Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Lewis Acid Catalyst-steered Divergent Synthesis of Functionalized Vicinal Amino Alcohols and Pyrroles from Tertiary Enamides

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Table of Contents

1. General information

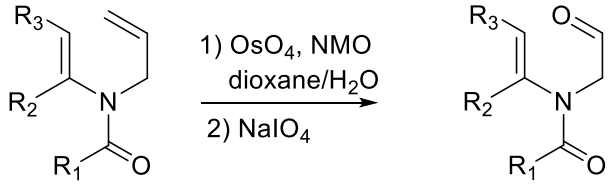
Reagents and solvents were purchased from commercial sources and preserved under argon. More sensitive compounds were stored in a desiccator or glove-box if required. Reagents were used without further purification unless otherwise noted. All reactions were performed under argon (or nitrogen) and stirring unless otherwise noted. When needed oven dried glassware was used (T°>100 °C) or under vacuum with a heat gun (T >200 °C).

Anhydrous solvents were purified and dried following standard procedures. Flash column chromatography was performed using Silicycle SiliaFlash® P60 230-400 mesh. TLC analysis was performed on pre-coated, glass-backed silica gel plates. TLC's were revealed by UV fluorescence (254 nm) then one of the following: $KMnO_4$, phosphomolybdic acid, ninhydrin, pancaldi, *p*-anisaldehyde, vanillin.

Melting points were uncorrected. The ^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECX-400 400 MHz spectrometers or ECX-300 300 MHz spectrometers. ^{1}H NMR chemical shifts were reported relative to residual $CDCl_3$ (7.26 ppm) or acetone-d6 (2.05 ppm). ^{13}C NMR chemical shifts were reported relative to the central line of $CDCl_3$ (77.2 ppm) or acetone-d_6 (29.8 ppm, 206.2 ppm). Abbreviations are used in the description of NMR data as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet), coupling constant (*J*, Hz). The high resolution mass spectra (HRMS) were recorded on a GCT-MS Micromass UK spectrometer or a micrOTOF-Q spectrometer. Infrared spectra were recorded using a PerkinElmer Spectrum 100 FT-IR spectrometer with KBr pellets in the 4000-400 cm^{-1} region.

2. Preparation of substrates 1

2.1 General procedure for the synthesis of substrates 1



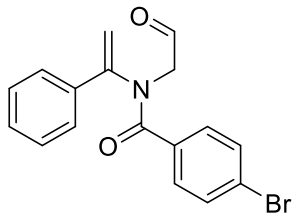
S1 **1**

The synthesis of compounds **S1** and **1** were completed according to a slightly modified literarure procedure[1-2]. To a mixture of **S1** (5 mmol) and aqueous NMO (50%) solution (15 mmol) in 1,4-dioxane/H_2O (60 mL, v/v=2:1) at rt was added OsO_4 (0.8 mL, 0.075 M in water, 0.06 mmol). After the mixture was stirred at rt overnight, $NaIO_4$ (2.14g, 10 mmol) was added. Upon stirring at rt for another 2 h, the reaction mixture was quenched with aqueous NaS_2O_3 and H_2O. The reaction mixture was extracted with EtOAc (3×20 mL) The organic extracts were washed with brine, dried over Na_2SO_4, filtered and concentrated in *vacuo*. The residue was purified by flash column chromatography on silica gel to afford the desired product **1**.

2.2 Characterization of substrates 1

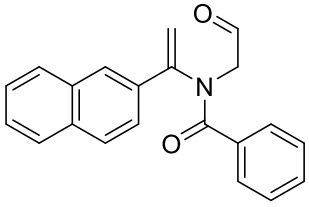
Compounds **1a-q**, **1c'** have been reported. The analytical data were in accordance with those reported in the literature[3]

4-bromo-*N*-(2-oxoethyl)-*N*-(1-phenylvinyl)benzamide (1n')



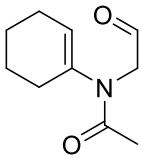
White solid (53% yield). **m.p.** 106-108 ℃; **IR** (KBr) ν 3429, 2912, 2865, 1749, 1723, 1644, 1589 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.69 (s, 1H), 7.51-7.38 (m, 9H), 5.45 (s, 1H), 4.99 (s, 1H), 4.32 (s, 2H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 195.9, 170.6, 147.7, 135.2, 133.3, 131.2, 129.7, 129.6, 129.2, 126.2, 125.2, 114.1, 57.7; **HRMS** (ESI) Calcd. for $C_{17}H_{15}NO_2Br$, $[M+H]^+$ 344.0281. Found: 344.0278.

***N*-(1-(naphthalen-2-yl)vinyl)-*N*-(2-oxoethyl)benzamide (1p')**



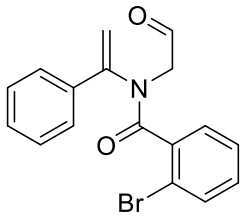
Light yellow solid (60% yield). **m.p.** 138-139 ℃; **IR** (KBr) ν 3051, 2816, 1747, 1720, 1636 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.74 (s, 1H), 8.01 (d, J = 0.8 Hz, 1H), 7.90-7.85 (m, 3H), 7.63-7.51 (m, 5H), 7.35-7.31 (m, 1H), 7.25-7.21 (m, 2H), 5.58 (s, 1H), 5.10 (s, 1H), 4.38 (s, 2H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 196.4, 171.9, 147.9, 134.5, 133.7, 133.4, 132.8, 130.8, 129.1, 128.6, 128.0, 127.96, 127.7, 127.0, 126.9, 125.6.3, 123.8, 114.8, 57.8; **HRMS** (ESI) Calcd. for $C_{21}H_{18}NO_2$, $[M+H]^+$ 316.1332. Found: 316.1328.

***N*-(cyclohex-1-en-1-yl)-N-(2-oxoethyl)acetamide (1q')**



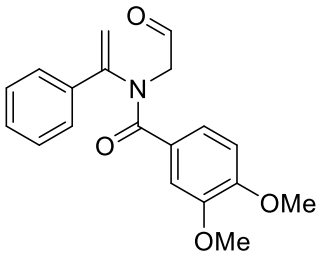
Light yellow oil (40% yield). **IR** (KBr) ν 3359, 2935, 2861, 1724, 1656 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.56 (s, 1H), 5.83-5.81 (m, 1H), 4.09 (s, 2H), 2.16-2.05 (m, 7H), 1.77-1.70 (m, 2H), 1.63-1.57 (m, 2H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 198.0, 170.7, 139.6, 128.2, 56.5, 28.0, 24.7, 22.7, 21.4, 21.0; **HRMS** (ESI) Calcd. for $C_{10}H_{16}NO_2$, $[M+H]^+$ 182.1176. Found: 182.1178.

2-bromo-*N*-(2-oxoethyl)-*N*-(1-phenylvinyl)benzamide (1r)



Light yellow oil (77% yield). **IR** (KBr) ν 3446, 3058, 1733, 1661, 1652, 1377, 1027, 776 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.73 (s, 1H), 7.44-7.42 (m, 1H), 7.36-7.32 (m, 2H), 7.31-7.28 (m, 3H), 7.18-7.15 (m, 1H), 7.10-7.03 (m, 2H), 5.33 (d, *J* = 0.9 Hz, 1H), 5.32 (d, *J* = 0.9 Hz, 1H), 4.39 (s, 2H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 196.2, 169.6, 146.8, 137.1, 135.7, 132.8, 130.4, 129.2, 128.8, 127.4, 126.7, 126.0, 120.4, 113.0, 57.5; **HRMS** (ESI) Calcd. for $C_{17}H_{14}BrNO_2$, $[M+H]^+$ 344.0281; Found: 344.0277.

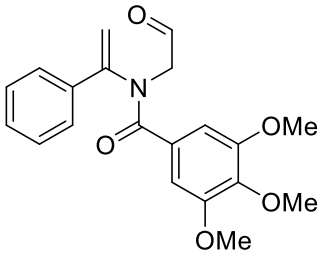
3,4-dimethoxy-*N*-(2-oxoethyl)-*N*-(1-phenylvinyl)benzamide (1s)



Light yellow solid (62% yield). **m.p.** 114-115 ℃; **IR** (KBr) ν 3429, 3006，2942, 2842, 1725, 1630 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.71 (s, 1H), 7.57-7.55

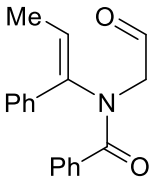
(m, 2H), 7.44-7.36 (m, 3H), 7.24 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.17 (d, *J* = 1.6 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 5.48 (s, 1H), 5.03 (s, 1H), 4.28 (s, 2H), 3.85 (s, 3H), 3.70 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 196.7, 171.3, 151.1, 148.2, 148.1, 135.5, 129.4, 129.1, 126.4, 126.1, 121.7, 113.6, 111.7, 109.9, 57.7, 55.9, 55.7; **HRMS** (ESI) Calcd. for $C_{19}H_{20}NO_4$, $[M+H]^+$ 326.1387. Found: 326.1384.

3,4,5-trimethoxy-*N*-(2-oxoethyl)-*N*-(1-phenylvinyl)benzamide (1t)



Light yellow oil (63% yield). **IR** (KBr) ν 3429, 2939，2837, 1732, 1646, 1585 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.72 (s, 1H), 7.55 (d, *J* = 7.2 Hz, 2H), 7.42-7.34 (m, 3H), 6.83 (s, 2H), 5.51 (s, 1H), 5.09 (s, 1H), 4.34 (s, 2H), 3.81 (s, 3H), 3.64 (s, 6H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 196.3, 171.4, 152.6, 147.8, 139.9, 135.4, 129.43, 129.38, 129.1, 125.9, 113.7, 105.5, 60.8, 57.8, 55.9; **HRMS** (ESI) Calcd. for $C_{20}H_{22}NO_5$, $[M+H]^+$ 356.1492. Found: 356.1488.

***N*-(2-oxoethyl)-N-(1-phenylprop-1-en-1-yl)benzamide (1u)**

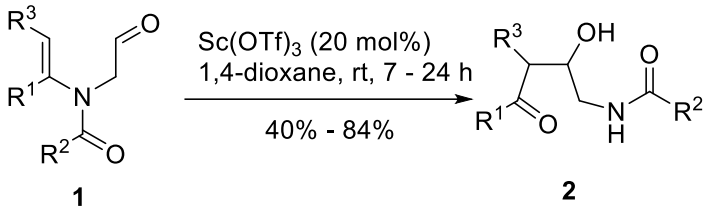


White solid (65% yield). **m.p.** 93-95 ℃; **IR** (KBr) ν 3445, 3058, 2813, 1735, 1652, 1626, 1589 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 9.73 (s, 1H), 7.64-7.62 (m, 2H), 7.53-7.51 (m, 2H), 7.44-7.34 (m, 4H), 7.27-7.23 (m, 2H), 5.86 (q, *J* = 6.8 Hz, 1H), 4.40 (d, *J* = 17.2 Hz, 1H), 3.95 (dd, *J* = 17.6, 0.8 Hz, 1H), 1.54 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 196.5, 171.5, 140.8, 136.3, 134.3, 130.9, 129.1, 128.9, 127.9, 127.7, 125.9, 122.9, 57.7, 14.3; **HRMS** (ESI) Calcd. for

$C_{18}H_{18}NO_2$, $[M+H]^+$ 280.1332. Found: 280.1331.

3. Scope of the reactions

3.1 General procedure for the synthesis of vicinal amino alcohols 2

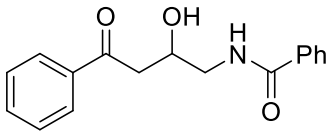


1 **2**

To a solution of **1** (0.3 mmol) in 1,4-dioxane (4 mL) was added $Sc(OTf)_3$ (30 mg, 0.06 mmol). The reaction mixture was stirred at ambient temperature until the disappearance of **1** (monitored by TLC). The reaction was quenched with saturated aqueous $NaHCO_3$ (5 mL), and extracted with CH_2Cl_2 (3×5 mL). The combined organic extracts were washed with brine, dried over $MgSO_4$. After filtration and concentration *in vacuo*, the residue was purified by flash column chromatography on silica gel to give the product **2**.

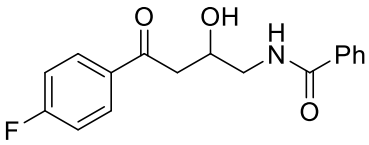
3.2. Characterization of vicinal amino alcohols 2

_N_-(2-hydroxy-4-oxo-4-phenylbutyl)benzamide (2a)



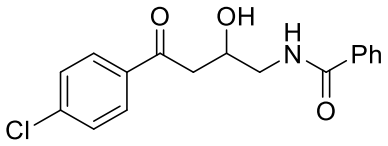
White solid (47 mg, 84% yield). **m.p.** 155-156 ℃; **IR** (KBr) ν 3378, 1685, 1623, 1531 cm^{-1}; **^{1}H NMR** (400MHz, CDCl3, TMS) δ (ppm) 7.97-7.94 (m, 2H), 7.83-7.80 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.55-7.42 (m, 5H), 6.73 (br, 1H), 4.45 (ddd, *J* = 12.0, 6.7, 3.3 Hz, 1H), 3.80 (ddd, *J* = 13.9, 6.2, 3.3 Hz, 1H), 3.57 (ddd, *J* = 13.8, 6.7, 5.6 Hz, 1H), 3.30 (dd, *J* = 17.9, 3.3 Hz, 1H), 3.16 (dd, *J* = 17.9, 8.8 Hz, 1H); **^{13}C NMR** (100MHz, Methanol-*d*$_4$, TMS) δ (ppm) 200.5, 170.7, 138.5, 135.6, 134.4, 132.70, 129.7, 129.5, 129.3, 128.3, 68.2, 46.8, 44.6; **HRMS** (ESI) Calcd. for $C_{17}H_{17}NO_3$, $[M+Na]^+$ 306.1101. found: 306.1103.

_N_-(4-(4-fluorophenyl)-2-hydroxy-4-oxobutyl)benzamide (2b)



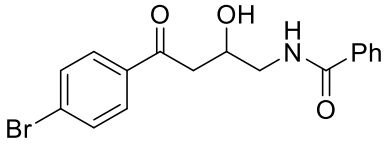
White solid (44 mg, 73% yield). **m.p.** 168-169 ℃; **IR** (KBr) ν 3390, 1688, 1625, 1597, 1534 cm^{-1}; **^{1}H NMR** (400MHz, Methanol-*d*$_4$, TMS) δ (ppm) 8.08-8.04 (m, 2H), 7.84-7.81 (m, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.20 (t, *J* = 8.8 Hz, 2H), 4.48-4.42 (m, 1H), 3.58 (dd, *J* = 13.6, 5.1 Hz, 1H), 3.52 (dd, *J* = 13.6, 6.6 Hz, 1H), 3.25-3.14 (m, 2H); **^{13}C NMR** (100MHz, Methanol-*d*$_4$, TMS) δ (ppm) 198.8, 170.7, 168.5, 166.0, 135.6, 135.2, 132.7, 132.2 (d, *J* = 37.2 Hz), 129.5, 128.3, 116.6 (d, *J* = 88 Hz), 68.2, 46.8; 44.5; **HRMS** (ESI) Calcd. for $C_{17}H_{16}NO_3F$, $[M+Na]^+$ 324.1006. found: 324.1007.

_N_-(4-(4-chlorophenyl)-2-hydroxy-4-oxobutyl)benzamide (2c)



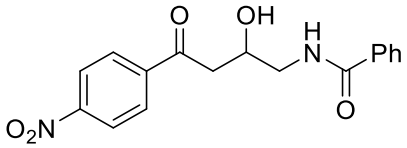
White solid (48 mg, 76% yield). **m.p.** 169-171 ℃; **IR** (KBr) ν 3382, 3354, 1685, 1624, 1528 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.89 (d, *J* = 8.3 Hz, 2H), 7.80 (d, *J* = 7.3 Hz, 2H), 7.53-7.44 (m, 5H), 6.69 (s, 1H), 4.43 (s, 1H), 3.82-3.75 (m, 2H), 3.62-3.55 (m, 1H), 3.24 (dd, *J* = 17.6, 3.0 Hz, 1H), 3.13 (dd, *J* = 17.7, 8.6 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 198.9, 168.9, 140.2, 134.9, 133.8, 131.8, 129.7, 129.0, 128.6, 127.1, 67.2, 45.1, 42.7; **HRMS** (ESI) Calcd. for $C_{17}H_{16}NO_3Cl$, $[M+Na]^+$ 340.0711. found: 340.0712.

N-(4-(4-bromophenyl)-2-hydroxy-4-oxobutyl)benzamide (2d)



White solid (53 mg, 73% yield). **m.p.** 172-173 ℃; **IR** (KBr) ν 3351, 3304, 1691, 1630, 1541 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.83-7.80 (m, 4H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 2H), 6.72 (s, 1H), 4.43 (s, 1H), 3.87 (s, 1H), 3.78 (ddd, *J* = 13.8, 6.1, 3.2 Hz, 1H), 3.61-3.54 (m, 1H), 3.24 (dd, *J* = 17.8, 3.2 Hz, 1H), 3.12 (dd, *J* = 17.9, 8.7 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 199.6, 168.3, 135.2, 134.3, 132.3, 131.9, 129.8, 129.3, 128.8, 127.1, 67.6, 44.9, 42.5; **HRMS** (ESI) Calcd. for $C_{17}H_{16}NO_3Br$, $[M+Na]^+$ 384.0206. found: 384.0207.

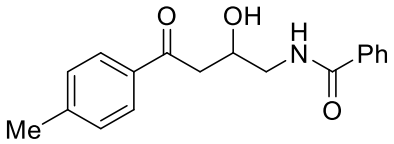
N-(2-hydroxy-4-(4-nitrophenyl)-4-oxobutyl)benzamide (2e)



Light yellow solid (30 mg, 46% yield). **m.p.** 180-182 ℃; **IR** (KBr) ν 3346, 1700, 1631, 1515 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 8.31 (d, *J* = 8.8 Hz, 2H), 8.11 (d, *J* = 8.9 Hz, 2H), 7.81-7.79 (m, 2H), 7.54-7.43 (m, 3H), 6.69 (s, 1H), 4.47 (ddd, *J* = 10.0, 6.9, 3.6 Hz, 1H), 3.78 (ddd, *J* = 14.0, 6.0, 3.3 Hz, 1H), 3.65-3.59 (m, 1H), 3.30

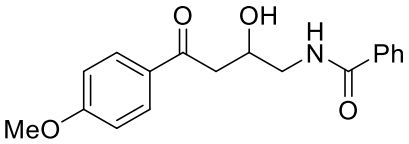
(dd, *J* = 17.9, 3.6 Hz, 1H), 3.22 (dd, *J* = 18.0, 8.3 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$+Methanol-d_4, TMS) δ (ppm) 198.2, 169.0, 150.5, 141.2, 133.8, 131.8, 129.3, 128.6, 127.1, 123.9, 67.0, 45.2, 43.5; **HRMS** (ESI) Calcd. for $C_{17}H_{16}N2O_5$, $[M+Na]^+$ 351.0951. found: 351.0955.

_N_-(2-hydroxy-4-oxo-4-p-tolylbutyl)benzamide (2f)



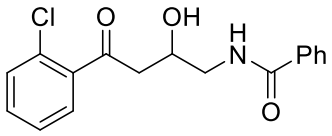
White solid (45 mg, 76% yield). **m.p.** 171-172 ℃; **IR** (KBr) ν 3383, 1681, 1625, 1531 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.85 (d, *J* = 8.2 Hz, 2H), 7.82-7.80 (m, 2H), 7.54-7.49 (m, 1H), 7.45-7.42 (m, 2H), 7.26 (t, *J* = 4.0 Hz, 3H), 6.79 (s, 1H), 4.43 (s, 1H), 4.04 (s, 1H), 3.78 (ddd, *J* = 13.8, 6.2, 3.3 Hz, 1H), 3.55 (ddd, *J* = 13.7, 6.7, 5.6 Hz, 1H), 3.26 (dd, *J* = 17.7, 3.2 Hz, 1H), 3.12 (dd, *J* = 17.7, 8.9 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 200.3, 168.2, 145.0, 134.4, 134.1, 131.8, 129.6, 128.7, 128.4, 127.1, 67.7, 44.9, 42.2, 21.9; **HRMS** (ESI) Calcd. for $C_{18}H_{19}NO_3$, $[M+Na]^+$ 320.1257. found: 320.1257.

_N_-(2-hydroxy-4-(4-methoxyphenyl)-4-oxobutyl)benzamide (2g)



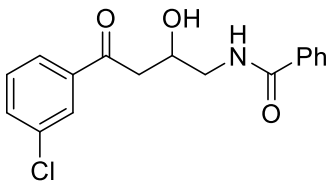
White solid (43 mg, 69% yield). **m.p.** 158-159 ℃; **IR** (KBr) ν 3386, 1678, 1626, 1601, 1532 cm^{-1}; **^{1}H NMR** (400MHz, Methanol-d_4, TMS) δ (ppm) 7.96 (d, *J* = 8.9 Hz, 2H), 7.83-7.80 (m, 2H), 7.54-7.49 (m, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 4.46-4.40 (m, 1H), 3.86 (s, 3H), 3.59 (dd, *J* = 13.6, 5.0 Hz, 1H), 3.51 (dd, *J* = 13.6, 6.6 Hz, 1H), 3.21-3.11 (m, 2H); **^{13}C NMR** (100MHz, Methanol-d_4, TMS) δ (ppm) 199.4, 170.7, 165.4, 135.7, 132.6, 131.7, 131.6, 129.5, 128.3, 114.9, 68.6, 56.1, 46.9, 44.3; **HRMS** (ESI) Calcd. for $C_{18}H_{19}NO_4$, $[M+Na]^+$ 336.1206. found: 336.1208.

_N_-(4-(2-chlorophenyl)-2-hydroxy-4-oxobutyl)benzamide (2h)



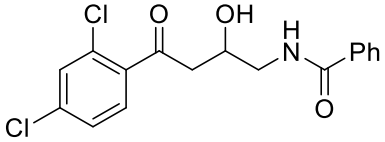
White solid (38 mg, 60% yield). **m.p.** 114-115 ℃; **IR** (KBr) ν 3317, 1702, 1633, 1544 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.81-7.78 (m, 2H), 7.53-7.49 (m, 2H), 7.46-7.41 (m, 4H), 7.37-7.32 (m, 1H), 6.72 (br, 1H), 4.43 (ddd, *J* = 11.8, 6.8, 3.3 Hz, 1H), 3.77 (ddd, J = 13.9, 6.2, 3.2 Hz, 1H), 3.53 (ddd, *J* = 13.8, 6.8, 5.4 Hz, 1H), 3.28 (dd, *J* = 17.8, 3.5 Hz, 1H), 3.15 (dd, *J* = 17.8, 8.6 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 203.3, 168.4, 138.4, 134.3, 132.5, 131.8, 131.3, 131.0, 129.4, 128.8, 127.2, 127.1, 67.8, 47.0, 45.1; **HRMS** (ESI) Calcd. for $C_{17}H_{16}ClNO_3$, $[M+Na]^+$ 340.0711. found: 340.0714.

_N_-(4-(3-chlorophenyl)-2-hydroxy-4-oxobutyl)benzamide (2i)



White solid (42 mg, 66% yield). **m.p.** 127-128 ℃; **IR** (KBr) ν 3339, 1693, 1631, 1538 cm^{-1}; **^{1}H NMR** (400MHz, Methanol-d_4, TMS) δ (ppm) 7.96-7.94 (m, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.84-7.72 (m, 2H), 7.61-7.59 (m, 1H), 7.55-7.44 (m, 4H), 4.48-4.42 (m, 1H), 3.60-3.50 (m, 2H), 3.20 (d, *J* = 6.2 Hz, 2H); **^{13}C NMR** (100MHz, Methanol-d_4, TMS) δ (ppm) 199.0, 170.7, 140.2, 135.9, 135.5, 134.1, 132.7, 131.4, 129.6, 129.1, 128.3, 127.7, 68.0, 46.7, 44.7; **HRMS** (ESI) Calcd. for $C_{17}H_{16}ClNO_3$, $[M+Na]^+$ 340.0711. found: 340.0711.

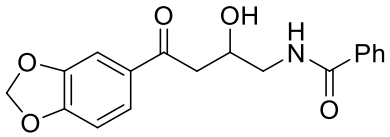
_N_-(4-(2,4-dichlorophenyl)-2-hydroxy-4-oxobutyl)benzamide (2j)



White solid (31 mg, 43% yield). **m.p.** 151-152 ℃; **IR** (KBr) ν 3339, 1704, 1632, 1543 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.85-7.78 (m, 2H), 7.53-7.50 (m, 2H),

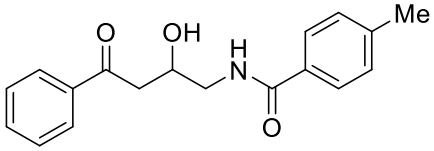
7.46-7.43 (m, 3H), 7.33 (dd, *J* = 8.3, 1.9 Hz, 1H), 6.71 (s, 1H), 4.42 (ddd, *J* = 11.7, 6.8, 3.3 Hz, 1H), 3.76 (ddd, *J* = 13.9, 6.2, 3.2 Hz, 1H), 3.57-3.51 (m, 1H), 3.25 (dd, *J* = 17.8, 3.4 Hz, 1H), 3.15 (dd, *J* = 17.8, 8.5 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 201.8, 168.4, 138.4, 136.5, 134.2, 132.6, 131.9, 130.9, 130.7, 128.8, 127.7, 127.1, 67.8, 47.0, 45.1; **HRMS** (ESI) Calcd. for $C_{17}H_{15}Cl_2NO_3$, $[M+Na]^+$ 374.0321. found: 374.0324.

_N_-(4-(benzo[_d_][1,3]dioxol-5-yl)-2-hydroxy-4-oxobutyl)benzamide (2k)



White solid (26 mg, 40% yield). **m.p.** 180-181 ℃; **IR** (KBr) ν 3370, 3313, 1671, 1633, 1542 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.77 (d, *J* = 7.7 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.42-7.38 (m, 3H), 6.82 (d, *J* = 8.2 Hz, 1H), 6.01 (s, 2H), 4.39-4.33 (m, 1H), 3.61 (dd, *J* = 13.8, 3.9 Hz, 1H), 3.47 (dd, *J* = 13.8, 6.8 Hz, 1H), 3.13-3.05 (m, 2H); **^{13}C NMR** (100MHz, $CDCl_3$+Methanol-d_4, TMS) δ (ppm) 198.2, 169.3, 152.5, 148.5, 134.1, 131.9, 131.6, 128.7, 127.3, 125.2, 108.1, 107.9, 102.2, 67.5, 45.4, 42.8; **HRMS** (ESI) Calcd. for $C_{18}H_{17}NO_5$, $[M+Na]^+$ 350.0999. found: 350.0999.

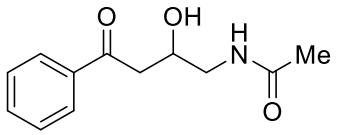
_N_-(2-hydroxy-4-oxo-4-phenylbutyl)-4-methylbenzamide (2l)



White solid (44 mg, 74% yield). **m.p.** 163-165 ℃; **IR** (KBr) ν 3378, 1685, 1621, 1539 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.71 (d, *J* = 8.2 Hz, 2H), 7.62-7.58 (m, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.23 (d, *J* = 6.7 Hz, 1H), 6.69 (s, 1H), 4.46-4.41 (m, 1H), 3.78 (ddd, *J* = 13.9, 6.1, 3.2 Hz, 1H), 3.60-3.53 (m, 1H), 3.29 (dd, *J* = 17.8, 3.3 Hz, 1H), 3.16 (dd, *J* = 17.9, 8.8 Hz, 1H), 2.40 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 200.7, 168.2, 142.3, 136.5, 134.0, 131.4, 129.4, 128.9, 128.3, 127.1,

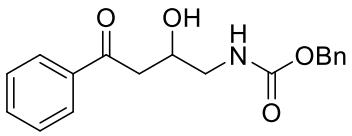
67.7, 44.9, 42.4, 21.6; **HRMS** (ESI) Calcd. for $C_{18}H_{19}NO_3$, $[M+H]^+$ 298.1438. found: 298.1435.

N-(2-hydroxy-4-oxo-4-phenylbutyl)acetamide (2m)



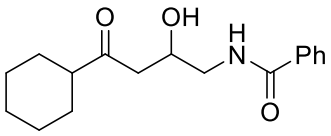
White solid (27 mg, 61% yield). **m.p.** 132-133 ℃; **IR** (KBr) ν 3354, 1680, 1664, 1551 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.96-7.94 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 6.09 (s, 1H), 4.36-4.30 (m, 1H), 3.58 (ddd, *J* = 13.8, 6.3, 3.2 Hz, 1H), 3.37-3.30 (m, 1H), 3.22 (dd, *J* = 17.8, 3.3 Hz, 1H), 3.10 (dd, *J* = 17.8, 8.7 Hz, 1H), 2.04 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 200.6, 171.0, 136.5, 134.0, 128.9, 128.3, 67.5, 44.6, 42.4, 23.4; **HRMS** (ESI) Calcd. for $C_{12}H_{15}NO_3$, $[M+H]^+$ 222.1125. found: 222.1127.

benzyl 2-hydroxy-4-oxo-4-phenylbutylcarbamate (2n)



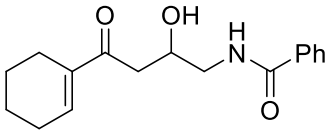
White solid (49 mg, 79% yield). **m.p.** 92-93 ℃; **IR** (KBr) ν 3432, 3358, 1713, 1680, 1535 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.93 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.37-7.30 (m, 5H), 5.32 (s, 1H), 5.12 (s, 2H), 4.36-4.31 (m, 1H), 3.66 (d, *J* = 2.1 Hz, 1H), 3.48 (ddd, *J* = 13.6, 6.1, 3.4 Hz, 1H), 3.34-3.27 (m, 1H), 3.20 (dd, *J* = 17.8, 2.6 Hz, 1H), 3.09 (dd, *J* = 17.8, 9.0 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 200.5, 157.1, 136.6, 136.5, 133.9, 128.9, 128.7, 128.3, 128.3, 128.2, 67.5, 67.0, 46.0, 42.2; **HRMS** (ESI) Calcd. for $C_{18}H_{19}NO_4$, $[M+Na]^+$ 336.1206. found: 336.1206.

N-(4-cyclohexyl-2-hydroxy-4-oxobutyl)benzamide (2o)



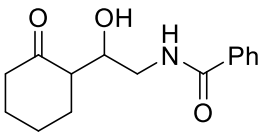
White solid (33 mg, 57% yield). **m.p.** 130-131 ℃; **IR** (KBr) ν 3405, 2926, 1710, 1628, 1528 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.78 (d, *J* = 7.3 Hz, 2H), 7.50 (t, *J* = 7.1 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 6.70 (s, 1H), 4.23-4.19 (m, 1H), 3.66 (ddd, *J* = 13.7, 6.1, 3.1 Hz, 1H), 3.45-3.38 (m, 1H), 2.74 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.61 (dd, *J* = 17.9, 8.9 Hz, 1H), 2.36-2.30 (m, 1H), 1.80 (dd, *J* = 25.8, 10.3 Hz, 4H), 1.66 (d, *J* = 10.9 Hz, 1H), 1.35-1.13 (m, 5H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 215.5, 168.1, 134.3, 131.8, 128.7, 127.1, 67.4, 51.5, 44.8, 44.1, 28.43, 28.37, 25.8, 25.6; **HRMS** (ESI) Calcd. for $C_{17}H_{23}NO_3$, $[M+Na]^+$ 312.1570. found: 312.1572.

N-(4-cyclohexenyl-2-hydroxy-4-oxobutyl)benzamide (2p)



White solid (40 mg, 69% yield). **m.p.** 127-128 ℃; **IR** (KBr) ν 3376, 2938, 1663, 1626, 1530 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.80 (d, *J* = 7.4 Hz, 2H), 7.47 (dt, *J* = 14.0, 7.6 Hz, 3H), 6.96 (s, 1H), 6.75 (br, 1H), 4.27 (ddd, *J* = 12.2, 6.5, 3.1 Hz, 1H), 4.02 (br, 1H), 3.74-3.69 (m, 1H), 3.50-3.43 (m, 1H), 2.96 (d, *J* = 17.3 Hz, 1H), 2.78 (dd, *J* = 17.4, 9.1 Hz, 1H), 2.23 (d, *J* = 18.5 Hz, 4H), 1.62 (br, 4H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 201.7, 168.1, 142.5, 139.3, 134.4, 131.7, 128.7, 127.1, 67.8, 44.9, 40.6, 26.3, 22.9, 21.9, 21.5; **HRMS** (ESI) Calcd. for $C_{17}H_{21}NO_3$, $[M+Na]^+$ 310.1414. found: 310.1416.

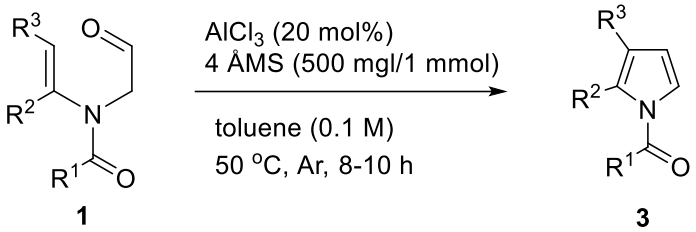
N-(2-hydroxy-2-(2-oxocyclohexyl)ethyl)benzamide (2q)



White solid (39 mg, 75% yield). **m.p.** 137-138 ℃; **IR** (KBr) ν 3303, 1701, 1633, 1551

cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.82 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 4.23 (dd, *J* = 11.9, 5.5 Hz, 1H), 3.51 (dd, *J* = 13.6, 4.7 Hz, 1H), 3.42 (dd, *J* = 13.6, 7.2 Hz, 1H), 2.53-2.48 (m, 1H), 2.41-2.25(m, 3H), 2.06-1.93 (m, 2H), 1.74-1.66 (m, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 214.2, 170.7, 135.6, 132.7, 129.5, 128.3, 69.0, 54.7, 45.1, 43.2, 29.3, 28.8, 25.5; **HRMS** (ESI) Calcd. for $C_{15}H_{19}NO_3$, $[M+Na]^+$ 284.1257. found: 284.1252.

3.3. General procedure for the synthesis of substituted pyrroles 3



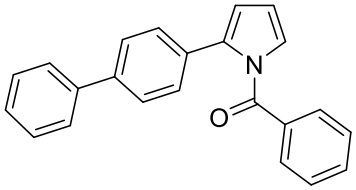
1 **3**

To a solution of **1** (0.5 mmol) in toluene (5 mL) was added $AlCl_3$ (0.1 mmol, 0.2 equiv) and 4 Å molecular sieves (250 mg). The reaction mixture was stirred at 50 °C until the disappearance of **1** (monitored by TLC). After filtration and concentration *in vacuo*, the residue was purified by flash column chromatography on silica gel to give the substituted pyrroles **3**.

3.4. Characterization of substituted pyrroles 3

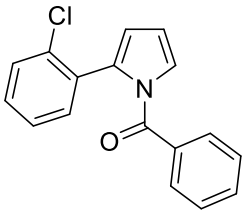
The products **3a-g**, **3k** and **3m** have been reported. The analytical data were in accordance with those reported in the literature[4].

(2-([1,1'-biphenyl]-4-yl)-1H-pyrrol-1-yl)(phenyl)methanone (3c')



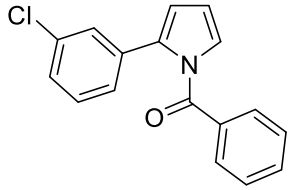
Yellow solid (158 mg, 98% yield). **m.p.** 143-145 ℃; **IR** (KBr) ν 3062, 1699, 1598, 1469, 1449 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.83-7.81 (m, 2H), 7.56 (t, *J* = 7.2 Hz, 3H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.46-7.31 (m, 7H), 7.08 (dd, *J* = 3.2, 1.6 Hz, 1H), 6.50 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.33 (t, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.8, 140.7, 139.6, 136.1, 133.3, 133.0, 132.0, 130.4, 128.7, 128.4, 128.3, 127.2, 127.0, 126.8, 124.9, 115.1, 111.2; **HRMS** (ESI) Calcd. for $C_{23}H_{18}NO$, $[M+H]^+$ 324.1383. Found: 324.1387.

(2-(2-chlorophenyl)-1H-pyrrol-1-yl)(phenyl)methanone (3h)



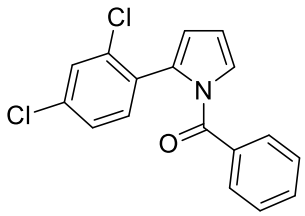
White solid (129 mg, 92% yield). **m.p.** 106-107 ℃; **IR** (KBr) ν 3382, 3105, 3061, 1700, 1598, 1449 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.79-7.77 (m, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 3H), 7.32-7.20 (m, 3H), 7.07 (dd, *J* = 3.2, 1.6 Hz, 1H), 6.40 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.30 (t, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.3, 133.4, 133.0, 132.7, 132.6, 131.3, 130.4, 129.3, 128.9, 128.3, 126.7, 124.0, 115.8, 110.9; **HRMS** (ESI) Calcd. for $C_{17}H_{13}NOCl$, $[M+H]^+$ 282.0680. Found: 282.0685.

(2-(3-chlorophenyl)-1H-pyrrol-1-yl)(phenyl)methanone (3i)



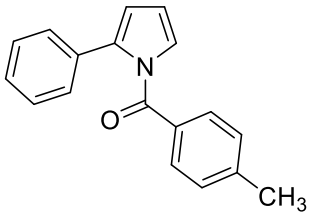
White solid (129 mg, 92% yield). **m.p.** 67-68 ℃; **IR** (KBr) ν 3057, 1695, 1598, 1492, 1447 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.78 (d, J = 7.6 Hz, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.30 (s, 1H), 7.19-7.12 (m, 3H), 7.08 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.46 (dd, *J* = 3.2, 2.0 Hz, 1H), 6.31 (t, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.5, 134.9, 134.8, 133.8, 133.1, 130.3, 129.2, 128.5, 127.9, 127.0, 126.2, 125.2, 115.7, 111.3; **HRMS** (ESI) Calcd. for $C_{17}H_{13}NOCl$, $[M+H]^+$ 282.0680. Found: 282.0685.

(2-(2,4-dichlorophenyl)-1H-pyrrol-1-yl)(phenyl)methanone (3j)



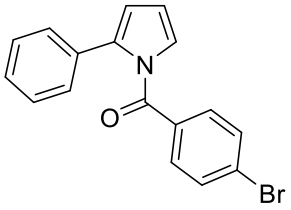
White solid (142 mg, 90% yield). **m.p.** 92-93 ℃; **IR** (KBr) ν 3063, 1704, 1599, 1560, 1489, 1448 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.79-7.77 (m, 2H), 7.60-7.56 (m, 1H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.37-7.34 (m, 2H), 7.27-7.25 (m, 1H), 7.06 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.39 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.32 (t, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.2, 134.1, 134.0, 132.9, 132.7, 131.9, 131.6, 131.4, 130.4, 129.2, 128.4, 127.0, 124.4, 116.2, 111.0; **HRMS** (ESI) Calcd. for $C_{17}H_{12}NOCl_2$, $[M+H]^+$ 316.0291. Found: 316.0294.

(2-phenyl-1H-pyrrol-1-yl)(p-tolyl)methanone (3l)



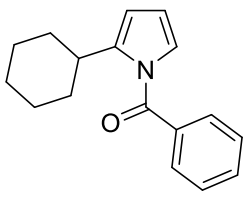
White solid (116mg, 89% yield). **m.p.** 103-105 ℃; **IR** (KBr) ν 3044, 1697, 1605, 1466 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.71 (d, *J* = 8.0 Hz, 2H), 7.31-7.18 (m, 7H), 7.06 (dd, *J* = 3.2, 2.0 Hz, 1H), 6.44 (dd, *J* = 3.2, 1.6 Hz, 1H), 6.29 (t, *J* = 3.2 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.7, 144.0, 136.4, 133.1, 130.7, 130.5, 129.1, 128.0, 127.9, 126.9, 124.8, 114.7, 110.9, 21.7; **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO$, $[M+H]^+$ 262.1226. Found: 262.1231.

(4-bromophenyl)(2-phenyl-1H-pyrrol-1-yl)methanone (3n')



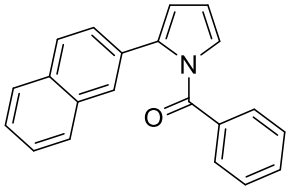
White solid (158mg, 97% yield). **m.p.** 90-91 ℃; **IR** (KBr) ν 3146, 3020, 1701, 1588, 1470 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.63 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.27-7.19 (m, 5H), 7.06 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.45 (dd, *J* = 3.2, 1.6 Hz, 1H), 6.32 (t, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 167.9, 136.4, 132.9, 132.2, 131.8, 131.7, 128.1, 128.0, 127.1, 124.4, 115.1, 111.5; **HRMS** (ESI) Calcd. for $C_{17}H_{13}NOBr$, $[M+H]^+$ 326.0175. Found: 326.0179.

(2-cyclohexyl-1H-pyrrol-1-yl)(phenyl)methanone (3o)



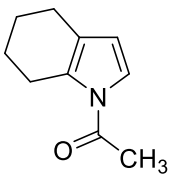
Light yellow oil (123 mg, 97% yield). **IR** (KBr) ν 3427, 2928, 2853, 1736, 1698, 1600, 1448 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.73 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.73 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.14-6.10 (m, 2H), 3.36-3.30 (m, 1H), 2.07 (d, *J* = 12.8 Hz, 2H), 1.80-1.71 (m, 3H), 1.47-1.17 (m, 5H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 169.6, 143.6, 134.7, 132.3, 129.8, 128.3, 123.2, 110.2, 109.6, 36.4, 33.6, 26.6, 26.4; **HRMS** (ESI) Calcd. for $C_{17}H_{20}NO$, $[M+H]^+$ 254.1539. Found: 254.1543.

(2-(naphthalen-2-yl)-1H-pyrrol-1-yl)(phenyl)methanone (3p')



Light yellow solid (146 mg, 98% yield). **m.p.** 144-145 ℃; **IR** (KBr) ν 3055, 1697, 1599, 1450 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.83-7.75 (m, 5H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.46-7.35 (m, 5H), 7.11 (dd, *J* = 3.2, 1.6 Hz, 1H), 6.55 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.35 (t, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.8, 136.5, 133.4, 133.2, 133.0, 132.3, 130.7, 130.4, 128.4, 127.9, 127.6, 127.5, 126.45, 126.41, 126.1, 125.8, 124.9, 115.4, 111.3; **HRMS** (ESI) Calcd. for $C_{21}H_{16}NO$, $[M+H]^+$ 298.1226. Found: 298.1231.

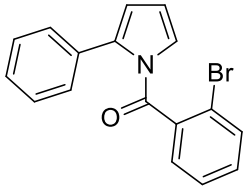
1-(4,5,6,7-tetrahydro-1H-indol-1-yl)ethan-1-one (3q')



White solid (75mg, 92% yield). **m.p.** 55-56 ℃; **IR** (KBr) ν 3405, 2934, 2855, 1713, 1497, 1433 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 6.96 (d, *J* = 3.2 Hz, 1H), 6.05 (d, *J* = 3.2 Hz, 1H), 2.91 (t, *J* = 6.0 Hz, 2H), 2.49 (s, 3H), 2.47-2.43 (m, 2H), 1.81-1.75 (m, 2H), 1.73-1.67 (m, 2H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.9,

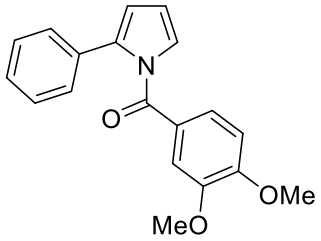
130.9, 122.9, 118.8, 112.6, 25.4, 23.8, 23.3, 23.2, 22.7; **HRMS** (ESI) Calcd. for $C_{10}H_{14}NO$, $[M+H]^+$ 164.1070. Found: 164.1074.

(2-bromophenyl)(2-phenyl-1H-pyrrol-1-yl)methanone (3r)



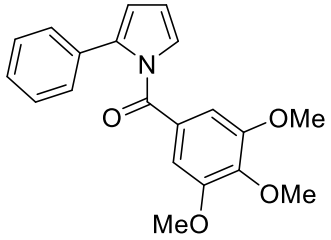
White solid (150mg, 92% yield). **m.p.** 85-87 ℃; **IR** (KBr) ν 3063, 1714, 1327, 760 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.54 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.44-7.39 (m, 3H), 7.33-7.23 (m, 5H), 7.01 (dd, *J* = 3.4, 1.7 Hz, 1H), 6.41 (dd, *J* = 3.3, 1.7 Hz, 1H), 6.34 (t, *J* = 3.3 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 166.9, 136.2, 135.8, 133.2, 133.0, 132.0, 130.1, 128.7, 127.7, 127.24, 127.19, 123.5, 120.5, 116.1, 112.2; **HRMS** (ESI) Calcd. for $C_{17}H_{12}BrNO$, $[M+H]^+$ 326.0175. Found: 326.0172.

(3,4-dimethoxyphenyl)(2-phenyl-1H-pyrrol-1-yl)methanone (3s)



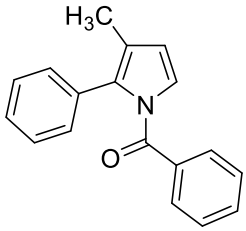
White solid (152mg, 99% yield). **m.p.** 146-147 ℃; **IR** (KBr) ν 3133, 2935, 2841, 1682, 1596, 1510, 1466 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.45 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.35 (d, *J* = 2.0 Hz, 1H), 7.31-7.24 (m, 4H), 7.22-7.18 (m, 1H), 7.11 (dd, *J* = 2.8, 1.6 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 1H), 6.46 (dd, *J* = 3.2, 1.2 Hz, 1H), 6.31 (t, *J* = 3.2 Hz, 1H), 3.93 (s, 3H), 3.88 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.3, 153.4, 148.9, 136.5, 133.2, 128.2, 127.9, 127.0, 125.6, 125.4, 124.9, 114.5, 113.1, 110.9, 110.1, 56.3, 56.1; **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_3$, $[M+H]^+$ 308.1281. Found: 308.1286.

(2-phenyl-1H-pyrrol-1-yl)(3,4,5-trimethoxyphenyl)methanone (3t)



White solid (157mg, 93% yield). **m.p.** 105-106 ℃; **IR** (KBr) ν 3007, 2936, 2837, 1697, 1582, 1502, 1462 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.29-7.24 (m, 4H), 7.22-7.16 (m, 2H), 7.03 (s, 2H), 6.47-6.46 (m, 1H), 6.33 (t, *J* = 3.2 Hz, 1H), 3.89 (s, 3H), 3.85 (s, 6H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.2, 152.8, 142.3, 136.4, 133.1, 128.1, 127.8, 127.0, 124.7, 114.7, 111.1, 108.1, 60.9, 56.3; **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_4$, $[M+H]^+$ 338.1387. Found: 338.1391.

(3-methyl-2-phenyl-1H-pyrrol-1-yl)(phenyl)methanone (3u)

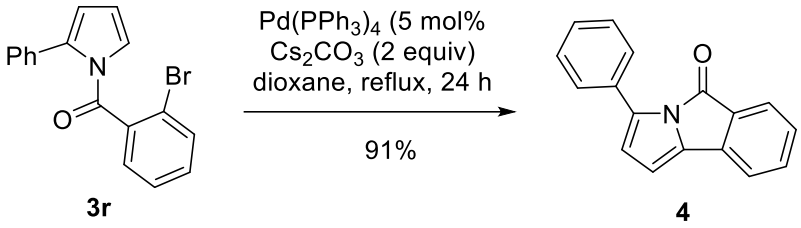


White solid (129mg, 99% yield). **m.p.** 83-84 ℃; **IR** (KBr) ν 3060, 2943, 1694, 1599, 1476 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.75-7.72 (m, 2H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.32-7.28 (m, 2H), 7.25-7.20 (m, 3H), 6.97 (d, *J* = 3.2 Hz, 1H), 6.19 (d, *J* = 3.2 Hz, 1H), 2.10 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 168.3, 133.8, 132.8, 132.5, 131.7, 130.2, 129.5, 128.3, 127.9, 126.8, 123.3, 113.7, 11.7; **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO$, $[M+H]^+$ 262.1226. Found: 262.1231.

4. Procedure for the gram-scale synthesis of compounds 3a, 3q' and 3u

To a solution of the corresponding substrate (**1a**, **1u** 5 mmol; **1q'** 7 mmol) in toluene (**1a**, **1u** 25 mL; **1q'** 35 mL) was added $AlCl_3$ (0.2 equiv, **1a**, **1u** 1 mmol; **1q'** 1.4 mmol) and 4 Å molecular sieve (**1a**, **1u** 2.5 g; **1q**' 3.5 g). The reaction mixture was stirred at 50 ℃ until the disappearance of the substrate (monitored by TLC). After filtration and concentration in vacuo, the residue was purified by flash column chromatography on silica gel to give the product **3a**, **3q'** and **3u**.

5. Synthetic application of 3r and characterization of compound 4



$Pd(PPh_3)_4$ (28.9 mg, 0.025 mmol), Cs_2CO_3 (32.5 mg, 1.0 mmol) and 3r (163.1 mg, 0.5 mmol) were added in a flame-dried round bottom flask fitted with a magnetic stir bar. The flask was purged with dry nitrogen for three times. Dry dioxane (5 mL) was added and the resulting solution was heated to 100 ^oC until the disappearance of **3r** (monitored by TLC). The reaction system was allowed to cool to room temperature and the solution was quenched with saturated NH_4Cl solution, extracted with EtOAc. The combined organic layers were washed with brine and dried over Na_2SO_4. The solvents were removed in vacuo and the residue was then purified by flash column chromatography (PE/EA, 50:1) to afford compound **4** as an organge solid in 91% yield. **m.p.** 114-116 ℃; **IR** (KBr) ν 3063, 1763, 1738, 1615, 1477, 1353, 1208, 753 cm^{-1}; **^{1}H NMR** (400MHz, $CDCl_3$, TMS) δ (ppm) 7.81 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.45-7.40 (m, 3H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 6.29 (d, *J* = 3.2 Hz, 1H), 6.27 (d, *J* = 3.2 Hz, 1H); **^{13}C NMR** (100MHz, $CDCl_3$, TMS) δ (ppm) 163.6, 137.1, 136.2, 135.9, 134.6, 132.1, 130.2, 128.4, 128.3, 127.4, 127.1, 125.9, 119.4, 116.8, 107.9; **HRMS** (ESI) Calcd. for $C_{17}H_{11}NO$, $[M+H]^+$ 246.0913. Found: 246.0911.

6. Crystallographic data and structure refinement of 4

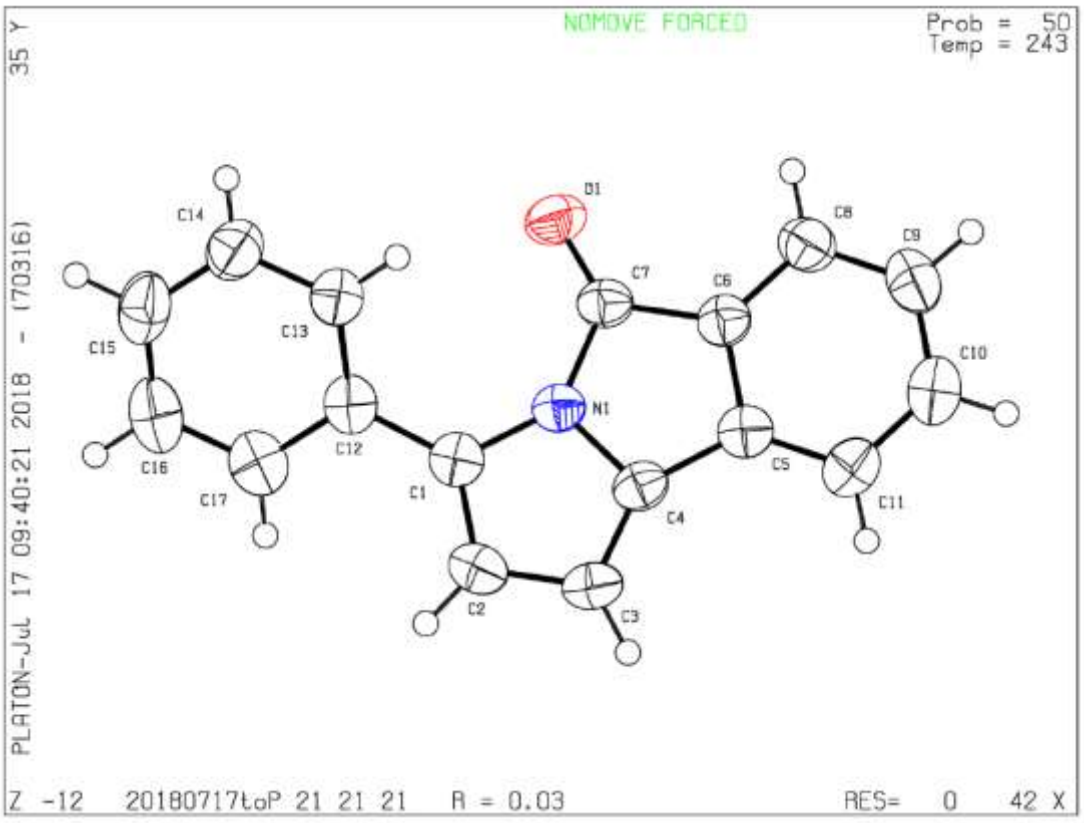


Figure S1. The structure of compound **4**

Indentification code	**4**
Empirical formular	$C_{17}H_{11}NO$
Formula weight	245.2810
Temperature	243.00(10)
Wavelength	1.54184 Å
Crystal system	orthorhombic
Space group	P 21 21 21
Unit cell dimen	a = 6.22900(10) Å α = 90.00°
	b = 13.6065(2) Å β = 90.00°
	c = 14.6177(3) Å γ = 90.00°
Volumn	1238.92(4) $Å^3$
Z	4
Crystal size	0.55×0.45×0.3 mm
CCDC Number 1860475	

7. References

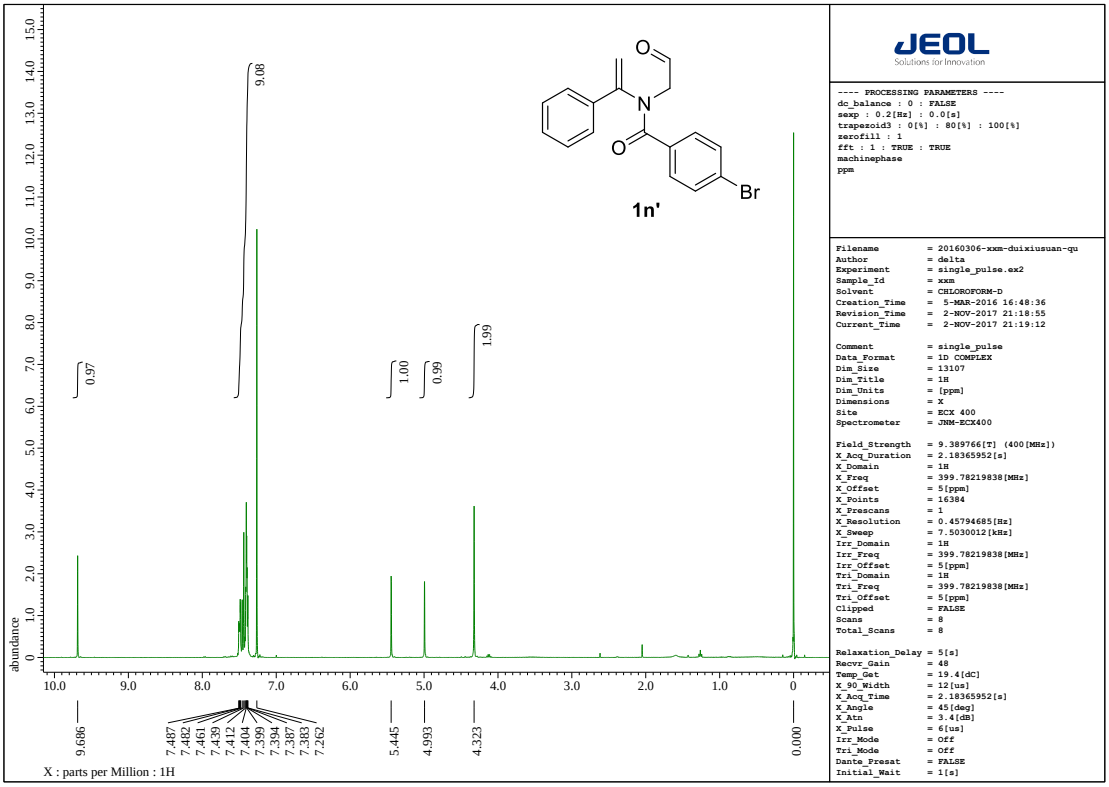
[1] (a) L. Yang, D.- X. Wang, Z.- T. Huang and M.- X. Wang, *J. Am. Chem. Soc.*, **2009**, *131*, 10390-10391. (b) L. Yang, C. - H. Lei, D.- X. Wang, Z.- T. Huang and M.- X. Wang, *Org. Lett.*, **2010**, *12*, 3918-3921.

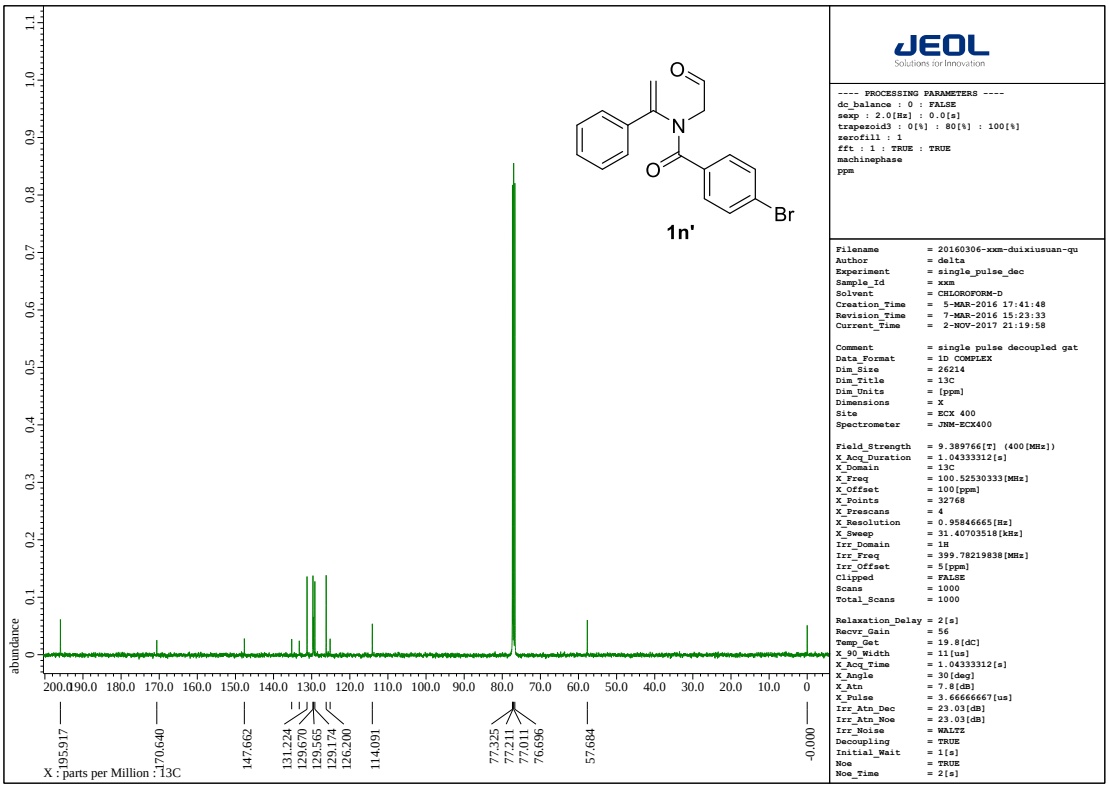
[2] C.-H. Lei, D.-X. Wang, L. Zhao, J. Zhu and M.-X. Wang, *J. Am. Chem. Soc.*, **2013**, *135*, 4708.

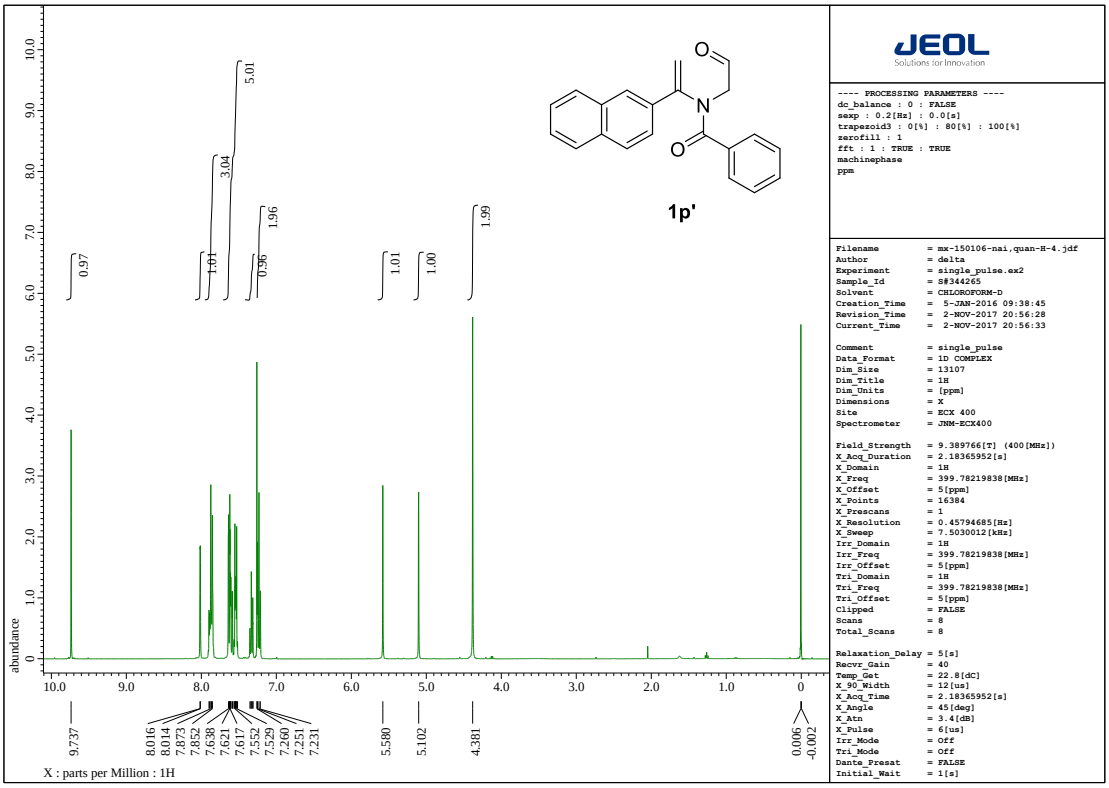
[3] C.-H. Lei, D.-X. Wang, L. Zhao, J. Zhu and M.-X. Wang, *Chem. Eur. J.*, **2013**, *19*, 16981.

[4] Ueda H., Tokuyama H., et al. *Org. Lett.*, **2014**, *16*, 4948.

8. Copies of ^{1}H and ^{13}C NMR spectra





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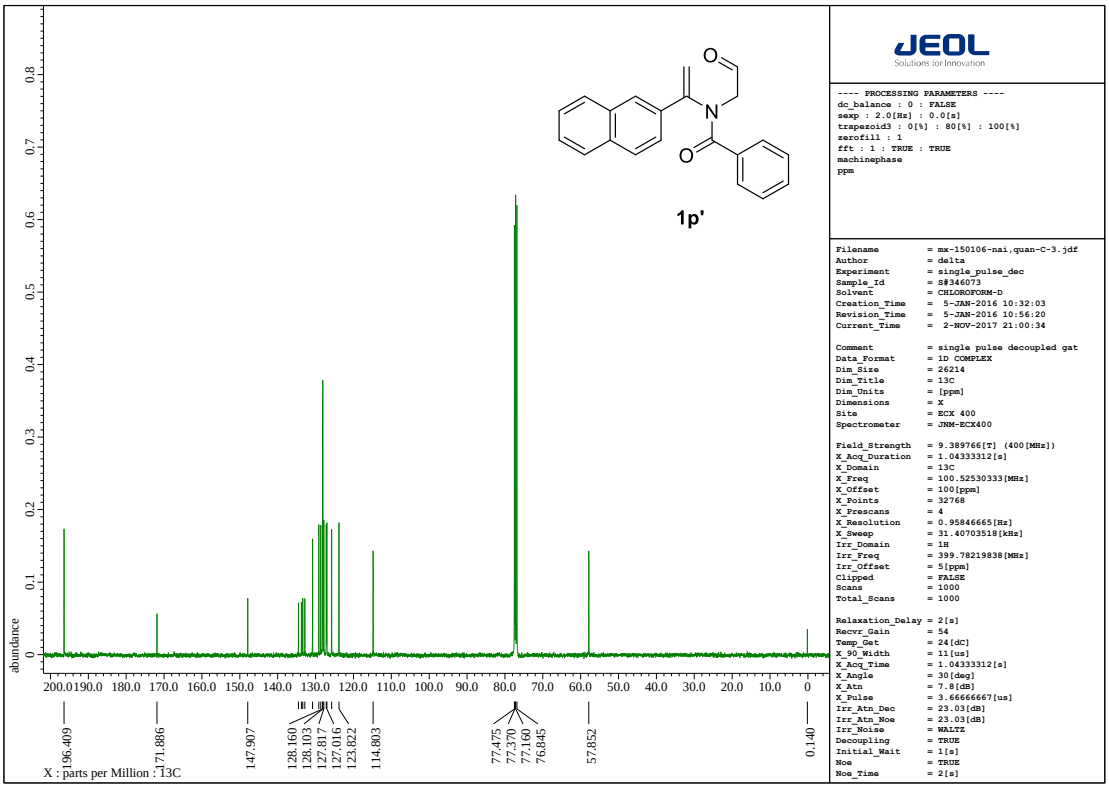


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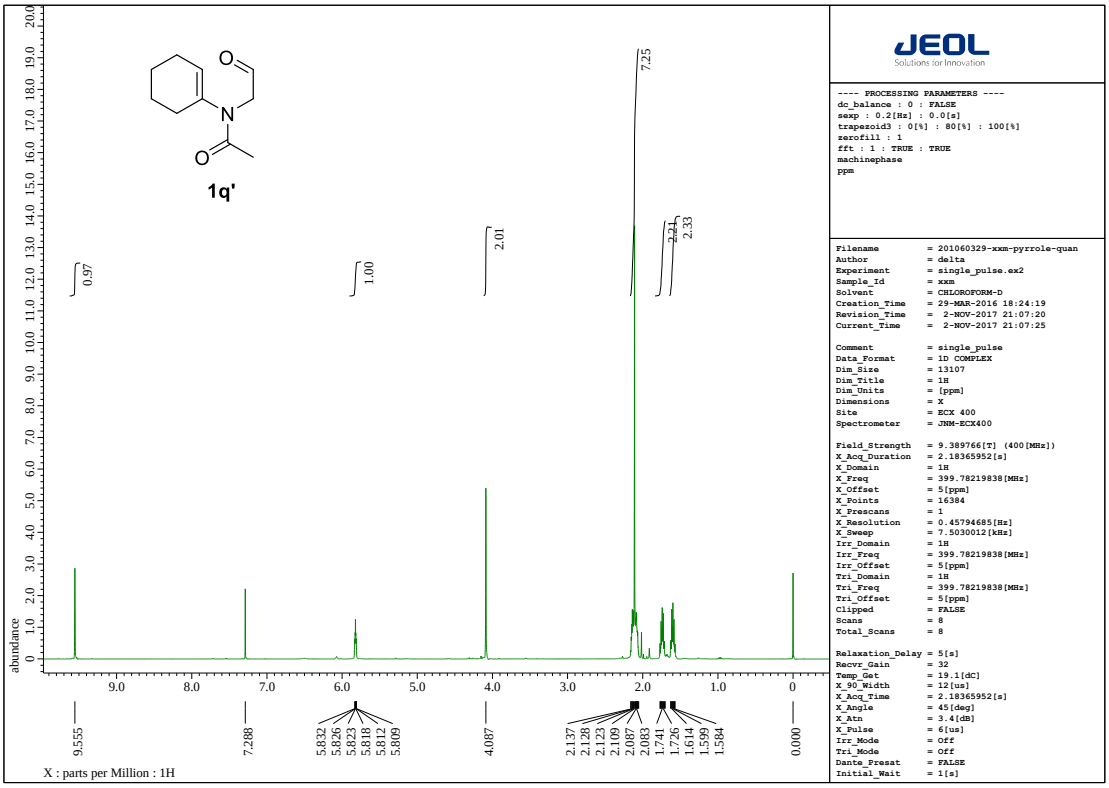
Noe_Time          = 2[s]
```



JEOL
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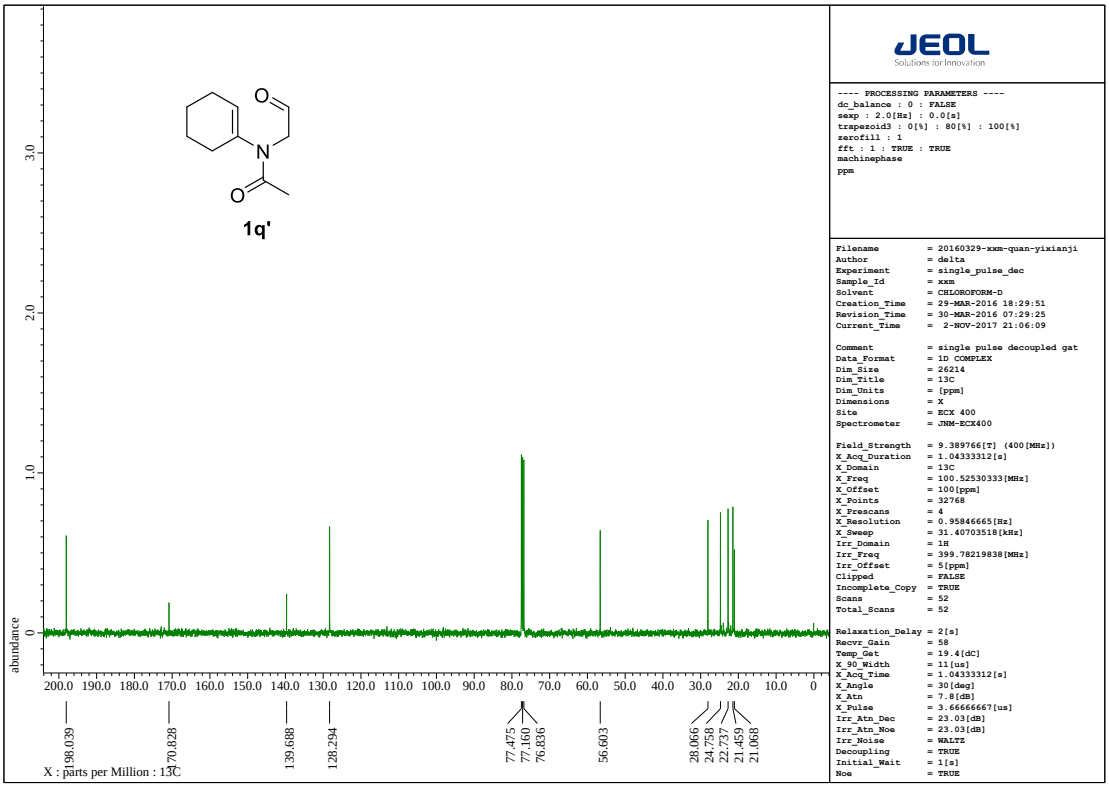
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Filename          = 201060329-xxm-pyrrole-quan
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 29-MAR-2016 18:24:19
Revision_Time     =  2-NOV-2017 21:07:20
Current_Time      =  2-NOV-2017 21:07:25

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 32
Temp_Get          = 19.1[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



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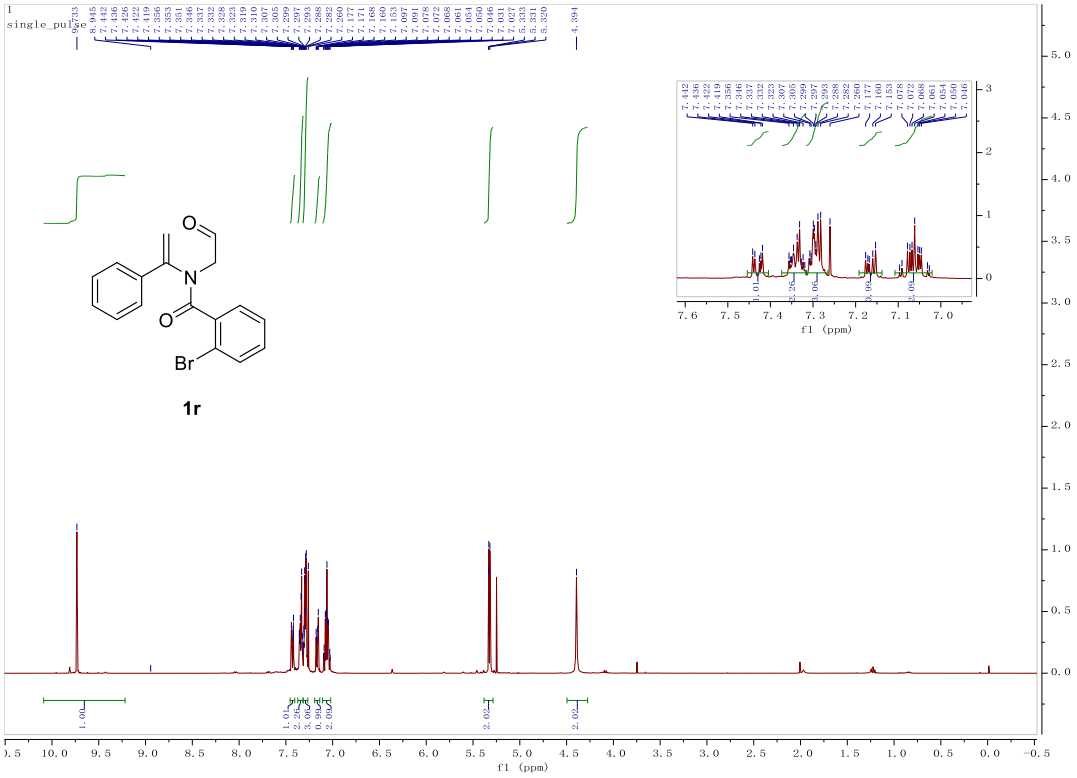
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

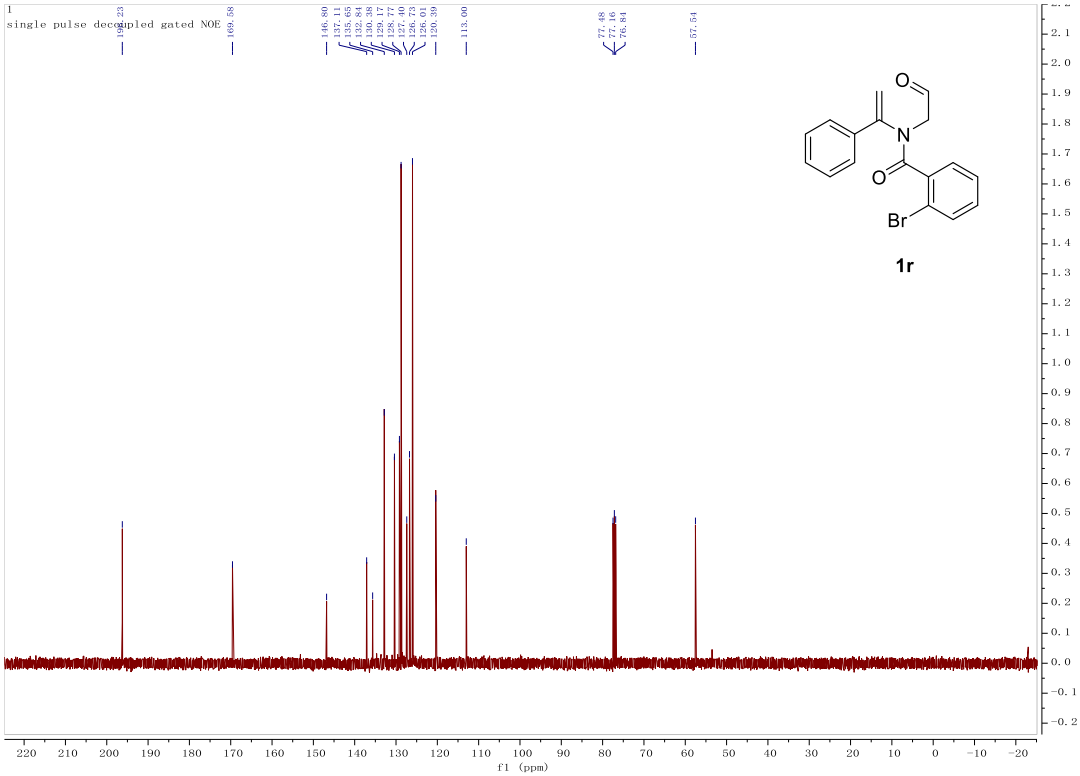
Filename          = 20160329-xxm-quan-yixianji
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 29-MAR-2016 18:29:51
Revision_Time     = 30-MAR-2016 07:29:25
Current_Time      =  2-NOV-2017 21:06:09

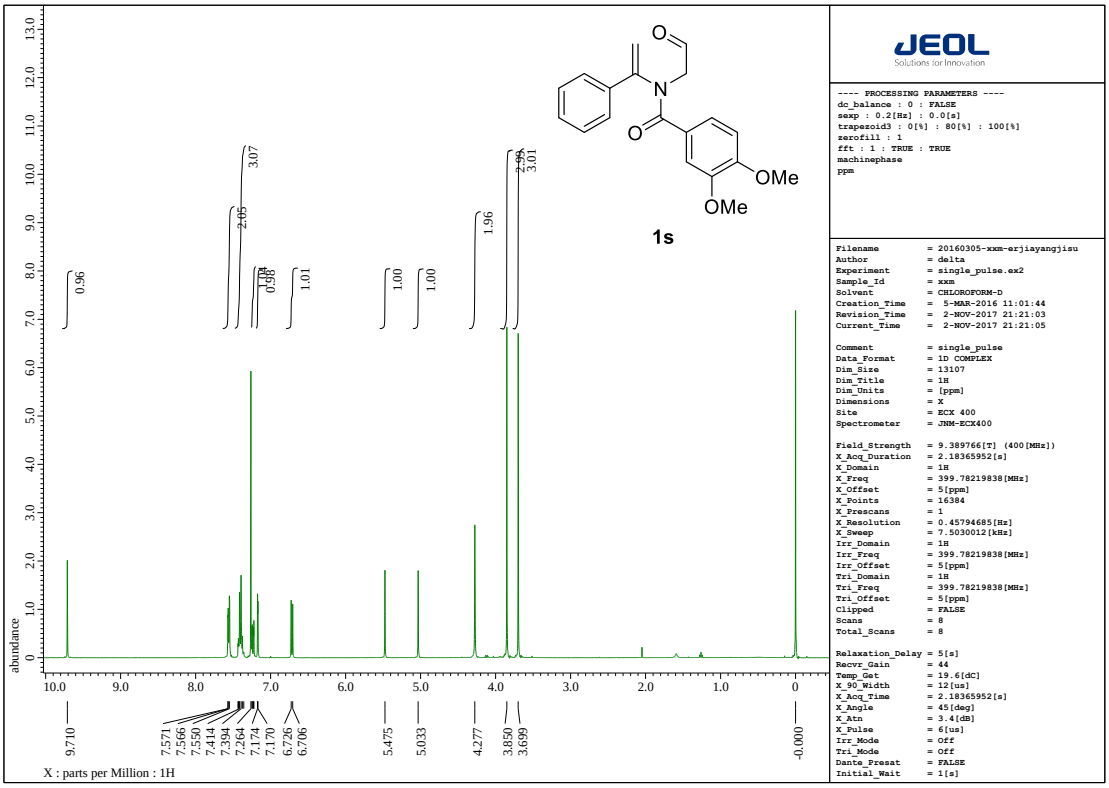
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Incomplete_Copy   = TRUE
Scans             = 52
Total_Scans       = 52

Relaxation_Delay = 2[s]
Recvr_Gain        = 58
Temp_Get          = 19.4[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```


single_pul
1r
f1 (ppm)


single pulse decoupled gated NOE
1r
f1 (ppm)



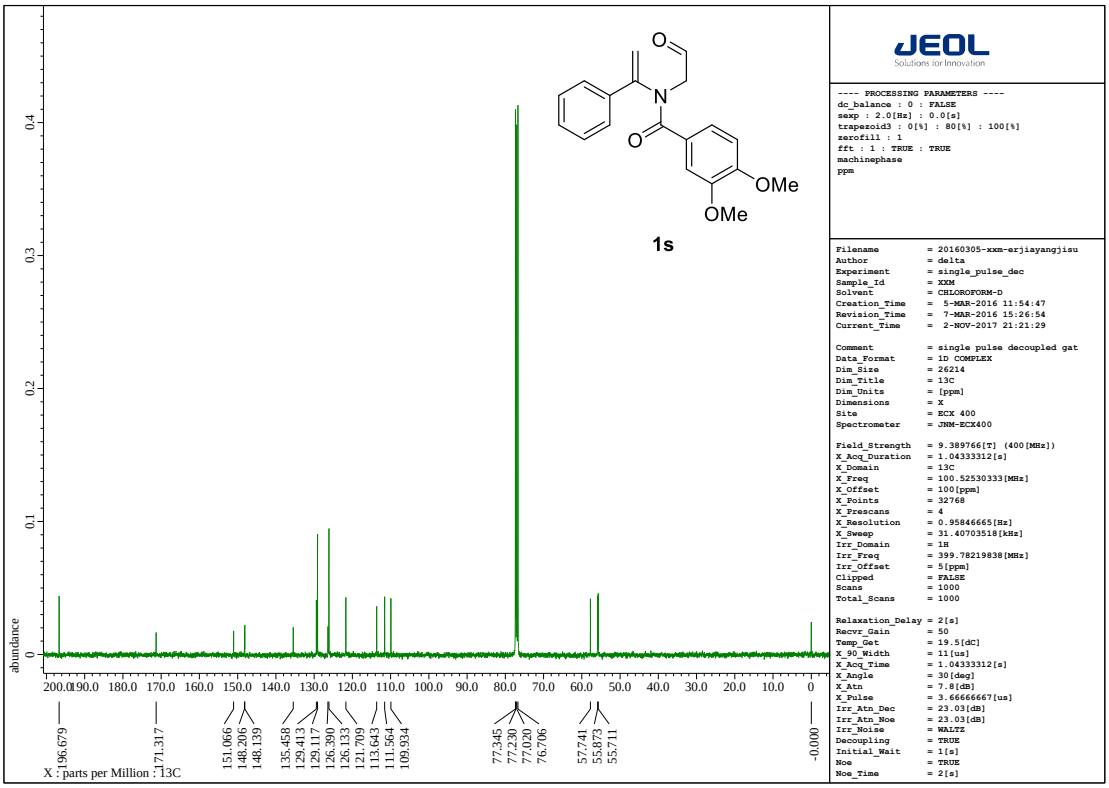

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Filename          = 20160305-xxm-erjiayangjisu
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2016 11:01:44
Revision_Time     =  2-NOV-2017 21:21:03
Current_Time      =  2-NOV-2017 21:21:05

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 44
Temp_Get          = 19.6[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



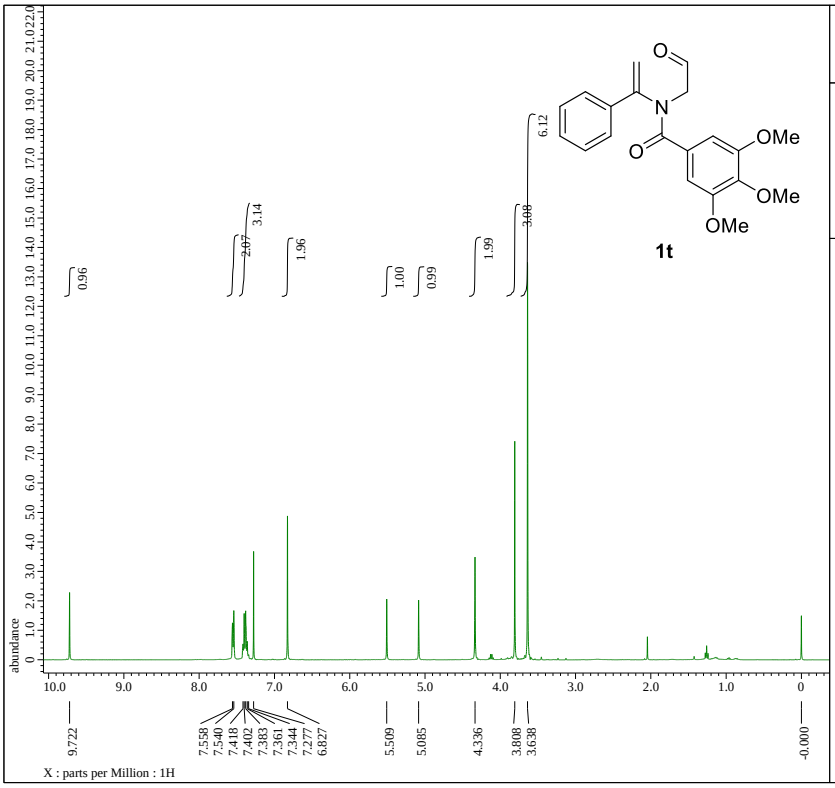

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Filename          = 20160305-xxm-erjiayangjisu
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = XXM
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2016 11:54:47
Revision_Time     =  7-MAR-2016 15:26:54
Current_Time      =  2-NOV-2017 21:21:29

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1000
Total_Scans       = 1000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 19.5[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



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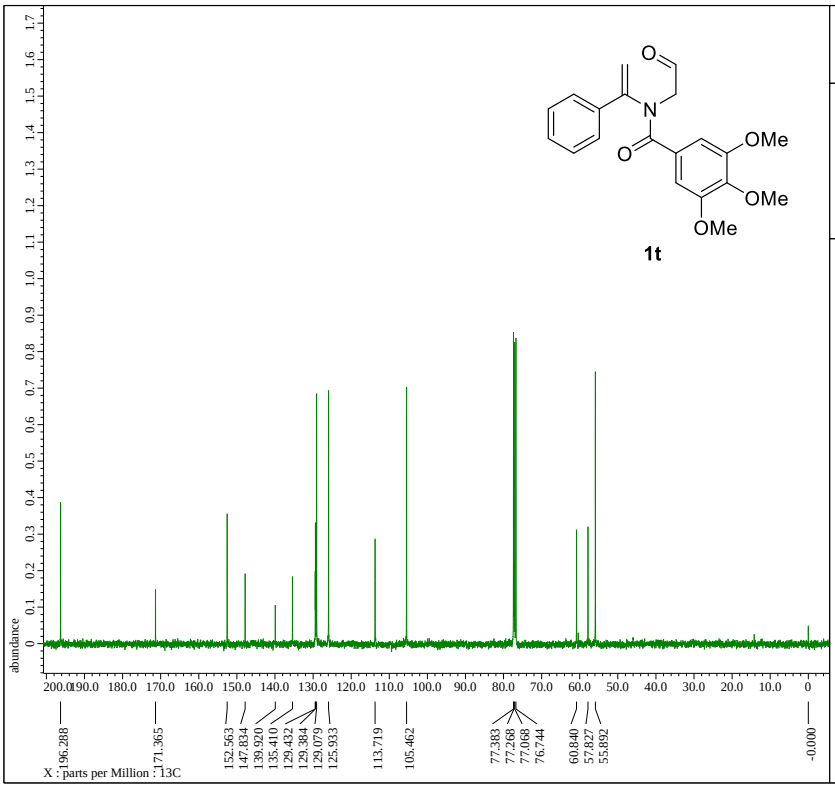
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

```
Filename          = 20160307-xxm-trioMequan-Hs
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     =  7-MAR-2016 15:01:09
Revision_Time     =  2-NOV-2017 21:22:09
Current_Time      =  2-NOV-2017 21:22:17

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 34
Temp_Get          = 19.3[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



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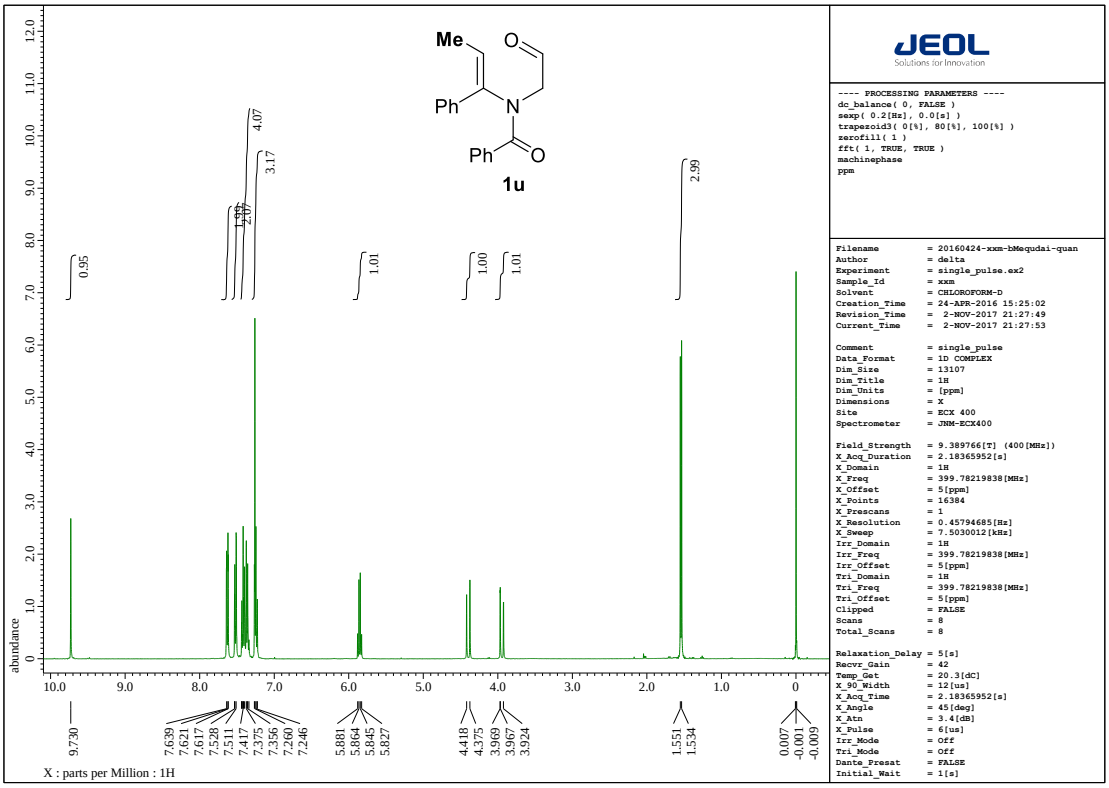
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

```
Filename          = 20160307-xxm-trioMesuanqua
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     =  7-MAR-2016 15:10:55
Revision_Time     =  7-MAR-2016 15:16:32
Current_Time      =  2-NOV-2017 21:23:04

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Incomplete_Copy   = TRUE
Scans             = 137
Total_Scans       = 137

Relaxation_Delay = 2[s]
Recvr_Gain        = 56
Temp_Get          = 19.6[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```


Me
O
Ph
N
Ph
O
1u
4.07
3.17
2.99
0.95
1.01
1.00
1.01
abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
9.730
7.639 7.621 7.617 7.528 7.511 7.417 7.375 7.356 7.260 7.246
5.881 5.864 5.845 5.827
4.418 4.375 3.969 3.967 3.924
1.551 1.534
0.007 -0.001 -0.009
X : parts per Million : 1H
JEOL
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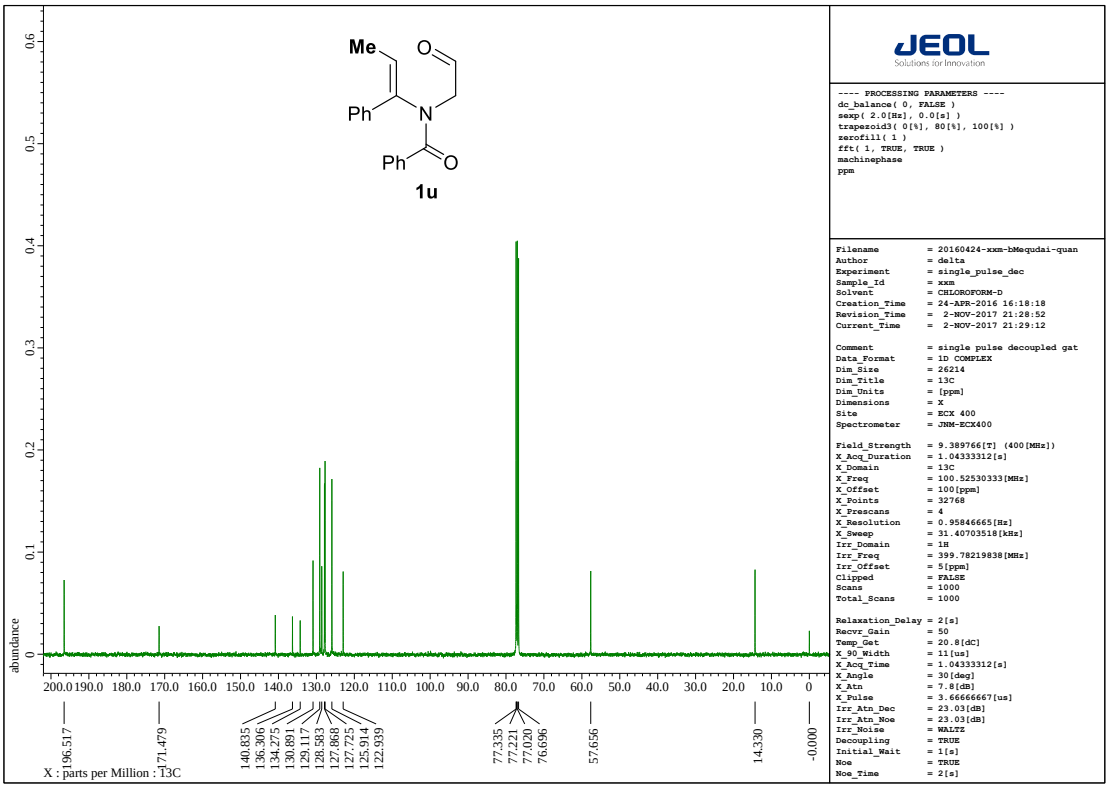
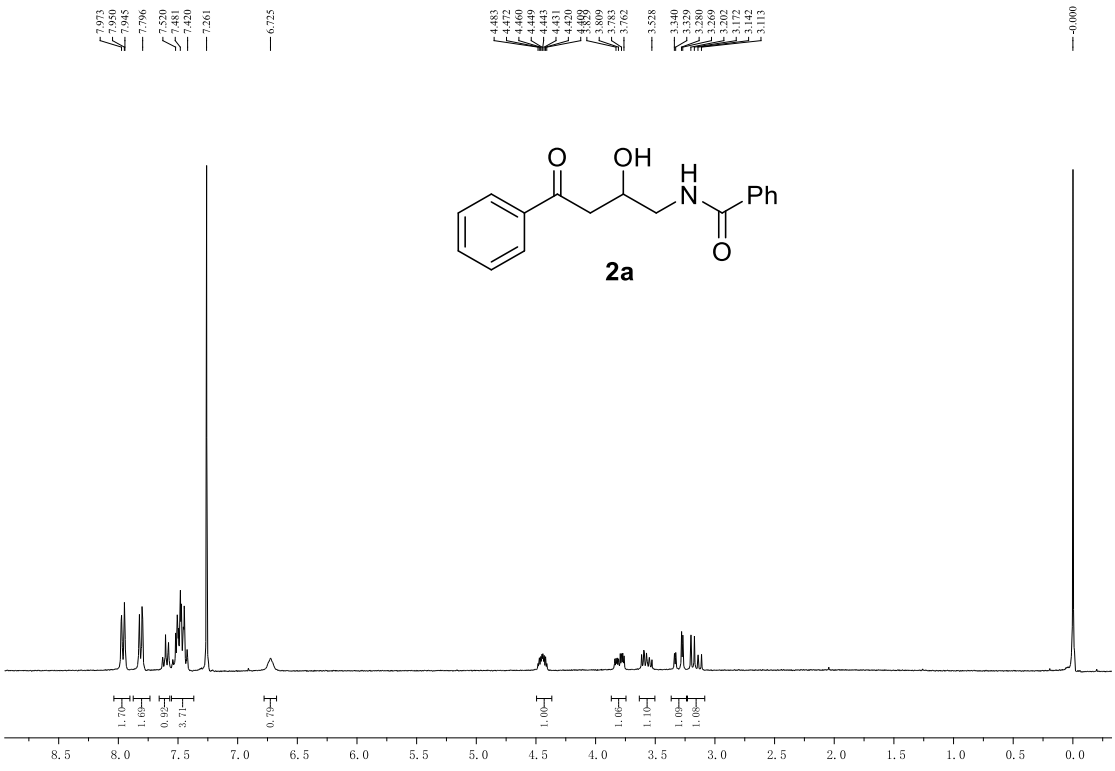
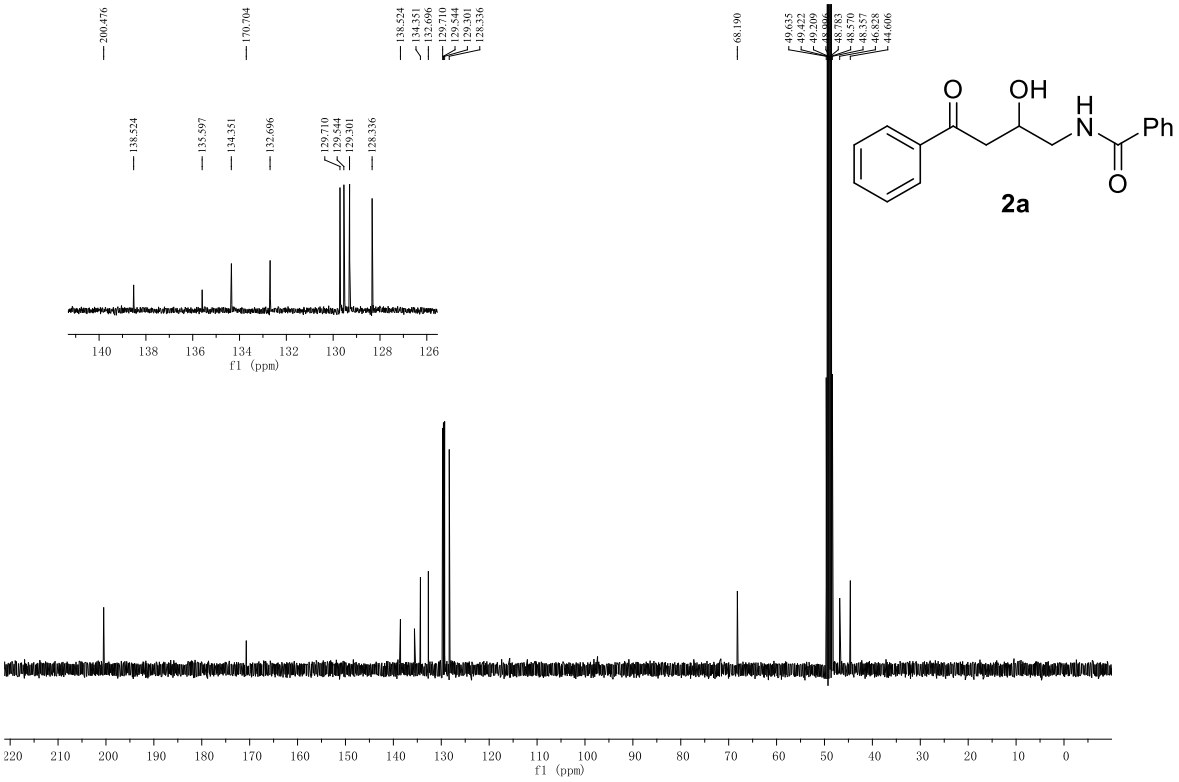
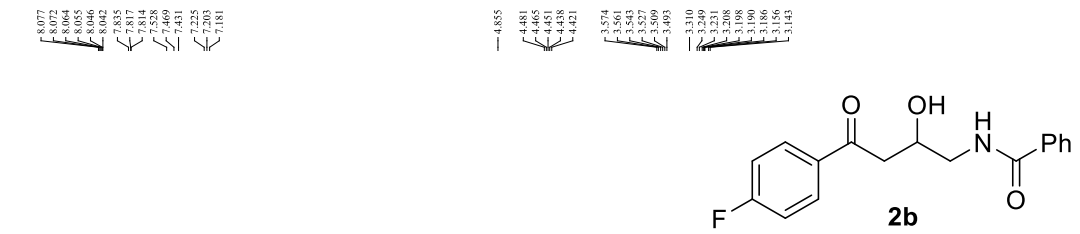
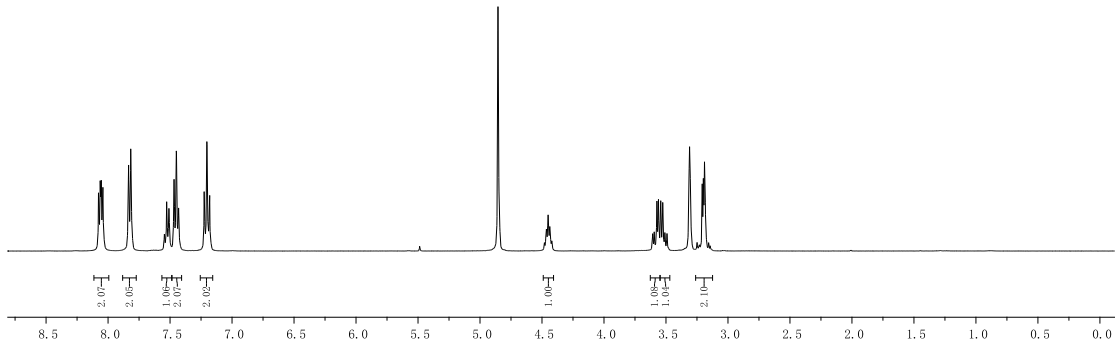
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160424-xxm-bMequdai-quan
Author = delta
Experiment = single_pulse.ex2
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 24-APR-2016 15:25:02
Revision_Time = 2-NOV-2017 21:27:49
Current_Time = 2-NOV-2017 21:27:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 20.3[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 3.4[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]


Me
O
Ph
N
Ph
O
1u
abundance
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
196.517
71.479
140.835 136.306 134.275 130.891 129.117 128.583 127.868 127.725 125.914 122.939
77.335 77.221 77.020 76.696
57.656
14.330
-0.000
X : parts per Million : 13C
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160424-xxm-bMequdai-quan
Author = delta
Experiment = single_pulse_dec
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 24-APR-2016 16:18:18
Revision_Time = 2-NOV-2017 21:28:52
Current_Time = 2-NOV-2017 21:29:12
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.8[dC]
X_90_Width = 11[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 3.66666667[us]
Irr_Atn_Dec = 23.03[dB]
Irr_Atn_Noe = 23.03[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]


7.973
7.950
7.945
7.796
7.520
7.481
7.420
7.261
6.725
4.483
4.472
4.460
4.449
4.443
4.431
4.420
3.809
3.783
3.762
3.528
3.340
3.329
3.280
3.269
3.202
3.172
3.142
3.113
-0.000
O
OH
H
N
Ph
O
2a
1.70
1.69
0.95
3.71
0.79
1.00
1.08
1.10
1.09
1.08
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


200.476
170.704
138.524
134.351
132.696
129.710
129.544
129.301
128.336
68.190
49.635
49.422
49.209
48.996
48.783
48.570
48.357
46.828
44.606
138.524
135.597
134.351
132.696
129.710
129.544
129.301
128.336
140
138
136
134
132
130
128
126
f1 (ppm)
O
OH
H
N
Ph
O
2a
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.077
8.072
8.064
8.055
8.046
8.042
7.835
7.817
7.814
7.528
7.469
7.431
7.225
7.203
7.181
4.855
4.481
4.465
4.451
4.438
4.421
3.574
3.561
3.543
3.527
3.509
3.493
3.310
3.249
3.231
3.208
3.198
3.190
3.186
3.156
3.143
O
OH
H
N
Ph
O
F
2b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2.08
1.06
2.07
2.02
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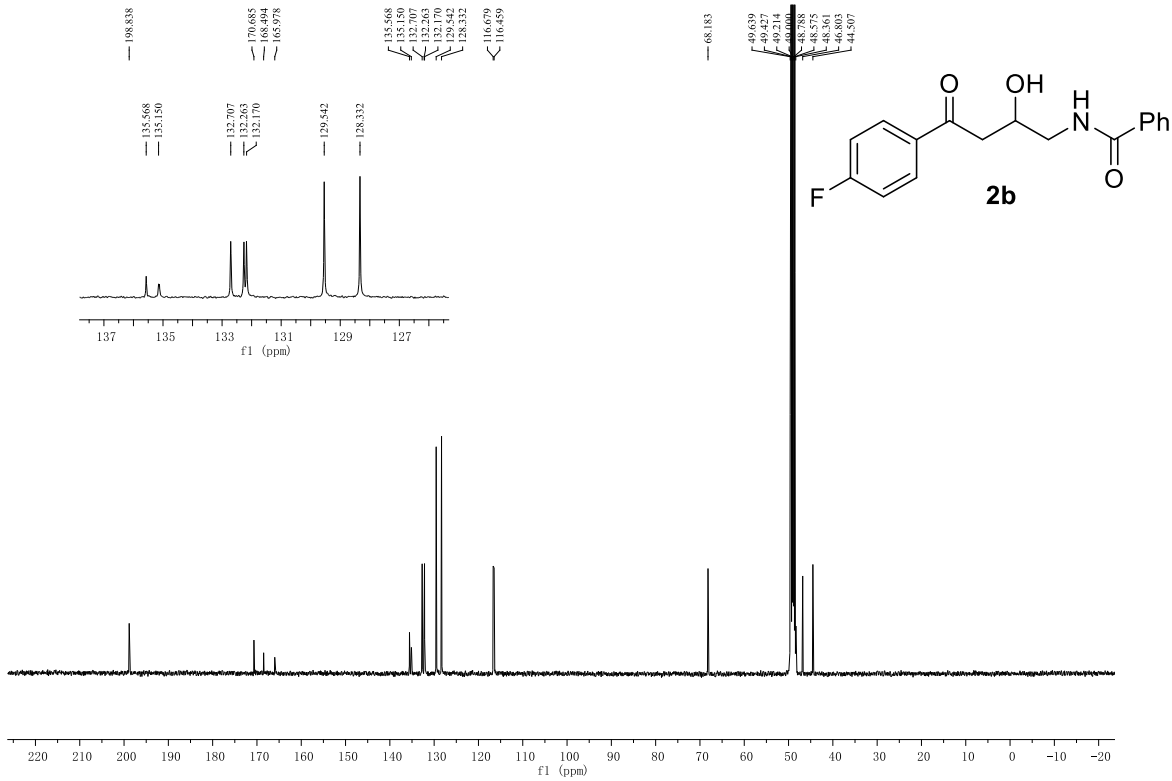
1.08
1.04
2.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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168.494
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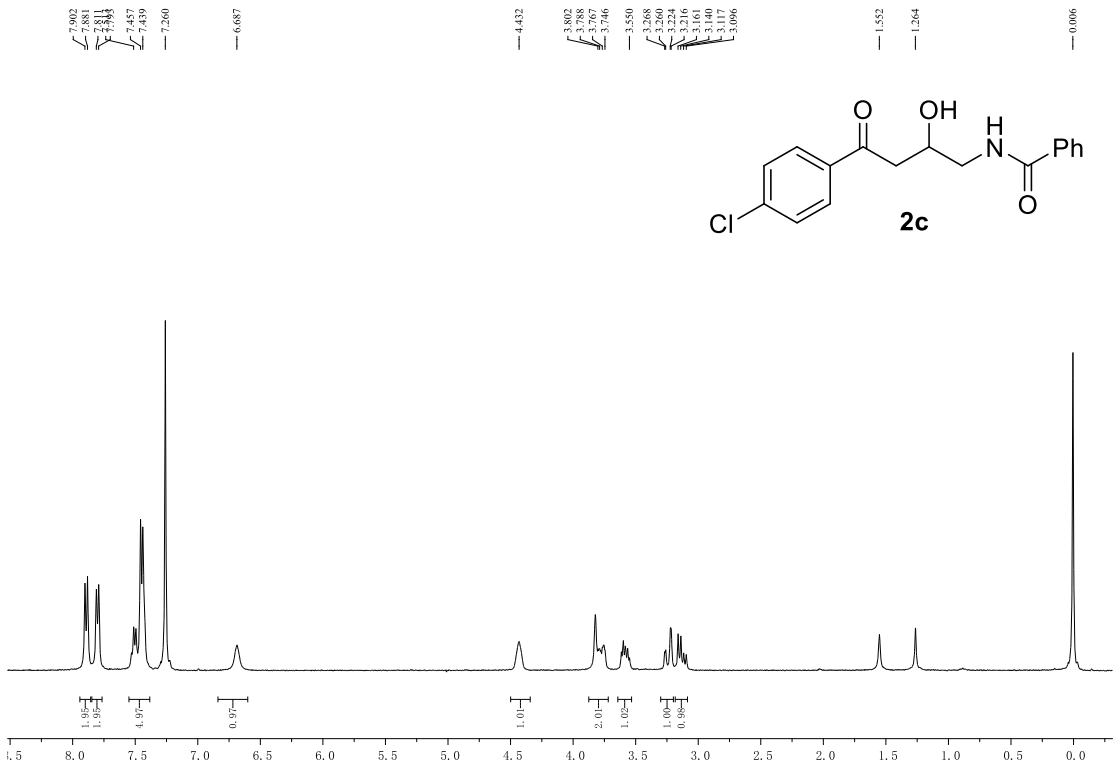
135.568
135.150
132.707
132.263
132.170
129.542
128.332
116.679
116.459
68.183
49.639
49.427
49.214
49.000
48.788
48.575
48.361
46.803
44.507
135.568
135.150
132.707
132.263
132.170
129.542
128.332
137
135
133
131
129
127
f1 (ppm)
O
OH
H
N
Ph
O
F
2b
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)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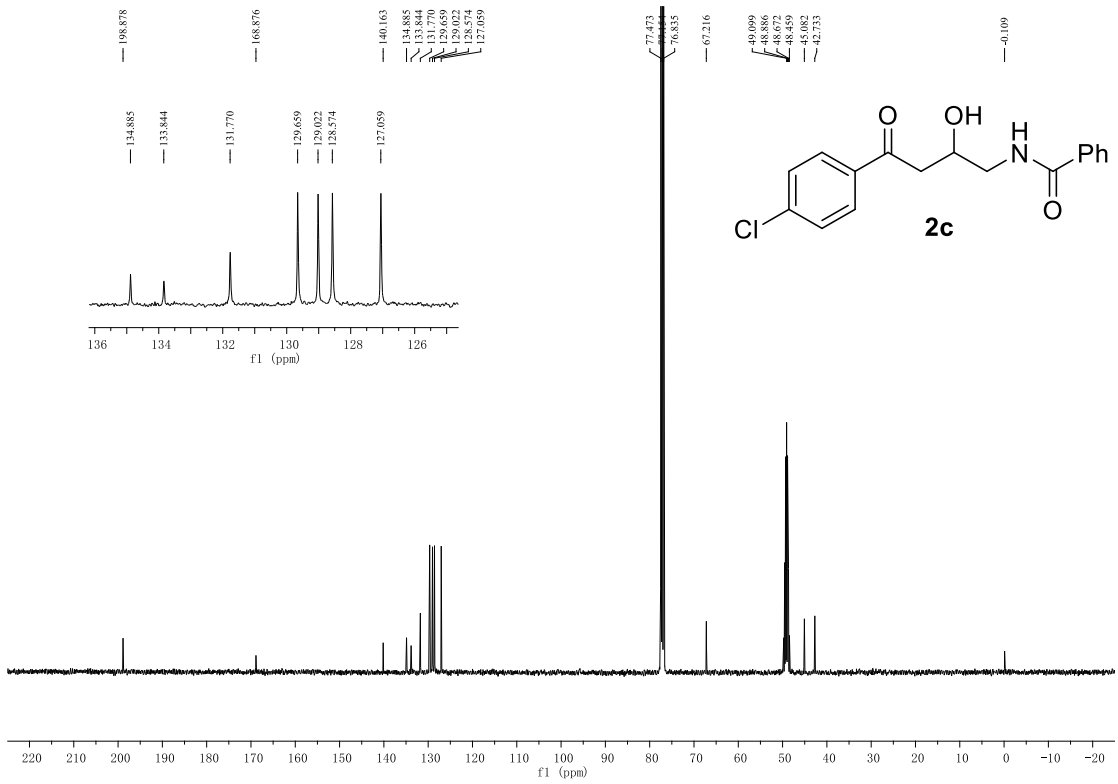
7.811
7.793
7.457
7.439
7.260
6.687
4.432
3.802
3.788
3.767
3.746
3.550
3.268
3.260
3.224
3.216
3.161
3.140
3.117
3.096
1.552
1.264
0.006
O
OH
H
N
Ph
O
Cl
2c
1.98
1.95
4.97
0.97
1.01
2.01
1.02
1.00
0.98
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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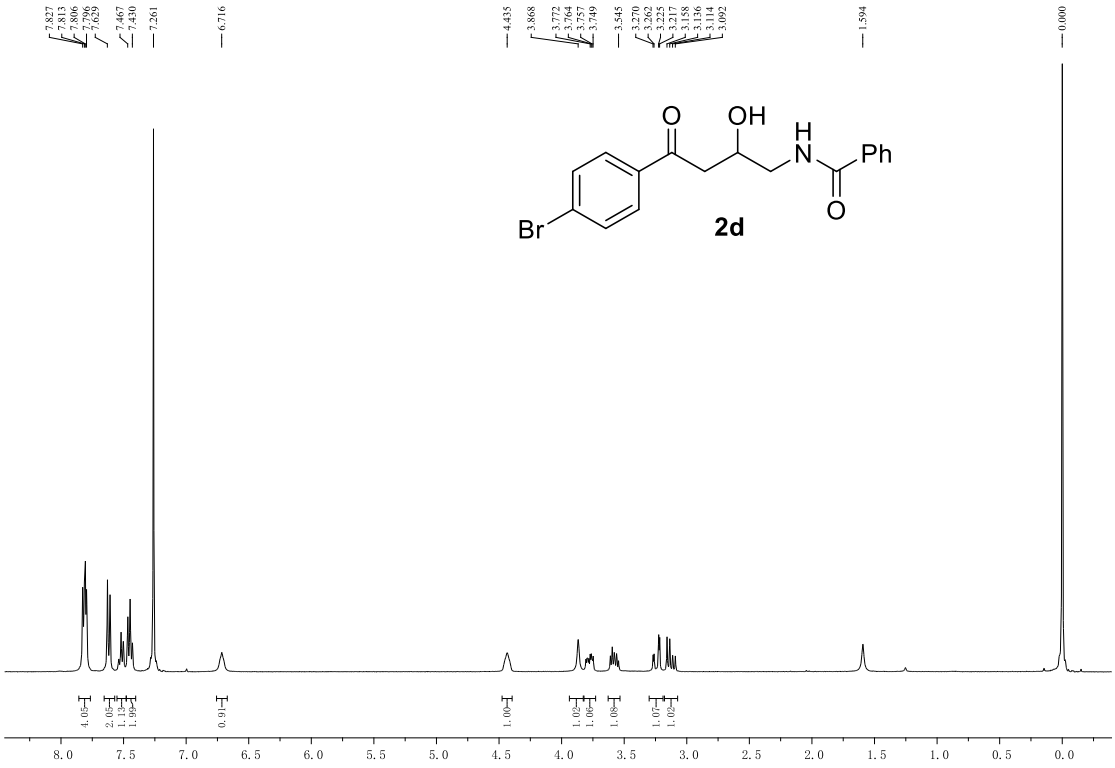
140.163
134.885
133.844
131.770
129.659
129.022
128.574
127.059
77.473
77.154
76.835
67.216
49.099
48.886
48.672
48.459
45.082
42.753
-0.109
O
OH
H
N
Ph
O
Cl
2c
136
134
132
130
128
126
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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7.813
7.806
7.796
7.629
7.467
7.430
7.261
6.716
4.435
3.868
3.772
3.764
3.757
3.749
3.545
3.270
3.262
3.255
3.217
3.158
3.136
3.114
3.092
1.594
0.000
O
OH
H
N
Ph
O
Br
2d
4.05
2.05
1.13
1.99
0.91
1.00
1.02
1.06
1.08
1.07
1.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
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2.0
1.5
1.0
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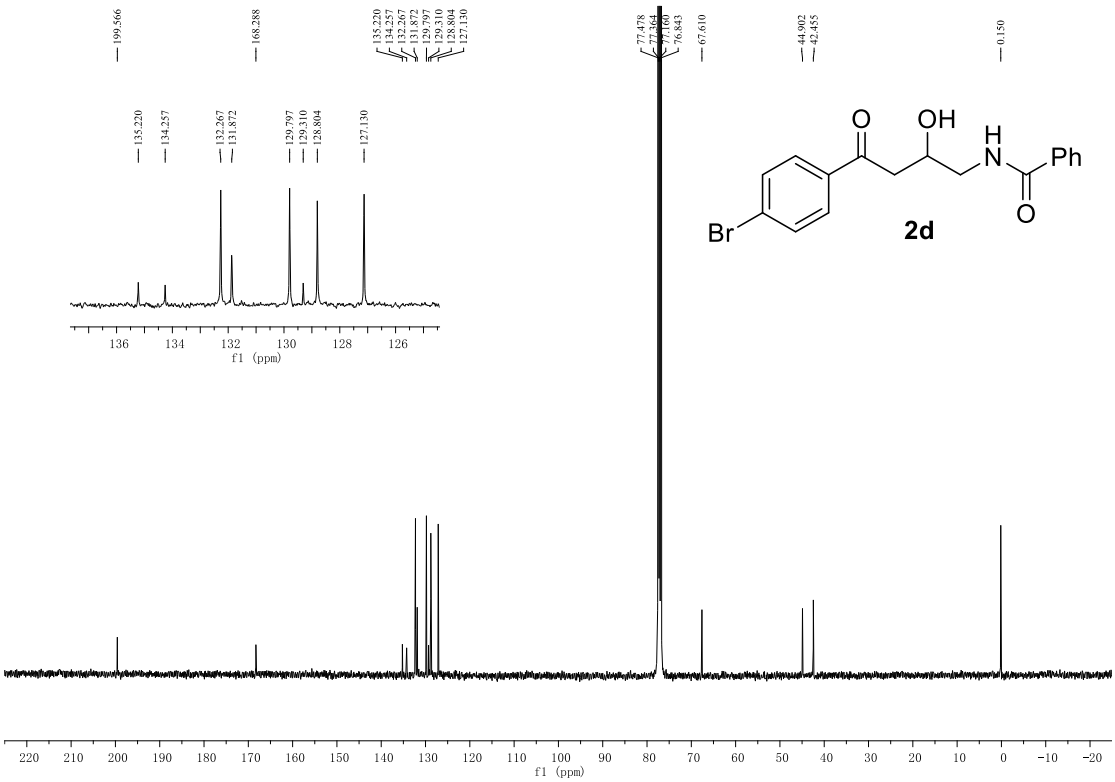
0.0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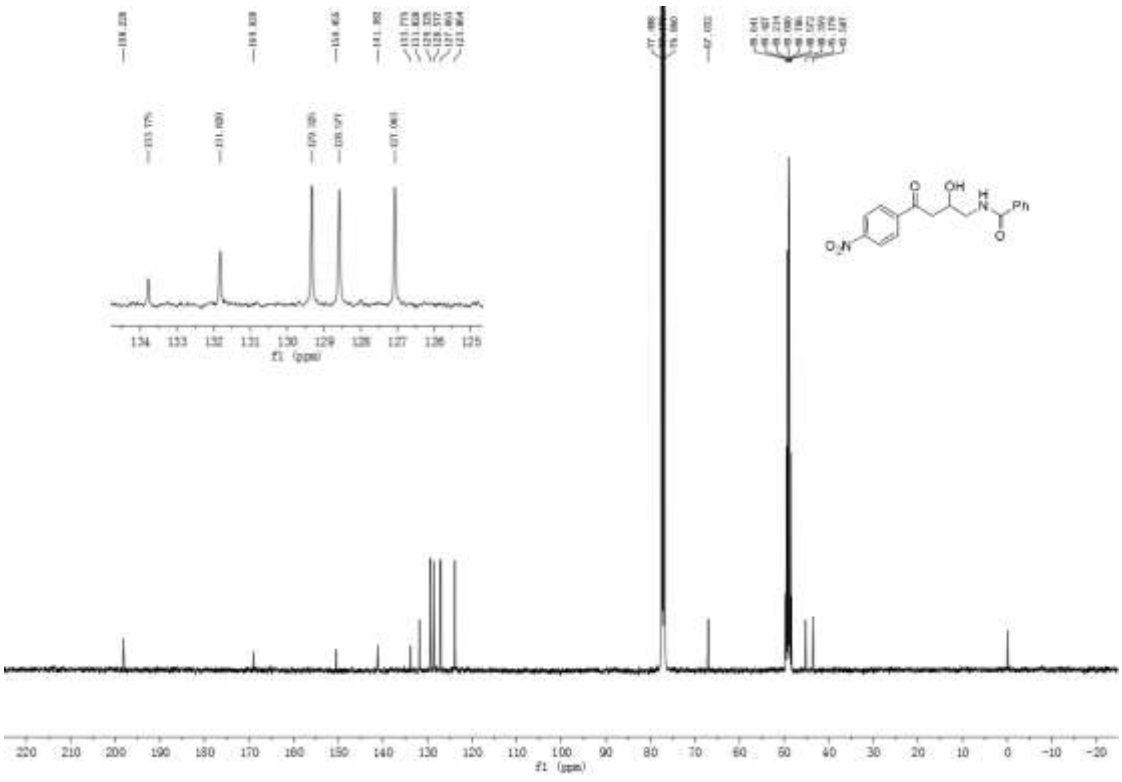
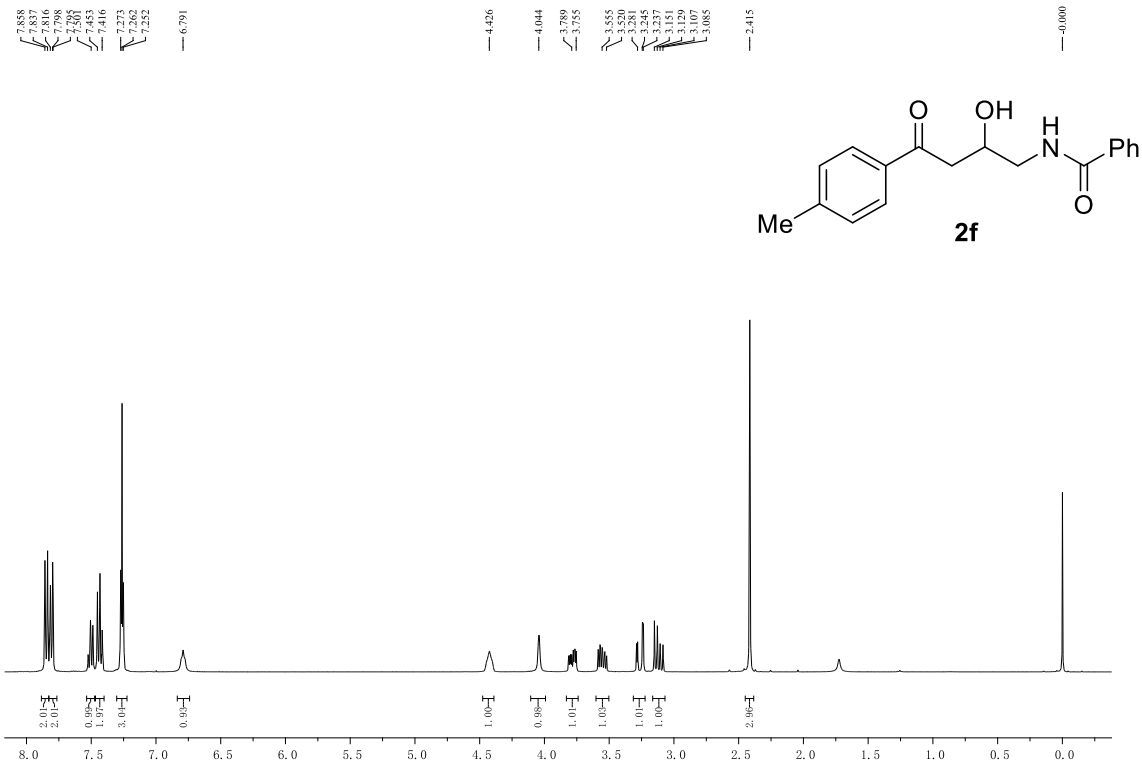
168.288
135.220
134.257
132.267
131.872
129.797
129.310
128.804
127.130
77.478
77.164
76.849
76.843
67.610
44.902
42.455
0.150
O
OH
H
N
Ph
O
Br
2d
136
134
132
130
128
126
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)

^{1}H NMR spectra of **2e**

^{13}C NMR spectra of **2e**

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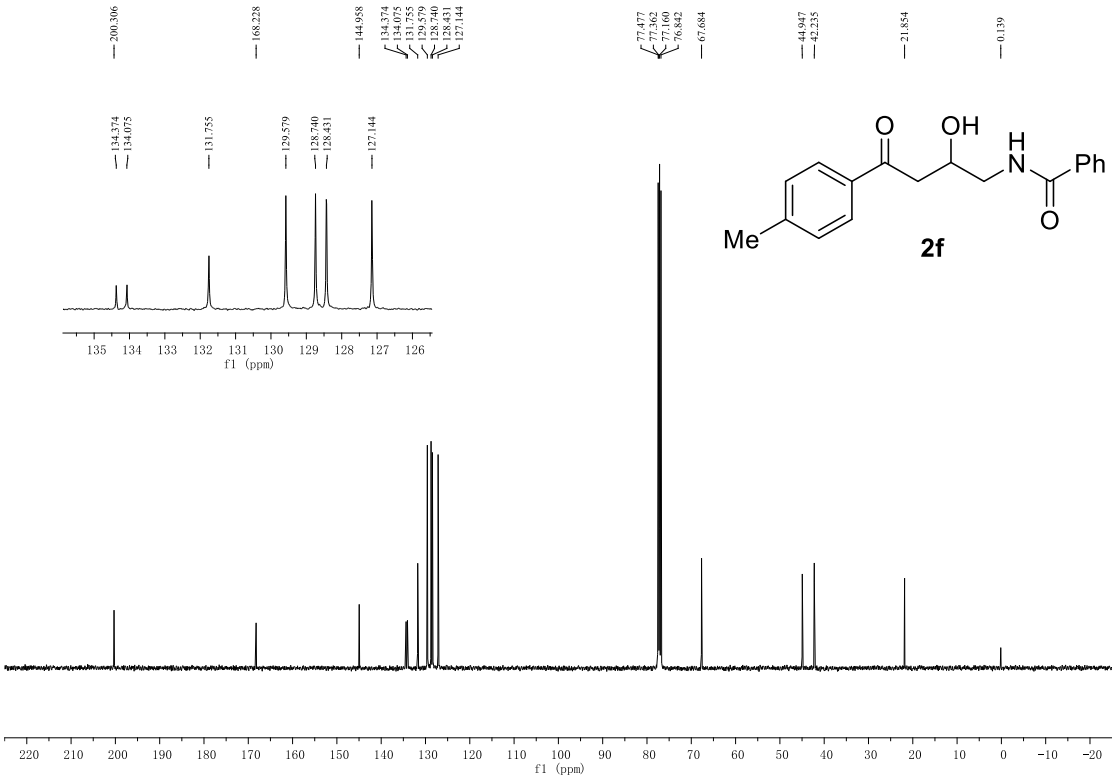
7.837
7.816
7.798
7.795
7.501
7.453
7.416
7.273
7.262
7.252
6.791
4.426
4.044
3.789
3.755
3.555
3.520
3.501
3.241
3.237
3.151
3.129
3.107
3.085
2.415
0.000
O
OH
H
N
Ph
O
Me
2f
2.01
2.01
0.98
1.97
3.04
0.98
1.00
0.98
1.01
1.00
1.01
1.00
2.96
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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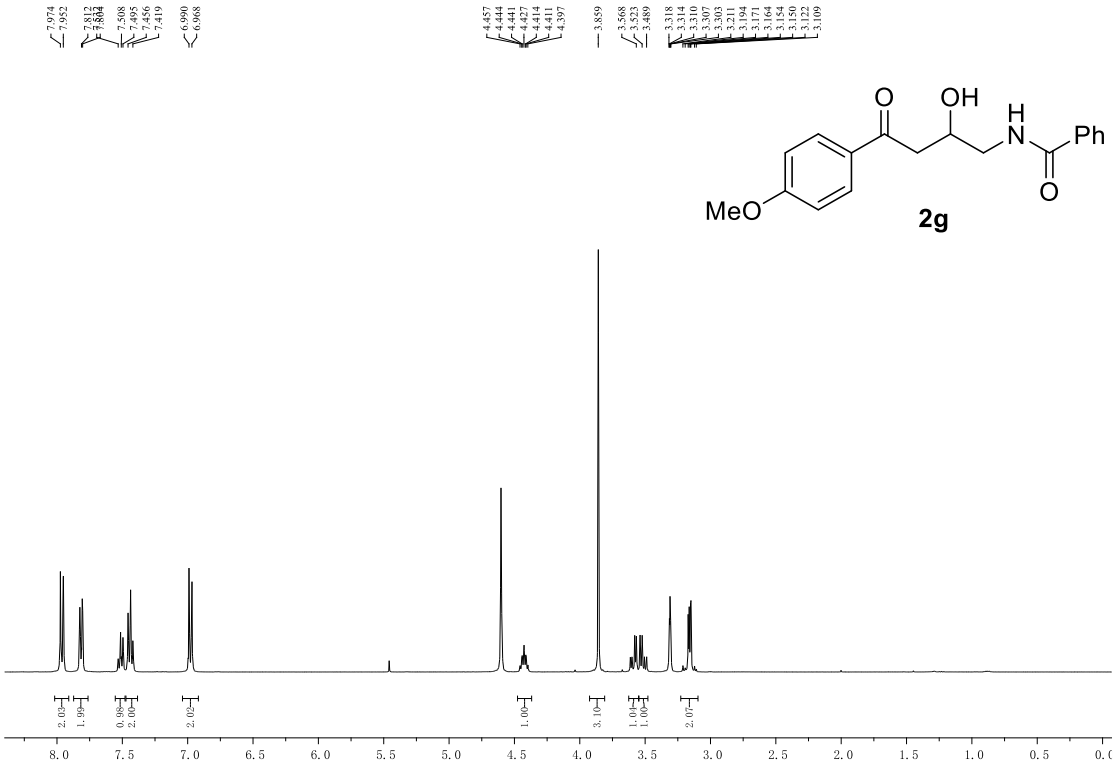
168.228
144.958
134.374
134.075
131.755
129.579
128.740
128.431
127.144
77.477
77.362
77.160
76.842
67.684
44.947
42.235
21.854
0.139
134.374
134.075
131.755
129.579
128.740
128.431
127.144
135
134
133
132
131
130
129
128
127
126
f1 (ppm)
O
OH
H
N
Ph
O
Me
2f
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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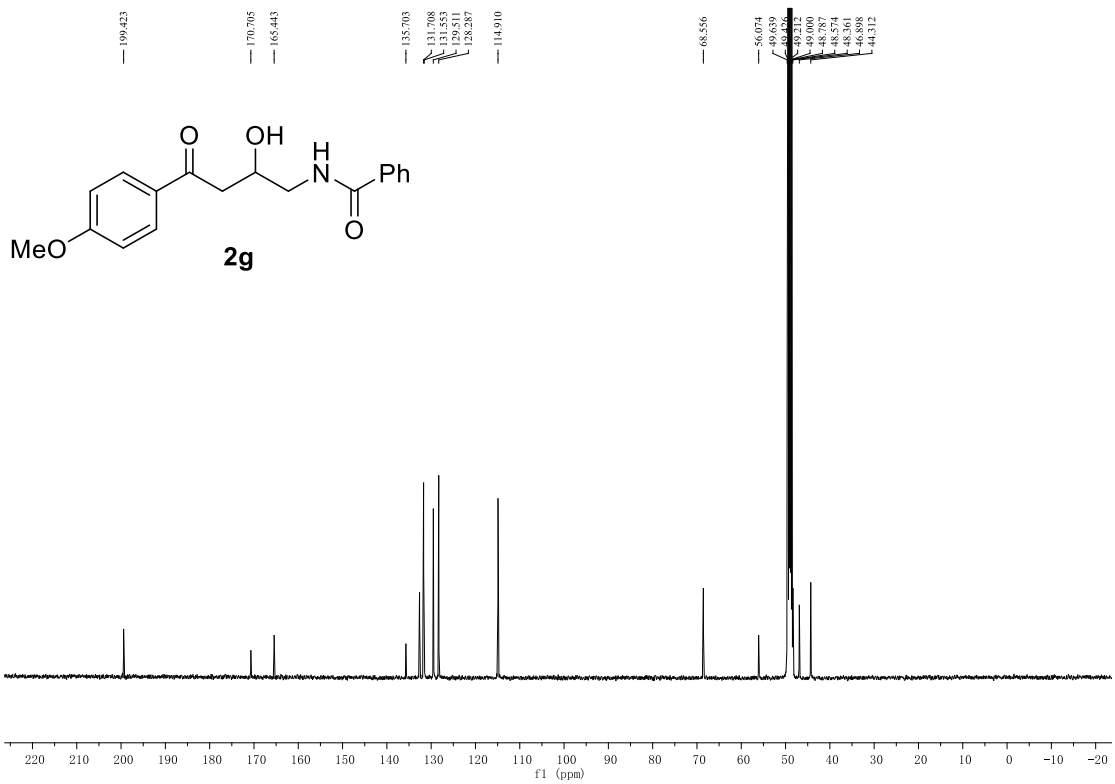
7.952
7.812
7.804
7.508
7.495
7.456
7.419
6.990
6.968
4.457
4.444
4.441
4.427
4.414
4.411
4.397
3.859
3.568
3.523
3.489
3.318
3.314
3.310
3.307
3.303
3.171
3.164
3.154
3.150
3.122
3.109
O
OH
H
N
Ph
O
MeO
2g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131.553
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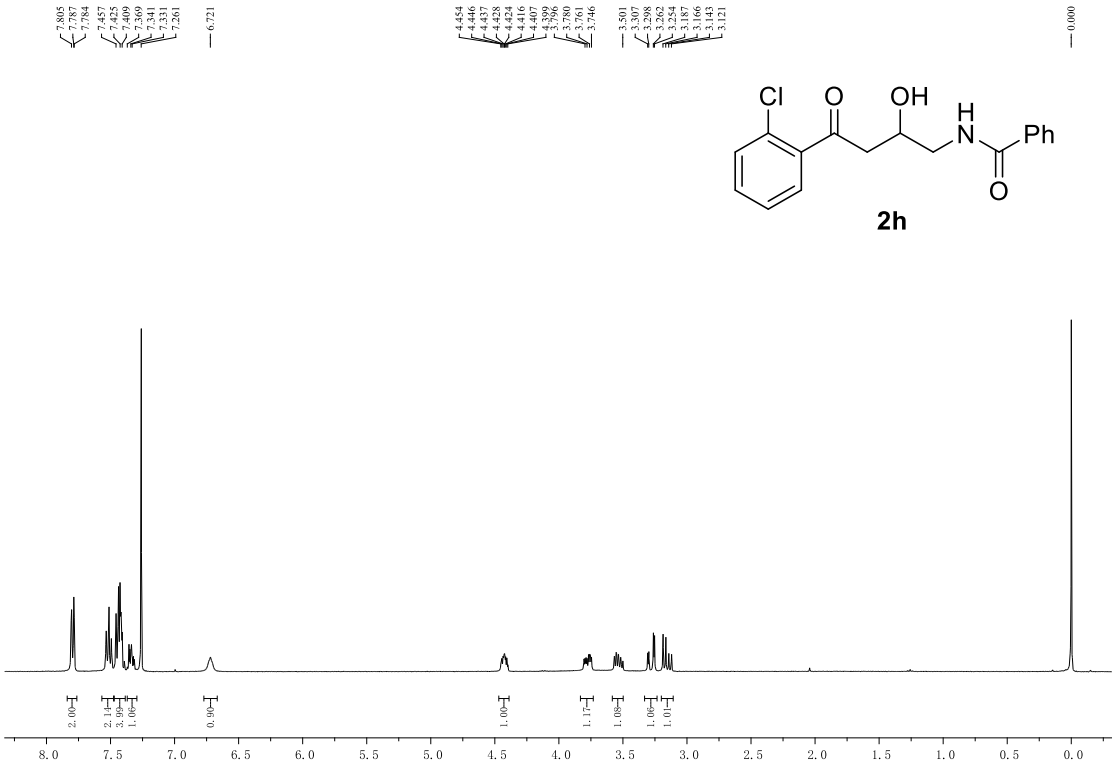
128.287
114.910
68.556
56.074
49.639
49.426
49.212
49.000
48.787
48.574
48.361
46.898
44.312
O
OH
H
N
Ph
O
MeO
2g
f1 (ppm)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7.457
7.455
7.403
7.369
7.341
7.331
7.261
6.721
4.454
4.446
4.437
4.428
4.424
4.416
4.407
4.399
3.796
3.780
3.761
3.746
3.501
3.307
3.298
3.262
3.254
3.187
3.166
3.143
3.121
0.000
Cl
O
OH
H
N
Ph
O
2h
2.00
2.14
3.98
1.06
0.98
1.00
1.17
1.08
1.06
1.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
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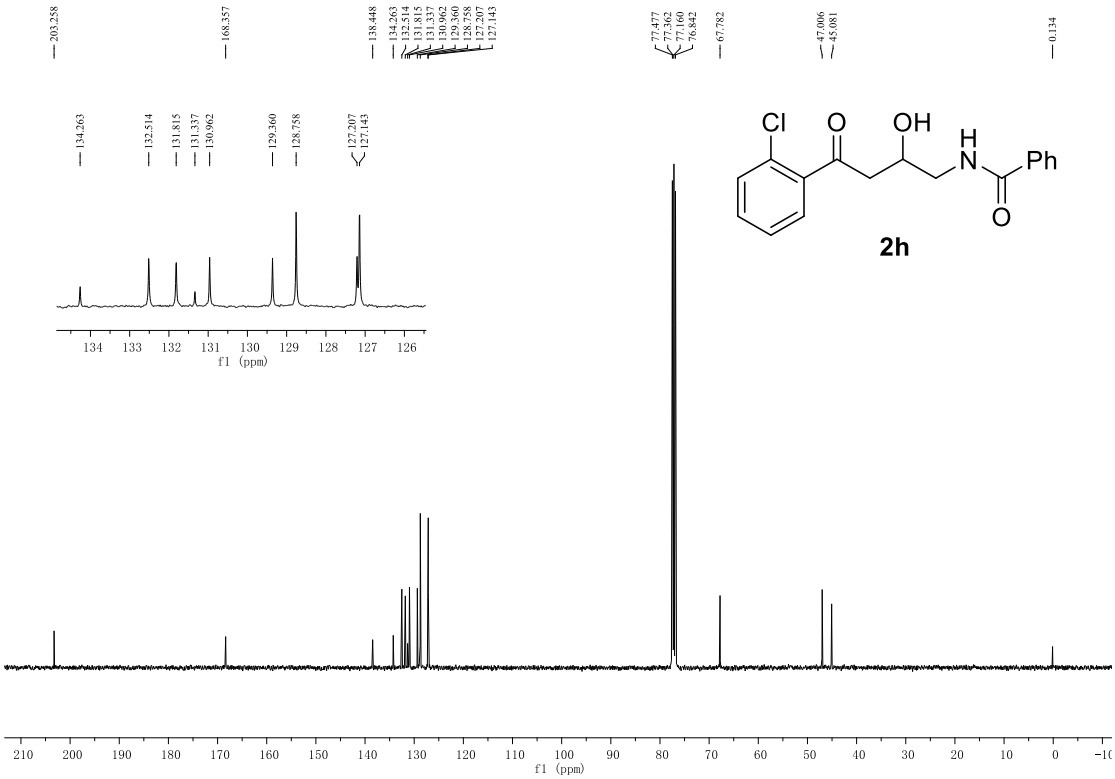
2.0
1.5
1.0
0.5
0.0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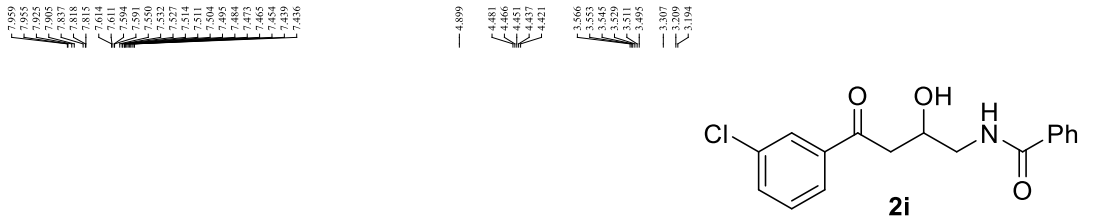
138.448
134.263
132.514
131.815
131.337
130.962
129.360
128.758
127.207
127.143
77.477
77.362
77.160
76.842
67.782
47.006
45.081
0.134
Cl
O
OH
H
N
Ph
O
2h
134
133
132
131
130
129
128
127
126
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.614
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7.594
7.591
7.550
7.532
7.527
7.514
7.511
7.504
7.495
7.484
7.473
7.465
7.454
7.439
7.436
4.899
4.481
4.466
4.451
4.437
4.421
3.566
3.555
3.545
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3.511
3.495
3.307
3.209
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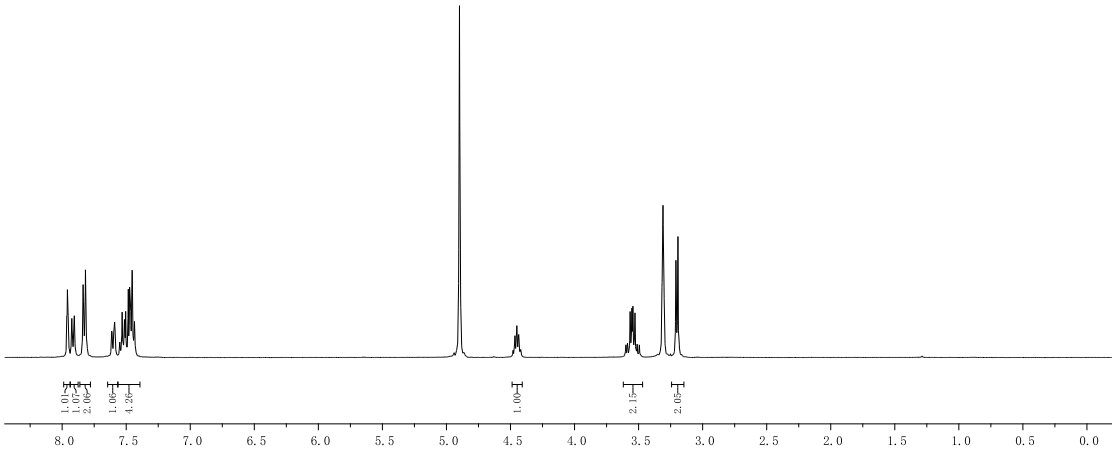
Cl
O
OH
H
N
Ph
O
2i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1.07
2.06
1.06
4.20
1.00
2.15
2.05
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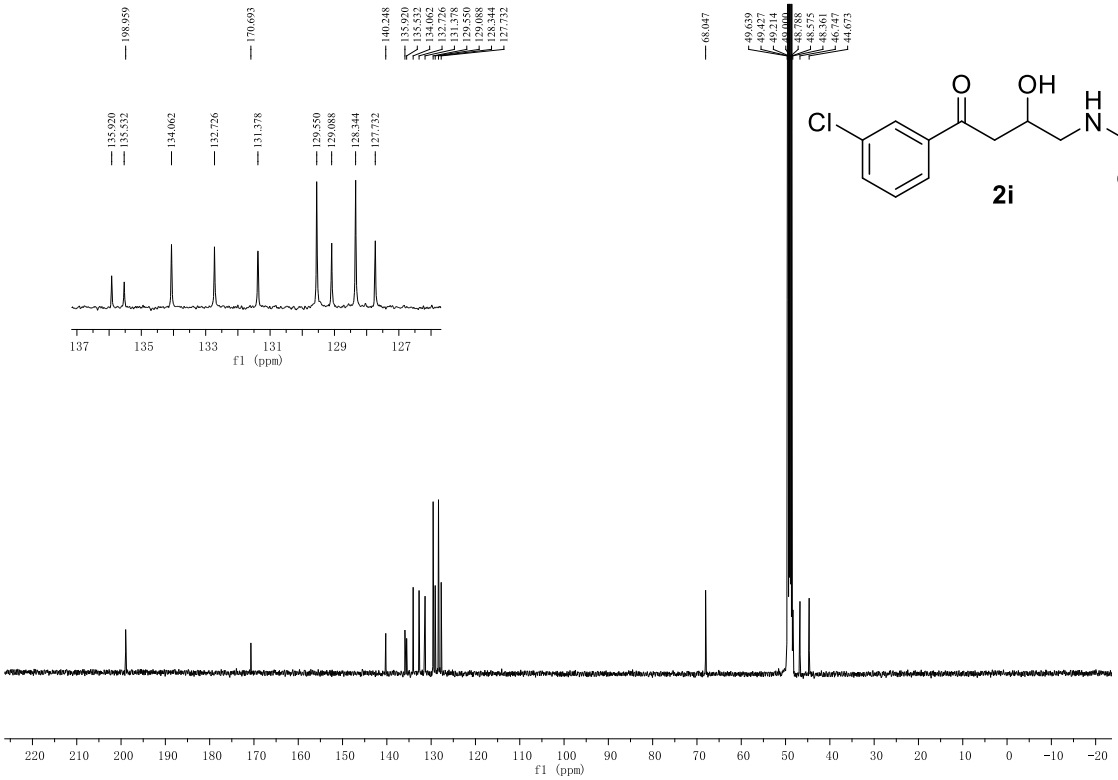
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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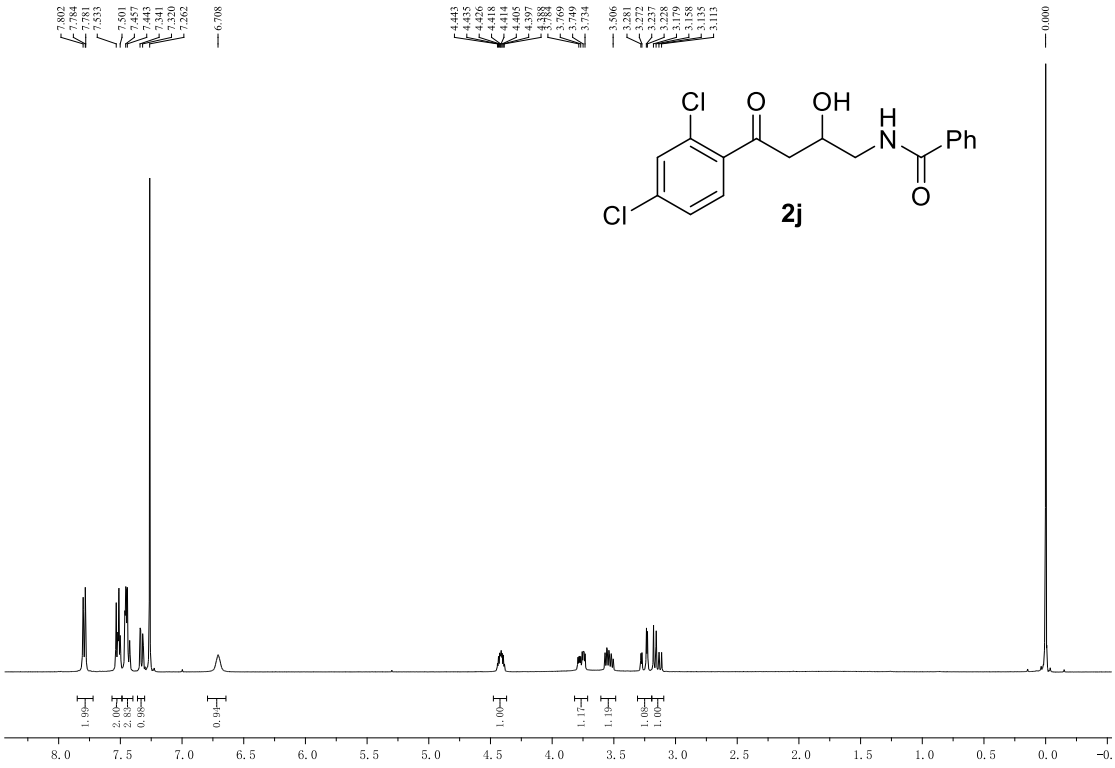
135.532
134.062
132.726
131.378
129.550
129.088
128.344
127.732
68.047
49.639
49.427
49.214
49.000
48.788
48.575
48.361
46.747
44.673
135.920
135.532
134.062
132.726
131.378
129.550
129.088
128.344
127.732
137
135
133
131
129
127
f1 (ppm)
Cl
O
OH
H
N
Ph
O
2i
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)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7.341
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7.262
6.708
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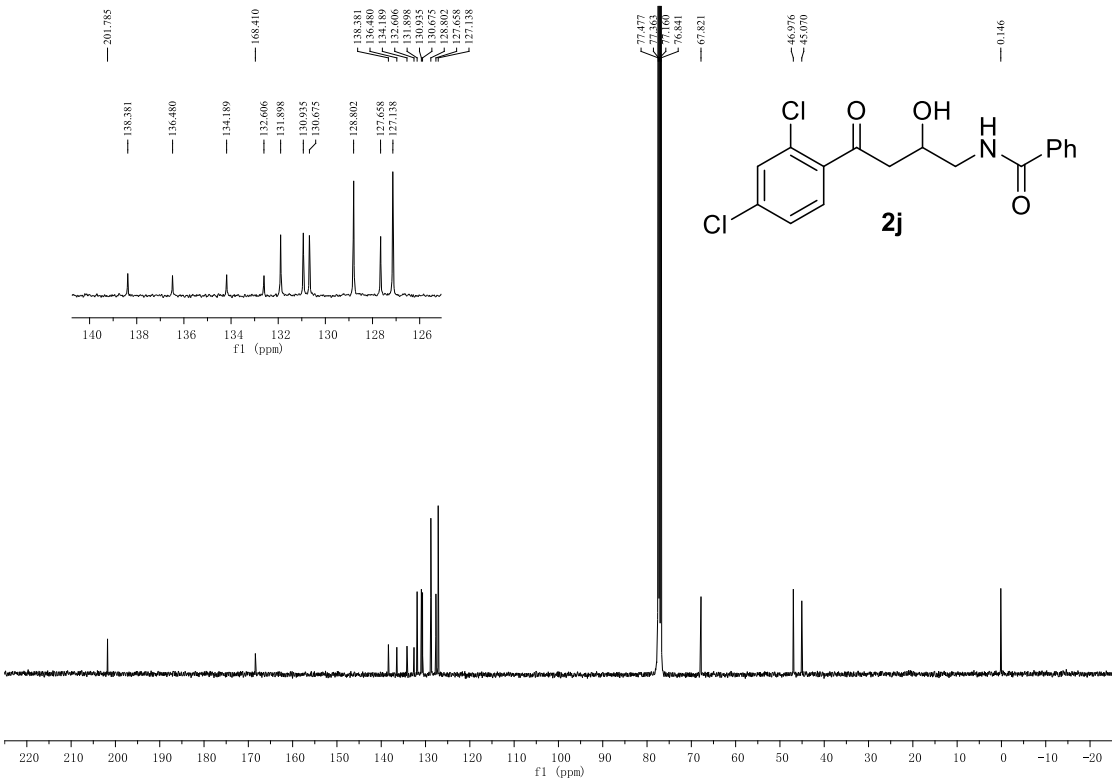
4.435
4.426
4.418
4.414
4.405
4.397
3.769
3.749
3.734
3.506
3.281
3.272
3.237
3.228
3.179
3.158
3.135
3.115
0.000
Cl
O
OH
H
N
Ph
O
Cl
2j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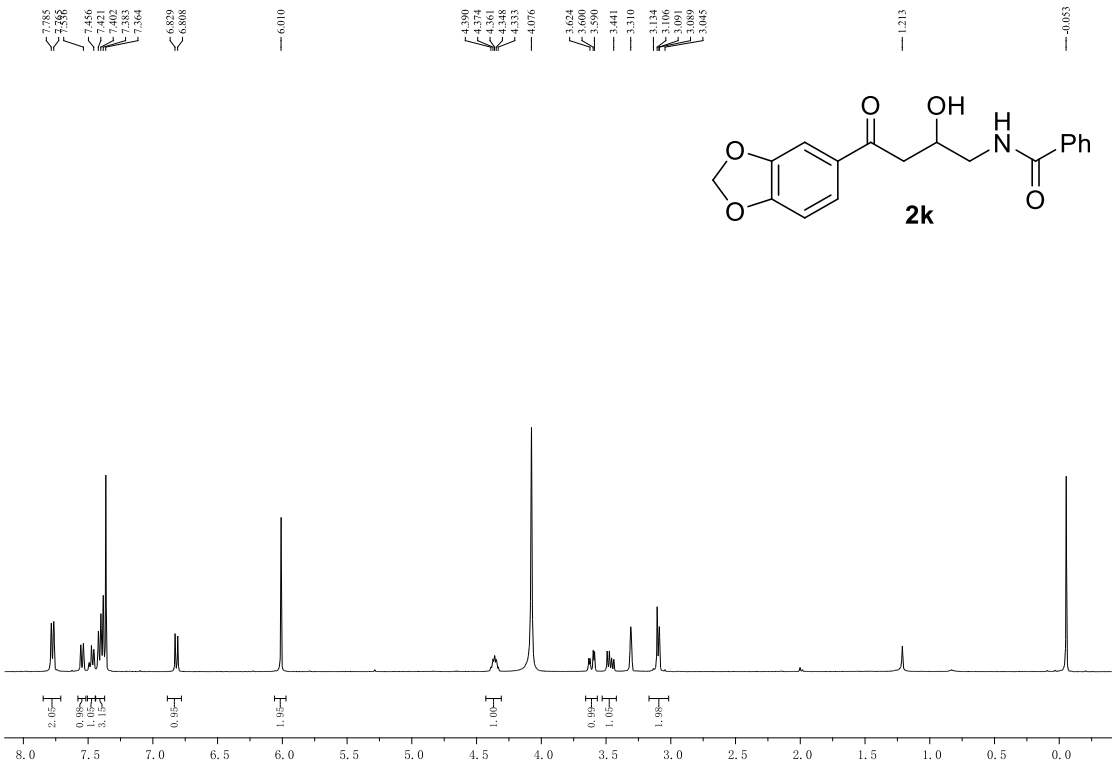
131.898
130.935
130.675
128.802
127.658
127.138
77.477
77.163
76.841
67.821
46.976
45.070
0.146
Cl
O
OH
H
N
Ph
O
Cl
2j
f1 (ppm)
f1 (ppm)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6.808
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4.361
4.348
4.333
4.076
3.624
3.600
3.590
3.441
3.310
3.134
3.106
3.091
3.089
3.045
1.213
0.053
O
OH
H
N
Ph
O
O
O
2k
2.05
0.98
1.05
3.15
0.99
1.95
1.00
0.99
1.05
1.98
8.0
7.5
7.0
6.5
6.0
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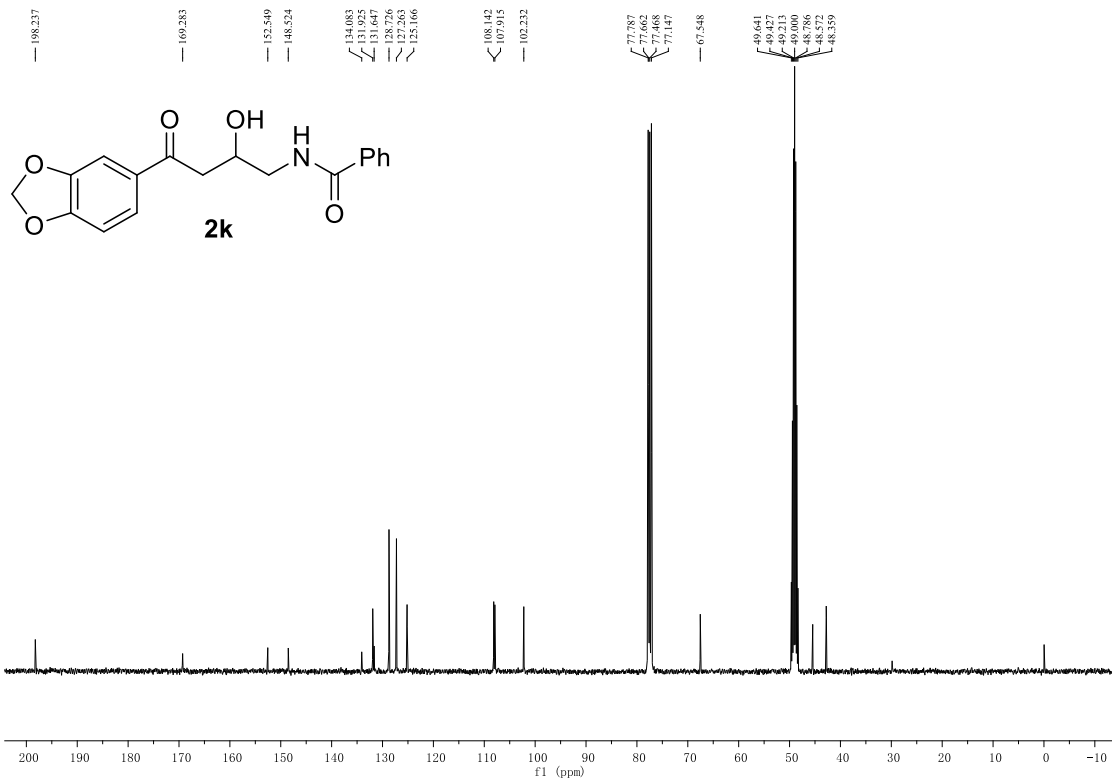
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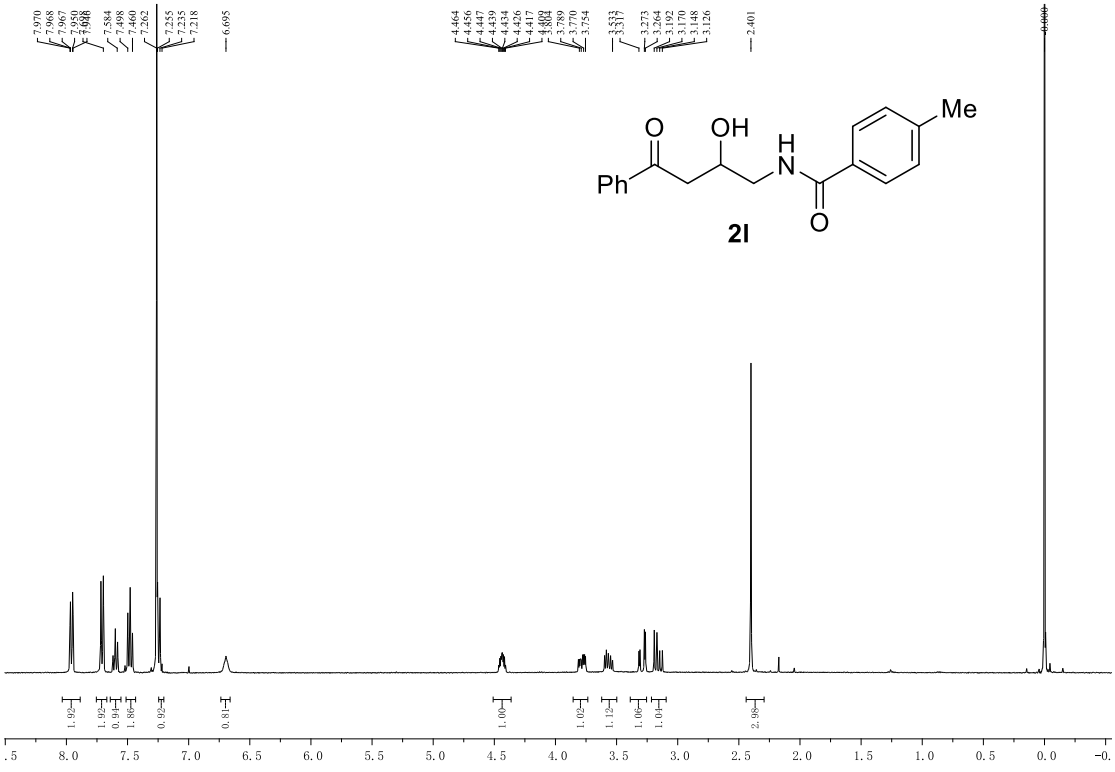
134.083
131.925
131.647
128.726
127.263
125.166
108.142
107.915
102.232
77.787
77.662
77.468
77.147
67.548
49.641
49.427
49.213
49.000
48.786
48.572
48.359
O
OH
H
N
Ph
O
O
O
2k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.262
7.255
7.235
7.218
6.695
4.464
4.456
4.447
4.439
4.434
4.426
4.417
3.789
3.770
3.754
3.533
3.317
3.273
3.264
3.192
3.170
3.148
3.126
2.401
O
OH
H
N
Ph
Me
O
2l
1.99
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1.80
0.92
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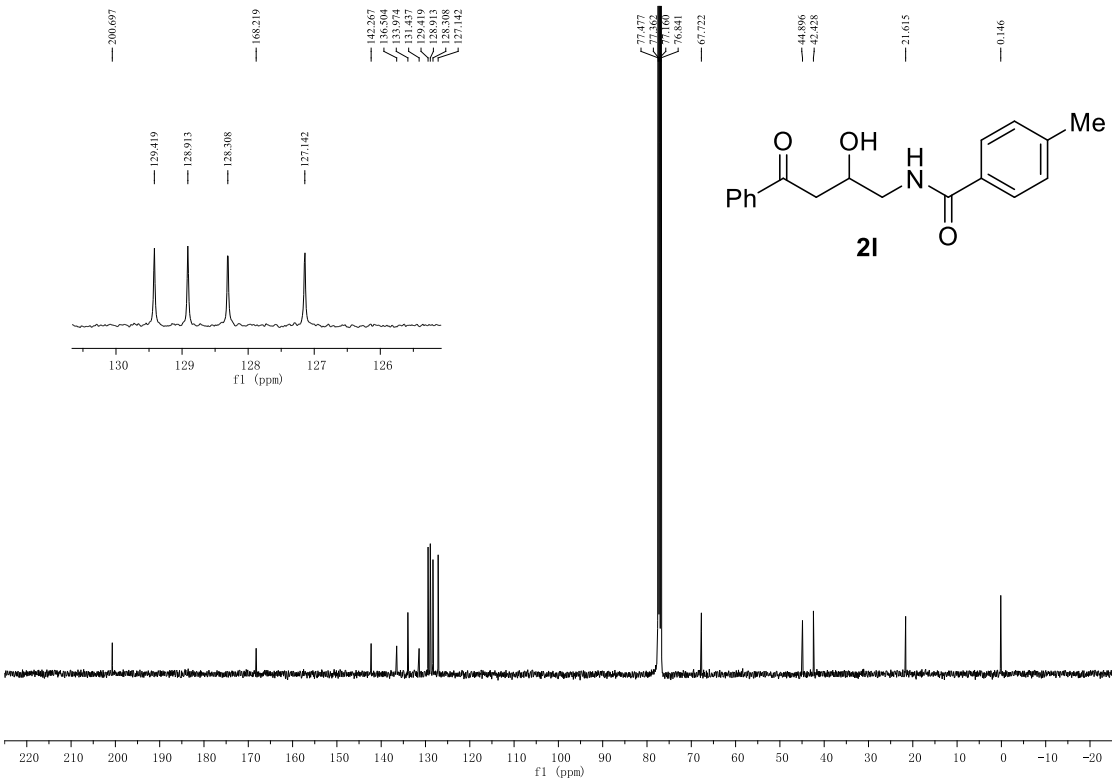
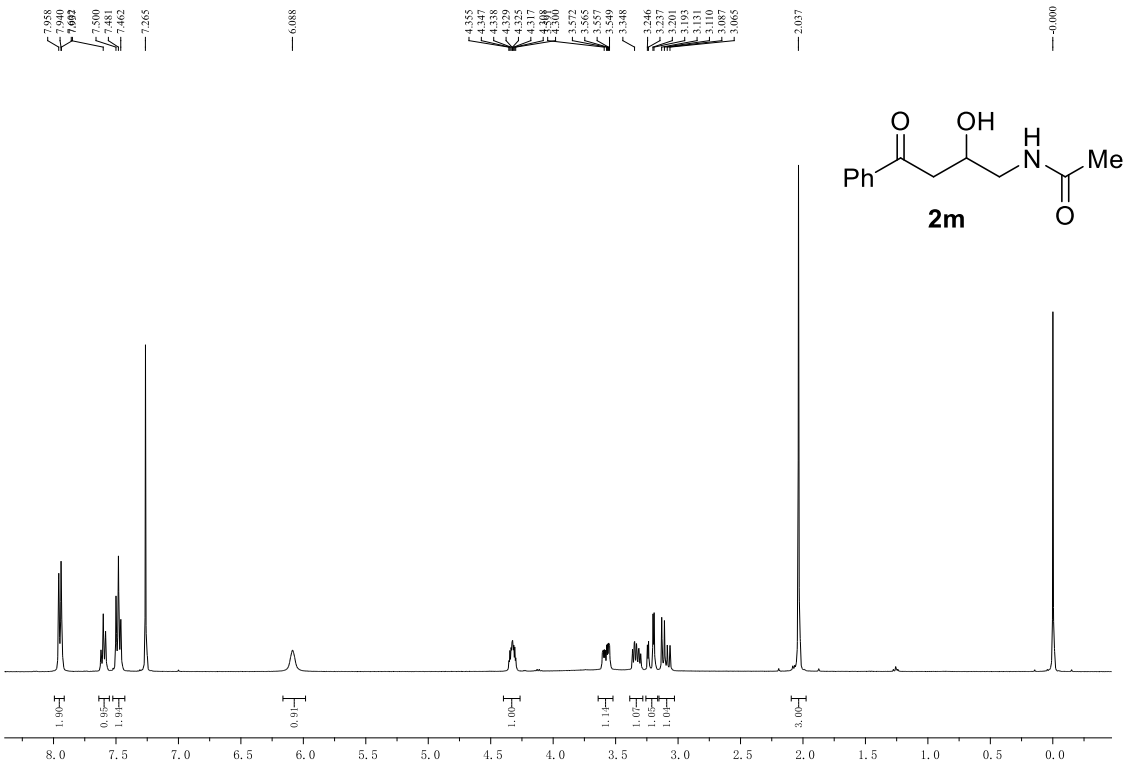
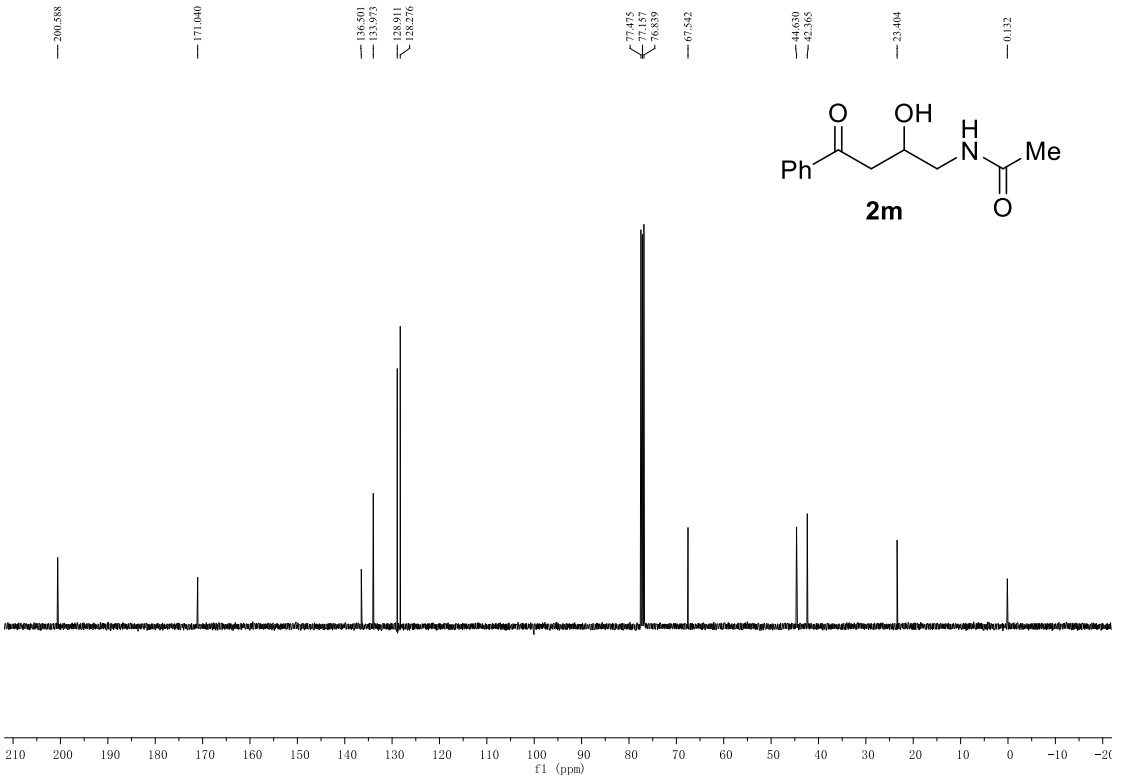
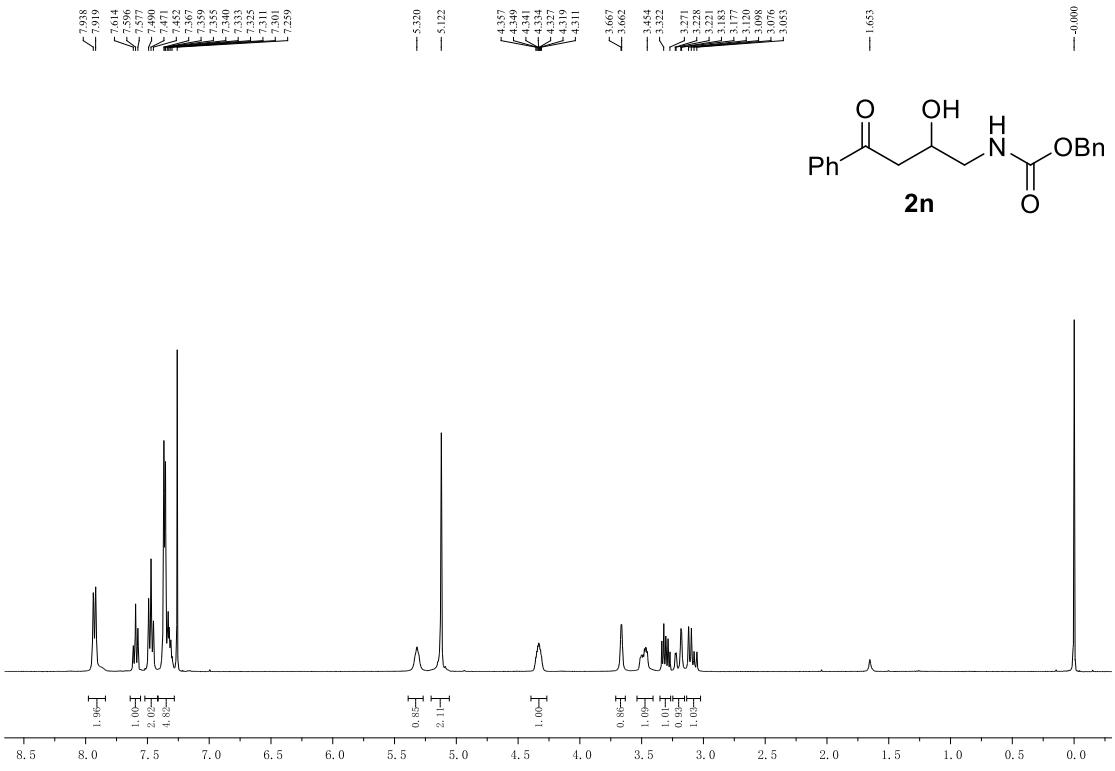
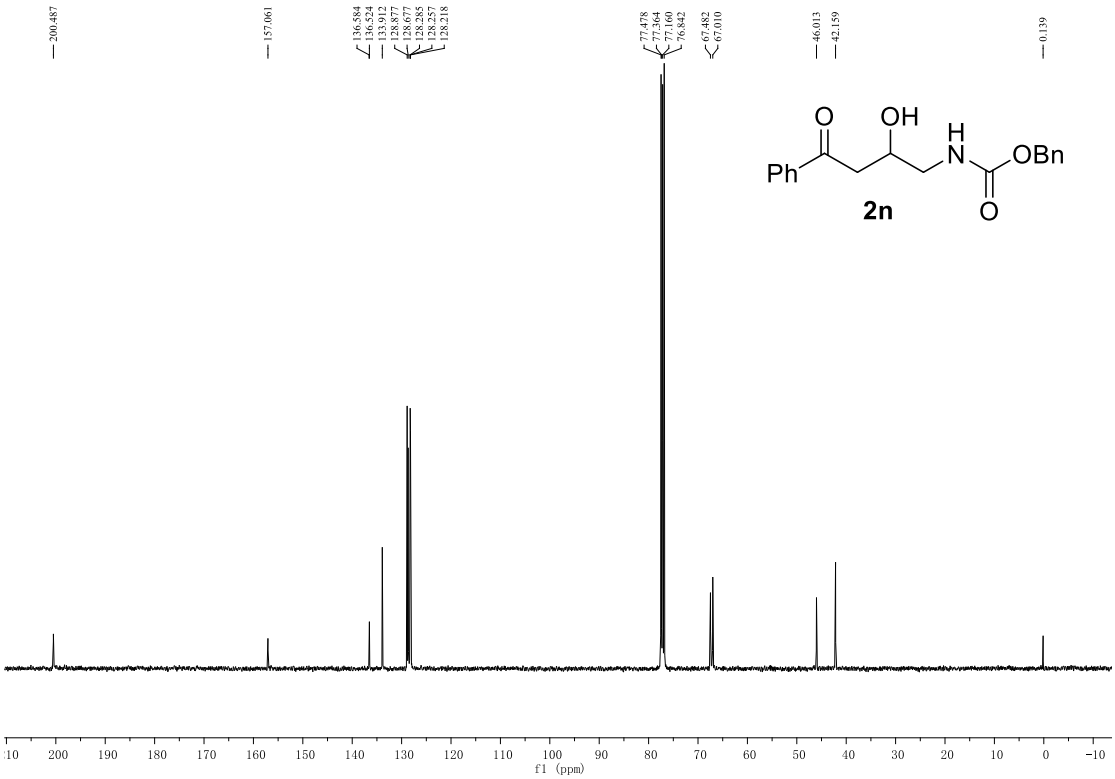
1.02
1.12
1.06
1.04
2.98

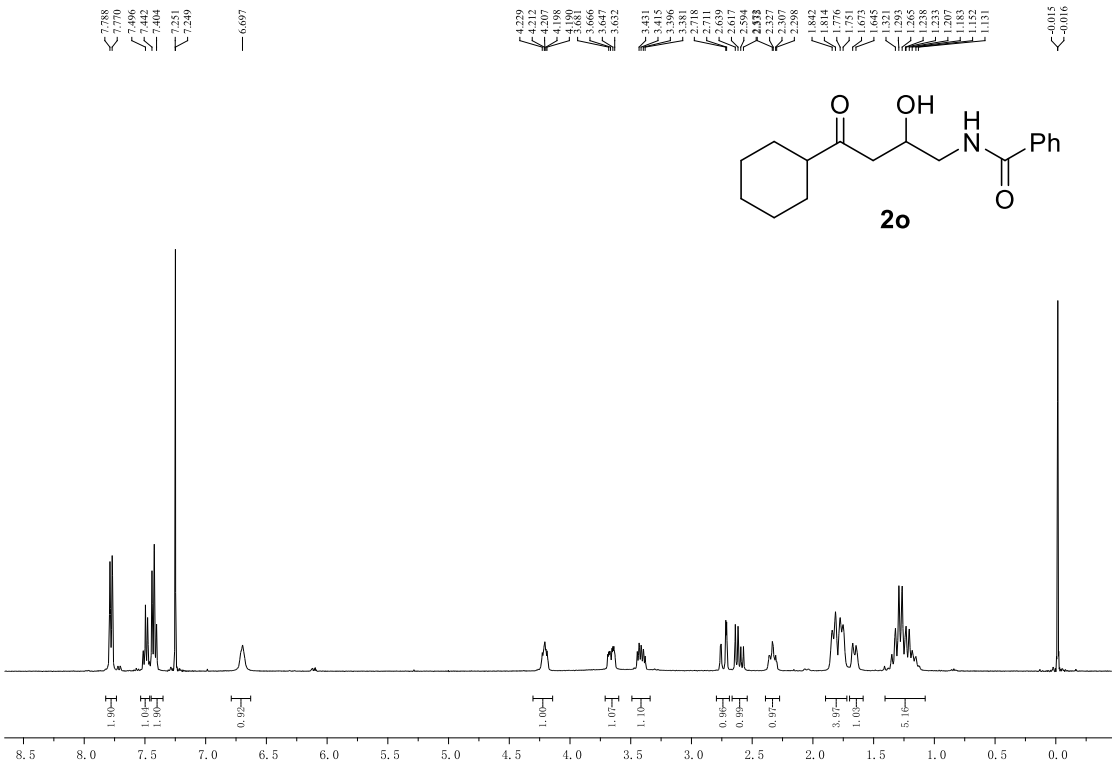

200.697
168.219
142.267
136.504
133.974
133.437
129.419
128.913
128.308
127.142
77.477
77.162
76.841
67.722
44.896
42.428
21.615
0.146
129.419
128.913
128.308
127.142
O
OH
H
N
Ph
Me
O
2l
f1 (ppm)
f1 (ppm)

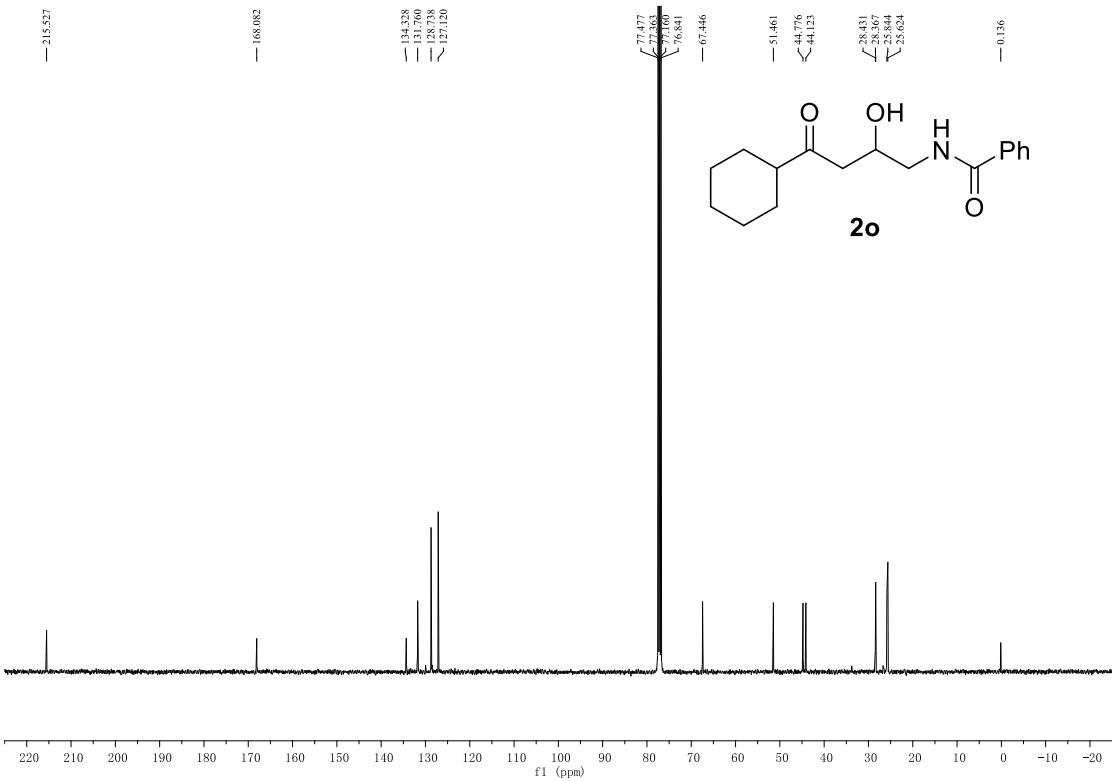

7.958
7.940
7.500
7.481
7.462
7.265
6.088
4.355
4.347
4.338
4.330
4.325
4.317
3.572
3.565
3.557
3.549
3.348
3.246
3.237
3.201
3.193
3.131
3.110
3.087
3.065
2.037
0.000
O
OH
H
N
Me
Ph
O
2m
1.90
0.95
1.94
0.91
1.00
1.11
1.07
1.05
1.04
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

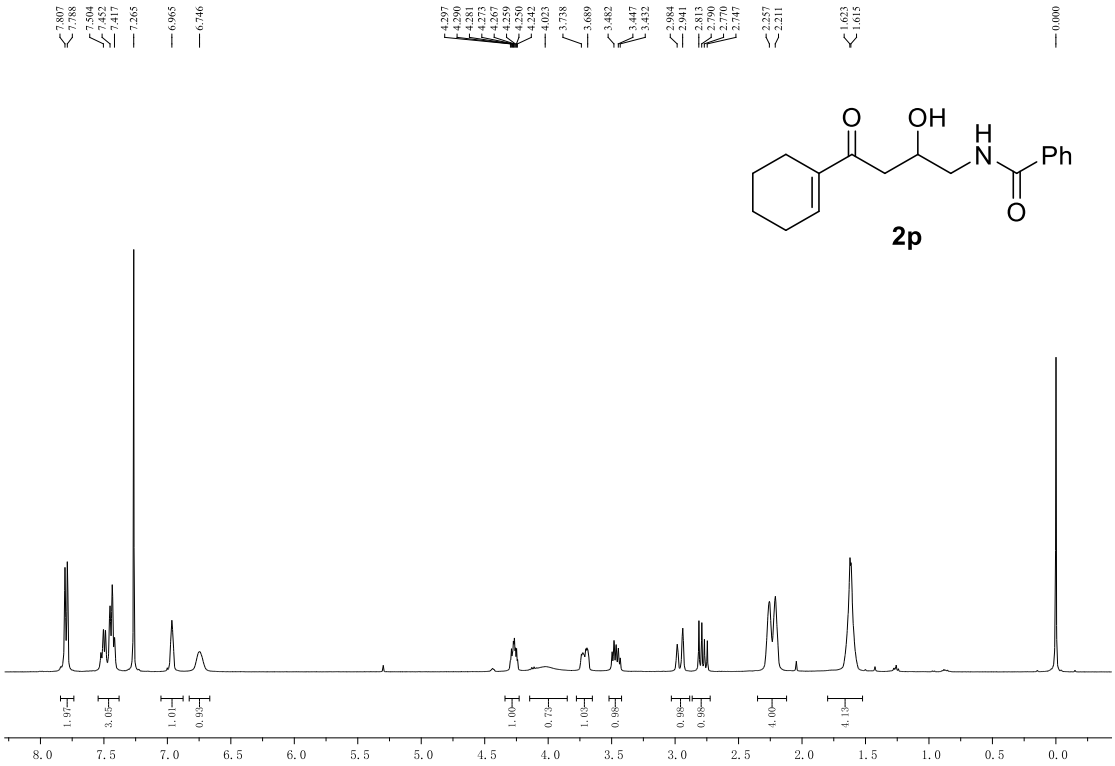

200.588
171.040
136.501
133.973
128.911
128.276
77.475
77.157
76.839
67.542
44.630
42.365
23.404
0.132
O
OH
H
N
Me
Ph
O
2m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)

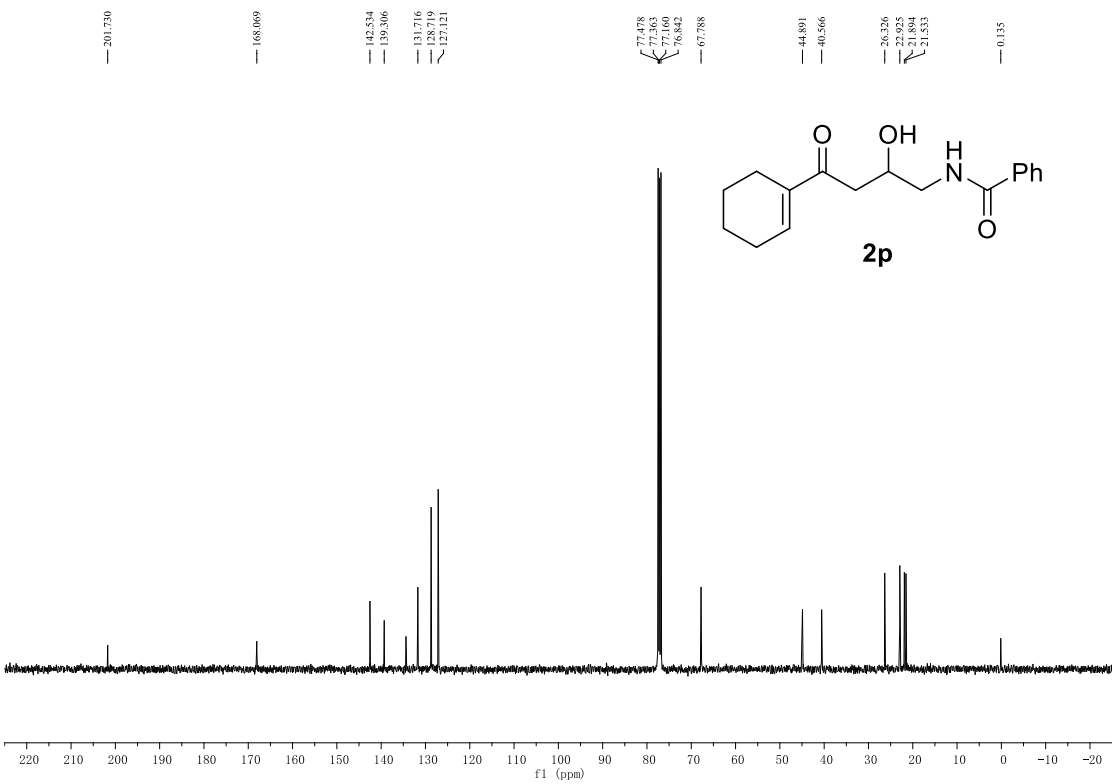

7.938
7.919
7.614
7.596
7.577
7.490
7.471
7.452
7.367
7.359
7.355
7.340
7.335
7.325
7.311
7.301
7.259
5.320
5.122
4.357
4.349
4.341
4.334
4.327
4.319
4.311
3.667
3.662
3.454
3.322
3.271
3.228
3.221
3.183
3.177
3.120
3.098
3.076
3.053
1.653
-0.000
O
OH
H
N
OBn
Ph
O
2n
1.96
1.00
2.02
4.82
0.85
2.11
1.00
0.86
1.08
1.01
0.93
1.05
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

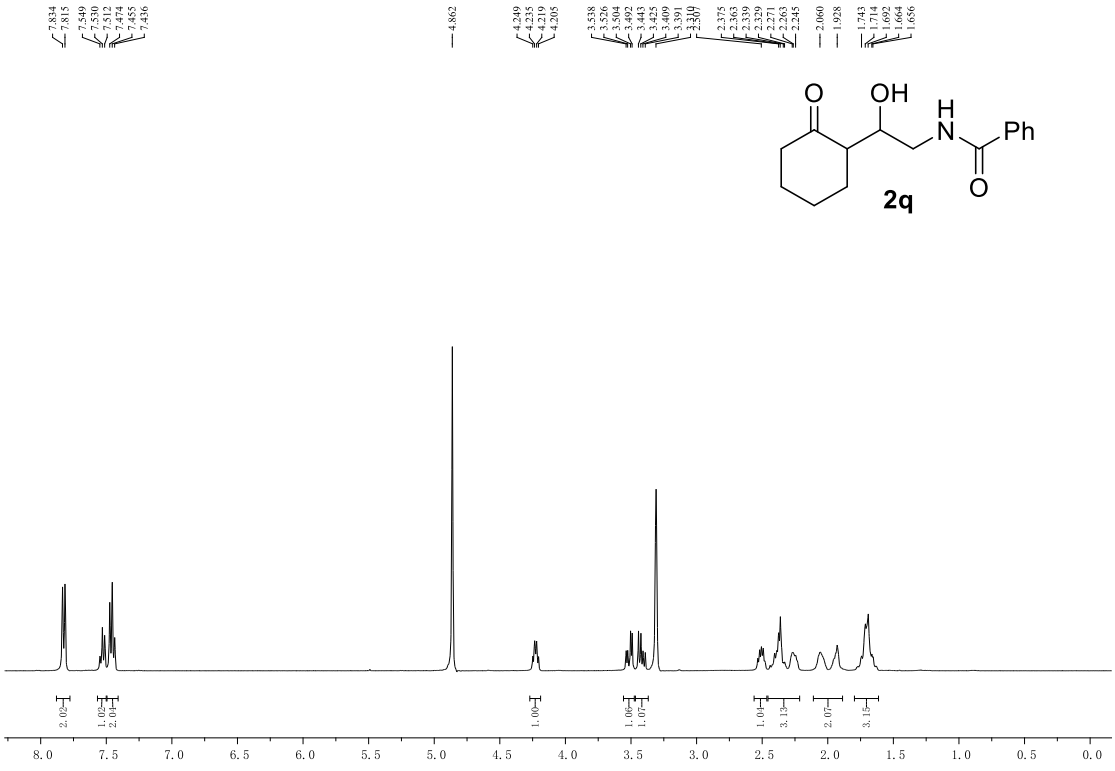

200.487
157.061
136.584
136.524
133.912
128.677
128.577
128.285
128.257
128.218
77.478
77.364
77.160
76.842
67.482
67.010
46.013
42.159
0.139
O
OH
H
N
OBn
Ph
O
2n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

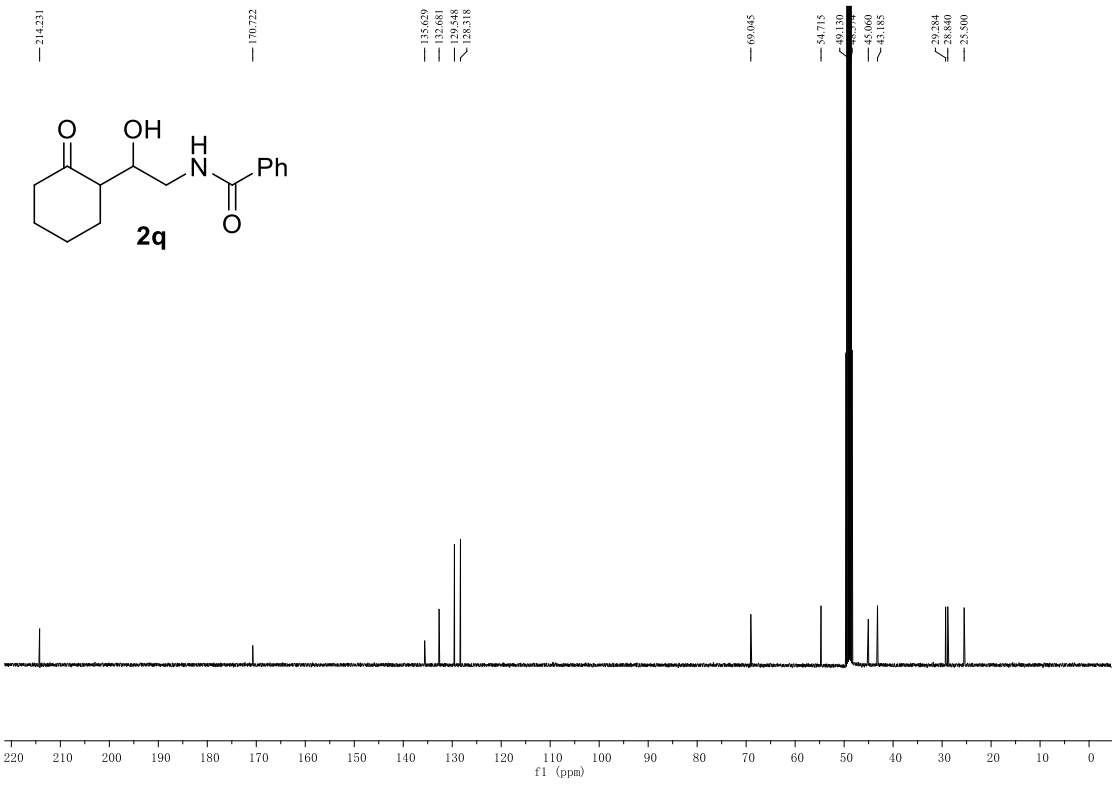

7.788
7.770
7.496
7.442
7.404
7.251
7.249
6.697
4.229
4.212
4.207
4.198
4.190
3.681
3.666
3.647
3.632
3.431
3.415
3.396
3.381
2.718
2.711
2.639
2.617
2.584
2.327
2.307
2.298
1.842
1.814
1.776
1.751
1.673
1.645
1.321
1.293
1.265
1.238
1.233
1.207
1.183
1.152
1.131
0.015
0.016
O
OH
H
N
Ph
O
2o
1.90
1.01
1.90
0.92
1.00
1.07
1.10
0.96
0.99
0.97
3.97
1.03
5.16
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

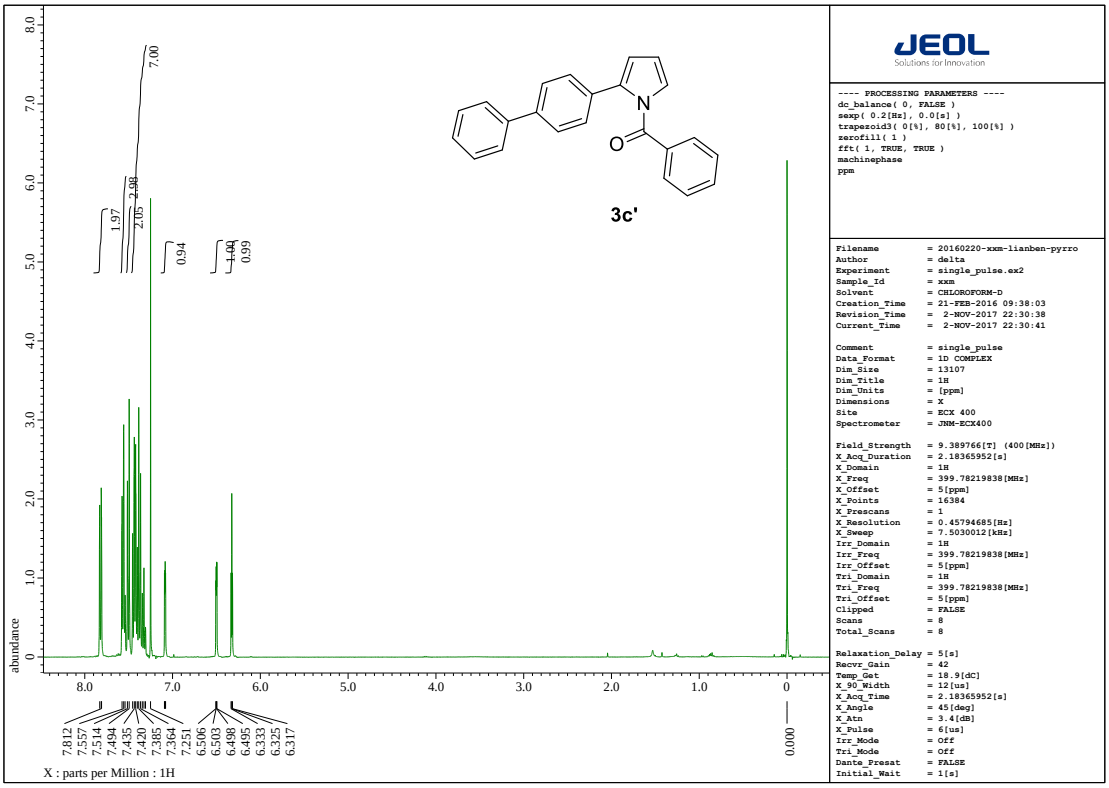

215.527
168.082
134.328
131.760
128.738
127.120
77.477
77.163
76.160
76.841
67.446
51.461
44.776
44.123
28.431
28.367
25.844
25.624
0.136
O
OH
H
N
Ph
O
2o
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)


7.807
7.788
7.504
7.452
7.417
7.265
6.965
6.746
4.297
4.290
4.281
4.273
4.267
4.259
4.250
4.242
4.023
3.738
3.689
3.482
3.447
3.432
2.984
2.941
2.813
2.790
2.770
2.747
2.257
2.211
1.623
1.615
0.000
O
OH
H
N
Ph
O
2p
1.97
3.05
1.01
0.93
1.00
0.73
1.04
0.98
0.98
0.98
4.00
4.13
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


201.730
168.069
142.534
139.306
131.716
128.719
127.121
77.478
77.363
77.160
76.842
67.788
44.891
40.566
26.326
22.925
21.904
21.533
0.135
O
OH
H
N
Ph
O
2p
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)


7.834
7.815
7.549
7.530
7.512
7.474
7.455
7.436
4.862
4.249
4.235
4.219
4.205
3.538
3.526
3.504
3.492
3.443
3.425
3.409
3.391
3.330
2.375
2.363
2.339
2.329
2.271
2.263
2.245
2.060
1.928
1.743
1.714
1.692
1.664
1.656
O
OH
H
N
Ph
O
2q
2.02
1.03
2.04
1.00
1.06
1.07
1.01
3.13
2.07
3.15
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


214.231
170.722
135.629
132.681
129.548
128.318
69.045
54.715
49.130
45.060
43.185
29.284
28.840
25.500
O
OH
H
N
Ph
O
2q
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



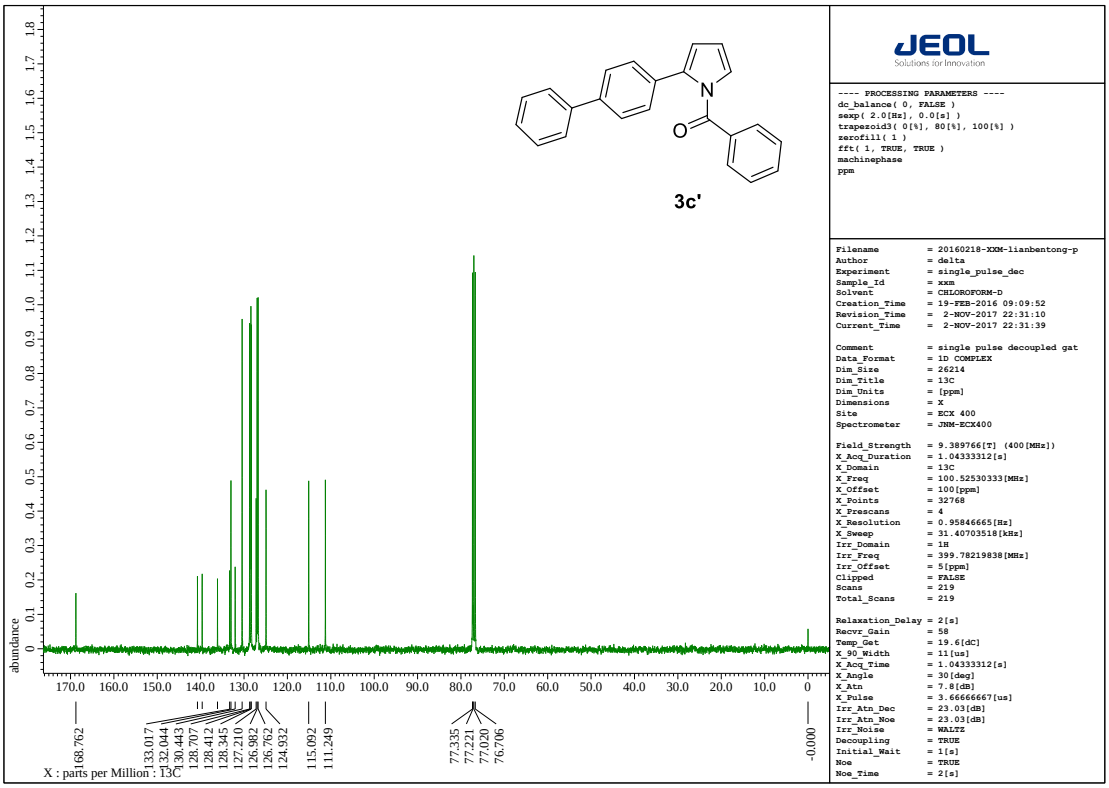

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename          = 20160220-xxm-lianben-pyrro
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 21-FEB-2016 09:38:03
Revision_Time     =  2-NOV-2017 22:30:38
Current_Time      =  2-NOV-2017 22:30:41

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 42
Temp_Get          = 18.9[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



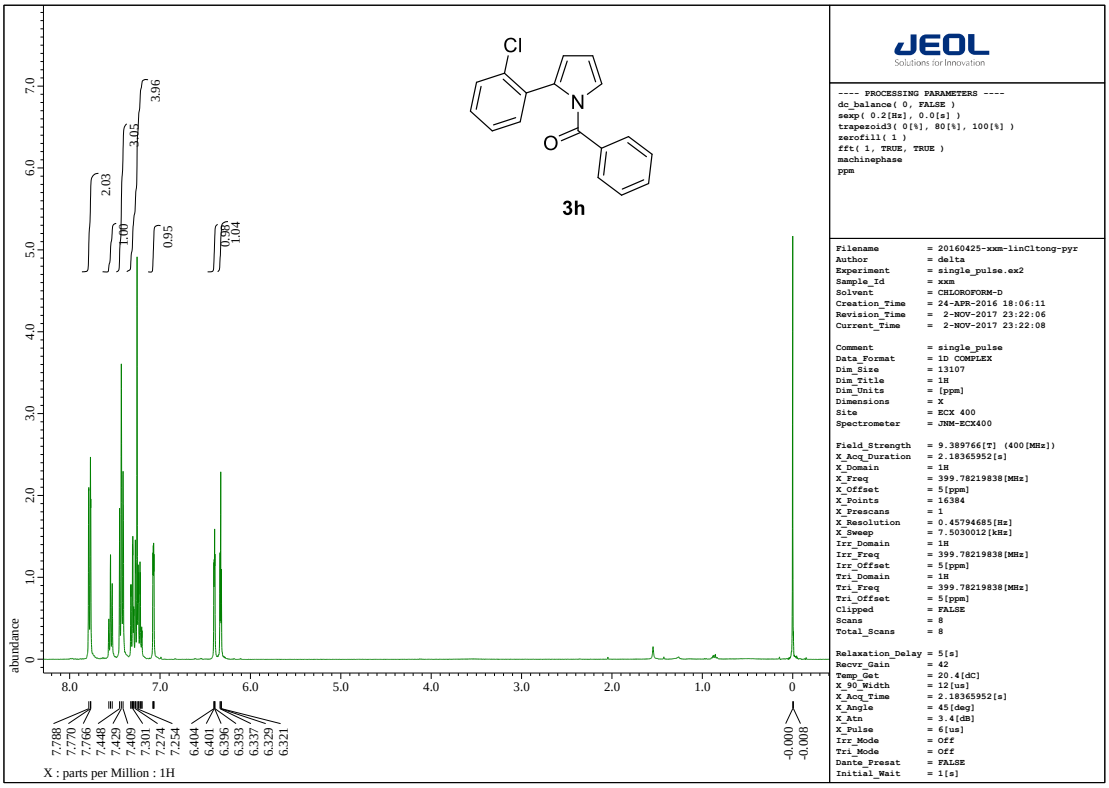

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename          = 20160218-XXM-lianbentong-p
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 19-FEB-2016 09:09:52
Revision_Time     =  2-NOV-2017 22:31:10
Current_Time      =  2-NOV-2017 22:31:39

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 219
Total_Scans       = 219

Relaxation_Delay = 2[s]
Recvr_Gain        = 58
Temp_Get          = 19.6[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



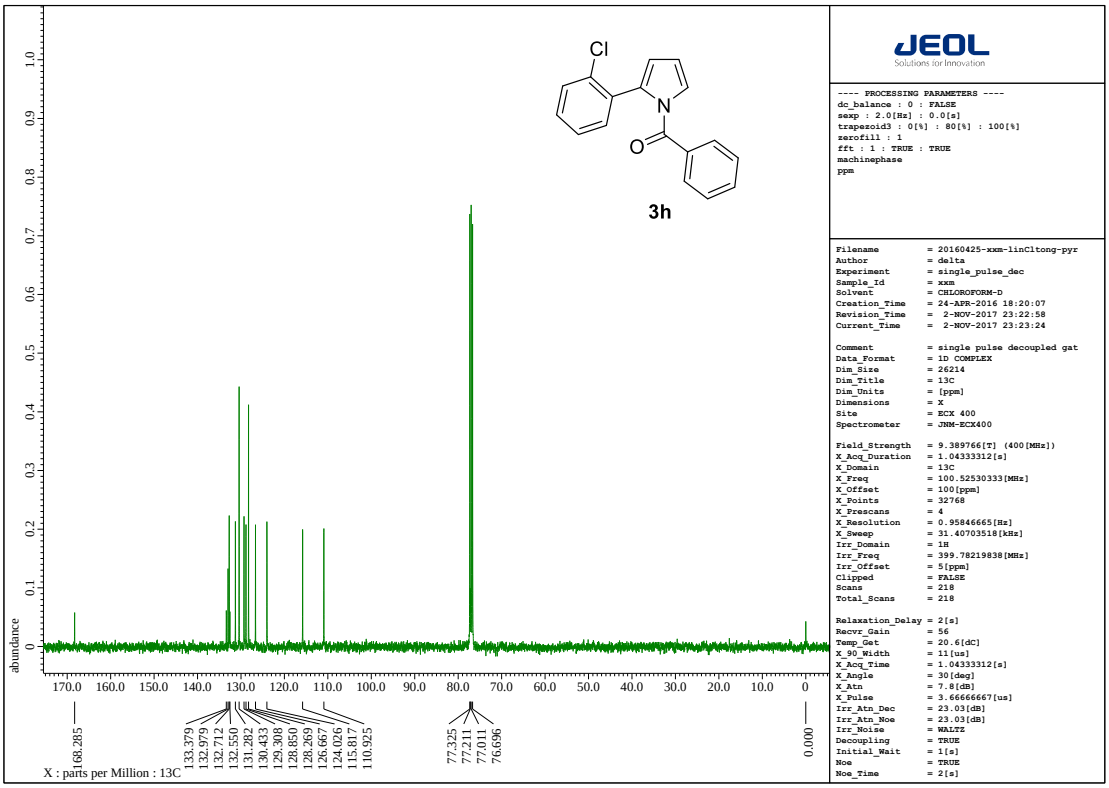

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160425-xxm-linCltong-pyr
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 24-APR-2016 18:06:11
Revision_Time     =  2-NOV-2017 23:22:06
Current_Time      =  2-NOV-2017 23:22:08

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 42
Temp_Get          = 20.4[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



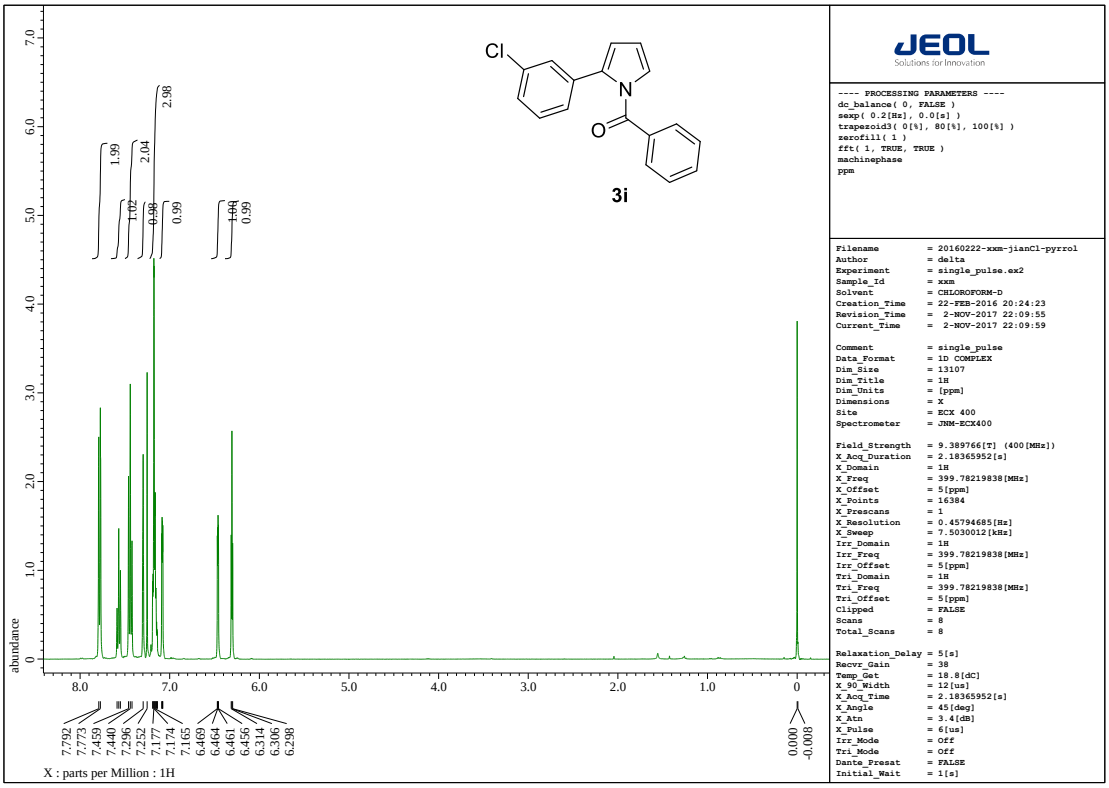

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

```
Filename          = 20160425-xxm-linCltong-pyr
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 24-APR-2016 18:20:07
Revision_Time     =  2-NOV-2017 23:22:58
Current_Time      =  2-NOV-2017 23:23:24

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 218
Total_Scans       = 218

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 20.6[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



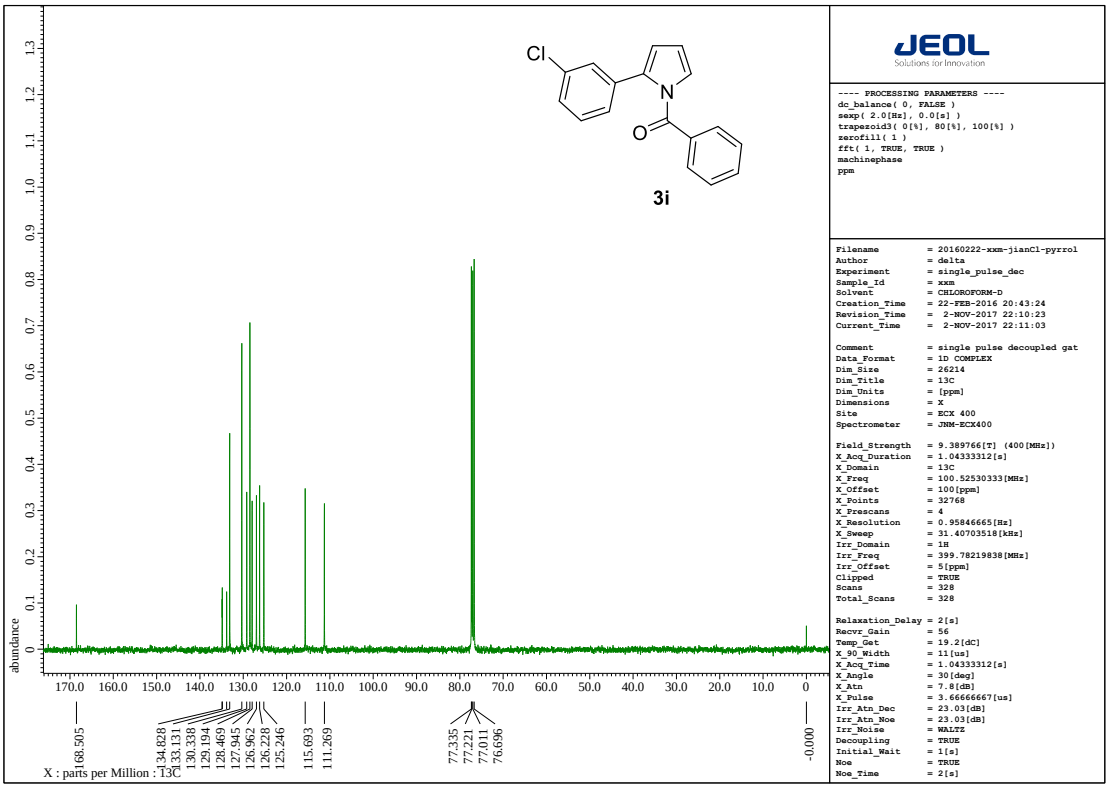

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160222-xxm-jianCl-pyrrol
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2016 20:24:23
Revision_Time     =  2-NOV-2017 22:09:55
Current_Time      =  2-NOV-2017 22:09:59

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 38
Temp_Get          = 18.8[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



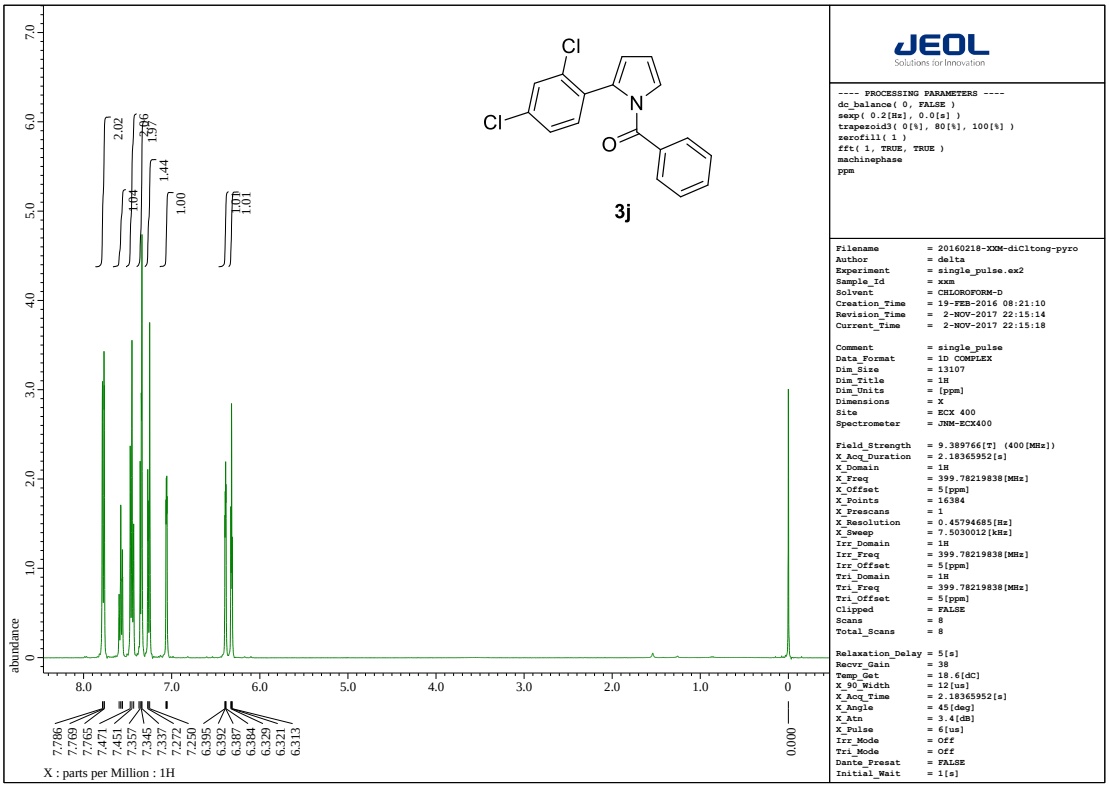

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160222-xxm-jianCl-pyrrol
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2016 20:43:24
Revision_Time     =  2-NOV-2017 22:10:23
Current_Time      =  2-NOV-2017 22:11:03

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 328
Total_Scans       = 328

Relaxation_Delay = 2[s]
Recvr_Gain        = 56
Temp_Get          = 19.2[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



JEOL Solutions for Innovation

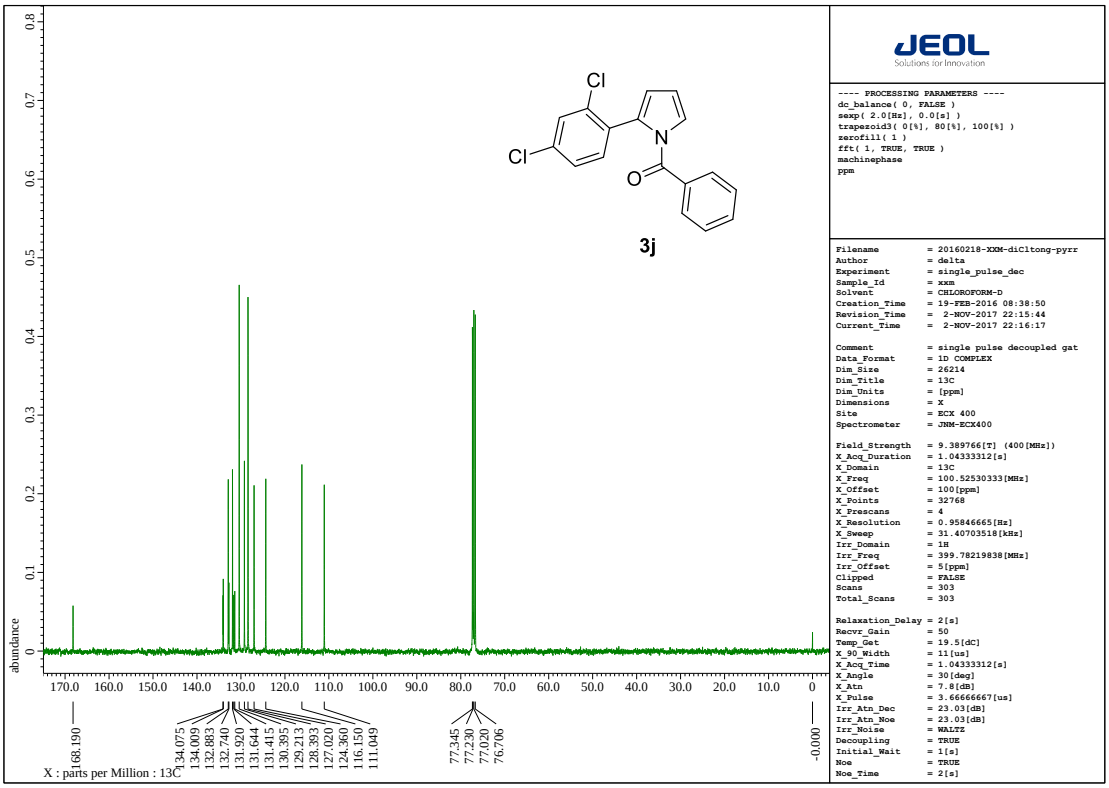
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160218-XXM-diCltong-pyro
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 19-FEB-2016 08:21:10
Revision_Time     =  2-NOV-2017 22:15:14
Current_Time      =  2-NOV-2017 22:15:18

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 38
Temp_Get          = 18.6[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



JEOL Solutions for Innovation

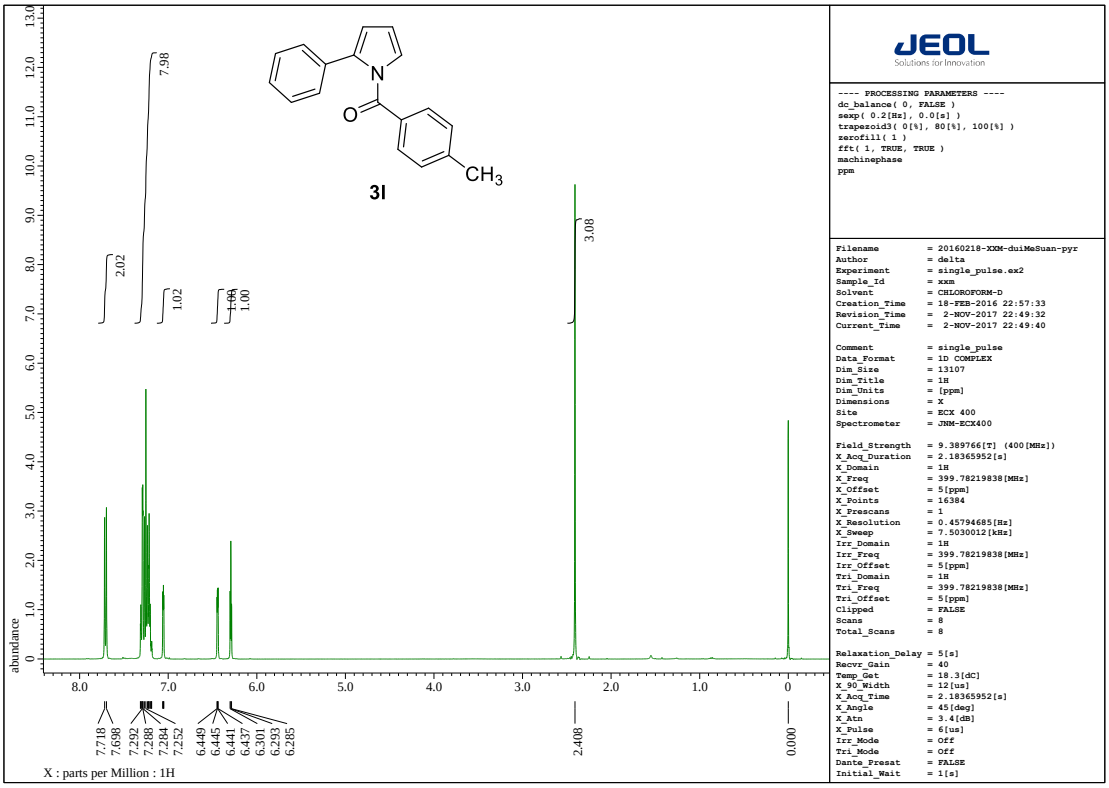
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160218-XXM-diCltong-pyrr
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 19-FEB-2016 08:38:50
Revision_Time     =  2-NOV-2017 22:15:44
Current_Time      =  2-NOV-2017 22:16:17

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 303
Total_Scans       = 303

Relaxation_Delay = 2[s]
Recvr_Gain        = 50
Temp_Get          = 19.5[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



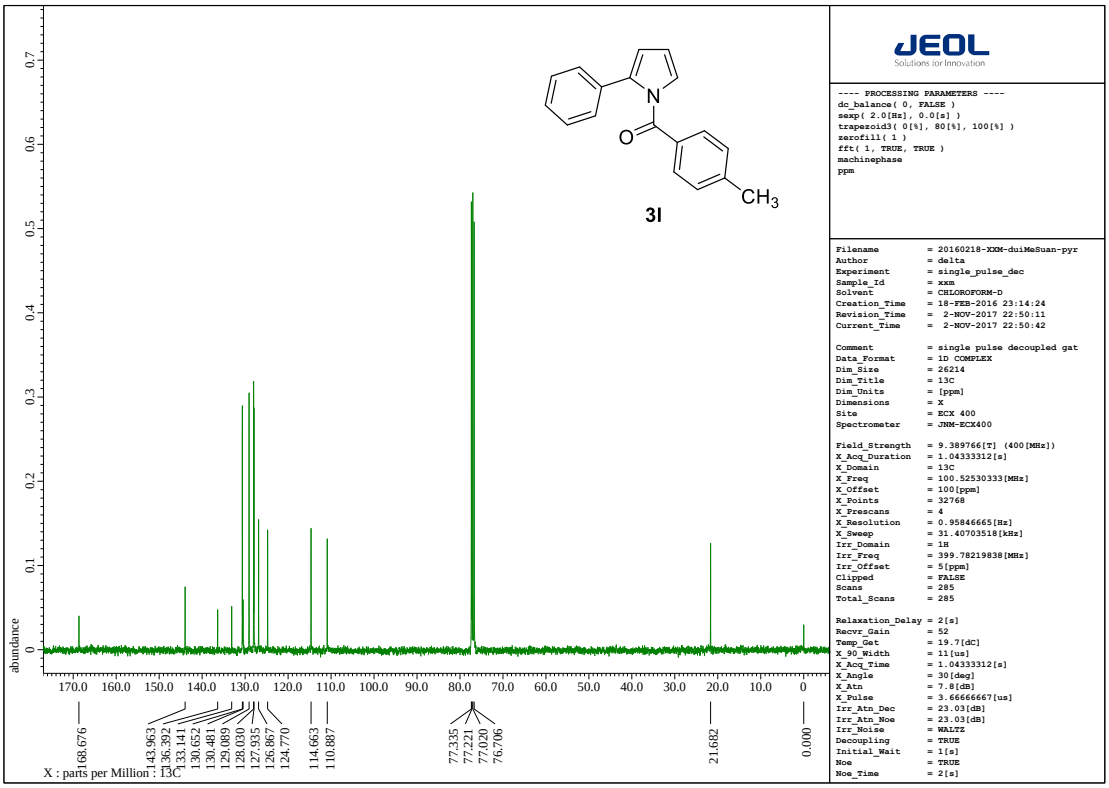

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160218-XXM-duiMeSuan-pyr
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 22:57:33
Revision_Time     =  2-NOV-2017 22:49:32
Current_Time      =  2-NOV-2017 22:49:40

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 40
Temp_Get          = 18.3[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



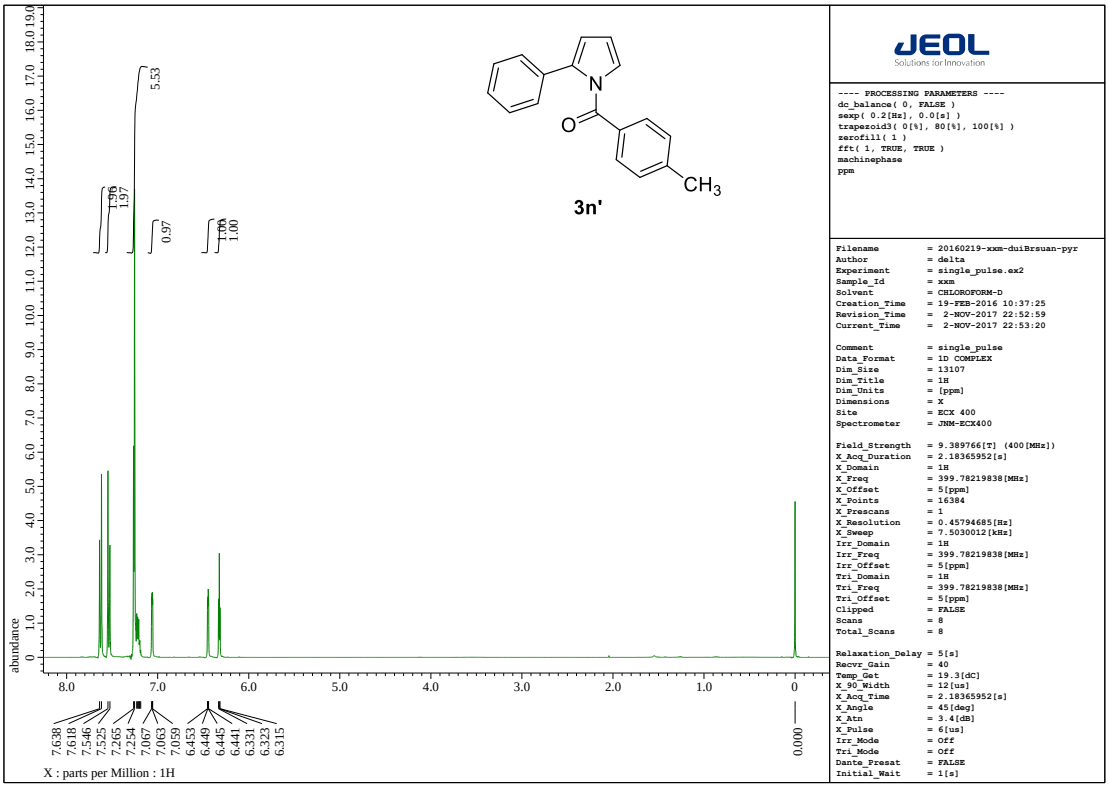

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 20160218-XXM-duiMeSuan-pyr
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 23:14:24
Revision_Time     =  2-NOV-2017 22:50:11
Current_Time      =  2-NOV-2017 22:50:42

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 285
Total_Scans       = 285

Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
Temp_Get          = 19.7[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



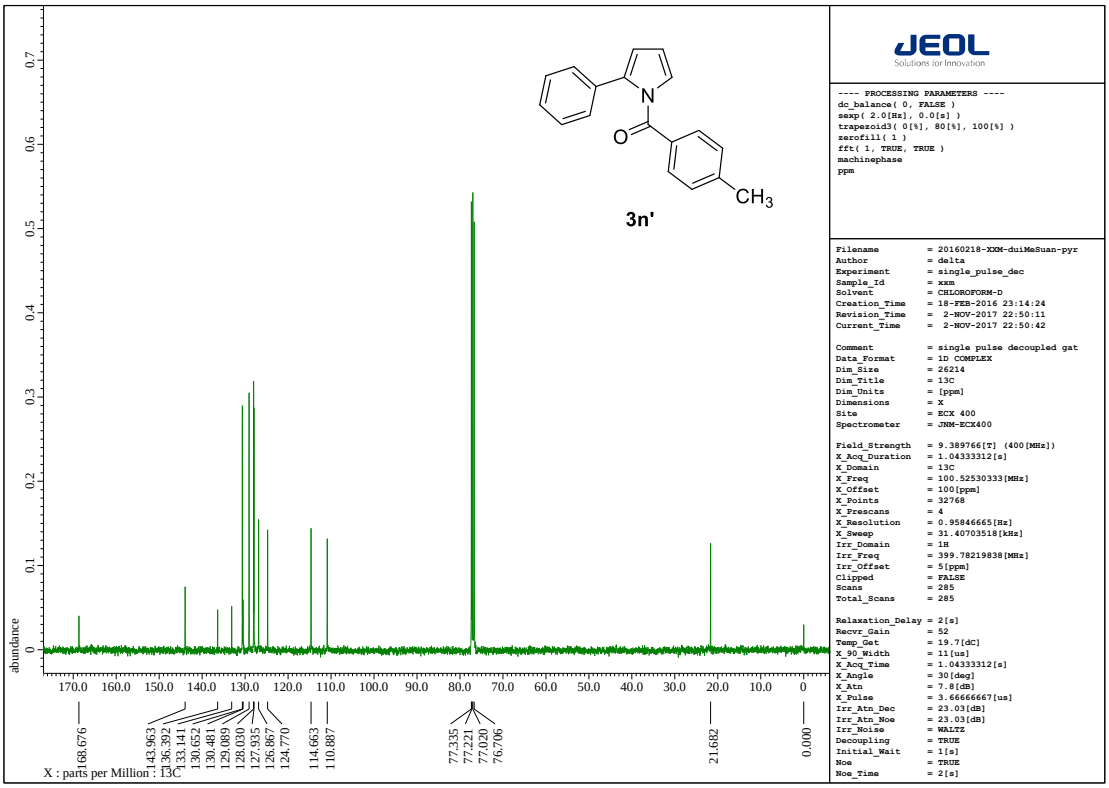

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename          = 20160219-xxm-duiBrsuan-pyr
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 19-FEB-2016 10:37:25
Revision_Time     =  2-NOV-2017 22:52:59
Current_Time      =  2-NOV-2017 22:53:20

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 40
Temp_Get          = 19.3[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



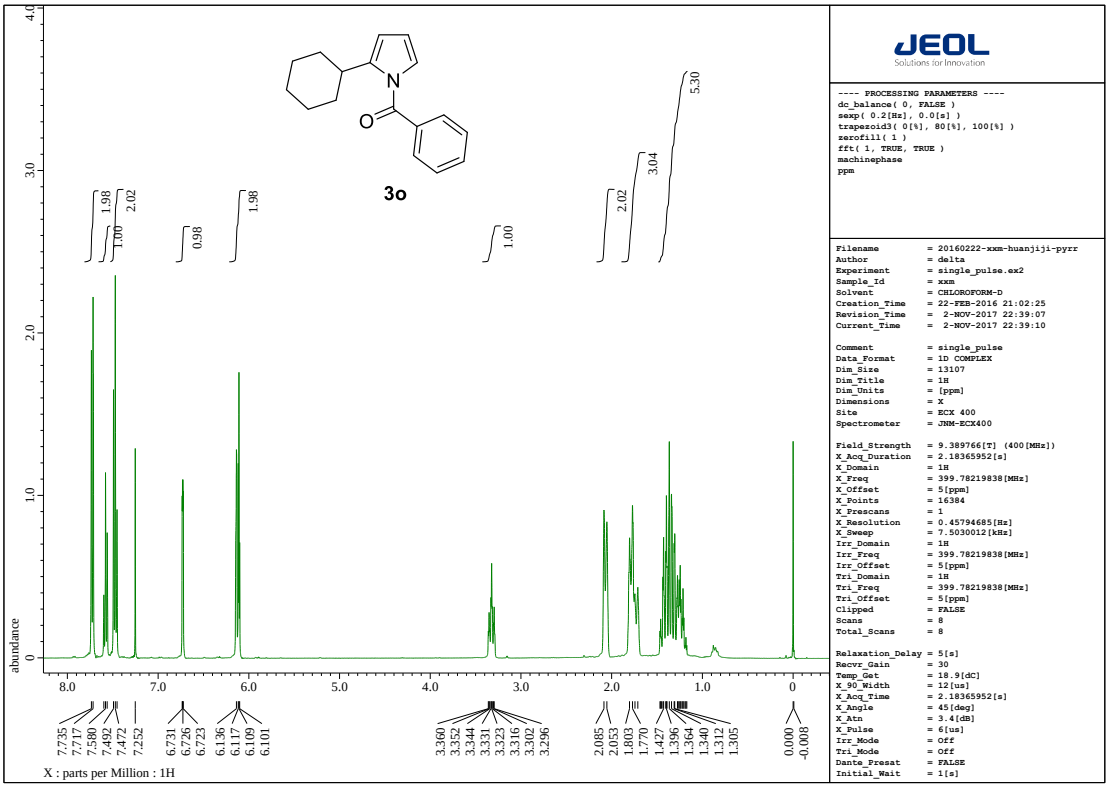

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

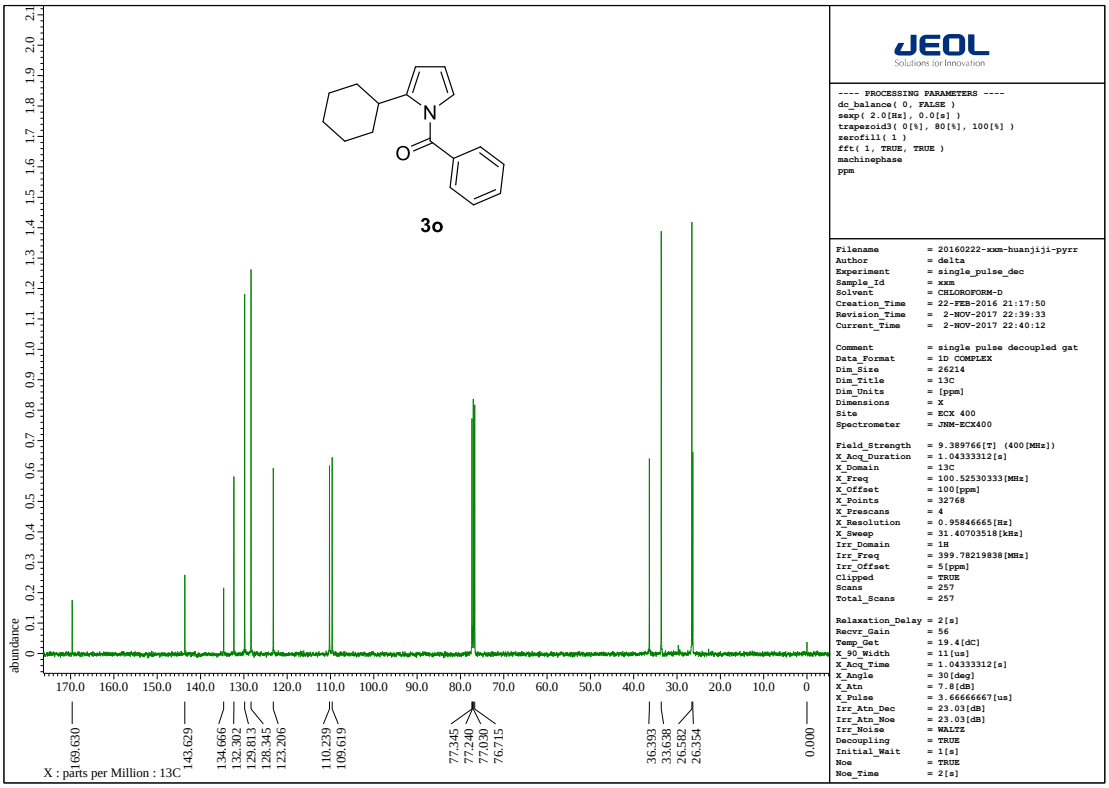
Filename          = 20160218-XXM-duiMeSuan-pyr
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 23:14:24
Revision_Time     =  2-NOV-2017 22:50:11
Current_Time      =  2-NOV-2017 22:50:42

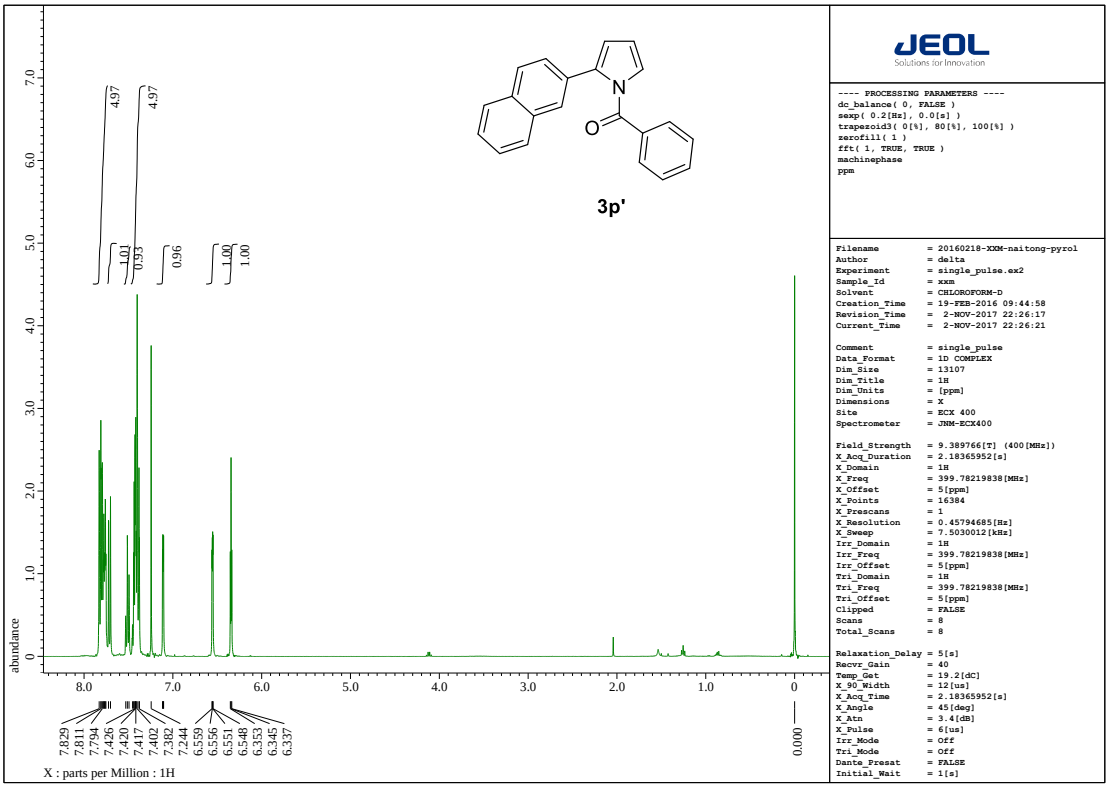
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

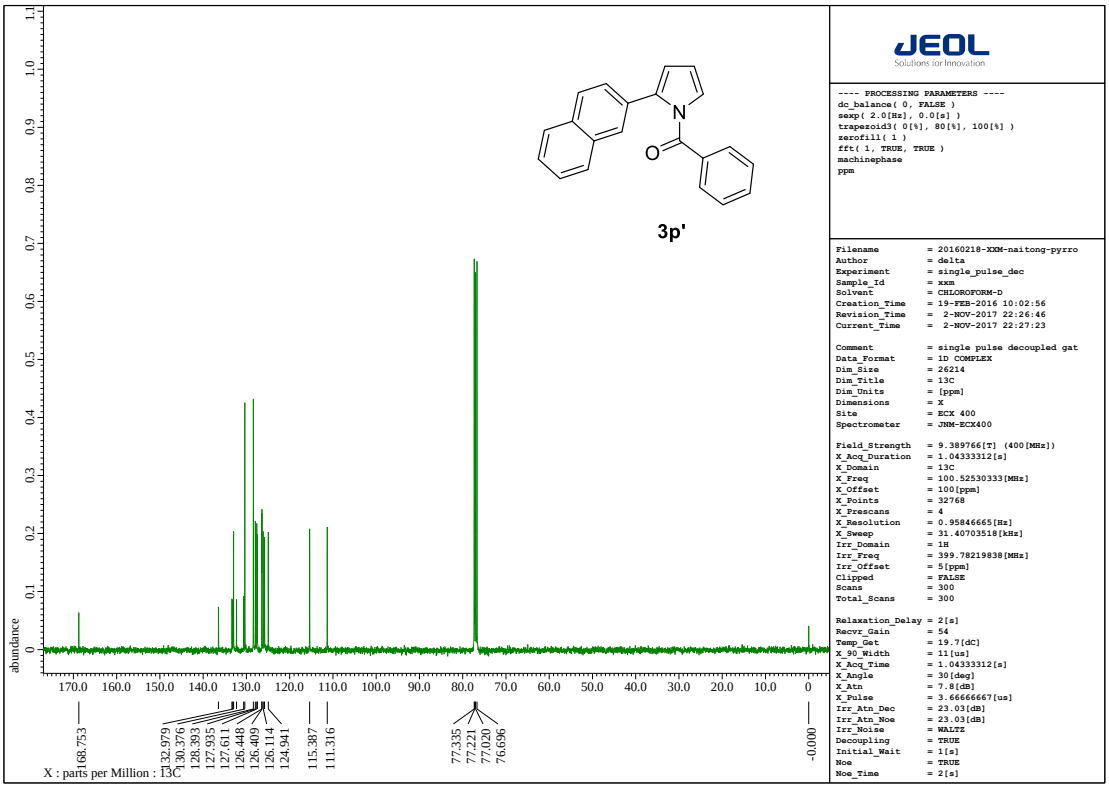
Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 285
Total_Scans       = 285

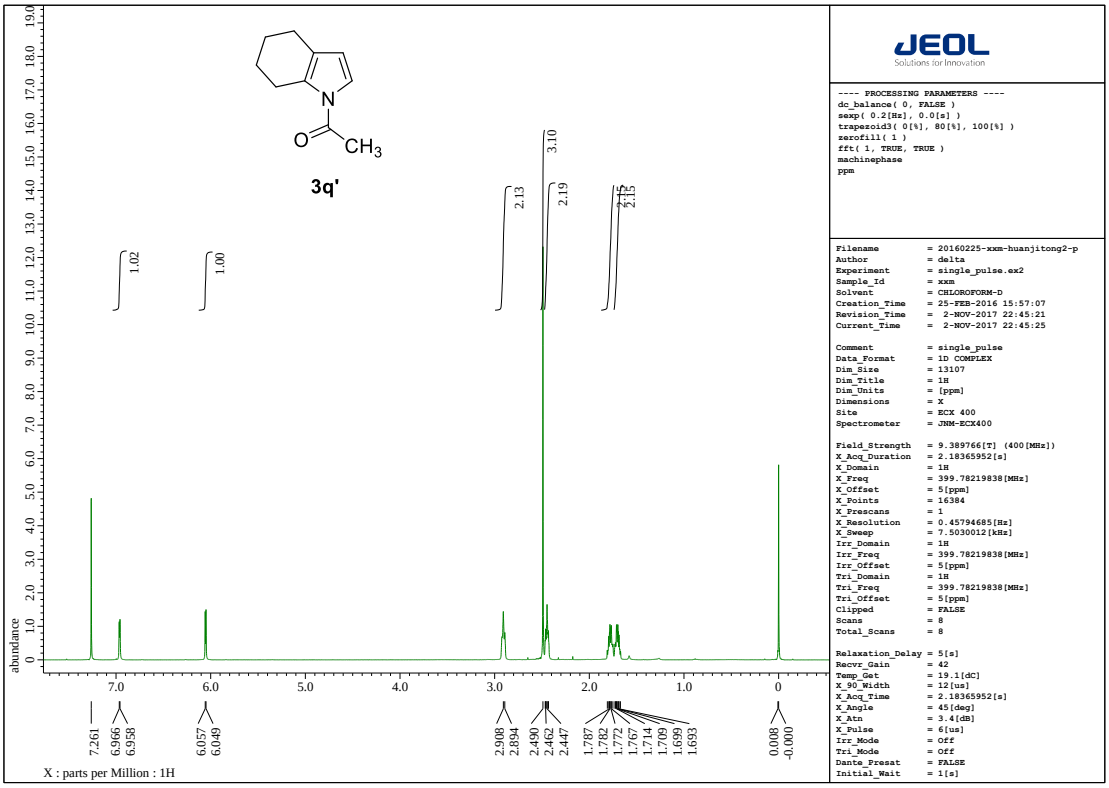
Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
Temp_Get          = 19.7[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```

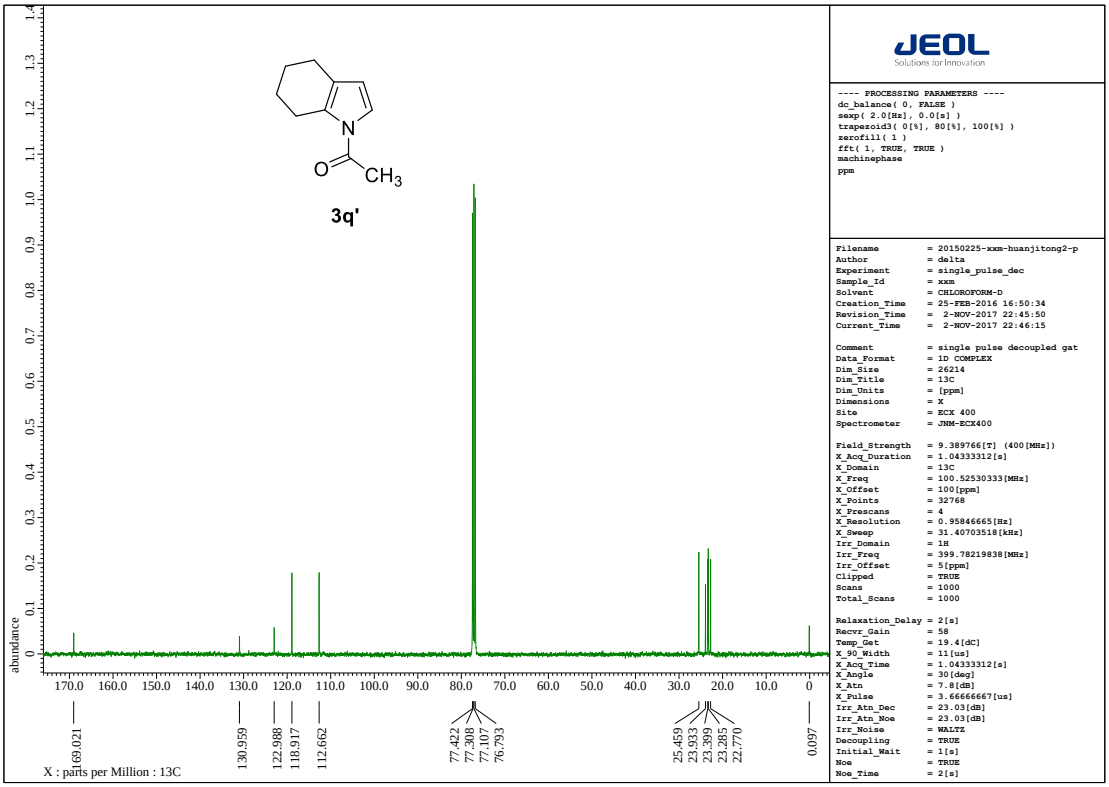

3o
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160222-xxm-huanjiji-pyrr
Author = delta
Experiment = single_pulse.ex2
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 22-FEB-2016 21:02:25
Revision_Time = 2-NOV-2017 22:39:07
Current_Time = 2-NOV-2017 22:39:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 18.9[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 3.4[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

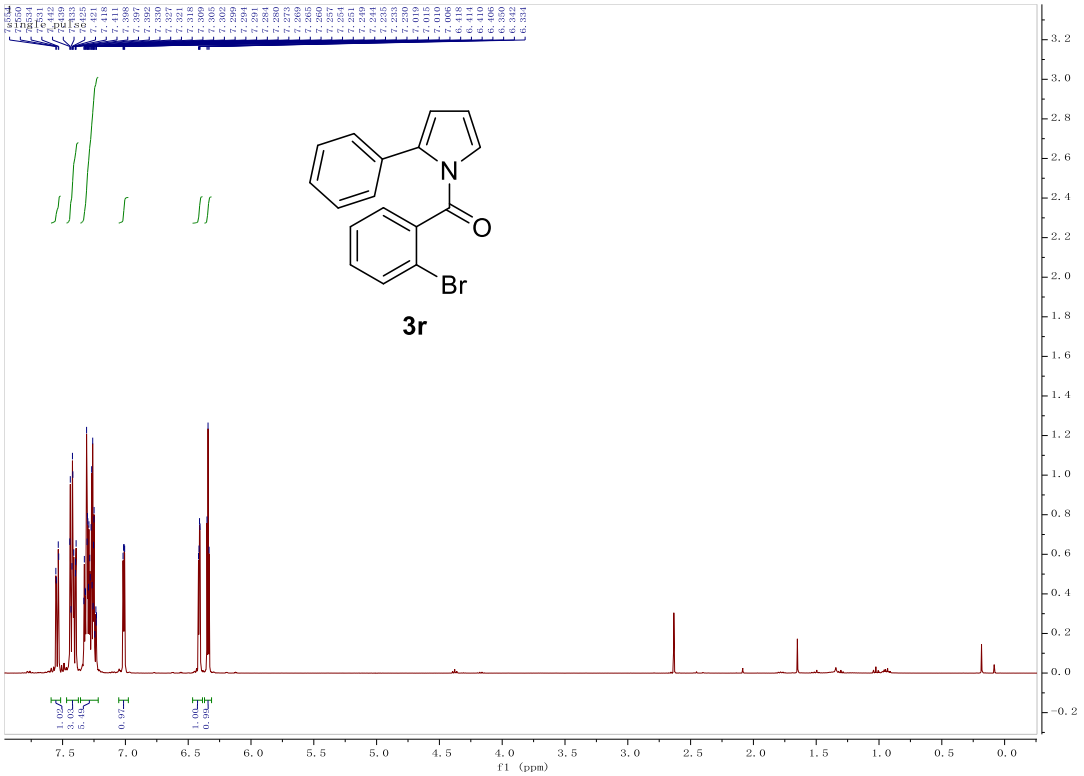

3o
X : parts per Million : 13C
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160222-xxm-huanjiji-pyrr
Author = delta
Experiment = single_pulse_dec
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 22-FEB-2016 21:17:50
Revision_Time = 2-NOV-2017 22:39:33
Current_Time = 2-NOV-2017 22:40:12
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 257
Total_Scans = 257
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 19.4[dC]
X_90_Width = 11[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 3.66666667[us]
Irr_Atn_Dec = 23.03[dB]
Irr_Atn_Noe = 23.03[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

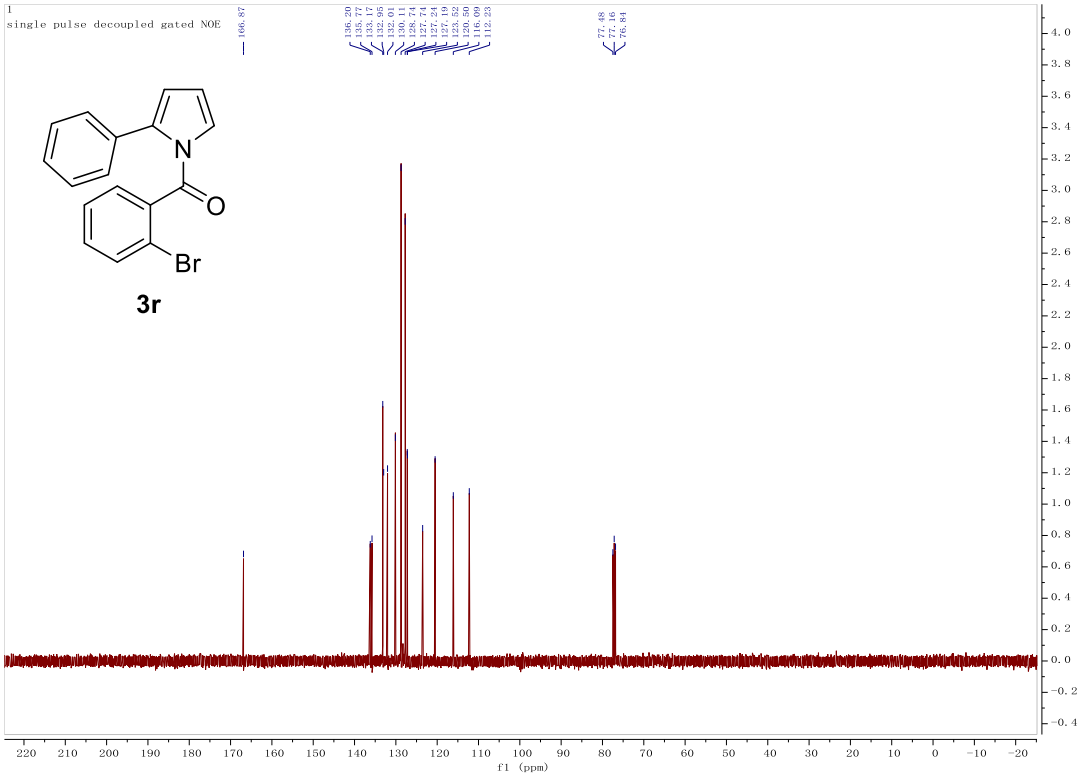

3p'
4.97
4.97
1.01
0.93
0.96
1.00
1.00
7.829
7.811
7.794
7.426
7.420
7.417
7.402
7.382
7.244
6.559
6.556
6.551
6.548
6.353
6.345
6.337
0.000
X : parts per Million : 1H
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160218-XXM-naitong-pyrol
Author = delta
Experiment = single_pulse.ex2
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 19-FEB-2016 09:44:58
Revision_Time = 2-NOV-2017 22:26:17
Current_Time = 2-NOV-2017 22:26:21
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 19.2[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 3.4[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

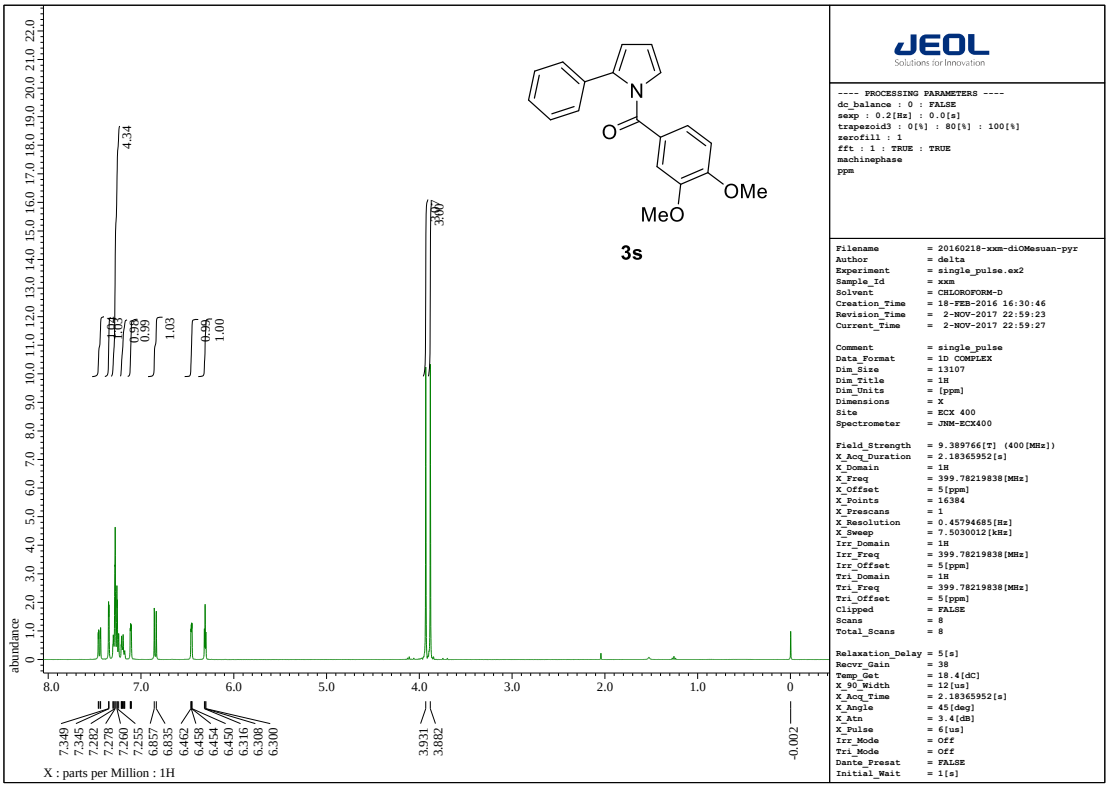

3p'
168.753
132.979
130.376
128.393
127.935
127.611
126.448
126.409
126.114
124.941
115.387
111.316
77.335
77.221
77.020
76.696
-0.000
X : parts per Million : 13C
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160218-XXM-naitong-pyrro
Author = delta
Experiment = single_pulse_dec
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 19-FEB-2016 10:02:56
Revision_Time = 2-NOV-2017 22:26:46
Current_Time = 2-NOV-2017 22:27:23
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 300
Total_Scans = 300
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 19.7[dC]
X_90_Width = 11[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 3.66666667[us]
Irr_Atn_Dec = 23.03[dB]
Irr_Atn_Noe = 23.03[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]


3q'
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160225-xxm-huanjitong2-p
Author = delta
Experiment = single_pulse.ex2
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 25-FEB-2016 15:57:07
Revision_Time = 2-NOV-2017 22:45:21
Current_Time = 2-NOV-2017 22:45:25
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 19.1[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 3.4[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]


3q'
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20150225-xxm-huanjitong2-p
Author = delta
Experiment = single_pulse_dec
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 25-FEB-2016 16:50:34
Revision_Time = 2-NOV-2017 22:45:50
Current_Time = 2-NOV-2017 22:46:15
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 19.4[dC]
X_90_Width = 11[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 3.66666667[us]
Irr_Atn_Dec = 23.03[dB]
Irr_Atn_Noe = 23.03[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]


3r
f1 (ppm)


single pulse decoupled gated NOE
3r
f1 (ppm)



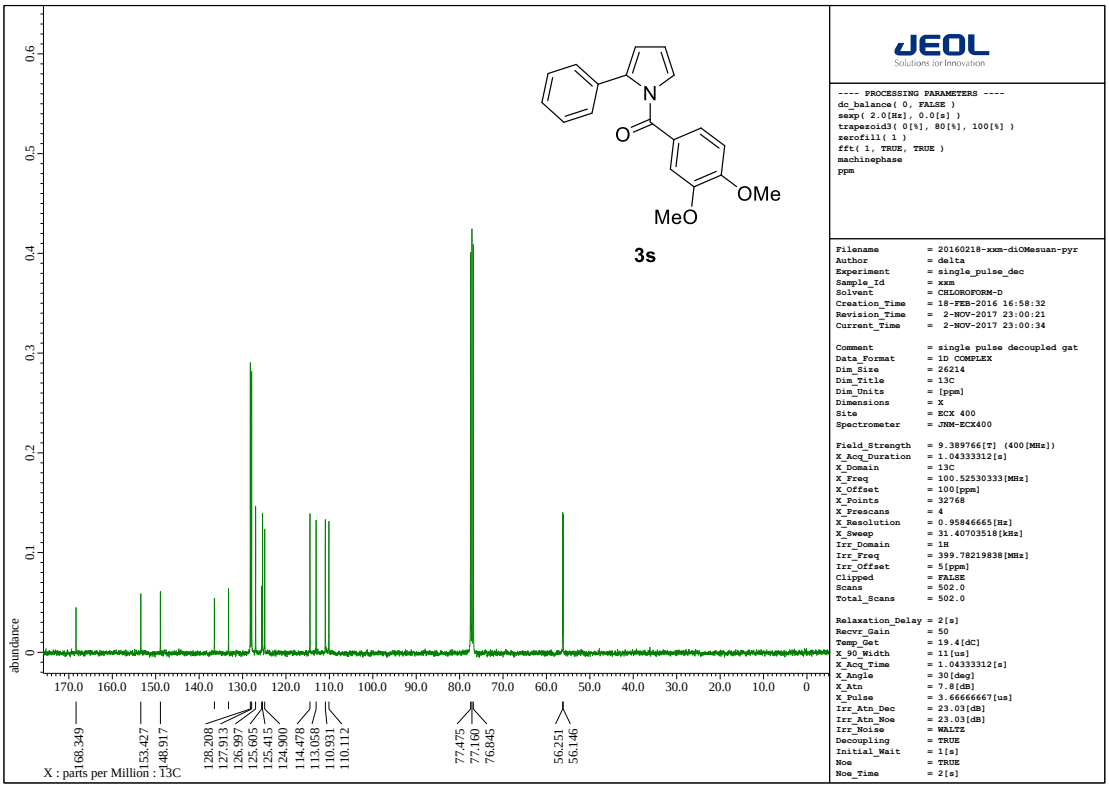

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Filename          = 20160218-xxm-diOMesuan-pyr
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 16:30:46
Revision_Time     =  2-NOV-2017 22:59:23
Current_Time      =  2-NOV-2017 22:59:27

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 38
Temp_Get          = 18.4[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



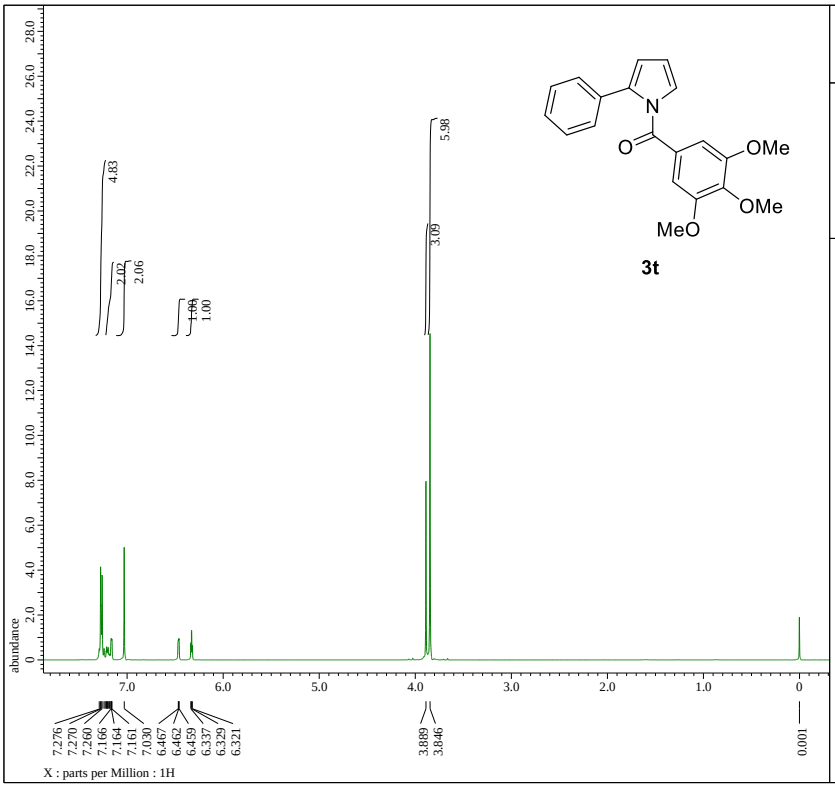

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename          = 20160218-xxm-diOMesuan-pyr
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 16:58:32
Revision_Time     =  2-NOV-2017 23:00:21
Current_Time      =  2-NOV-2017 23:00:34

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 502.0
Total_Scans       = 502.0

Relaxation_Delay = 2[s]
Recvr_Gain        = 50
Temp_Get          = 19.4[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



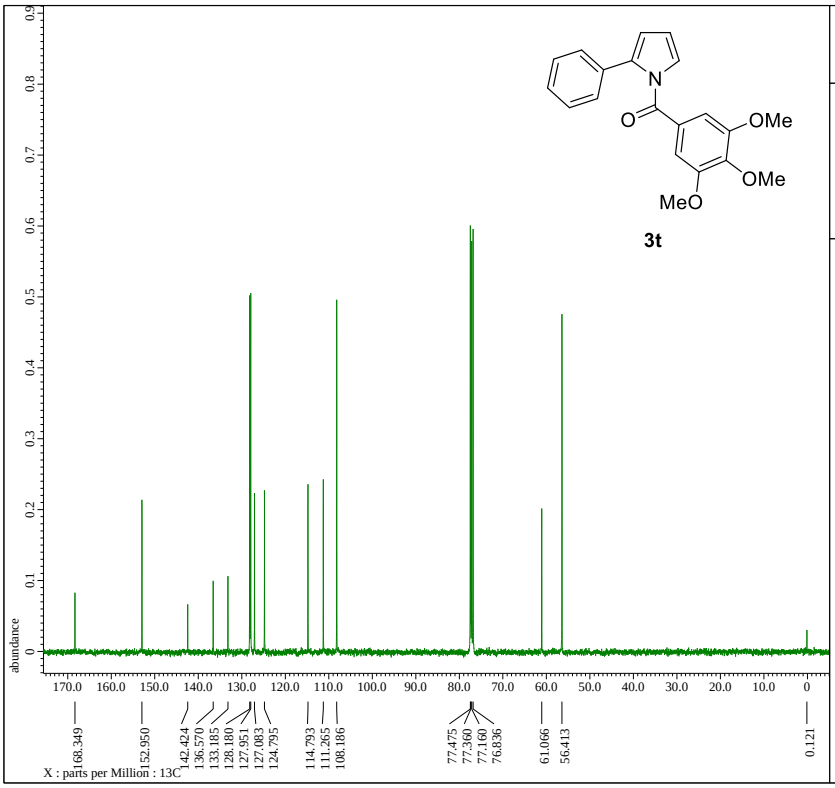

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Filename          = 20160218-xxm-triOMesuan-py
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 16:00:58
Revision_Time     =  2-NOV-2017 23:02:13
Current_Time      =  2-NOV-2017 23:02:17

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 36
Temp_Get          = 19.2[dC]
X_90_Width        = 12[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.4[dB]
X_Pulse           = 6[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



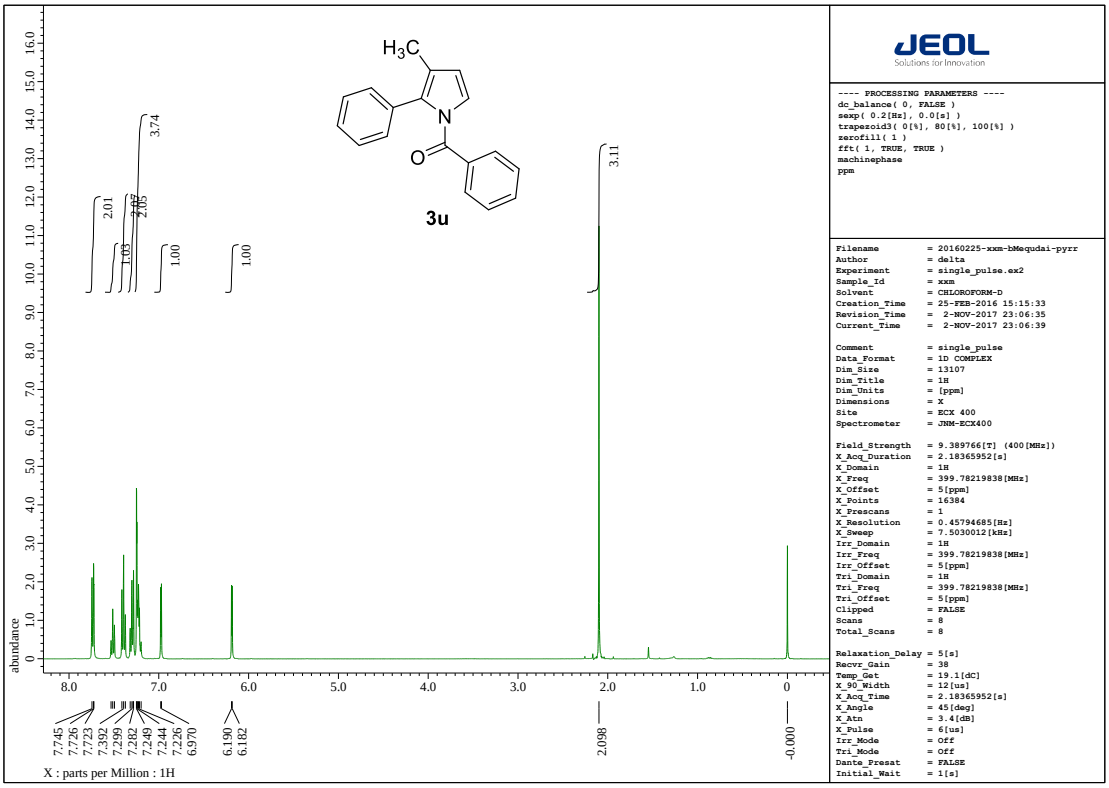

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

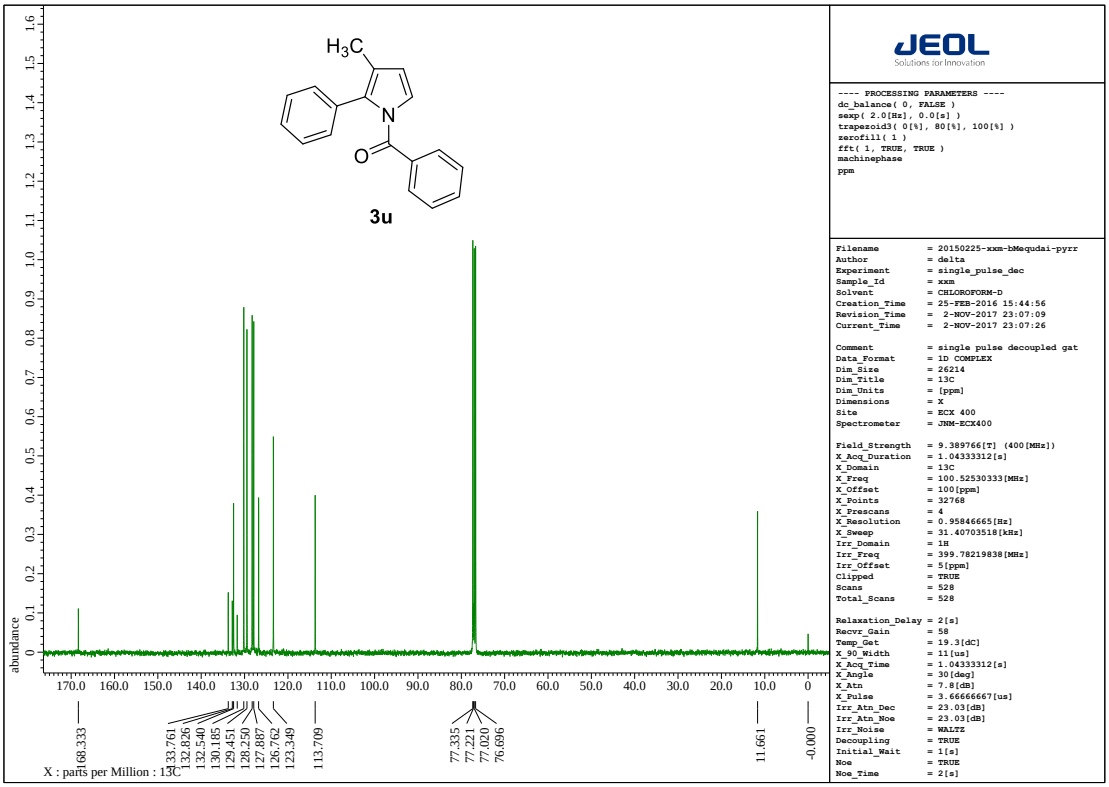
Filename          = 20160218-xxm-triOMesuan-py
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = xxm
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2016 16:19:32
Revision_Time     = 18-FEB-2016 16:50:09
Current_Time      =  2-NOV-2017 23:02:38

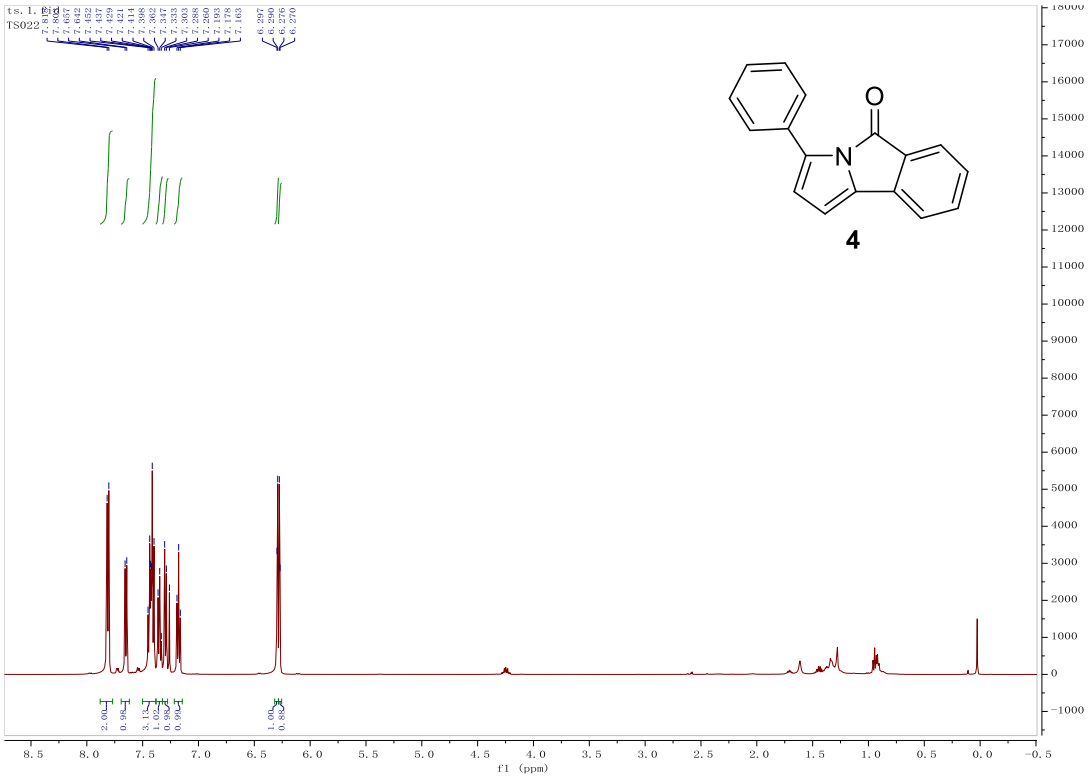
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

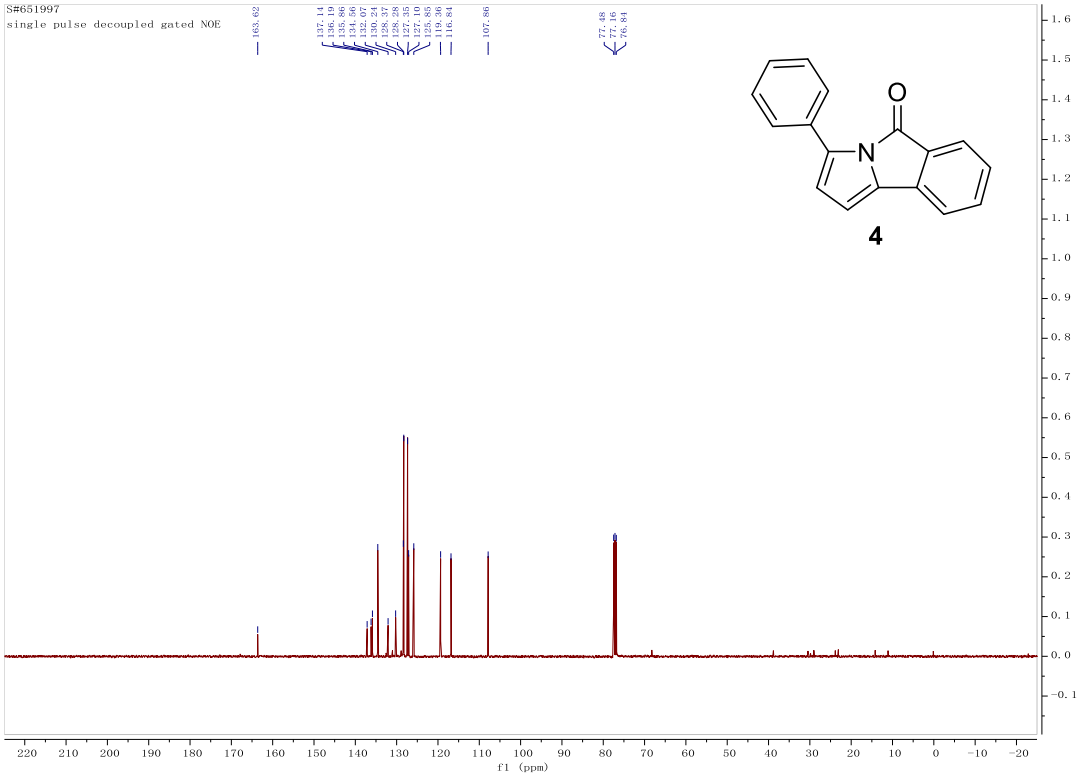
Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 302
Total_Scans       = 302

Relaxation_Delay = 2[s]
Recvr_Gain        = 52
Temp_Get          = 19.6[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 7.8[dB]
X_Pulse           = 3.66666667[us]
Irr_Atn_Dec       = 23.03[dB]
Irr_Atn_Noe       = 23.03[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```


3u
abundance
X : parts per Million : 1H
7.745
7.726
7.723
7.392
7.299
7.282
7.249
7.244
7.226
6.970
6.190
6.182
2.098
-0.000
2.01
1.03
3.74
2.02
2.05
1.00
1.00
3.11
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20160225-xxm-bMequdai-pyrr
Author = delta
Experiment = single_pulse.ex2
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 25-FEB-2016 15:15:33
Revision_Time = 2-NOV-2017 23:06:35
Current_Time = 2-NOV-2017 23:06:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 19.1[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 3.4[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]


3u
abundance
X : parts per Million : 13C
168.333
133.761
132.826
132.540
130.185
129.451
128.250
127.887
126.762
123.349
113.709
77.335
77.221
77.020
76.696
11.661
-0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20150225-xxm-bMequdai-pyrr
Author = delta
Experiment = single_pulse_dec
Sample_Id = xxm
Solvent = CHLOROFORM-D
Creation_Time = 25-FEB-2016 15:44:56
Revision_Time = 2-NOV-2017 23:07:09
Current_Time = 2-NOV-2017 23:07:26
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 528
Total_Scans = 528
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 19.3[dC]
X_90_Width = 11[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 7.8[dB]
X_Pulse = 3.66666667[us]
Irr_Atn_Dec = 23.03[dB]
Irr_Atn_Noe = 23.03[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]


ts. I. H
TS022
4
f1 (ppm)


S#651997
single pulse decoupled gated NOE
4
f1 (ppm)