Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.


# Supporting Information

# δ-Cyano Substituted *para*-Quinone Methides Enables Access to Unsymmetric Tri- and Tetraarylmethanes Containing All-Carbon Quaternary Stereocenters

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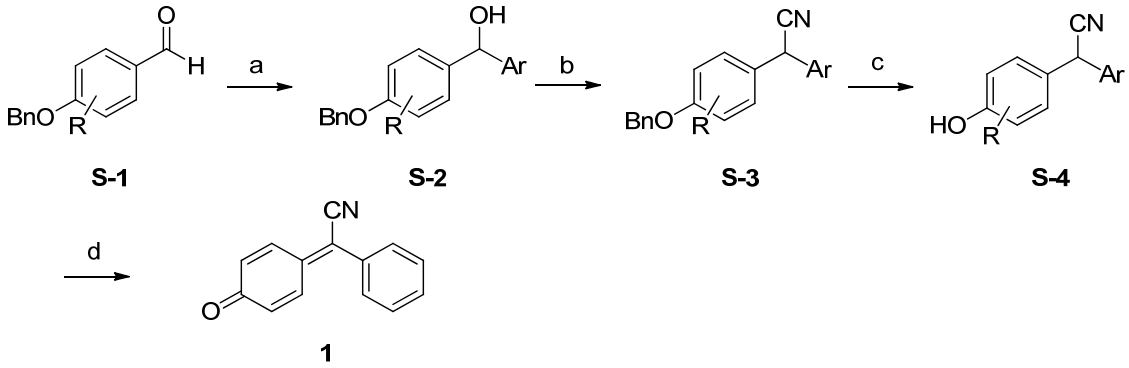
## General information

Proton ($^{1}$H NMR) nuclear magnetic resonance spectra were recorded at 500 MHz respectively. Carbon ($^{13}$C NMR) nuclear magnetic resonance spectra were recorded at 126 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: $CDCl_3$ = 7.26 ppm, $(CD_3)_2CO$ = 2.05 ppm; for $^{13}$C NMR: $CDCl_3$ = 77.23 ppm, $(CD_3)_2CO$ = 206.23 ppm/29.82ppm. Analytical TLC was performed on precoated silica gel GF254 plates. Column chromatography was carried out on silica gel (200–300 mesh). HRMS were carried out on an Orbitrap analyzer.

**Substrate preparation**



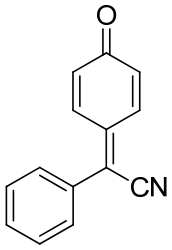

**Regent and condition:**(**a**) ArMgBr (1.0 equiv), THF, 0 °C; (**b**) $InCl_3$ (0.1 equiv), TMSCN (1.3 equiv), $CH_2Cl_2$, 0 °C; (**c**) Pd/C (10%), MeOH, hydrogen balloon, r.t; (**d**) DDQ (1.0 equiv), $CH_2Cl_2$, rt.

To a solution of S-**1** (10.0 mmol, 1.0 equiv) in anhydrous THF at 0 ºC was added a freshly prepared solution of ArMgBr (1.0 M, 10 mL) in THF dropwise under $N_2$. After stirred at the same temperature for 0.5h, the reaction was warmed up to room temperature slowly and stirred for 2 h. Upon completion, the mixture was quenched dropwise by a saturated aqueous $NH_4Cl$ solution (15 mL). The organic layer was extracted with ethyl acetate (3×20 mL) and the combined organic layers were washed with saturated brine, dried over anhydrous $MgSO_4$, filtered and removed under vacuum to afford crude **S-2**.

To a mixture of $InCl_3$ (1.0 mmol, 0.1 equiv) and TMSCN (13.0 mmol, 1.3 equiv) in anhydrous $CH_2Cl_2$ (20 mL) was added a solution of **S-2** in anhydrous $CH_2Cl_2$ (10 mL) dropwise at 0 ºC. The reaction was stirred at the same temperature and monitored by TLC until the complete conversion. Then it was quenched by saturated aqueous $NaHCO_3$ solution (20 mL) and extracted with $CH_2Cl_2$ (3×20 mL). The combined organic layers were washed with saturated brine, dried over anhydrous $MgSO_4$, filtered and removed under vacuum. The residue was purified by a column chromatography on silica gel using ethyl acetate/petroleum ether as eluent to give **S-3**. The product **S-3** was dissolved in 20 mL MeOH solution, and 10% Pd/C (10 wt % of the substrate) was added. The mixture was stirred overnight under a hydrogen balloon at room temperature before it was filtered through a Celite pad. The solvent was

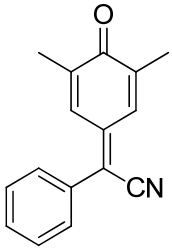
removed under vacuum and the residue was purified by a column chromatography on silica gel using ethyl acetate/petroleum ether as eluent to give **S-4**.

To a solution of **S-4** in $CH_2Cl_2$ (20.0 mL) was added DDQ (1.0 equiv) and it was stirred at room temperature for 1 h. Then the solvent was removed under vacuum and the residue was purified by silica gel chromatography using ethyl acetate/petroleum ether as eluent to afford product **1**.



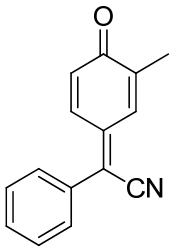

**2-(4-Oxocyclohexa-2,5-dien-1-ylidene)-2-phenylacetonitrile (1a)**

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.59–7.50 (m, 5H), 7.48 (dd, *J* = 10.1, 2.7 Hz, 1H), 6.62 (dd, *J* = 10.0, 1.9 Hz, 1H), 6.49 (dd, *J* = 10.1, 1.9 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.6, 139.8, 137.1, 134.6, 132.1, 131.6, 131.5, 131.4, 130.6, 129.5, 124.1, 117.3; HRMS (ESI) m/z calculated for $C_{14}H_{10}NO$ $[M + H]^+$ 208.0757, found 208.0752.



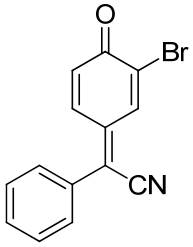

**2-(3,5-Dimethyl-4-oxocyclohexa-2,5-dien-1-ylidene)-2-phenylacetonitrile (1b)**

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 2.6, 1.4 Hz, 1H), 7.53–7.47 (m, 5H), 7.21 (dd, *J* = 2.6, 1.4 Hz, 1H), 2.13 (d, *J* = 1.4 Hz, 3H), 2.02 (d, *J* = 1.4 Hz, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 187.1, 140.6, 139.9, 139.9, 133.3, 132.6, 130.7, 130.7, 130.6, 129.3, 120.1, 117.9, 17.0, 16.7; HRMS (ESI) m/z calculated for $C_{16}H_{14}NO$ $[M + H]^+$ 236.1070, found 236.1073.



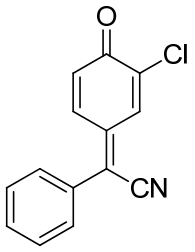

**2-(3-Methyl-4-oxocyclohexa-2,5-dien-1-ylidene)-2-phenylacetonitrile (1c)**

**1c** was obtained as a 1:1 mixture of the Z/E isomers. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 9.9, 2.7 Hz, 1H), 7.69–7.65 (m, 1H), 7.61–7.47 (m, 9H), 7.40 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.32–7.27 (m, 1H), 6.60 (d, *J* = 9.9 Hz, 1H), 6.47 (d, *J* = 10.0 Hz, 1H), 2.15 (d, *J* = 1.4 Hz, 3H), 2.03 (d, *J* = 1.4 Hz, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.9, 186.8, 140.5, 140.4, 140.3, 140.2, 136.7, 134.2, 133.6, 132.4, 132.3, 131.3, 131.3, 131.0, 130.6, 130.5, 129.4, 129.4, 122.0, 117.6, 16.8, 16.4; HRMS (ESI) m/z calculated for $C_{15}H_{12}NO$ $[M + H]^+$ 222.0913, found 222.0909.



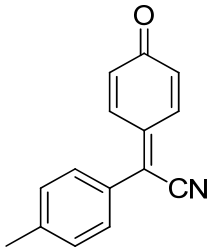

**2-(3-bromo-4-oxocyclohexa-2,5-dien-1-ylidene)-2-phenylacetonitrile (1d)**

**1d** was obtained as a 1:1 mixture of the Z/E isomers. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 2.5 Hz, 1H), 7.92 (d, *J* = 2.5 Hz, 1H), 7.85 (dd, *J* = 9.8, 2.5 Hz, 1H), 7.66–7.42 (m, 11H), 6.75 (d, *J* = 9.9 Hz, 1H), 6.63 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 179.1, 179.1, 139.6, 139.4, 138.4, 137.0, 136.1, 134.7, 131.9, 131.9, 131.9, 130.7, 130.7, 130.7, 130.6, 130.5, 130.2, 129.7, 129.6, 124.7, 124.6, 117.1, 117.0, 100.1; HRMS (ESI) m/z calculated for $C_{14}H_9BrNO$ $[M + H]^+$ 285.9862, found 285.9865.



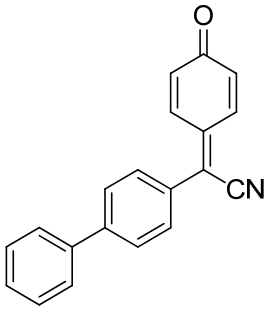

**2-(3-Chloro-4-oxocyclohexa-2,5-dien-1-ylidene)-2-phenylacetonitrile (1e)**

**1e** was obtained as a 1:1 mixture of the Z/E isomers. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 2.5 Hz, 1H), 7.83 (dd, *J* = 9.9, 2.5 Hz, 1H), 7.65 (d, *J* = 2.5 Hz, 1H), 7.60–7.54 (m, 5H), 7.54–7.49 (m, 5H), 7.48 (dd, *J* = 10.0, 2.5 Hz, 1H), 6.71 (d, *J* = 9.9 Hz, 1H), 6.60 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 179.1, 179.0, 139.2, 139.0, 137.5, 137.3, 136.9, 134.7, 134.3, 132.1, 131.9, 131.8, 131.1, 131.1, 130.7, 130.6, 129.7, 129.6, 124.9, 124.8, 117.0, 116.9; HRMS (ESI) m/z calculated for $C_{14}H_9ClNO$ $[M + H]^+$ 242.0367, found 242.0372.



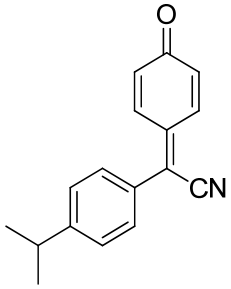

**2-(4-Oxocyclohexa-2,5-dien-1-ylidene)-2-(p-tolyl)acetonitrile (4a)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.51 (dd, *J* = 10.1, 2.7 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.60 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.48 (dd, *J* = 10.1, 1.8 Hz, 1H), 2.45 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.7, 142.5, 139.2, 137.3, 134.9, 131.4, 131.4, 130.7, 130.2, 129.4, 124.5, 117.4, 21.8; HRMS (ESI) m/z calculated for $C_{15}H_{12}NO$ $[M + H]^+$ 222.0913, found222.0916.



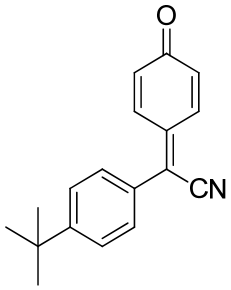

**2-([1,1'-Biphenyl]-4-yl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4b)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.66–7.60 (m, 4H), 7.58 (dd, *J* = 10.1, 2.7 Hz, 1H), 7.53–7.48 (m, 2H), 7.46–7.41 (m, 1H), 6.63 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.52 (dd, *J* = 10.1, 1.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.7, 144.5, 139.6, 139.5, 137.2, 134.7, 131.5, 131.3, 131.0, 129.3, 128.7, 128.1, 127.4, 123.9, 117.3; HRMS (ESI) m/z calculated for $C_{20}H_{14}NO$ $[M + H]^+$ 284.1070, found 284.1066.



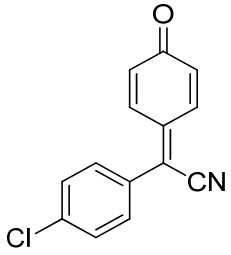

**2-(4-Isopropylphenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4c)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.53 (dd, *J* = 10.1, 2.7 Hz, 1H), 7.48–7.43 (m, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 6.60 (dd, *J* = 10.0, 1.9 Hz, 1H), 6.48 (dd, *J* = 10.1, 1.9 Hz, 1H), 2.99 (hept, *J* = 6.9 Hz, 1H), 1.29 (d, *J* = 6.9 Hz, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.6, 153.0, 139.0, 137.1, 134.7, 131.2, 131.2, 130.7, 129. 6, 127.5, 124.4, 117.2, 34.2, 23.7; HRMS (ESI) m/z calculated for $C_{17}H_{16}NO$ $[M + H]^+$ 250.1226, found 250.1229.



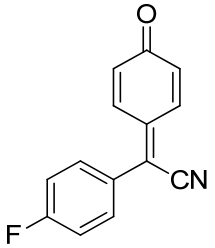

**2-(4-(*tert*-Butyl)phenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4d)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.59–7.51 (m, 3H), 7.49–7.44 (m, 2H), 6.61 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.49 (dd, *J* = 10.1, 1.8 Hz, 1H), 1.37 (s, 9H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.7, 155.5, 139.2, 137.2, 134.9, 131.3, 131.3, 130.6, 129.4, 126.5, 124.4, 117.3, 35.3, 31.2; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO$ $[M + H]^+$ 264.1383, found 264.1378.



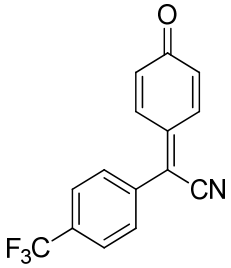

**2-(4-Chlorophenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4e)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 10.0, 2.6 Hz, 1H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.43 (dd, *J* = 10.1, 2.6 Hz, 1H), 6.62 (dd, *J* = 10.0, 1.6 Hz, 1H), 6.50 (dd, *J* = 10.1, 1.5 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.5, 140.1, 138.1, 136.9, 134.1, 131.8, 131.8, 130.5, 129.9, 122.6, 116.9; HRMS (ESI) m/z calculated for $C_{14}H_9ClNO$ $[M + H]^+$ 242.0367, found 242.0365.



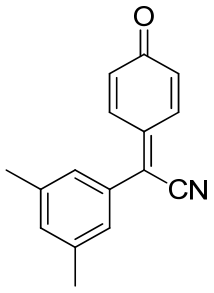

**2-(4-Fluorophenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4f)**

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.56–7.51 (m, 2H), 7.44 (dd, *J* = 10.1, 2.7 Hz, 1H), 7.27–7.23 (m, 2H), 6.62 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.50 (dd, *J* = 10.1, 1.9 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.6, 164.3 (d, *J* = 255.0 Hz), 139.9, 136.9, 134.2, 132.9, 132.8, 131.7 (d, *J* = 2.8 Hz), 128.2 (d, *J* = 3.6 Hz), 117.1, 116.9 (d, *J* = 22.3 Hz); HRMS (ESI) m/z calculated for $C_{14}H_9FNO$ $[M + H]^+$ 226.0663, found 226.0666.




**2-(4-Oxocyclohexa-2,5-dien-1-ylidene)-2-(4-(trifluoromethyl)phenyl)acetonitrile (4g)**

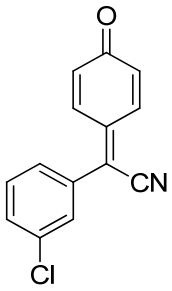
$^1$H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.38 (dd, *J* = 10.1, 2.7 Hz, 1H), 6.62 (dd, *J* = 10.0, 1.7 Hz, 1H), 6.48 (dd, *J* = 10.1, 1.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.4, 141.2, 136.7, 135.4, 133.8, 133.1 (q, *J* = 33.2 Hz), 132.2, 132.1, 130.9, 126.6 (q, *J* = 3.7 Hz), 123.6 (q, *J* = 272.6 Hz), 121. 9, 116.8; HRMS (ESI) m/z calculated for $C_{15}H_9F_3NO$ $[M + H]^+$ 276.0631, found 276.0635.




**2-(3,5-Dimethylphenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4h)**

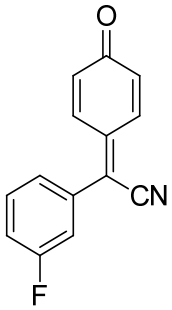
$^1$H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 10.0, 2.6 Hz, 1H), 7.50 (dd, *J* = 10.1, 2.6 Hz, 1H), 7.17 (s, 1H), 7.12 (s, 2H), 6.60 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.48 (dd, *J* = 10.1, 1.8 Hz, 1H), 2.39 (s, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.8, 139.5, 139.4, 137.2,

135.0, 133.3, 132.1, 131.5, 131.3, 128.4, 124.79, 117.4, 21.5; HRMS (ESI) m/z calculated for $C_{16}H_{14}NO$ $[M + H]^+$ 236.1070, found 236.1067.



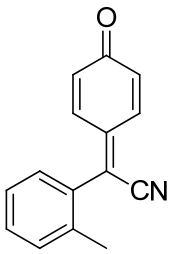

**2-(3-Chlorophenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4i)**

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.48–7.40 (m, 3H), 7.37–7.31 (m, 2H), 6.56 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.44 (dd, *J* = 10.1, 1.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.5, 140.7, 136.8 135.7, 134.0, 133.6, 132.0, 131.9, 131.5, 130.8, 130.3, 128.7, 122.1, 116.9; HRMS (ESI) m/z calculated for $C_{14}H_9ClNO$ $[M + H]^+$ 242.0367, found 242.0365.



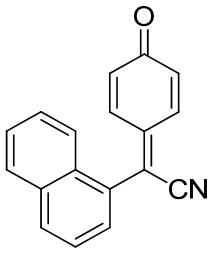

**2-(3-Fluorophenyl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4j)**

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.38 (dd, *J* = 10.1, 2.7 Hz, 1H), 6.65 (dd, *J* = 10.0, 1.9 Hz, 1H), 6.50 (dd, *J* = 10.1, 1.9 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.4, 162.8 (d, *J* = 250.3 Hz), 140.6, 136.8, 134.1, 133.7 (d, *J* = 7.9 Hz), 131.9, 131.8, 131.2 (d, *J* = 8.3 Hz), 126.3 (d, *J* = 3.2 Hz), 122.2, 118.4 (d, *J* = 21.1 Hz), 117.4 (d, *J* = 23.4 Hz), 116.9; HRMS (ESI) m/z calculated for $C_{14}H_9FNO$ $[M + H]^+$ 226.0663, found 226.0667.



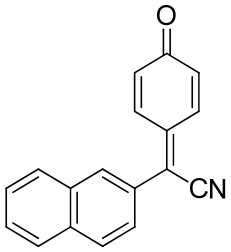

**2-(4-Oxocyclohexa-2,5-dien-1-ylidene)-2-(o-tolyl)acetonitrile (4k)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 10.0, 2.6 Hz, 1H), 7.42 (td, *J* = 7.6, 1.2 Hz, 1H), 7.32 (dd, *J* = 16.8, 8.0 Hz, 2H), 7.18 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.08 (dd, *J* = 10.1, 2.6 Hz, 1H), 6.61 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.39 (dd, *J* = 10.1, 1.9 Hz, 1H), 2.37 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.7, 141.6, 137.4, 136.4, 134.5, 131.9, 131.5, 131.4, 131.0, 130.9, 130.7, 126.7, 123.4, 116.4, 20.2; HRMS (ESI) m/z calculated for $C_{15}H_{12}NO$ $[M+H]^+$ 222.0913, found 222.0915.




**2-(Naphthalen-1-yl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4l)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.3 Hz, 1H), 8.01–7.93 (m, 2H), 7.86 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.67–7.54 (m, 3H), 7.47 (dd, *J* = 7.1, 0.9 Hz, 1H), 7.08 (dd, *J* = 10.1, 2.6 Hz, 1H), 6.67 (dd, *J* = 10.0, 1.9 Hz, 1H), 6.34 (dd, *J* = 10.1, 1.9 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.7, 142.5, 136.4, 136.0, 134.8, 134.3, 133.9, 133.3, 131.9, 131.8, 131.7, 131.3, 131.1, 130.0, 129.6, 129.3, 129.1, 129.0, 128.8, 128.8, 128.2, 127.6, 127.4, 126.7, 125.3, 124.9, 124.7, 124.2, 122.2, 120.8, 117.0; HRMS (ESI) m/z calculated for $C_{18}H_{12}NO$ $[M+H]^+$ 258.0913, found 258.0910.



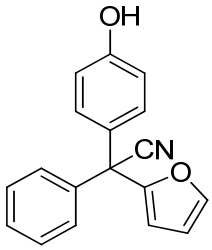

**2-(Naphthalen-2-yl)-2-(4-oxocyclohexa-2,5-dien-1-ylidene)acetonitrile (4m)**

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.04–7.97 (m, 2H), 7.96–7.87 (m, 3H), 7.6 –7.55 (m, 4H), 6.64 (dd, *J* = 10.0, 1.8 Hz, 1H), 6.52 (dd, *J* = 10.1, 1.8 Hz, 1H);$^{13}$C NMR (126 MHz, $CDCl_3$) δ 186.6, 139.8, 137.2, 134.9, 134.2, 132.9, 131.7, 131.6, 131.6, 129.5, 129.5, 129.0, 128.8, 128.1, 127.8, 126.5, 124.3, 117.4; HRMS (ESI) m/z calculated for $C_{18}H_{12}NO$ $[M + H]^+$ 258.0913, found 258.0917.

**General procedure**

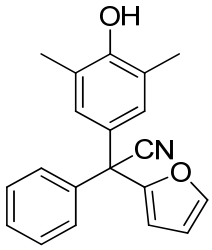
To a solution of **1** (0.1 mmol, 1.0 equiv) in $CH_2Cl_2$ (3.0 mL) was successively added $Bi(OTf)_3$ (0.01 mmol, 0.1 equiv) and **2** (0.12 mmol, 1.2 equiv) at rt. The mixture was stirred at the same temperature for 20 min. Then the mixture was concentrated and purified by a flash column chromatography to give the desired product.

**Analytical data for products**



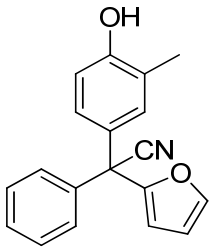

**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (3a)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **3a** (25.3 mg, 93%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.52–7.45 (m, 1H), 7.42–7.34 (m, 3H), 7.29–7.26 (m, 2H), 7.16–7.05 (m, 2H), 6.86–6.78 (m, 2H), 6.41–6.32 (m, 1H), 6.04 (dd, *J* = 3.3, 0.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 139.6, 134.0, 132.1, 131.5, 130.1, 129.6, 129.6, 129.2, 129.1, 129.0, 129.0, 128.9, 128.6, 128.1, 128.0, 126.9, 126.4, 124.1, 122.2, 115.8, 112.5, 106.3, 51.9; HRMS (ESI) m/z calculated for $C_{18}H_{12}NO_2$ $[M - H]^-$ 274.0874, found 274.0878.



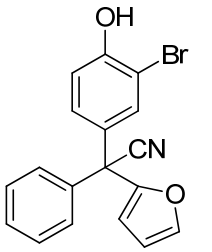

**2-(Furan-2-yl)-2-(4-hydroxy-3,5-dimethylphenyl)-2-phenylacetonitrile (3b)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **3b** (25.7 mg, 90%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 1.0 Hz, 1H), 7.40–7.34 (m, 3H), 7.30–7.26 (m, 2H), 6.85 (s, 2H), 6.38–6.34 (m, 1H), 6.03 (d, *J* = 3.3 Hz, 1H), 4.74 (s, 1H), 2.21 (s, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 152.3, 151.4, 143.7, 138.7, 129.6, 128.7, 128.3, 128.1, 127.9, 123.3, 120.7, 111.0, 110.4, 52.0, 16.0; HRMS (ESI) m/z calculated for $C_{20}H_{16}NO_2$ $[M - H]^-$ 302.1187, found 302.1182.



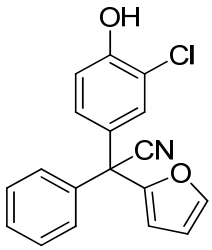

**2-(Furan-2-yl)-2-(4-hydroxy-3-methylphenyl)-2-phenylacetonitrile (3c)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **3c** (24.8 mg, 92%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 1.0 Hz, 1H), 7.41–7.36 (m, 3H), 7.32–7.27 (m, 2H), 7.04 (d, *J* = 2.3 Hz, 1H), 6.90 (dd, *J* = 8.4, 2.5 Hz, 1H), 6.77 (d, *J* = 8.4 Hz, 1H), 6.41–6.35 (m, 1H), 6.04 (d, *J* = 3.3 Hz, 1H), 2.22 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 154.2, 151.2, 143.8, 138.6, 130.5, 130.0, 128.8, 128.4, 127.9, 126.7, 124.6, 120.7, 115.1, 111.2, 110.5, 52.1, 16.0; HRMS (ESI) m/z calculated for $C_{19}H_{14}NO_2$ $[M - H]^-$ 288.1030, found 288.1034.



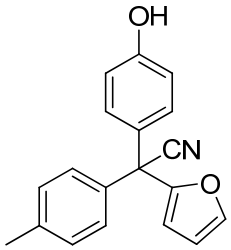

**2-(3-Bromo-4-hydroxyphenyl)-2-(furan-2-yl)-2-phenylacetonitrile (3d)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **3d** (29.7 mg, 91%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.56–7.48 (m, 1H), 7.43–7.37 (m, 4H), 7.30–7.25 (m, 2H), 7.12 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.44–6.35 (m, 1H), 6.14–6.06 (m, 1H), 5.89 (s, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 152.8, 150.7, 144.3, 138.1, 132.0, 131.7, 129.1, 129.1, 129.0, 128.0, 120.2, 116.5, 111.6, 110.8, 110.7, 51.9; HRMS (ESI) m/z calculated for $C_{18}H_{11}BrNO_2$ $[M - H]^-$ 351.9979, found 351.9976.



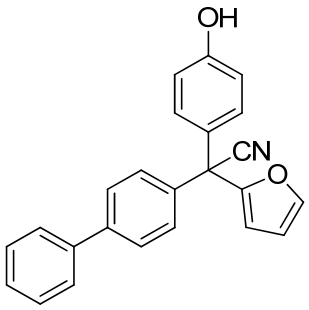

**2-(3-Chloro-4-hydroxyphenyl)-2-(furan-2-yl)-2-phenylacetonitrile (3e)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **3e** (27.2 mg, 88%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.43–7.41 (m, 1H), 7.33–7.29 (m, 3H), 7.20–7.17 (m, 2H), 7.14 (d, *J* = 2.3 Hz, 1H), 7.00 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.93 (d, *J* = 8.6 Hz, 1H), 6.33–6.28 (m, 1H), 6.00 (dd, *J* = 3.3, 0.8 Hz, 1H), 5.69 (s, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 139.6, 134.0, 132.1, 131.5, 130.1, 129.6, 129.6, 129.2, 129.1, 129.0, 129.0, 128.9, 128.6, 128.1, 128.0, 126.9, 126.4, 124.1, 122.2, 115.8, 112.5, 106.3, 51.9; HRMS (ESI) m/z calculated for $C_{18}H_{11}ClNO_2$ $[M - H]^-$ 308.0484, found 308.0480.



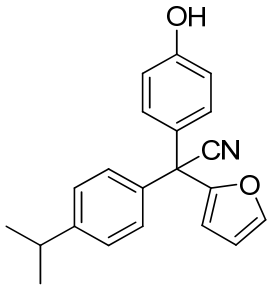

**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-(p-tolyl)acetonitrile (5a)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5a** (25.7 mg, 91%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.50–7.44 (m, 1H), 7.19–7.10 (m, 6H), 6.84–6.79 (m, 2H), 6.38–6.32 (m, 1H), 6.03 (d, *J* = 3.3 Hz, 1H), 2.36 (s, 3H);$^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.7, 151.4, 143.7, 138.3, 135.6, 130.7, 129.4, 129.4, 127.7, 120.6, 115.5, 111.0, 110.4, 51.7, 21.0; HRMS (ESI) m/z calculated for $C_{19}H_{14}NO_2$ $[M - H]^-$ 288.1030, found 288.1033.



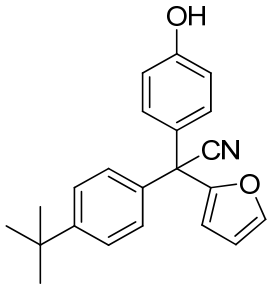

**2-([1,1'-Biphenyl]-4-yl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5b)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5b** (30.9 mg, 90%). $^{1}$H NMR (500 MHz, Acetone) δ 7.77–7.74 (m, 2H), 7.72–7.68 (m, 3H), 7.51–7.47 (m, 2H), 7.42–7.39 (m, 1H), 7.37–7.34 (m, 2H), 7.16–7.11 (m, 2H), 6.95–6.90 (m, 2H), 6.51 (m, 1H), 6.11 (dd, *J* = 3.3, 0.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 139.6, 134.0, 132.1, 131.5, 130.1, 129.6, 129.6, 129.2, 129.1, 129.0, 129.0, 128.9, 128.6, 128.1, 128.0, 126.9, 126.4, 124.1, 122.2, 115.8, 112.5, 106.3, 51.9; HRMS (ESI) m/z calculated for $C_{24}H_{16}NO_2$ $[M - H]^-$ 350.1187, found 350.1185.



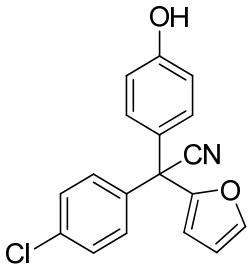

**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-(4-isopropylphenyl)acetonitrile (5c)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5c** (27.9 mg, 90%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.50–7.45 (m, 1H), 7.23–7.20 (m, 2H), 7.18–7.15 (m, 2H), 7.14–7.09 (m, 2H), 6.84–6.79 (m, 2H), 6.39–6.31 (m, 1H), 6.03 (dd, *J* = 3.3, 0.8 Hz, 1H), 2.95–2.87 (m, 1H), 1.25 (d, *J* = 6.9 Hz, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 151.6, 149.4, 143.9, 135.9, 130.7, 129.5, 127.9, 127.0, 120.8, 115.8, 111.2, 110.7, 51.9, 33.9, 24.1; HRMS (ESI) m/z calculated for $C_{21}H_{18}NO_2$ $[M - H]^-$ 316.1343, found 316.1348.



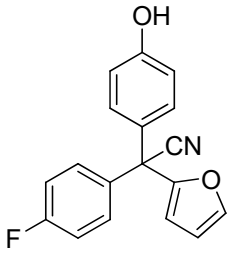

**2-(4-(Tert-butyl)phenyl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5d)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5d** (28.7 mg, 89%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.39–7.35 (m, 2H), 7.20–7.11 (m, 4H), 6.84–6.80 (m, 2H), 6.38–6.32 (m, 1H), 6.04 (dd, *J* = 3.3, 0.8 Hz, 1H), 1.31 (s, 9H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.1, 151.9, 151.9, 144.2, 135.9, 131.1, 129.8, 127.9, 126.1, 121.0, 116.0, 111.4, 110.9, 52.1, 35.0, 31.7; HRMS (ESI) m/z calculated for $C_{22}H_{20}NO_2$ $[M - H]^-$ 330.1500, found 330.1504.



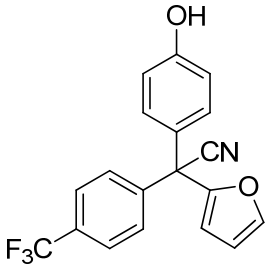

**2-(4-Chlorophenyl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5e)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5e** (27.2 mg, 91%). $^{1}$H NMR (500 MHz, Acetone) δ 8.75 (s, 1H), 7.70 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.55–7.48 (m, 2H), 7.32–7.25 (m, 2H), 7.11–7.05 (m, 2H), 6.94–6.88 (m, 2H), 6.53–6.48 (m, 1H), 6.09 (dd, *J* = 3.3, 0.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.1, 150.8, 144.2, 137.3, 134.8, 130.1, 129.5, 129.5, 129.1, 120.3, 115.9, 111.5, 110.8, 51.7; HRMS (ESI) m/z calculated for $C_{18}H_{11}ClNO_2$ $[M - H]^-$ 308.0484, found 308.0487.



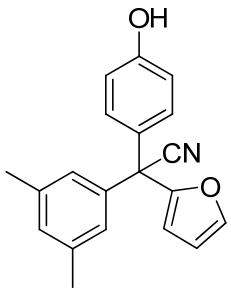

**2-(4-Fluorophenyl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5f)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5f** (27.0 mg,93%). $^{1}$H NMR (500 MHz, Acetone) δ 8.75 (s, 1H), 7.71–7.67 (m, 1H), 7.32–7.27 (m, 2H), 7.26–7.20 (m, 2H), 7.09–7.04 (m, 2H), 6.94–6.89 (m, 2H), 6.52–6.44 (m, 1H), 6.07 (dd, *J* = 3.3, 0.7 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ162.6 (d, *J* = 248.8 Hz), 156.2, 151.0, 144.1, 134.4 (d, *J* = 3.3 Hz), 130.2, 129.8 (d, *J* = 8.3 Hz), 129.4, 120.6, 116.0, 115.8 (d, *J* = 21.9 Hz), 111.4, 110.7, 51.6; HRMS (ESI) m/z calculated for $C_{18}H_{11}FNO_2$ $[M - H]^-$ 292.0779, found 292.0776.



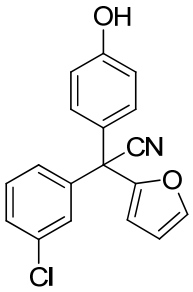

**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-(4-(trifluoromethyl)phenyl)acetonitrile (5g)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5g** (29.3 mg, 89%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.54–7.47 (m, 1H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.14–7.07 (m, 2H), 6.87–6.80 (m, 2H), 6.41–6.35 (m, 1H), 6.09 (dd, *J* = 3.3, 0.8 Hz, 1H), 5.08 (s, 1H); $^{13}$C NMR (126 MHz, Acetone) δ 156.1, 150.4, 144.4, 142.6, 131.1, 129.9, 129.6, 128.6, 126.0 (q, *J* = 3.7 Hz), 120.0, 116.0, 111.6, 110.9, 52.1; HRMS (ESI) m/z calculated for $C_{19}H_{11}F_3NO_2$ $[M - H]^-$ 342.0747, found 342.0743.



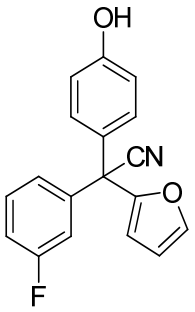

**2-(3,5-Dimethylphenyl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5h)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5h** (26.7 mg, 94%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.51–7.43 (m, 1H), 7.14–7.08 (m, 2H), 6.98 (s, 1H), 6.89–6.77 (m, 4H), 6.40–6.32 (m, 1H), 6.07–6.01 (m, 1H), 2.28 (s, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.6, 151.4, 143.7, 138.4, 138.2, 130.7, 130.1, 129.4, 128.7, 127.9, 125.6, 120.7, 115.5, 111.0, 110.4, 51.9, 21.4; HRMS (ESI) m/z calculated for $C_{20}H_{16}NO_2$ $[M - H]^-$ 302.1187, found 302.1192.



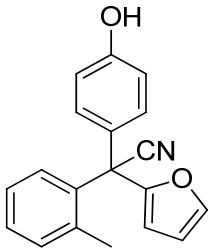

**2-(3-Chlorophenyl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5i)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5i** (27.2 mg, 92%). $^{1}$H NMR (500 MHz, Acetone) δ 8.76 (s, 1H), 7.78–7.65 (m, 1H), 7.56–7.43 (m, 2H), 7.33–7.20 (m, 2H), 7.15–7.06 (m, 2H), 6.97–6.88 (m, 2H), 6.57–6.46 (m, 1H), 6.13 (dd, $J$ = 3.3, 0.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.1, 150.3, 144.1, 140.4, 134.8, 130.0, 129.5, 129.3, 128.8, 128.0, 126.1, 120.0, 115.8, 111.4, 110.6, 51.7; HRMS (ESI) m/z calculated for $C_{18}H_{11}ClNO_2$ $[M - H]^-$ 308.0484, found 308.0493.




**2-(3-Fluorophenyl)-2-(furan-2-yl)-2-(4-hydroxyphenyl)acetonitrile (5j)**

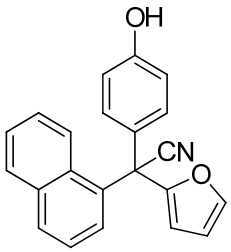
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5j** (26.6 mg, 93%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.51–7.48 (m, 1H), 7.38–7.32 (m, 1H), 7.14–7.02 (m, 4H), 6.98–6.90 (m, 1H), 6.89–6.79 (m, 2H), 6.42–6.33 (m, 1H), 6.07 (dd, *J* = 3.3, 0.7 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ162.9 (d, *J* = 247.6 Hz), 156.1, 150.7, 144.2, 141.1 (d, *J* = 7.1 Hz), 130.5 (d, *J* = 8.3 Hz), 130.0, 129.5, 123.8 (d, *J* = 3.1 Hz), 120.2, 115.9, 115.8 (d, *J* = 21.1 Hz), 115.5 (d, *J* = 23.8 Hz), 111.5, 110.8, 51.9; HRMS (ESI) m/z calculated for $C_{18}H_{11}FNO_2$ $[M-H]^-$ 292.0779, found 292.0766.




**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-(o-tolyl)acetonitrile (5k)**

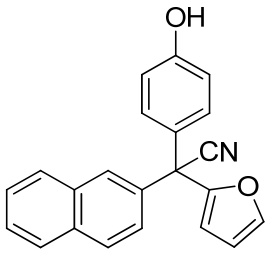
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5k** (26.1 mg, 91%). $^{1}$H NMR (500 MHz, Acetone) δ 8.73 (s, 1H), 7.72 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.34–7.27 (m, 2H), 7.23–7.19 (m, 1H), 7.13–7.09 (m, 2H), 6.94–6.89 (m, 2H), 6.56 (dd, *J* = 7.9, 0.9 Hz, 1H), 6.51–6.47 (m, 1H), 5.97 (dd, *J* = 3.3, 0.8 Hz, 1H), 2.19 (s, 3H); $^{13}$C NMR (126 MHz, Acetone) δ 158.4, 152.5, 144.9, 138.0, 137.8, 133.4, 129.6, 129.6, 129.1, 129.0, 127.0, 120.3, 116.5, 116.4, 112.0,

111.7, 51.8, 20.9; HRMS (ESI) m/z calculated for $C_{19}H_{14}NO_2$ [M - H]$^-$ 288.1030, found 288.1042.




**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-(naphthalen-1-yl)acetonitrile (5l)**

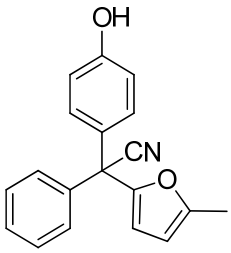
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:9) as eluent to afford **5l** (29.7 mg, 86%). $^1$H NMR (500 MHz, Acetone) δ 8.73 (s, 1H), 8.03–7.95 (m, 3H), 7.78–7.74 (m, 1H), 7.54–7.48 (m, 2H), 7.46–7.42 (m, 1H), 7.17 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.9 Hz, 2H), 6.81 (dd, *J* = 7.4, 0.9 Hz, 1H), 6.56–6.52 (m, 1H), 6.04 (d, *J* = 3.3 Hz, 1H);$^{13}$C NMR (126 MHz, Acetone) δ 158.4, 152.5, 144.9, 135.6, 135.1, 131.1, 130.8, 130.0, 129.6, 129.5, 128.1, 126.9, 126.7, 126.2, 125.8, 120.8, 116.6, 112.2, 111.8, 51.9; HRMS (ESI) m/z calculated for $C_{22}H_{14}NO_2$ [M - H]$^-$ 324.1030, found 324.1020.




**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-(naphthalen-2-yl)acetonitrile (5m)**

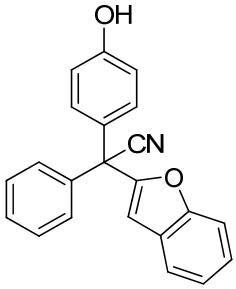
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **5m** (27.8 mg, 89%). $^1$H NMR (500 MHz, $CDCl_3$) δ 7.86–7.79 (m, 3H), 7.70 (d, *J* = 1.8 Hz, 1H), 7.55–7.50 (m, 3H), 7.40–7.37 (m, 1H), 7.18–7.13 (m, 2H), 6.85–6.81 (m, 2H), 6.40–6.35 (m, 1H), 6.10 (dd, *J* = 3.3, 0.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.0, 151.0, 143.9, 135.7, 132.9, 132.9, 130.1, 129.5, 128.7, 128.4, 127.6,

127.0, 127.0, 126.7, 125.4, 120.6, 115.7, 111.3, 110.6, 52.2; HRMS (ESI) m/z calculated for $C_{22}H_{14}NO_2$ [M - H]$^-$ 324.1030, found 324.1036.




**2-(4-Hydroxyphenyl)-2-(5-methylfuran-2-yl)-2-phenylacetonitrile (7a)**

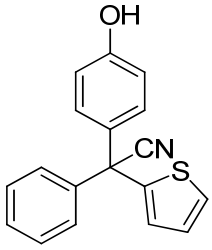
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7a** (24.7 mg, 90%). $^1$H NMR (500 MHz, $CDCl_3$) δ 7.40–7.34 (m, 3H), 7.29–7.26 (m, 2H), 7.15–7.08 (m, 2H), 6.85–6.79 (m, 2H), 5.95–5.91 (m, 1H), 5.82 (d, *J* = 3.2 Hz, 1H), 2.29 (d, *J* = 0.4 Hz, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.0, 154.1, 149.2, 138.8, 130.6, 129.5, 128.9, 128.5, 128.0, 121.0, 115.7, 112.3, 106.6, 52.3, 13.8; HRMS (ESI) m/z calculated for $C_{19}H_{14}NO_2$ [M - H]$^-$ 288.1030, found 288.1039.




**2-(Benzofuran-2-yl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7b)**

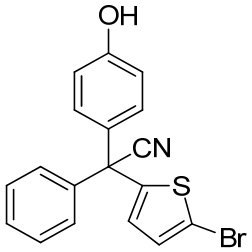
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7b** (27.6 mg, 91%). $^1$H NMR (500 MHz, Acetone) δ 8.77 (s, 1H), 7.65 (d, *J* = 7.7 Hz, 1H), 7.54 (dd, *J* = 8.3, 0.6 Hz, 1H), 7.51–7.44 (m, 3H), 7.40–7.35 (m, 3H), 7.31–7.27 (m, 1H), 7.19 7.15 (m, 2H), 6.96–6.92 (m, 2H), 6.50 (d, *J* = 0.8 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.1, 155.7, 154.1, 138.1, 136.6, 130.0, 129.7, 129.1,

128.8, 128.2, 127.6, 125.3, 123.5, 121.5, 120.4, 115.9, 111.9, 108.4, 52.7; HRMS (ESI) m/z calculated for $C_{22}H_{14}NO_2$ [M - H]$^-$ 324.1030, found 324.1023.



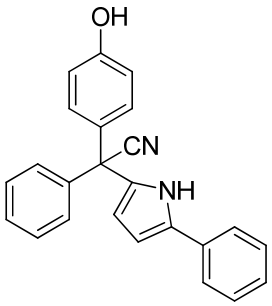

**2-(4-Hydroxyphenyl)-2-phenyl-2-(thiophen-2-yl)acetonitrile (7c)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7c** (24.7 mg, 89%). $^1$H NMR (500 MHz, Acetone) δ 8.73 (s, 1H), 7.57 (dd, *J* = 5.2, 1.1 Hz, 1H), 7.49–7.40 (m, 3H), 7.36–7.29 (m, 2H), 7.16–7.07 (m, 3H), 6.96–6.88 (m, 3H);$^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 144.6, 140.8, 132.8, 129.7, 128.9, 128.7, 128.6, 128.1, 127.1, 127.1, 122.6, 115.7, 53.1; HRMS (ESI) m/z calculated for $C_{18}H_{12}NOS$ [M - H]$^-$ 290.0645, found 290.0649.



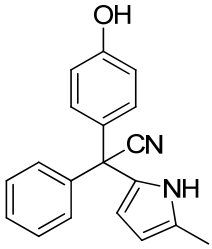

**2-(5-Bromothiophen-2-yl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7d)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7d** (29.7 mg, 86%). $^1$H NMR (500 MHz, Acetone) δ 8.80 (s, 1H), 7.50–7.42 (m, 3H), 7.38–7.32 (m, 2H), 7.17–7.11 (m, 3H), 6.94–6.89 (m, 2H), 6.79 (d, *J* = 3.9 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 156.1, 145.8, 140.1, 132.0, 129.9, 129.6, 129.0, 128.9, 128.9, 128.0, 122.0, 115.8, 114.2, 53.3; HRMS (ESI) m/z calculated for $C_{18}H_{11}BrNOS$ [M - H]$^-$ 367.9750, found 367.9755.



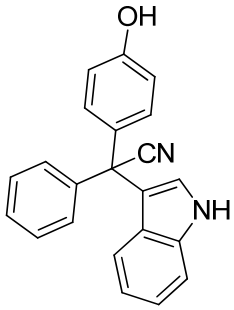

**2-(4-Hydroxyphenyl)-2-phenyl-2-(5-phenyl-1H-pyrrol-2-yl)acetonitrile (7e)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7e** (30.1 mg, 90%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.36–7.22 (m, 9H), 7.17–7.11 (m, 1H), 7.09–7.03 (m, 2H), 6.77–6.71 (m, 2H), 6.43–6.25 (m, 1H), 5.79–5.73 (m, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 139.6, 134.0, 132.1, 131.5, 130.1, 129.7, 129.6, 129.2, 129.1, 129.0, 129.0, 128.9, 128.6, 128.1, 128.0, 126.9, 126.4, 124.1, 122.2, 115.8, 112.5, 106.3, 51.9; HRMS (ESI) m/z calculated for $C_{24}H_{17}N_2O$ $[M - H]^-$ 349.1346, found 349.1341.



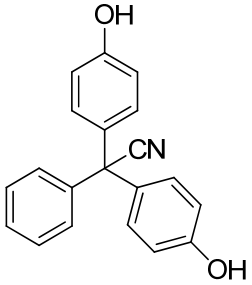

**2-(4-Hydroxyphenyl)-2-(5-methyl-1H-pyrrol-2-yl)-2-phenylacetonitrile (7f)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7f** (25.4 mg, 92%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.40–7.32 (m, 3H), 7.31–7.26 (m, 2H), 7.19–7.06 (m, 2H), 6.86–6.72 (m, 2H), 5.87–5.74 (m, 1H), 5.65 (t, $J$ = 3.0 Hz, 1H), 5.12 (s, 1H), 2.24 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.9, 139.6, 134.0, 132.1, 131.5, 130.1, 129.6, 129.6, 129.2, 129.1, 129.0, 129.0, 128.9, 128.6, 128.1, 128.0, 126.9, 126.4, 124.1, 122.2, 115.8, 112.5, 106.3, 51.9; HRMS (ESI) m/z calculated for $C_{19}H_{15}N_2O$ $[M - H]^-$ 287.1190, found 287.1195.



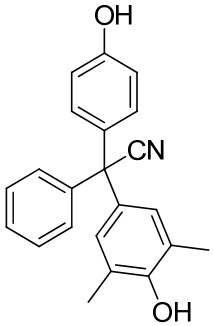

**2-(4-Hydroxyphenyl)-2-(1H-indol-3-yl)-2-phenylacetonitrile (7g)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7g** (29.5 mg, 91%). $^{1}$H NMR (400 MHz, DMSO) δ 11.26 (s, 1H), 9.68 (s, 1H), 7.48–7.36 (m, 4H), 7.31–7.26 (m, 2H), 7.15–7.10 (m, 1H), 7.06 (d, *J* = 8.7 Hz, 3H), 6.97–6.92 (m, 1H), 6.82–6.76 (m, 2H), 6.51 (d, *J* = 2.6 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 157.1, 140.1, 137.1, 129.7, 128.8, 128.8, 128.0, 127.5, 126.1, 124.7, 122.6, 121.8, 119.4, 119.3, 115.5, 114.5, 112.2, 50.1. HRMS (ESI) m/z calculated for $C_{22}H_{15}N_2O$ $[M - H]^-$ 323.1190, found 323.1187.



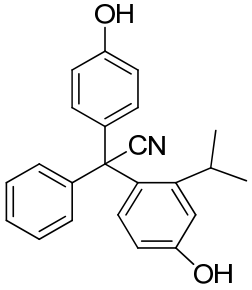

**2,2-Bis(4-hydroxyphenyl)-2-phenylacetonitrile (7h)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7h** (25.0 mg, 87%). $^{1}$H NMR (500 MHz, Acetone) δ 8.67 (s, 2H), 7.47–7.35 (m, 3H), 7.28–7.18 (m, 2H), 7.07–6.98 (m, 4H), 6.90–6.85 (m, 4H);$^{13}$C NMR (126 MHz, Acetone) δ 158.0, 157.9, 142.2, 132.3, 130.6, 129.4, 129.2, 128.7, 124.5, 116.2, 116.1, 56.8; HRMS (ESI) m/z calculated for $C_{20}H_{14}NO_2$ $[M - H]^-$ 300.1030, found 300.1027.



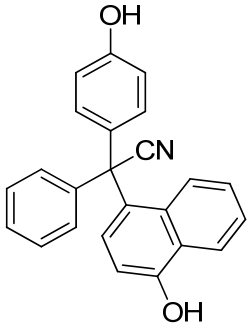

**2-(4-Hydroxy-3,5-dimethylphenyl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7i)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7i** (28.3 mg, 90%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.37–7.30 (m, 3H), 7.25–7.17 (m, 2H), 7.07–6.99 (m, 2H), 6.84–6.75 (m, 4H), 4.92 (s, 1H), 2.18 (s, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 155.6, 152.1, 140.9, 132.6, 131.8, 130.3, 129.0, 128.8, 128.7, 128.1, 124.2, 123.5, 115.6, 56.3, 16.3; HRMS (ESI) m/z calculated for $C_{22}H_{18}NO_2$ $[M - H]^-$ 328.1343, found 328.1347.



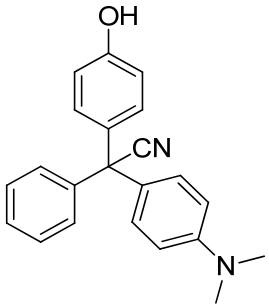

**2-(4-Hydroxy-2-isopropylphenyl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7j)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7j** (31.6 mg, 95%). $^{1}$H NMR (500 MHz, Acetone) δ 8.64 (s, 1H), 8.56 (s, 1H), 7.43–7.34 (m, 3H), 7.26–7.19 (m, 2H), 7.06–6.99 (m, 3H), 6.89–6.83 (m, 3H), 6.77 (dd, $J$ = 8.4, 2.5 Hz, 1H), 3.34–3.23 (m, 1H), 1.14 (d, $J$ = 6.9 Hz, 3H), 1.13 (d, $J$ = 6.9 Hz, 3H); $^{13}$C NMR (126 MHz, Acetone) δ 157.9, 154.9, 142.3, 135.6, 132.5, 132.3, 130.6, 129.3, 129.2, 128.6, 127.6, 127.4, 124.5, 116.1, 115.7, 57.0, 27.7, 22.5; HRMS (ESI) m/z calculated for $C_{23}H_{20}NO_2$ $[M - H]^-$ 342.1500, found 342.1503.



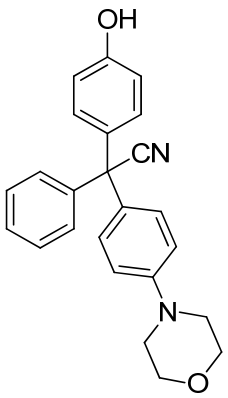

**2-(4-Hydroxynaphthalen-1-yl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7k)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7k** (28.1 mg, 93%). $^{1}$H NMR (500 MHz, Acetone) δ 9.44 (s, 1H), 8.68 (s, 1H), 8.36 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.51–7.37 (m, 5H), 7.28 (d, *J* = 7.1 Hz, 2H), 7.08 (d, *J* = 8.6 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H), 6.79 (d, *J* = 8.1 Hz, 1H), 6.51 (d, *J* = 8.1 Hz, 1H);$^{13}$C NMR (126 MHz, Acetone) δ 158.1, 155.1, 141.9, 132.5, 132.0, 130.8, 130.2, 129.7, 129.4, 128.8, 127.7, 127.0, 126.9, 125.5, 124.1, 123.8, 116.4, 107.4, 62.8, 56.0; HRMS (ESI) m/z calculated for $C_{24}H_{16}NO_2$ $[M - H]^-$ 350.1187, found 350.1182.



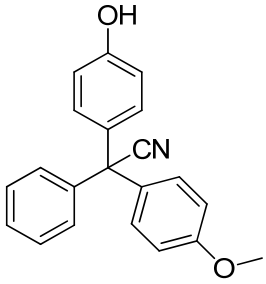

**2-(4-(Dimethylamino)phenyl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7l)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:4) as eluent to afford **7l** (27.0 mg, 86%). $^{1}$H NMR (500 MHz, Acetone) δ 8.62 (s, 1H), 7.44–7.34 (m, 3H), 7.25–7.17 (m, 2H), 7.03–6.95 (m, 4H), 6.88–6.83 (m, 2H), 6.76–6.72 (m, 2H), 2.95 (s, 6H); $^{13}$C NMR (126 MHz, Acetone) δ 158.0, 151.1, 142.6, 132.8, 130.7, 130.0, 129.4, 129.3, 128.7, 128.6, 124.7, 116.2, 112.9, 56.8, 40.4; HRMS (ESI) m/z calculated for $C_{22}H_{19}N_2O$ $[M - H]^-$ 327.1503, found 327.1506.



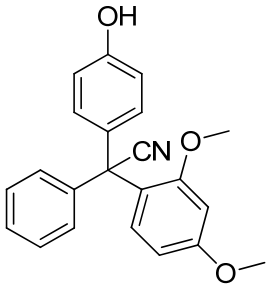

**2-(4-Hydroxyphenyl)-2-(4-morpholinophenyl)-2-phenylacetonitrile (7m)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:4) as eluent to afford **7m** (30.7 mg, 85%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.36–7.31 (m, 3H), 7.24–7.20 (m, 2H), 7.09 (d, *J* = 8.8 Hz, 2H), 7.05–7.01 (m, 2H), 6.88 (d, *J* = 7.9 Hz, 2H), 6.79–6.75 (m, 2H), 6.06 (s, 1H), 3.91–3.84 (m, 4H), 3.23–3.15 (m, 4H); $^{13}$C NMR (126 MHz, Acetone) δ 158.1, 151.9, 142.3, 132.4, 131.7, 130.6, 130.1, 129.5, 129.3, 128.8, 124.5, 116.2, 116.1, 115.7, 67.2, 62.8, 56.8, 49.2; HRMS (ESI) m/z calculated for $C_{24}H_{21}N_2O_2$ $[M - H]^-$ 369.1609, found 369.1604.




**2-(4-Hydroxyphenyl)-2-(4-methoxyphenyl)-2-phenylacetonitrile (7n)**

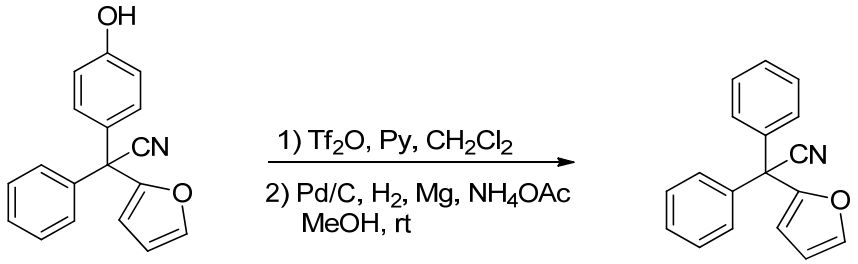
It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7n** (25.3 mg, 83%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.37–7.31 (m, 3H), 7.24–7.19 (m, 2H), 7.13–7.09 (m, 2H), 7.07–7.02 (m, 2H), 6.89–6.84 (m, 2H), 6.82–6.78 (m, 2H), 3.81 (s, 3H);$^{13}$C NMR (126 MHz, $CDCl_3$) δ 159.4, 155.7, 140.8, 132.7, 132.6, 130.3, 130.1, 128.8, 128.2, 124.0, 115.6, 114.12, 56.31, 55.6; HRMS (ESI) m/z calculated for $C_{21}H_{16}NO_2$ $[M - H]^-$ 314.1187, found 314.1191.




**2-(2,4-Dimethoxyphenyl)-2-(4-hydroxyphenyl)-2-phenylacetonitrile (7o)**

It was synthesized following the general procedure and purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:6) as eluent to afford **7o** (30.4 mg, 92%). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.37–7.29 (m, 3H), 7.23–7.15 (m, 2H), 7.08–7.00 (m, 2H), 6.82–6.76 (m, 2H), 6.52 (d, *J* = 2.3 Hz, 1H), 6.42–6.29 (m, 2H), 5.44 (s, 1H), 3.80 (s, 3H), 3.67 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 161.4, 158.5, 155.7, 140.4, 131.8, 130.9, 129.9, 128.6, 128.4, 127.8, 123.3, 121.5, 115.6, 104.2, 100.0, 55.9, 55.6, 53.1; HRMS (ESI) m/z calculated for $C_{22}H_{18}NO_3$ $[M - H]^-$ 344.1292, found 344.1295.

**Synthetic utilities**

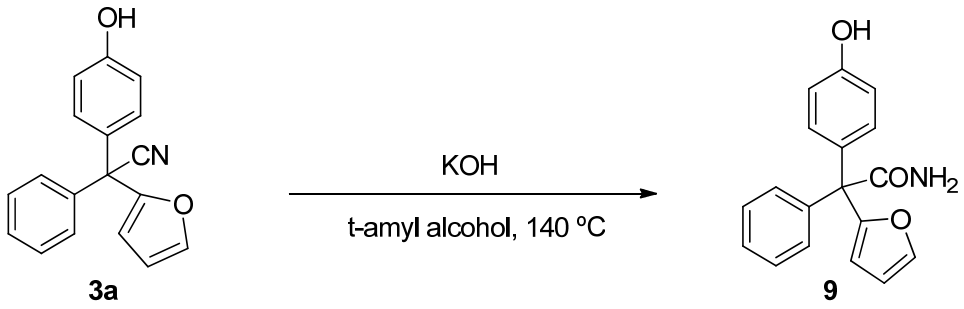



**3a** **8**

**2-(Furan-2-yl)-2,2-diphenylacetonitrile (8)**

To a solution of **3a** (0.1 mmol, 1.0 equiv) in $CH_2Cl_2$ (5 mL) were added pyridine (0.2 mmol, 2.0 equiv) and a solution of $Tf_2O$ (0.115 mmol, 1.15 equiv) in $CH_2Cl_2$ (0.5 mL) sequentially. The reaction mixture was stirred for 2 h. Then water (10 mL) was added. The layers were separated, and the aqueous layer was extracted with ethyl acetate (10 mL×3). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash

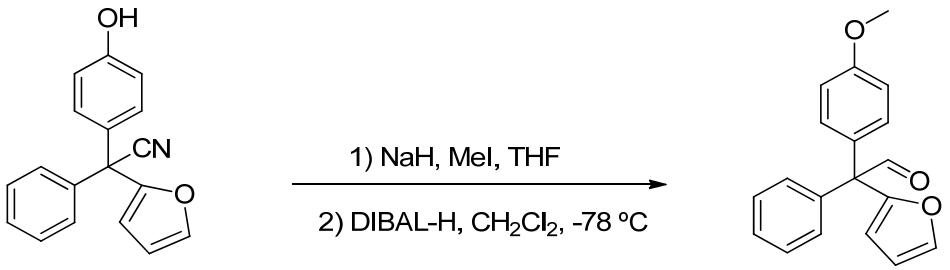
chromatography on silica gel using ethyl acetate/petroleum ether (1:10) as eluent to afford the trifluoromethanesulfonate ester. Then a mixture of the trifluoromethanesulfonate ester, 10% Pd/C (9.3 mg, 10 wt %), $NH_4OAc$ (15.4 mg), and Mg (12.0 mg) in methanol (5.0 mL) was stirred at room temperature under hydrogen balloon for 12 h. The mixture was passed through a short length of silica gel using ethyl acetate/petroleum ether (1:10) as eluent to afford **8** (29.0 mg, 87% yield) as an oil.




**3a** **9**

**2-(Furan-2-yl)-2-(4-hydroxyphenyl)-2-phenylacetamide (9)** [1]

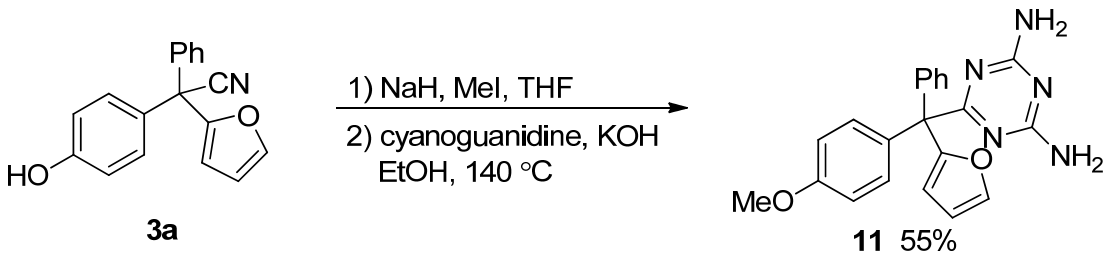
To a solution of **3a** (0.1 mmol, 1.0 equiv) in *t*-amyl alcohol (1 mL) was added KOH (0.5 mmol, 5.0 equiv) and the mixture was heated to 140 °C for 48 h. After cooling to room temperature, the mixture was passed through a pad of celite. Then the filtrate was removed under vacuum and the residue was purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:3) as eluent to afford **9** (24.4 mg, 92% yield). $^1$H NMR (500 MHz, Acetone) δ 8.39 (s, 1H), 7.70–7.56 (m, 1H), 7.35–7.27 (m, 3H), 7.20–7.15 (m, 2H), 7.02–6.96 (m, 2H), 6.86–6.73 (m, 3H), 6.50 (s, 1H), 6.46–6.39 (m, 1H), 6.01 (dd, $J$ = 3.3, 0.7 Hz, 1H); $^{13}$C NMR (126 MHz, Acetone) δ 173.0, 156.4, 156.4, 142.9, 142.6, 133.1, 130.5, 129.4, 127.6, 126.9, 114.5, 111.5, 110.2, 62.8; HRMS (ESI) m/z calculated for $C_{18}H_{15}NNaO_3$ $[M+Na]^+$ 316.0944, found 316.0947.




**3a** **10**

**2-(Furan-2-yl)-2-(4-methoxyphenyl)-2-phenylacetaldehyde (10)** [1]

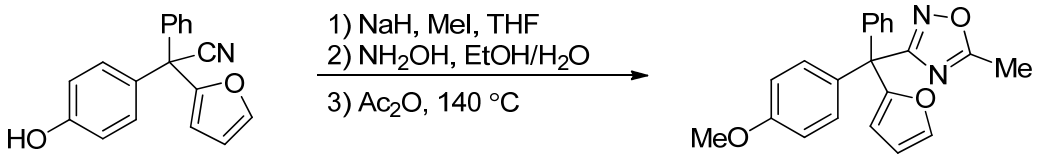
To a solution of **3a** (0.1 mmol, 1.0 equiv) in THF (5 mL) was added NaH (60% in mineral oil, 0.24 mmol, 2.4 equiv) and the reaction mixture was stirred for 30 min. Then iodomethane (0.3 mmol, 3.0 equiv) was added and the mixture was refluxed for 4h. After completion, water (5 mL) was added and the layers were separated, and the aqueous layer was extracted with ethyl acetate (10 mL×3). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:10) as eluent. Then to a solution of the product in $CH_2Cl_2$ (5 mL) was added di-isobutyl aluminium hydride (1 M in toluene, 0.3 mmol, 3.0 equiv) at -78 °C under nitrogen. The reaction mixture was stirred at the same temperature overnight and warmed to room temperature. The mixture was quenched by a saturated aqueous $NH_4Cl$ solution. The organic layer was extracted with ethyl acetate and the combined organic layers were washed with saturated aqueous NaCl solution, dried over anhydrous $MgSO_4$, filtered and removed under vacuum. The residue was purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:10) as eluent to afford **10** (22.2 mg, 83% yield). $^1$H NMR (500 MHz, $CDCl_3$) δ 10.15 (s, 1H), 7.54–7.48 (m, 1H), 7.38–7.33 (m, 3H), 7.06–7.03 (m, 2H), 6.97–6.94 (m, 2H), 6.91–6.87 (m, 2H), 6.40–6.36 (m, 1H), 6.06 (dd, $J$ = 3.3, 0.8 Hz, 1H), 3.81 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 195.9, 159.1, 153.7, 143.0, 138.7, 130.8, 130.3, 129.6, 128.5, 127.8, 113.9, 111.3, 110.2, 66.0, 55.3; HRMS (ESI) m/z calculated for $C_{19}H_{17}O_3$ $[M + H]^+$ 293.1172, found 293.1176.




**3a** **11** 55%

**6-(Furan-2-yl(4-methoxyphenyl)(phenyl)methyl)-1,3,5-triazine-2,4-diamine (11)** [1]

To a solution of **3a** (0.1 mmol, 1.0 equiv) in THF (5 mL) was added NaH (60% in mineral oil, 0.24 mmol, 2.4 equiv) and the reaction mixture was stirred for 30 min. Then iodomethane (0.3 mmol, 3.0 equiv) was added and the mixture was refluxed for 4h. After completion, water (5 mL) was added and the layers were separated, and the aqueous layer was extracted with ethyl acetate (10 mL×3). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:10) as eluent to afford the product. To a flame-dried 10 mL sealable glass vessel containing a magnetic stirring bar were added the product (0.1 mmol, 1.0 equiv), cyanoguanidine (0.125 mmol, 1.25 equiv), KOH (0.07 mmol, 0.7 equiv) and ethanol (0.5 mL) and then the vessel was sealed. The mixture was stirred at 140 °C for 10 h. After cooling to room temperature, the reaction mixture was diluted with water (1 mL) and extracted with ethyl acetate (3 ×15 mL). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:1) as eluent to afford **11** (20.5 mg, 55% yield). $^1$H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, $J$ = 0.8 Hz, 1H), 7.31–7.19 (m, 3H), 7.13–7.05 (m, 2H), 7.01 (d, $J$ = 8.9 Hz, 2H), 6.77 (d, $J$ = 8.9 Hz, 2H), 6.31 (dd, $J$ = 3.1, 1.8 Hz, 1H), 6.21 (d, $J$ = 3.2 Hz, 1H), 5.91 (brs, 2H), 4.93 (brs, 2H), 3.75 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$, rotamers seen) δ 180.1, 166.7, 158.4, 157.2, 143.7, 142.6, 142.3, 135.3, 131.3, 131.2, 130.1, 123.0, 127.9, 127.7, 127.1, 126.9, 113.1, 111.2, 110.9, 110.2, 110.0, 63.0, 55.5, 55.3; HRMS (ESI) m/z calculated for $C_{21}H_{20}N_5O_2$ $[M + H]^+$ 374.1612, found 374.1609.




**3a** **12** 53%

**3-(Furan-2-yl(4-methoxyphenyl)(phenyl)methyl)-5-methyl-1,2,4-oxadiazole (12)** [1]

To a solution of **3a** (0.1 mmol, 1.0 equiv) in THF (5 mL) was added NaH (60% in mineral oil, 0.24 mmol, 2.4 equiv) and the reaction mixture was stirred for 30 min. Then iodomethane (0.3 mmol, 3.0 equiv) was added and the mixture was refluxed for 4h. After completion, water (5 mL) was added and the layers were separated, and the aqueous layer was extracted with ethyl acetate (10 mL×3). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash chromatography on silica gel using ethyl acetate/petroleum ether (1:10) as eluent to afford the product. To a flame-dried 10 mL sealable glass vessel containing a magnetic stirring bar were added the product (0.1 mmol, 1.0 equiv), $NH_2OH$ (66 μL, 50% in $H_2O$), and ethanol (0.5 mL) and then the vessel was sealed. The mixture was stirred at 140 °C for 10 h. After cooling to room temperature, the reaction mixture was diluted with water (1 mL) and extracted with ethyl acetate (3 ×15 mL). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The resulting crude product was treated with acetic anhydride (0.5 mL) in a flame-dried 10 mL sealable glass vessel and the reaction mixture was stirred at 140 °C for 10 h. After cooling to room temperature, the reaction mixture was diluted with water (1 mL) and extracted with ethyl acetate (3 ×15 mL). The combined organic layers were washed with brine (10 mL), dried over anhydrous $Na_2SO_4$, filtered, and concentrated. The residue was purified by flash chromatography on silica gel using ethyl acetate /petroleum ether (1:10) as eluent to afford **12** (18.3 mg, 53%).

## Computation details

Density functional theory (DFT) calculations were conducted with Gaussian 09 package.[2] The geometries of all stationary points were optimized using the B3LYP functional[3] with the 6-31G(d)[4] basis set for all of atoms in the gas phase. The vibrational frequencies were carried out at the same level of theory to verify stationary points (no imaginary frequency). To get the electronic properties, we performed natural bond orbital (NBO) analysis[5] using the NBO 3.1 version[6] of the Gaussian 09 at the B3LYP/6-311+g(d,p) level. The electrostatic potential (ESP) maps were implemented by Multiwfn program.[7]

**Notes and references**

1. Nambo, M.; Yar, M.; Smith, J. D.; Crudden, C. M. *Org. Lett*. **2015**, *17*, 50.

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(b) A. E. Reed, L. A.Curtiss and F. Weinhold, *Chem. Rev*. **1988**, *88*, 899.

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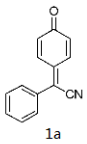
## NMR spectra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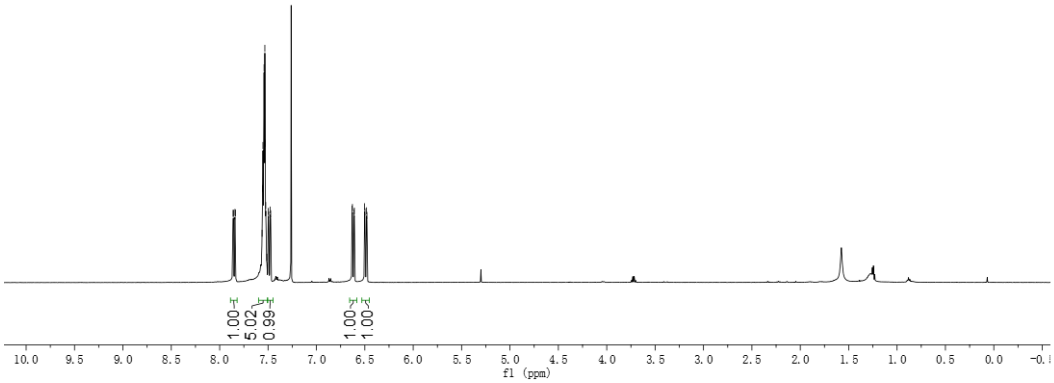


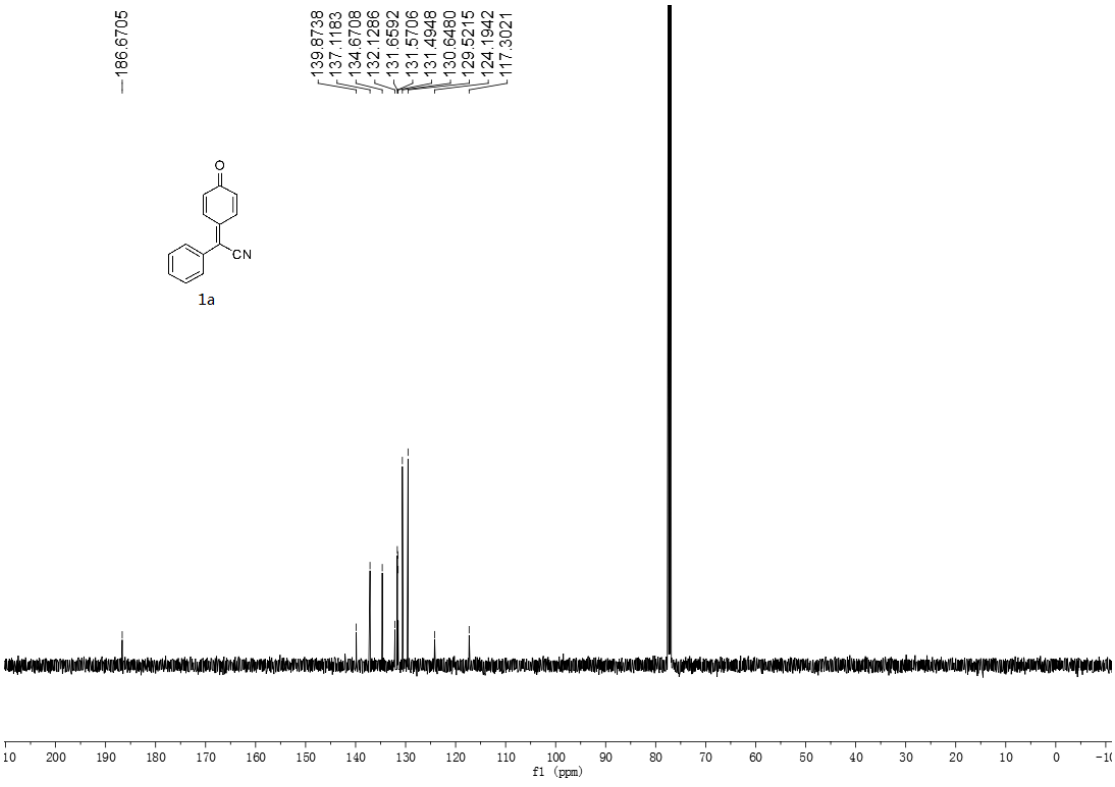

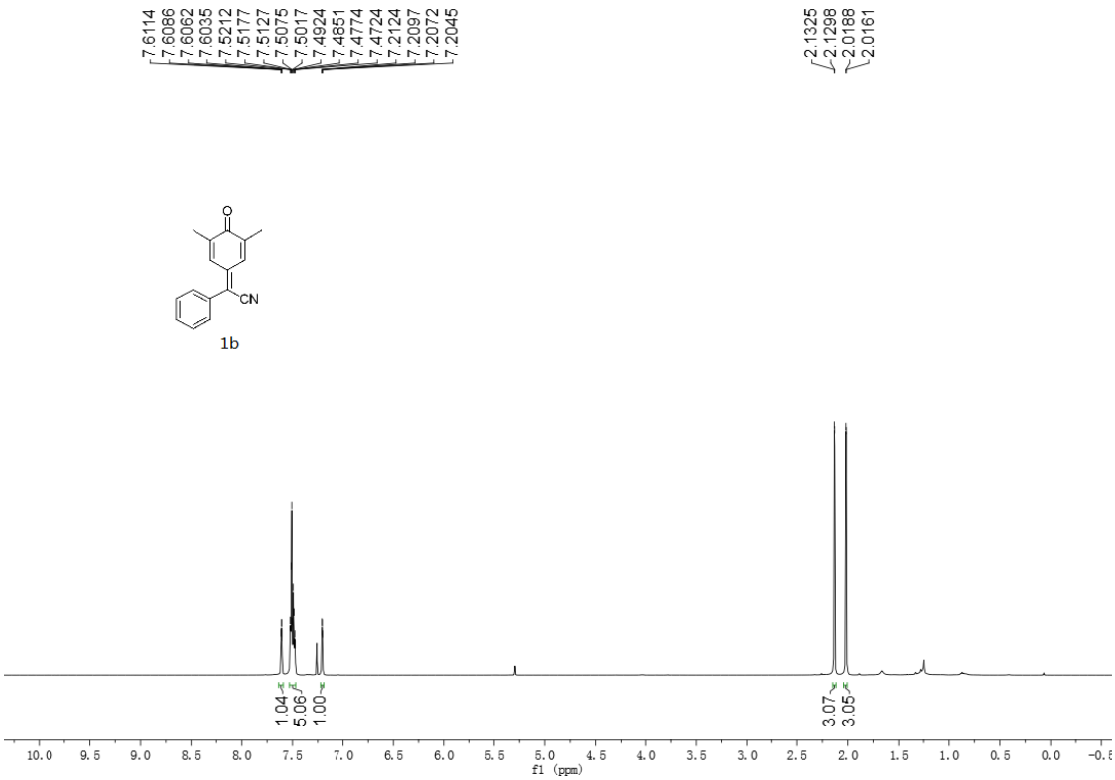
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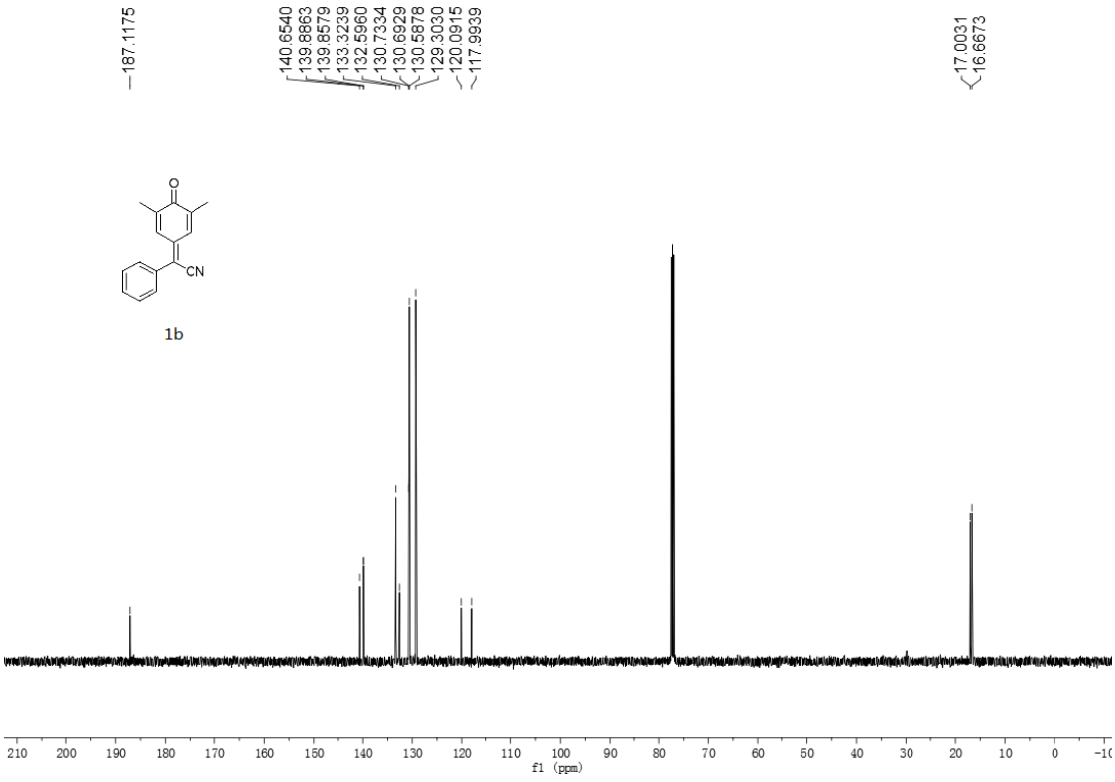
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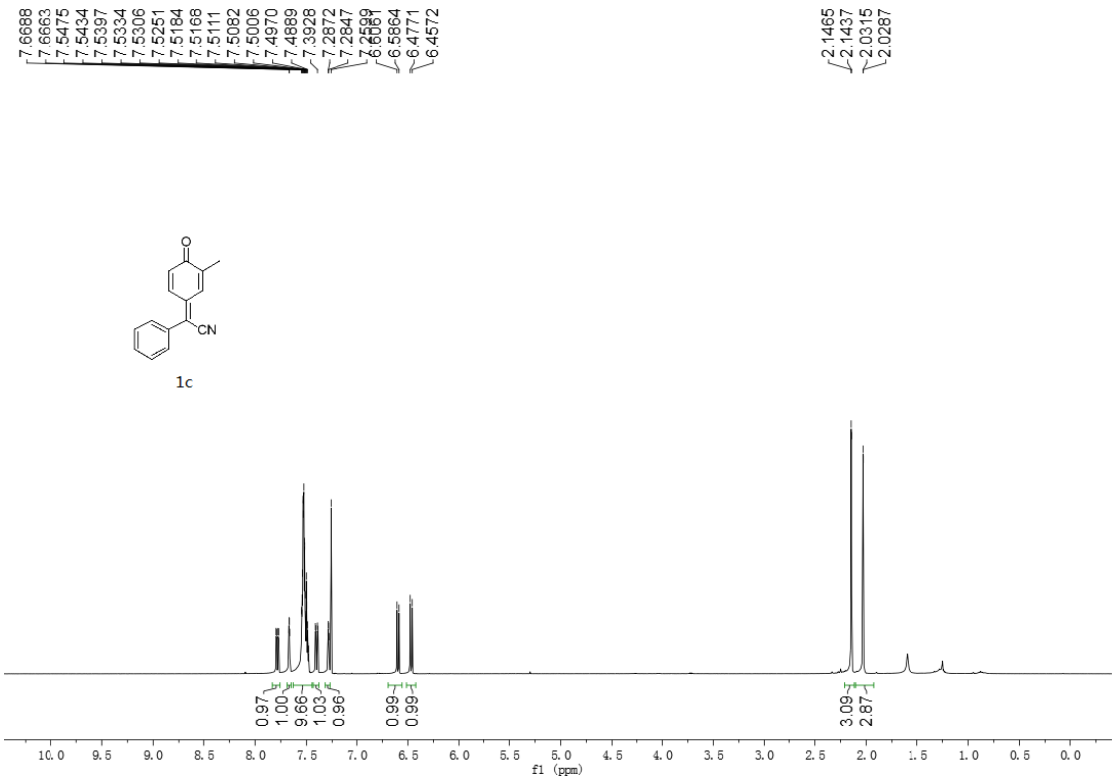
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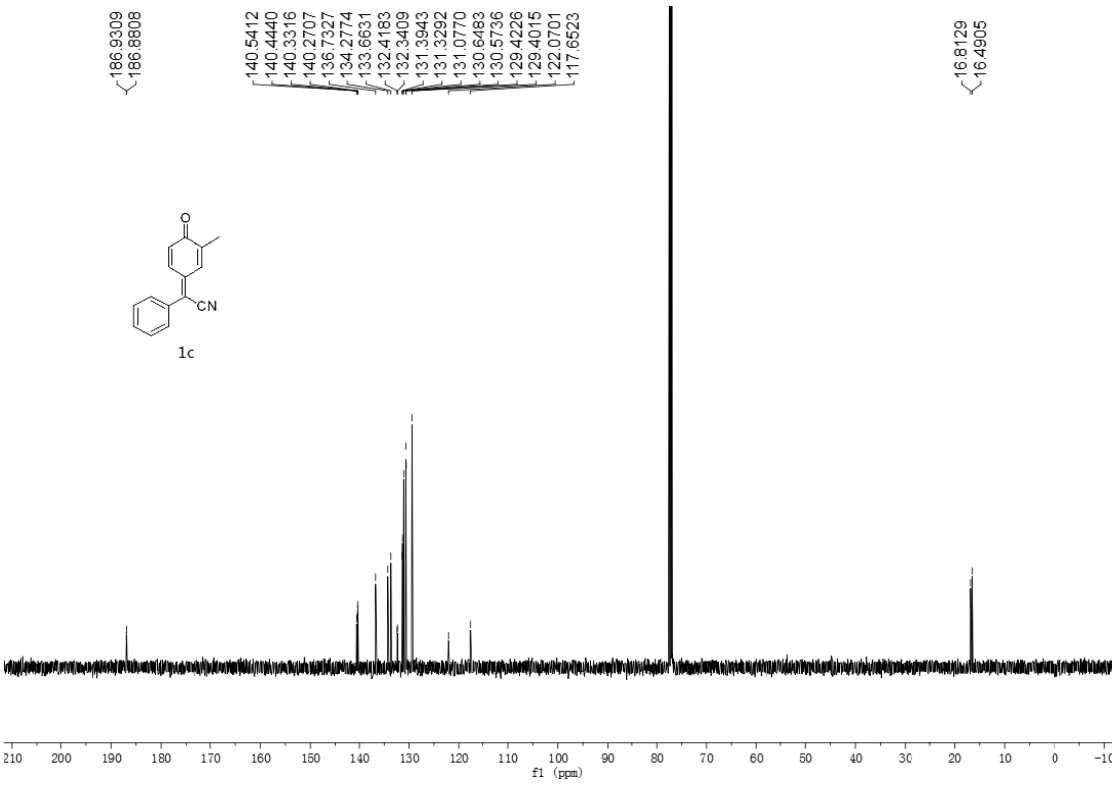
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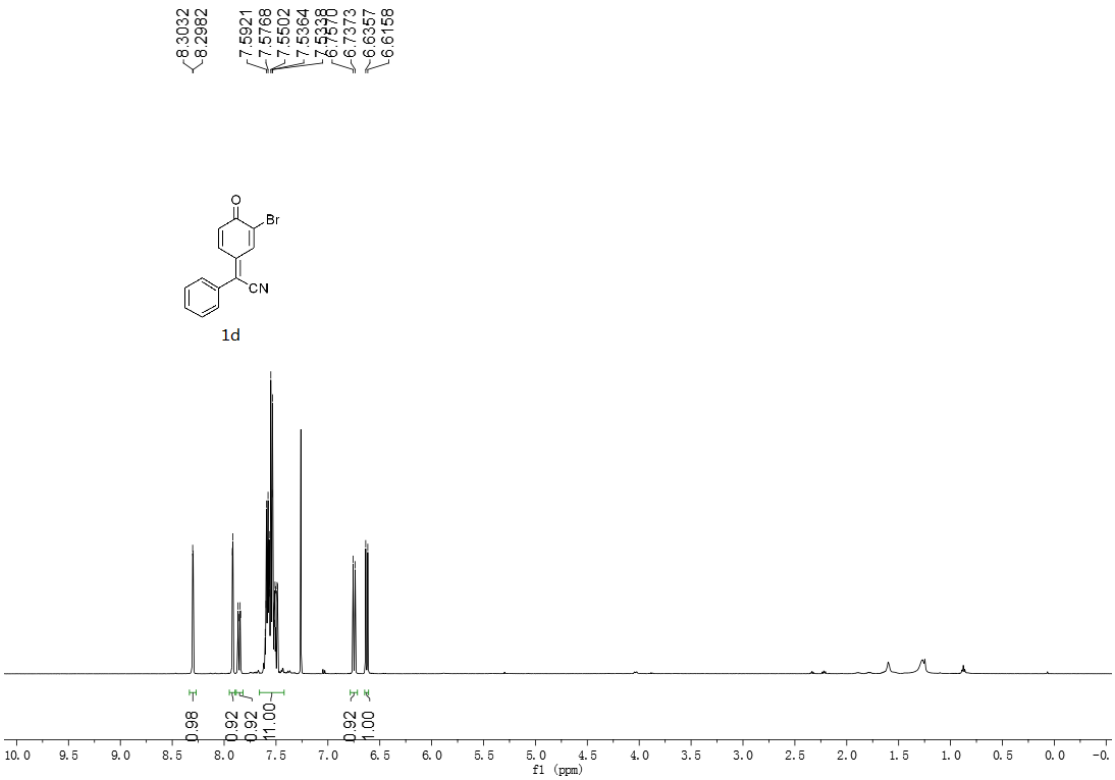
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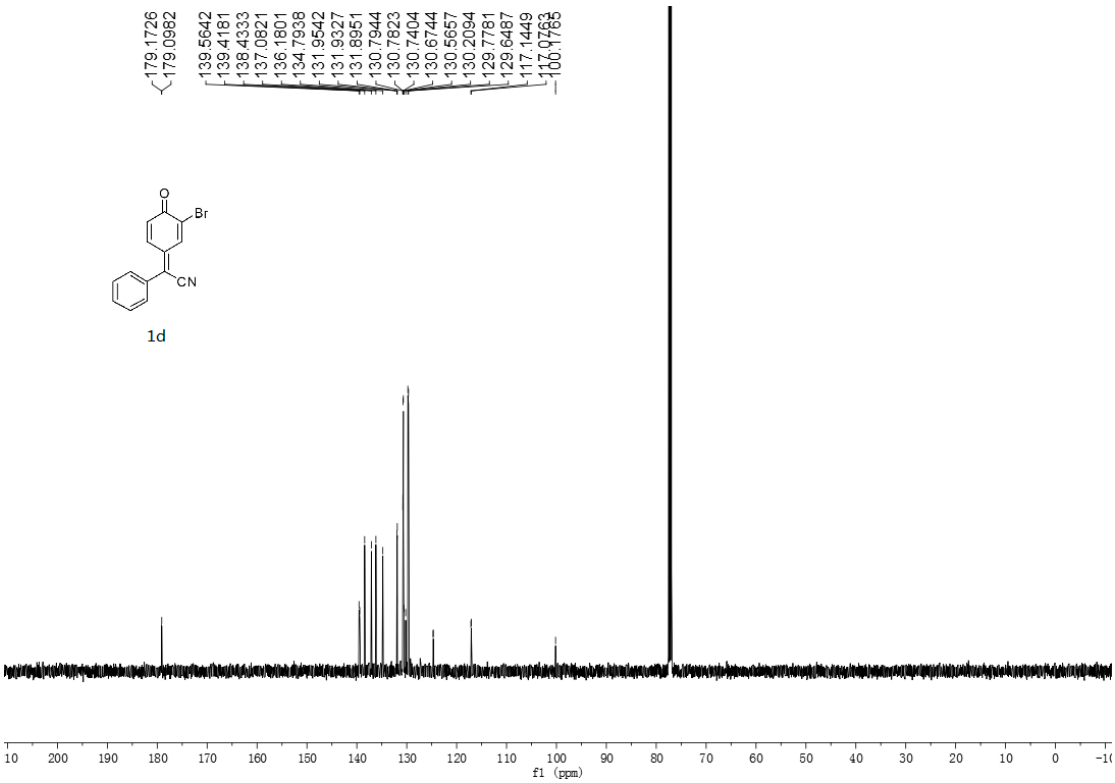
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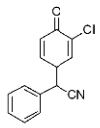
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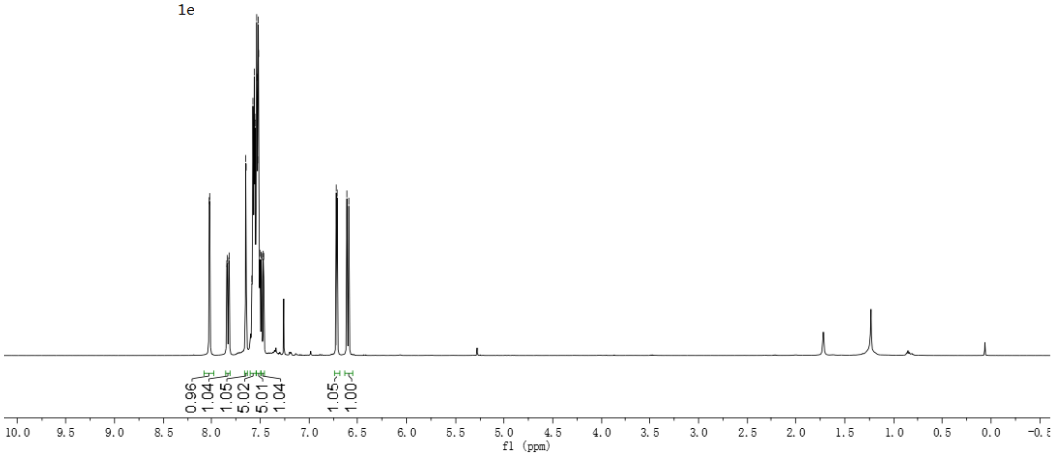
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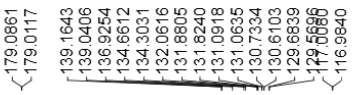
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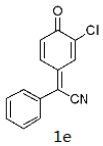
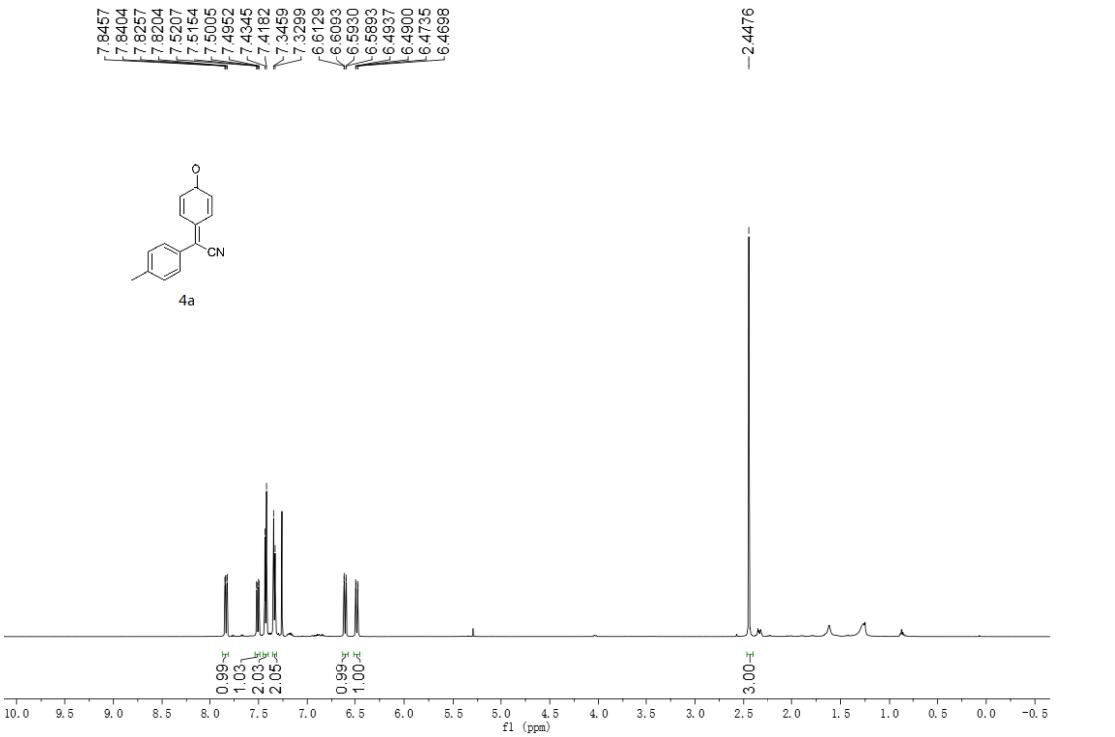

O
Cl
CN

1e


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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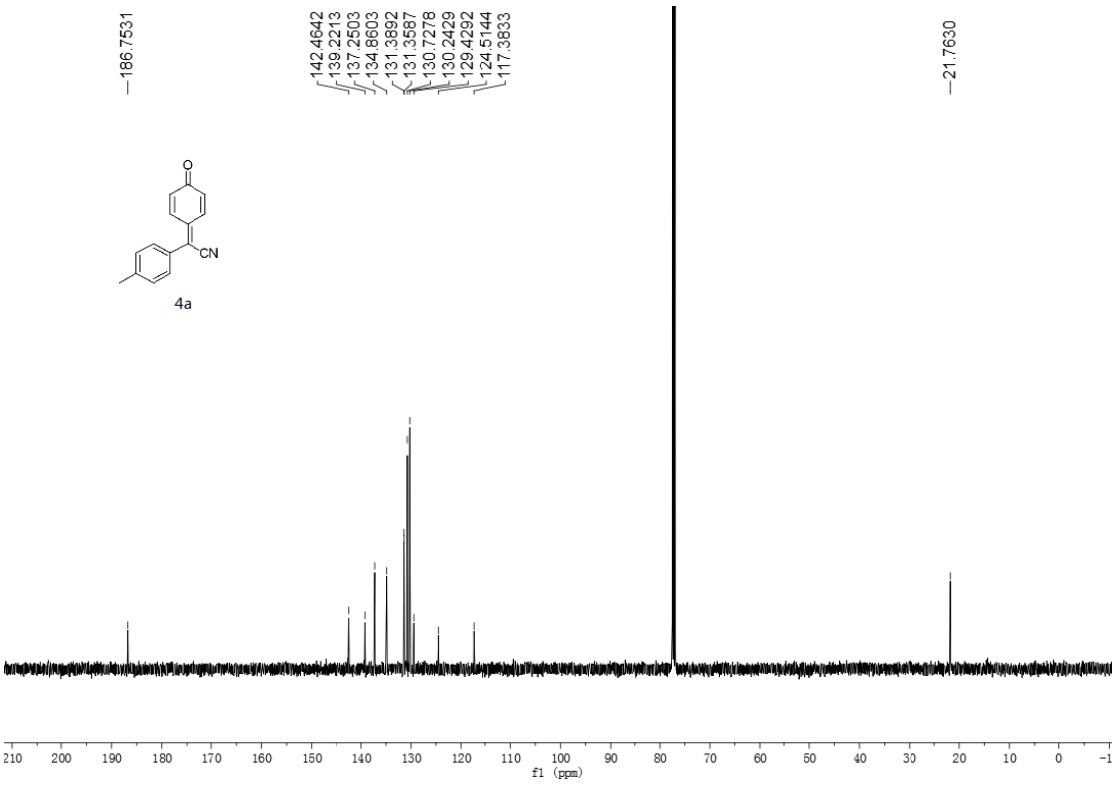
7.8257
7.8204
7.5207
7.5154
7.5005
7.4952
7.4345
7.4182
7.3459
7.3299
6.6129
6.6093
6.5930
6.5893
6.4937
6.4900
6.4735
6.4698
2.4476
O
CN
4a
0.99
1.03
2.03
2.05
0.99
1.00
3.00
f1 (ppm)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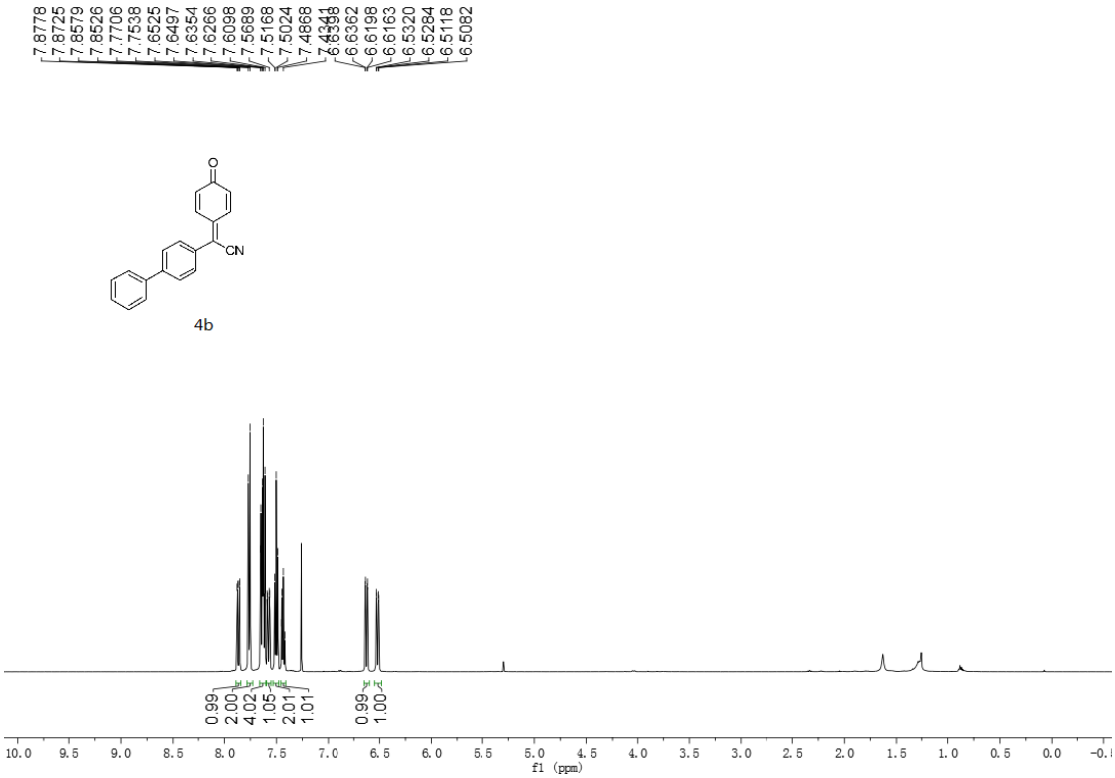
142.4642
139.2213
137.2503
134.8603
131.3892
131.3567
130.7278
130.2429
129.4292
124.5144
117.3833
21.7630
O
CN
4a
f1 (ppm)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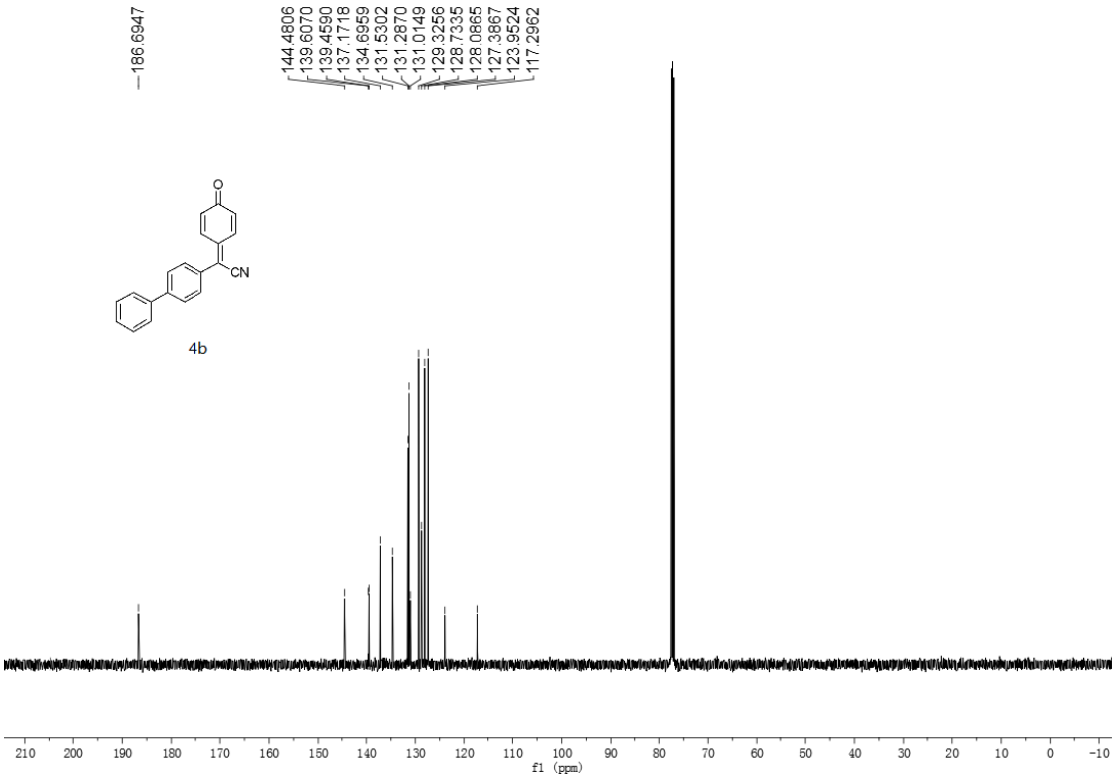
7.8579
7.8526
7.7706
7.7538
7.6525
7.6497
7.6354
7.6266
7.6098
7.5689
7.5168
7.5024
7.4868
6.6362
6.6198
6.6163
6.5320
6.5284
6.5118
6.5082
O
CN
4b
0.99
2.00
4.02
1.05
2.01
1.01
0.99
1.00
f1 (ppm)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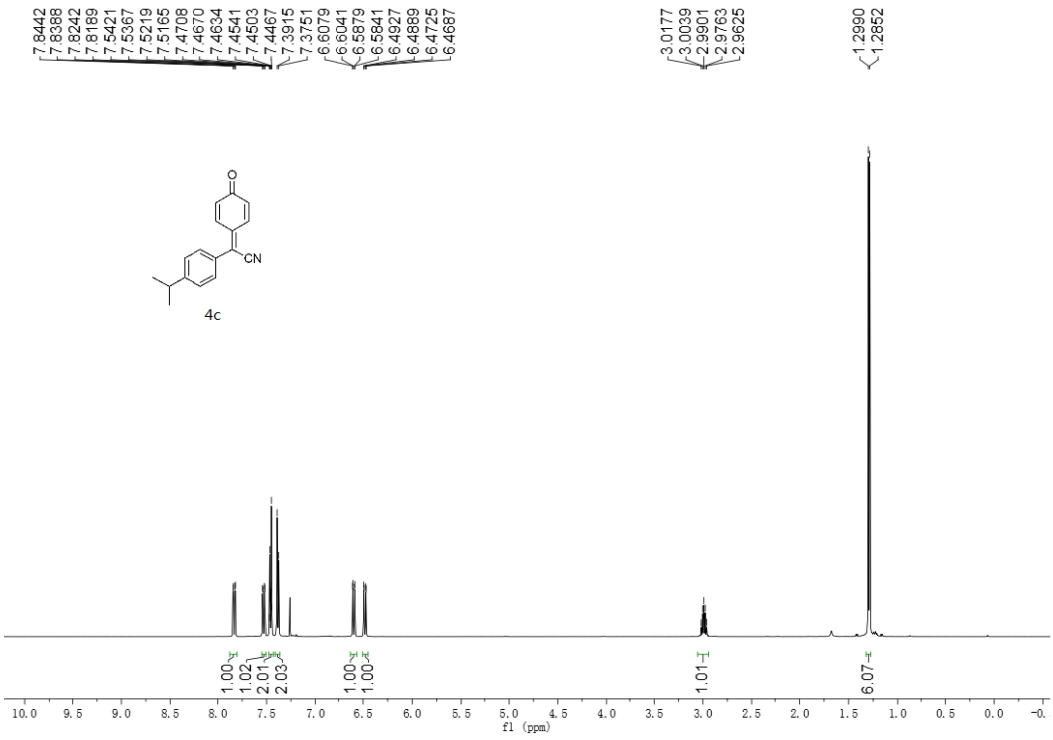
144.4806
139.6070
139.4590
137.1718
134.6959
131.5302
131.2870
131.0149
129.3256
128.7335
128.0865
127.3867
123.9524
117.2962
O
CN
4b
f1 (ppm)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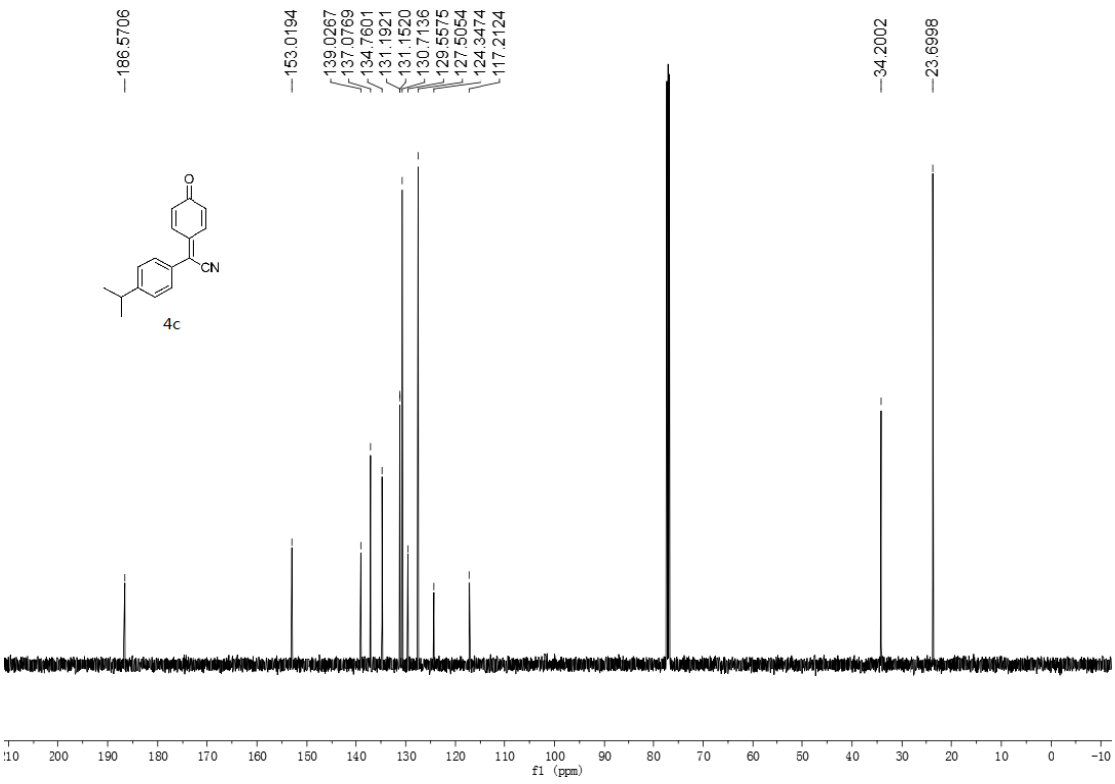
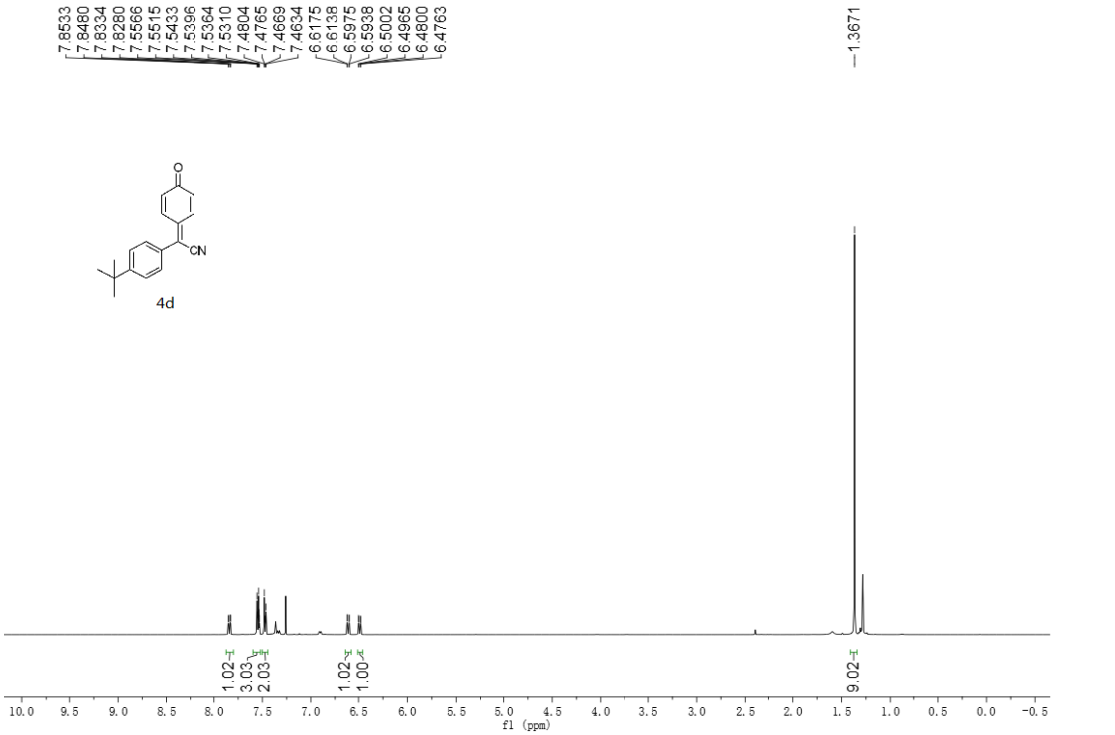
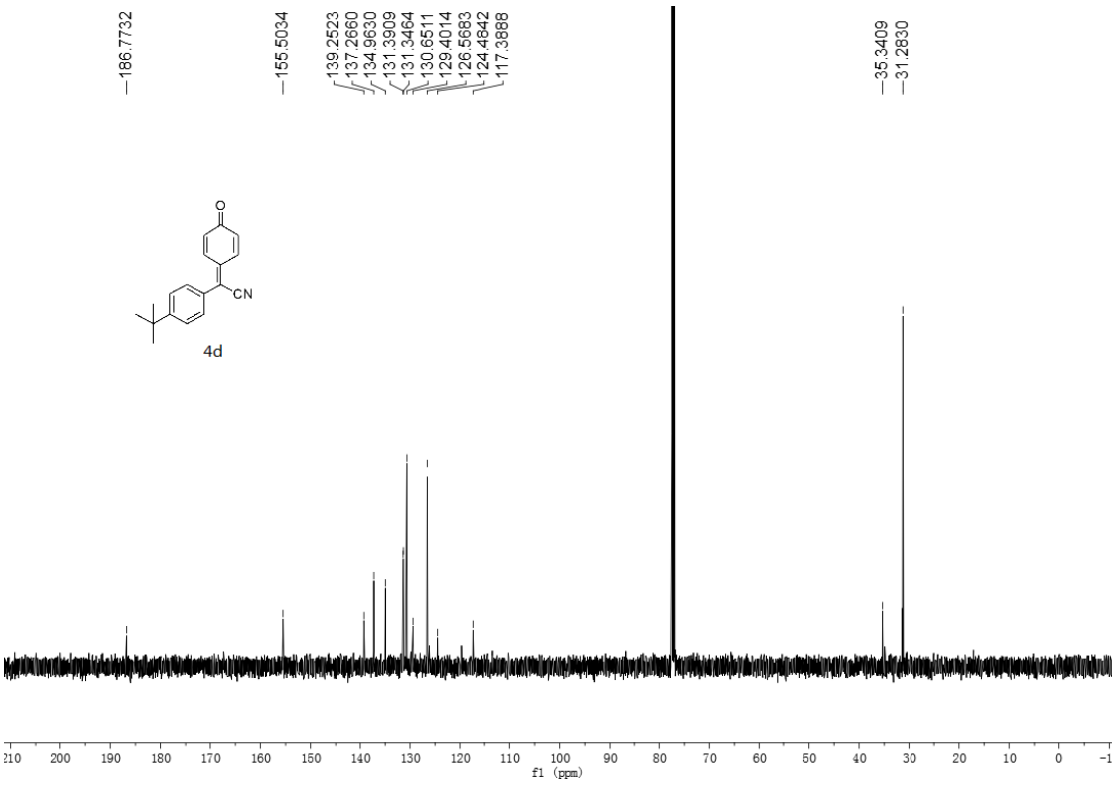
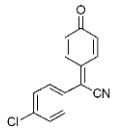
7.8388
7.8242
7.8189
7.5421
7.5367
7.5219
7.5165
7.4708
7.4670
7.4634
7.4541
7.4503
7.4467
7.3915
7.3751
6.6079
6.6041
6.5879
6.5841
6.4927
6.4889
6.4725
6.4687
3.0177
3.0039
2.9901
2.9763
2.9625
1.2990
1.2852
O
CN
4c
1.00
1.02
2.01
2.03
1.00
1.00
1.01
6.07
f1 (ppm)


186.5706
153.0194
139.0267
137.0769
134.7601
131.1921
131.1520
130.7136
129.5575
127.5054
124.3474
117.2124
34.2002
23.6998
O
CN
4c
f1 (ppm)

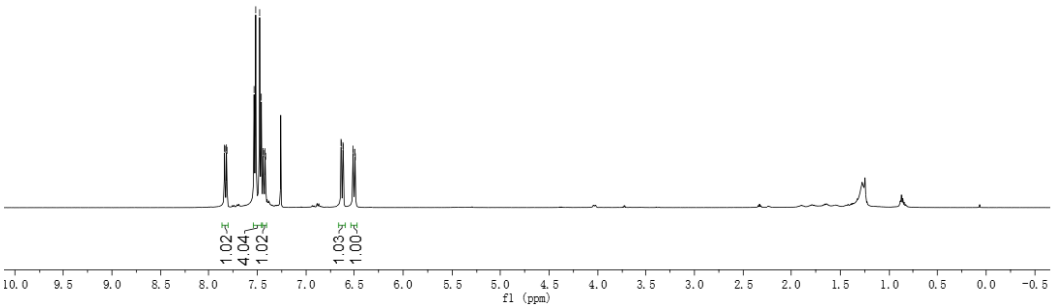

7.8533
7.8480
7.8334
7.8280
7.5566
7.5515
7.5433
7.5396
7.5364
7.5310
7.4804
7.4765
7.4669
7.4634
6.6175
6.6138
6.5975
6.5938
6.5002
6.4965
6.4800
6.4763
1.3671
O
CN
4d
1.02
3.03
2.03
1.02
1.00
9.02
f1 (ppm)

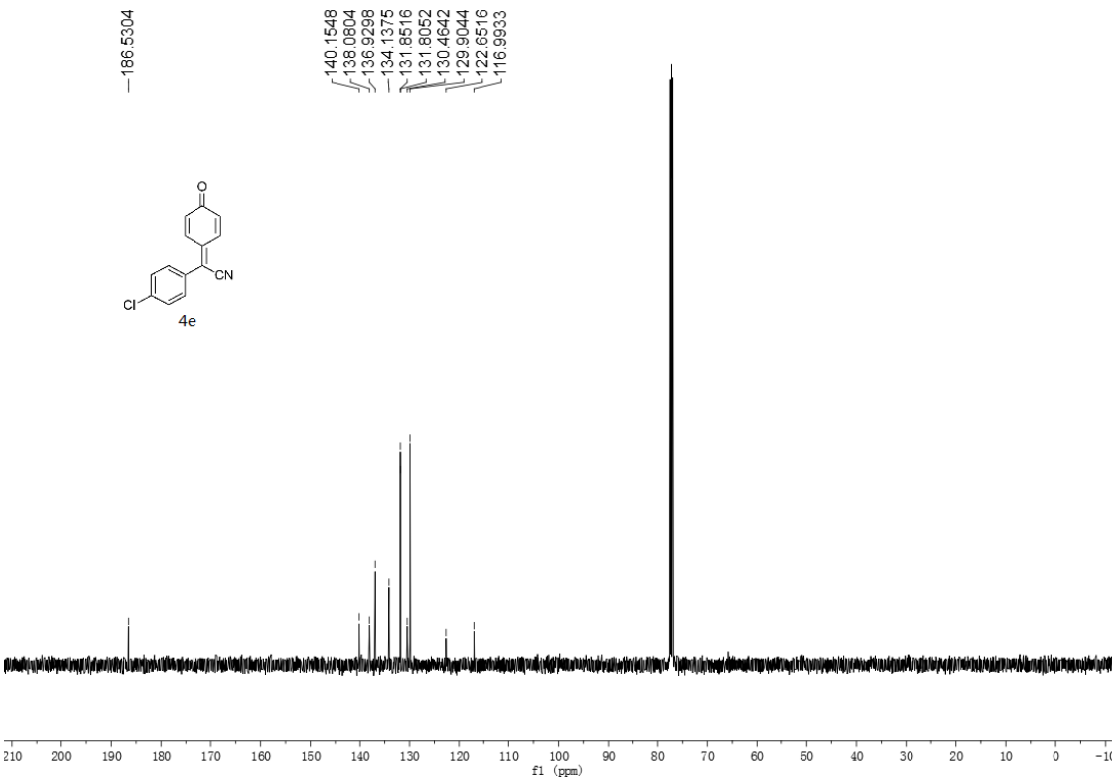

186.7732
155.5034
139.2523
137.2660
134.9630
131.3909
131.3464
130.6511
129.4014
126.5683
124.4842
117.3888
35.3409
31.2830
O
CN
4d
f1 (ppm)


7.8361
7.8309
7.8161
7.8109
7.5334
7.5164
7.4763
7.4592
7.4404
7.4353
7.4202
7.4150
6.6325
6.6293
6.6125
6.6093
6.5096
6.5066
6.4895
6.4864


O
CN
Cl

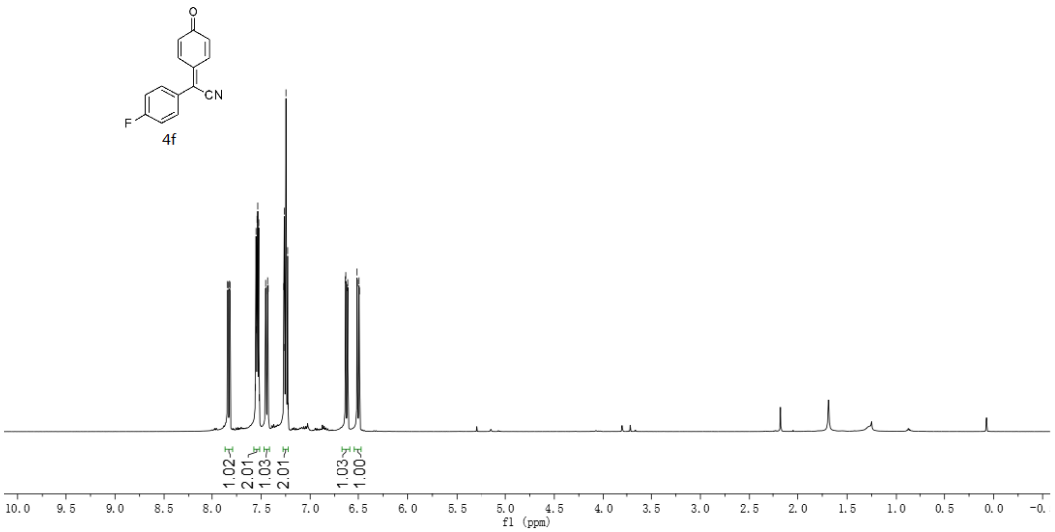
4e

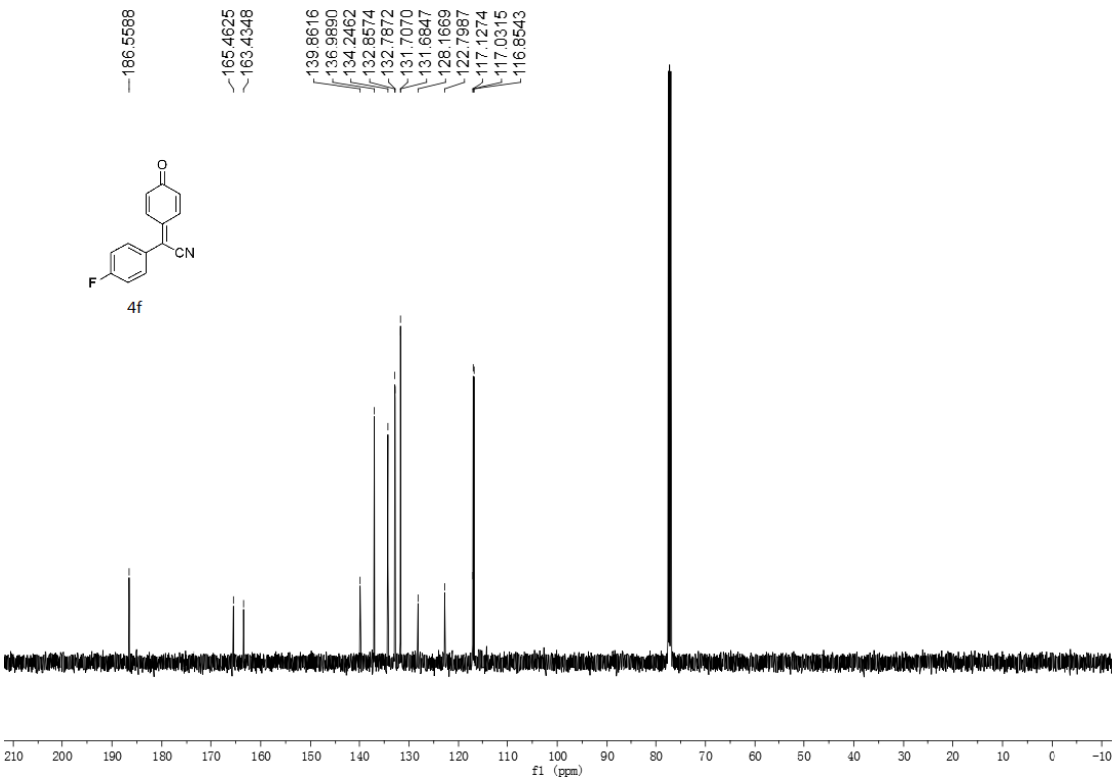

1.02
4.04
1.02
1.03
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


186.5304
140.1548
138.0804
136.9298
134.1375
131.8516
131.8052
130.4642
129.9044
122.6516
116.9933
O
CN
Cl
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)

4e


7.8425
7.8372
7.8225
7.8172
7.5519
7.5416
7.5381
7.5343
7.5241
7.4537
7.4483
7.4335
7.4281
7.2687
7.2635
7.2466
7.2295
6.6307
6.6270
6.6107
6.6070
6.5129
6.5092
6.4927
6.4890


O
CN
F
4f
1.02
2.01
1.03
2.01
1.03
1.00
f1 (ppm)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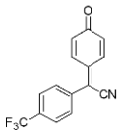
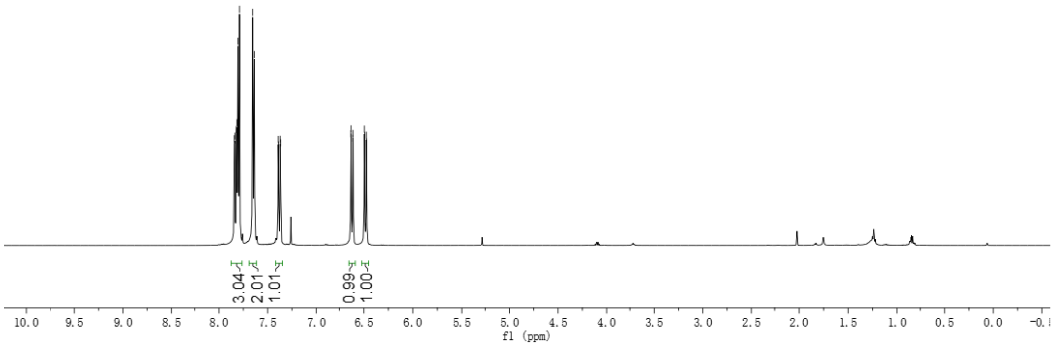
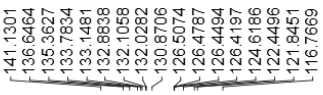
165.4625
163.4348
139.8616
136.9890
134.2462
132.8574
132.7872
131.7070
131.6847
128.1669
122.7987
117.1274
117.0315
116.8543
O
CN
F
4f
f1 (ppm)

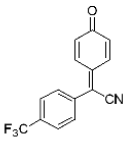

7.8420
7.8367
7.8219
7.8166
7.8058
7.7894
7.6536
7.6373
7.3912
7.3859
7.3709
7.3656
6.6338
6.6303
6.6138
6.6103
6.4957
6.4922
6.4755
6.4719


O
CN
F3C

4g

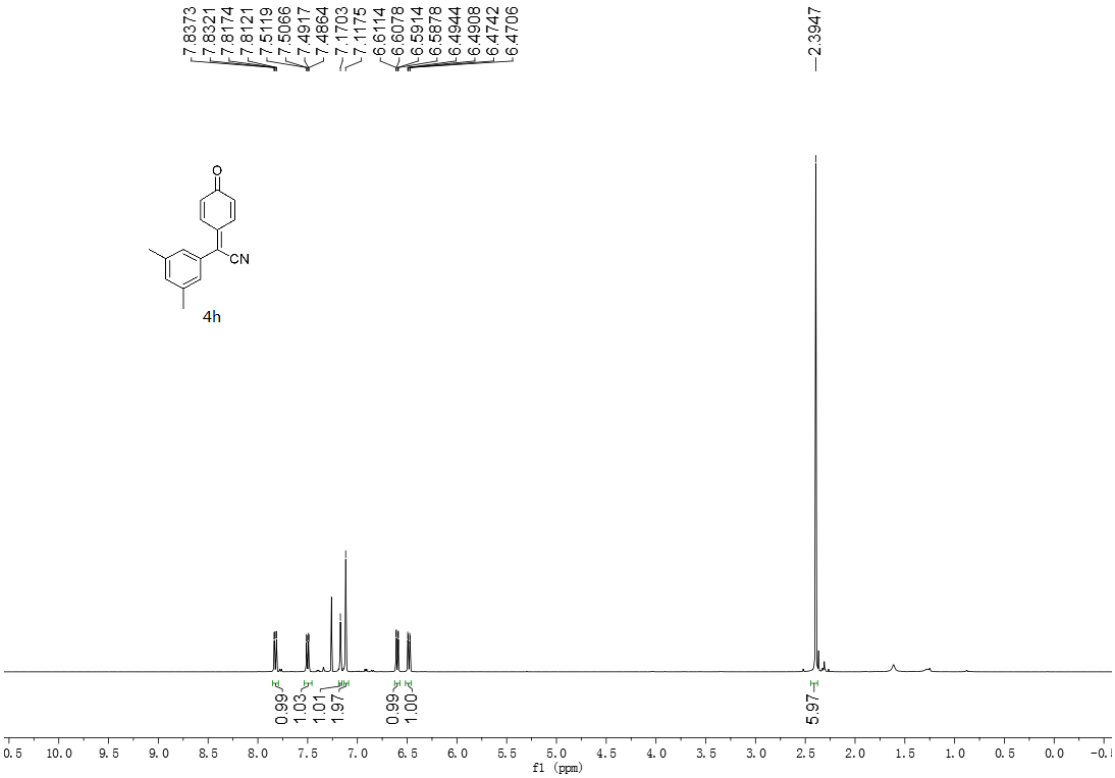

3.04
2.01
1.01
0.99
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

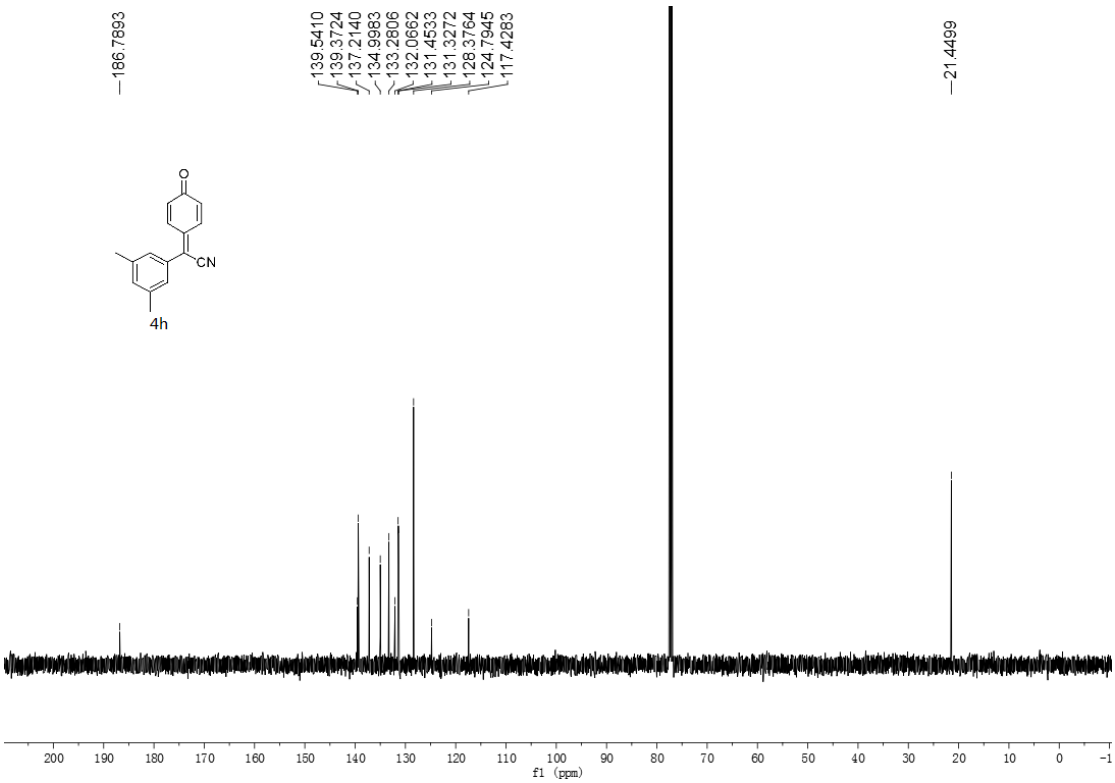

141.1301
136.6464
135.3627
133.7834
133.1481
132.8838
132.1058
132.0282
130.8706
126.5074
126.4787
126.4494
126.4197
124.6186
122.4496
121.8451
116.7669


O
CN
F3C

4g


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


7.8373
7.8321
7.8174
7.8121
7.5119
7.5066
7.4917
7.4864
7.1703
7.1175
6.6114
6.6078
6.5914
6.5878
6.4944
6.4908
6.4742
6.4706
2.3947
O
CN
4h
0.99
1.03
1.01
1.97
0.99
1.00
5.97
f1 (ppm)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139.5410
139.3724
137.2140
134.9983
133.2806
132.0662
131.4533
131.3272
128.3764
124.7945
117.4283
21.4499
O
CN
4h
f1 (ppm)


7.8332
7.8279
7.8132
7.8078
7.5207
7.5183
7.5101
7.5069
7.5034
7.4993
7.4838
7.4324
7.4270
7.4121
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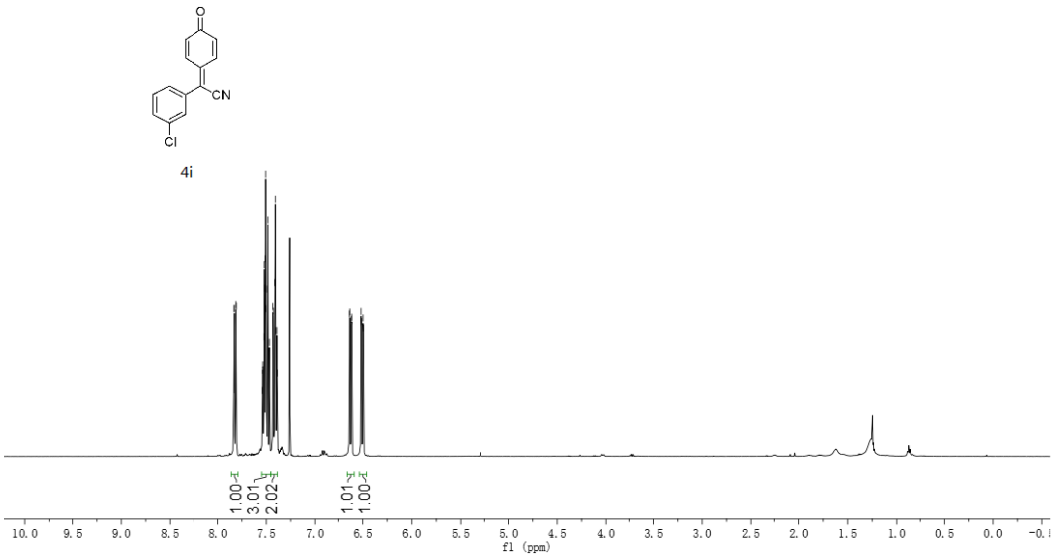
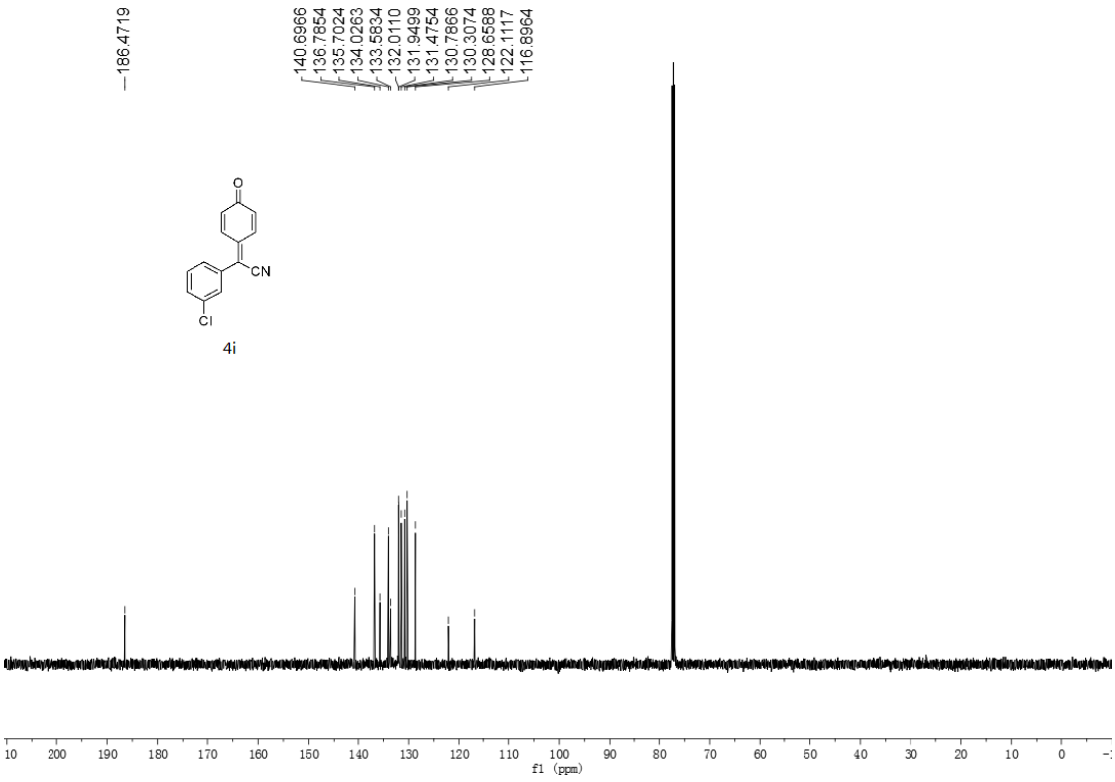
7.4023
6.6327
6.6162
6.6127
6.5166
6.5131
6.4964
6.4928


O
CN
Cl
4i
1.00
3.01
2.02
1.01
1.00
f1 (ppm)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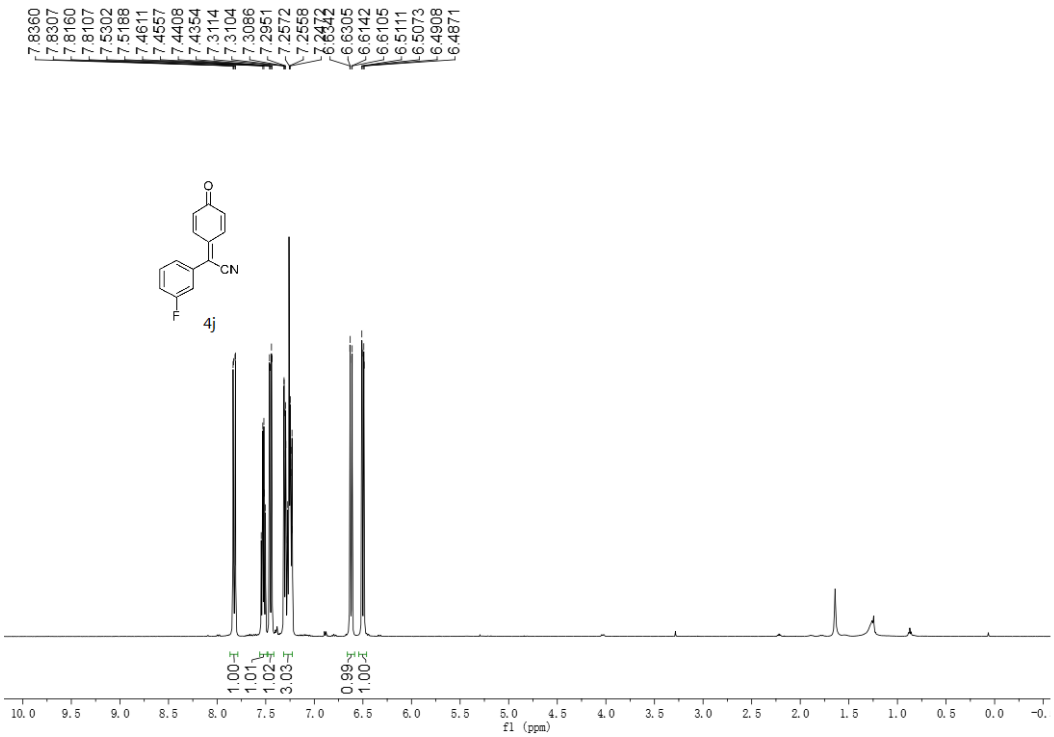
136.7854
135.7024
134.0263
133.5834
132.0110
131.9499
131.4754
130.7866
130.3074
128.6588
122.1117
116.8964
O
CN
Cl
4i
f1 (ppm)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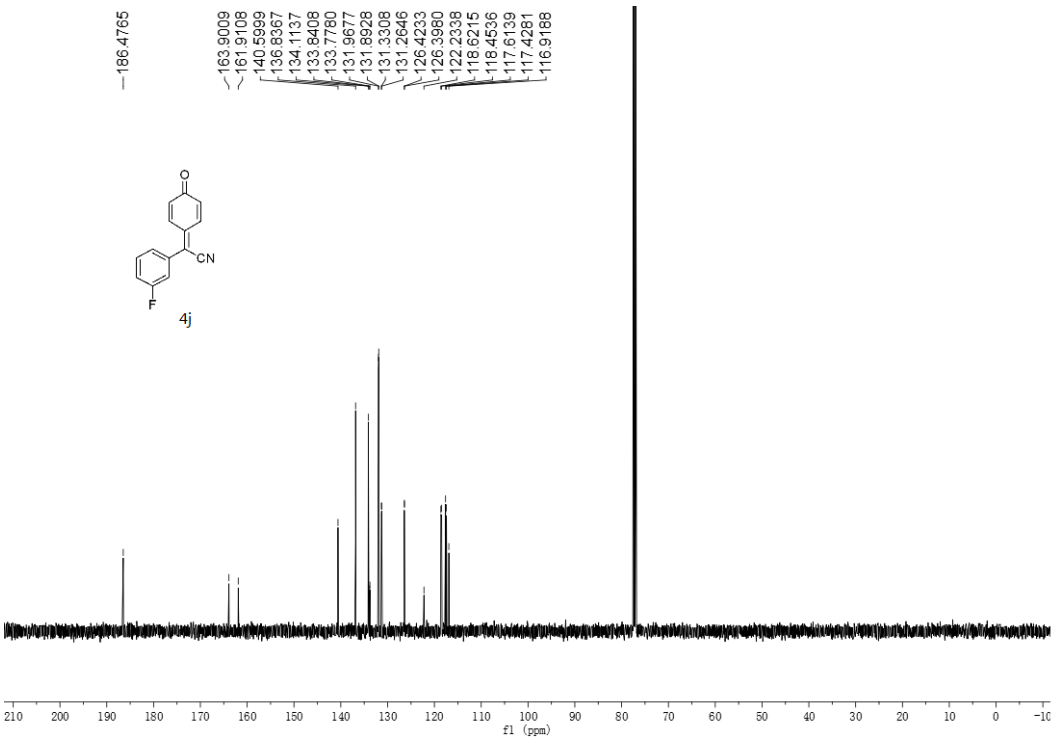
7.8307
7.8160
7.8107
7.5302
7.5188
7.4611
7.4557
7.4408
7.4354
7.3114
7.3104
7.3086
7.2951
7.2572
7.2558
6.6305
6.6142
6.6105
6.5111
6.5073
6.4908
6.4871
O
CN
F
4j
1.00
1.01
1.02
3.03
0.99
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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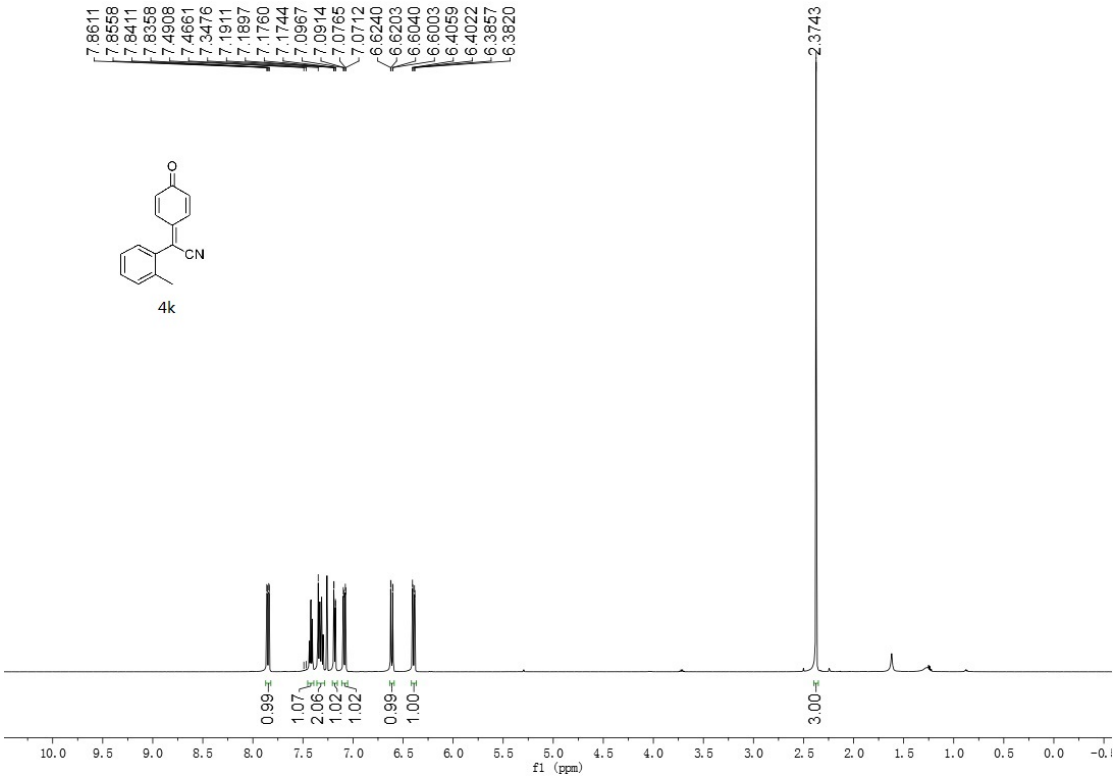
161.9108
140.5999
136.8367
134.1137
133.8408
133.7780
131.9677
131.8928
131.3308
131.2646
126.4233
126.3980
122.2338
118.6215
118.4536
117.6139
117.4281
116.9188
O
CN
F
4j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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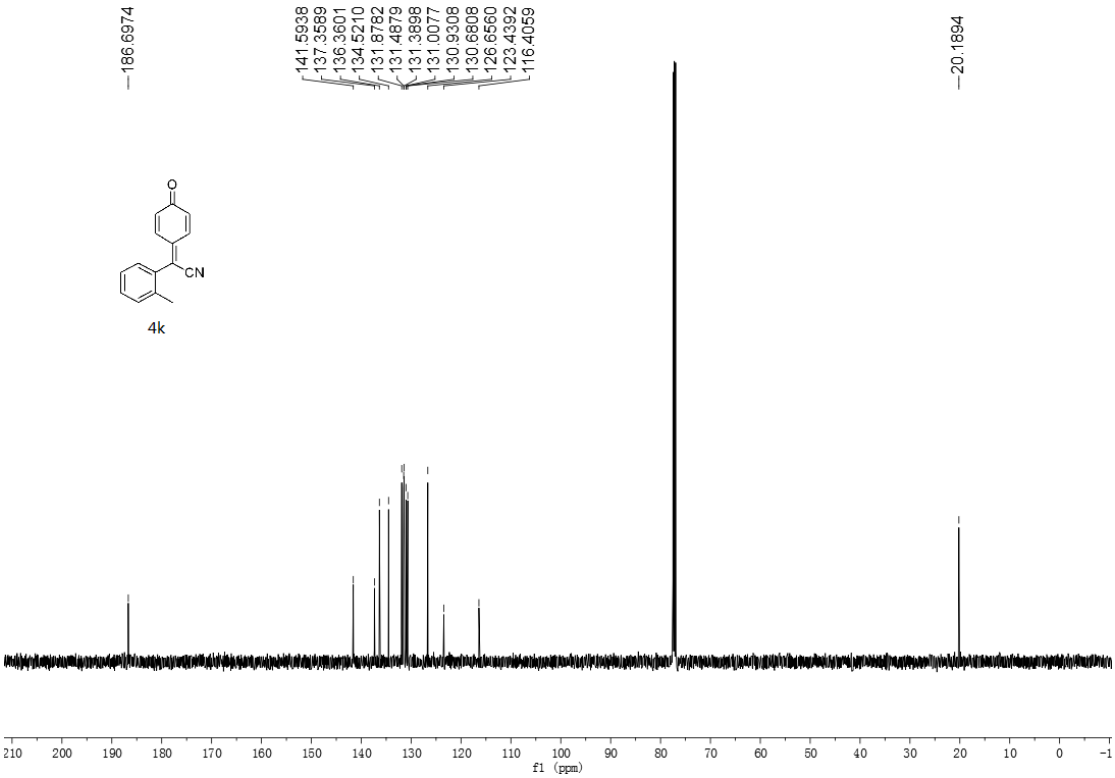
7.8558
7.8411
7.8358
7.4908
7.4661
7.3476
7.1911
7.1897
7.1760
7.1744
7.0967
7.0914
7.0765
7.0712
6.6240
6.6203
6.6040
6.6003
6.4059
6.4022
6.3857
6.3820
2.3743
O
CN
4k
0.99
1.07
2.06
1.02
1.02
0.99
1.00
3.00
f1 (ppm)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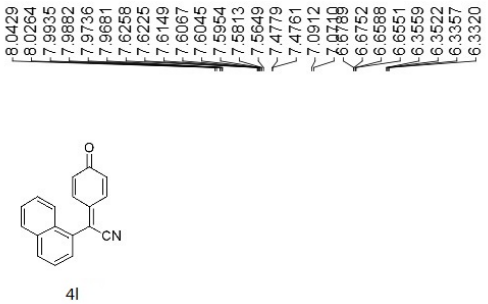
136.3601
134.5210
131.8782
131.4879
131.3898
131.0077
130.9308
130.6808
126.6560
123.4392
116.4059
20.1894
O
CN
4k
f1 (ppm)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8.0264
7.9935
7.9882
7.9736
7.9681
7.6258
7.6225
7.6149
7.6067
7.6045
7.5954
7.5813
7.5649
7.4779
7.4761
7.0912
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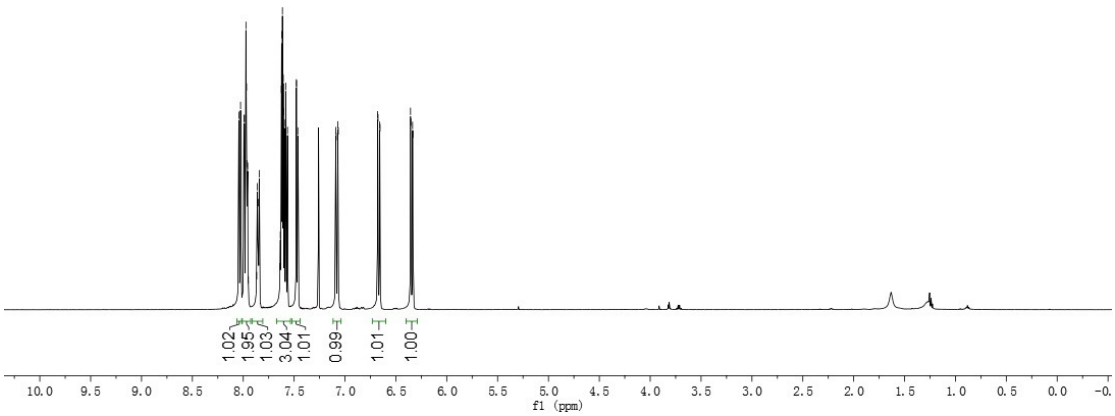
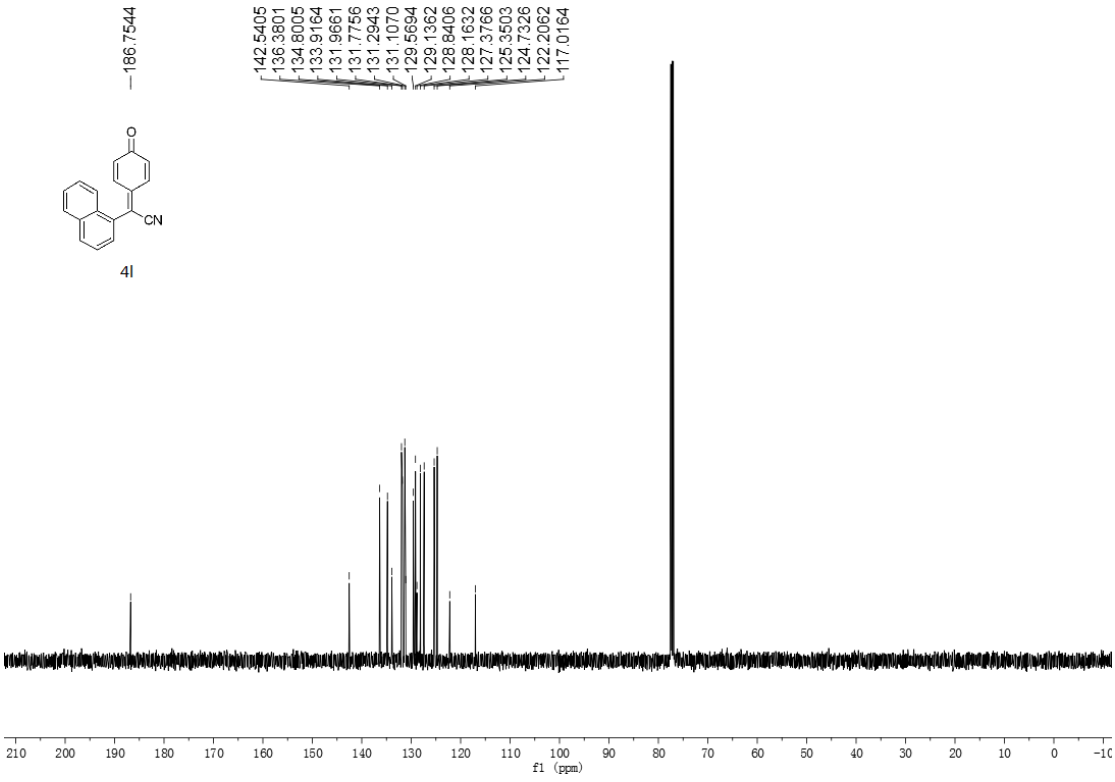
6.6588
6.6551
6.3559
6.3522
6.3357
6.3320
O
CN

4l


1.02
1.95
1.03
3.04
1.01
0.99
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.3801
134.8005
133.9164
131.9661
131.7756
131.2943
131.1070
129.5694
129.1362
128.8406
128.1632
127.3766
125.3503
124.7326
122.2062
117.0164
O
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4l


8.0237
7.9945
7.9774
7.9483
7.9299
7.9102
7.9048
7.8900
7.8847
7.6476
7.6298
7.6140
7.6124
7.6044
7.6009
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6.5285
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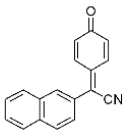
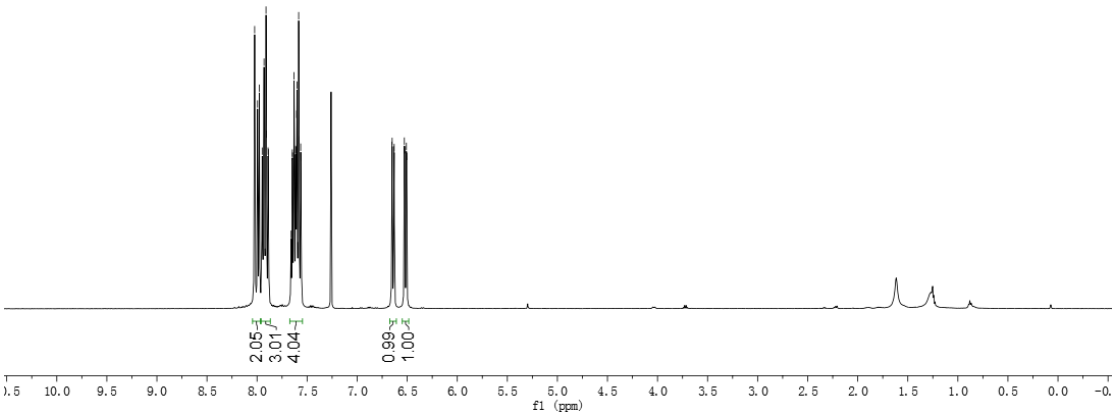
6.5083
6.5048


O
CN

4m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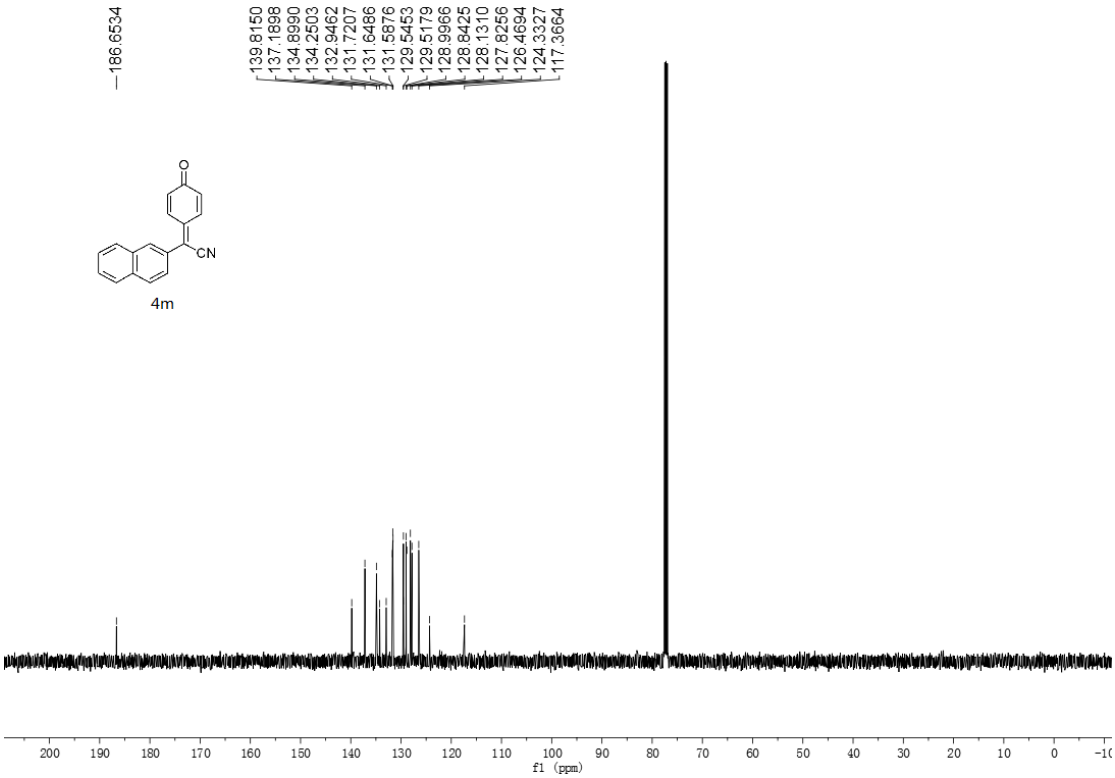
3.01
4.04
0.99
1.00
f1 (ppm)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137.1898
134.8990
134.2503
132.9462
131.7207
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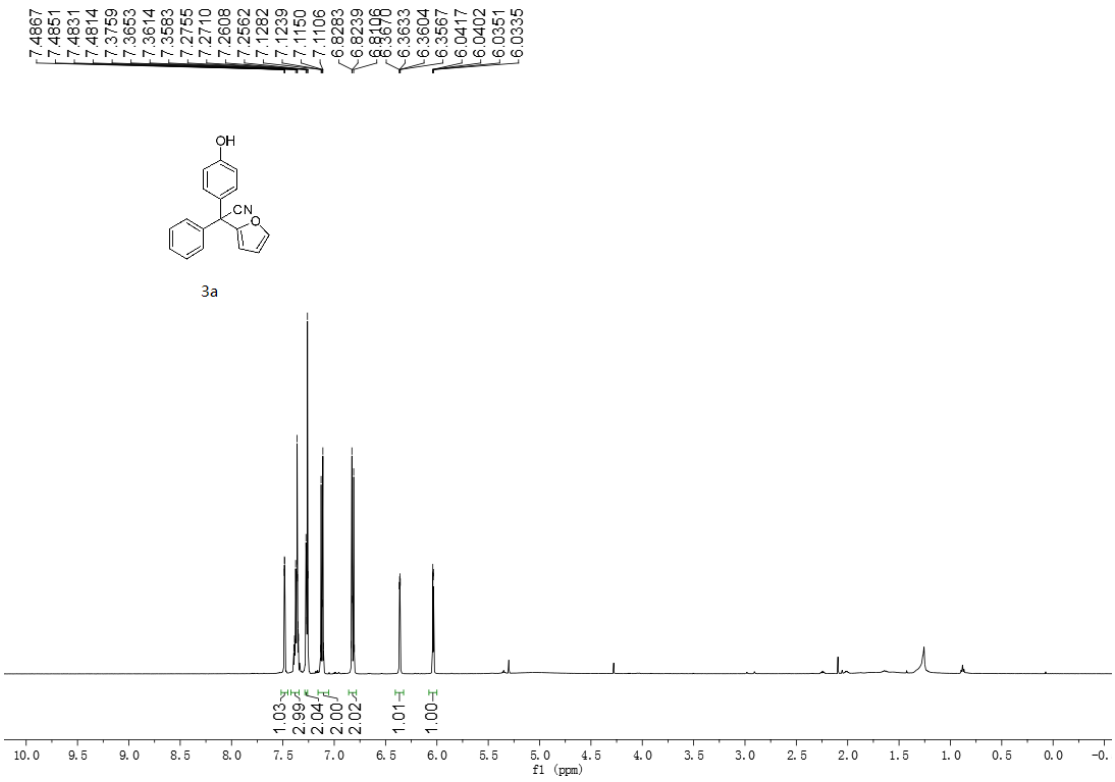
131.5876
129.5453
129.5179
128.9966
128.8425
128.1310
127.8256
126.4694
124.3327
117.3664
O
CN
f1 (ppm)

4m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7.3614
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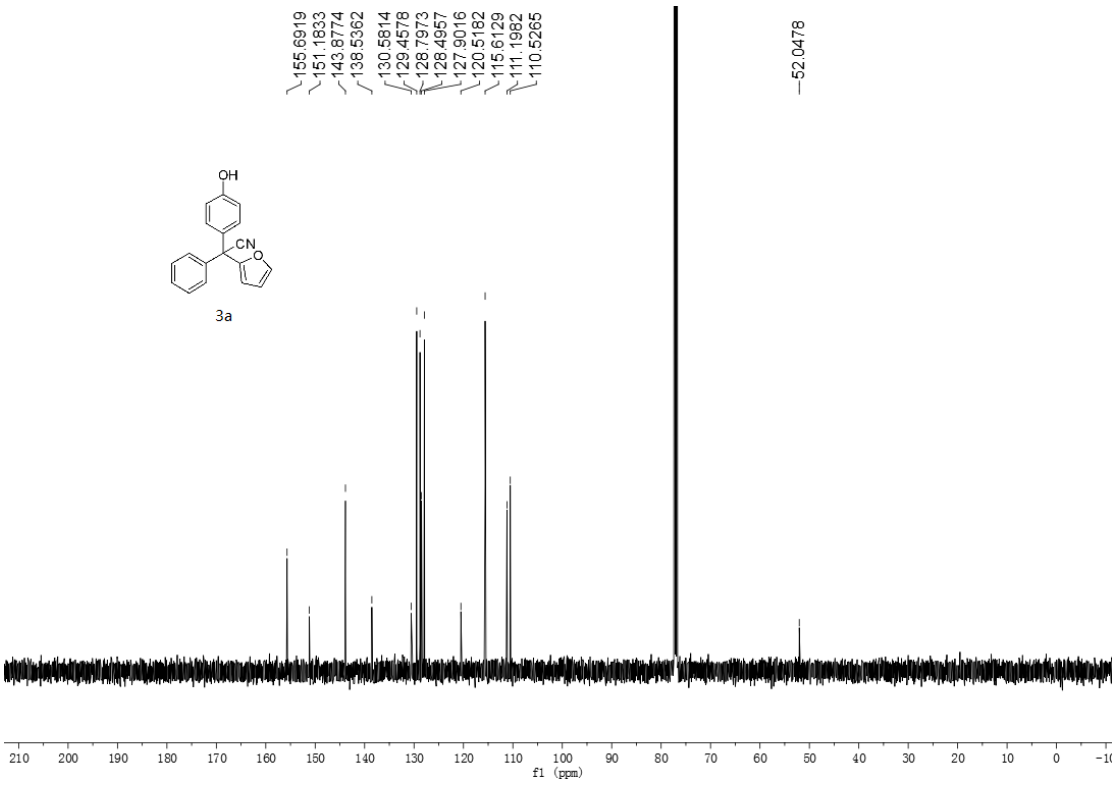
7.2755
7.2710
7.2608
7.2562
7.1282
7.1239
7.1150
7.1106
6.8283
6.8239
6.8106
6.8070
6.3633
6.3604
6.3567
6.0417
6.0402
6.0351
6.0335
OH
CN
O
3a
1.03
2.99
2.04
2.00
2.02
1.01
1.00
f1 (ppm)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138.5362
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128.7973
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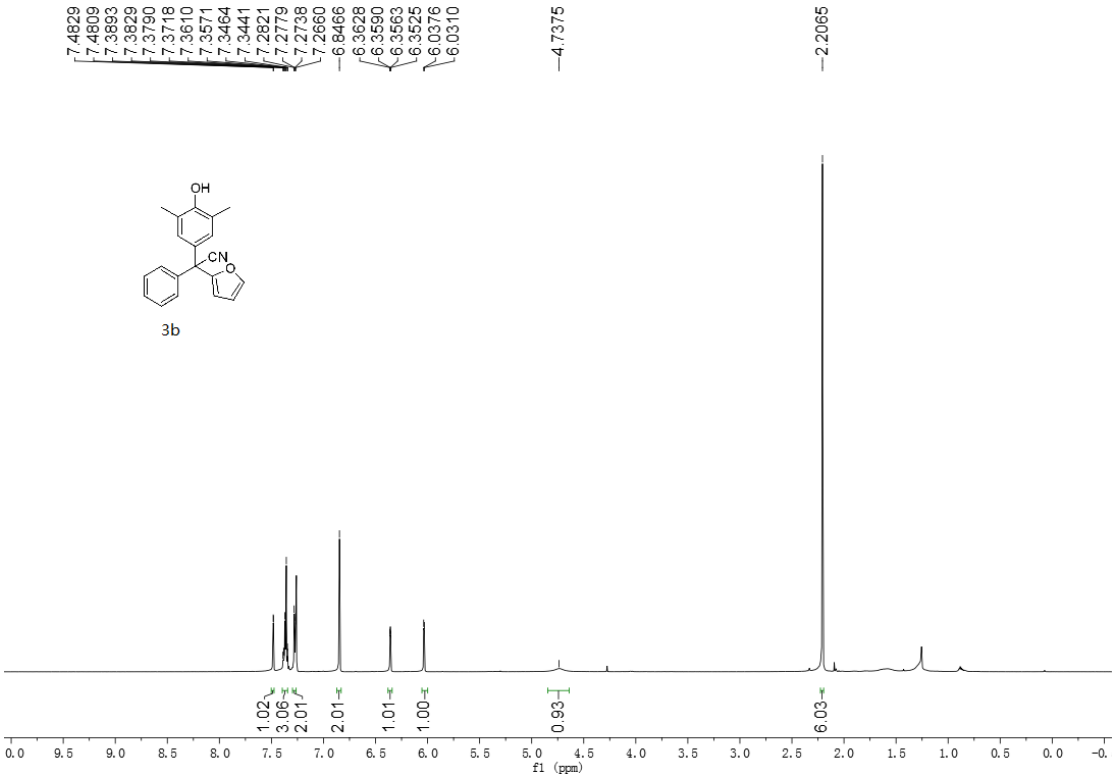
115.6129
111.1982
110.5265
52.0478
OH
CN
O
3a
f1 (ppm)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7.3718
7.3610
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7.3464
7.3441
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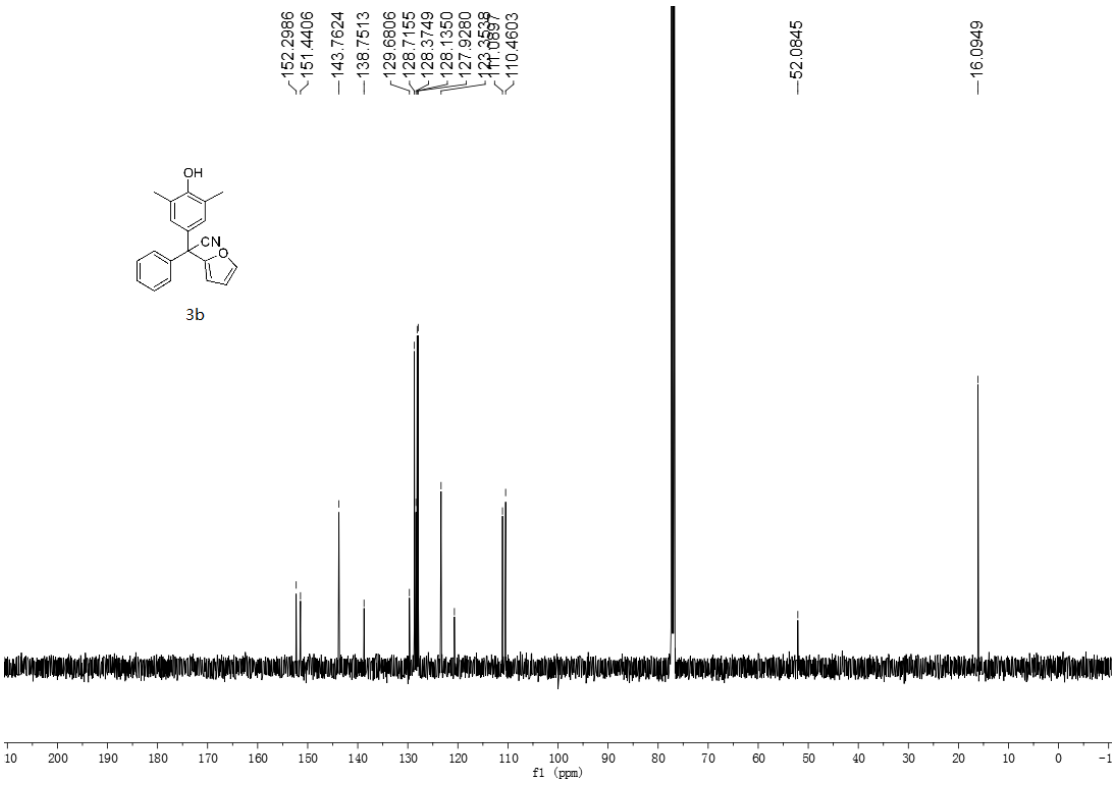
7.2779
7.2738
7.2660
6.8466
6.3628
6.3590
6.3563
6.3525
6.0376
6.0310
4.7375
2.2065
OH
CN
O
3b
1.02
3.06
2.01
2.01
1.01
1.00
0.93
6.03
f1 (ppm)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138.7513
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128.7155
128.3749
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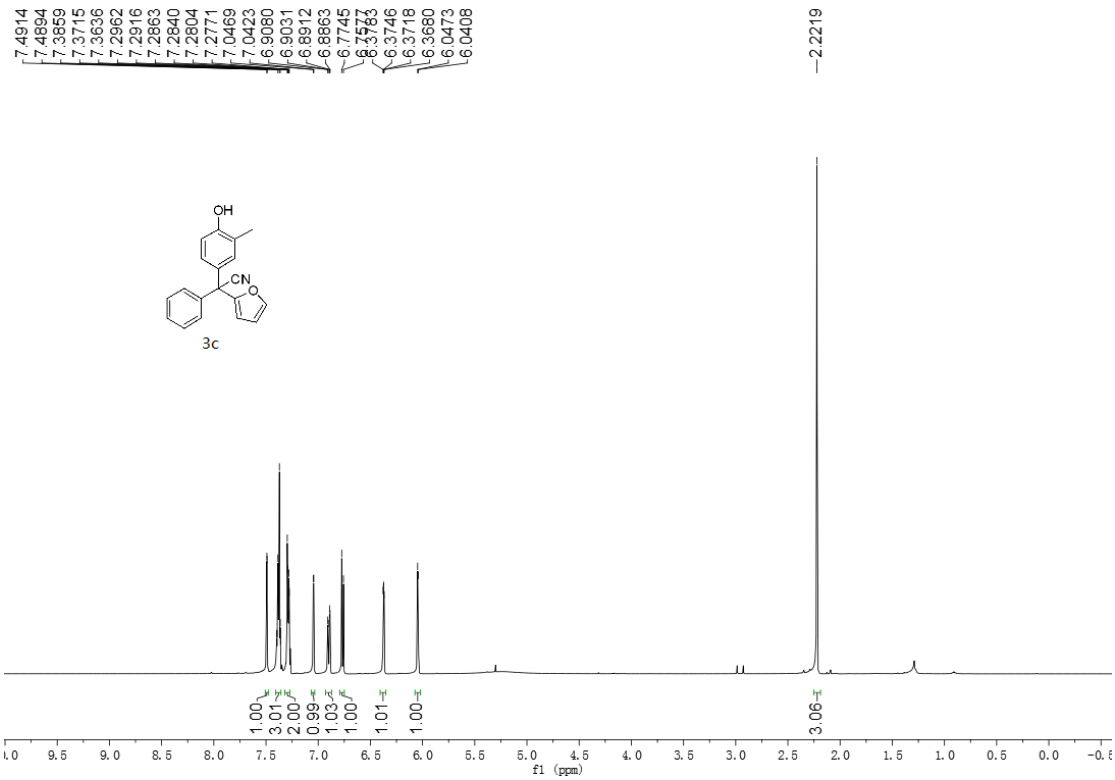
127.9280
123.3538
111.0897
110.4603
52.0845
16.0949
OH
CN
O
3b
f1 (ppm)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7.3715
7.3636
7.2962
7.2916
7.2863
7.2840
7.2804
7.2771
7.0469
7.0423
6.9080
6.9031
6.8912
6.8863
6.7745
6.7577
6.3783
6.3746
6.3718
6.3680
6.0473
6.0408
2.2219
OH
CN
O
3c
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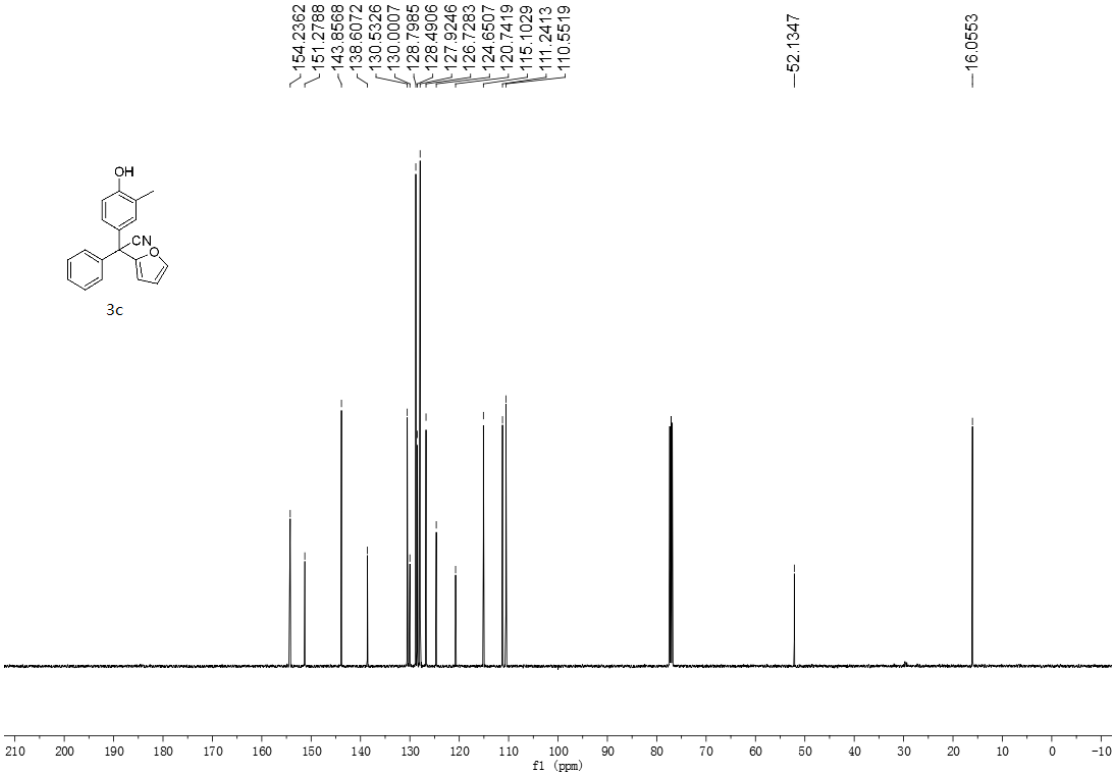
3.01
2.00
0.99
1.03
1.00
1.01
1.00
3.06
f1 (ppm)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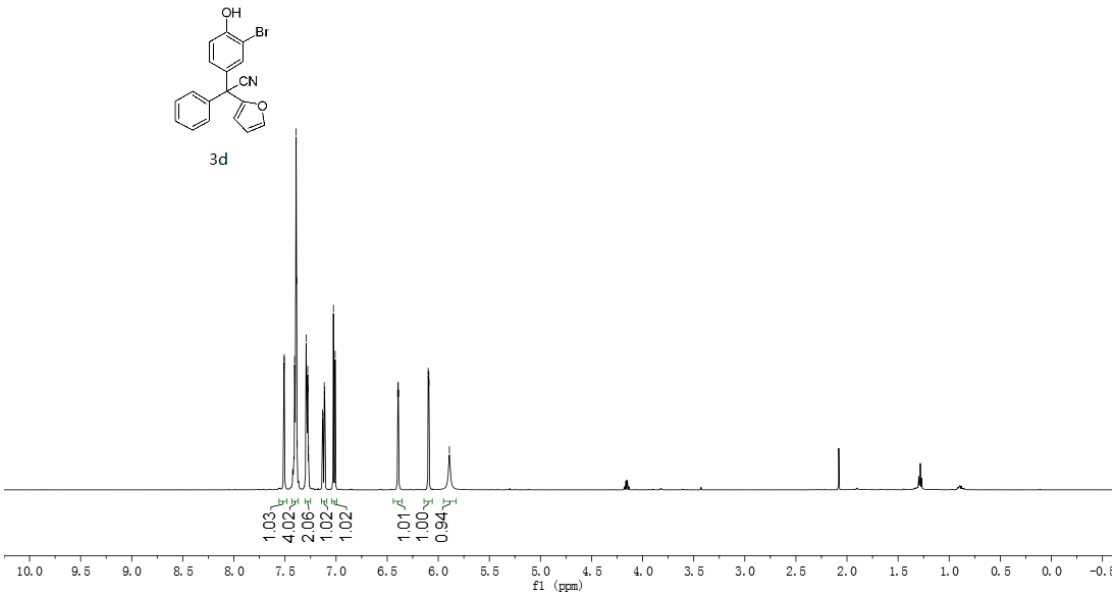
130.5326
130.0007
128.7985
128.4906
127.9246
126.7283
124.6507
120.7419
115.1029
111.2413
110.5519
52.1347
16.0553
OH
CN
O
3c
f1 (ppm)


7.5095
7.5081
7.5060
7.4060
7.3934
7.3907
7.3856
7.2935
7.2888
7.2844
7.2813
7.2776
7.2743
7.1330
7.1283
7.1158
7.1111
7.0264
6.3941
6.3912
6.3875
6.0991
6.0978
6.0924
6.0912
5.8910


OH
Br
CN
O
3d
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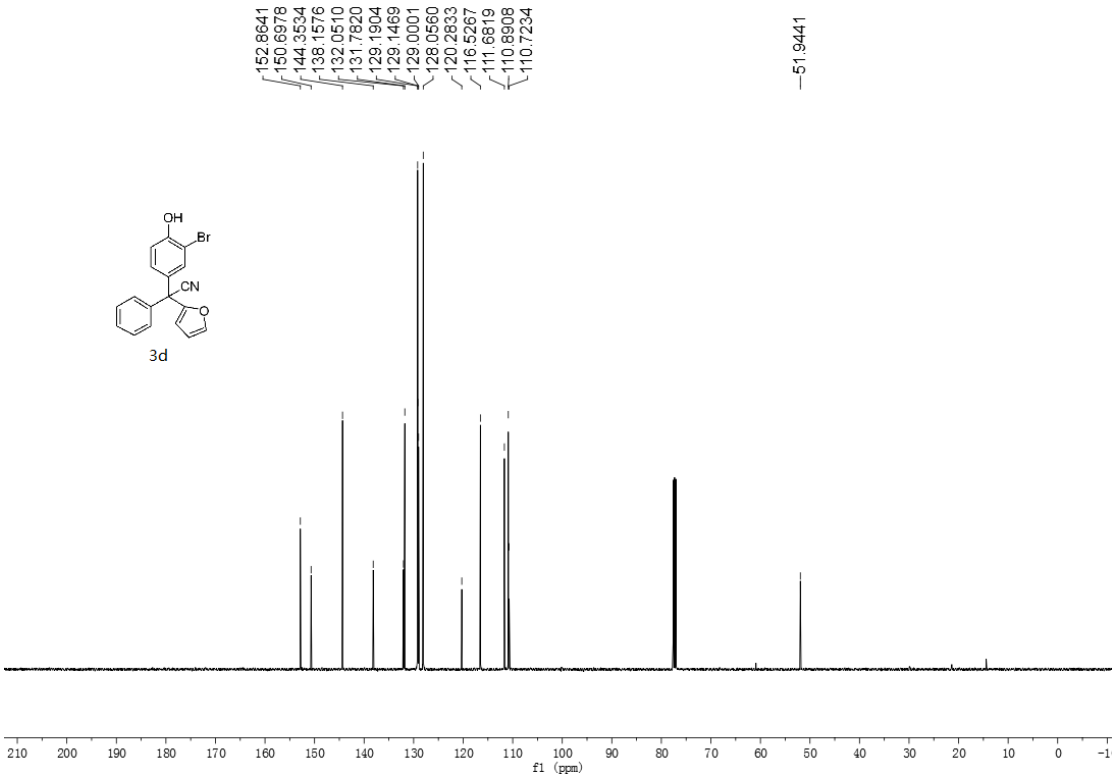
4.02
2.06
1.02
1.02
1.01
1.00
0.94
f1 (ppm)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132.0510
131.7820
129.1904
129.1469
129.0001
128.0560
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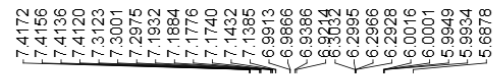
111.6819
110.8908
110.7234
51.9441
OH
Br
CN
O
3d
f1 (ppm)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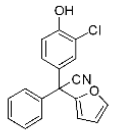
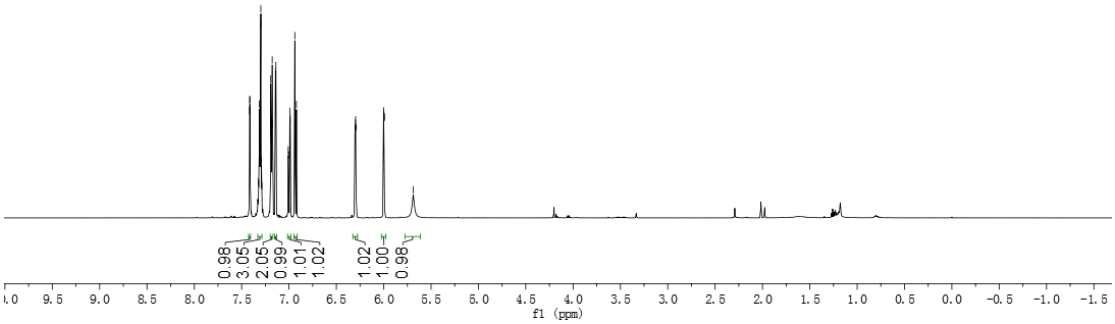
7.4156
7.4136
7.4120
7.3123
7.3001
7.2975
7.1932
7.1884
7.1776
7.1740
7.1432
7.1385
6.9913
6.9866
6.9386
6.9214
6.2995
6.2966
6.2928
6.0016
6.0001
5.9949
5.9934
5.6878


OH
Cl
CN
O

3e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3.05
2.05
0.99
1.01
1.02
1.02
1.00
0.98
f1 (ppm)


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150.6576
144.2842
138.1076
131.7357
129.1229
128.9266
128.7836
128.3734
128.0044
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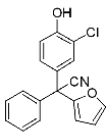
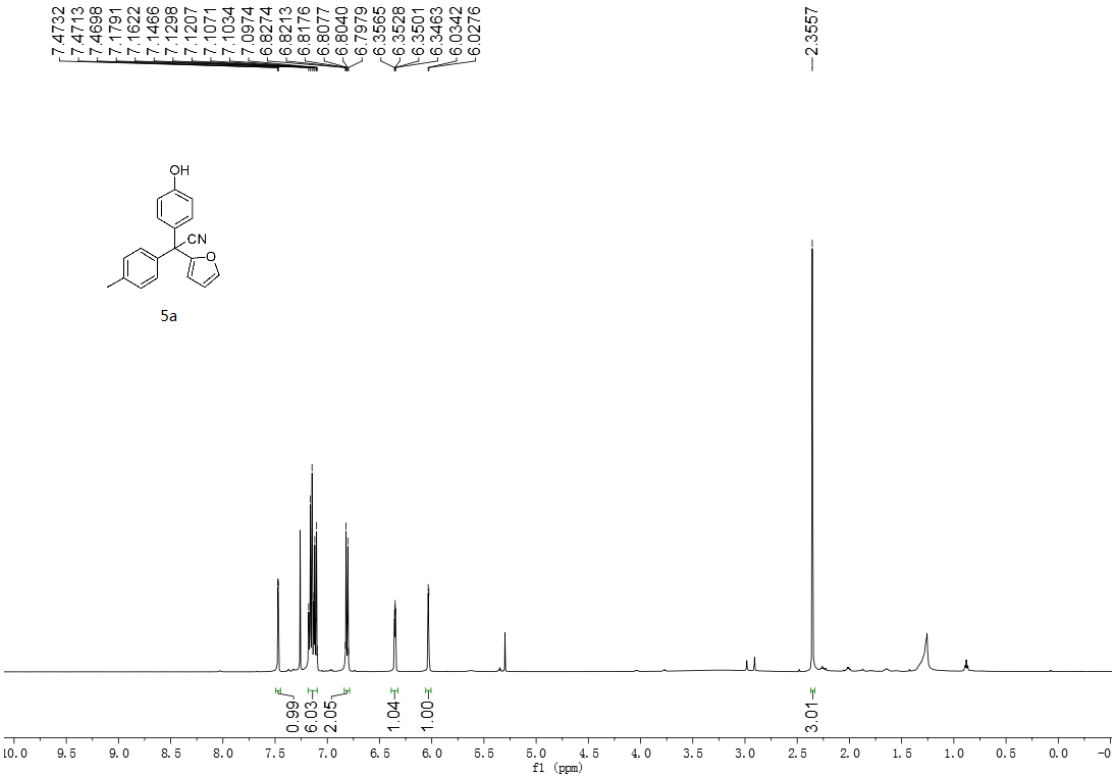
120.1993
116.6581
111.5858
110.8116
51.9902


OH
Cl
CN
O

3e


f1 (ppm)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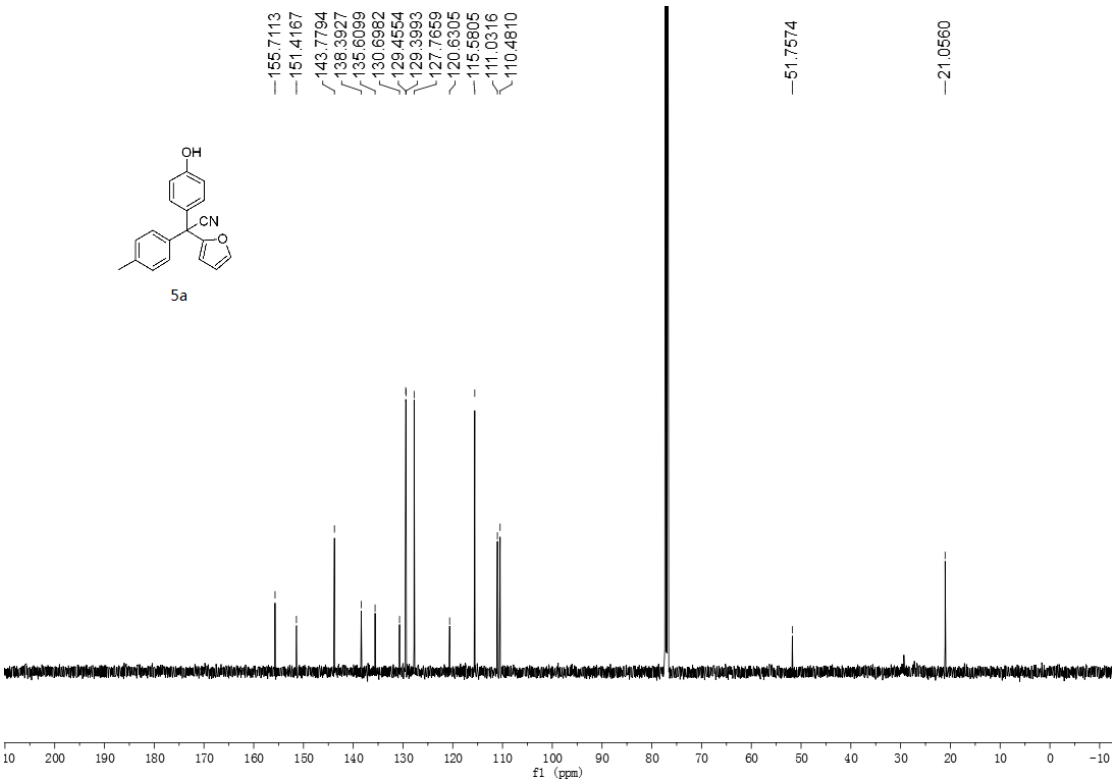
7.1622
7.1466
7.1298
7.1207
7.1071
7.1034
7.0974
6.8274
6.8213
6.8176
6.8077
6.8040
6.7979
6.3565
6.3528
6.3501
6.3463
6.0342
6.0276
2.3557
OH
CN
O
5a
0.99
6.03
2.05
1.04
1.00
3.01
f1 (ppm)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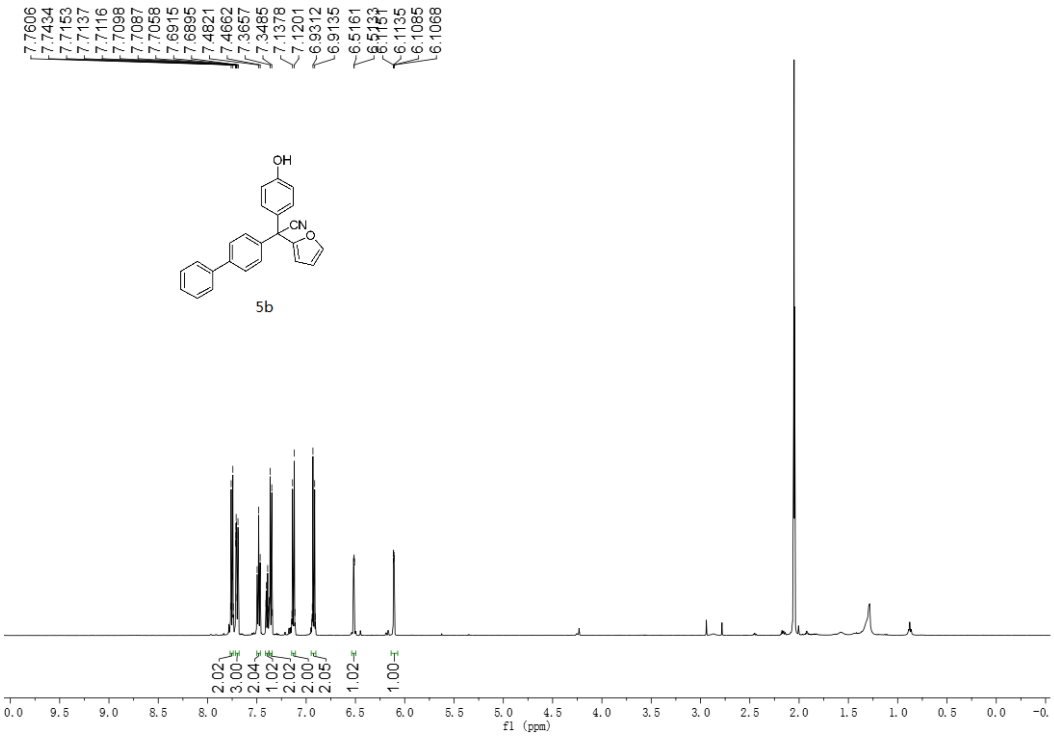
138.3927
135.6099
130.6982
129.4554
129.3993
127.7659
120.6305
115.5805
111.0316
110.4810
51.7574
21.0560
OH
CN
O
5a
f1 (ppm)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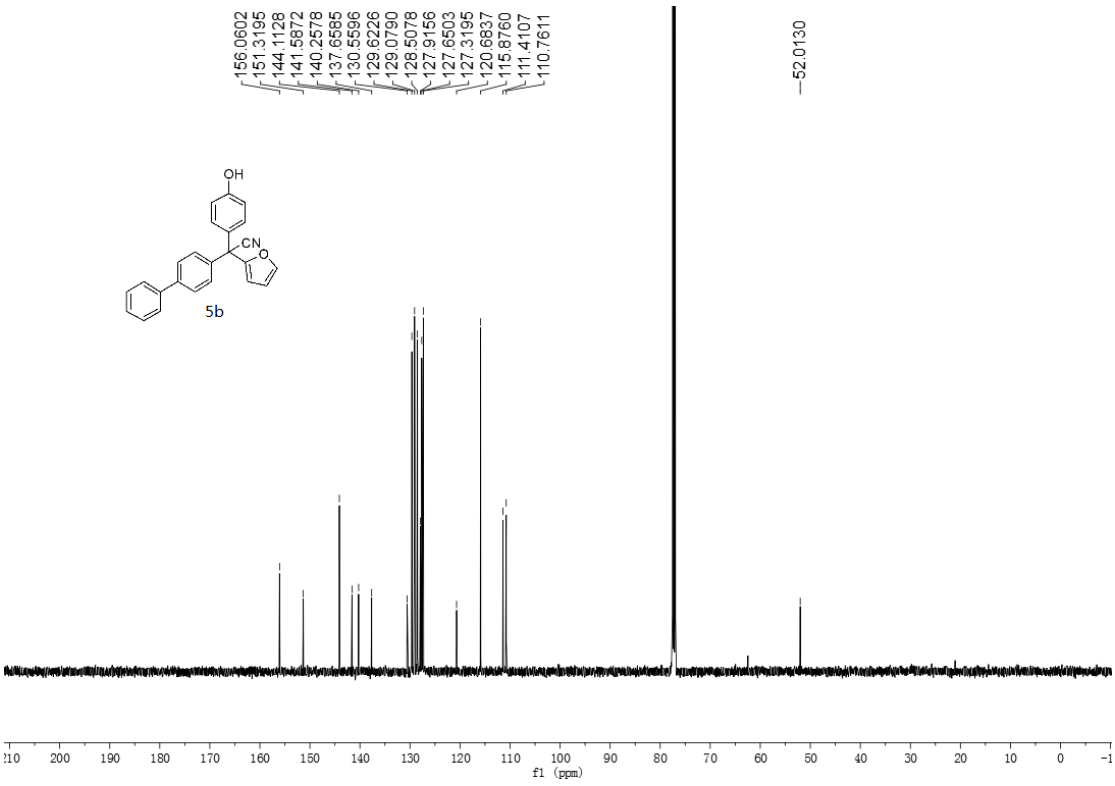
7.7153
7.7137
7.7116
7.7098
7.7087
7.7058
7.6915
7.6895
7.4821
7.4662
7.3657
7.3485
7.1378
7.1201
6.9312
6.9135
6.5161
6.5133
6.1151
6.1135
6.1085
6.1068
OH
CN
O
5b
2.02
3.00
2.04
1.02
2.02
2.00
2.05
1.02
1.00
f1 (ppm)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141.5872
140.2578
137.6585
130.5596
129.6226
129.0790
128.5078
127.9156
127.6503
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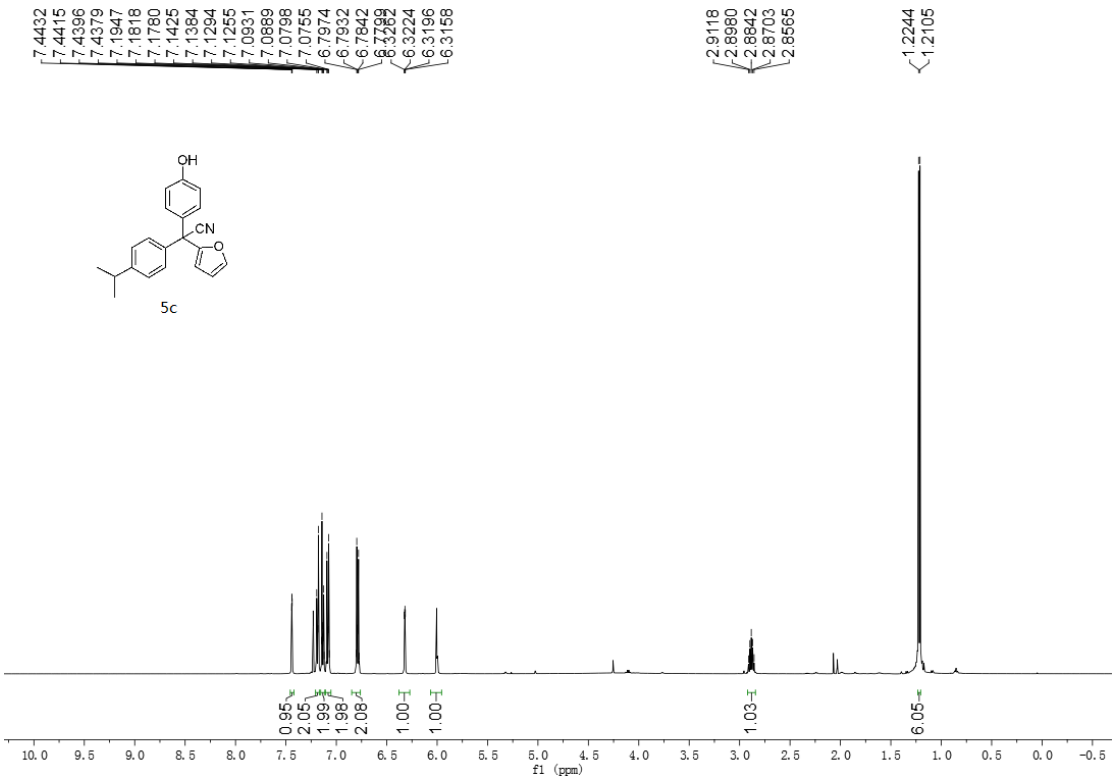
120.6837
115.8760
111.4107
110.7611
52.0130
OH
CN
O
5b
f1 (ppm)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7.4379
7.1947
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7.1425
7.1384
7.1294
7.1255
7.0931
7.0889
7.0798
7.0755
6.7974
6.7932
6.7842
6.3224
6.3196
6.3158
2.9118
2.8980
2.8842
2.8703
2.8565
1.2244
1.2105
OH
CN
O
5c
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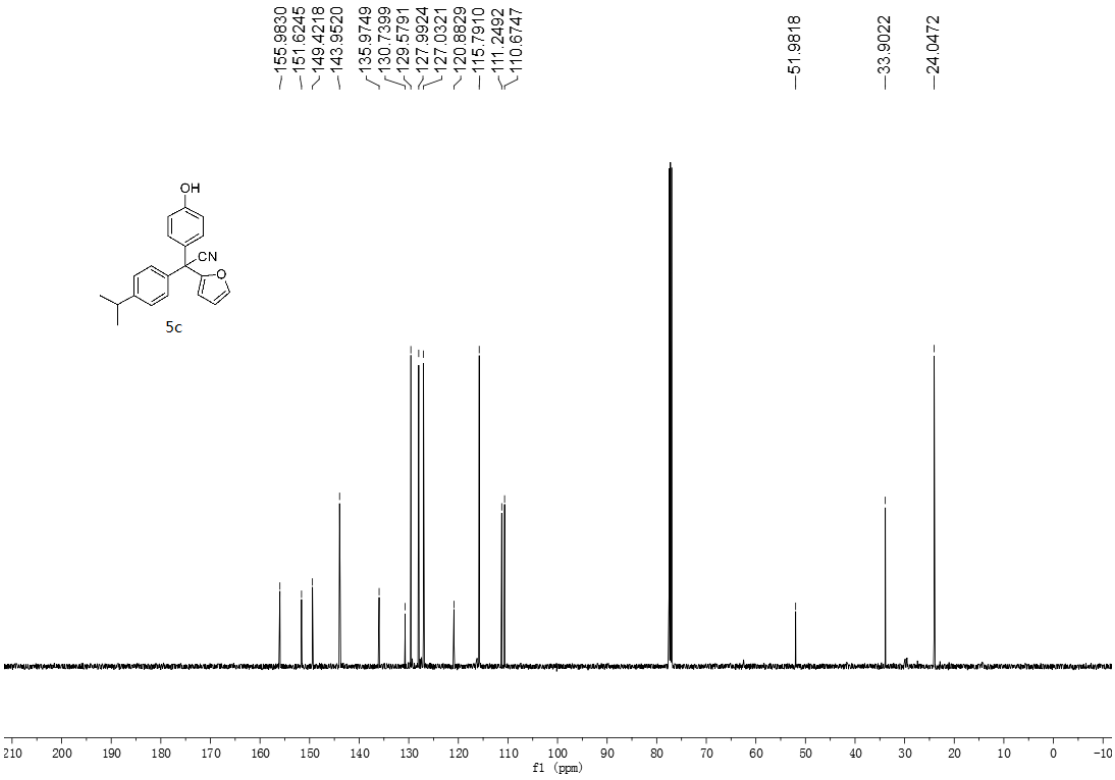
2.05
1.99
1.98
2.08
1.00
1.00
1.03
6.05
f1 (ppm)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130.7399
129.5791
127.9924
127.0321
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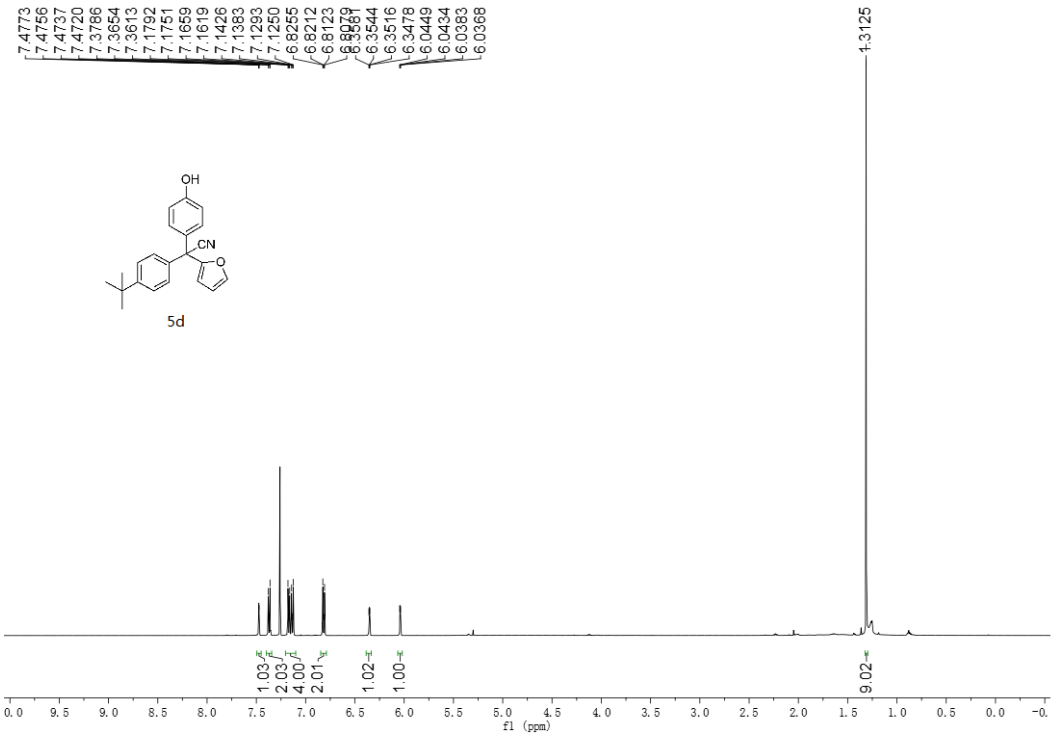
111.2492
110.6747
51.9818
33.9022
24.0472
OH
CN
O
5c
f1 (ppm)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7.1751
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7.1426
7.1383
7.1293
7.1250
6.8255
6.8212
6.8123
6.3581
6.3544
6.3516
6.3478
6.0449
6.0434
6.0383
6.0368
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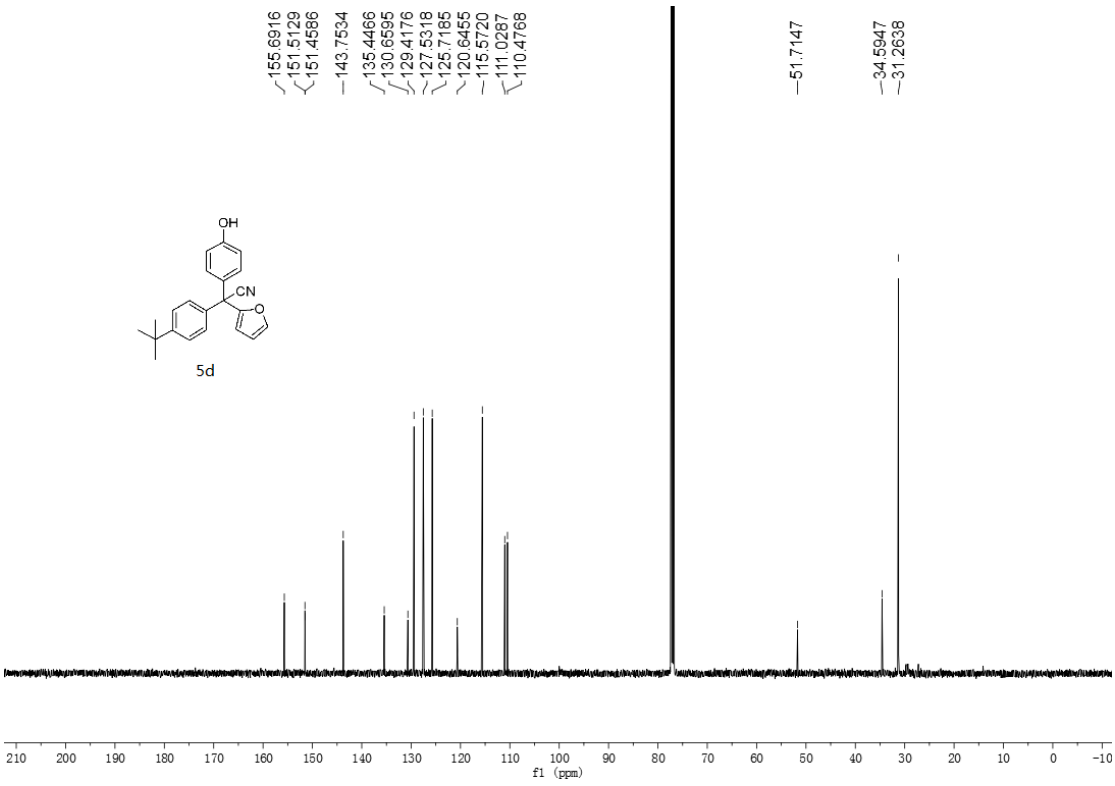
OH
CN
O
5d
1.03
2.03
4.00
2.01
1.02
1.00
9.02
f1 (ppm)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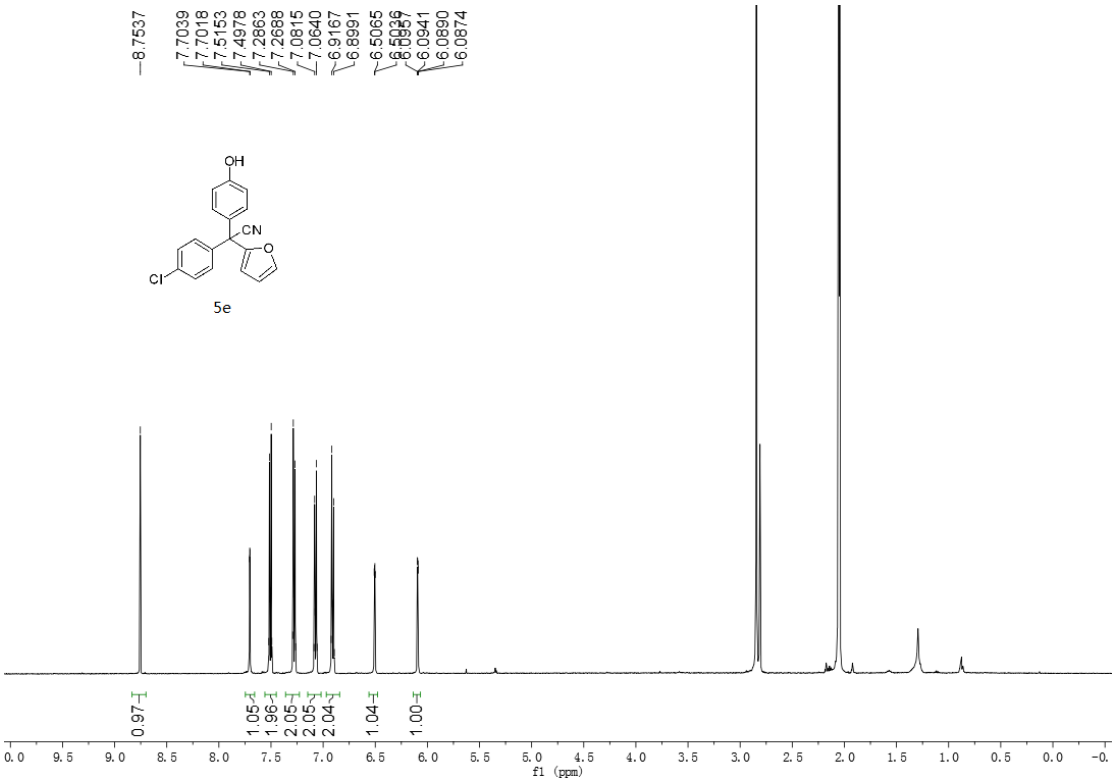
34.5947
31.2638
OH
CN
O
5d
f1 (ppm)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7.0640
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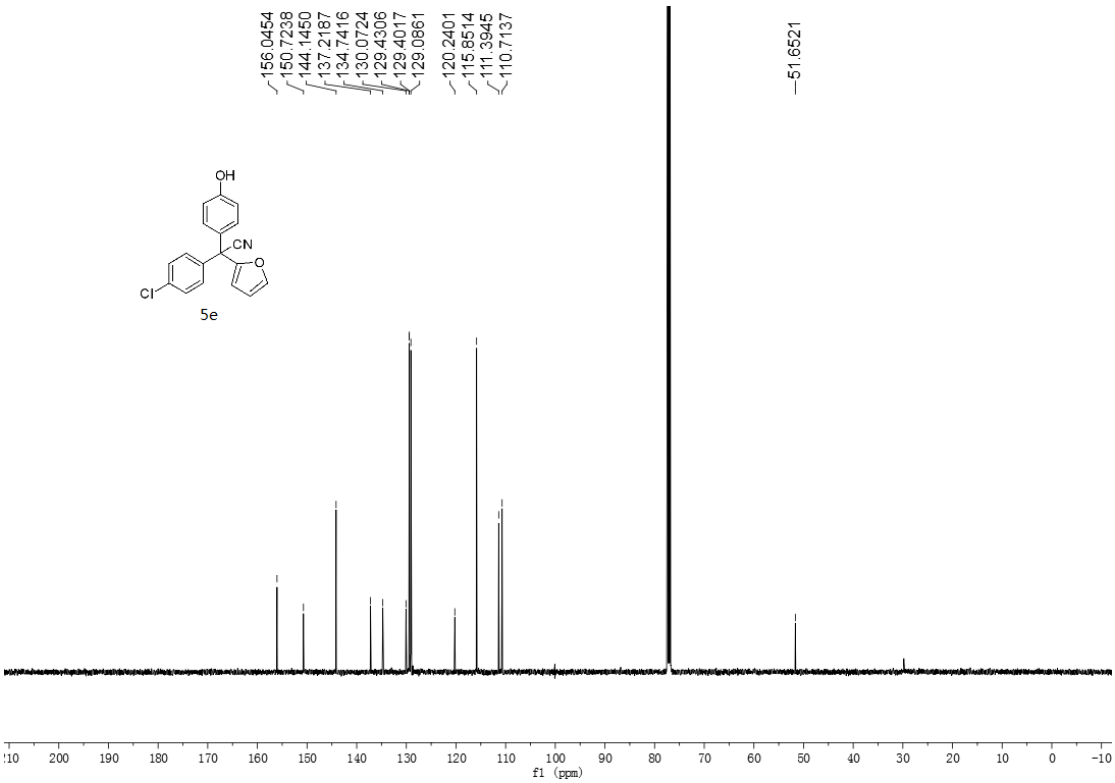
6.8991
6.5065
6.0941
6.0890
6.0874
OH
CN
O
Cl
5e
0.97
1.05
1.96
2.05
2.05
2.04
1.04
1.00
f1 (ppm)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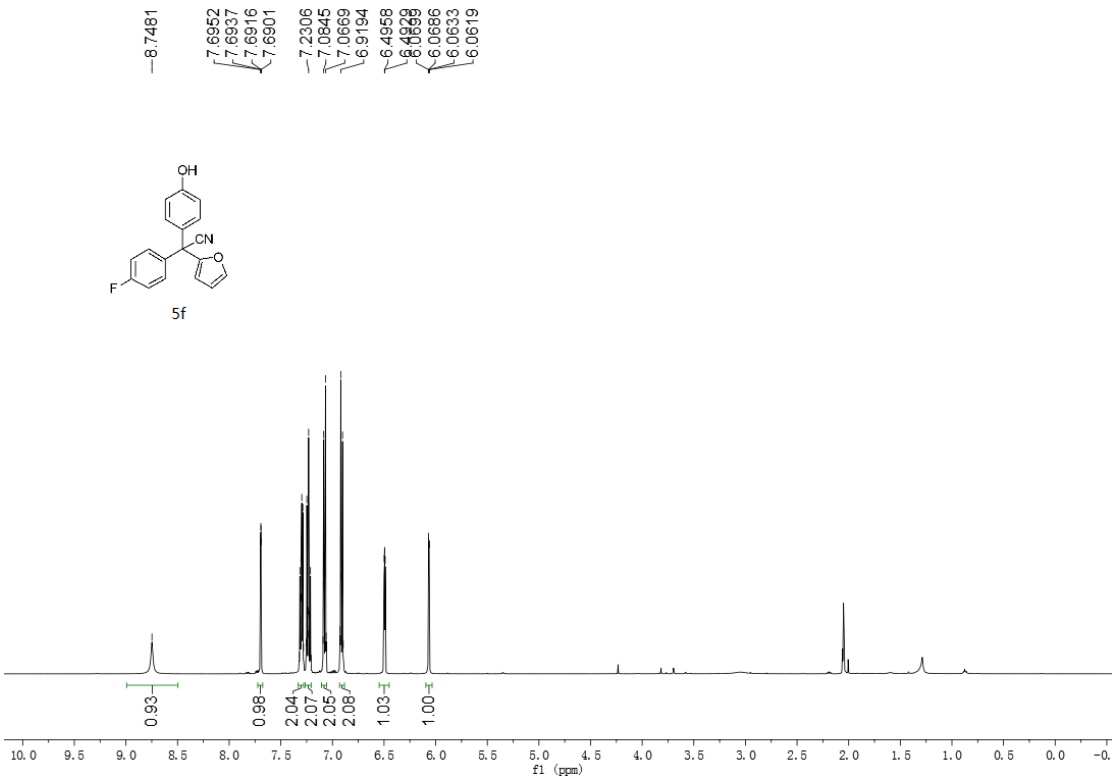
CN
O
Cl
5e
f1 (ppm)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6.0686
6.0633
6.0619
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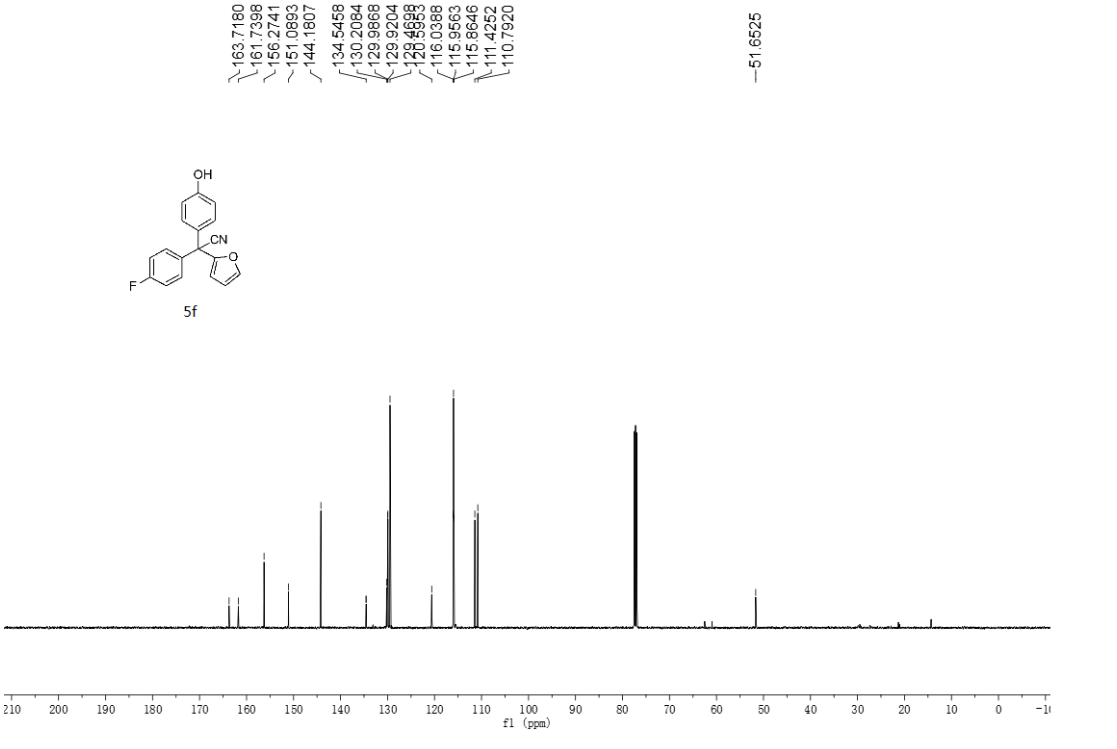
CN
F
5f
0.93
0.98
2.04
2.07
2.05
2.08
1.03
1.00
f1 (ppm)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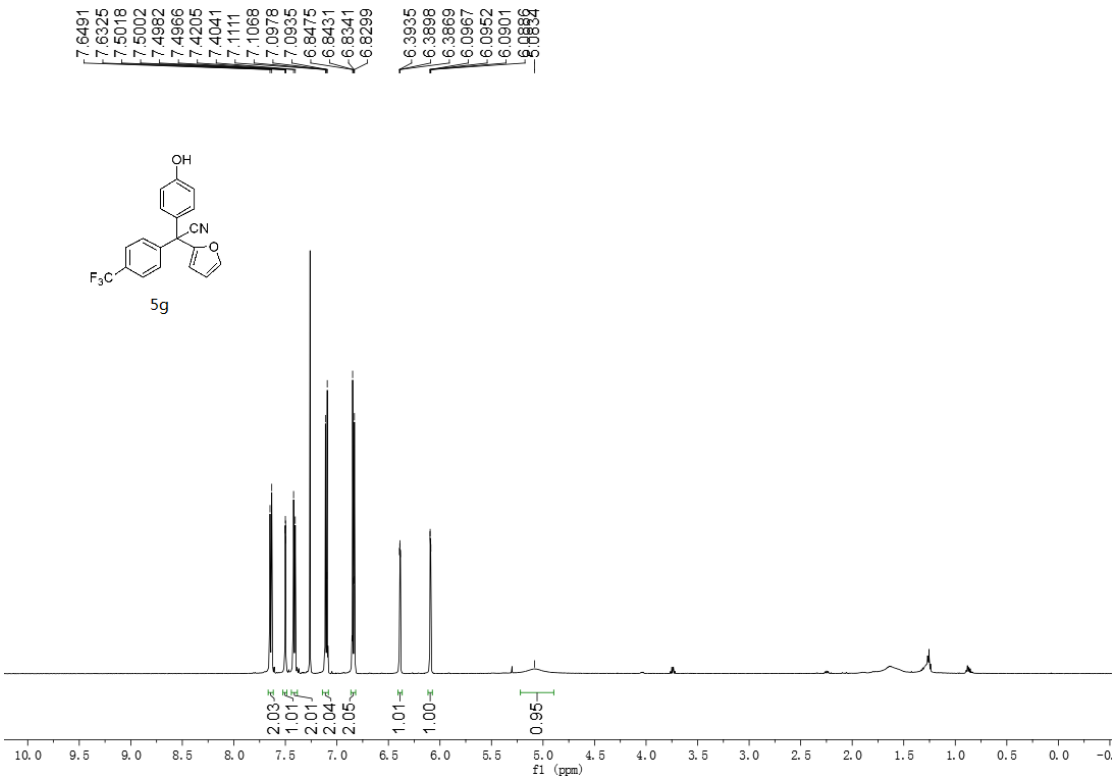
111.4252
110.7920
51.6525
OH
CN
F
5f
f1 (ppm)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7.0978
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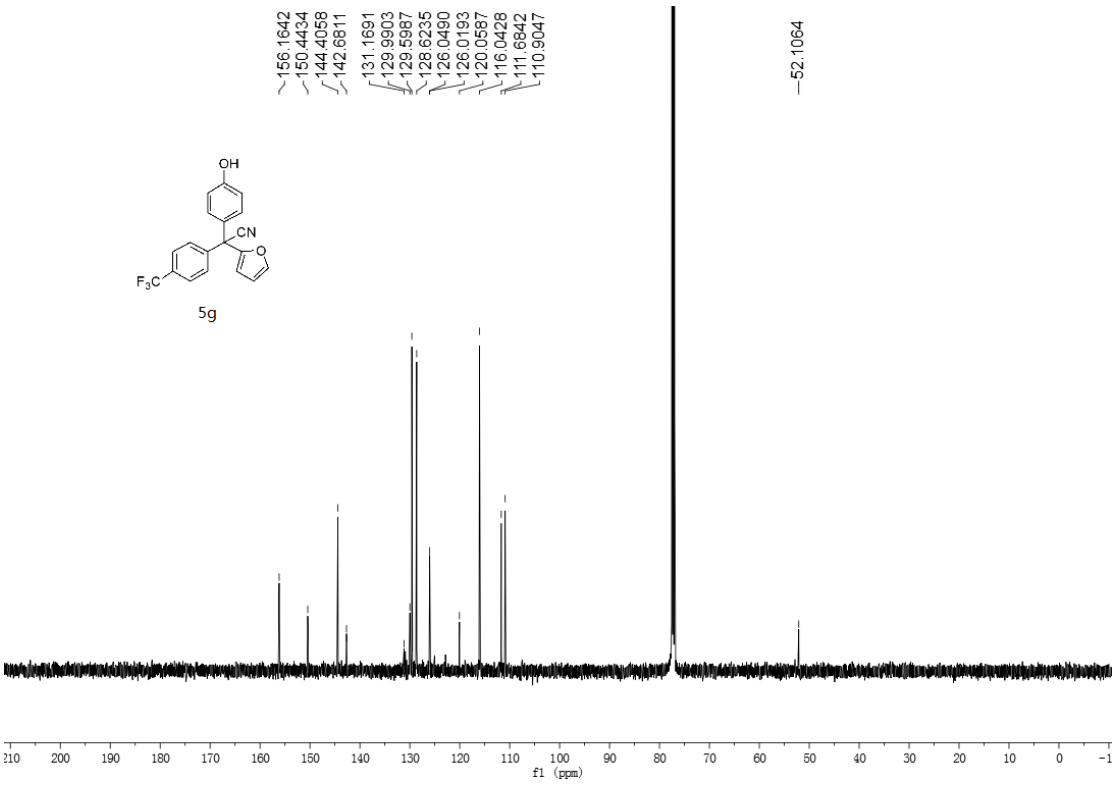
6.8475
6.8431
6.8341
6.8299
6.3935
6.3898
6.3869
6.0967
6.0952
6.0901
OH
CN
O
F3C
5g
2.03
1.01
2.01
2.04
2.05
1.01
1.00
0.95
f1 (ppm)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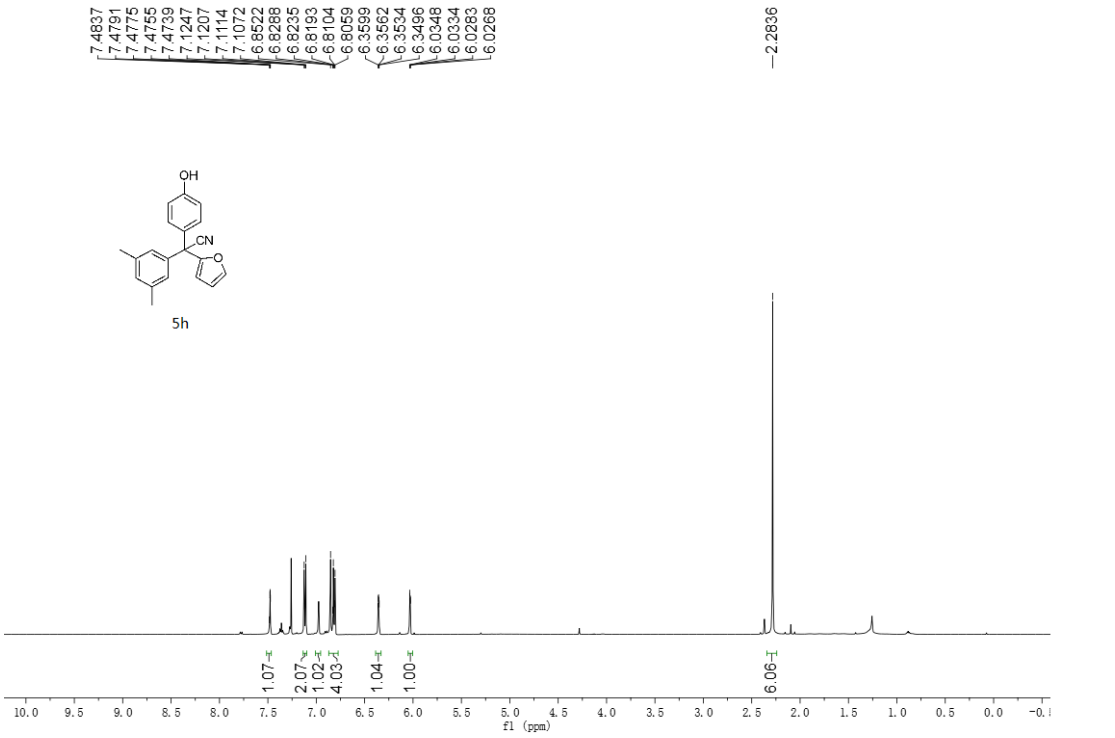
OH
CN
O
F3C
5g
f1 (ppm)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7.1072
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6.8288
6.8235
6.8193
6.8104
6.8059
6.3599
6.3562
6.3534
6.3496
6.0348
6.0334
6.0283
6.0268
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O
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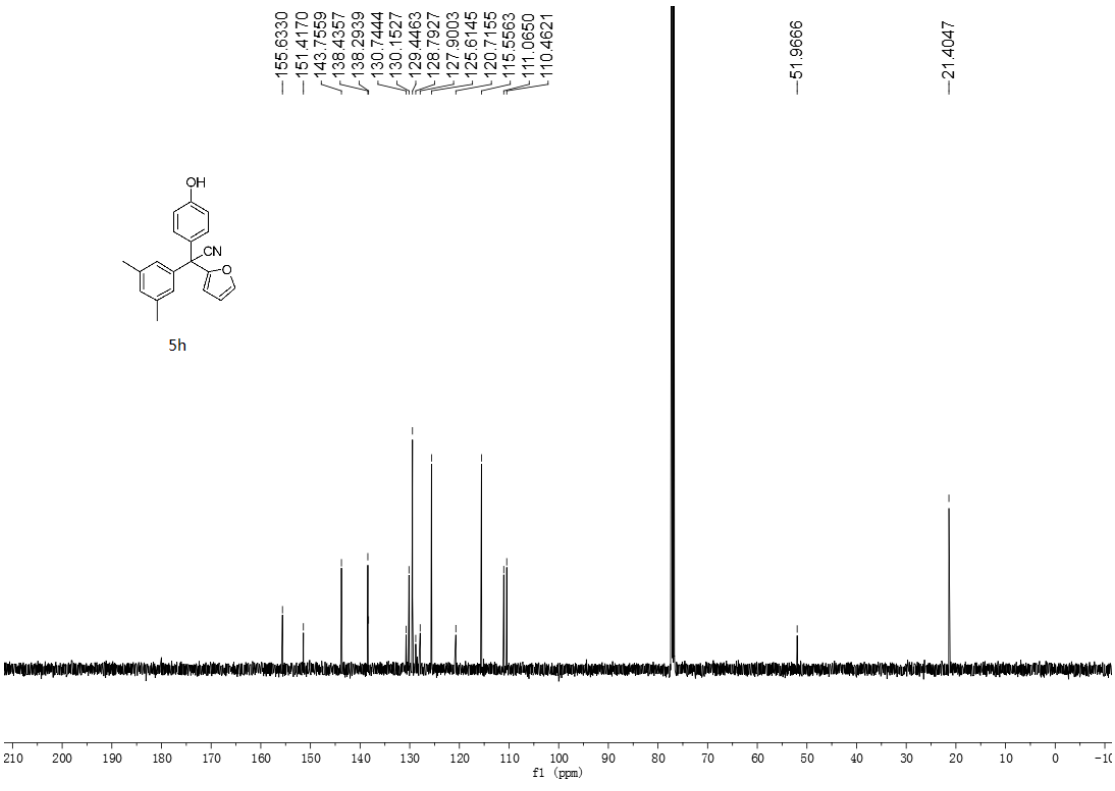
2.07
1.02
4.03
1.04
1.00
6.06
f1 (ppm)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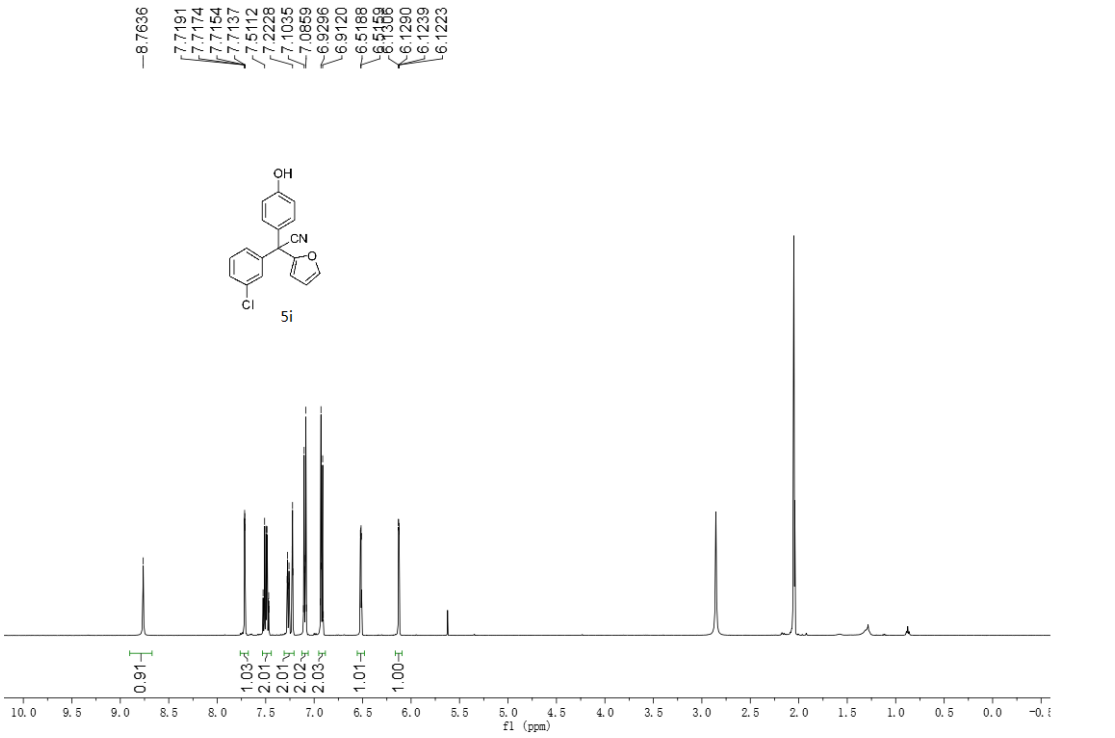
51.9666
21.4047
OH
CN
O
5h
f1 (ppm)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7.7154
7.7137
7.5112
7.2228
7.1035
7.0859
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6.9120
6.5188
6.5159
6.1290
6.1239
6.1223
OH
CN
O
Cl
5i
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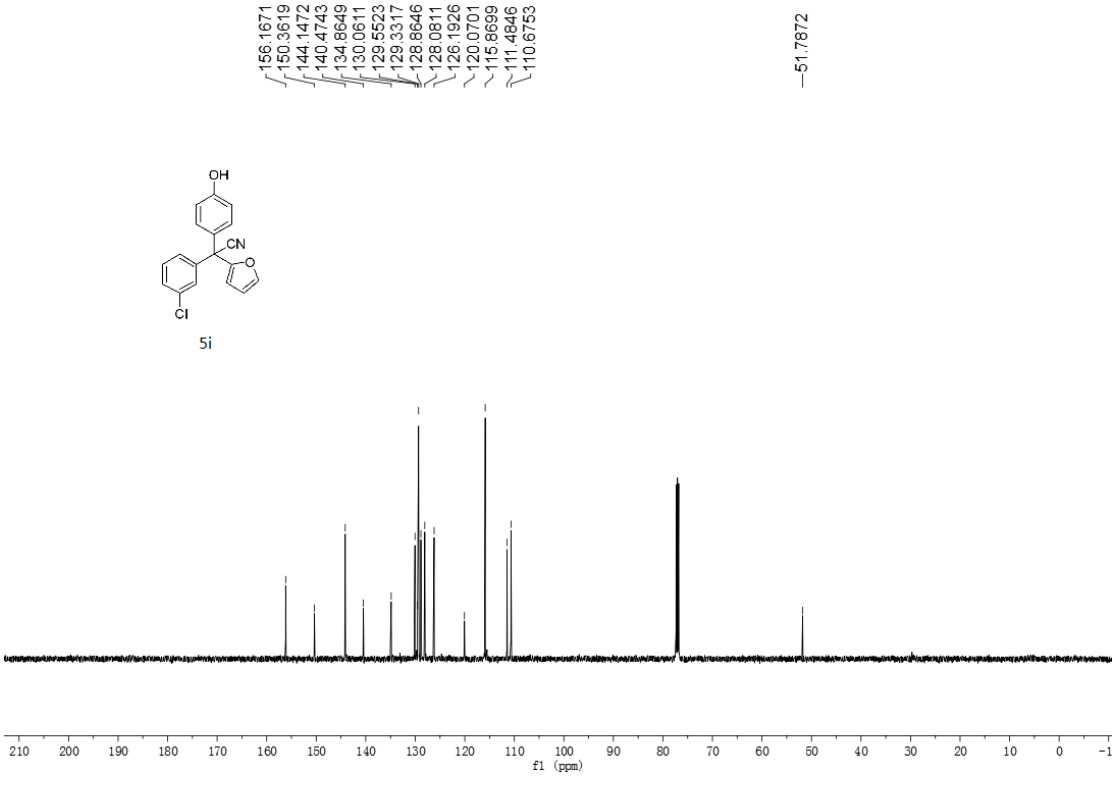
1.03
2.01
2.01
2.02
2.03
1.01
1.00
f1 (ppm)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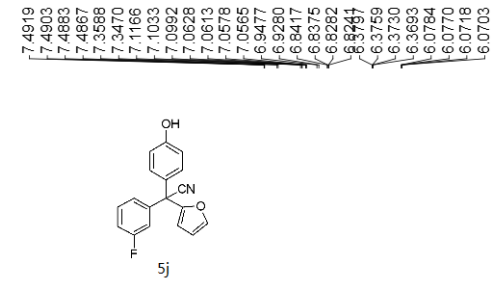
115.8699
111.4846
110.6753
51.7872
OH
CN
O
Cl
5i
f1 (ppm)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7.0992
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7.0578
7.0565
6.9477
6.9280
6.8417
6.8375
6.8282
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6.3693
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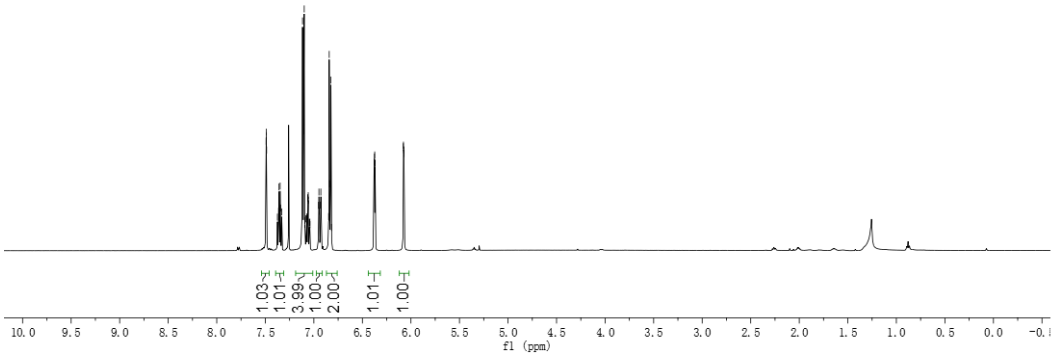
6.0770
6.0718
6.0703
OH
CN
O
F
5j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3.99
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1.00
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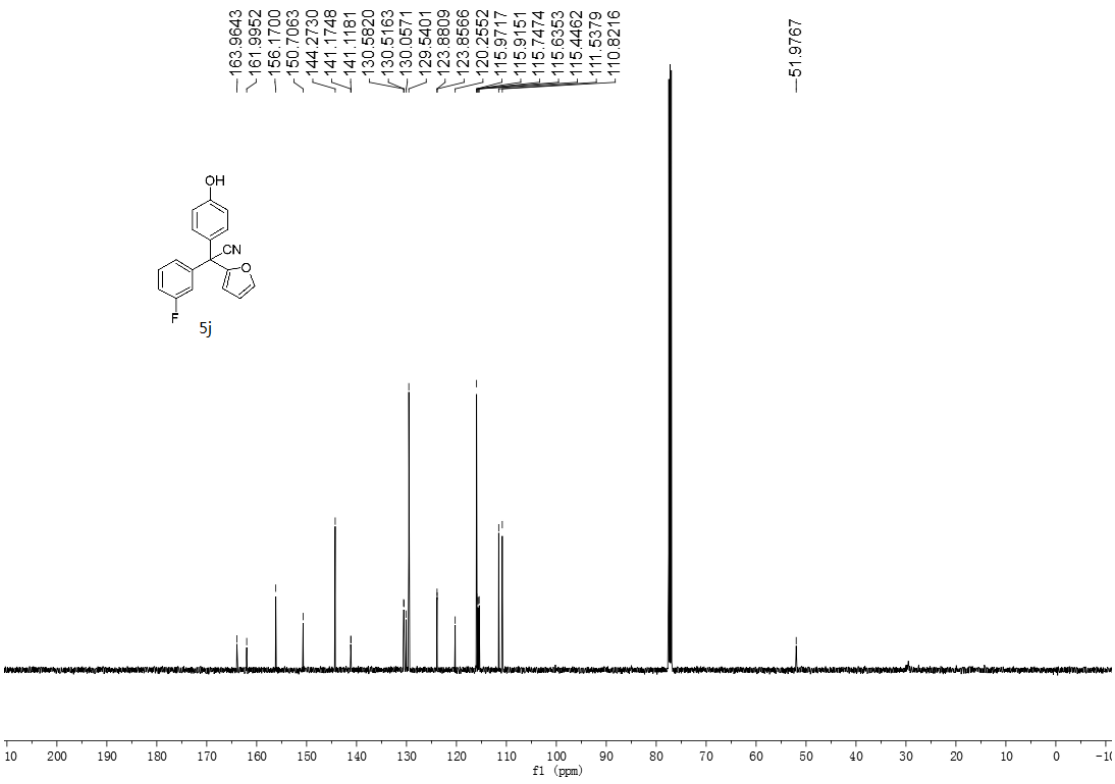
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141.1748
141.1181
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130.5163
130.0571
129.5401
123.8809
123.8566
120.2552
115.9717
115.9151
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115.6353
115.4462
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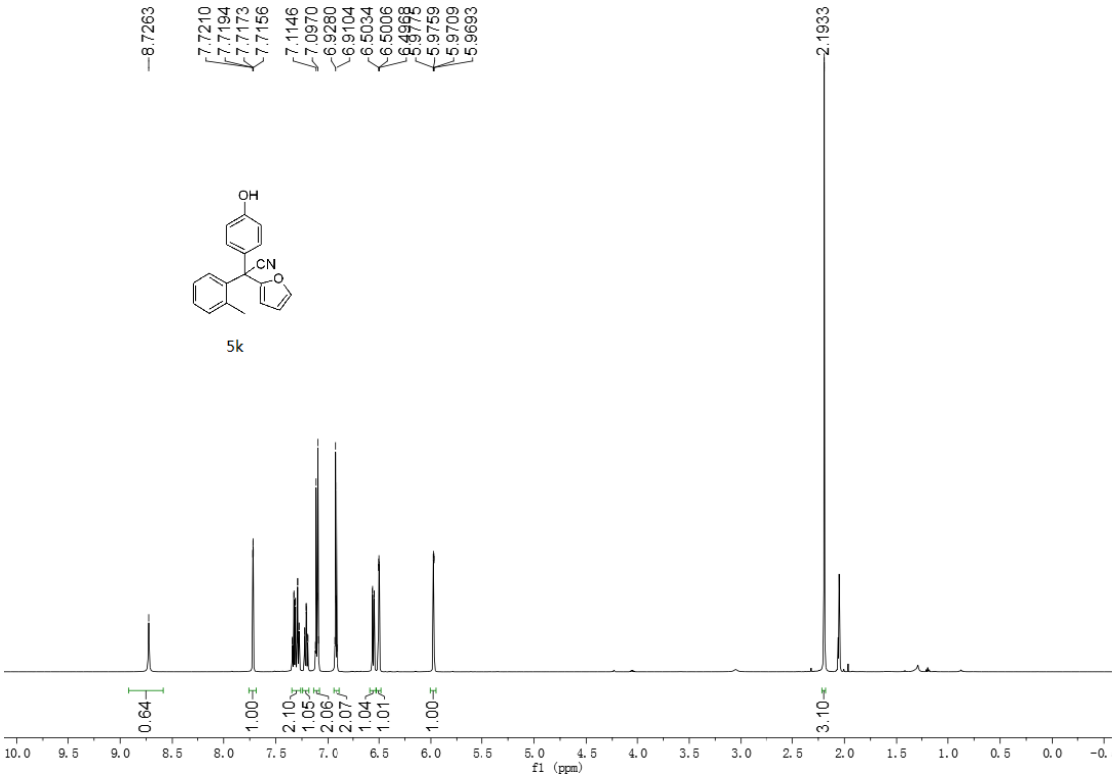
OH
CN
O
F
5j
f1 (ppm)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7.0970
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6.9104
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6.5006
5.9759
5.9709
5.9693
2.1933
OH
CN
O
5k
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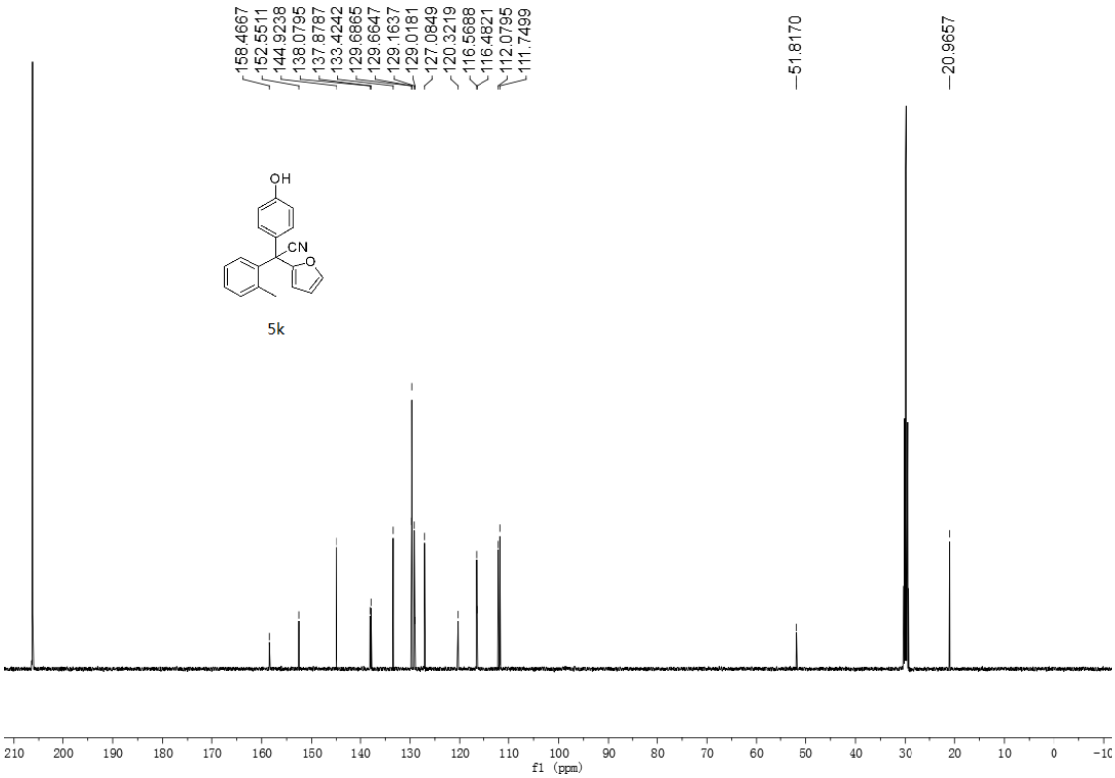
2.10
1.05
2.06
2.07
1.04
1.01
1.00
3.10
f1 (ppm)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127.0849
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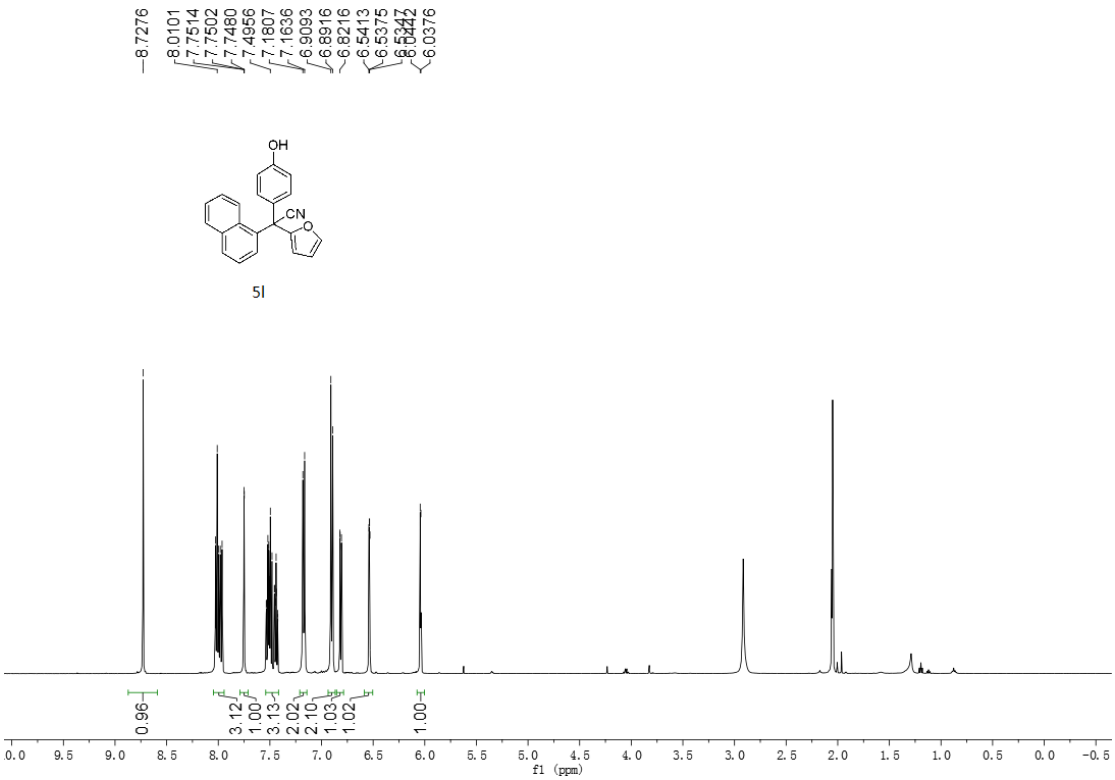
116.4821
112.0795
111.7499
51.8170
20.9657
OH
CN
O
5k
f1 (ppm)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7.1636
6.9093
6.8916
6.8216
6.5413
6.5375
6.0376
OH
CN
O
5l
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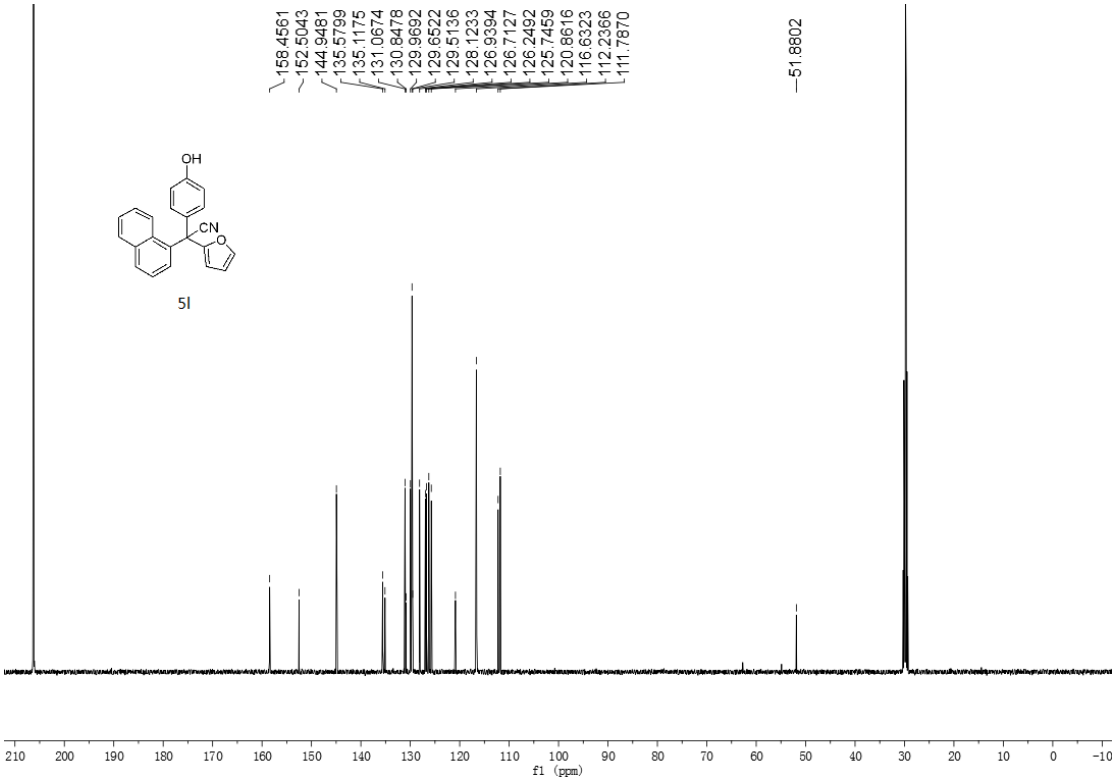
3.12
1.00
3.13
2.02
2.10
1.03
1.02
1.00
f1 (ppm)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131.0674
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129.6522
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128.1233
126.9394
126.7127
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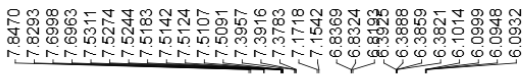
120.8616
116.6323
112.2366
111.7870
51.8802
OH
CN
O
5l
f1 (ppm)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7.6998
7.6963
7.5311
7.5274
7.5244
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7.5142
7.5124
7.5107
7.5091
7.3957
7.3916
7.3783
7.1718
7.1542
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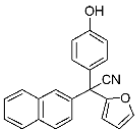
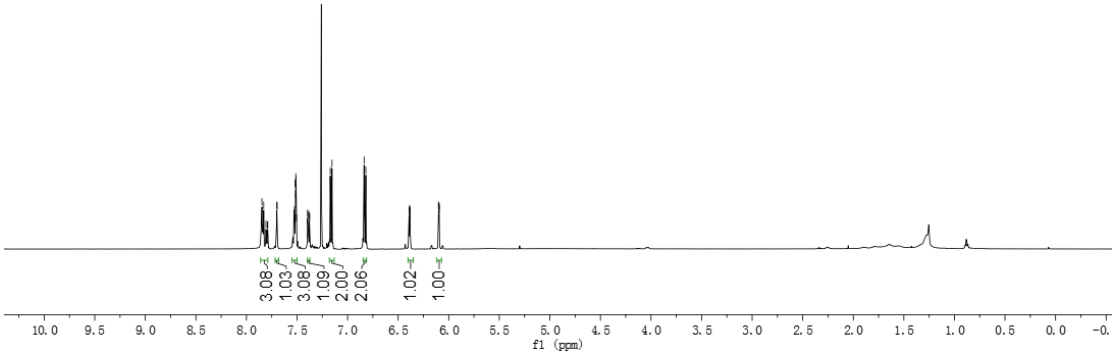
6.3821
6.1014
6.0999
6.0948
6.0932


OH
CN
O

5m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1.03
3.08
1.09
2.00
2.06
1.02
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


156.0945
151.0436
143.9791
135.7533
132.9376
132.9258
130.1023
129.5169
128.7844
128.4202
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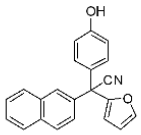
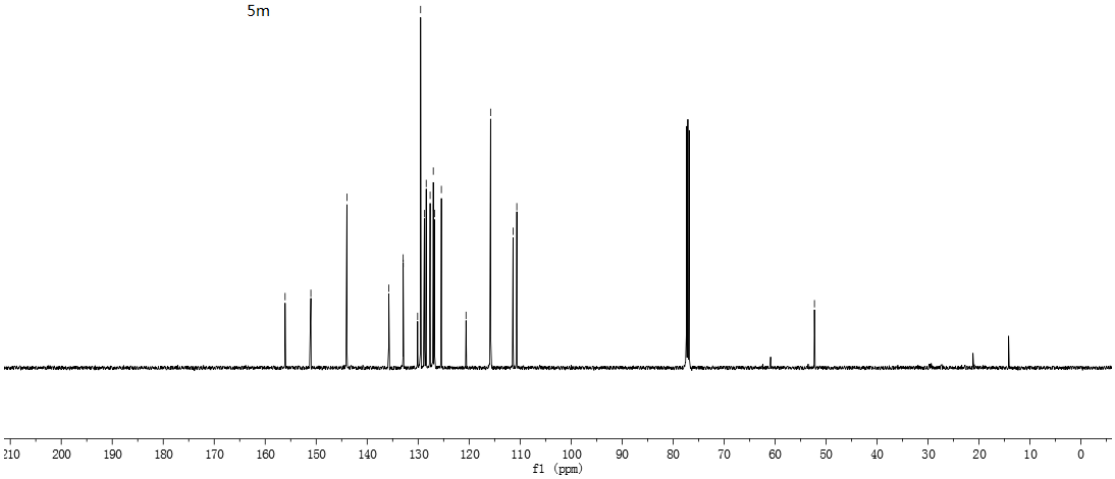
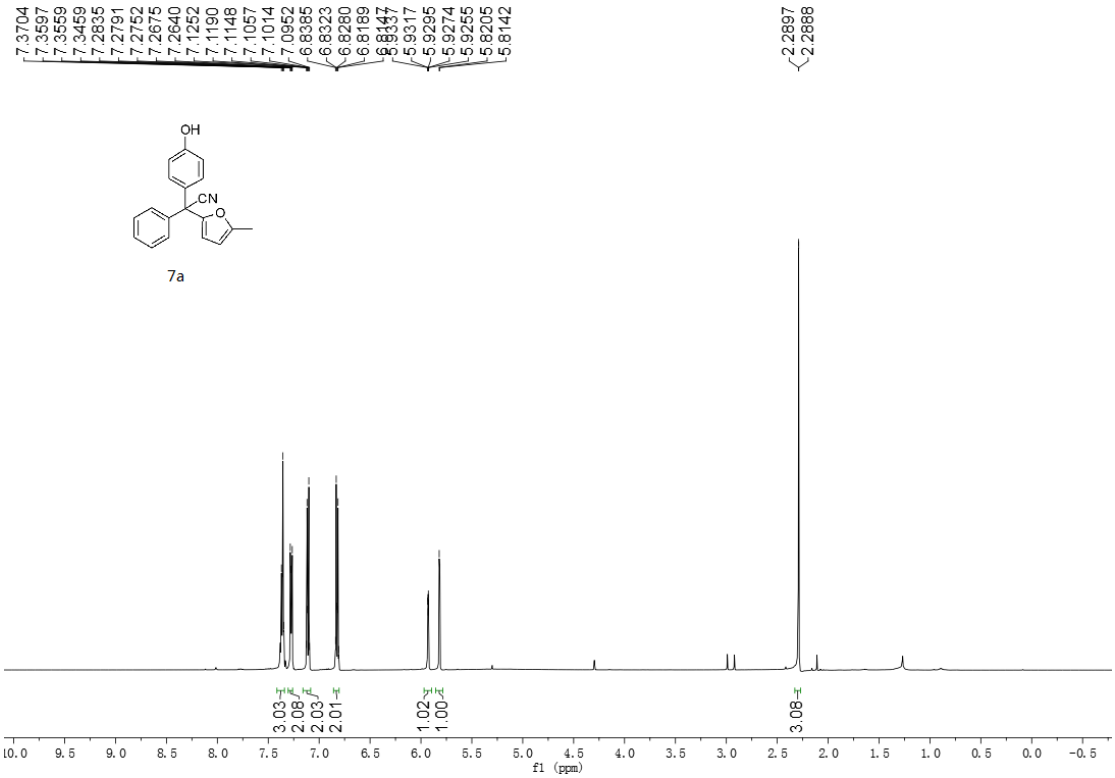
110.6530


52.2737


OH
CN
O

5m


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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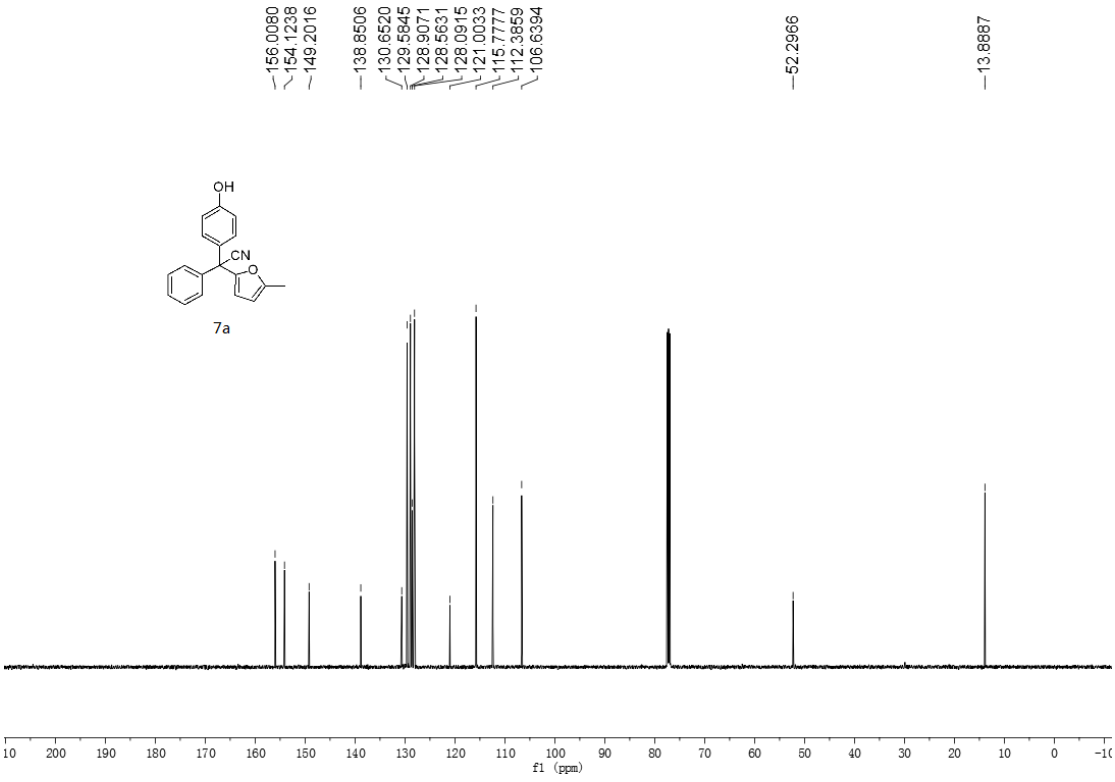
7.1190
7.1148
7.1057
7.1014
7.0952
6.8385
6.8323
6.8280
6.8189
5.9317
5.9295
5.9274
5.9255
5.8205
5.8142
2.2897
2.2888
OH
CN
O
7a
3.03
2.08
2.03
2.01
1.02
1.00
3.08
f1 (ppm)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149.2016
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128.9071
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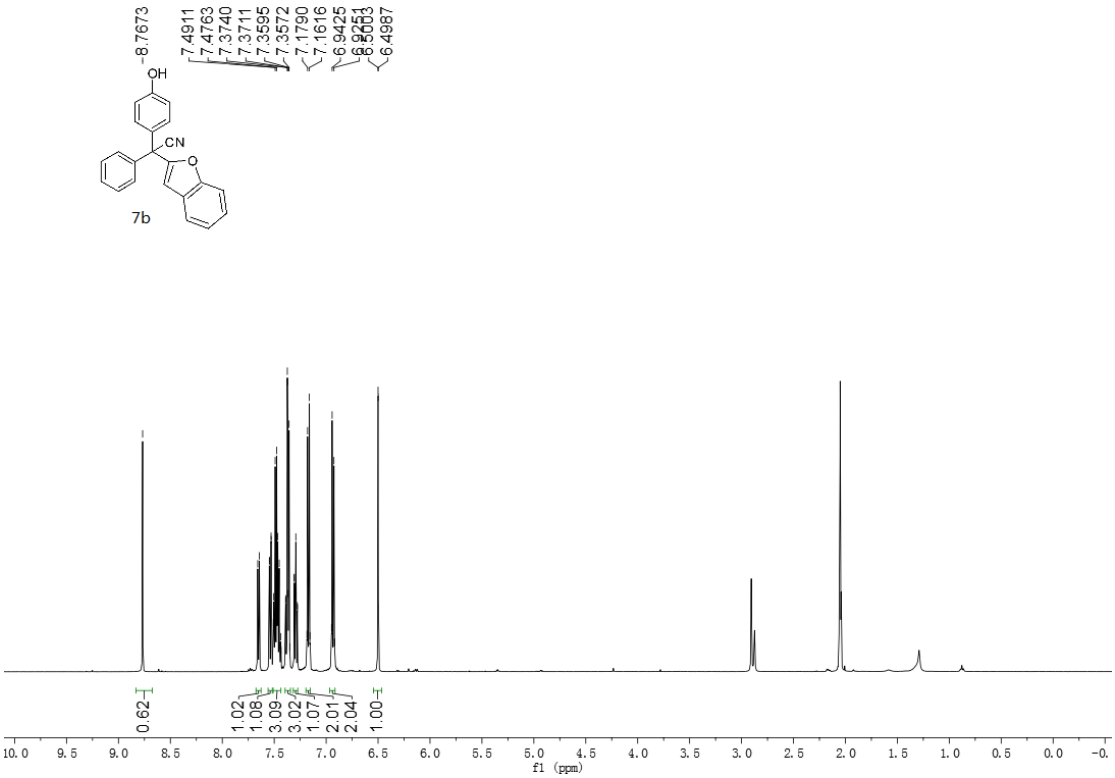
112.3859
106.6394
52.2966
13.8887
OH
CN
O
7a
f1 (ppm)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7.3711
7.3595
7.3572
7.1790
7.1616
6.9425
6.4987
OH
CN
O
7b
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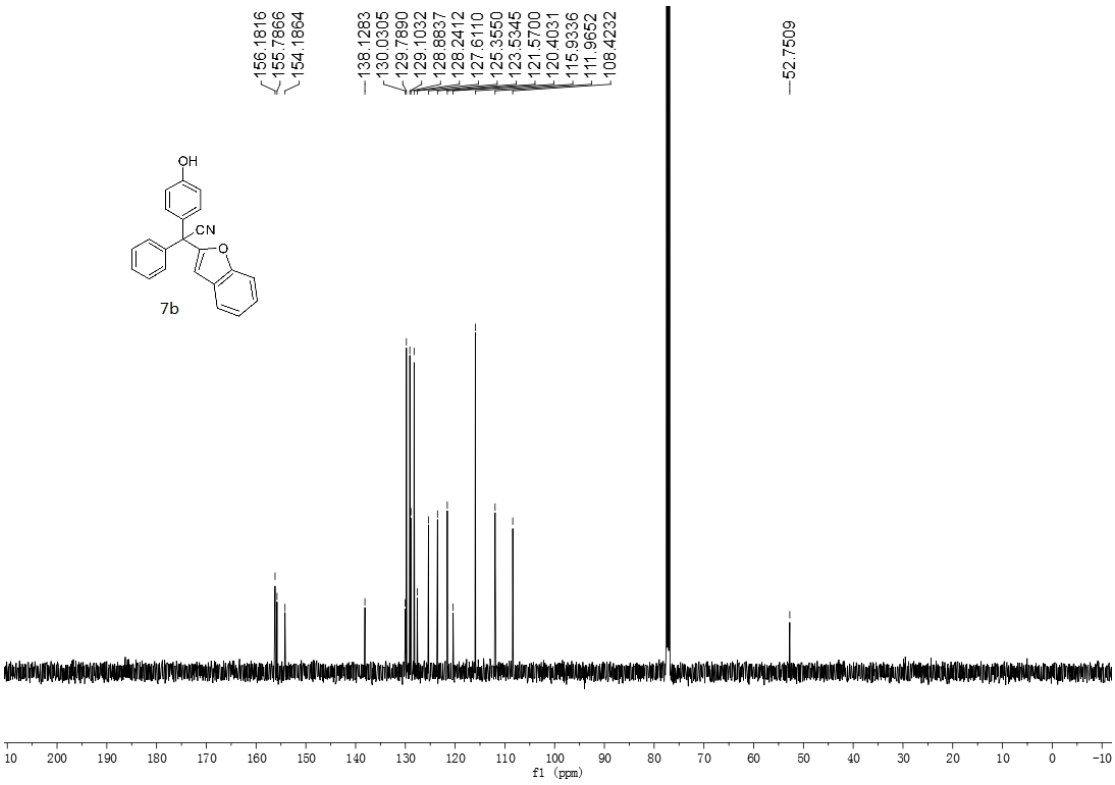
1.02
1.08
3.09
3.02
1.07
2.01
2.04
1.00
f1 (ppm)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154.1864
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129.7890
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128.8837
128.2412
127.6110
125.3550
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120.4031
115.9336
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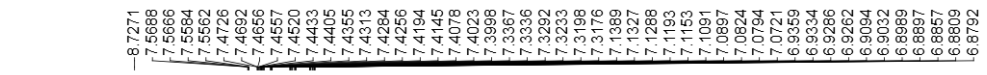
OH
CN
O
7b
f1 (ppm)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7.4405
7.4355
7.4313
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7.4256
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7.3292
7.3233
7.3198
7.3176
7.1389
7.1327
7.1288
7.1193
7.1153
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7.0897
7.0824
7.0794
7.0721
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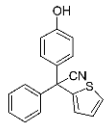
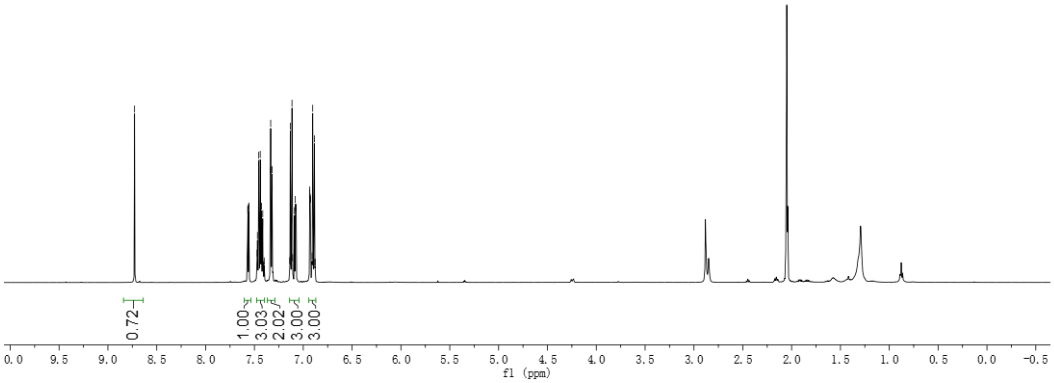
6.8792


OH
CN
S

7c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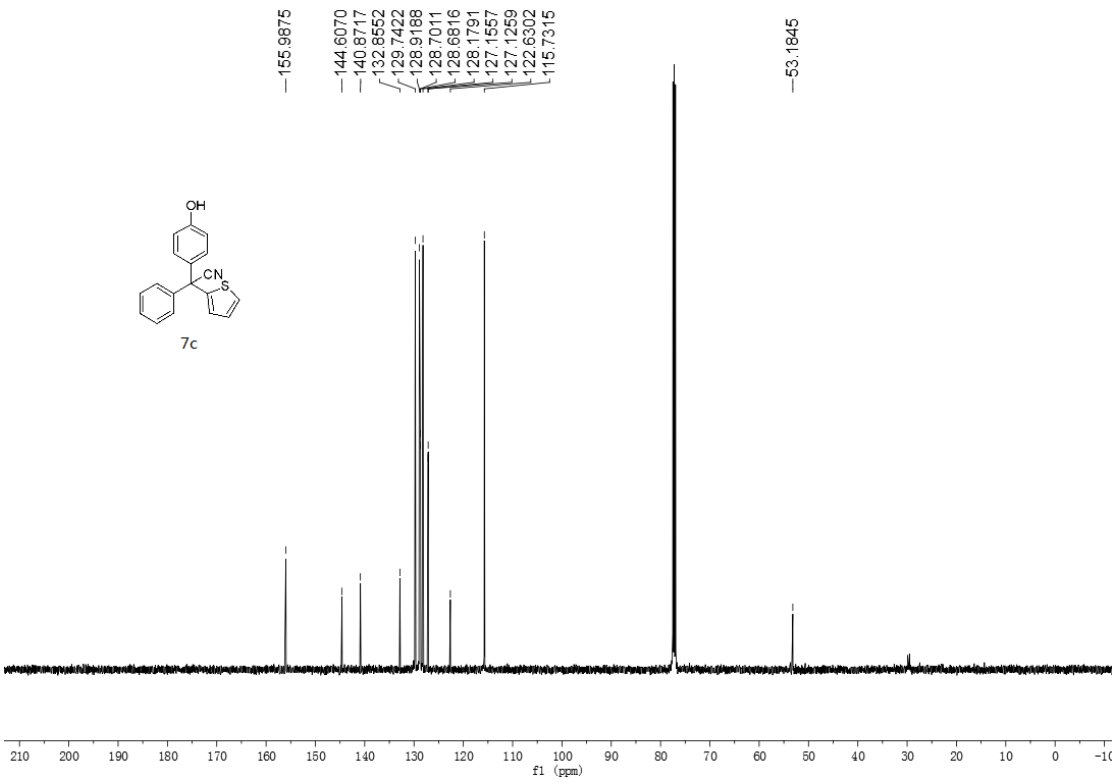
2.02
3.00
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.1557
127.1259
122.6302
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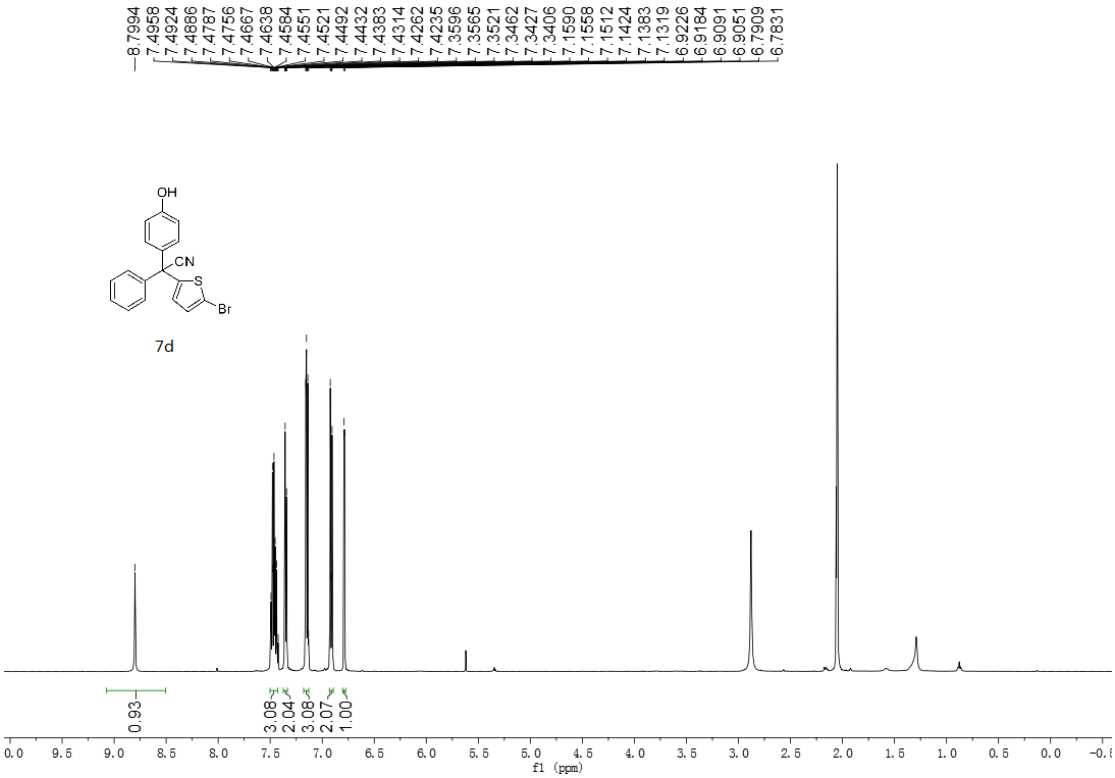
53.1845
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OH
CN
S

7c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7.4432
7.4383
7.4314
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7.3462
7.3427
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7.1590
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7.1512
7.1424
7.1383
7.1319
6.9226
6.9184
6.9091
6.9051
6.7909
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CN
S
Br
7d
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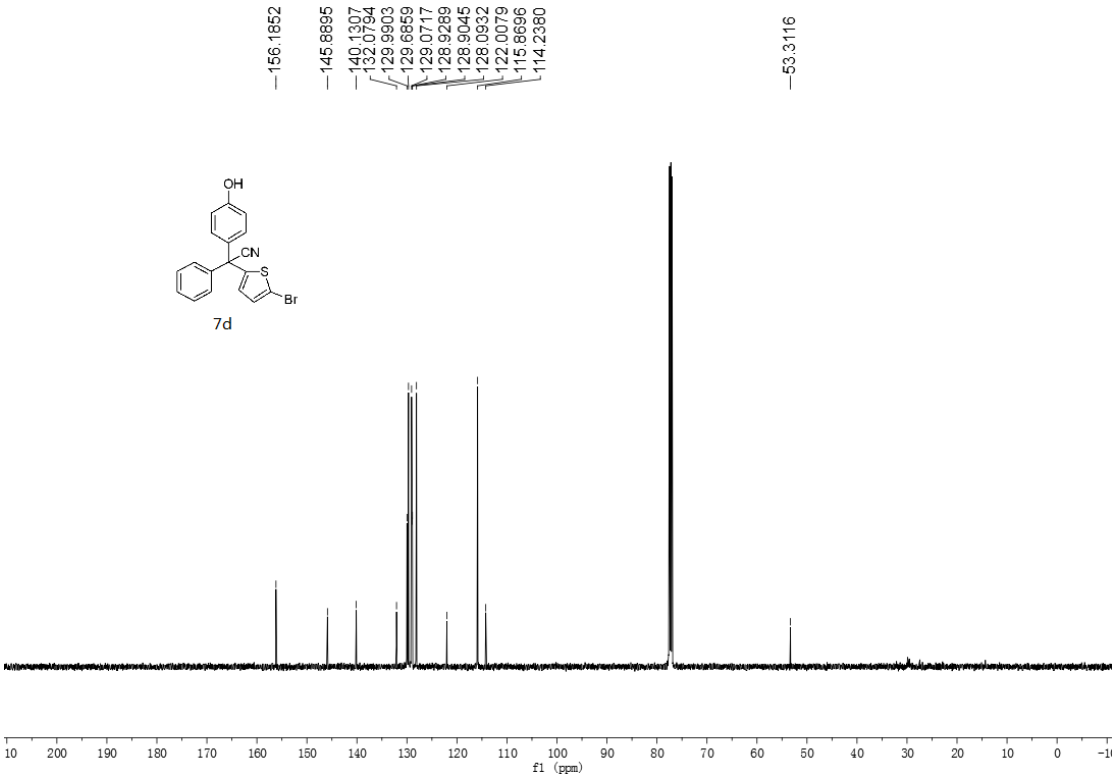
2.04
3.08
2.07
1.00
f1 (ppm)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122.0079
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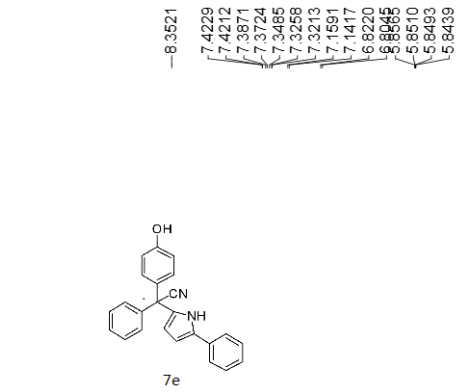
OH
CN
S
Br
7d
f1 (ppm)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5.8493
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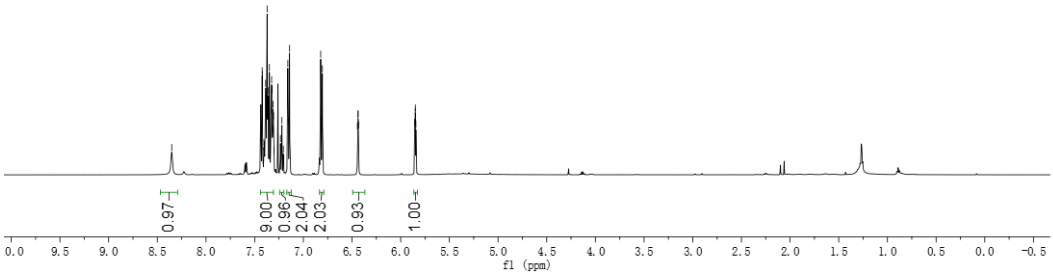
OH
CN
NH
7e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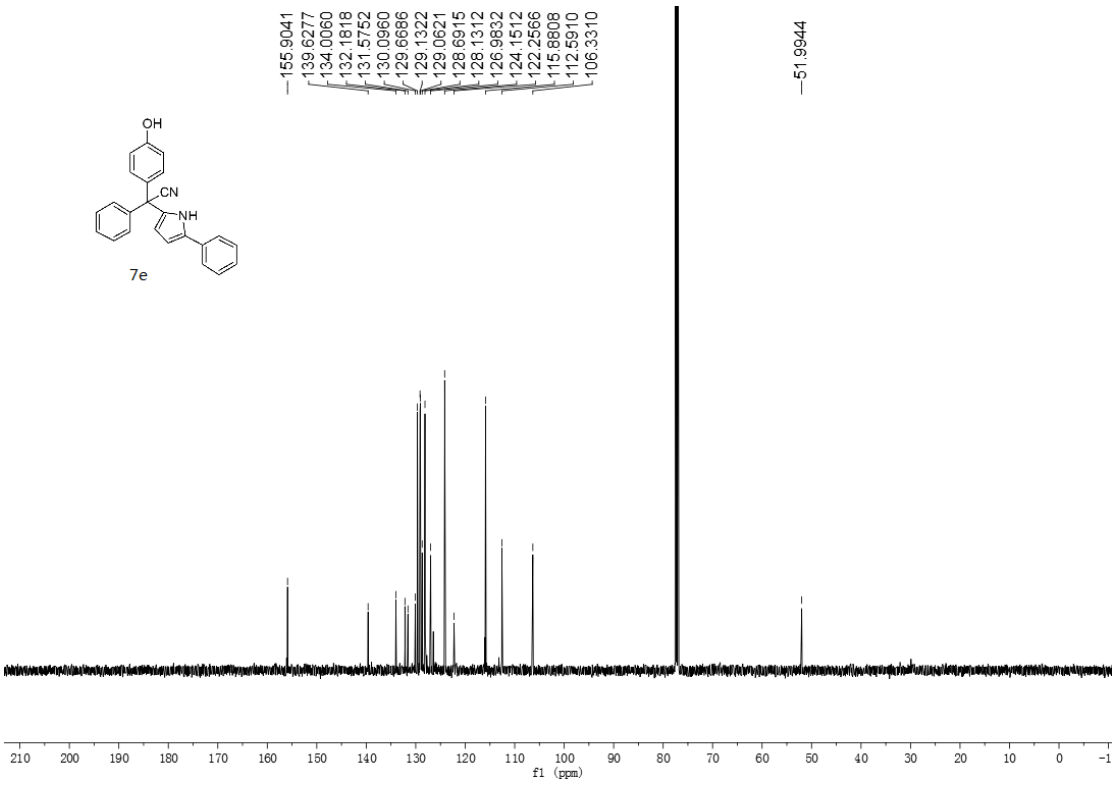
1.00
f1 (ppm)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51.9944
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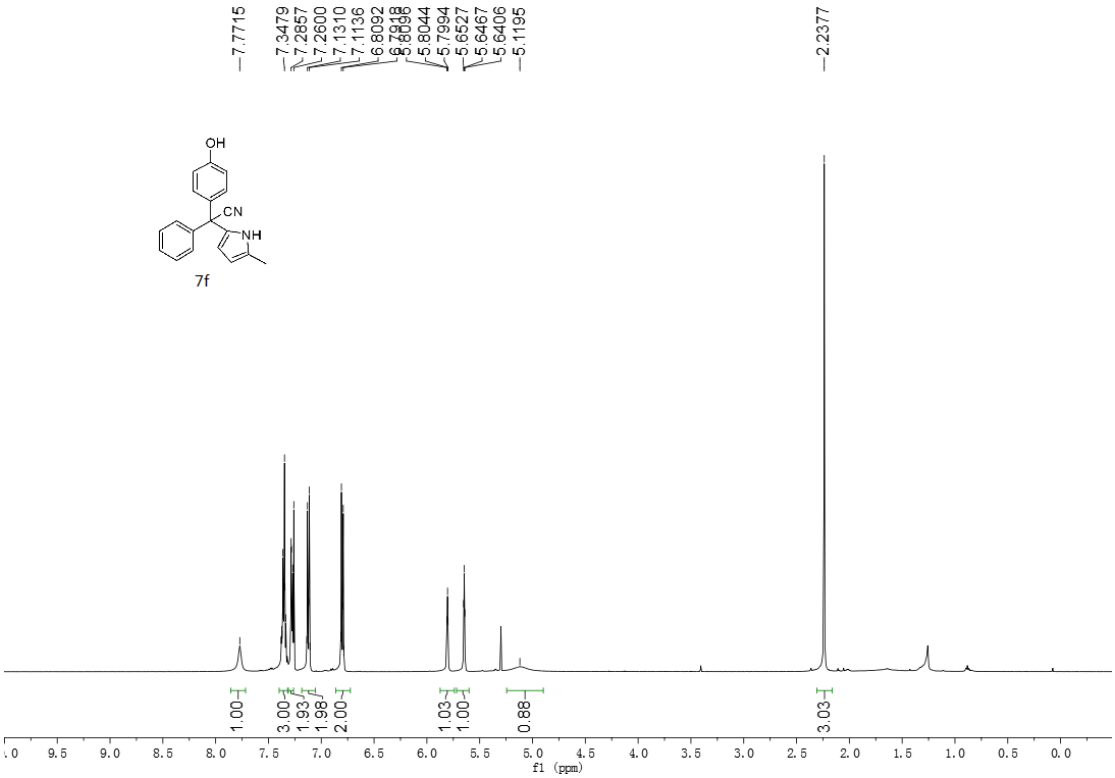
CN
NH
7e
f1 (ppm)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2.2377
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7f
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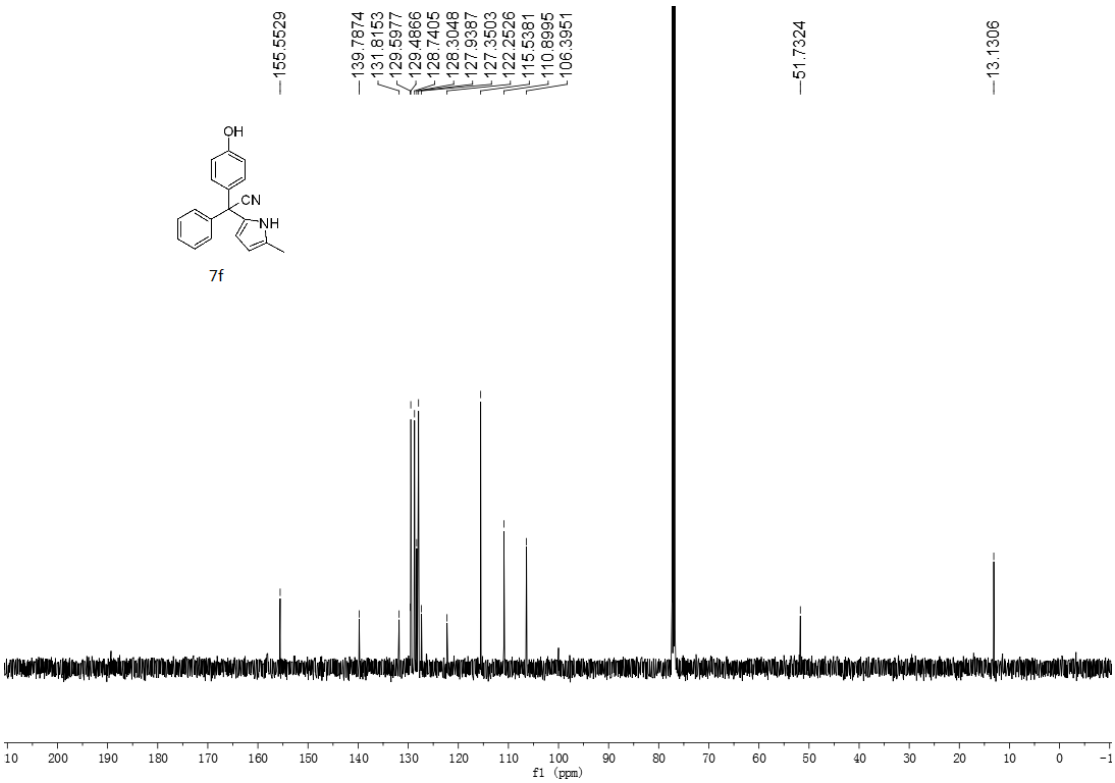
3.03
f1 (ppm)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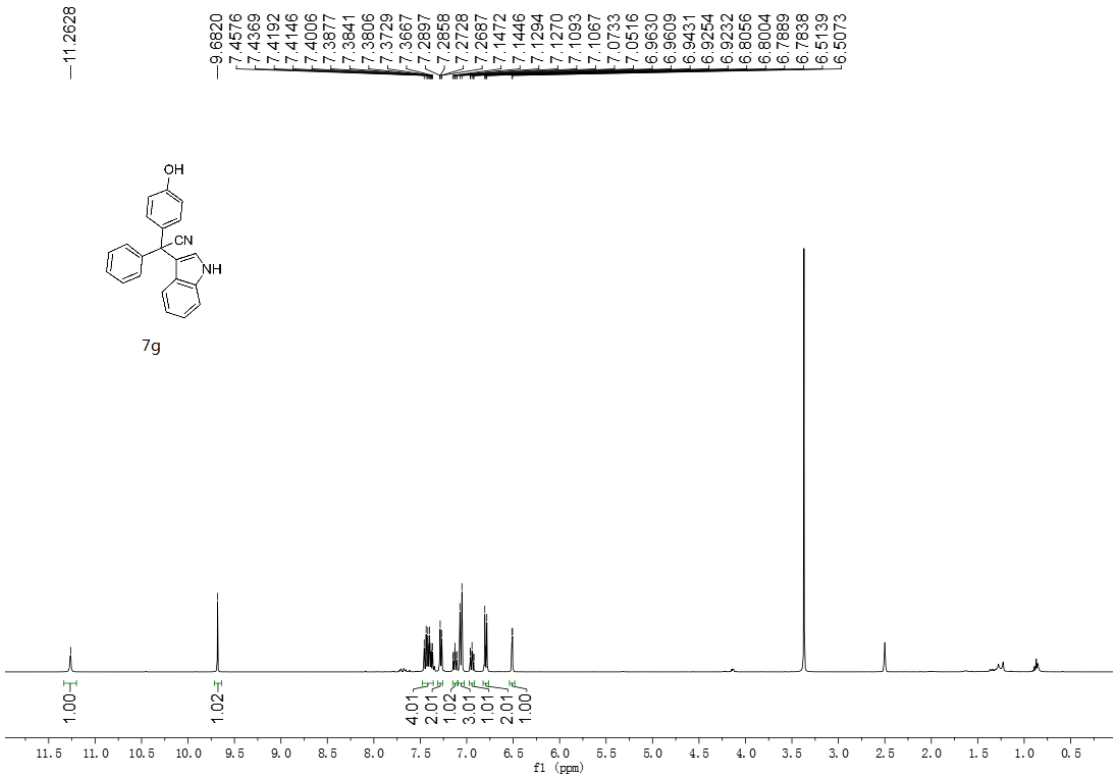
CN
NH
7f
f1 (ppm)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4.01
2.01
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3.01
1.01
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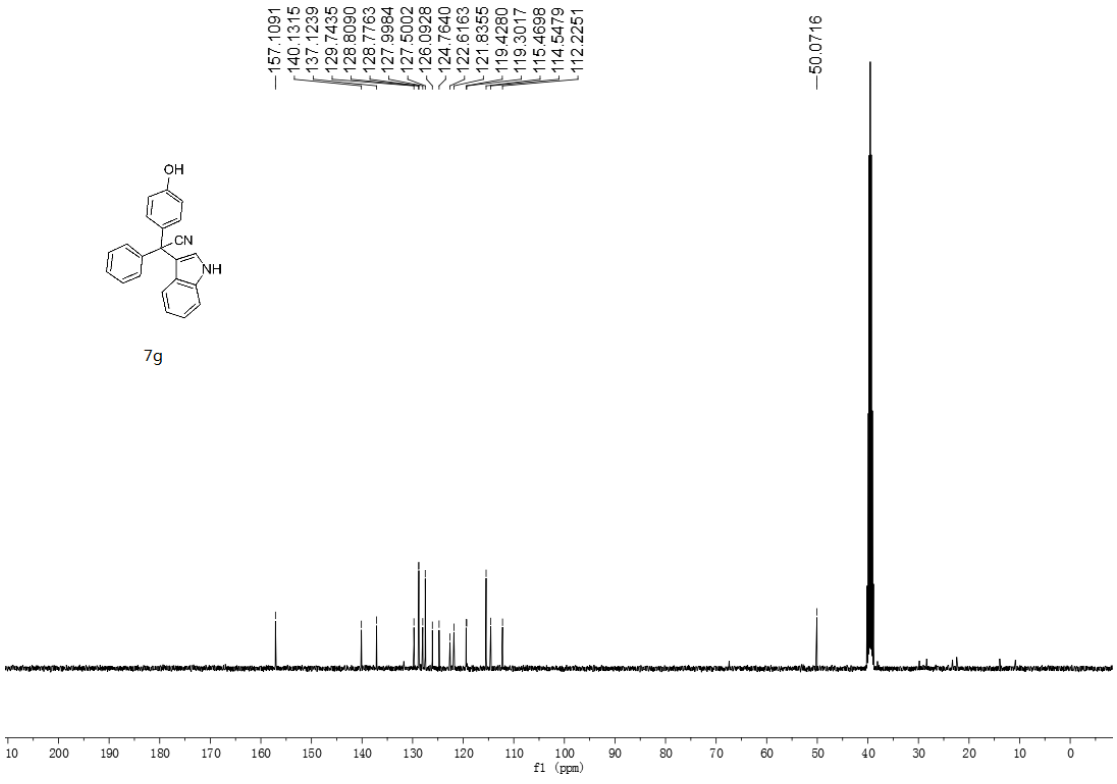
1.00
f1 (ppm)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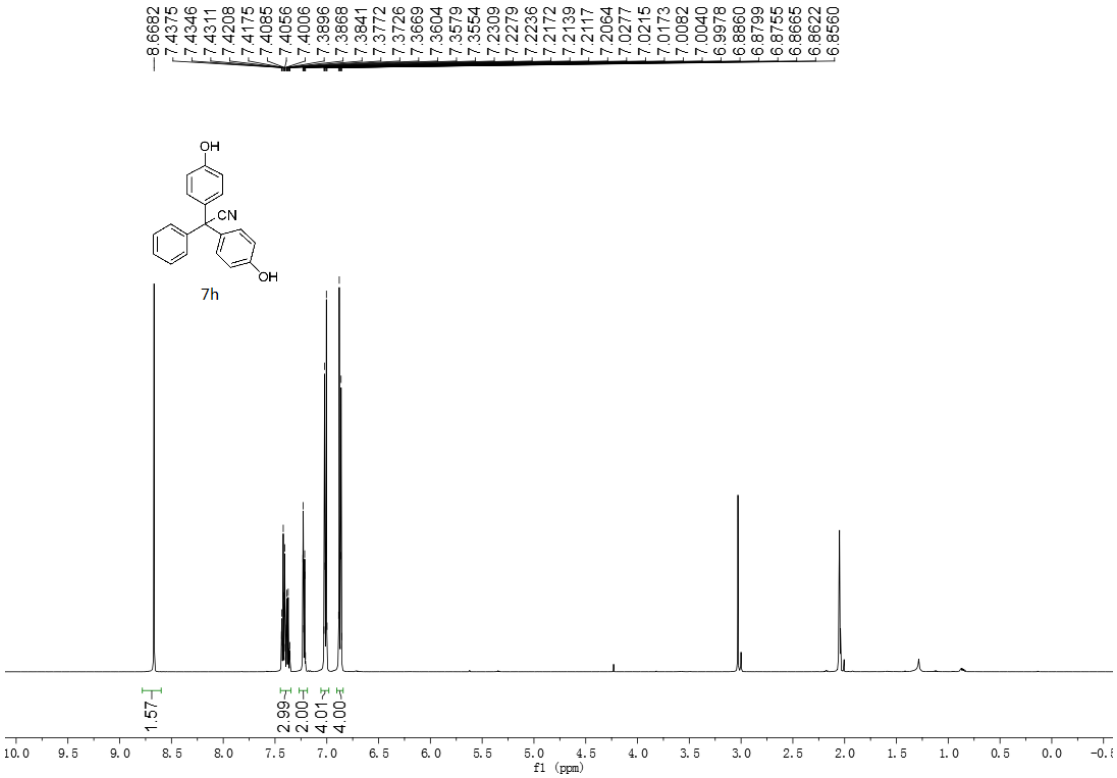
114.5479
112.2251
50.0716
OH
CN
NH
7g
f1 (ppm)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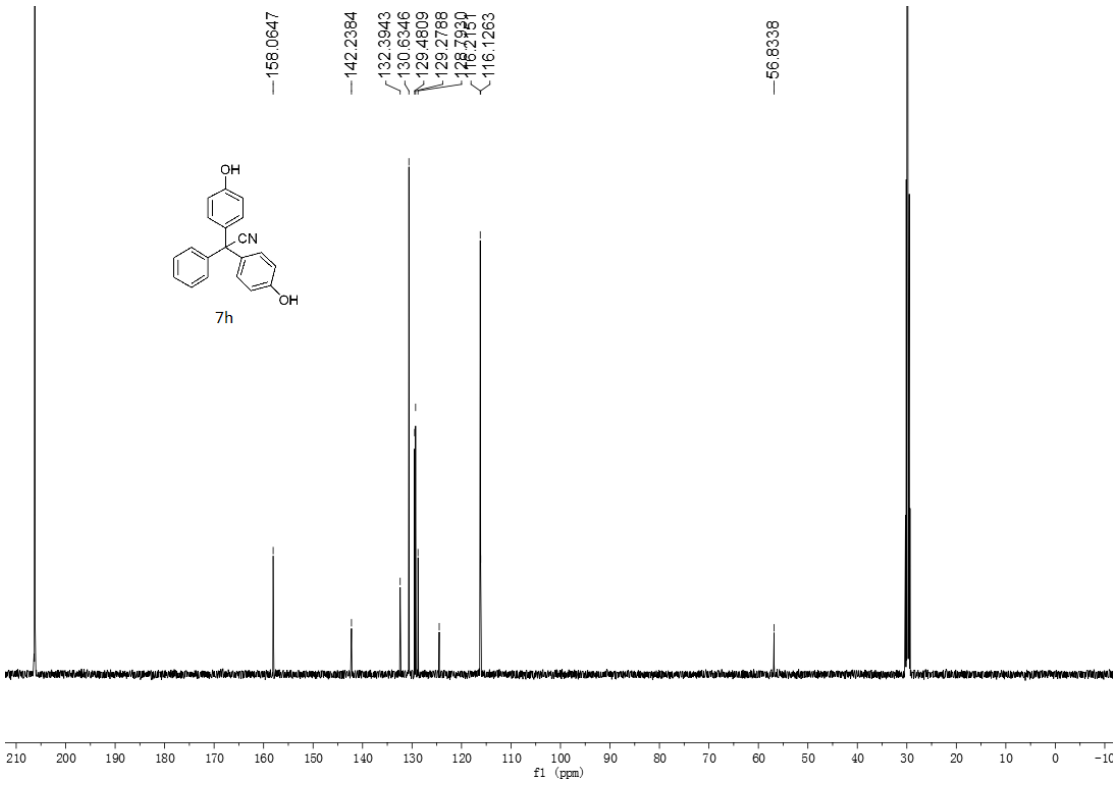
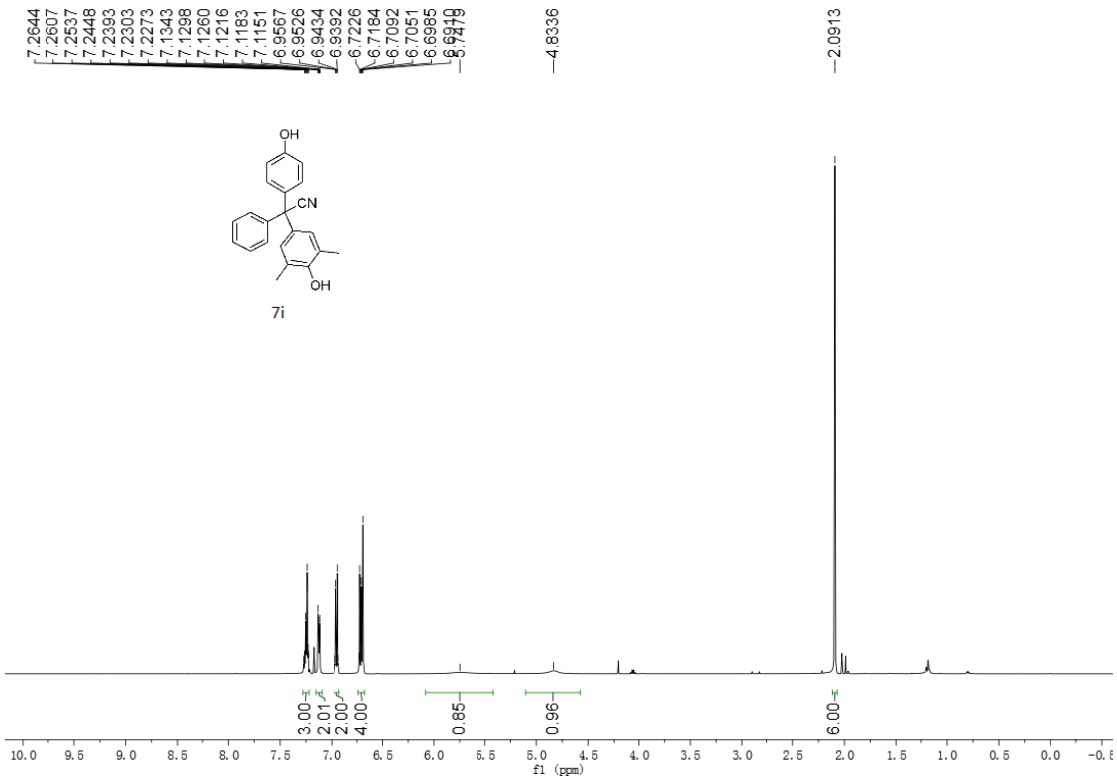
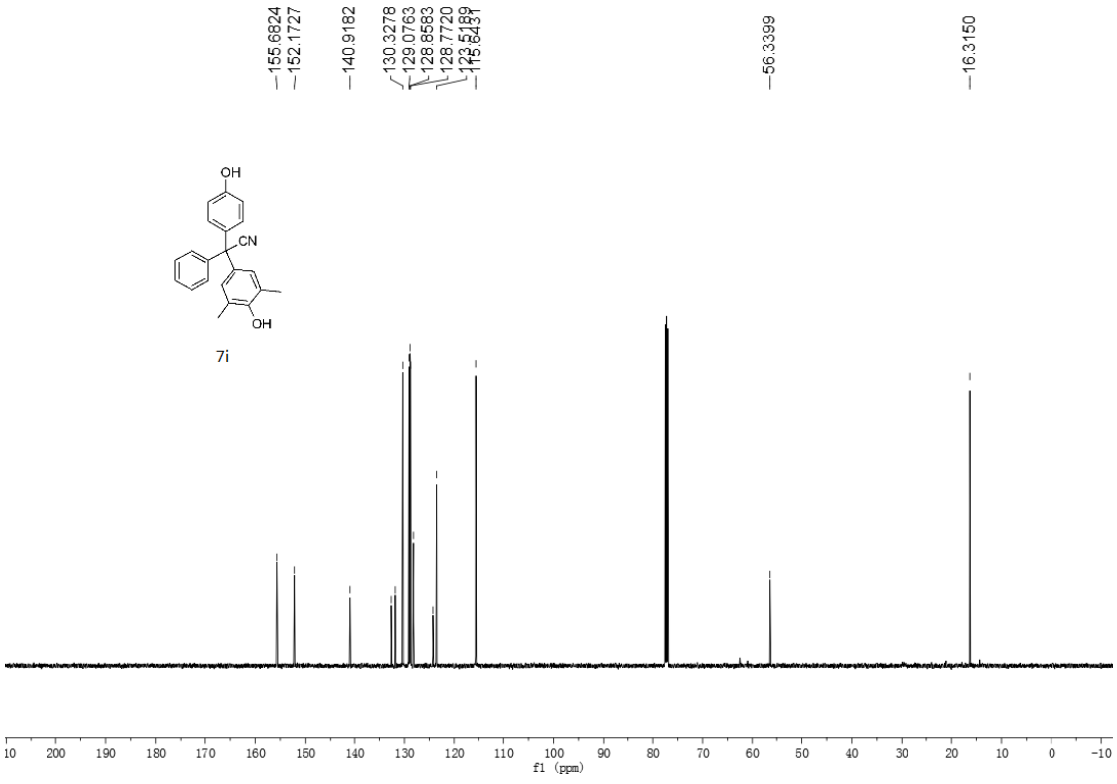
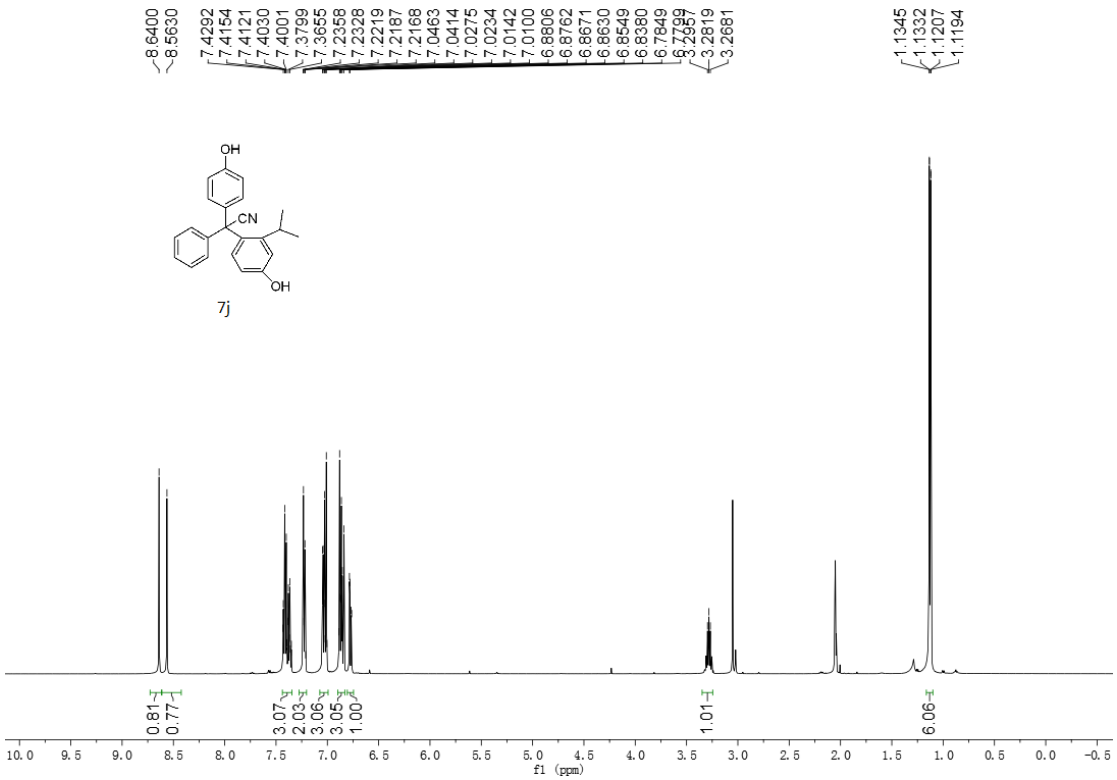
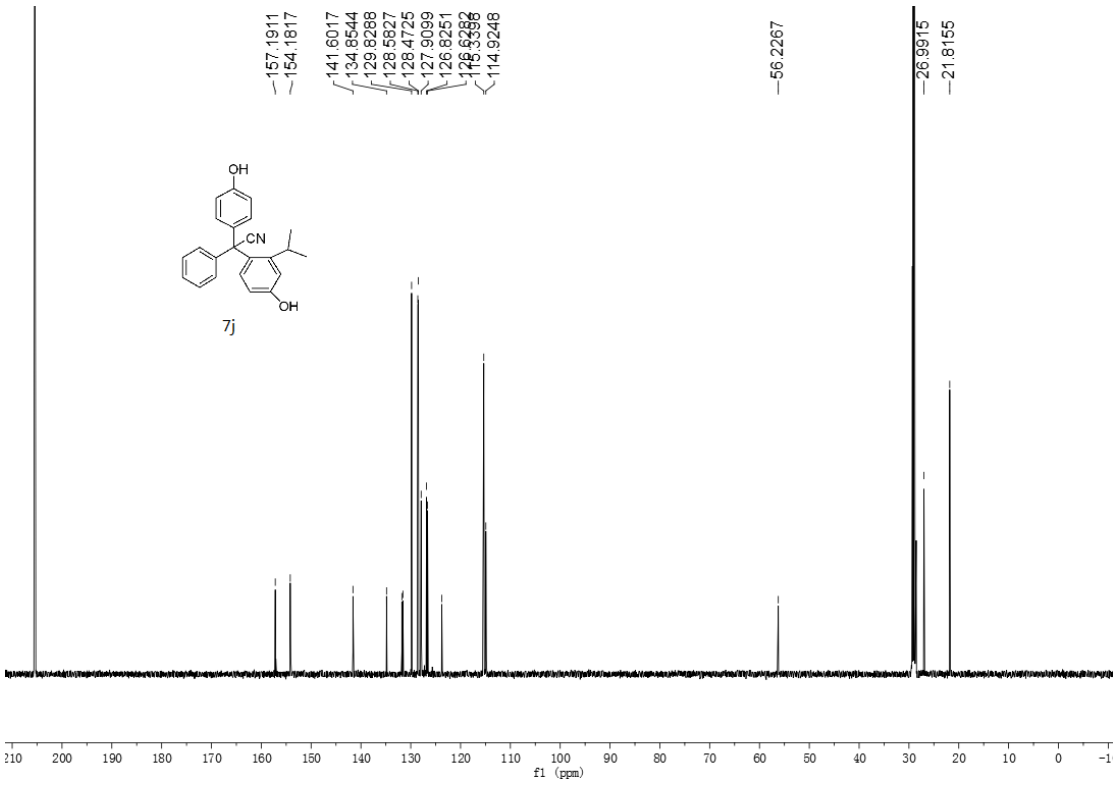
7.4346
7.4311
7.4208
7.4175
7.4085
7.4056
7.4006
7.3896
7.3868
7.3841
7.3772
7.3726
7.3669
7.3604
7.3579
7.3554
7.2309
7.2279
7.2236
7.2172
7.2139
7.2117
7.2064
7.0277
7.0215
7.0173
7.0082
7.0040
6.9978
6.8860
6.8799
6.8755
6.8665
6.8622
6.8560
OH
CN
OH
7h
1.57
2.99
2.00
4.01
4.00
f1 (ppm)


158.0647
142.2384
132.3943
130.6346
129.4809
129.2788
128.7930
116.1263
56.8338
OH
CN
OH
7h
f1 (ppm)


7.2644
7.2607
7.2537
7.2448
7.2393
7.2303
7.2273
7.1343
7.1298
7.1260
7.1216
7.1183
7.1151
6.9567
6.9526
6.9434
6.9392
6.7226
6.7184
6.7092
6.7051
6.6985
4.8336
2.0913
OH
CN
OH
7i
3.00
2.01
2.00
4.00
0.85
0.96
6.00
f1 (ppm)


155.6824
152.1727
140.9182
130.3278
129.0763
128.8583
128.7720
56.3399
16.3150
OH
CN
OH
7i
f1 (ppm)


8.6400
8.5630
7.4292
7.4154
7.4121
7.4030
7.4001
7.3799
7.3655
7.2358
7.2328
7.2219
7.2187
7.2168
7.0463
7.0414
7.0275
7.0234
7.0142
7.0100
6.8806
6.8762
6.8671
6.8630
6.8549
6.8380
6.7849
6.7799
3.2957
3.2819
3.2681
1.1345
1.1332
1.1207
1.1194
OH
CN
OH
7j
0.81
0.77
3.07
2.03
3.06
3.05
1.00
1.01
6.06
f1 (ppm)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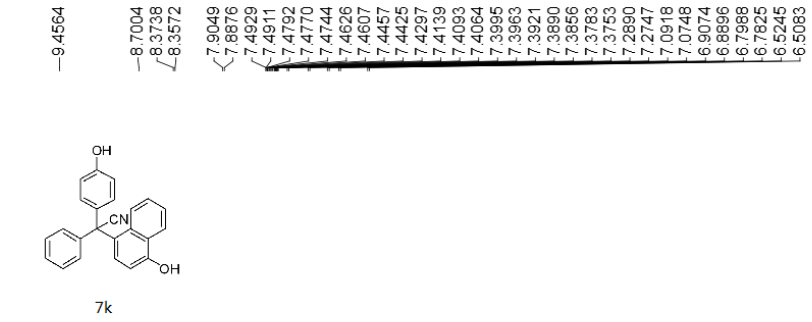
154.1817
141.6017
134.8544
129.8288
128.5827
128.4725
127.9099
126.8251
115.3398
114.9248
56.2267
26.9915
21.8155
OH
CN
OH
7j
f1 (ppm)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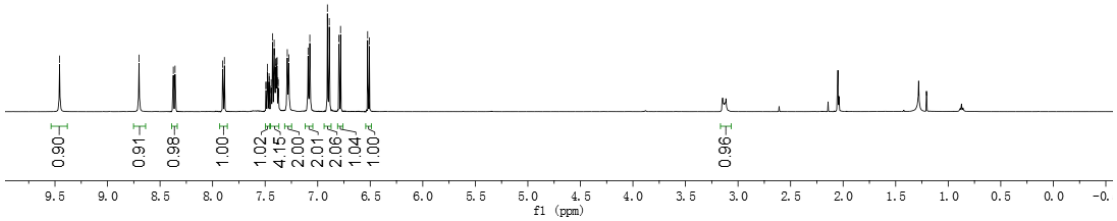
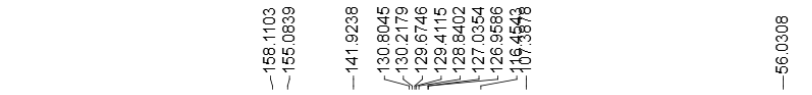
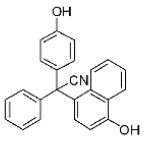
8.7004
8.3738
8.3572
7.9049
7.8876
7.4929
7.4911
7.4792
7.4770
7.4744
7.4626
7.4607
7.4457
7.4425
7.4297
7.4139
7.4093
7.4064
7.3995
7.3963
7.3921
7.3890
7.3856
7.3783
7.3753
7.2890
7.2747
7.0918
7.0748
6.9074
6.8896
6.7988
6.7825
6.5245
6.5083


OH
CN
OH

7k

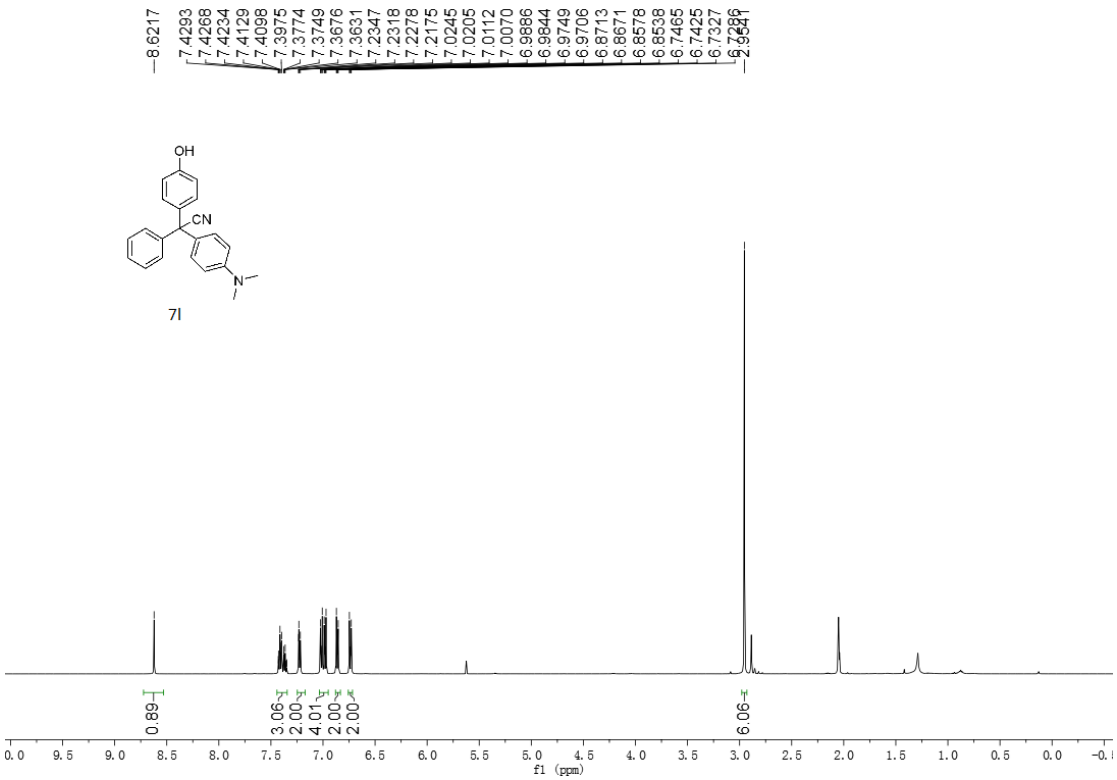

0.90
0.91
0.98
1.00
1.02
4.15
2.00
2.01
2.06
1.04
1.00
0.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


158.1103
155.0839
141.9238
130.8045
130.2179
129.6746
129.4115
128.8402
127.0354
126.9586
116.4543
107.3878
56.0308


OH
CN
OH

7k


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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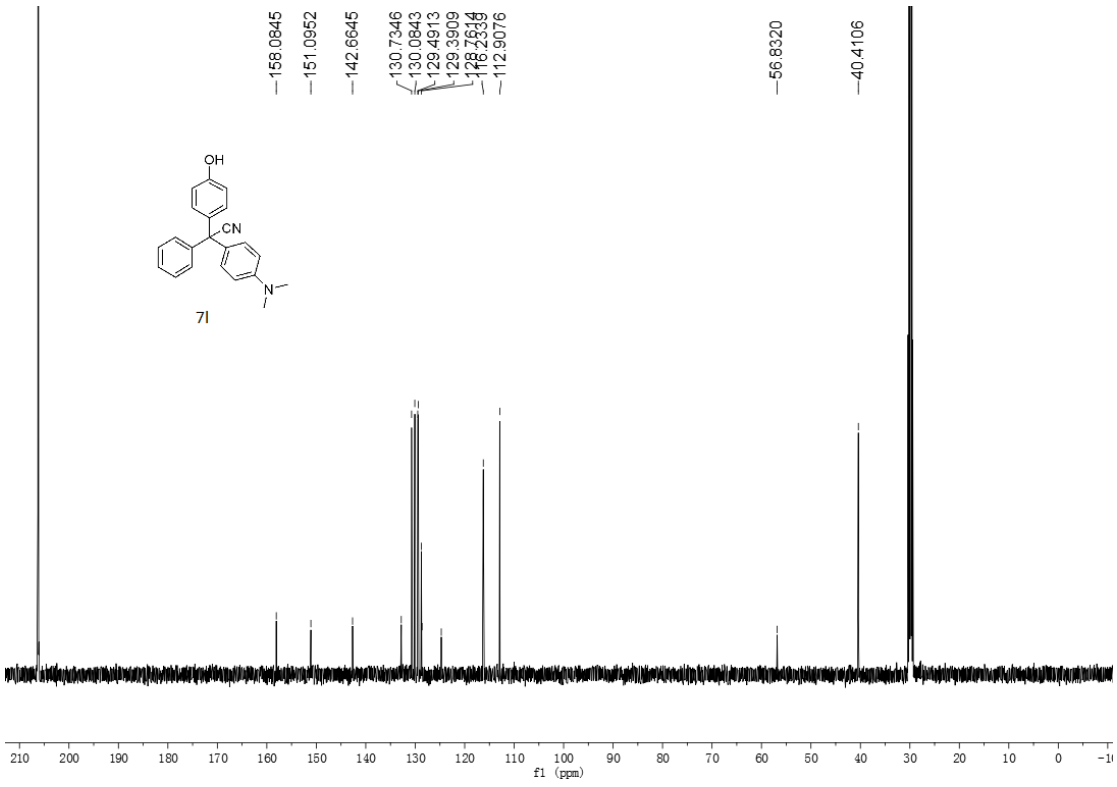
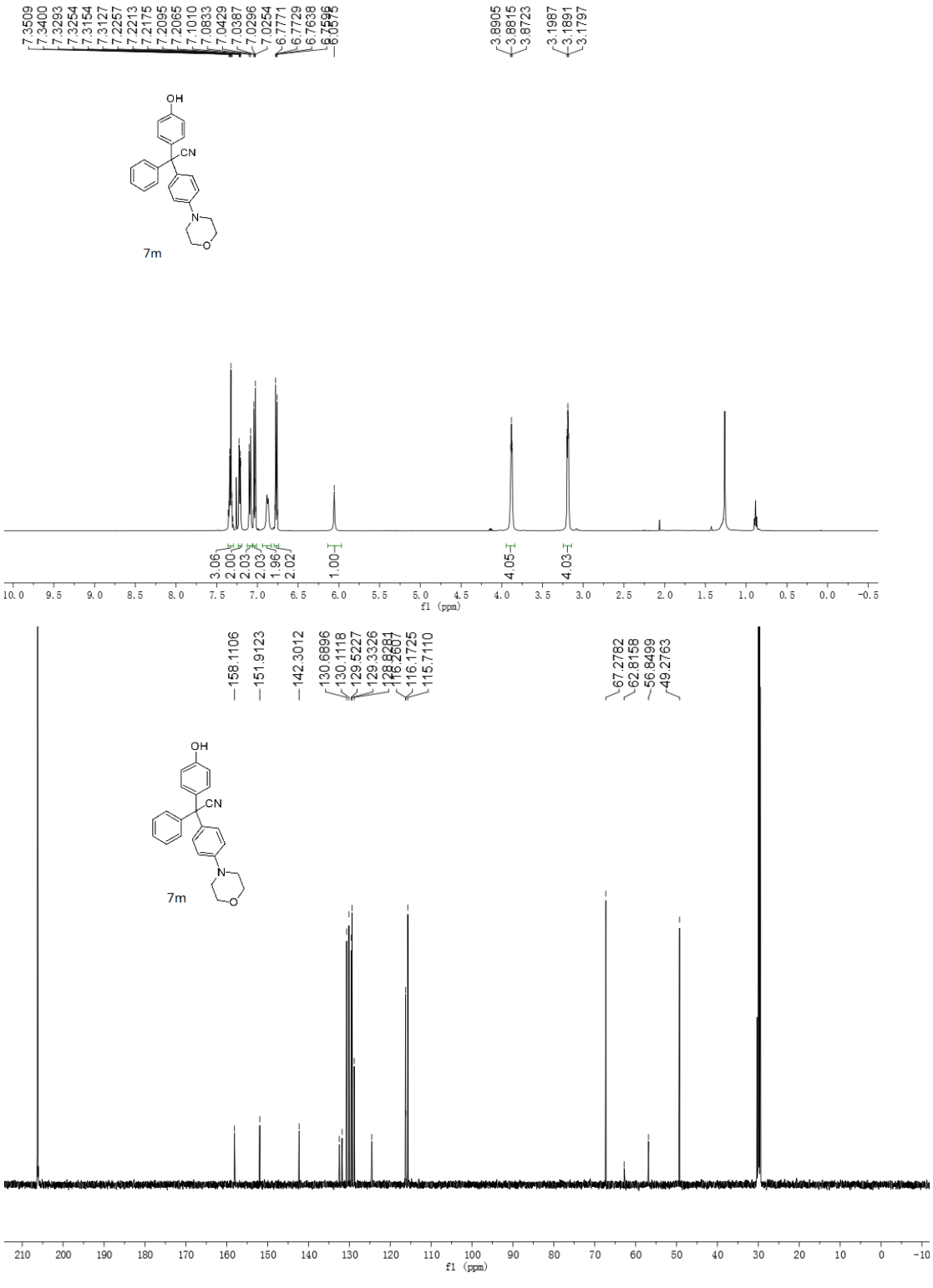
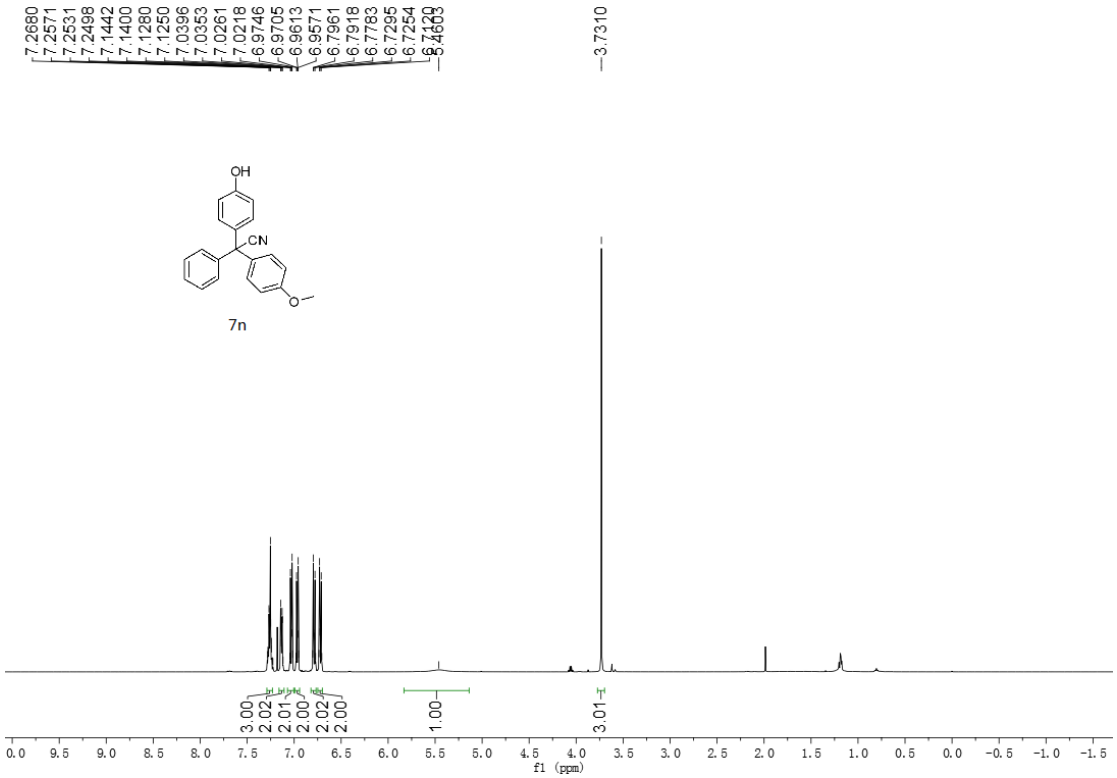
7.4293
7.4268
7.4234
7.4129
7.4098
7.3975
7.3774
7.3749
7.3676
7.3631
7.2347
7.2318
7.2278
7.2175
7.0245
7.0205
7.0112
7.0070
6.9886
6.9844
6.9749
6.9706
6.8713
6.8671
6.8578
6.8538
6.7465
6.7425
6.7327
2.9541
OH
CN
N
7l
0.89
3.06
2.00
4.01
2.00
2.00
6.06
f1 (ppm)


158.0845
151.0952
142.6645
130.7346
130.0843
129.4913
129.3909
128.7614
116.2339
112.9076
56.8320
40.4106
OH
CN
N
7l
f1 (ppm)


7.3509
7.3400
7.3293
7.3254
7.3154
7.3127
7.2257
7.2213
7.2175
7.2095
7.2065
7.1010
7.0833
7.0429
7.0387
7.0296
7.0254
6.7771
6.7729
6.7638
3.8905
3.8815
3.8723
3.1987
3.1891
3.1797
OH
CN
N
O
7m
3.06
2.00
2.03
2.03
1.96
2.02
1.00
4.05
4.03
f1 (ppm)
158.1106
151.9123
142.3012
130.6896
130.1118
129.5227
129.3326
116.2607
116.1725
115.7110
67.2782
62.8158
56.8499
49.2763
OH
CN
N
O
7m
f1 (ppm)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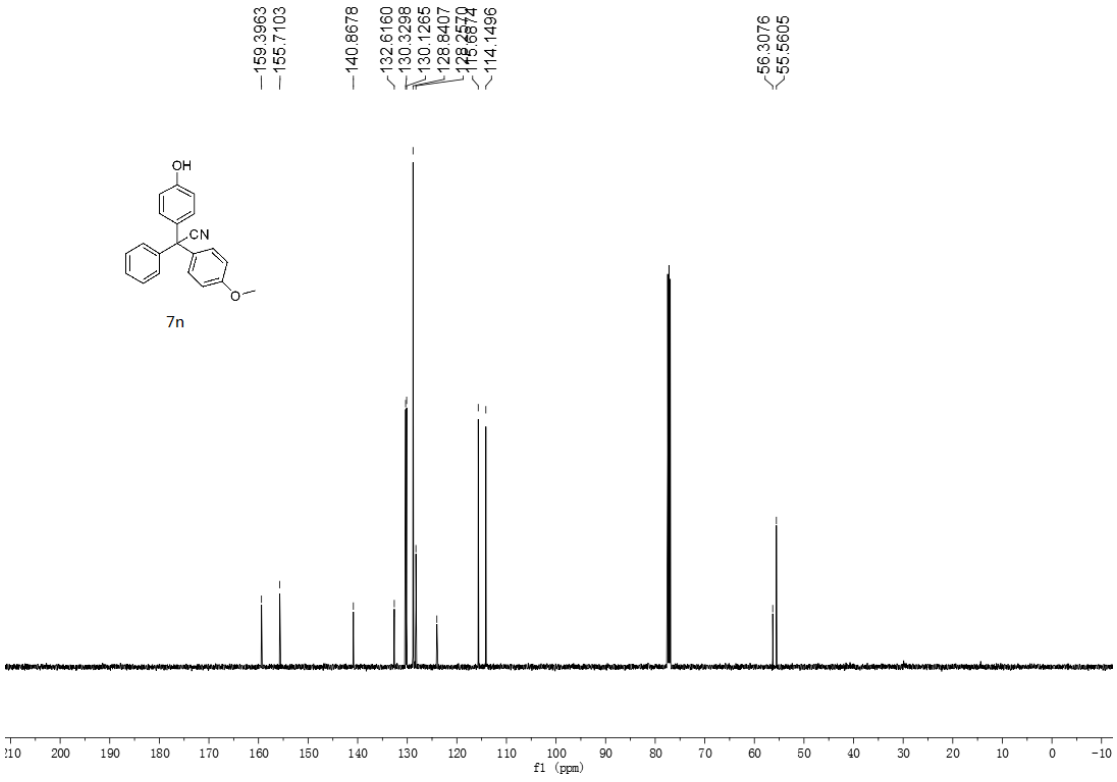
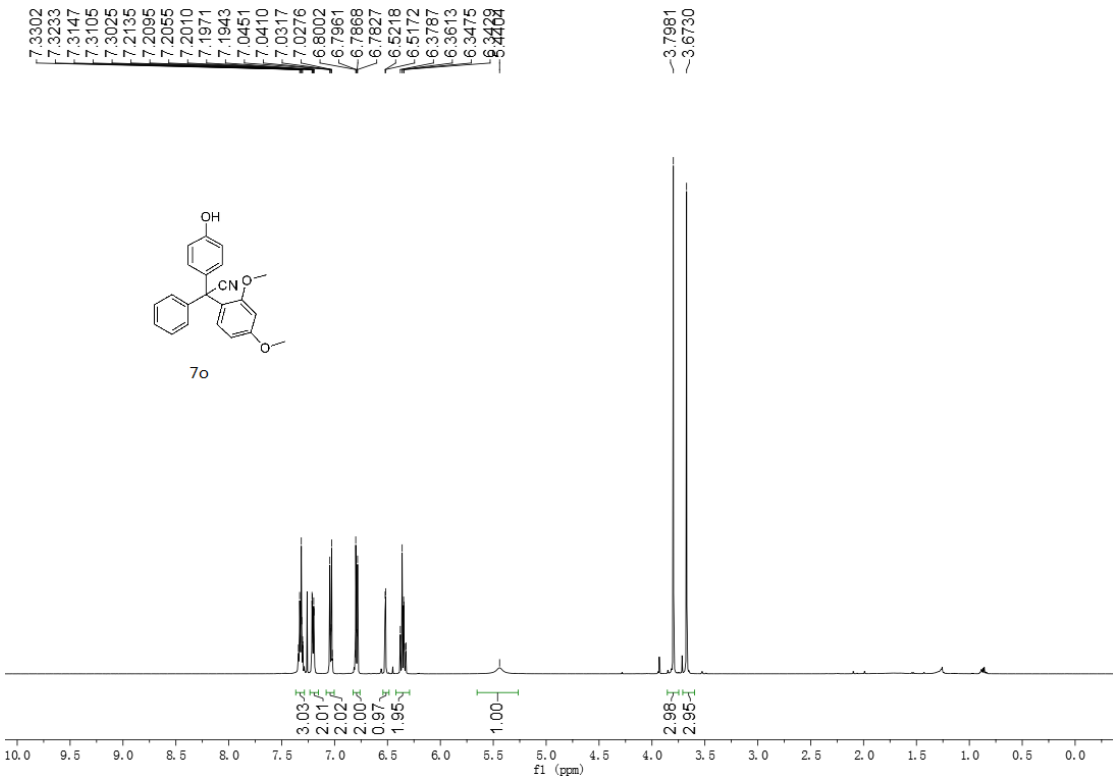
7.2571
7.2531
7.2498
7.1442
7.1400
7.1280
7.1250
7.0396
7.0353
7.0261
7.0218
6.9746
6.9705
6.9613
6.9571
6.7961
6.7918
6.7783
6.7295
6.7254
6.7129
6.4603
3.7310
OH
CN
O
7n
3.00
2.02
2.01
2.00
2.02
2.00
1.00
3.01
f1 (ppm)


159.3963
155.7103
140.8678
132.6160
130.3298
130.1265
128.8407
114.1496
56.3076
55.5605
OH
CN
O
7n
f1 (ppm)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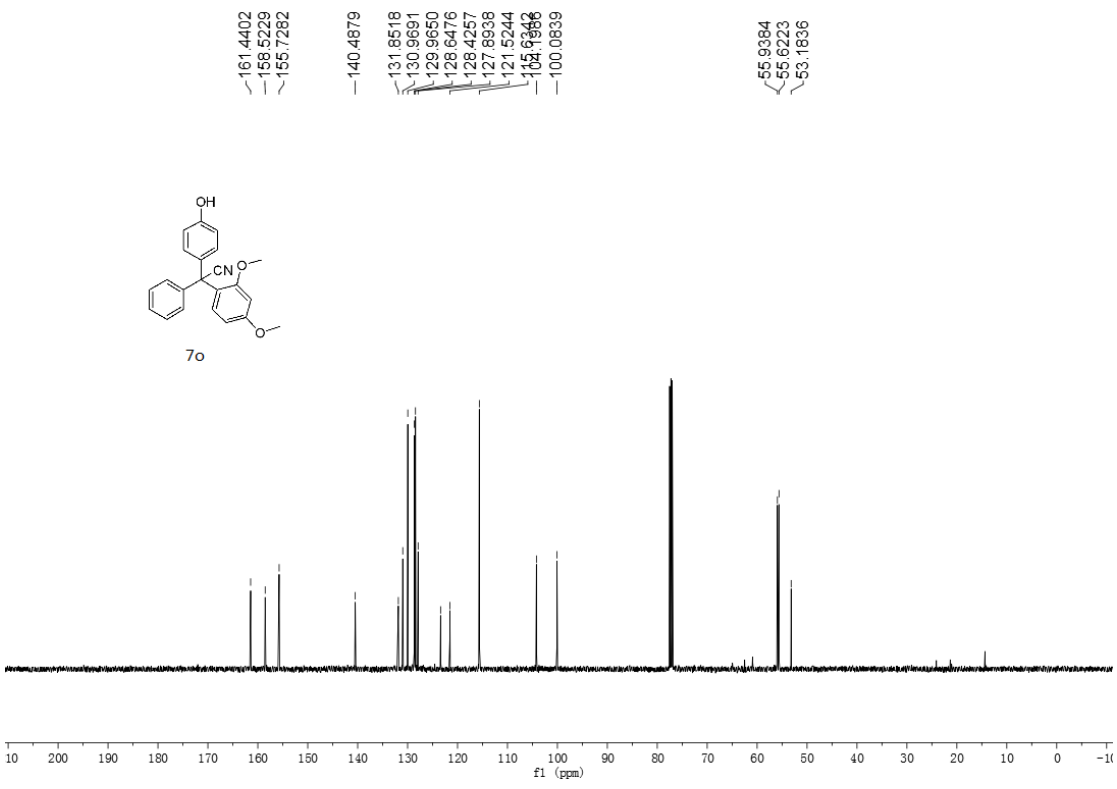
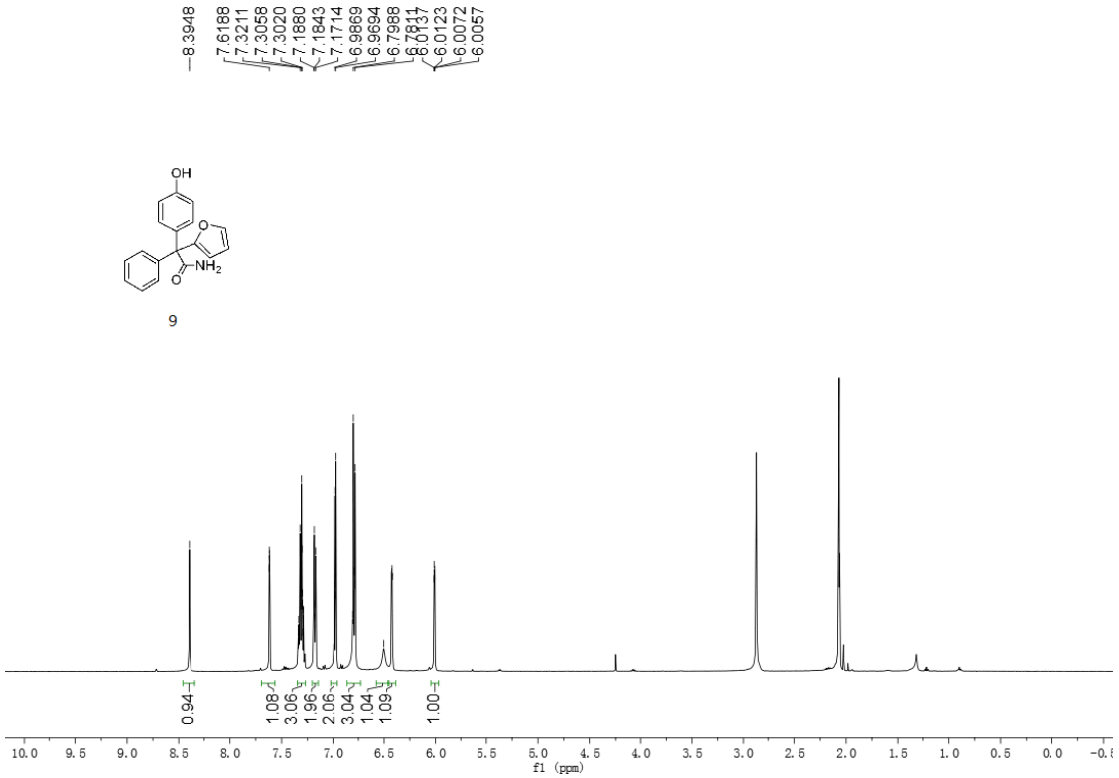
7.3233
7.3147
7.3105
7.3025
7.2135
7.2095
7.2055
7.2010
7.1971
7.1943
7.0451
7.0410
7.0317
7.0276
6.8002
6.7961
6.7868
6.7827
6.5218
6.5172
6.3787
6.3613
6.3475
3.7981
3.6730
OH
CN
O
O
3.03
2.01
2.02
2.00
0.97
1.95
1.00
2.98
2.95
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

7o


161.4402
158.5229
155.7282
140.4879
131.8518
130.9691
129.9650
128.6476
128.4257
127.8938
121.5244
100.0839
55.9384
55.6223
53.1836
OH
CN
O
O
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

7o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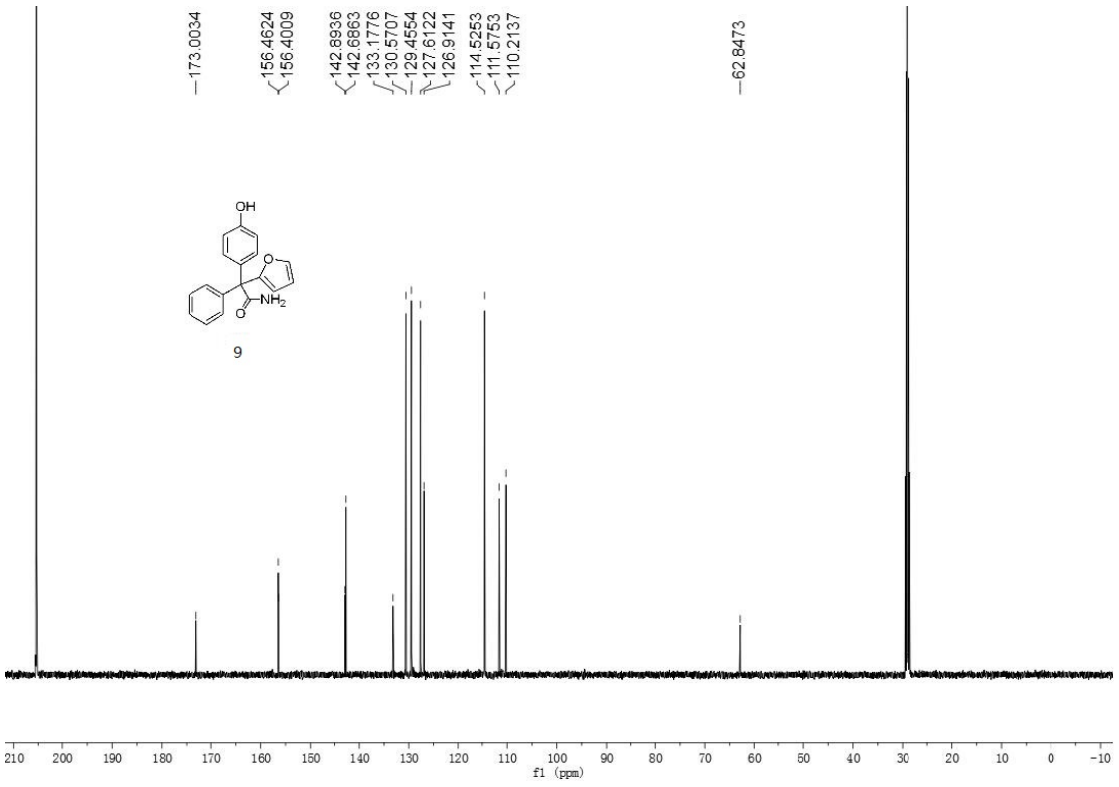
7.3211
7.3058
7.3020
7.1880
7.1843
7.1714
6.9869
6.9694
6.7988
6.7811
6.0137
6.0123
6.0072
6.0057
OH
O
NH2
O
9
0.94
1.08
3.06
1.96
2.06
3.04
1.04
1.09
1.00
f1 (ppm)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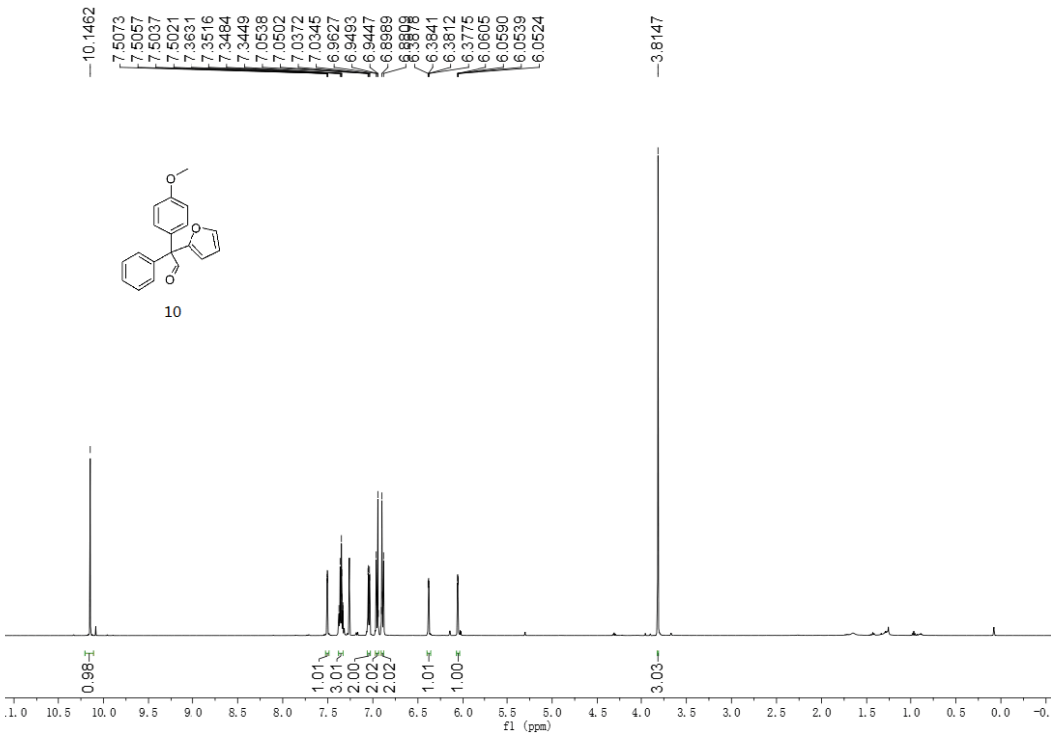
156.4009
142.8936
142.6863
133.1776
130.5707
129.4554
127.6122
126.9141
114.5253
111.5753
110.2137
62.8473
OH
O
NH2
O
9
f1 (ppm)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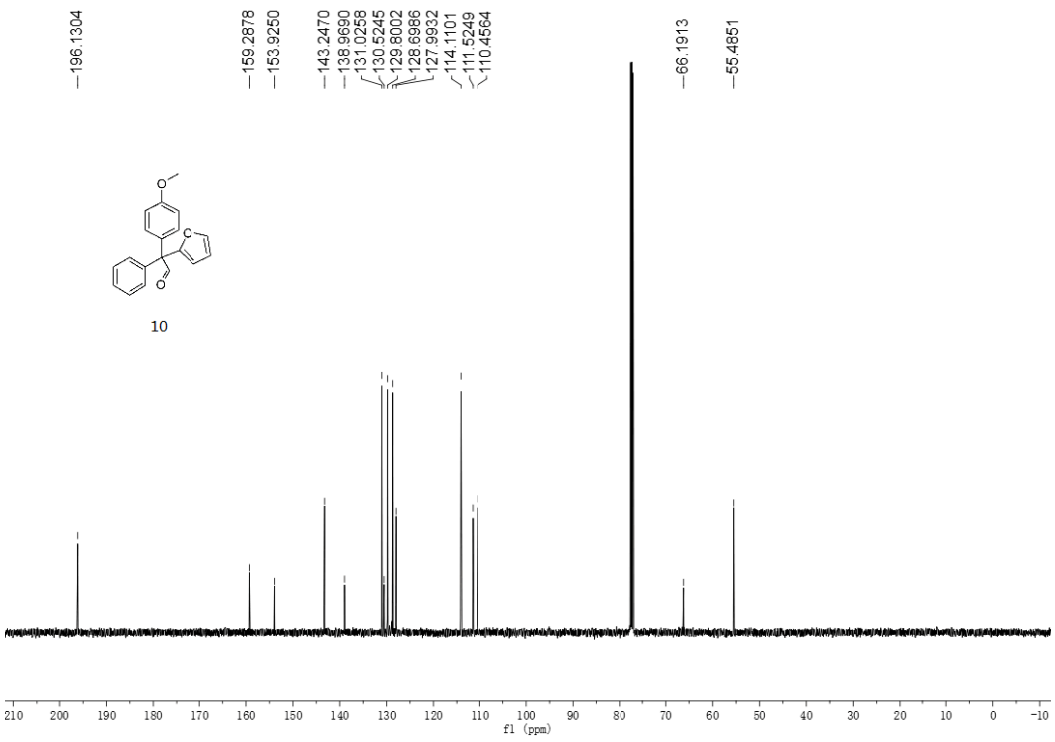
7.5057
7.5037
7.5021
7.3631
7.3516
7.3484
7.3449
7.0538
7.0502
7.0372
7.0345
6.9627
6.9493
6.9447
6.8989
6.3841
6.3812
6.3775
6.0605
6.0590
6.0539
6.0524
3.8147
0.98
1.01
3.01
2.00
2.02
2.02
1.01
1.00
3.03
f1 (ppm)

10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153.9250
143.2470
138.9690
131.0258
130.5245
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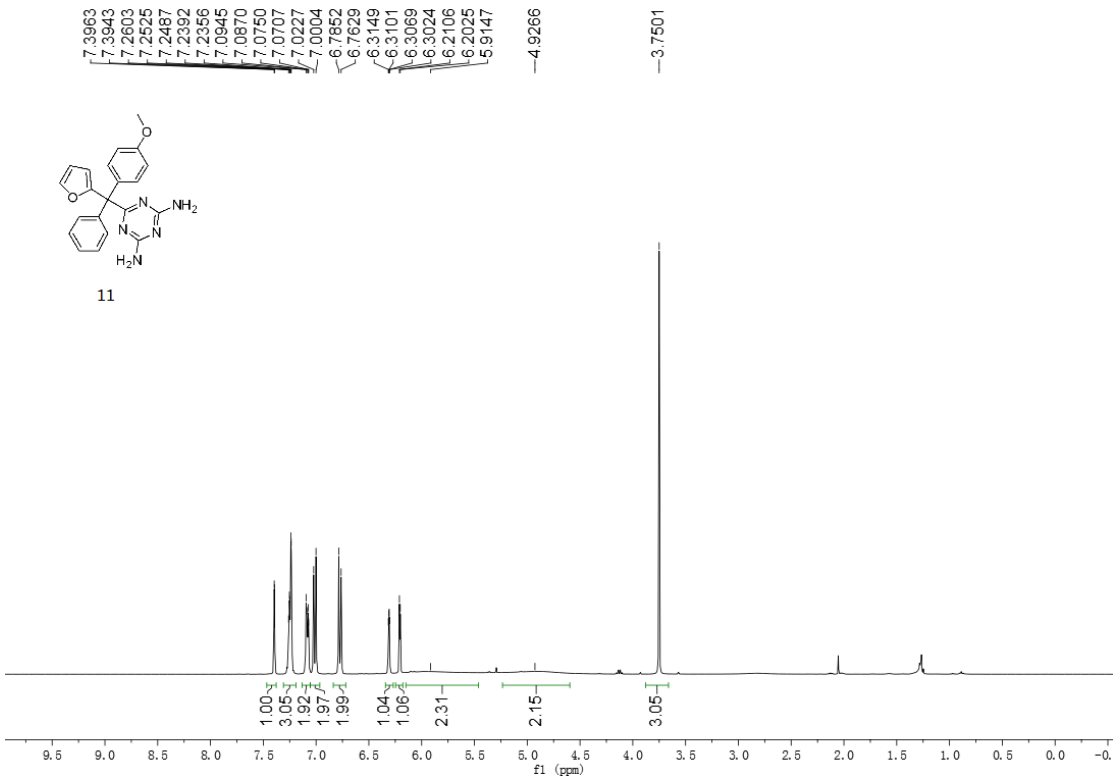
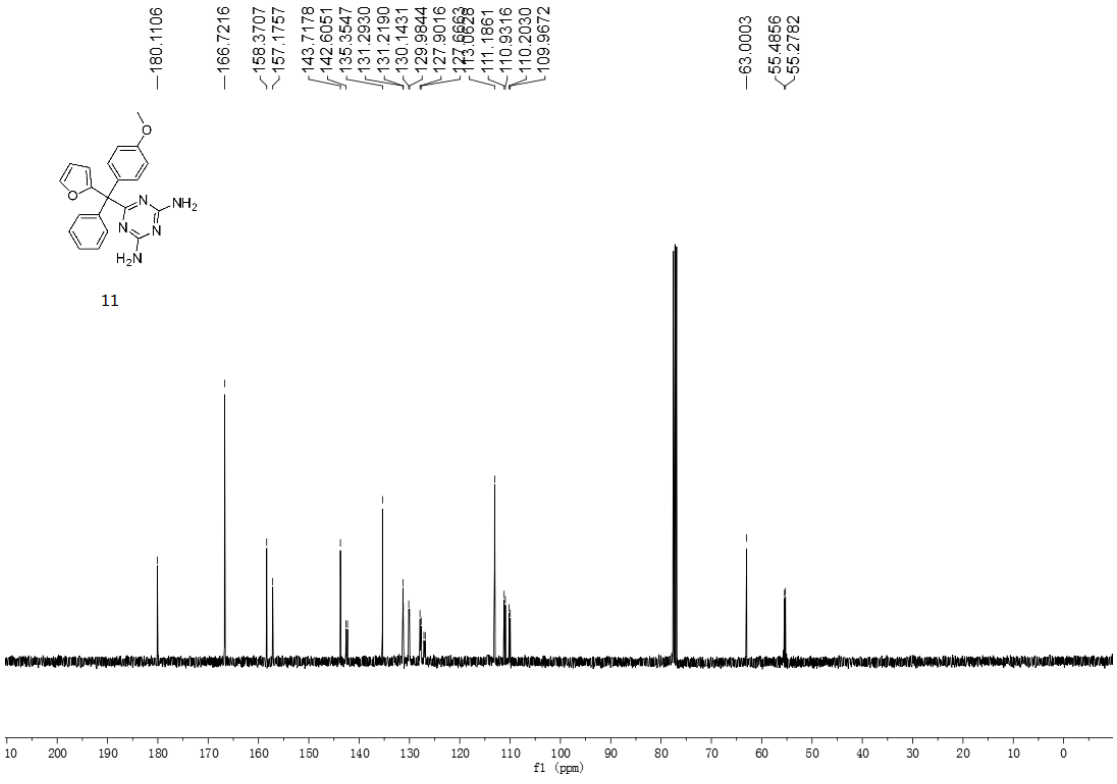
127.9932
114.1101
111.5249
110.4564
66.1913
55.4851
f1 (ppm)

10


7.3963
7.3943
7.2603
7.2525
7.2487
7.2392
7.2356
7.0945
7.0870
7.0750
7.0707
7.0227
7.0004
6.7852
6.7629
6.3149
6.3101
6.3069
6.3024
6.2106
6.2025
5.9147
4.9266
3.7501
O
NH2
N
N
N
H2N
1.00
3.05
1.92
1.97
1.99
1.04
1.06
2.31
2.15
3.05
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 -0.
f1 (ppm)

11


180.1106
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157.1757
143.7178
142.6051
135.3547
131.2930
131.2190
130.1431
129.9844
127.9016
127.6663
113.0828
111.1861
110.9316
110.2030
109.9672
63.0003
55.4856
55.2782
O
NH2
N
N
N
H2N
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

11