Supporting Information

Palladium-catalyzed direct addition of arylboronic acids to 2-aminobenzonitrile derivatives: synthesis, biological evaluation and *in silico* analysis of 2-aminobenzophenones, 7-benzoyl-2-oxoindolines, and 7-benzoylindoles

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1. General information

Melting points are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were measured on a 500 MHz spectrometer (^{1}H at 500 MHz, ^{13}C at 125 MHz), using DMSO-d_6 or $CDCl_3$ as the solvent with tetramethylsilane (TMS) as an internal standard at room temperature. Chemical shifts are given n δ relative to TMS, and the coupling constants J are given in hertz. High-resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Other commercially obtained reagents were used without further purification. All reactions were conducted using standard Schlenk techniques. Column chromatography was performed using EM silica gel 60 (300−400 mesh).

Activity Assay. The modified MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide] assay was performed. The cells were seeded in 96-well plate with a concentration of 5.0×10^4 cells per mL and a volume of 100 μL per well. Different concentrations of compounds were applied to culture wells in triplicate after the cells incubated at 37 ºC in a humidified incubator with 5% CO_2 for 24 h. After incubation for another 48 h, 10 μL MTT solutions (5 mg/mL in PBS) was added to each well and the plate incubated for another 3 h at 37ºC. The culture medium was then removed and 200 μL DMSO was added to dissolve the MTT crystals. The plate was shaken for 20 min and the absorbance was read on 570 nm using a multi-well plate reader (Model 680, Bio-Rad Laboratories). The half maximal inhibitory concentration (IC_{50}) was calculated, as the compound concentrations required reducing the MTT signal by 50% compared with untreated control cultures.

Molecular Docking. The complex crystal structure of tubulin with its destabilizing drug BAL27862 was retrieved from the PDB database[18] under the accession ID: 4O2A. The active site of tubulin was defined by its co-crystallized BAL27862. First, the BAL27862, water molecules and other cofactors were manually removed from the crystal structure and hydrogen atoms were added to protein by using REDUCE program.[19] Then the atoms of protein receptor and compound ligands were assigned with Kollman[20] and Gasteiger[21] charges, respectively. The AutoDock Tools[22] were employed to set the center and size of grid boxes covering the identified ligand-binding site in tubulin, and to prepare the *pdbqt* files for protein and compound ligands. The docking calculations were implemented with AutoDock Vina,[23] which utilized Lamarckian genetic algorithm (LGA) to explore the conformational space of ligand molecule within the active pocket of protein receptor.

2. General procedure

General procedure for the synthesis of 2-aminobenzophenones. A Schlenk tube was charged with 2-aminobenzonitriles **1** (0.4 mmol), arylboronic acids **2** (0.8 mmol), $Pd(O_2CCF_3)_2$ (5 mol %), MsOH (10 equiv), **L2** (7.5 mol %), 2-MeTHF (2 mL), and H_2O (1 mL) at room temperature. The reaction mixture was stirred vigorously at 80 °C for 36 h. The mixture was poured into ethyl acetate, which was washed with saturated $NaHCO_3$ (2 × 10 mL) and then brine (1 × 10 mL). After the aqueous layer was extracted with ethyl acetate, the combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under a vacuum. The residue was purified by flash column chromatography (hexane/ethyl acetate as eluent) to afford the desired products **3**.

General procedure for the synthesis of 7-benzoyl-2-oxoindolines and 7-benzoylindoles. A Schlenk tube was charged with 2-oxoindoline-7-carbonitrile (**1l**) or indole-7-carbonitrile (**1j**) (0.4 mmol), arylboronic acids **2** (0.8 mmol), $Pd(O_2CCF_3)_2$ (10 mol %), **L2** (15 mol %), 2-MeTHF (2 mL), and H_2O (1 mL) at room temperature. The reaction mixture was stirred vigorously at 80 °C for 36 h. The mixture was poured into ethyl acetate, which was washed with saturated $NaHCO_3$ (2 × 10 mL) and then brine (1 × 10 mL). After the aqueous layer was extracted with ethyl acetate, the combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under a vacuum. The residue was purified by flash column chromatography (hexane/ethyl acetate as eluent) to afford the desired products **4** or **5**.

3. The dose-response curves of 4e against the different cancer cell lines

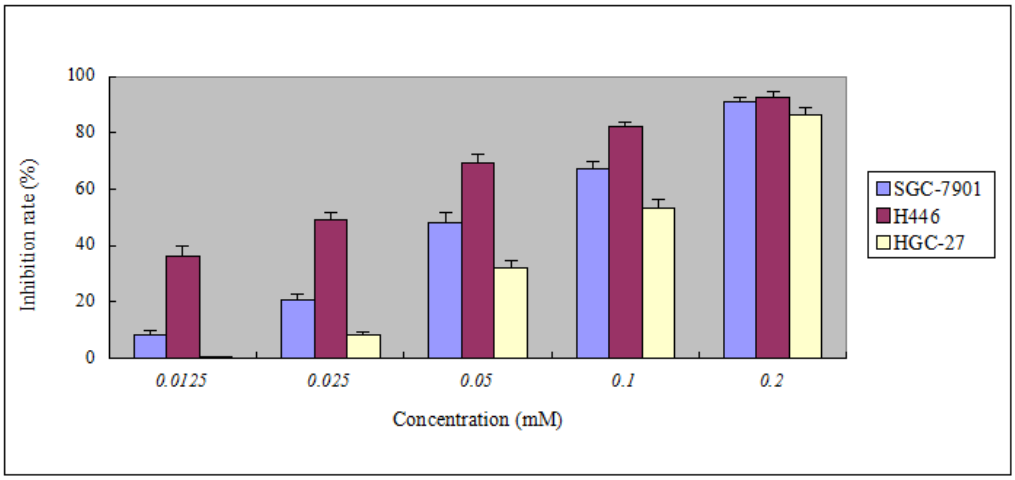

Fig. S1 The dose-response curves of **4e** against the different cancer cell lines

4. Analytical data for all products

*2-Aminobenzophenone (**3aa**)*. Yellow solid (73.3 mg, 93% yield), mp 111-112 °C (Lit.[1] 109-111 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.63 (d, *J* = 7.1 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.47-7.44 (m, 3H), 7.28 (t, *J* = 7.0 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 6.60 (t, *J* = 7.6 Hz, 1H), 6.09 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 199.1, 150.9, 140.1, 134.6, 134.2, 131.0, 129.1, 128.1, 118.2, 117.0, 115.5.

*(2-Aminophenyl)(p-tolyl)methanone (**3ab**)*. Yellow solid (75.1 mg, 89% yield), mp 92-93 °C (Lit.[2] 92-93 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.56 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.30-7.25 (m, 3H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.60 (t, *J* = 7.5 Hz, 1H), 6.00 (s, 2H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.8, 150.7, 141.7, 137.2, 134.4, 134.0, 129.4, 128.7, 118.6, 116.9, 115.5, 21.5.

*(2-Aminophenyl)(m-tolyl)methanone (**3ac**).* Yellow solid (96.8 mg, 91% yield), mp 56-57 °C (Lit.[3] 57 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.46 (d, *J* = 6.2 Hz, 2H), 7.43-7.41 (m, 1H), 7.34-7.31 (m, 2H), 7.30 (t, *J* = 7.7 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 6.64-6.59 (m, 1H), 6.09 (s, 2H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.8, 150.7, 141.7, 137.2, 134.4, 134.0, 129.4, 128.7, 118.6, 116.9, 115.5, 21.5. δ 198.8, 150.4, 139.7, 137.4, 134.1, 133.6, 131.3, 129.1, 127.4, 125.8, 117.9, 116.5, 115.0, 20.8.

*(2-Aminophenyl)(o-tolyl)methanone (**3ad**)*. Yellow solid (48.1 mg, 57% yield), mp 79-81 °C (Lit.[4] 84 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.34 (t, *J* = 7.1 Hz, 1H), 7.29-7.27 (m, 1H), 7.25-7.20 (m, 4H), 6.71 (d, *J* = 8.3 Hz, 1H), 6.52 (t, *J* = 7.6 Hz, 1H), 6.41 (s, 2H), 2.27 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 200.8, 150.7, 140.1, 134.6, 134.3, 134.2, 130.0, 128.7, 126.6, 124.7, 117.9, 116.4, 115.1, 19.0.

*(2-Aminophenyl)(4-methoxyphenyl)methanone (**3ae**)*. Yellow solid (80.0 mg, 88% yield), mp 77-78 °C (Lit.[5] 75-76 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.68 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 8.3 Hz, 1H), 6.62 (t, *J* = 7.1 Hz, 1H), 5.86 (s, 2H), 3.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.8, 162.3, 150.4, 134.0, 133.7, 131.8, 122.2, 199.0, 117.0, 115.6, 113.4, 55.4.

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*(2-Aminophenyl)(3-methoxyphenyl)methanone (**3af**)*.[6] Light yellow oil (80.9 mg, 89% yield); ^{1}HNMR ($CDCl_3$, 500 MHz) δ 7.47 (d, *J*=8.1 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.19-7.17 (m, 2H), 7.06 (d, *J* = 8.2 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 6.60 (t, *J* = 7.6 Hz 1H), 6.10 (s, 2H), 3.35 (s, 3H); ^{13}CNMR ($CDCl_3$, 125 MHz) δ 198.3, 158.9, 150.4, 140.9, 134.1, 133.8, 128.5, 121.1, 117.7, 116.8, 116.5, 115.0, 113.3, 54.9.

*(2-Aminophenyl)(3,4-dimethoxyphenyl)methanone (**3ag**)*. Yellow solid (96.7 mg, 94% yield), mp 80-81 °C (Lit.[7] 79-81 °C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.48 (d, *J* = 8.0 Hz, 1H), 7.32-7.31 (m, 1H), 7.30-7.25 (m, 2H), 6.89 (d, *J* = 8.3 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 6.63 (t, *J* = 7.5 Hz, 1H), 5.86 (s, 2H), 3.95 (s, 3H), 3.92 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.7, 152.0, 150.4, 148.8, 134.0, 133.7, 132.4, 124.1, 118.9, 117.0, 115.6, 112.1, 109.8, 56.1, 55.0.

*(2-Aminophenyl)(3,4,5-trimethoxyphenyl)methanone (**3ah**)*.[8] Yellow solid (125.5 mg, 81% yield), 55-57 ^{o}C (not reported); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.50 (d, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 6.91 (s, 2H), 6.75 (d, *J* = 8.3 Hz, 1H), 6.63 (t, *J* = 7.5 Hz, 1H), 6.00 (s, *2*H), 3.93 (s, 3H), 3.88 (s, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.1, 152.8, 150.8, 140.8, 135.2, 134.2, 134.2, 118.3, 117.1, 115.5, 106.9, 61.0, 56.3.

*(2-Aminophenyl)(4-fluorophenyl)methanone (**3ai**)*.[9] Yellow solid (69.7 mg, 81% yield), mp 128-129 °C (not reported); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.69-7.66 (m, 2H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 7.14 (t, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 8.3 Hz, 1H), 6.62 (t, *J* = 7.6 Hz, 1H), 6.03 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.5, 165.5 (d, $^1J_{C\text{-}F}$ = 252 Hz, 1C), 150.8, 136.1, 134.3, 134.2, 131.7 (d, $^3J_{C\text{-}F}$=8.9 Hz, 1C), 118.1, 117.1, 115.6, 115.3 (d, $^2J_{C\text{-}F}$=22 Hz, 1C).

*(2-Aminophenyl)(4-chlorophenyl)methanone (**3aj**)*. Yellow solid (78.8 mg, 85% yield), mp 100-101 °C (Lit.[10] 98-100 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.59 (d, *J* = 8.5 Hz, 2H), 7.44-7.39 (m, 3H), 7.30 (t, *J* = 7.7 Hz, 1H), 6.73(d, *J* = 8.9 Hz, 1H), 6.60 (t, *J* = 7.6 Hz, 1H), 6.08 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.9, 151.0, 138.4, 137.4, 134.5, 134.3, 130.6, 128.4, 117.9, 117.2, 115.7.

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*(2-Aminophenyl)(4-bromophenyl)methanone (**3ak**)*.[11] Yellow solid (83.9 mg, 76% yield), mp 108-109 °C (not reported); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.61 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 6.61 (t, *J* = 7.6 Hz, 1H), 6.10 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.8, 151.0, 138.8, 134.5, 134.2, 131.4, 130.7, 125.8, 117.7, 117.1, 115.6.

*(2-Aminophenyl)(4-iodophenyl)methanone (**3al**)*. Yellow solid (91.7 mg, 71% yield), mp 102-103 °C; IR (KBr) 3420, 3331, 1623, 1595, 1541, 1508, 1460, 1261, 1172, 837, 769 cm^{-1}; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.41-7.36 (m, 3H), 7.30 (t, *J* = 7.7 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 6.60 (t, *J* = 7.6 Hz, 1H), 6.10 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.0, 151.1, 139.5, 137.4, 134.6, 134.3, 130.7, 117.7, 117.2, 115.7, 98.1. HRMS (ESI) *m*/*z* calcd for $C_{13}H_{11}INO^+$ $[M + H]^+$ 323.9880, found 323.9874.

*(2-Aminophenyl)(4-(methylthio)phenyl)methanone (**3am**)*. Yellow solid (52.6 mg, 54% yield), mp 87-88 °C; IR (KBr) 3432, 3326, 1627, 1586, 1538, 1467, 1421, 1141, 824, 758 cm^{-1}. ^{1}H NMR ($CDCl_3$, 500MHz): δ 7.60 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.29-7.26 (m, 3H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.60 (t, *J* = 7.5 Hz, 1H), 5.97 (s, 2H), 2.53 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.0, 150.7, 143.5, 136.2, 134.2, 134.1, 130.0, 125.0, 118.5, 117.1, 115.6, 15.1. HRMS (ESI) *m*/*z* calcd for $C_{14}H_{14}NOS^+$ $[M + H]^+$ 244.0791, found 244.0798.

*(2-Aminophenyl)(thiophen-3-yl)methanone (**3an**)*. Yellow solid (29.2 mg, 36% yield), mp 81-82 °C (Lit.[12] 82-85 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.78-7.79 (m, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 5.0 Hz, 1H), 7.35-7.36 (m, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.65 (t, *J* = 7.6 Hz, 1H), 5.94 (s, 2H); ^{13}C NMR ($CDCl_3$, 125MHz) δ 191.4, 149.8, 142.0, 133.5, 132.9, 130.9, 128.1, 125.1, 118.8, 116.5, 115.3.

*(2-Aminophenyl)(biphenyl-4-yl)methanone (**3ao**)*. Yellow solid (100.6 mg, 92% yield), mp 141-142 °C (Lit.[13] 142-144 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.68-7.64 (m, 4H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 6.74 (d, *J* = 7.6 Hz, 1H), 6.63 (t, *J* = 7.6 Hz, 1H), 6.07 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.7, 150.9, 144.0, 140.3, 138.8, 134.5, 134.3, 129.9, 129.0, 128.0, 127.3,

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126.9, 118.4, 117.1, 115.6.

*(2-Aminophenyl)(naphthalen-2-yl)methanone (**3ap**)*. Yellow solid (80.1 mg, 81% yield), mp 107-108 °C (Lit.[14] 110-111 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.12 (s, 1H), 7.93-7.89 (m, 3H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.60-7.51 (m, 3H), 7.31 (t, *J* = 7.7 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 6.62 (t, *J* = 7.1 Hz, 1H), 6.09 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 199.0, 150.9, 137.3, 134.6, 134.6, 134.2, 132.3, 130.1, 129.1, 128.0, 127.8, 127.7, 126.7, 125.8, 118.5, 117.1, 115.6.

*(2-Amino-4-methylphenyl)(phenyl)methanone (**3ba**)*. Yellow solid (76.9 mg, 91% yield), mp 63-64 °C (Lit.[15] 66-67 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.61 (d, *J*=8.4 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.33 (d, *J* = 8.2 Hz, 1H), 6.54 (s, 1H), 6.41 (d, *J* = 7.3 Hz, 1H), 6.12 (s, 2H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.7, 151.3, 145.4, 140.5, 134.8, 130.8, 129.0, 128.1, 117.1, 117.0, 116.0, 21.8.

*(2-Amino-4-methylphenyl)(4-fluorophenyl)methanone (**3bi**)*. Yellow solid (84.4 mg, 92% yield), mp 106-107 °C; IR (KBr) 3412, 3330, 1617, 1595, 1538, 1463, 1421, 1261, 1149, 874, 768 cm^{-1}. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.62-7.64 (m, 2H), 7.31-7.29 (m, 1H), 7.11-7.13 (m, 2H), 6.55 (s, 1H), 6.41-6.42 (m, 1H), 6.06 (s, 2H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.2, 165.4, 163.4, 151.2, 145.5, 136.4, 134.4, 131.5, 131.5, 117.1, 115.9, 115.2, 115.1, 21.8. HRMS (ESI) *m*/*z* calcd for $C_{14}H_{12}FNO^+$ $[M + H]^+$ 230.0976, found 230.0969.

*(2-Amino-4-chlorophenyl)(phenyl)methanone (**3ca**)*. Yellow solid(84.3 mg, 91% yield), mp 82-84 °C (Lit.[16] 83-85 °C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.60 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.38 (d, *J* = 8.6 Hz, 1H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.55-6.57 (m, 1H), 6.21 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.3, 151.7, 140.3, 139.7, 135.9, 131.3, 129.0, 128.2, 116.6, 116.2, 116.0.

*(2-Amino-5-fluorophenyl)(phenyl)methanone (**3da**)*. Yellow solid (73.2 mg, 85% yield), mp 115-117 °C (Lit.[17] 118 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.64 (d, *J*=8.4 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.13-7.16 (m, 1H), 7.05-7.09 (m, 1H), 6.70-6.72 (m, 1H), 5.91 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.0, 153.1 (d, $^1J_{C\text{-}F}$ = 233.6 Hz, 1C), 147.3, 139.4, 131.5, 129.1, 128.3, 122.2 (d, $^2J_{C\text{-}F}$ = 23.5 Hz, 1C), 118.5 (d, $^2J_{C\text{-}F}$ = 22.5 Hz, 1C), 118.2 (d, $^1J_{C\text{-}F}$ = 6.7 Hz,

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1C), 117.9.

*(2-Amino-5-chlorophenyl)(phenyl)methanone (**3ea**)*. Yellow solid (88.9 mg, 96% yield), mp 97-98 °C (Lit.[18] 98-100 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 2.5 Hz, 1H), 7.23-7.25 (m, 1H), 6.69 (d, *J* = 8.8 Hz, 1H), 6.07 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.0, 149.4, 139.3, 134.2, 133.3, 131.6, 129.1, 128.4, 120.0, 118.8, 118.5.

*(2-Amino-5-bromophenyl)(phenyl)methanone (**3fa**)*. Yellow solid (103.8 mg, 94% yield), mp 108-109 °C (Lit.[19] 110 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.58-7.55 (m, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.35-7.37 (m, 1H), 6.65 (d, *J* = 8.8 Hz, 1H), 6.10 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.0, 149.8, 139.4, 136.9, 136.3, 131.7, 129.2, 128.5, 119.6, 118.9, 106.7.

*(2-Amino-5-chlorophenyl)(2-fluorophenyl)methanone (**3eq**)*.[20] Yellow solid (63.9 mg, 64% yield), mp 96-97 °C (not reported); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.52-7.47 (m, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.28-7.23 (m, 3H), 7.17 (t, *J* = 9.0 Hz, 1H), 6.68 (d, *J* = 8.8 Hz, 1H), 6.39 (s, 2H); ^{13}CNMR ($CDCl_3$, 125 MHz) δ 194.5, 160.0, 158.1, 149.6, 135.1, 133.2, 133.2, 132.3, 132.2, 129.7, 129.7, 128.0, 127.9, 124.4, 124.3, 120.1, 118.6, 118.3, 116.4, 116.2.

*(2-Amino-5-chlorophenyl)(2-chlorophenyl)methanone (**3er**)*.[21] Yellow solid (55.3 mg, 52% yield), mp 88-89 °C (not reported); ^{1}H NMR ($CDCl_3$, 500MHz): δ 7.47-7.35 (m, 3H), 7.31-7.23 (m, 2H), 7.11 (s, 1H), 6.69-6.67 (m, 1H), 6.47 (s, 2H); ^{13}CNMR ($CDCl_3$, 125 MHz) δ 196.4, 149.9, 139.0, 135.3, 133.2, 130.8, 130.7, 130.1, 128.4, 126.8, 120.1, 118.4, 118.0.

*(2-Amino-5-nitrophenyl)(phenyl)methanone (**3ga**)*. Yellow solid (94.4 mg, 97% yield), mp 153-154 °C (Lit.[22] 152 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.48 (s, 1H), 8.16-8.18 (m, 1H), 7.66 (d, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 6.90 (s, 2H), 6.77-6.75 (d, *J* = 9.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.0, 155.3, 138.5, 136.7, 132.2, 131.6, 129.3, 129.2, 128.7, 116.8, 116.1.

*(2-Amino-4,5-dimethoxyphenyl)(phenyl)methanone (**3ha**)*. Yellow solid (100.8 mg, 98% yield), mp 78-79 °C (Lit.[23] 78-80 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.61 (d, *J*=8.4 Hz, 2H), 7.50 (t, *J* = 7.3

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Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 2H), 6.92 (s, 1H), 6.25 (s, 2H), 6.20 (s, 1H), 3.88 (s, 3H), 3.65 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.2, 155.5, 148.6, 140.7, 139.7, 130.6, 128.7, 128.1, 116.7, 110.0, 99.3, 56.6, 55.9.

*(2-Amino-4,5-dimethoxyphenyl)(3,4-dimethoxyphenyl)methanone (**3hg**)*.[24] Yellow oil (118.0 mg, 93% yield), (not reported); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.28-7.27 (m, 2H), 7.02 (s, 1H), 6.92 (d, *J* = 8.8Hz, 1H), 6.23 (s, 1H), 6.05 (s, 2H), 3.96 (s, 3H), 3.92 (d, *J* = 8.8 Hz, 6H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.1, 155.0, 151.5, 148.7, 139.6, 133.1, 123.2, 116.4, 112.0, 110.4, 109.9, 99.4, 56.6, 56.0, 56.0, 55.9.

*(2-Amino-4,5-dimethoxyphenyl)(3,4,5-trimethoxyphenyl)methanone (**3hh**)*.[25] Yellow solid (127.8 mg, 92% yield), mp 163-165 °C (not reported); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 6.99 (s, 1H), 6.87 (s, 2H), 6.21 (s, 1H), 6.15 (s, 2H), 3.90-3.89 (m, 6H), 3.86 (s, 6H), 3.68 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.1, 155.4, 152.8, 148.5, 140.3, 139.7, 135.8, 116.3, 109.8, 106.4, 99.4, 61.0, 56.6, 56.2, 55.9.

*(2-Aminopyridin-3-yl)(phenyl)methanone (**3ia**)*. Yellow solid (65.0 mg, 82% yield), mp 146-147 °C (Lit.[26] 140 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.25 (d, *J* = 4.8 Hz, 2H), 7.77 (dd, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H) , 6.81 (s, 2H), 6.59-6.62 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.8, 159.8, 153.9, 143.0, 139.2, 131.6, 129.1, 128.4, 112.9, 112.1.

*(2-Aminopyridin-3-yl)(3,4-dimethoxyphenyl)methanone (**3ig**)*. Yellow solid (94.0 mg, 91% yield), mp 162-163 °C (Lit.[27] 163 °C); ^{1}H NMR($CDCl_3$, 500MHz): δ 8.16 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.21 (s, 1H), 7.15 (d, *J* = 8.3 Hz, 2H), 6.84 (d, *J* = 8.3 Hz, 1H), 6.62 (s, 1H), 6.56-6.54 (m, 1H), 3.89 (s, 3H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.3, 159.6, 153.2, 152.4, 149.0, 142.3, 131.5, 124.0, 113.4, 112.0, 111.9, 109.9, 56.1, 56.1.

*(3-Aminopyridin-4-yl)(3,4-dimethoxyphenyl)methanone (**3jg**)*.[28] Yellow solid (83.7 mg, 81% yield), mp 144-146 °C (not reported); ^{1}H NMR ($CDCl_3$, 500MHz): δ 8.28 (s, 1H), 7.97-7.96 (m, 1H), 7.37-7.27 (m, 3H), 6.92 (d, *J* = 8.4 Hz, 1H), 5.57 (s, 2H), 3.97 (s, 3H), 3.94 (s, 3H); ^{13}C

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NMR ($CDCl_3$, 125MHz) δ 196.3, 153.1, 149.1, 143.9, 140.9, 136.9, 130.5, 124.8, 124.6, 123.5, 111.9, 109.9, 56.1, 56.1.

*(4-Aminopyrimidin-5-yl)(3,4,5-trimethoxyphenyl)methanone (**3kh**)*. Yellow solid (82.1 mg, 71% yield), mp 136-138 °C; IR (KBr) 3444, 3331, 3013, 1629, 1613, 1580, 1527, 1503, 1450, 1407, 1238, 1135, 993, 921, 801, 776, 666, 540 cm^{-1}; ^1H NMR ($CDCl_3$, 500MHz) δ 8.66-8.63 (m, 2H), 8.32 (s, 1H), 6.89 (s, 2H), 6.11 (s, 1H), 3.93 (s, 3H), 3.89 (s, 6H); ^{13}C NMR ($CDCl_3$, 125MHz) δ 195.5, 162.8, 161.1, 160.9, 153.2, 141.9, 132.9, 111.4, 106.8, 61.1, 56.4. HRMS (ESI) *m*/*z* calcd for $C_{14}H_{16}N_3O_4^+$ $[M + H]^+$ 290.1135, found 290.1144.

*7-Benzoyl-2-oxoindoline (**4a**)*. Yellow solid (84.5 mg, 89% yield), mp 153-154 °C (Lit.[29] 154 °C); ^{1}HNMR ($CDCl_3$, 500 MHz) δ 9.57 (s, 1H), 7.72-7.71 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.55-7.49 (m, 3H), 7.43 (d, *J* = 7.3 Hz, 1H), 7.04 (t, *J* = 7.7 Hz, 1H), 3.57 (s, 2H); ^{13}CNMR ($CDCl_3$, 125MHz) δ 196.8, 176.7, 145.6, 138.0, 132.2, 131.1, 129.3, 129.0, 128.4, 127.0, 121.0, 117.9, 35.1.

*7-(4-Bromobenzoyl)-2-oxoindoline (**4b**)*. Yellow solid (89.7 mg, 71% yield), mp 195-196 °C (Lit.[30] 196-198 °C); ^1H NMR ($CDCl_3$,500MHz) δ 9.49 (s, 1H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 7.3 Hz, 1H), 7.04 (t, *J* = 7.7 Hz, 1H), 3.57 (s, 2H); ^{13}C NMR ($CDCl_3$, 125MHz) δ 195.6, 176.4, 145.7, 136.7, 131.7, 130.9, 130.7, 129.2, 127.2, 121.1, 117.6, 112.0, 35.1.

*7-(3-Methoxybenzoyl)-2-oxoindoline (**4c**)*. Yellow solid (82.3 mg, 77% yield), mp 131-133 °C; IR (KBr) 3318, 1728, 1712, 1651, 1583, 1509, 1418, 1338, 1168, 1122, 868, 688 cm^{-1}; ^{1}HNMR ($CDCl_3$, 500 MHz) δ 9.69 (s, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.43-7.38 (m, 2H), 7.29-7.26 (m, 2H), 7.14-7.12 (m, 1H), 7.04 (t, *J* = 7.7 Hz, 1H), 3.85 (s, 3H), 3.57 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.4, 176.8, 159.6, 145.5, 139.2, 131.0, 129.3, 129.0, 127.0, 121.9, 121.0, 118.3, 118.0, 114.0, 55.5, 35.1; HRMS (ESI) *m*/*z* calcd for $C_{16}H_{14}NO_3^+$ $[M + H]^+$ 268.0968, found 268.0961.

*7-(3,4-Dimethoxybenzoyl)-2-oxoindoline (**4d**)*. Yellow solid (101.1 mg, 85% yield), mp 154-156 °C; IR (KBr) 3308, 1712, 1712, 1651, 1583, 1513, 1418, 1338,1165, 868, 771, 681 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 9.36 (s, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.40 (d, *J* = 7.3 Hz, 1H), 7.36-7.34 (m,

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2H), 7.04 (t, *J* = 7.7Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 3.56 (s, 2H); ^{13}C NMR ($CDCl_3$, 125MHz) δ 195.1, 176.5, 152.9, 149.1, 145.3, 130.6, 130.5, 128.5, 127.0, 124.5, 120.8, 118.4, 112.0, 109.9, 56.1, 56.1, 35.3. HRMS (ESI) *m/z* calcd for $C_{17}H_{16}NO_4^+$ $[M + H]^+$ 298.1074, found 298.1066.

*7-(3,4,5-Trimethoxybenzoyl)-2-oxoindoline (**4e**)*. Yellow solid (73.3 mg, 56% yield), mp 156-158 °C; IR (KBr, cm−1) 3311, 2961, 1722, 1702, 1649, 1580, 1503, 1411, 1338, 1314, 1165, 1122, 862, 764, 698 cm^{-1}; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 9.45 (s, 1H), 7.59 (d, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 7.3Hz, 1H), 7.05 (t, *J* = 7.4 Hz, 1H), 6.97 (s, 2H), 3.93 (s, 3H), 3.88 (s, 6H), 3.58 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 195.7, 176.5, 153.0, 145.5, 141.8, 133.0, 130.7, 128.9, 127.1, 120.9, 118.0, 107.1, 61.0, 56.3, 35.2. HRMS (ESI) *m/z* calcd for $C_{18}H_{18}NO_5^+$ $[M + H]^+$ 328.1179, found 328.1183.

*7-(4-Fluorobenzoyl)indole (**5a**)*. Yellow solid (68.9 mg, 72% yield), mp 101-102 °C (Lit.[31] 103-104 °C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.40 (s, 1H), 7.94 (d, *J* = 7.8Hz, 1H), 7.83-7.80 (m, 2H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.40 (s, 1H), 7.22-7.16 (m, 3H), 6.66 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.7, 135.7, 131.9, 131.9, 129.6, 127.9, 127.4, 126.5, 126.1, 125.9, 125.9, 119.7, 119.2, 118.7, 115.5, 103.8, 102.7.

*7-(4-Chlorobenzoyl)indole (**5b**)*. Yellow solid (76.7 mg, 75% yield), mp 149 °C (Lit.[32] 149-151 °C); ^{1}H NMR ($CDCl_3$, 500 MHz): δ 10.38 (s, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 7.4 Hz, 1H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.40 (s, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 6.66 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.8, 137.8, 137.4, 135.6, 130.8, 129.6, 128.6, 127.9, 127.5, 125.9, 119.1, 118.7, 102.7.

*7-(4-Methoxybenzoyl)indole (**5c**)*. Yellow solid (76.4 mg, 76% yield), mp 156-158 °C; IR (KBr) 3358, 1628, 1586, 1586, 1513, 1406, 1265, 1035, 872, 856 cm^{-1}. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.36 (s, 1H), 7.91 (d, *J* = 7.8Hz, 1H), 7.82 (d, *J* = 8.7Hz, 2H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.37 (s, 1H), 7.17 (t, *J* = 7.7 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 2H), 6.65 (s, 1H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.8, 162.6, 135.8, 131.9, 131.6, 129.4, 127.6, 126.7, 125.7, 119.8, 118.6, 113.6, 102.5, 55.5. HRMS (ESI) *m/z* calcd for $C_{16}H_{14}NO_2^+$ $[M + H]^+$ 252.1019, found 252.1026.

*7-(3,4-Dimethoxybenzoyl)indole (**5d**)*. Yellow solid (91.1 mg, 81% yield), mp 98-100 °C; IR (KBr)

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3351, 2914, 1626, 1596, 1580, 1510, 1404, 1265, 1139, 1023, 888, 867, 734, 627 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 10.32 (s, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.44-7.42 (m, 2H), 7.37 (s, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 6.95-6.92 (m, 1H), 6.65 (s, 1H), 3.97 (s, 3H), 3.95 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 196.7, 152.3, 148.9, 135.8, 131.6, 129.5, 127.5, 126.7, 125.7, 124.3, 119.2, 118.4, 112.2, 109.9, 102.6, 56.1, 56.1. HRMS (ESI) *m*/*z* calcd for $C_{17}H_{16}NO_3^+$ $[M + H]^+$ 282.1125, found 282.1132.

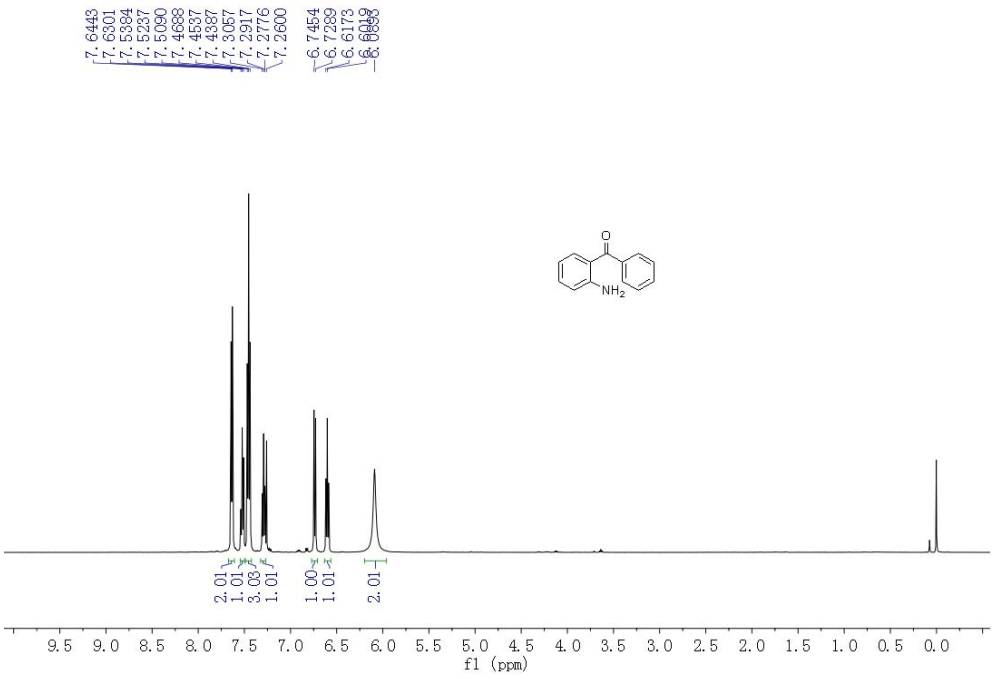
*7-(3,4,5-Trimethoxybenzoyl)indole (**5e**)*. Yellow solid (88.4 mg, 71% yield), mp 112-113 °C (Lit.[33] 114.1-115.2 °C); ^1H NMR ($CDCl_3$, 500 MHz): δ 10.36 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.39-7.38 (m, 1H), 7.17 (t, *J* = 7.7 Hz, 1H), 7.04 (s, 2H), 6.67-6.65 (m, 1H), 3.95 (s, 3H), 3.90 (s, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 197.1, 152.9, 141.1, 135.7, 134.2, 129.5, 127.7, 127.1, 125.9, 119.4, 118.6, 107.1, 102.7, 61.0, 56.3.

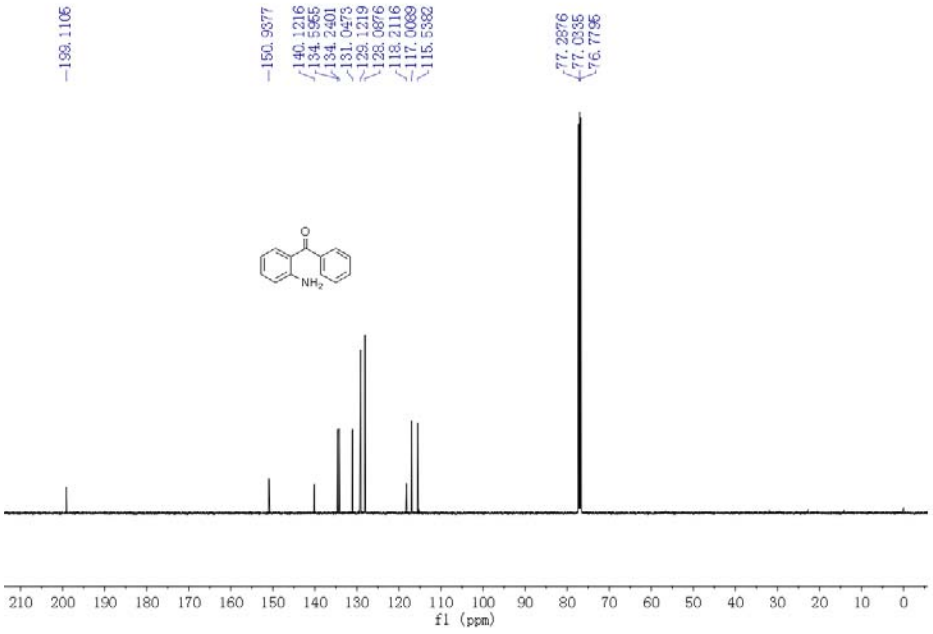
*7-(4-Phenylbenzoyl)indole (**5f**)*. Yellow solid (102.3 mg, 86% yield), mp 155-157 °C; IR (KBr) 3361, 1636, 1581, 1576, 1532, 1404, 1143, 1013, 877, 721, 636 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ 10.48 (s, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.70-7.68 (m, 3H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.44-7.40 (m, 2H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.69 (s, 1H); ^{13}C NMR ($CDCl_3$, 125MHz) δ 197.8, 144.4, 140.2, 137.8, 135.7, 130.1, 129.5, 129.0, 128.1, 127.2, 126.5, 125.9, 119.7, 119.5, 118.7, 103.7, 102.7. HRMS (ESI) *m*/*z* calcd for $C_{21}H_{16}NO^+$ $[M + H]^+$ 298.1226, found 298.1231.

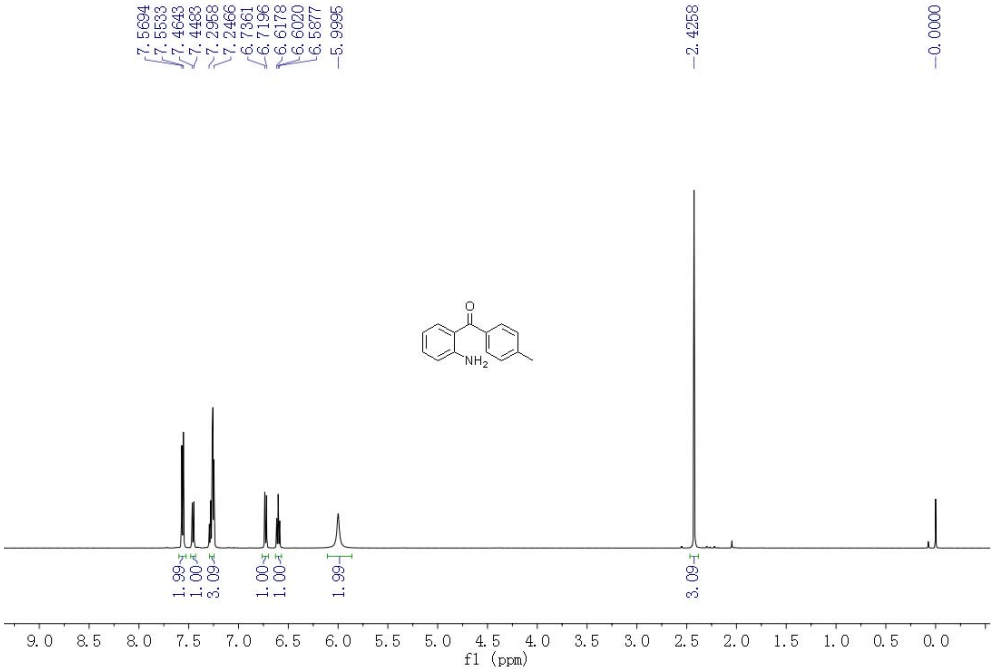
*7-(2-Naphthalenoyl)indole (**5g**)*. Yellow solid (98.7 mg, 91% yield), mp 87-89 °C; IR (KBr) 3345, 1631, 1592, 1570, 1512, 1408, 1255, 1141, 1033, 871, 743, 631 cm^{-1}; ^1H NMR ($CDCl_3$, 500MHz): δ 10.48 (s, 1H), 8.27 (s, 1H), 8.00-7.93 (m, 4H), 7.90-7.87 (m, 2H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.43 (s, 1H), 7.32 (s, 1H), 7.15-7.20 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 198.1, 136.3, 134.8, 132.3, 130.5, 129.5, 129.2, 128.2, 127.9, 127.2, 126.8, 126.5, 126.1, 125.9, 125.8, 119.7, 118.7. HRMS (ESI) *m*/*z* calcd for $C_{19}H_{14}NO^+$ $[M + H]^+$ 272.1070, found 272.1076.

[33] Liou, J.-P.; Wu, C.-Y.; Hsieh, H.-P.; Chang, C.-Y.; Chen, C.-M.; Kuo, C.-C.; Chang, J.-Y. *J. Med. Chem.* **2007**, *50*, 4548.

5. Copies of ^{1}H NMR and ^{13}C NMR for all products



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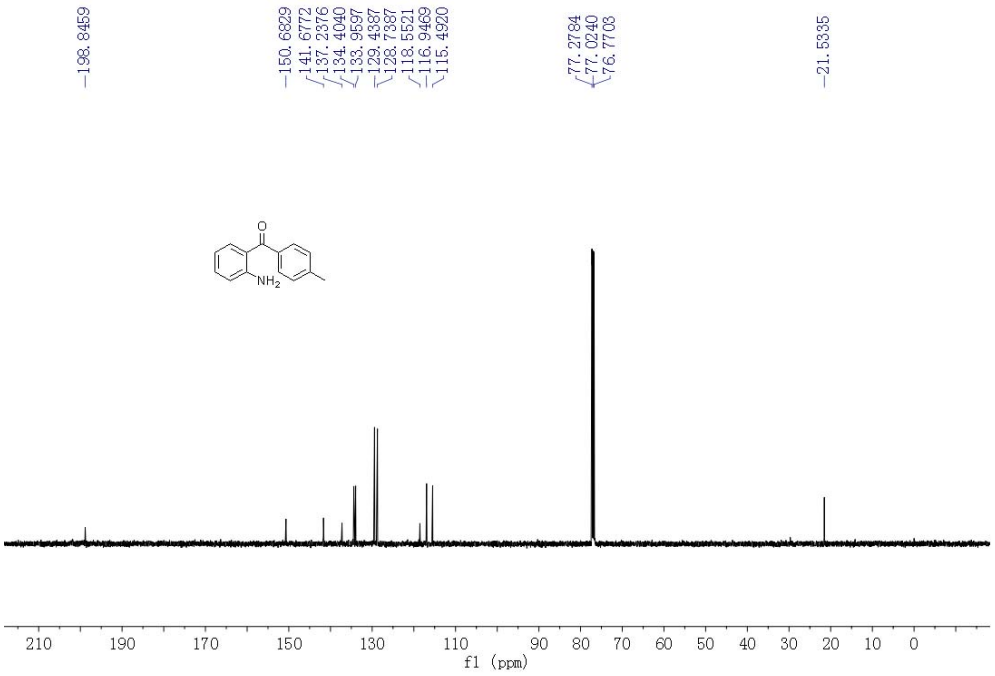
3.09
f1 (ppm)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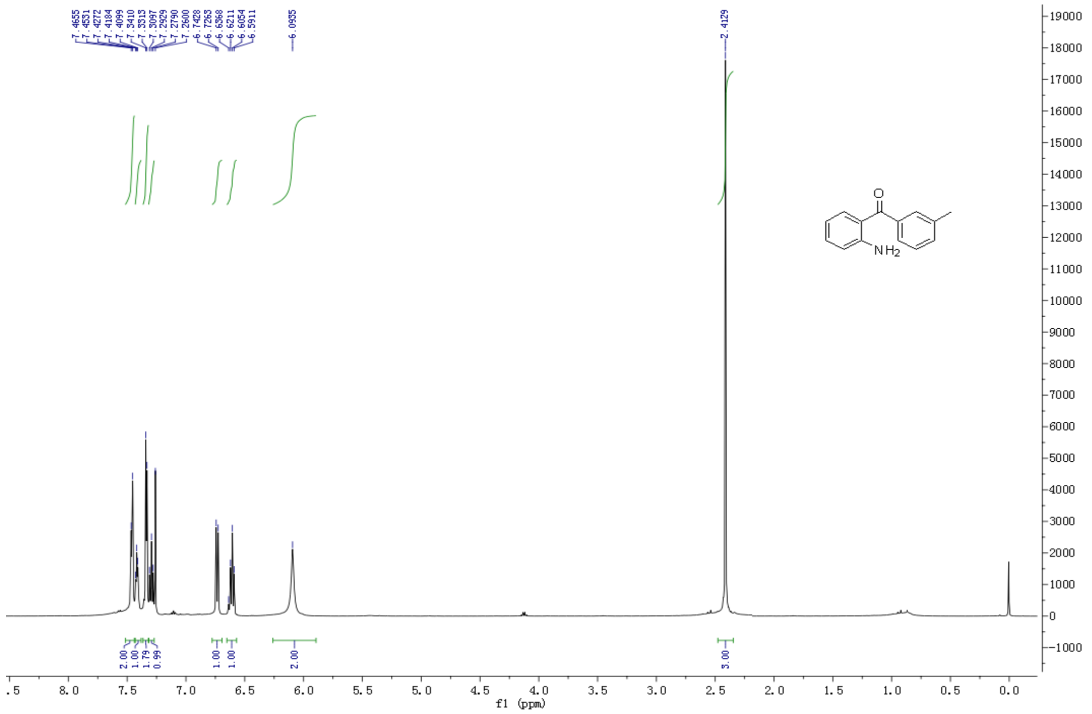
137.2376
134.4040
133.9597
129.4387
128.7387
118.5521
116.9469
115.4920
77.2784
77.0240
76.7703
21.5335
f1 (ppm)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7.4272
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7.4099
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7.3313
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7.2929
7.2790
7.2600
6.7428
6.7263
6.6368
6.6211
6.6054
6.5911
6.0935
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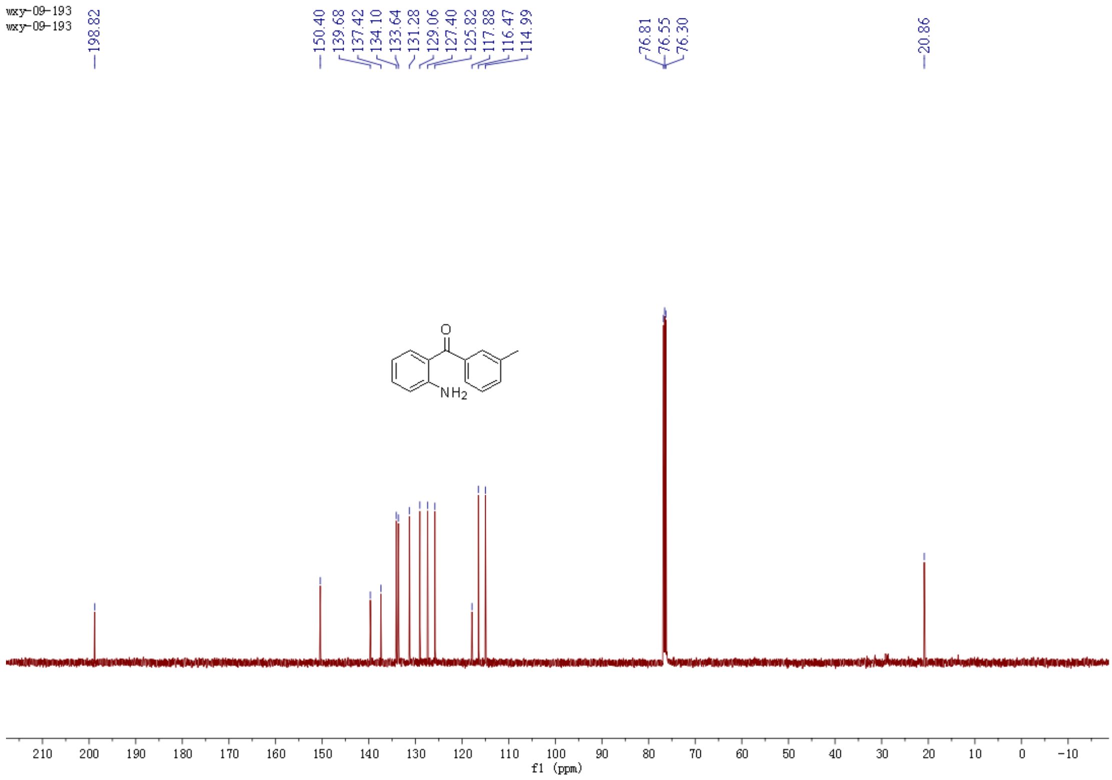
O
NH2
2.00
1.00
1.79
0.99
1.00
1.00
2.00
3.00
f1 (ppm)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wxy-09-193
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139.68
137.42
134.10
133.64
131.28
129.06
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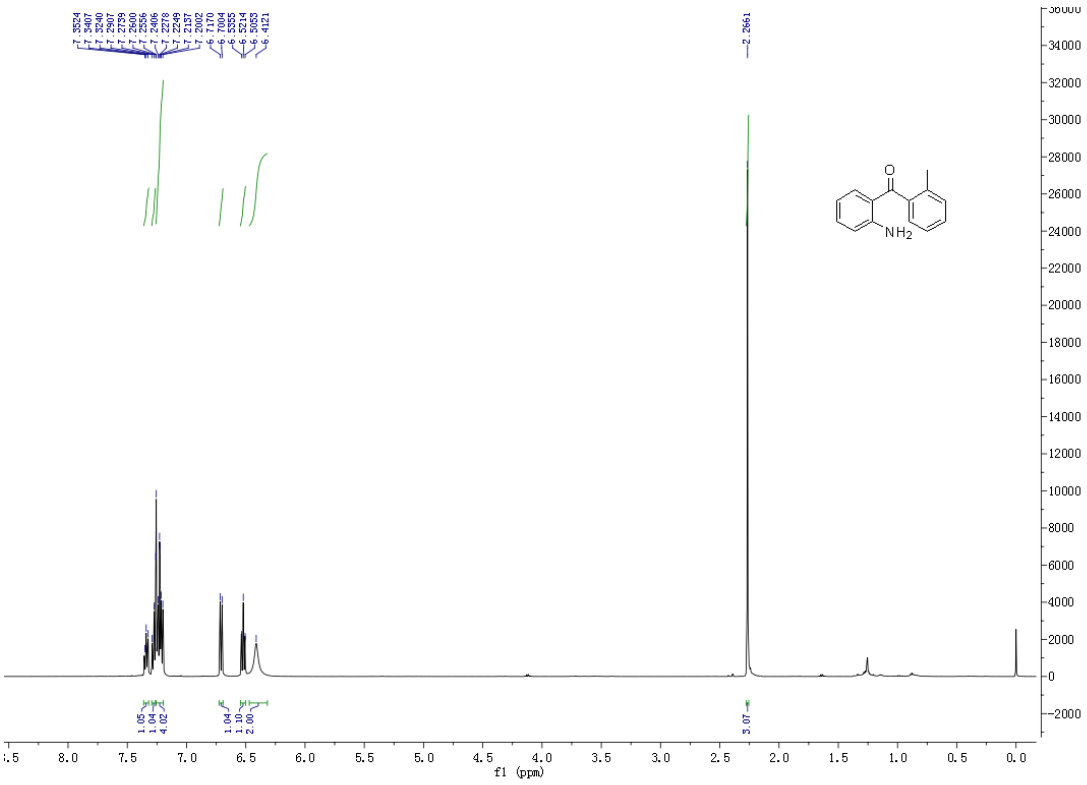
117.88
116.47
114.99
76.81
76.55
76.30
20.86
O
NH2
f1 (ppm)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7.3290
7.2907
7.2739
7.2600
7.2536
7.2496
7.2278
7.2249
7.2157
7.2002
7.1770
6.7004
6.5355
6.5214
6.5055
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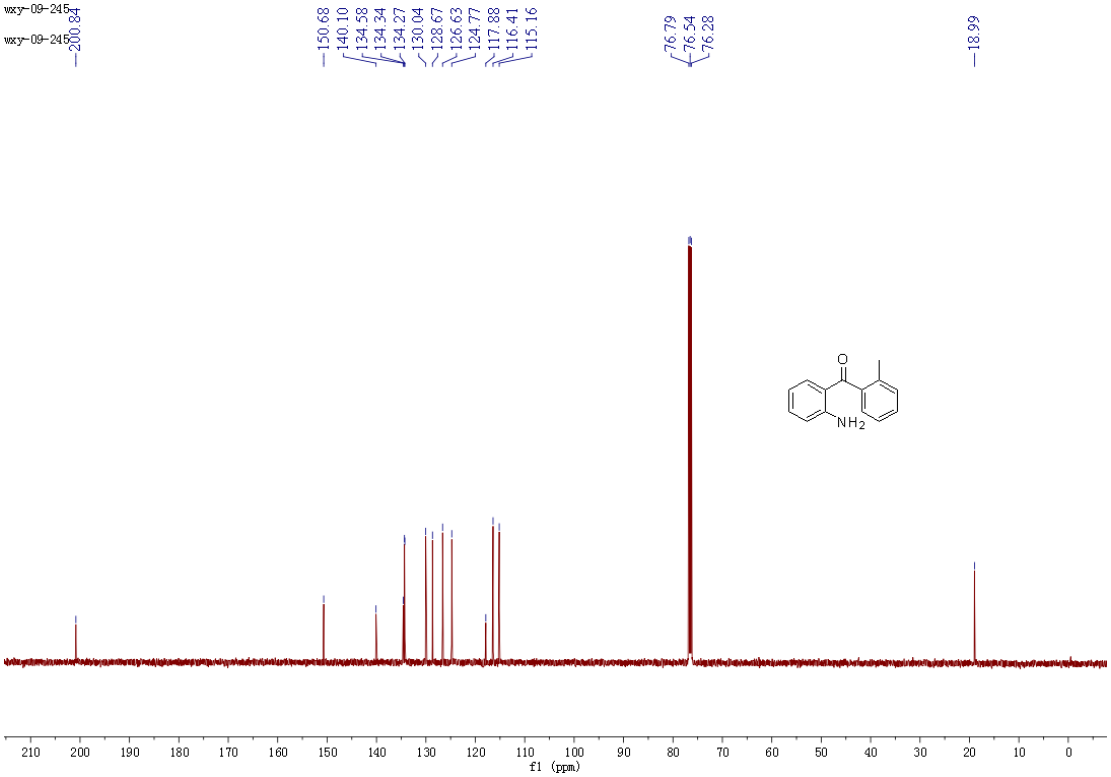
NH2
1.05
1.04
4.02
1.04
1.10
2.00
3.07
f1 (ppm)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134.34
134.27
130.04
128.67
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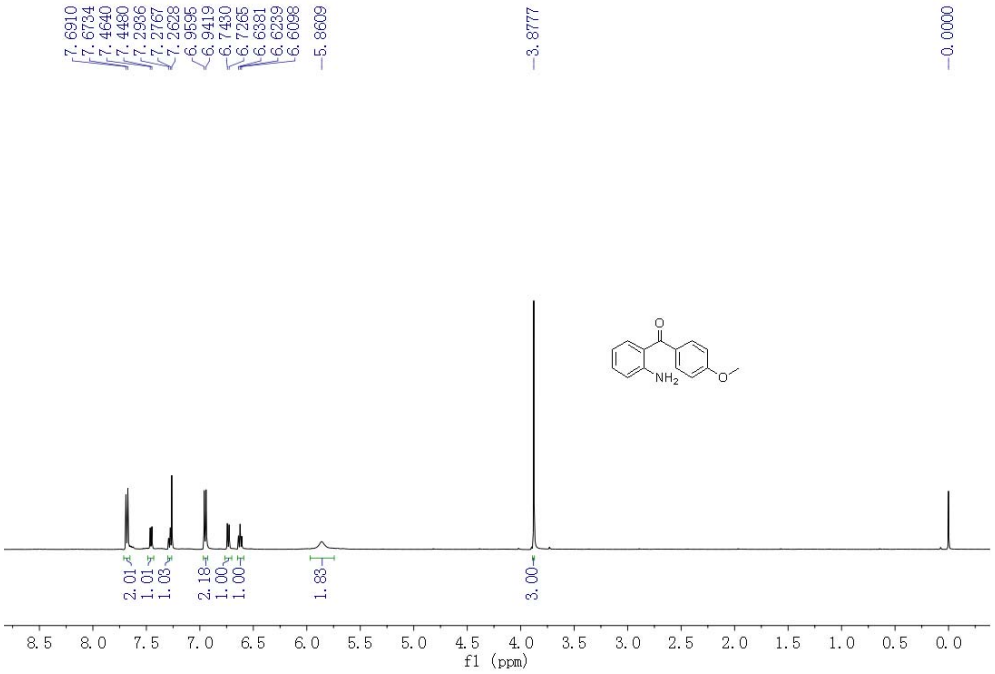
117.88
116.41
115.16
76.79
76.54
76.28
18.99
O
NH2
f1 (ppm)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7.2936
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7.2628
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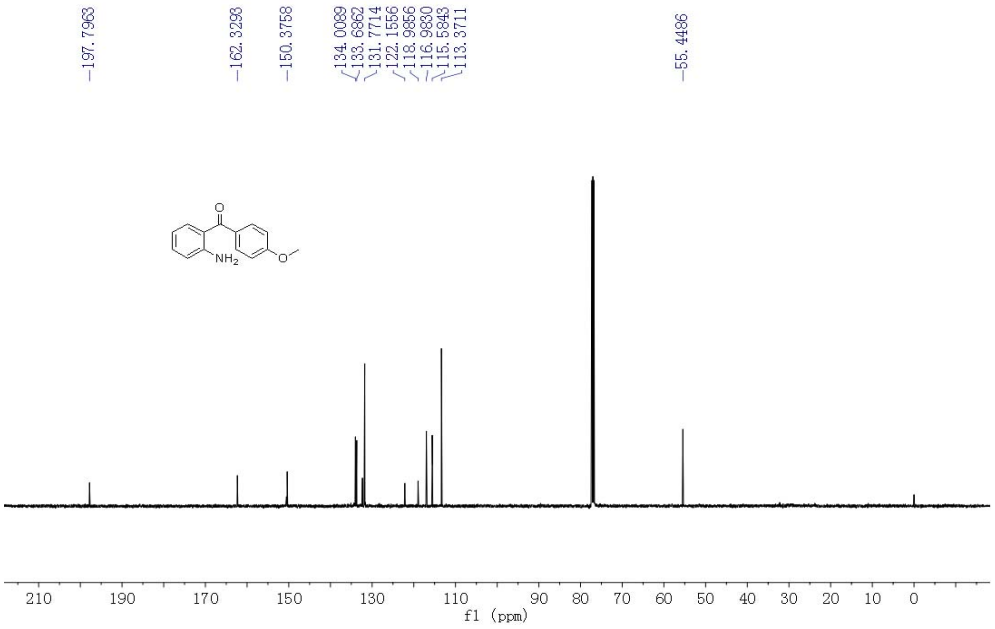
6.9419
6.7430
6.7265
6.6381
6.6239
6.6098
5.8609
3.8777
0.0000
2.01
1.01
1.03
2.18
1.00
1.00
1.83
3.00
O
NH2
O
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.6862
131.7714
122.1556
118.9866
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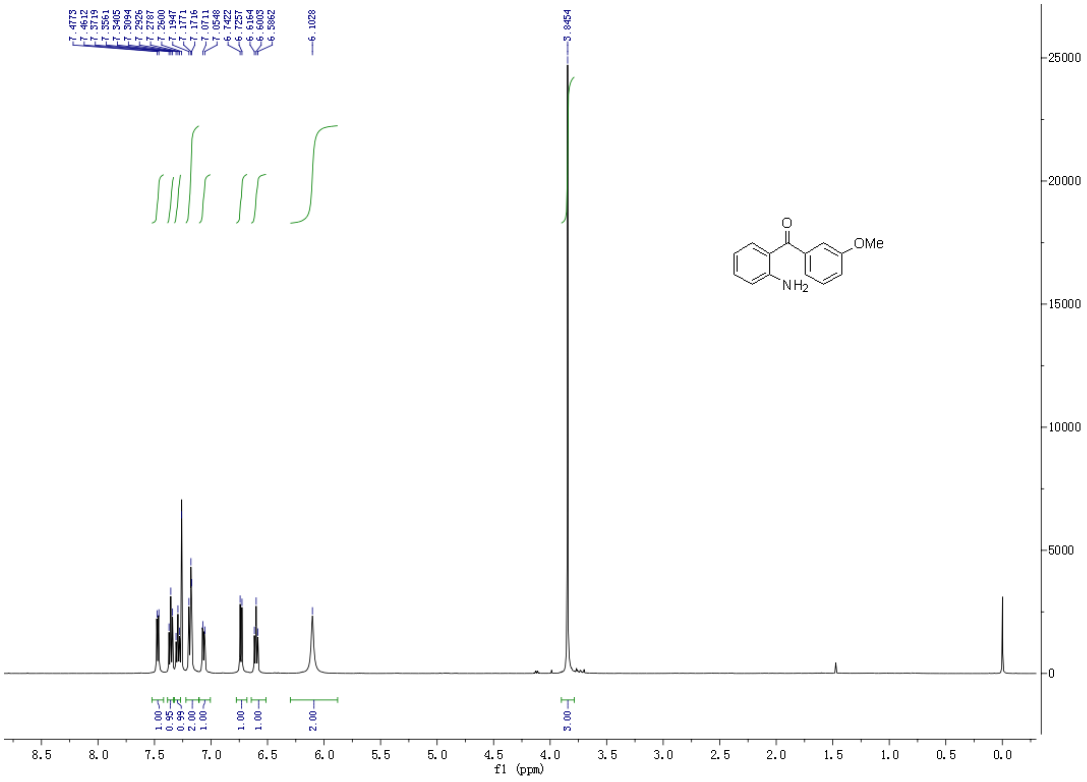
113.3711
55.4486
O
NH2
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2926
7.2787
7.2600
7.1947
7.1771
7.1716
7.0711
7.0548
6.7422
6.7253
6.6164
6.6003
6.5862
6.1028
3.8454
O
OMe
NH2
25000
20000
15000
10000
5000
0
1.00
0.95
0.99
2.00
1.00
1.00
1.00
2.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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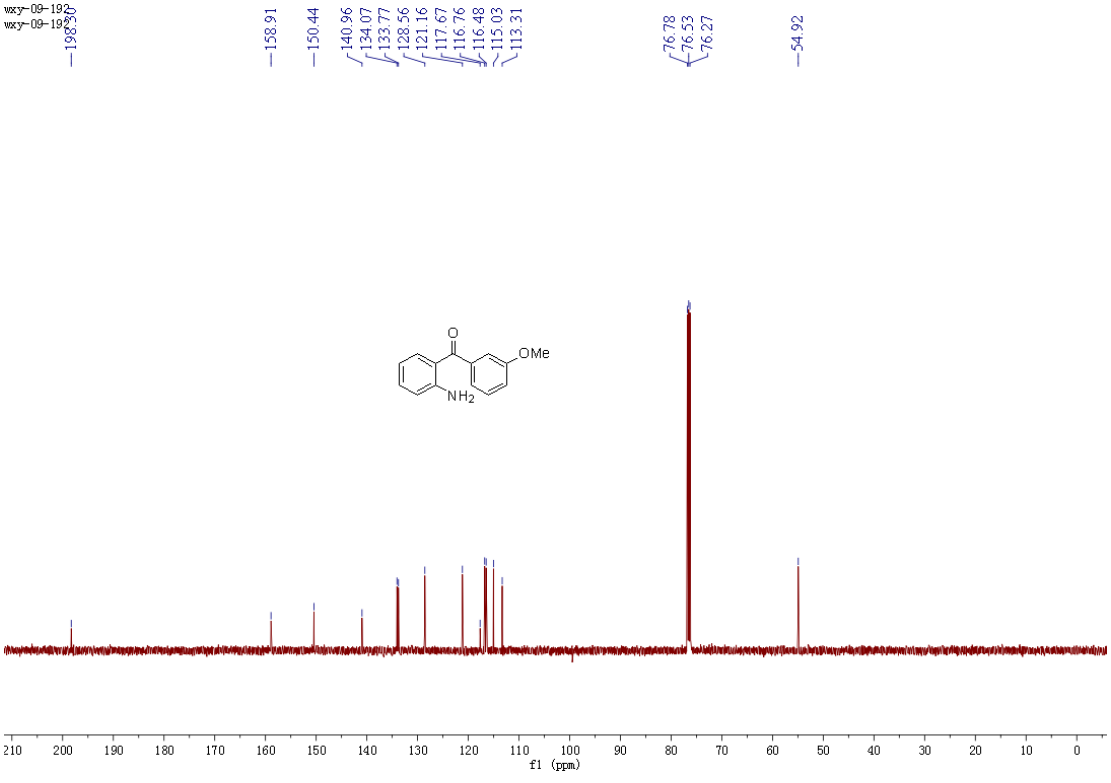
0.0
f1 (ppm)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wxy-09-192
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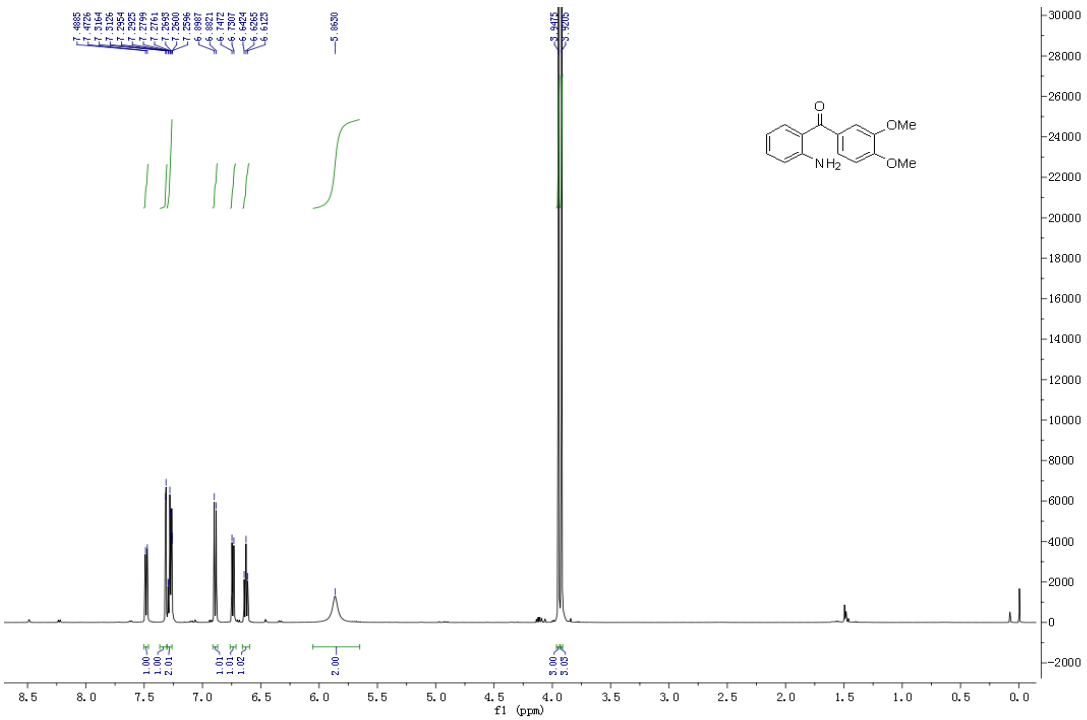
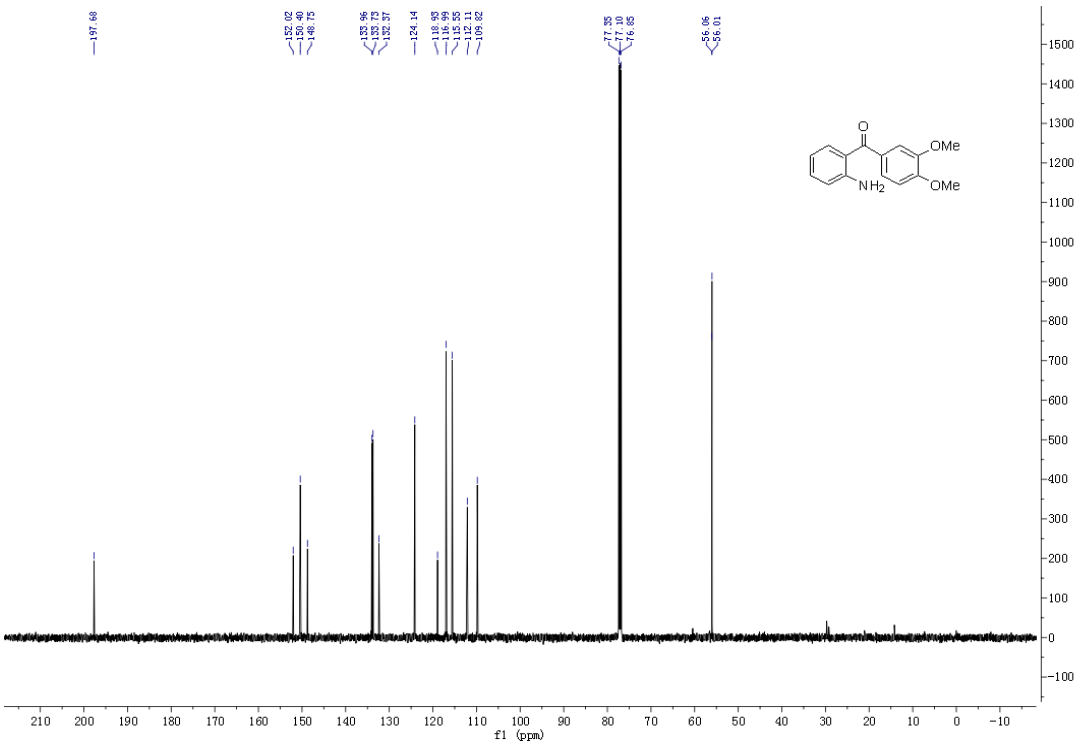
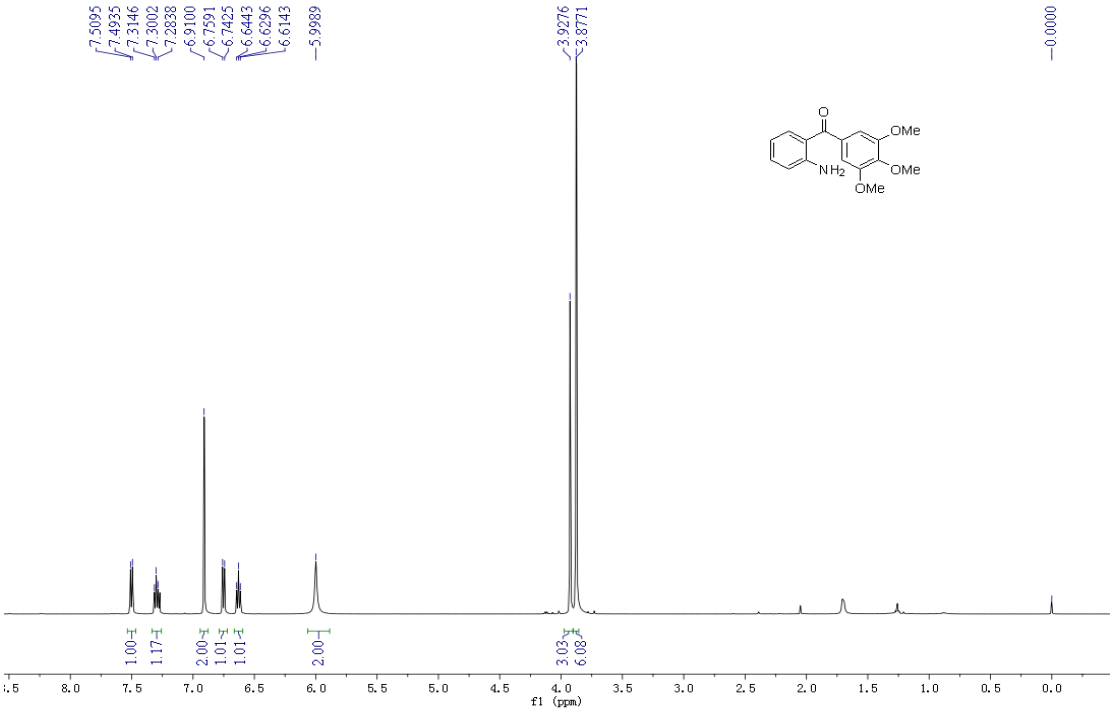
140.96
134.07
133.77
128.56
121.16
117.67
116.76
116.48
115.03
113.31
76.78
76.53
76.27
54.92
O
OMe
NH2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
OMe
NH2
f1 (ppm)


OMe
OMe
NH2
f1 (ppm)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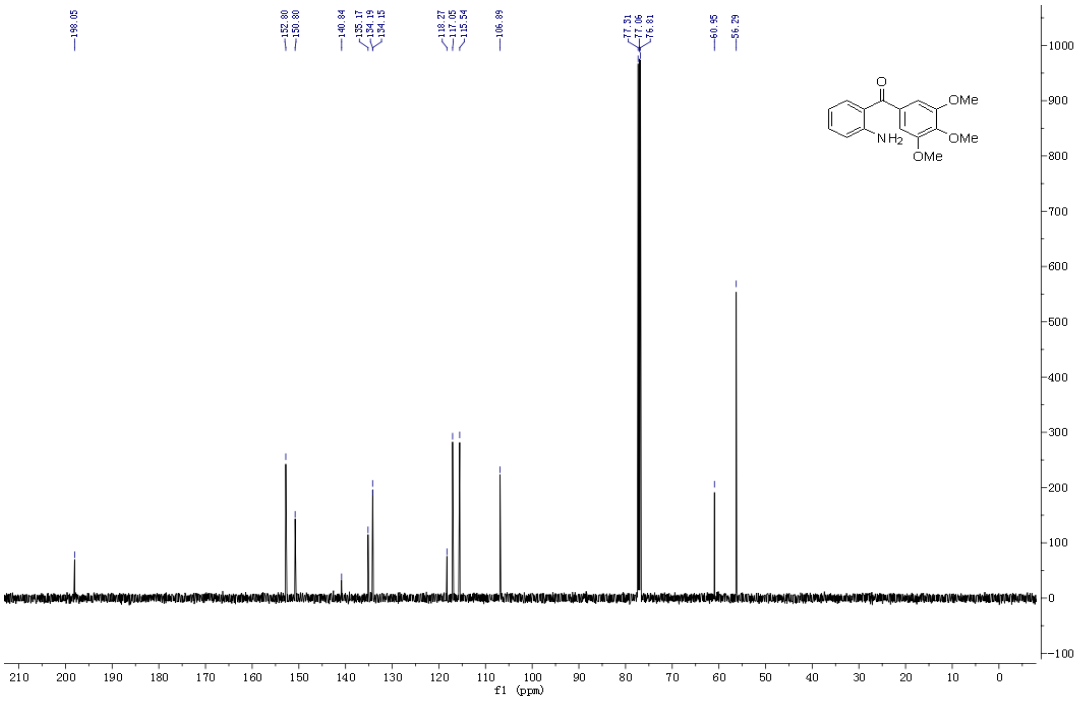
7.3146
7.3002
7.2838
6.9100
6.7591
6.7425
6.6443
6.6296
6.6143
5.9989
3.9276
3.8771
0.0000
1.00
1.17
2.00
1.01
1.01
2.00
3.03
6.08
f1 (ppm)
O
NH2
OMe
OMe
OMe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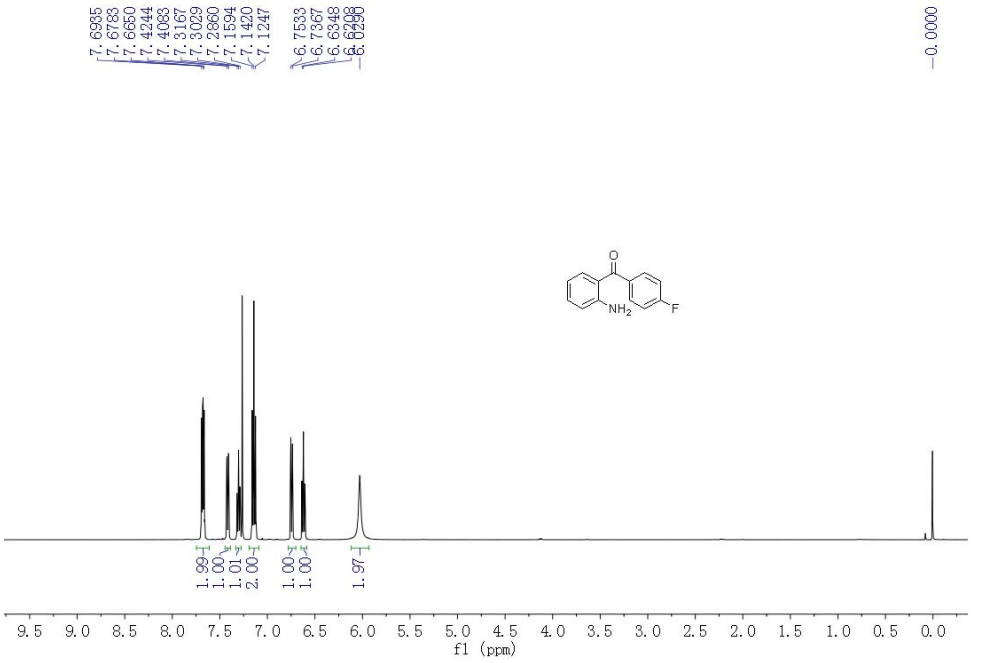
150.80
140.84
135.17
134.19
134.15
118.27
117.05
115.54
106.89
77.31
77.06
76.81
60.95
56.29
f1 (ppm)
O
NH2
OMe
OMe
OMe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7.3029
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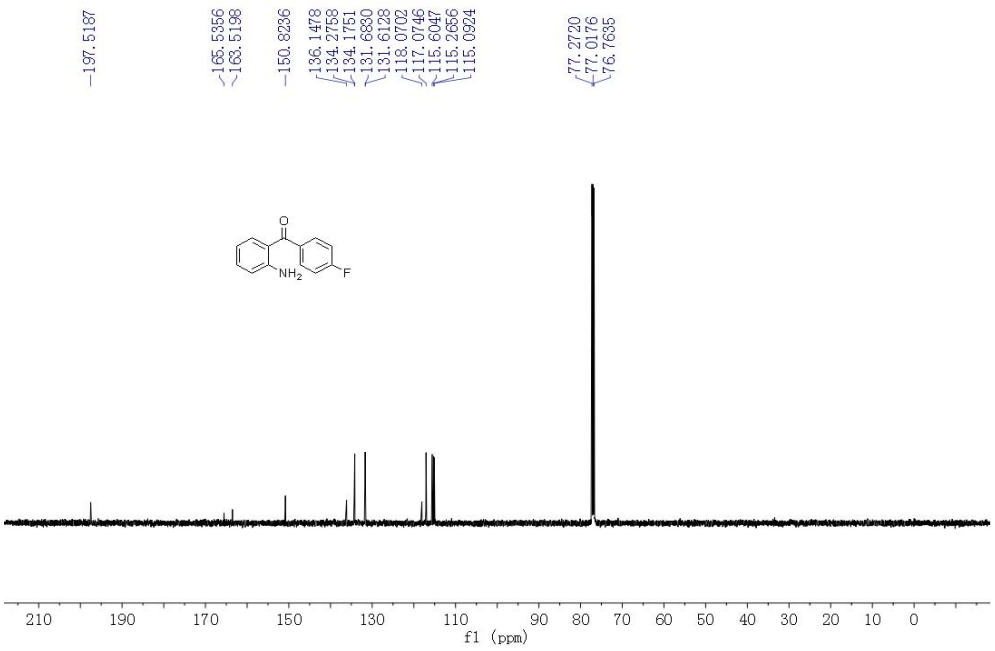
7.1594
7.1420
7.1247
6.7533
6.7367
6.6348
6.6208
6.6090
0.0000
O
NH2
F
1.99
1.00
1.01
2.00
1.00
1.00
1.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.6128
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115.6047
115.2656
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77.0176
76.7635
O
NH2
F
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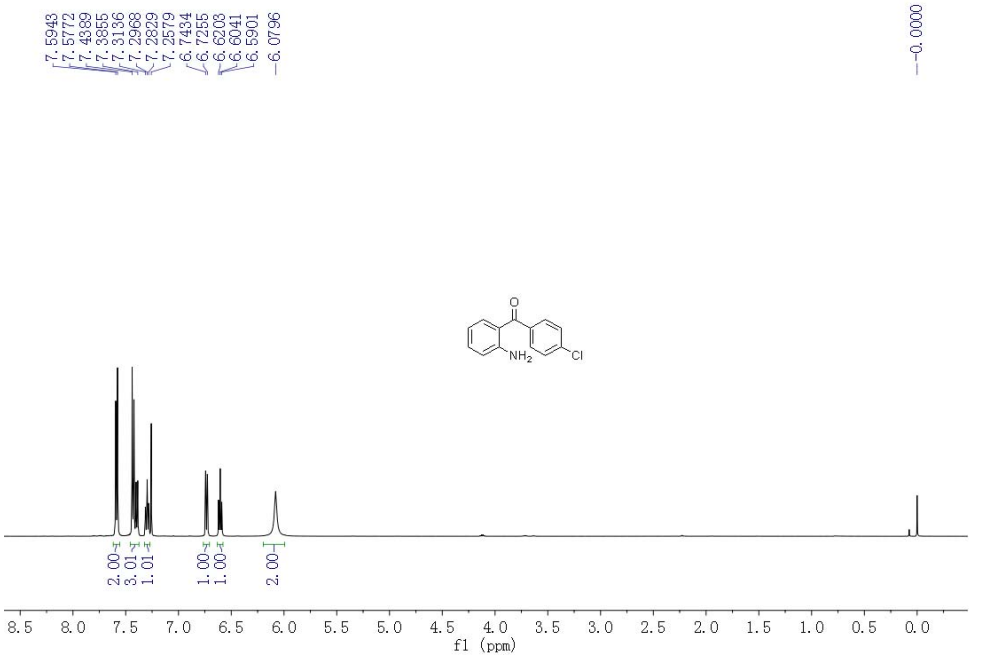
f1 (ppm)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7.3136
7.2968
7.2829
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6.7434
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6.6203
6.6041
6.5901
6.0796
0.0000
O
NH2
Cl
2.00
3.01
1.01
1.00
1.00
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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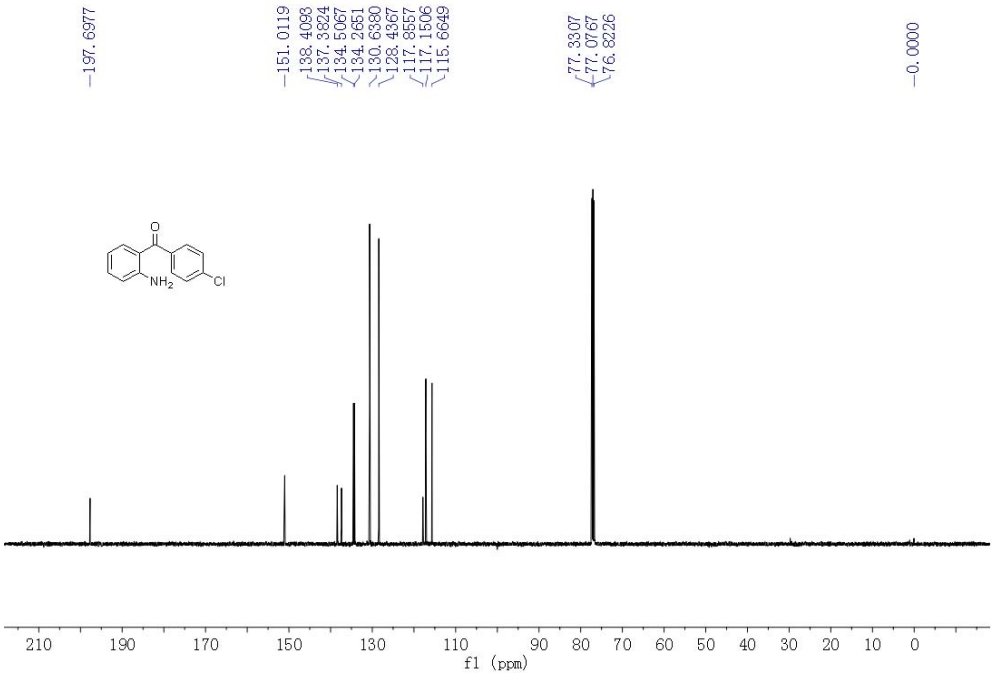
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76.8226
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NH2
Cl
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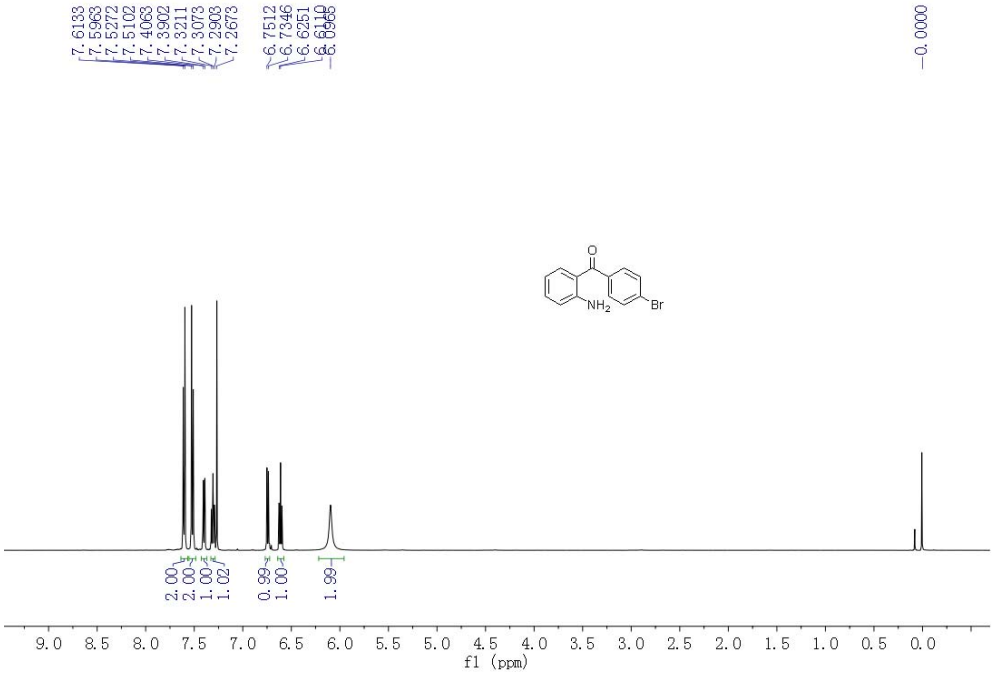
f1 (ppm)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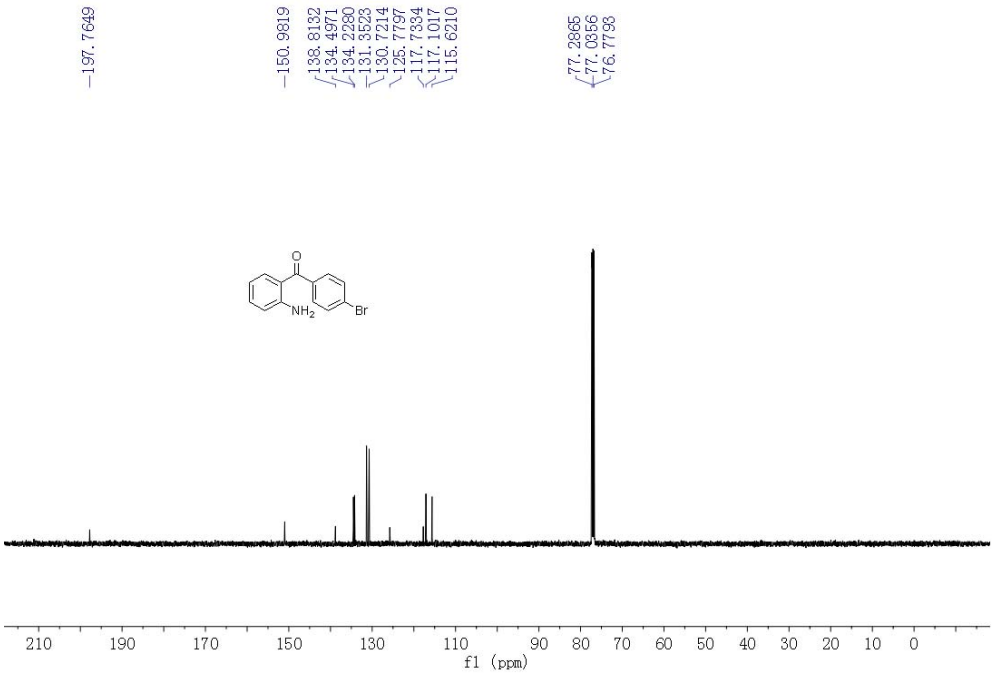
6.7512
6.7346
6.6251
6.6110
6.0968
0.0000
2.00
2.00
1.00
1.02
0.99
1.00
1.99
O
NH2
Br
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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117.1017
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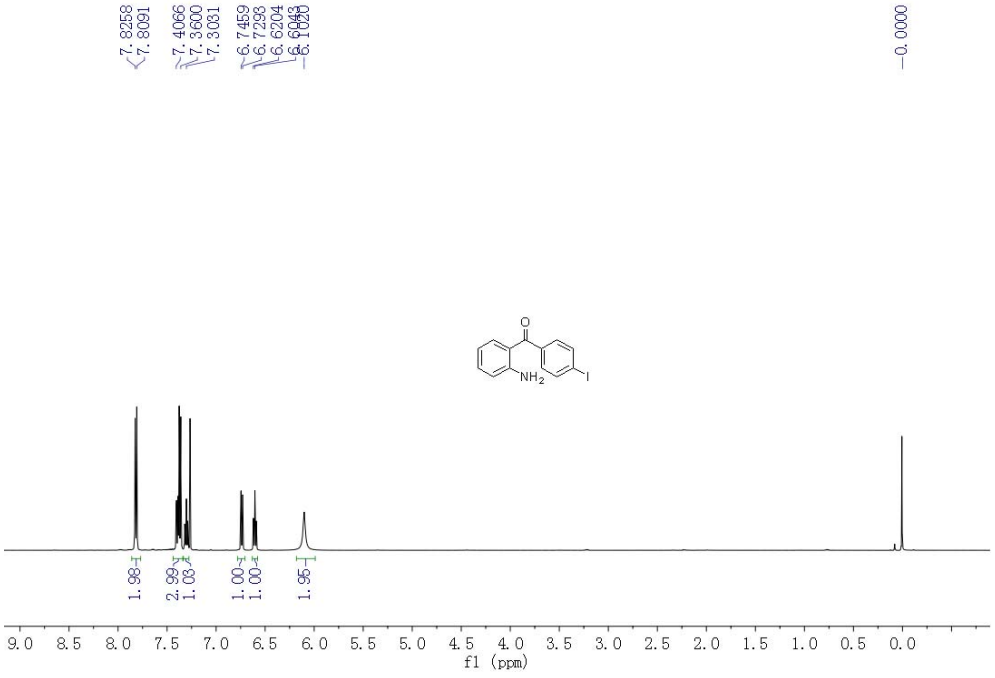
O
NH2
Br
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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6.7293
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1.00
1.00
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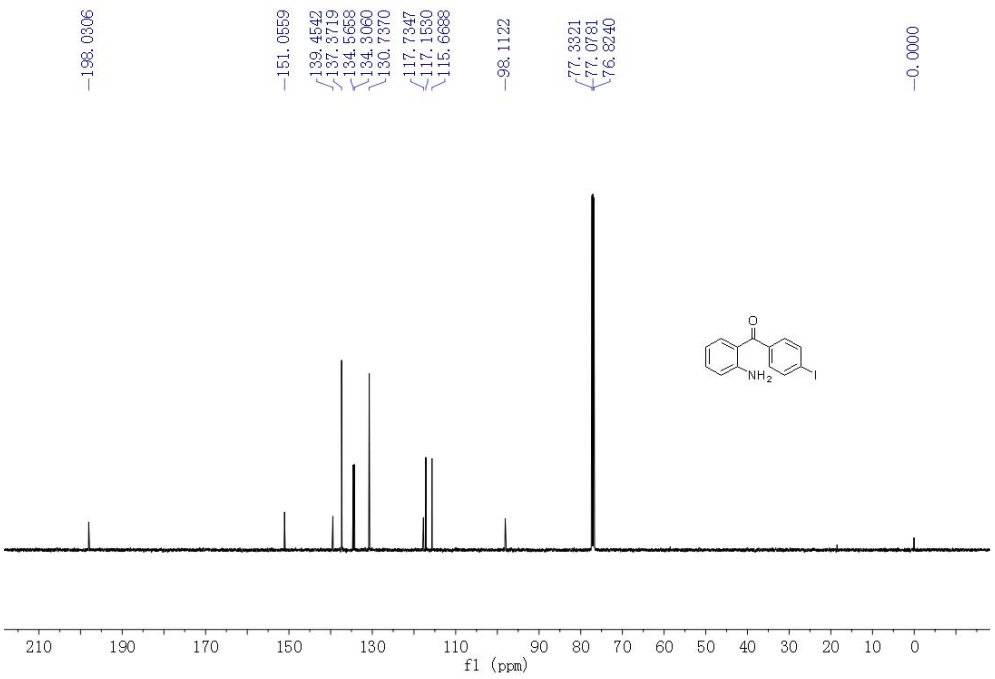
f1 (ppm)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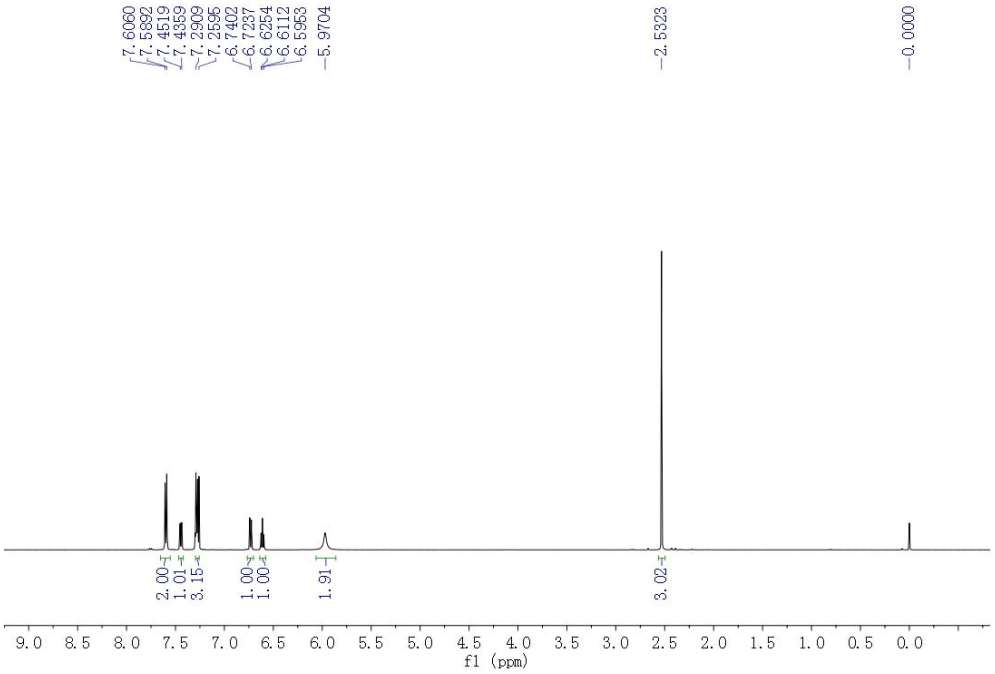
f1 (ppm)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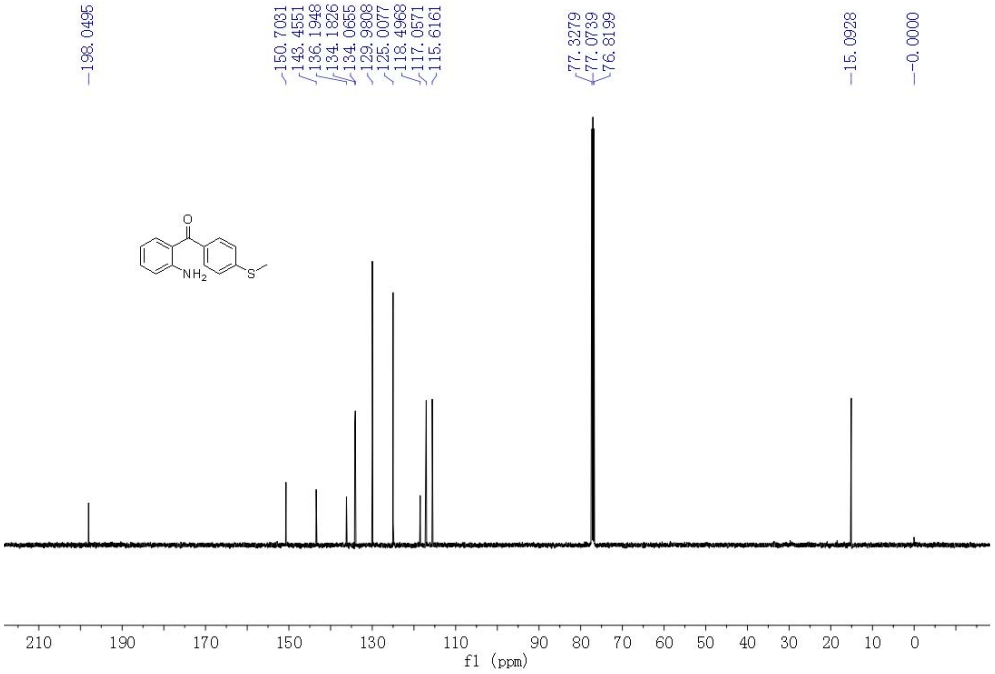
6.6254
6.6112
6.5963
5.9704
2.5323
0.0000
2.00
1.01
3.15
1.00
1.00
1.91
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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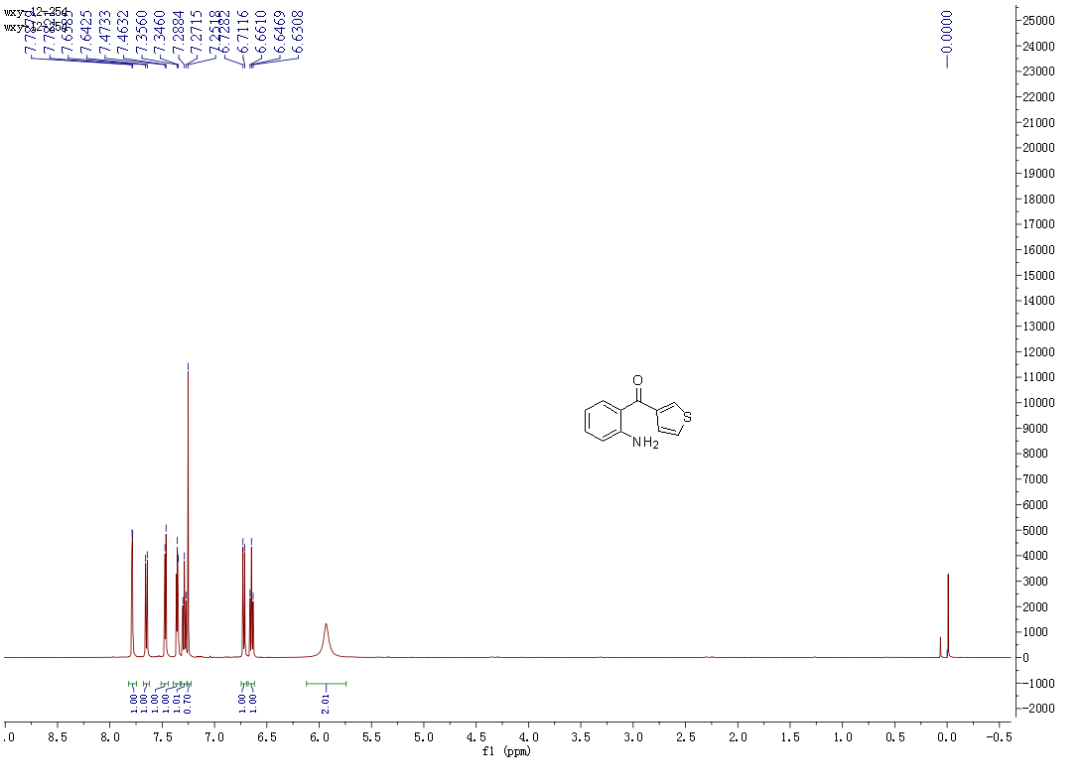
O
NH2
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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wxy-12-254
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7.2588
7.2282
6.7116
6.6610
6.6469
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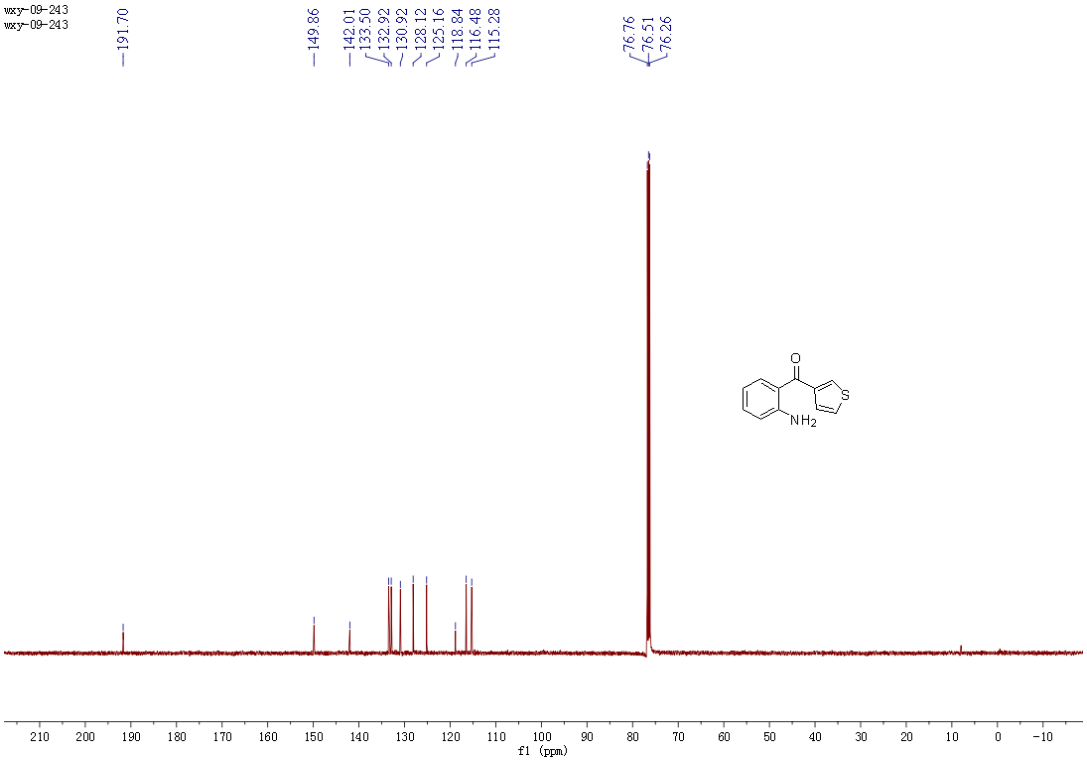
f1 (ppm)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wxy-09-243
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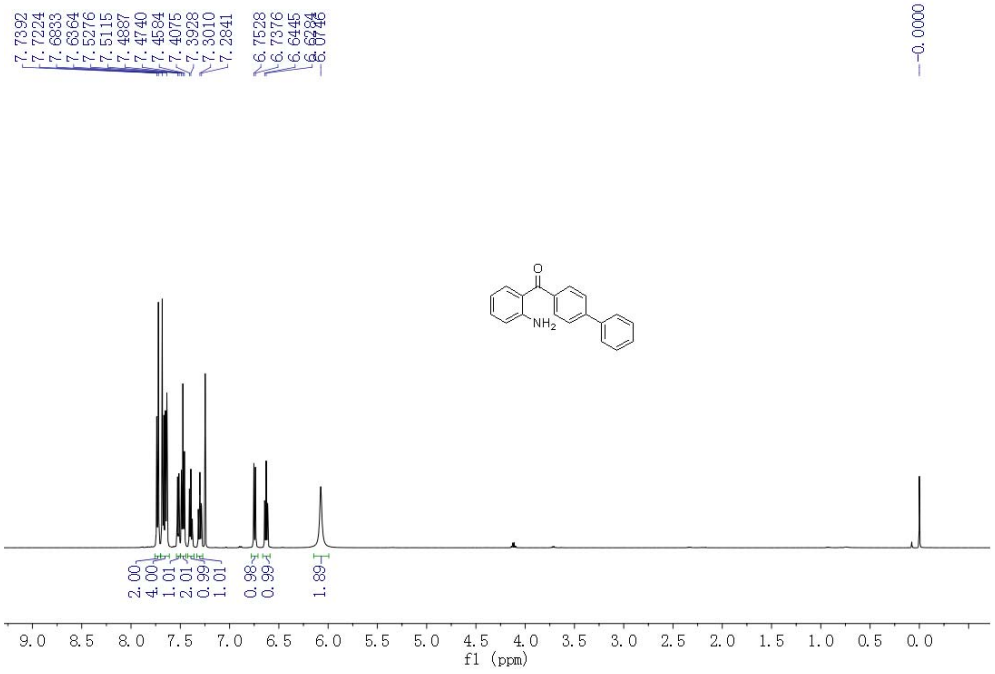
f1 (ppm)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7.3010
7.2841
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6.7376
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6.6284
6.6140
0.0000
2.00
4.00
1.01
2.01
0.99
1.01
0.98
0.99
1.89
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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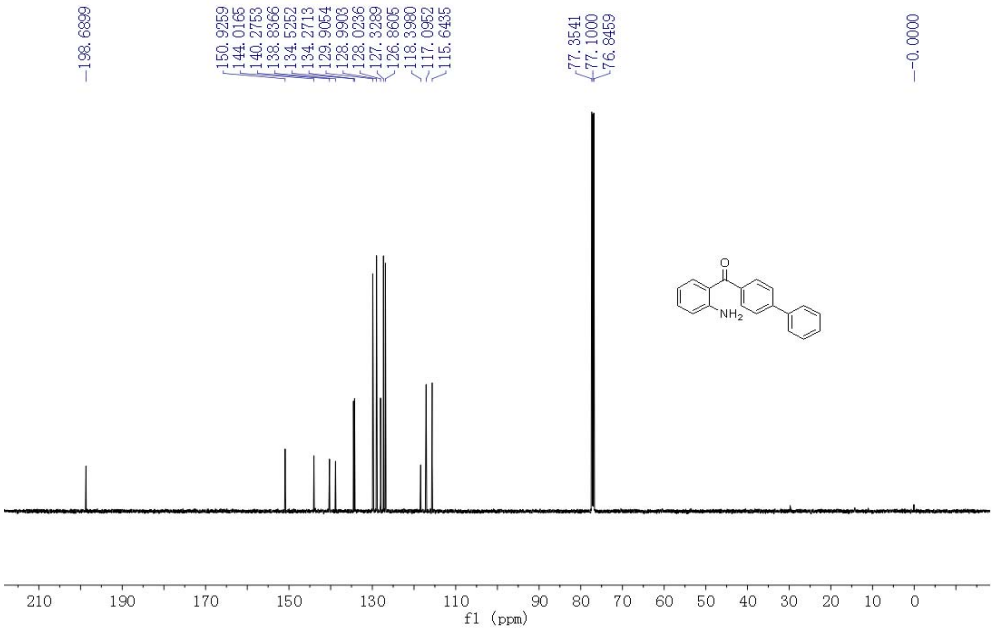
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126.8605
118.3980
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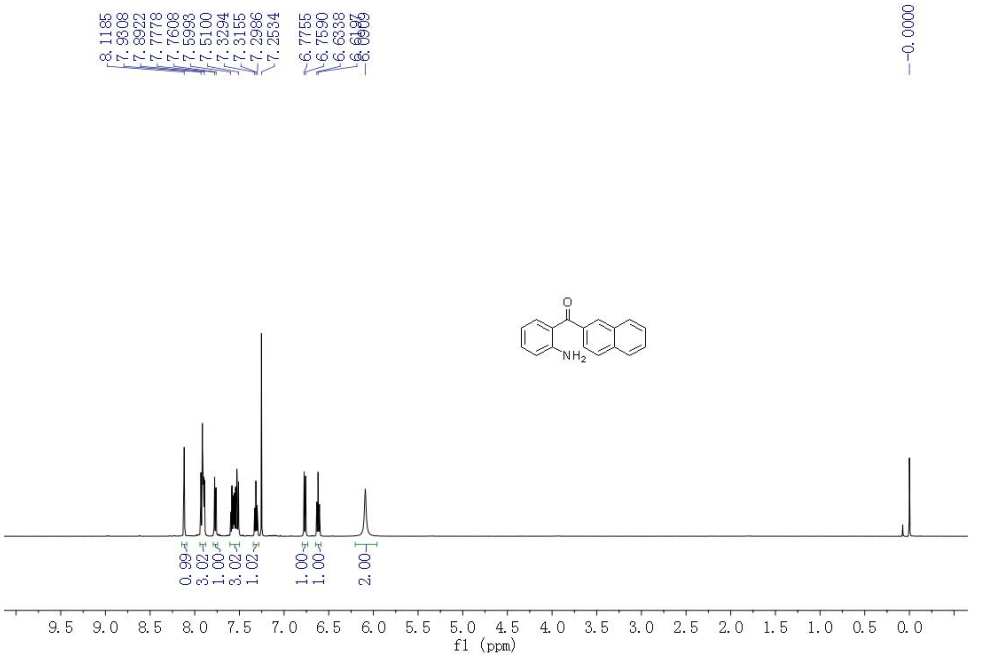
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2986
7.2634
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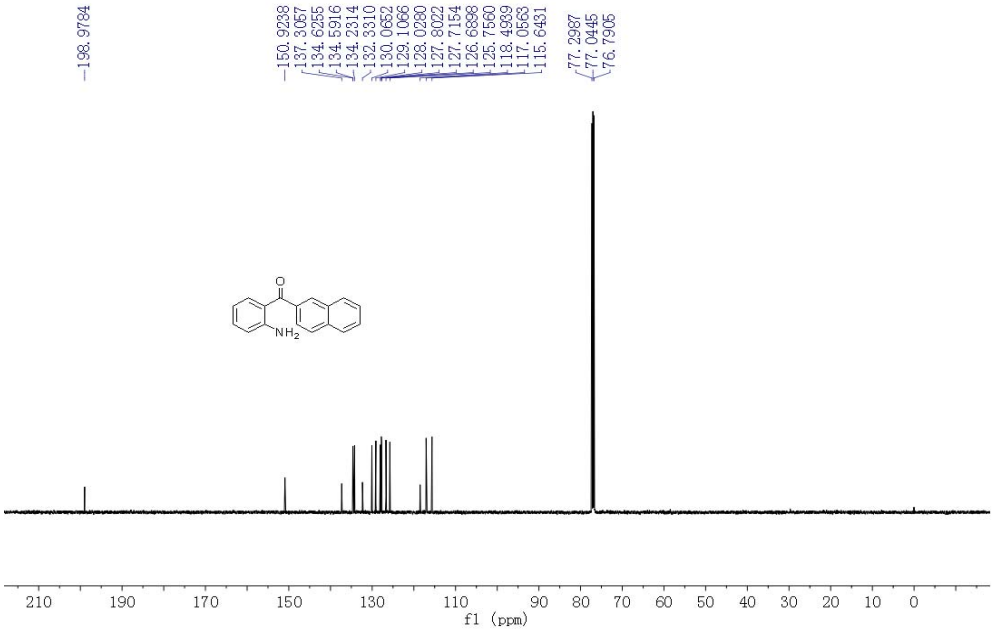
6.7590
6.6338
6.6087
0.0000
O
NH2
0.99
3.02
1.00
3.02
1.02
1.00
1.00
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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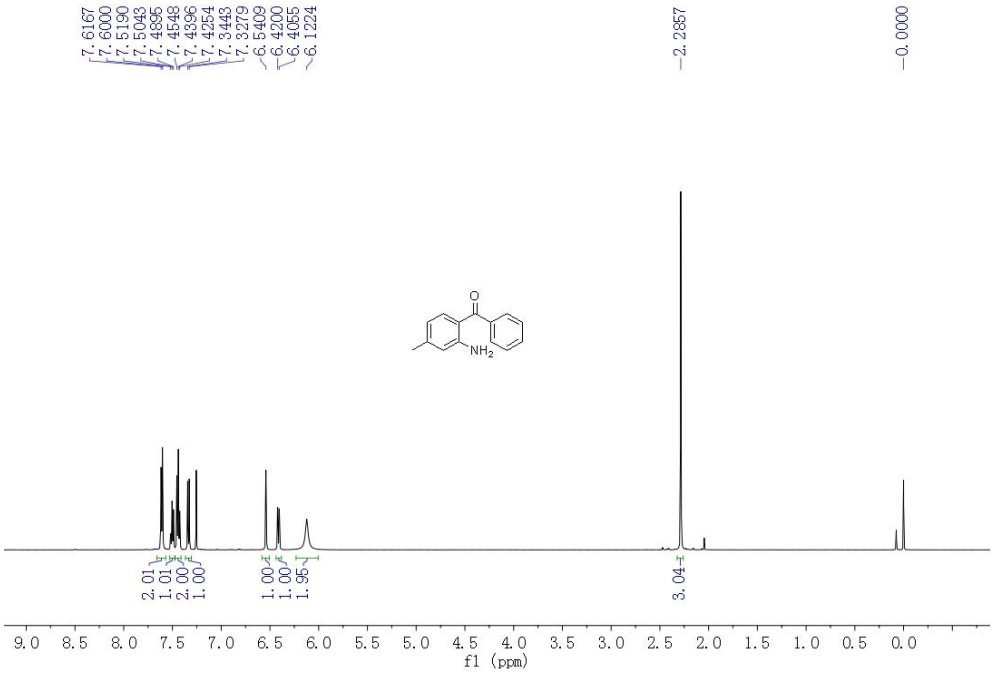
O
NH2
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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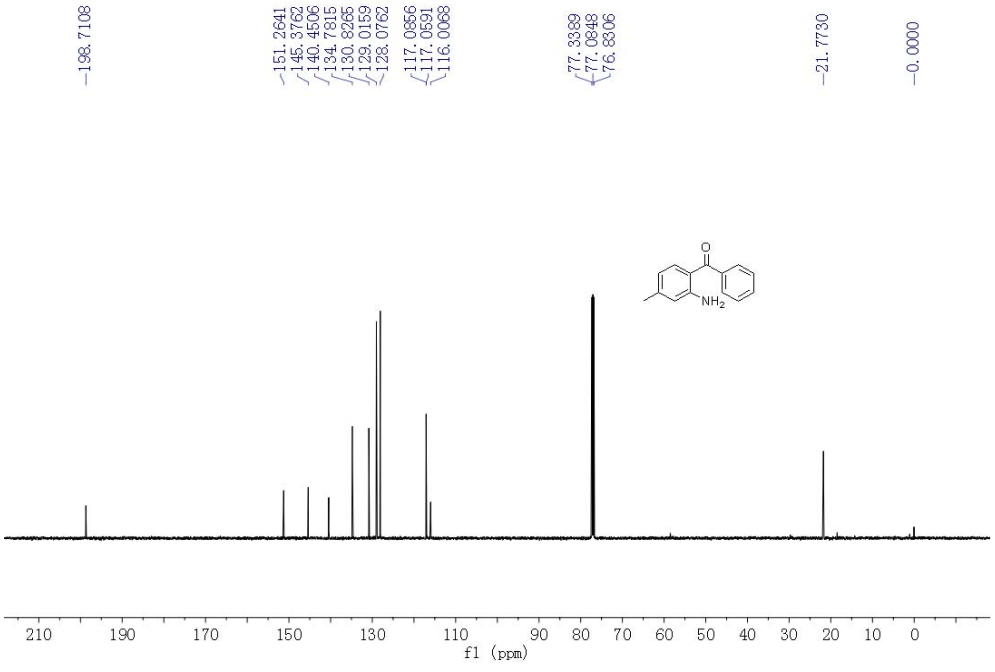
6.4065
6.1224
2.2857
0.0000
O
NH2
2.01
1.01
2.00
1.00
1.00
1.00
1.95
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.4506
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130.8265
129.0159
128.0762
117.0856
117.0591
116.0068
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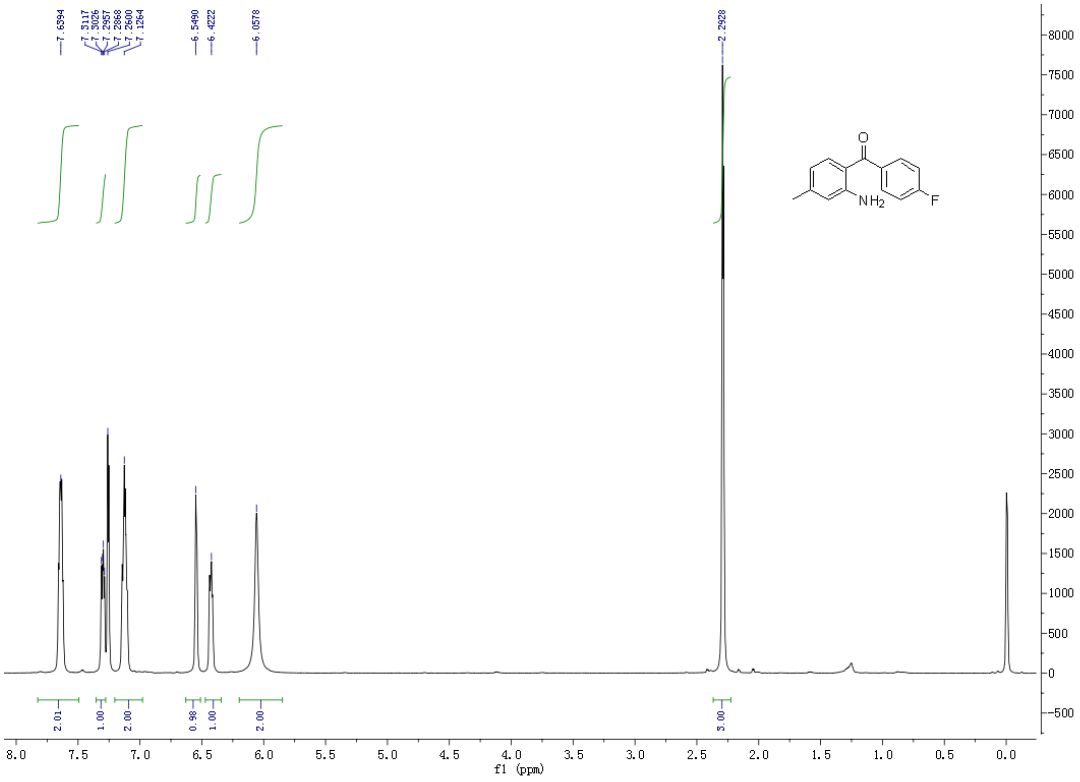
77.0848
76.8306
21.7730
0.0000
O
NH2
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.3026
7.2957
7.2868
7.2600
7.1844
6.5490
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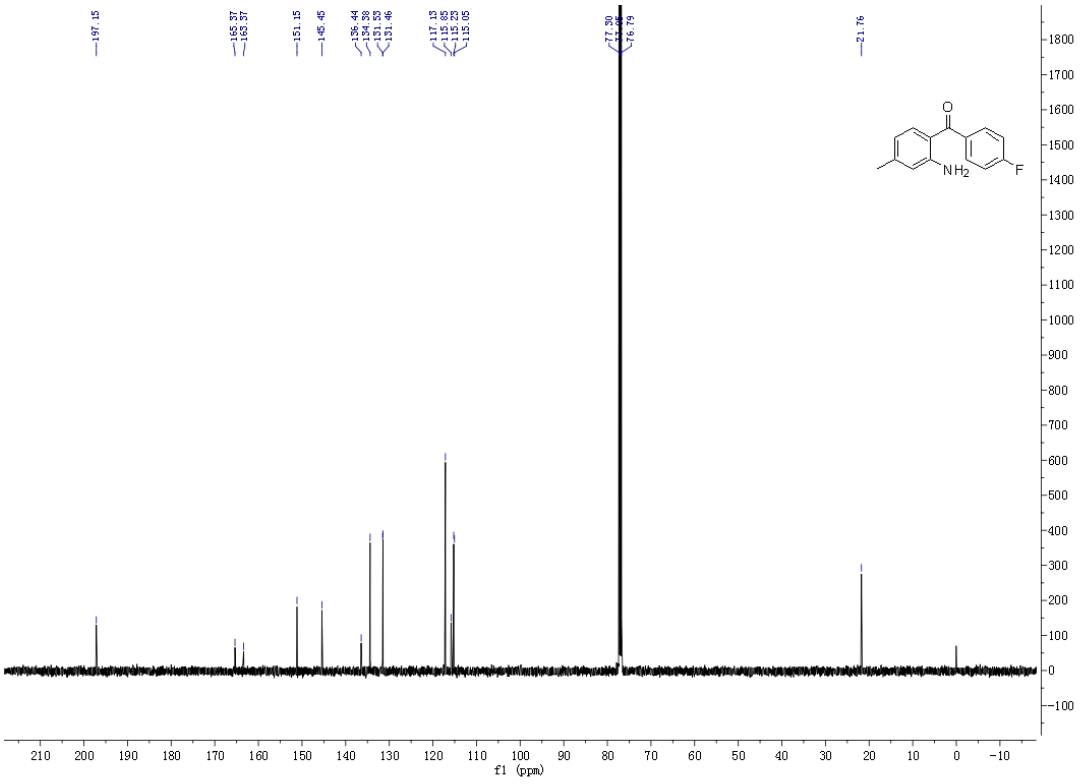
2.2928
2.01
1.00
2.00
0.98
1.00
2.00
3.00
f1 (ppm)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163.57
151.15
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136.44
134.58
131.53
131.46
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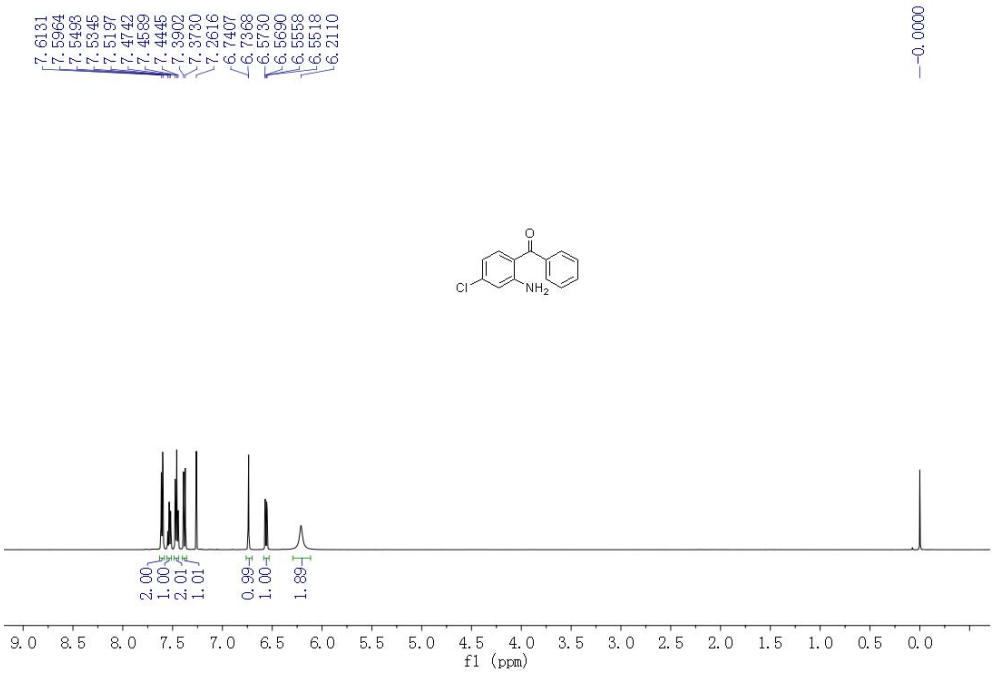
115.85
115.23
115.05
77.30
77.04
76.79
21.76
f1 (ppm)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7.5493
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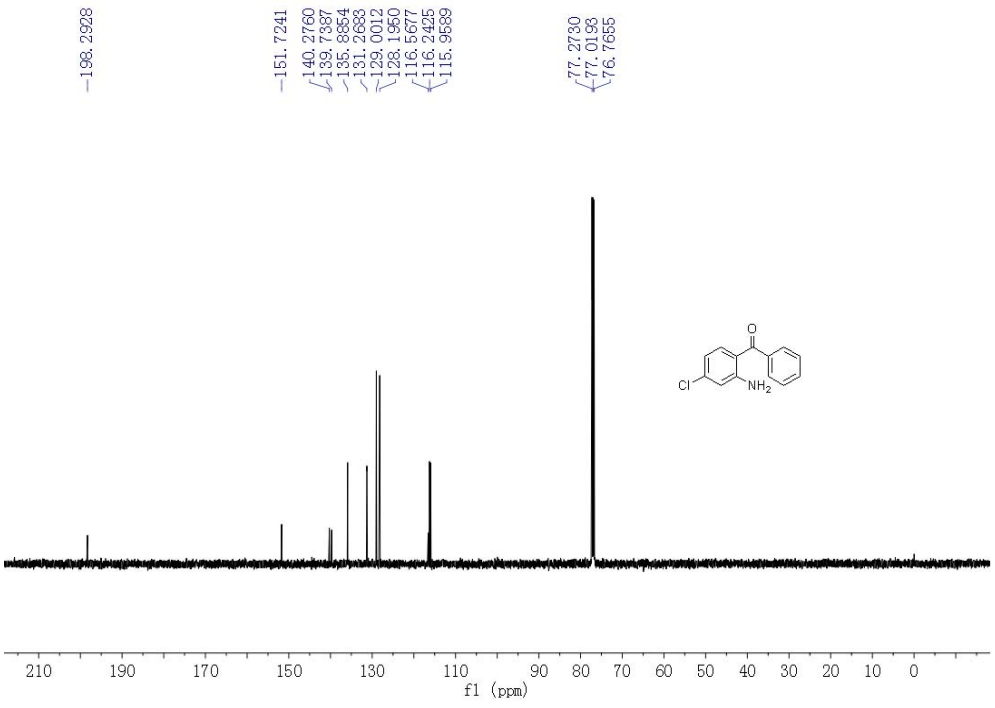
7.5197
7.4742
7.4589
7.4445
7.3902
7.3730
7.2616
6.7407
6.7368
6.5730
6.5690
6.5558
6.5518
6.2110
0.0000
Cl
NH2
2.00
1.00
2.01
1.01
0.99
1.00
1.89
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.2730
77.0193
76.7655
Cl
NH2
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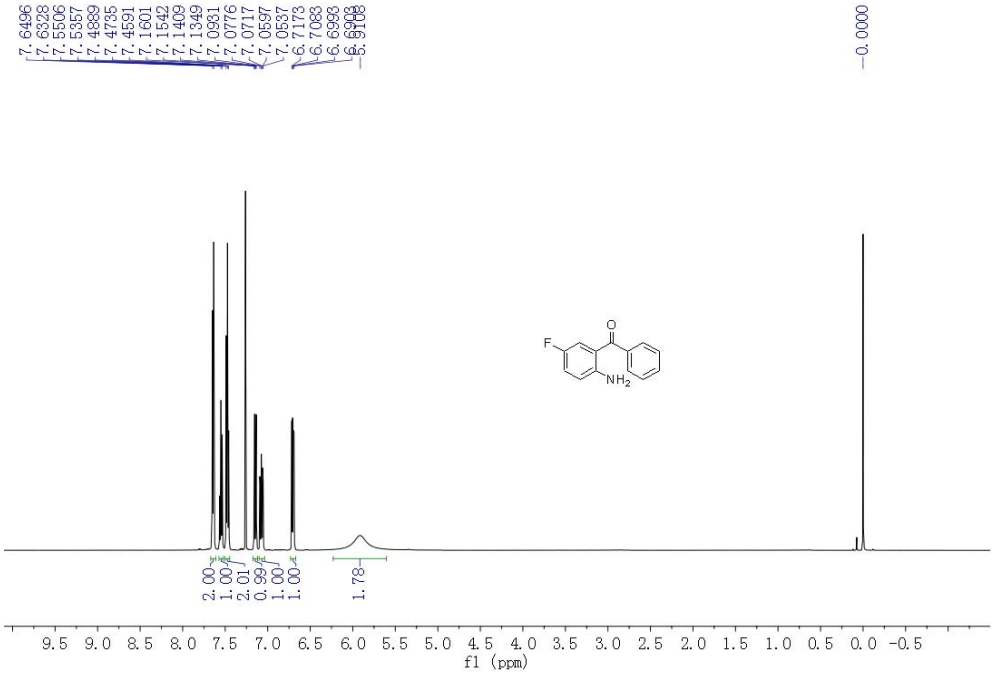
f1 (ppm)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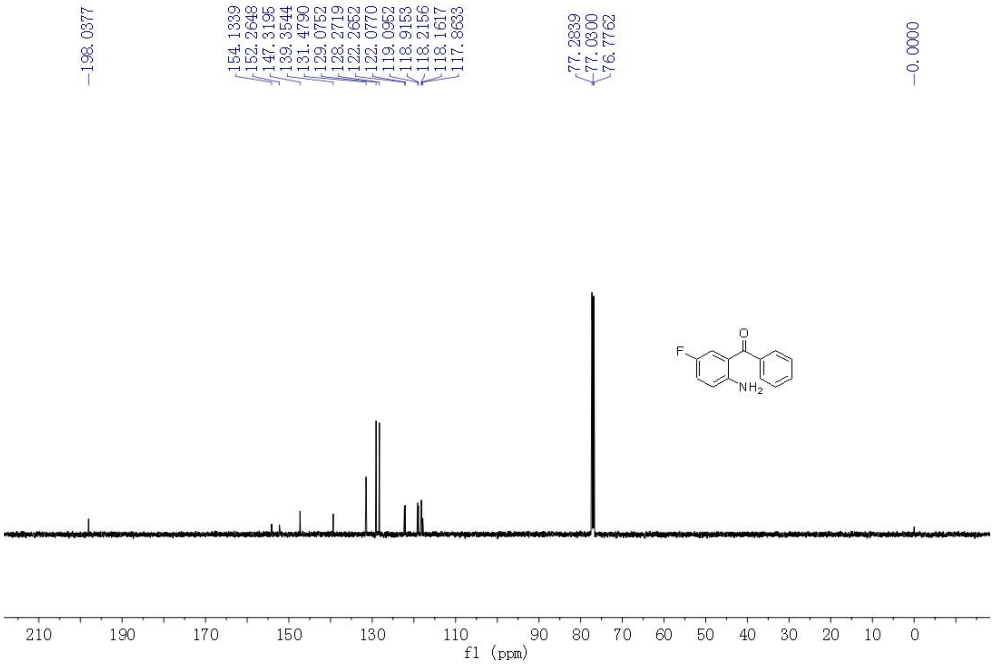
7.4735
7.4591
7.1601
7.1542
7.1409
7.1349
7.0931
7.0776
7.0717
7.0597
7.0537
6.7173
6.7083
6.6993
6.6903
0.0000
2.00
1.00
2.01
0.99
1.00
1.00
1.78
F
O
NH2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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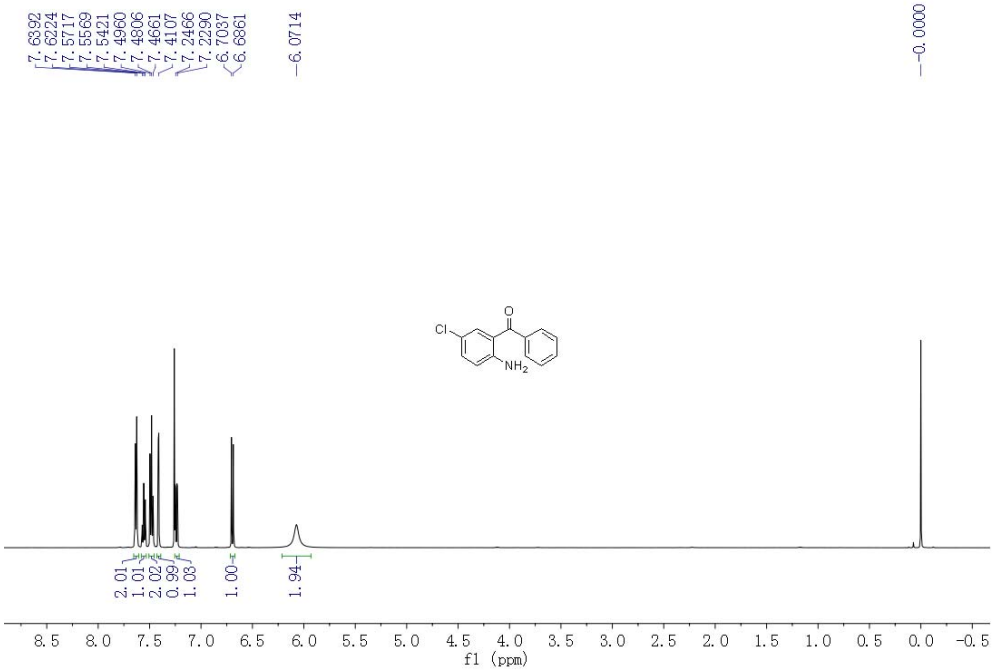
128.2719
122.2652
122.0770
119.0952
118.9153
118.2156
118.1617
117.8633
77.2839
77.0300
76.7762
0.0000
F
O
NH2
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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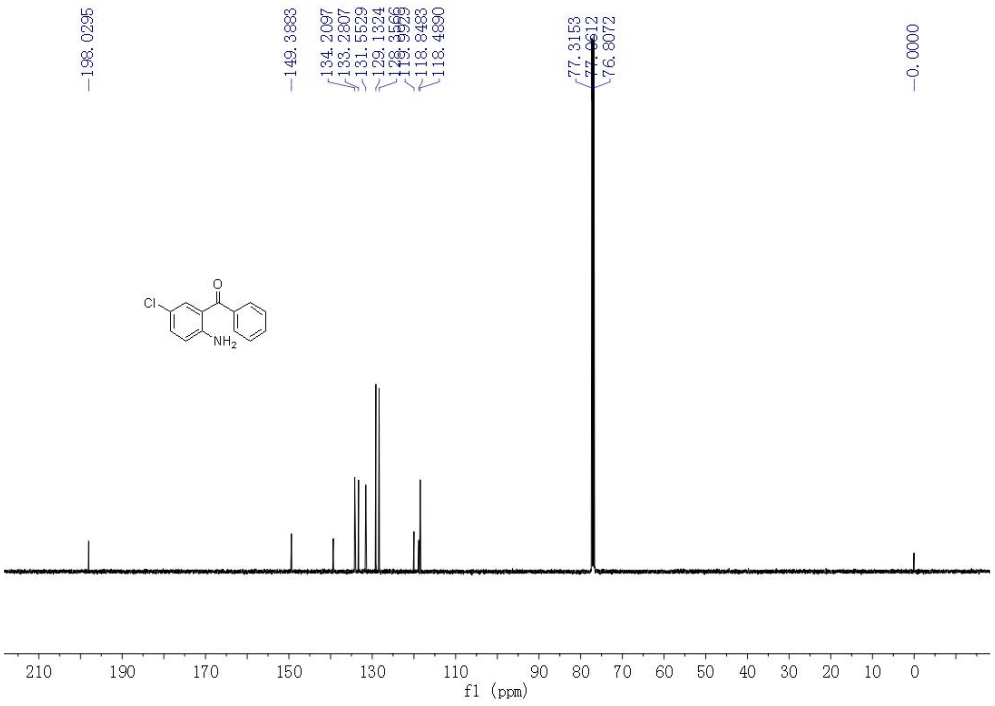
7.5717
7.5569
7.5421
7.4960
7.4806
7.4661
7.4107
7.2466
7.2290
6.7037
6.6861
6.0714
0.0000
Cl
O
NH2
2.01
1.01
2.02
0.99
1.03
1.00
1.94
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.1324
118.8483
118.4890
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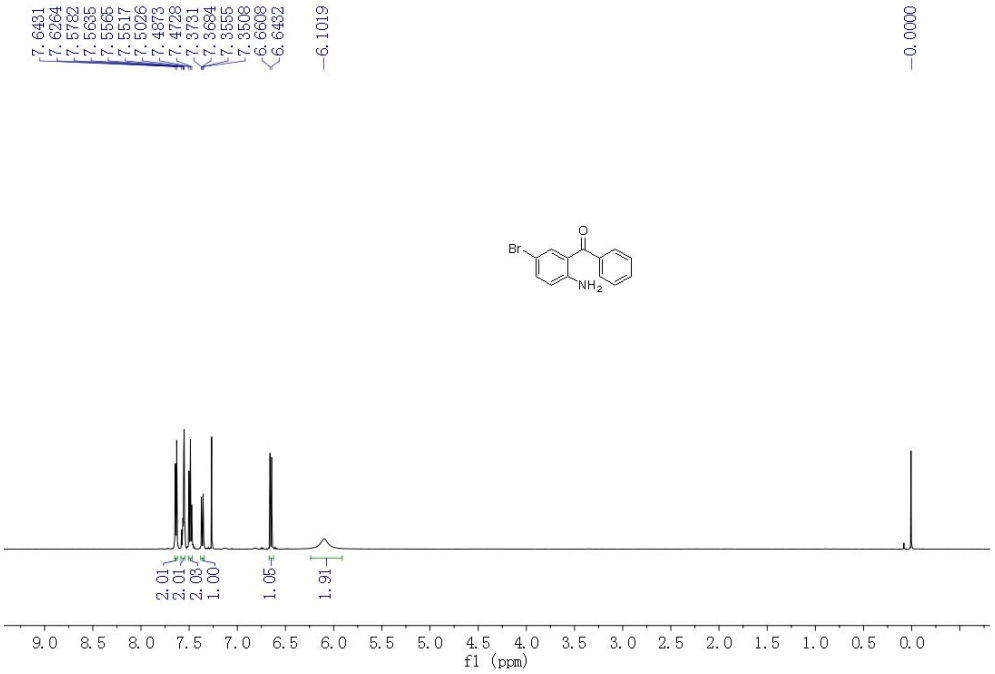
76.8072
0.0000
Cl
O
NH2
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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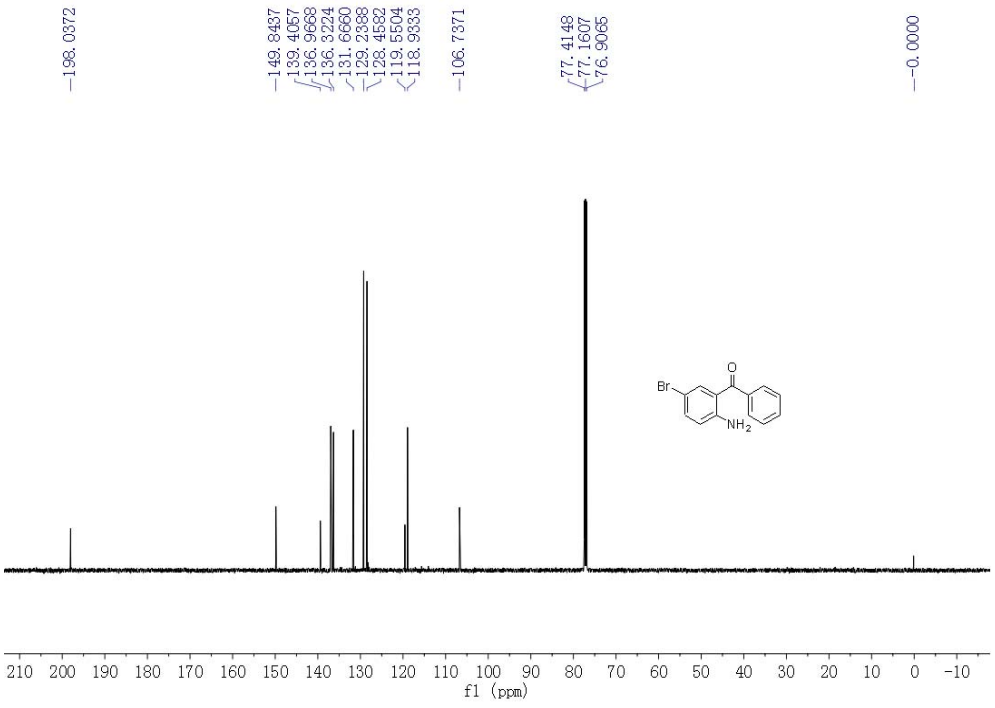
7.6264
7.5782
7.5635
7.5565
7.5517
7.5026
7.4873
7.4728
7.3731
7.3684
7.3555
7.3508
6.6608
6.6432
6.1019
0.0000
Br
O
NH2
2.01
2.01
2.03
1.00
1.05
1.91
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.3224
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129.2388
128.4582
119.5504
118.9333
106.7371
77.4148
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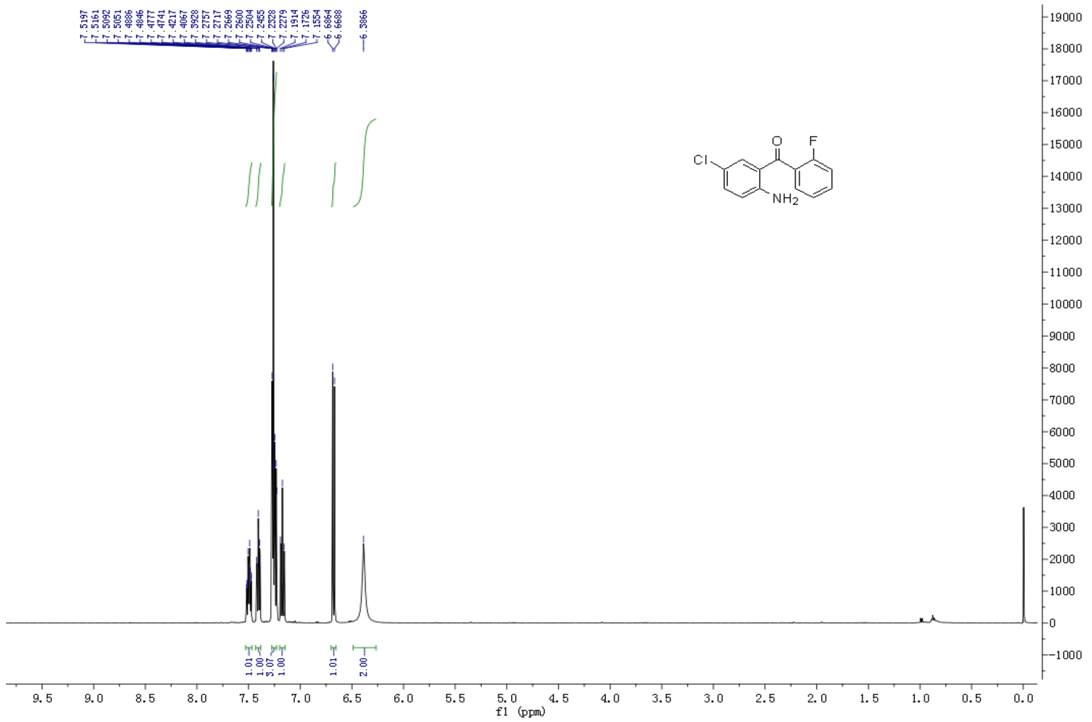
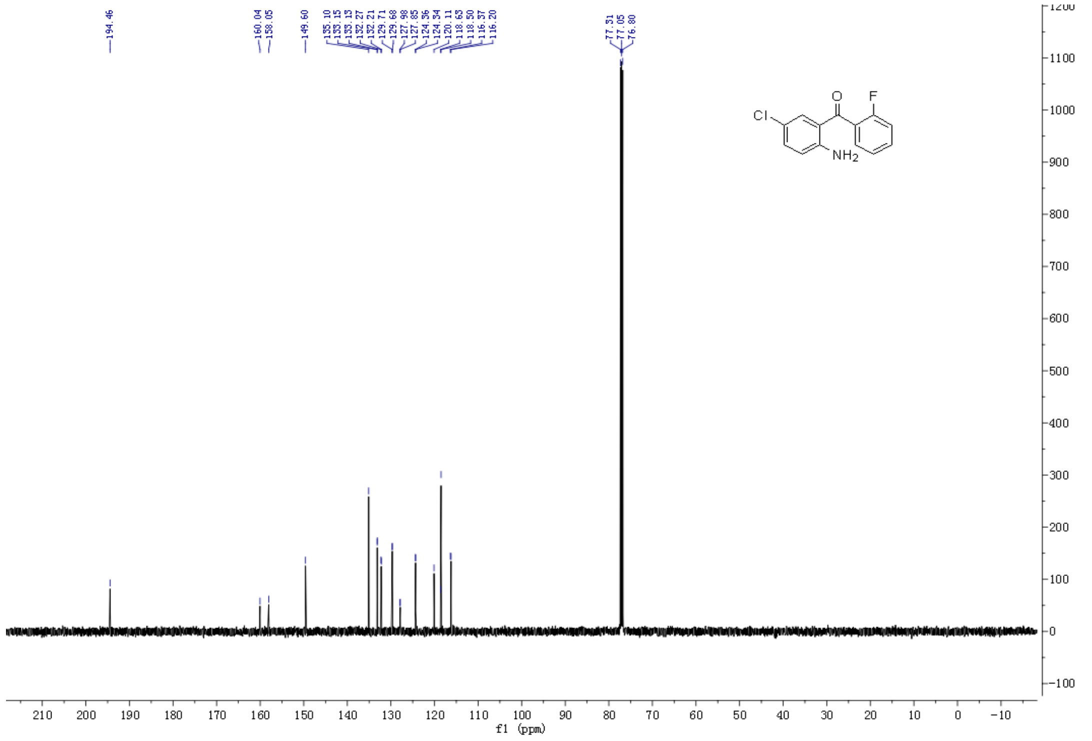
76.9065
0.0000
Br
O
NH2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Cl
O
F
NH2
f1 (ppm)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160.04
158.05
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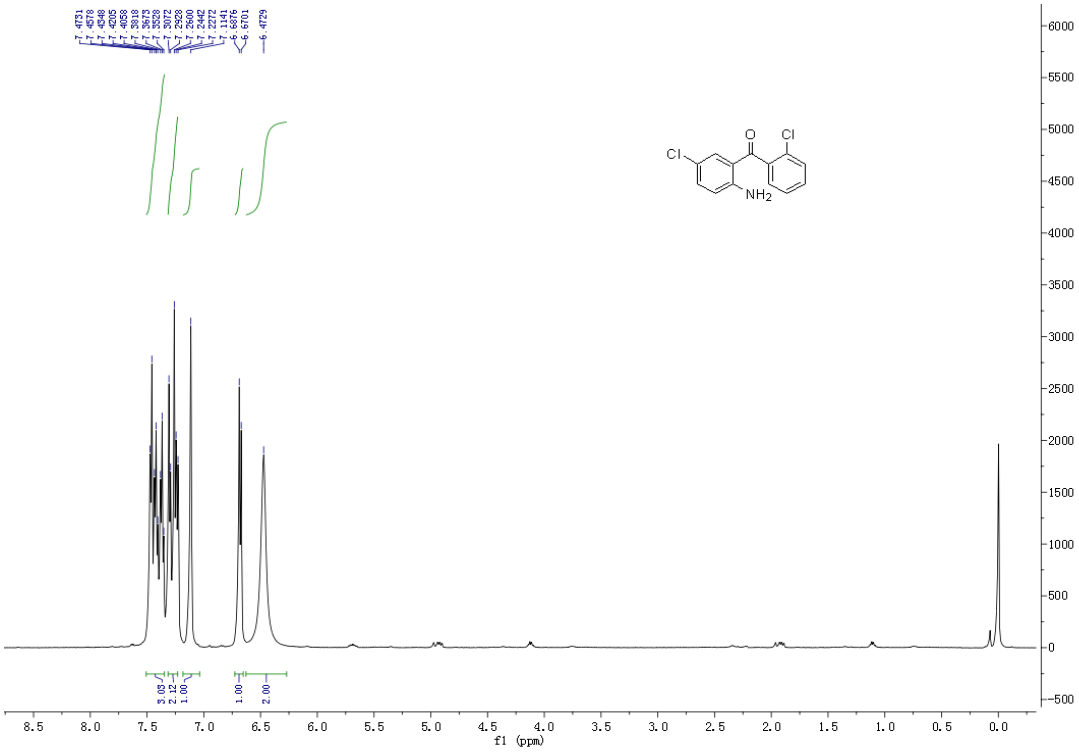
77.31
77.05
76.80
Cl
O
F
NH2
f1 (ppm)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7.4546
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7.4058
7.3918
7.3673
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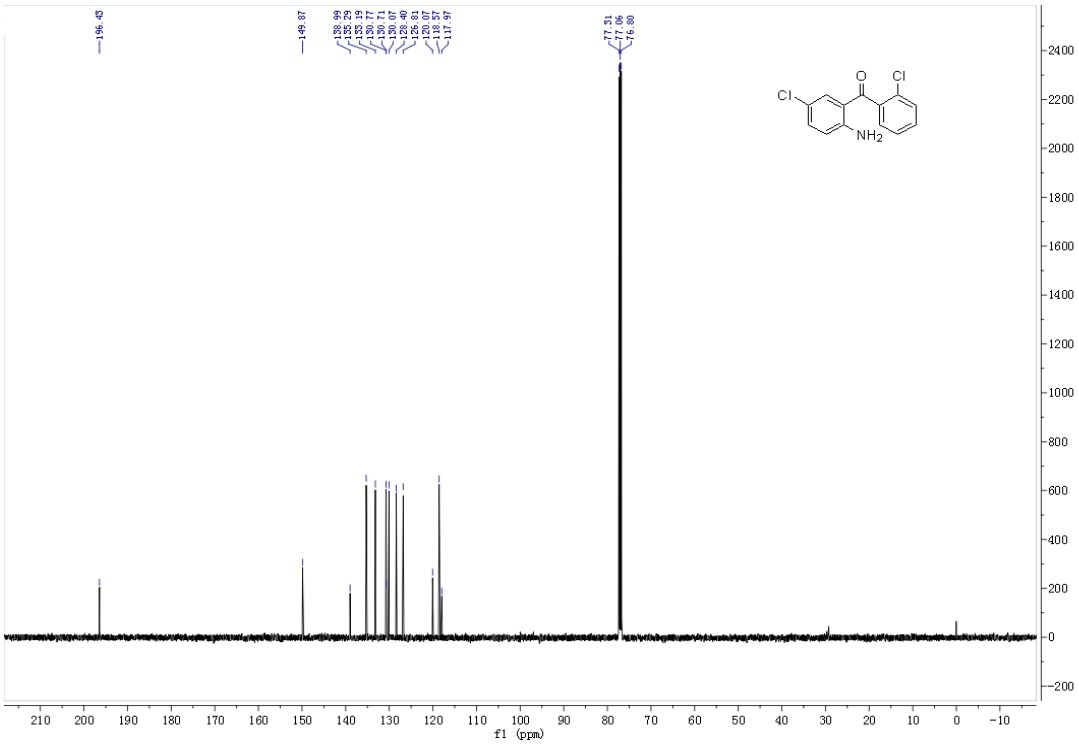
7.3072
7.2928
7.2600
7.2442
7.2272
7.1441
6.6876
6.6701
6.4729
O
Cl
Cl
NH2
3.05
2.12
1.00
1.00
2.00
f1 (ppm)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138.99
135.29
133.19
130.77
130.71
130.07
128.40
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120.07
118.57
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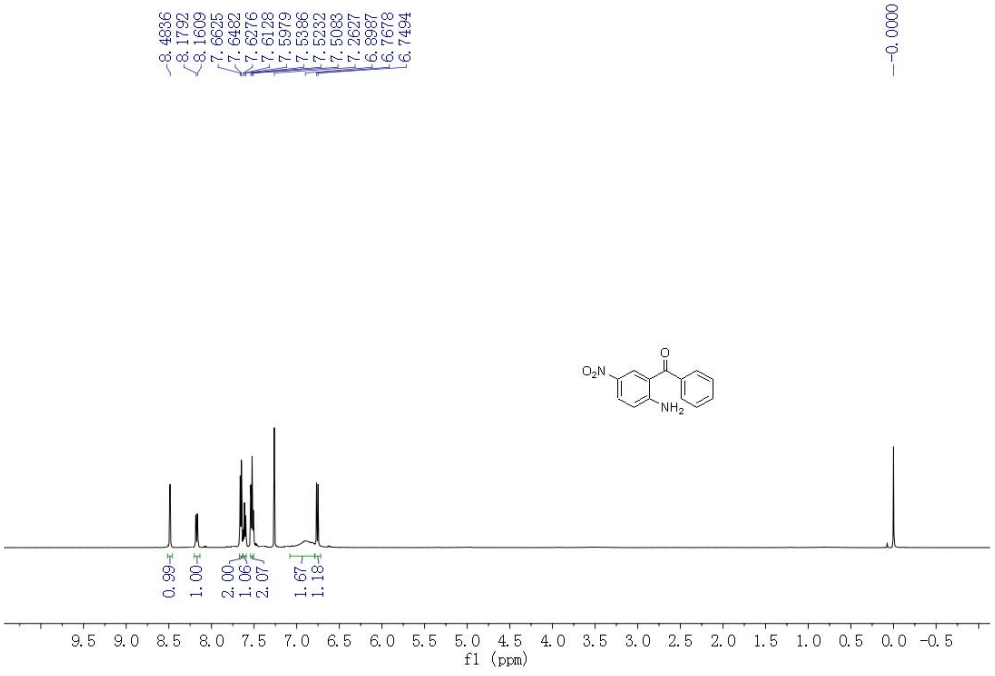
77.06
76.80
O
Cl
Cl
NH2
f1 (ppm)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8.1609
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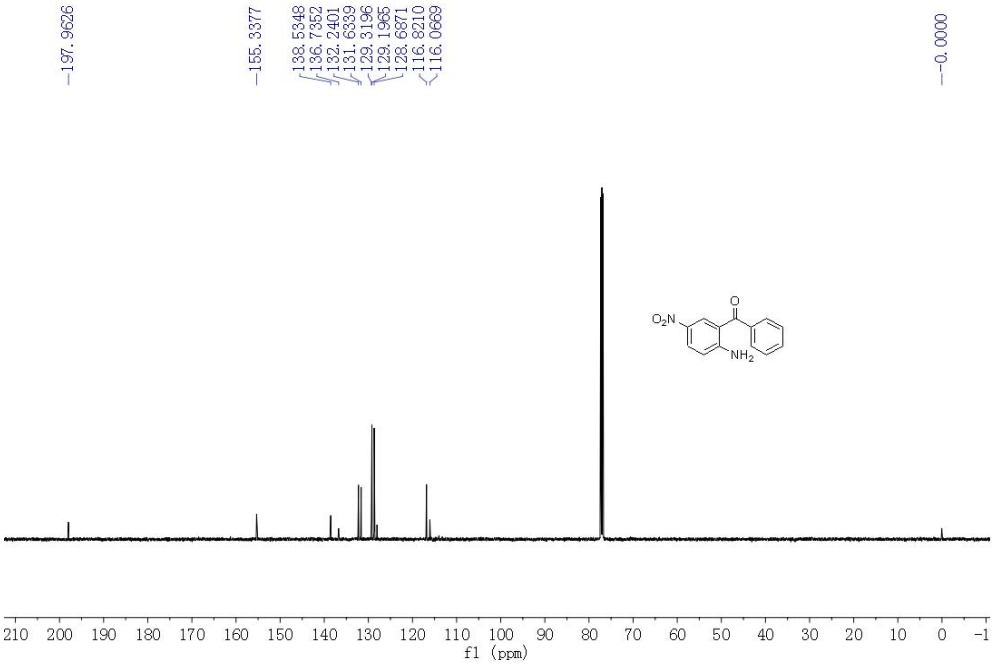
7.6482
7.6276
7.6128
7.5979
7.5386
7.5232
7.5083
7.2627
6.8987
6.7678
6.7494
0.0000
O2N
O
NH2
0.99
1.00
2.00
1.06
2.07
1.67
1.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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132.2401
131.6339
129.3196
129.1965
128.6871
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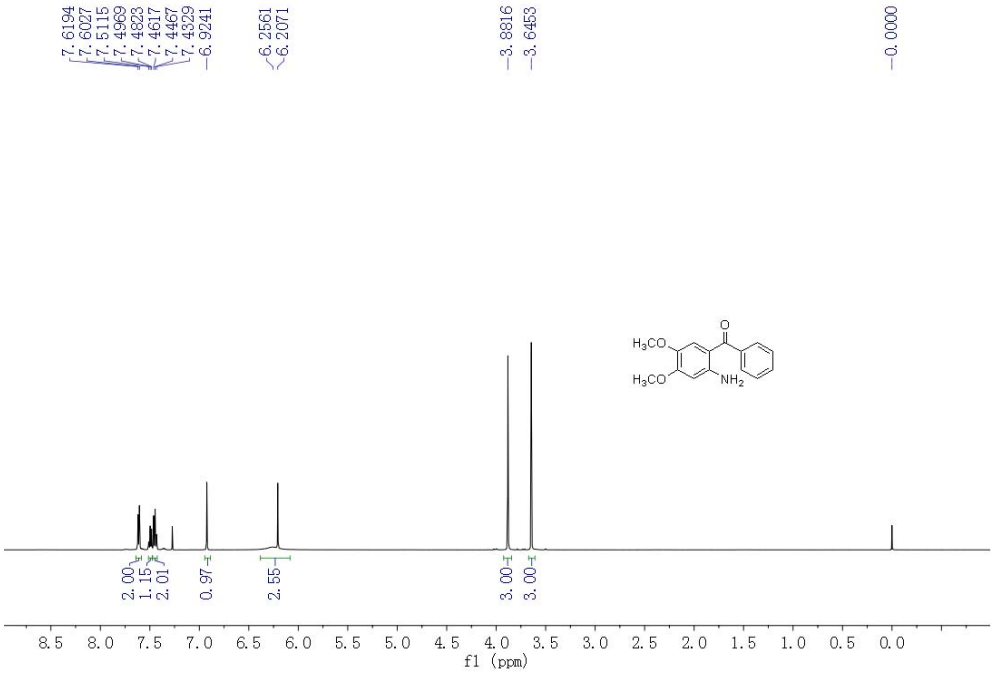
0.0000
O2N
O
NH2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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7.4823
7.4617
7.4467
7.4329
6.9241
6.2561
6.2071
3.8816
3.6453
0.0000
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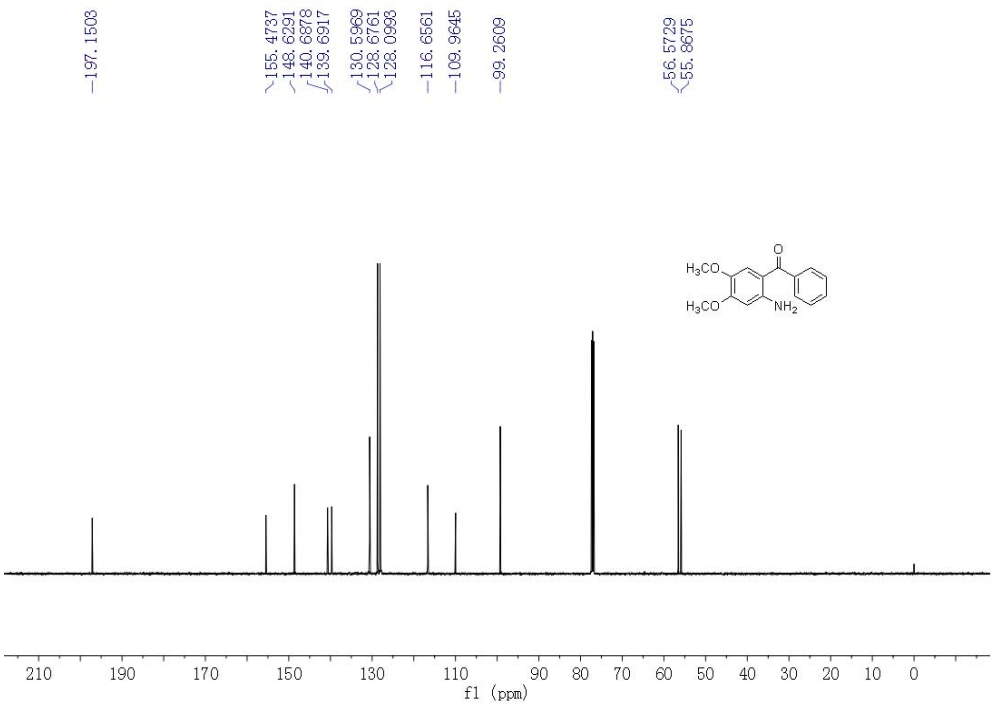
H3CO
O
NH2
2.00
1.15
2.01
0.97
2.55
3.00
3.00
f1 (ppm)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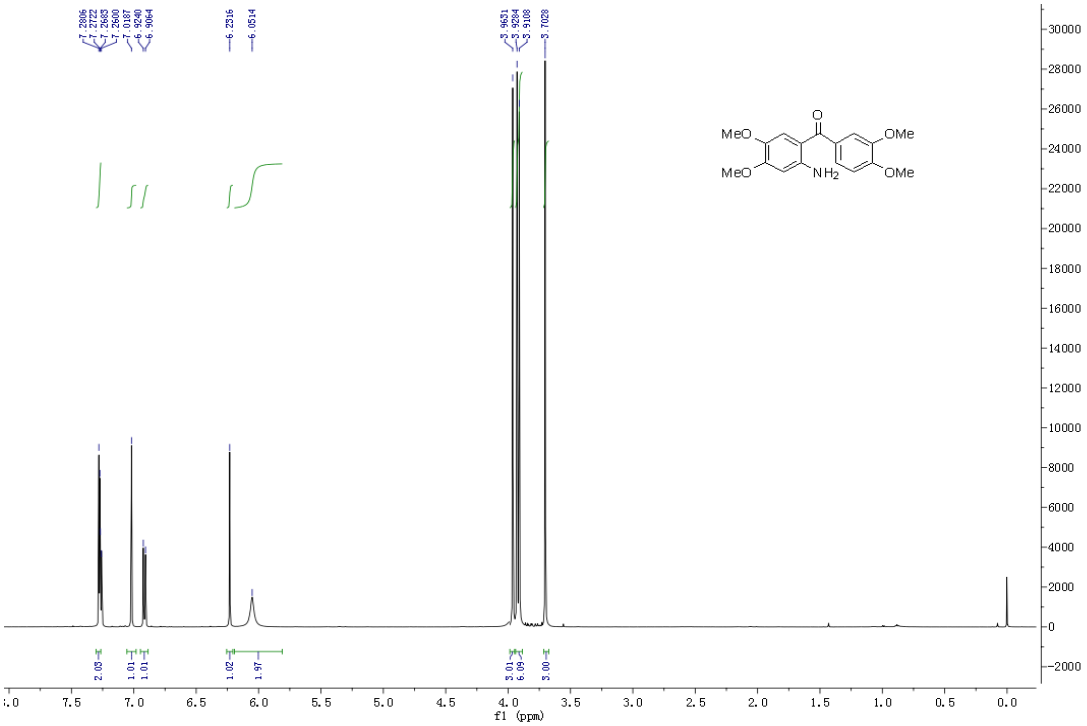
55.8675
H3CO
H3CO
O
NH2
f1 (ppm)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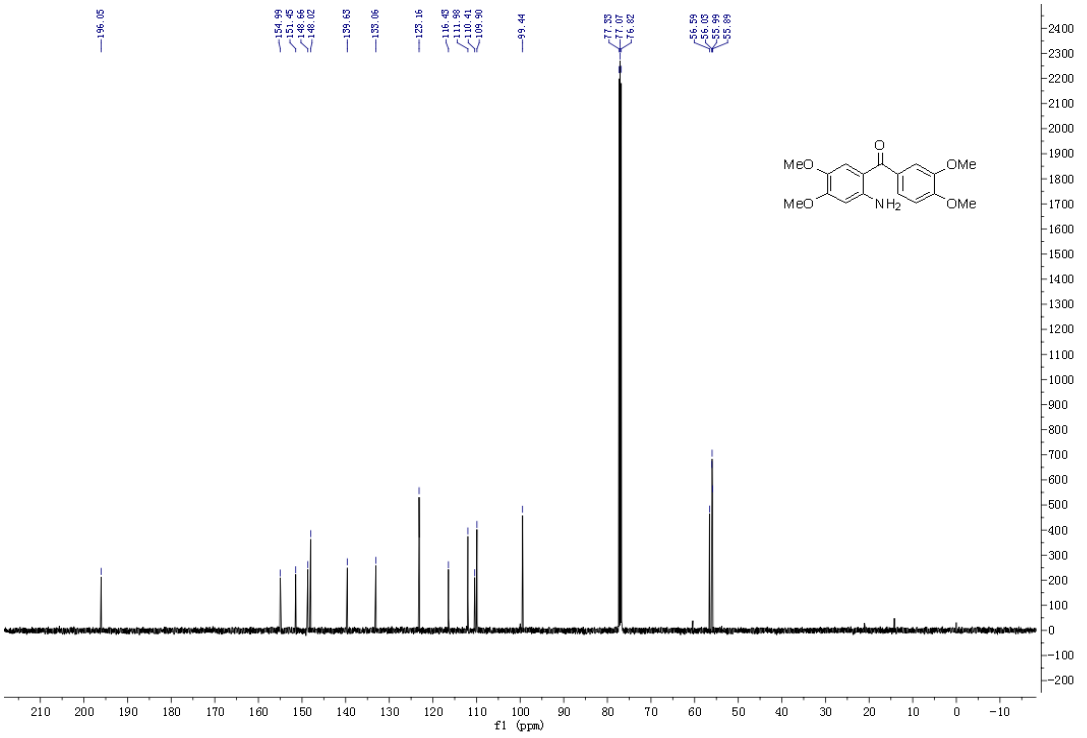
7.1057
7.1035
6.9240
6.9064
6.2316
6.0514
3.9651
3.9284
3.9108
3.7028
MeO
OMe
MeO
OMe
NH2
O
2.03
1.01
1.01
1.02
1.97
3.01
6.09
3.00
f1 (ppm)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139.63
133.06
125.16
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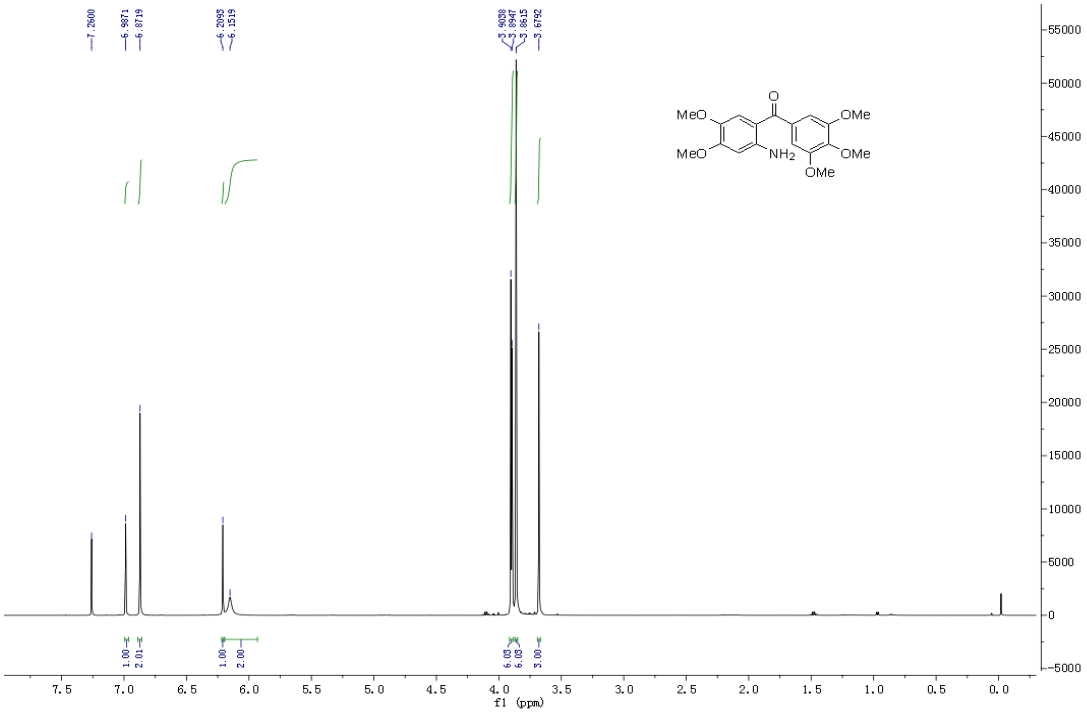
111.98
110.41
109.90
99.44
77.33
77.07
76.82
56.59
56.03
55.98
55.89
MeO
OMe
MeO
OMe
NH2
O
f1 (ppm)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6.8719
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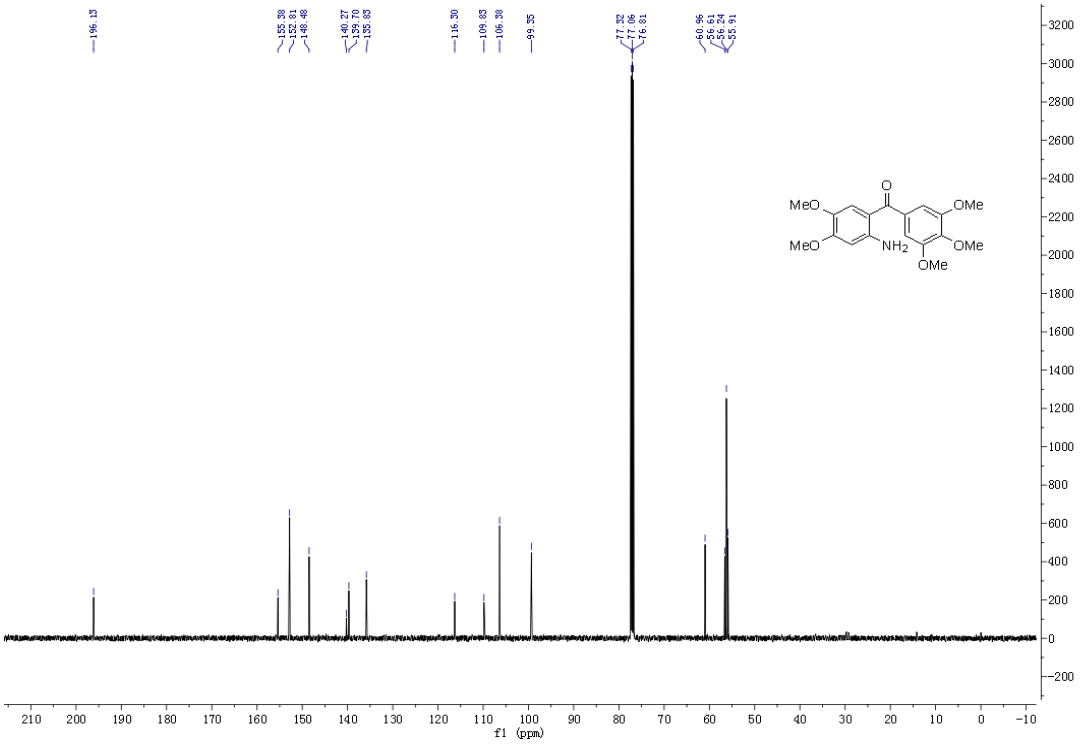
3.8947
3.8615
3.6792
MeO
MeO
NH2
OMe
OMe
OMe
f1 (ppm)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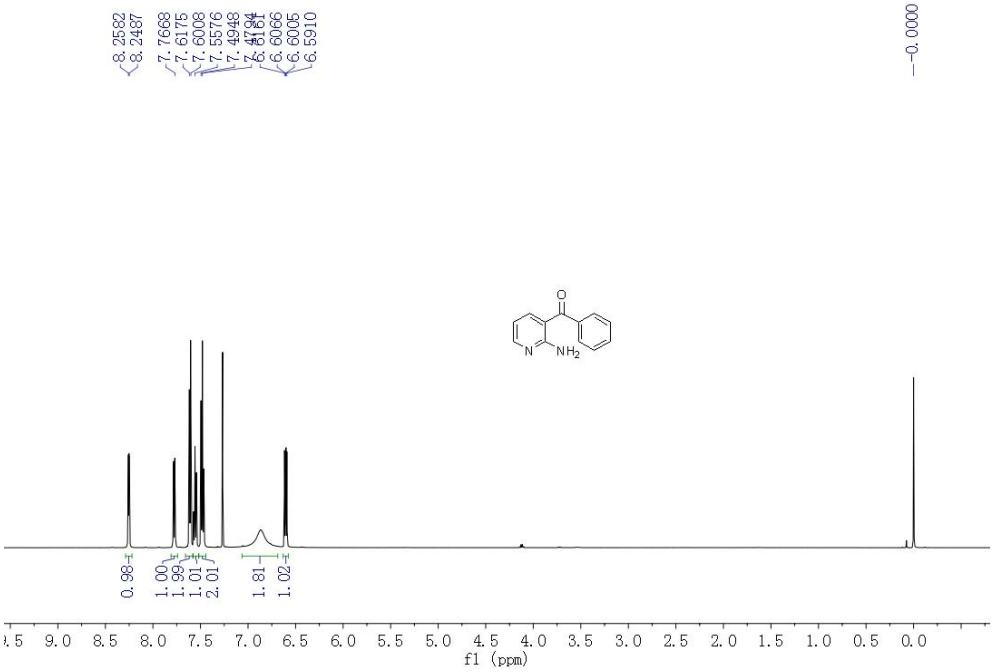
140.27
139.70
135.83
116.30
109.83
106.39
99.35
77.32
77.06
76.81
60.96
56.61
56.24
55.91
MeO
MeO
NH2
OMe
OMe
OMe
f1 (ppm)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8.2487
7.7668
7.6175
7.6008
7.5576
7.4948
7.4794
7.4161
6.6066
6.6005
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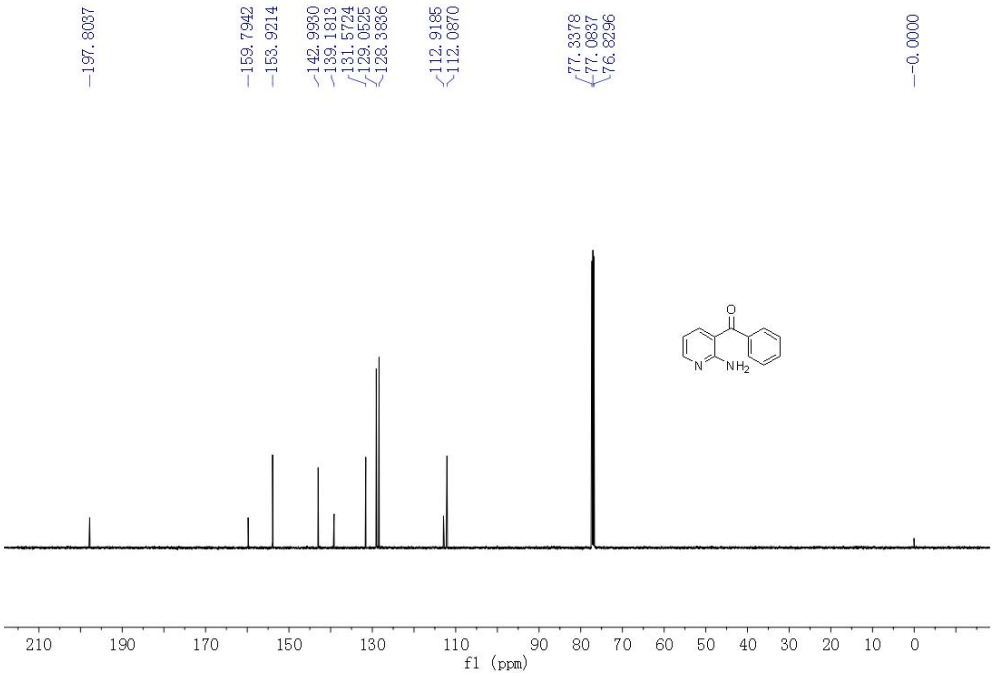
0.0000
0.98
1.00
1.99
1.01
2.01
1.81
1.02
f1 (ppm)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142.9930
139.1813
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112.0870
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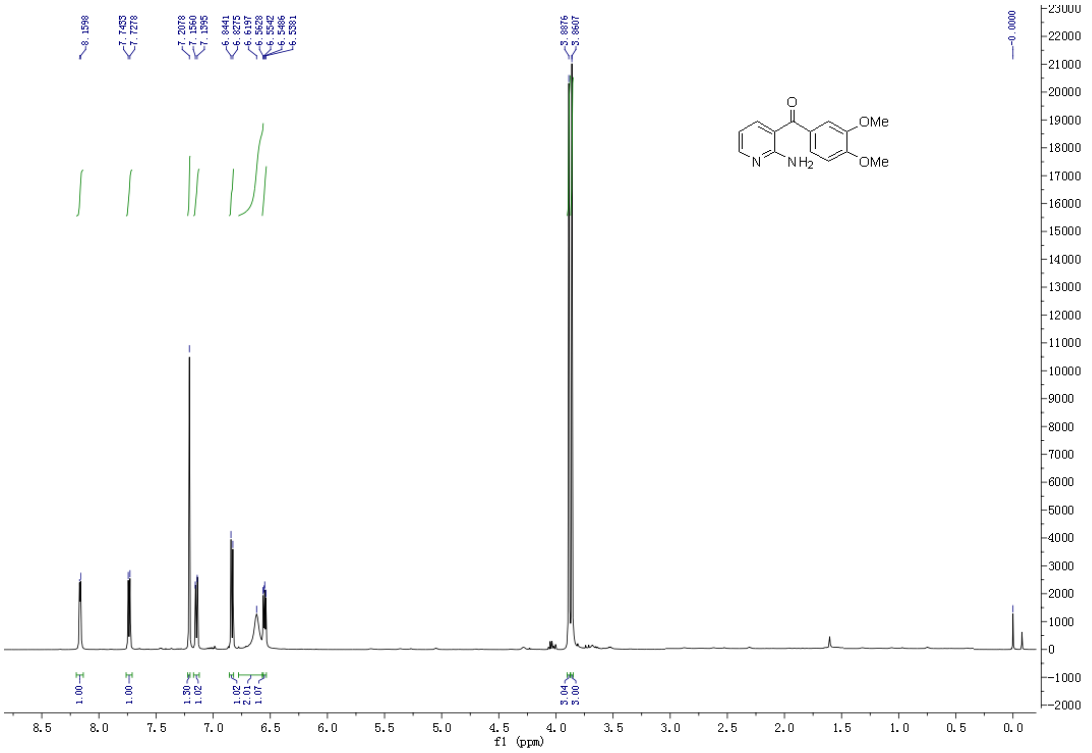
77.0837
76.8296
0.0000
f1 (ppm)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7.2078
7.1560
7.1395
6.8441
6.8275
6.6197
6.5628
6.5542
6.5466
6.5381
3.8876
3.8697
-0.0000
OMe
OMe
NH2
N
O
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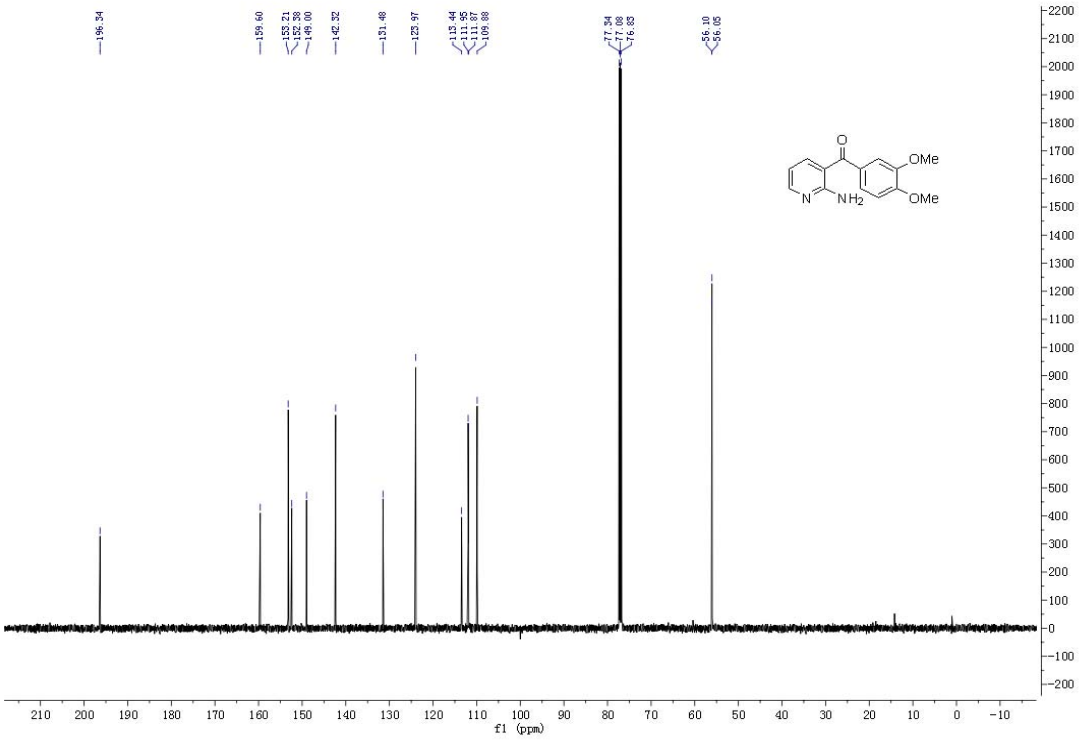
1.00
1.30
1.02
1.02
2.01
1.07
3.04
3.00
f1 (ppm)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125.97
113.44
111.95
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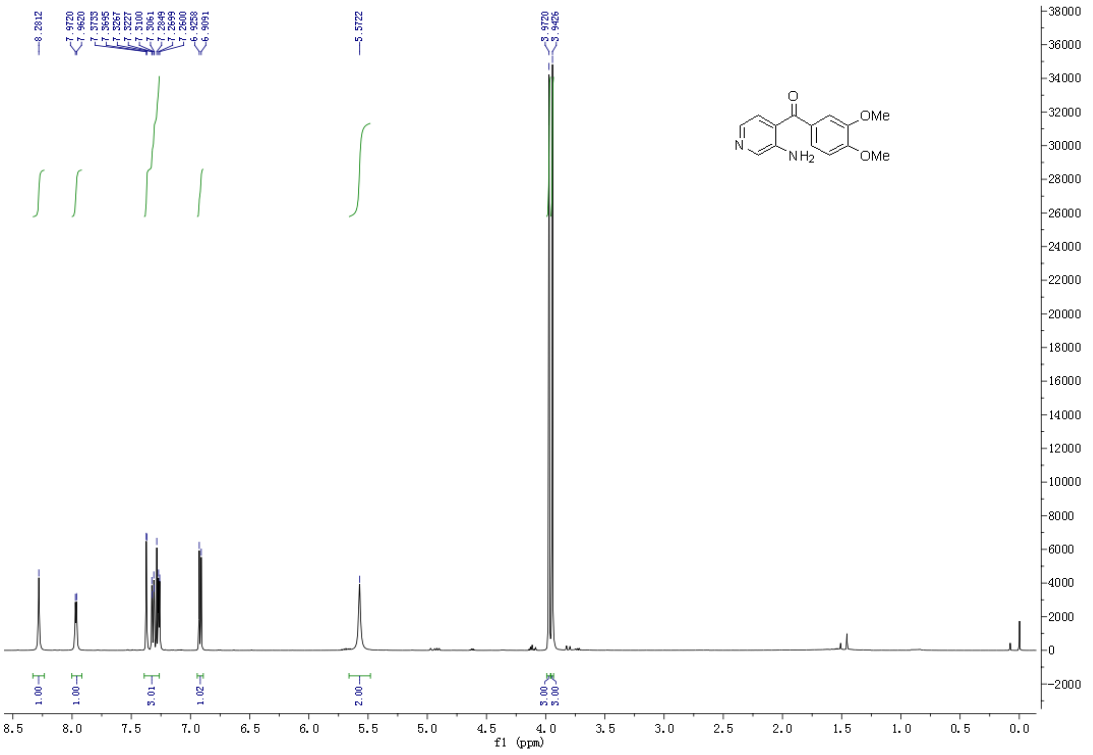
77.34
77.08
76.83
56.10
56.05
OMe
OMe
NH2
N
O
f1 (ppm)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7.3733
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7.3257
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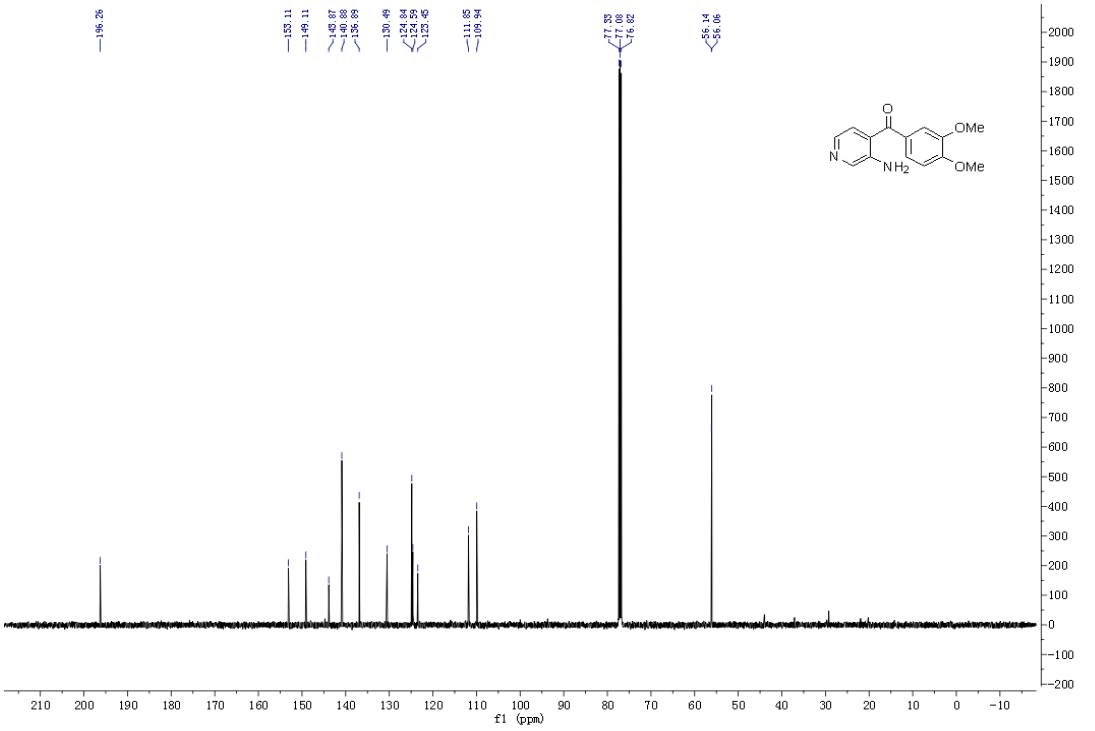
7.3061
7.2849
7.2699
7.2650
7.2598
6.9091
5.5722
3.9720
3.9426
O
OMe
OMe
N
NH2
1.00
1.00
3.01
1.02
2.00
3.00
3.00
f1 (ppm)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136.89
130.49
124.84
124.59
123.45
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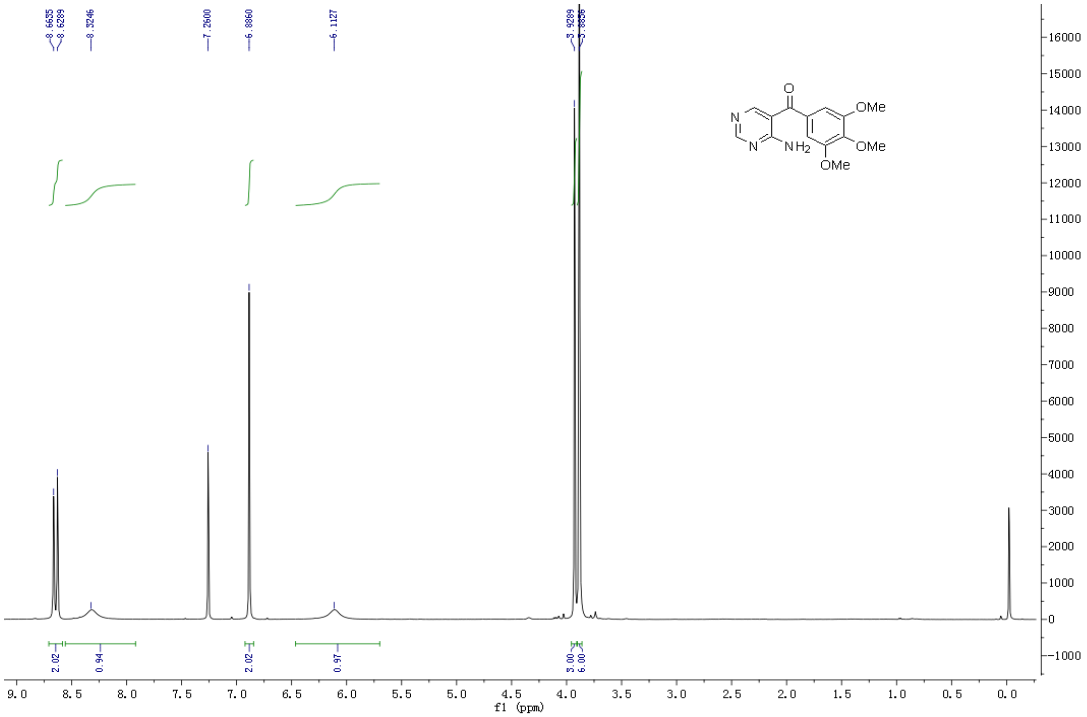
56.06
O
OMe
OMe
N
NH2
f1 (ppm)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8.3246
7.2600
6.8860
6.1127
3.9289
3.8835
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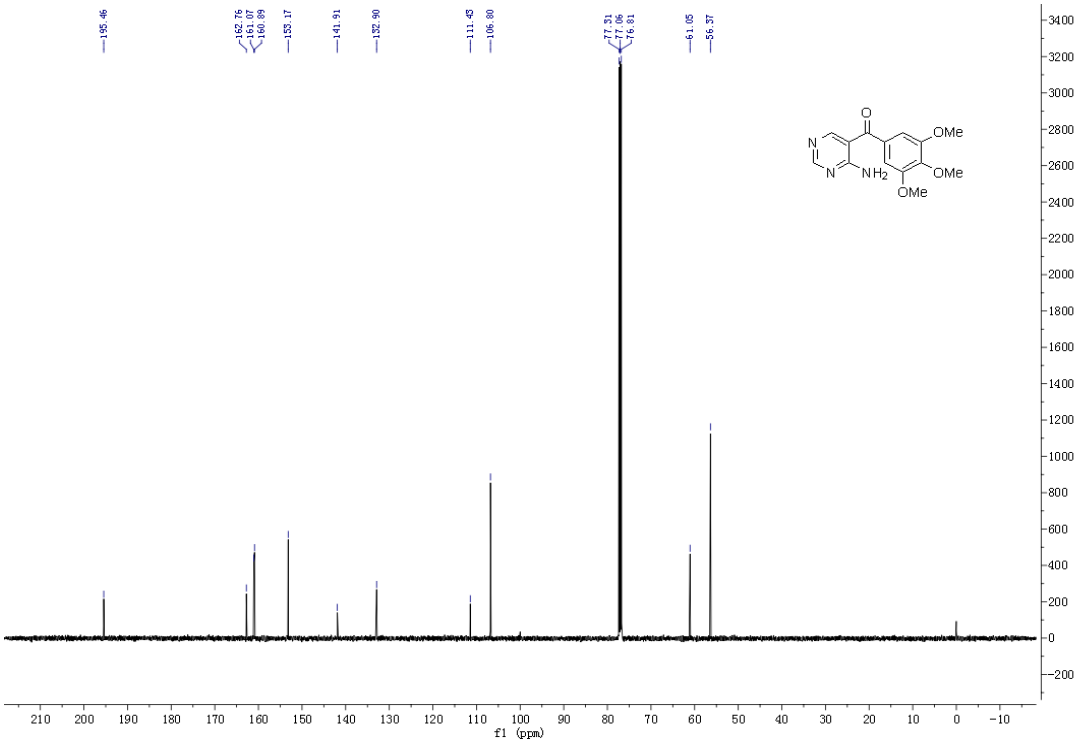
2.02
0.97
3.00
6.00
f1 (ppm)
O
N
N
NH2
OMe
OMe
OMe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162.76
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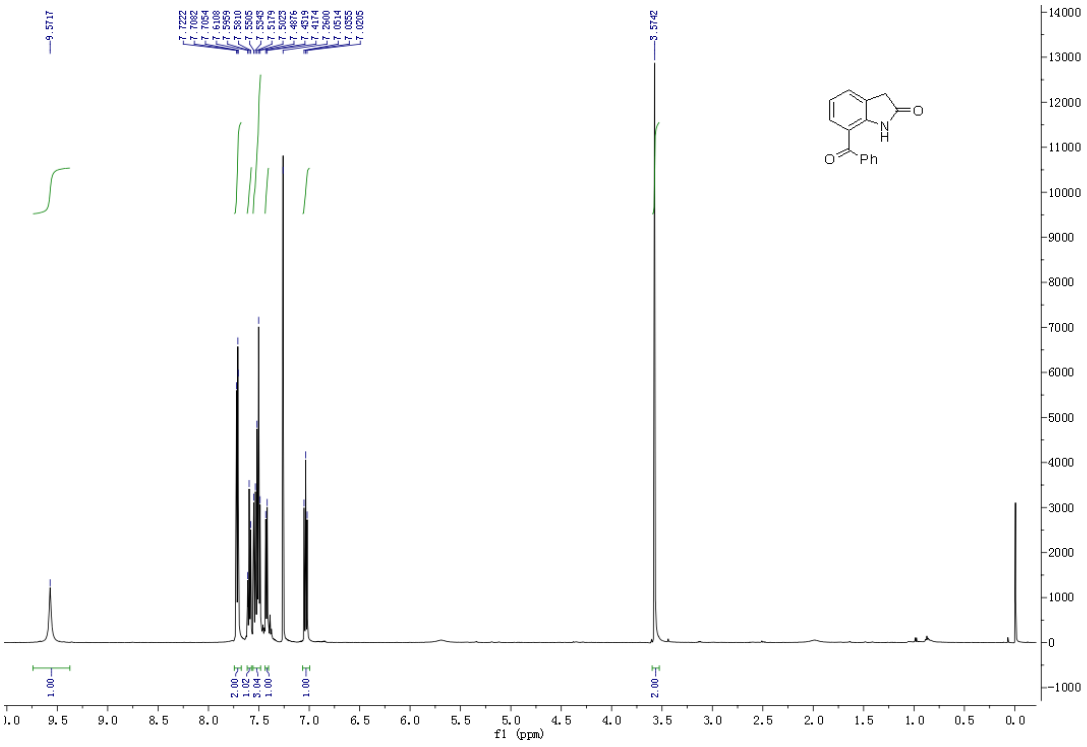
153.17
141.91
132.90
111.43
106.80
77.31
77.06
76.81
61.05
56.37
f1 (ppm)
O
N
N
NH2
OMe
OMe
OMe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7.4819
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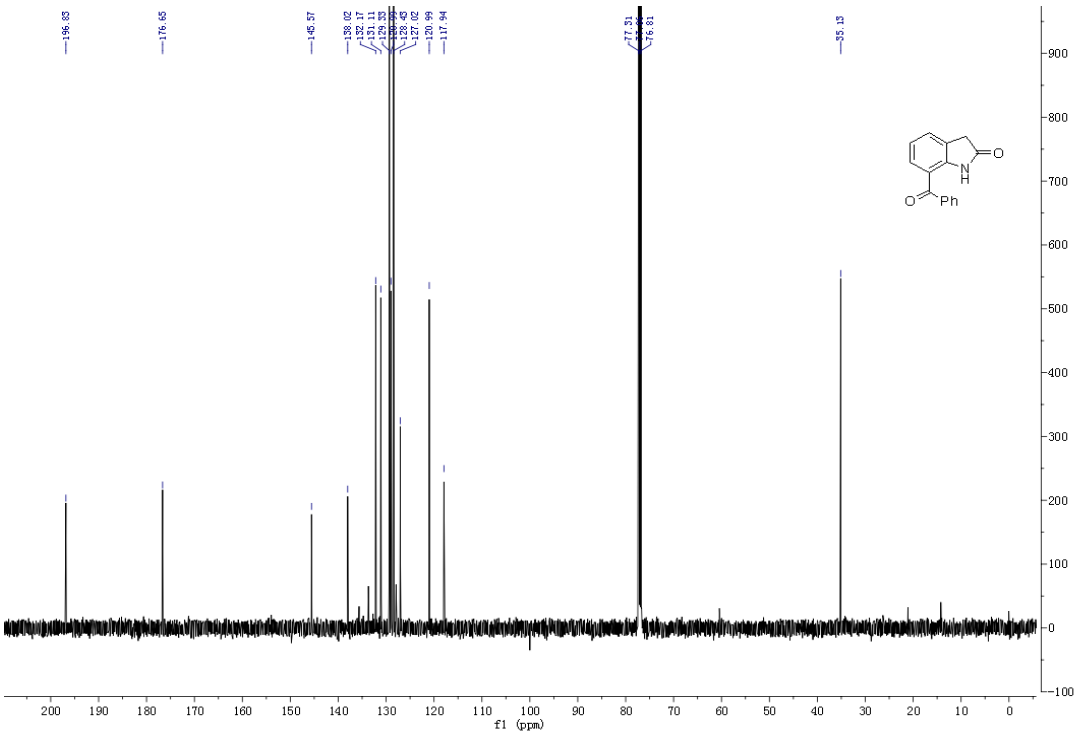
H
O
Ph
f1 (ppm)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117.94
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76.81
55.13
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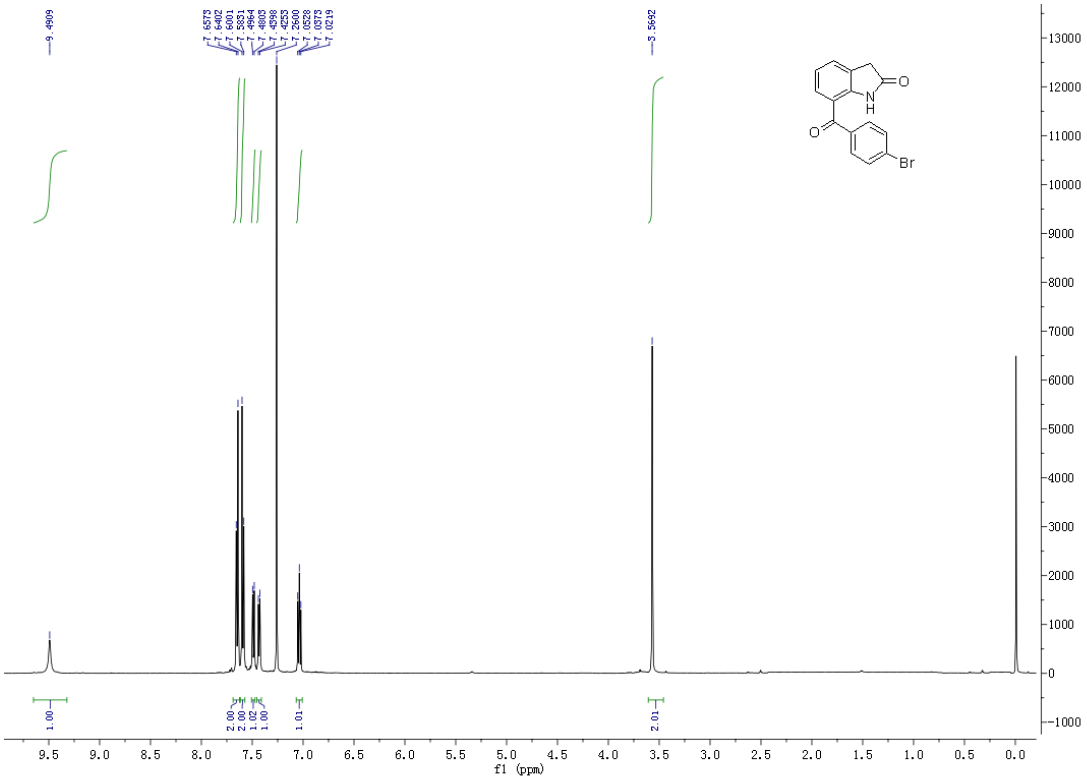
N
H
O
Ph
f1 (ppm)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7.0529
7.0373
7.0219
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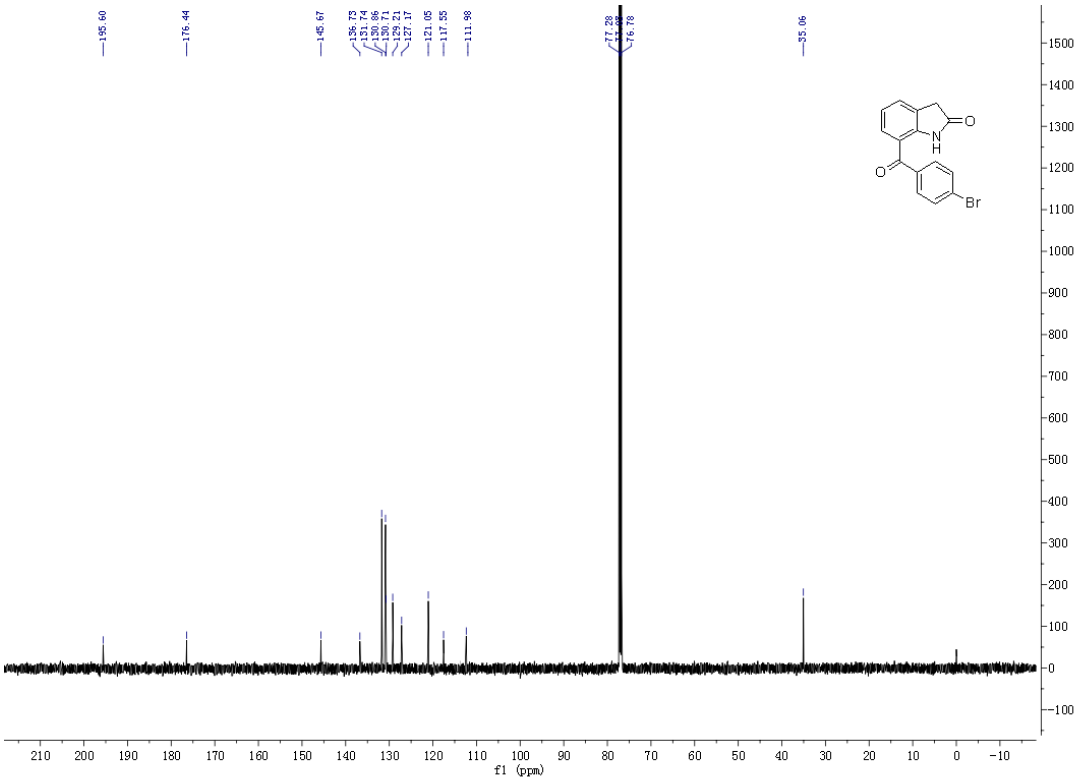
H
O
Br
1.00
2.00
2.00
1.07
1.00
1.01
2.01
f1 (ppm)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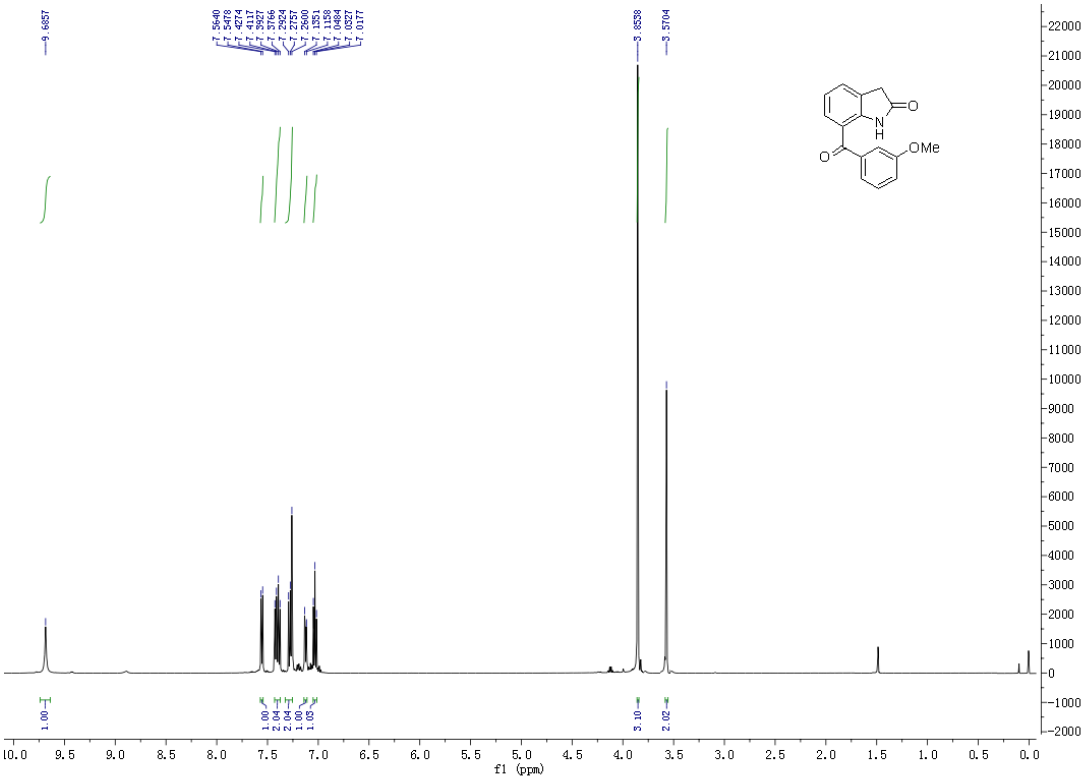
N
H
O
Br
f1 (ppm)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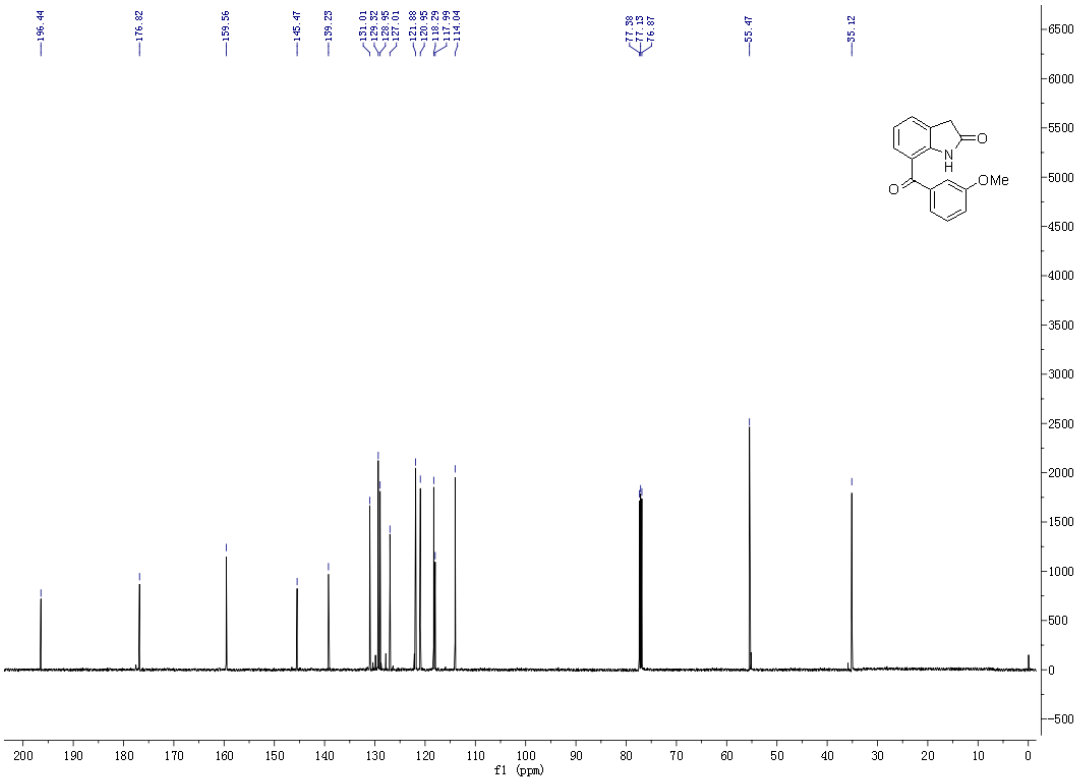
OMe
f1 (ppm)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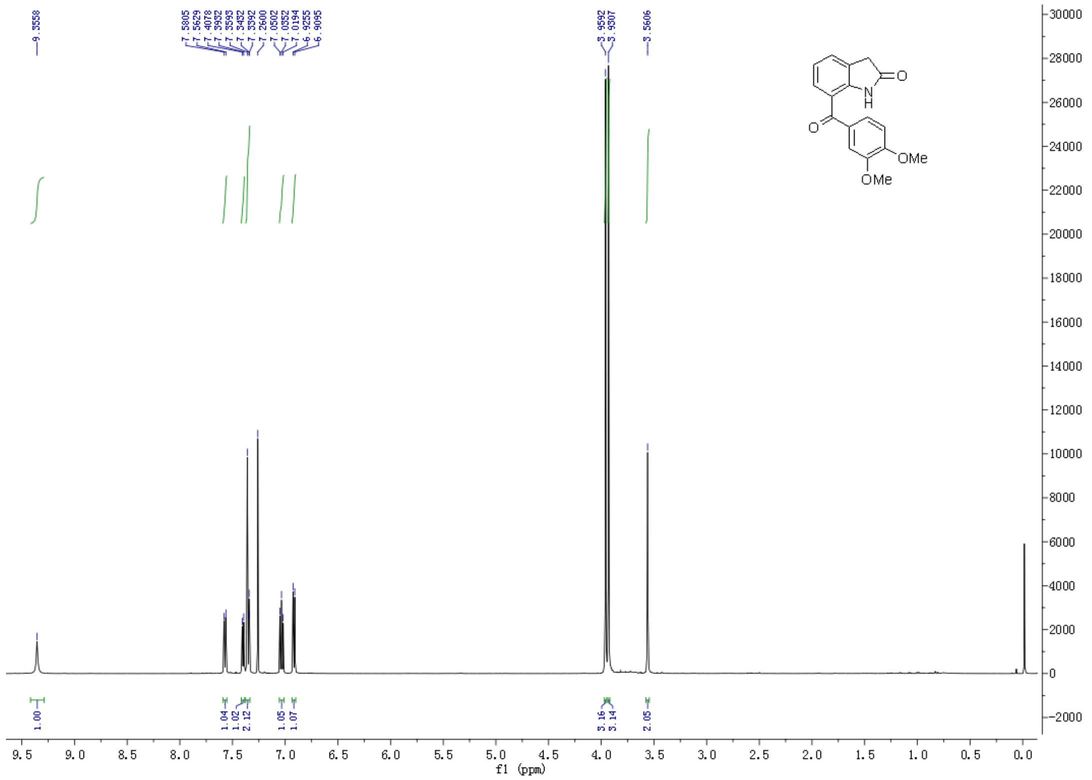
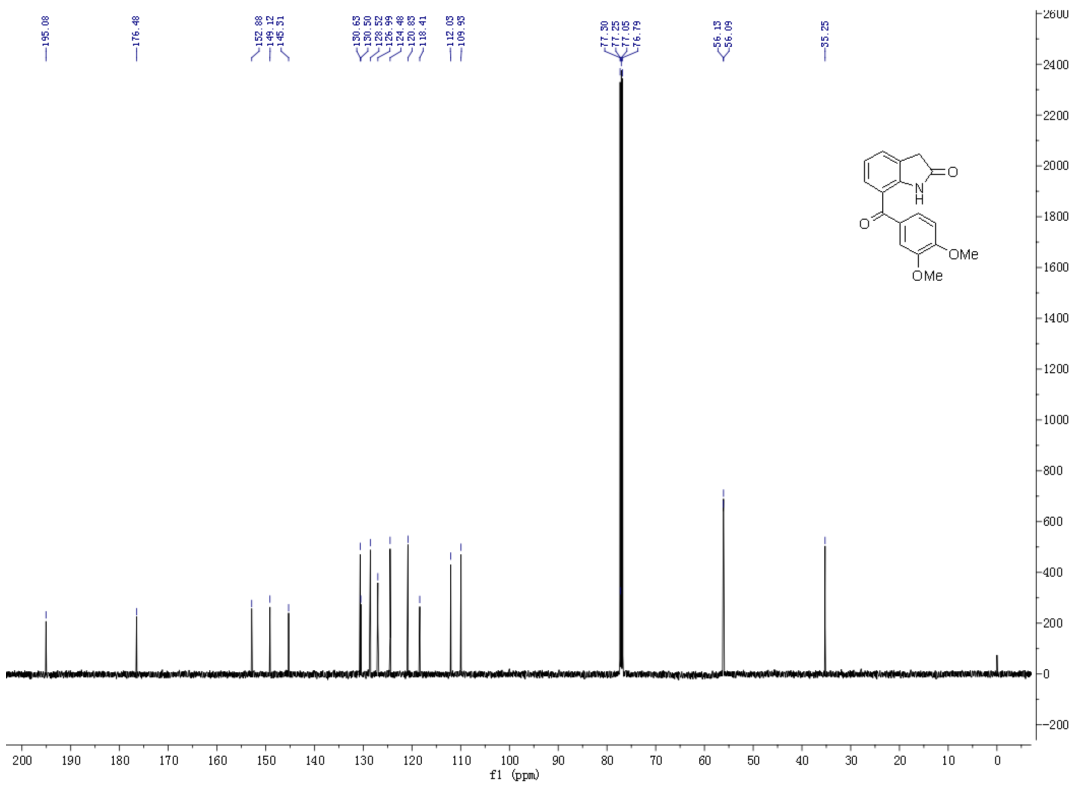
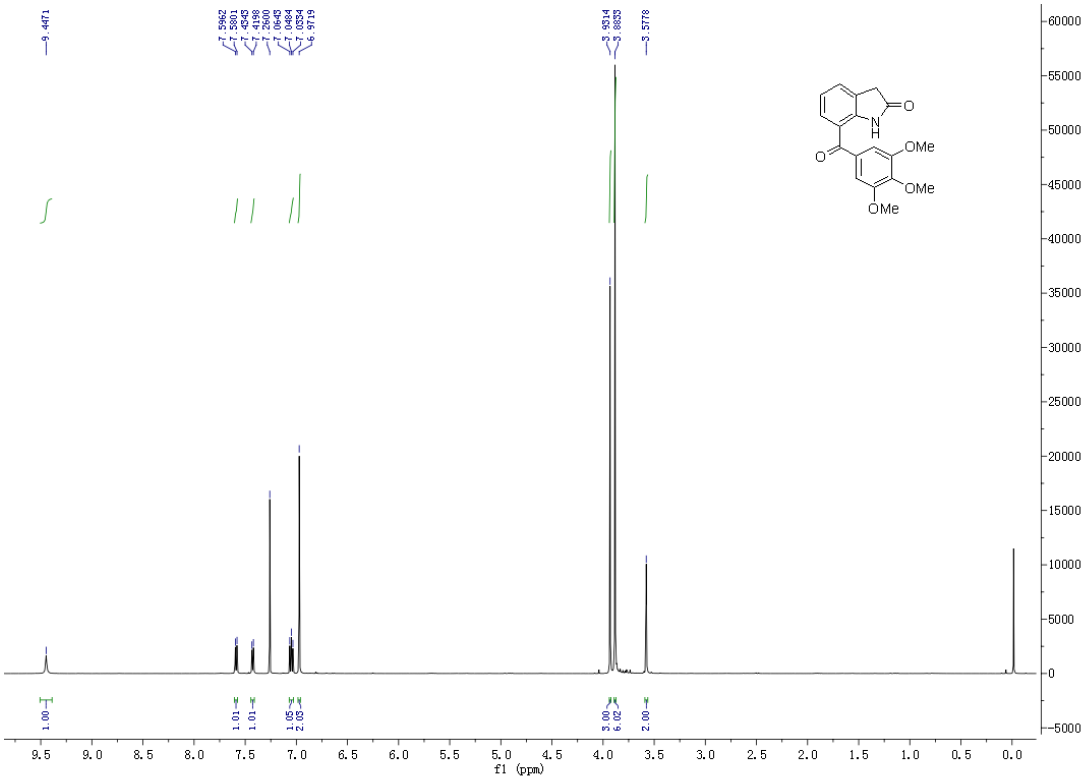
OMe
f1 (ppm)



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7.0354
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3.9314
3.8635
3.5778
O
N
H
O
OMe
OMe
OMe
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1.01
1.01
1.05
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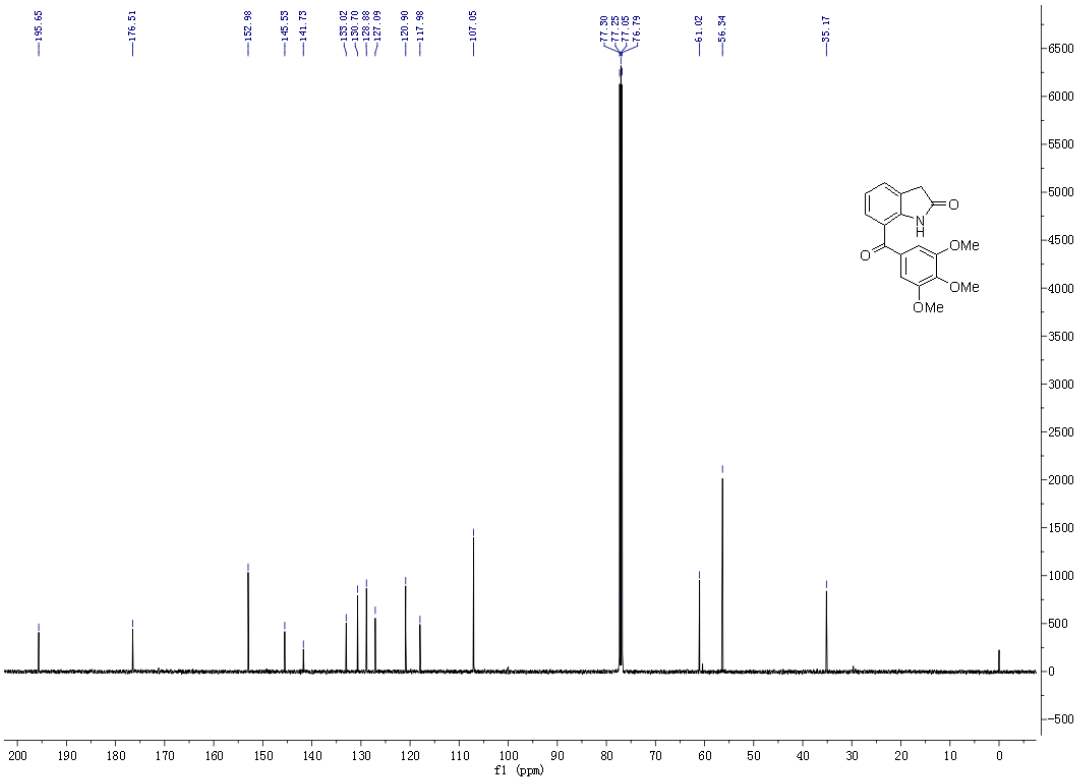
3.00
6.02
2.00
f1 (ppm)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130.70
129.88
127.09
120.90
117.98
107.05
77.30
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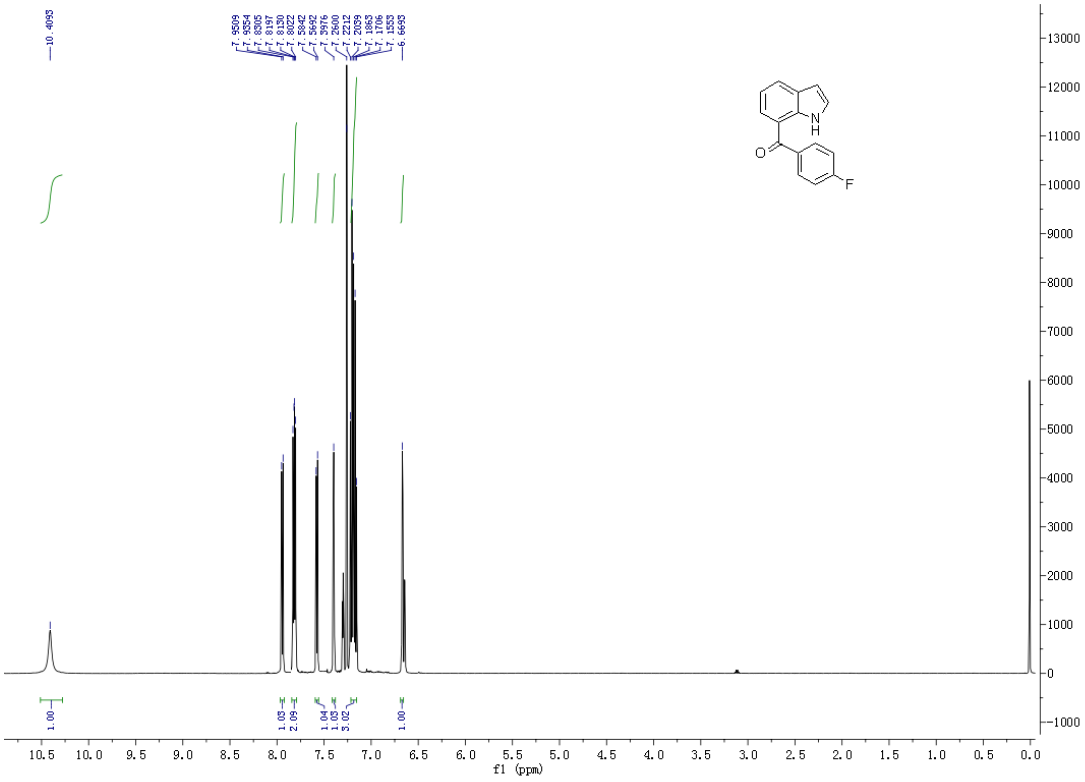
77.05
76.79
61.02
56.34
35.17
O
N
H
O
OMe
OMe
OMe
f1 (ppm)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7.2212
7.2039
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1.03
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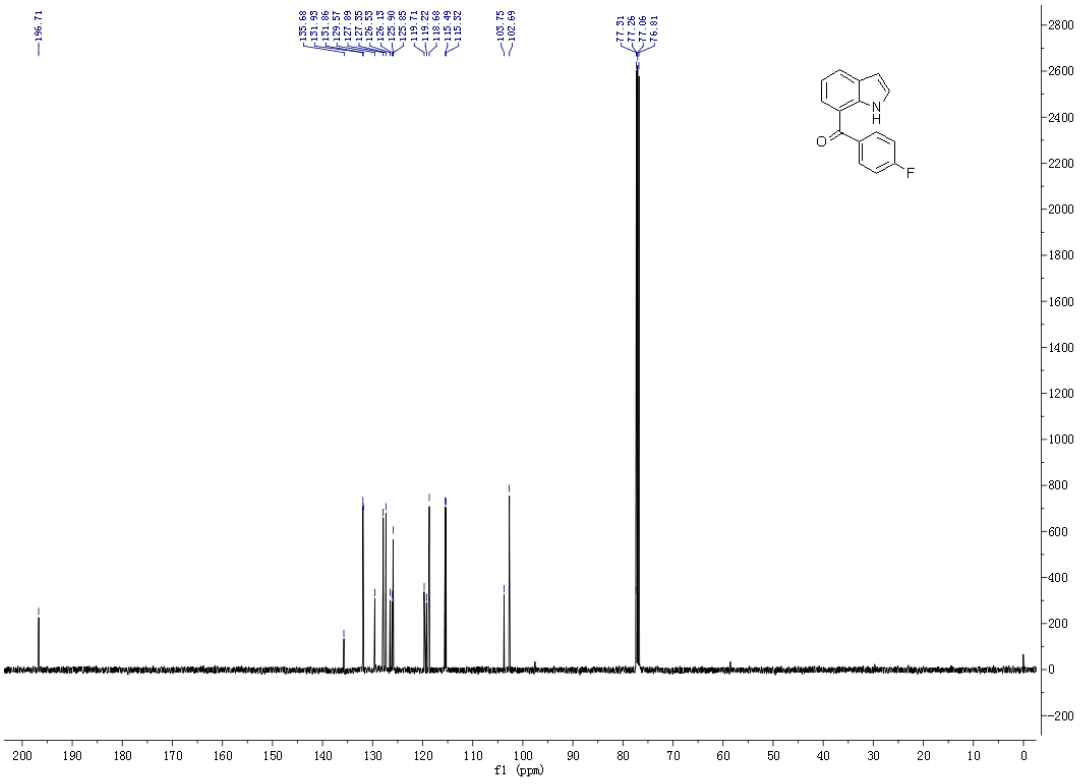
1.00
f1 (ppm)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126.53
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126.30
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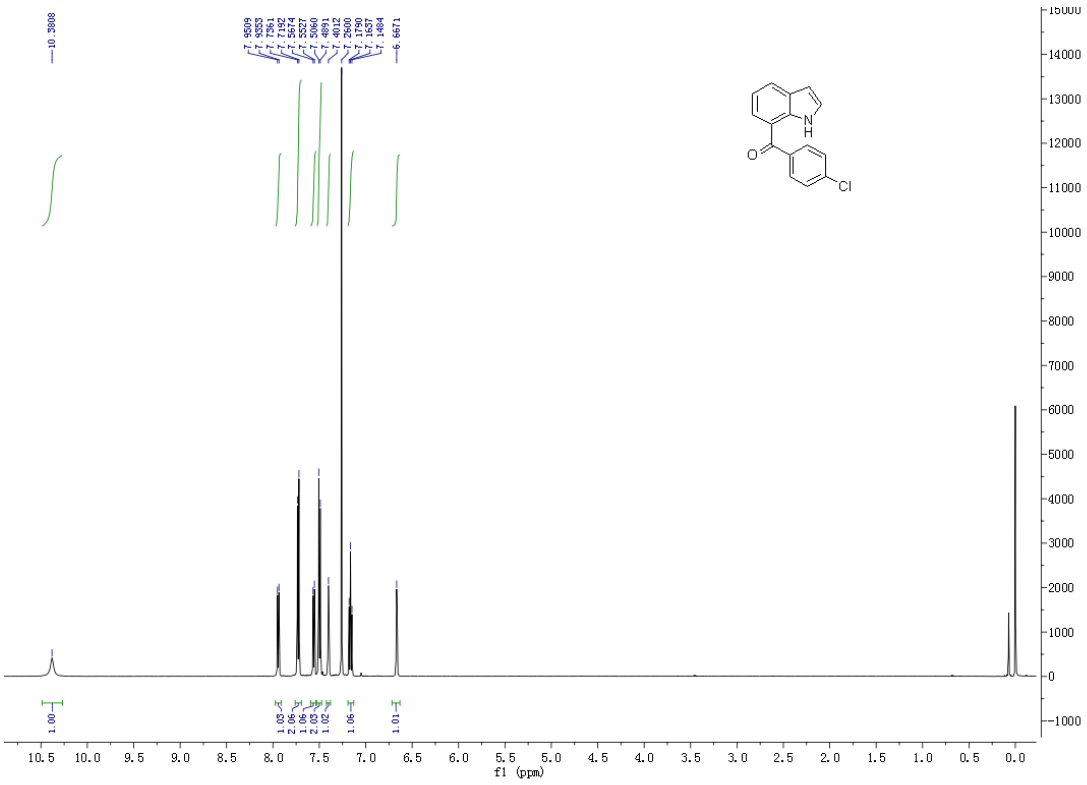
77.26
77.06
76.81
f1 (ppm)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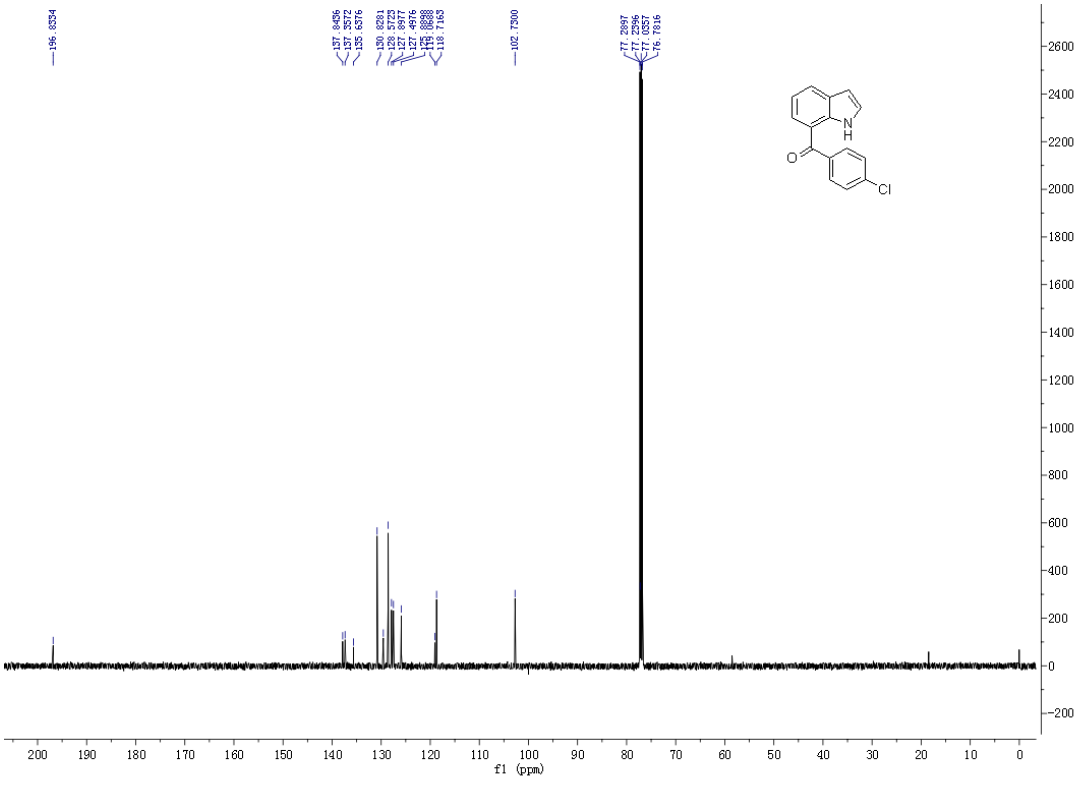
2.06
1.06
2.03
1.02
1.06
1.01
f1 (ppm)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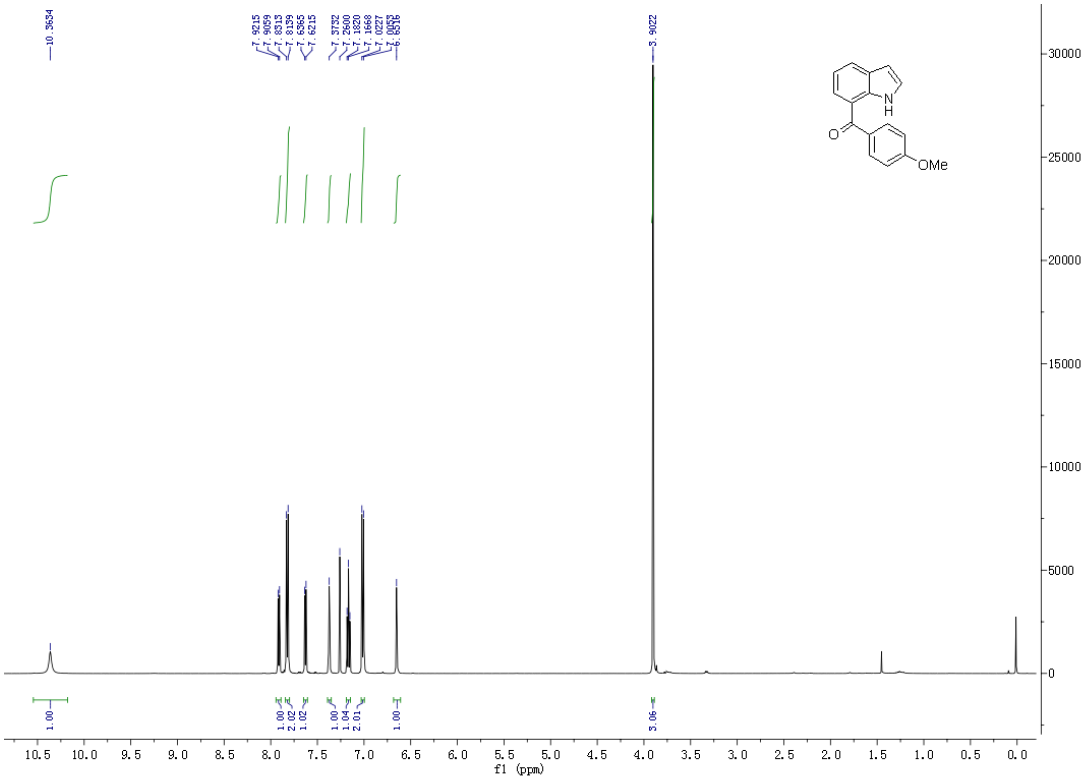
76.7916
f1 (ppm)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7.2600
7.1820
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7.0277
7.0053
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1.02
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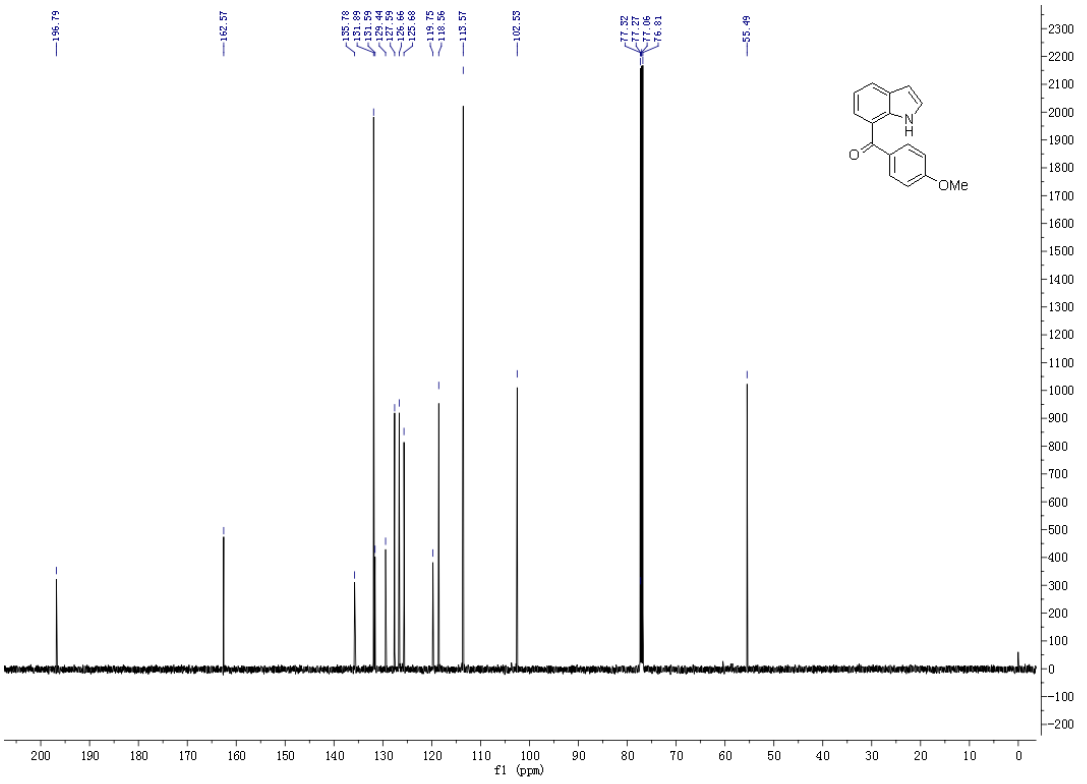
3.06
f1 (ppm)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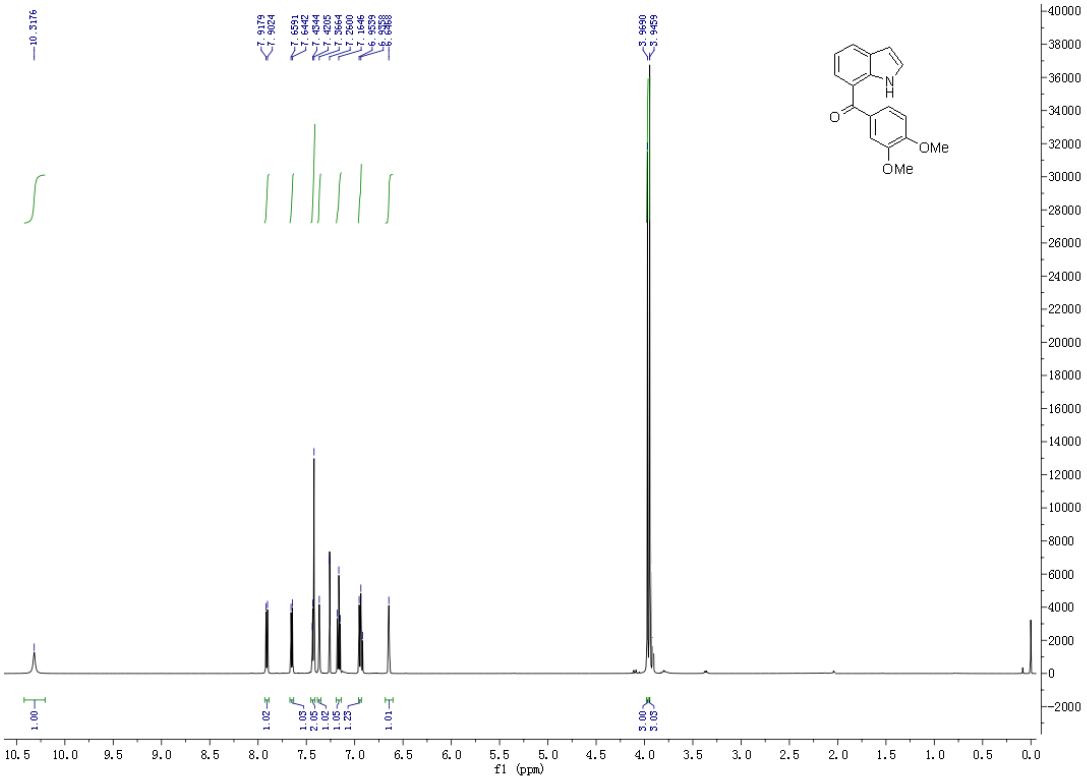
77.06
76.81
55.49
f1 (ppm)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6.9539
6.9388
6.9238
3.9690
3.9459
OMe
OMe
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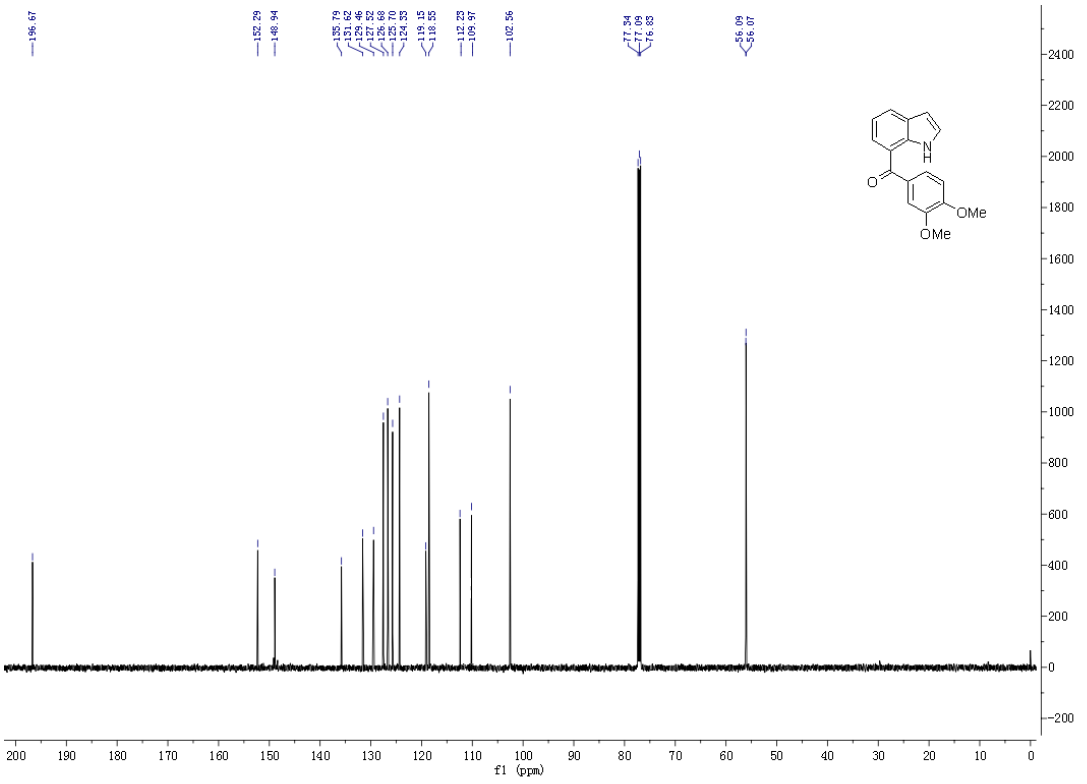
1.03
2.05
1.02
1.05
1.23
1.01
3.00
3.03
f1 (ppm)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124.33
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102.56
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77.09
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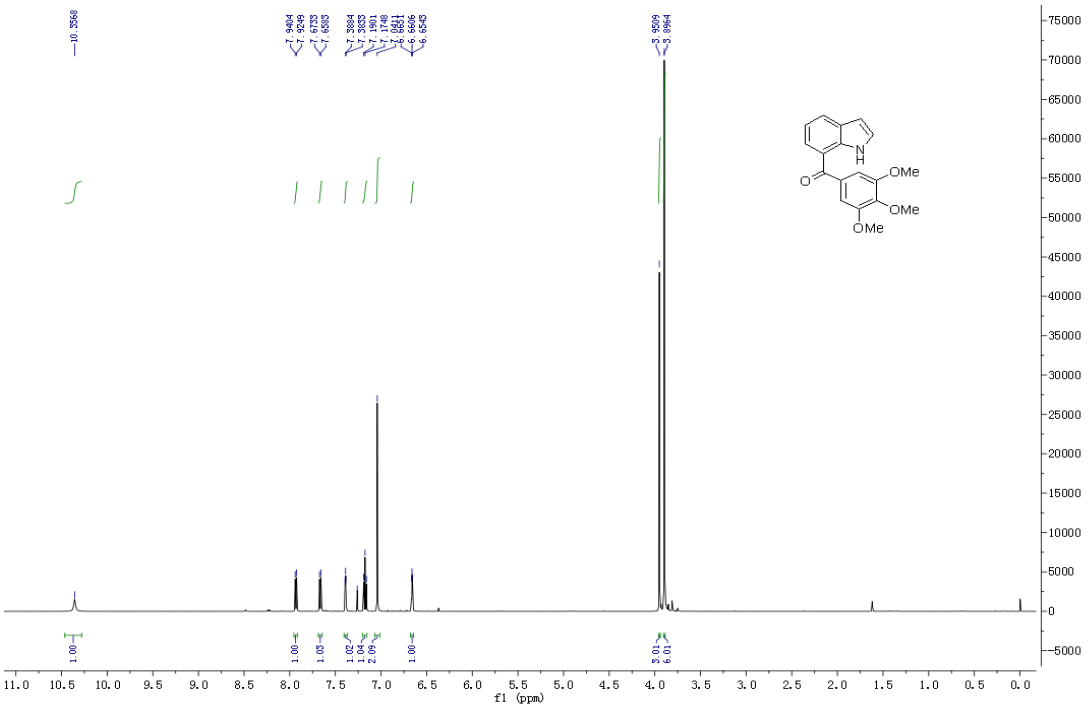
56.09
56.07
OMe
OMe
f1 (ppm)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6.6345
3.9599
3.8964
OMe
OMe
OMe
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1.00
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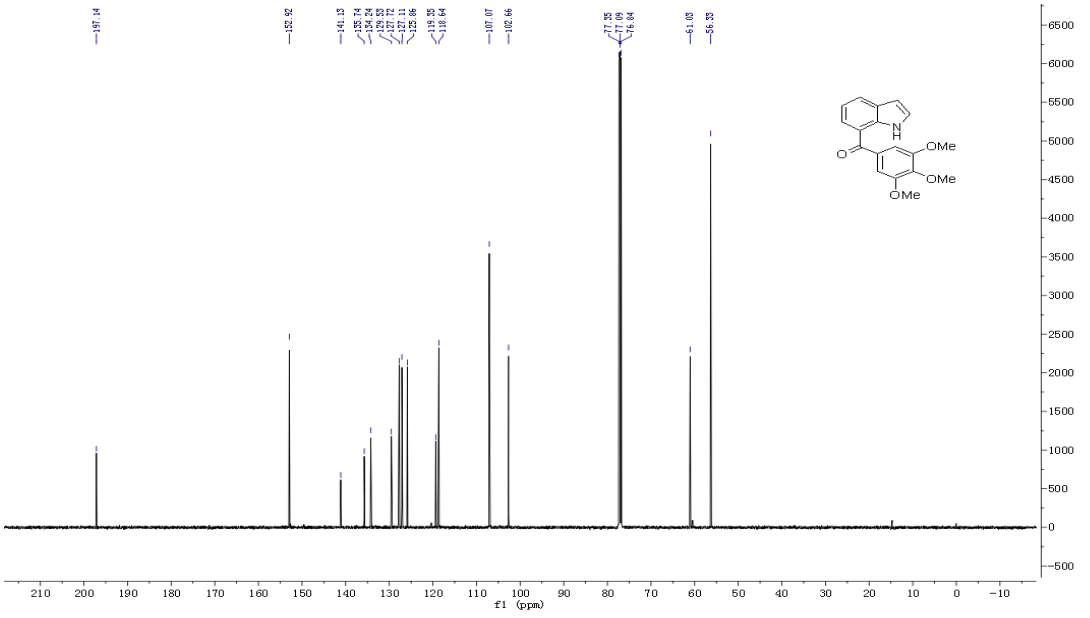
1.04
2.09
1.00
3.01
6.01
f1 (ppm)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119.35
110.64
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77.09
76.84
61.05
56.53
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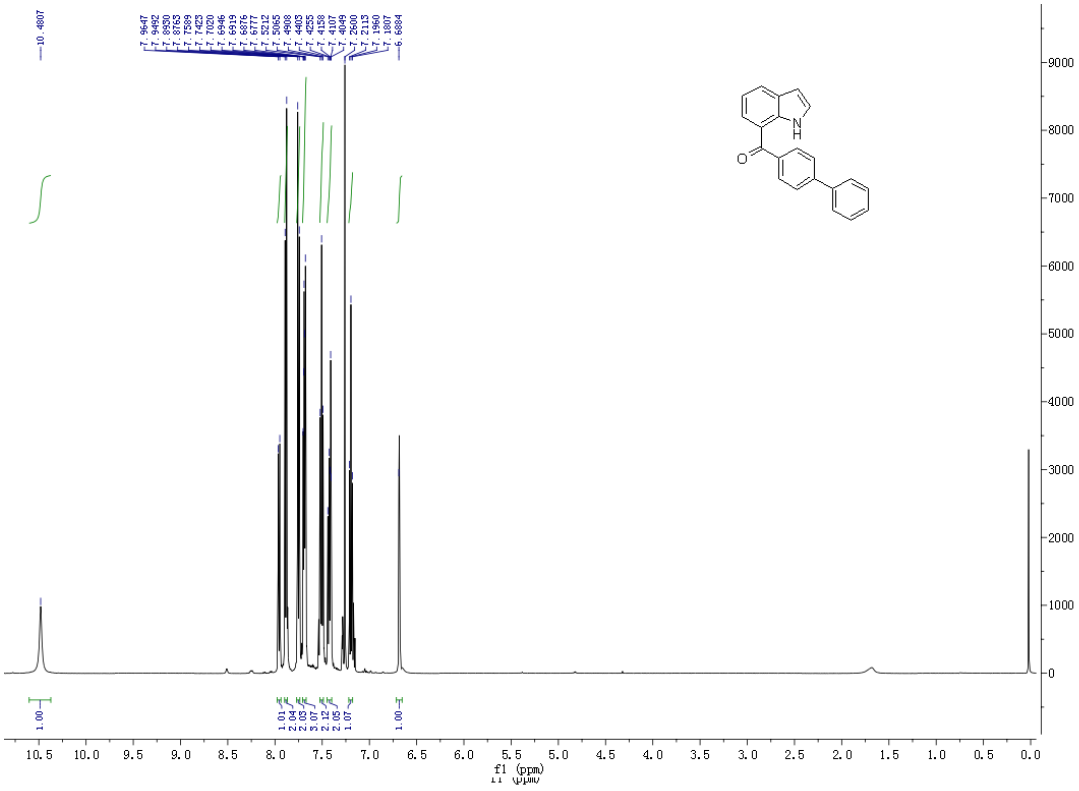
OMe
OMe
N
H
O
f1 (ppm)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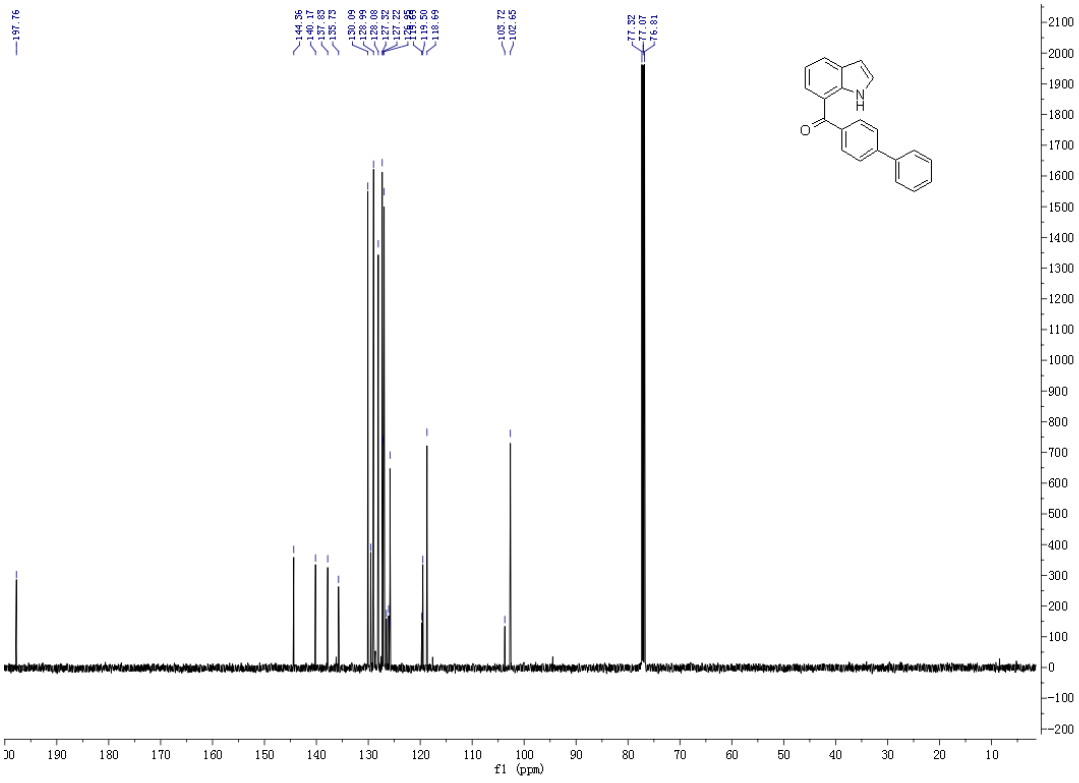
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118.69
103.72
102.65
77.32
77.07
76.81
fl (ppm)