.00
134.15
129.71
128.90
128.84
124.54
f1 (ppm)

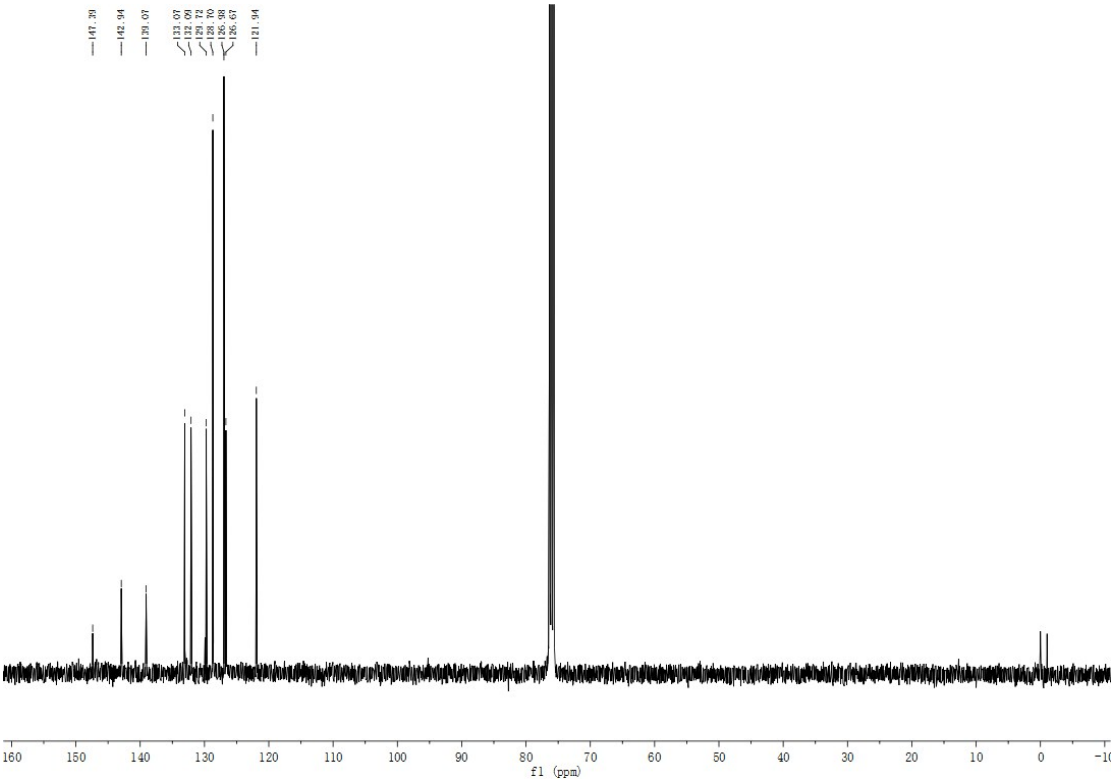

Me
O
O
S


8.25
8.24
8.23
8.23
7.90
7.88
7.88
7.61
7.60
7.60
7.59
7.58
7.58
7.58
7.54
7.52
7.51
7.49
7.49
7.44
7.42
7.41
7.26
7.25
2.47
0.95
1.88
1.01
2.88
1.10
1.00
3.00
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
-1.0
f1 (ppm)


141.41
139.32
136.01
133.57
132.37
132.05
131.45
129.00
127.65
126.46
20.16
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
O
S
NO2


8.71
8.37
8.34
8.23
8.21
7.94
7.92
7.69
7.67
7.65
7.59
7.58
7.56
7.52
7.50
7.48
7.46
0.93
0.95
1.00
1.97
1.18
1.02
2.22
f1 (ppm)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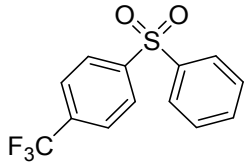
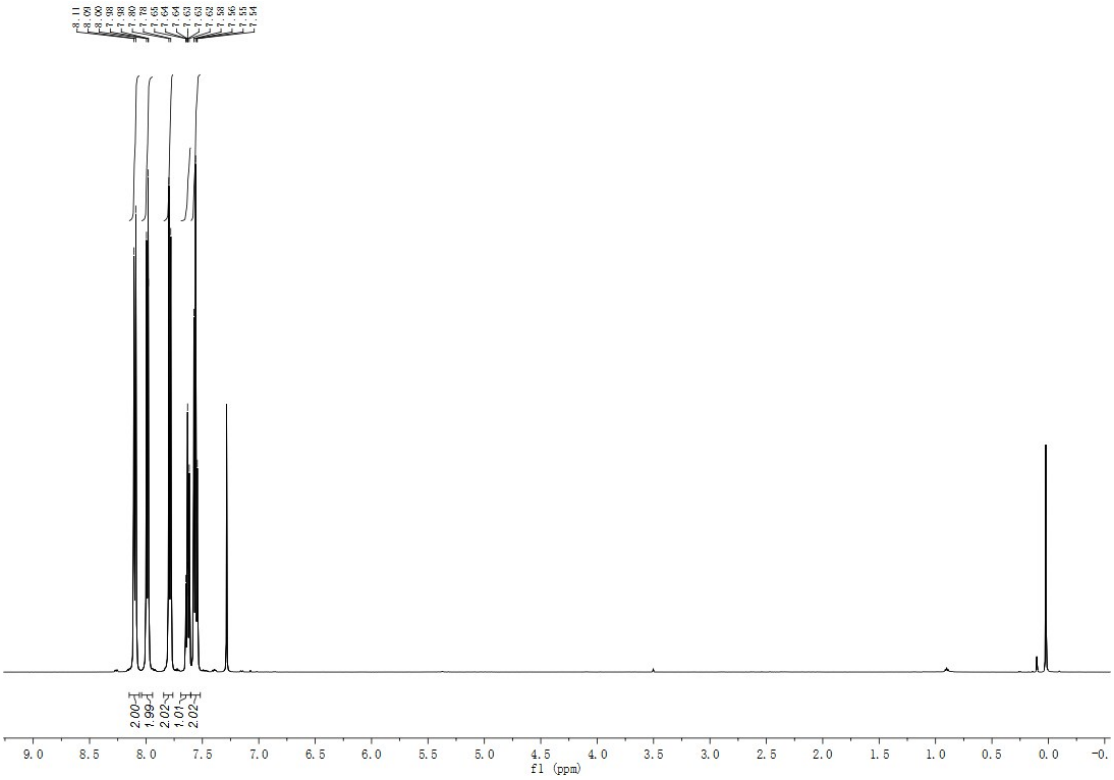
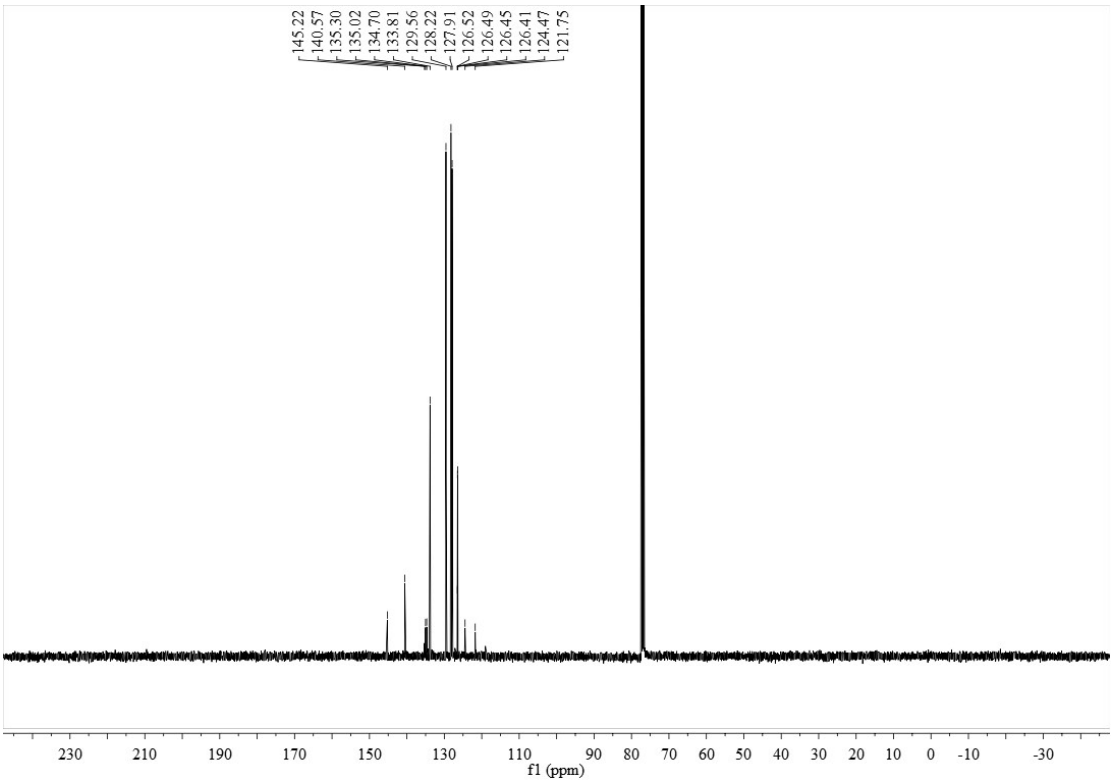
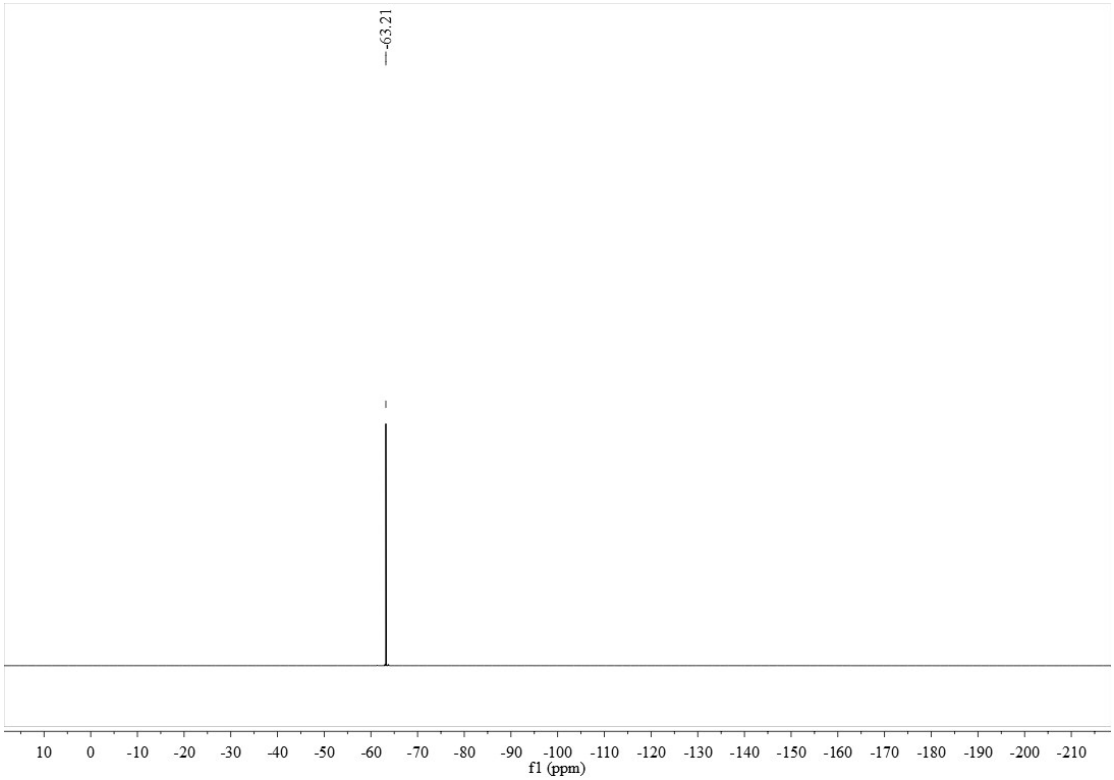
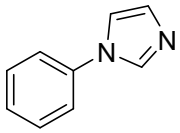
142.94
139.07
133.07
132.09
129.72
128.70
126.98
126.67
121.94
f1 (ppm)

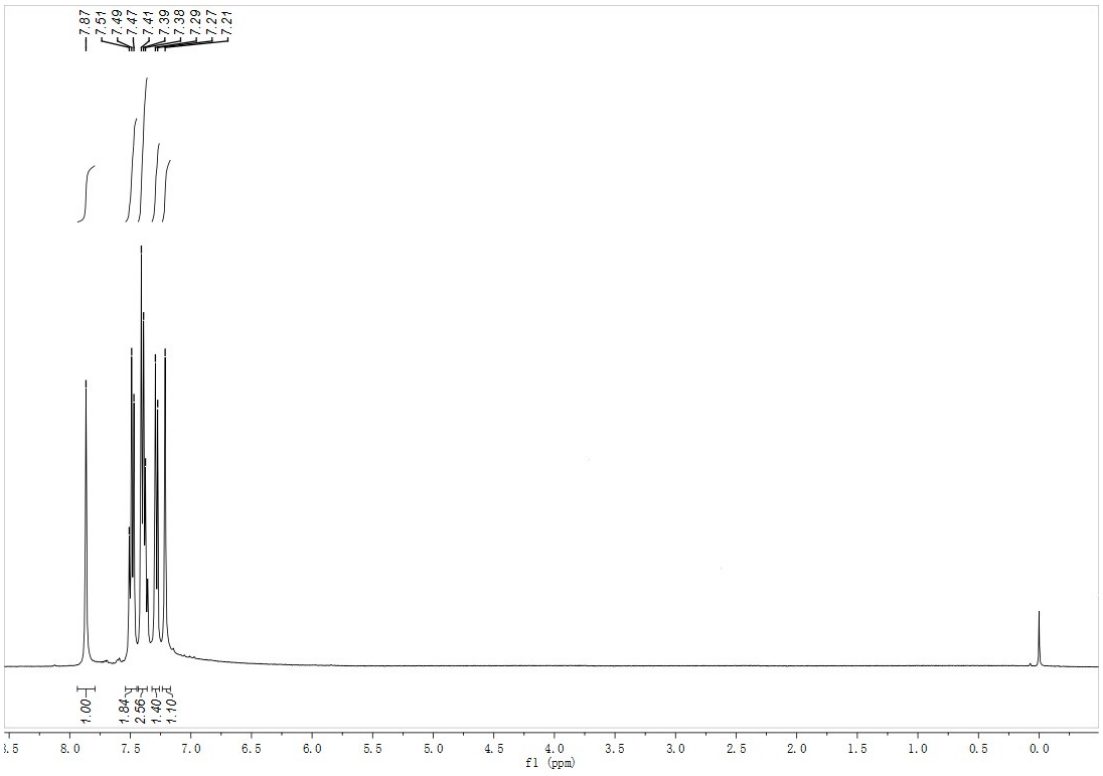

O
O
S
F3C

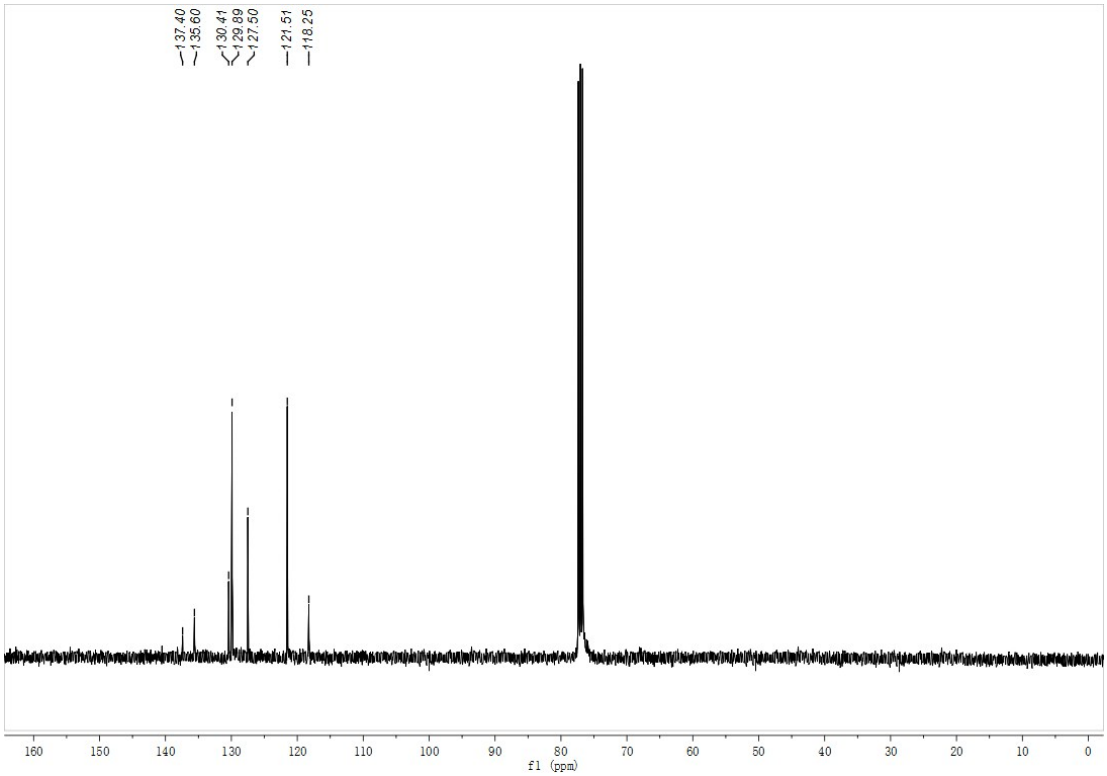

8.11
8.09
8.08
7.98
7.98
7.80
7.78
7.65
7.64
7.64
7.63
7.62
7.62
7.58
7.56
7.55
7.54
2.00
1.99
2.02
1.01
2.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


145.22
140.57
135.30
135.02
134.70
133.81
129.56
128.22
127.91
126.52
126.49
126.45
126.41
124.47
121.75
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
f1 (ppm)


-63.21
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)




7.87
7.51
7.49
7.47
7.41
7.39
7.38
7.29
7.27
7.21
1.00
1.84
2.56
1.40
1.10
f1 (ppm)


137.40
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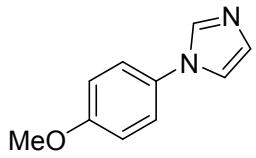
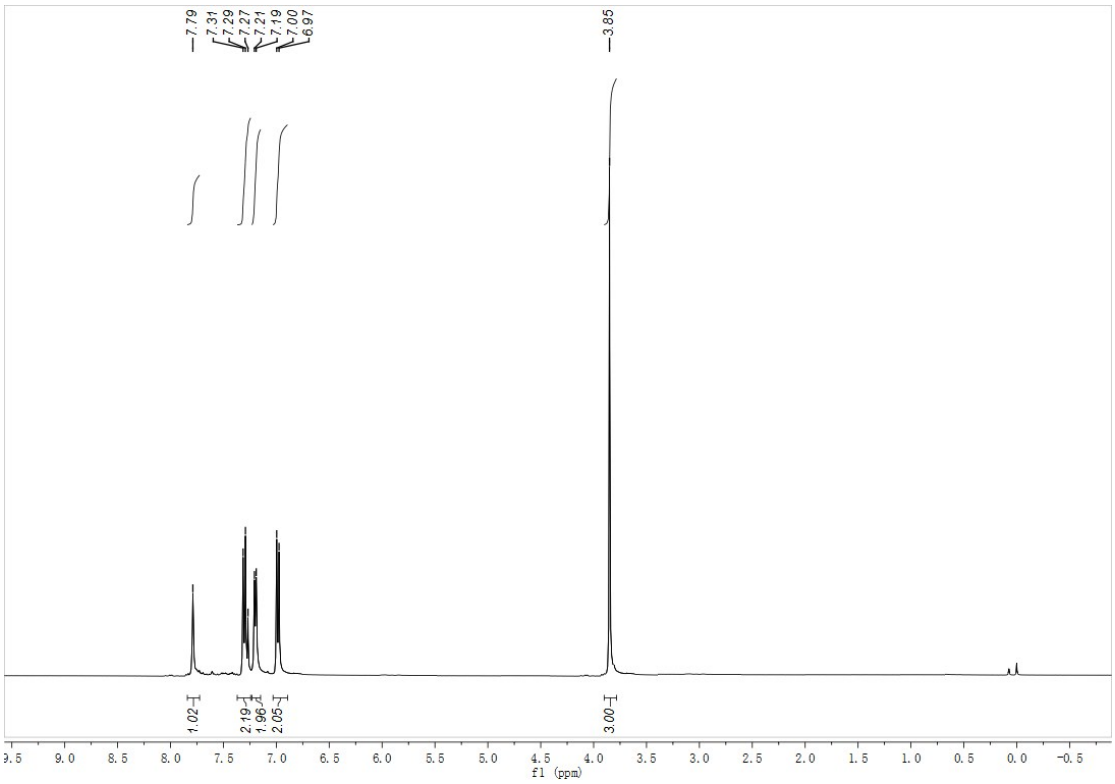
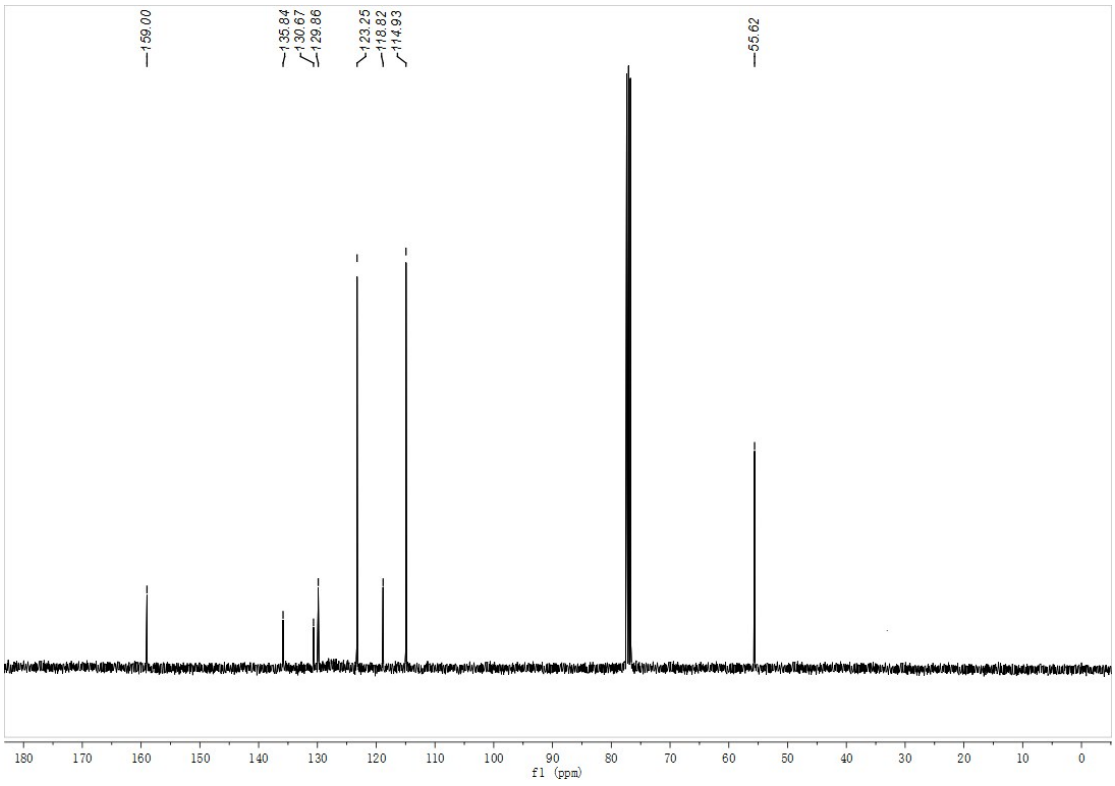
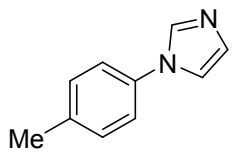
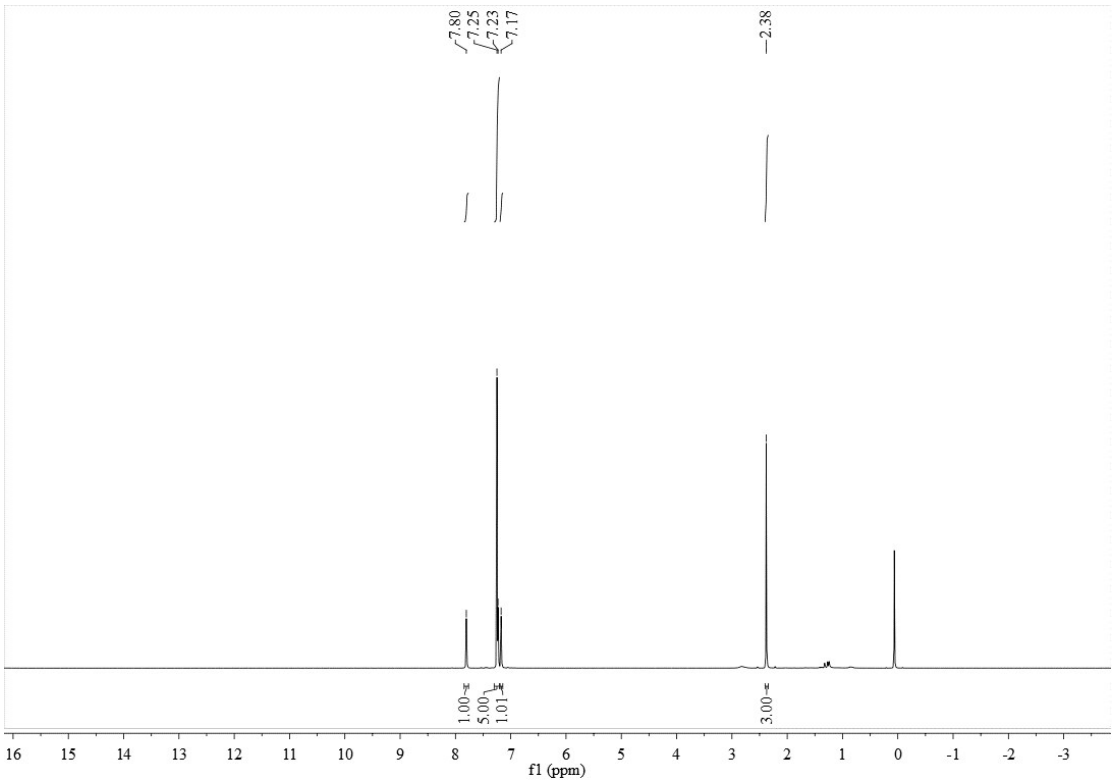
130.41
129.89
127.50
121.51
118.25
f1 (ppm)

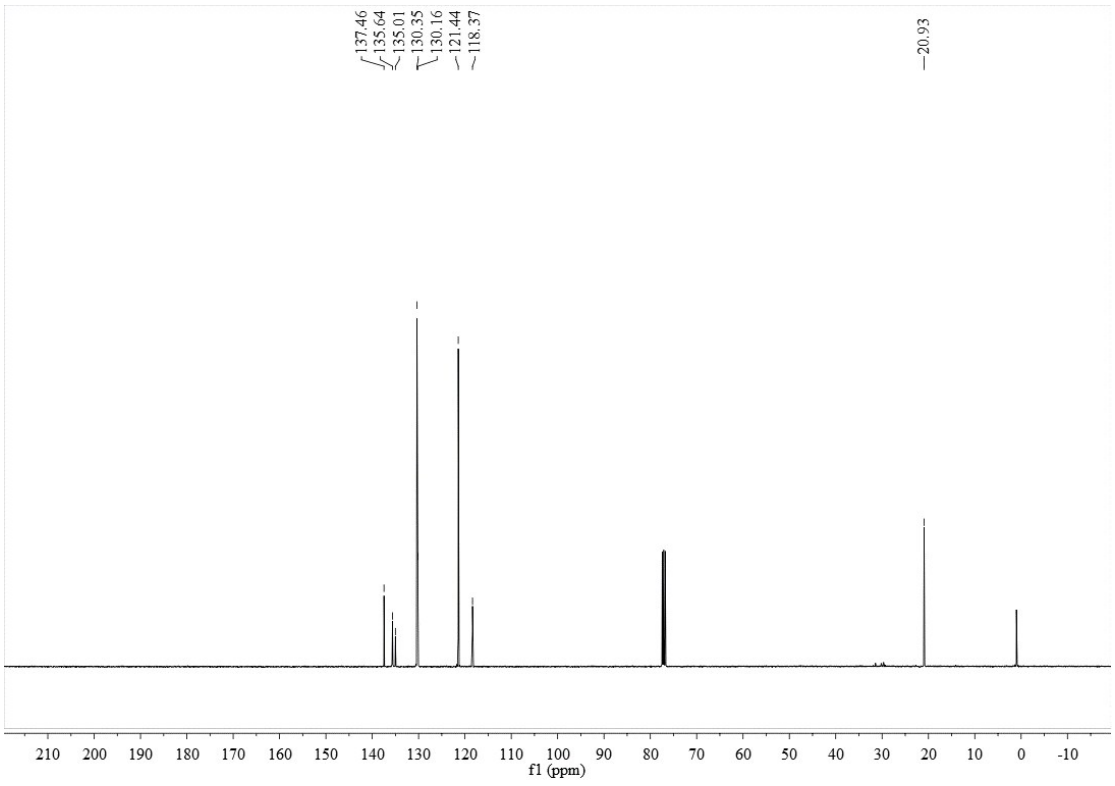

N
N
MeO

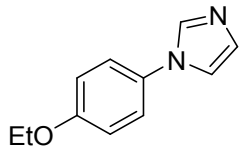

7.79
7.31
7.29
7.27
7.21
7.19
7.00
6.97
3.85
1.02
2.19
1.96
2.05
3.00
f1 (ppm)


159.00
135.84
130.67
129.86
123.25
118.82
114.93
55.62
f1 (ppm)


N
N
Me


7.80
7.25
7.23
7.17
2.38
1.00
5.00
1.01
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


137.46
135.64
135.01
130.35
130.16
121.44
118.37
20.93
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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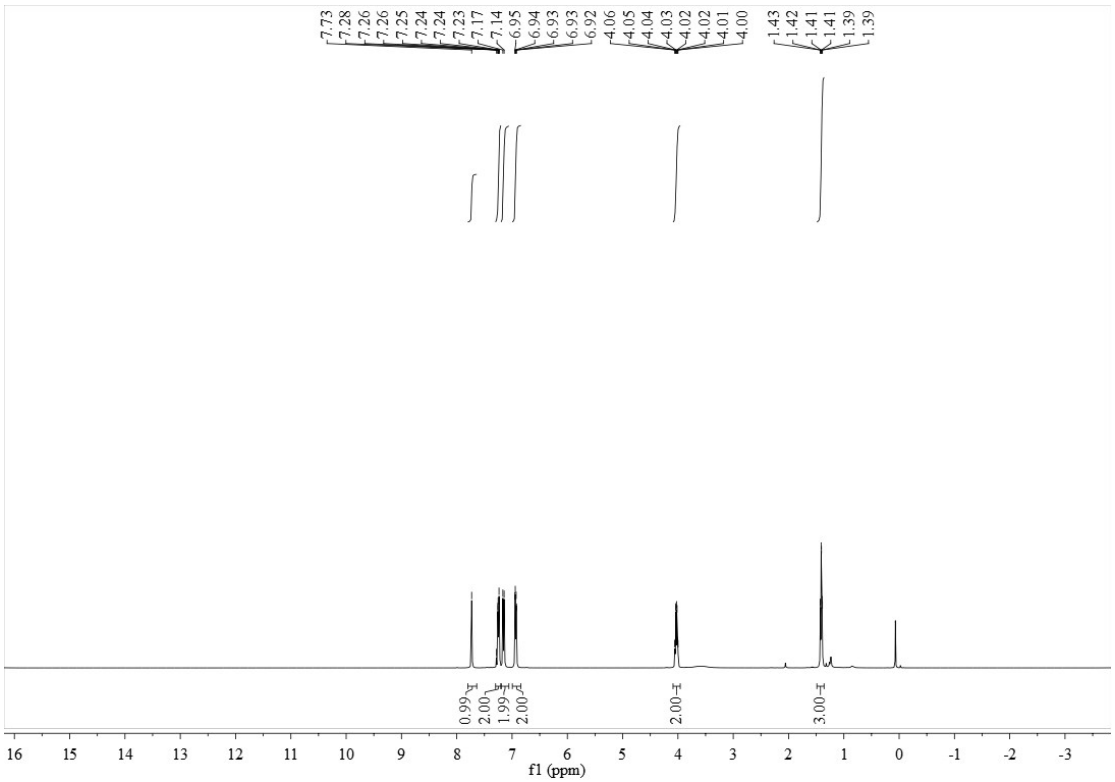
EtO


7.73
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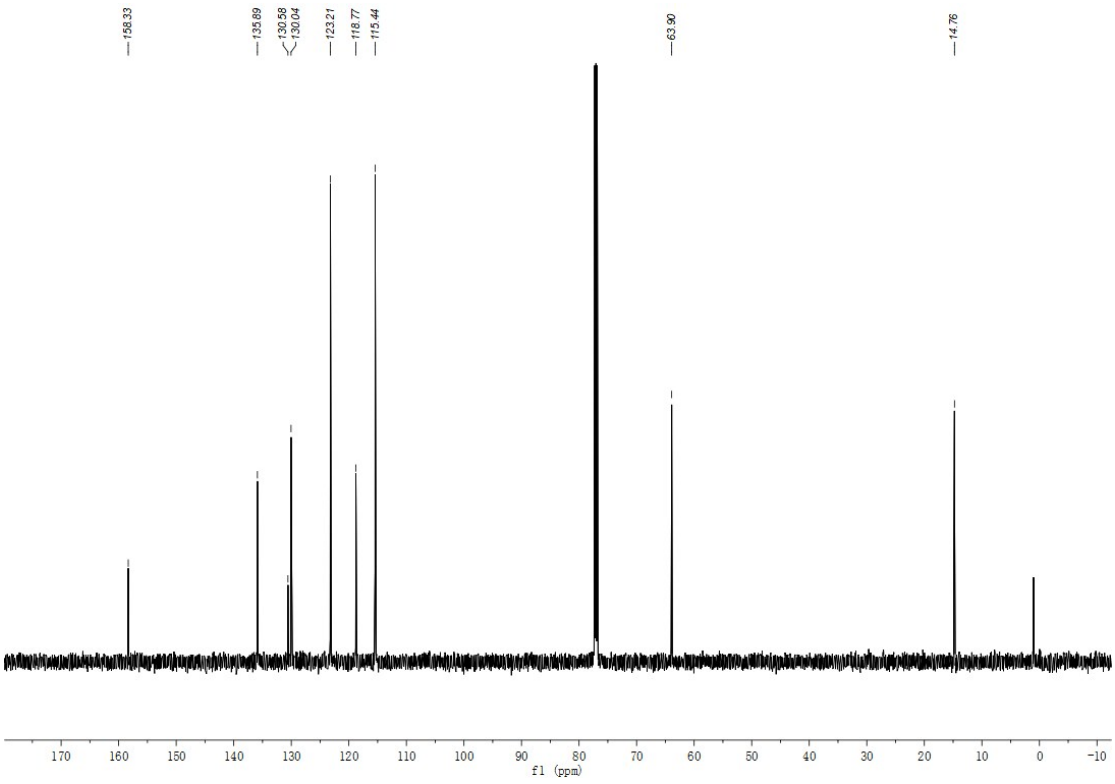
7.24
7.24
7.23
7.17
7.14
6.95
6.94
6.93
6.93
6.92
4.06
4.05
4.04
4.03
4.02
4.02
4.01
4.00
1.43
1.42
1.41
1.41
1.39
1.39
0.99
2.00
1.99
2.00
2.00
3.00
f1 (ppm)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130.04
123.21
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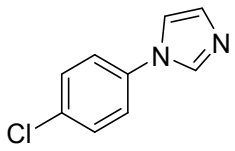
115.44
63.90
14.76
f1 (ppm)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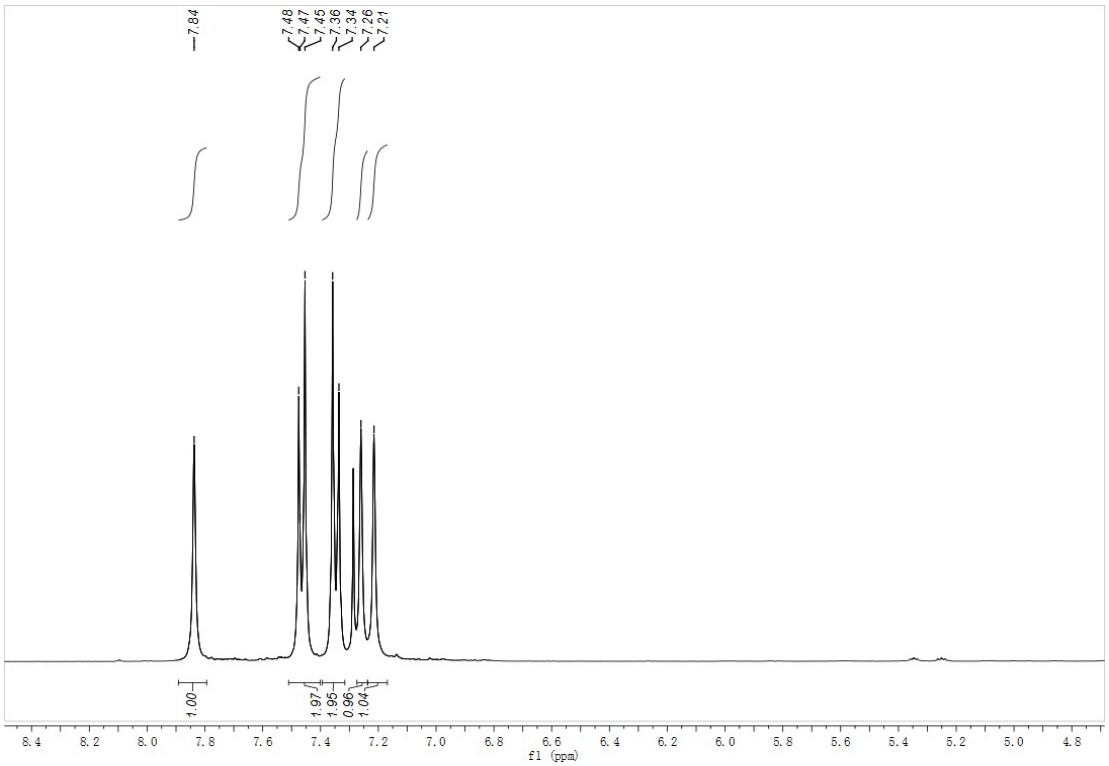
N
Cl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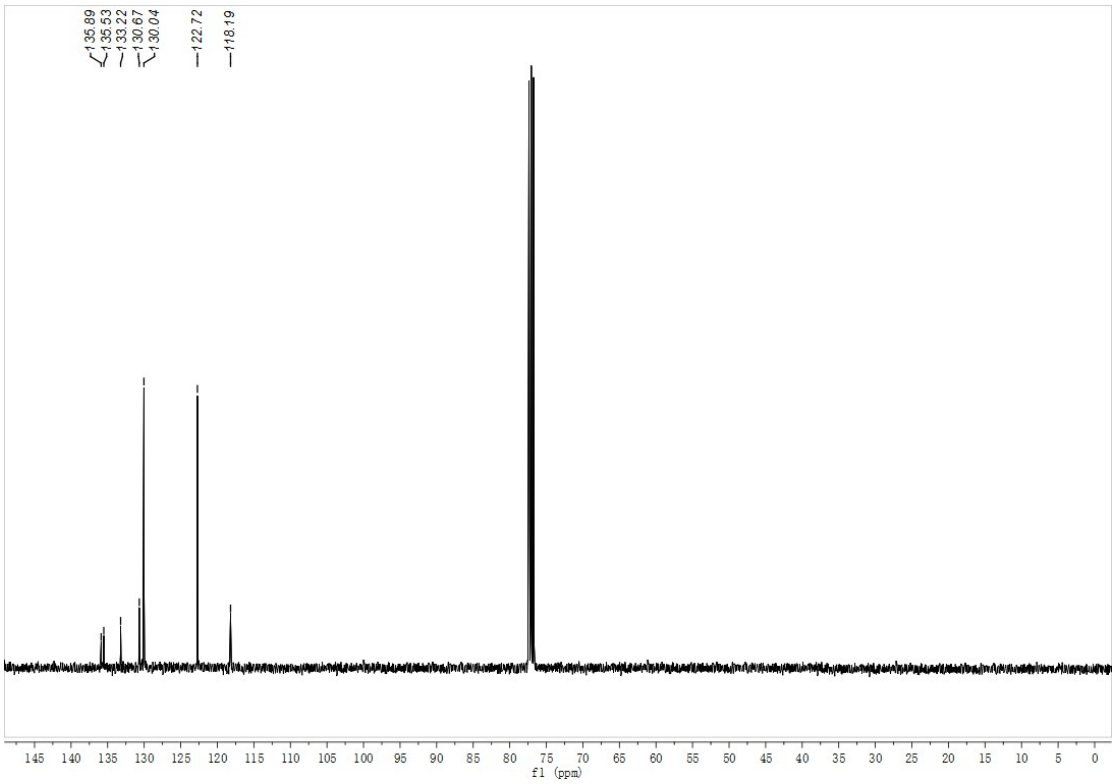
7.34
7.26
7.21
1.00
1.97
1.95
0.96
1.04
f1 (ppm)


135.89
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133.22
130.67
130.04
122.72
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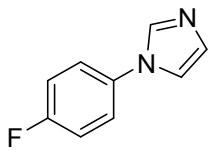
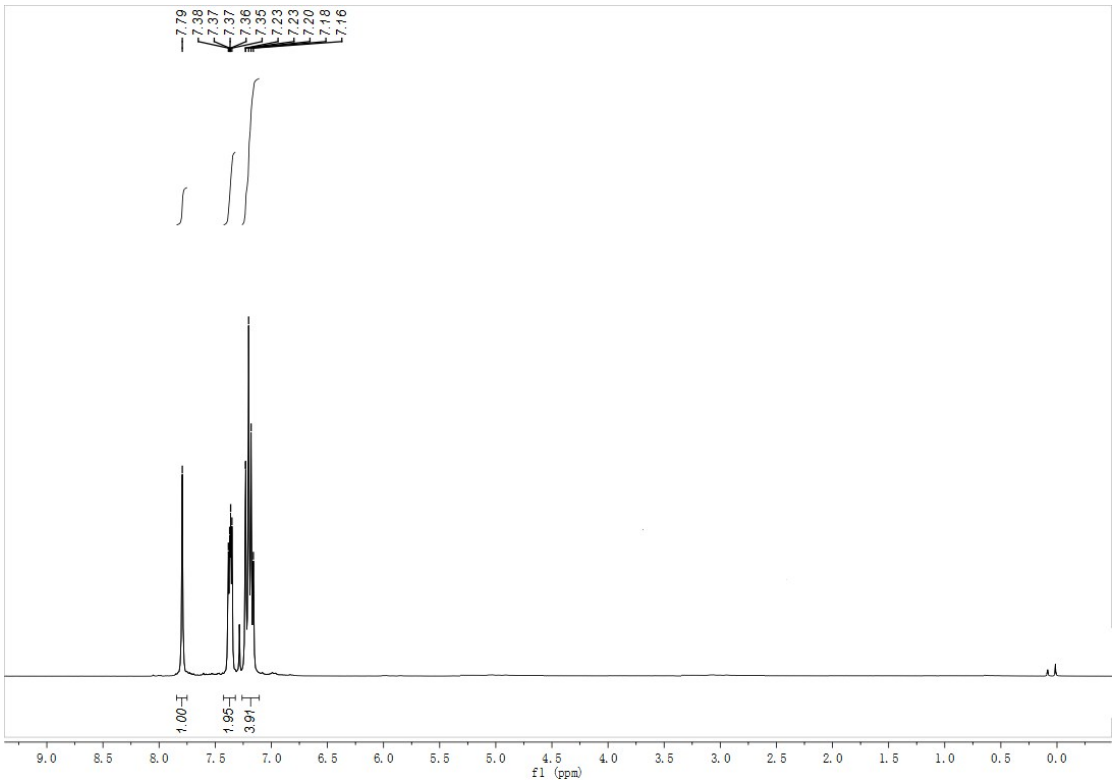
f1 (ppm)


N
N
F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7.23
7.23
7.20
7.18
7.16
1.00
1.95
3.91
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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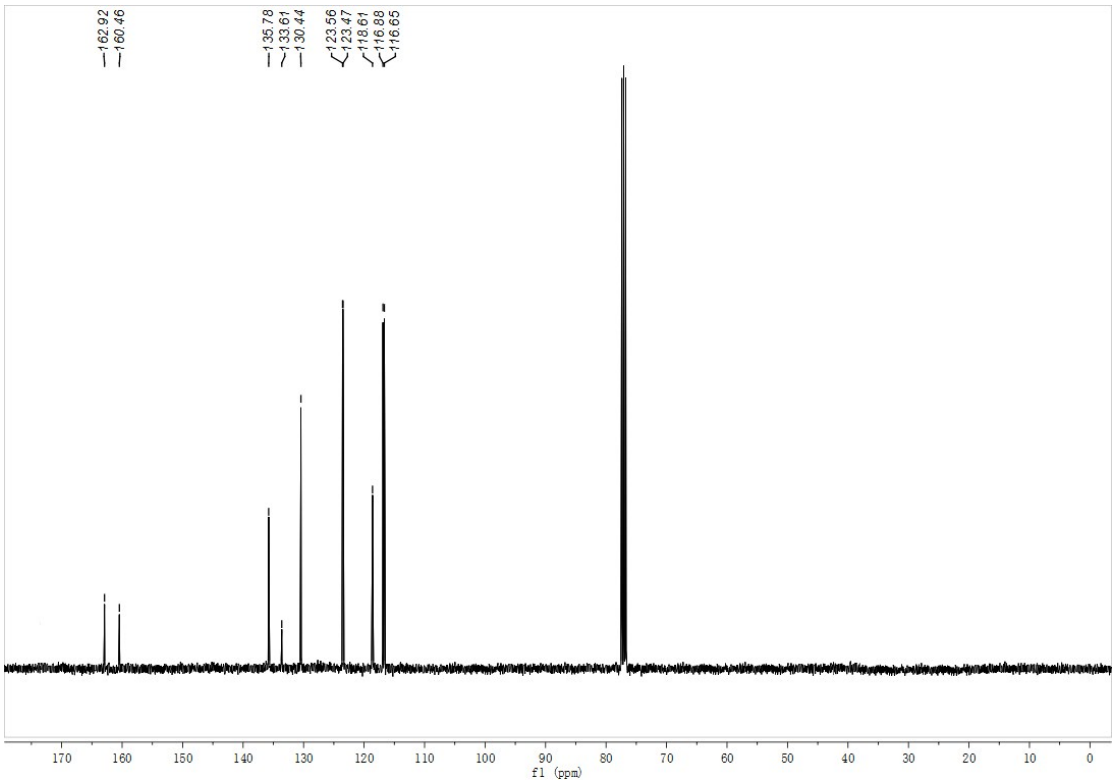
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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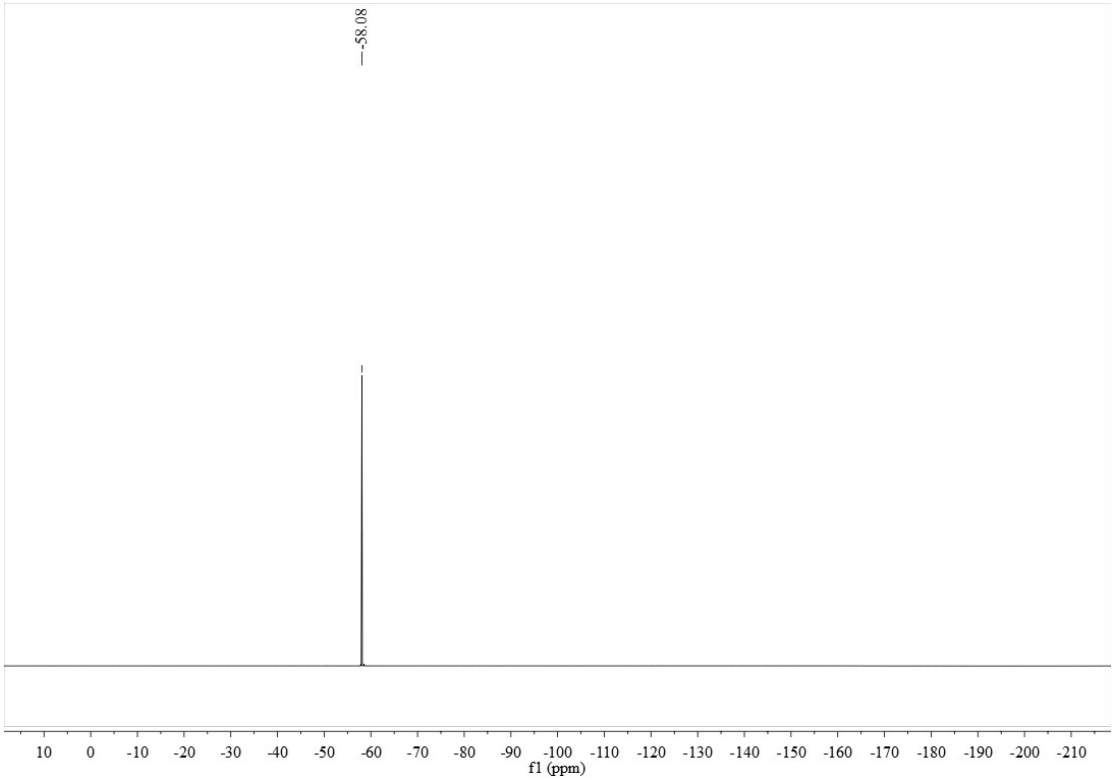
160.46
135.78
133.61
130.44
123.56
123.47
118.61
116.88
116.65
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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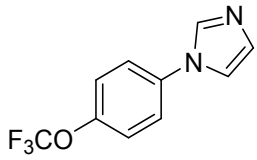
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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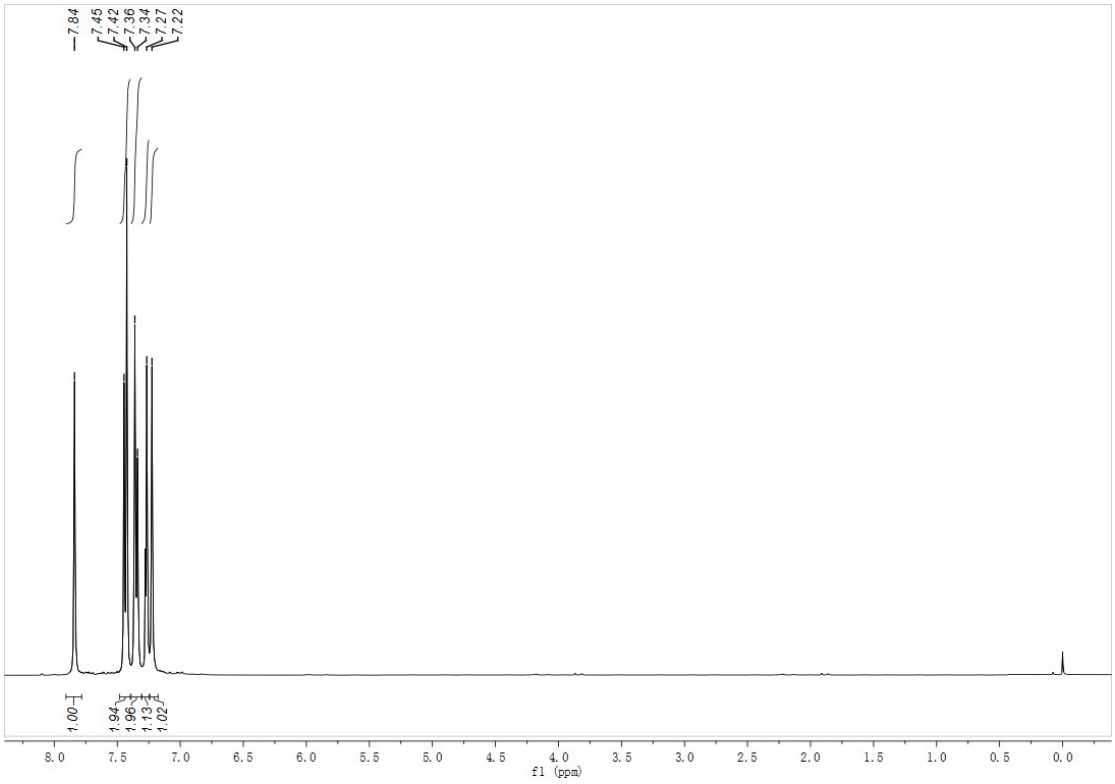
N
F3CO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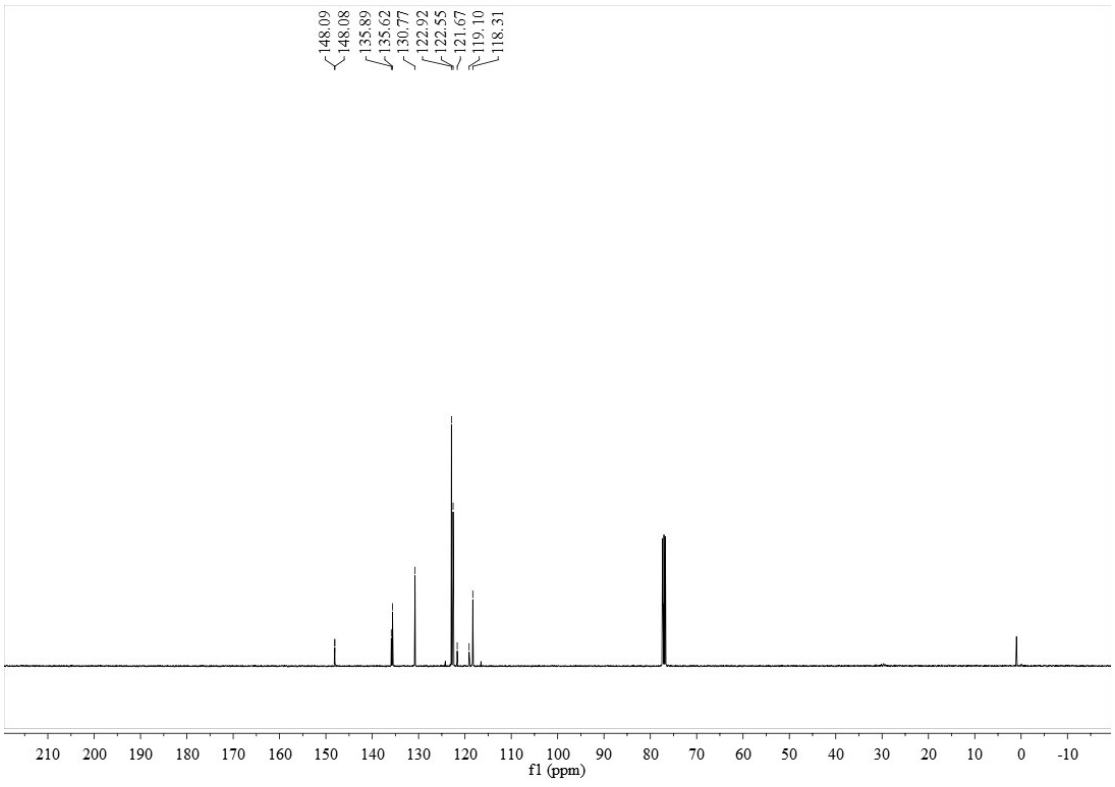
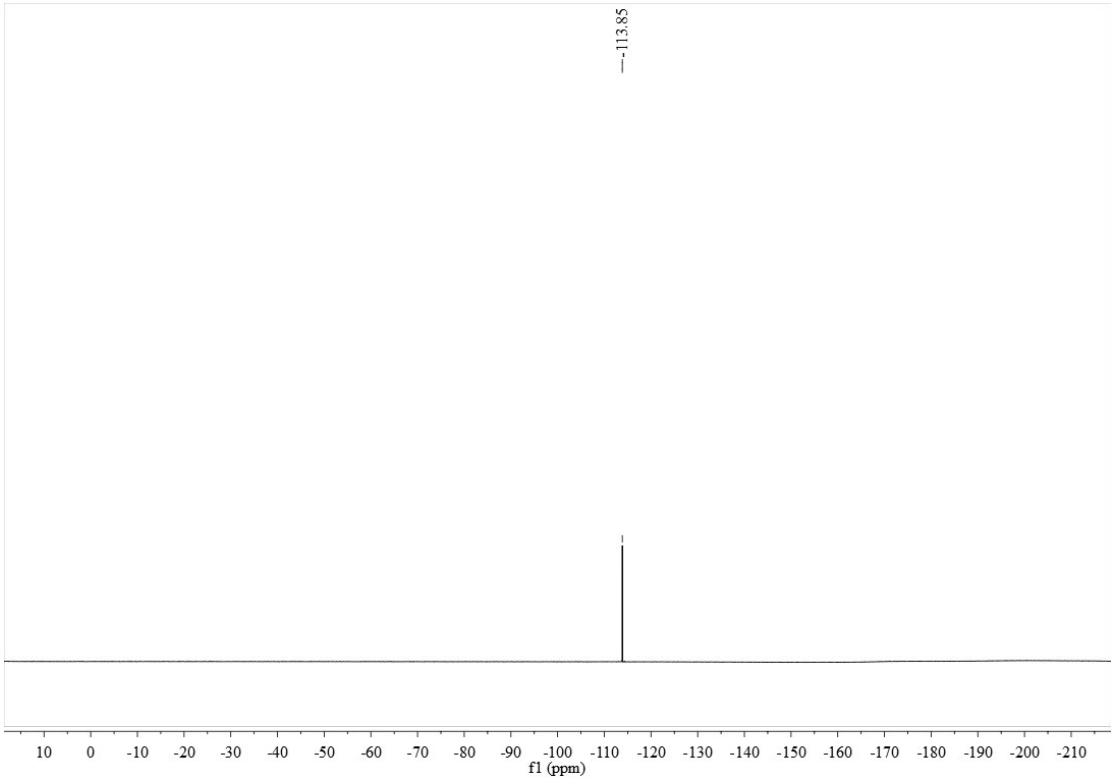
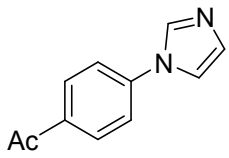
7.45
7.42
7.36
7.34
7.27
7.22
1.00
1.94
1.96
1.13
1.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.09
148.08
135.89
135.62
130.77
122.92
122.55
121.67
119.10
118.31
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)


-113.85
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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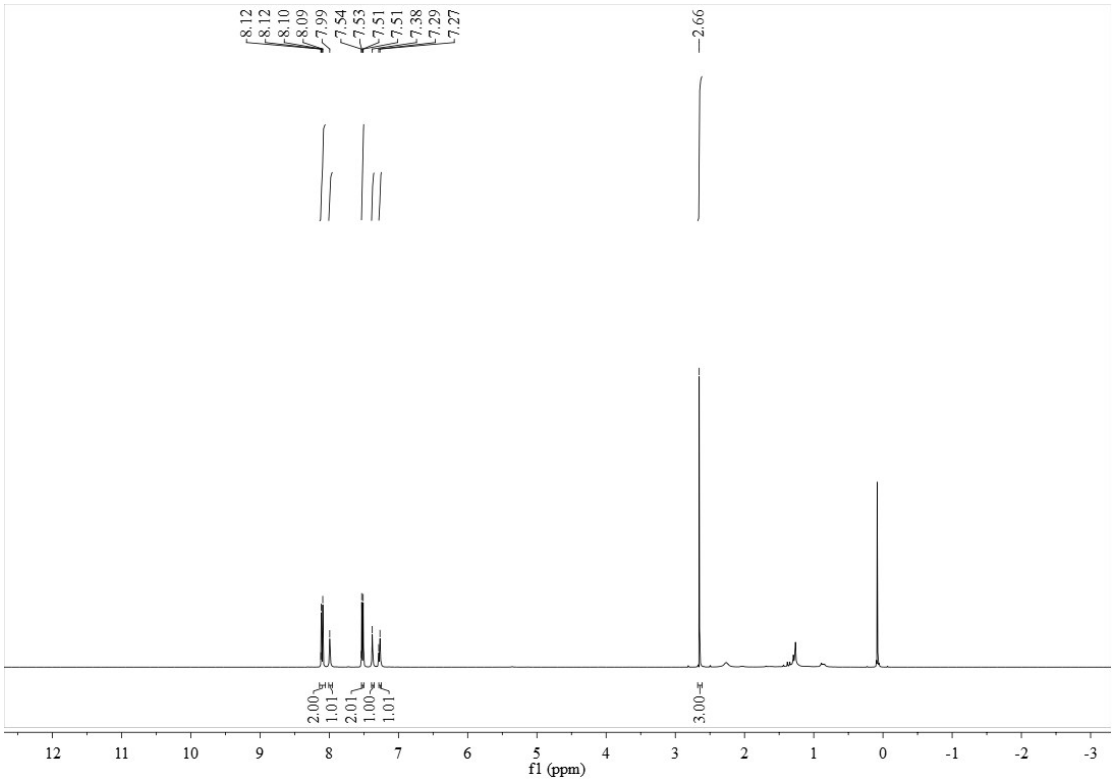
N
Ac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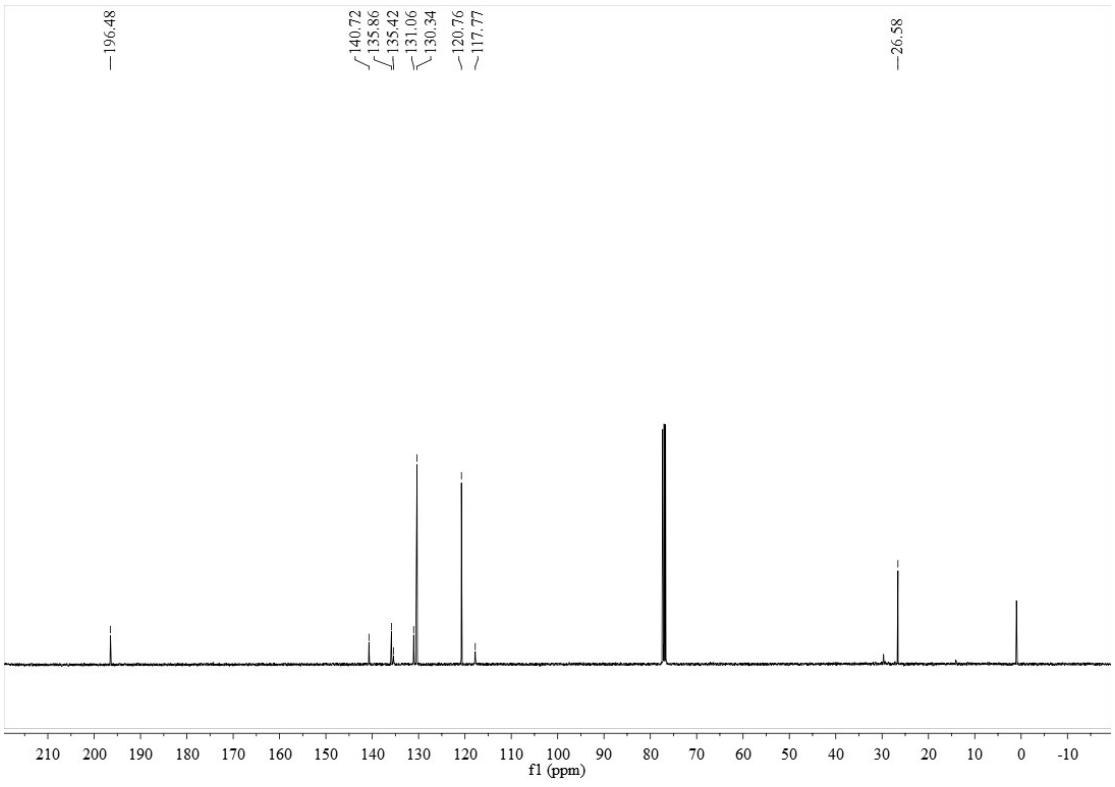
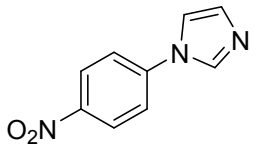
8.12
8.10
8.09
7.99
7.54
7.53
7.51
7.51
7.38
7.29
7.27
2.66
2.00
1.01
2.01
1.00
1.01
3.00
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


196.48
140.72
135.86
135.42
131.06
130.34
120.76
117.77
26.58
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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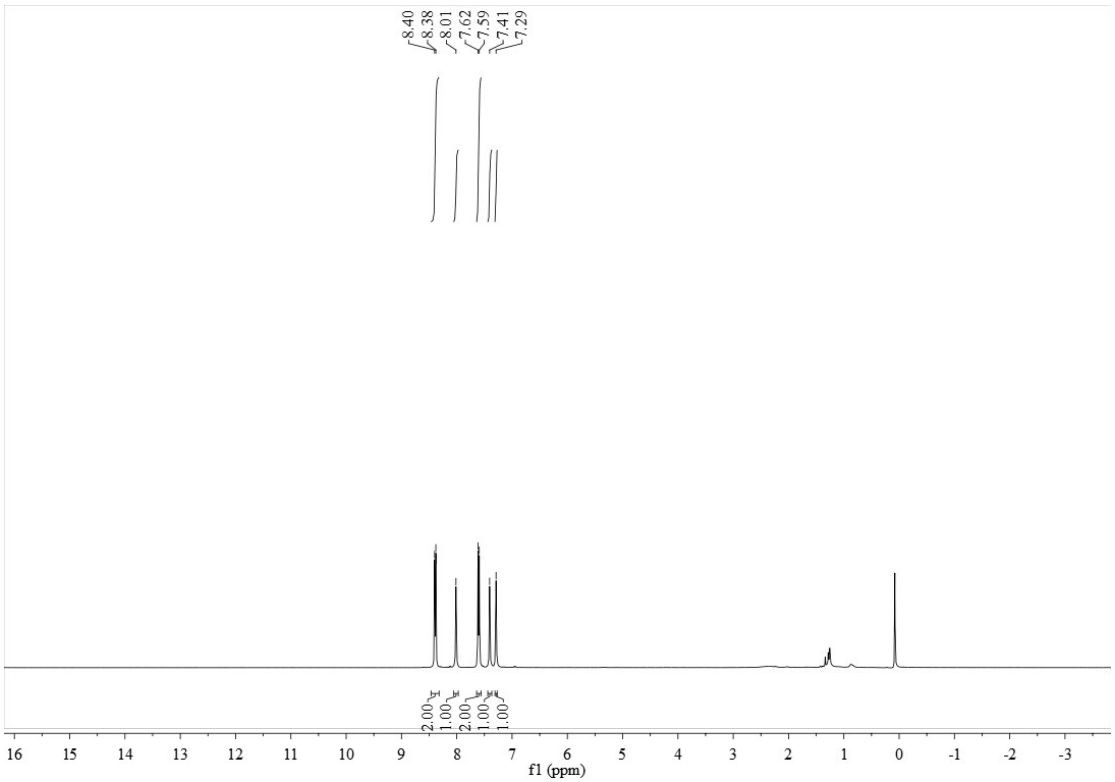
N
O2N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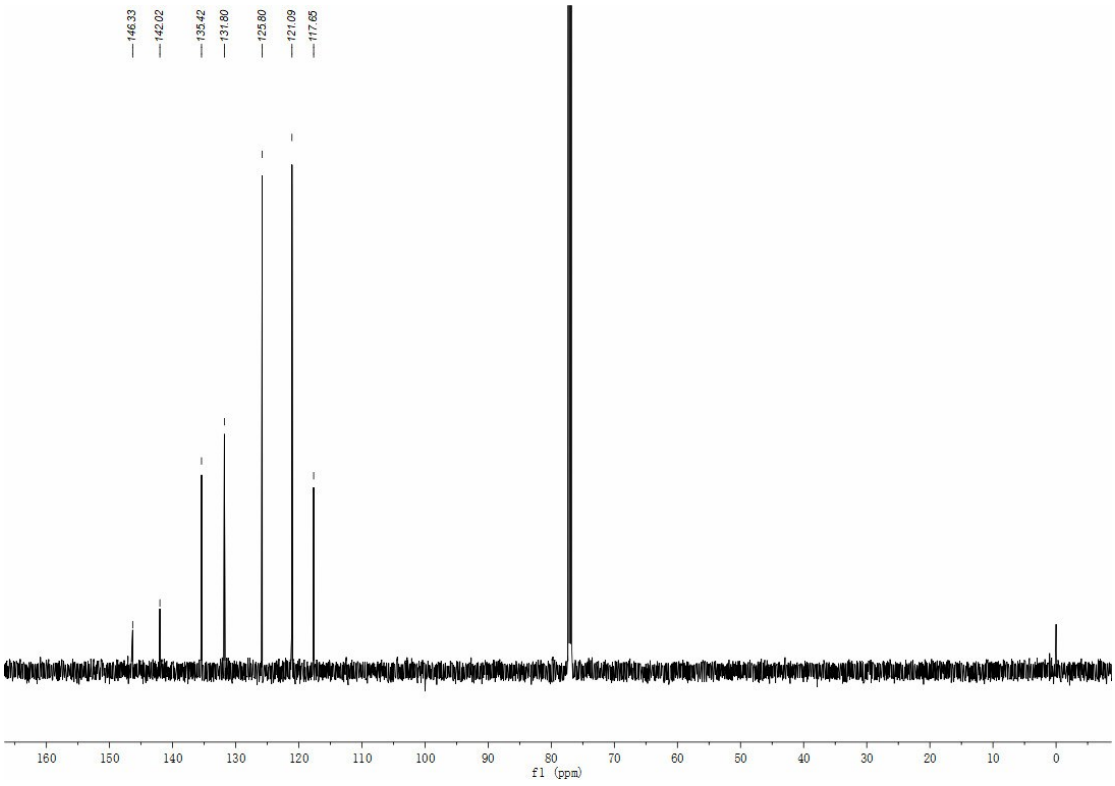
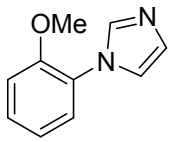
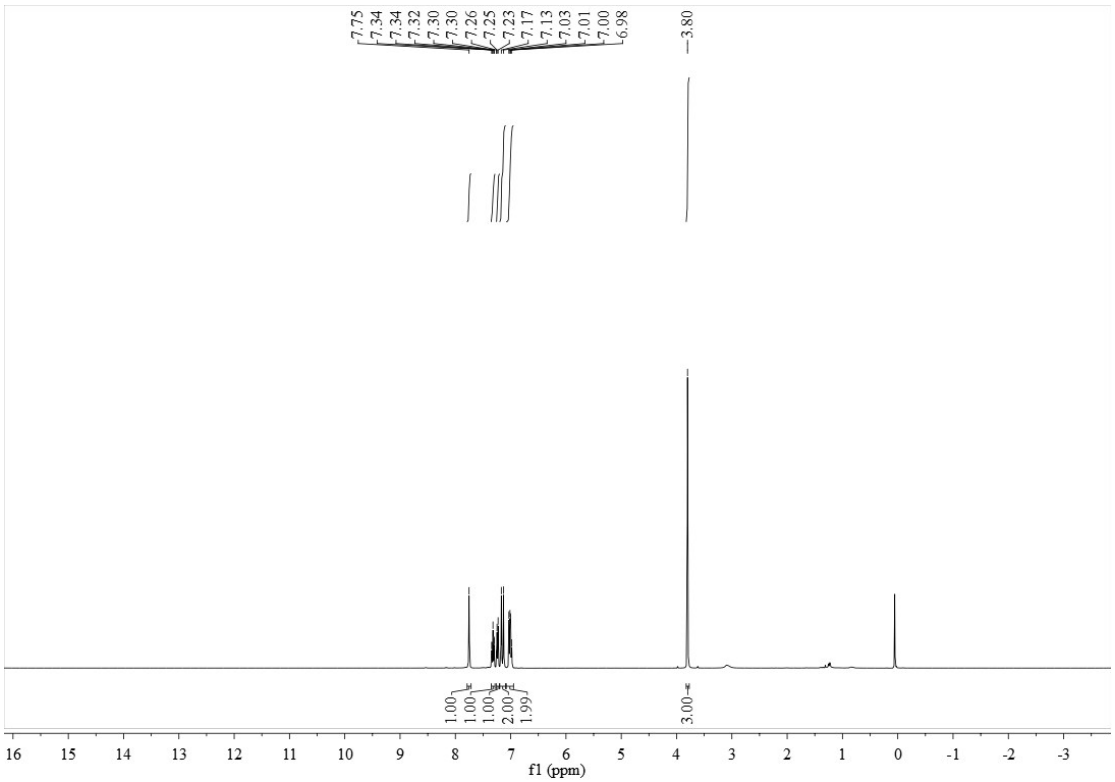
8.38
8.01
7.62
7.59
7.41
7.29
2.00
1.00
2.00
1.00
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


146.33
142.02
135.42
131.80
125.80
121.09
117.65
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
N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7.34
7.34
7.32
7.30
7.30
7.26
7.25
7.23
7.17
7.13
7.03
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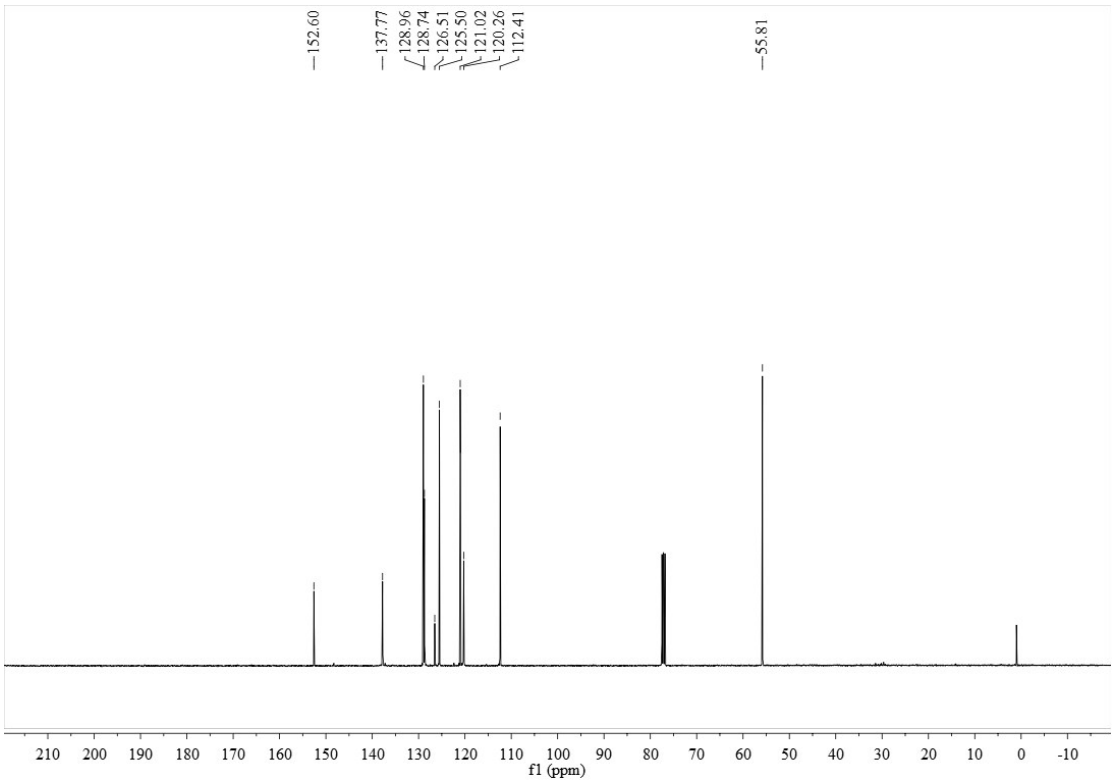
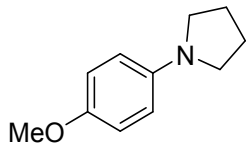
1.00
2.00
1.99
3.00
f1 (ppm)


152.60
137.77
128.96
128.74
126.51
125.50
121.02
120.26
112.41
55.81
f1 (ppm)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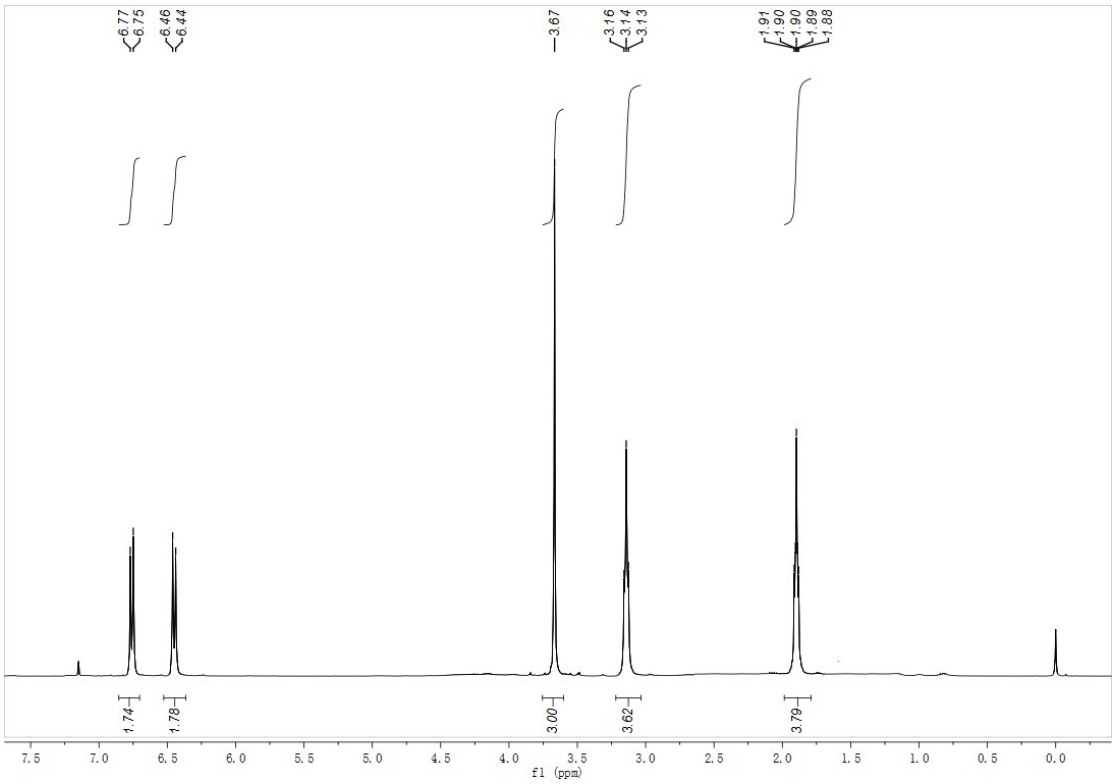
MeO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3.67
3.16
3.14
3.13
1.91
1.90
1.90
1.89
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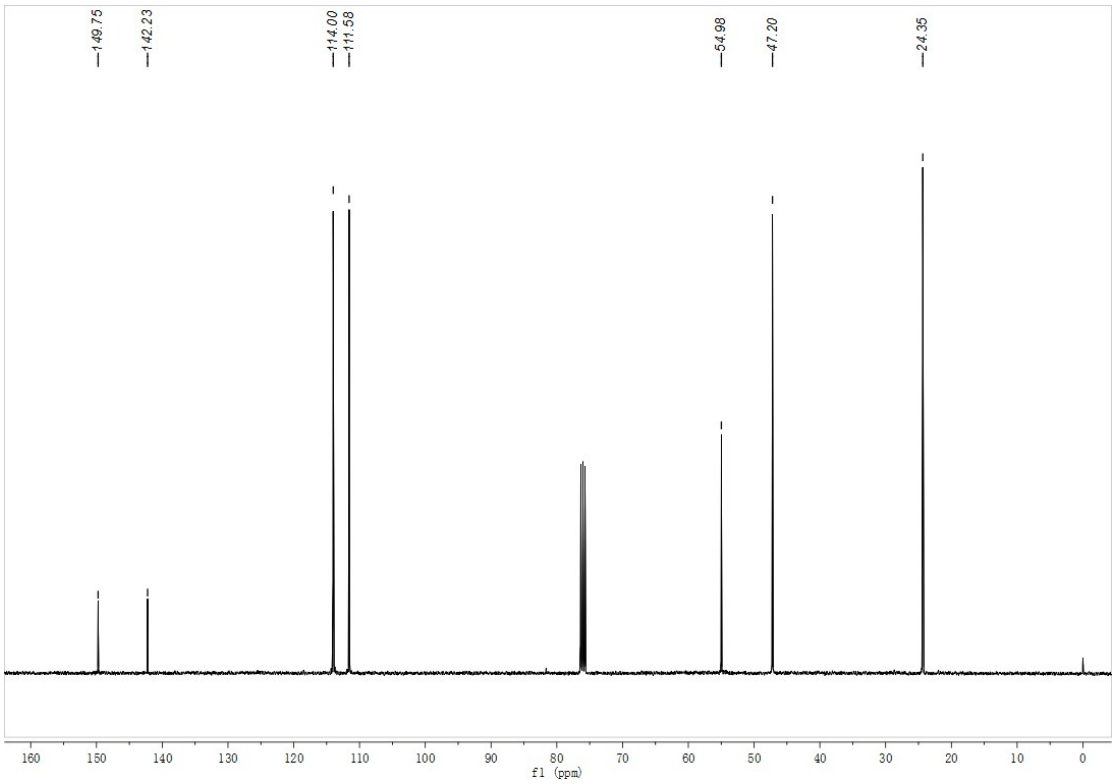
1.78
3.00
3.62
3.79
f1 (ppm)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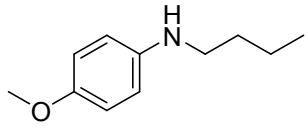
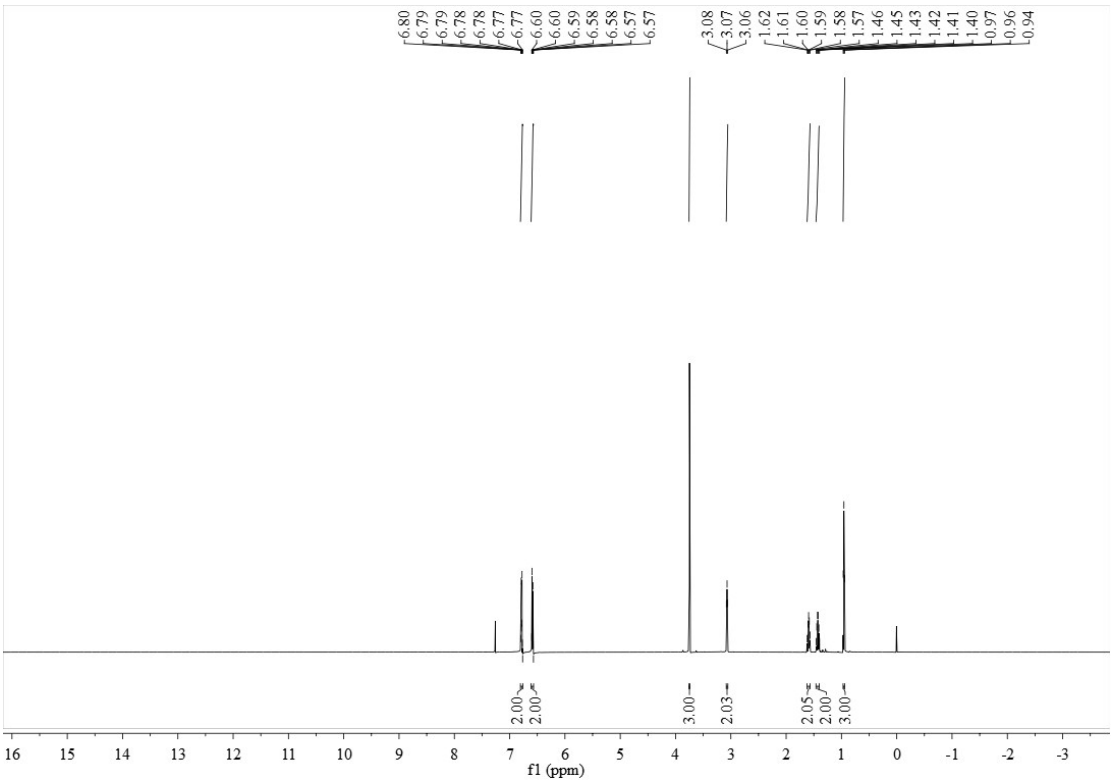
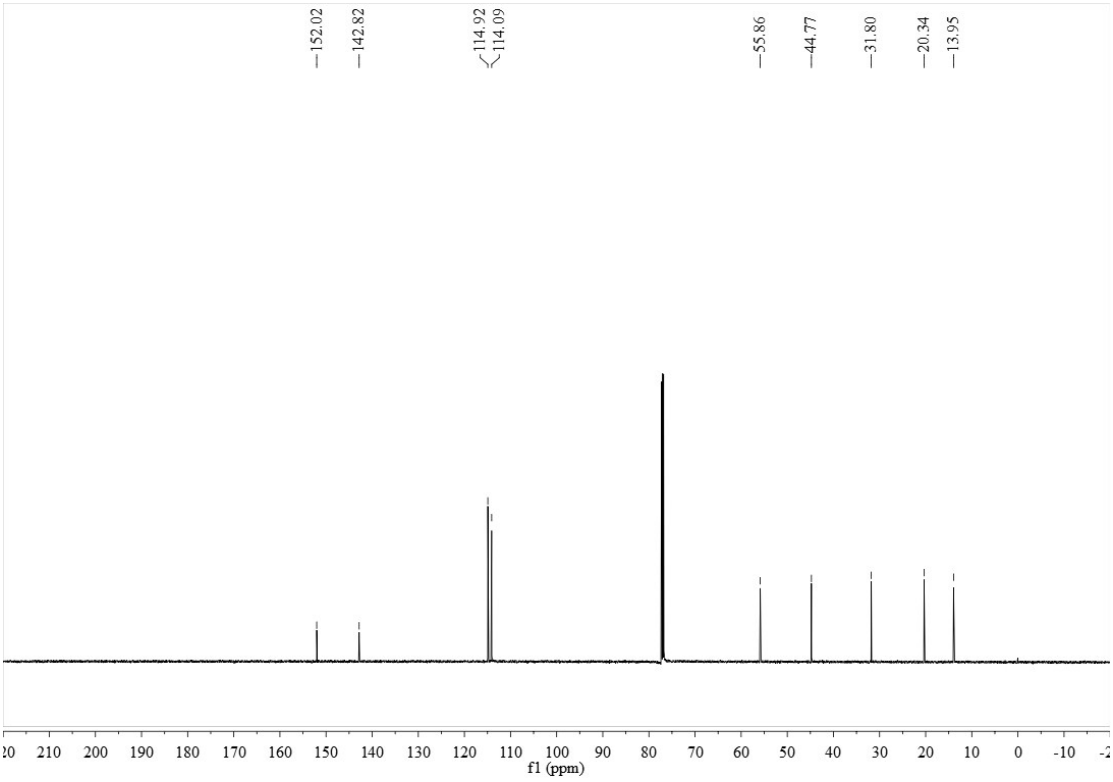
142.23
114.00
111.58
54.98
47.20
24.35
f1 (ppm)




6.80
6.79
6.79
6.78
6.78
6.77
6.77
6.60
6.60
6.59
6.58
6.58
6.57
6.57
3.08
3.07
3.06
1.62
1.61
1.60
1.59
1.58
1.57
1.46
1.45
1.43
1.42
1.41
1.40
0.97
0.96
0.94
2.00
2.00
3.00
2.03
2.05
2.00
3.00
f1 (ppm)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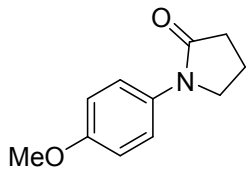
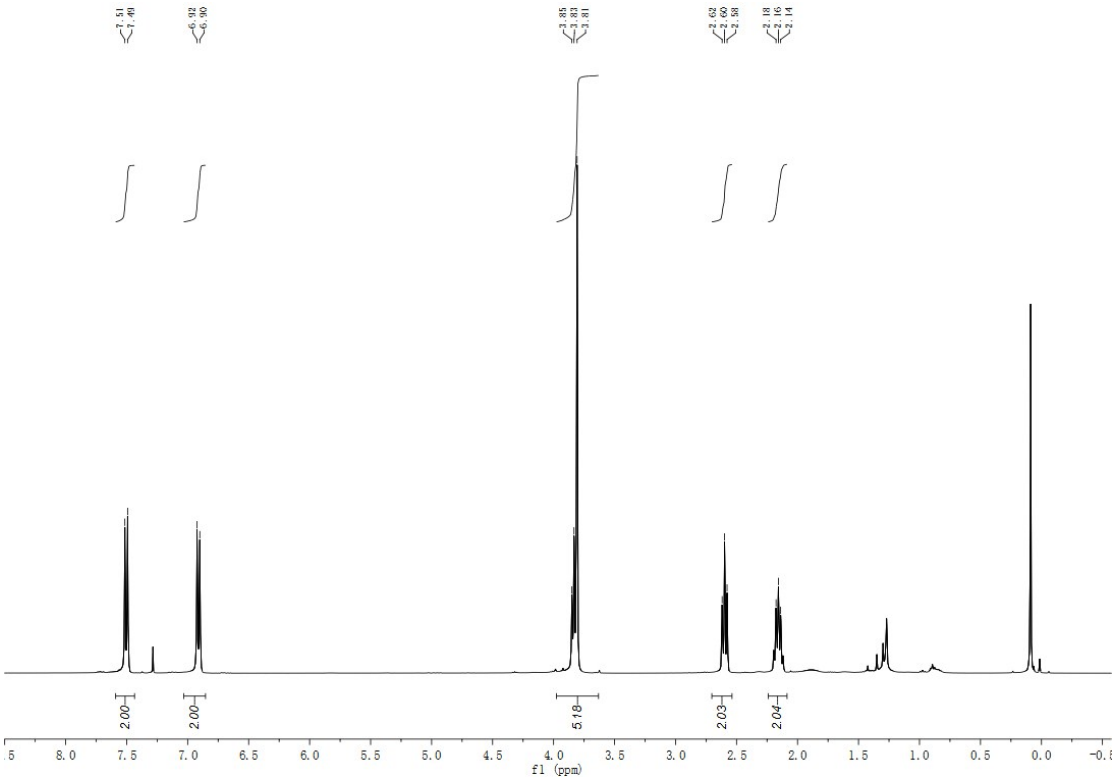
44.77
31.80
20.34
13.95
f1 (ppm)


O
N
MeO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7.49
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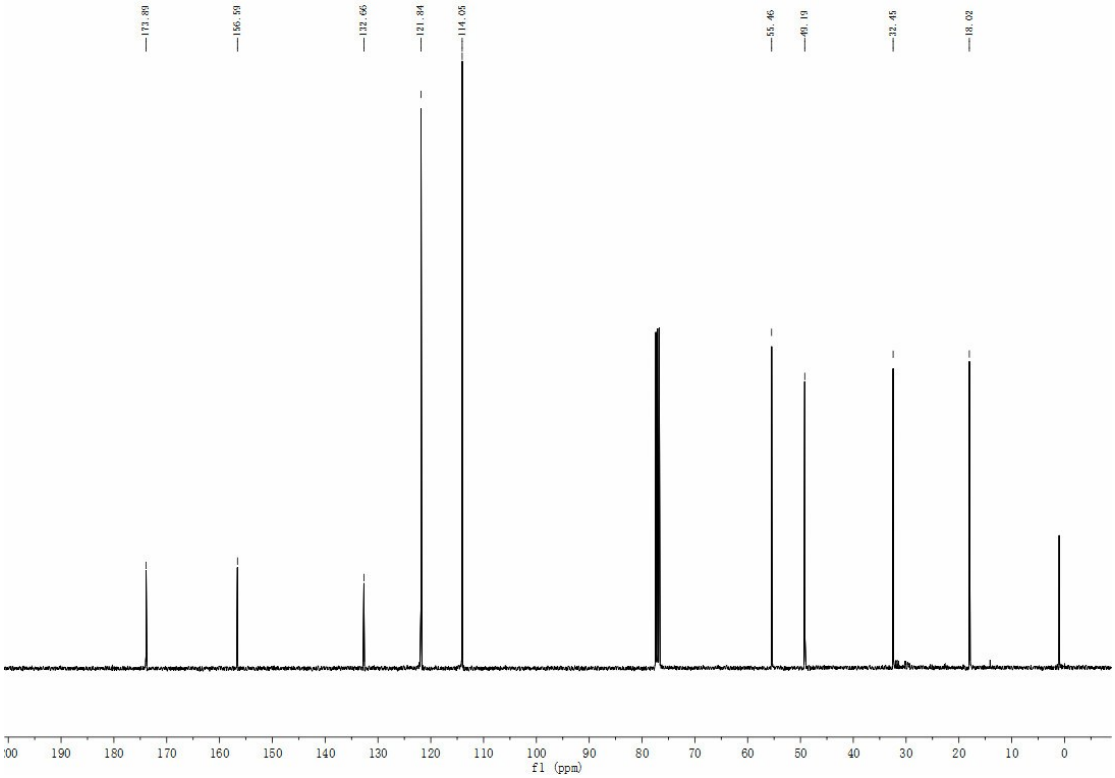
6.90
3.85
3.83
3.81
2.62
2.60
2.58
2.18
2.16
2.14
2.00
2.00
5.18
2.03
2.04
f1 (ppm)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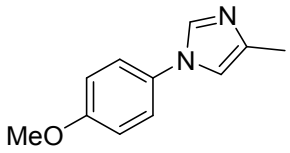
121.84
114.05
55.46
49.19
32.45
18.02
f1 (ppm)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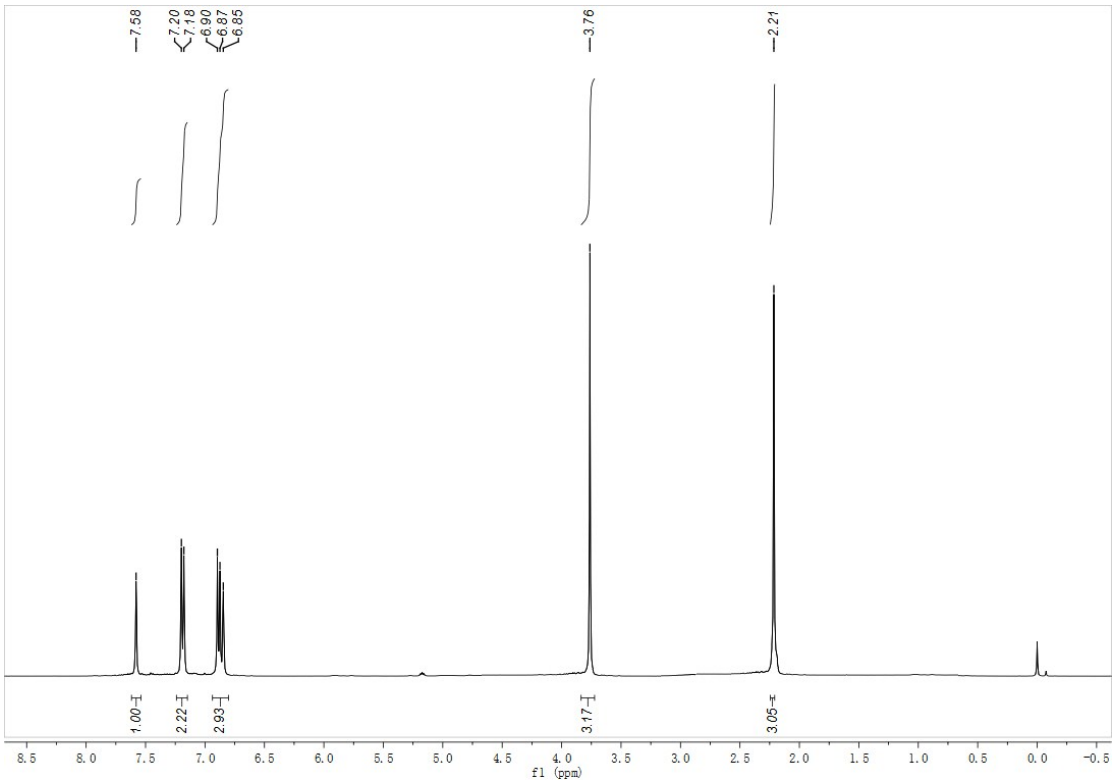
N
MeO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2.21
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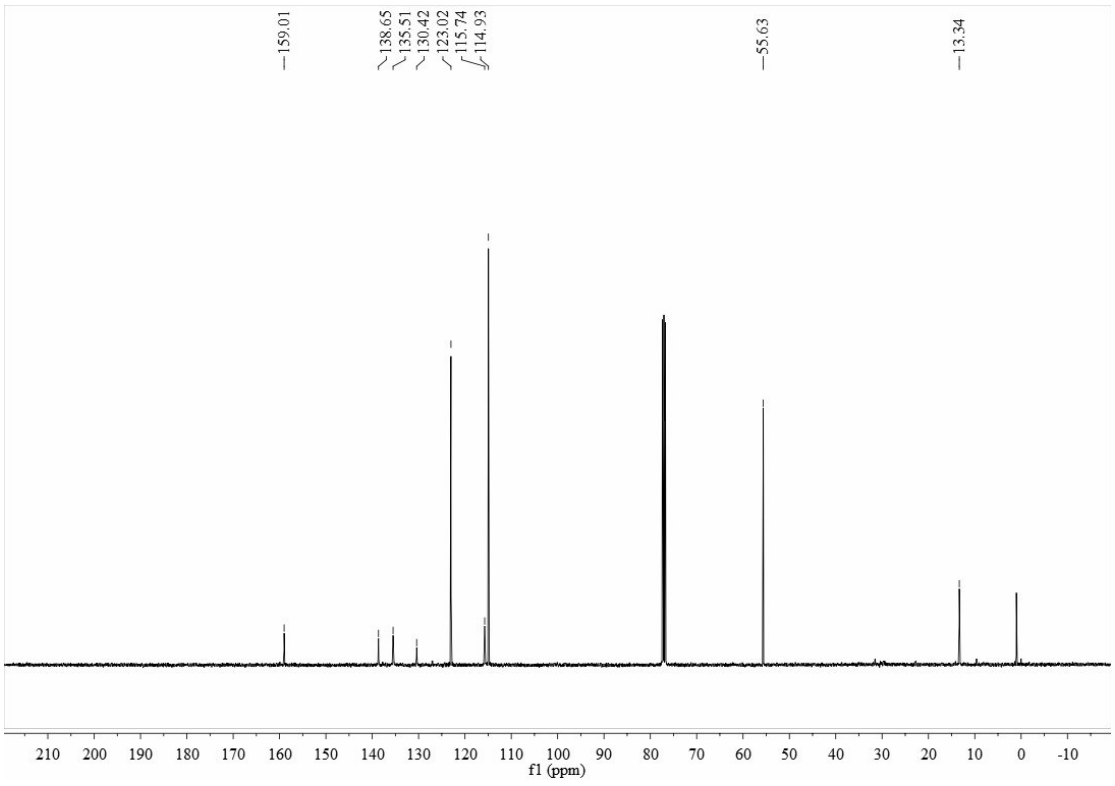
2.22
2.93
3.17
3.05
f1 (ppm)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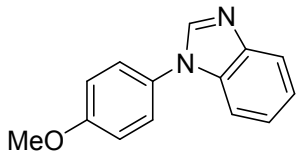
130.42
123.02
115.74
114.93
55.63
13.34
f1 (ppm)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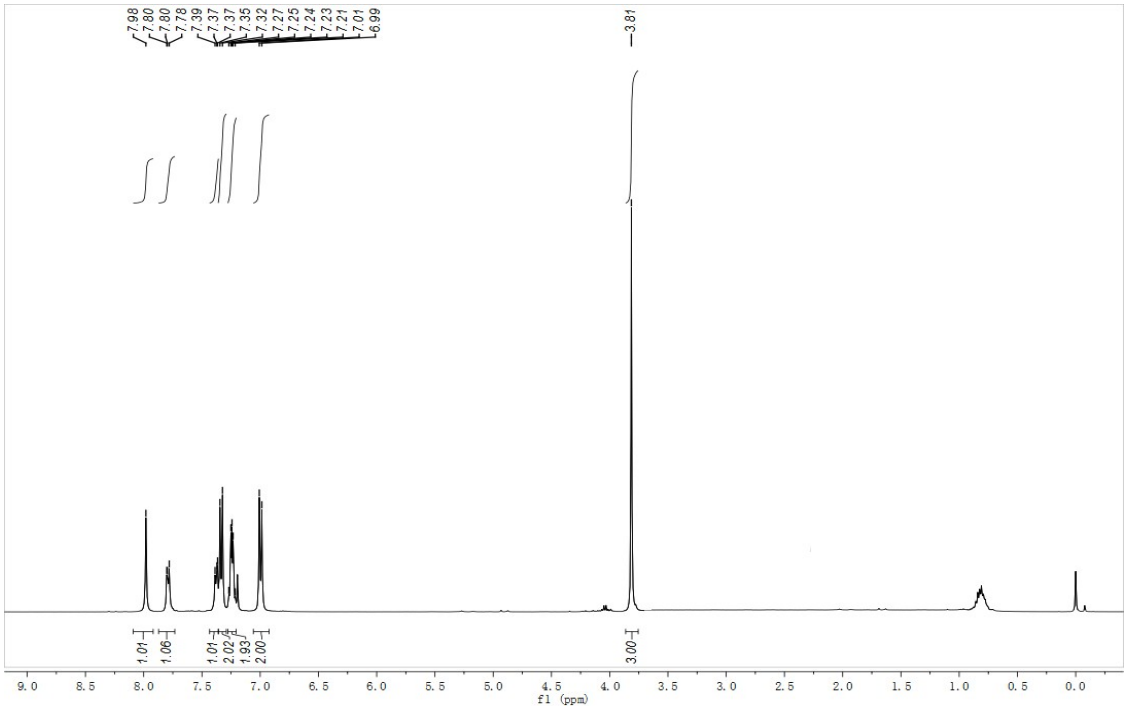
MeO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7.35
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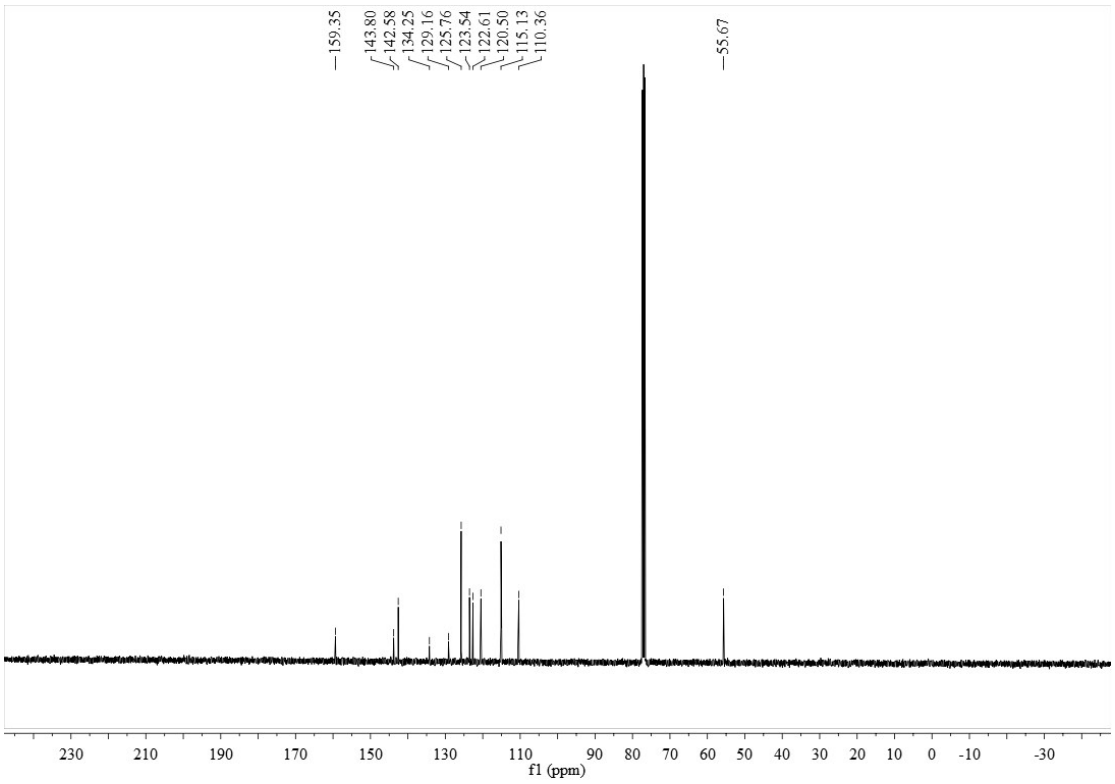
7.27
7.25
7.24
7.23
7.21
7.01
6.99
3.81
1.01
1.06
1.01
2.02
1.93
2.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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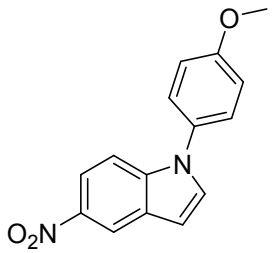
143.80
142.58
134.25
129.16
125.76
123.54
122.61
120.50
115.13
110.36
55.67
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -30
f1 (ppm)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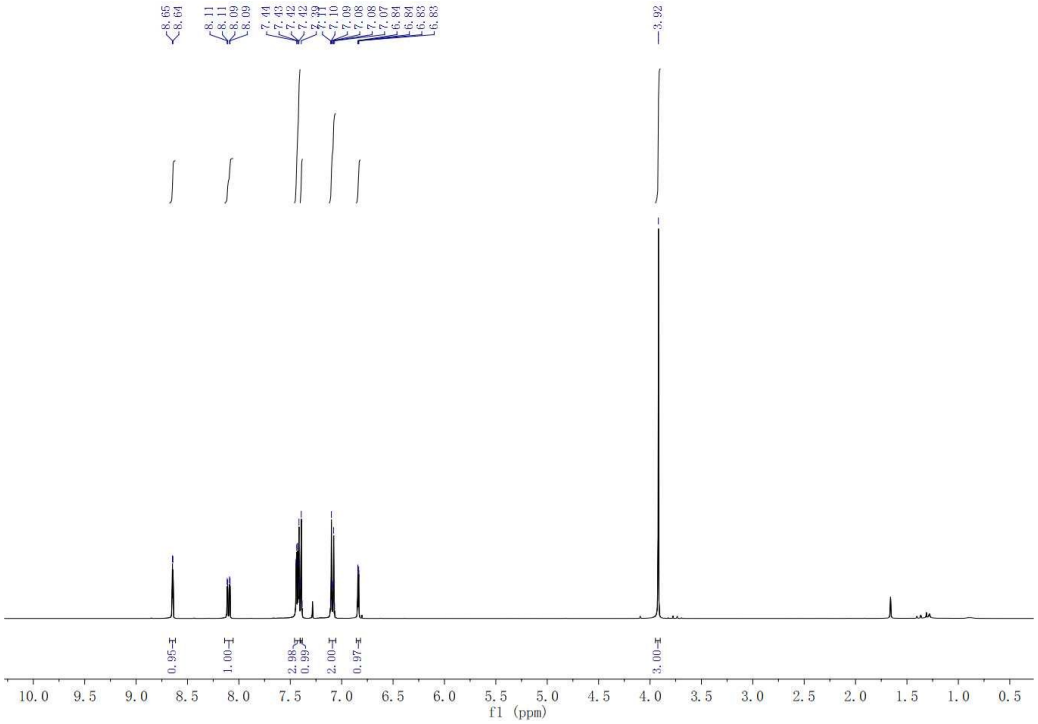
O_2N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7.43
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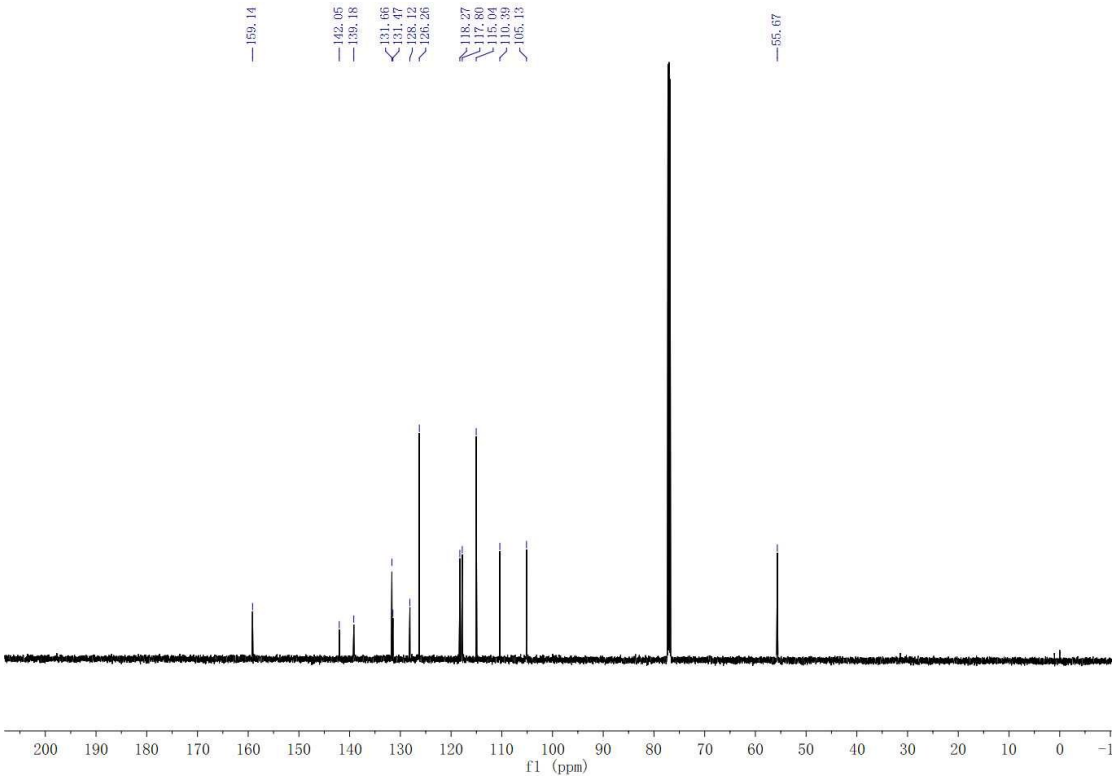
7.42
7.39
7.11
7.10
7.09
7.08
7.08
7.07
6.84
6.84
6.83
6.83
3.92
0.95
1.00
2.98
0.99
2.00
0.97
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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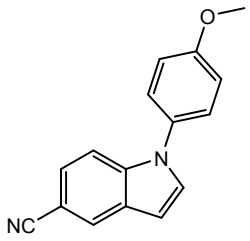
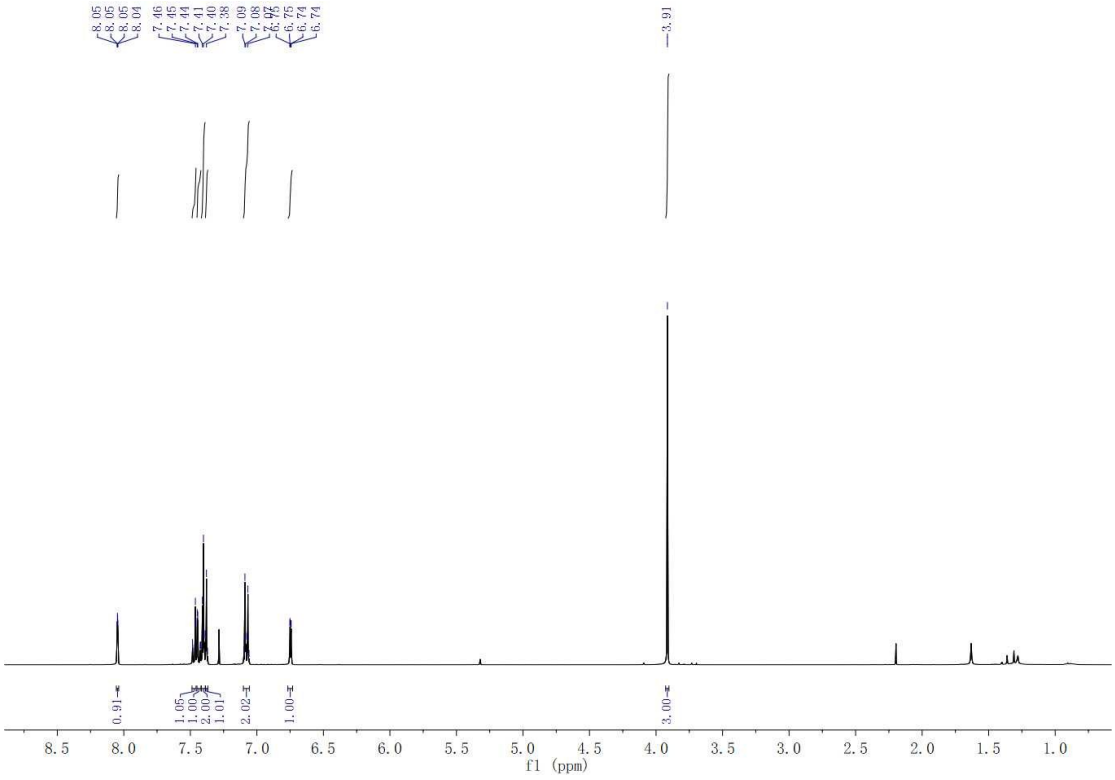
131.66
131.47
128.12
126.26
118.27
117.80
115.94
110.39
105.13
55.67
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


O
N
NC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8.05
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7.41
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7.38
7.09
7.08
6.75
6.74
6.74
3.91
0.91
1.05
1.00
2.00
1.01
2.02
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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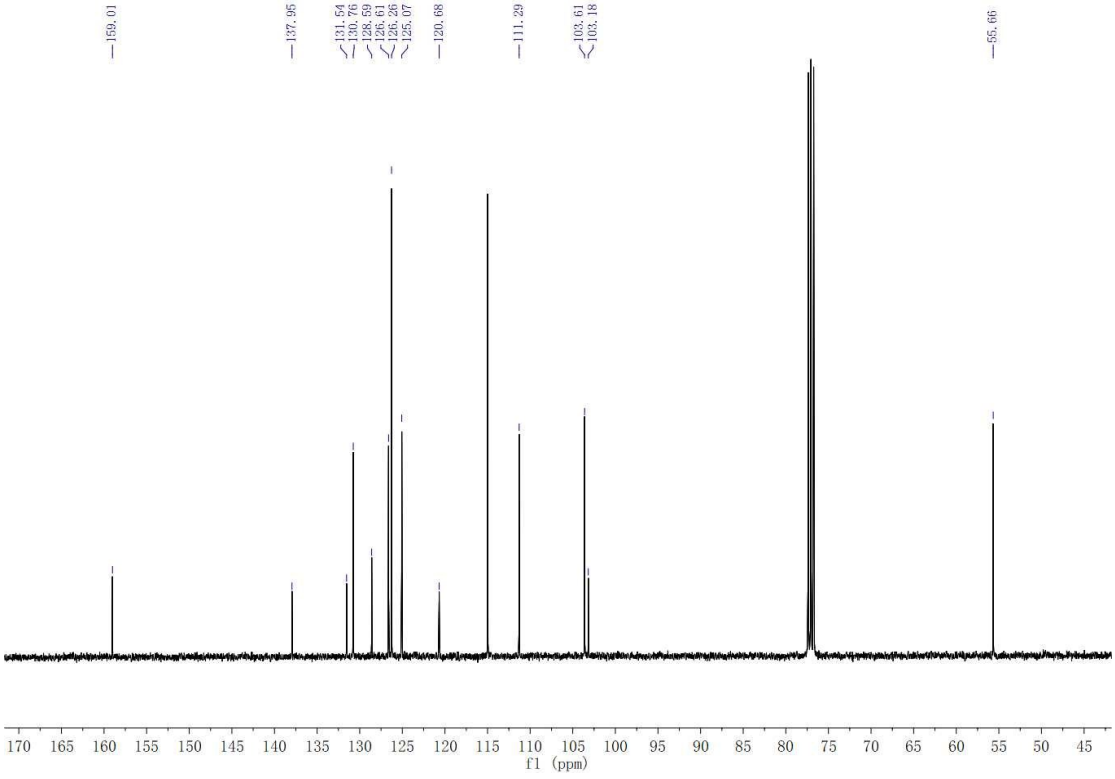
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)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160
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150
145
140
135
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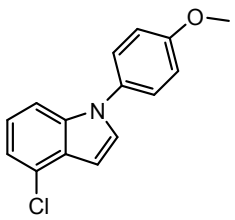
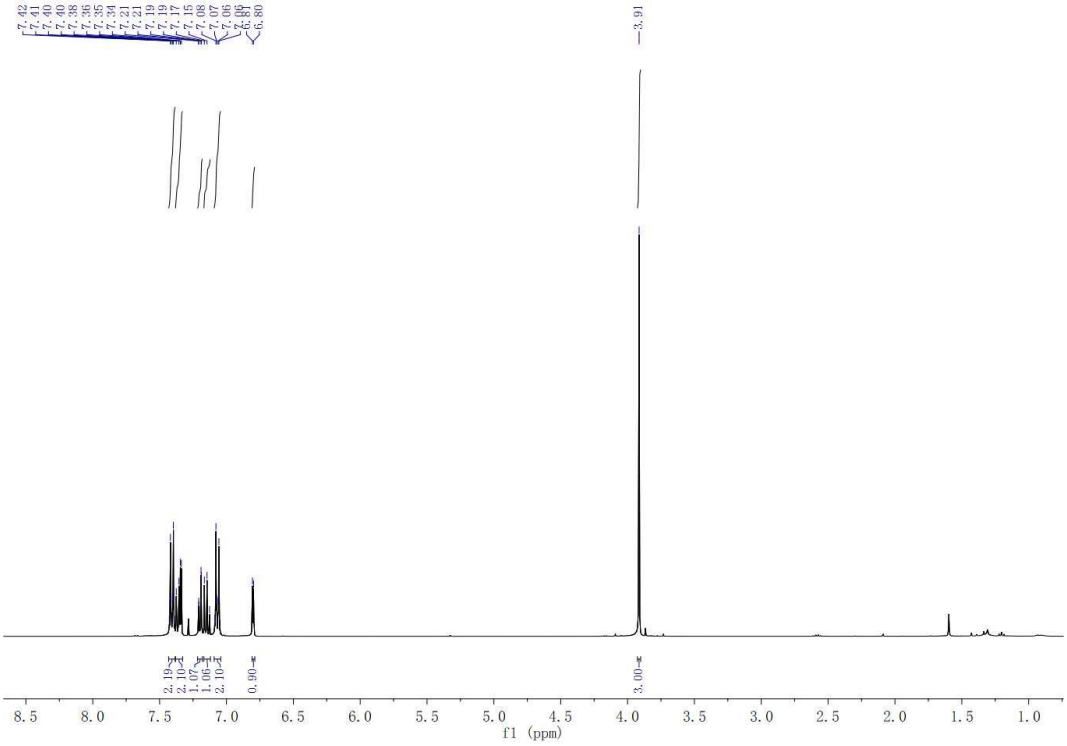
70
65
60
55
50
45
f1 (ppm)


O
N
Cl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7.15
7.08
7.07
7.06
6.81
6.80
3.91
2.19
2.10
1.07
1.06
2.10
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3.00
8.5
8.0
7.5
7.0
6.5
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4.0
3.5
3.0
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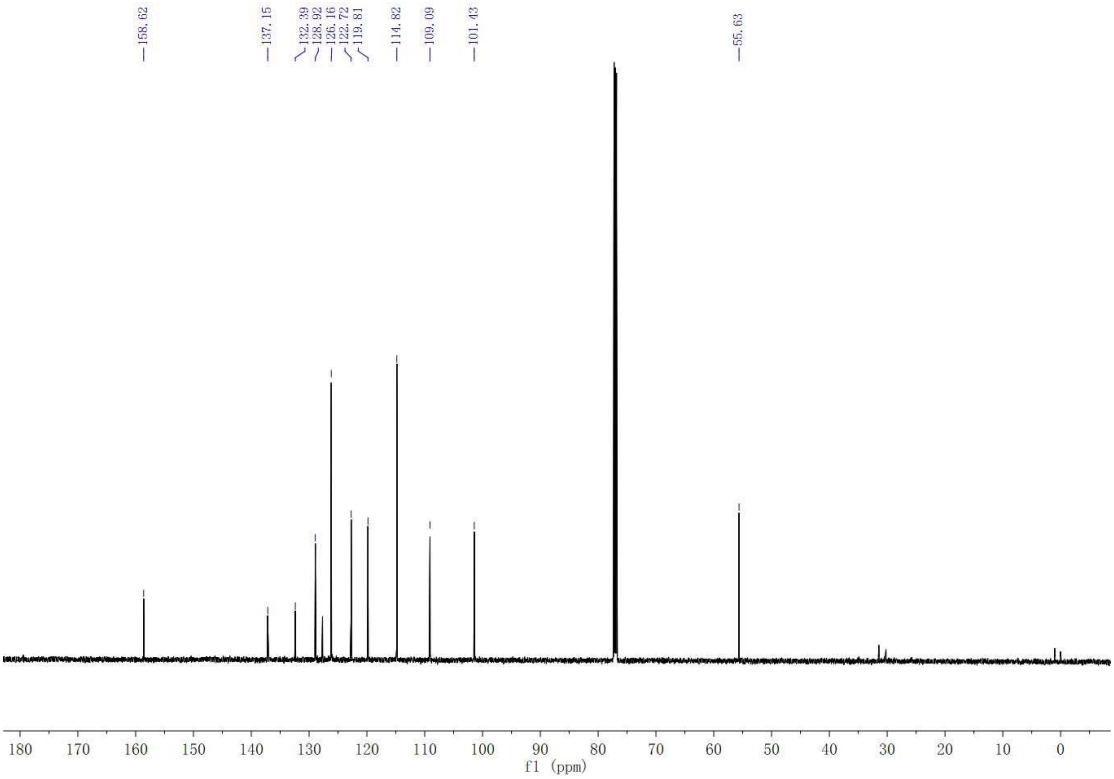
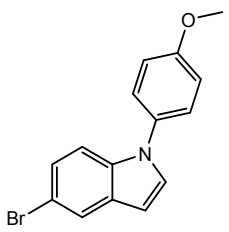
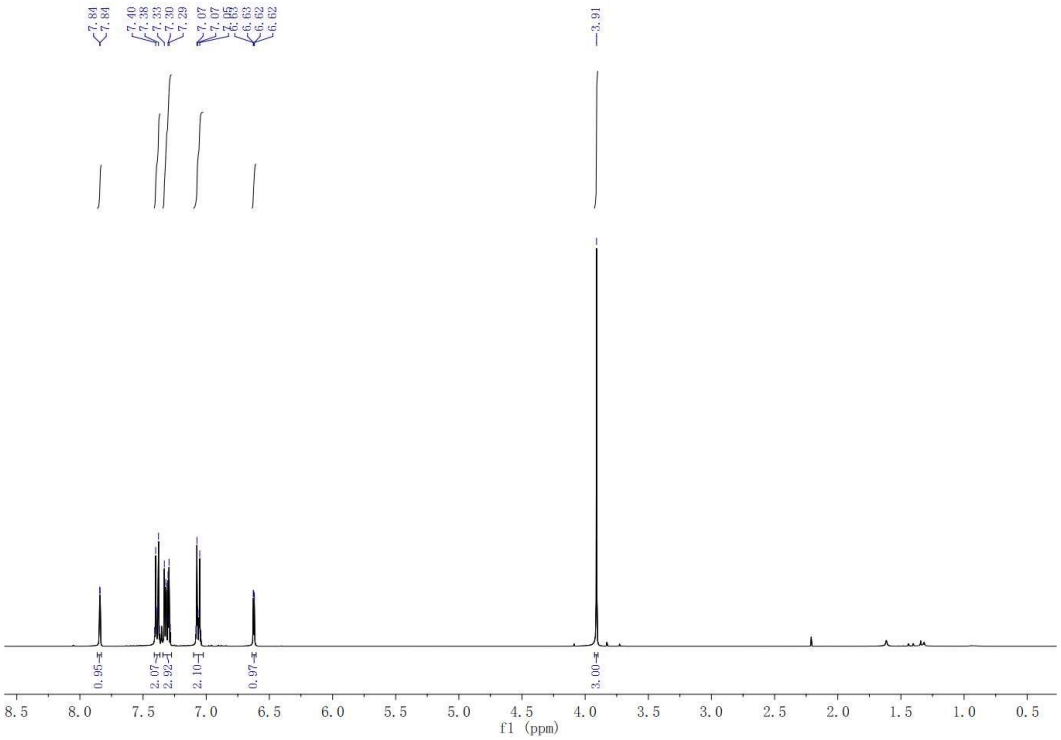
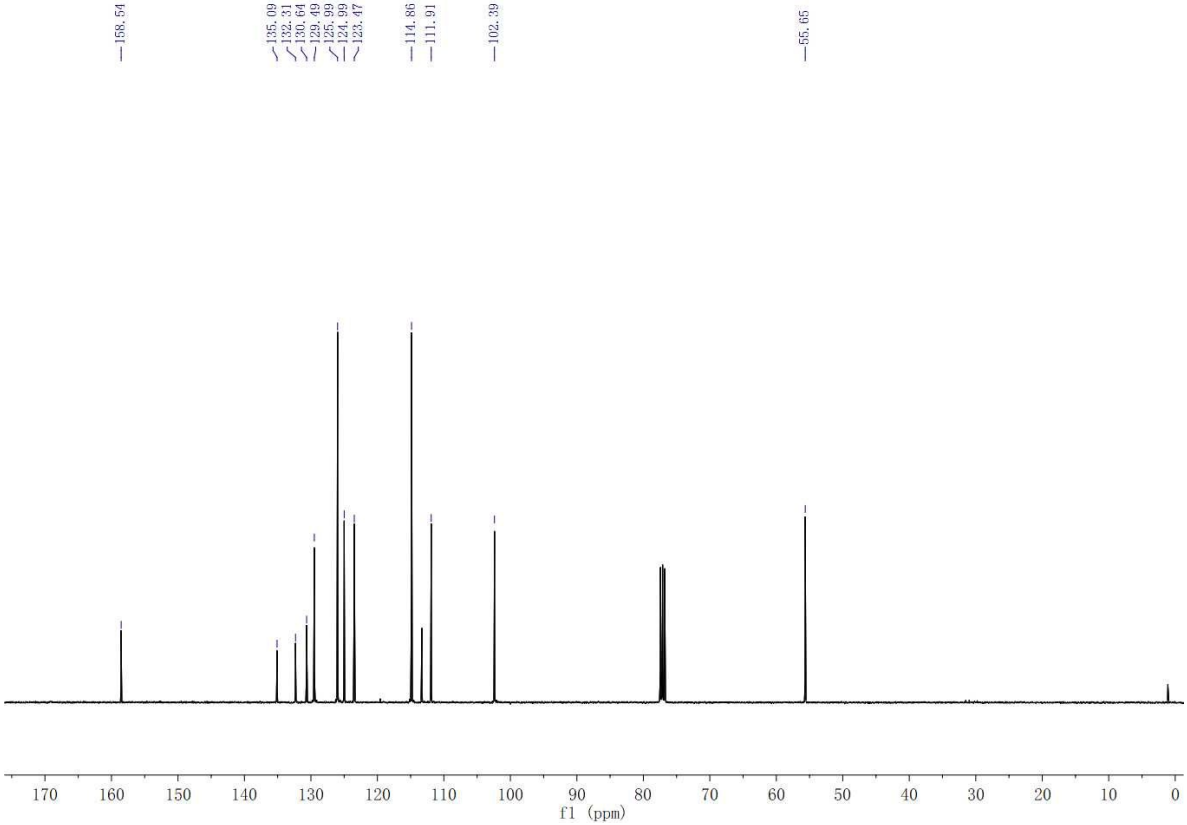
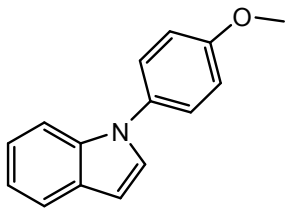
2.0
1.5
1.0
f1 (ppm)

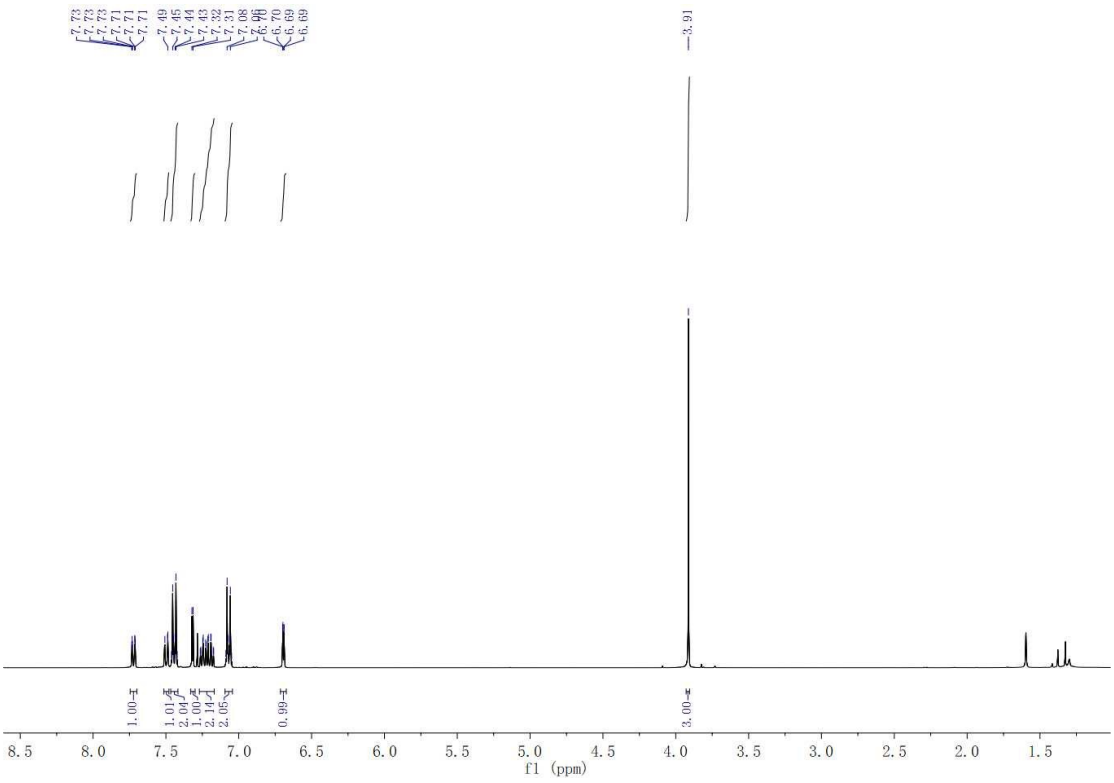

158.62
137.15
132.39
128.92
126.16
122.72
119.81
114.82
109.09
101.43
55.63
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

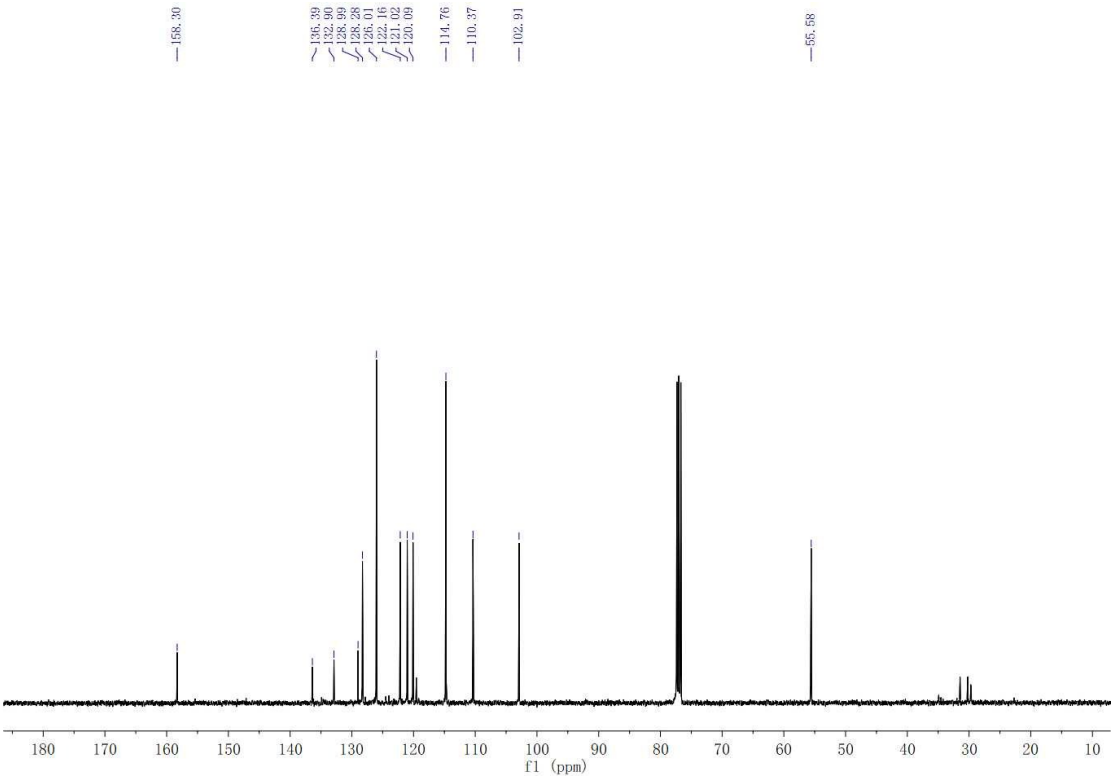

O
N
Br


7.84
7.84
7.40
7.38
7.33
7.30
7.29
7.07
7.07
6.63
6.62
6.62
3.91
0.95
2.07
2.02
2.10
0.97
3.00
f1 (ppm)


158.54
135.09
132.31
130.64
129.49
125.99
124.99
123.47
114.86
111.91
102.39
55.65
f1 (ppm)


O
N


7.73
7.73
7.73
7.71
7.71
7.71
7.49
7.45
7.44
7.43
7.32
7.31
7.08
6.70
6.69
6.69
3.91
1.00
1.01
2.04
1.00
1.14
2.05
0.99
3.00
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
f1 (ppm)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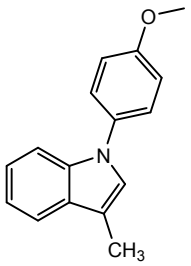
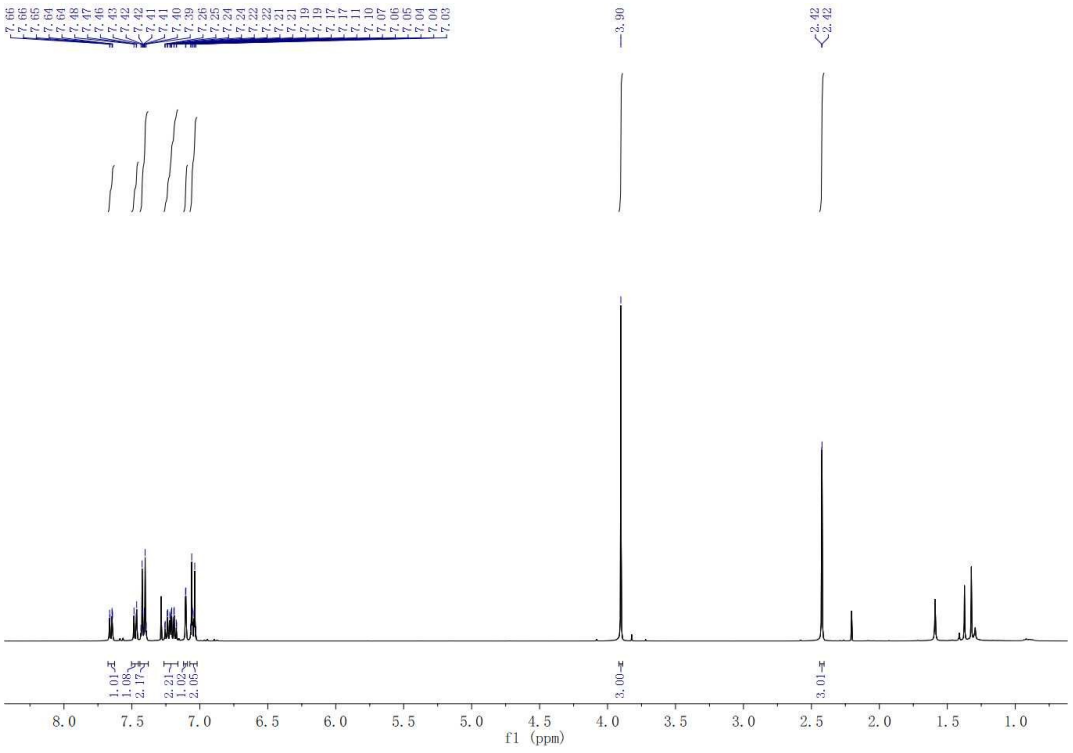
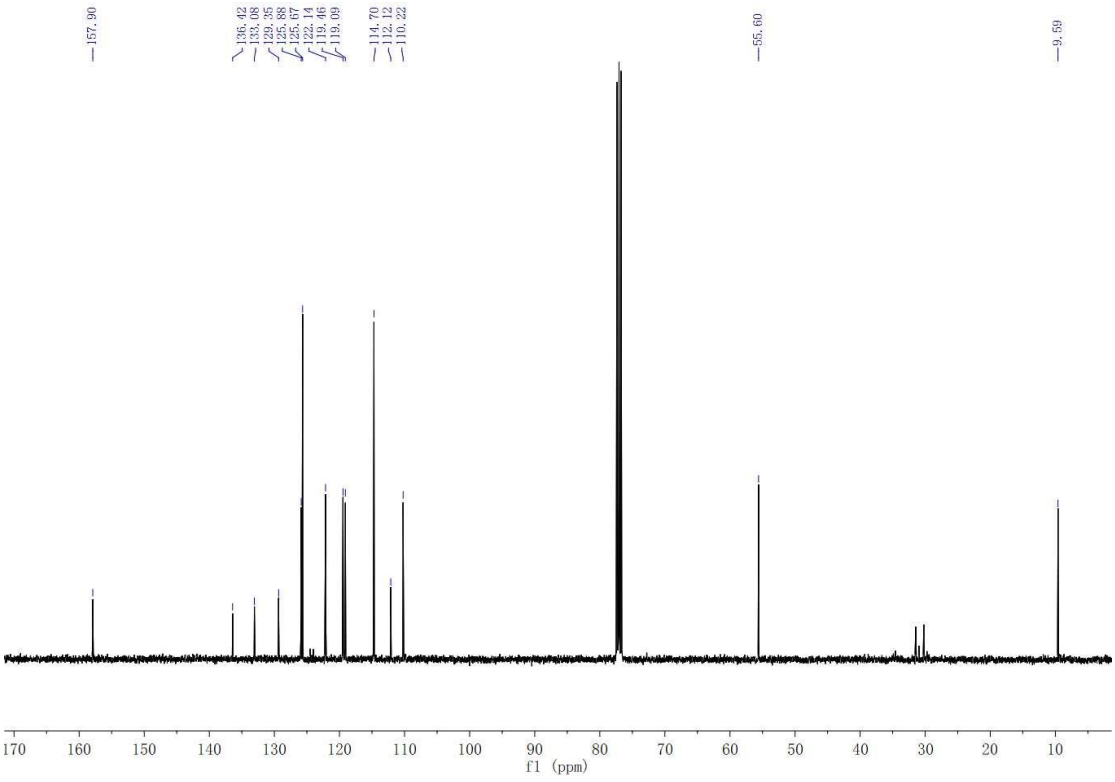
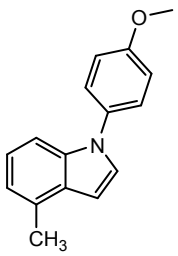
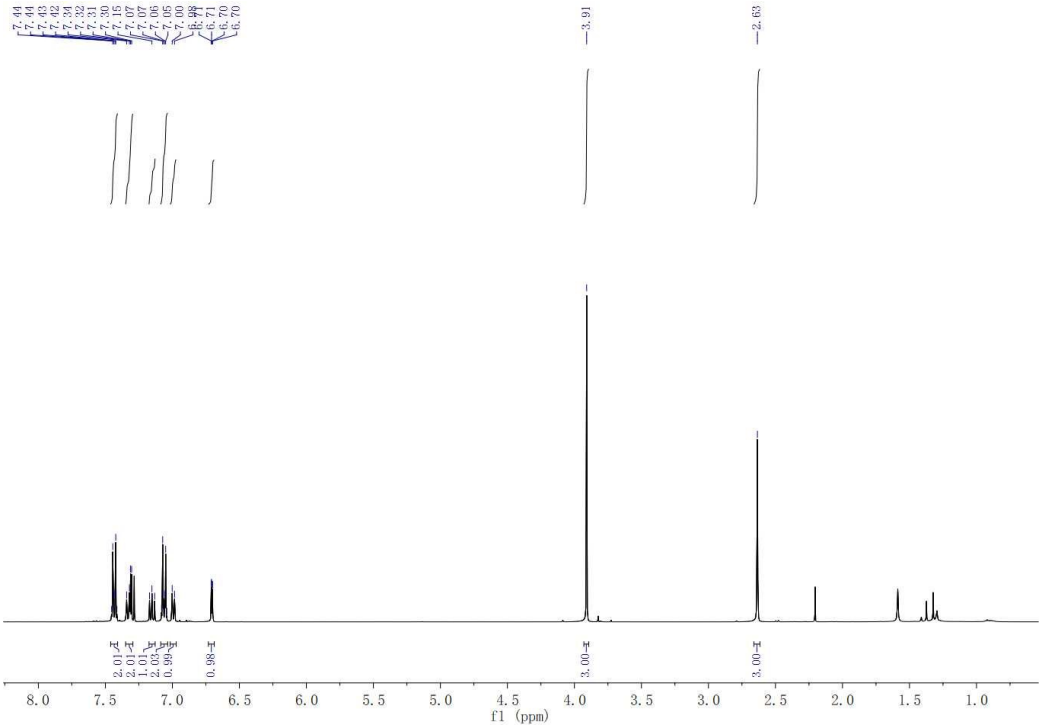
136.39
132.90
128.99
128.28
126.01
122.16
121.02
120.09
114.76
110.37
102.91
55.58
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

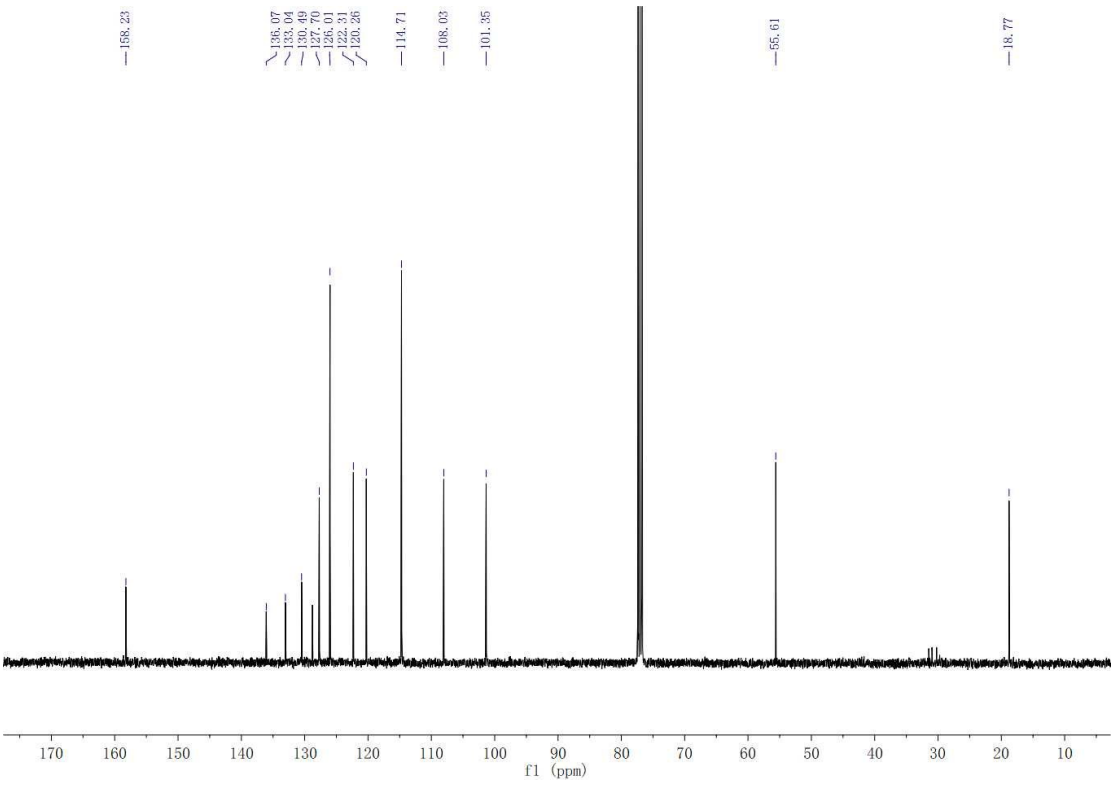

O
N
CH3


7.66
7.66
7.65
7.64
7.64
7.48
7.47
7.46
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.26
7.25
7.24
7.24
7.22
7.22
7.21
7.21
7.19
7.19
7.17
7.17
7.11
7.10
7.07
7.06
7.05
7.04
7.04
7.03
3.90
2.42
2.42
1.01
1.08
2.17
2.21
1.02
2.05
3.00
3.01
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
f1 (ppm)


157.90
136.42
133.08
129.35
125.88
125.67
122.14
119.46
119.09
114.70
112.12
110.22
55.60
9.59
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
N
CH3


7.44
7.44
7.43
7.42
7.34
7.32
7.31
7.30
7.15
7.07
7.07
7.05
7.00
6.98
6.71
6.70
6.70
3.91
2.63
2.01
2.01
1.01
2.03
0.99
0.98
3.00
3.00
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
f1 (ppm)


158.23
136.07
133.04
130.49
127.70
126.01
122.31
120.26
114.71
108.03
101.35
55.61
18.77
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

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