Supplementary Information

Pivalophenone N–H Imine as a Benzonitrile Surrogate for Directed C–H Bond Functionalization

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Material and Methods

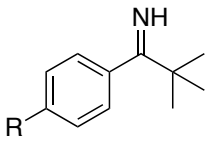
General. All reactions dealing with air- and moisture-sensitive compounds were carried out in oven-dried reaction vessels under nitrogen atmosphere. Analytical thin-layer chromatography (TLC) was performed on Merck 60 F254 silica gel plates. Flash column chromatography was performed using 40-63μm silica gel (Si 60, Merck). ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on a JEOL ECA-400 (400 MHz), Bruker AV-300 (300 MHz), or AV-400 (400 MHz) NMR spectrometers. ^{1}H and ^{13}C NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm), and ^{31}P NMR spectra are reported in reference to an external standard, 85% phosphoric acid (0 ppm). Gas chromatography (GC) analysis was performed on a Shimadzu GC-2010 system equipped with glass capillary column DB-5 (Agilent J&W, 0.25 mm i.d. x 30 m, 0.25 μm film thickness). High-resolution mass spectra (HRMS) were obtained with a Q-Tof Premier LC HR mass spectrometer. Melting points were determined using a capillary melting point apparatus and are uncorrected.

Materials. Unless otherwise noted, commercial reagents were purchased from Aldrich, Alfa Aesar, and other commercial suppliers and were used as received. THF was distilled over Na/benzophenone. Grignard reagents were prepared from the corresponding alkyl halides and magnesium turnings in THF, and titrated before use. $CoBr_2$ (99%) was purchased from Sigma-Aldrich and used as received. $Co(acac)_3$ was purchased from Alfa Aesar and used as received. *N*,*N*-Diisopropylimidazolinium tetrafluoroborate (**L1**) was purchased from Sigma-Aldrich and used as received.

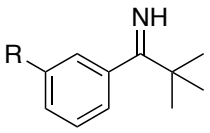
Preparation of Starting Materials and Ligand

Pivalophenone N–H Imines

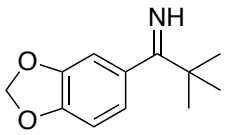
All imines shown below were synthesized from the corresponding aryl nitriles and *t*-BuLi according to the literature procedures,[1] and purified by recrystallization or distillation. Spectral data for **1a**,[2] **1d**,[1] **1f**,[3] and **1g**[1] showed good agreement with the literature data.



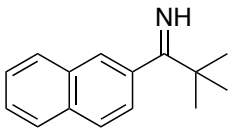
1a (R = H)
1b (R = Me)
1c (R = Ph)
1d (R = OMe)
1e (R = OCF_3)
1f (R = SMe)
1g (R = NMe_2)
1h (R = F)



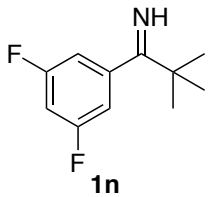
1i (R = Me)
1j (R = CF_3)
1k (R = OMe)



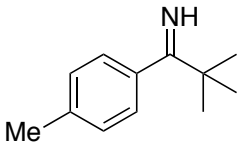
1l



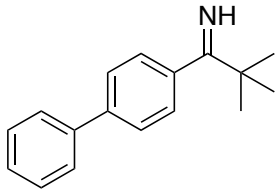
1m



1n

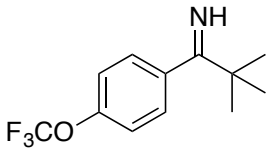


2,2-Dimethyl-1-(*p*-tolyl)propan-1-imine (1b): Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.13 (brs, 1H), 7.14 – 7.08 (m, 4H), 2.35 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.5, 139.7, 137.8, 128.7, 126.5, 40.2, 28.7, 21.3; HRMS (ESI) Calcd for $C_{12}H_{18}N$ $[M + H]^+$ 176.1439, found 176.1435.

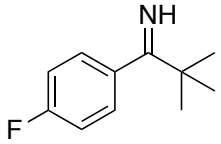


1-([1,1'-Biphenyl]-4-yl)-2,2-dimethylpropan-1-imine (1c): White solid; M.p. 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.27 (brs, 1H), 7.62 – 7.56 (m, 4H), 7.48 – 7.42 (m, 2H), 7.39 – 7.34 (m, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 141.0, 140.6, 129.0 (two signals overlapped), 127.7, 127.2, 127.1, 126.8, 28.6; HRMS (ESI) Calcd for

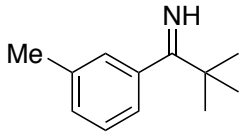
$C_{17}H_{20}N$ $[M + H]^+$ 238.1596, found 238.1586.



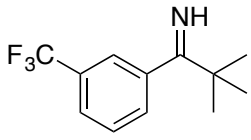
2,2-Dimethyl-1-(4-(trifluoromethoxy)phenyl)propan-1-imine (1e): Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.16 (brs, 1H), 7.28 – 7.17 (m, 4H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.1, 149.1, 141.0, 128.3, 120.7, 120.6 (q, $^1J_{C\text{-}F}$ = 257.5 Hz), 40.5, 28.5; HRMS (ESI) Calcd for $C_{12}H_{15}NOF_3$ $[M + H]^+$ 246.1106, found 246.1105.



1-(4-Fluorophenyl)-2,2-dimethylpropan-1-imine (1h): Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.12 (brs, 1H), 7.14 (brs, 2H), 6.99 – 6.94 (m, 2H), 1.18 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.4, 162.4 (d, $^1J_{C\text{-}F}$ = 247.2 Hz), 138.4, 128.3, 115.0 (d, $^2J_{C\text{-}F}$ = 21.4 Hz), 40.5, 28.4; HRMS (ESI) Calcd for $C_{11}H_{15}NF$ $[M + H]^+$ 180.1189, found 180.1196.

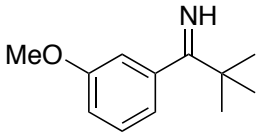


2,2-Dimethyl-1-(*m*-tolyl)propan-1-imine (1i): Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.13 (brs, 1H), 7.19 (t, J = 7.9 Hz, 1H), 7.12 (d, J = 7.3 Hz, 1H), 6.99 – 6.95 (m, 2H), 2.34 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 142.4, 137.7, 128.7, 127.8, 127.1, 123.5, 40.1, 28.6, 21.5; HRMS (ESI) Calcd for $C_{12}H_{18}N$ $[M + H]^+$ 176.1439, found 176.1437.

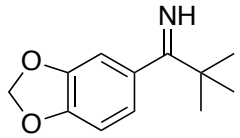


2,2-Dimethyl-1-(3-(trifluoromethyl)phenyl)propan-1-imine (1j): Light yellow liquid; ^{1}H

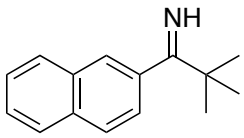
NMR (400 MHz, $CDCl_3$): δ 9.20 (brs, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.52 – 7.33 (m, 3H), 1.21 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8, 143.0, 130.6 (q, $^{2}J_{C\text{-}F}$ = 32.1 Hz), 129.9, 128.7, 124.9 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 124.0 (q, $^{1}J_{C\text{-}F}$ = 272.2 Hz), 123.3, 40.4, 28.3; HRMS (ESI) Calcd for $C_{12}H_{15}NF_3$ $[M + H]^+$ 230.1157, found 230.1161.



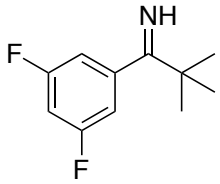
1-(3-Methoxyphenyl)-2,2-dimethylpropan-1-imine (1k): Light yellow liquid; ^1H NMR (400 MHz, $CDCl_3$): δ 9.18 (brs, 1H), 7.25 (t, J = 8.3 Hz, 1H), 6.87 (dd, J = 8.3, 2.3 Hz, 1H), 6.78 (d, J = 7.5 Hz, 1H), 6.73 (s, 1H), 3.81 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.2, 159.2, 143.7, 129.3, 119.0, 113.4, 112.6, 55.4, 40.9, 28.7; HRMS (ESI) Calcd for $C_{12}H_{18}NO$ $[M + H]^+$ 192.1389, found 192.1388.



1-(Benzo[*d*][1,3]dioxol-5-yl)-2,2-dimethylpropan-1-imine (1l): Light yellow liquid; ^1H NMR (400 MHz, $CDCl_3$): δ 9.13 (brs, 1H), 6.75 – 6.71 (m, 1H), 6.68 (s, 1H), 6.65 (d, J = 7.8 Hz, 1H), 5.92 (s, 2H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.5, 147.4, 147.1, 136.2, 120.3, 108.0, 107.5, 101.2, 40.3, 28.7; HRMS (ESI) Calcd for $C_{12}H_{16}NO_2$ $[M + H]^+$ 206.1181, found 206.1182.

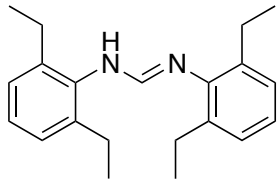


2,2-Dimethyl-1-(naphthalen-2-yl)propan-1-imine (1m): Light yellow liquid; ^1H NMR (400 MHz, $CDCl_3$): δ 9.35 (brs, 1H), 7.86 – 7.80 (m, 3H), 7.68 (s, 1H), 7.54 – 7.48 (m, 2H), 7.35 (d, J = 8.1 Hz, 1H), 1.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.3, 145.8, 139.9, 132.8, 128.3, 127.8, 127.7, 126.6, 126.5, 125.4, 124.8, 40.4, 28.7; HRMS (ESI) Calcd for $C_{15}H_{18}N$ $[M + H]^+$ 212.1439, found 212.1447.

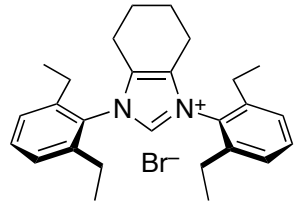


1-(3,5-Difluorophenyl)-2,2-dimethylpropan-1-imine (1n): Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.17 (brs, 1H), 6.89 – 6.58 (m, 3H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.0, 162.6 (dd, $^{1}J_{C\text{-}F}$ = 250.1 Hz, $^{3}J_{C\text{-}F}$ = 12.5 Hz), 145.3 (d, $^{3}J_{C\text{-}F}$ = 15.4 Hz), 110.3, 103.6 (t, $^{2}J_{C\text{-}F}$ = 25.0 Hz), 40.2, 28.4; HRMS (ESI) Calcd for $C_{11}H_{14}NF_2$ $[M + H]^+$ 198.1094, found 198.1096.

Preparation of L2•HBr



(*E*)-*N*,*N*'-Bis(2,6-diethylphenyl)formamidine: The formamidine was prepared as follows according to the method described by Grubbs et al.[4] A mixture of 2,6-diethylaniline (8.95 g, 60 mmol, 2 equiv), triethylorthoformate (4.45g, 30 mmol, 1 equiv), and glacial acetic acid (0.1 mL, 1.5 mmol, 0.05 equiv) was heated at 140 °C overnight. The crude solid was triturated, washed with cold *n*-pentane, and filtered through a glass frit. The solid was dried under the reduced pressure to give the title compound as a pale yellow solid (4.62 g, 50%). The ^{1}H and ^{13}C NMR spectra showed good agreement with the literature data.[5]



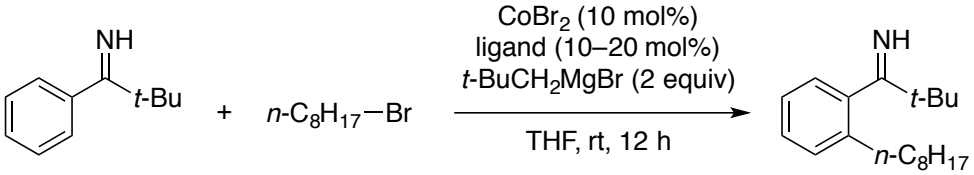
1,3-Bis-(2,6-diethylphenyl)-4,5,6,7-tetrahydro-3*H*-benzoimidazol-1-ium bromide (L2•HBr): The synthesis was performed according to the procedure reported by Glorius and cowokers.[6] To a suspension of *N,N'*-bis(2,6-diethylphenyl)formamidine (1.39 g, 4.5 mmol, 1 equiv) in

acetonitrile (9 mL) were added diisopropylethylamine (0.90 mL, 5.4 mmol, 1.2 equiv) and 2-bromocyclohexanone (1.59 g, 9.0 mmol, 2 equiv). The resulting mixture was stirred at 110 °C for 20 h. The reaction progress was monitored by TLC (CH_2Cl_2/MeOH 10:1). After full consumption of the formamidine, the volatiles were removed under reduced pressure. The residue was suspended in toluene (11 mL), followed by the addition of acetic anhydride (1.30 mL, 13.5 mmol, 3 equiv) and 48% HBr in acetic acid (0.77 mL, 6.8 mmol, 1.5 equiv). The resulting mixture was stirred at 90 °C for 24 h. The mixture was then transferred into a separatory funnel containing CH_2Cl_2 and H_2O (50 mL each). After separation of the two layers, the aqueous layer was extracted with CH_2Cl_2 (50 mL x 3). The combined organic extracts were dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: CH_2Cl_2/MeOH = 100/1 to 10/1). The collected solids were dried under vacuum and then dissolved in hot acetonitrile. The solution was stirred vigorously with charcoal powder for 5 min, followed by filtration and recrystallization from CH_2Cl_2/Et_2O to afford the title compound as a white powder (589 mg, 28%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.78–10.68 (m, 1H), 7.48 (t, J = 7.7 Hz, 2H), 7.29 (d, J = 7.7 Hz, 4H), 2.48–2.37 (m, 8H), 2.31 (brs, 4H), 1.92 (brs, 4H), 1.23–1.19 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 137.7, 131.8, 131.2, 130.0, 127.6, 24.5, 21.8, 20.4, 14.6; HRMS (ESI) Calcd for $C_{27}H_{36}N_2Br$ $[M + H]^+$ 467.2062, found 467.2066.

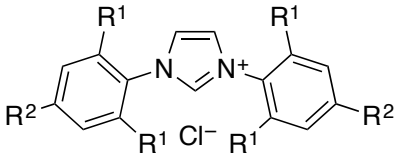
Cobalt-Catalyzed *ortho*-Alkylation of Pivalophenone N–H Imines with Alkyl Bromides

Table S1. Screening of Reaction Conditions

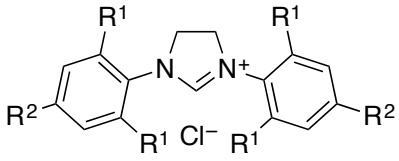


1a **2a** (1.5 equiv) **3aa**

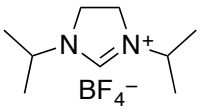
entry	ligand (mol%)	yield (%)[a]
1	PPh_3 (20)	26
2	PCy_3 (20)	5
3	dppe (10)	6
4	IMes•HCl (10)	4
5	IPr•HCl (10)	6
6	SIMes•HCl (10)	3
7	SIPr•HCl (10)	4
8	**L1**•HBF_4 (10)	90[b]
9	**L3**•HBF_4 (10)	35
10	**L4**•HBr (10)	76
11[c]	**L1**•HBF_4 (10)	55



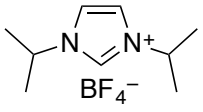
IMes•HCl (R^1 = R^2 = Me)
IPr•HCl (R^1 = *i*-Pr, R^2 = H)



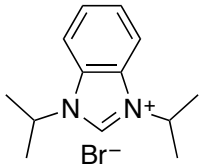
SIMes•HCl (R^1 = R^2 = Me)
SIPr•HCl (R^1 = *i*-Pr, R^2 = H)



L1•HBF_4

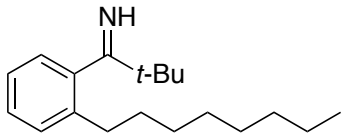


L3•HBF_4



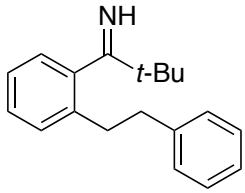
L4•HBr

[a] Determined by GC using *n*-tridecane as an internal standard. [b] Isolated yield. [c] *n*-Octyl chloride was used instead of *n*-octyl bromide.

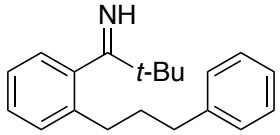


General Procedure: 2,2-Dimethyl-1-(2-octylphenyl)propan-1-imine (3aa). In a Schlenk tube were placed **L1**•HBF_4 (4.9 mg, 0.020 mmol), a freshly prepared THF solution of $CoBr_2$ (0.20 M, 0.10 mL, 0.020 mmol), and THF (0.3 mL). The resulting solution was cooled in an ice bath, followed by the addition of *t*-$BuCH_2MgBr$ (2.0 M in THF, 0.20 mL, 0.40 mmol). After stirring for 30 min, 2,2-dimethyl-1-phenylpropan-1-imine (**1a**, 33 mg, 0.20 mmol) and 1-bromooctane (**2a**, 52 μL, 0.30 mmol) were added sequentially. The resulting mixture was warmed to room temperature and stirred for 12 h, and then filtered through a short pad of silica gel, which was washed with ethyl acetate (5 mL). The filtrate was concentrated under reduced pressure. Silica gel chromatography (eluent: hexane/EtOAc/NEt_3 = 100/1/1) of the crude product afforded the title compound as a colorless oil (49 mg, 90%).

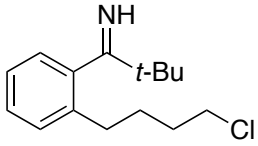
R_f 0.60 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.19 (brs, 1H), 7.26 – 7.23 (m, 2H), 7.15 – 7.10 (m, 1H), 7.01 (d, J = 7.5 Hz, 1H), 2.48 – 2.44 (m, 2H), 1.60 – 1.52 (m, 2H), 1.37 – 1.20 (m, 19H), 0.87 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.9, 141.6, 139.0, 129.4, 127.9, 126.2, 125.1, 40.6, 33.9, 32.1, 32.0, 30.0, 29.7, 29.5, 28.9, 22.9, 14.3; HRMS (ESI) Calcd for $C_{19}H_{32}N$ $[M + H]^+$ 274.2535, found 274.2535.



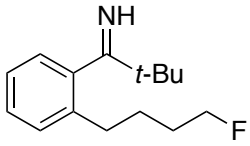
2,2-Dimethyl-1-(2-phenethylphenyl)propan-1-imine (3ab): Light yellow oil (44 mg, 83%); R_f 0.51 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96 (s, 1H), 7.35 – 7.25 (m, 4H), 7.22 – 7.11 (m, 4H), 7.02 (d, J = 7.6 Hz, 1H), 2.91 – 2.87 (m, 2H), 2. 80 – 2.76 (m, 2H), 1.21 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 141.7, 137.7, 136.1, 129.5, 128.7 (two signals overlapped), 128.0, 126.4, 126.3, 125.5, 40.6, 38.3, 36.1, 28.9; HRMS (ESI) Calcd for $C_{19}H_{24}N$ $[M + H]^+$ 266.1909, found 266.1908.



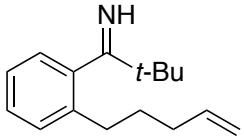
2,2-Dimethyl-1-(2-(3-phenylpropyl)phenyl)propan-1-imine (3ac): Light yellow oil (51 mg, 91%); R_f 0.50 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.20 (brs, 1H), 7.31 – 7.23 (m, 4H), 7.20 – 7.11 (m, 4H), 7.01 (d, J = 7.5 Hz, 1H), 2.67 (t, J = 7.6 Hz, 2H), 2.53 – 2.49 (m, 2H), 1.97 – 1.87 (m, 2H), 1.18 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.7, 142.1, 141.6, 138.4, 129.3, 128.7, 128.6, 128.0, 126.3, 126.0, 125.3, 40.6, 36.2, 33.44 (two signals overlapped), 28.8; HRMS (ESI) Calcd for $C_{20}H_{26}N$ $[M + H]^+$ 280.2065, found 280.2065.



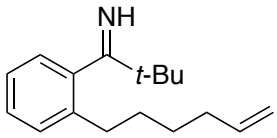
1-(2-(4-Chlorobutyl)phenyl)-2,2-dimethylpropan-1-imine (3ad): Light yellow oil (38 mg, 75%); R_f 0.49 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.07 (brs, 1H), 7.27 – 7.23 (m, 2H), 7.19 – 7.12 (m, 1H), 7.03 (d, J = 7.6 Hz, 1H), 3.54 (t, J = 6.4 Hz, 2H), 2.54 – 2.48 (m, 2H), 1.86 – 1.65 (m, 4H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 141.5, 137.95, 129.3, 128.1, 126.4, 125.4, 45.0, 40.7, 33.0, 32.7, 29.0, 28.9; HRMS (ESI) Calcd for $C_{15}H_{23}NCl$ $[M + H]^+$ 252.1519, found 252.1517.



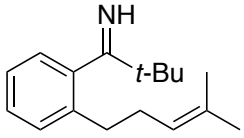
1-(2-(4-Fluorobutyl)phenyl)-2,2-dimethylpropan-1-imine (3ae): Light yellow oil (38 mg, 80%); R_f 0.50 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.09 (brs, 1H), 7.26 – 7.25 (m, 2H), 7.19 – 7.12 (m, 1H), 7.03 (d, J = 7.7 Hz, 1H), 4.53 – 4.49 (m, 1H), 4.40 – 4.38 (m, 1H), 2.55 – 2.51 (m, 2H), 1.80 – 1.65 (m, 4H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 141.4, 138.1, 129.3, 128.1, 126.4, 125.4, 84.1 (d, $^1J_{C\text{-}F}$ = 164.8 Hz), 40.7, 33.4, 30.6 (d, $^2J_{C\text{-}F}$ = 19.6 Hz), 28.9, 27.5 (d, $^3J_{C\text{-}F}$ = 4.7 Hz); HRMS (ESI) Calcd for $C_{15}H_{23}NF$ $[M + H]^+$ 236.1815, found 236.1811.



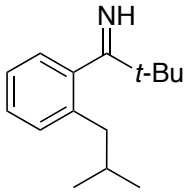
2,2-Dimethyl-1-(2-(pent-4-en-1-yl)phenyl)propan-1-imine (3af): Light yellow oil (38 mg, 82%); R_f 0.62 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.18 (brs, 1H), 7.28 – 7.21 (m, 2H), 7.16 – 7.11 (m, 1H), 7.02 (d, J = 7.6 Hz, 1H), 5.86 – 5.75 (m, 1H), 5.06 – 4.94 (m, 2H), 2.51 – 2.46 (m, 2H), 2.12 – 2.07 (m, 2H), 1.72– 1.64 (m, 2H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 141.6, 138.5 (two signals overlapped), 129.4, 128.0, 126.3, 125.2, 115.2, 40.6, 34.0, 33.3, 31.0, 28.9; HRMS (ESI) Calcd for $C_{16}H_{24}N$ $[M + H]^+$ 230.1909, found 230.1911.



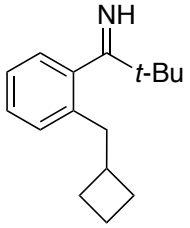
1-(2-(Hex-5-en-1-yl)phenyl)-2,2-dimethylpropan-1-imine (3ag): Light yellow oil (34 mg, 70%); R_f 0.65 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.10 (brs, 1H), 7.27 – 7.22 (m, 2H), 7.17 – 7.17 (m, 1H), 7.01 (d, J = 7.7 Hz, 1H), 5.85 – 5.74 (m, 1H), 5.03 – 4.91 (m, 2H), 2.52 – 2.43 (m, 2H), 2.10 – 2.03 (m, 2H), 1.65 – 1.55 (m, 2H), 1.47 – 1.39 (m, 2H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 141.6, 138.9, 138.7, 129.4, 128.0, 126.2, 125.2, 114.8, 40.6, 39.9, 33.8 (two signals overlapped), 31.4, 28.9; HRMS (ESI) Calcd for $C_{17}H_{26}N$ $[M + H]^+$ 244.2065, found 244.2067.



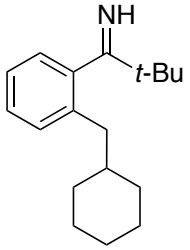
2,2-Dimethyl-1-(2-(4-methylpent-3-en-1-yl)phenyl)propan-1-imine (3ah): Light yellow oil (37 mg, 75%); R_f 0.50 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.14 (brs, 1H), 7.30 – 7.22 (m, 2H), 7.17 – 7.11 (m, 1H), 7.01 (d, J = 7.3 Hz, 1H), 5.17 – 5.10 (m, 1H), 2.52 – 2.48 (m, 2H), 2.28 – 2.22 (m, 2H), 1.68 (s, 3H), 1.55 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.7, 141.6, 138.4, 132.8, 129.5, 127.9, 126.2, 125.2, 123.8, 40.6, 34.0, 30.4, 28.9, 25.9, 17.9; HRMS (ESI) Calcd for $C_{17}H_{26}N$ $[M + H]^+$ 244.2065, found 244.2070.



1-(2-Isobutylphenyl)-2,2-dimethylpropan-1-imine (3ai): Light yellow oil (35 mg, 81%); R_f 0.62 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.16 (brs, 1H), 7.26 – 7.20 (m, 2H), 7.14 (t, J = 7.2 Hz, 1H), 7.01 (d, J = 7.6 Hz, 1H), 2.36 (d, J = 7.3 Hz, 2H), 1.95 – 1.87 (m, 1H), 1.21 (s, 9H), 0.88 (d, J = 6.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 142.1, 137.6, 129.8, 127.8, 126.3, 125.2, 43.0, 40.6, 30.0, 29.0, 22.7; HRMS (ESI) Calcd for $C_{15}H_{24}N$ $[M + H]^+$ 218.1909, found 218.1914.

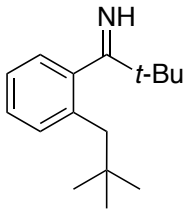


1-(2-(Cyclobutylmethyl)phenyl)-2,2-dimethylpropan-1-imine (3aj): Light yellow oil (41 mg, 90%); R_f 0.63 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.12 (brs, 1H), 7.25 – 7.17 (m, 2H), 7.13 (td, J = 7.3, 1.8 Hz, 1H), 7.00 (d, J = 7.4 Hz, 1H), 2.62 – 2.50 (m, 3H), 2.09 – 2.00 (m, 2H), 1.89 – 1.64 (m, 4H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.9, 141.7, 137.3, 129.1, 127.8, 126.2, 125.2, 40.6 (two signals overlapped), 37.1, 28.9 (two signals overlapped), 18.6; HRMS (ESI) Calcd for $C_{16}H_{24}N$ $[M + H]^+$ 230.1909, found 230.1915.

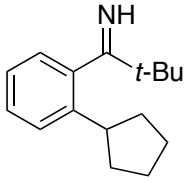


1-(2-(Cyclohexylmethyl)phenyl)-2,2-dimethylpropan-1-imine (3ak):[3] Light yellow oil (45 mg, 87%); R_f 0.64 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.13 (brs, 1H), 7.25 – 7.19 (m, 2H), 7.13 (td, J = 7.2, 2.0 Hz, 1H), 7.00 (d, J = 7.6 Hz, 1H), 2.36 (d, J = 7.1 Hz,

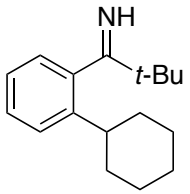
2H), 1.72 – 1.49 (m, 6H), 1.26 – 1.10 (m, 12H), 0.98 – 0.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 142.1, 137.2, 129.9, 127.6, 126.2, 125.1, 41.7, 40.6, 39.6, 33.5, 29.0, 26.7, 26.6; HRMS (ESI) Calcd for $C_{18}H_{28}N$ $[M + H]^+$ 258.2222, found 258.2222.



2,2-Dimethyl-1-(2-neopentylphenyl)propan-1-imine (3al): Light yellow oil (42 mg, 91%); R_f 0.67 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.26 (brs, 1H), 7.28 – 7.20 (m, 2H), 7.16 (td, J = 7.3, 1.7 Hz, 1H), 6.97 (d, J = 7.3 Hz, 1H), 2.43 (s, 2H), 1.17 (s, 9H), 0.92 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.9, 142.6, 135.8, 130.9, 127.1, 126.7, 125.7, 47.4, 40.7, 32.8, 30.3, 29.2; HRMS (ESI) Calcd for $C_{16}H_{26}N$ $[M + H]^+$ 232.2065, found 232.2058.

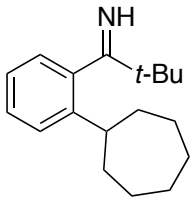


1-(2-Cyclopentylphenyl)-2,2-dimethylpropan-1-imine (3am): Light yellow oil (39 mg, 85%); R_f 0.56 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.11 (s, 1H), 7.34 – 7.25 (m, 2H), 7.11 (td, J = 7.5, 1.4 Hz, 1H), 6.99 (dd, J = 7.6, 1.2 Hz, 1H), 2.85 – 2.73 (m, 1H), 2.03 – 1.92 (m, 2H), 1.87 – 1.76 (m, 2H), 1.70 – 1.50 (m, 4H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 143.5, 141.6, 128.3, 126.9, 125.9, 124.9, 43.4, 40.6, 28.9 (two signals overlapped), 26.4; HRMS (ESI) Calcd for $C_{16}H_{24}N$ $[M + H]^+$ 230.1909, found 230.1901.

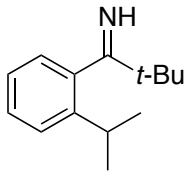


1-(2-Cyclohexylphenyl)-2,2-dimethylpropan-1-imine (3an): Light yellow oil (42 mg, 87%); R_f 0.56 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.13 (brs, 1H), 7.32 – 7.24

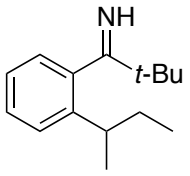
(m, 2H), 7.14 – 7.10 (m, 1H), 7.00 – 6.96 (m, 1H), 2.36 (tt, J = 11.7, 3.1 Hz, 1H), 1.86 – 1.65 (m, 6H), 1.37 – 1.19 (m, 13H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 144.0, 141.0, 128.1, 127.0, 126.2, 125.2, 42.3, 40.6, 29.0, 27.1 (two signals overlapped), 26.3; HRMS (ESI) Calcd for $C_{17}H_{26}N$ $[M + H]^+$ 244.2065, found 244.2070.



1-(2-Cycloheptylphenyl)-2,2-dimethylpropan-1-imine (3ao): Light yellow oil (43 mg, 84%); R_f 0.56 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.14 (brs, 1H), 7.27 – 7.26 (m, 2H), 7.14 – 7.07 (m, 1H), 6.97 (d, J = 7.7 Hz, 1H), 2.52 (t, J = 10.1 Hz, 1H), 1.85 – 1.41 (m, 12H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.2, 146.3, 142.6, 128.3, 127.0, 126.0, 124.9, 43.7, 40.6, 29.0, 28.0 (two signals overlapped), 27.7; HRMS (ESI) Calcd for $C_{18}H_{28}N$ $[M + H]^+$ 258.2222, found 258.2228.

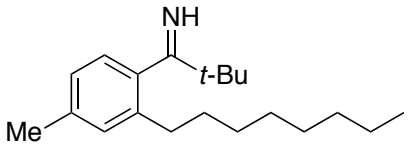


1-(2-Isopropylphenyl)-2,2-dimethylpropan-1-imine (3ap): Light yellow oil (21 mg, 51%); R_f 0.62 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.17 (brs, 1H), 7.34 – 7.27 (m, 2H), 7.13 (td, J = 7.6, 1.5 Hz, 1H), 6.99 (dd, J = 7.6, 0.8 Hz, 1H), 2.78 (hept, J = 6.9 Hz, 1H), 1.27 – 1.18 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 145.2, 140.7, 128.3, 126.2 (two signals overlapped), 125.2, 47.4, 40.7, 31.4, 28.9; HRMS (ESI) Calcd for $C_{14}H_{22}N$ $[M + H]^+$ 204.1752, found 204.1757.

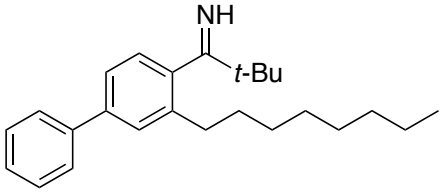


1-(2-(*sec*-Butyl)phenyl)-2,2-dimethylpropan-1-imine (3aq): Light yellow oil (24 mg, 53%); R_f

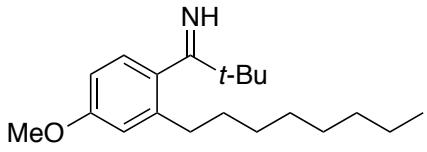
0.59 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.14 (brs, 1H), 7.31 – 7.25 (m, 2H), 7.16 – 7.10 (m, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 2.56 – 2.43 (m, 1H), 1.58 (d, *J* = 6.5 Hz, 2H), 1.23 (s, 9H), 1.19 (d, *J* = 7.0 Hz, 3H), 0.85 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 144.3, 141.3, 128.2, 126.4, 126.2, 125.1, 40.6, 38.2, 30.4, 29.2, 29.1, 22.2, 12.6; HRMS (ESI) Calcd for $C_{15}H_{24}N$ $[M + H]^+$ 218.1909, found 218.1904.



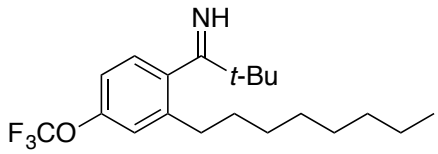
2,2-dimethyl-1-(4-methyl-2-octylphenyl)propan-1-imine (3ba): Light yellow oil (50 mg, 87%); R_f 0.62 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.09 (brs, 1H), 7.05 (s, 1H), 6.94 (d, *J* = 7.8 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 1H), 2.45 – 2.38 (m, 2H), 2.32 (s, 3H), 1.60 – 1.50 (m, 2H), 1.38 – 1.18 (m, 19H), 0.89– 0.86 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 138.9 (two signals overlapped), 137.5, 130.0, 126.1, 125.8, 40.6, 33.9, 32.1, 30.1, 29.7, 29.5, 28.97, 22.9, 21.4, 14.3; HRMS (ESI) Calcd for $C_{20}H_{34}N$ $[M + H]^+$ 288.2691, found 288.2700.



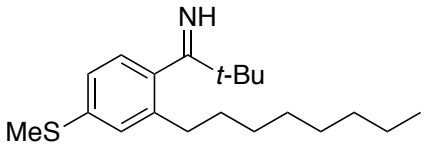
2,2-Dimethyl-1-(3-octyl-[1,1'-biphenyl]-4-yl)propan-1-imine (3ca): Light yellow oil (60 mg, 87%); R_f 0.57 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.27 (brs, 1H), 7.62 – 7.58 (m, 2H), 7.50 – 7.42 (m, 3H), 7.39 – 7.33 (m, 2H), 7.10 (d, *J* = 7.9 Hz, 1H), 2.57 – 2.51 (m, 1H), 1.69 – 1.59 (m, 1H), 1.42 – 1.22 (m, 19H), 0.89 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.7, 141.0 (two signals overlapped), 140.8, 139.5, 129.0, 128.1, 127.6, 127.3, 126.7, 123.9, 40.7, 34.1, 32.1, 30.1, 29.7, 29.4, 29.0, 22.9 (two signals overlapped), 14.3; HRMS (ESI) Calcd for $C_{25}H_{36}N$ $[M + H]^+$ 350.2848, found 350.2856.



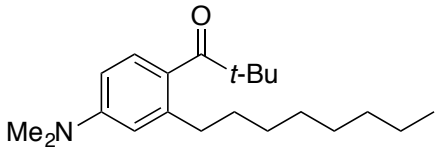
2,2-Dimethyl-1-(3-octyl-[1,1'-biphenyl]-4-yl)propan-1-imine (3da): Light yellow oil (60 mg, 87%); R_f 0.50 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.05 (brs, 1H), 6.93 (d, J = 8.4 Hz, 1H), 6.77 (d, J = 2.5 Hz, 1H), 6.67 (dd, J = 8.4, 2.6 Hz, 1H), 3.79 (s, 3H), 2.46 – 2.39 (m, 2H), 1.61 – 1.51 (m, 2H), 1.34 – 1.18 (m, 19H), 0.87 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.7, 159.1, 140.8, 131.2, 127.3, 114.7, 110.4, 55.4, 40.7, 34.1, 32.1, 31.9, 30.0, 29.7, 29.4, 28.9, 22.9, 14.3; HRMS (ESI) Calcd for $C_{20}H_{34}NO$ $[M + H]^+$ 304.2640, found 304.2640.



2,2-Dimethyl-1-(2-octyl-4-(trifluoromethoxy)phenyl)propan-1-imine (3ea): Light yellow oil (63 mg, 88%); R_f 0.52 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.20 (brs, 1H), 7.09 (s, 1H), 7.05 – 6.97 (m, 2H), 2.50 – 2.43 (m, 2H), 1.62 – 1.51 (m, 2H), 1.37 – 1.15 (m, 19H), 0.87 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.7, 148.9, 141.7, 140.0, 127.6, 121.6, 120.7 (q, $^1J_{C\text{-}F}$ = 120.71 Hz), 117.6, 40.7, 33.8, 32.1, 31.6, 29.9, 29.6, 29.4, 28.8, 22.9, 14.3; HRMS (ESI) Calcd for $C_{20}H_{31}NOF_3$ $[M + H]^+$ 358.2358, found 358.2355.

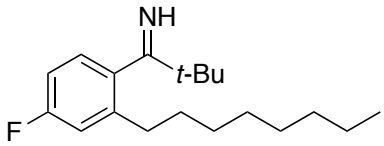


2,2-Dimethyl-1-(4-(methylthio)-2-octylphenyl)propan-1-imine (3fa): Light yellow oil (51 mg, 88%); R_f 0.60 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.15 (brs, 1H), 7.13 (d, J = 1.6 Hz, 1H), 7.02 (dd, J = 8.0, 1.8 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 2.48 (s, 3H), 2.45 – 2.39 (m, 2H), 1.59 – 1.51 (m, 2H), 1.37 – 1.18 (m, 19H), 0.87 (t, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 139.8, 138.5, 138.0, 127.4, 126.7, 123.1, 40.7, 33.9, 32.1, 31.9, 30.0, 29.6, 29.4, 28.9, 22.9, 15.9, 14.3; HRMS (ESI) Calcd for $C_{20}H_{34}NS$ $[M + H]^+$ 320.2412, found 320.2411.

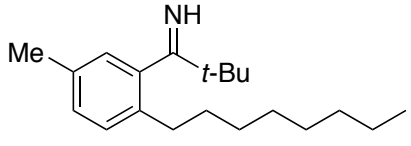


1-(4-(Dimethylamino)-2-octylphenyl)-2,2-dimethylpropan-1-one (3ga): The crude reaction mixture was hydrolyzed with HCl (3 M, 1 mL). The mixture was neutralized and extracted with ethyl acetate. The extracts were concentrated under reduced pressure, and the residue was subjected to silica gel chromatography (eluent: hexane/EtOAc = 50/1) to afford the title compound as a light yellow oil (52 mg, 82%).

R_f 0.55 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20 (d, J = 8.6 Hz, 1H), 6.54 (d, J = 2.6 Hz, 1H), 6.48 (dd, J = 8.6, 2.6 Hz, 1H), 2.97 (s, 6H), 2.53 – 2.47 (m, 2H), 1.61 – 1.51 (m, 2H), 1.37 – 1.22 (m, 19H), 0.91 – 0.85 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 213.8, 150.9, 142.4, 128.5, 127.2, 113.6, 108.4, 45.0, 40.5, 34.6, 32.4, 32.2, 30.1, 29.8, 29.5, 28.4, 22.9, 14.4, 1.3; HRMS (ESI) Calcd for $C_{21}H_{35}NO$ $[M + H]^+$ 317.2719, found 317.2721.

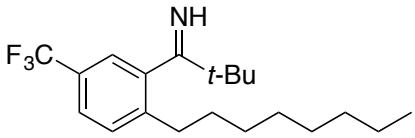


1-(4-Fluoro-2-octylphenyl)-2,2-dimethylpropan-1-imine (3ha): Light yellow oil (50 mg, 85%); R_f 0.58 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96 (brs, 1H), 7.01 – 6.91 (m, 2H), 6.86 – 6.79 (m, 1H), 2.48 – 2.41 (m, 2H), 1.60 – 1.51 (m, 2H), 1.36 – 1.17 (m, 19H), 0.89 – 0.85 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.0, 162.4 (d, $^1J_{C\text{-}F}$ = 246.0 Hz), 141.9, 137.4, 127.8 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 115.8 (d, $^2J_{C\text{-}F}$ = 21.0 Hz), 112.2 (d, $^2J_{C\text{-}F}$ = 21.5 Hz), 40.7, 33.9, 32.1, 31.5, 29.9, 29.6, 29.4, 28.8, 22.9, 14.3; HRMS (ESI) Calcd for $C_{19}H_{31}NF$ $[M + H]^+$ 292.2441, found 292.2444.

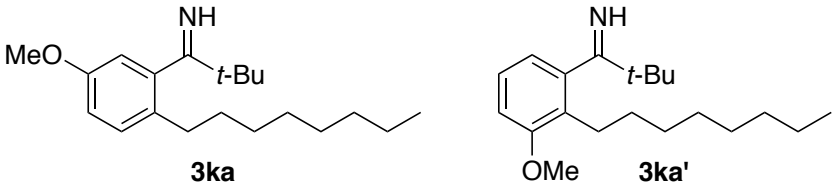


2,2-Dimethyl-1-(5-methyl-2-octylphenyl)propan-1-imine (3ia): Light yellow oil (50 mg, 86%); R_f 0.61 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.89 (brs, 1H),

7.13 (d, J = 7.9 Hz, 1H), 7.05 (dd, J = 8.1, 1.2 Hz, 1H), 6.81 (s, 1H), 2.45 – 2.38 (m, 2H), 2.30 (s, 3H), 1.58 – 1.49 (m, 2H), 1.36 – 1.18 (m, 19H), 0.87 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 135.9, 134.5, 129.2 (two signals overlapped), 128.7, 126.7, 40.5, 33.5, 32.1, 32.7, 30.0, 29.7, 29.5, 29.0, 22.9, 21.2, 14.3; HRMS (ESI) Calcd for $C_{20}H_{34}N$ $[M + H]^+$ 288.2691, found 288.2690.

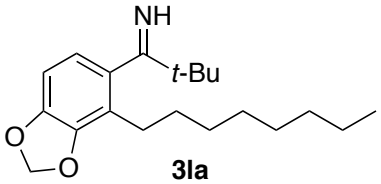


2,2-dimethyl-1-(2-octyl-5-(trifluoromethyl)phenyl)propan-1-imine (3ja): Light yellow oil (53 mg, 77%); R_f 0.60 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.22 (brs, 1H), 7.50 (d, J = 7.9 Hz, 1H), 7.37 (d, J = 8.2 Hz, 1H), 7.27 – 7.26 (m, 1H), 2.55 – 2.48 (m, 2H), 1.63 – 1.53 (m, 2H), 1.39 – 1.19 (m, 19H), 0.91 – 0.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.3, 143.5, 141.8, 129.9, 127.6 (q, $^2J_{C\text{-}F}$ = 32.7 Hz), 124.75 (q, $^3J_{C\text{-}F}$ = 3.5 Hz), 124.3 (d, $^1J_{C\text{-}F}$ = 274.0 Hz), 123.19 (d, $^3J_{C\text{-}F}$ = 5.8 Hz), 40.7, 33.9, 32.1, 31.7, 30.0, 29.6, 29.4, 28.8, 22.9, 14.3; HRMS (ESI) Calcd for $C_{20}H_{31}NF_3$ $[M + H]^+$ 342.2409, found 342.2407.

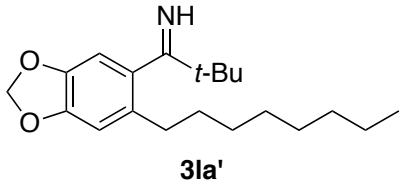


2,2-Dimethyl-1-(5-methyl-2-octylphenyl)propan-1-imine (3ka): Silica gel chromatography (eluent: hexane/EtOAc/NEt_3 = 50/1/1) of the crude product afforded a mixture of the title compound and its regioisomer **3ka'** as a light yellow oil (52 mg, 85%). The ratio of **3ka** and **3ka'** was determined to be 4:1 by ^{1}H NMR analysis.

R_f 0.50 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (**3ka**, 400 MHz, $CDCl_3$): δ 7.15 (d, J = 8.6 Hz, 1H), 6.80 (dd, J = 8.6, 2.7 Hz, 1H), 6.54 (d, J = 2.7 Hz, 1H), 3.77 (s, 3H), 2.42 – 2.35 (m, 2H), 1.58 – 1.47 (m, 2H), 1.34 – 1.19 (m, 19H), 0.87 (t, J = 6.8 Hz, 3H); ^{13}C NMR (**3ka**, 100 MHz, $CDCl_3$): δ 190.7, 156.8, 142.4, 131.1, 130.4, 113.4, 111.9, 55.5, 40.5, 33.1, 32.2, 32.1, 30.0, 29.7, 29.0, 22.9, 14.3; HRMS (ESI) Calcd for $C_{20}H_{34}NO$ $[M + H]^+$ 304.2640, found 304.2645.



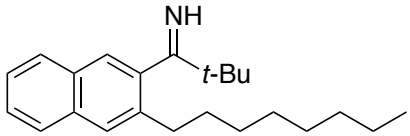
3la



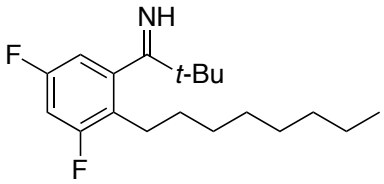
3la'

2,2-Dimethyl-1-(4-octylbenzo[*d*][1,3]dioxol-5-yl)propan-1-imine (3la): Silica gel chromatography (eluent: hexane/EtOAc/NEt_3 = 50/1/1) of the crude product afforded a mixture of the title compound and its regioisomer **3la'** as a light yellow oil (52 mg, 82%). The ratio of **3la** and **3la'** was determined to be 3:2 by ^{1}H NMR analysis.

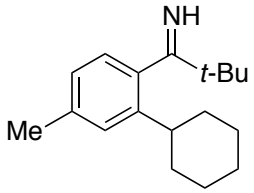
R_f 0.50 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.16 (s, 1H for each isomer), 6.70 (s, 1H for **3la'**), 6.62 (d, J = 8.0 Hz, 1H for **3la**), 6.50 (d, J = 8.1 Hz, 1H for each isomer), 5.94 (s, 2H for **3la**), 5.92 (s, 2H for **3la'**), 2.44 – 2.32 (m, 2H for each isomer), 1.56 – 1.47 (m, 2H for each isomer), 1.37 – 1.17 (m, 19H for each isomer), 0.86 (t, J = 6.6 Hz, 3H for each isomer); ^{13}C NMR (both isomers, 100 MHz, $CDCl_3$): δ 190.4, 190.0, 147.3, 146.5, 146.3, 144.9, 136.0, 132.9, 121.8, 119.4, 109.2, 106.5, 105.6, 101.2, 101.0, 40.6, 33.8, 32.2, 32.1, 30.6, 30.2, 29.9, 29.7, 29.6, 29.4, 29.1, 29.0, 22.9, 14.3; HRMS (ESI) Calcd for $C_{20}H_{32}NO_2$ $[M + H]^+$ 318.2433, found 318.2435.



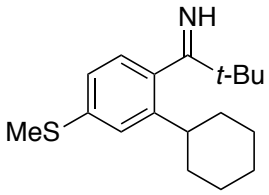
2,2-Dimethyl-1-(3-octylnaphthalen-2-yl)propan-1-imine (3ma): Light yellow oil (55 mg, 85%); R_f 0.58 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.89 (brs, 1H), 7.78 (dd, J = 7.5, 1.9 Hz, 2H), 7.71 (s, 1H), 7.49 (s, 1H), 7.48 – 7.41 (m, 2H), 2.67 – 2.60 (m, 2H), 1.74 – 1.62 (m, 2H), 1.46 – 1.21 (m, 19H), 0.89 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.9, 140.5, 137.3, 133.1, 131.2, 127.9, 127.6, 127.4, 126.4, 125.9, 124.8, 40.8, 34.0, 32.1, 31.8, 30.0, 29.7, 29.5, 29.0, 22.9, 14.3; HRMS (ESI) Calcd for $C_{23}H_{34}N$ $[M + H]^+$ 324.2691, found 324.2686.



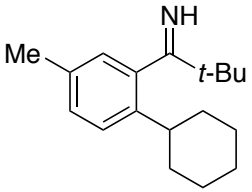
1-(3,5-Difluoro-2-octylphenyl)-2,2-dimethylpropan-1-imine (3na): Light yellow oil (48 mg, 78%); R_f 0.58 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.23 (brs, 1H), 6.76 – 6.71 (m, 1H), 6.58 (d, J = 8.4 Hz, 1H), 2.48 – 2.33 (s, 2H), 1.54 – 1.42 (m, 2H), 1.36 – 1.17 (m, 19H), 0.87 (t, J = 6.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.4, 161.9 (dd, $^1J_{C\text{-}F}$ = 248.8 Hz, $^3J_{C\text{-}F}$ = 12.2 Hz), 160.4 (dd, $^1J_{C\text{-}F}$ = 247.3 Hz, $^2J_{C\text{-}F}$ = 12.8 Hz), 144.0, 122.9, 109.2 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 103.3 (t, $^2J_{C\text{-}F}$ = 25.9 Hz), 40.6, 32.1, 30.9, 30.2, 29.5, 29.4, 28.9, 28.1, 22.9, 14.3; HRMS (ESI) Calcd for $C_{19}H_{30}NF_2$ $[M + H]^+$ 310.2346, found 310.2343.



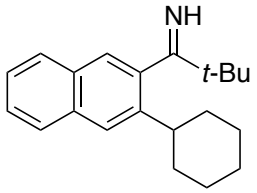
1-(2-Cyclohexyl-4-methylphenyl)-2,2-dimethylpropan-1-imine (3bn): Light yellow oil (43 mg, 83%); R_f 0.57 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.09 (brs, 1H), 7.10 (s, 1H), 6.94 (d, J = 7.7 Hz, 1H), 6.88 (d, J = 7.8 Hz, 1H), 2.38 – 2.28 (m, 4H), 1.83 – 1.66 (m, 4H), 1.56 – 1.18 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.2, 144.0, 138.4, 137.6, 127.6, 126.1, 125.9, 42.2, 40.6, 29.0, 27.1 (two signals overlapped), 26.3, 21.6; HRMS (ESI) Calcd for $C_{18}H_{28}N$ $[M + H]^+$ 258.2222, found 258.2224.



1-(2-Cyclohexyl-4-(methylthio)phenyl)-2,2-dimethylpropan-1-imine (3fn): Light yellow oil (39 mg, 68%); R_f 0.53 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.16 (brs, 1H), 7.18 (d, J = 1.9 Hz, 1H), 7.01 (dd, J = 8.1, 1.9 Hz, 1H), 6.92 (d, J = 8.1 Hz, 1H), 2.49 (s, 3H), 2.38 – 2.30 (m, 1H), 1.83 – 1.69 (m, 4H), 1.46 – 1.24 (m, 6H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.6, 144.8, 138.1 (two signals overlapped), 126.8, 125.3, 123.2, 42.3, 40.7, 28.9, 27.0 (two signals overlapped), 26.3, 16.0; HRMS (ESI) Calcd for $C_{18}H_{28}NS$ $[M + H]^+$ 290.1942, found 290.1938.



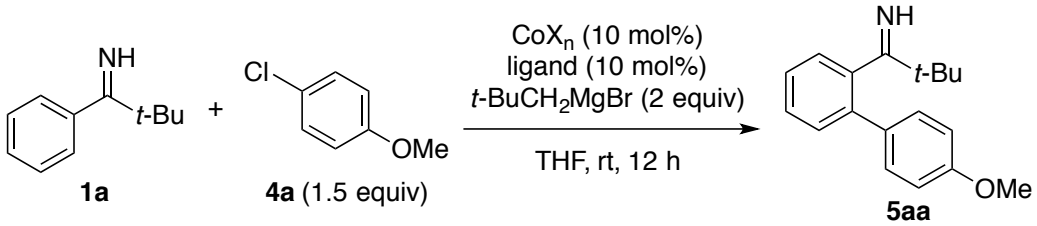
1-(2-Cyclohexyl-5-methylphenyl)-2,2-dimethylpropan-1-imine (3in): Light yellow oil (37 mg, 71%); R_f 0.61 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.10 (brs, 1H), 7.18 (d, J = 8.0 Hz, 1H), 7.09 (dd, J = 7.8, 1.6 Hz, 1H), 6.79 (d, J = 1.0 Hz, 1H), 2.37 – 2.27 (m, 4H), 1.79 – 1.70 (m, 4H), 1.51 – 1.19 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.2, 141.1, 134.6, 128.9 (two signals overlapped), 126.8, 126.6, 41.9, 40.5, 29.0, 27.2 (two signals overlapped), 26.35, 21.21; HRMS (ESI) Calcd for $C_{18}H_{28}N$ $[M + H]^+$ 258.2222, found 258.2224.



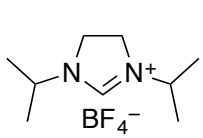
1-(3-Cyclohexylnaphthalen-2-yl)-2,2-dimethylpropan-1-imine (3mn): Light yellow oil (48 mg, 81%); R_f 0.58 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.24 (brs, 1H), 7.78 (t, J = 7.0 Hz, 2H), 7.75 (s, 1H), 7.49 – 7.40 (m, 3H), 2.46 (t, J = 11.5 Hz, 1H), 1.95 – 1.73 (m, 6H), 1.46 – 1.24 (m, 13H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 142.6, 140.3, 133.1, 131.1, 127.7, 127.4, 126.2, 125.8, 125.4, 124.6, 42.3, 40.7, 28.9, 27.2 (two signals overlapped), 26.2; HRMS (ESI) Calcd for $C_{21}H_{28}N$ $[M + H]^+$ 294.2222, found 294.2224.

Cobalt-Catalyzed *ortho*-Arylation of Pivalophenone N–H Imines with Aryl Chlorides

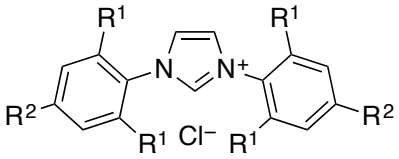
Table S2. Screening of Reaction Conditions



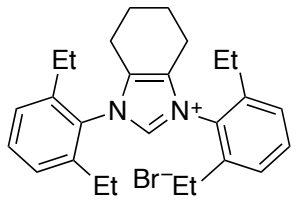
entry	CoX_n	ligand	yield (%)[a]
1	$CoBr_2$	**L1**•HBF_4	trace
2	$CoBr_2$	IMes•HCl	22
3	$CoBr_2$	IPr•HCl	16
4	$CoBr_2$	IEt•HCl	24
5	$CoBr_2$	**L2**•HBr	22
6	$Co(acac)_2$	IEt•HCl	32
7	$Co(acac)_3$	IEt•HCl	37
8[b]	$Co(acac)_3$	IEt•HCl	42
9[b,c]	$Co(acac)_3$	IEt•HCl	55
10[b,c]	$Co(acac)_3$	IMes•HCl	50
11[b,c]	$Co(acac)_3$	**L2**•HBr	84[d]



L1•HBF_4

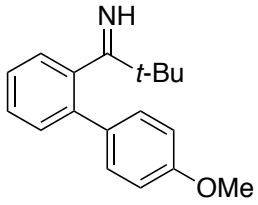


IMes•HCl (R^1 = R^2 = Me)
IPr•HCl (R^1 = *i*-Pr, R^2 = H)
IEt•HCl (R^1 = Et, R^2 = H)



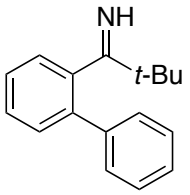
L2•HBr

[a] Determined by GC using *n*-tridecane as an internal standard. [b] 2.5 equiv of *t*-$BuCH_2MgBr$ was used. [c] TMEDA (80 mol%) was added. [d] Isolated yield.

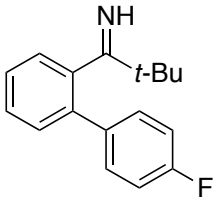


General Procedure: 1-(4'-Methoxy-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5aa). In a Schlenk tube were placed **L2**•HBr (7.5 mg, 0.020 mmol), $Co(acac)_3$ (6.8 mg, 0.020 mmol), and THF (0.3 mL). The resulting solution was cooled in an ice bath, followed by the addition of *t*-$BuCH_2MgBr$ (2.0 M in THF, 0.25 mL, 0.50 mmol). After stirring for 30 min, TMEDA (24 μL, 0.16 mmol), 2,2-dimethyl-1-phenylpropan-1-imine (**1a**, 33 mg, 0.20 mmol), and 1-bromo-4-methoxybenzene (**4a**, 37 μL, 0.30 mmol) were added sequentially. The resulting mixture was warmed to room temperature and stirred for 12 h, and then filtered through a short pad of silica gel, which was washed with ethyl acetate (5 mL). The filtrate was concentrated under reduced pressure. Silica gel chromatography (eluent: hexane/EtOAc/NEt_3 = 30/1/1) of the crude product afforded the title compound as a colorless oil (45 mg, 84%).

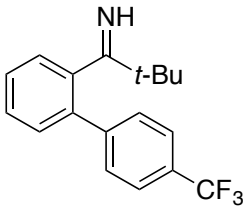
R_f 0.24 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.63 (brs, 1H), 7.44 – 7.25 (m, 5H), 7.16 – 7.08 (m, 1H), 6.96 – 6.86 (m, 2H), 3.82 (s, 3H), 0.89 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.8, 159.1, 141.2, 138.2, 134.2, 131.2, 130.2, 128.2, 127.8, 126.6, 113.7, 55.4, 40.6, 28.8; HRMS (ESI) Calcd for $C_{18}H_{22}NO$ $[M + H]^+$ 268.1701, found 268.1704.



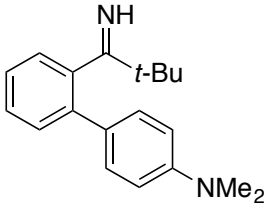
2,2-Dimethyl-1-(4'-methyl-[1,1'-biphenyl]-2-yl)propan-1-imine (5ac): Light yellow oil (42 mg, 83%); R_f 0.46 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.27 (brs, 1H), 7.41 – 7.24 (m, 5H), 7.16 (d, J = 7.8 Hz, 2H), 7.12 (d, J = 7.4 Hz, 1H), 2.37 (s, 3H), 0.89 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.7, 141.2, 138.8, 138.6, 137.2, 130.4, 130.0, 129.1, 128.2, 127.8, 126.8, 40.6, 28.9, 21.4; HRMS (ESI) Calcd for $C_{18}H_{22}N$ $[M + H]^+$ 252.1752, found 252.1754.



1-(4'-Fluoro-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ad): Light yellow oil (40 mg, 79%); R_f 0.41 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (brs, 1H), 7.41 – 7.30 (m, 5H), 7.13 (d, J = 7.7 Hz, 1H), 7.08 – 7.01 (m, 2H), 0.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.4, 162.4 (d, $^1J_{C\text{-}F}$ = 246.9 Hz), 141.2, 137.7 (d, $^4J_{C\text{-}F}$ = 3.3 Hz), 137.6, 131.8 (d, $^3J_{C\text{-}F}$ = 7.9 Hz), 130.3, 128.3, 128.0, 127.1, 115.3 (d, $^2J_{C\text{-}F}$ = 21.4 Hz), 40.7, 28.8; HRMS (ESI) Calcd for $C_{17}H_{19}NF$ $[M + H]^+$ 256.1502, found 256.1507.

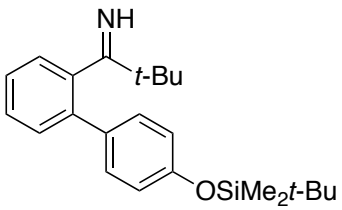


2,2-Dimethyl-1-(4'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)propan-1-imine (5ae): Light yellow oil (42 mg, 68%); R_f 0.40 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (brs, 1H), 7.62 (d, J = 8.2 Hz, 2H), 7.51 (d, J = 7.9 Hz, 2H), 7.43 – 7.33 (m, 3H), 7.20 – 7.16 (m, 1H), 0.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 145.4, 141.0, 137.3, 130.6, 130.31, 129.7 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 128.5, 128.1, 127.8, 125.3 (q, $^3J_{C\text{-}F}$ = 3.4 Hz), 124.4 (q, $^1J_{C\text{-}F}$ = 272.0 Hz), 40.8, 28.8; HRMS (ESI) Calcd for $C_{18}H_{19}NF_3$ $[M + H]^+$ 306.1470, found 306.1472.

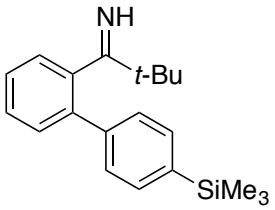


2'-(1-Imino-2,2-dimethylpropyl)-*N*,*N*-dimethyl-[1,1'-biphenyl]-4-amine (5af): Light yellow oil (45 mg, 81%); R_f 0.35 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.28 (brs, 1H), 7.39 – 7.31 (m, 2H), 7.28 – 7.23 (m, 3H), 7.09 (d, J = 7.4 Hz, 1H), 6.74 – 6.69 (m, 2H), 2.97 (s, 6H), 0.91 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.4, 149.9, 141.2, 138.8, 130.8, 130.2, 129.8, 128.2, 127.9, 126.0, 112.3, 40.7, 40.6, 29.0; HRMS (ESI) Calcd for $C_{19}H_{25}N_2$ [M +

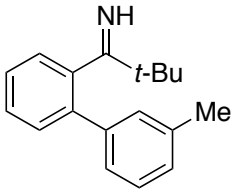
H]$^+$ 281.2018, found 281.2016.



1-(4'-((*tert*-Butyldimethylsilyl)oxy)-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ag): Light yellow oil (57 mg, 78%); R_f 0.34 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.25 (brs, 1H), 7.39 – 7.27 (m, 3H), 7.23 (d, J = 8.5 Hz, 2H), 7.11 – 7.08 (m, 1H), 6.85 – 6.81 (m, 2H), 0.99 (s, 9H), 0.87 (s, 9H), 0.20 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.0, 155.4, 138.3, 134.9, 131.3, 130.2, 128.2, 127.9, 126.9, 126.6, 120.1, 40.6, 28.9, 28.1, 26.0, -4.2; HRMS (ESI) Calcd for $C_{23}H_{34}NOSi$ [M + H]$^+$ 368.2410, found 368.2409.

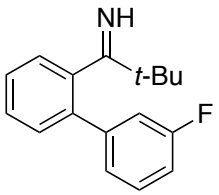


2,2-Dimethyl-1-(4'-(trimethylsilyl)-[1,1'-biphenyl]-2-yl)propan-1-imine (5ah): Light yellow oil (50 mg, 81%); R_f 0.46 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (brs, 1H), 7.53 – 7.48 (m, 2H), 7.43 – 7.29 (m, 1H), 7.14 (d, J = 7.3 Hz, 5H), 0.88 (s, 9H), 0.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.5, 142.0, 141.3, 139.5, 138.6, 133.3, 130.4, 129.5, 128.2, 127.8, 127.0, 40.6, 28.9, -0.9; HRMS (ESI) Calcd for $C_{20}H_{28}NSi$ [M + H]$^+$ 310.1991, found 310.1997.

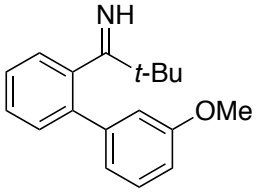


2,2-Dimethyl-1-(3'-methyl-[1,1'-biphenyl]-2-yl)propan-1-imine (5ai): Light yellow oil (41 mg, 82%); R_f 0.45 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (brs, 1H), 7.40 – 7.29 (m, 3H), 7.26 – 7.21 (m, 1H), 7.20 – 7.14 (m, 2H), 7.12 (d, J = 7.4 Hz, 2H), 2.36 (s,

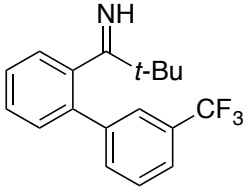
3H), 0.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.7, 141.6, 141.3, 138.6, 137.9, 130.9, 130.3, 128.2, 128.2, 128.2, 127.8, 127.3, 126.9, 40.6, 29.0, 21.7; HRMS (ESI) Calcd for $C_{18}H_{22}N$ $[M + H]^+$ 252.1752, found 252.1756.



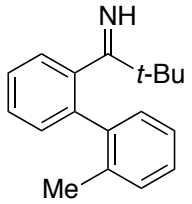
1-(3'-Fluoro-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5aj): Light yellow oil (38 mg, 75%); R_f 0.45 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.65 (brs, 1H), 7.43 – 7.29 (m, 4H), 7.18 – 7.09 (m, 3H), 7.05 – 6.98 (m, 1H), 0.90 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 162.6 (d, $^1J_{C\text{-}F}$ = 246.1 Hz), 143.7 (d, $^4J_{C\text{-}F}$ = 8.1 Hz), 137.2, 130.1, 129.7 (d, $^3J_{C\text{-}F}$ = 8.3 Hz), 128.2, 128.0 (d, $^3J_{C\text{-}F}$ = 8.5 Hz), 127.3, 126.7, 125.9 (d, $^4J_{C\text{-}F}$ = 2.4 Hz), 117.0 (d, $^2J_{C\text{-}F}$ = 21.8 Hz), 114.2 (d, $^2J_{C\text{-}F}$ = 21.0 Hz), 40.6, 28.7; HRMS (ESI) Calcd for $C_{17}H_{19}NF$ $[M + H]^+$ 256.1502, found 256.1498.



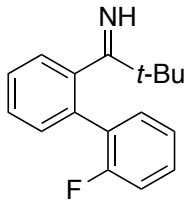
1-(3'-Methoxy-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ak): Light yellow oil (45 mg, 84%); R_f 0.30 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.58 (brs, 1H), 7.41 – 7.30 (m, 3H), 7.27 (t, J = 7.9 Hz, 1H), 7.13 (d, J = 7.4 Hz, 1H), 6.99 – 6.93 (m, 2H), 6.88 – 6.84 (m, 1H), 3.80 (s, 3H), 0.90 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.7, 159.5, 143.1, 141.2, 138.4, 130.2, 129.4, 128.2, 128.0, 127.1, 122.7, 115.6, 113.3, 55.5, 40.7, 28.9; HRMS (ESI) Calcd for $C_{18}H_{22}NO$ $[M + H]^+$ 268.1701, found 268.1702.



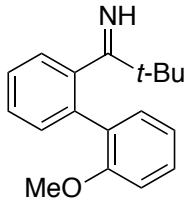
2,2-Dimethyl-1-(3'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)propan-1-imine (5al): Light yellow oil (37 mg, 61%); R_f 0.45 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (brs, 1H), 7.67 (s, 1H), 7.58 (d, J = 7.7 Hz, 2H), 7.51 – 7.34 (m, 4H), 7.18 (d, J = 7.4 Hz, 1H), 0.87 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.9, 142.4, 137.2, 133.6, 130.8 (q, $^2J_{C\text{-}F}$ = 32.2 Hz), 130.6, 130.3, 128.8, 128.5, 128.1, 127.7, 127.0 (q, $^3J_{C\text{-}F}$ = 3.2 Hz), 124.3 (q, $^1J_{C\text{-}F}$ = 272.4 Hz), 124.2 (q, $^3J_{C\text{-}F}$ = 3.6 Hz), 40.8, 28.8; HRMS (ESI) Calcd for $C_{18}H_{19}NF_3$ $[M + H]^+$ 306.1470, found 306.1471.



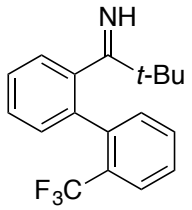
2,2-Dimethyl-1-(2'-methyl-[1,1'-biphenyl]-2-yl)propan-1-imine (5am): Light yellow oil (34 mg, 67%); R_f 0.45 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.14 (brs, 1H), 7.38 – 7.30 (m, 2H), 7.25 – 7.21 (m, 3H), 7.18 – 7.14 (m, 3H), 2.21 (s, 3H), 0.91 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 142.1, 140.4, 137.7, 136.1, 131.4, 131.1, 130.5, 127.8, 127.6, 127.5, 126.9, 125.3, 40.3, 29.1, 20.8; HRMS (ESI) Calcd for $C_{18}H_{22}N$ $[M + H]^+$ 252.1752, found 252.1749.



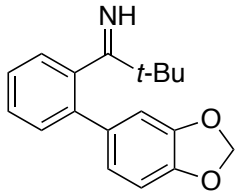
1-(2'-Fluoro-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5an): Light yellow oil (33 mg, 65%); R_f 0.46 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.54 (brs, 1H), 7.41 – 7.24 (m, 5H), 7.20 – 7.16 (m, 1H), 7.15 – 7.07 (m, 2H), 0.93 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 159.8 (d, $^1J_{C\text{-}F}$ = 246.0 Hz), 142.0, 132.9, 132.4, 131.2, 129.8 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 128.9 (d, $^2J_{C\text{-}F}$ = 15.6 Hz), 127.8, 127.6, 127.4, 123.8 (d, $^3J_{C\text{-}F}$ = 3.3 Hz), 115.9 (d, $^2J_{C\text{-}F}$ = 22.8 Hz), 40.4, 28.9; HRMS (ESI) Calcd for $C_{17}H_{19}NF$ $[M + H]^+$ 256.1502, found 256.1500.



1-(2'-Methoxy-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ao): Light yellow oil (38 mg, 71%); R_f 0.35 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.29 (brs, 1H), 7.38 – 7.26 (m, 4H), 7.15 – 7.13 (m, 2H), 6.96 – 6.93 (m, 1H), 6.90 (d, J = 8.3 Hz, 1H), 3.75 (s, 3H), 0.94 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 156.7, 135.4, 132.2, 131.2, 130.3, 129.3, 127.6, 126.9 (two signals overlapped), 126.7, 120.2, 110.8, 55.4, 40.0, 29.2; HRMS (ESI) Calcd for $C_{18}H_{22}NO$ $[M + H]^+$ 268.1701, found 268.1700.

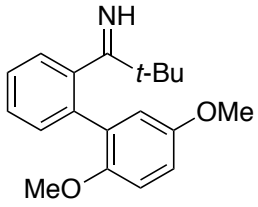


2,2-Dimethyl-1-(2'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)propan-1-imine (5ap): Light yellow oil (28 mg, 45%); R_f 0.45 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.42 (brs, 1H), 7.74 – 7.71 (m, 1H), 7.52 – 7.42 (m, 2H), 7.38 – 7.29 (m, 4H), 7.24 – 7.20 (m, 1H), 1.02 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.8, 141.5, 139.4, 135.8, 132.9, 131.1, 131.0, 129.2 (q, $^2J_{C\text{-}F}$ = 29.4 Hz), 128.0, 127.5, 127.3, 127.2, 127.0 (q, $^3J_{C\text{-}F}$ = 5.2 Hz), 124.4 (q, $^1J_{C\text{-}F}$ = 274.1 Hz), 40.2, 29.4; HRMS (ESI) Calcd for $C_{18}H_{19}NF_3$ $[M + H]^+$ 306.1470, found 306.1469.

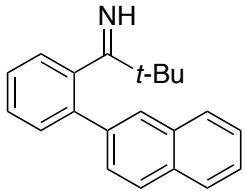


1-(2-(Benzo[*d*][1,3]dioxol-5-yl)phenyl)-2,2-dimethylpropan-1-imine (5aq): Light yellow oil (47 mg, 84%); R_f 0.33 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.58 (brs, 1H), 7.39 – 7.27 (m, 3H), 7.13 – 7.08 (m, 1H), 6.89 – 6.78 (m, 3H), 5.98 (s, 2H), 0.92 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.7, 147.7, 147.1, 141.2, 138.2, 135.7, 130.3, 128.3, 128.0,

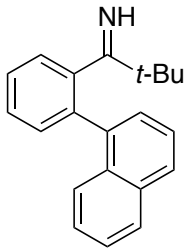
126.8, 123.9, 110.6, 108.2, 101.3, 40.7, 29.0; HRMS (ESI) Calcd for $C_{18}H_{20}NO_2$ $[M + H]^+$ 282.1494, found 282.1499.



1-(2',5'-Dimethoxy-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ar): Light yellow oil (47 mg, 79%); R_f 0.31 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.40 (brs, 1H), 7.38 – 7.25 (m, 3H), 7.14 (dd, J = 7.1, 1.2 Hz, 1H), 6.86 – 6.79 (m, 2H), 6.74 (d, J = 2.6 Hz, 1H), 3.75 (s, 3H), 3.70 (s, 3H), 0.96 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 153.1, 151.0, 135.7, 131.1, 131.0, 127.6, 127.0, 126.8, 118.1, 114.1, 111.7 (two signals overlapped), 56.1, 55.8, 40.0, 29.2; HRMS (ESI) Calcd for $C_{19}H_{24}NO_2$ $[M + H]^+$ 298.1807, found 298.1805.

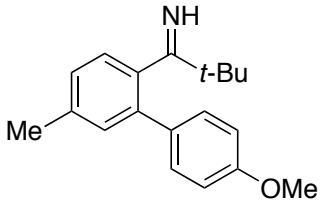


2,2-Dimethyl-1-(2-(naphthalen-2-yl)phenyl)propan-1-imine (5as): Light yellow oil (41 mg, 72%); R_f 0.41 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.71 (brs, 1H), 7.88 – 7.81 (m, 4H), 7.57 – 7.41 (m, 5H), 7.37 (td, J = 7.3, 1.9 Hz, 1H), 7.19 (d, J = 7.6 Hz, 1H), 0.86 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.6, 141.4, 139.2, 138.5, 133.3, 132.6, 130.7, 129.2, 128.4, 128.3 (two signals overlapped), 128.0, 128.0, 127.8, 127.1, 126.5, 126.4, 40.7, 29.0; HRMS (ESI) Calcd for $C_{21}H_{22}N$ $[M + H]^+$ 288.1752, found 288.1755.

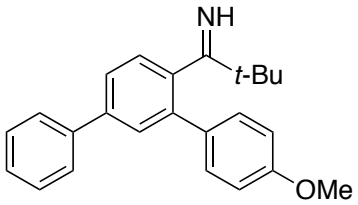


2,2-Dimethyl-1-(2-(naphthalen-1-yl)phenyl)propan-1-imine (5at): Light yellow oil (29 mg,

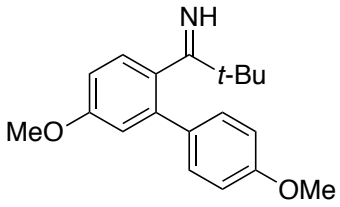
52%); R_f 0.41 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.44 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.3 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.49 – 7.34 (m, 7H), 7.28 – 7.24 (m, 1H), 0.82 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.6, 142.7, 138.4, 136.6, 133.9, 132.6, 132.0, 129.0, 128.6, 128.2, 127.7, 127.4, 127.2, 126.4, 126.3, 125.9, 125.0, 40.3, 29.2; HRMS (ESI) Calcd for $C_{21}H_{22}N$ $[M + H]^+$ 288.1752, found 288.1748.



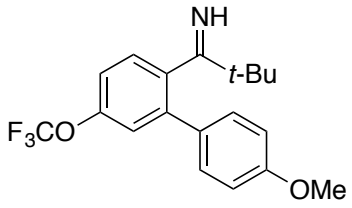
1-(4'-Methoxy-5-methyl-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ba): Light yellow oil (45 mg, 80%); R_f 0.36 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.50 (brs, 1H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.14 (s, 1H), 7.12 – 7.08 (m, 1H), 7.00 (d, *J* = 7.7 Hz, 1H), 6.91 – 6.86 (m, 2H), 3.82 (s, 3H), 2.39 (s, 3H), 0.89 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.0, 159.1, 138.1, 137.9 (two signals overlapped), 134.4, 131.2, 131.0, 127.8, 127.2, 113.7, 55.5, 40.6, 28.9, 21.4; HRMS (ESI) Calcd for $C_{19}H_{24}NO$ $[M + H]^+$ 282.1858, found 282.1859.



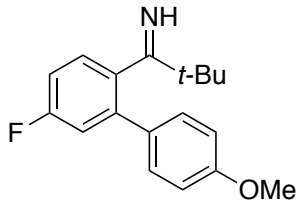
1-(4''-Methoxy-[1,1':3',1''-terphenyl]-4'-yl)-2,2-dimethylpropan-1-imine (5ca): Light yellow oil (53 mg, 78%); R_f 0.35 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (brs, 1H), 7.65 – 7.61 (m, 2H), 7.56 (d, *J* = 1.8 Hz, 1H), 7.53 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.32 (m, 3H), 7.19 (d, *J* = 7.9 Hz, 1H), 6.94 – 6.90 (m, 2H), 3.84 (s, 3H), 0.93 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.8, 159.2, 141.1, 140.6, 140.1, 138.8, 134.2, 131.3, 129.1 (two signals overlapped), 128.5, 127.8, 127.3, 125.2, 113.9, 55.5, 40.8, 28.9; HRMS (ESI) Calcd for $C_{24}H_{26}NO$ $[M + H]^+$ 344.2014, found 344.2019.



1-(4',5-Dimethoxy-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5da): Light yellow oil (48 mg, 81%); R_f 0.25 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.50 (brs, 1H), 7.29 (d, J = 8.5 Hz, 2H), 7.03 (d, J = 8.1 Hz, 1H), 6.92 – 6.81 (m, 4H), 3.83 (s, 3H), 3.82 (s, 3H), 0.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.8, 159.2, 139.8, 134.2, 134.0, 131.1, 129.1 (two signals overlapped), 115.5, 113.8, 112.1, 55.5, 55.5, 40.7, 28.9; HRMS (ESI) Calcd for $C_{19}H_{24}NO_2$ $[M + H]^+$ 298.1807, found 298.1805.

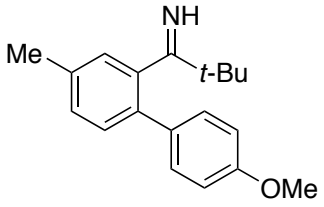


1-(4'-Methoxy-5-(trifluoromethoxy)-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ea): Light yellow oil (55 mg, 78%); R_f 0.27 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.68 (brs, 1H), 7.30 (d, J = 7.5 Hz, 2H), 7.18 (s, 1H), 7.14 (s, 2H), 6.90 (dd, J = 8.5, 1.6 Hz, 2H), 3.83 (s, 3H), 0.87 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 159.6, 148.9, 140.0 (d, $^2J_{C\text{-}F}$ = 87.9 Hz), 132.8, 131.2, 129.5, 122.5, 120.7 (d, $^1J_{C\text{-}F}$ = 257.6 Hz), 118.8, 114.0, 55.5, 40.8, 28.8; HRMS (ESI) Calcd for $C_{19}H_{21}NO_2F_3$ $[M + H]^+$ 352.1524, found 352.1530.

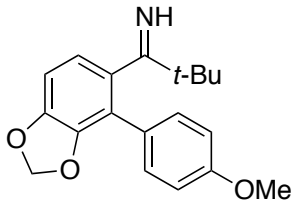


1-(5-Fluoro-4'-methoxy-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ha): Light yellow oil (45 mg, 79%); R_f 0.35 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (brs, 1H), 7.29 (d, J = 8.4 Hz, 2H), 7.10 – 6.96 (m, 3H), 6.92 – 6.87 (m, 2H), 3.82 (s, 3H), 0.87 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 162.3 (d, $^1J_{C\text{-}F}$ = 247.1 Hz), 159.5, 140.6, 137.2, 133.1, 131.1, 129.6 (d, $^3J_{C\text{-}F}$ = 8.1 Hz), 116.9 (d, $^2J_{C\text{-}F}$ = 21.3 Hz), 113.9, 113.4 (d, $^2J_{C\text{-}F}$ =

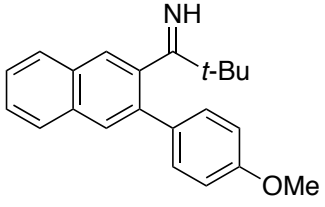
21.1 Hz), 55.5, 40.8, 28.8; HRMS (ESI) Calcd for $C_{18}H_{21}NOF$ $[M + H]^+$ 286.1607, found 286.1613.



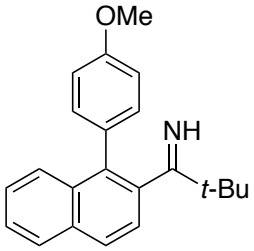
1-(4'-Methoxy-4-methyl-[1,1'-biphenyl]-2-yl)-2,2-dimethylpropan-1-imine (5ia): Light yellow oil (41 mg, 73%); R_f 0.37 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (brs, 1H), 7.30 – 7.25 (m, 2H), 7.22 – 7.16 (m, 2H), 6.91 – 6.86 (m, 3H), 3.82 (s, 3H), 2.38 (s, 3H), 0.88 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.1, 159.0, 141.1, 136.3, 135.4, 134.3, 131.2, 130.2, 129.0, 128.5, 113.8, 55.5, 40.6, 29.0, 21.3; HRMS (ESI) Calcd for $C_{19}H_{24}NO$ $[M + H]^+$ 282.1858, found 282.1861.



1-(4-(4-Methoxyphenyl)benzo[*d*][1,3]dioxol-5-yl)-2,2-dimethylpropan-1-imine (5la): Light yellow oil (51 mg, 82%); R_f 0.31 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.52 (brs, 1H), 7.33 (d, J = 8.7 Hz, 2H), 6.94 – 6.88 (m, 2H), 6.76 (d, J = 8.0 Hz, 1H), 6.61 (d, J = 8.0 Hz, 1H), 5.96 (s, 2H), 3.82 (s, 3H), 0.89 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 159.4, 147.0, 145.3, 136.0, 131.9, 127.3, 121.2, 120.8, 113.9, 107.0, 101.2, 55.5, 40.6, 29.0; HRMS (ESI) Calcd for $C_{19}H_{22}NO_3$ $[M + H]^+$ 312.1600, found 312.1596.



5na



5na'

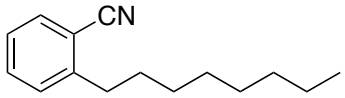
1-(3-(4-Methoxyphenyl)naphthalen-2-yl)-2,2-dimethylpropan-1-imine (5na): Silica gel chromatography (eluent: hexane/EtOAc/NEt_3 = 30/1/1) of the crude product afforded a mixture of the title compound and its regioisomer **5na'** as a light yellow oil (48 mg, 75%). The ratio of **5na** and **5na'** was determined to be 3:2 by ^{1}H NMR analysis.

R_f 0.35 (hexane/EtOAc/NEt_3 = 10/1/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H for each isomer), 7.90 – 7.80 (m, 4H for each isomer), 7.79 (s, 1H for **5na**), 7.65 (d, J = 8.5 Hz, 1H for **5na'**), 7.59 (s, 1H for **5na**), 7.54 – 7.46 (m, 4H for each isomer), 7.43 – 7.37 (m, 3Hfor each isomer), 7.29 – 7.24 (m, 2H for each isomer), 7.00 – 6.92 (m, 4H for each isomer), 3.87 (s, 3H for **5na'**), 3.85 (s, 3H for **5na**), 0.97 (s, 9H for **5na'**), 0.95 – 0.89 (m, 9H for **5na**); ^{13}C NMR (both isomers, 100 MHz, $CDCl_3$): δ 192.1, 191.3, 159.2, 159.2, 140.2, 139.8, 136.7, 135.1, 134.2, 133.16, 133.15, 133.13, 133.12, 133.11, 131.8, 131.6, 130.5, 129.0, 128.1, 127.9, 127.2, 127.1, 126.8, 126.7, 126.6, 126.6, 126.2, 124.8, 113.9, 113.5, 55.53, 55.51, 40.7, 40.2, 29.4, 29.0; HRMS (ESI) Calcd for $C_{22}H_{24}NO$ $[M + H]^+$ 318.1858, found 318.1860.

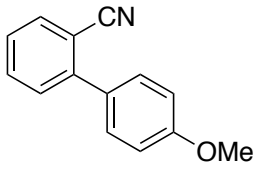
Synthesis of *ortho*-Substituted Benzonitriles

Conditions A: 3aa or **5aa** (0.20 mmol) was weighed in a 4 mL vial containing a stir bar, and then dissolved in *t*-BuOO*t*-Bu (0.5 mL). The vial was placed in Luzchem LZC-4V photoreactor and irradiated at 254 nm for 12 h. The mixture was concentrated under reduced pressure, and the residue was subjected to silica gel chromatography (eluent: hexane/EtOAc = 100/1 for *ortho*-alkylbenzonitrile, 30/1 for *ortho*-arylbenzonitrile) to afford the desired benzonitrile derivative.

Conditions B: In a 10 mL Schlenk tube containing a stir bar were placed **3aa** or **5aa** (0.20 mmol) and $Cu(OAc)_2$ (3.6 mg, 0.020 mmol), followed by the addition of DMF (2 mL). An oxygen balloon was attached to the Schlenk tube, and the reaction mixture was stirred at 80 °C for 12 h. The mixture was concentrated under reduced pressure, and the residue was subjected to silica gel chromatography (eluent: hexane/EtOAc = 100/1 for *ortho*-alkylbenzonitrile, 30/1 for *ortho*-arylbenzonitrile) to afford the desired benzonitrile derivative.

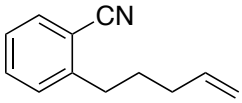


2-Octylbenzonitrile (7a):[7] Colorless oil; R_f 0.65 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, J = 7.7 Hz, 1H), 7.50 (t, J = 7.7 Hz, 1H), 7.32 – 7.24 (m, 2H), 2.86 – 2.80 (m, 2H), 1.70 – 1.63 (m, 2H), 1.40 – 1.21 (m, 10H), 0.88 (t, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.1, 133.0, 132.9, 129.7, 126.5, 118.4, 112.6, 34.9, 32.1, 31.2, 29.6, 29.5, 29.4, 22.9, 14.3; HRMS (ESI) Calcd for $C_{15}H_{22}N$ $[M + H]^+$ 216.1752, found 216.1760.



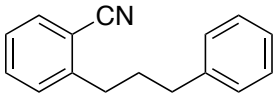
4'-Methoxy-[1,1'-biphenyl]-2-carbonitrile (7b):[8] Colorless oil; R_f 0.32 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (dd, J = 7.8, 1.2 Hz, 1H), 7.62 (td, J = 7.8, 1.3 Hz, 1H), 7.53 – 7.47 (m, 3H), 7.40 (td, J = 7.6, 1.0 Hz, 1H), 7.04 – 7.00 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 145.4, 134.0, 133.0, 130.8, 130.2, 130.1, 127.3, 119.2, 114.4, 111.3, 55.6; HRMS (ESI) Calcd for $C_{14}H_{12}NO$ $[M + H]^+$ 210.0919, found 210.0915.

Two-Step Synthesis of *ortho*-Substituted Benzonitriles



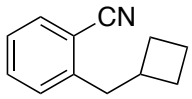
Procedure A: 2-(Pent-4-en-1-yl)benzonitrile (7d). The reaction of 2,2-dimethyl-1-phenylpropan-1-imine (**1a**, 33 mg, 0.20 mmol) and 5-bromopent-1-ene (**2g**, 36 μL, 0.30 mmol) was performed according to the typical procedure described above. The reaction mixture was filtered through a short pad of silica gel, washing with ethyl acetate (5 mL). The filtrate was concentrated under reduced pressure. The residue was dissolved in a small amount (ca. 1 mL) of CH_2Cl_2, transferred to a 4 mL vial, and then concentrated again under reduced pressure. A stir bar was placed in this vial, and *t*-BuOO*t*-Bu (0.5 mL) was added. The vial was placed in Luzchem LZC-4V photoreactor and irradiated at 254 nm for 12 h. The mixture was concentrated under reduced pressure, and the residue was subjected to silica gel chromatography (eluent: hexane/EtOAc = 100/1) to afford the title compound as a colorless oil (27 mg, 78%).

R_f 0.62 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, J = 7.7 Hz, 1H), 7.50 (td, J = 7.7, 1.2 Hz, 1H), 7.33 – 7.28 (m, 2H), 5.88 – 5.78 (m, 1H), 5.09 – 4.97 (m, 2H), 2.85 (t, J = 14.3 Hz, 2H), 2.14 (dd, J = 14.3, 7.1 Hz, 2H), 1.82 – 1.74 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.6, 138.1, 133.0, 132.9, 129.8, 126.6, 118.3, 115.5, 112.6, 34.2, 33.4, 30.2; HRMS (ESI) Calcd for $C_{12}H_{14}N$ $[M + H]^+$ 172.1126, found 172.1124.

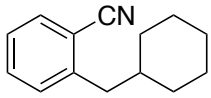


Procedure B: 2-(3-Phenylpropyl)benzonitrile (7c). [9] The reaction of 2,2-dimethyl-1-phenylpropan-1-imine (**1a**, 33 mg, 0.20 mmol) and (3-bromopropyl)benzene (**2c**, 46 μL, 0.30 mmol) was performed according to the typical procedure described above. The reaction mixture was filtered through a short pad of silica gel, washing with ethyl acetate (5 mL). The filtrate was concentrated under reduced pressure. The residue was dissolved in DMF (1 mL) and then transferred into a 10 mL Schelenk tube containing a stir bar, followed by the addition of $Cu(OAc)_2$ (3.6 mg, 0.020 mmol) and DMF (1 mL). The reaction mixture was stirred under oxygen atmosphere (using a balloon) at 80 °C for 12 h. The mixture was concentrated under reduced pressure, and the residue was subjected to silica gel chromatography (eluent: hexane/EtOAc = 100/1) to afford the title compound as a colorless oil (36 mg, 81%).

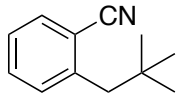
R_f 0.60 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, J = 7.7 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.33 – 7.27 (m, 4H), 7.21 (d, J = 7.3 Hz, 3H), 2.90 (t, J = 7.6 Hz, 2H), 2.72 (t, J = 7.7 Hz, 2H), 2.07 – 1.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.5, 141.8, 133.1, 133.0, 129.70, 128.6 (two signals overlapped), 126.7, 126.2, 118.3, 112.6, 35.7, 34.4, 32.6; HRMS (ESI) Calcd for $C_{16}H_{16}N$ $[M + H]^+$ 222.1283, found 222.1288.



2-(Cyclobutylmethyl)benzonitrile (7e): Light yellow oil (28 mg, 82%, procedure A); R_f 0.60 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (dd, J = 8.0, 1.4 Hz, 1H), 7.48 (td, J = 7.7, 1.4 Hz, 1H), 7.29 – 7.24 (m, 2H), 2.93 (d, J = 7.6 Hz, 2H), 2.71 – 2.60 (m, 1H), 2.09 – 1.98 (m, 2H), 1.91 – 1.73 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 133.0, 132.8, 129.7, 126.6, 118.6, 112.6, 41.3, 36.9, 28.3, 18.5; HRMS (ESI) Calcd for $C_{12}H_{14}N$ $[M + H]^+$ 172.1126, found 172.1126.

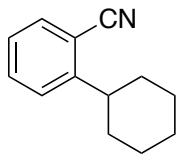


2-(Cyclohexylmethyl)benzonitrile (7f): Light yellow oil (32 mg, 81%, procedure A); R_f 0.61 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (dd, J = 8.0, 1.4 Hz, 1H), 7.49 (td, J = 7.7, 1.4 Hz, 1H), 7.29 – 7.25 (m, 2H), 2.72 (d, J = 6.9 Hz, 2H), 1.74 – 1.60 (m, 5H), 1.23 – 1.13 (m, 4H), 1.08 – 0.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.7, 132.9, 132.6, 130.6, 126.5, 118.7, 113.1, 42.6, 39.8, 33.2, 26.6, 26.4; HRMS (ESI) Calcd for $C_{14}H_{18}N$ $[M + H]^+$ 200.1439, found 200.1436.

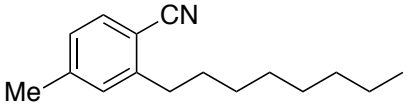


2-Neopentylbenzonitrile (7g): Light yellow oil (29 mg, 85%, procedure A); R_f 0.61 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (dd, J = 7.7, 1.2 Hz, 1H), 7.49 (td, J = 7.8, 1.4 Hz, 1H), 7.32 – 7.26 (m, 2H), 2.78 (s, 2H), 0.98 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.9, 133.0, 132.1, 131.8, 126.7, 119.3, 114.2, 48.0, 33.4, 29.6; HRMS (ESI) Calcd

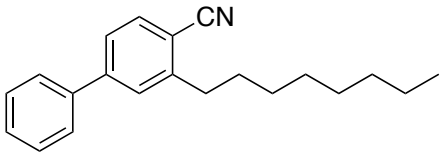
for $C_{12}H_{16}N$ $[M + H]^+$ 174.1283, found 174.1286.



2-Cyclohexylbenzonitrile (7h):[10] Light yellow oil (30 mg, 82%, procedure A); R_f 0.57 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (dd, J = 7.7, 1.5 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.36 (dd, J = 8.0, 0.5 Hz, 1H), 7.28 – 7.24 (m, 1H), 3.03 – 2.92 (m, 1H), 1.93 – 1.84 (m, 4H), 1.83 – 1.73 (m, 2H), 1.51 – 1.41 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 133.2, 133.1, 126.8, 126.5, 118.5, 112.1, 43.0, 33.9, 26.8, 26.2; HRMS (ESI) Calcd for $C_{13}H_{16}N$ $[M + H]^+$ 186.1283, found 186.1283.

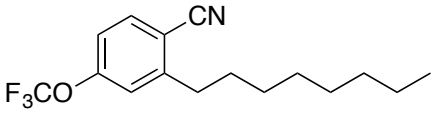


4-Methyl-2-octylbenzonitrile (7i): Light yellow oil (35 mg, 77%, procedure B); R_f 0.62 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, J = 7.9 Hz, 1H), 7.11 (s, 1H), 7.07 (d, J = 8.1 Hz, 1H), 2.81 – 2.74 (m, 2H), 2.38 (s, 3H), 1.69 – 1.60 (m, 2H), 1.40 – 1.20 (m, 10H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.0, 143.7, 132.9, 130.4, 127.4, 118.8, 109.5, 34.8, 32.1, 31.2, 29.6, 29.5, 29.4, 22.9, 22.0, 14.3; HRMS (ESI) Calcd for $C_{16}H_{24}N$ $[M + H]^+$ 230.1909, found 230.1911.

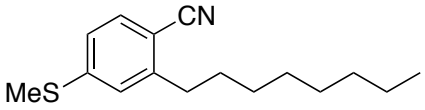


3-Octyl-[1,1'-biphenyl]-4-carbonitrile (7j): Light yellow oil (46 mg, 79%, procedure A); R_f 0.55 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, J = 8.0 Hz, 1H), 7.60 – 7.57 (m, 2H), 7.52 – 7.49 (m, 2H), 7.48 – 7.45 (m, 2H), 7.44 – 7.41 (m, 1H), 2.92 – 2.86 (m, 2H), 1.76 – 1.67 (m, 2H), 1.44 – 1.24 (m, 10H), 0.90 – 0.86 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.6, 145.8, 139.8, 133.4, 129.3, 128.7, 128.4, 127.5, 125.3, 118.6, 111.2, 35.0, 32.1, 31.3, 29.6 (two signals overlapped), 29.4, 22.9, 14.3; HRMS (ESI) Calcd for $C_{21}H_{26}N$ $[M + H]^+$ 292.2065,

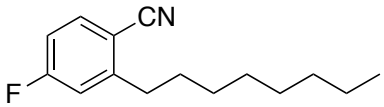
found 292.2070.



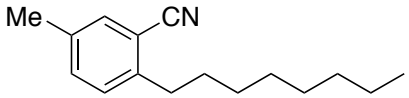
2-Octyl-4-(trifluoromethoxy)benzonitrile (7k): Light yellow oil (48 mg, 81%, procedure A); R_f 0.50 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (d, J = 8.4 Hz, 1H), 7.15 – 7.11 (m, 2H), 2.88 – 2.82 (m, 2H), 1.71 – 1.64 (m, 2H), 1.42 – 1.22 (m, 10H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.3, 150.0, 134.8, 122.2 (d, $^1J_{C\text{-}F}$ = 238.5 Hz), 121.6, 118.6, 117.3, 111.0, 34.9, 32.0, 30.9, 30.8, 29.5, 29.4, 22.9, 14.3; HRMS (ESI) Calcd for $C_{16}H_{21}NOF_3$ $[M + H]^+$ 300.1575, found 300.1577.



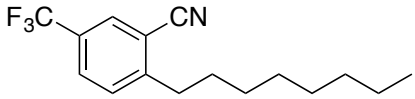
4-(Methylthio)-2-octylbenzonitrile (7l): Light yellow oil (37 mg, 71%, procedure A); R_f 0.60 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, J = 8.2 Hz, 1H), 7.10 (d, J = 1.6 Hz, 1H), 7.07 (dd, J = 8.2, 1.9 Hz, 1H), 2.81 – 2.75 (m, 2H), 2.50 (s, 3H), 1.69 – 1.61 (m, 2H), 1.40 – 1.23 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 145.9, 133.0, 126.1, 123.1, 118.6, 108.2, 34.9, 32.8, 31.1, 29.6, 29.5, 29.4, 22.9, 15.0, 14.3; HRMS (ESI) Calcd for $C_{16}H_{24}NS$ $[M + H]^+$ 262.1629, found 262.1633.



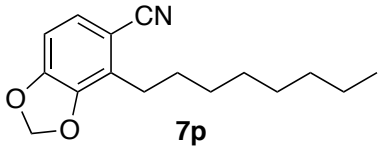
4-Fluoro-2-octylbenzonitrile (7m): Light yellow oil (37 mg, 79%, procedure B); R_f 0.58 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (dd, J = 8.5, 5.5 Hz, 1H), 7.04 – 6.95 (m, 2H), 2.86 – 2.80 (m, 2H), 1.70 – 1.62 (m, 2H), 1.40 – 1.23 (m, 10H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2 (d, $^1J_{C\text{-}F}$ = 256.0 Hz), 150.6 (d, $^3J_{C\text{-}F}$ = 8.8 Hz), 135.2 (d, $^3J_{C\text{-}F}$ = 9.6 Hz), 117.7, 117.0 (d, $^2J_{C\text{-}F}$ = 22.3 Hz), 114.3 (d, $^2J_{C\text{-}F}$ = 22.8 Hz), 108.7, 34.8, 32.0, 30.8, 29.5, 29.4, 22.9, 14.3; HRMS (ESI) Calcd for $C_{15}H_{21}NF$ $[M + H]^+$ 234.1658, found 234.1665.



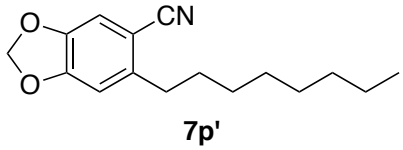
5-Methyl-2-octylbenzonitrile (7n): Light yellow oil (35 mg, 77%, procedure B); R_f 0.61 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (d, J = 0.6 Hz, 1H), 7.30 (dd, J = 7.9, 1.6 Hz, 1H), 7.19 (d, J = 7.9 Hz, 1H), 2.81 – 2.75 (m, 2H), 2.34 (s, 3H), 1.67 – 1.60 (m, 2H), 1.38 – 1.23 (m, 10H), 0.87 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.1, 136.3, 133.8, 133.2, 129.6, 118.6, 112.3, 34.4, 32.1, 31.2, 29.6, 29.5, 22.9, 20.9, 14.3; HRMS (ESI) Calcd for $C_{16}H_{24}N$ $[M + H]^+$ 230.1909, found 230.1916.



2-Octyl-5-(trifluoromethyl)benzonitrile (7o): Light yellow oil (34 mg, 61%, procedure A); R_f 0.60 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, J = 1.5 Hz, 1H), 7.75 (dd, J = 8.3, 1.5 Hz, 1H), 7.46 (d, J = 8.1 Hz, 1H), 2.93 – 2.87 (m, 2H), 1.73 – 1.64 (m, 2H), 1.30 – 1.26 (m, 10H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 130.4, 129.9 (q, $^3J_{C\text{-}F}$ = 3.7 Hz), 129.5 (q, $^3J_{C\text{-}F}$ = 3.2 Hz), 128.8 (q, $^2J_{C\text{-}F}$ = 111.8 Hz), 123.4 (q, $^1J_{C\text{-}F}$ = 272.3 Hz), 117.0, 113.5, 34.9, 32.0, 30.9, 29.5, 29.4, 29.4, 22.9, 14.3; HRMS (ESI) Calcd for $C_{16}H_{21}NF_3$ $[M + H]^+$ 284.1626, found 284.1629.



7p

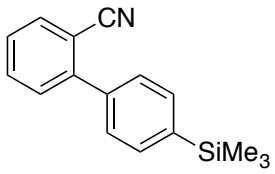


7p'

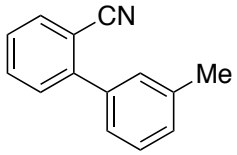
4-Octylbenzo[*d*][1,3]dioxole-5-carbonitrile (7p): Procedure A was applied. Silica gel chromatography (eluent: hexane/EtOAc = 50/1) of the crude product afforded a mixture of the title compound and its regioisomer **7p'** as a light yellow oil (39 mg, 75%). The ratio of **7p** and **7p'** was determined to be 3:2 by ^{1}H NMR analysis.

R_f 0.50 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (d, J = 8.1 Hz, 1H for **7q**), 6.96 (s, 1H for **7q'**), 6.74 (s, 1H for **7q'**), 6.72 (d, J = 8.1 Hz, 1H for **7q**), 6.04 (s, 2H for **7q**), 6.02 (s, 2H for **7q'**), 2.78 – 2.70 (m, 2H for each isomer), 1.68 – 1.60 (m, 2H for each isomer), 1.38 – 1.22 (m, 10H for each isomer), 0.88 (t, J = 6.7 Hz, 3H for each isomer); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 150.9, 146.4, 146.2, 143.9, 128.7, 127.8, 118.6, 118.4, 111.5, 109.8,

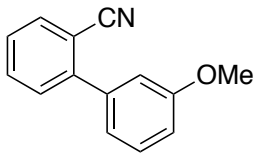
107.2, 106.1, 104.3, 102.3, 102.1, 34.8, 32.1, 31.3, 29.6, 29.4, 29.4, 28.6, 22.9, 14.3; HRMS (ESI) Calcd for $C_{16}H_{22}NO_2$ $[M + H]^+$ 260.1651, found 260.1645.



4'-(Trimethylsilyl)-[1,1'-biphenyl]-2-carbonitrile (7q): Light yellow oil (31 mg, 61%, procedure A); R_f 0.46 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 – 7.76 (m, 1H), 7.67 – 7.62 (m, 3H), 7.57 – 7.51 (m, 3H), 7.47 – 7.42 (m, 1H), 0.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.7, 141.5, 138.6, 134.1, 134.0, 133.1, 130.3, 128.2, 127.8, 119.0, 111.5, -0.9; HRMS (ESI) Calcd for $C_{16}H_{18}NSi$ $[M + H]^+$ 252.1209, found 252.1213.

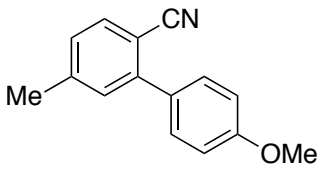


3'-Methyl-[1,1'-biphenyl]-2-carbonitrile (7r): [11] Light yellow oil (24 mg, 61%, procedure B); R_f 0.45 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 – 7.74 (m, 1H), 7.66 – 7.61 (m, 1H), 7.52 – 7.50 (m, 1H), 7.45 – 7.40 (m, 1H), 7.39 – 7.35 (m, 3H), 7.28 – 7.25 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.9, 138.6, 138.4, 133.9, 133.0, 130.3, 129.7 (two signals overlapped), 128.8, 127.6, 126.1, 119.0, 111.5, 21.7; HRMS (ESI) Calcd for $C_{14}H_{12}N$ $[M + H]^+$ 194.0970, found 194.0972.

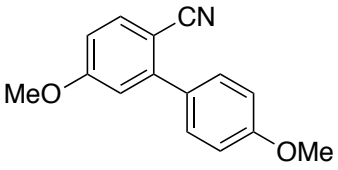


3'-Methoxy-[1,1'-biphenyl]-2-carbonitrile (7s): [12] Light yellow oil (24 mg, 58%, procedure B); R_f 0.31 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.74 (m, 1H), 7.67 – 7.61 (m, 1H), 7.54 – 7.51 (m, 1H), 7.47 – 7.37 (m, 2H), 7.15 – 7.12 (m, 1H), 7.10 – 7.08 (m, 1H), 7.01 – 6.97 (m, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9, 145.6, 139.7, 138.4, 134.0, 133.0, 130.3, 130.0, 127.8, 121.4, 114.7, 114.5, 111.6, 55.6; HRMS (ESI) Calcd for

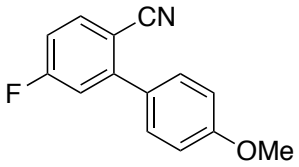
$C_{14}H_{12}NO$ $[M + H]^+$ 210.0919, found 210.0920.



4'-Methoxy-5-methyl-[1,1'-biphenyl]-2-carbonitrile (7t): Light yellow oil (27 mg, 60%, procedure B); R_f 0.36 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, J = 7.9 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.29 (s, 1H), 7.22 – 7.18 (m, 1H), 7.03 – 6.98 (m, 2H), 3.86 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.2, 145.3, 143.8, 133.9, 130.9, 130.8, 130.2, 128.1, 119.5, 114.4, 108.3, 55.6, 22.1; HRMS (ESI) Calcd for $C_{15}H_{14}NO$ $[M + H]^+$ 224.1075, found 224.1077.



4',5-Dimethoxy-[1,1'-biphenyl]-2-carbonitrile (7u): Light yellow oil (27 mg, 57%, procedure A); R_f 0.23 (hexane/EtOAc = 10/1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, J = 8.6 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.04 – 6.98 (m, 2H), 6.96 (d, J = 2.6 Hz, 1H), 6.90 (dd, J = 8.6, 2.5 Hz, 1H), 3.89 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9, 160.4, 147.5, 135.7, 130.8, 130.1, 119.6, 115.5, 114.4, 113.3, 103.2, 55.8, 55.6; HRMS (ESI) Calcd for $C_{15}H_{14}NO_2$ $[M + H]^+$ 240.1025, found 240.1015.



5-Fluoro-4'-methoxy-[1,1'-biphenyl]-2-carbonitrile (7v): White solid (24 mg, 54%, procedure A); R_f 0.34 (hexane/EtOAc = 10/1); M.p. 146-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (dd, J = 8.6, 5.6 Hz, 1H), 7.53 – 7.49 (m, 2H), 7.19 (dd, J = 9.5, 2.5 Hz, 1H), 7.10 (td, J = 8.2, 2.5 Hz, 1H), 7.05 – 7.00 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1 (d, $^1J_{C\text{-}F}$ = 249.0 Hz), 160.7, 148.5 (d, $^3J_{C\text{-}F}$ = 7.6 Hz), 136.3 (d, $^3J_{C\text{-}F}$ = 4.6 Hz), 130.1, 129.6, 118.6, 117.3 (d, $^2J_{C\text{-}}$

$_F$ = 22.9 Hz), 114.9 (d, $^2J_{C\text{-}F}$ = 22.9 Hz), 114.6, 107.4, 55.6; HRMS (ESI) Calcd for $C_{14}H_{11}NOF$ $[M + H]^+$ 228.0825, found 228.0822.

Reaction of 1i with *t*-BuCH$_2$MgBr

Imine **1i** (35 mg, 0.20 mmol) was placed in a J. Young NMR tube, and dissolved in [D$_8$]-THF (0.6 mL). After measurement of ^{1}H and ^{13}C NMR spectra, to this sample was added a THF solution of *t*-BuCH$_2$MgBr (0.20 mL, 1.5 M, 0.30 mmol) under nitrogen atmosphere at room temperature. The stopcock was closed and the resulting mixture was kept standing for 0.5 h. The sample was then subjected to ^{1}H and ^{13}C NMR measurements (Figure S1; the full spectra are attached to the bottom of this Supporting Information).

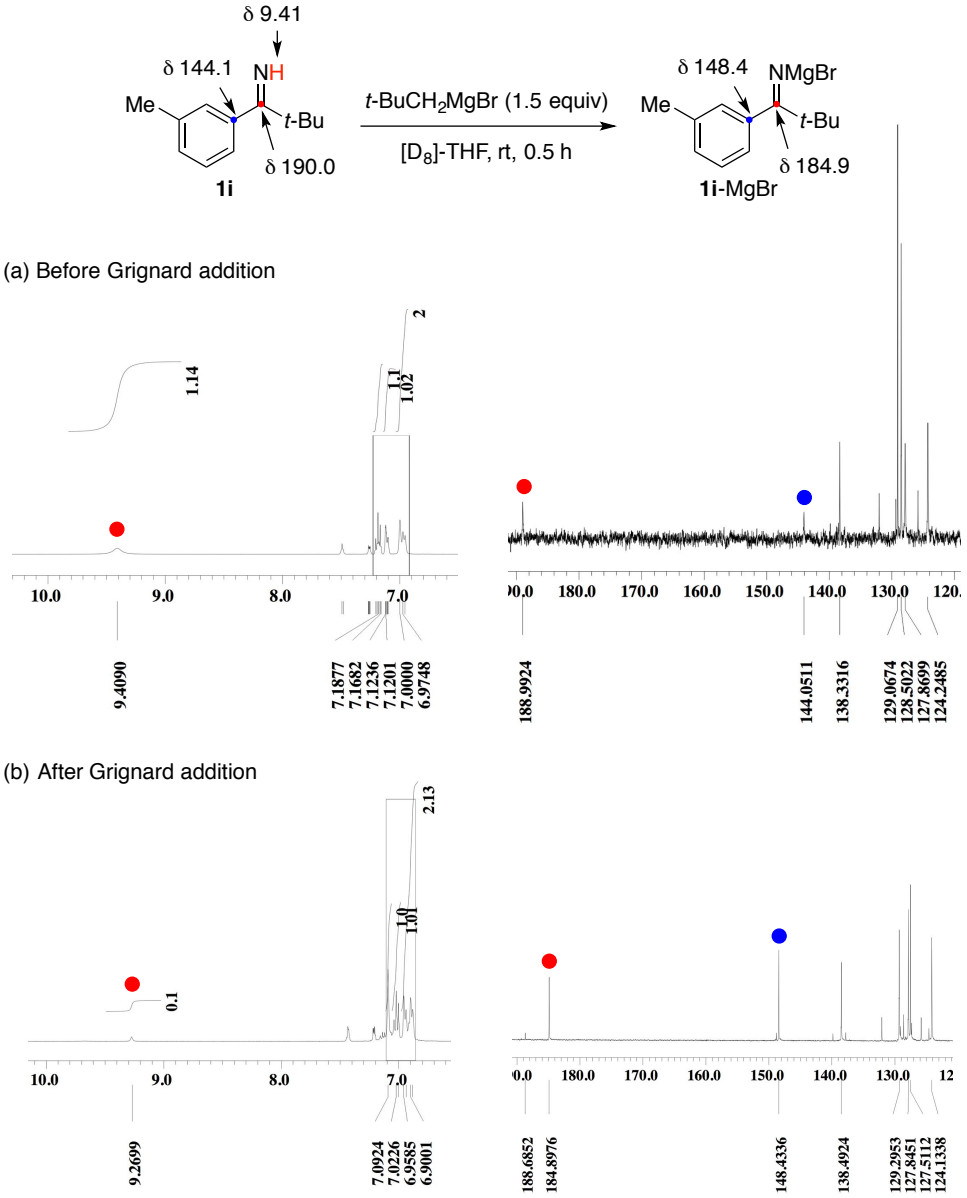


Figure S1. Imine/aromatic regions of ^{1}H (left) and ^{13}C (right) NMR spectra of **1i** before (a) and after (b) the addition of *t*-BuCH$_2$MgBr.

References

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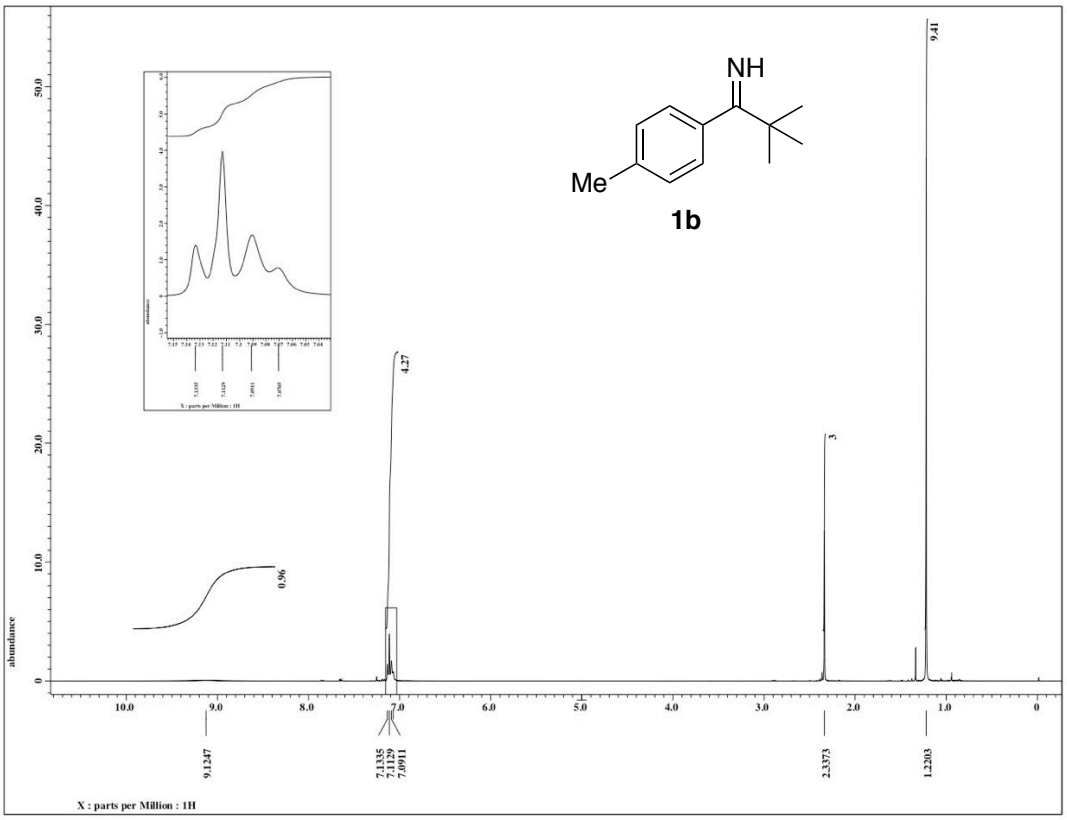
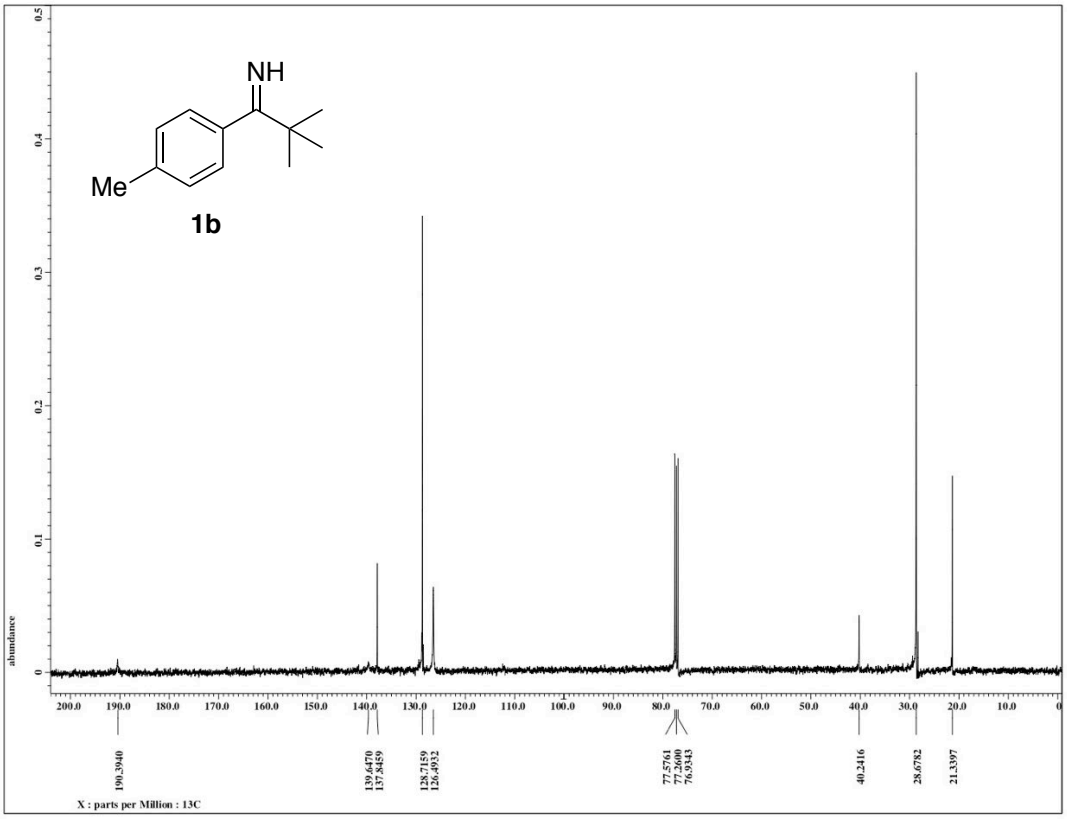
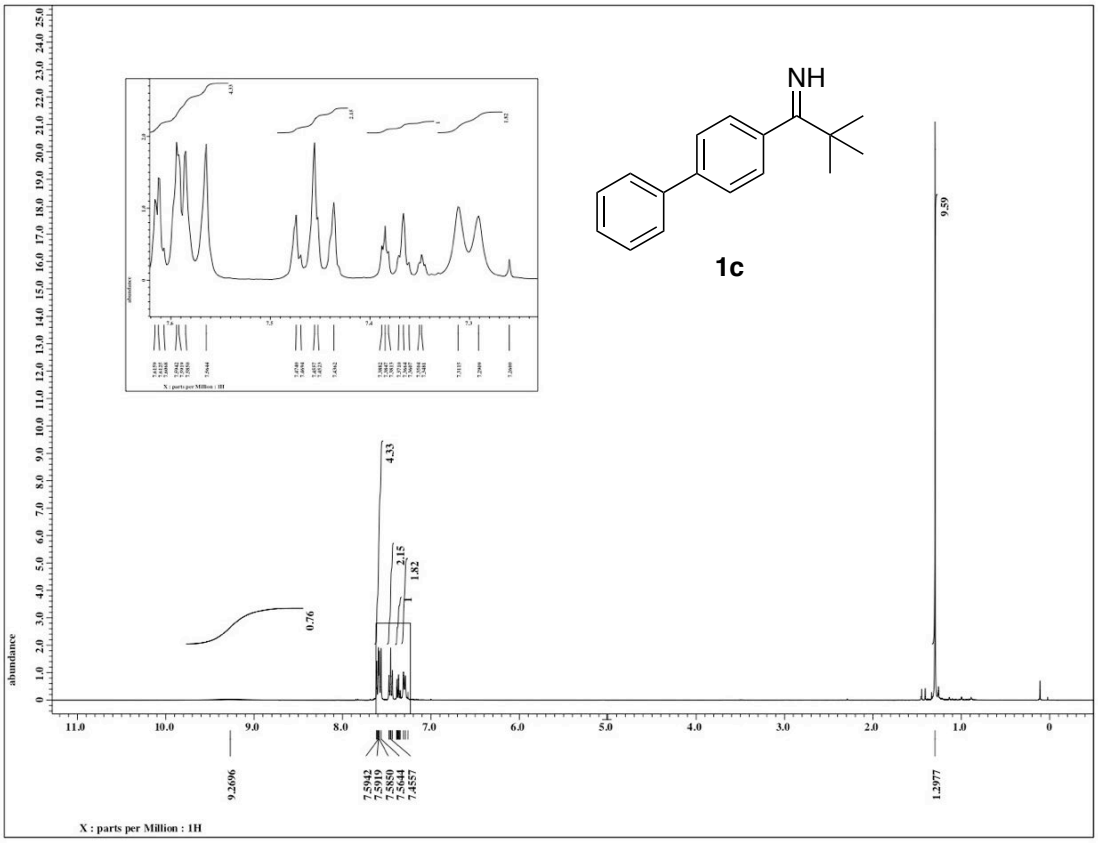
^{1}H and ^{13}C NMR Spectra



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7.4557
1.2977
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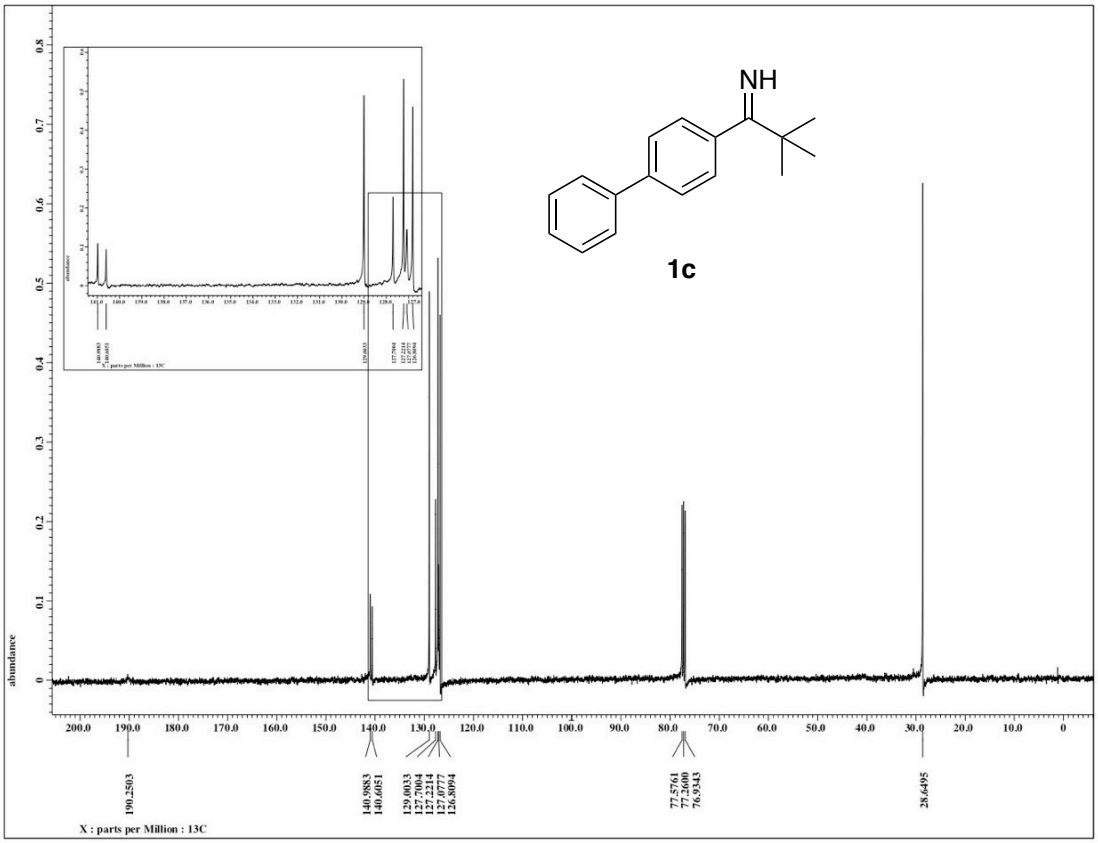
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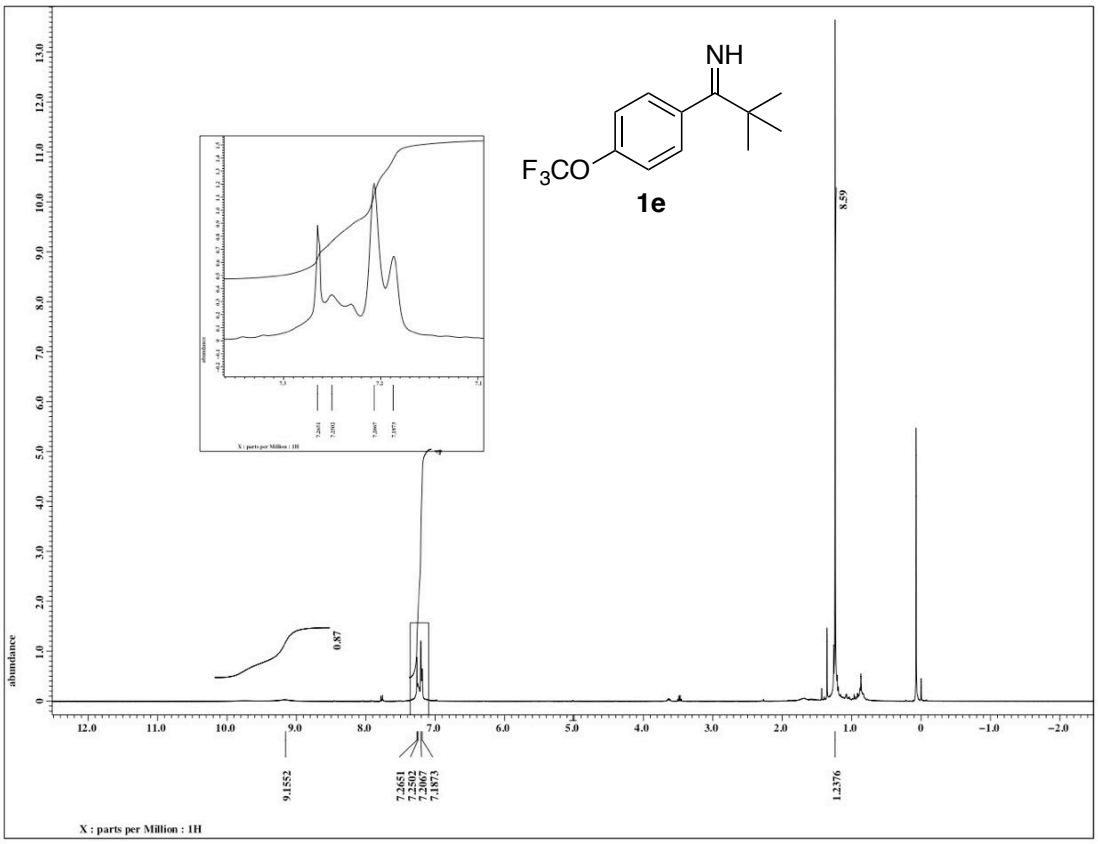
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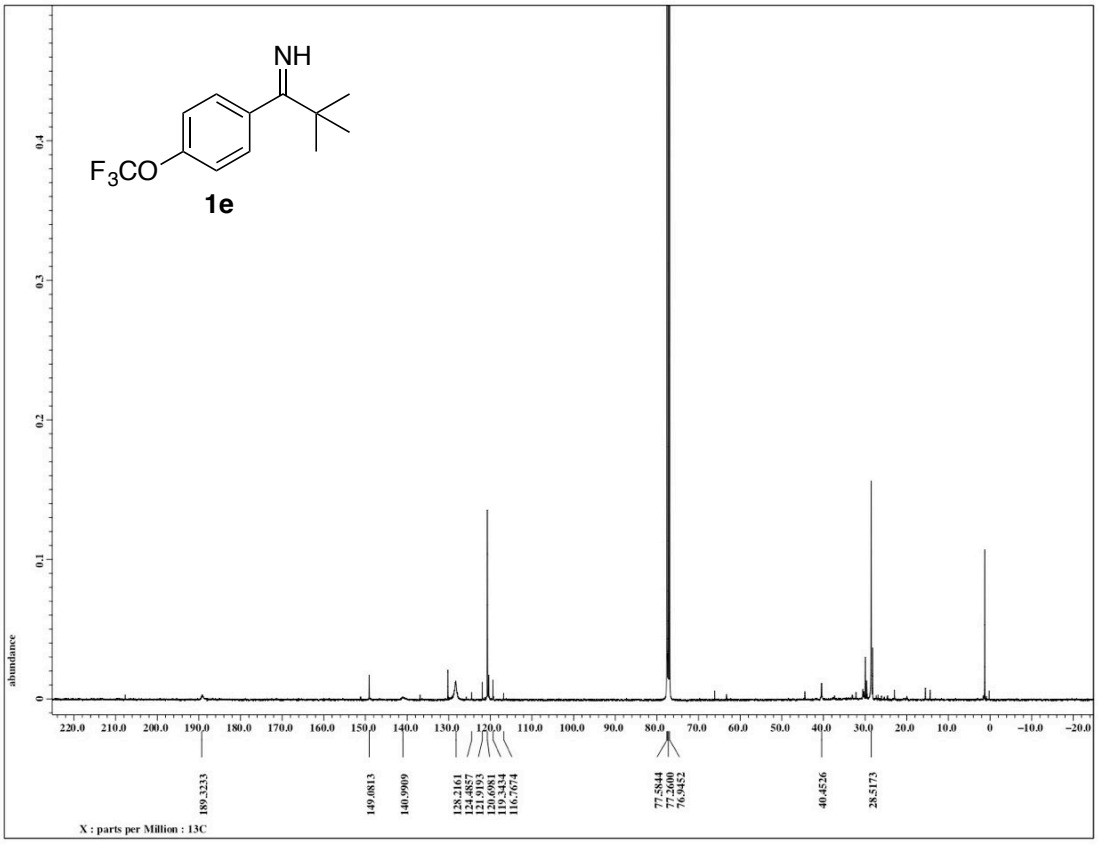
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abundance
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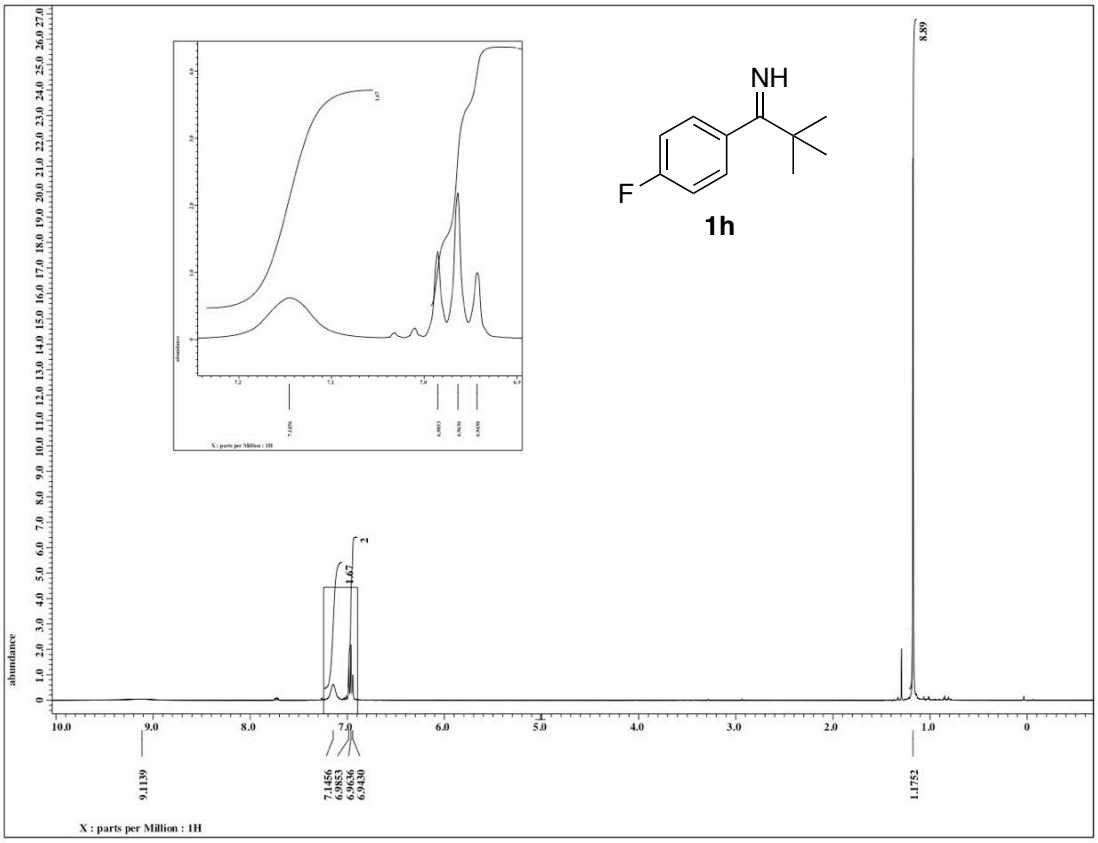
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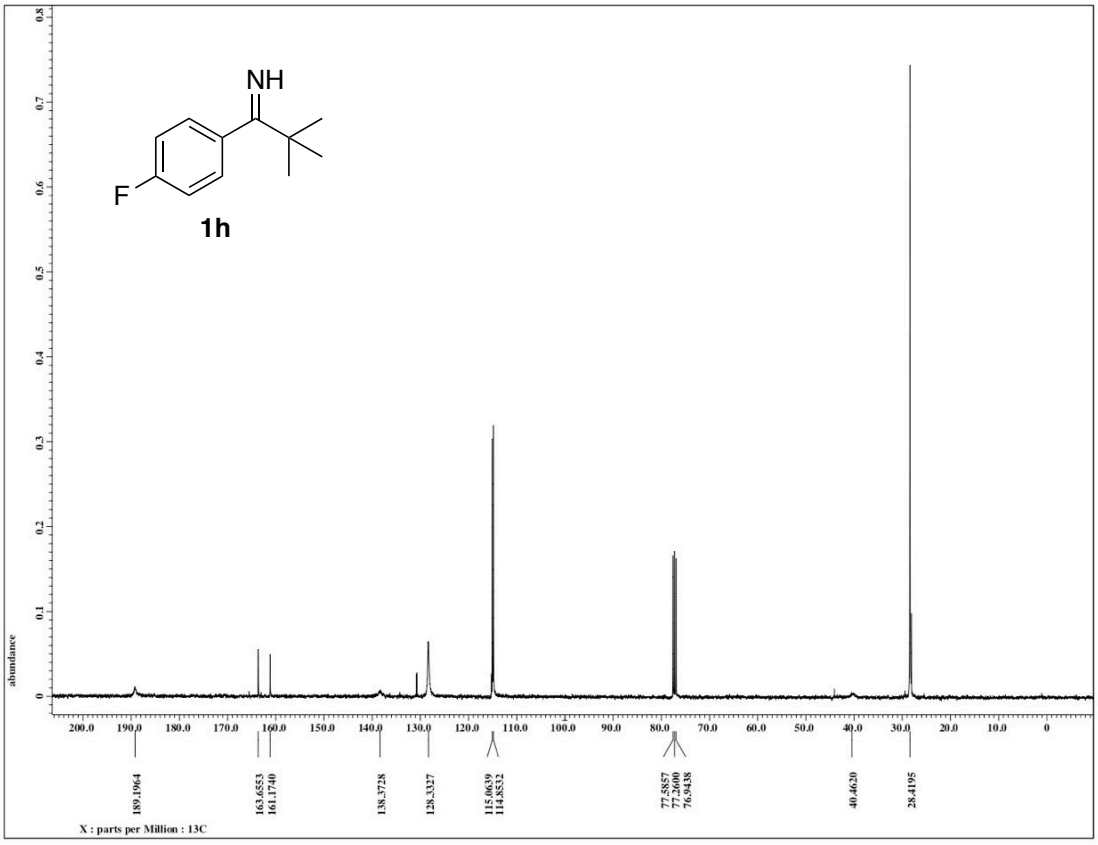
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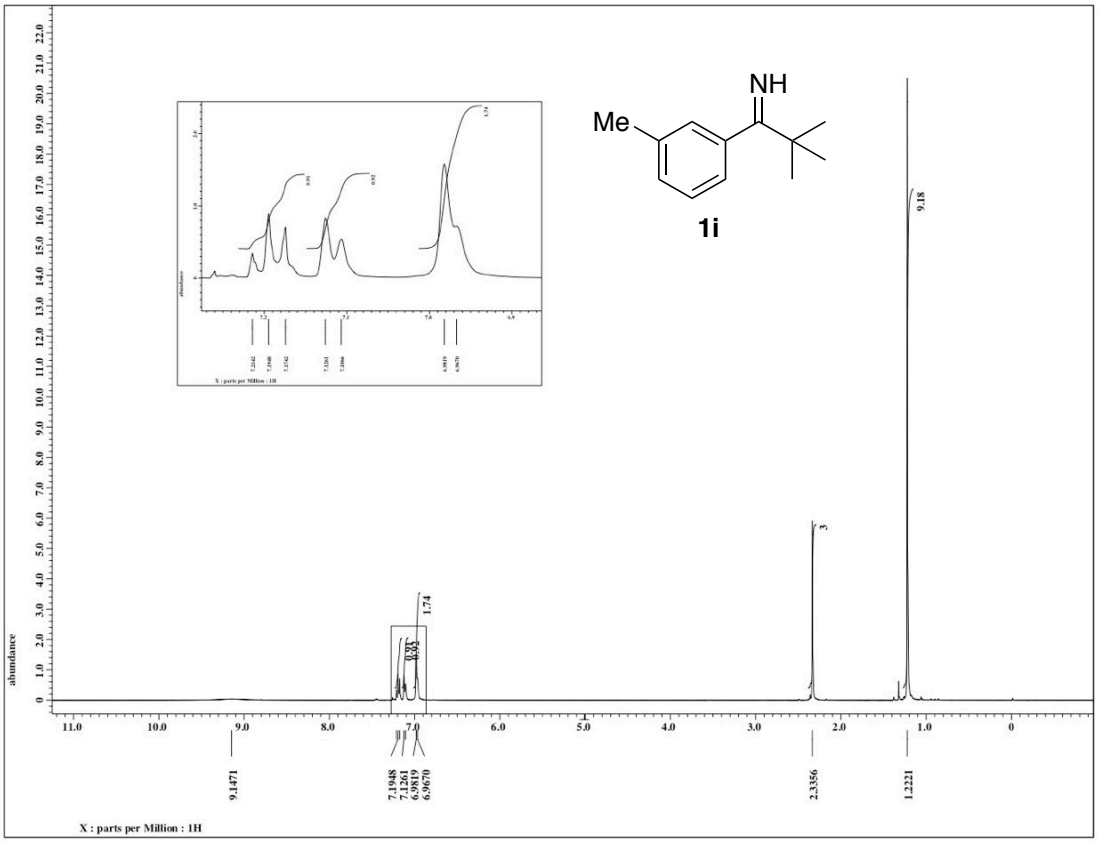
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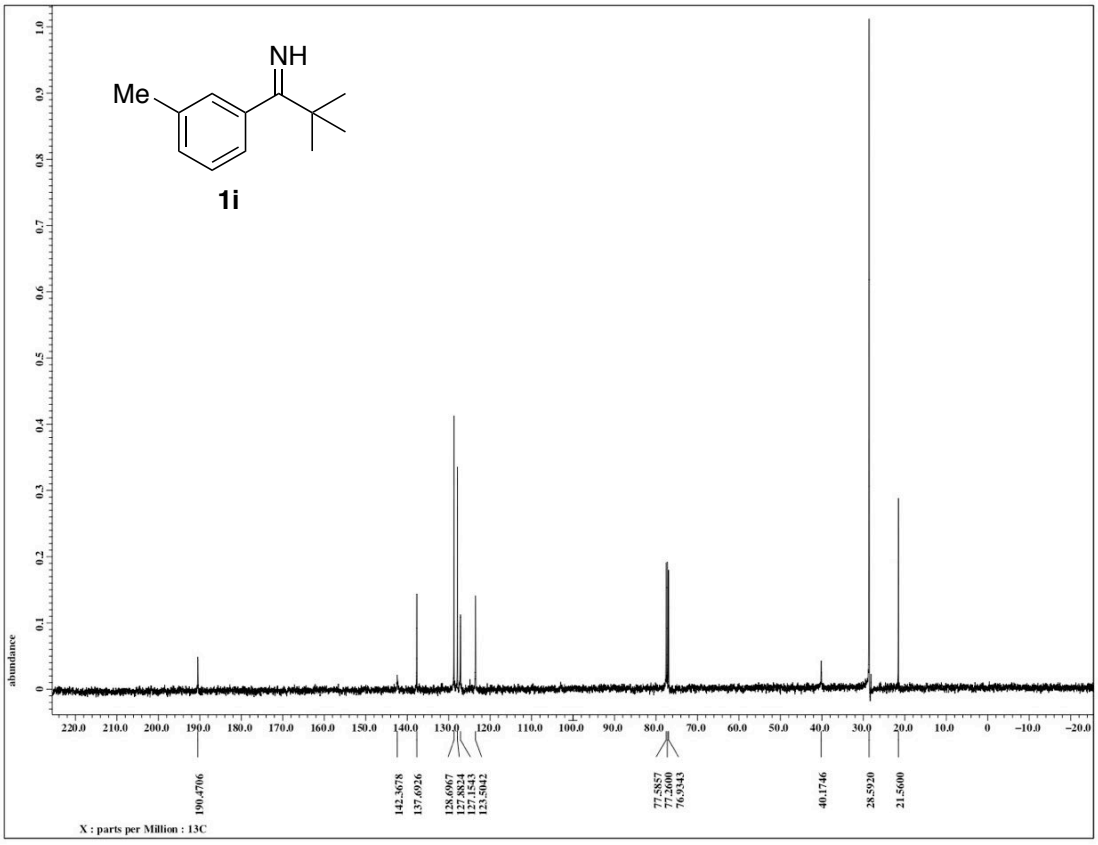
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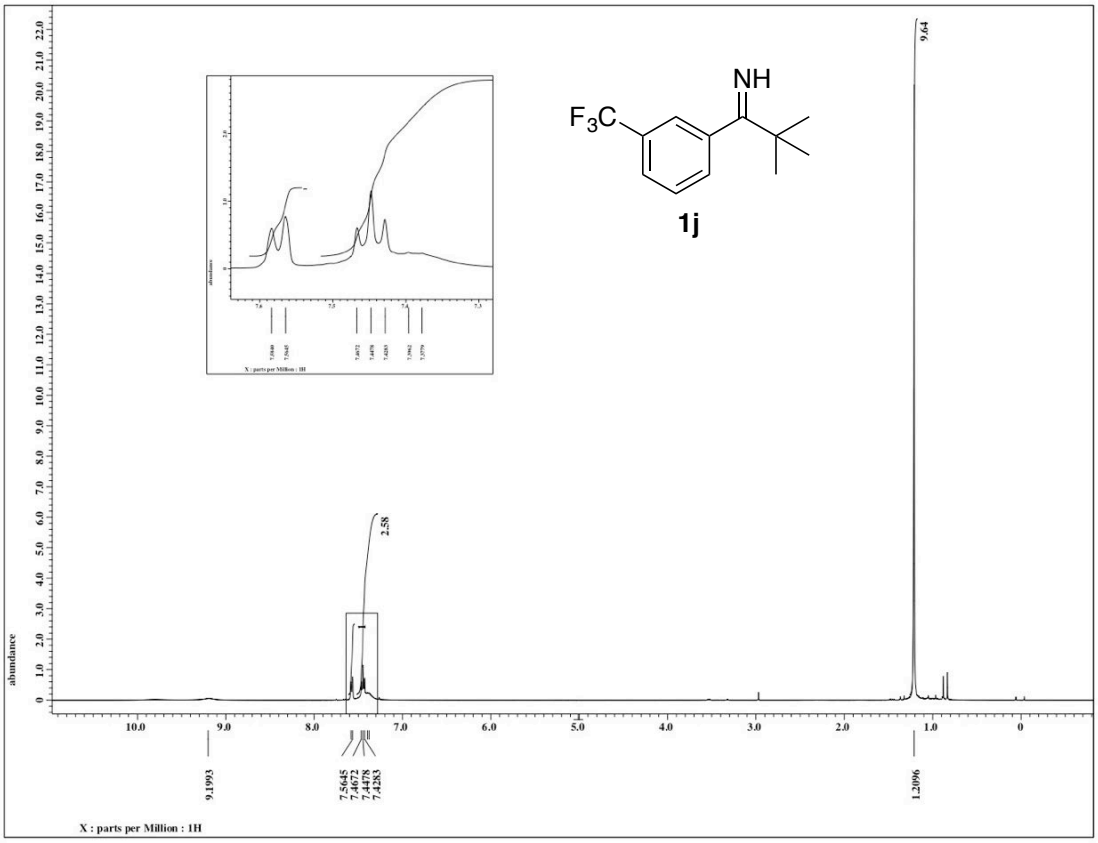
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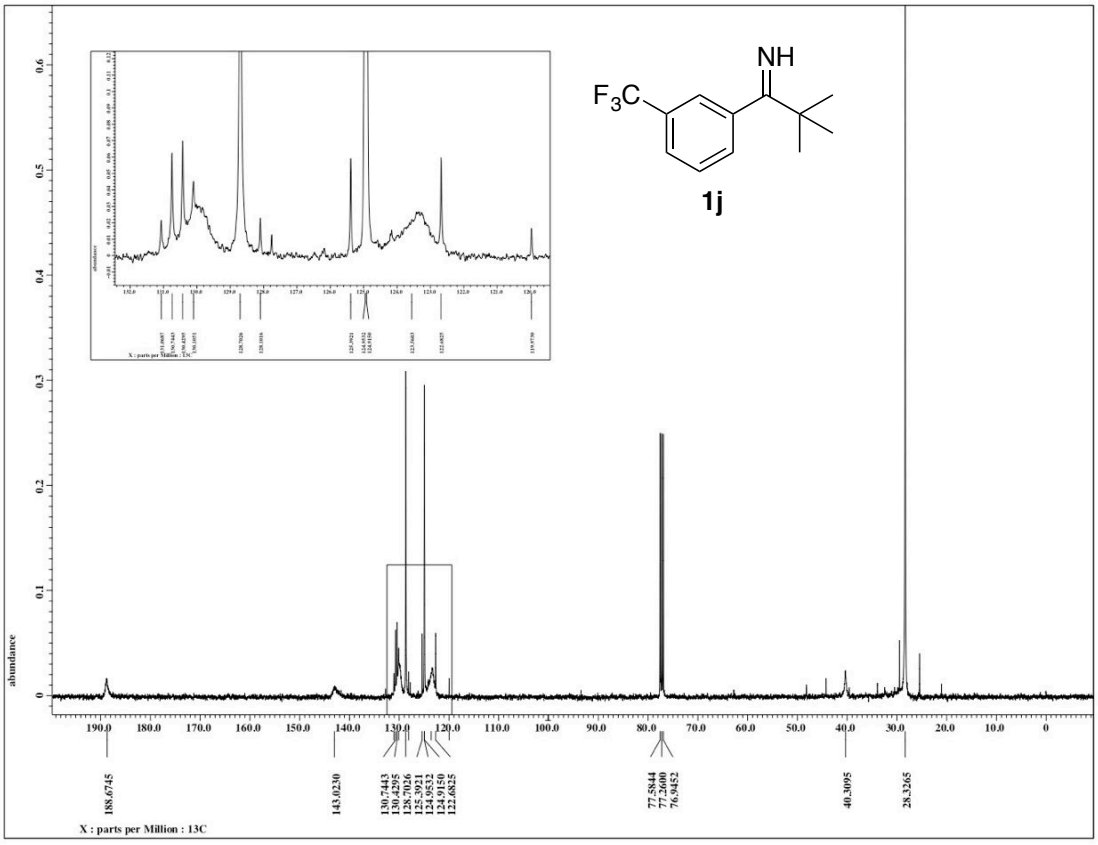
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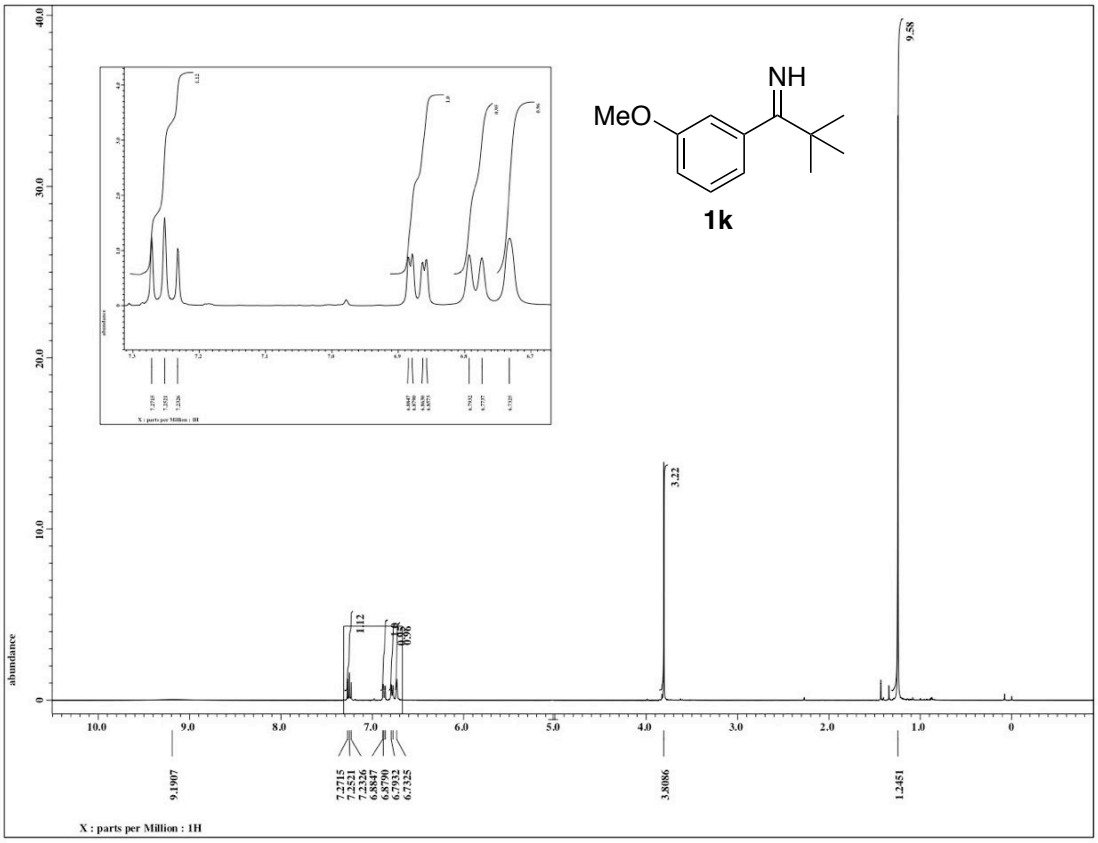
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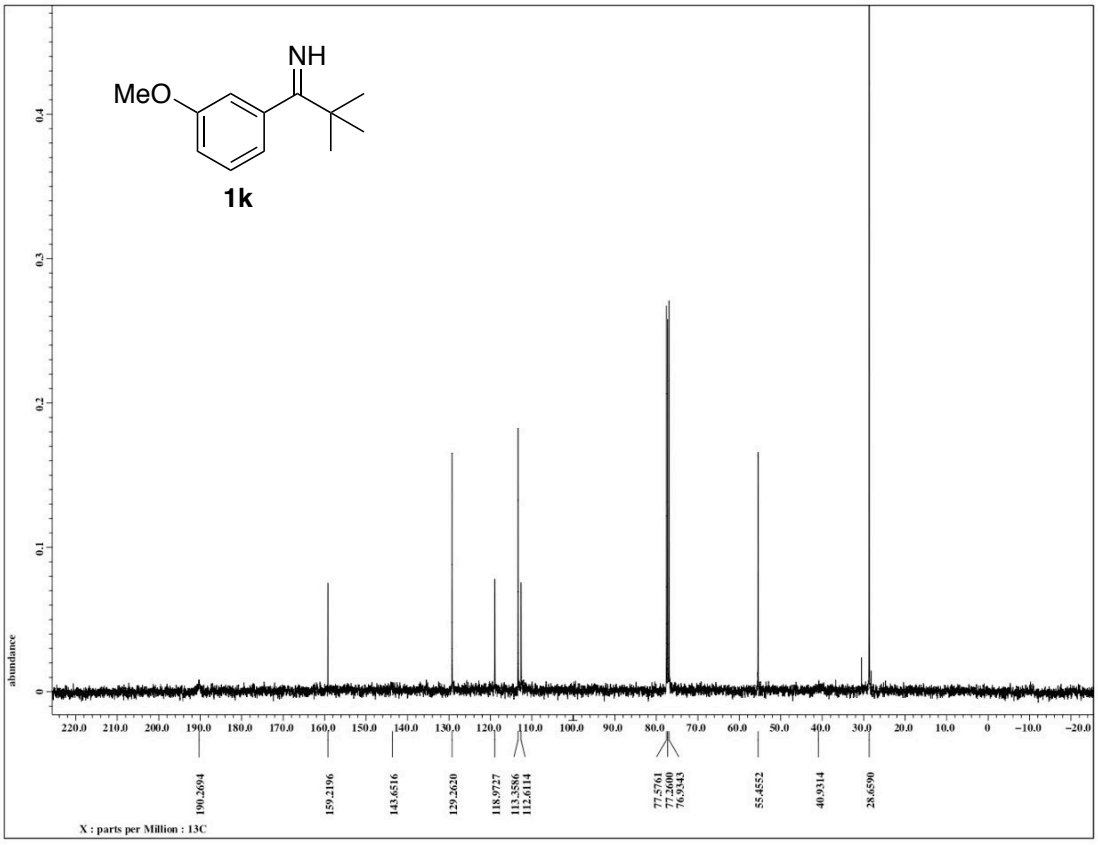
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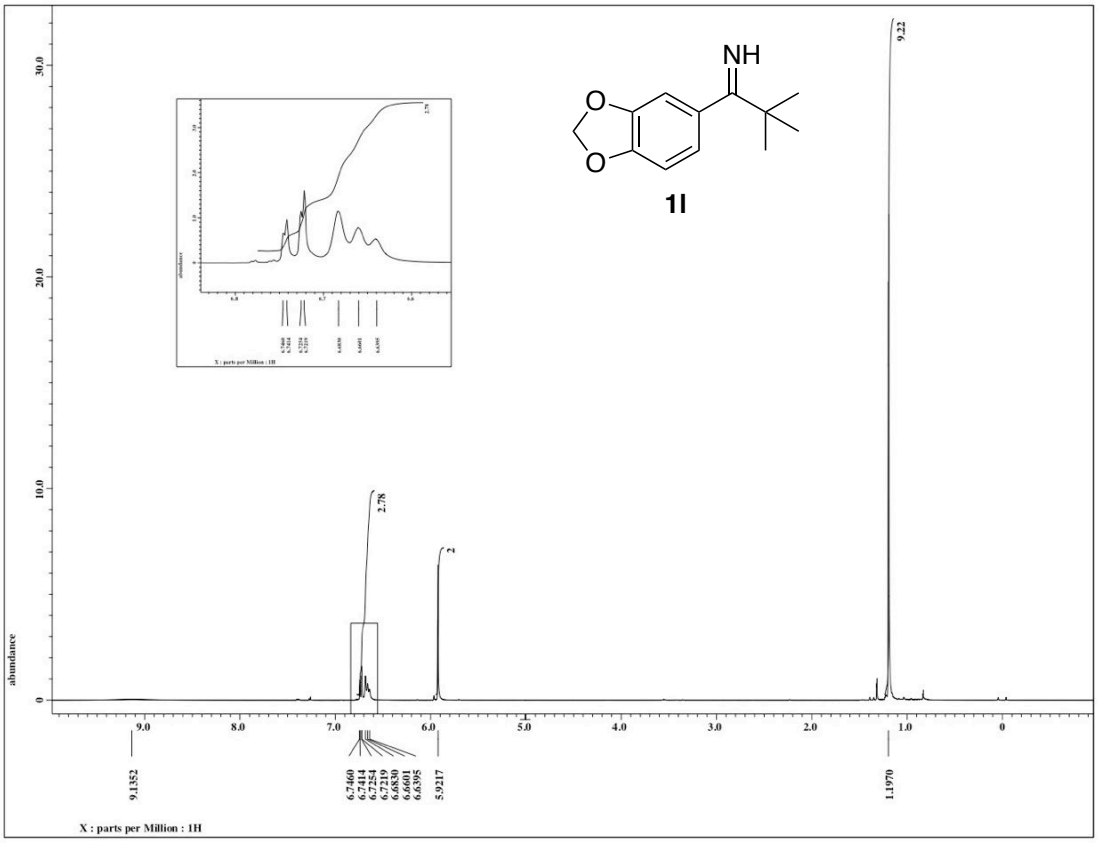

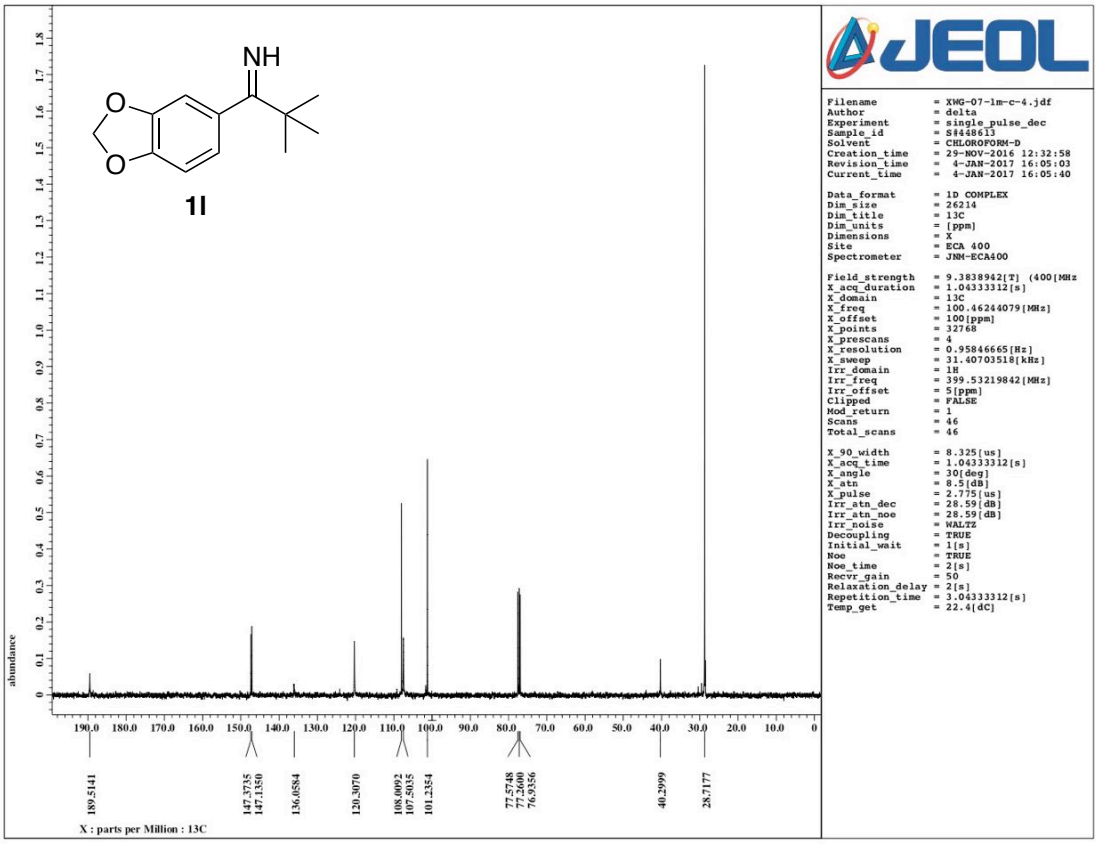

JEOL

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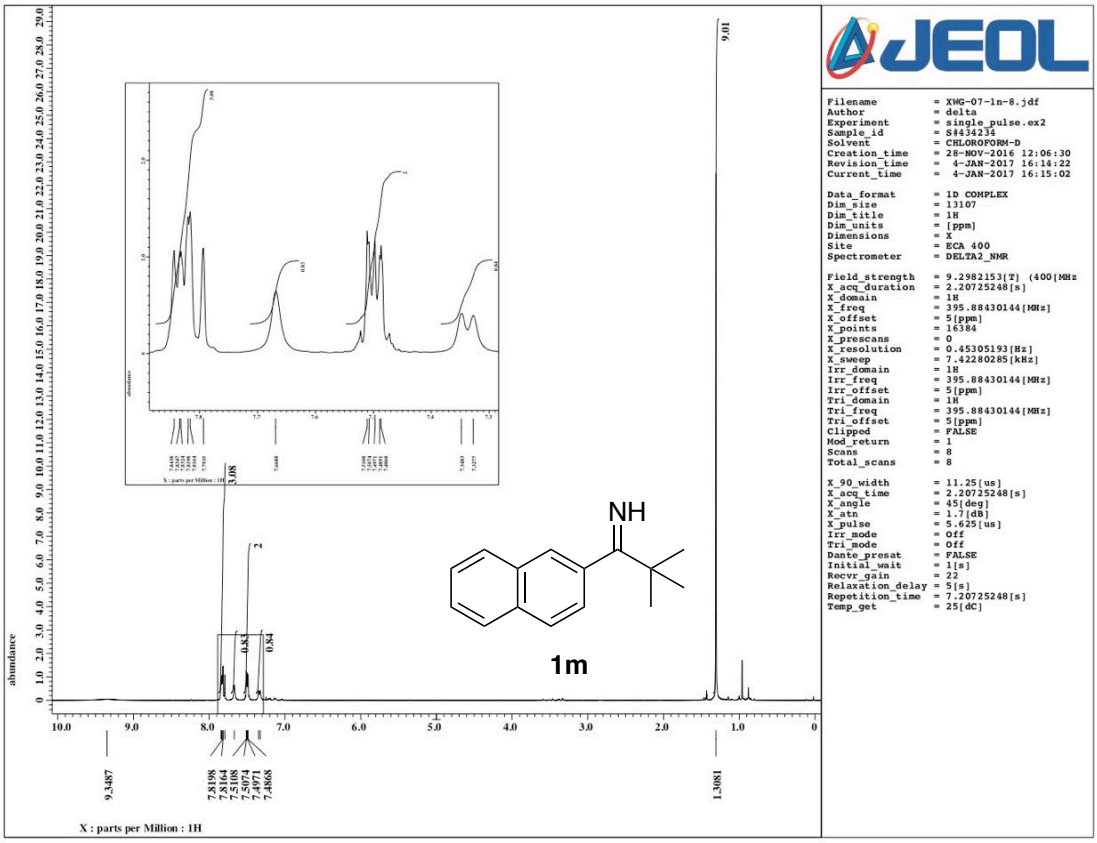


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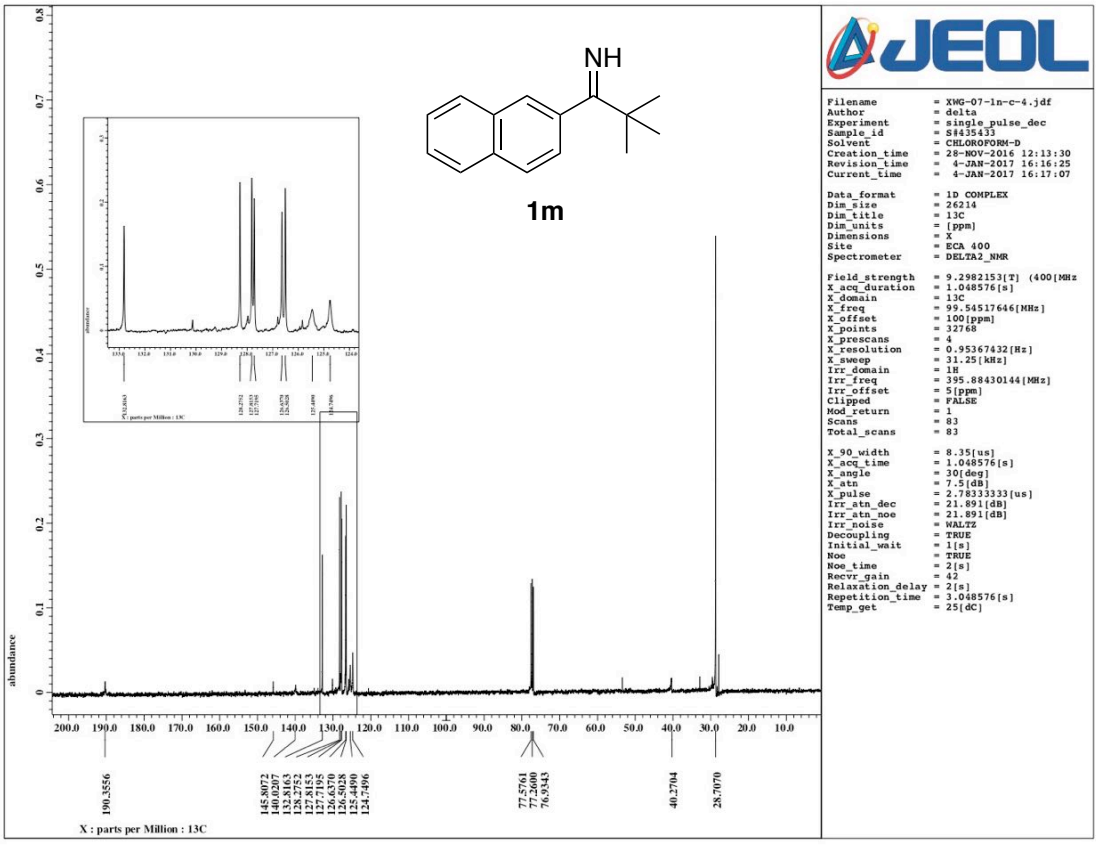


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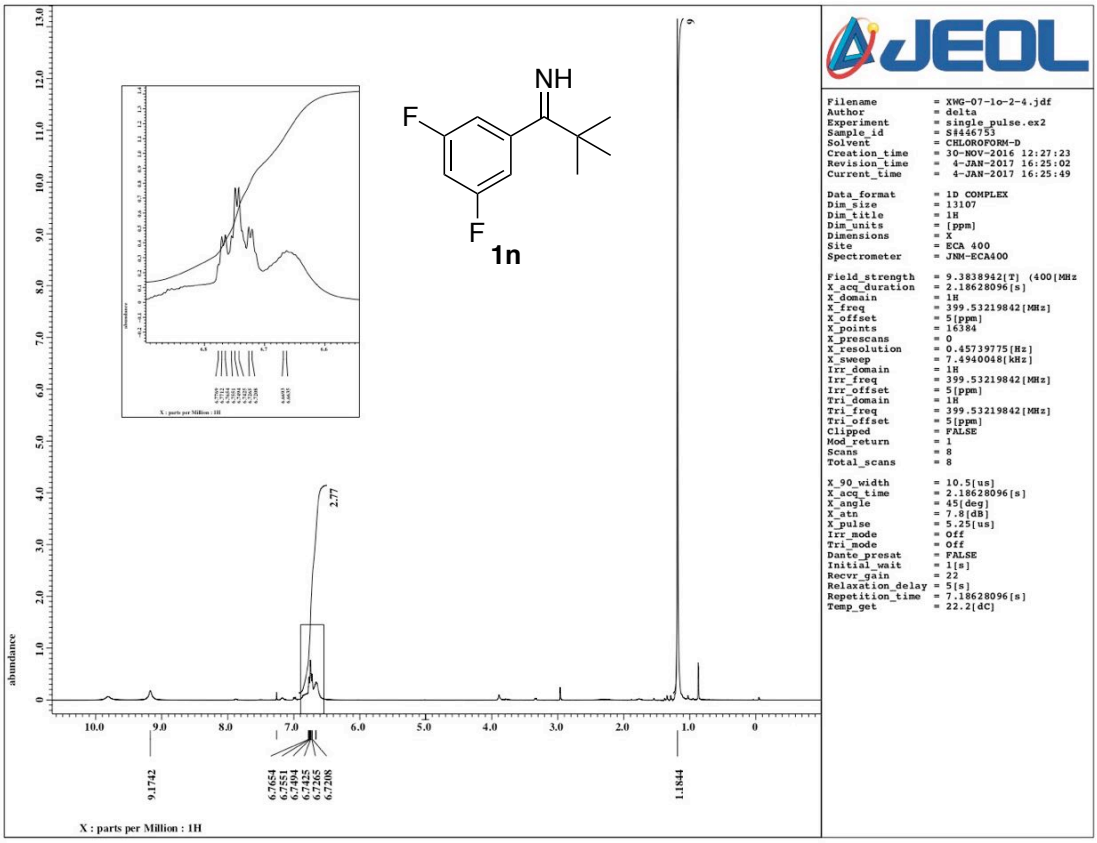

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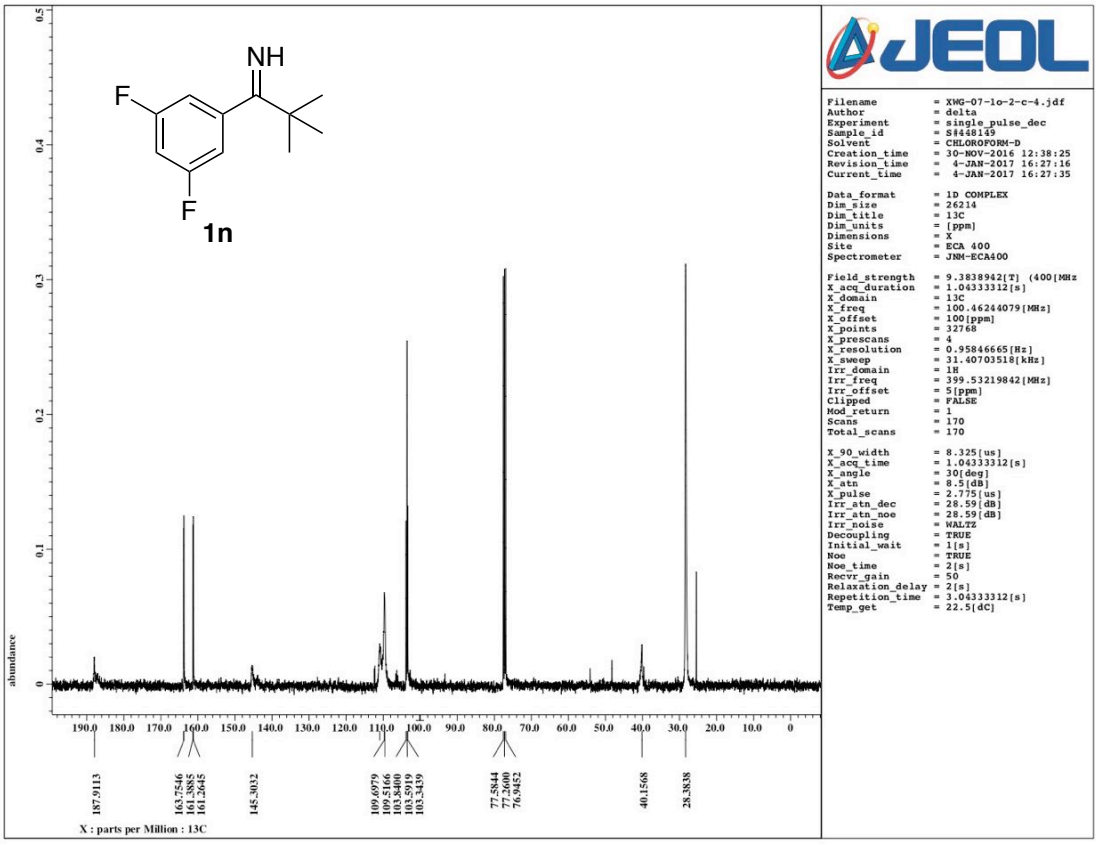
Repetition_time = 7.18628096[s]
Temp_get = 22.2[dC]

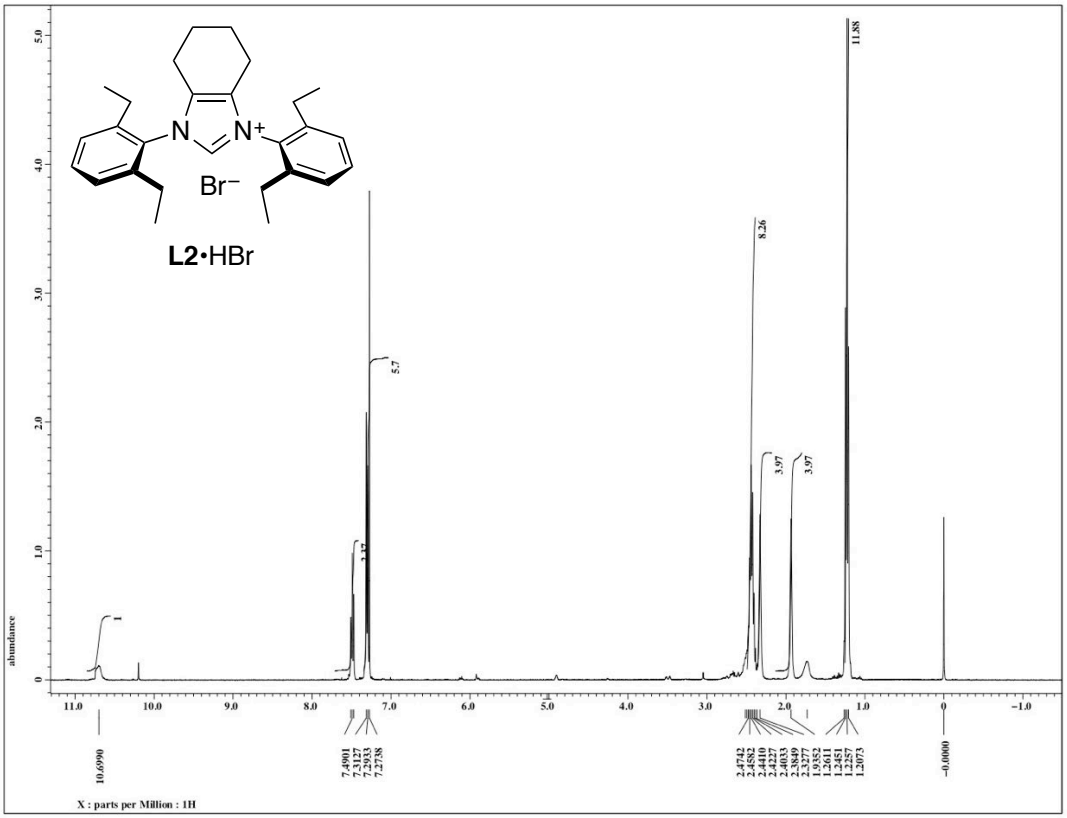


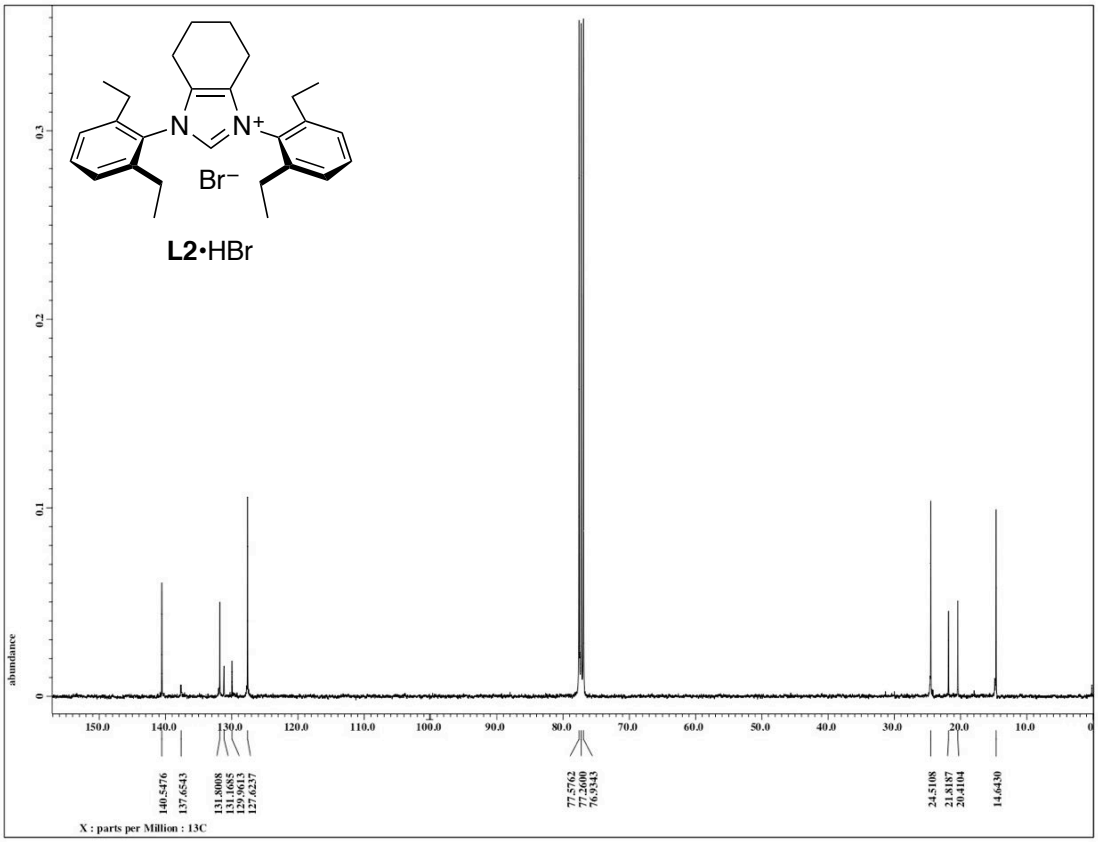
Filename = XWG-07-1o-2-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#448149
Solvent = CHLOROFORM-D
Creation_time = 30-NOV-2016 12:38:25
Revision_time = 4-JAN-2017 16:27:16
Current_time = 4-JAN-2017 16:27:35

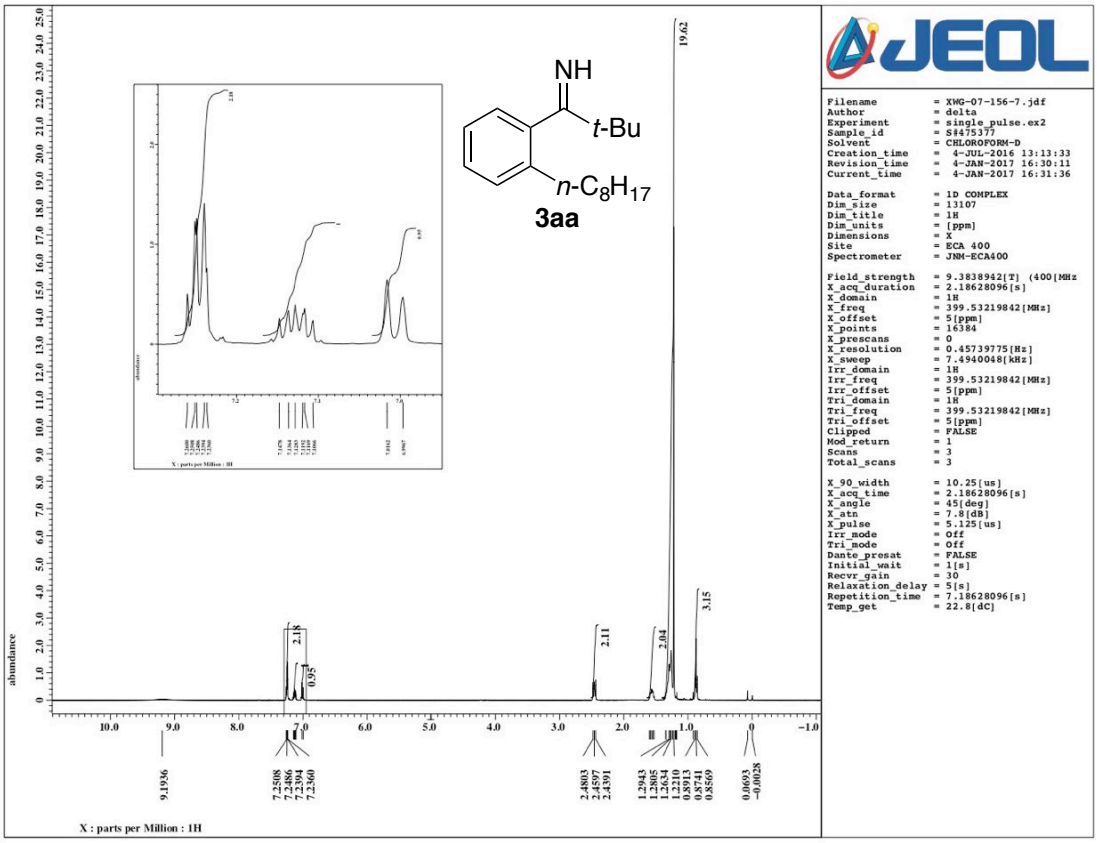
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400

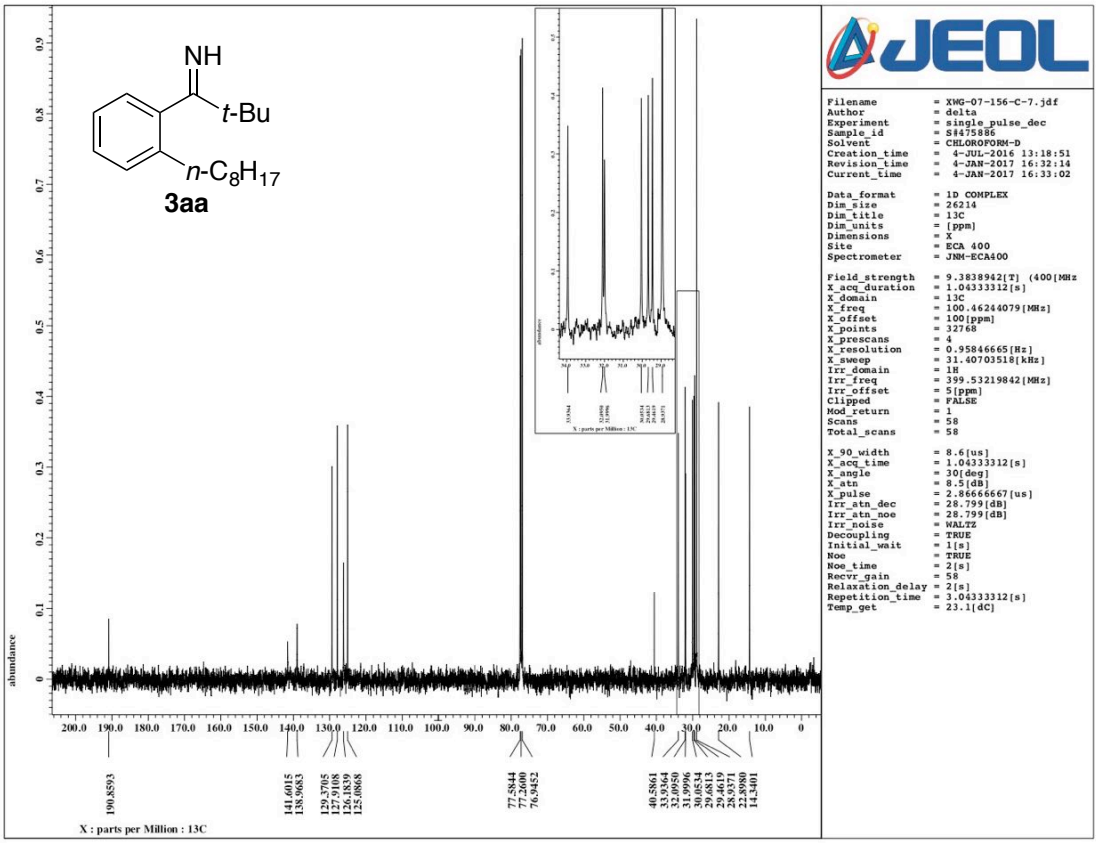
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 170
Total_scans = 170

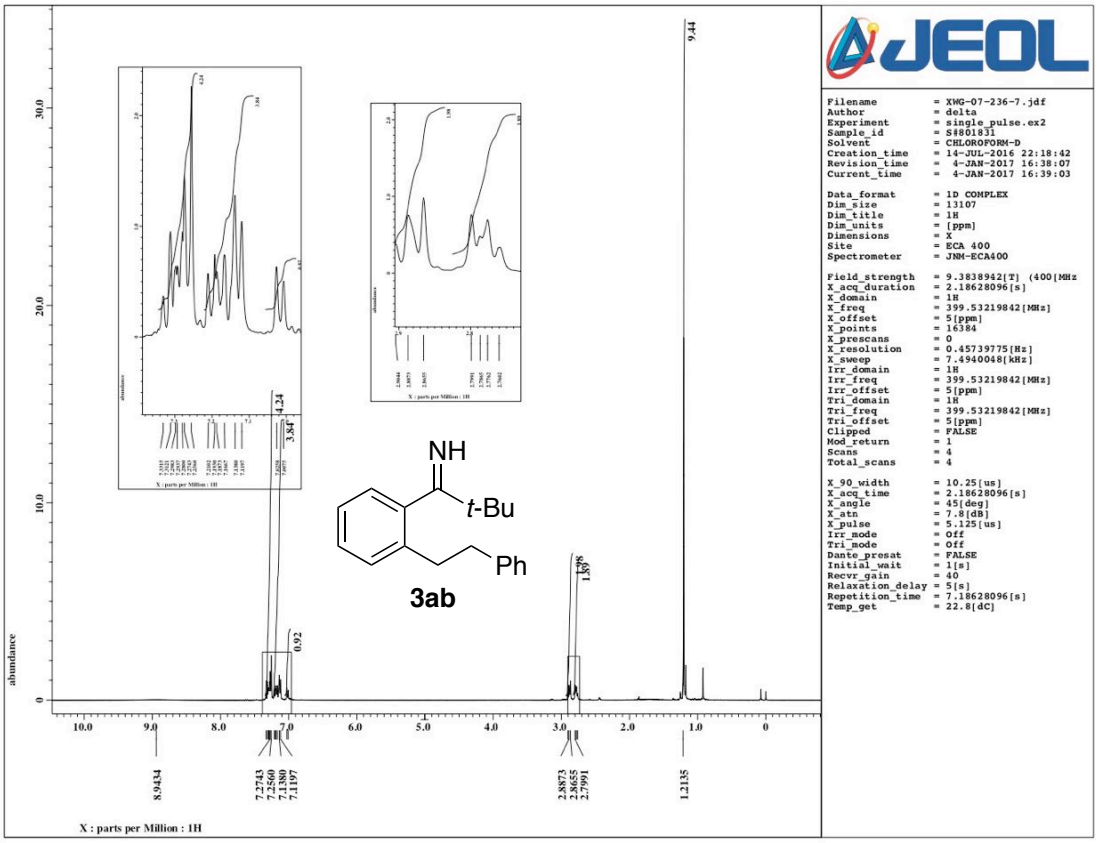
X_90_width = 8.325[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.775[us]
Irr_atn_dec = 28.59[dB]
Irr_atn_noe = 28.59[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.5[dC]


N
N+
Br−
L2•HBr
11.88
8.26
5.7
3.97
3.97
3.17
1
abundance
X : parts per Million : 1H

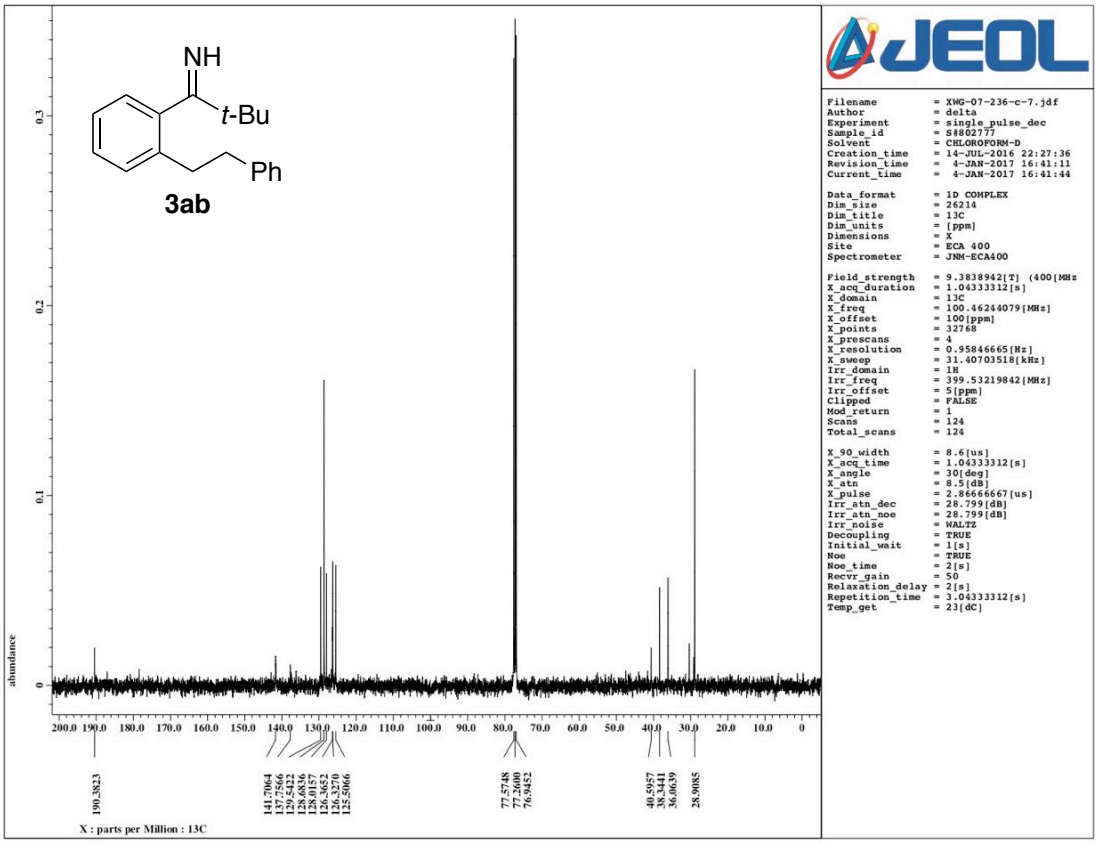

N
N+
Br−
L2•HBr
abundance
X : parts per Million : 13C


NH
t-Bu
n-C8H17
3aa
abundance
X : parts per Million : 1H

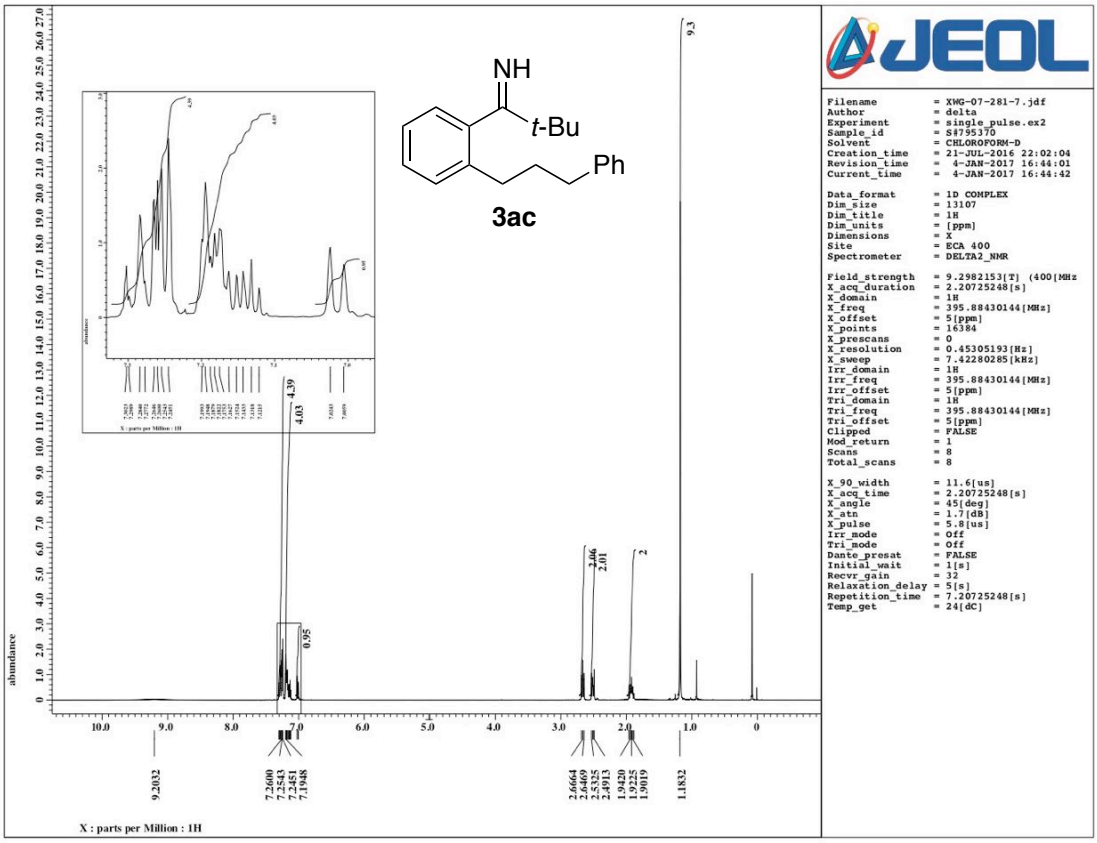

NH
t-Bu
n-C8H17
3aa
abundance
X : parts per Million : 13C

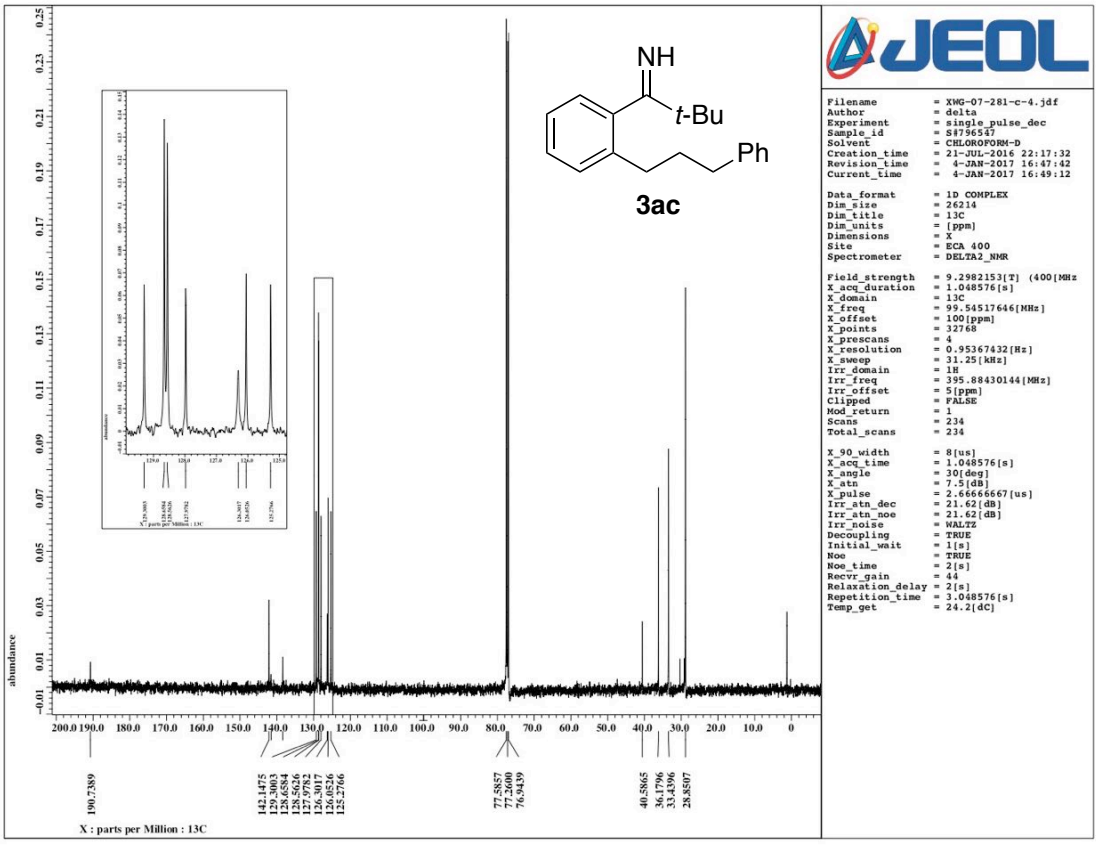


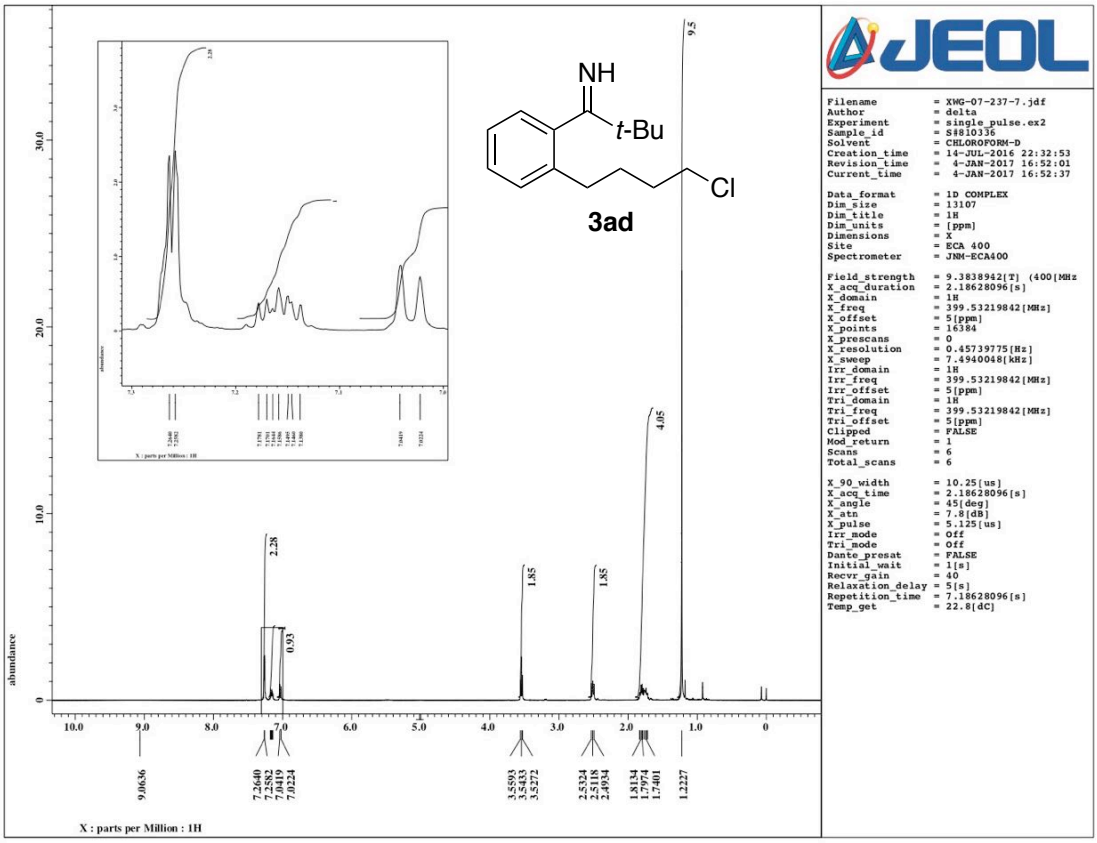

```
Filename        = XWG-07-236-7.jdf
Author          = delta
Experiment      = single_pulse.ex2
Sample_id       = S#801831
Solvent         = CHLOROFORM-D
Creation_time   = 14-JUL-2016 22:18:42
Revision_time   =  4-JAN-2017 16:38:07
Current_time    =  4-JAN-2017 16:39:03

Data_format     = 1D COMPLEX
Dim_size        = 13107
Dim_title       = 1H
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = JNM-ECA400

Field_strength  = 9.3838942[T] (400[MHz
X_acq_duration  = 2.18628096[s]
X_domain        = 1H
X_freq          = 399.53219842[MHz]
X_offset        = 5[ppm]
X_points        = 16384
X_prescans      = 0
X_resolution    = 0.45739775[Hz]
X_sweep         = 7.4940048[kHz]
Irr_domain      = 1H
Irr_freq        = 399.53219842[MHz]
Irr_offset      = 5[ppm]
Tri_domain      = 1H
Tri_freq        = 399.53219842[MHz]
Tri_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 4
Total_scans     = 4

X_90_width      = 10.25[us]
X_acq_time      = 2.18628096[s]
X_angle         = 45[deg]
X_atn           = 7.8[dB]
X_pulse         = 5.125[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 40
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get        = 22.8[dC]
```



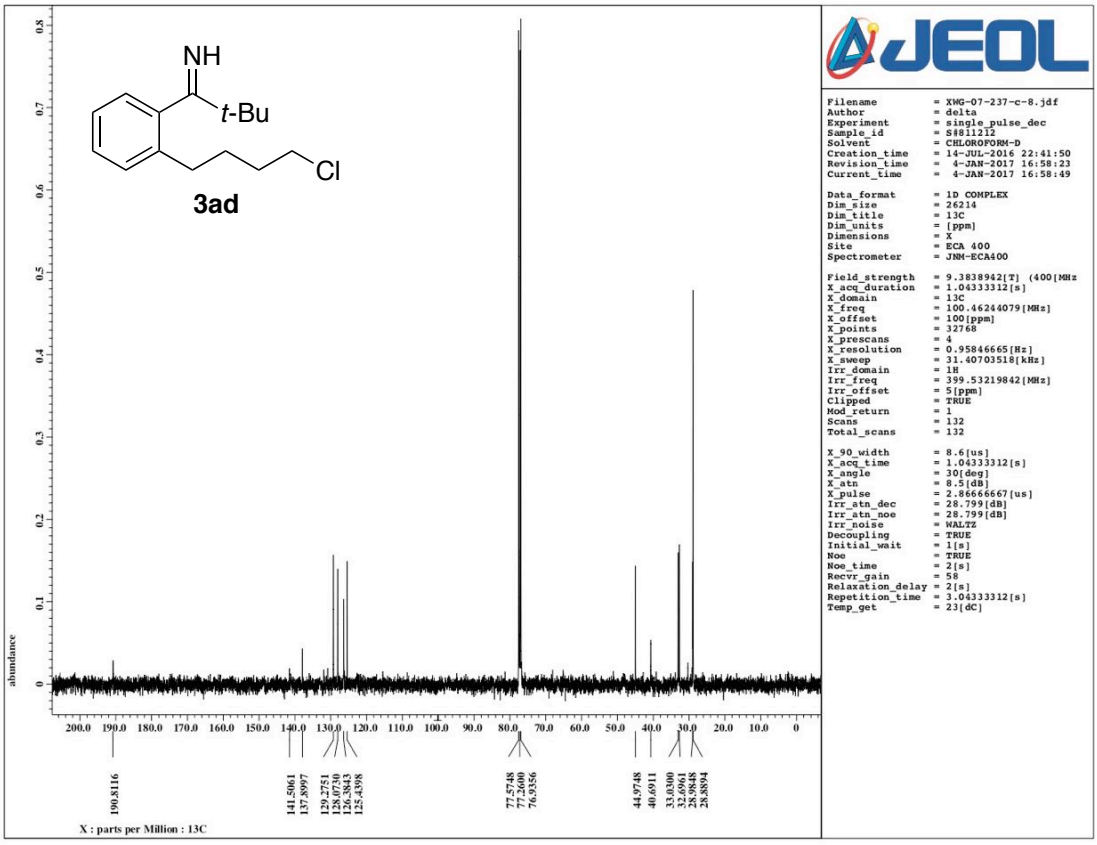

```
Filename        = XWG-07-236-c-7.jdf
Author          = delta
Experiment      = single_pulse_dec
Sample_id       = S#802777
Solvent         = CHLOROFORM-D
Creation_time   = 14-JUL-2016 22:27:36
Revision_time   =  4-JAN-2017 16:41:11
Current_time    =  4-JAN-2017 16:41:44

Data_format     = 1D COMPLEX
Dim_size        = 26214
Dim_title       = 13C
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = JNM-ECA400

Field_strength  = 9.3838942[T] (400[MHz
X_acq_duration  = 1.04333312[s]
X_domain        = 13C
X_freq          = 100.46244079[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        = 399.53219842[MHz]
Irr_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 124
Total_scans     = 124

X_90_width      = 8.6[us]
X_acq_time      = 1.04333312[s]
X_angle         = 30[deg]
X_atn           = 8.5[dB]
X_pulse         = 2.86666667[us]
Irr_atn_dec     = 28.799[dB]
Irr_atn_noe     = 28.799[dB]
Irr_noise       = WALTZ
Decoupling      = TRUE
Initial_wait    = 1[s]
Noe             = TRUE
Noe_time        = 2[s]
Recvr_gain      = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get        = 23[dC]
```


NH
t-Bu
Ph
3ac
abundance
X : parts per Million : 1H
9.2032
7.2690
7.2543
7.2451
7.1948
2.6664
2.6469
2.5325
2.4913
1.9420
1.9225
1.9019
1.1832
Filename = XWG-07-281-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#795370
Solvent = CHLOROFORM-D
Creation_time = 21-JUL-2016 22:02:04
Revision_time = 4-JAN-2017 16:44:01
Current_time = 4-JAN-2017 16:44:42
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.207725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24[dC]

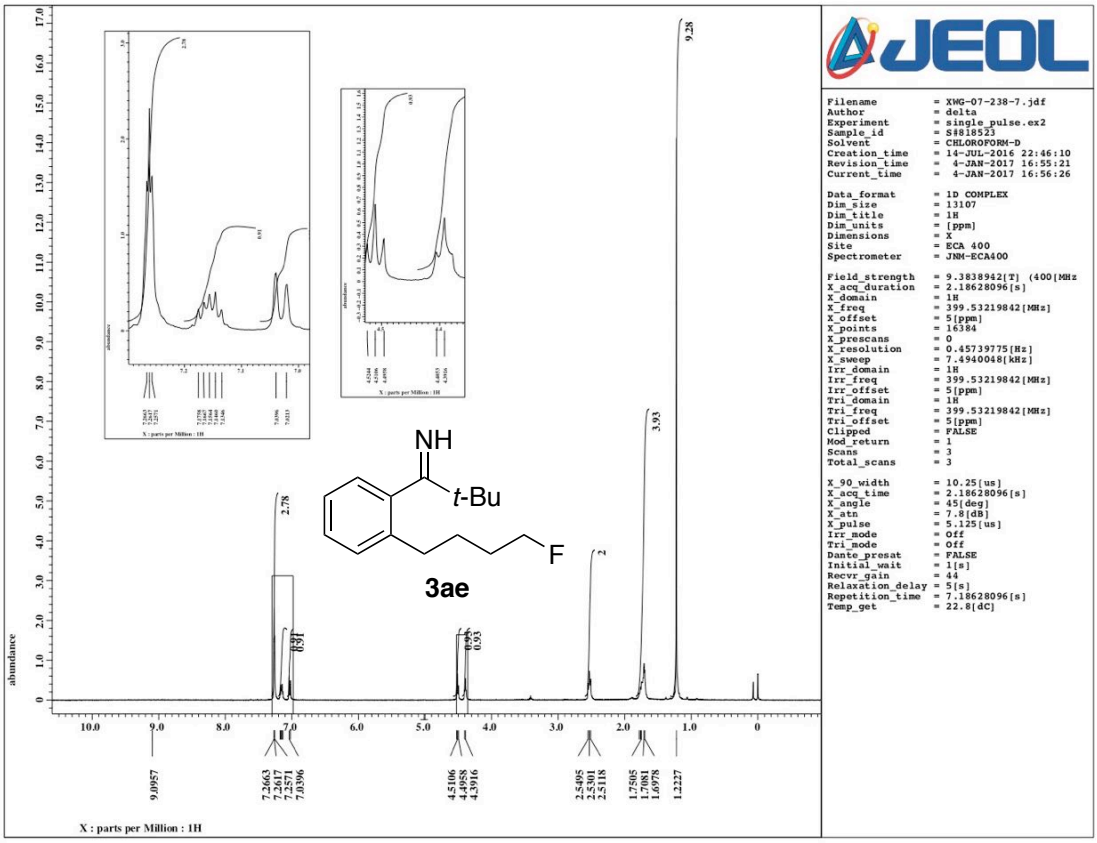

NH
t-Bu
Ph
3ac
abundance
X : parts per Million : 13C
190.7389
142.1475
129.3003
128.5624
127.9782
126.3017
126.0526
125.2766
77.5857
77.2690
76.9439
40.5865
36.1796
33.4396
28.8507
Filename = XWG-07-281-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#796547
Solvent = CHLOROFORM-D
Creation_time = 21-JUL-2016 22:17:32
Revision_time = 4-JAN-2017 16:47:42
Current_time = 4-JAN-2017 16:49:12
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 234
Total_scans = 234
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.2[dC]

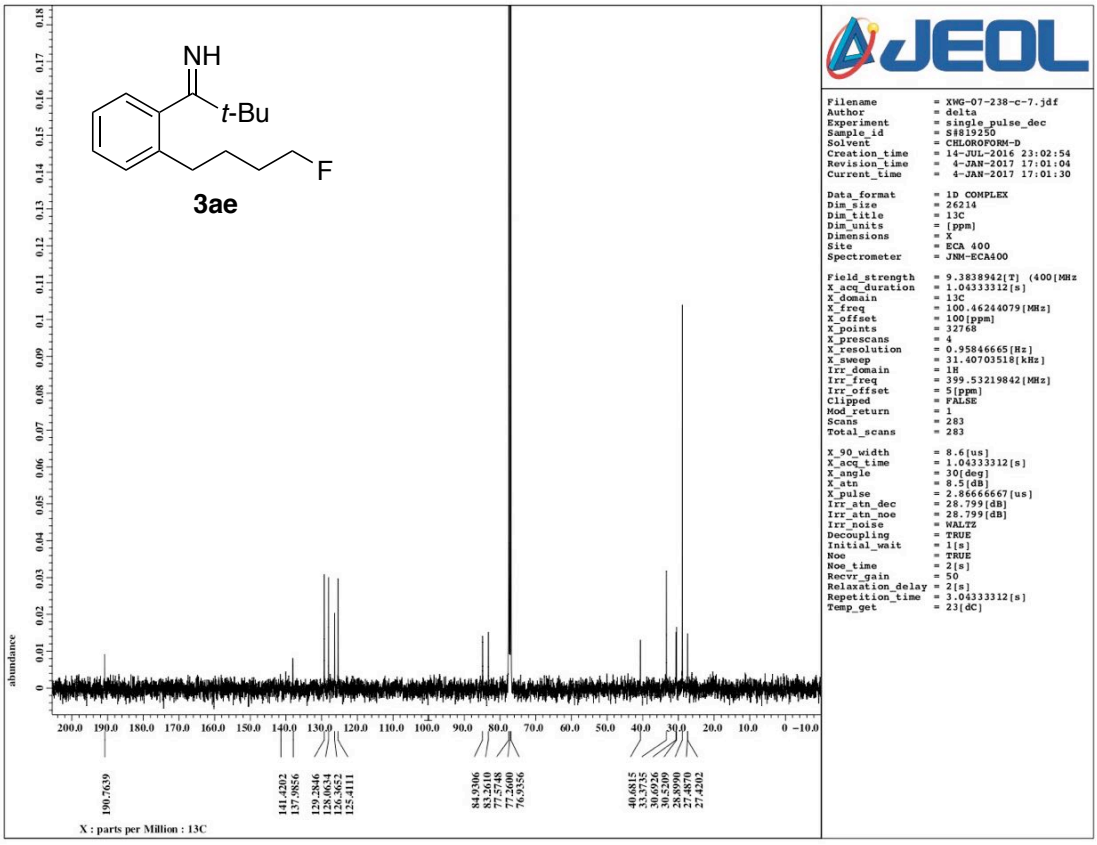


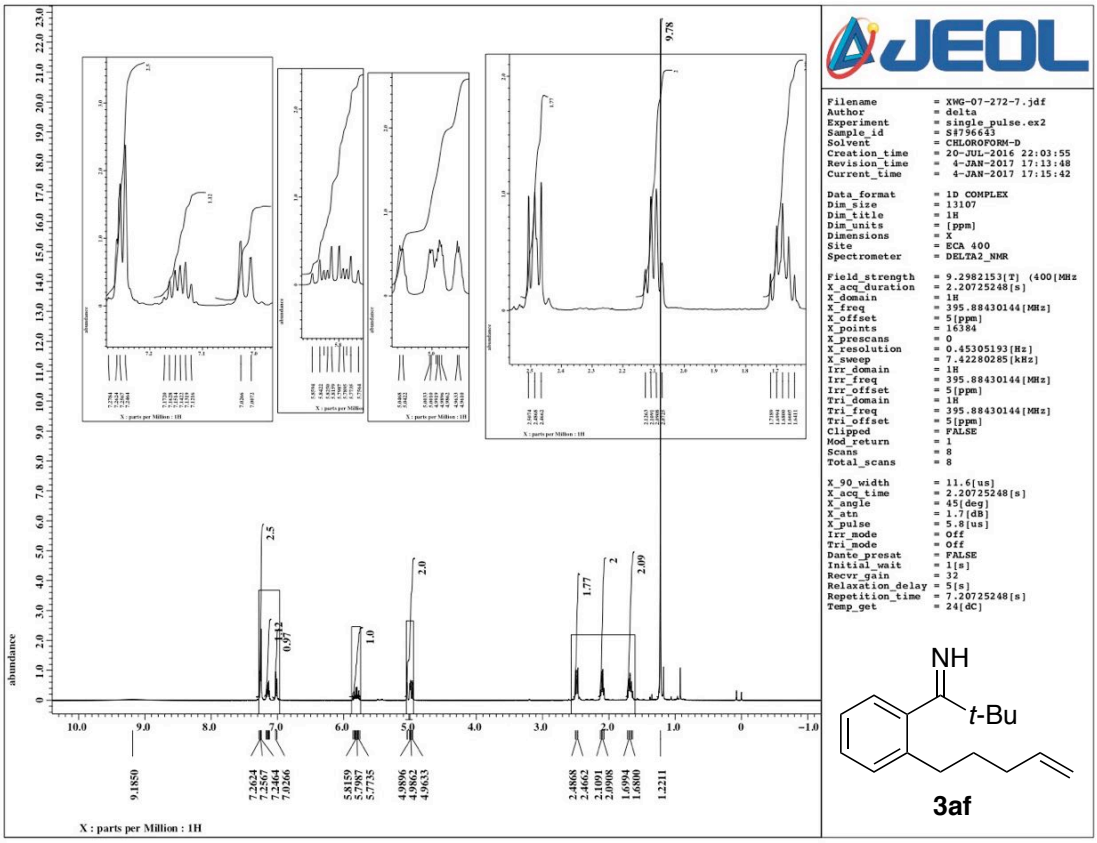

```
Filename          = XWG-07-237-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#810336
Solvent           = CHLOROFORM-D
Creation_time     = 14-JUL-2016 22:32:53
Revision_time     =  4-JAN-2017 16:52:01
Current_time      =  4-JAN-2017 16:52:37

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 2.18628096[s]
X_domain          = 1H
X_freq            = 399.53219842[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45739775[Hz]
X_sweep           = 7.4940048[kHz]
Irr_domain        = 1H
Irr_freq          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.53219842[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 6
Total_scans       = 6

X_90_width        = 10.25[us]
X_acq_time        = 2.18628096[s]
X_angle           = 45[deg]
X_atn             = 7.8[dB]
X_pulse           = 5.125[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 7.18628096[s]
Temp_get          = 22.8[dC]
```




```
Filename          = XWG-07-237-c-8.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#811212
Solvent           = CHLOROFORM-D
Creation_time     = 14-JUL-2016 22:41:50
Revision_time     =  4-JAN-2017 16:58:23
Current_time      =  4-JAN-2017 16:58:49

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.46244079[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          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 132
Total_scans       = 132

X_90_width        = 8.6[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 8.5[dB]
X_pulse           = 2.86666667[us]
Irr_atn_dec       = 28.799[dB]
Irr_atn_noe       = 28.799[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 23[dC]
```


NH
t-Bu
F
3ae
abundance
X : parts per Million : 1H
9.0957
7.2663
7.2617
7.2571
7.0396
4.5106
4.4958
4.3916
2.5095
2.5001
2.5118
1.7505
1.7081
1.6978
1.2227
Filename = XWG-07-238-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#818523
Solvent = CHLOROFORM-D
Creation_time = 14-JUL-2016 22:46:10
Revision_time = 4-JAN-2017 16:55:21
Current_time = 4-JAN-2017 16:56:26
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3
Total_scans = 3
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.8[dC]


NH
t-Bu
F
3ae
abundance
X : parts per Million : 13C
190.7639
141.4202
137.9856
129.2846
128.0634
126.3455
125.4111
84.9306
83.3610
77.5748
77.2600
76.8586
40.6815
33.3735
30.6926
30.5209
25.4870
25.4690
27.4202
Filename = XWG-07-238-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#819250
Solvent = CHLOROFORM-D
Creation_time = 14-JUL-2016 23:02:54
Revision_time = 4-JAN-2017 17:01:04
Current_time = 4-JAN-2017 17:01:30
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 283
Total_scans = 283
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 23[dC]

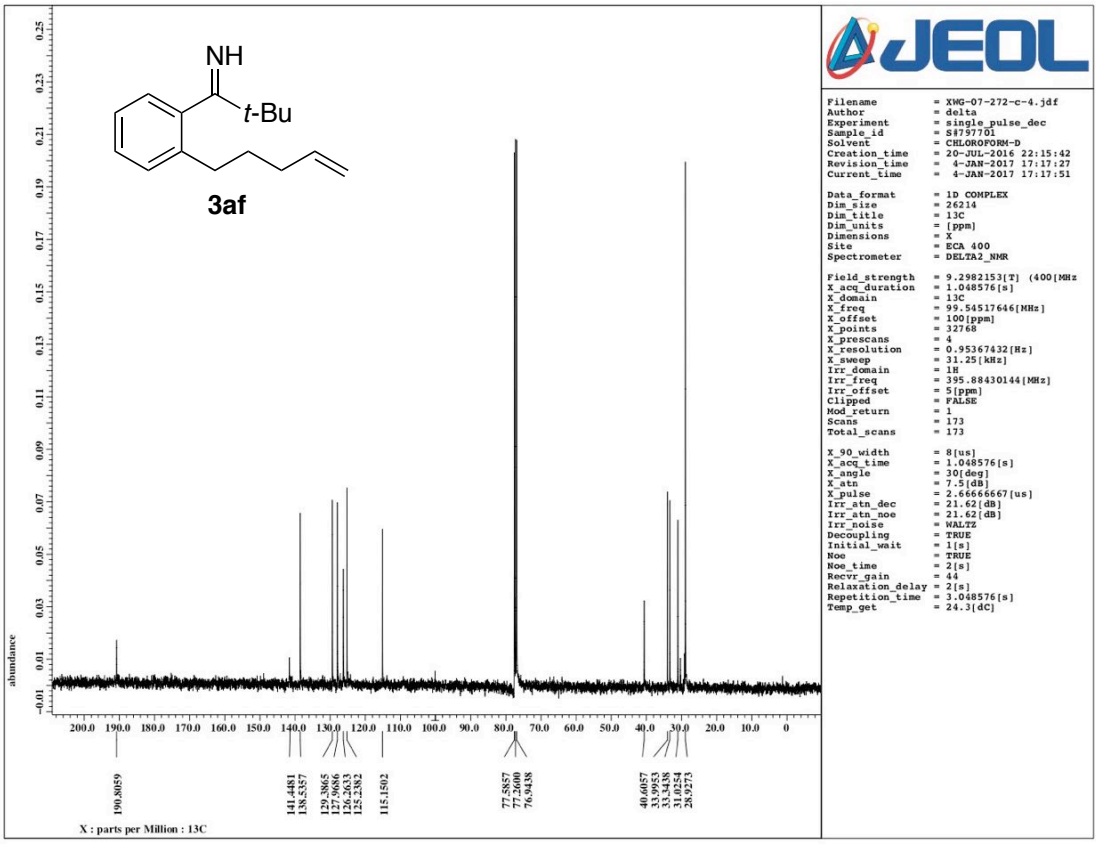


Filename = XWG-07-272-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#796643
Solvent = CHLOROFORM-D
Creation_time = 20-JUL-2016 22:03:55
Revision_time = 4-JAN-2017 17:13:48
Current_time = 4-JAN-2017 17:15:42

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR

Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24[dC]

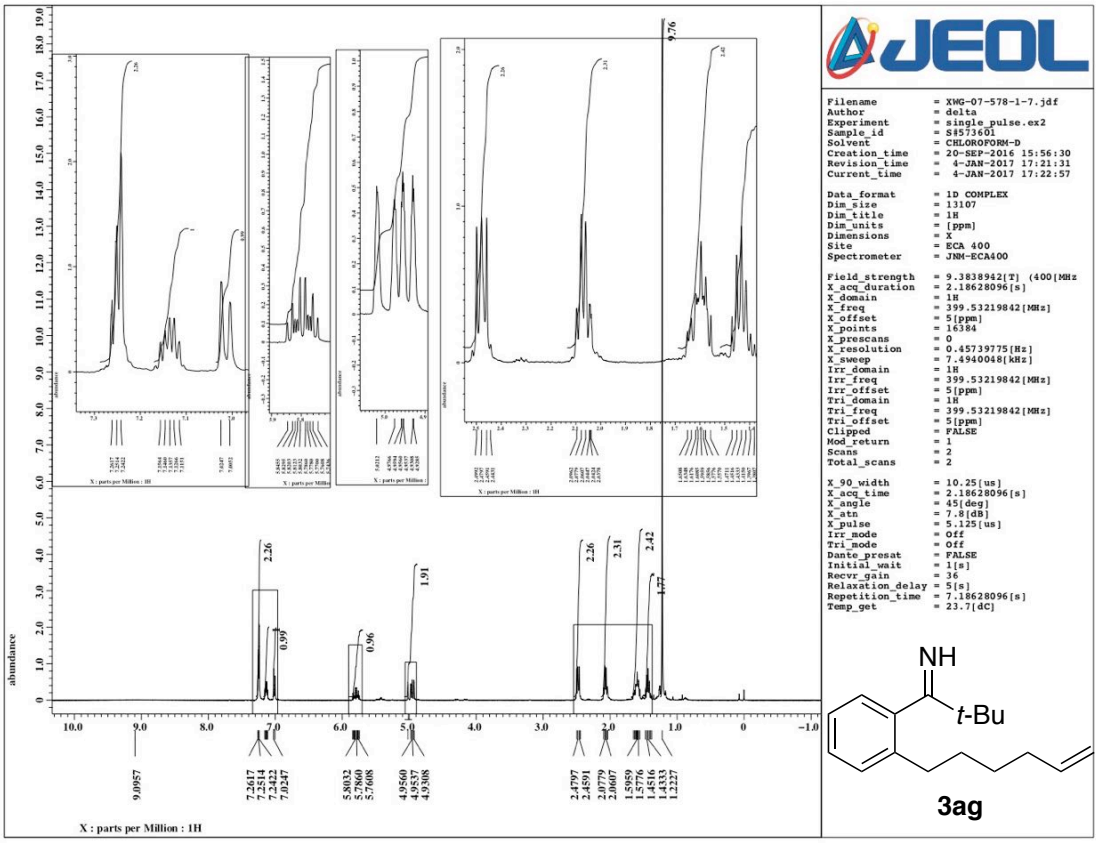


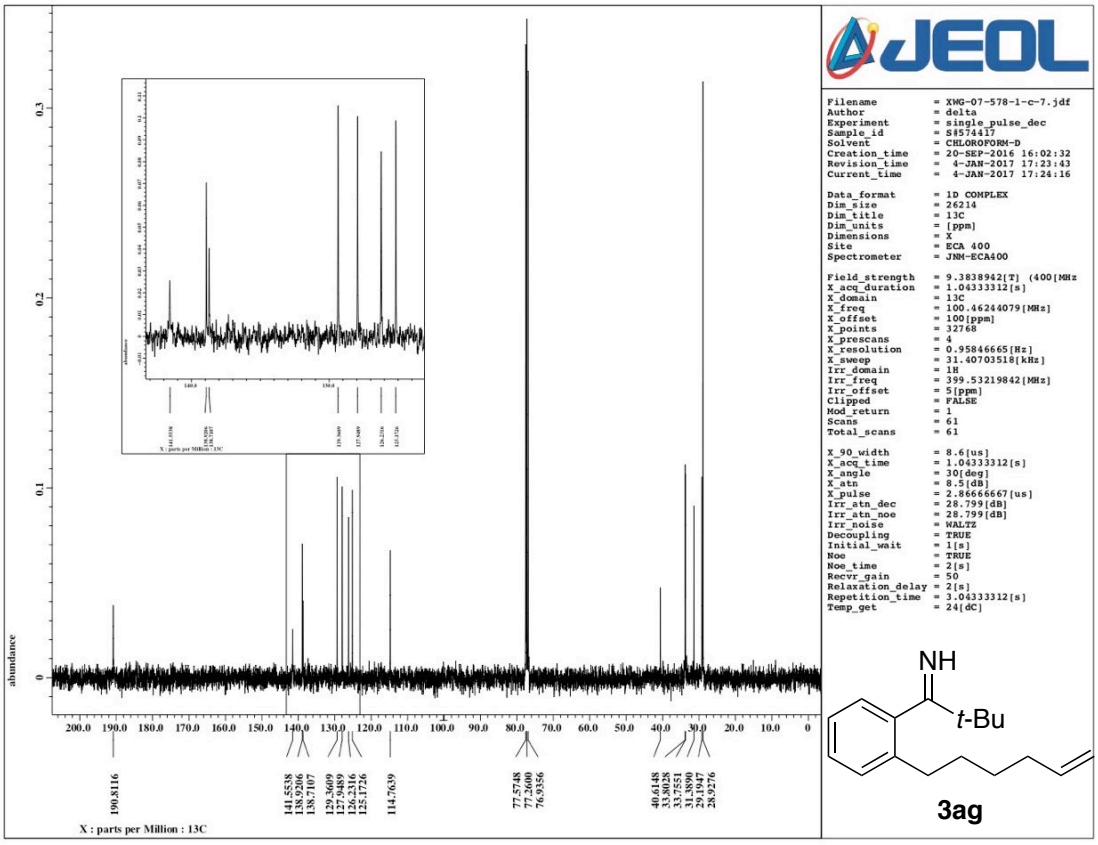
Filename = XWG-07-272-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#797701
Solvent = CHLOROFORM-D
Creation_time = 20-JUL-2016 22:15:42
Revision_time = 4-JAN-2017 17:17:27
Current_time = 4-JAN-2017 17:17:51

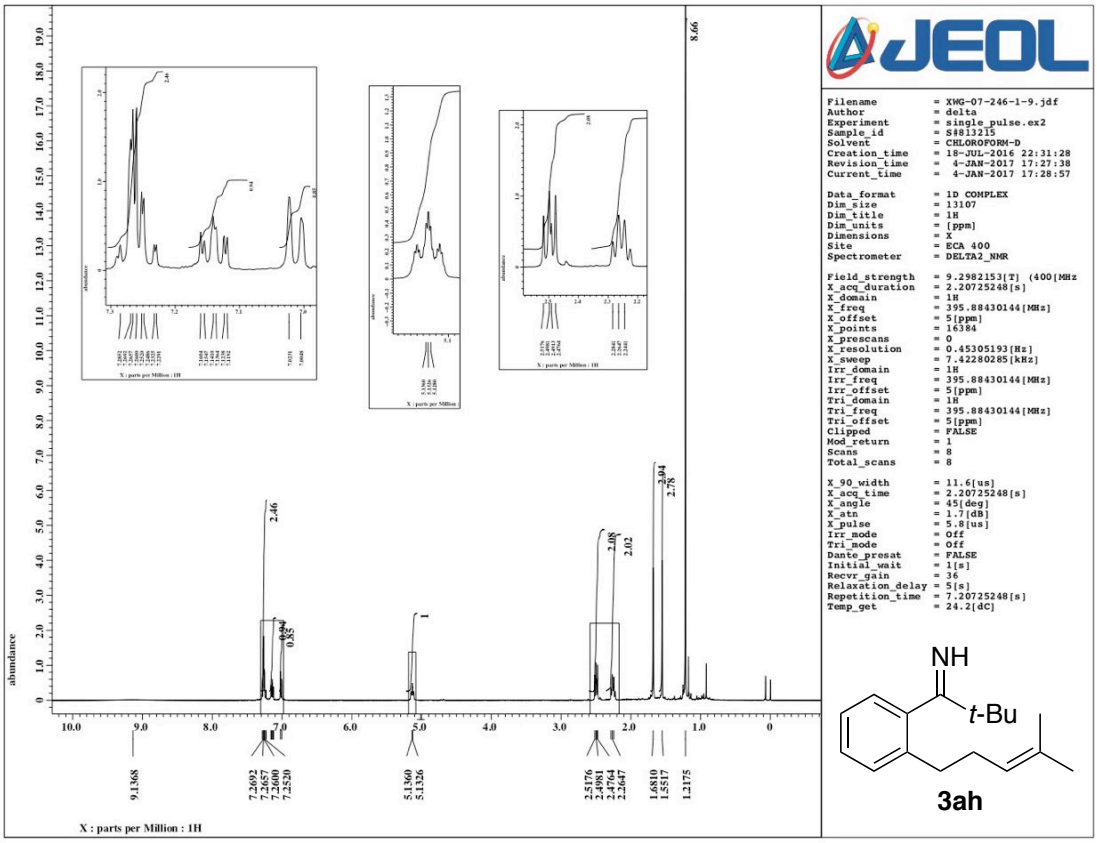
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR

Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 173
Total_scans = 173

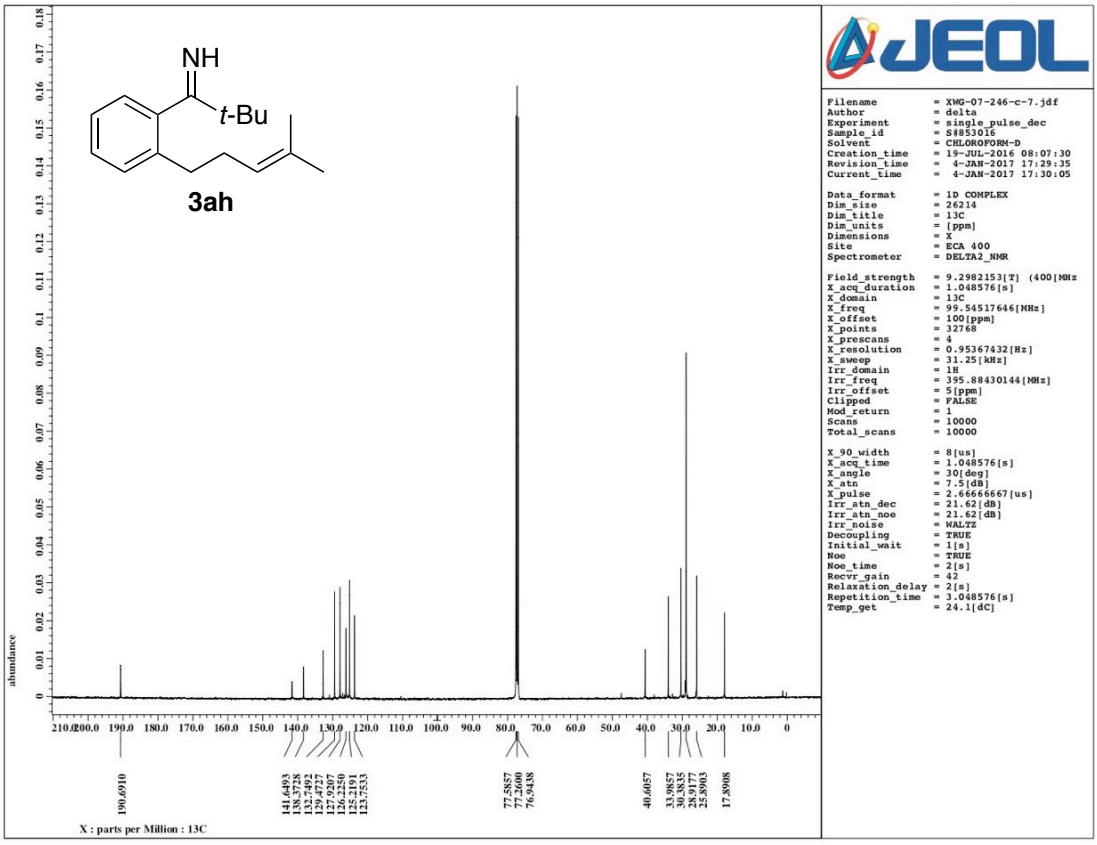
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.3[dC]


JEOL
Filename = XWG-07-578-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#573601
Solvent = CHLOROFORM-D
Creation_time = 20-SEP-2016 15:56:30
Revision_time = 4-JAN-2017 17:21:31
Current_time = 4-JAN-2017 17:22:57
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 2
Total_scans = 2
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 23.7[dC]
NH
t-Bu
3ag
abundance
X : parts per Million : 1H

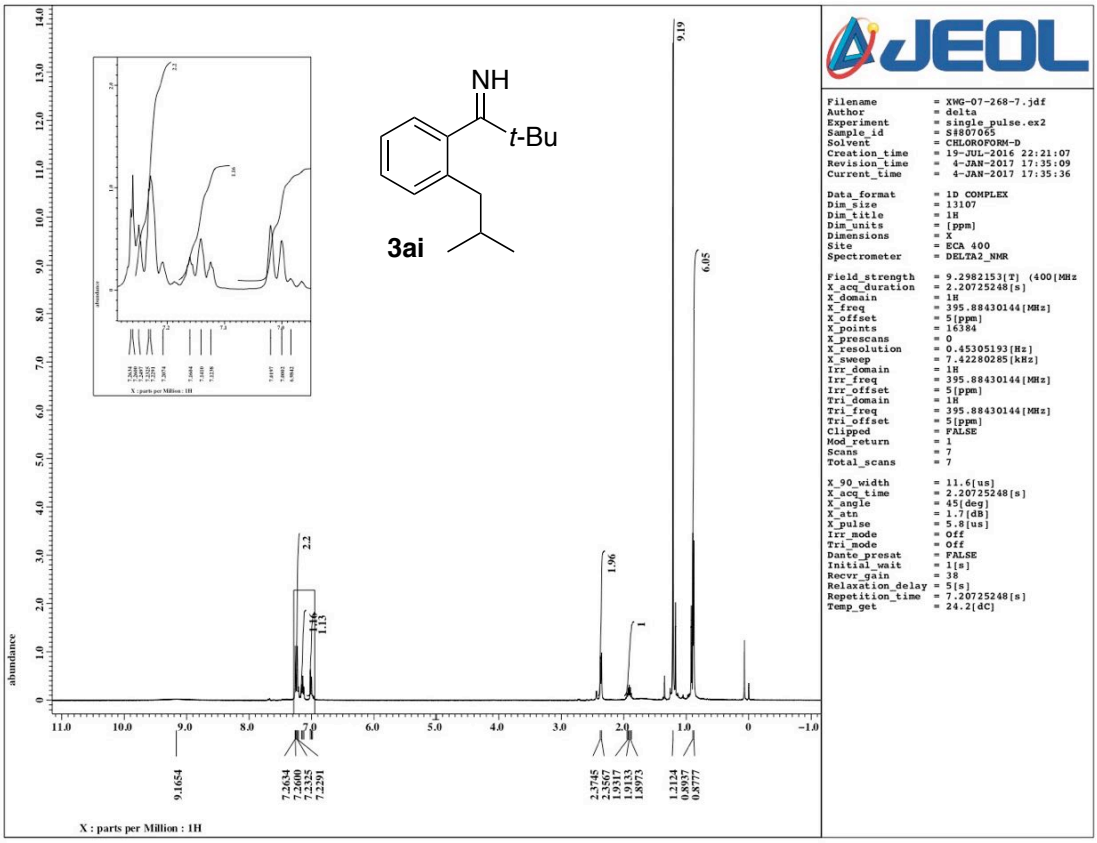

JEOL
Filename = XWG-07-578-1-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#574417
Solvent = CHLOROFORM-D
Creation_time = 20-SEP-2016 16:02:32
Revision_time = 4-JAN-2017 17:23:43
Current_time = 4-JAN-2017 17:24:16
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 61
Total_scans = 61
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24[dC]
NH
t-Bu
3ag
abundance
X : parts per Million : 13C

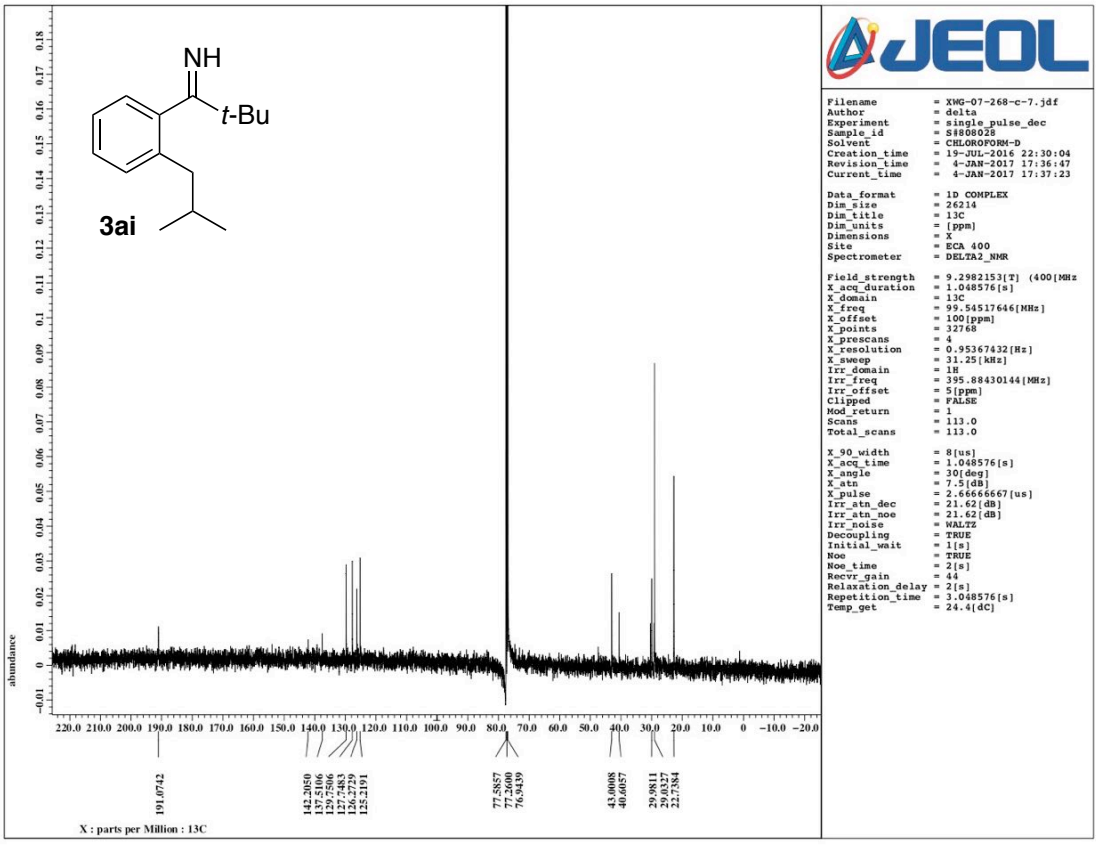

8.66
2.46
0.94
0.85
1
2.08
2.02
3.04
2.78
abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
9.1368
7.2692 7.2657 7.2600 7.2520
5.1360 5.1326
2.5176 2.4981 2.4764 2.2647
1.6810 1.5517
1.2175
X : parts per Million : 1H

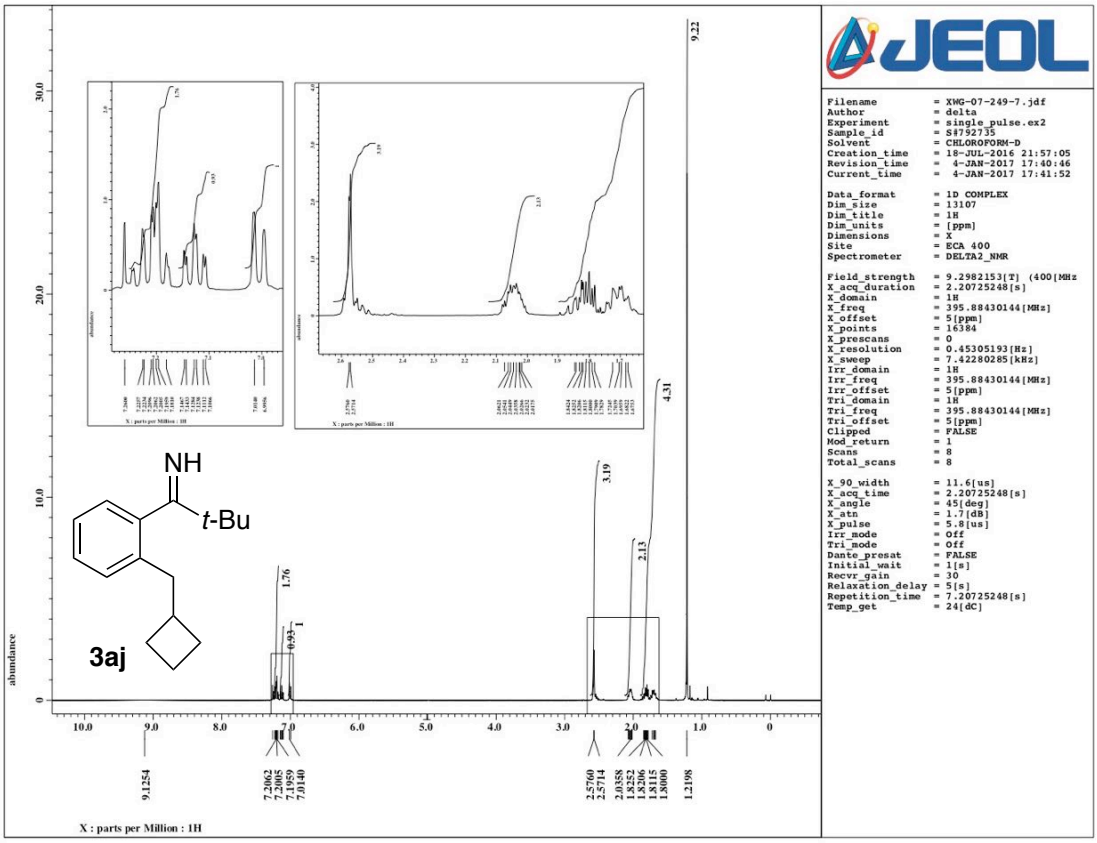
JEOL
Filename = XWG-07-246-1-9.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#813215
Solvent = CHLOROFORM-D
Creation_time = 18-JUL-2016 22:31:28
Revision_time = 4-JAN-2017 17:27:38
Current_time = 4-JAN-2017 17:28:57
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24.2[dC]
NH
t-Bu
3ah


NH
t-Bu
3ah
abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
190.6910
141.6493
138.3725
132.7492
129.4727
127.9207
126.2250
125.2191
123.7533
77.5857
77.2600
76.9438
40.6057
33.9857
30.3835
28.9177
25.8903
17.8908
X : parts per Million : 13C

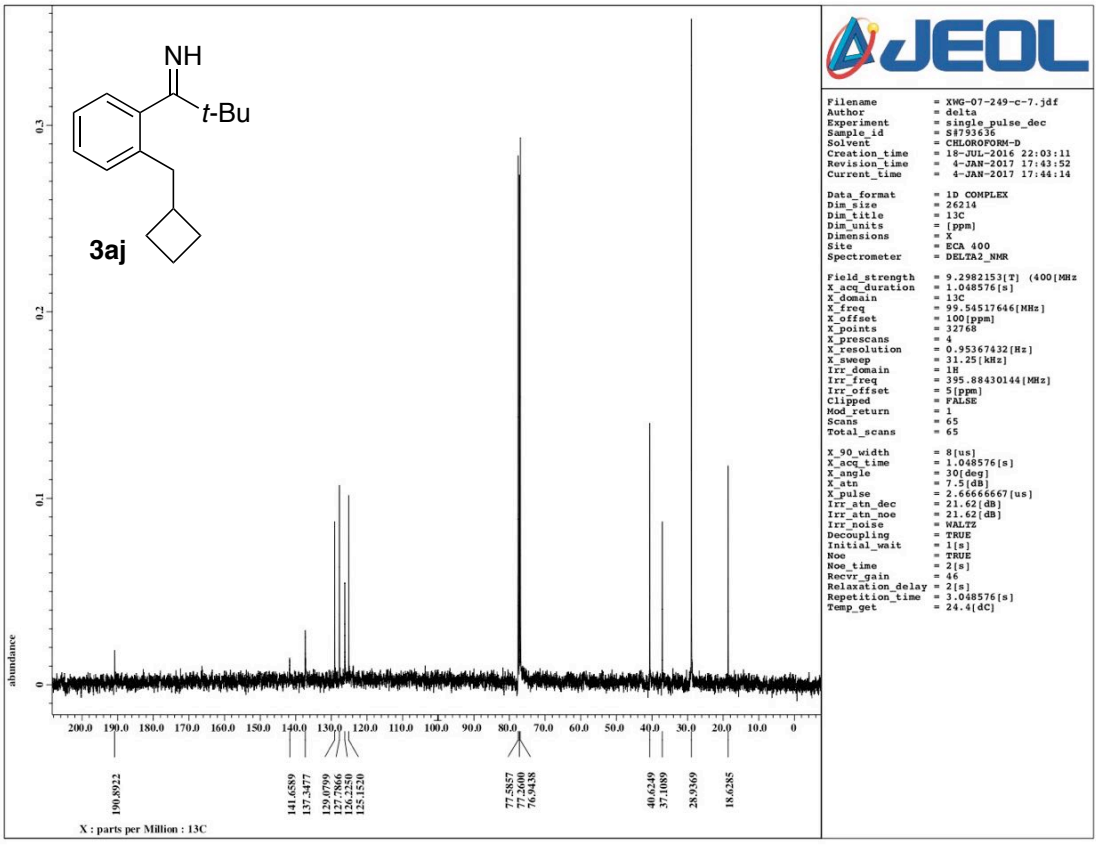
JEOL
Filename = XWG-07-246-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#853016
Solvent = CHLOROFORM-D
Creation_time = 19-JUL-2016 08:07:30
Revision_time = 4-JAN-2017 17:29:35
Current_time = 4-JAN-2017 17:30:05
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 42
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.1[dC]


NH
t-Bu
3ai
9.19
6.05
2.2
1.96
1
1.16
1.15
abundance
X : parts per Million : 1H
Filename = XWG-07-268-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#807065
Solvent = CHLOROFORM-D
Creation_time = 19-JUL-2016 22:21:07
Revision_time = 4-JAN-2017 17:35:09
Current_time = 4-JAN-2017 17:35:36
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 7
Total_scans = 7
X_90_width = 11.6[us]
X_acq_time = 2.207725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.207725248[s]
Temp_get = 24.2[dC]

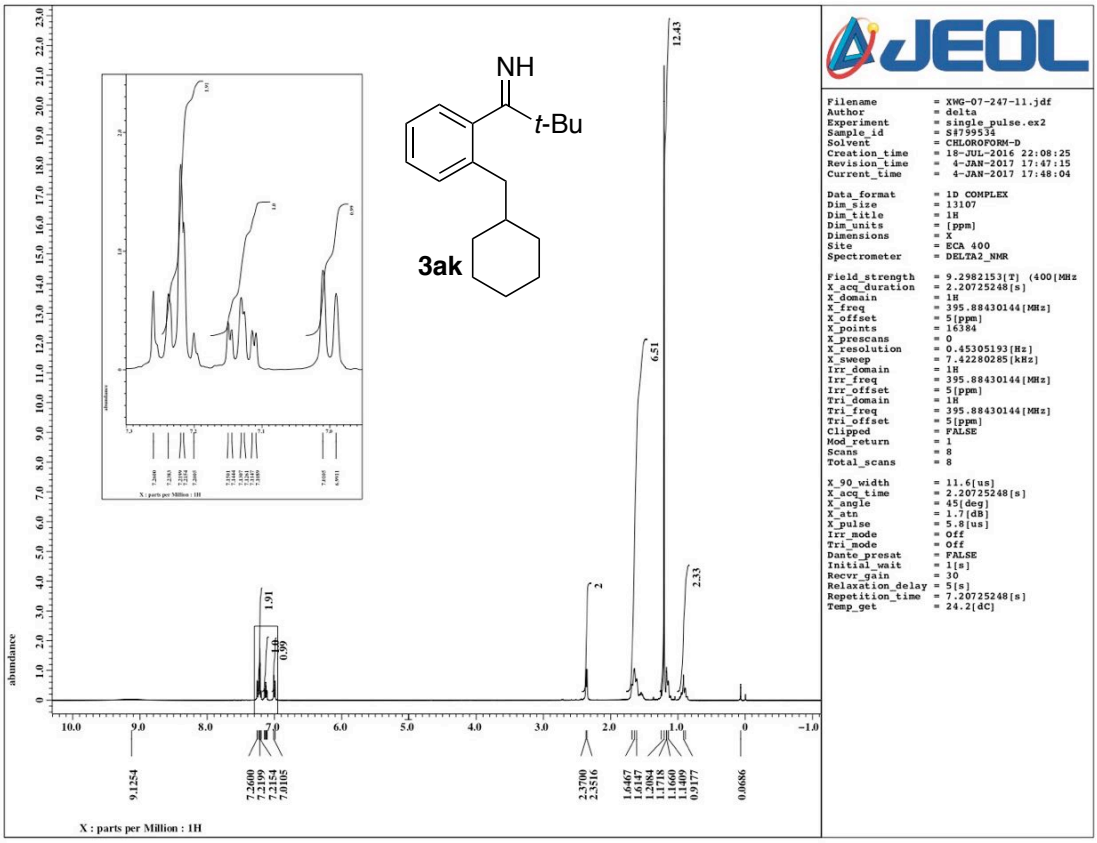

NH
t-Bu
3ai
abundance
X : parts per Million : 13C
Filename = XWG-07-268-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#808028
Solvent = CHLOROFORM-D
Creation_time = 19-JUL-2016 22:30:04
Revision_time = 4-JAN-2017 17:36:47
Current_time = 4-JAN-2017 17:37:23
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 113.0
Total_scans = 113.0
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.4[dC]



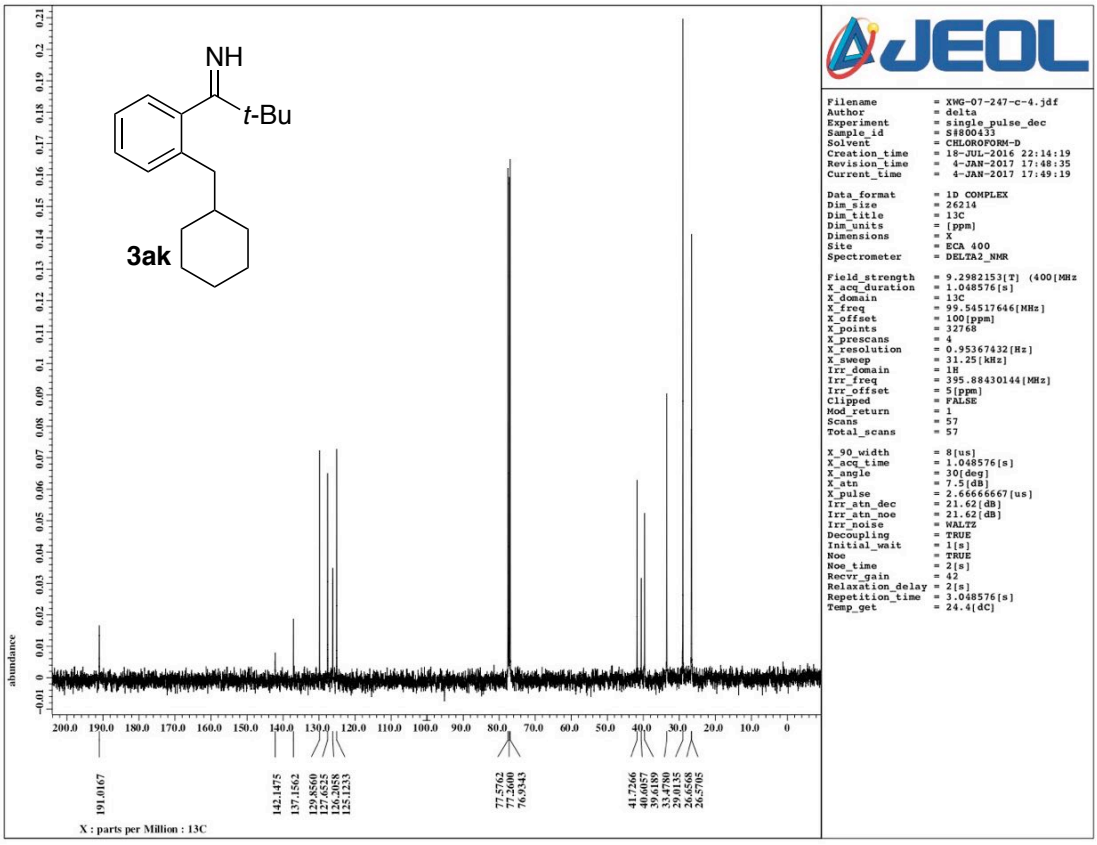

```
Filename          = XWG-07-249-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#792735
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2016 21:57:05
Revision_time     =  4-JAN-2017 17:40:46
Current_time      =  4-JAN-2017 17:41:52

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 24[dC]
```



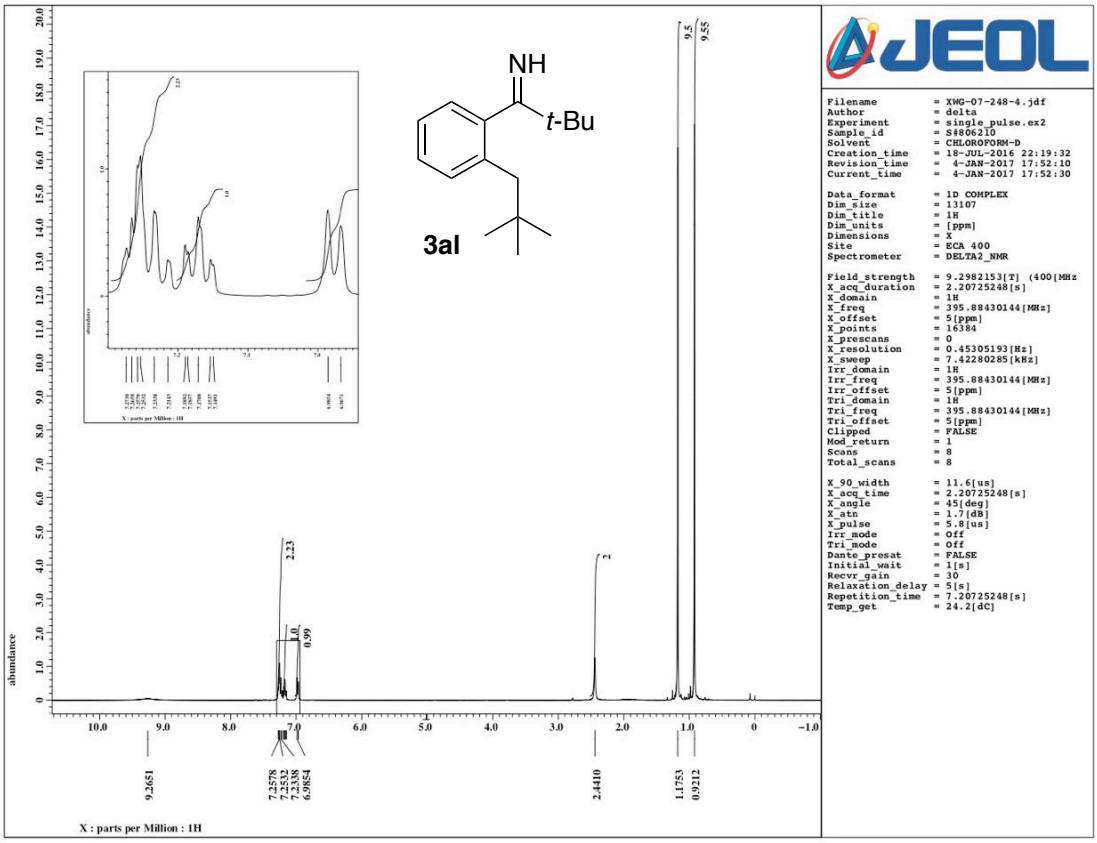

```
Filename          = XWG-07-249-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#793636
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2016 22:03:11
Revision_time     =  4-JAN-2017 17:43:52
Current_time      =  4-JAN-2017 17:44:14

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 65
Total_scans       = 65

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 46
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 24.4[dC]
```

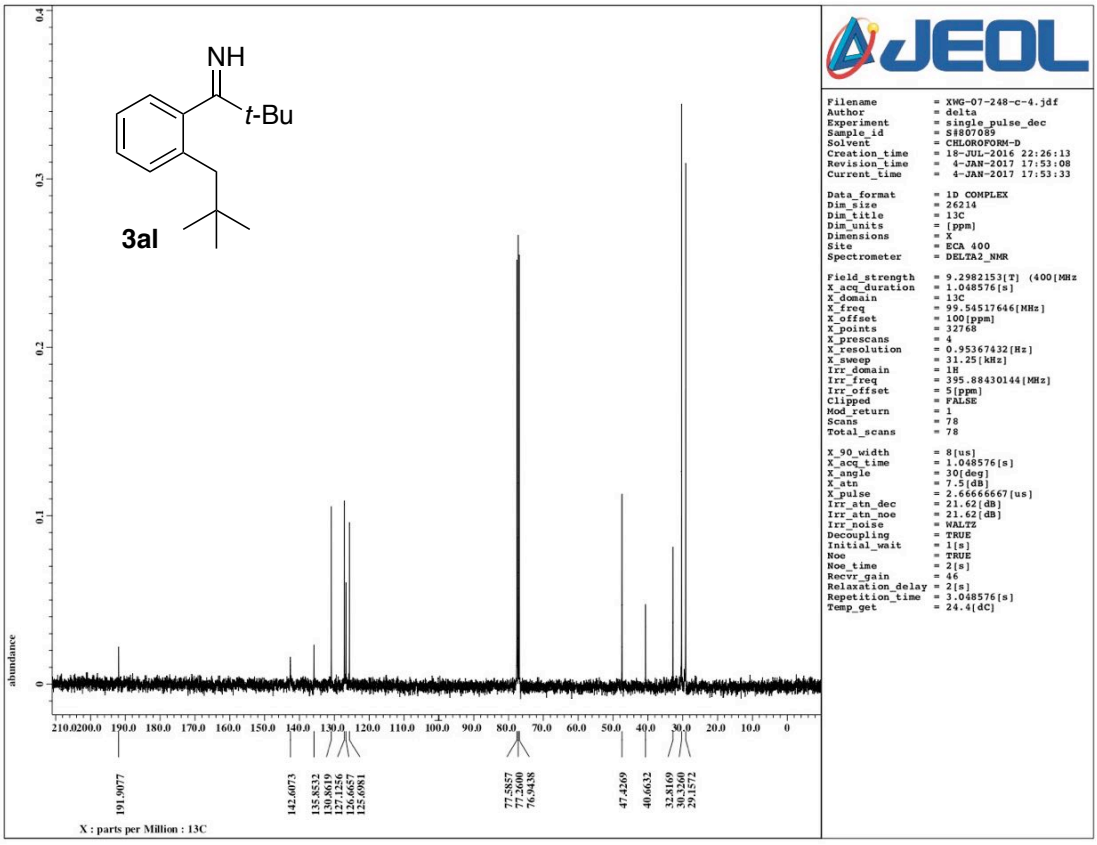


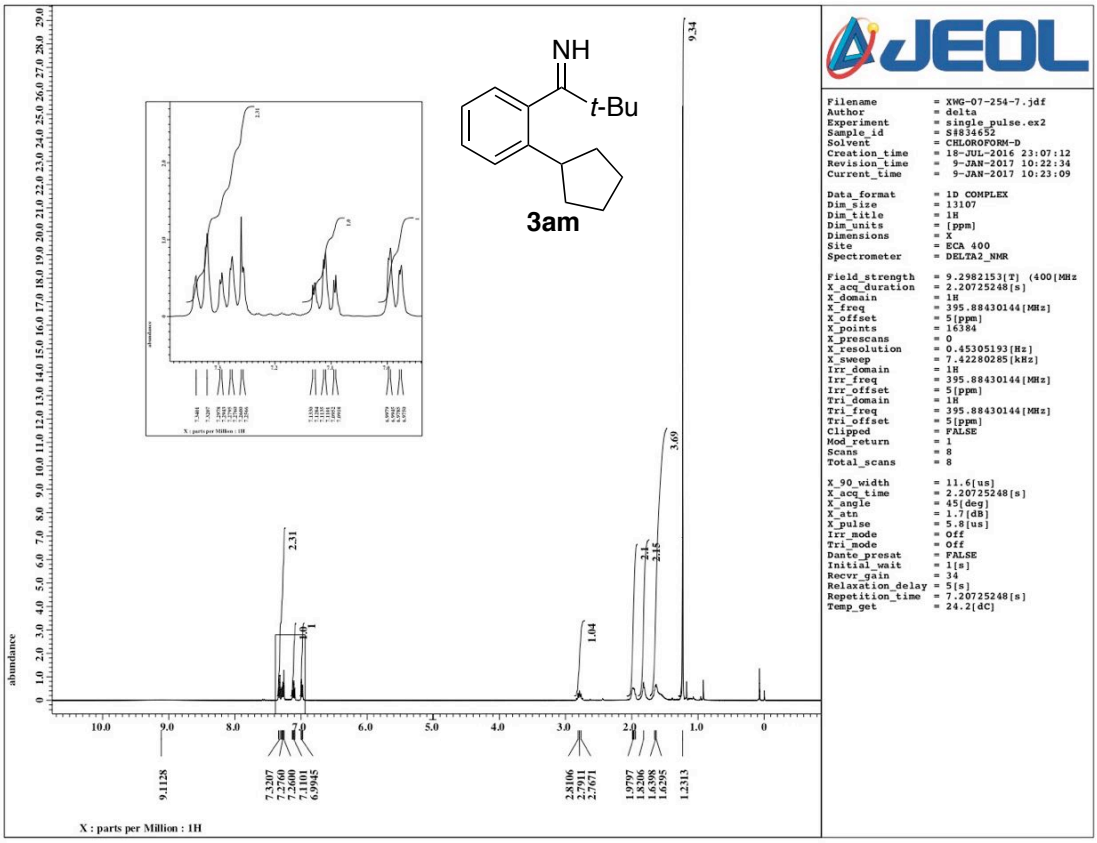

```
Filename          = XWG-07-247-11.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8799534
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2016 22:08:25
Revision_time     =  4-JAN-2017 17:47:15
Current_time      =  4-JAN-2017 17:48:04

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 24.2[dC]
```




```
Filename          = XWG-07-247-c-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8800433
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2016 22:14:19
Revision_time     =  4-JAN-2017 17:48:35
Current_time      =  4-JAN-2017 17:49:19

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 57
Total_scans       = 57

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 42
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 24.4[dC]
```


NH
t-Bu
3aI
abundance
X : parts per Million : 1H
9.2651
7.2578
7.1533
7.1336
6.9854
2.4410
1.1753
0.9212
Filename = XWG-07-248-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#806210
Solvent = CHLOROFORM-D
Creation_time = 18-JUL-2016 22:19:32
Revision_time = 4-JAN-2017 17:52:10
Current_time = 4-JAN-2017 17:52:30
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24.2[dC]


NH
t-Bu
3aI
abundance
X : parts per Million : 13C
191.9077
142.6073
135.8532
130.8619
127.1256
126.6657
125.6981
77.5857
77.2690
76.9438
47.4269
40.6632
32.8169
30.3260
29.1572
Filename = XWG-07-248-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#807089
Solvent = CHLOROFORM-D
Creation_time = 18-JUL-2016 22:26:13
Revision_time = 4-JAN-2017 17:53:08
Current_time = 4-JAN-2017 17:53:33
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 78
Total_scans = 78
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 46
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.4[dC]

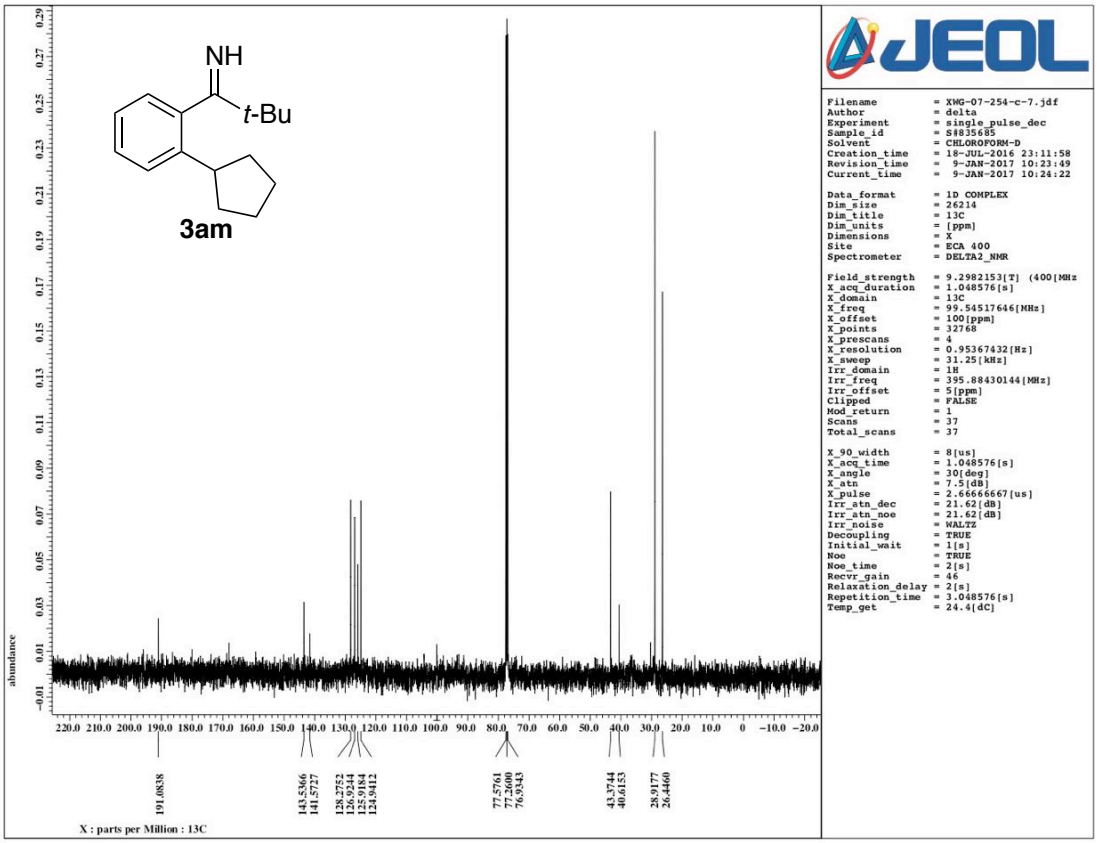


Filename = XWG-07-254-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#834652
Solvent = CHLOROFORM-D
Creation_time = 18-JUL-2016 23:07:12
Revision_time = 9-JAN-2017 10:22:34
Current_time = 9-JAN-2017 10:23:09

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR

Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.6[us]
X_acq_time = 2.207725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24.2[dC]

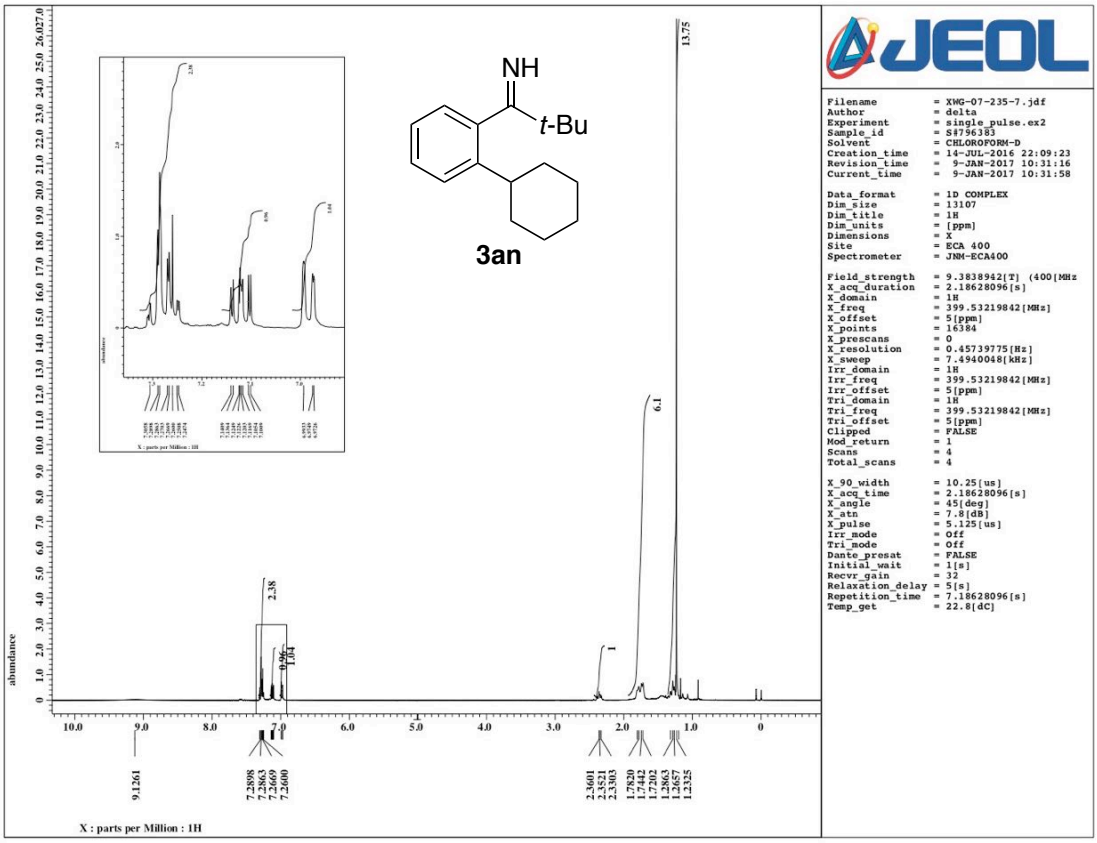


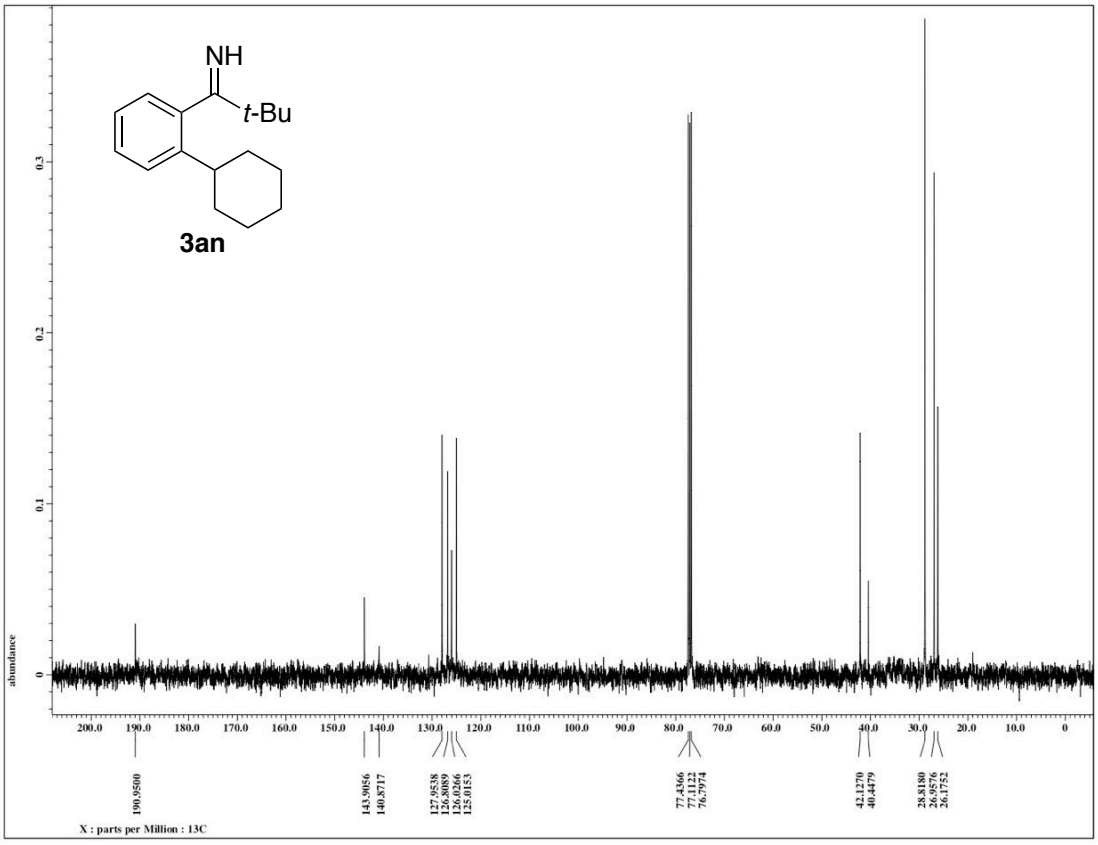
Filename = XWG-07-254-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#835685
Solvent = CHLOROFORM-D
Creation_time = 18-JUL-2016 23:11:58
Revision_time = 9-JAN-2017 10:23:49
Current_time = 9-JAN-2017 10:24:22

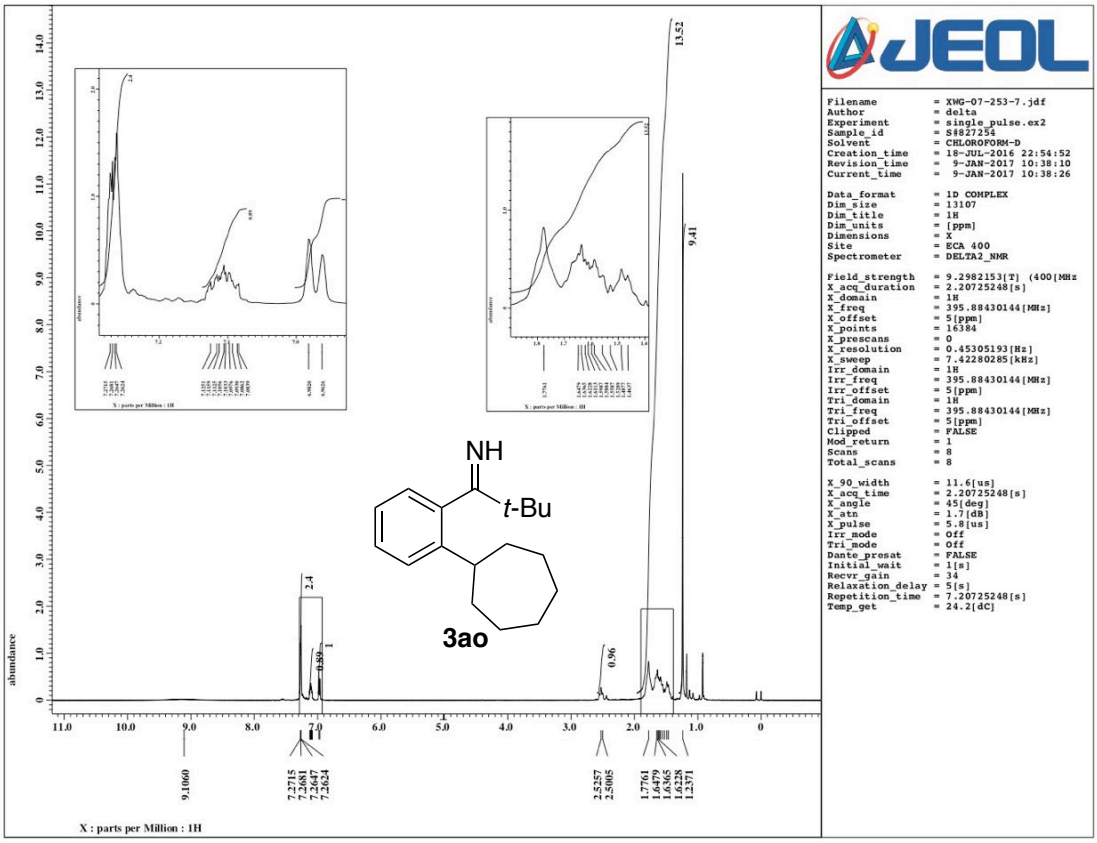
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR

Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 37
Total_scans = 37

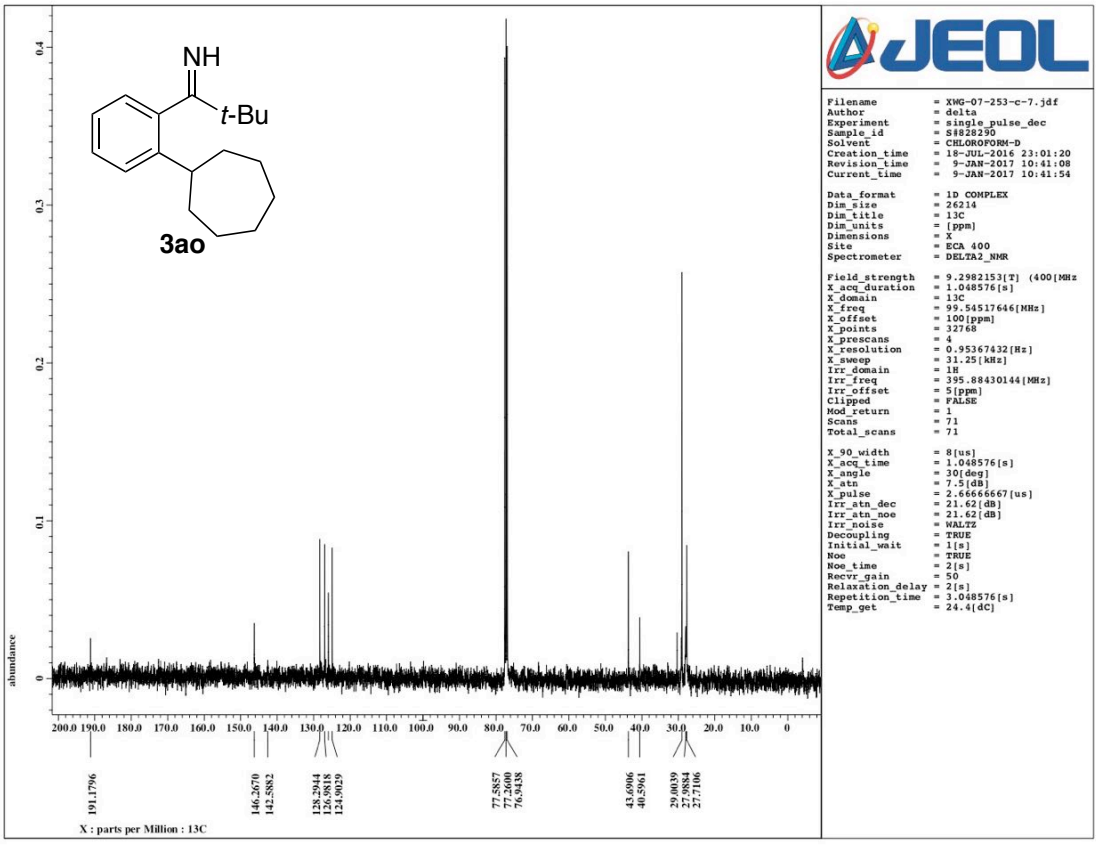
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 46
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.4[dC]


NH
t-Bu
3an
13.75
6.1
2.38
1.04
0.96
1
abundance
9.1261
7.2898
7.2863
7.2669
7.2660
2.3601
2.3521
2.3303
1.7820
1.7442
1.7202
1.2863
1.2657
1.2325
X : parts per Million : 1H
Filename = XWG-07-235-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#796383
Solvent = CHLOROFORM-D
Creation_time = 14-JUL-2016 22:09:23
Revision_time = 9-JAN-2017 10:31:16
Current_time = 9-JAN-2017 10:31:58
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.8[dC]

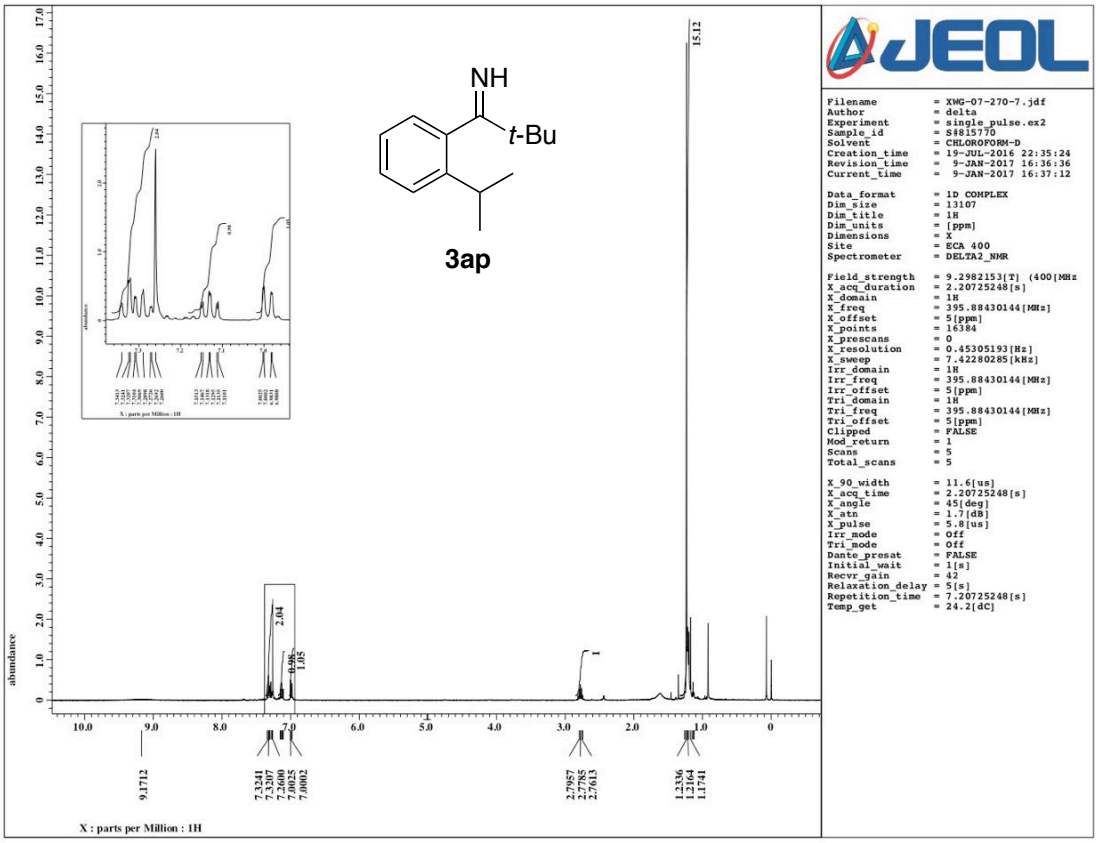

NH
t-Bu
3an
abundance
190.9500
143.9056
140.8717
127.9538
126.8089
126.0266
125.0153
77.4366
77.1122
76.7914
42.1270
40.4479
28.8180
26.9576
26.1752
X : parts per Million : 13C



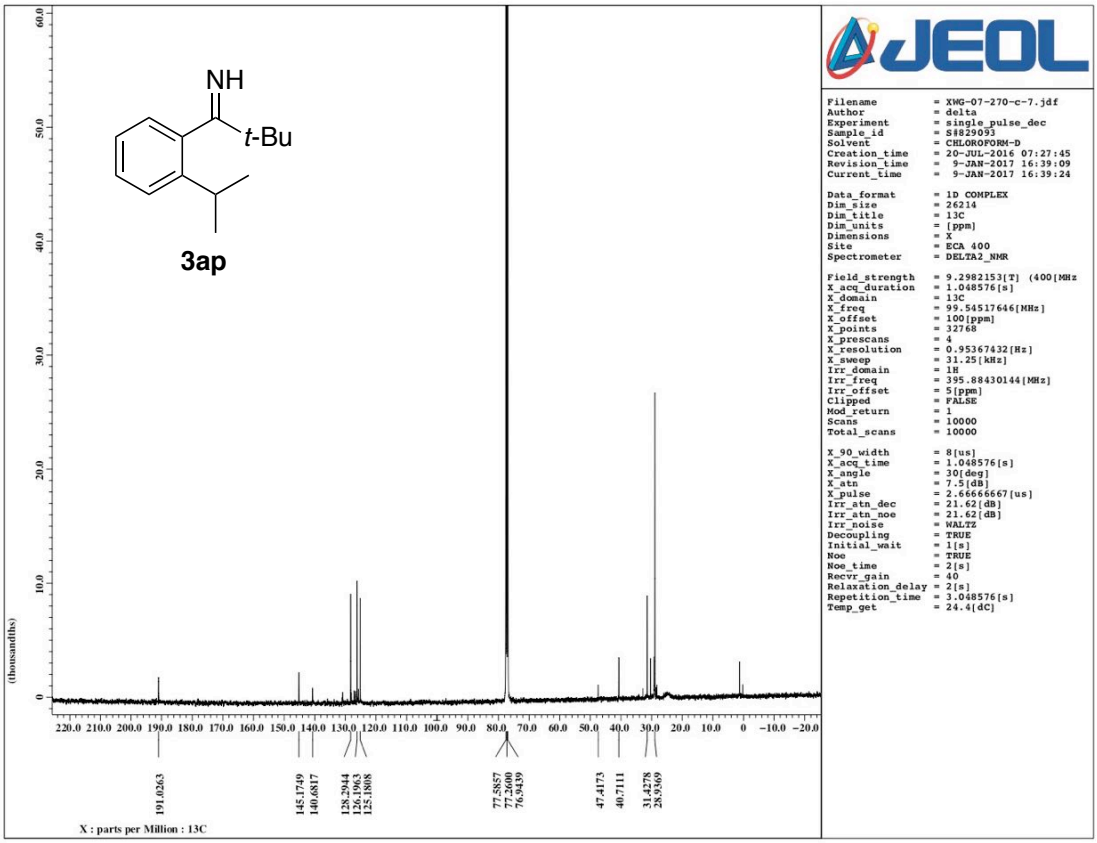

```
Filename          = XWG-07-253-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8827254
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2016 22:54:52
Revision_time     =  9-JAN-2017 10:38:10
Current_time      =  9-JAN-2017 10:38:26

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 24.2[dC]
```



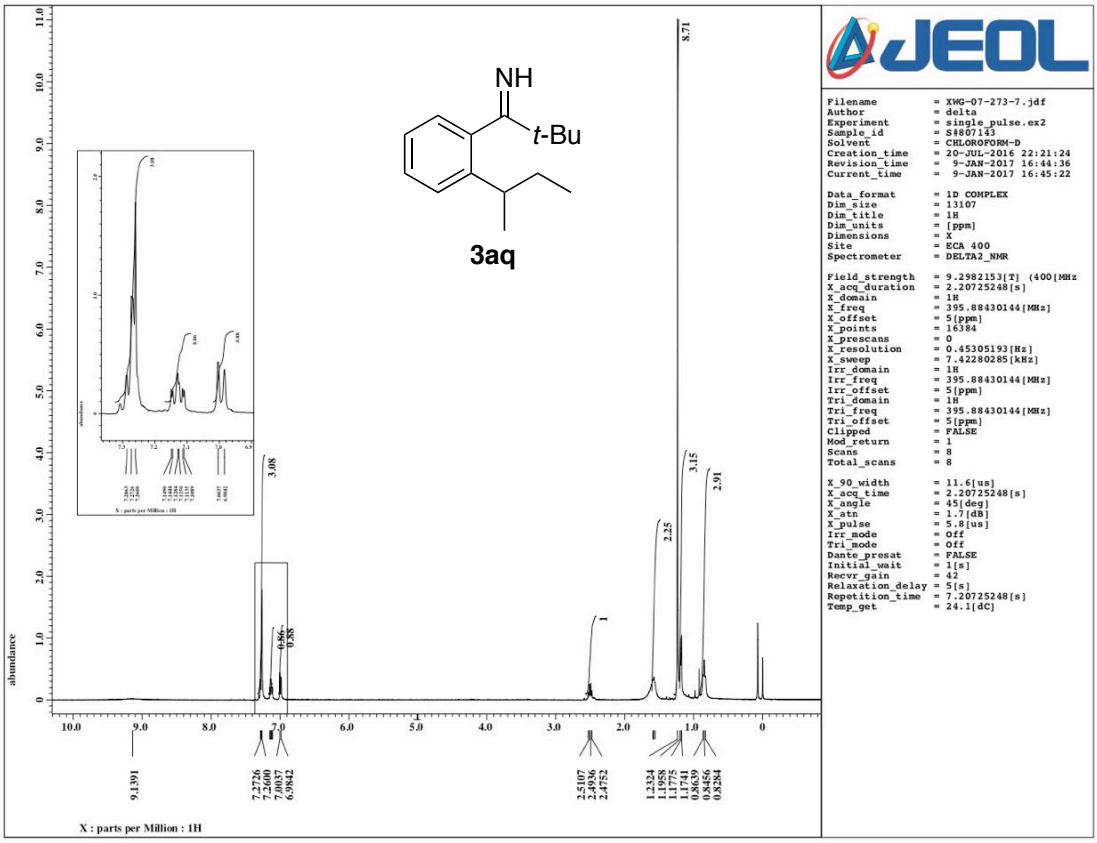

```
Filename          = XWG-07-253-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8828290
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2016 23:01:20
Revision_time     =  9-JAN-2017 10:41:08
Current_time      =  9-JAN-2017 10:41:54

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 71
Total_scans       = 71

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 24.4[dC]
```

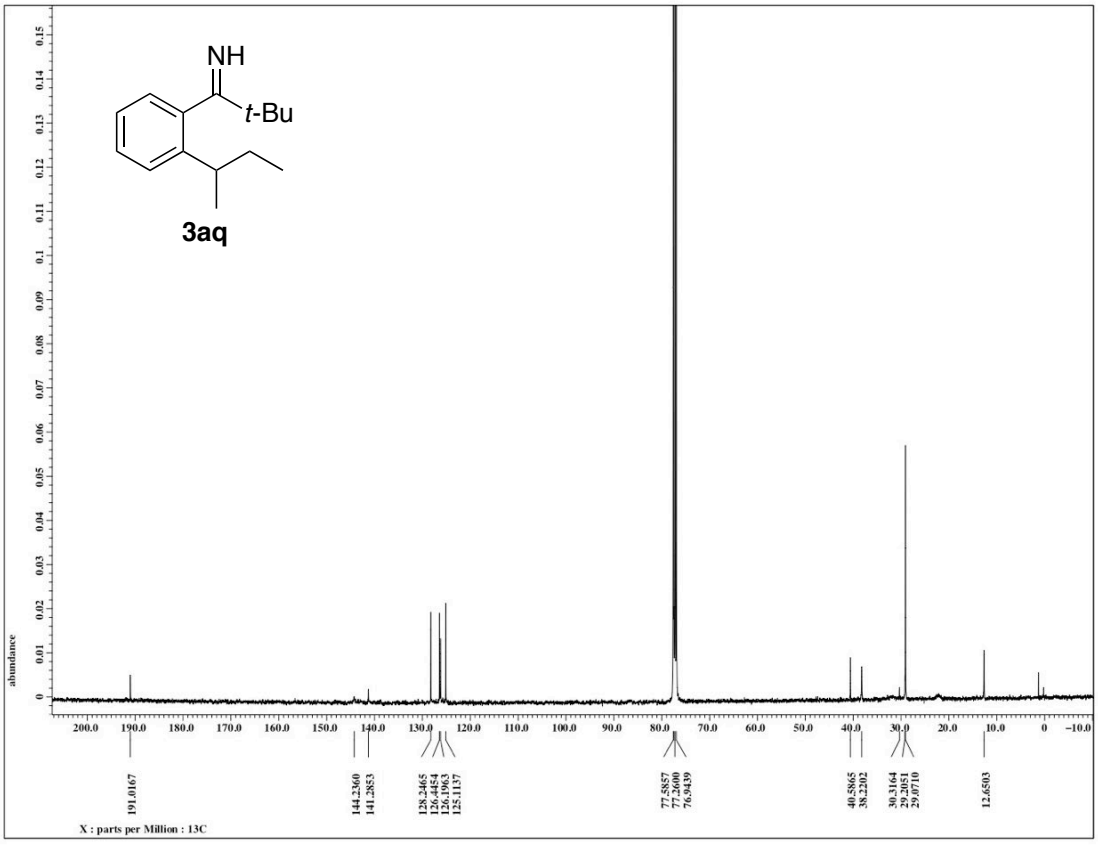


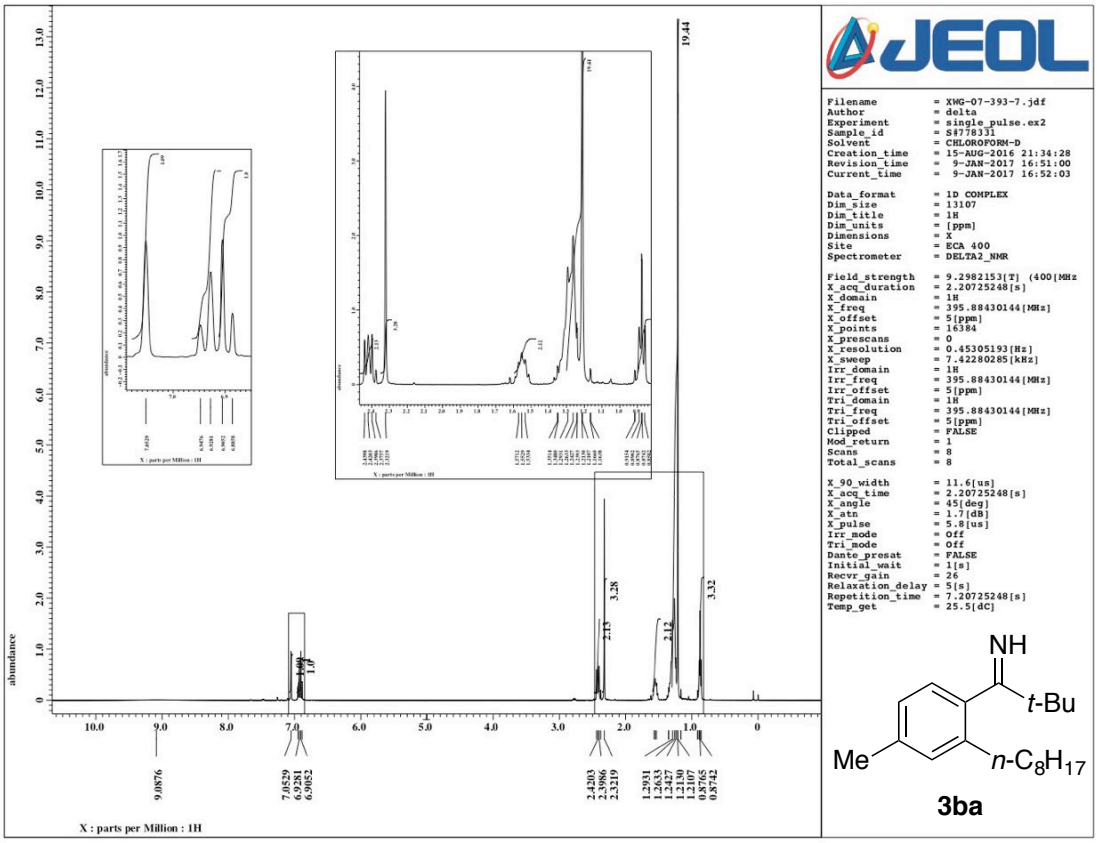

```
Filename          = XWG-07-270-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8815770
Solvent           = CHLOROFORM-D
Creation_time     = 19-JUL-2016 22:35:24
Revision_time     =  9-JAN-2017 16:36:36
Current_time      =  9-JAN-2017 16:37:12

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 5
Total_scans       = 5

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 24.2[dC]
```

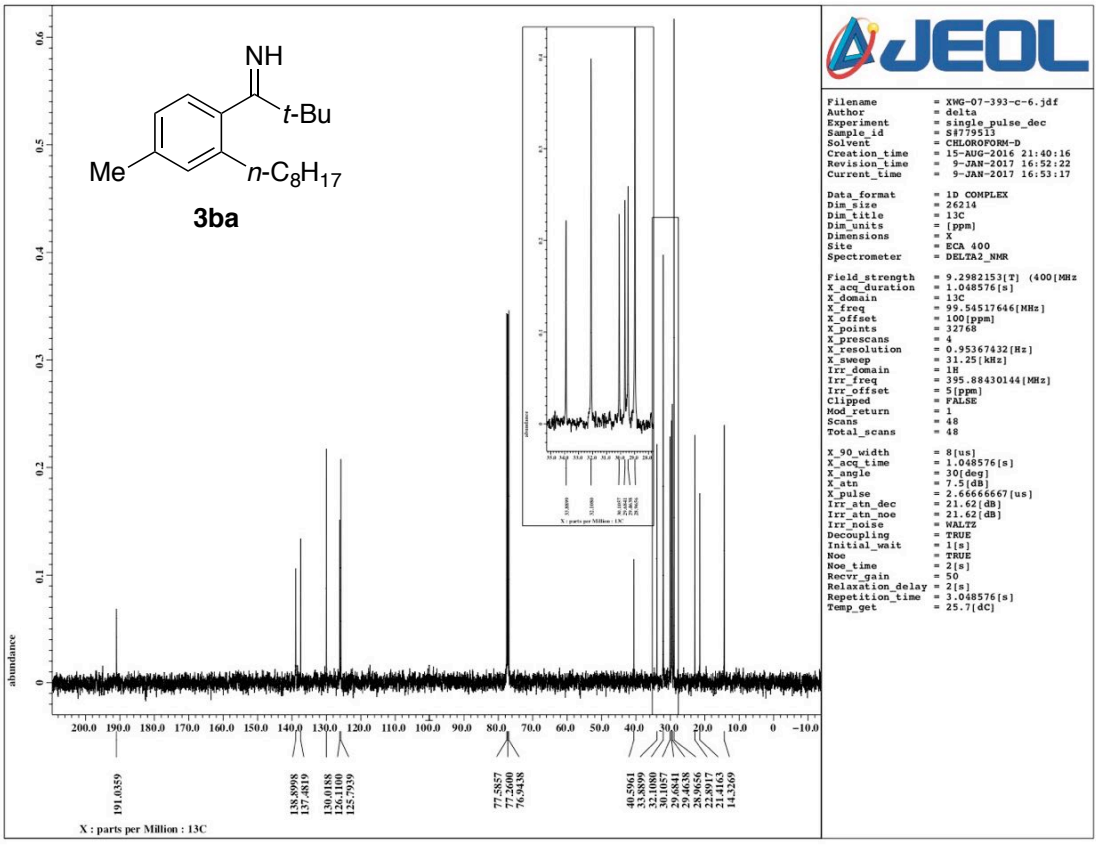


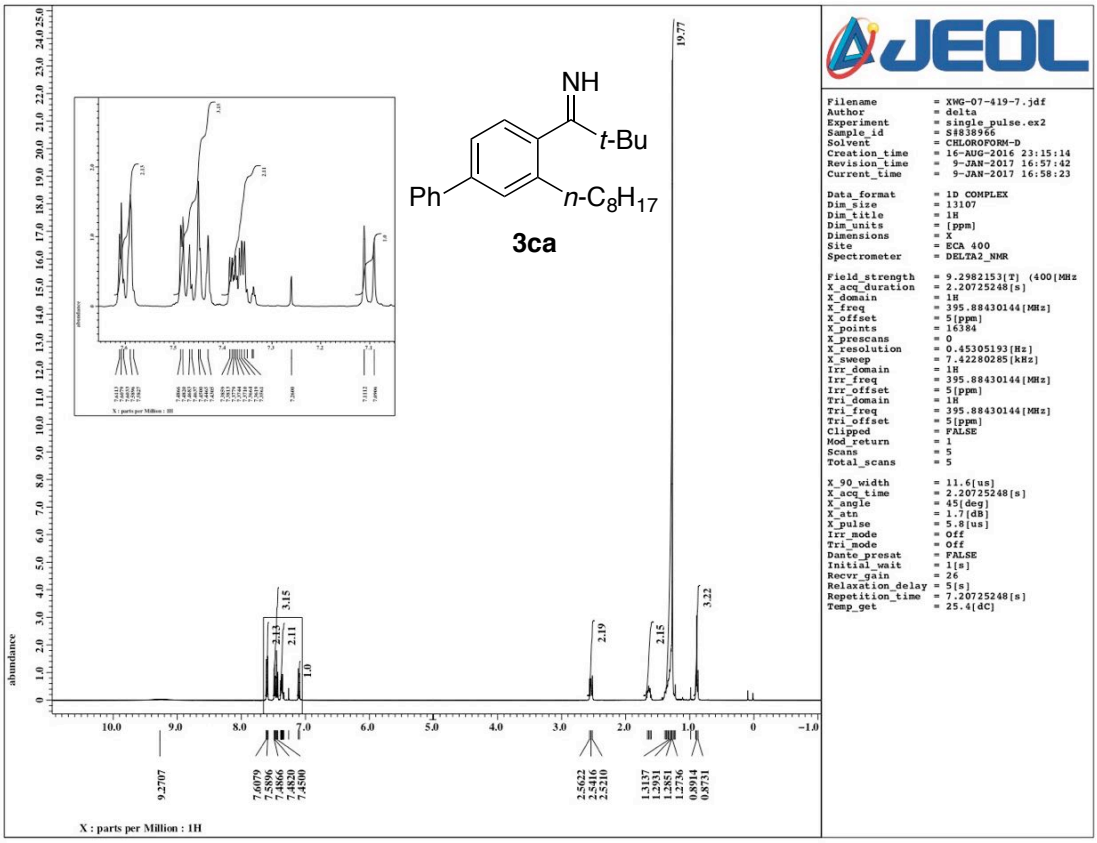

```
Filename          = XWG-07-270-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8829093
Solvent           = CHLOROFORM-D
Creation_time     = 20-JUL-2016 07:27:45
Revision_time     =  9-JAN-2017 16:39:09
Current_time      =  9-JAN-2017 16:39:24

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10000
Total_scans       = 10000

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 40
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 24.4[dC]
```

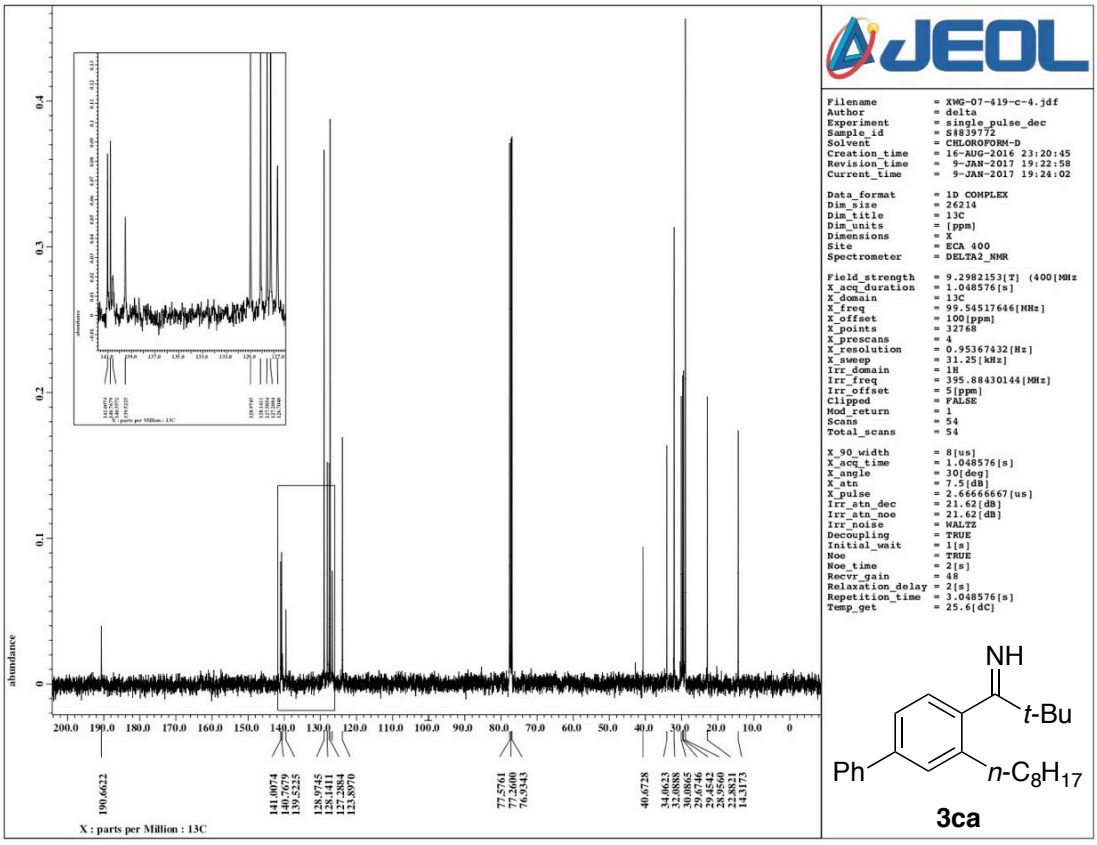

NH
t-Bu
3aq
abundance
X : parts per Million : 1H
Filename = XWG-07-273-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8807143
Solvent = CHLOROFORM-D
Creation_time = 20-JUL-2016 22:21:24
Revision_time = 9-JAN-2017 16:44:36
Current_time = 9-JAN-2017 16:45:22
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153(T) (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24.1[dC]

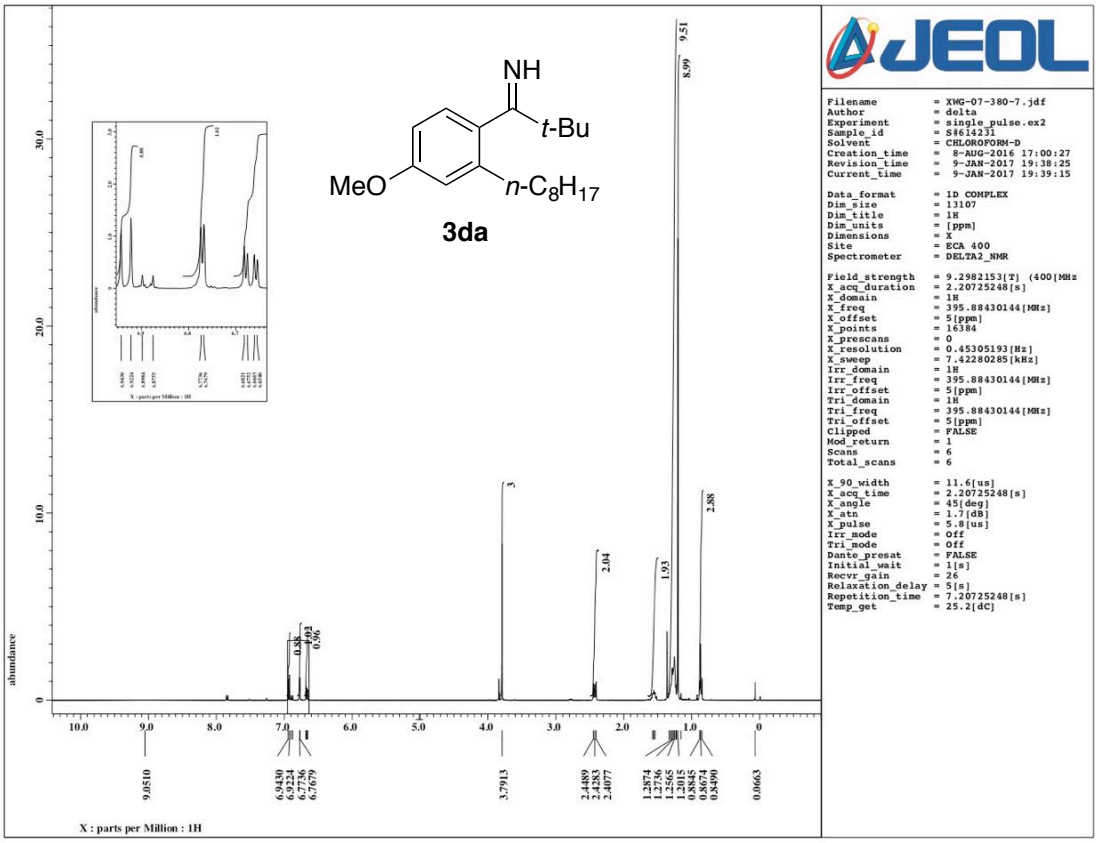

NH
t-Bu
3aq
abundance
X : parts per Million : 13C

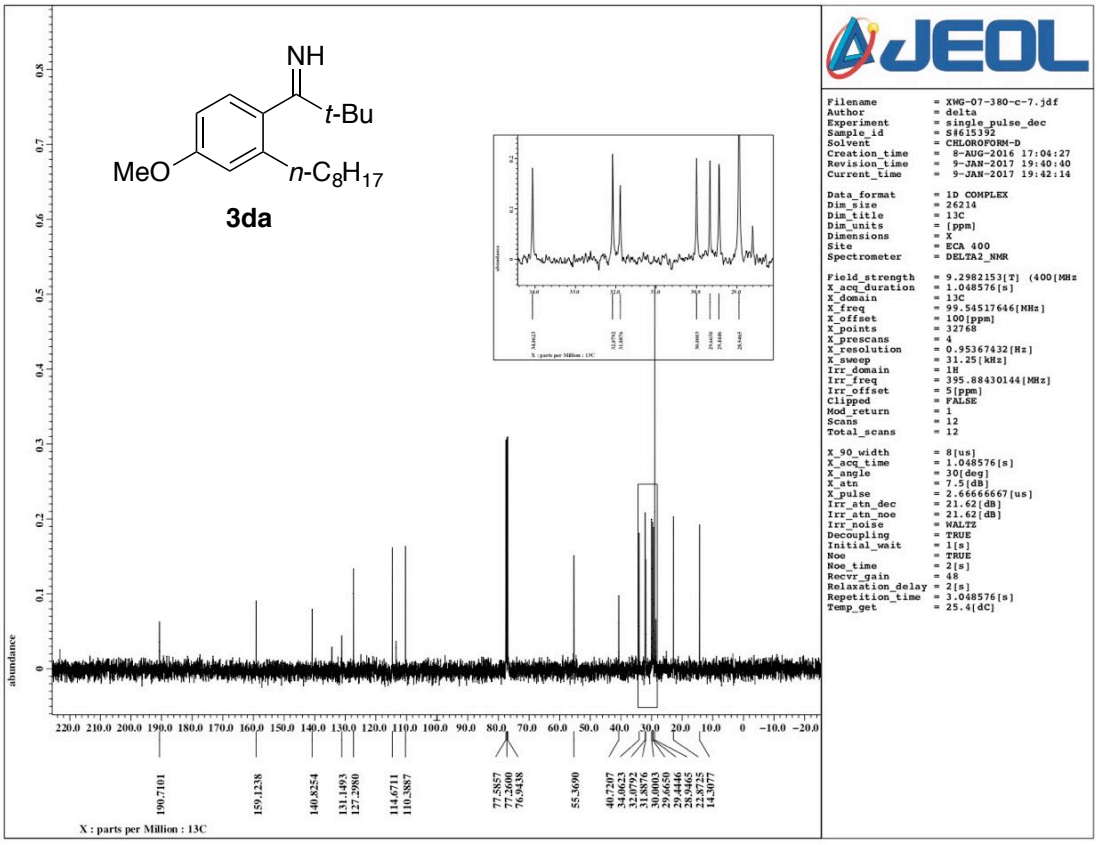

Filename = XWG-07-393-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#778331
Solvent = CHLOROFORM-D
Creation_time = 15-AUG-2016 21:34:28
Revision_time = 9-JAN-2017 16:51:00
Current_time = 9-JAN-2017 16:52:03
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 26
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]
NH
t-Bu
Me
n-C8H17
3ba
abundance
X : parts per Million : 1H

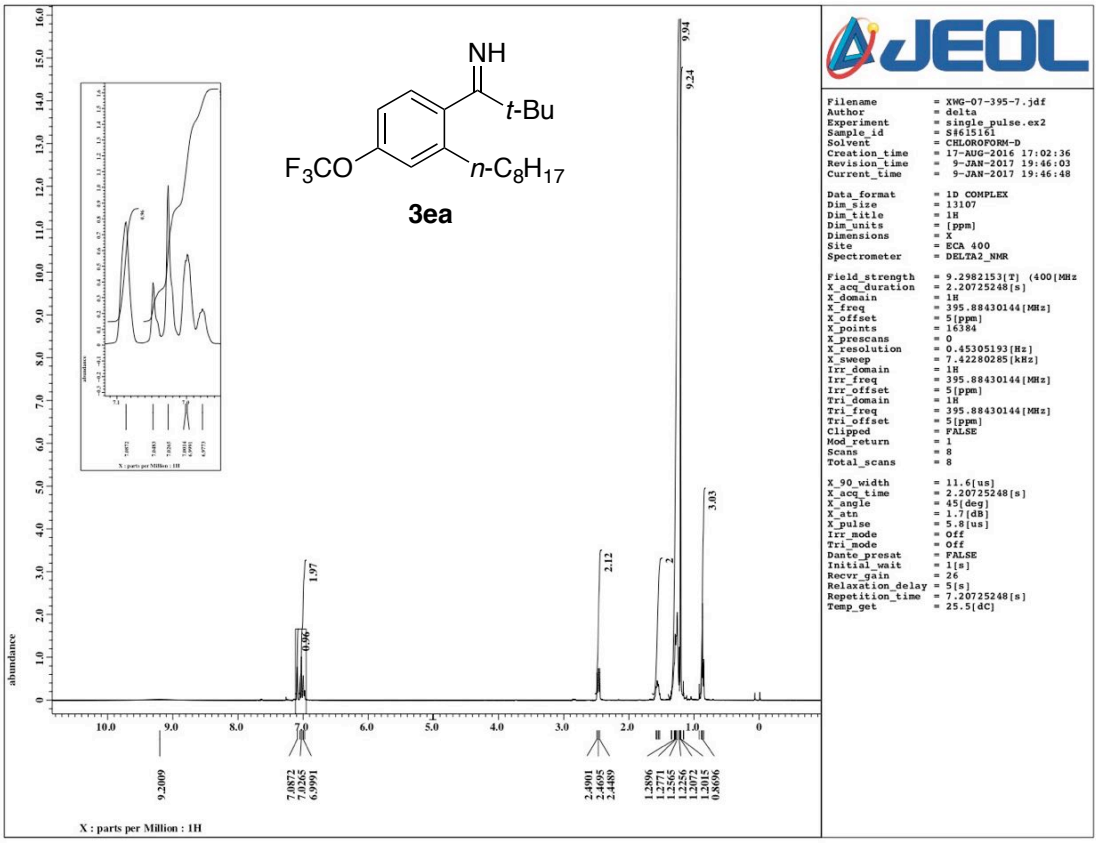

NH
t-Bu
Me
n-C8H17
3ba
Filename = XWG-07-393-c-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#779513
Solvent = CHLOROFORM-D
Creation_time = 15-AUG-2016 21:40:16
Revision_time = 9-JAN-2017 16:52:22
Current_time = 9-JAN-2017 16:53:17
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 48
Total_scans = 48
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]
abundance
X : parts per Million : 13C


NH
t-Bu
Ph
n-C8H17
3ca
19.77
3.15
2.13
2.11
1.0
2.19
2.15
3.22
abundance
X : parts per Million : 1H
Filename = XWG-07-419-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#838966
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 23:15:14
Revision_time = 9-JAN-2017 16:57:42
Current_time = 9-JAN-2017 16:58:23
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 26
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]

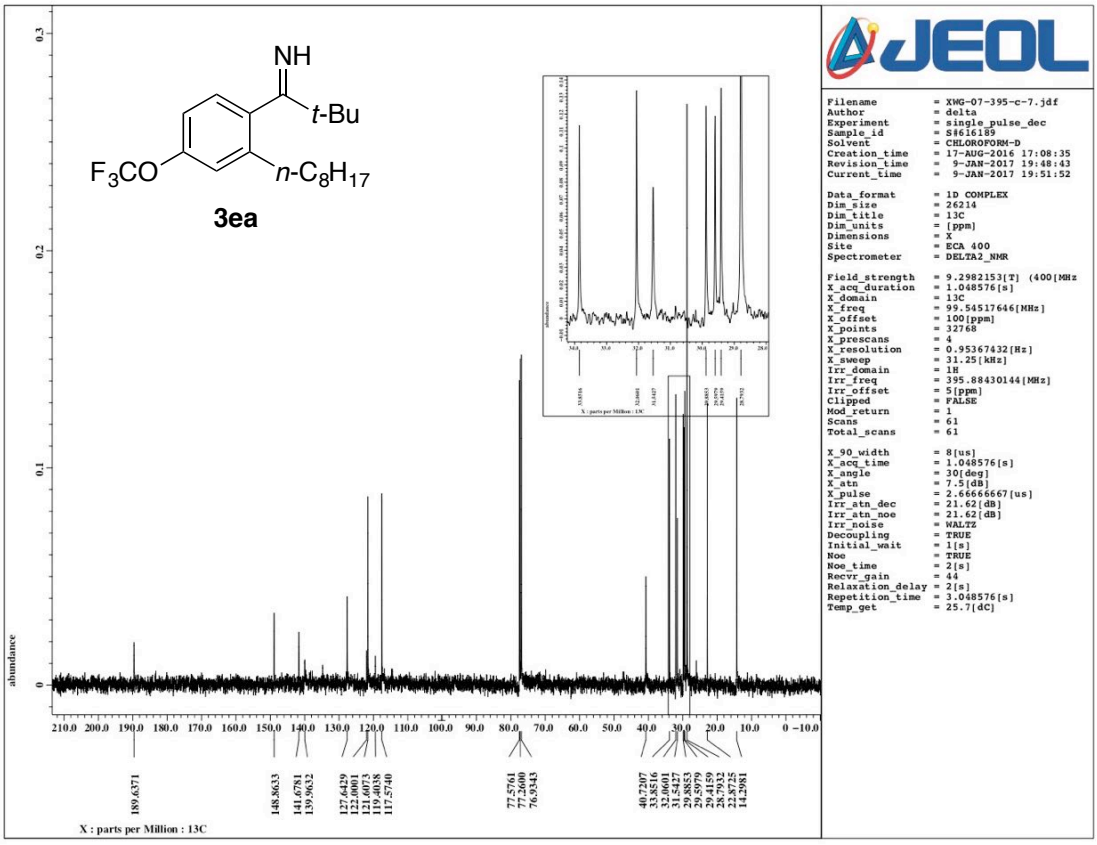

abundance
X : parts per Million : 13C
Filename = XWG-07-419-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#839772
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 23:20:45
Revision_time = 9-JAN-2017 19:22:58
Current_time = 9-JAN-2017 19:24:02
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 54
Total_scans = 54
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 48
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
NH
t-Bu
Ph
n-C8H17
3ca


NH
t-Bu
MeO
n-C8H17
3da
abundance
X : parts per Million : 1H
Filename = XWG-07-380-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8614231
Solvent = CHLOROFORM-D
Creation_time = 8-AUG-2016 17:00:27
Revision_time = 9-JAN-2017 19:38:25
Current_time = 9-JAN-2017 19:39:15
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 26
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.2[dC]

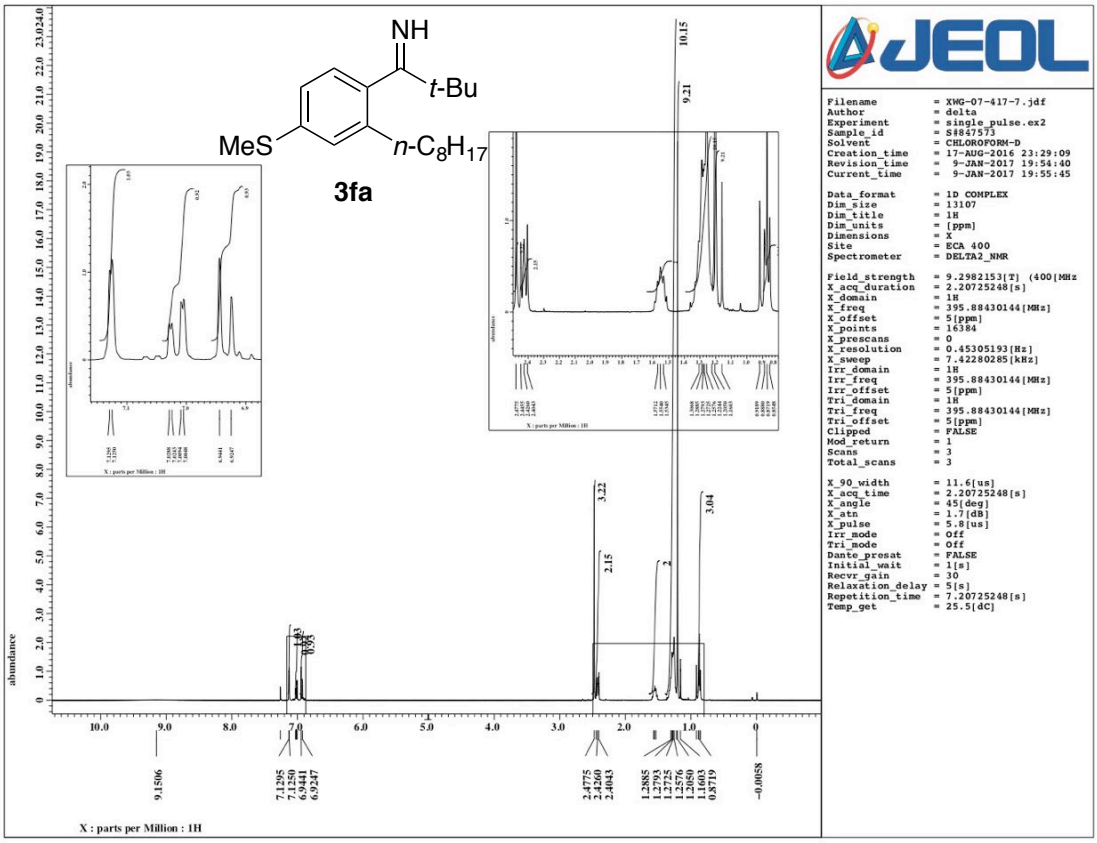

NH
t-Bu
MeO
n-C8H17
3da
abundance
X : parts per Million : 13C
Filename = XWG-07-380-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8615392
Solvent = CHLOROFORM-D
Creation_time = 8-AUG-2016 17:04:27
Revision_time = 9-JAN-2017 19:40:40
Current_time = 9-JAN-2017 19:42:14
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 12
Total_scans = 12
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 48
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.4[dC]



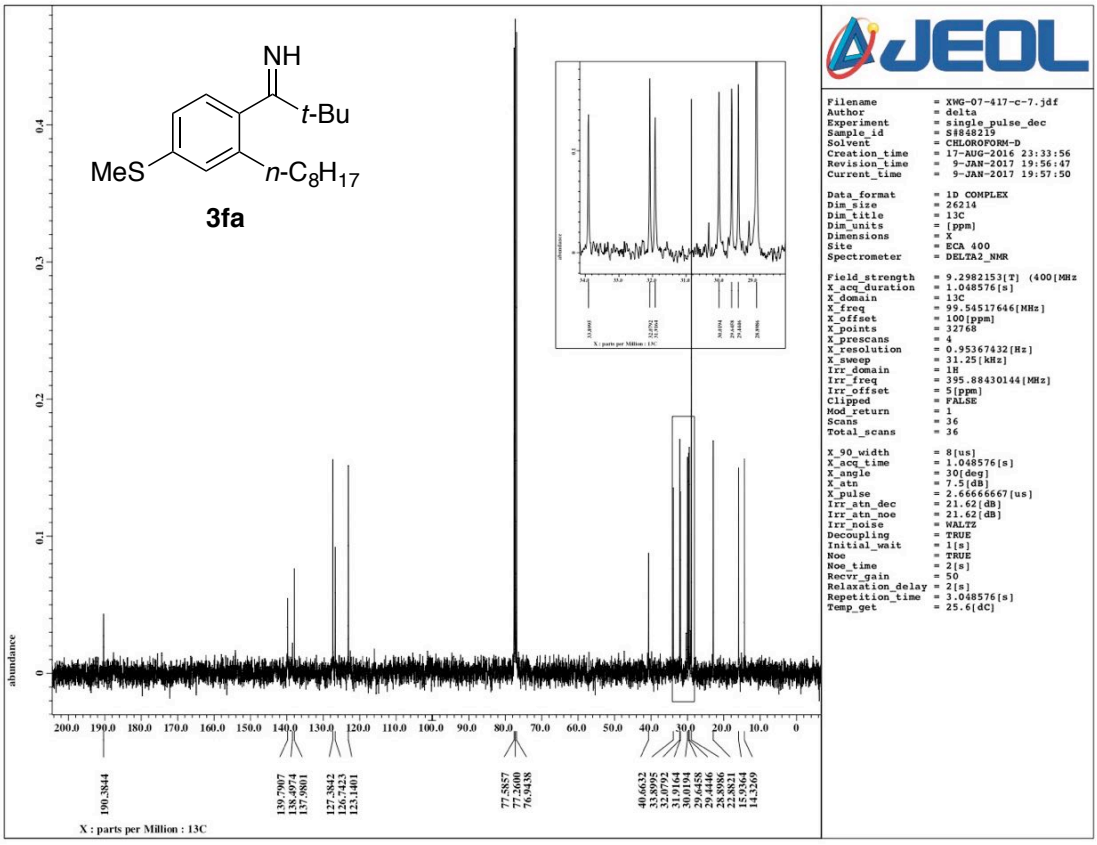

```
Filename        = XWG-07-395-7.jdf
Author          = delta
Experiment      = single_pulse.ex2
Sample_id       = S#615161
Solvent         = CHLOROFORM-D
Creation_time   = 17-AUG-2016 17:02:36
Revision_time   =  9-JAN-2017 19:46:03
Current_time    =  9-JAN-2017 19:46:48

Data_format     = 1D COMPLEX
Dim_size        = 13107
Dim_title       = 1H
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = DELTA2_NMR

Field_strength  = 9.2982153[T] (400[MHz
X_acq_duration  = 2.20725248[s]
X_domain        = 1H
X_freq          = 395.88430144[MHz]
X_offset        = 5[ppm]
X_points        = 16384
X_prescans      = 0
X_resolution    = 0.45305193[Hz]
X_sweep         = 7.42280285[kHz]
Irr_domain      = 1H
Irr_freq        = 395.88430144[MHz]
Irr_offset      = 5[ppm]
Tri_domain      = 1H
Tri_freq        = 395.88430144[MHz]
Tri_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 8
Total_scans     = 8

X_90_width      = 11.6[us]
X_acq_time      = 2.20725248[s]
X_angle         = 45[deg]
X_atn           = 1.7[dB]
X_pulse         = 5.8[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 26
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get        = 25.5[dC]
```



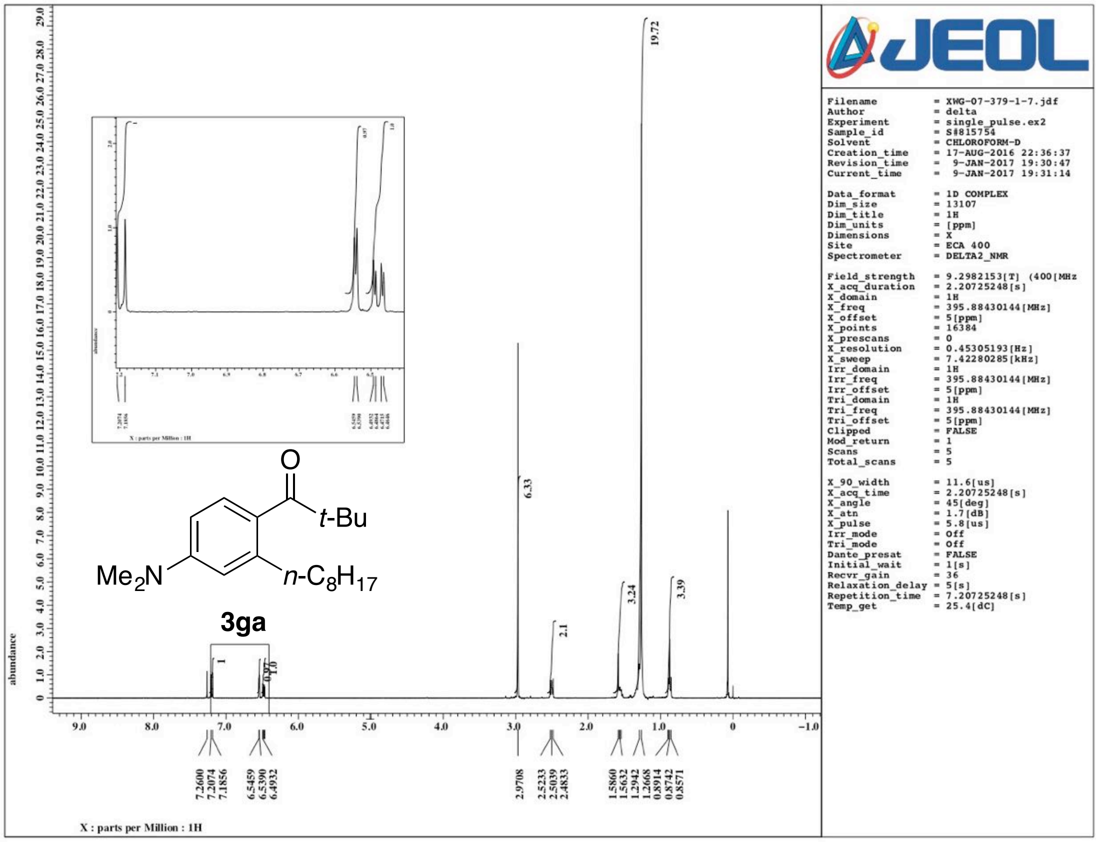

```
Filename        = XWG-07-395-c-7.jdf
Author          = delta
Experiment      = single_pulse_dec
Sample_id       = S#616189
Solvent         = CHLOROFORM-D
Creation_time   = 17-AUG-2016 17:08:35
Revision_time   =  9-JAN-2017 19:48:43
Current_time    =  9-JAN-2017 19:51:52

Data_format     = 1D COMPLEX
Dim_size        = 26214
Dim_title       = 13C
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = DELTA2_NMR

Field_strength  = 9.2982153[T] (400[MHz
X_acq_duration  = 1.048576[s]
X_domain        = 13C
X_freq          = 99.54517646[MHz]
X_offset        = 100[ppm]
X_points        = 32768
X_prescans      = 4
X_resolution    = 0.95367432[Hz]
X_sweep         = 31.25[kHz]
Irr_domain      = 1H
Irr_freq        = 395.88430144[MHz]
Irr_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 61
Total_scans     = 61

X_90_width      = 8[us]
X_acq_time      = 1.048576[s]
X_angle         = 30[deg]
X_atn           = 7.5[dB]
X_pulse         = 2.66666667[us]
Irr_atn_dec     = 21.62[dB]
Irr_atn_noe     = 21.62[dB]
Irr_noise       = WALTZ
Decoupling      = TRUE
Initial_wait    = 1[s]
Noe             = TRUE
Noe_time        = 2[s]
Recvr_gain      = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get        = 25.7[dC]
```

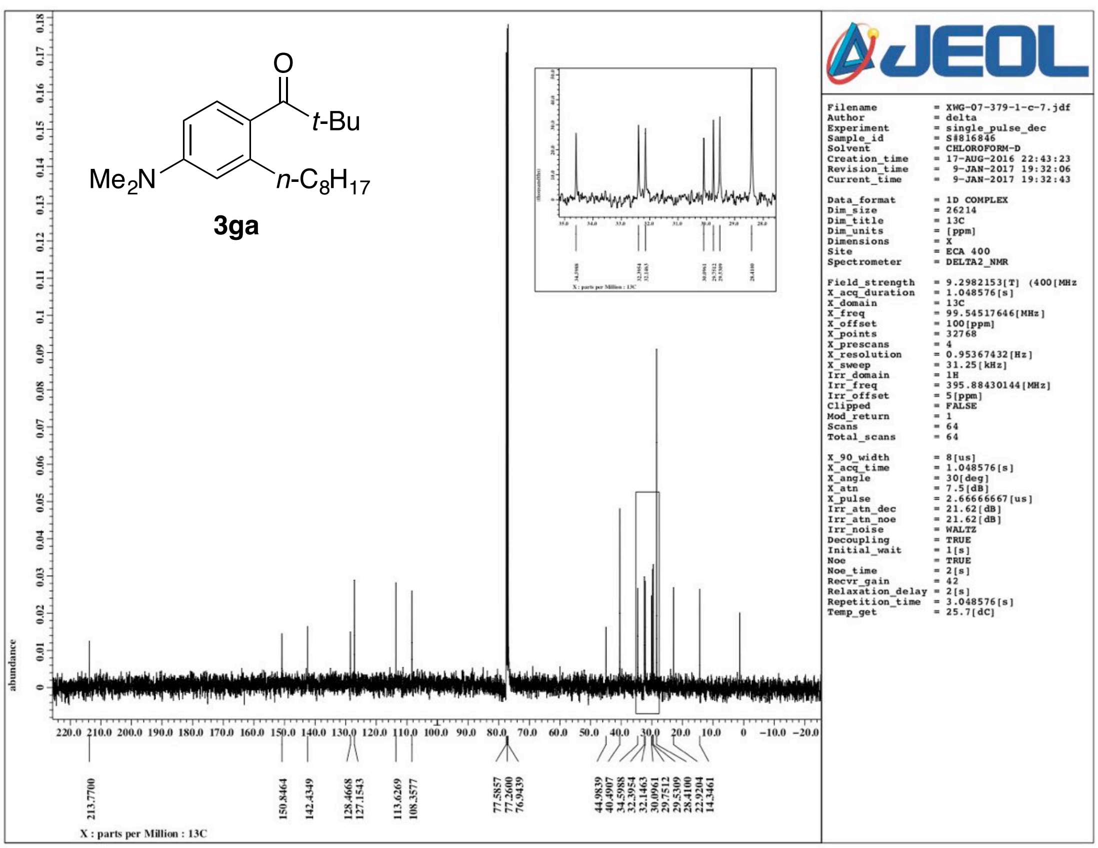


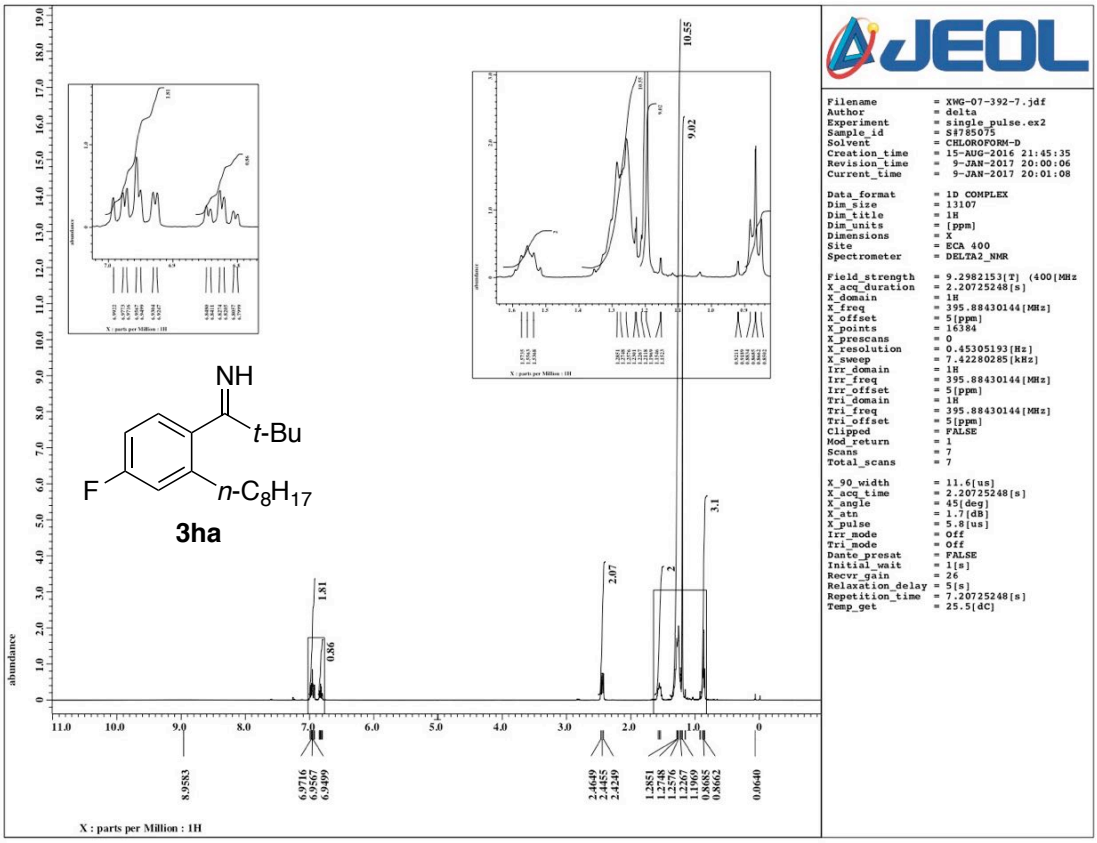

```
Filename          = XWG-07-417-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8847573
Solvent           = CHLOROFORM-D
Creation_time     = 17-AUG-2016 23:29:09
Revision_time     =  9-JAN-2017 19:54:40
Current_time      =  9-JAN-2017 19:55:45

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 3
Total_scans       = 3

X_90_width        = 11.6[us]
X_acq_time        = 2.207252485[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 5[s]
Repetition_time   = 7.207252485[s]
Temp_get          = 25.5[dC]
```

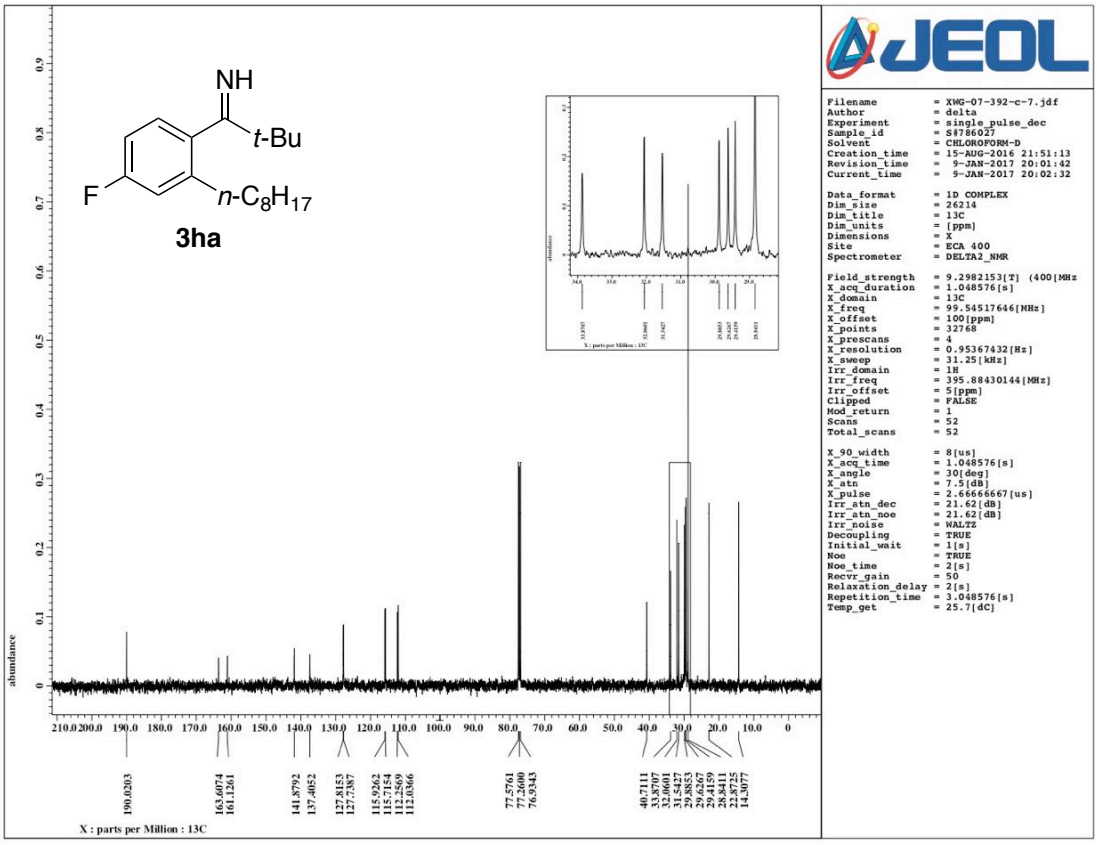


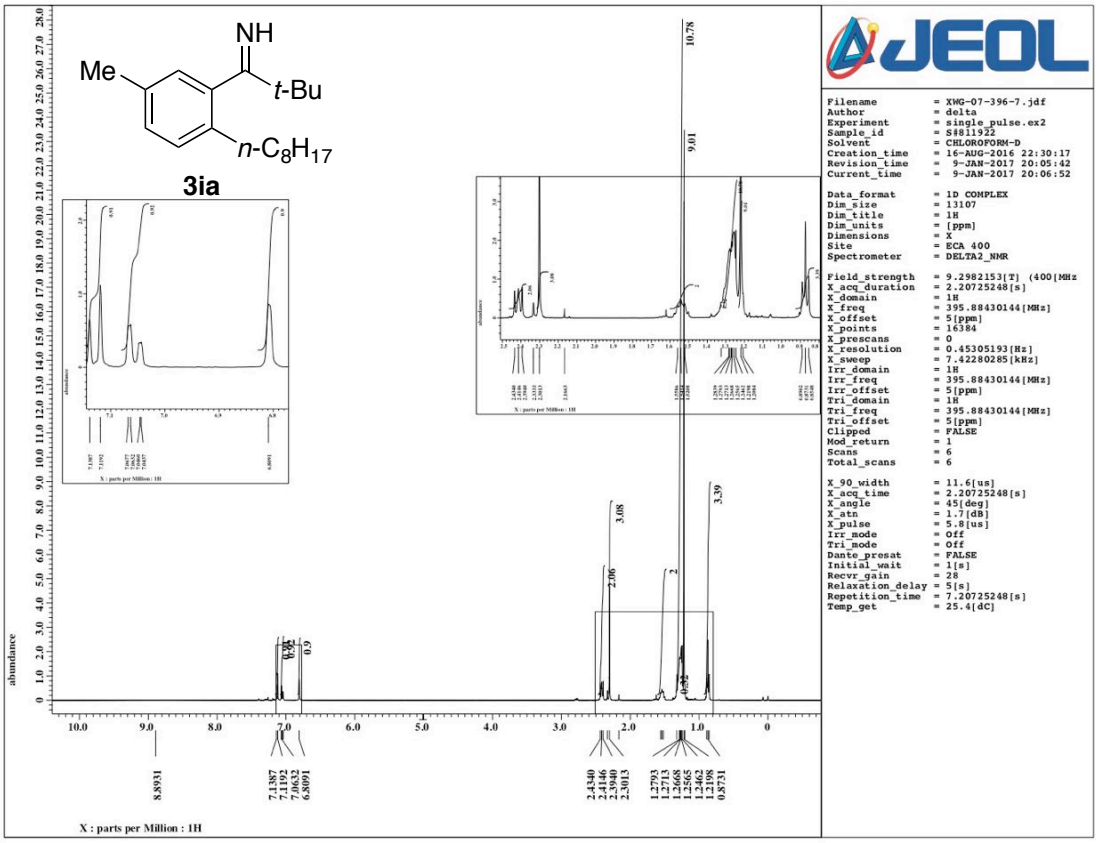

```
Filename          = XWG-07-417-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8848219
Solvent           = CHLOROFORM-D
Creation_time     = 17-AUG-2016 23:33:56
Revision_time     =  9-JAN-2017 19:56:47
Current_time      =  9-JAN-2017 19:57:50

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 36
Total_scans       = 36

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.6[dC]
```

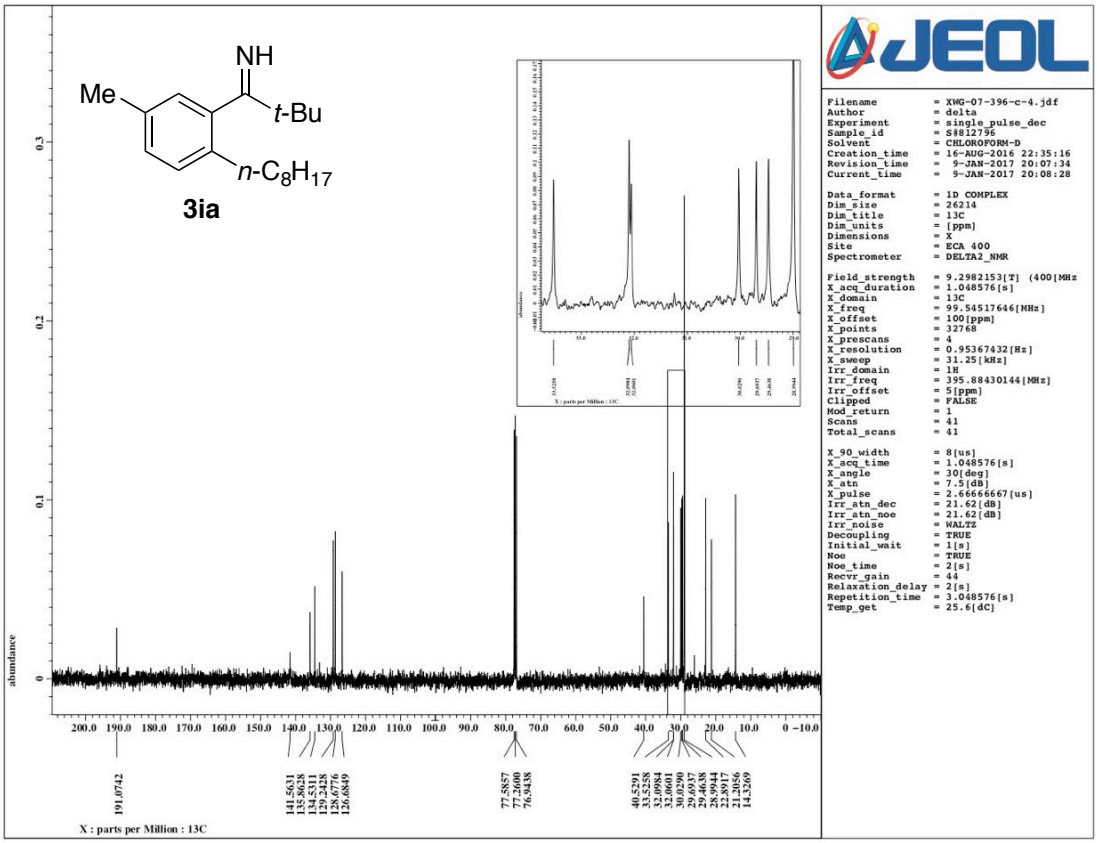

JEOL
O
t-Bu
Me2N
n-C8H17
3ga
abundance
X : parts per Million : 1H
19.72
6.33
3.24
3.39
2.1
1
0.97
1.0
7.2600
7.2074
7.1856
6.5459
6.5390
6.4932
2.9708
2.5233
2.5039
2.4833
1.5860
1.5632
1.2942
1.2668
0.8914
0.8742
0.8571

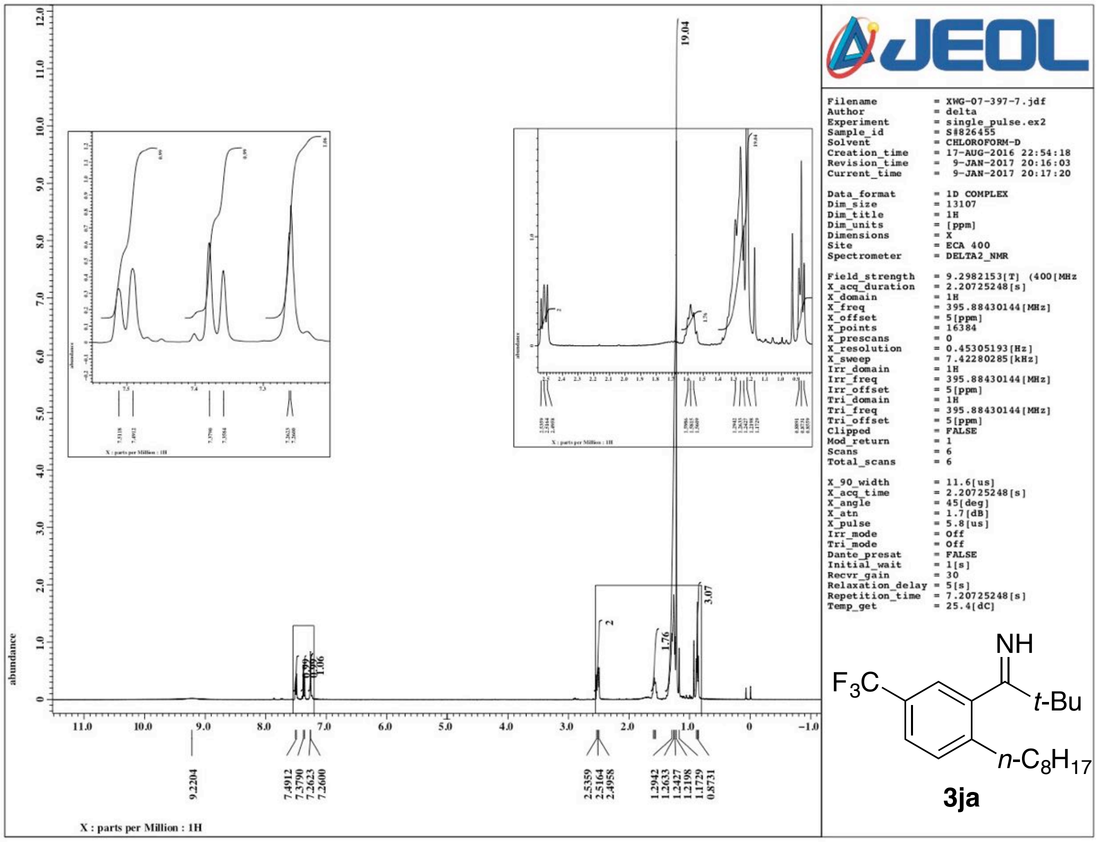

JEOL
O
t-Bu
Me2N
n-C8H17
3ga
abundance
X : parts per Million : 13C
213.7700
150.8464
142.4349
128.4668
127.1543
113.6269
108.3577
77.5857
77.2600
76.9439
44.9839
40.4907
34.5988
32.3954
32.1463
30.0961
29.7512
29.5309
28.4100
22.9204
14.3461

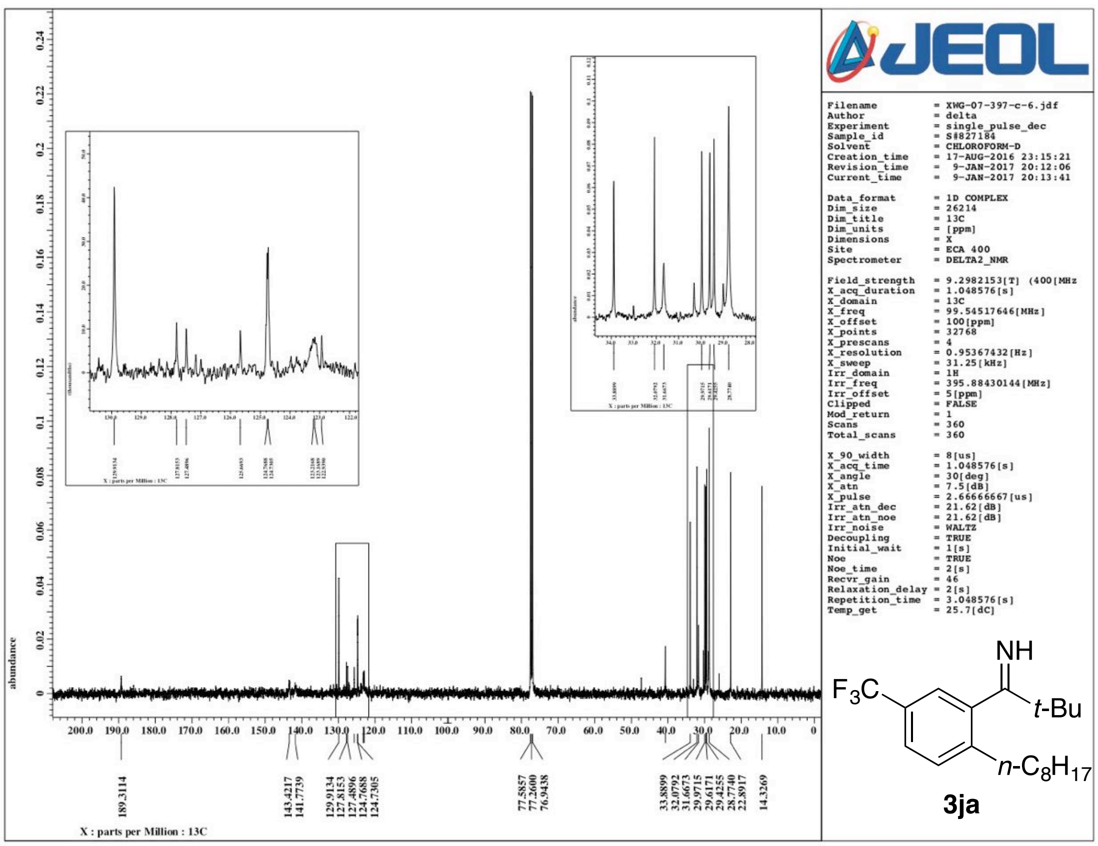

NH
t-Bu
F
n-C8H17
3ha
abundance
X : parts per Million : 1H
Filename = XWG-07-392-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#785075
Solvent = CHLOROFORM-D
Creation_time = 15-AUG-2016 21:45:35
Revision_time = 9-JAN-2017 20:00:06
Current_time = 9-JAN-2017 20:01:08
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 7
Total_scans = 7
X_90_width = 11.6[us]
X_acq_time = 2.207252248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 26
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]

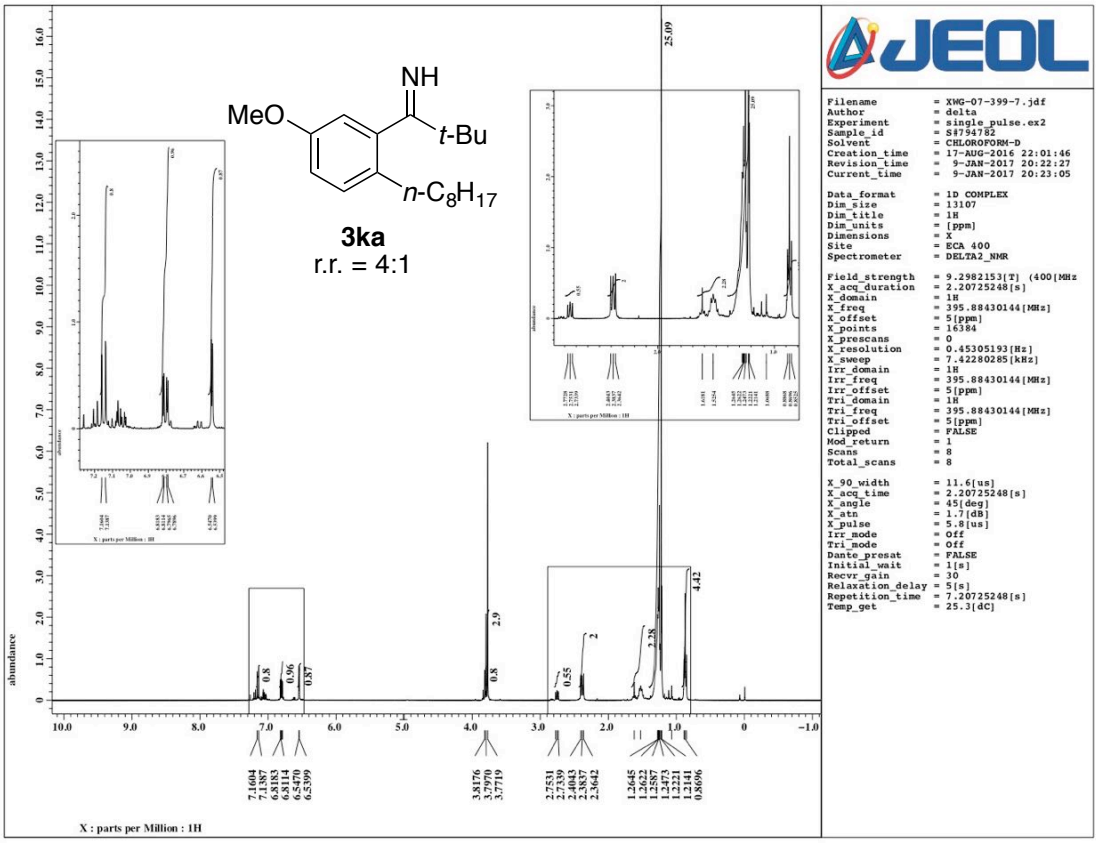

NH
t-Bu
F
n-C8H17
3ha
abundance
X : parts per Million : 13C
Filename = XWG-07-392-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#786027
Solvent = CHLOROFORM-D
Creation_time = 15-AUG-2016 21:51:13
Revision_time = 9-JAN-2017 20:01:42
Current_time = 9-JAN-2017 20:02:32
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 52
Total_scans = 52
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]

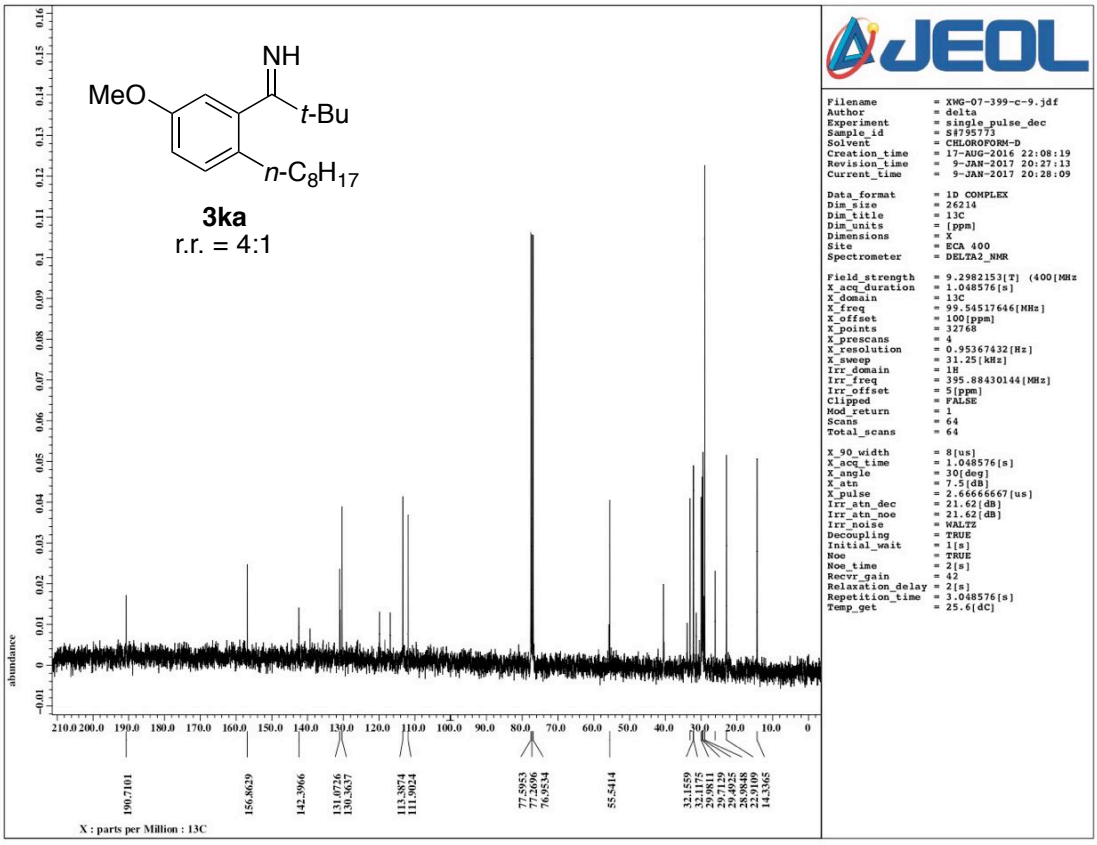

NH
Me
t-Bu
n-C8H17
3ia
abundance
X : parts per Million : 1H
Filename = XWG-07-396-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#811922
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 22:30:17
Revision_time = 9-JAN-2017 20:05:42
Current_time = 9-JAN-2017 20:06:52
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 28
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]

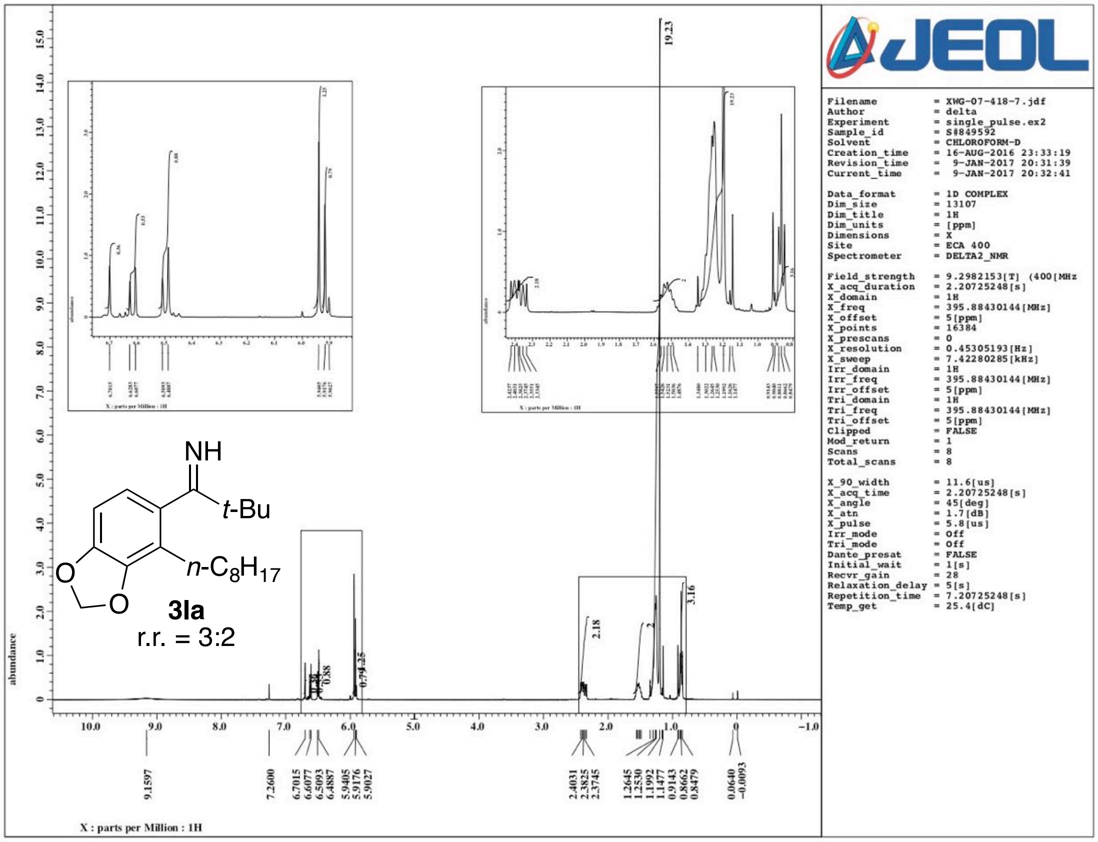

NH
Me
t-Bu
n-C8H17
3ia
abundance
X : parts per Million : 13C
Filename = XWG-07-396-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#812796
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 22:35:16
Revision_time = 9-JAN-2017 20:07:34
Current_time = 9-JAN-2017 20:08:28
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 41
Total_scans = 41
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]

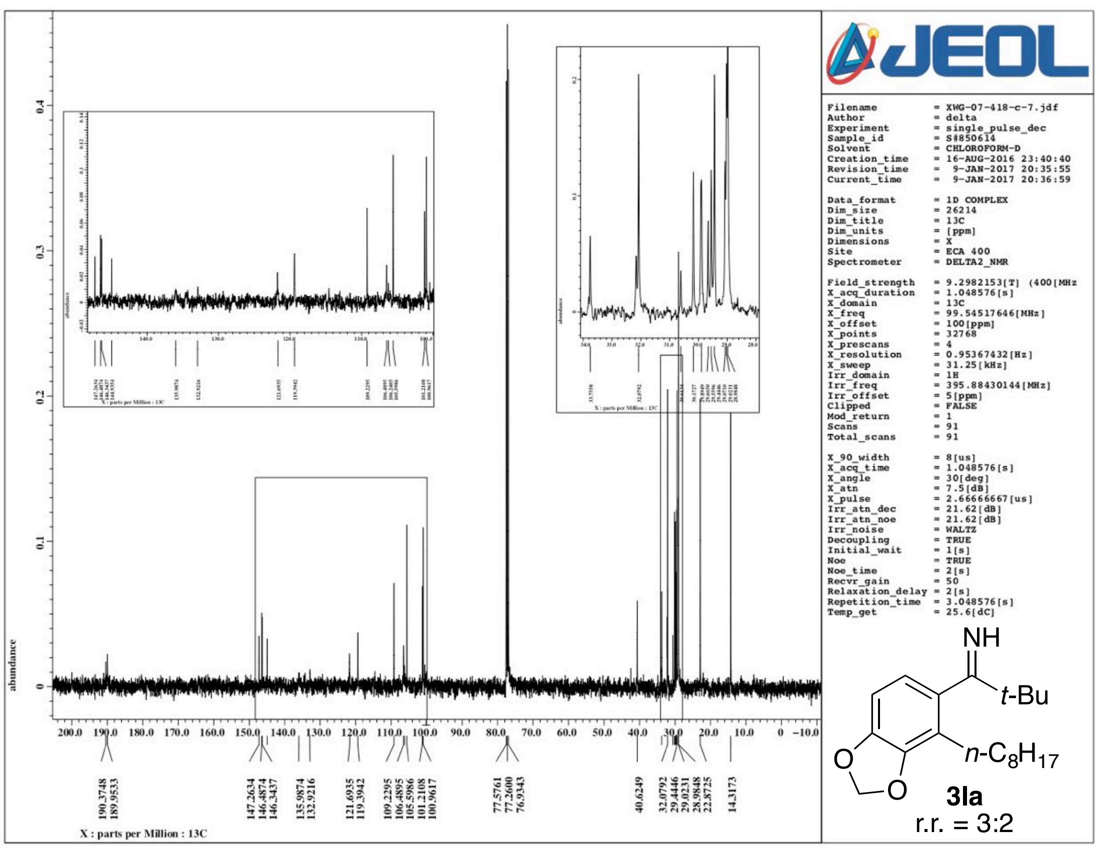

Filename = XWG-07-397-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#826455
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2016 22:54:18
Revision_time = 9-JAN-2017 20:16:03
Current_time = 9-JAN-2017 20:17:20
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]
X : parts per Million : 1H
abundance
9.2204
7.4912
7.3790
7.2623
7.2600
2.5359
2.5164
2.4958
1.2942
1.2633
1.2427
1.2198
1.1729
0.8731
19.04
3.07
2
1.76
1.06
NH
F_3C
t-Bu
n-C_8H_{17}
3ja

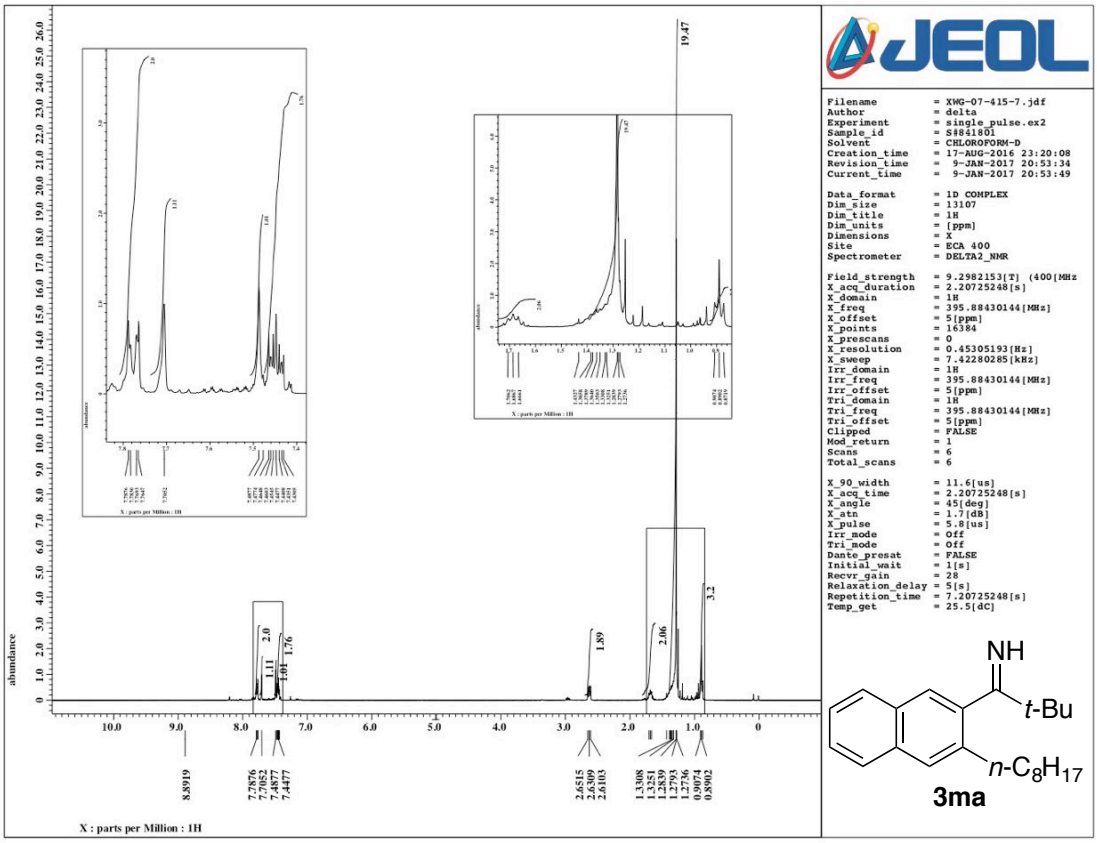

Filename = XWG-07-397-c-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#827184
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2016 23:15:21
Revision_time = 9-JAN-2017 20:12:06
Current_time = 9-JAN-2017 20:13:41
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 360
Total_scans = 360
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 46
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]
X : parts per Million : 13C
abundance
189.3114
143.4217
141.7739
129.9134
127.8153
127.4896
124.7688
124.7305
77.5857
77.2600
76.9438
33.8899
32.0792
31.6673
29.9715
29.6171
29.4255
28.7740
22.8917
14.3269
NH
F_3C
t-Bu
n-C_8H_{17}
3ja

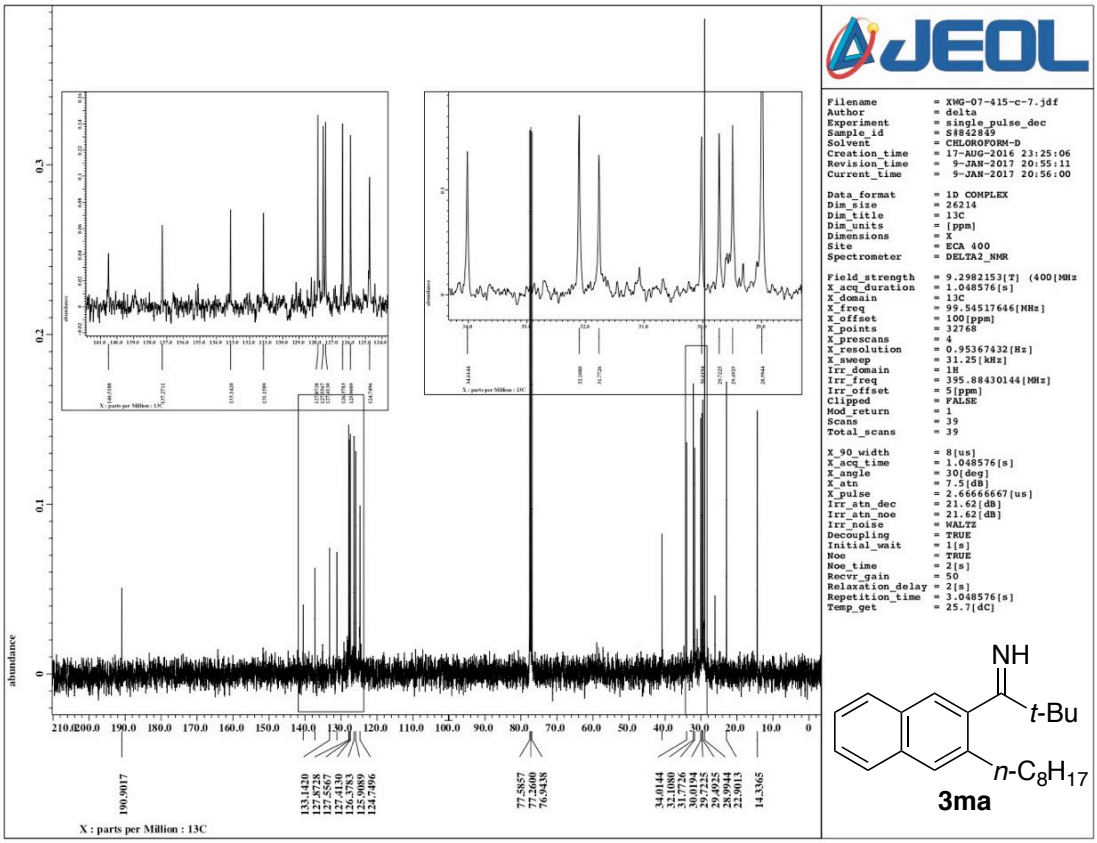

NH
MeO
t-Bu
n-C8H17
3ka
r.r. = 4:1
abundance
X : parts per Million : 1H
Filename = XWG-07-399-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#794782
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2016 22:01:46
Revision_time = 9-JAN-2017 20:22:27
Current_time = 9-JAN-2017 20:23:05
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.207252248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.3[dC]

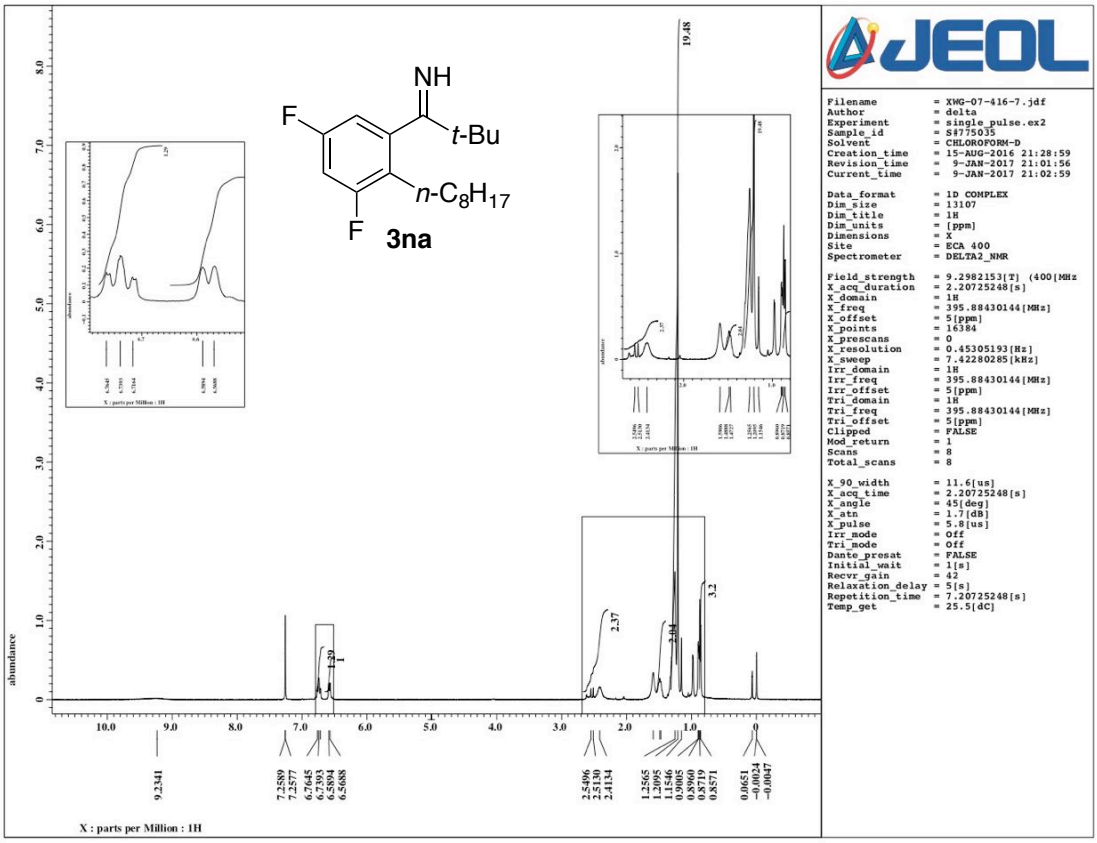

NH
MeO
t-Bu
n-C8H17
3ka
r.r. = 4:1
abundance
X : parts per Million : 13C
Filename = XWG-07-399-c-9.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#795773
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2016 22:08:19
Revision_time = 9-JAN-2017 20:27:13
Current_time = 9-JAN-2017 20:28:09
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 64
Total_scans = 64
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 42
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]

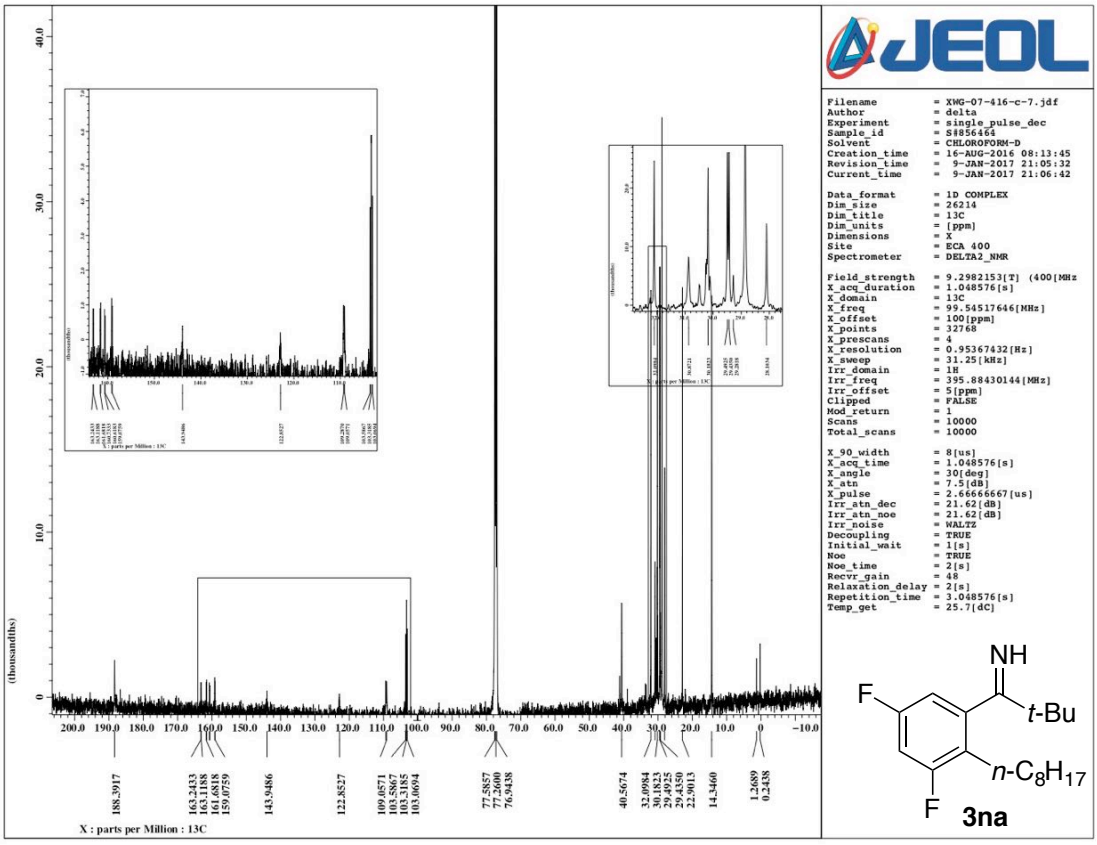

JEOL
Filename = XWG-07-418-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8849592
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 23:33:19
Revision_time = 9-JAN-2017 20:31:39
Current_time = 9-JAN-2017 20:32:41
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 28
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]
NH
t-Bu
n-C8H17
3la
r.r. = 3:2
abundance
X : parts per Million : 1H
9.1597
7.2600
6.7015
6.6077
6.5093
6.4887
5.9405
5.9176
5.9027
2.4031
2.3825
2.3745
1.2645
1.2530
1.1992
1.1477
0.9143
0.8662
0.8479
0.0640
−0.0093
19.23
2.18
3.16
0.88

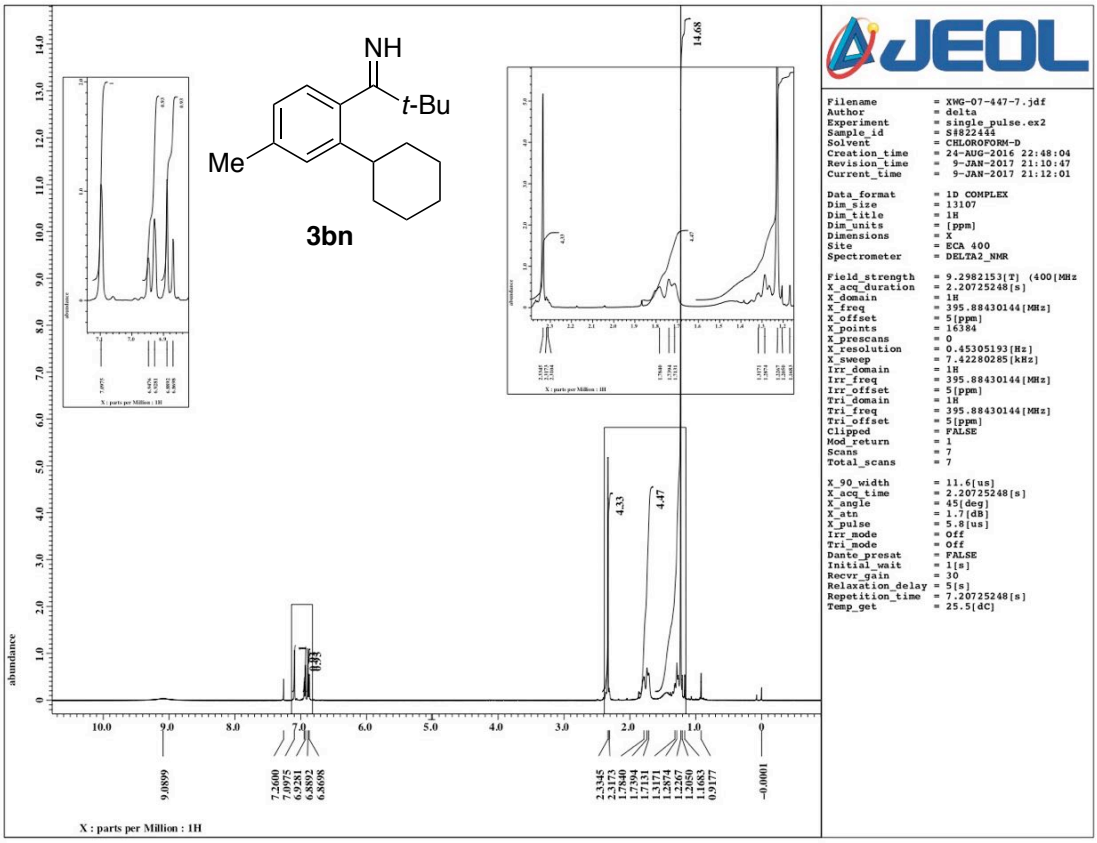

JEOL
Filename = XWG-07-418-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8850614
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 23:40:40
Revision_time = 9-JAN-2017 20:35:55
Current_time = 9-JAN-2017 20:36:59
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 91
Total_scans = 91
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
NH
t-Bu
n-C8H17
3la
r.r. = 3:2
abundance
X : parts per Million : 13C
190.3748
189.9533
147.2634
146.4874
146.3437
135.9874
132.9216
121.6935
119.3942
109.2295
106.4895
105.5986
101.2108
100.9617
77.5761
77.2600
76.9343
40.6249
32.0792
29.4446
29.0231
28.9848
22.8725
14.3173

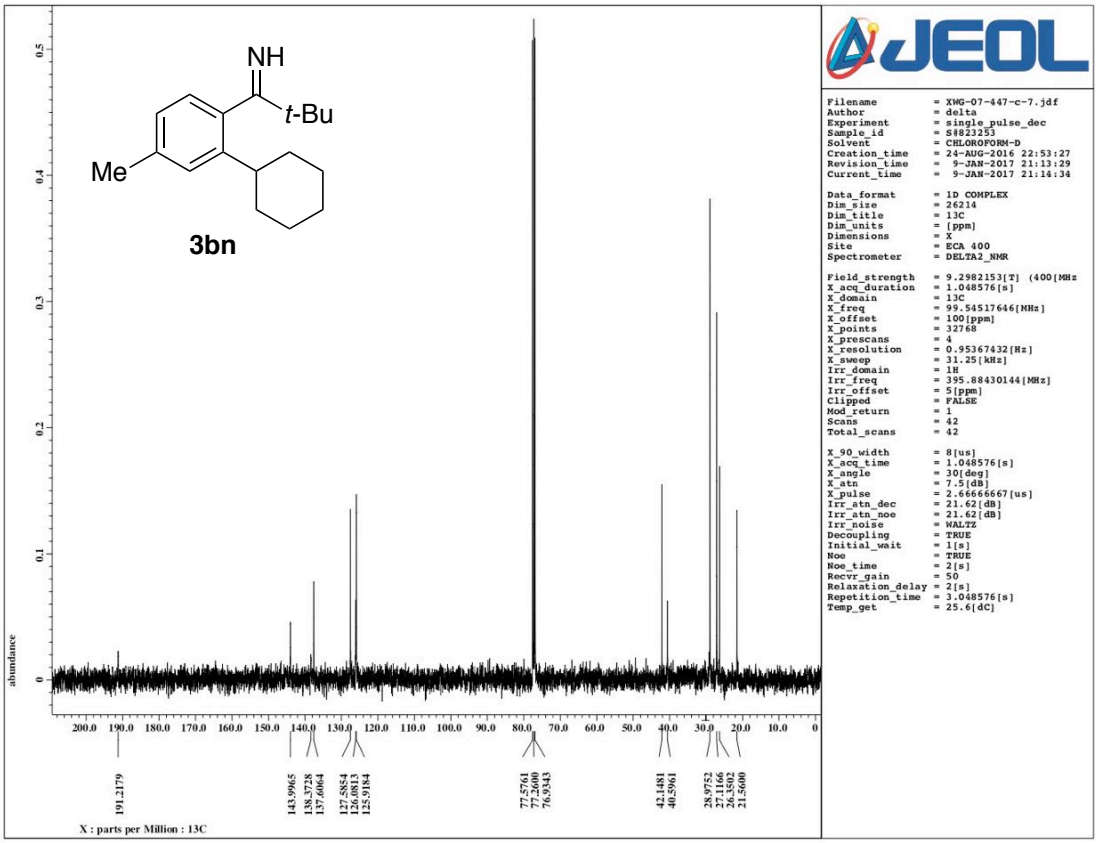

JEOL
Filename = XWG-07-415-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#841801
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2016 23:20:08
Revision_time = 9-JAN-2017 20:53:34
Current_time = 9-JAN-2017 20:53:49
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 28
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]
NH
t-Bu
n-C8H17
3ma
abundance
X : parts per Million : 1H
8.8919
7.7876
7.7052
7.4877
7.4477
2.6515
2.6300
2.6103
1.3308
1.3251
1.2930
1.2793
1.2736
0.9074
0.8902

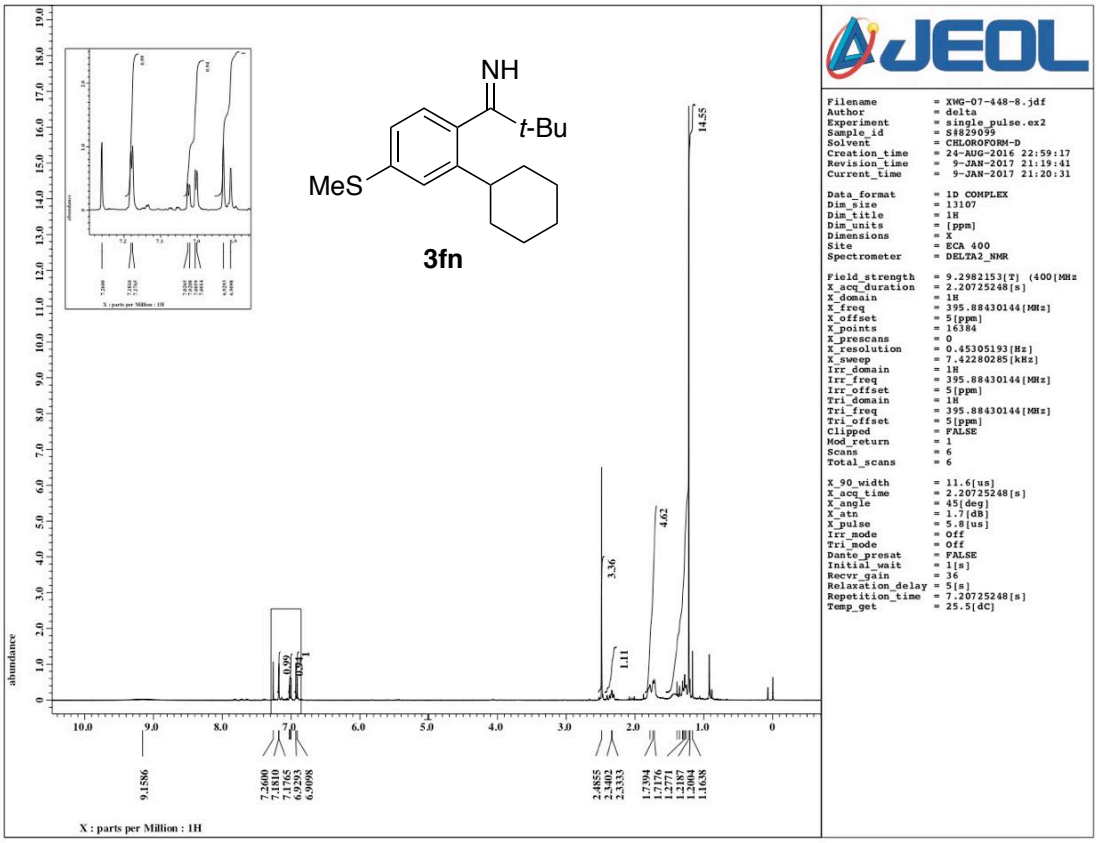

JEOL
Filename = XWG-07-415-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#842849
Solvent = CHLOROFORM-D
Creation_time = 17-AUG-2016 23:25:06
Revision_time = 9-JAN-2017 20:55:11
Current_time = 9-JAN-2017 20:56:00
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 39
Total_scans = 39
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]
NH
t-Bu
n-C8H17
3ma
abundance
X : parts per Million : 13C
190.9017
133.1420
127.8728
127.5867
127.4110
126.3783
125.9089
124.7496
77.5857
77.2600
76.9438
34.0144
32.1080
31.7726
30.0194
29.7125
29.4925
28.9944
22.9013
14.3365


NH
F
t-Bu
n-C8H17
F
3na
abundance
X : parts per Million : 1H
9.2341
7.2589
7.2577
6.7645
6.7393
6.5894
6.5688
2.5496
2.5130
2.4134
1.2565
1.2095
1.1546
0.9005
0.8769
0.8571
0.0651
-0.0024
-0.0047
Filename = XWG-07-416-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#775035
Solvent = CHLOROFORM-D
Creation_time = 15-AUG-2016 21:28:59
Revision_time = 9-JAN-2017 21:01:56
Current_time = 9-JAN-2017 21:02:59
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]

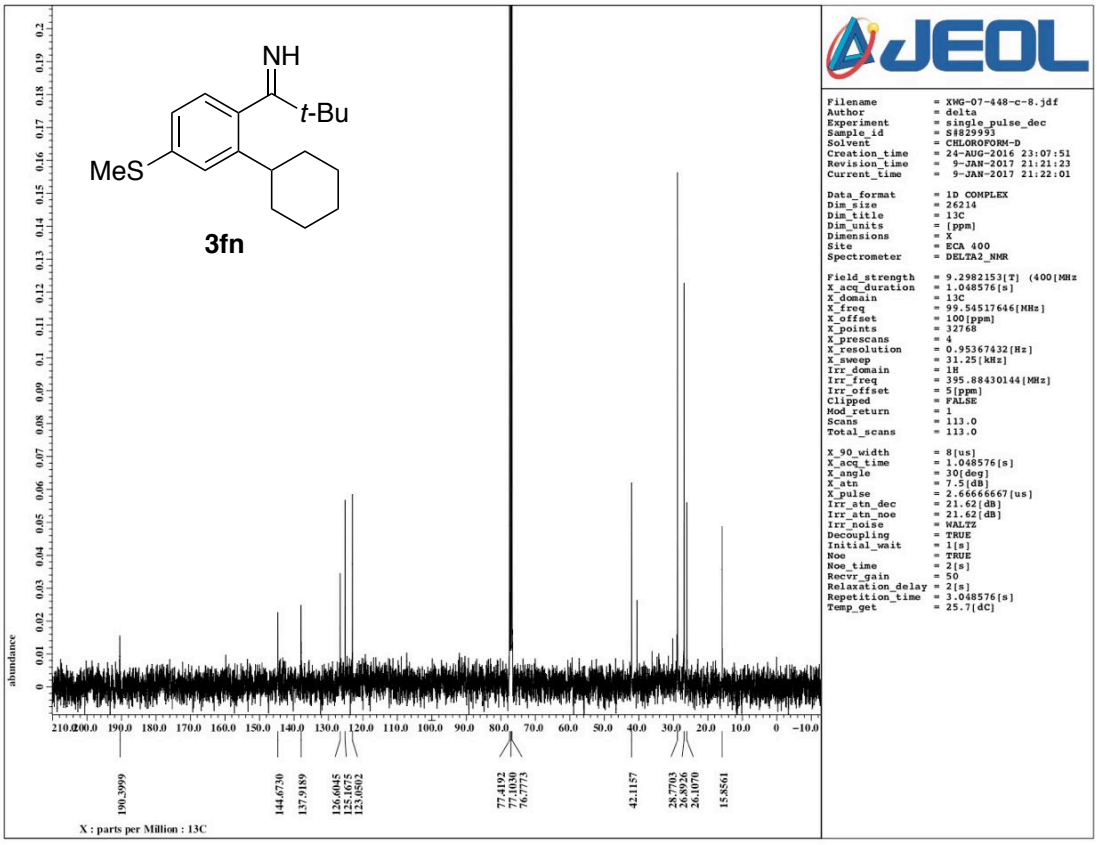

(thousandths)
X : parts per Million : 13C
188.3917
163.2433
163.1188
161.6818
159.0759
143.9486
122.8527
109.0871
103.5867
103.3185
103.0694
77.5857
77.2600
76.9438
40.5674
32.0984
30.1823
29.4925
29.4350
22.9013
14.3460
1.2689
0.2438
Filename = XWG-07-416-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#856464
Solvent = CHLOROFORM-D
Creation_time = 16-AUG-2016 08:13:45
Revision_time = 9-JAN-2017 21:05:32
Current_time = 9-JAN-2017 21:06:42
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 48
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]
NH
F
t-Bu
n-C8H17
F
3na


NH
t-Bu
Me
3bn
14.68
4.33
4.47
abundance
X : parts per Million : 1H
9.0899
7.2600
7.0975
6.9291
6.8892
6.8698
2.3345
2.3173
1.7840
1.7004
1.7133
1.3171
1.2874
1.2267
1.0980
1.1683
0.9177
0.0001
Filename = XWG-07-447-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#822444
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 22:48:04
Revision_time = 9-JAN-2017 21:10:47
Current_time = 9-JAN-2017 21:12:01
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 7
Total_scans = 7
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]

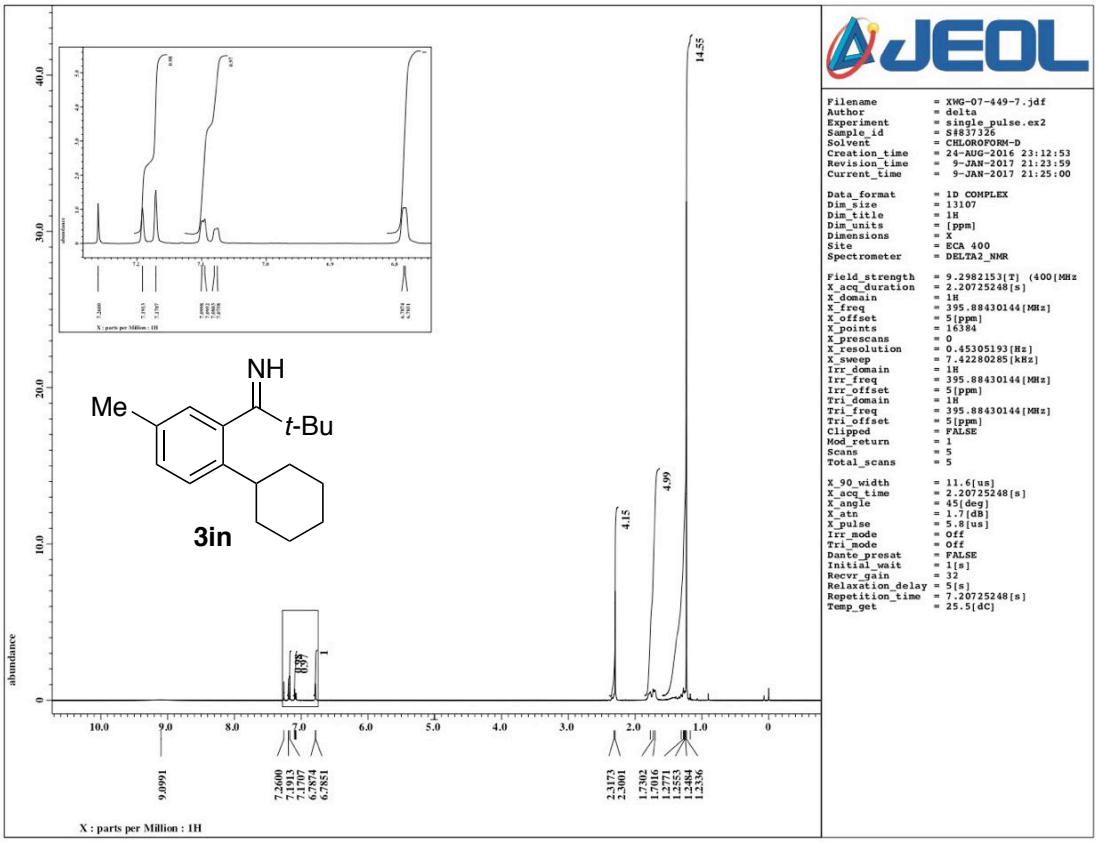

NH
t-Bu
Me
3bn
abundance
X : parts per Million : 13C
191.2179
143.9965
138.3728
137.6064
127.5854
126.6813
125.9184
77.5761
77.2600
76.9343
42.1481
40.5961
28.9752
27.1166
25.5502
21.5600
Filename = XWG-07-447-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#823253
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 22:53:27
Revision_time = 9-JAN-2017 21:13:29
Current_time = 9-JAN-2017 21:14:34
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 42
Total_scans = 42
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]

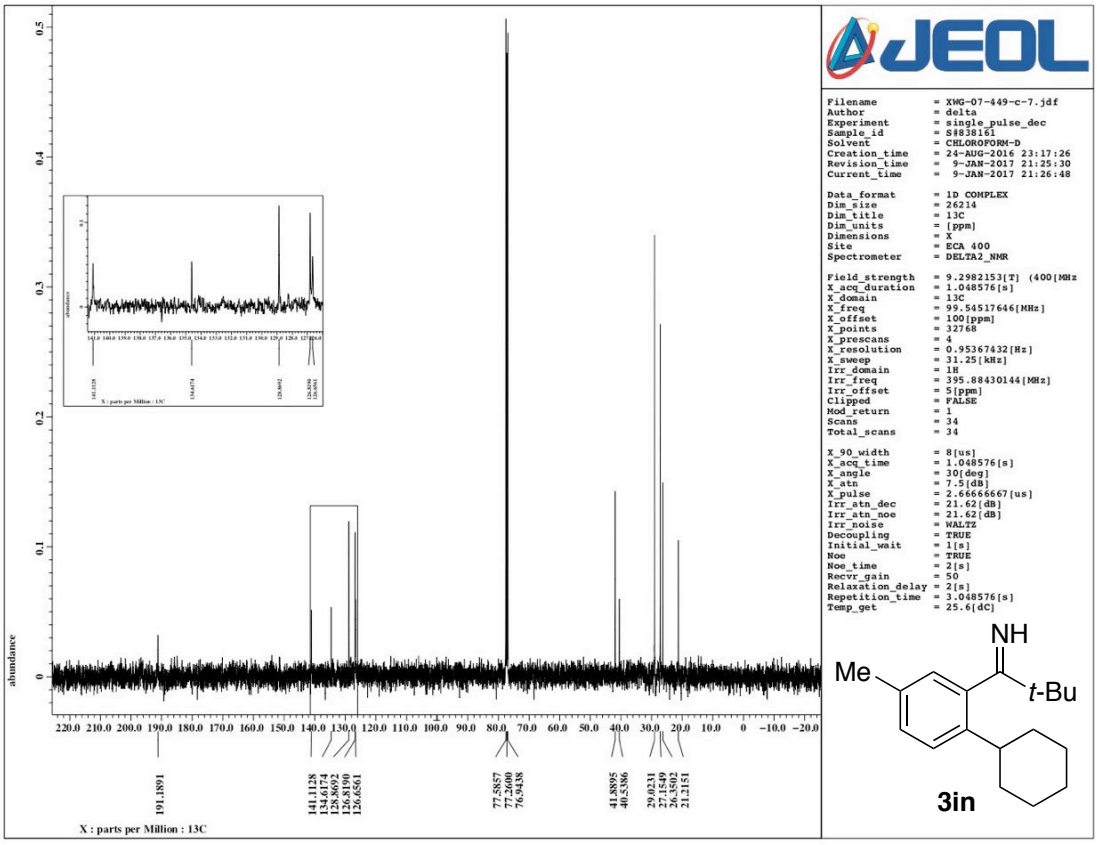


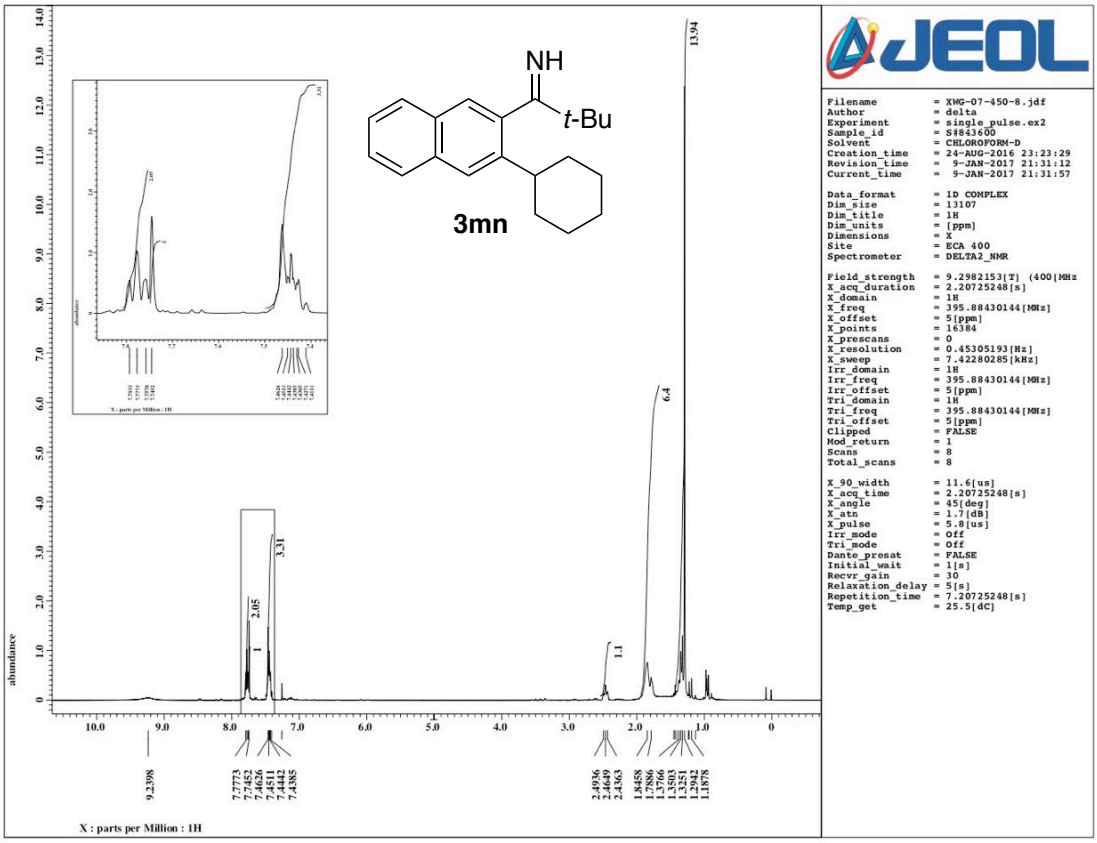

```
Filename          = XWG-07-448-8.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8829099
Solvent           = CHLOROFORM-D
Creation_time     = 24-AUG-2016 22:59:17
Revision_time     =  9-JAN-2017 21:19:41
Current_time      =  9-JAN-2017 21:20:31

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 6
Total_scans       = 6

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.5[dC]
```

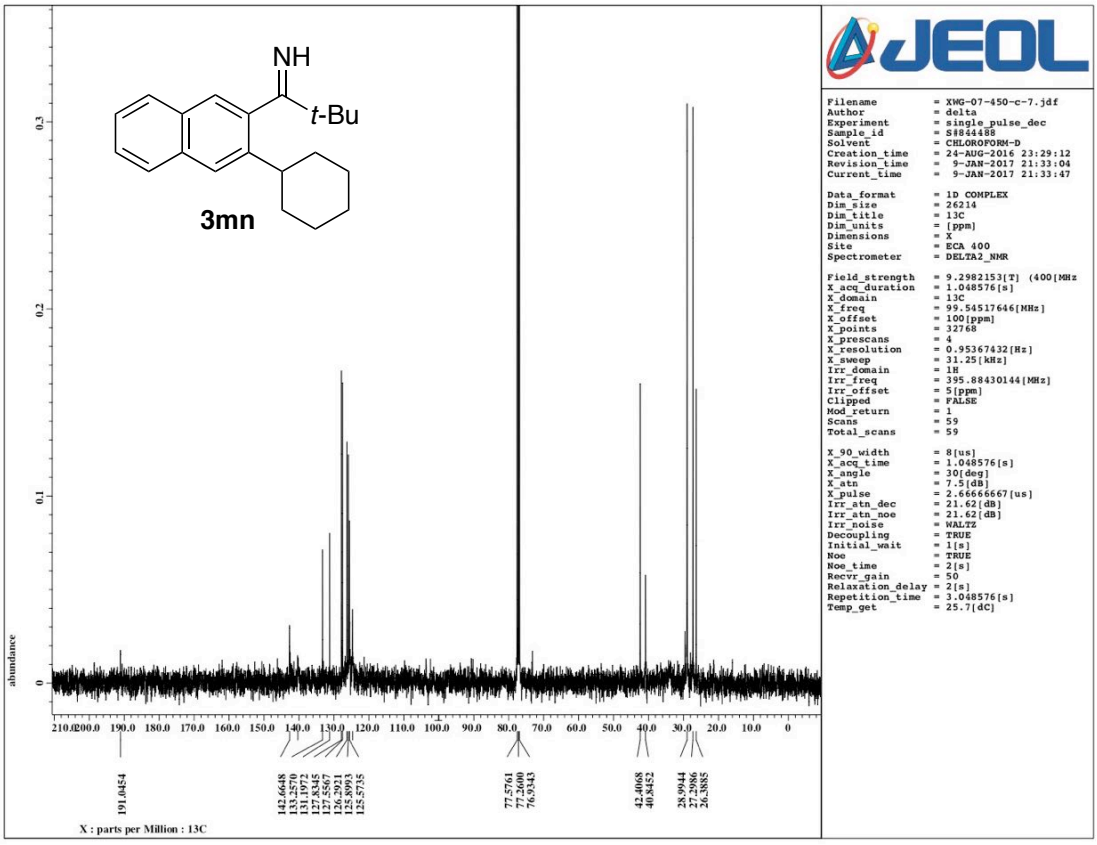


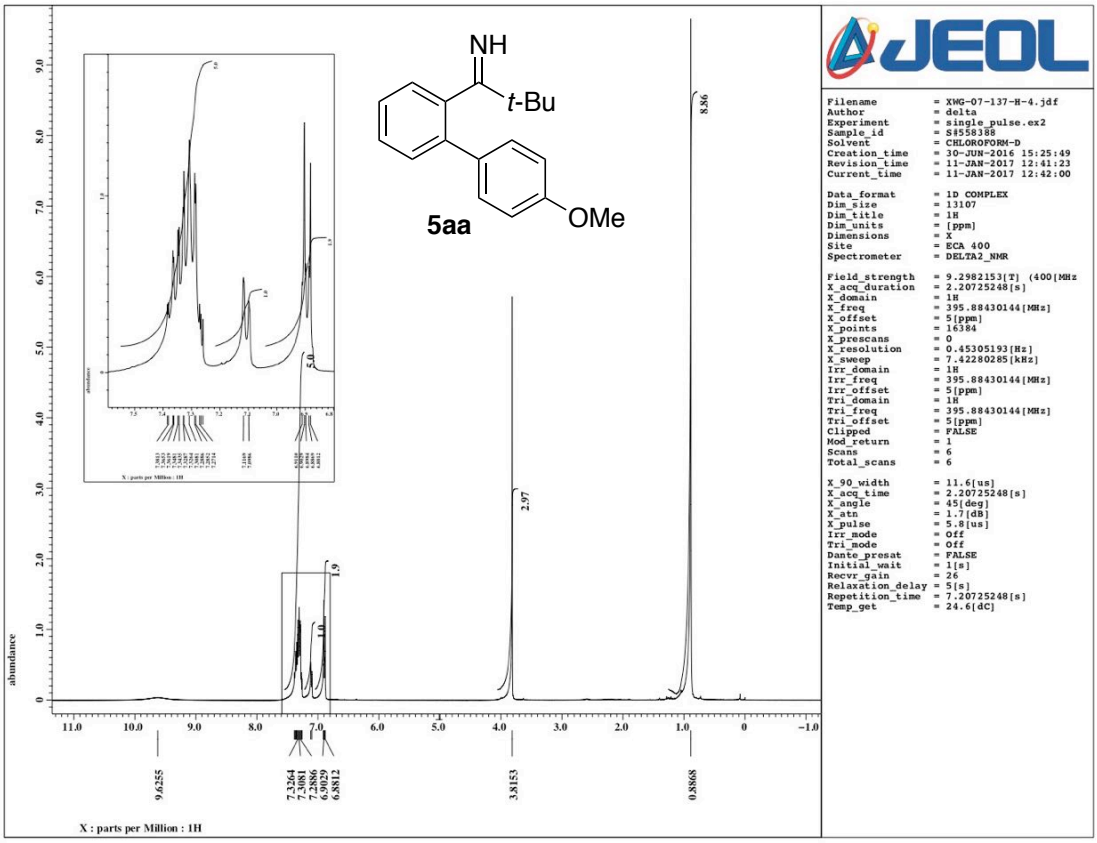

```
Filename          = XWG-07-448-c-8.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8829993
Solvent           = CHLOROFORM-D
Creation_time     = 24-AUG-2016 23:07:51
Revision_time     =  9-JAN-2017 21:21:23
Current_time      =  9-JAN-2017 21:22:01

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 113.0
Total_scans       = 113.0

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.7[dC]
```


Filename = XWG-07-449-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#837326
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 23:12:53
Revision_time = 9-JAN-2017 21:23:59
Current_time = 9-JAN-2017 21:25:00
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]
NH
Me
t-Bu
3in
abundance
14.55
4.99
4.15
9.0991
7.2600
7.1913
7.1707
6.7854
6.7851
2.3173
2.3001
1.7302
1.7016
1.2771
1.2583
1.2404
1.2336
X : parts per Million : 1H

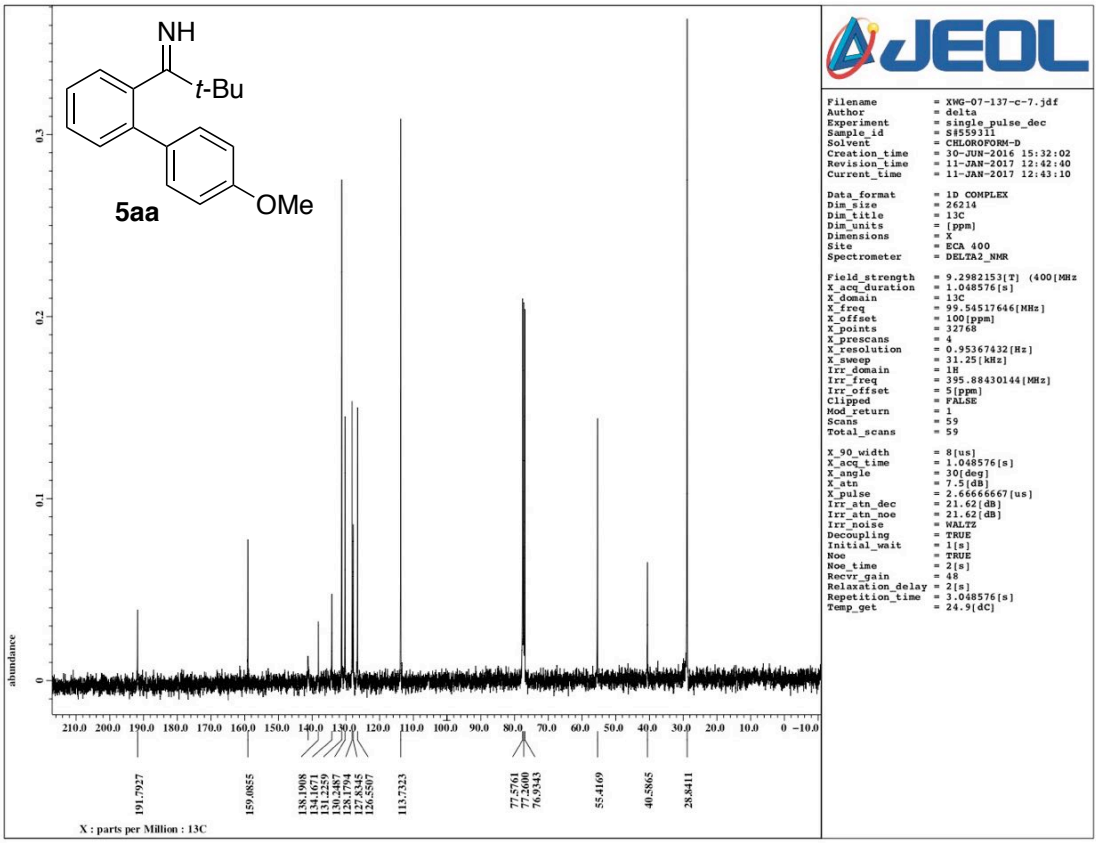

Filename = XWG-07-449-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#838161
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 23:17:26
Revision_time = 9-JAN-2017 21:25:30
Current_time = 9-JAN-2017 21:26:48
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 34
Total_scans = 34
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
NH
Me
t-Bu
3in
abundance
191.1891
141.1128
134.6174
128.8692
126.8190
126.6561
77.5857
77.1740
76.7438
41.8895
40.5386
29.0231
27.1549
26.3502
21.2151
X : parts per Million : 13C


NH
t-Bu
3mn
13.94
6.4
3.31
2.05
1
1.1
abundance
9.2398
7.7773
7.7452
7.4626
7.4511
7.4441
7.4385
2.4936
2.4669
2.4365
1.8458
1.7866
1.7066
1.3503
1.3251
1.2942
1.1878
X : parts per Million : 1H
Filename = XWG-07-450-8.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8843600
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 23:23:29
Revision_time = 9-JAN-2017 21:31:12
Current_time = 9-JAN-2017 21:31:57
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.207252248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.207252248[s]
Temp_get = 25.5[dC]

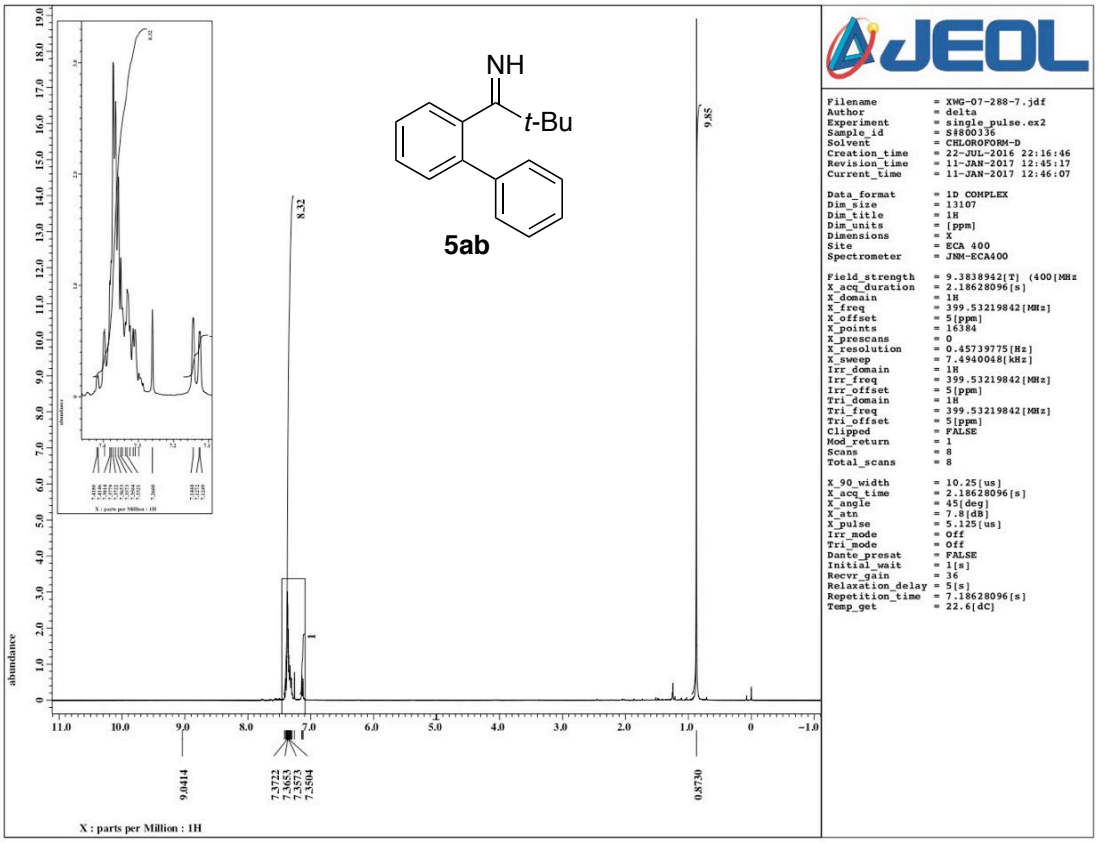

NH
t-Bu
3mn
abundance
191.0454
142.6648
133.2570
131.1972
127.8345
127.5567
126.2931
125.8993
125.5735
77.5761
77.2600
76.9343
42.4068
40.8452
28.9944
27.2986
26.3885
X : parts per Million : 13C
Filename = XWG-07-450-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8844488
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 23:29:12
Revision_time = 9-JAN-2017 21:33:04
Current_time = 9-JAN-2017 21:33:47
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 59
Total_scans = 59
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]

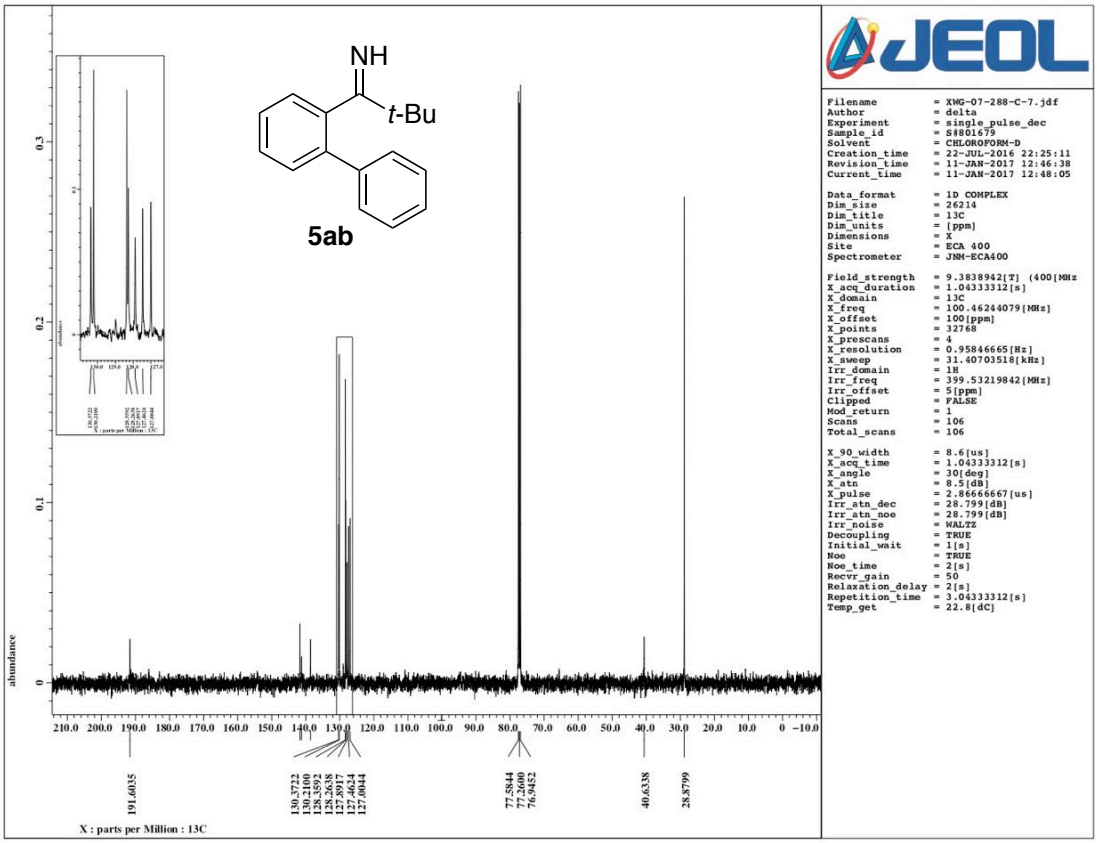


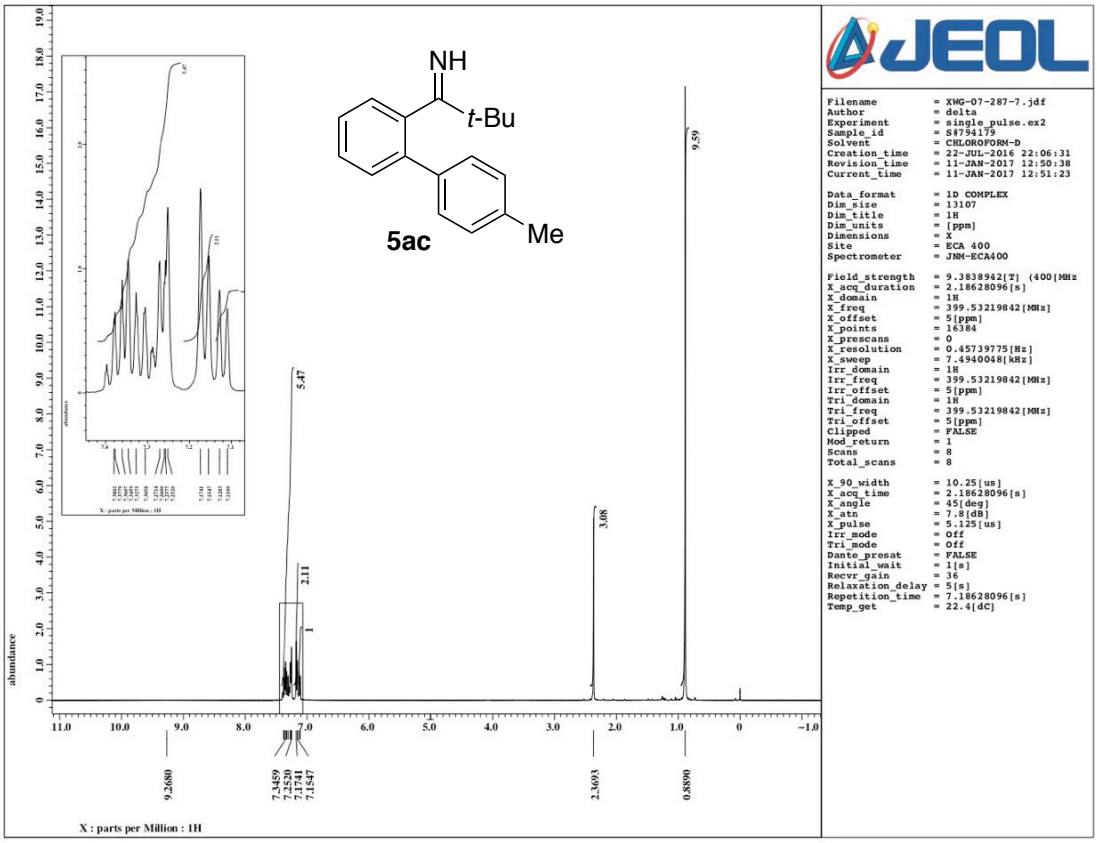

```
Filename          = XWG-07-137-H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#558388
Solvent           = CHLOROFORM-D
Creation_time     = 30-JUN-2016 15:25:49
Revision_time     = 11-JAN-2017 12:41:23
Current_time      = 11-JAN-2017 12:42:00

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 6
Total_scans       = 6

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 26
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 24.6[dC]
```

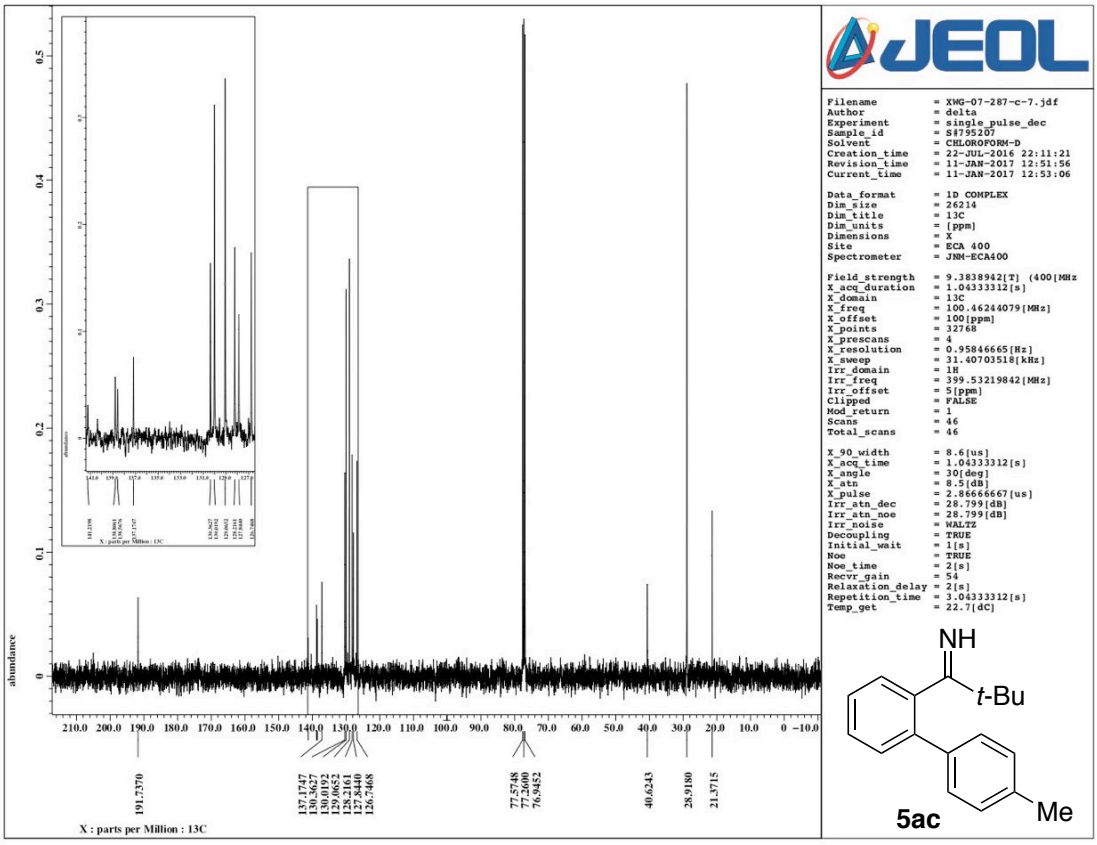


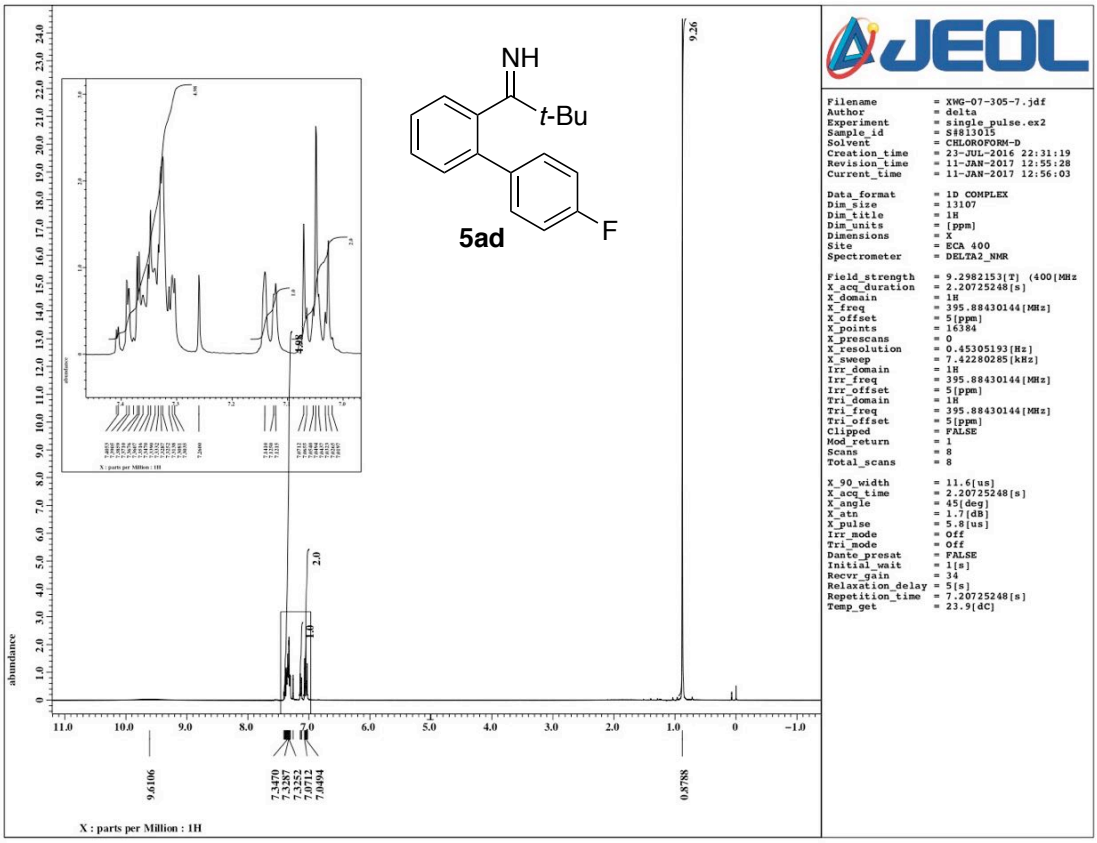

```
Filename          = XWG-07-137-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#559311
Solvent           = CHLOROFORM-D
Creation_time     = 30-JUN-2016 15:32:02
Revision_time     = 11-JAN-2017 12:42:40
Current_time      = 11-JAN-2017 12:43:10

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 59
Total_scans       = 59

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 48
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 24.9[dC]
```


NH
t-Bu
5ab
8.32
9.85
1
abundance
X : parts per Million : 1H
9.0414
7.3722
7.3653
7.3583
7.3504
0.8730
Filename = XWG-07-288-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#800336
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:16:46
Revision_time = 11-JAN-2017 12:45:17
Current_time = 11-JAN-2017 12:46:07
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.6[dC]

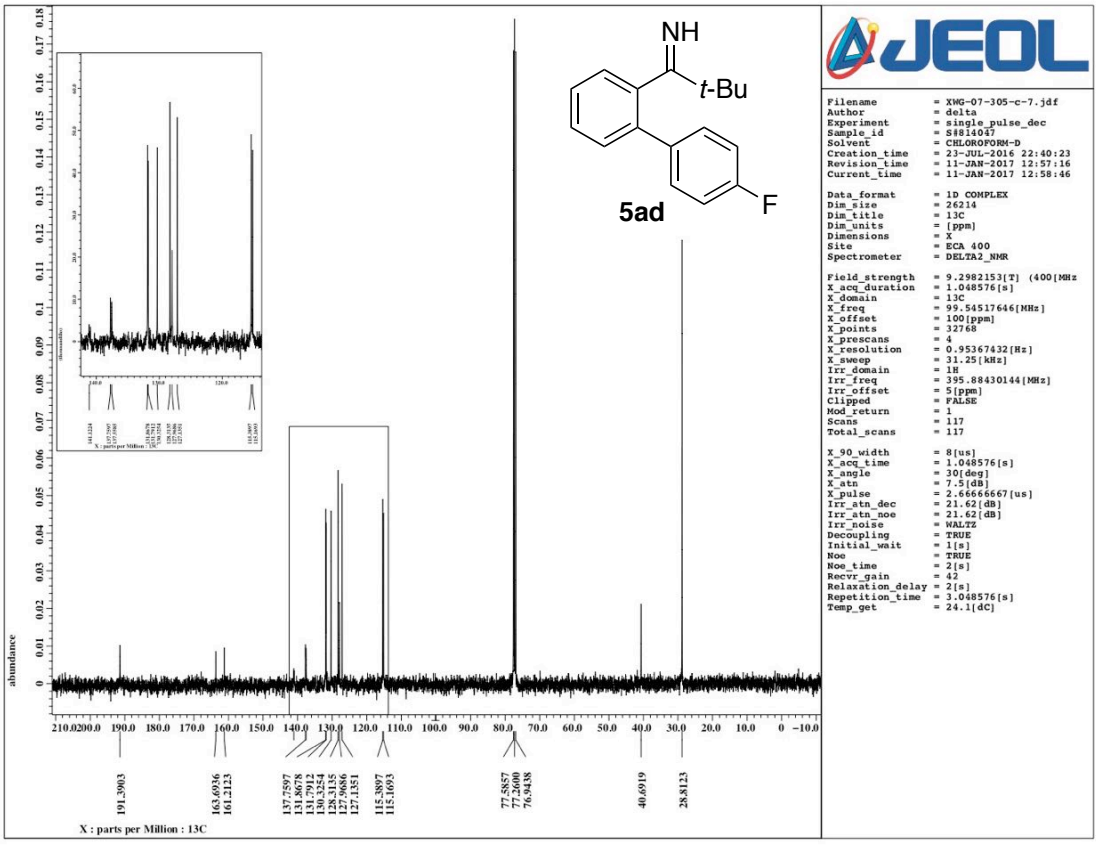

NH
t-Bu
5ab
abundance
X : parts per Million : 13C
191.6035
130.3722
130.2100
128.3592
128.2638
127.5037
127.4624
127.0044
77.5844
77.2660
76.9452
40.6338
28.8799
Filename = XWG-07-288-C-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#801679
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:25:11
Revision_time = 11-JAN-2017 12:46:38
Current_time = 11-JAN-2017 12:48:05
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 106
Total_scans = 106
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.8[dC]


NH
t-Bu
Me
5ac
9.59
5.47
2.11
3.08
abundance
X : parts per Million : 1H
9.2680
7.3459
7.2520
7.1741
7.1547
2.3693
0.8890
Filename = XWG-07-287-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#794179
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:06:31
Revision_time = 11-JAN-2017 12:50:38
Current_time = 11-JAN-2017 12:51:23
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.4[dC]

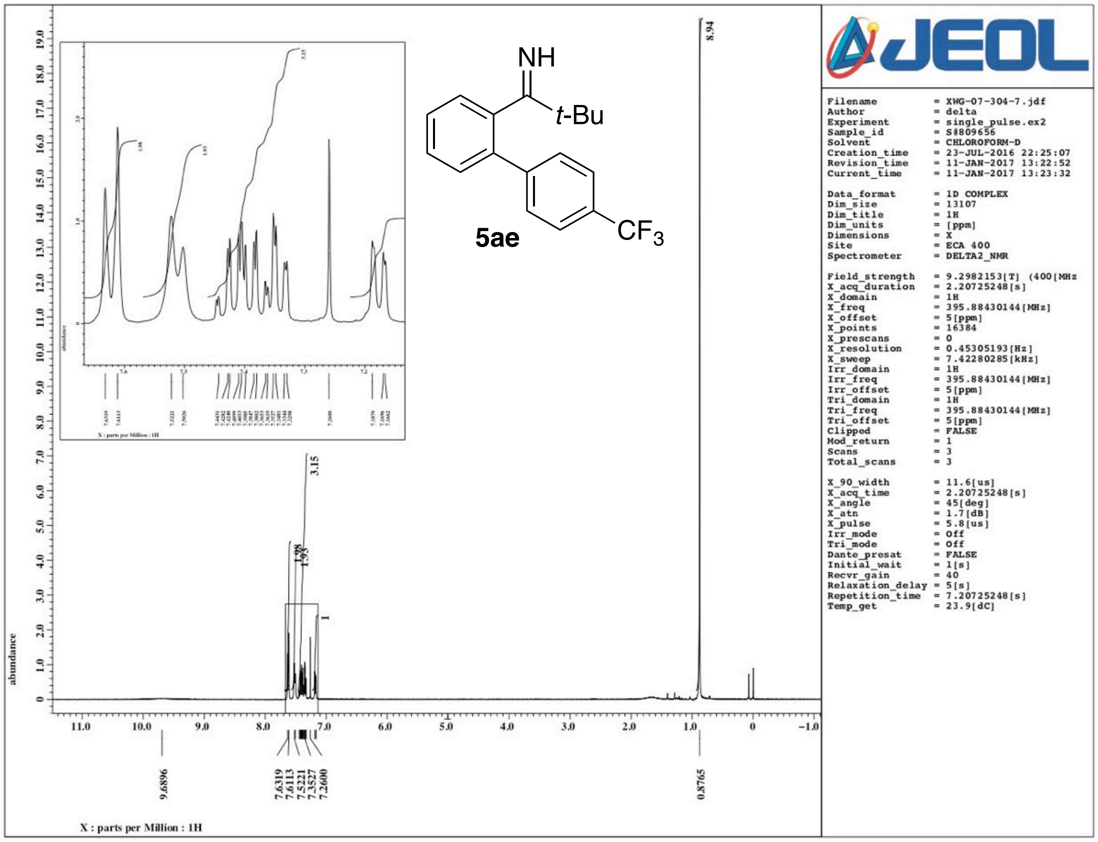

abundance
X : parts per Million : 13C
191.7370
137.1747
130.3627
130.0192
129.0652
128.2161
127.8440
126.7468
77.5748
77.2600
76.9452
40.6243
28.9180
21.3715
Filename = XWG-07-287-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#795207
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:11:21
Revision_time = 11-JAN-2017 12:51:56
Current_time = 11-JAN-2017 12:53:06
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 46
Total_scans = 46
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 54
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.7[dC]
NH
t-Bu
Me
5ac

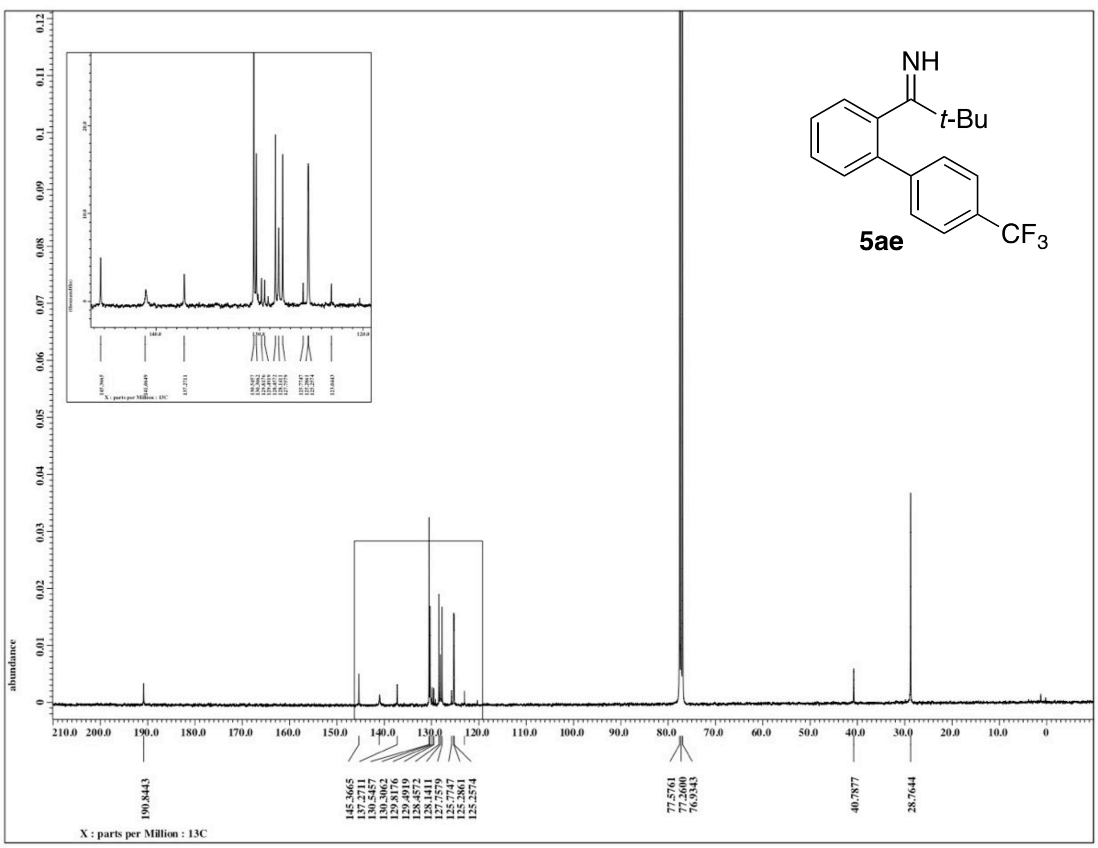


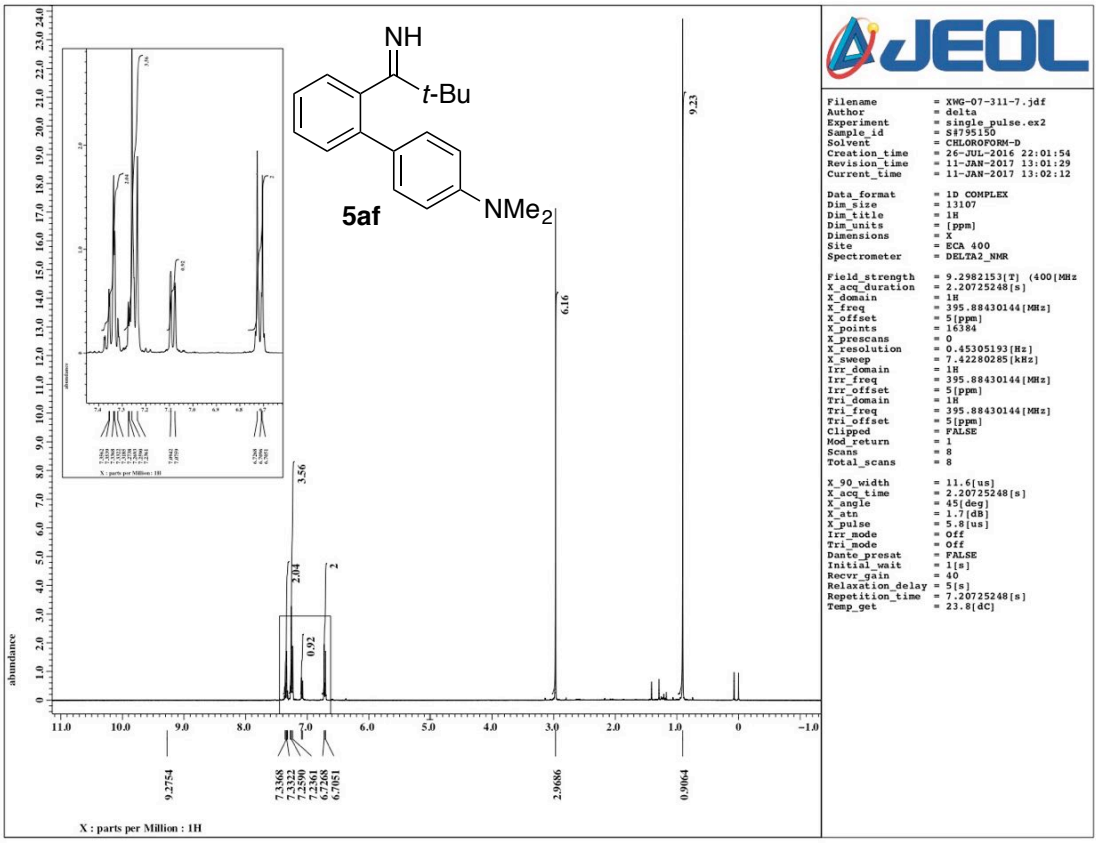

```
Filename          = XWG-07-305-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8813015
Solvent           = CHLOROFORM-D
Creation_time     = 23-JUL-2016 22:31:19
Revision_time     = 11-JAN-2017 12:55:28
Current_time      = 11-JAN-2017 12:56:03

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 2.207725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 5[s]
Repetition_time   = 7.207725248[s]
Temp_get          = 23.9[dC]
```

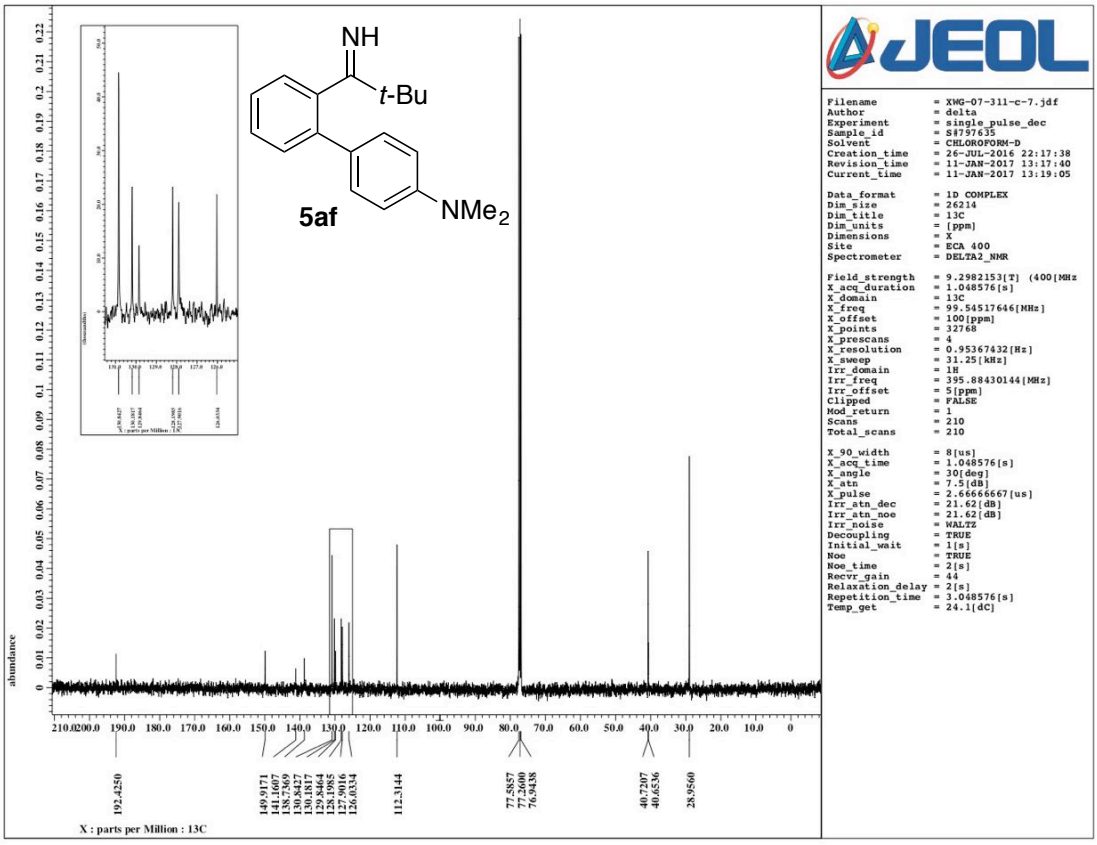


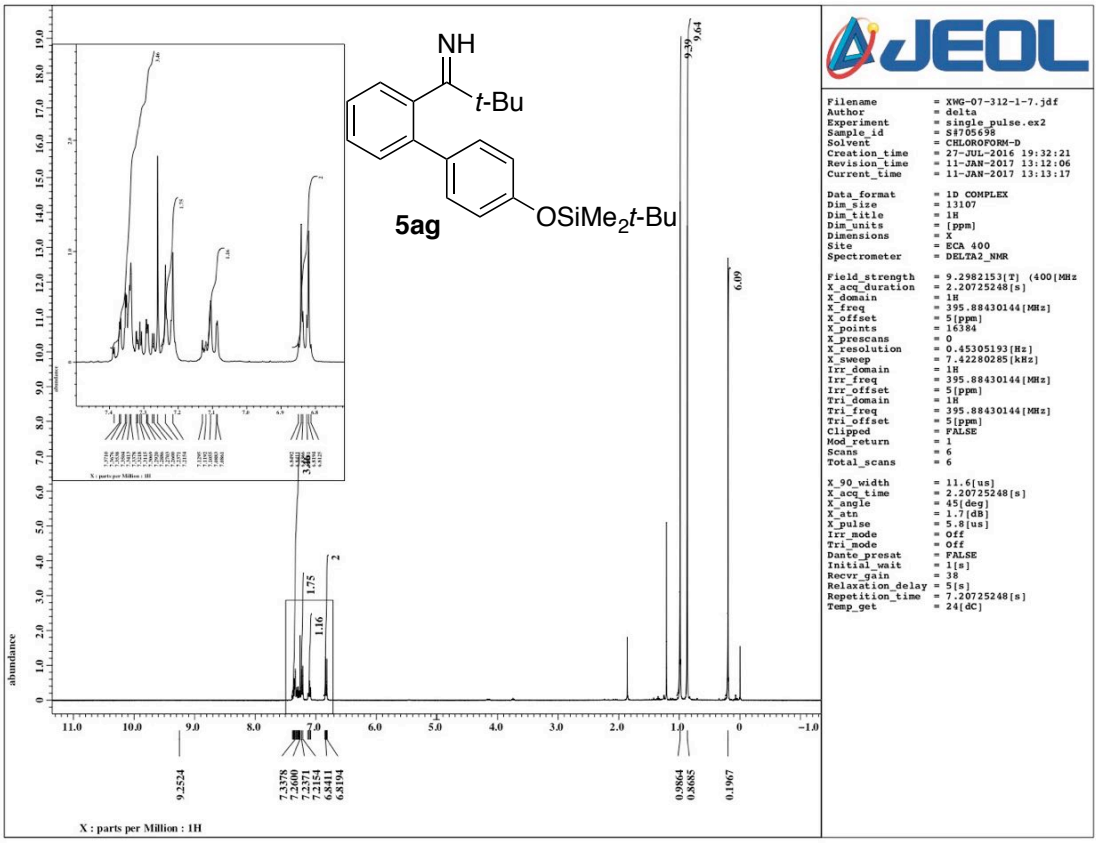

```
Filename          = XWG-07-305-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8814047
Solvent           = CHLOROFORM-D
Creation_time     = 23-JUL-2016 22:40:23
Revision_time     = 11-JAN-2017 12:57:16
Current_time      = 11-JAN-2017 12:58:46

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 117
Total_scans       = 117

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 42
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 24.1[dC]
```

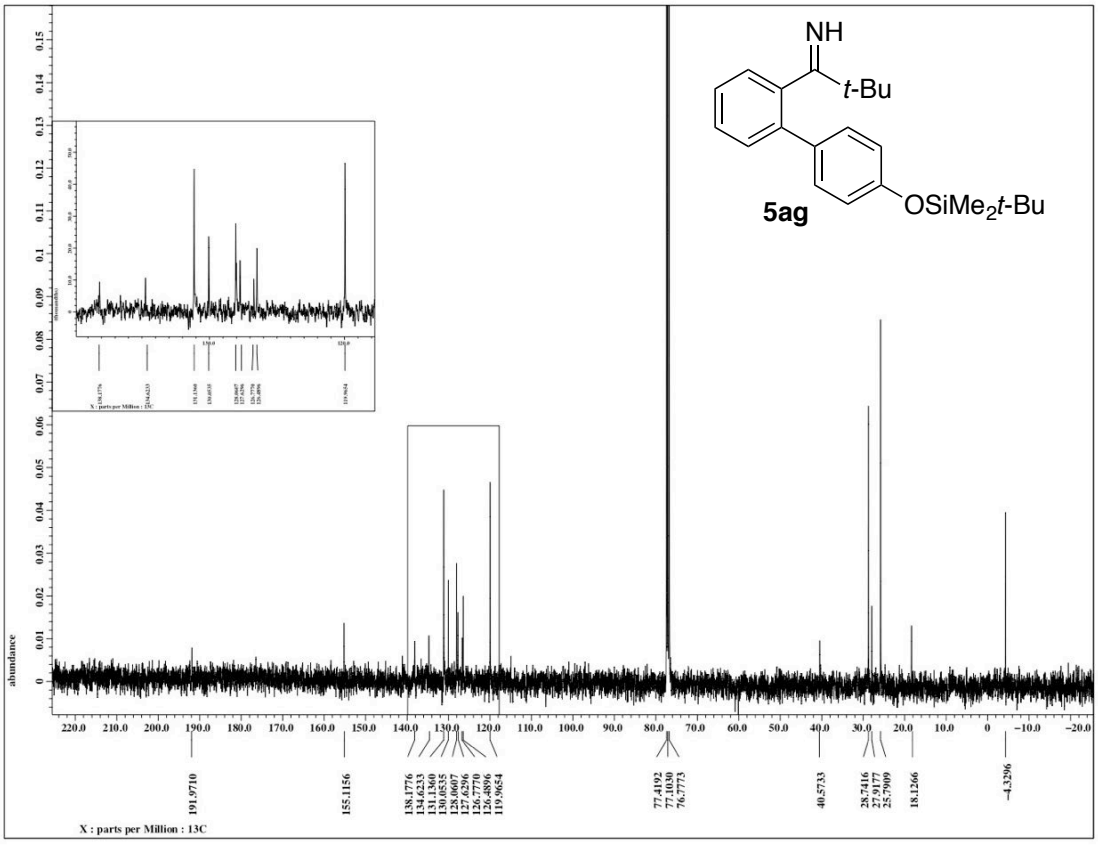

NH
t-Bu
CF3
5ae
JEOL
Filename = XWG-07-304-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#809656
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2016 22:25:07
Revision_time = 11-JAN-2017 13:22:52
Current_time = 11-JAN-2017 13:23:32
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3
Total_scans = 3
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 23.9[dC]
8.94
3.15
1.98
1.93
1
9.6896
7.6319
7.6113
7.5221
7.3527
7.2600
0.8765
abundance
X : parts per Million : 1H

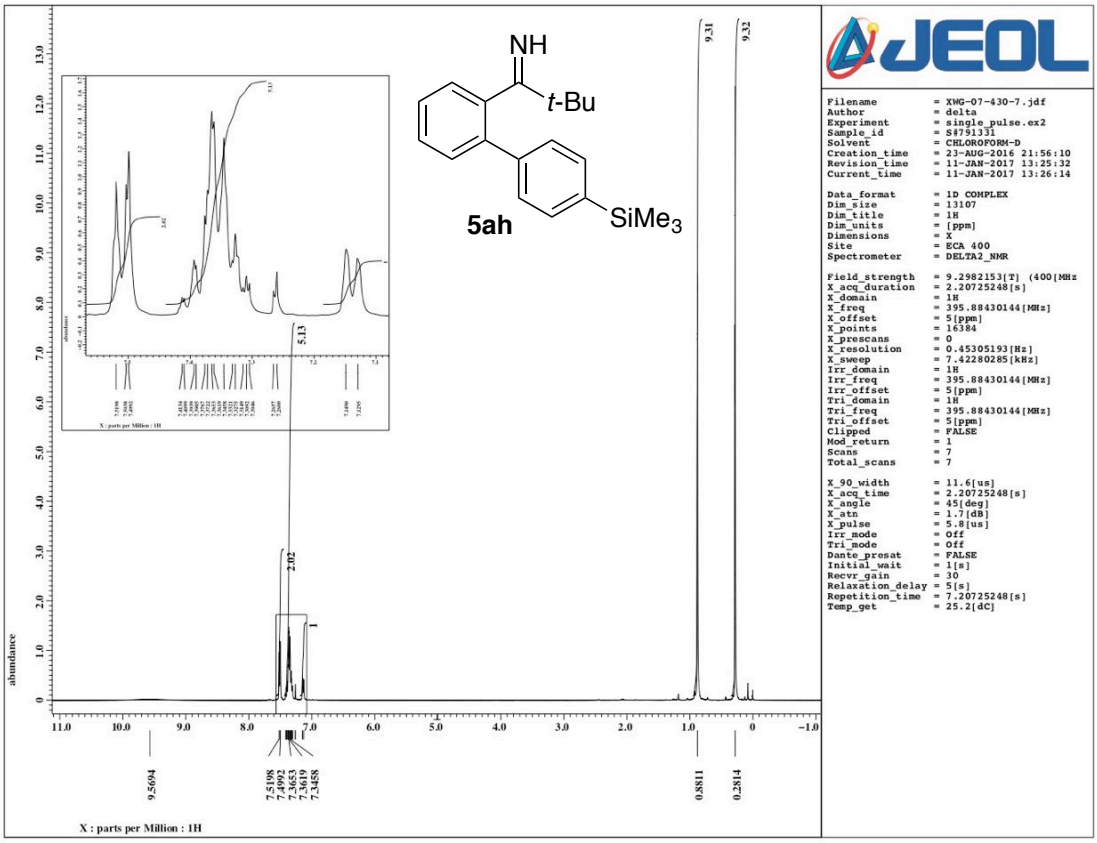

NH
t-Bu
CF3
5ae
190.8443
145.3665
137.2711
130.5457
130.3062
129.8176
129.4919
128.4572
128.1411
127.7579
125.7747
125.2861
125.2574
77.5761
77.2600
76.9343
40.7877
28.7644
abundance
X : parts per Million : 13C

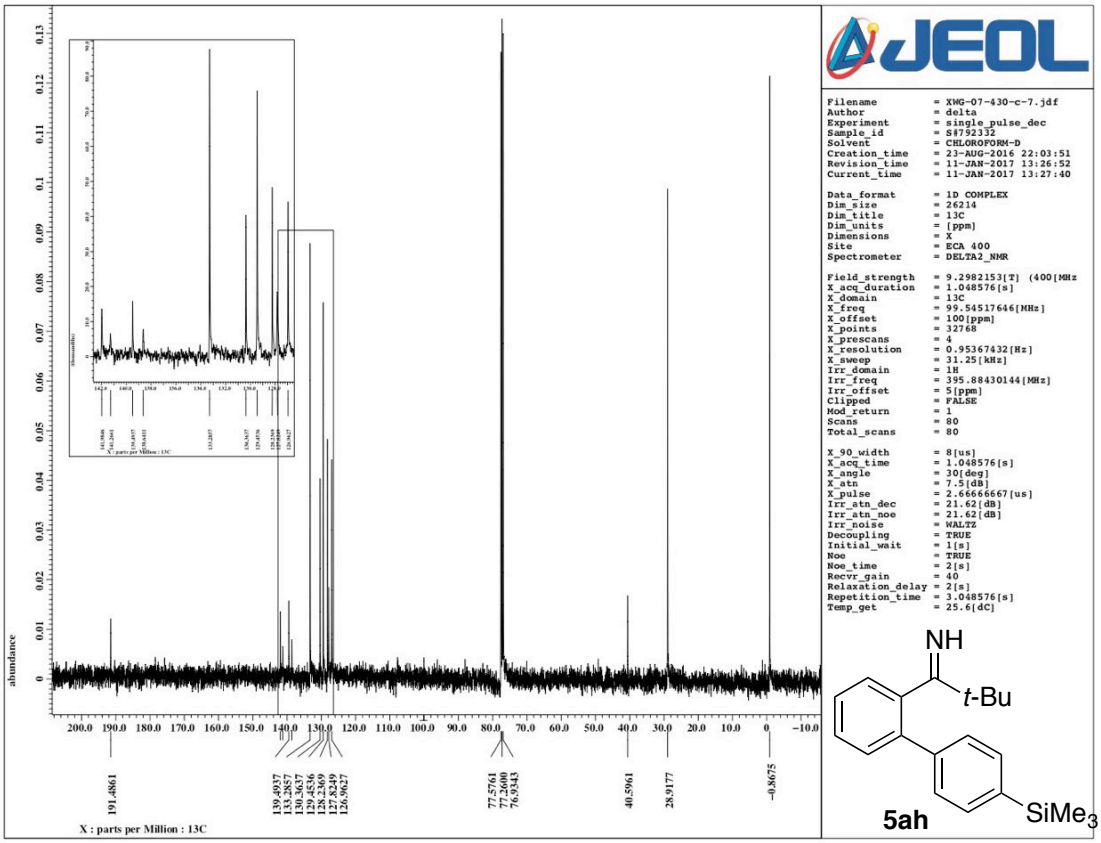

NH
t-Bu
NMe2
5af
9.23
6.16
3.56
2.04
2
0.92
abundance
X : parts per Million : 1H
9.2754
7.3368
7.3322
7.2590
7.2561
6.7068
6.7051
2.9686
0.9064
Filename = XWG-07-311-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#795150
Solvent = CHLOROFORM-D
Creation_time = 26-JUL-2016 22:01:54
Revision_time = 11-JAN-2017 13:01:29
Current_time = 11-JAN-2017 13:02:12
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.207725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 23.8[dC]

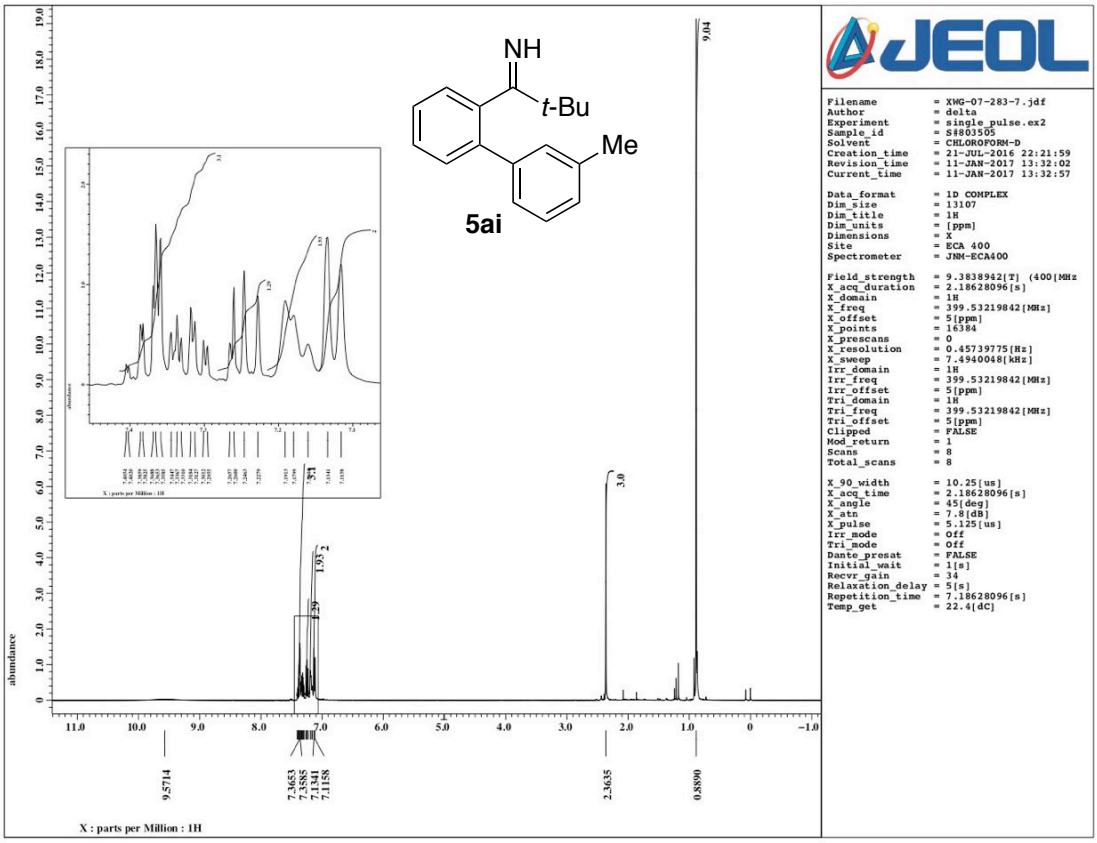

NH
t-Bu
NMe2
5af
abundance
X : parts per Million : 13C
192.4250
149.9171
141.1607
138.7369
130.3417
130.1817
129.8464
128.1985
127.9016
126.0534
112.3144
77.5857
77.2690
76.9438
40.7207
40.6536
28.9560
Filename = XWG-07-311-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#797635
Solvent = CHLOROFORM-D
Creation_time = 26-JUL-2016 22:17:38
Revision_time = 11-JAN-2017 13:17:40
Current_time = 11-JAN-2017 13:19:05
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 210
Total_scans = 210
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.1[dC]

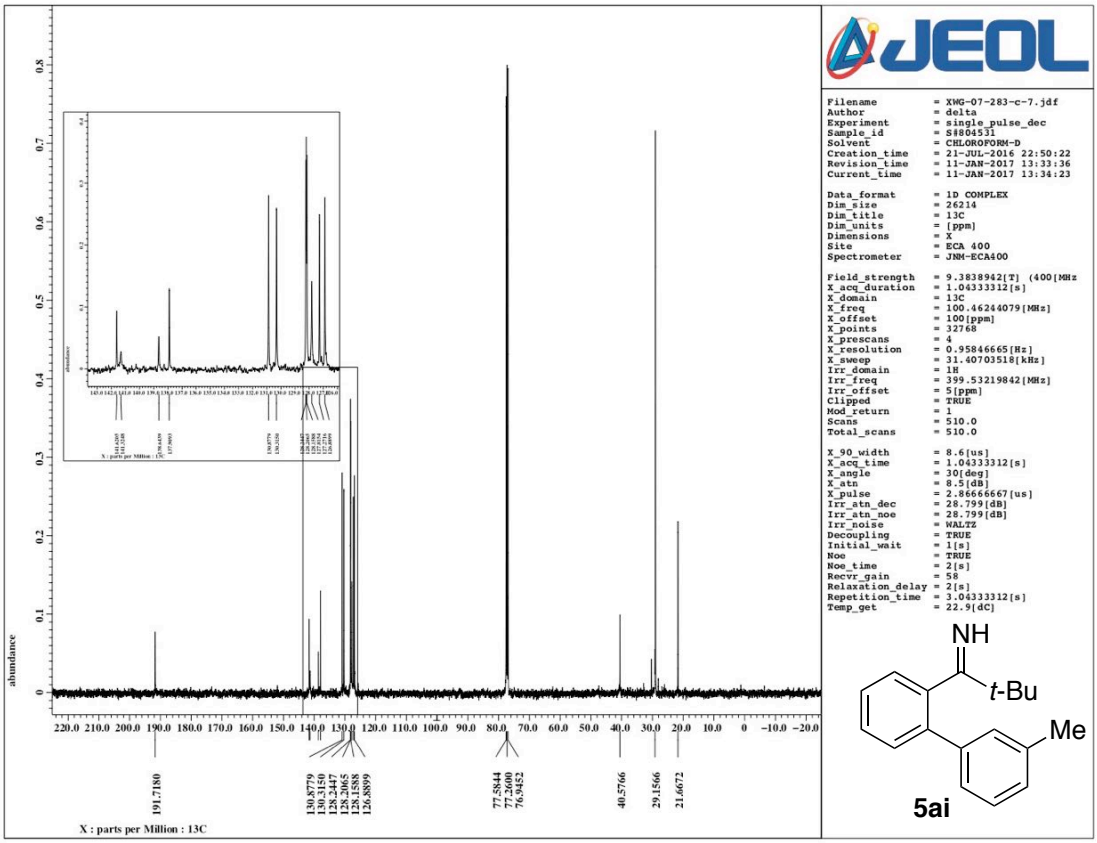

NH
t-Bu
OSiMe2t-Bu
5ag
JEOL
Filename = XWG-07-312-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8705698
Solvent = CHLOROFORM-D
Creation_time = 27-JUL-2016 19:32:21
Revision_time = 11-JAN-2017 13:12:06
Current_time = 11-JAN-2017 13:13:17
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153(T) (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 11.6[us]
X_acq_time = 2.207252 48[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 24[dC]
abundance
X : parts per Million : 1H
9.2524
7.3378
7.2600
7.2371
7.2154
6.8411
6.8194
0.9864
0.8685
0.1967
9.39
9.64
6.09
1.75
1.16

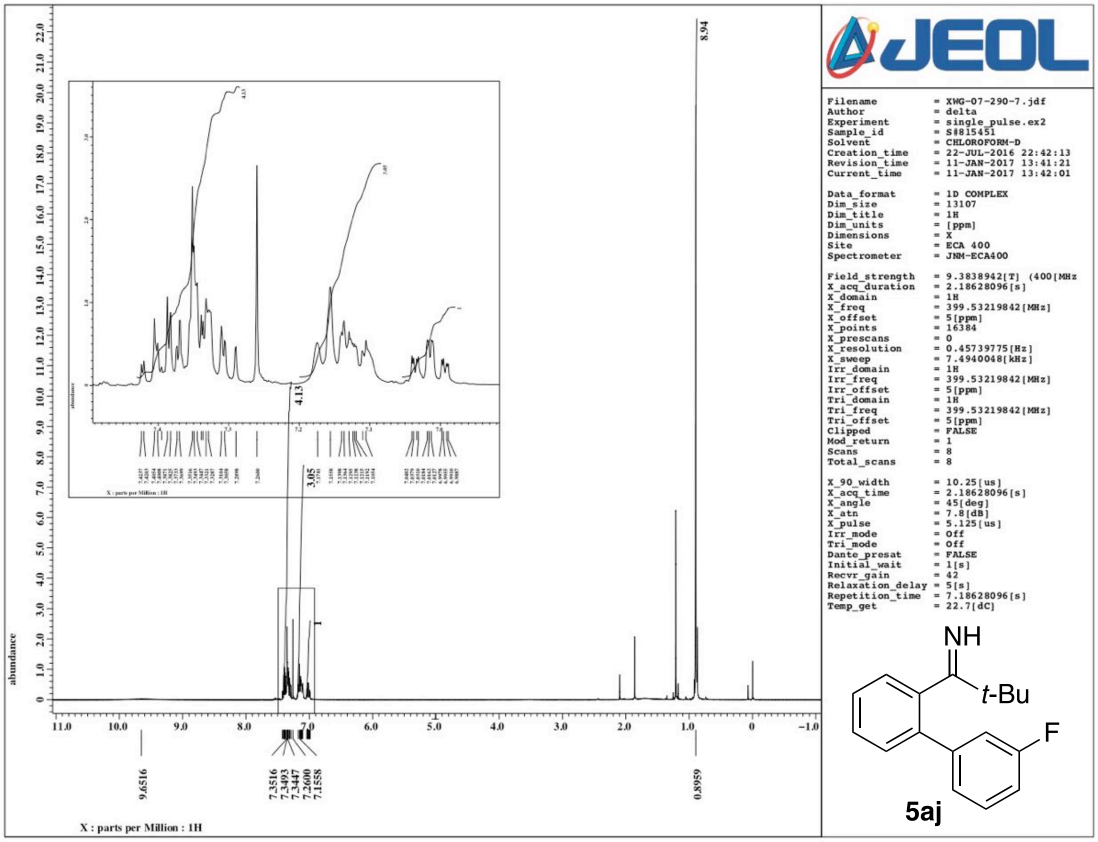

NH
t-Bu
OSiMe2t-Bu
5ag
abundance
X : parts per Million : 13C
191.9710
155.1156
138.1776
134.6233
131.1360
130.0535
128.0607
127.7936
126.7770
126.4896
119.9654
77.4192
77.1030
76.7773
40.5733
28.7416
27.9177
25.7909
18.1266
-4.3296

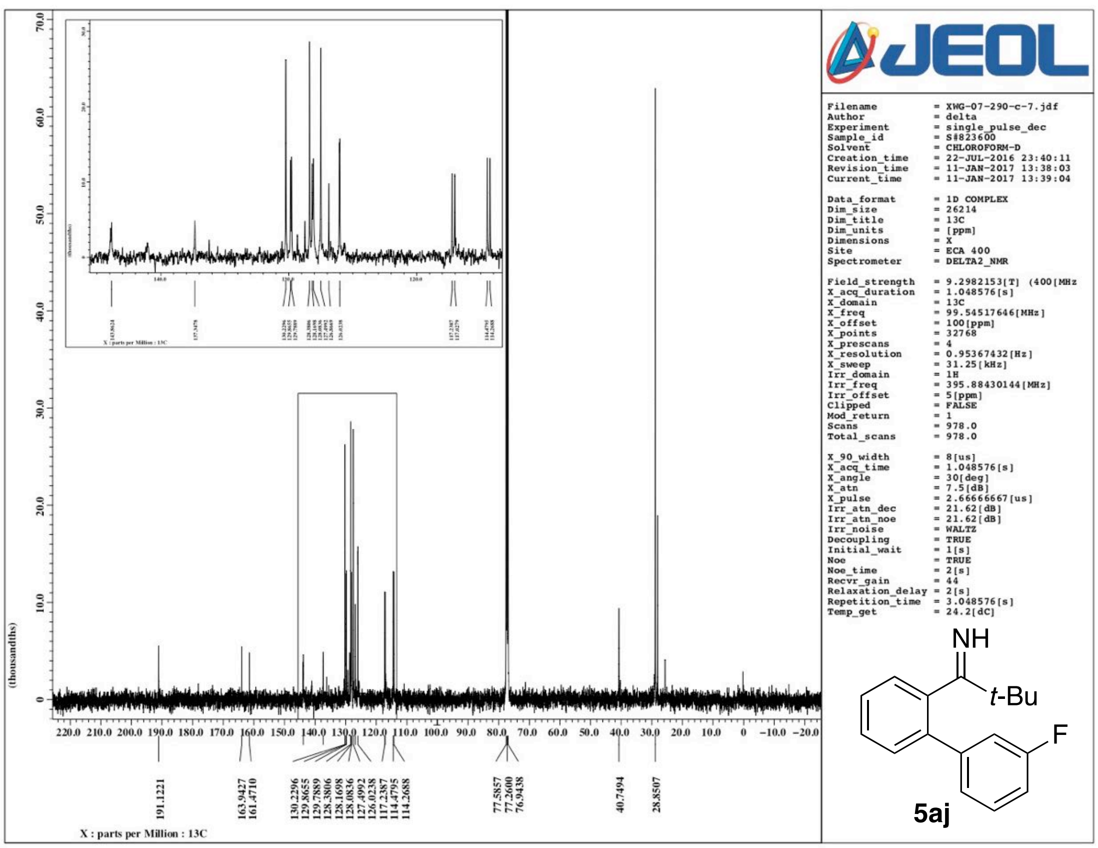

NH
t-Bu
SiMe3
5ah
9.31
9.32
2.02
1
5.13
abundance
X : parts per Million : 1H
9.5694
7.5198
7.4992
7.3653
7.3619
7.3458
0.8811
0.2814
Filename = XWG-07-430-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#791331
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 21:56:10
Revision_time = 11-JAN-2017 13:25:32
Current_time = 11-JAN-2017 13:26:14
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 7
Total_scans = 7
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.2[dC]

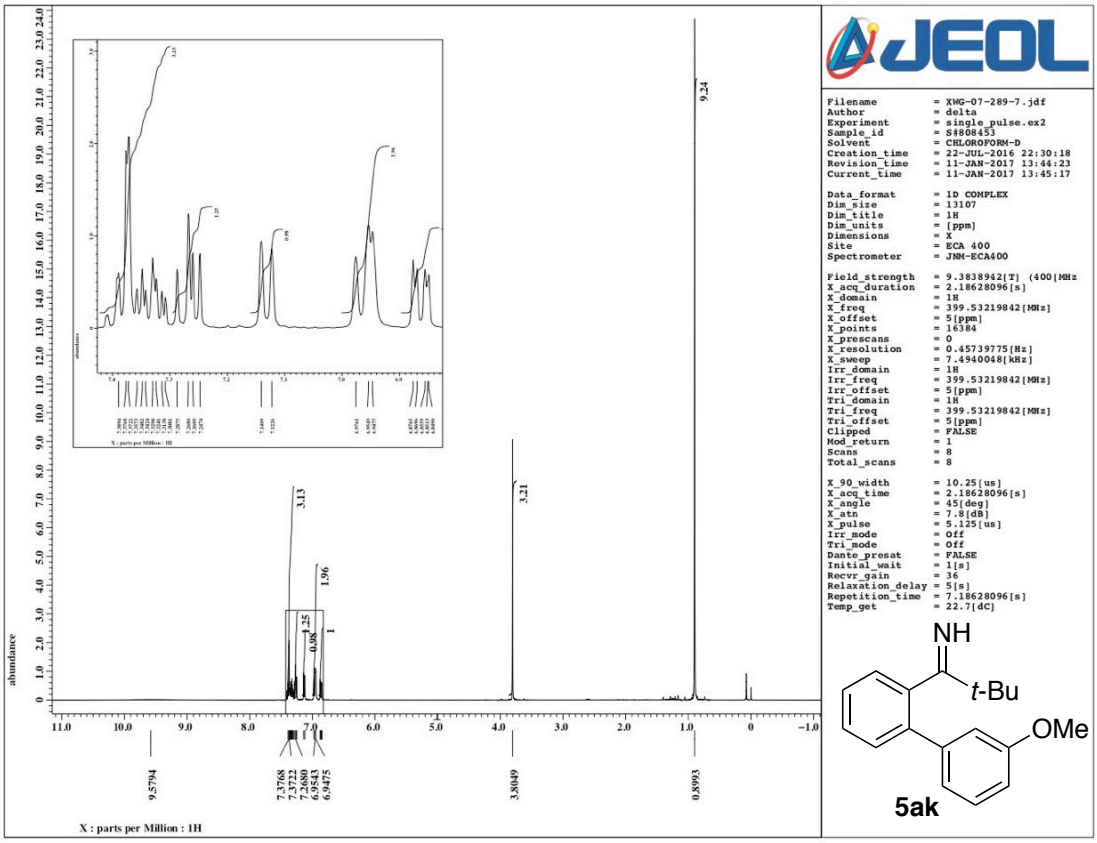

abundance
X : parts per Million : 13C
191.4861
139.4937
133.2857
130.3837
128.2456
128.2369
127.8249
126.9627
77.5761
77.2600
76.9343
40.5961
28.9177
−0.8675
Filename = XWG-07-430-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#792332
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 22:03:51
Revision_time = 11-JAN-2017 13:26:52
Current_time = 11-JAN-2017 13:27:40
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 80
Total_scans = 80
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 40
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
NH
t-Bu
SiMe3
5ah

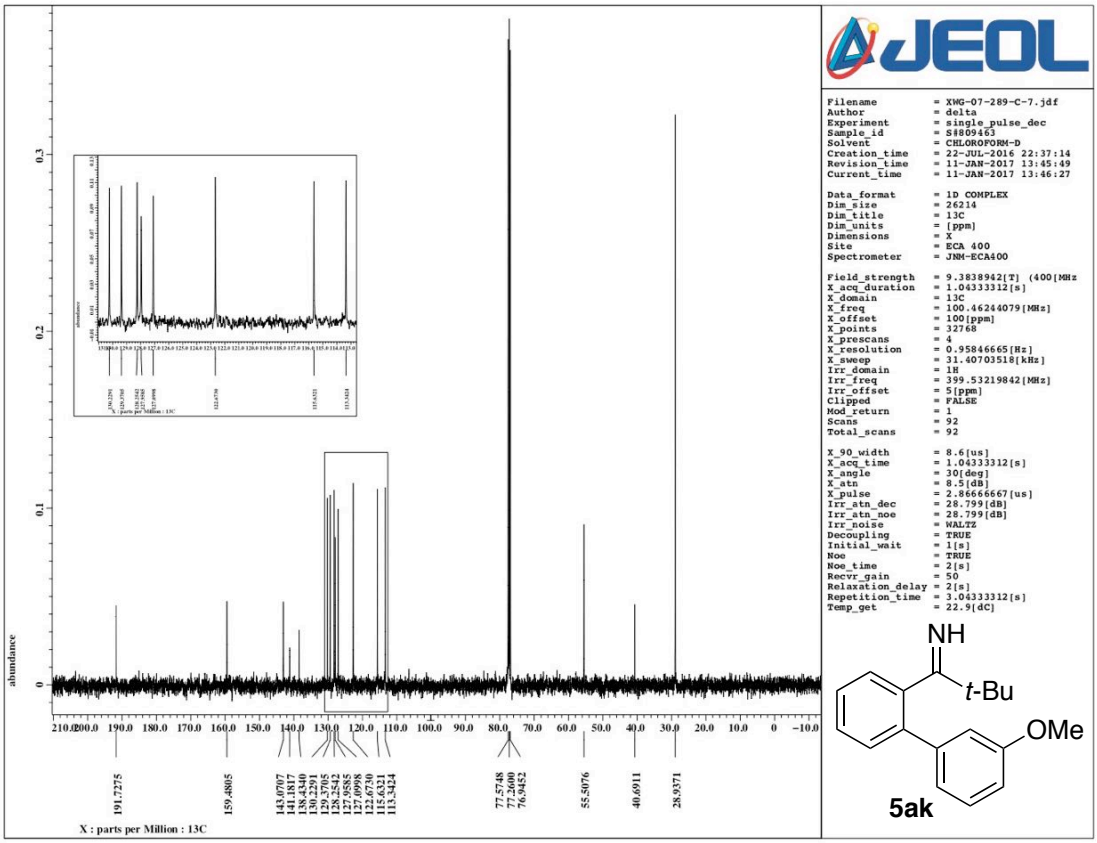

NH
t-Bu
Me
5ai
abundance
X : parts per Million : 1H
9.5714
7.3653
7.3585
7.1341
7.1158
2.3635
0.8890
Filename = XWG-07-283-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#803505
Solvent = CHLOROFORM-D
Creation_time = 21-JUL-2016 22:21:59
Revision_time = 11-JAN-2017 13:32:02
Current_time = 11-JAN-2017 13:32:57
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.4[dC]

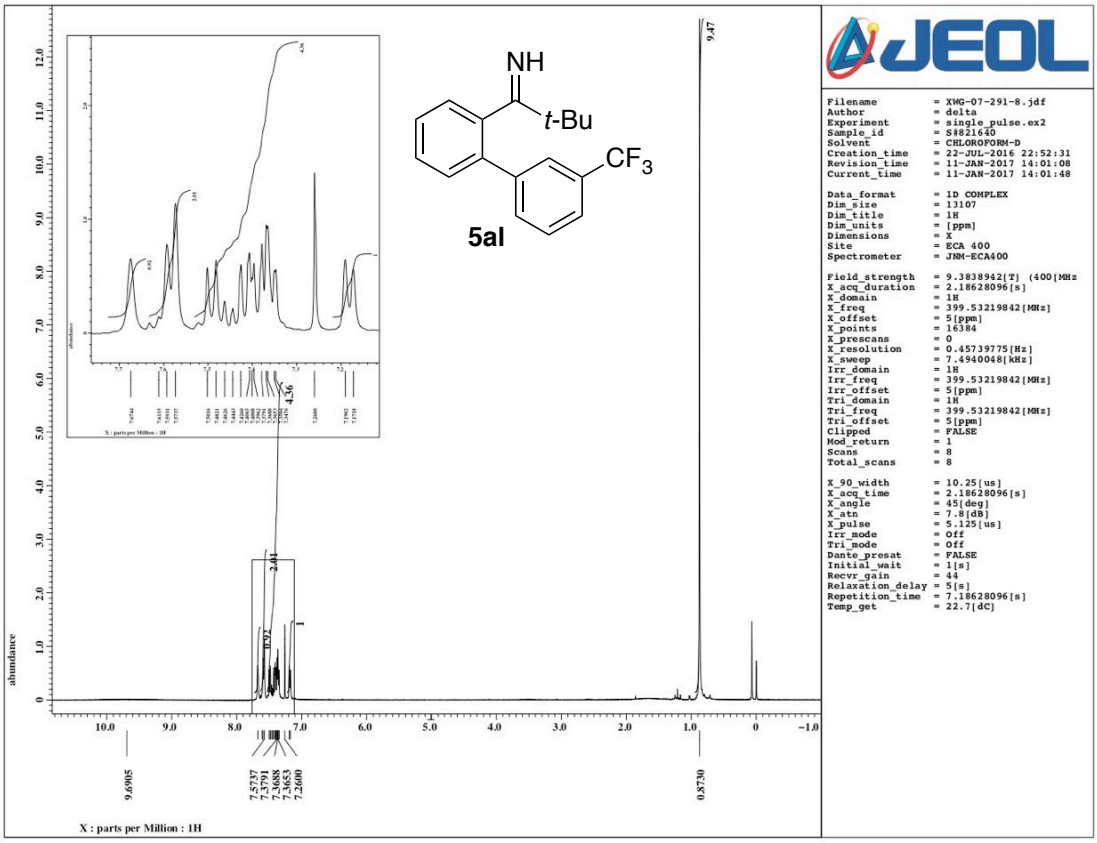

abundance
X : parts per Million : 13C
191.7180
130.8779
130.3150
128.2447
128.2065
128.1586
126.8899
77.5844
77.1660
76.7452
40.5766
29.1566
21.6672
Filename = XWG-07-283-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#804531
Solvent = CHLOROFORM-D
Creation_time = 21-JUL-2016 22:50:22
Revision_time = 11-JAN-2017 13:33:36
Current_time = 11-JAN-2017 13:34:23
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 510.0
Total_scans = 510.0
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 58
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.9[dC]
NH
t-Bu
Me
5ai

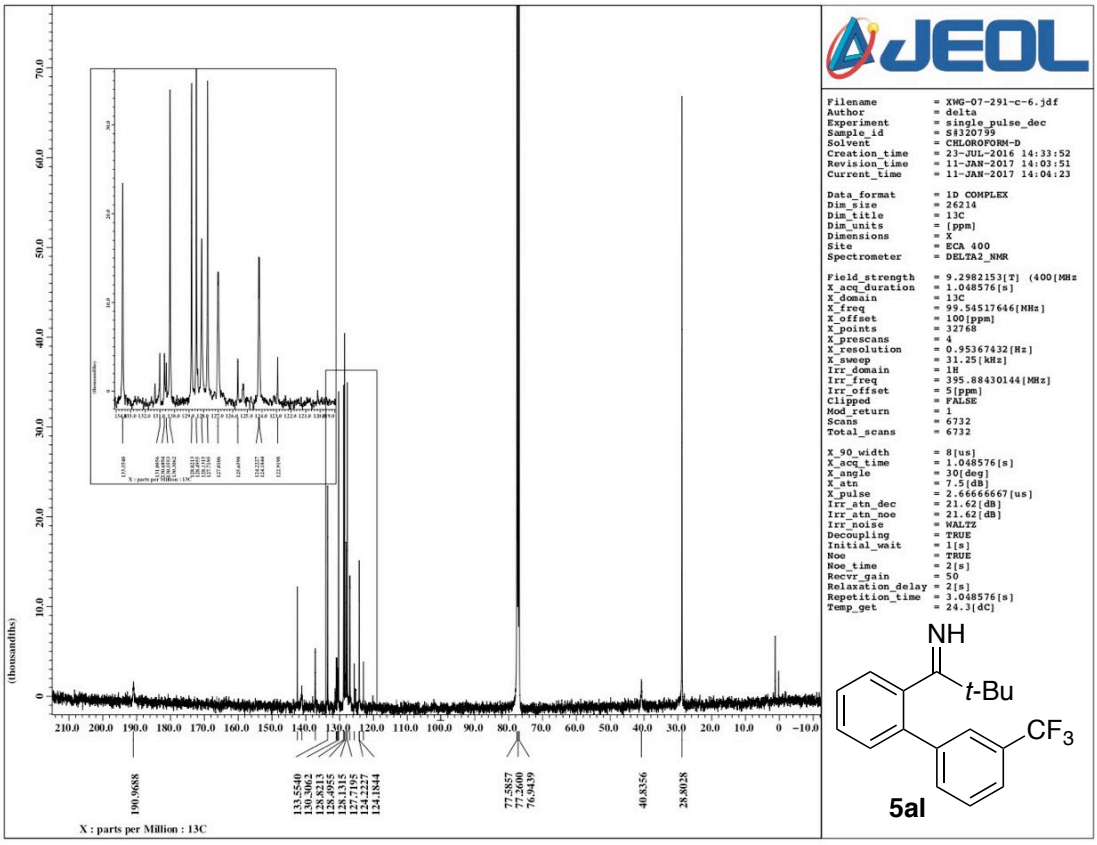

JEOL
Filename = XWG-07-290-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#815451
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:42:13
Revision_time = 11-JAN-2017 13:41:21
Current_time = 11-JAN-2017 13:42:01
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.7[dC]
NH
t-Bu
F
5aj
8.94
4.13
3.05
abundance
9.6516
7.3516
7.3493
7.3447
7.2600
7.1558
0.8959
X : parts per Million : 1H

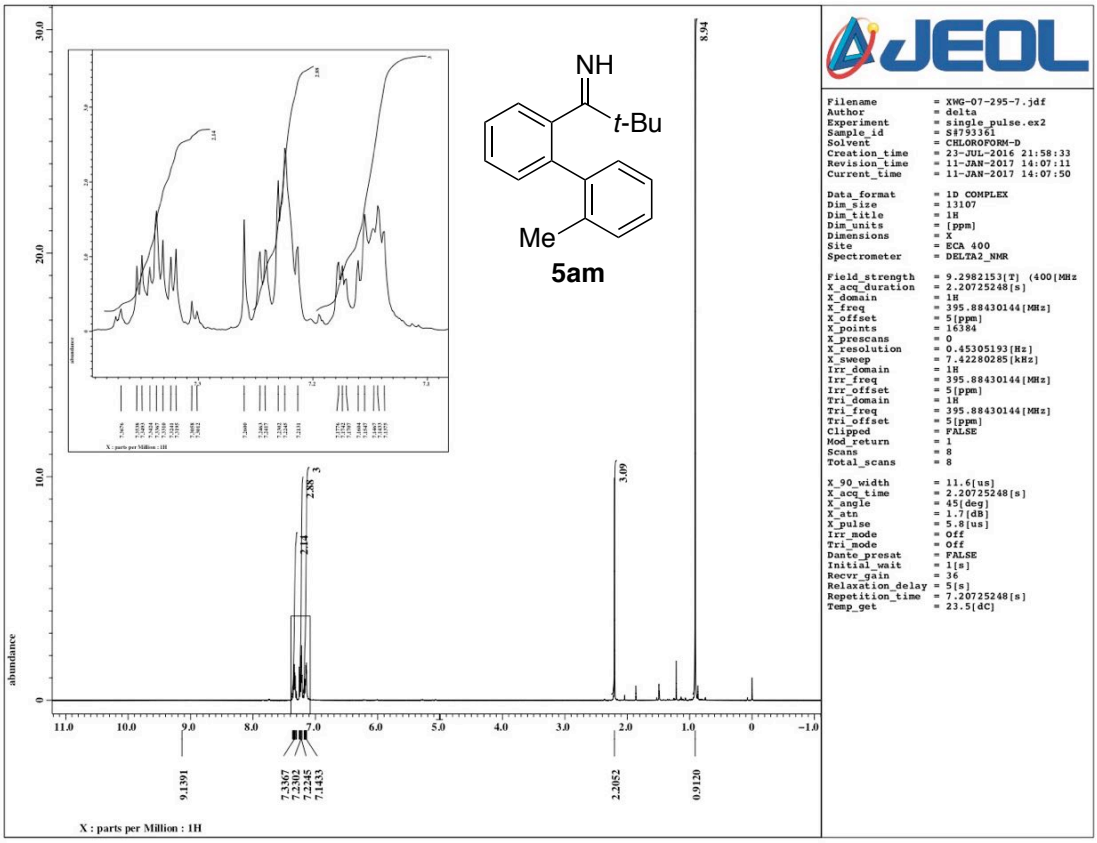

JEOL
Filename = XWG-07-290-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#823600
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 23:40:11
Revision_time = 11-JAN-2017 13:38:03
Current_time = 11-JAN-2017 13:39:04
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 978.0
Total_scans = 978.0
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.2[dC]
NH
t-Bu
F
5aj
(thousandths)
191.1221
163.9427
161.4710
130.2296
129.8655
129.7889
128.3806
128.1698
128.0836
127.4992
126.0238
117.2387
114.4795
114.2688
77.5857
77.2600
76.9438
40.7494
28.8507
X : parts per Million : 13C


Filename = XWG-07-289-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#808453
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:30:18
Revision_time = 11-JAN-2017 13:44:23
Current_time = 11-JAN-2017 13:45:17
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.7[dC]
NH
t-Bu
OMe
5ak
abundance
X : parts per Million : 1H
9.5794
7.3768
7.3722
7.2680
6.9543
6.9475
3.8049
0.8993

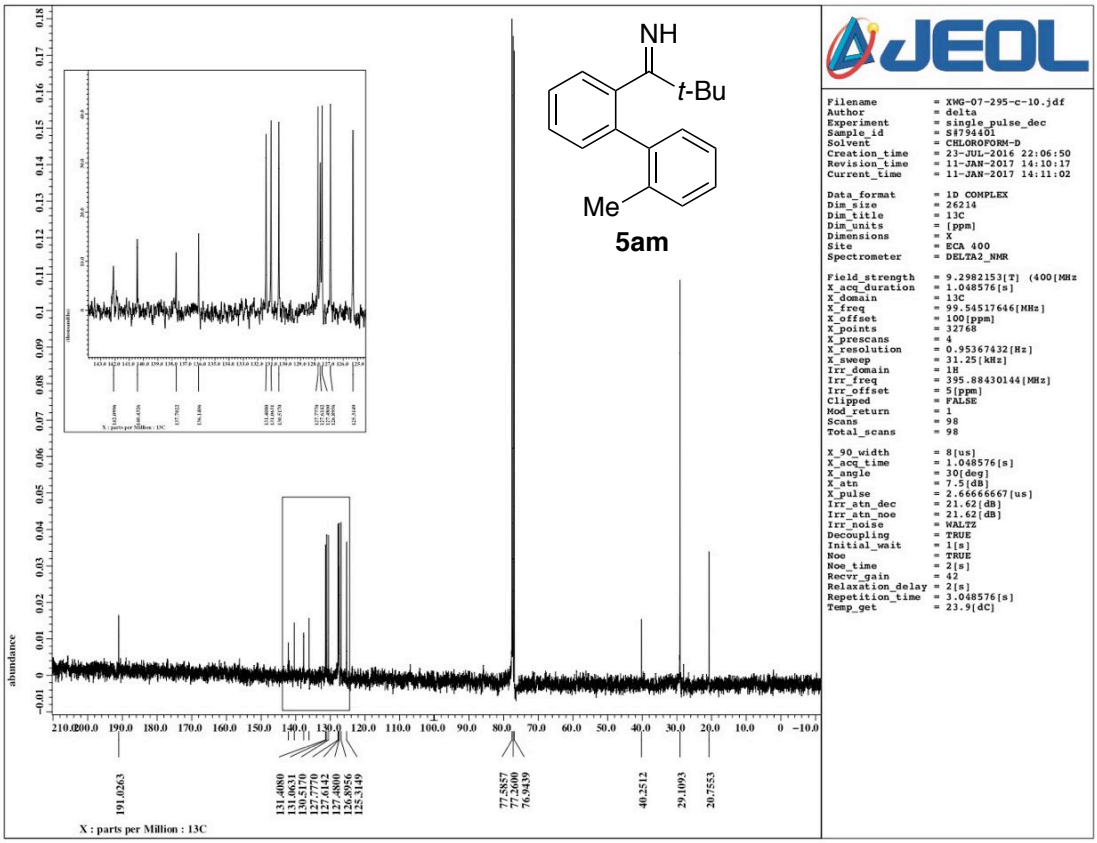

Filename = XWG-07-289-C-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#809463
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:37:14
Revision_time = 11-JAN-2017 13:45:49
Current_time = 11-JAN-2017 13:46:27
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 92
Total_scans = 92
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.9[dC]
NH
t-Bu
OMe
5ak
abundance
X : parts per Million : 13C
191.7275
159.4805
143.0707
141.1817
138.4340
130.2291
128.7705
126.2542
127.9585
127.0998
122.6730
113.6431
113.3424
77.5748
77.2600
76.9452
55.5076
40.6911
28.9371


NH
t-Bu
CF3
5al
abundance
X : parts per Million : 1H
9.6905
7.5737
7.3791
7.3688
7.3653
7.2600
0.8730
Filename = XWG-07-291-8.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8821640
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 22:52:31
Revision_time = 11-JAN-2017 14:01:08
Current_time = 11-JAN-2017 14:01:48
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.7[dC]

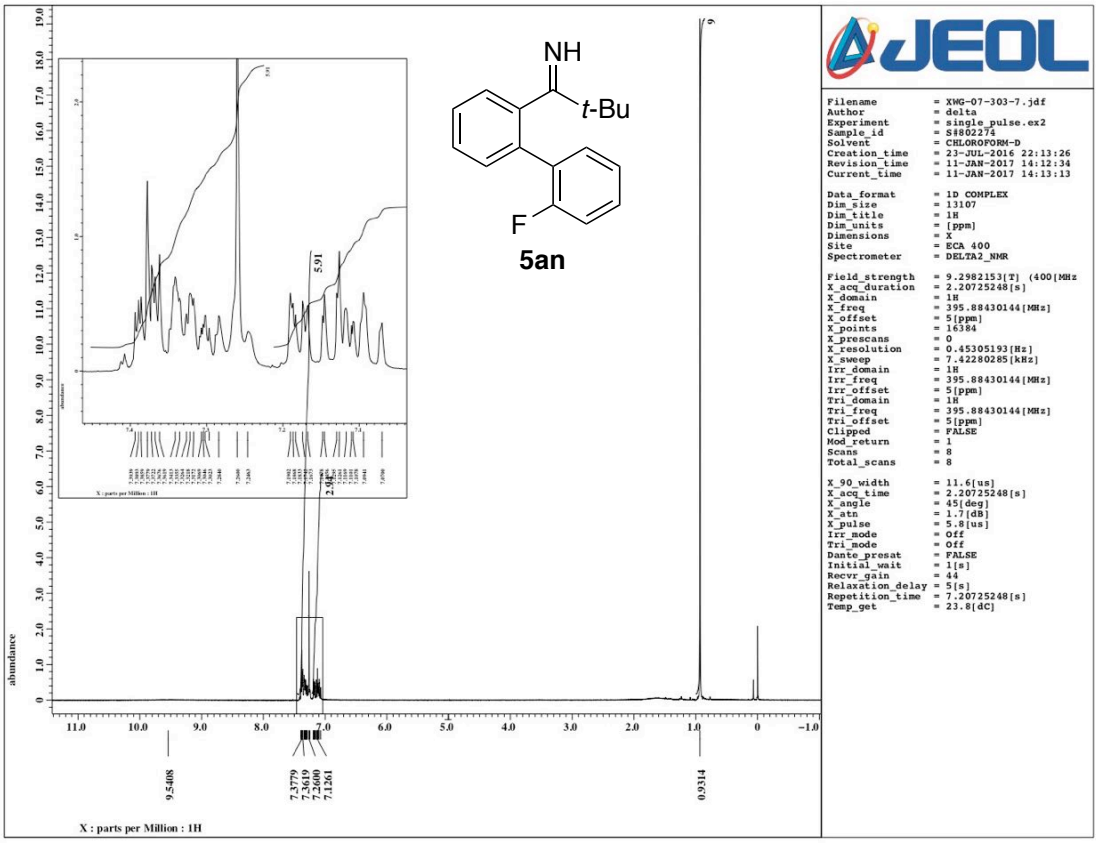

(thousandths)
X : parts per Million : 13C
190.9688
133.5540
130.3062
128.8213
128.4955
128.1315
127.7195
124.2227
124.1844
77.5857
77.2690
76.9439
40.8356
28.8028
Filename = XWG-07-291-c-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8320799
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2016 14:33:52
Revision_time = 11-JAN-2017 14:03:51
Current_time = 11-JAN-2017 14:04:23
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6732
Total_scans = 6732
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 24.3[dC]
NH
t-Bu
CF3
5al

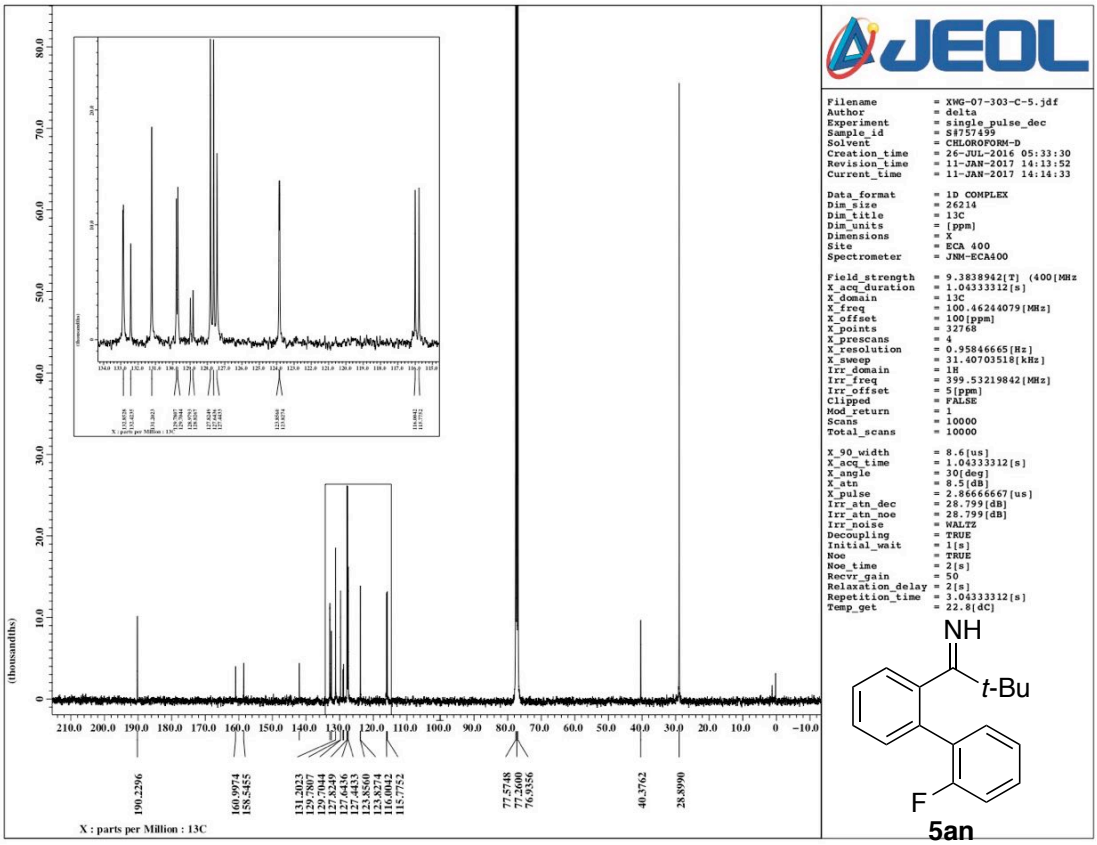


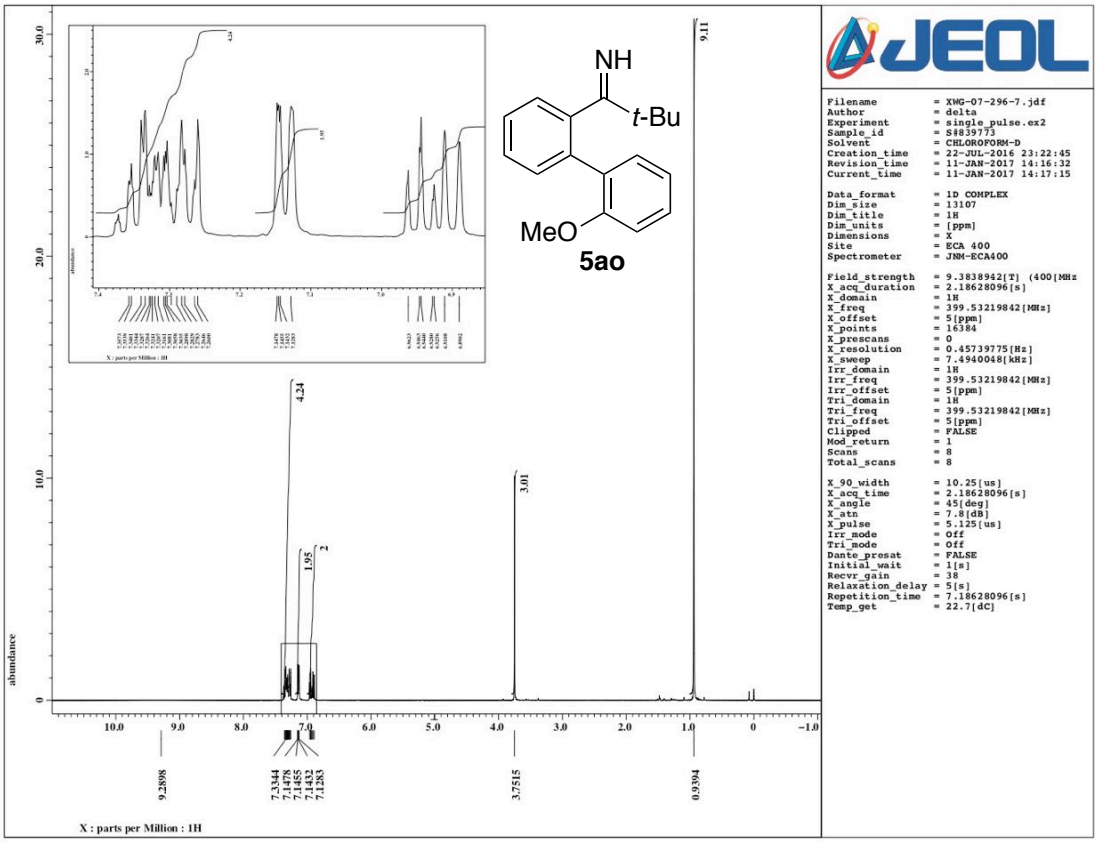

```
Filename        = XWG-07-295-7.jdf
Author          = delta
Experiment      = single_pulse.ex2
Sample_id       = S#793361
Solvent         = CHLOROFORM-D
Creation_time   = 23-JUL-2016 21:58:33
Revision_time   = 11-JAN-2017 14:07:11
Current_time    = 11-JAN-2017 14:07:50

Data_format     = 1D COMPLEX
Dim_size        = 13107
Dim_title       = 1H
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = DELTA2_NMR

Field_strength  = 9.2982153[T] (400[MHz
X_acq_duration  = 2.20725248[s]
X_domain        = 1H
X_freq          = 395.88430144[MHz]
X_offset        = 5[ppm]
X_points        = 16384
X_prescans      = 0
X_resolution    = 0.45305193[Hz]
X_sweep         = 7.42280285[kHz]
Irr_domain      = 1H
Irr_freq        = 395.88430144[MHz]
Irr_offset      = 5[ppm]
Tri_domain      = 1H
Tri_freq        = 395.88430144[MHz]
Tri_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 8
Total_scans     = 8

X_90_width      = 11.6[us]
X_acq_time      = 2.207725248[s]
X_angle         = 45[deg]
X_atn           = 1.7[dB]
X_pulse         = 5.8[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 36
Relaxation_delay = 5[s]
Repetition_time = 7.207725248[s]
Temp_get        = 23.5[dC]
```



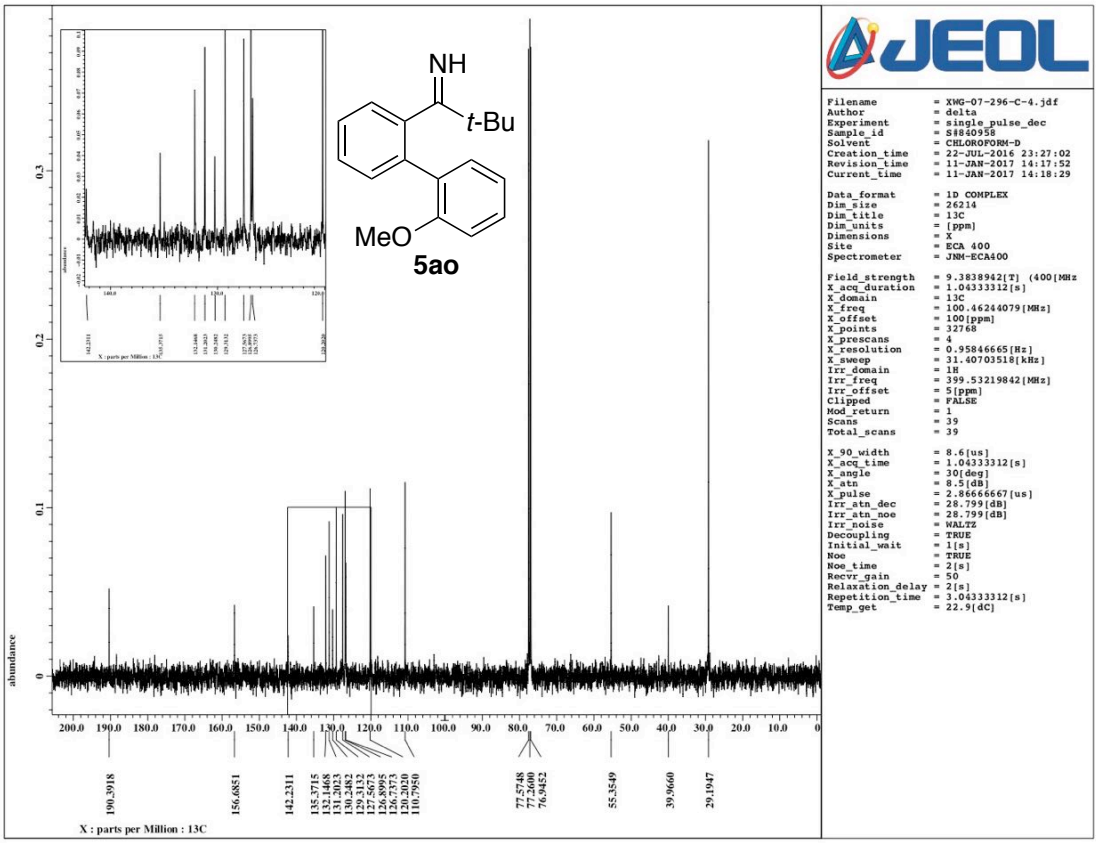

```
Filename        = XWG-07-295-c-10.jdf
Author          = delta
Experiment      = single_pulse_dec
Sample_id       = S#794401
Solvent         = CHLOROFORM-D
Creation_time   = 23-JUL-2016 22:06:50
Revision_time   = 11-JAN-2017 14:10:17
Current_time    = 11-JAN-2017 14:11:02

Data_format     = 1D COMPLEX
Dim_size        = 26214
Dim_title       = 13C
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = DELTA2_NMR

Field_strength  = 9.2982153[T] (400[MHz
X_acq_duration  = 1.048576[s]
X_domain        = 13C
X_freq          = 99.54517646[MHz]
X_offset        = 100[ppm]
X_points        = 32768
X_prescans      = 4
X_resolution    = 0.95367432[Hz]
X_sweep         = 31.25[kHz]
Irr_domain      = 1H
Irr_freq        = 395.88430144[MHz]
Irr_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 98
Total_scans     = 98

X_90_width      = 8[us]
X_acq_time      = 1.048576[s]
X_angle         = 30[deg]
X_atn           = 7.5[dB]
X_pulse         = 2.66666667[us]
Irr_atn_dec     = 21.62[dB]
Irr_atn_noe     = 21.62[dB]
Irr_noise       = WALTZ
Decoupling      = TRUE
Initial_wait    = 1[s]
Noe             = TRUE
Noe_time        = 2[s]
Recvr_gain      = 42
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get        = 23.9[dC]
```


NH
t-Bu
F
5an
abundance
X : parts per Million : 1H
9.5408
7.3779
7.3619
7.2600
7.1261
0.9314
Filename = XWG-07-303-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#802274
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2016 22:13:26
Revision_time = 11-JAN-2017 14:12:34
Current_time = 11-JAN-2017 14:13:13
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 23.8[dC]

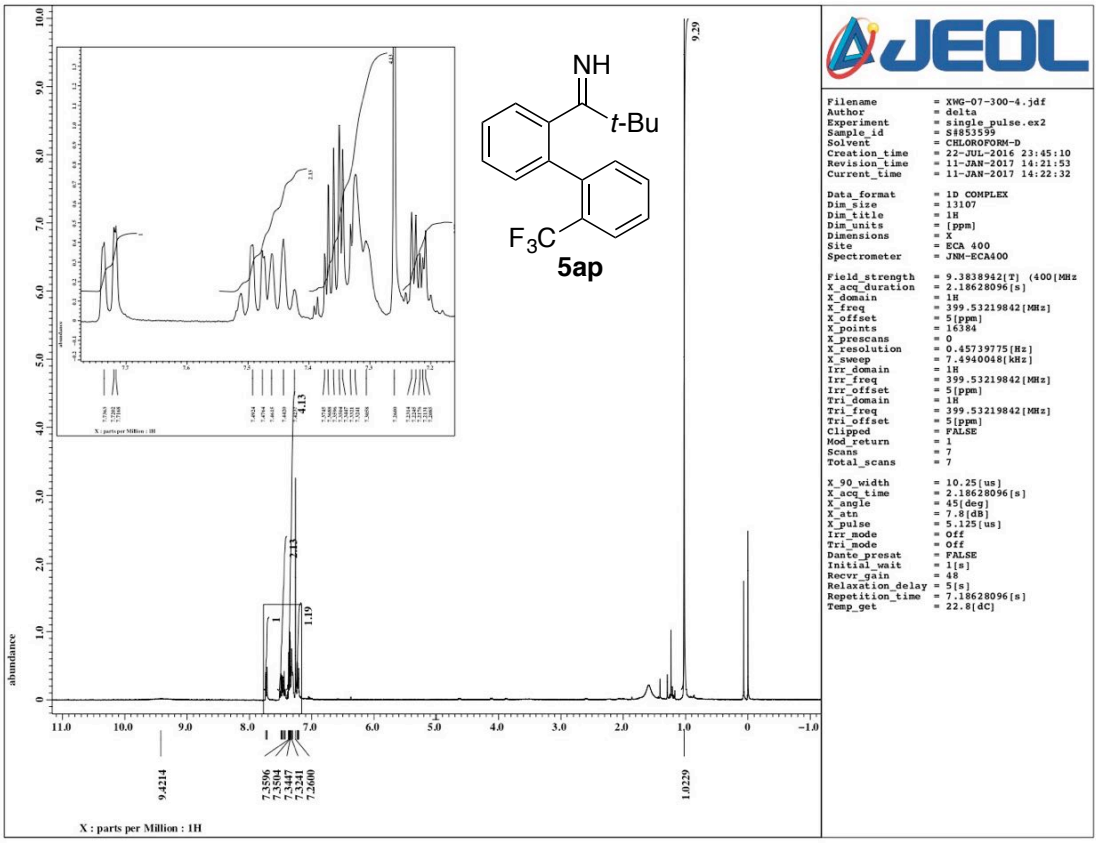

(thousandths)
X : parts per Million : 13C
190.2296
160.9974
158.5455
131.2023
129.2027
129.7044
127.8249
127.6436
123.8560
123.8274
116.0042
115.7752
77.5748
77.2600
76.9356
40.3762
28.8990
Filename = XWG-07-303-C-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#757499
Solvent = CHLOROFORM-D
Creation_time = 26-JUL-2016 05:33:30
Revision_time = 11-JAN-2017 14:13:52
Current_time = 11-JAN-2017 14:14:33
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.8[dC]
NH
t-Bu
F
5an

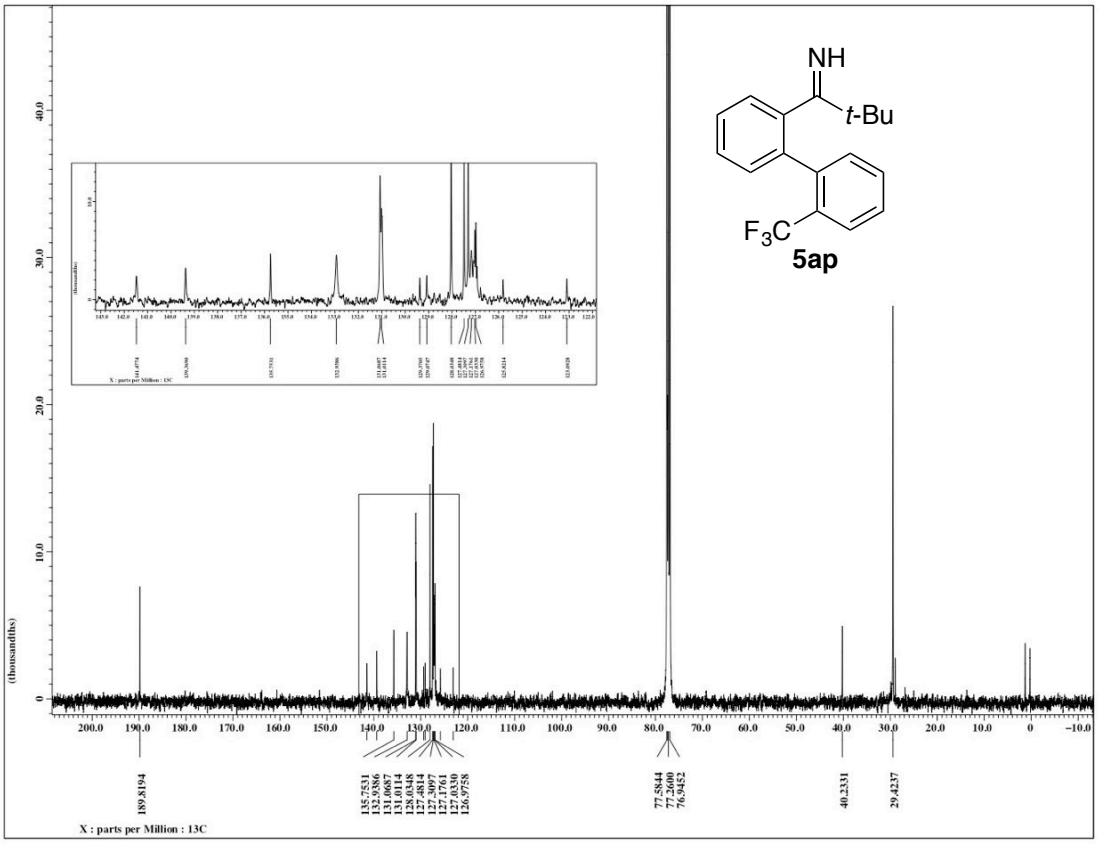


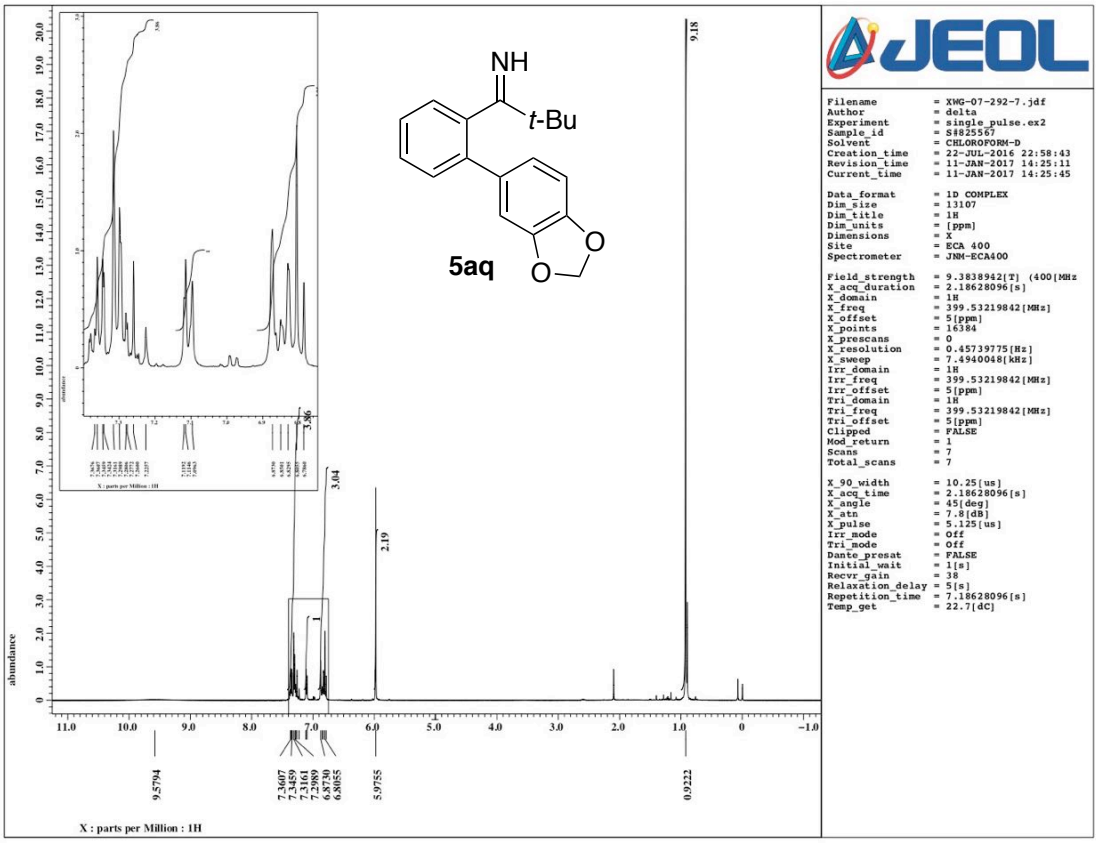

```
Filename          = XWG-07-296-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#839773
Solvent           = CHLOROFORM-D
Creation_time     = 22-JUL-2016 23:22:45
Revision_time     = 11-JAN-2017 14:16:32
Current_time      = 11-JAN-2017 14:17:15

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 2.18628096[s]
X_domain          = 1H
X_freq            = 399.53219842[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45739775[Hz]
X_sweep           = 7.4940048[kHz]
Irr_domain        = 1H
Irr_freq          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.53219842[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10.25[us]
X_acq_time        = 2.18628096[s]
X_angle           = 45[deg]
X_atn             = 7.8[dB]
X_pulse           = 5.125[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18628096[s]
Temp_get          = 22.7[dC]
```



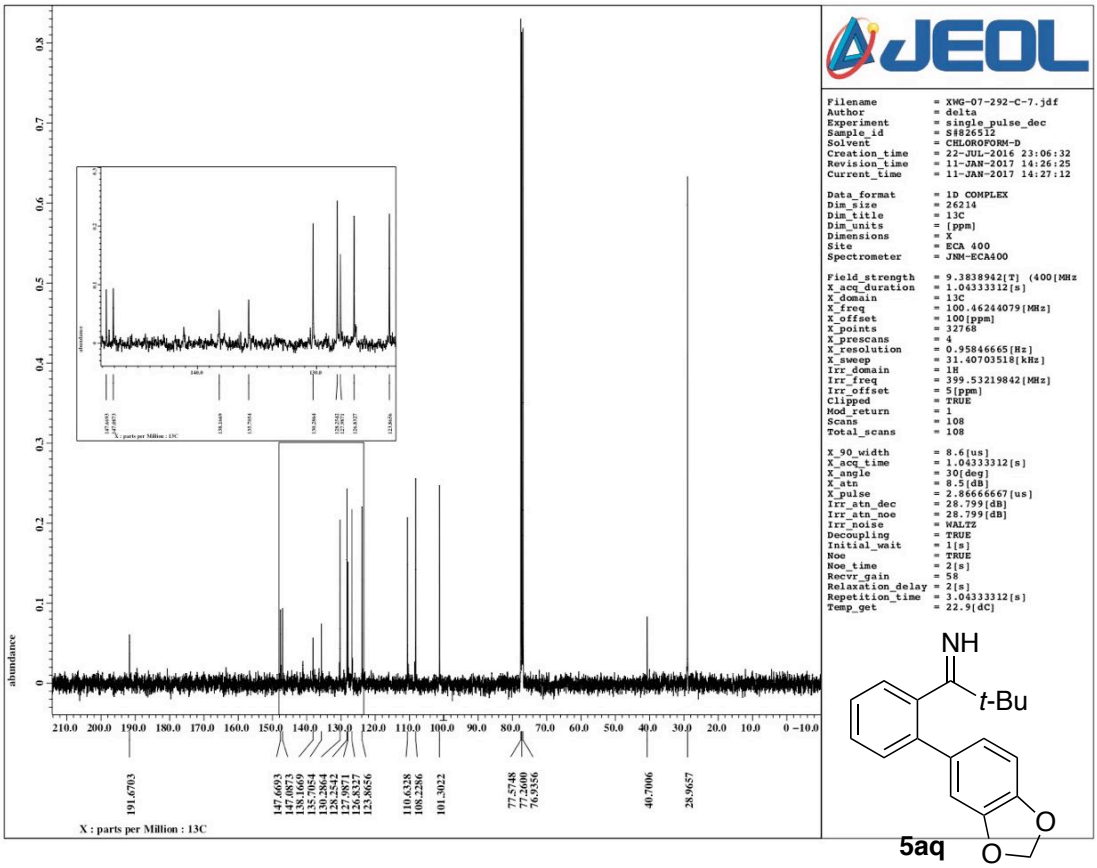

```
Filename          = XWG-07-296-C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#840958
Solvent           = CHLOROFORM-D
Creation_time     = 22-JUL-2016 23:27:02
Revision_time     = 11-JAN-2017 14:17:52
Current_time      = 11-JAN-2017 14:18:29

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.46244079[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          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 39
Total_scans       = 39

X_90_width        = 8.6[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 8.5[dB]
X_pulse           = 2.86666667[us]
Irr_atn_dec       = 28.799[dB]
Irr_atn_noe       = 28.799[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 22.9[dC]
```


NH
t-Bu
F3C
5ap
9.29
4.13
2.13
1.19
1
abundance
X : parts per Million : 1H
9.4214
7.3596
7.3504
7.3447
7.3241
7.2600
1.0229
Filename = XWG-07-300-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#853599
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 23:45:10
Revision_time = 11-JAN-2017 14:21:53
Current_time = 11-JAN-2017 14:22:32
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 7
Total_scans = 7
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 48
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.8[dC]

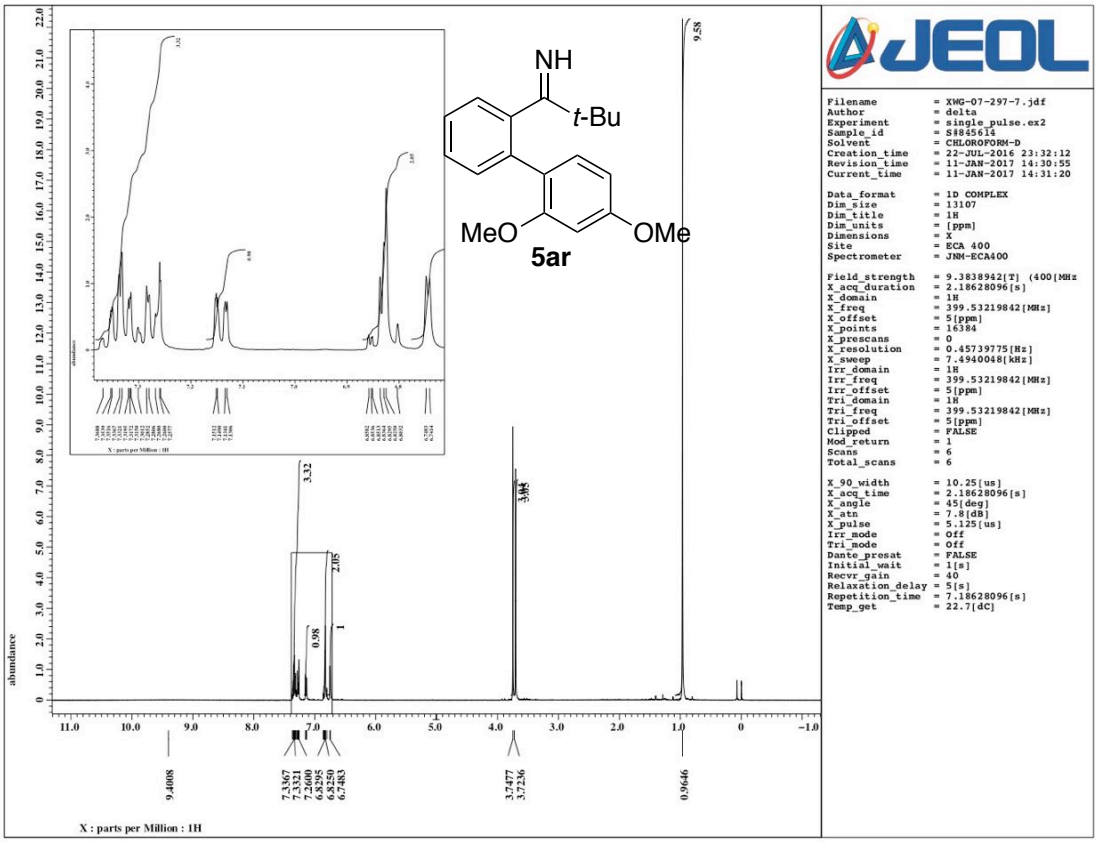

NH
t-Bu
F3C
5ap
(thousandths)
X : parts per Million : 13C
189.8194
135.7531
132.9386
131.0687
131.0114
130.4834
127.4814
127.3097
127.1761
127.0530
126.9758
77.5844
77.2600
76.9452
40.2331
29.4237

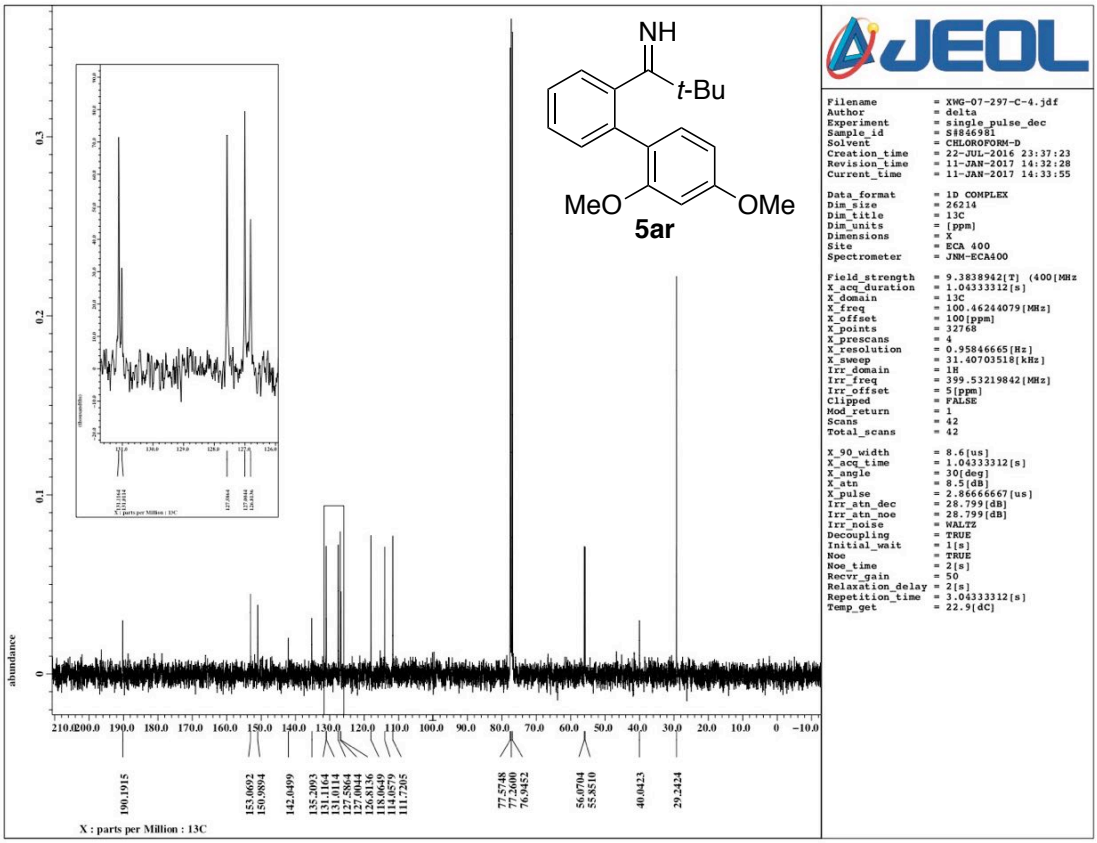


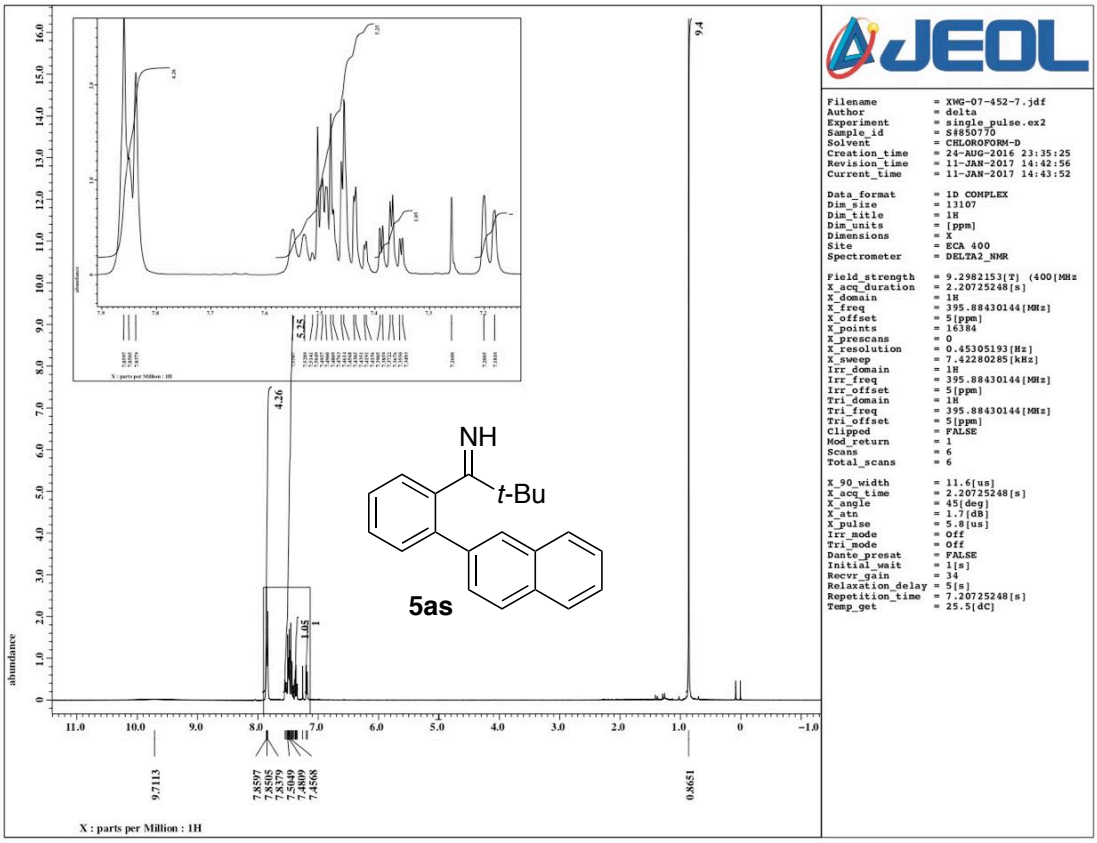

```
Filename          = XWG-07-292-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#825567
Solvent           = CHLOROFORM-D
Creation_time     = 22-JUL-2016 22:58:43
Revision_time     = 11-JAN-2017 14:25:11
Current_time      = 11-JAN-2017 14:25:45

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 2.18628096[s]
X_domain          = 1H
X_freq            = 399.53219842[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45739775[Hz]
X_sweep           = 7.4940048[kHz]
Irr_domain        = 1H
Irr_freq          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.53219842[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 7
Total_scans       = 7

X_90_width        = 10.25[us]
X_acq_time        = 2.18628096[s]
X_angle           = 45[deg]
X_atn             = 7.8[dB]
X_pulse           = 5.125[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18628096[s]
Temp_get          = 22.7[dC]
```

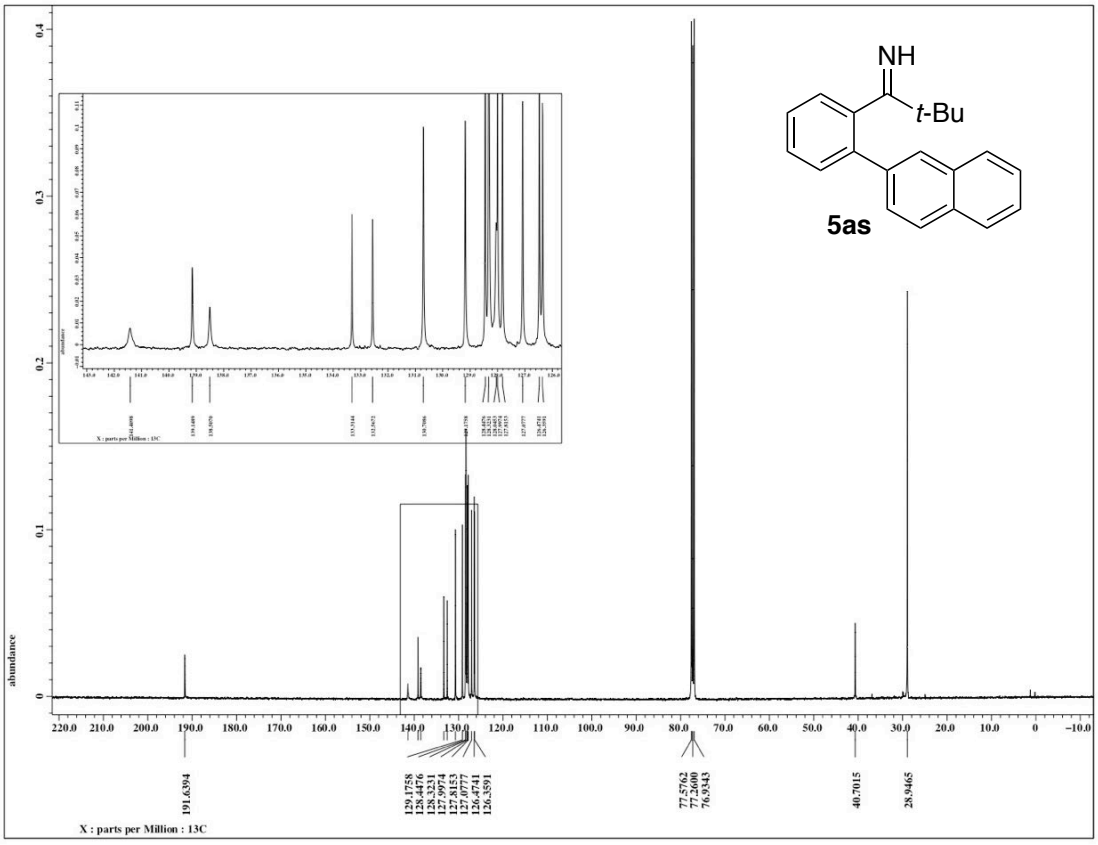


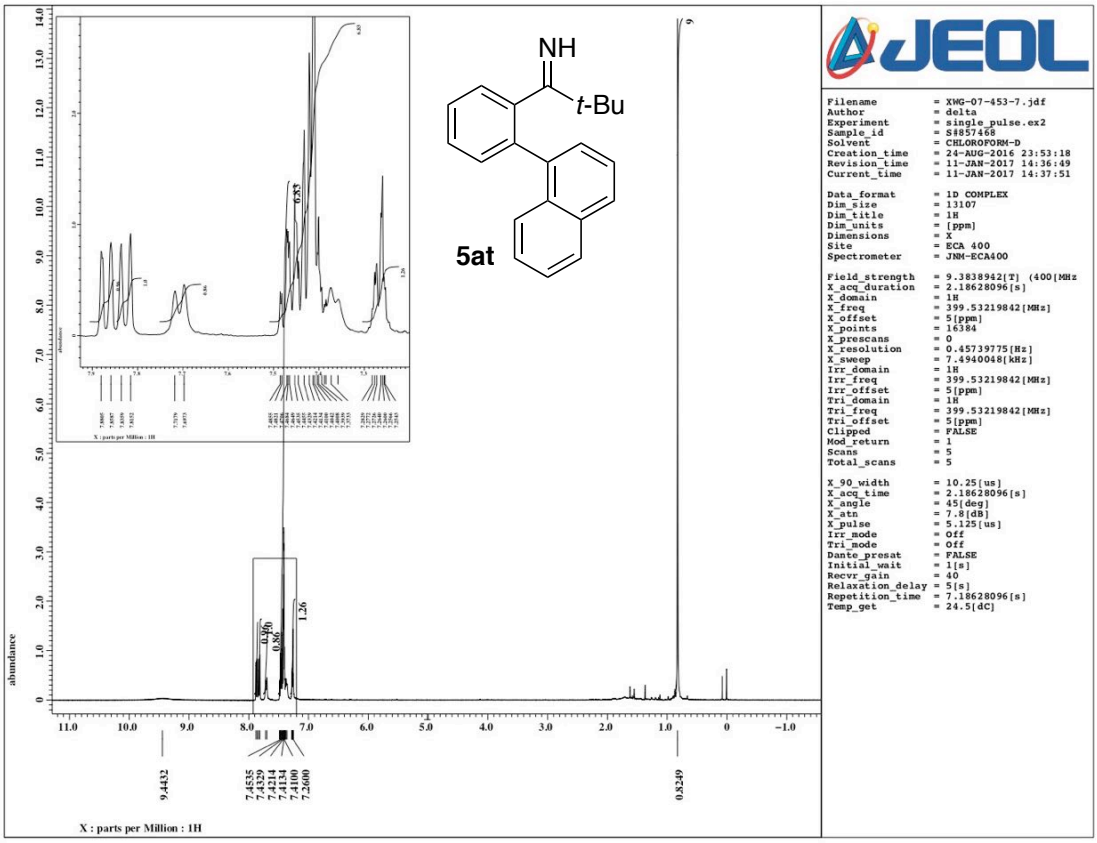

```
Filename          = XWG-07-292-C-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#826512
Solvent           = CHLOROFORM-D
Creation_time     = 22-JUL-2016 23:06:32
Revision_time     = 11-JAN-2017 14:26:25
Current_time      = 11-JAN-2017 14:27:12

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.46244079[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          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 108
Total_scans       = 108

X_90_width        = 8.6[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 8.5[dB]
X_pulse           = 2.86666667[us]
Irr_atn_dec       = 28.799[dB]
Irr_atn_noe       = 28.799[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 22.9[dC]
```

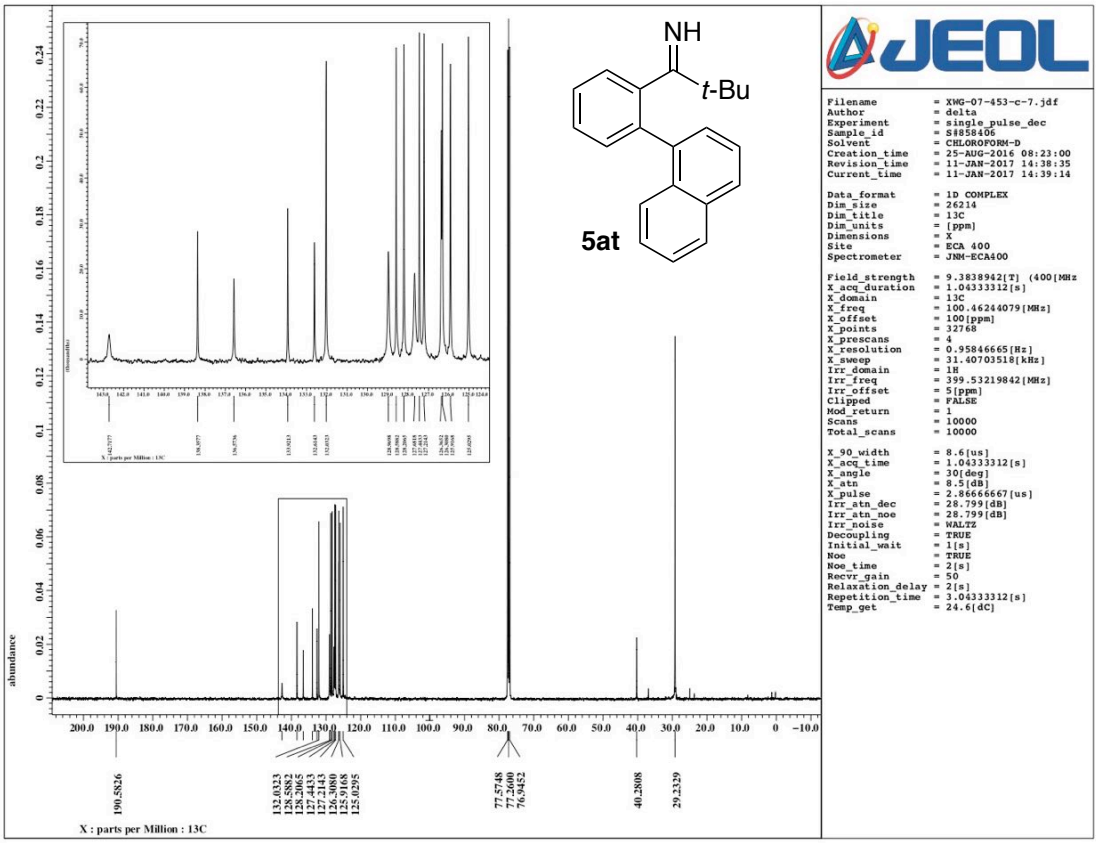

NH
t-Bu
MeO
OMe
5ar
abundance
X : parts per Million : 1H
Filename = XWG-07-297-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8845614
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 23:32:12
Revision_time = 11-JAN-2017 14:30:55
Current_time = 11-JAN-2017 14:31:20
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.7[dC]

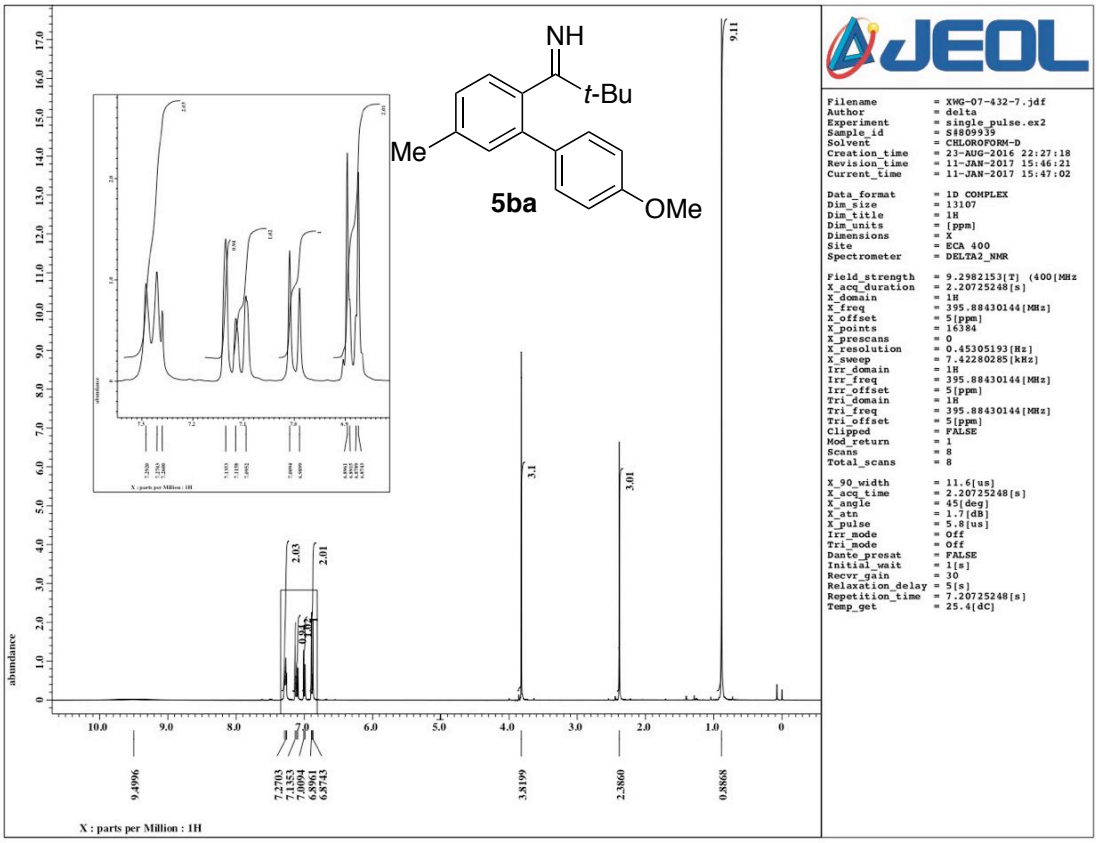

NH
t-Bu
MeO
OMe
5ar
abundance
X : parts per Million : 13C
Filename = XWG-07-297-C-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8846981
Solvent = CHLOROFORM-D
Creation_time = 22-JUL-2016 23:37:23
Revision_time = 11-JAN-2017 14:32:28
Current_time = 11-JAN-2017 14:33:55
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 42
Total_scans = 42
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.9[dC]

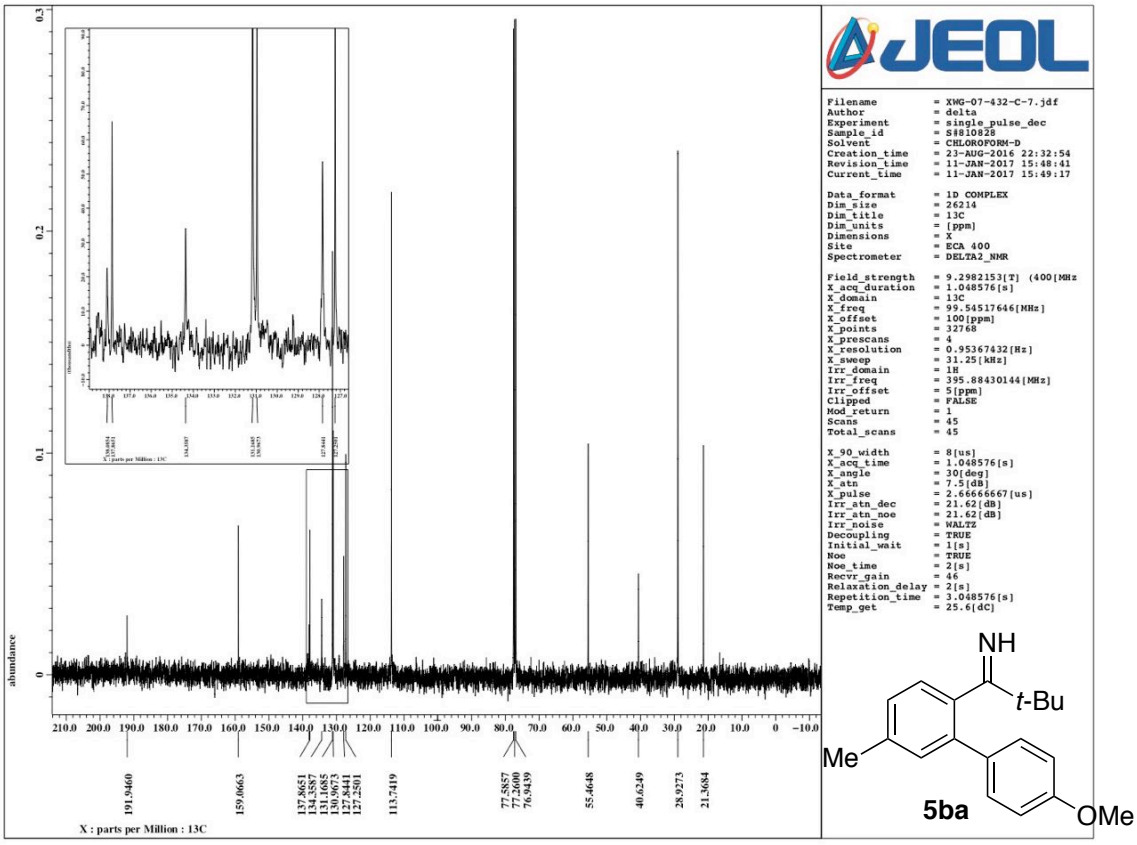

NH
t-Bu
5as
abundance
X : parts per Million : 1H
9.7113
7.8597
7.8505
7.8379
7.5049
7.4809
7.4568
0.8651

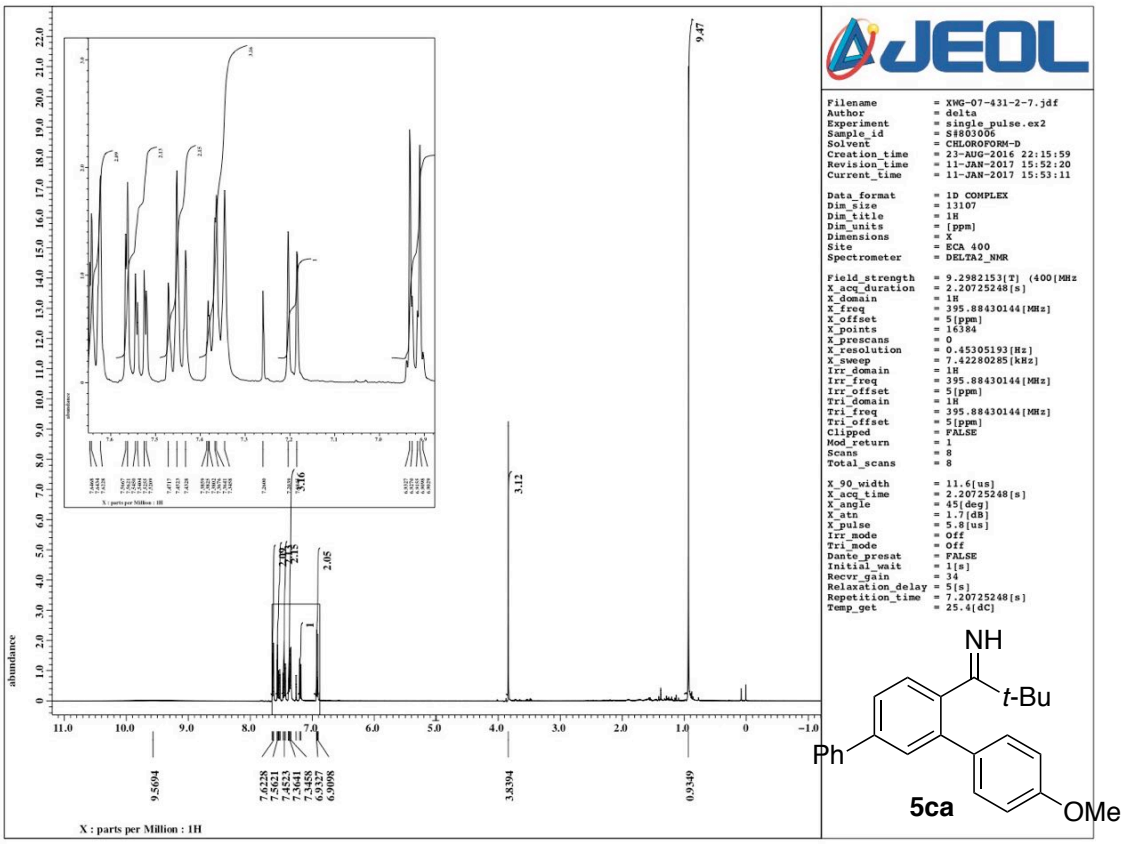

NH
t-Bu
5as
abundance
X : parts per Million : 13C
191.6394
139.1758
138.4476
138.3231
137.9974
137.8153
137.6777
126.4741
126.3591
77.5762
77.2600
76.9343
40.7015
28.9465

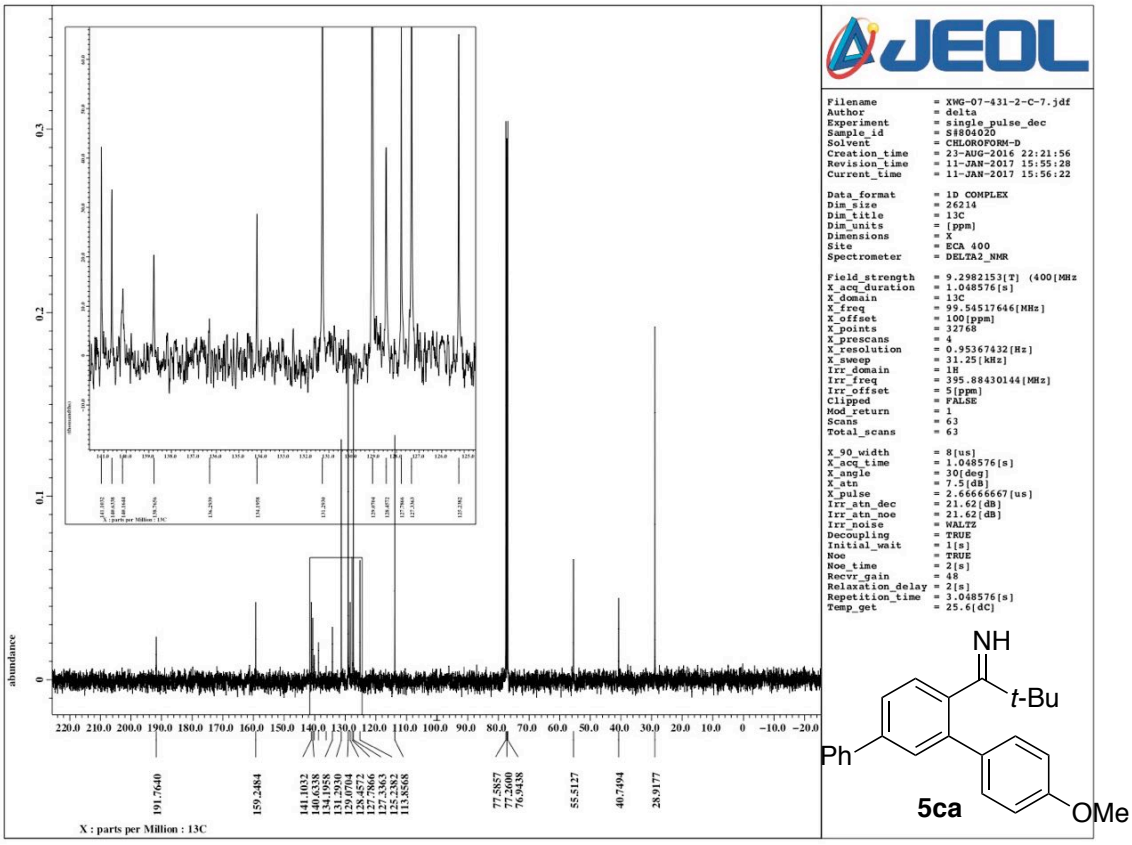

NH
t-Bu
5at
abundance
X : parts per Million : 1H
9.4432
7.4535
7.4329
7.4214
7.4114
7.4100
7.2600
0.8249
1.26
0.86
0.86
Filename = XWG-07-453-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#857468
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 23:53:18
Revision_time = 11-JAN-2017 14:36:49
Current_time = 11-JAN-2017 14:37:51
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.5[dC]

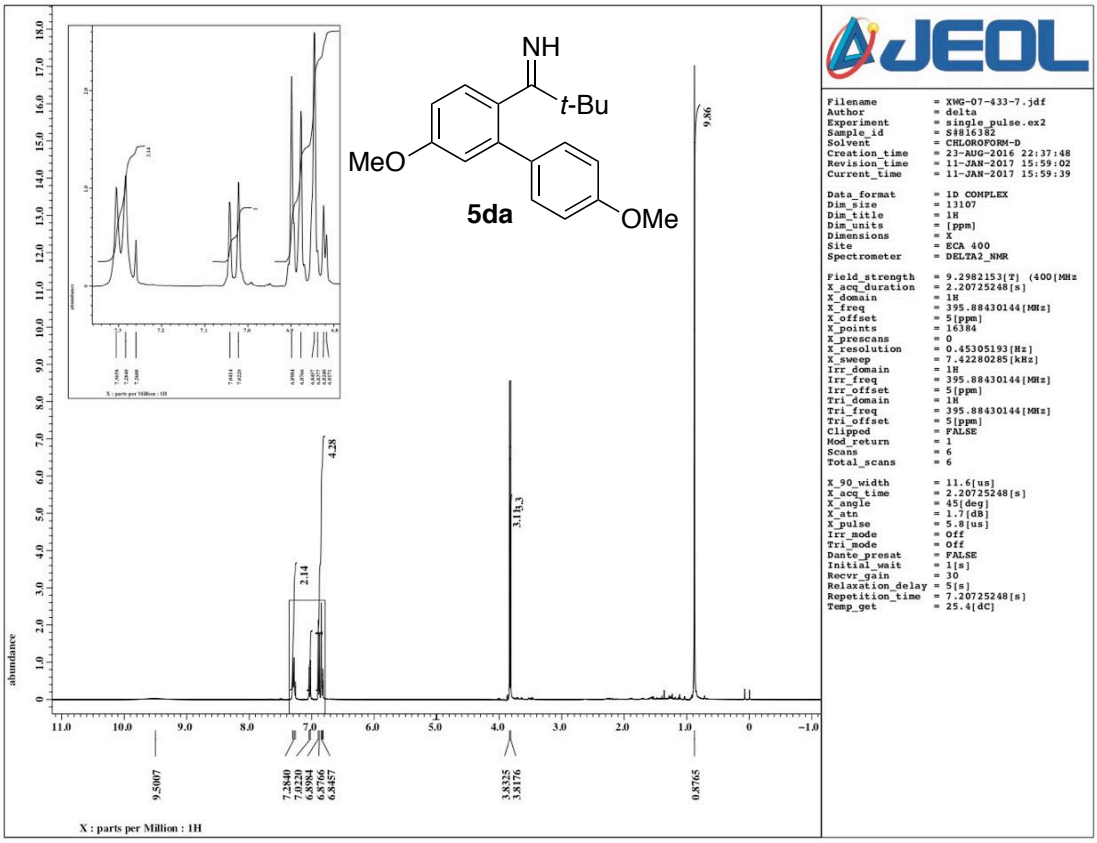

NH
t-Bu
5at
abundance
X : parts per Million : 13C
190.5826
132.0323
128.5882
128.2085
127.4453
127.2143
126.3080
125.9168
125.0295
77.5748
77.2600
76.9452
40.2898
29.2329
Filename = XWG-07-453-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#858406
Solvent = CHLOROFORM-D
Creation_time = 25-AUG-2016 08:23:00
Revision_time = 11-JAN-2017 14:38:35
Current_time = 11-JAN-2017 14:39:14
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.6[dC]


NH
t-Bu
Me
OMe
5ba
abundance
X : parts per Million : 1H
9.4996
7.2703
7.1353
7.0094
6.9961
6.8743
3.8199
2.3860
0.8868
Filename = XWG-07-432-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#809939
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 22:27:18
Revision_time = 11-JAN-2017 15:46:21
Current_time = 11-JAN-2017 15:47:02
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]

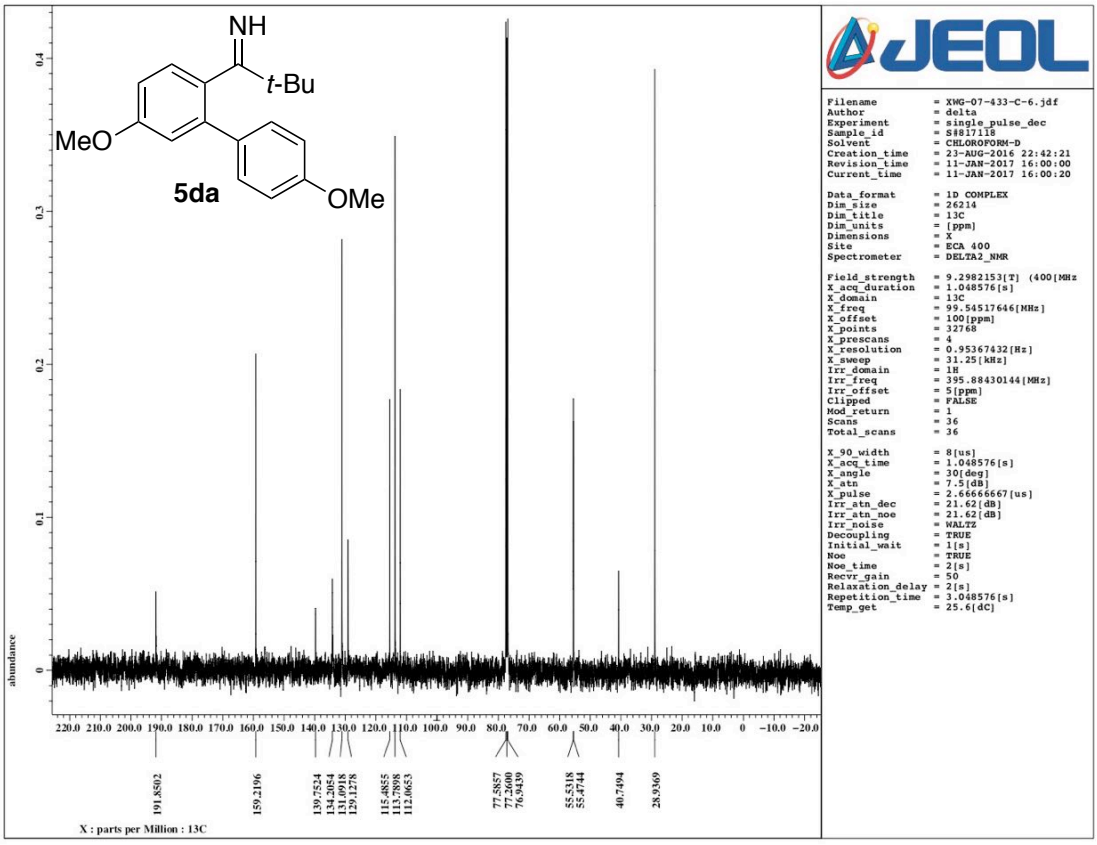

abundance
X : parts per Million : 13C
191.9460
159.0663
137.8651
134.3557
131.1685
130.9673
127.8441
127.2501
113.7419
77.5857
77.3600
76.9439
55.4648
40.6249
28.9273
21.3684
Filename = XWG-07-432-C-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#810828
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 22:32:54
Revision_time = 11-JAN-2017 15:48:41
Current_time = 11-JAN-2017 15:49:17
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 45
Total_scans = 45
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 46
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
NH
t-Bu
Me
OMe
5ba


JEOL
Filename = XWG-07-431-2-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#803006
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 22:15:59
Revision_time = 11-JAN-2017 15:52:20
Current_time = 11-JAN-2017 15:53:11
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]
NH
t-Bu
Ph
OMe
5ca
abundance
X : parts per Million : 1H

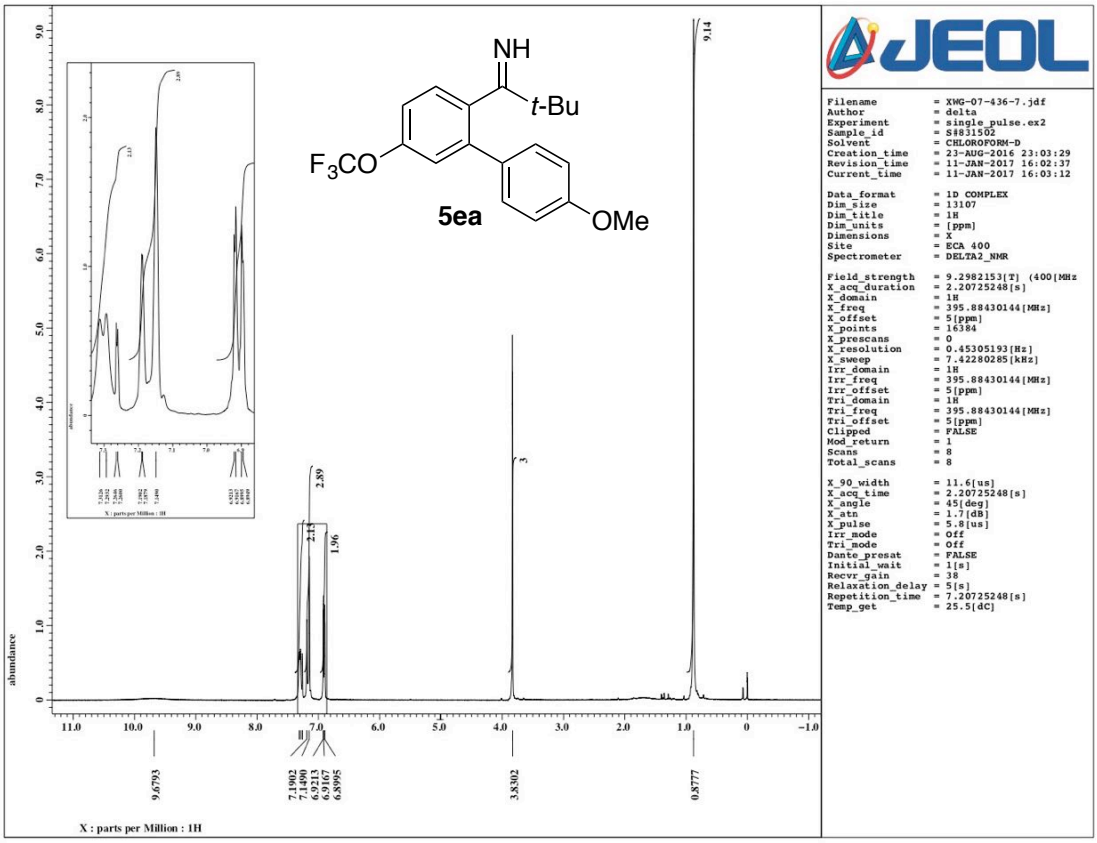

JEOL
Filename = XWG-07-431-2-C-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#804020
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 22:21:56
Revision_time = 11-JAN-2017 15:55:28
Current_time = 11-JAN-2017 15:56:22
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 63
Total_scans = 63
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 48
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
NH
t-Bu
Ph
OMe
5ca
abundance
X : parts per Million : 13C



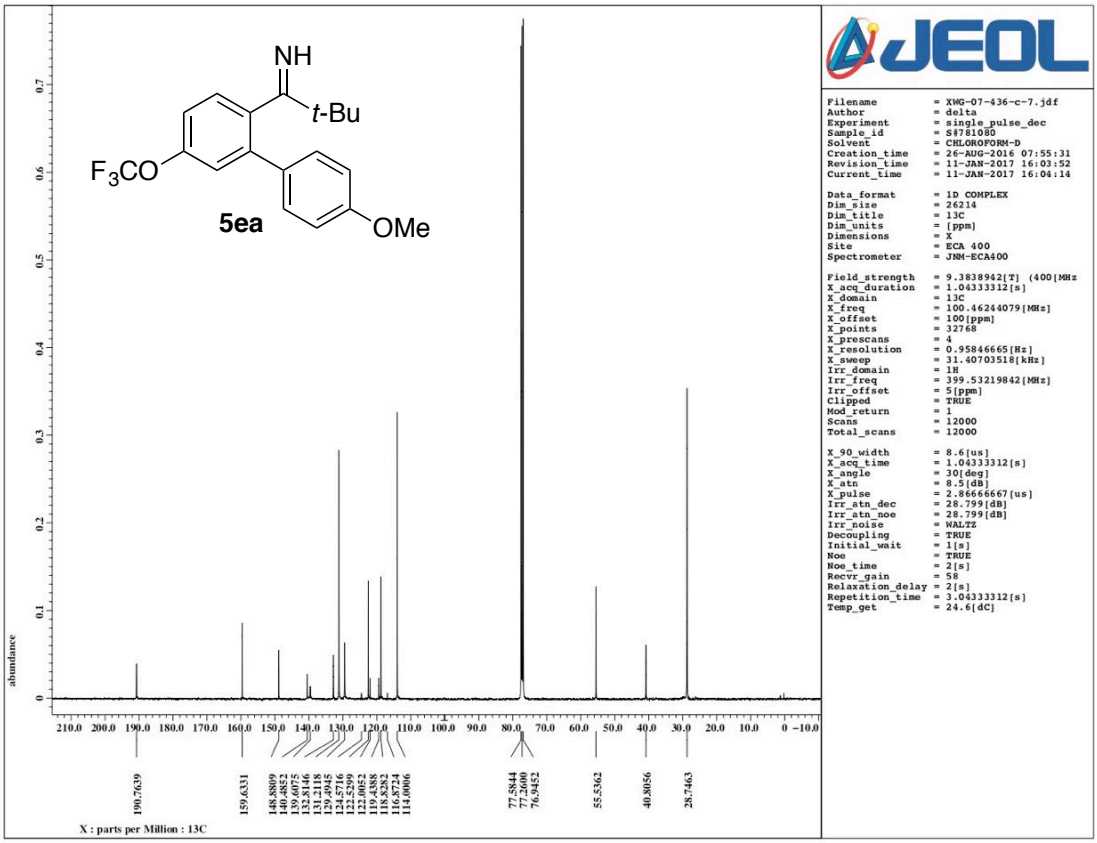

```
Filename          = XWG-07-433-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8816382
Solvent           = CHLOROFORM-D
Creation_time     = 23-AUG-2016 22:37:48
Revision_time     = 11-JAN-2017 15:59:02
Current_time      = 11-JAN-2017 15:59:39

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 6
Total_scans       = 6

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.4[dC]
```



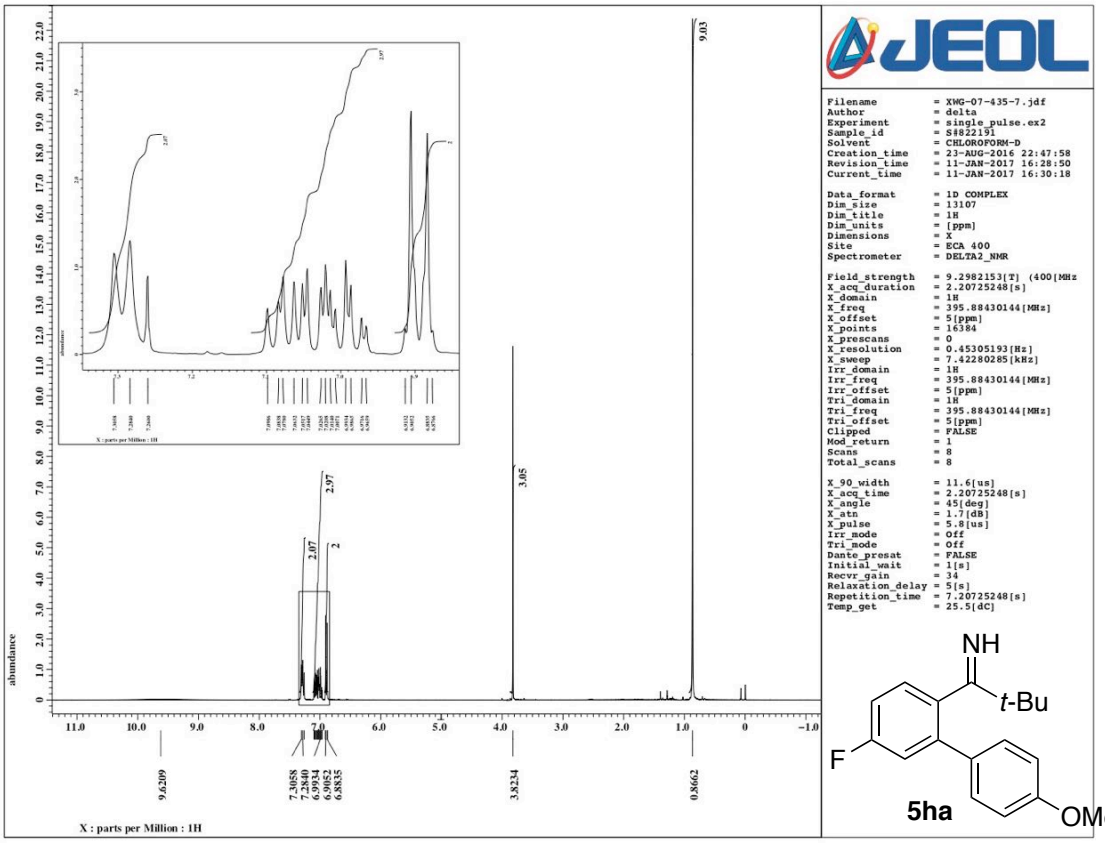

```
Filename          = XWG-07-433-C-6.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8817118
Solvent           = CHLOROFORM-D
Creation_time     = 23-AUG-2016 22:42:21
Revision_time     = 11-JAN-2017 16:00:00
Current_time      = 11-JAN-2017 16:00:20

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 36
Total_scans       = 36

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.6[dC]
```

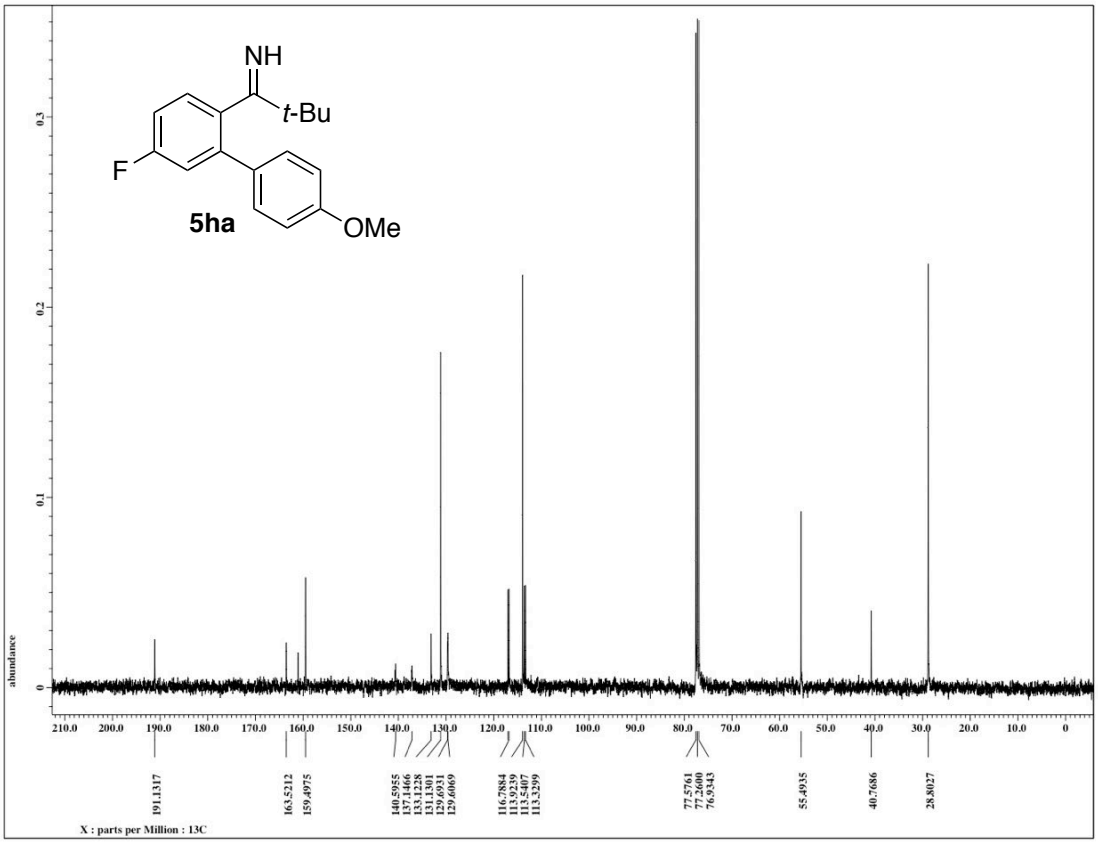


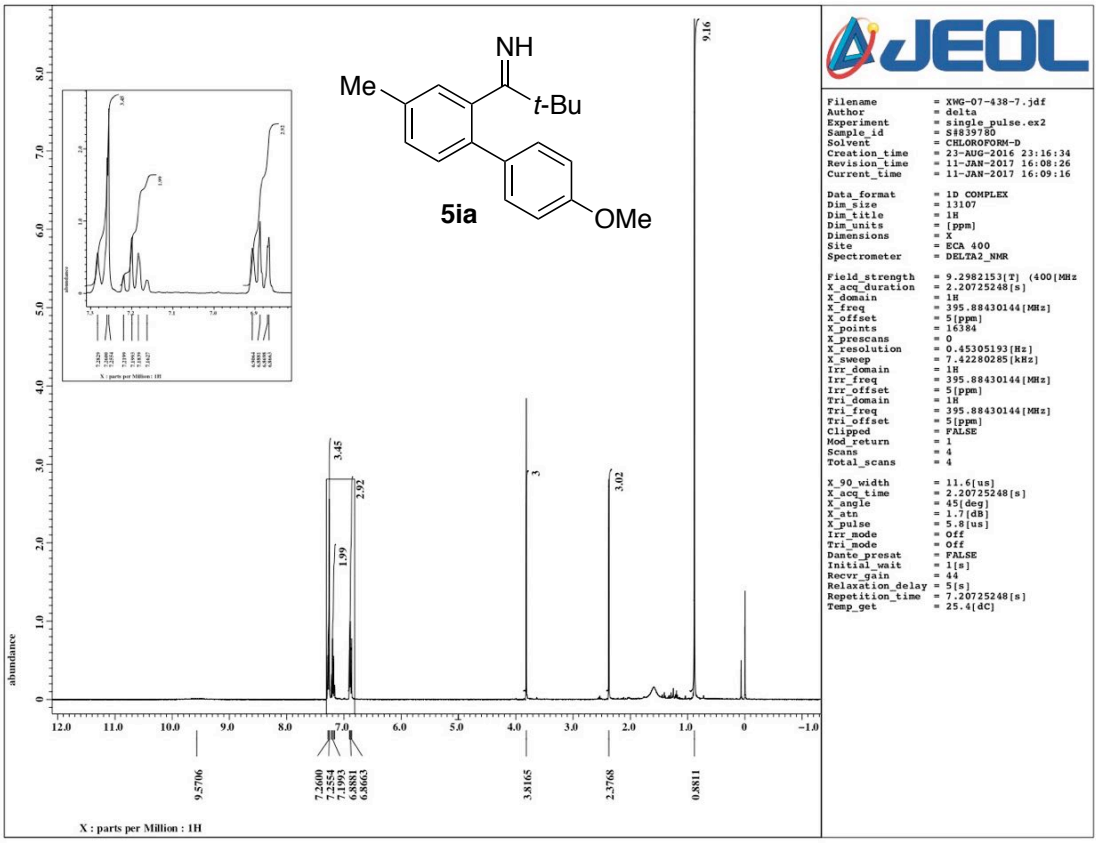

```
Filename          = XWG-07-436-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8831502
Solvent           = CHLOROFORM-D
Creation_time     = 23-AUG-2016 23:03:29
Revision_time     = 11-JAN-2017 16:02:37
Current_time      = 11-JAN-2017 16:03:12

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.5[dC]
```

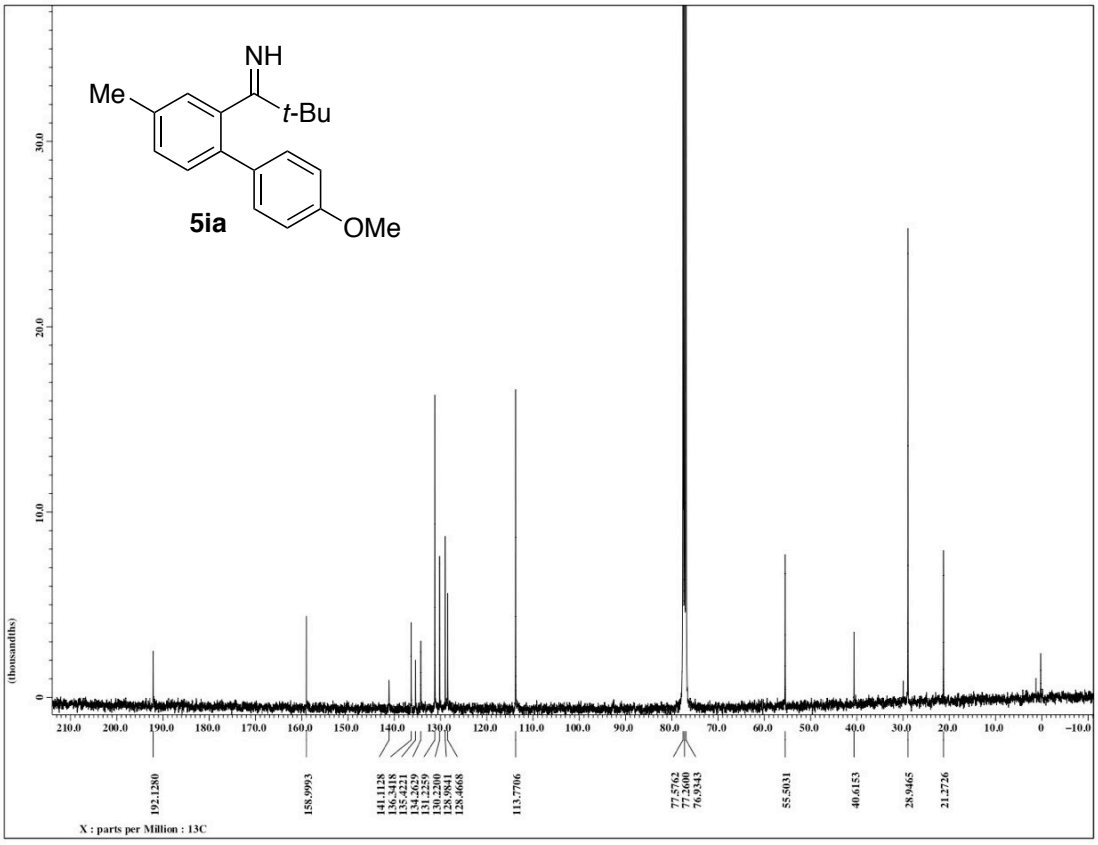


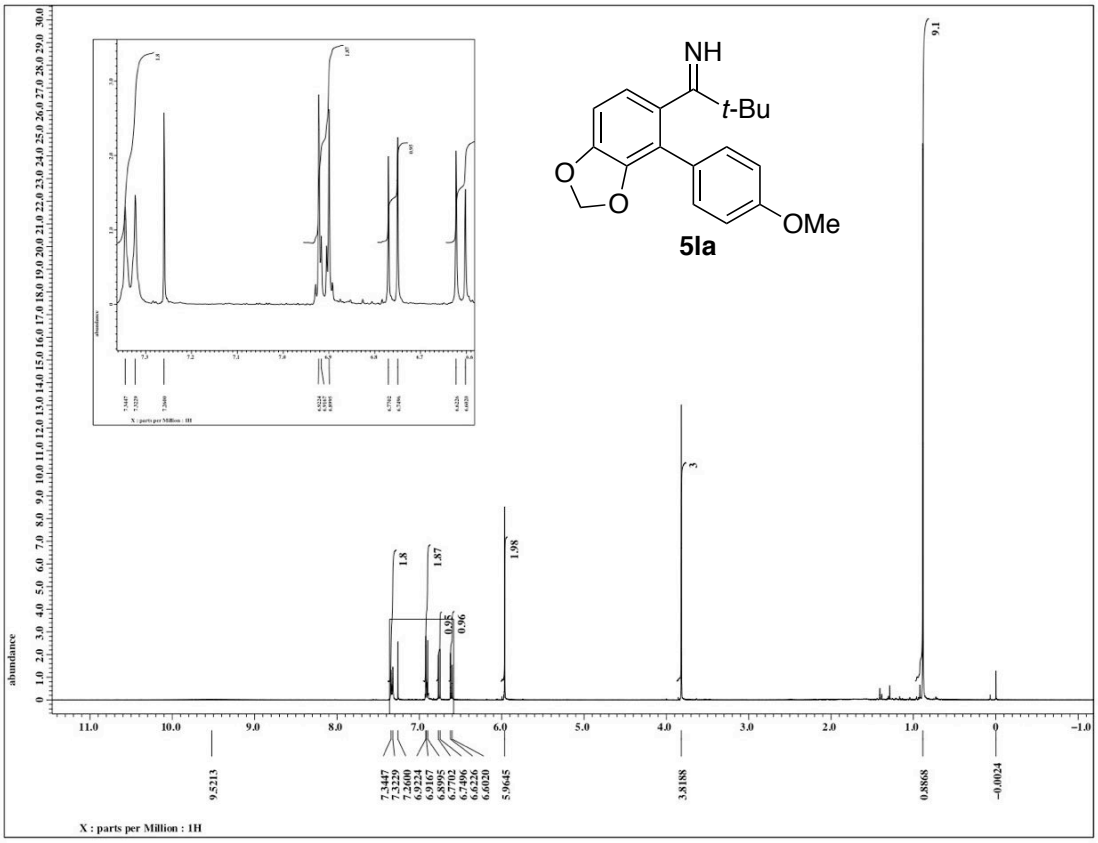

```
Filename          = XWG-07-436-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8781080
Solvent           = CHLOROFORM-D
Creation_time     = 26-AUG-2016 07:55:31
Revision_time     = 11-JAN-2017 16:03:52
Current_time      = 11-JAN-2017 16:04:14

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.46244079[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          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 12000
Total_scans       = 12000

X_90_width        = 8.6[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 8.5[dB]
X_pulse           = 2.86666667[us]
Irr_atn_dec       = 28.799[dB]
Irr_atn_noe       = 28.799[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 24.6[dC]
```

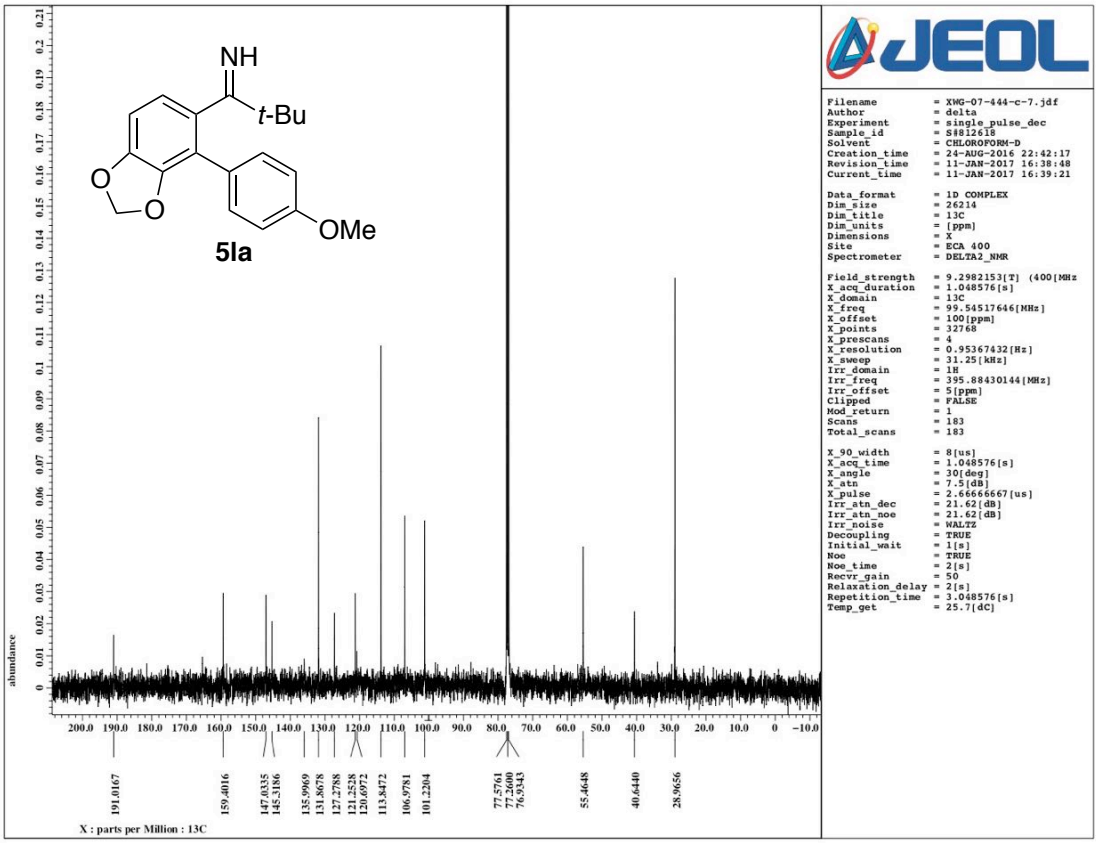

Filename = XWG-07-435-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8822191
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 22:47:58
Revision_time = 11-JAN-2017 16:28:50
Current_time = 11-JAN-2017 16:30:18
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.5[dC]
NH
t-Bu
F
OMe
5ha
abundance
9.6209
7.3058
7.2840
6.9934
6.9852
6.8835
3.8234
0.8662
X : parts per Million : 1H

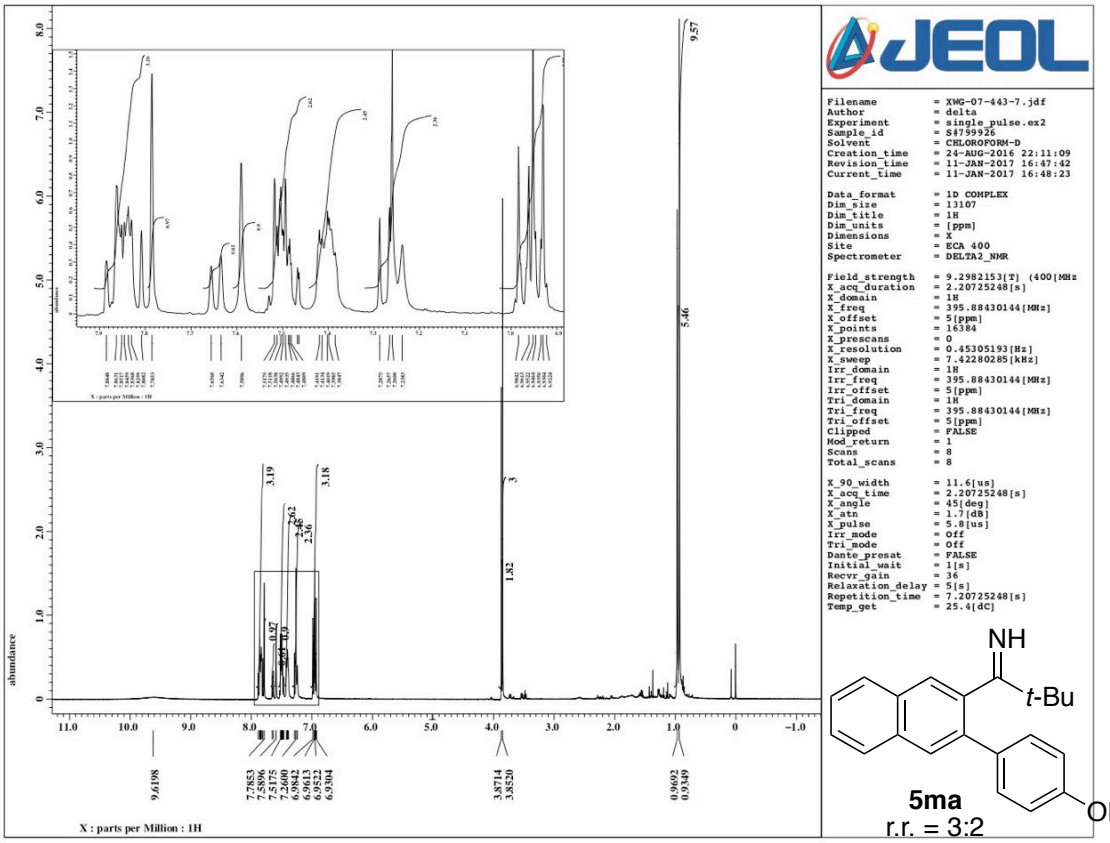

NH
t-Bu
F
OMe
5ha
abundance
191.1317
163.5212
159.4975
140.5955
137.1466
133.1228
131.1301
129.6931
129.6069
116.7884
113.9239
113.5407
113.3299
77.5761
77.2600
76.9343
55.4935
40.7686
28.8027
X : parts per Million : 13C

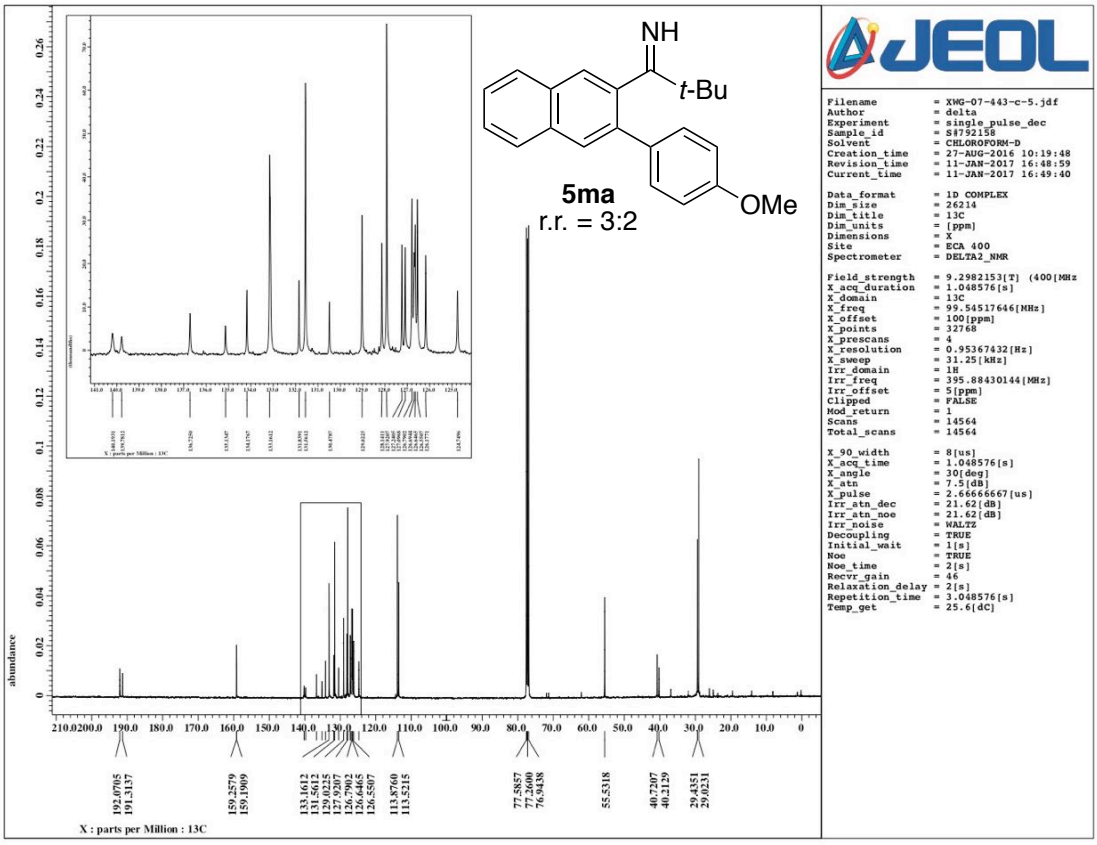

NH
Me
t-Bu
OMe
5ia
abundance
9.16
3.45
2.92
1.99
3
3.02
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 −1.0
9.5706
7.2600
7.2554
7.1993
6.8881
6.8663
3.8165
2.3768
0.8811
X : parts per Million : 1H
JEOL
Filename = XWG-07-438-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8839780
Solvent = CHLOROFORM-D
Creation_time = 23-AUG-2016 23:16:34
Revision_time = 11-JAN-2017 16:08:26
Current_time = 11-JAN-2017 16:09:16
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]

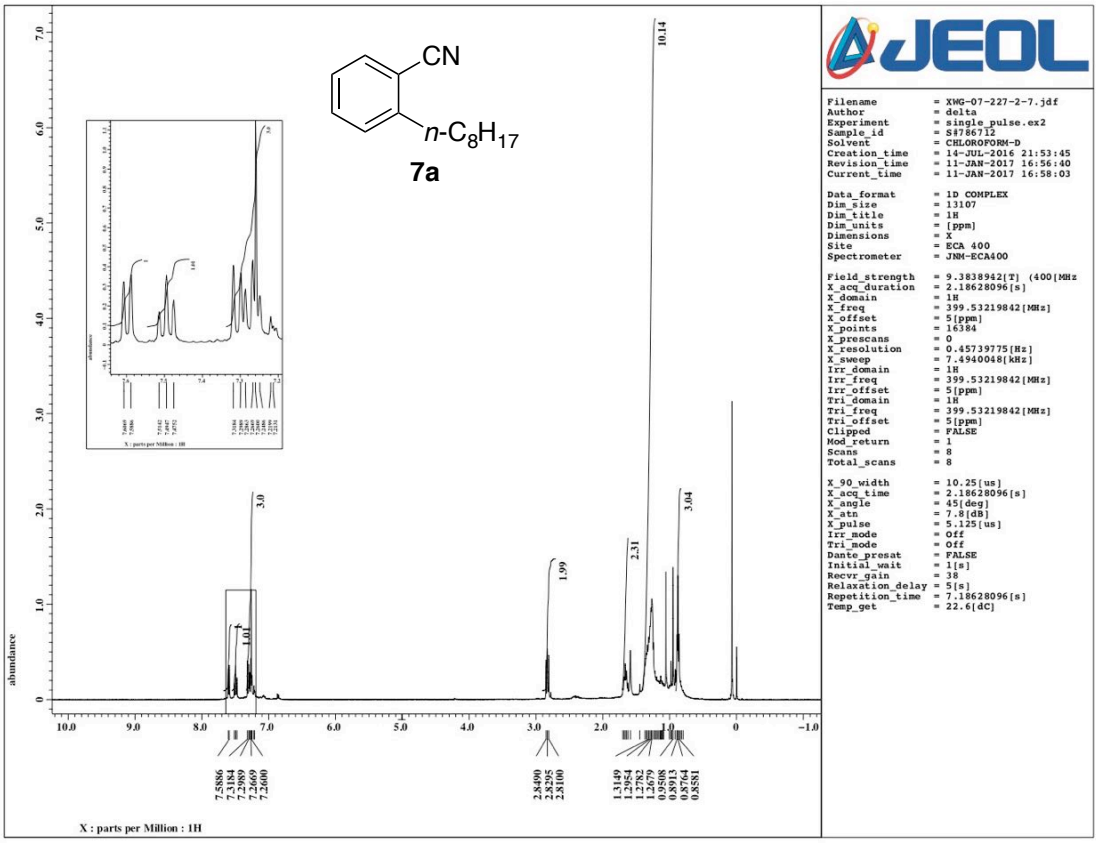

NH
Me
t-Bu
OMe
5ia
(thousandths)
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
192.1280
158.9993
141.1128
136.3418
135.4221
134.2629
131.2259
130.2700
128.9841
128.4668
113.7706
77.5762
77.2600
76.9343
55.5031
40.6153
28.9465
21.2726
X : parts per Million : 13C


NH
t-Bu
O
O
OMe
5la
abundance
X : parts per Million : 1H


NH
t-Bu
O
O
OMe
5la
abundance
X : parts per Million : 13C
Filename = XWG-07-444-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8812618
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 22:42:17
Revision_time = 11-JAN-2017 16:38:48
Current_time = 11-JAN-2017 16:39:21
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 183
Total_scans = 183
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.7[dC]


Filename = XWG-07-443-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#799926
Solvent = CHLOROFORM-D
Creation_time = 24-AUG-2016 22:11:09
Revision_time = 11-JAN-2017 16:47:42
Current_time = 11-JAN-2017 16:48:23
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.4[dC]
NH
t-Bu
OMe
5ma
r.r. = 3:2
abundance
X : parts per Million : 1H


NH
t-Bu
OMe
5ma
r.r. = 3:2
Filename = XWG-07-443-c-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#792158
Solvent = CHLOROFORM-D
Creation_time = 27-AUG-2016 10:19:48
Revision_time = 11-JAN-2017 16:48:59
Current_time = 11-JAN-2017 16:49:40
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 14564
Total_scans = 14564
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 46
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.6[dC]
abundance
X : parts per Million : 13C

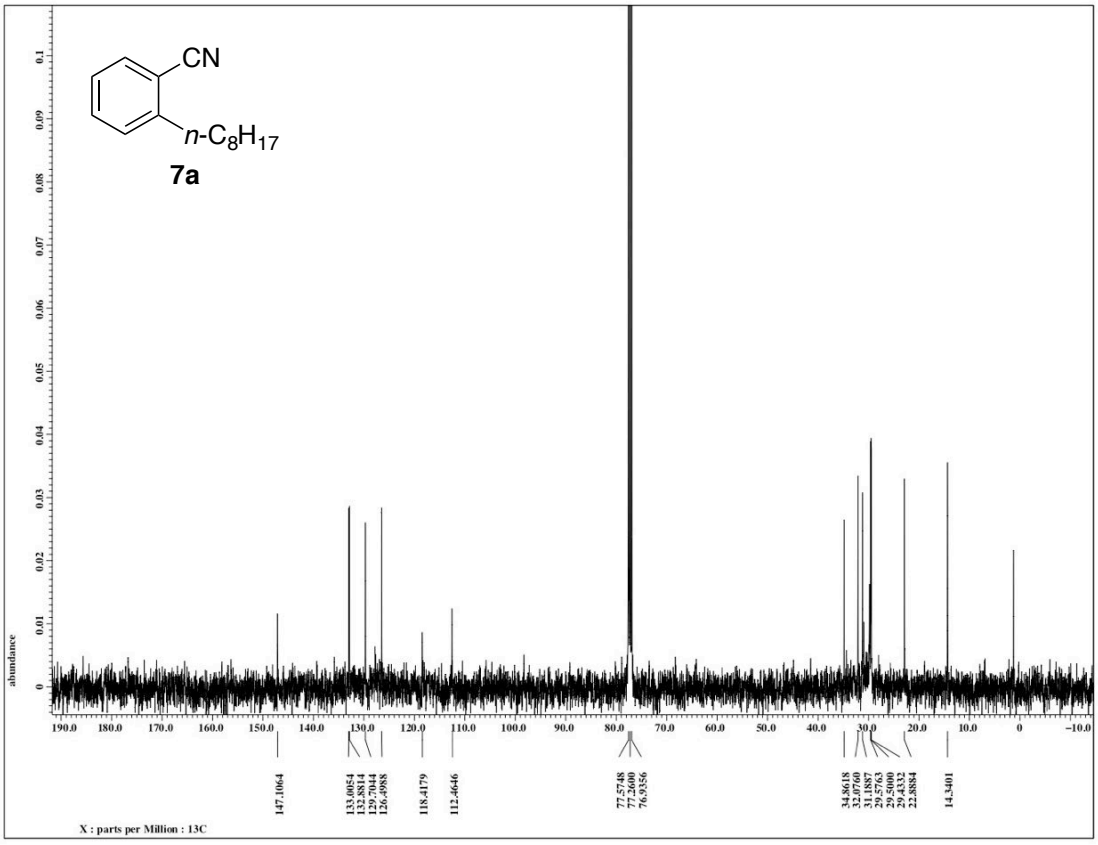


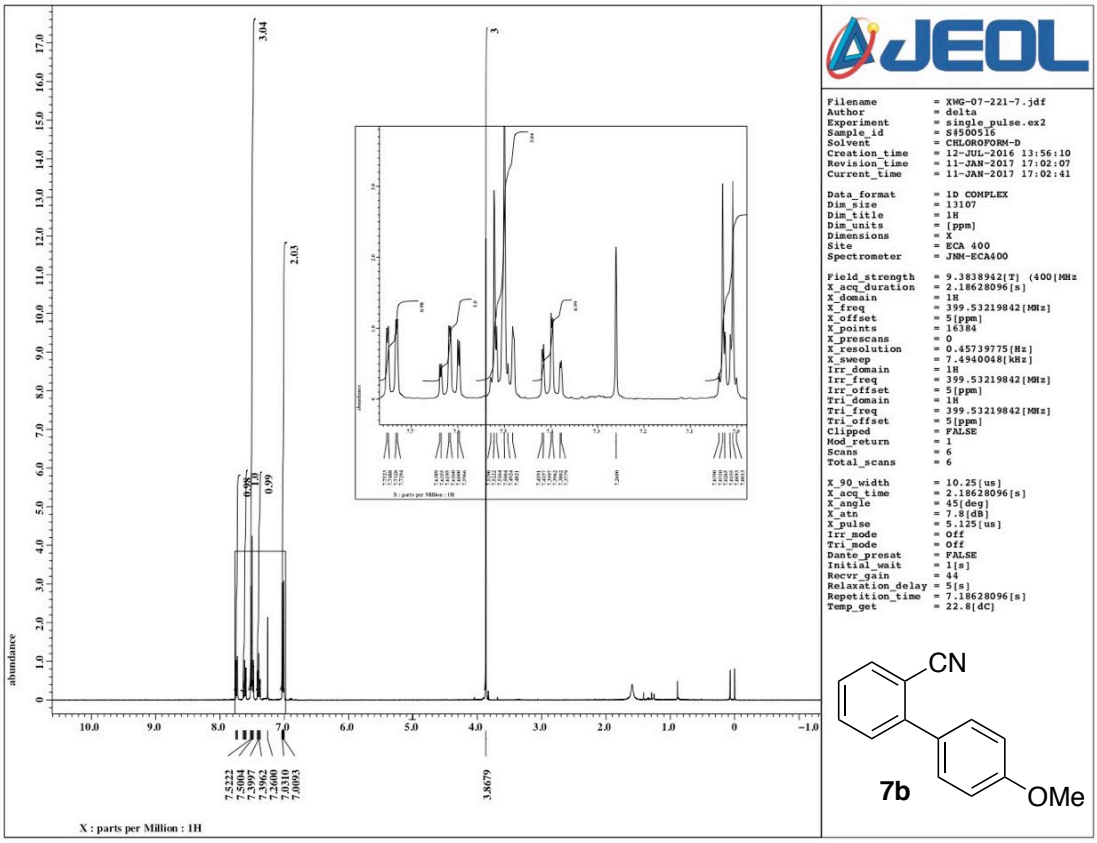
Filename = XWG-07-227-2-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8786712
Solvent = CHLOROFORM-D
Creation_time = 14-JUL-2016 21:53:45
Revision_time = 11-JAN-2017 16:56:40
Current_time = 11-JAN-2017 16:58:03

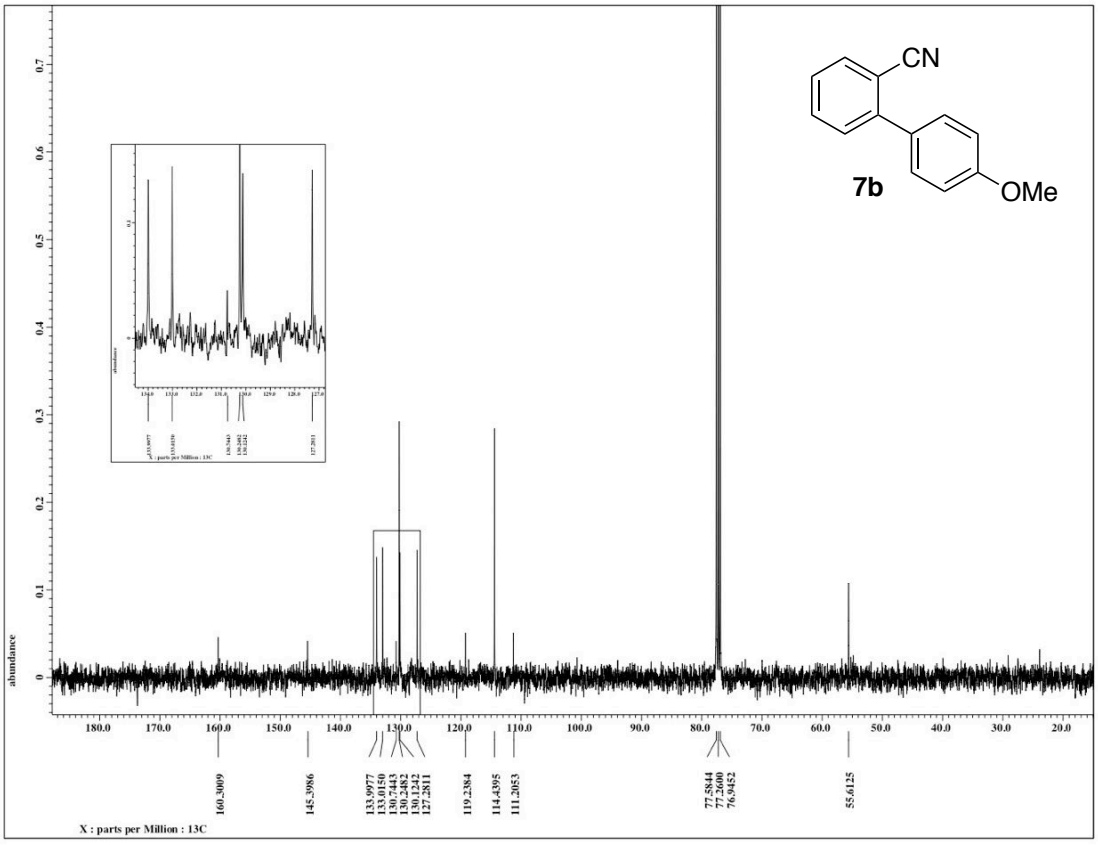
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400

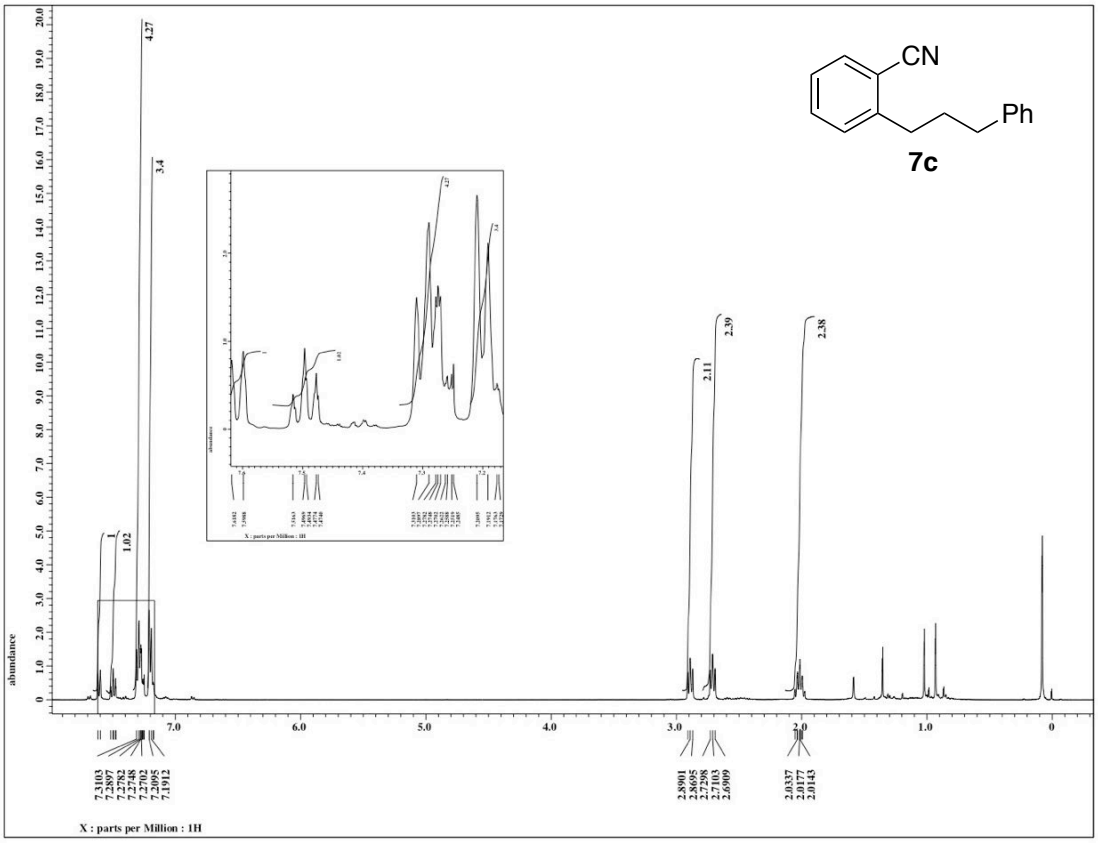
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

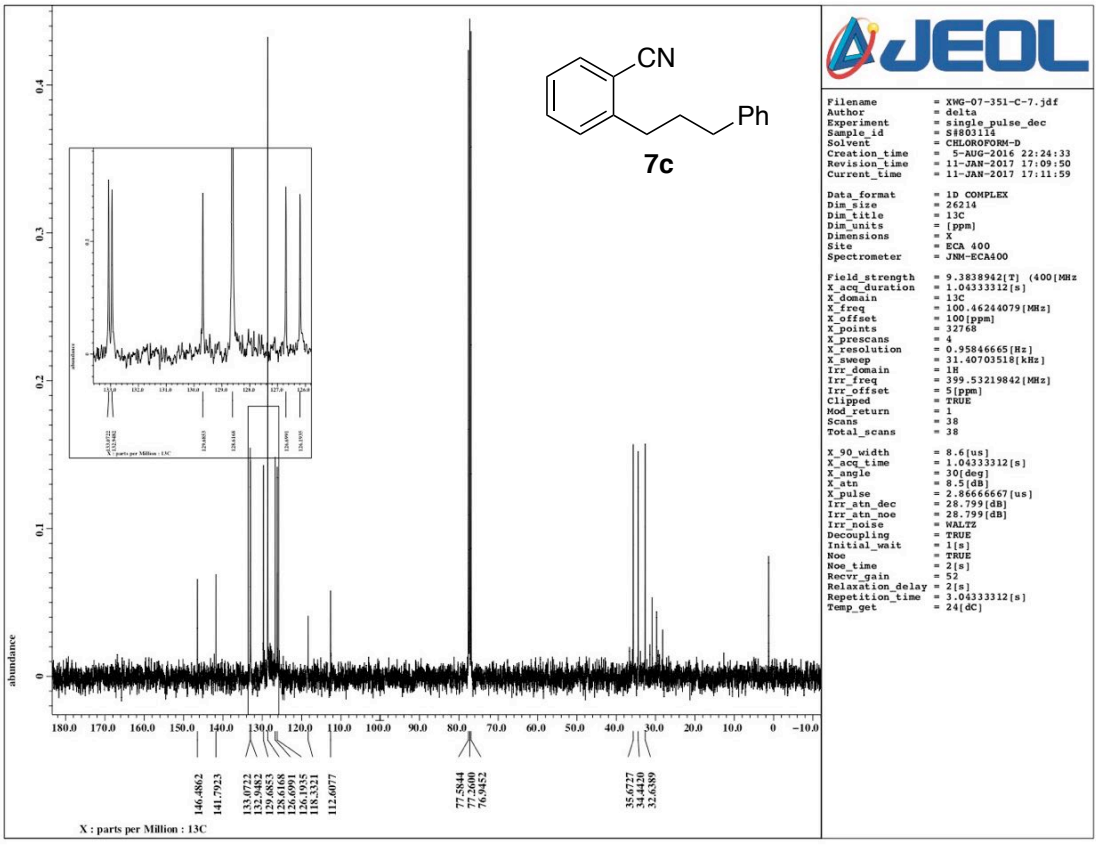
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.6[dC]

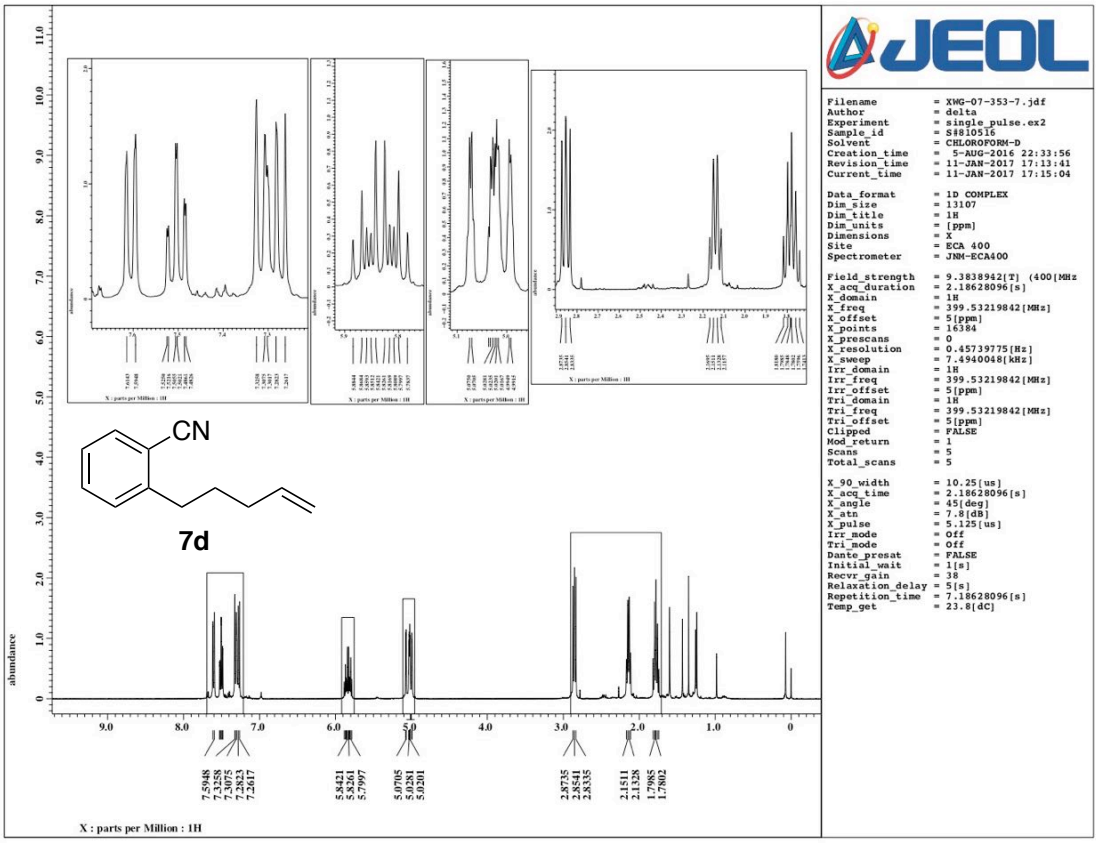



JEOL
Filename = XWG-07-221-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#500516
Solvent = CHLOROFORM-D
Creation_time = 12-JUL-2016 13:56:10
Revision_time = 11-JAN-2017 17:02:07
Current_time = 11-JAN-2017 17:02:41
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 22.8[dC]
CN
7b
OMe
abundance
X : parts per Million : 1H
7.5322
7.5084
7.3997
7.3962
7.2600
7.0310
7.0095
3.5679

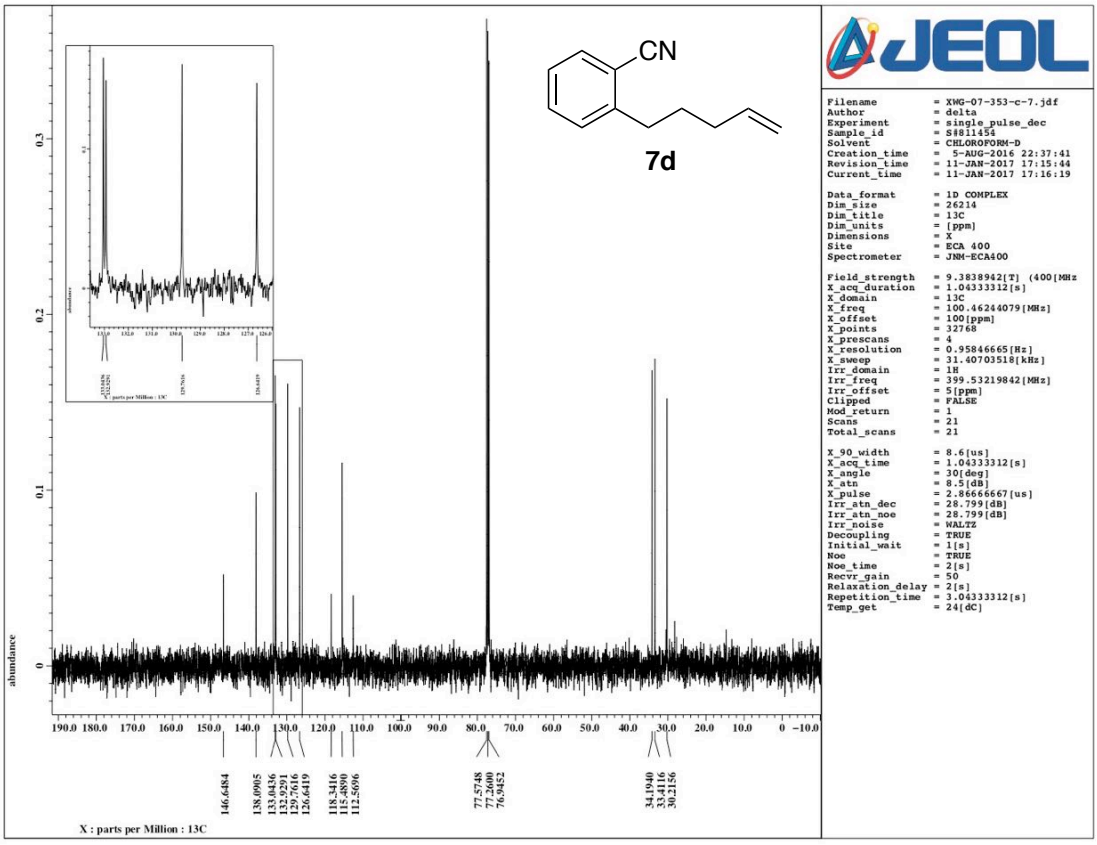

CN
7b
OMe
abundance
X : parts per Million : 13C
160.3009
145.3986
133.9977
131.0155
130.7443
130.2482
130.1242
127.2811
119.2384
114.4395
111.2053
77.5844
77.2600
76.9452
55.6125


CN
Ph
7c
4.27
3.4
1.02
2.11
2.39
2.38
abundance
X : parts per Million : 1H

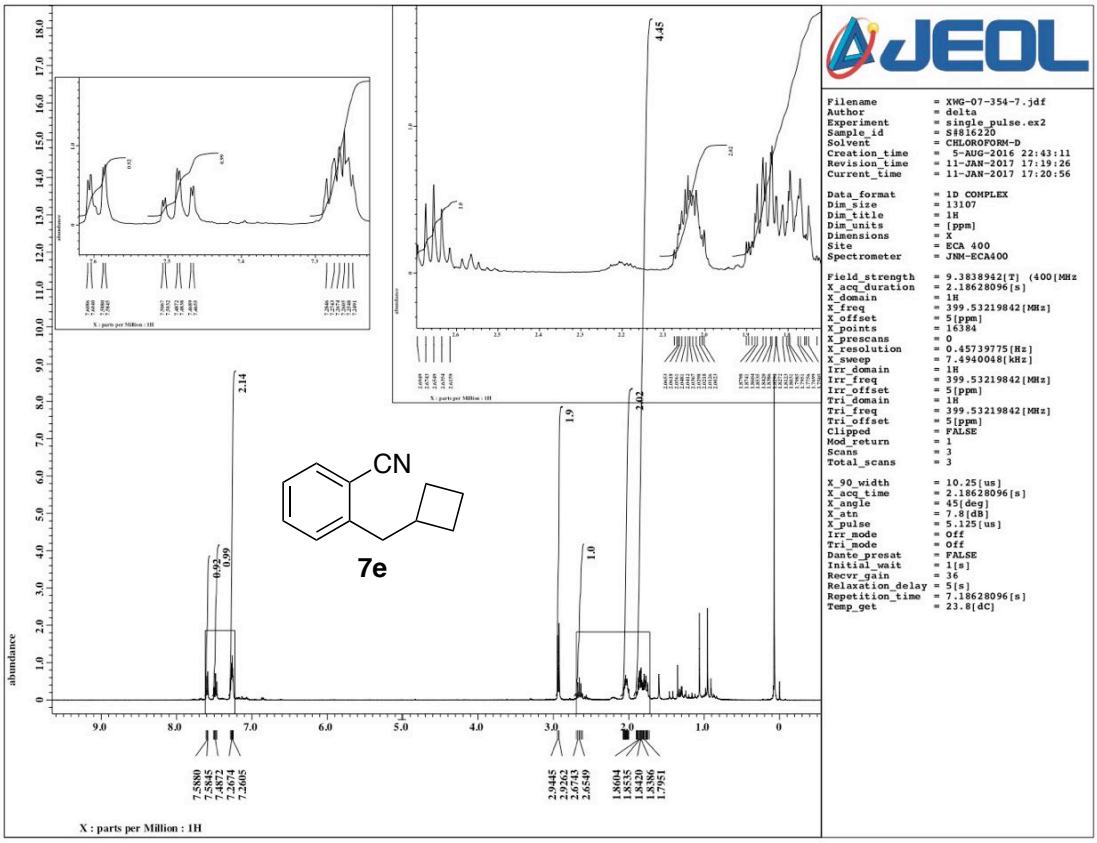

CN
Ph
7c
abundance
X : parts per Million : 13C
Filename = XWG-07-351-C-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S8803114
Solvent = CHLOROFORM-D
Creation_time = 5-AUG-2016 22:24:33
Revision_time = 11-JAN-2017 17:09:50
Current_time = 11-JAN-2017 17:11:59
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 38
Total_scans = 38
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 52
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24[dC]

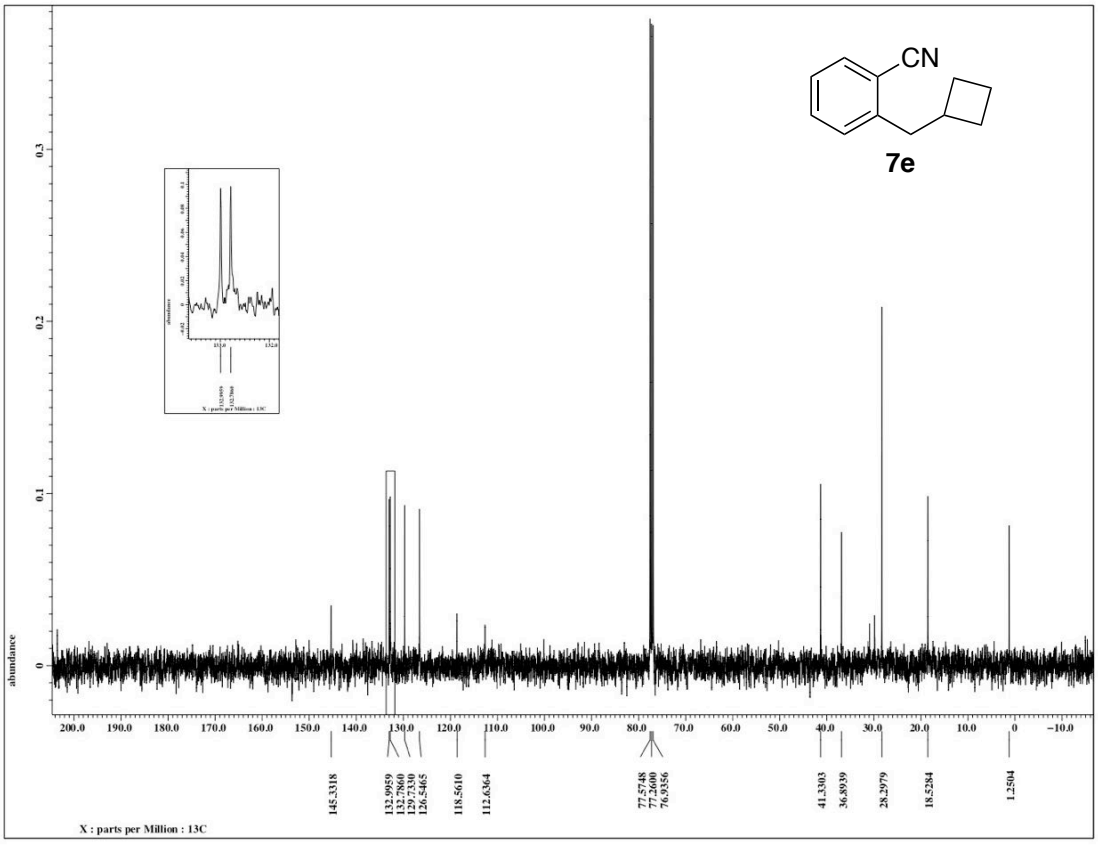


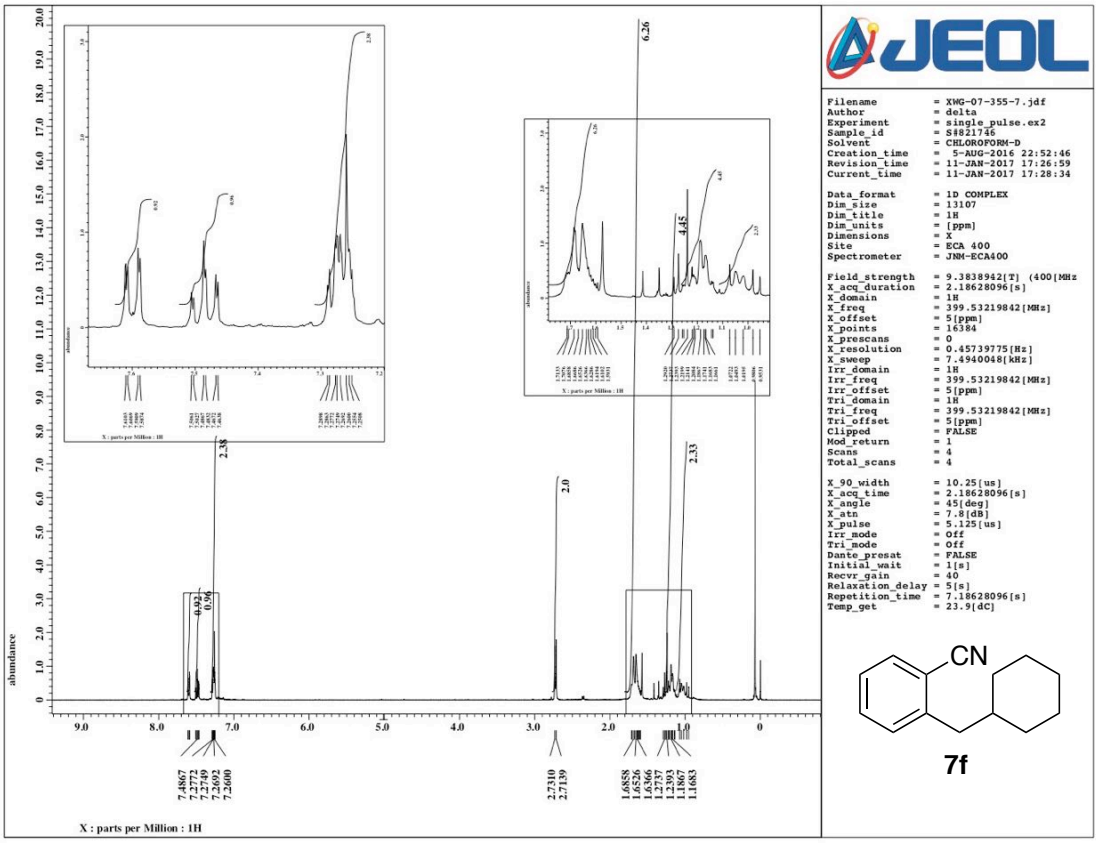

```
Filename          = XWG-07-353-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#810516
Solvent           = CHLOROFORM-D
Creation_time     =  5-AUG-2016 22:33:56
Revision_time     = 11-JAN-2017 17:13:41
Current_time      = 11-JAN-2017 17:15:04

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 2.18628096[s]
X_domain          = 1H
X_freq            = 399.53219842[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45739775[Hz]
X_sweep           = 7.4940048[kHz]
Irr_domain        = 1H
Irr_freq          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.53219842[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 5
Total_scans       = 5

X_90_width        = 10.25[us]
X_acq_time        = 2.18628096[s]
X_angle           = 45[deg]
X_atn             = 7.8[dB]
X_pulse           = 5.125[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18628096[s]
Temp_get          = 23.8[dC]
```



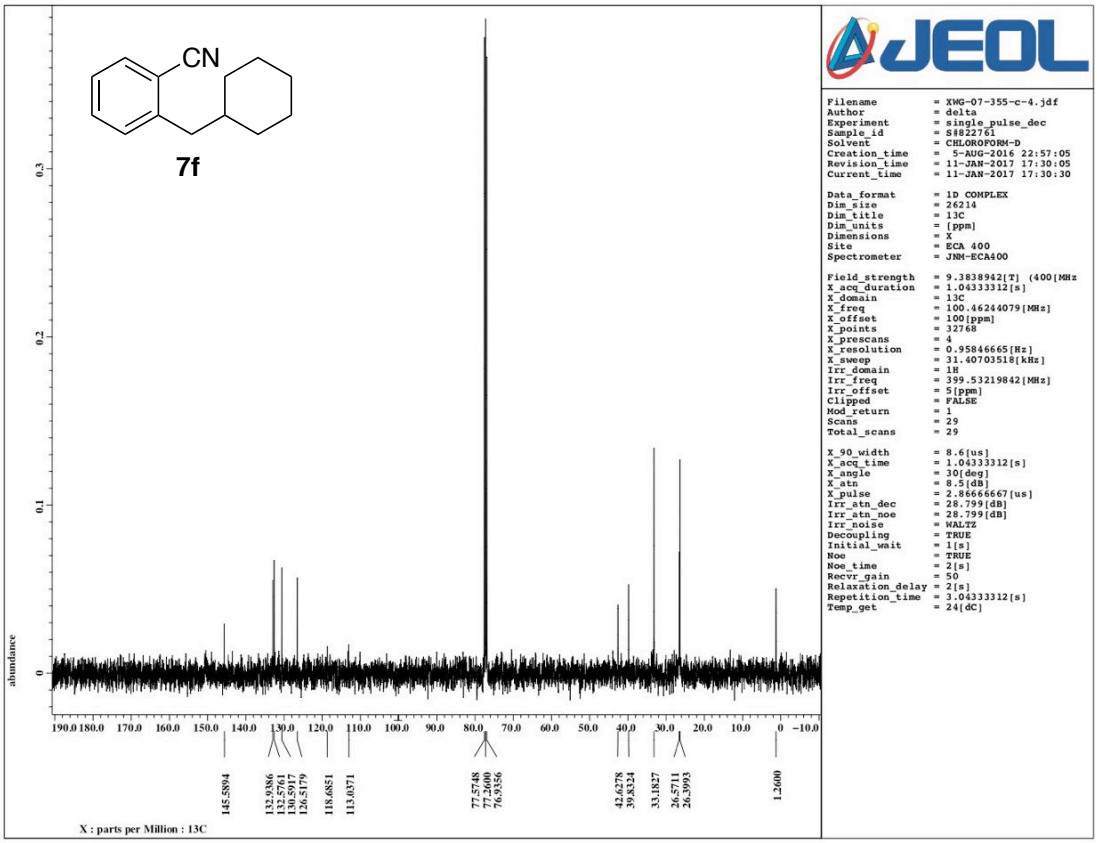

```
Filename          = XWG-07-353-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#811454
Solvent           = CHLOROFORM-D
Creation_time     =  5-AUG-2016 22:37:41
Revision_time     = 11-JAN-2017 17:15:44
Current_time      = 11-JAN-2017 17:16:19

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.46244079[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          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 21
Total_scans       = 21

X_90_width        = 8.6[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 8.5[dB]
X_pulse           = 2.86666667[us]
Irr_atn_dec       = 28.799[dB]
Irr_atn_noe       = 28.799[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 24[dC]
```


JEOL
Filename = XWG-07-354-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S8816220
Solvent = CHLOROFORM-D
Creation_time = 5-AUG-2016 22:43:11
Revision_time = 11-JAN-2017 17:19:26
Current_time = 11-JAN-2017 17:20:56
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3
Total_scans = 3
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 23.8[dC]
CN
7e
abundance
X : parts per Million : 1H

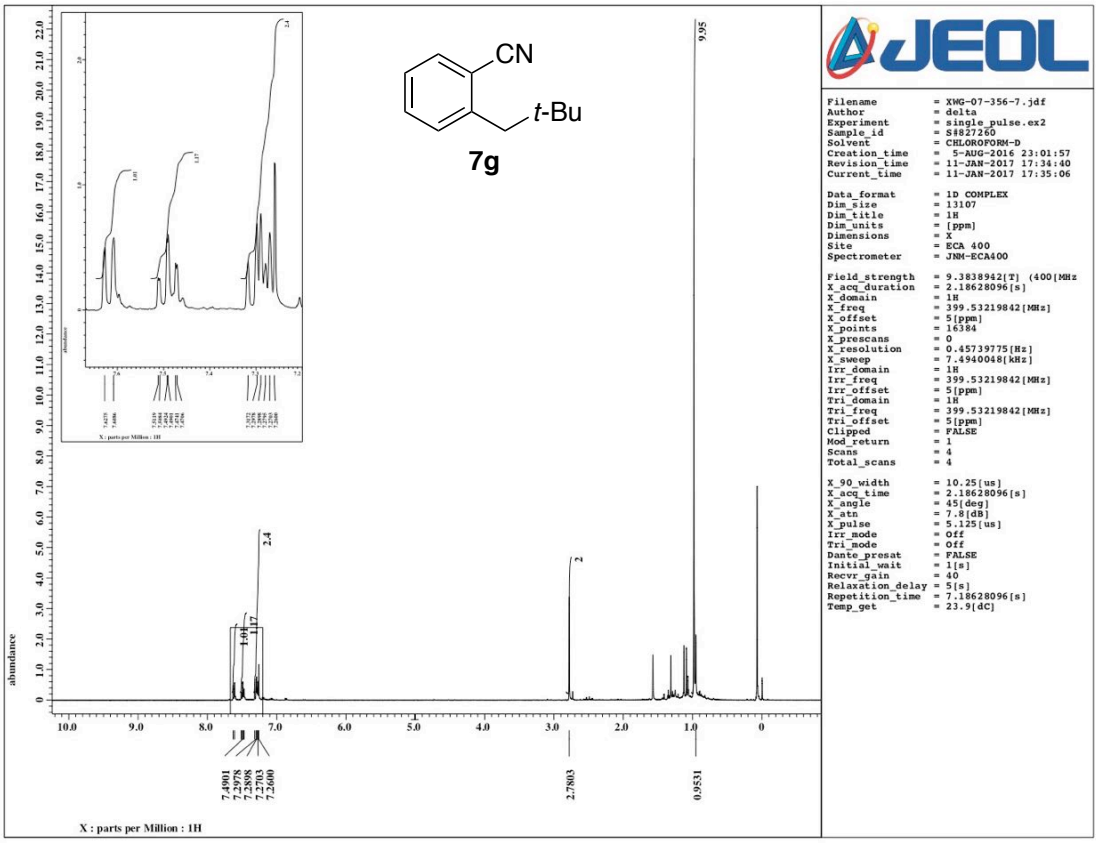

CN
7e
abundance
X : parts per Million : 13C


abundance
X : parts per Million : 1H
7.4867
7.2772
7.2749
7.2692
7.2660
2.7310
2.7139
1.6858
1.6526
1.6366
1.2757
1.2393
1.1867
1.1683
2.38
2.33
2.0
6.26
4.45
0.92
0.96

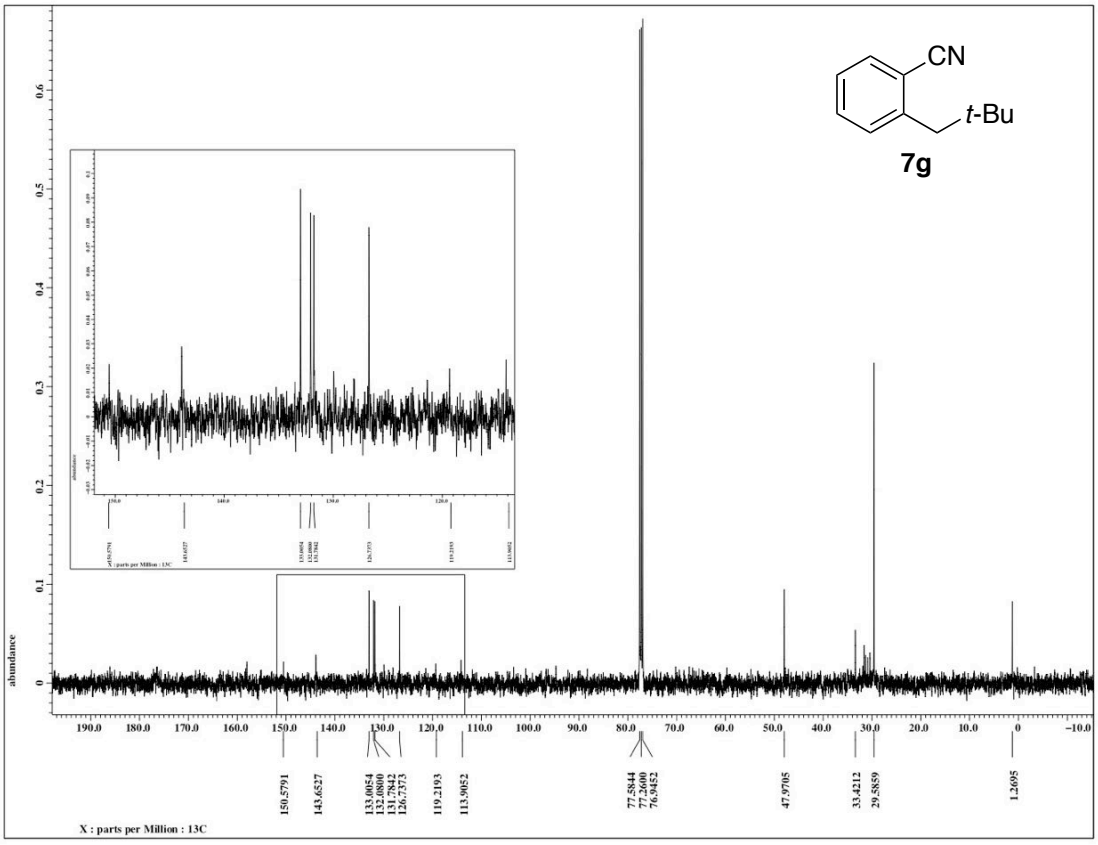
JEOL
Filename = XWG-07-355-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#821746
Solvent = CHLOROFORM-D
Creation_time = 5-AUG-2016 22:52:46
Revision_time = 11-JAN-2017 17:26:59
Current_time = 11-JAN-2017 17:28:34
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 23.9[dC]
CN
7f

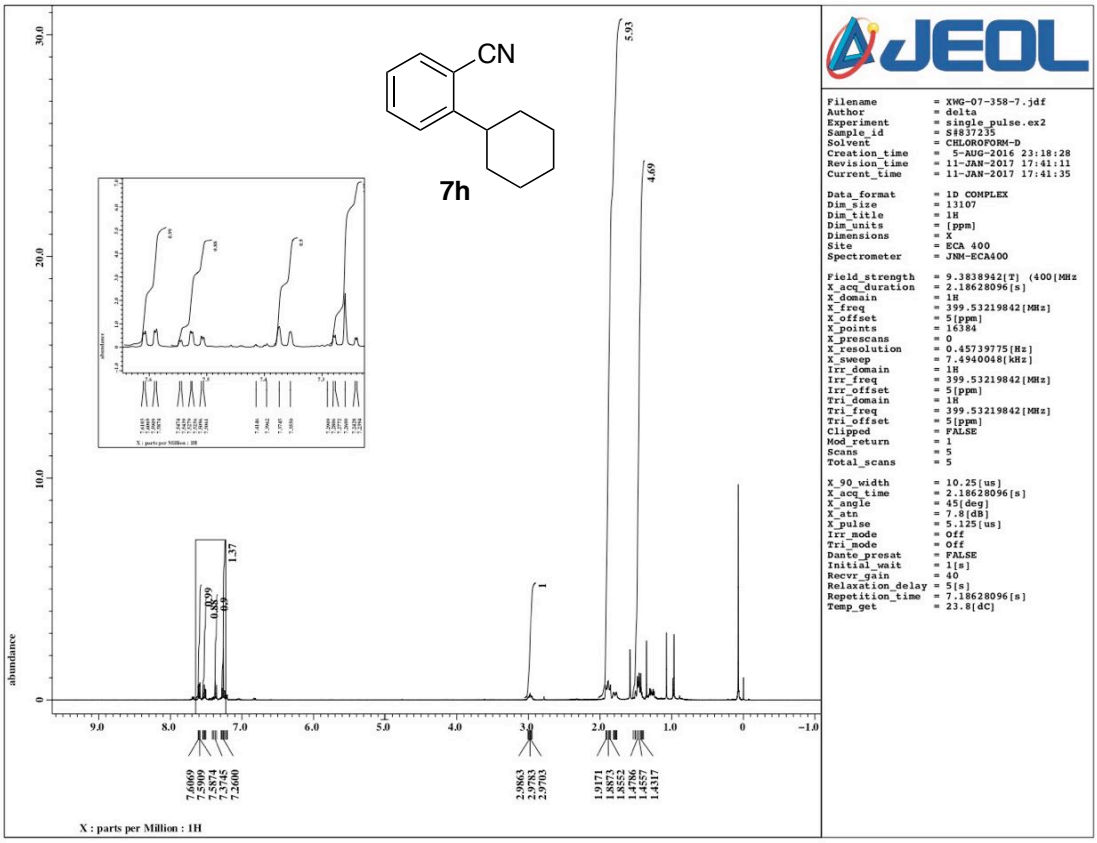

CN
7f
abundance
X : parts per Million : 13C
145.5894
133.9386
132.5761
130.5917
126.5179
118.6851
113.0371
77.5748
77.2600
76.9356
42.6278
39.8324
33.1827
26.5711
26.3993
1.2600

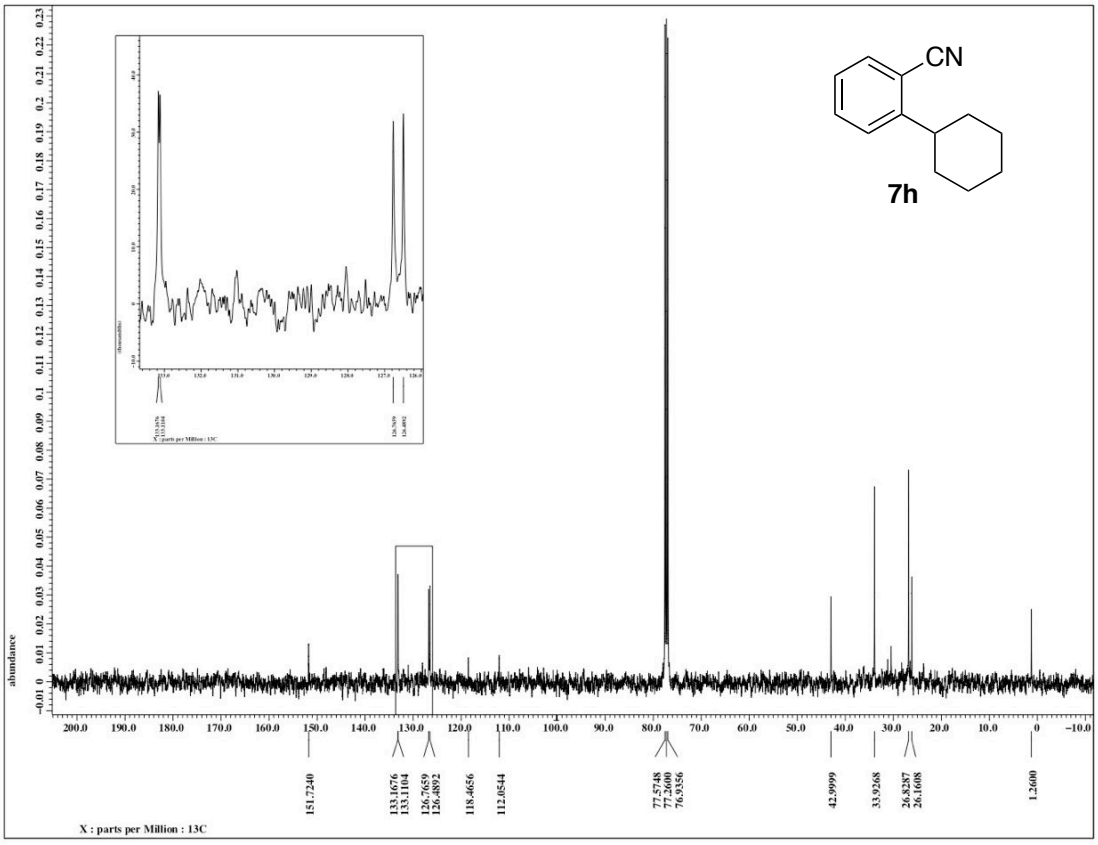
JEOL
Filename = XWG-07-355-c-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#822761
Solvent = CHLOROFORM-D
Creation_time = 5-AUG-2016 22:57:05
Revision_time = 11-JAN-2017 17:30:05
Current_time = 11-JAN-2017 17:30:30
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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_f_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 29
Total_scans = 29
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24[dC]

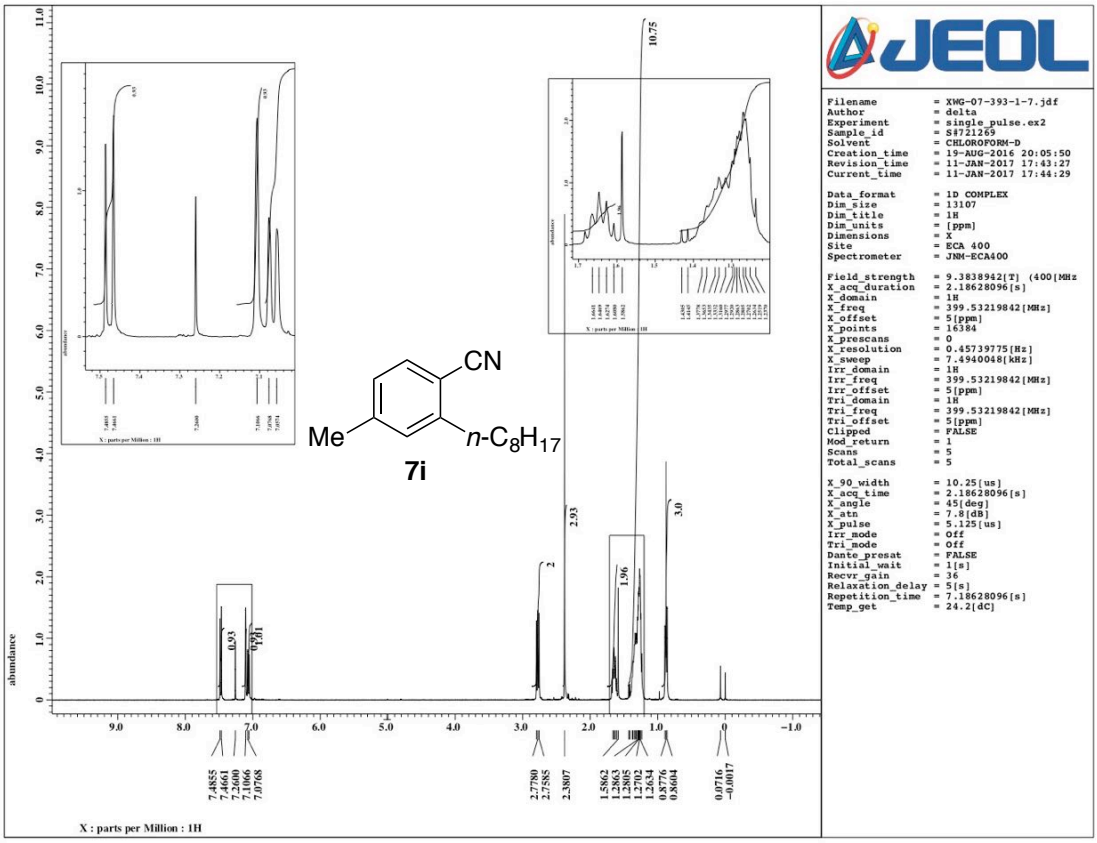



```
Filename          = XWG-07-356-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8827260
Solvent           = CHLOROFORM-D
Creation_time     =  5-AUG-2016 23:01:57
Revision_time     = 11-JAN-2017 17:34:40
Current_time      = 11-JAN-2017 17:35:06

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 2.18628096[s]
X_domain          = 1H
X_freq            = 399.53219842[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45739775[Hz]
X_sweep           = 7.4940048[kHz]
Irr_domain        = 1H
Irr_freq          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.53219842[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 4
Total_scans       = 4

X_90_width        = 10.25[us]
X_acq_time        = 2.18628096[s]
X_angle           = 45[deg]
X_atn             = 7.8[dB]
X_pulse           = 5.125[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 7.18628096[s]
Temp_get          = 23.9[dC]
```

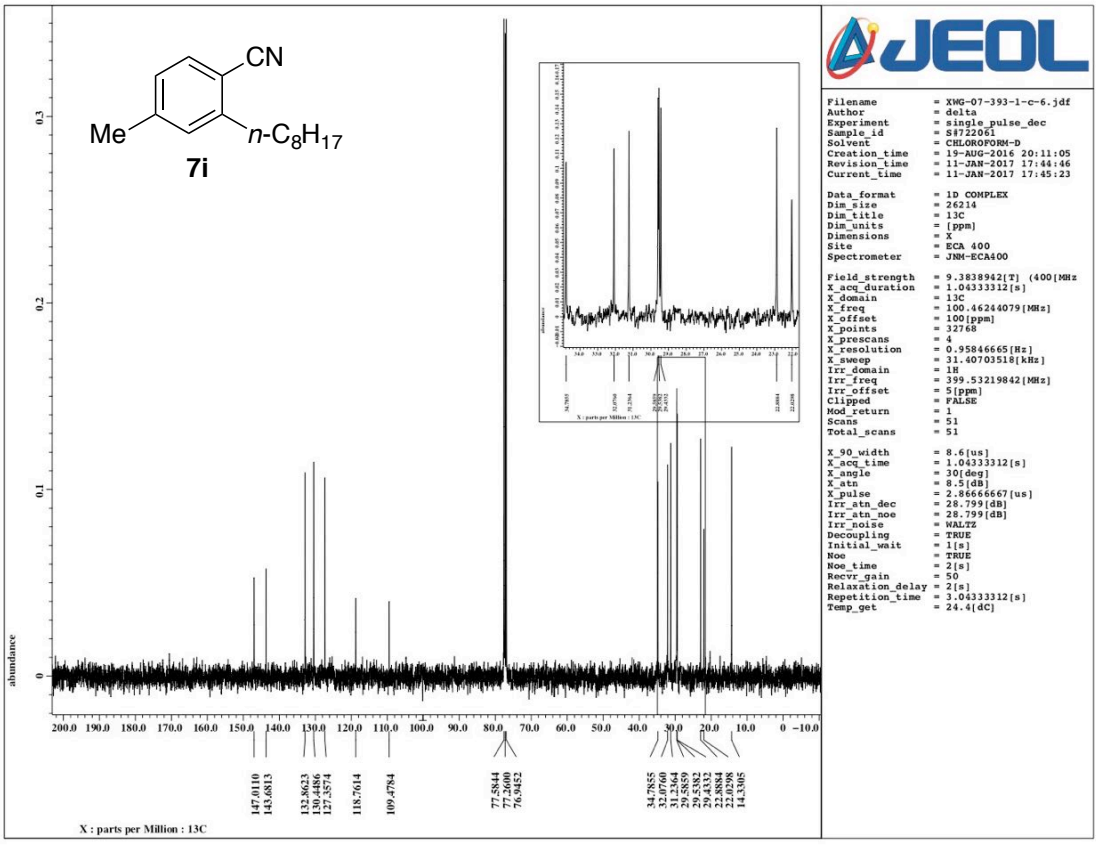



CN
7h
5.93
4.69
1.37
1
abundance
X : parts per Million : 1H
Filename = XWG-07-358-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#837235
Solvent = CHLOROFORM-D
Creation_time = 5-AUG-2016 23:18:28
Revision_time = 11-JAN-2017 17:41:11
Current_time = 11-JAN-2017 17:41:35
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 23.8[dC]

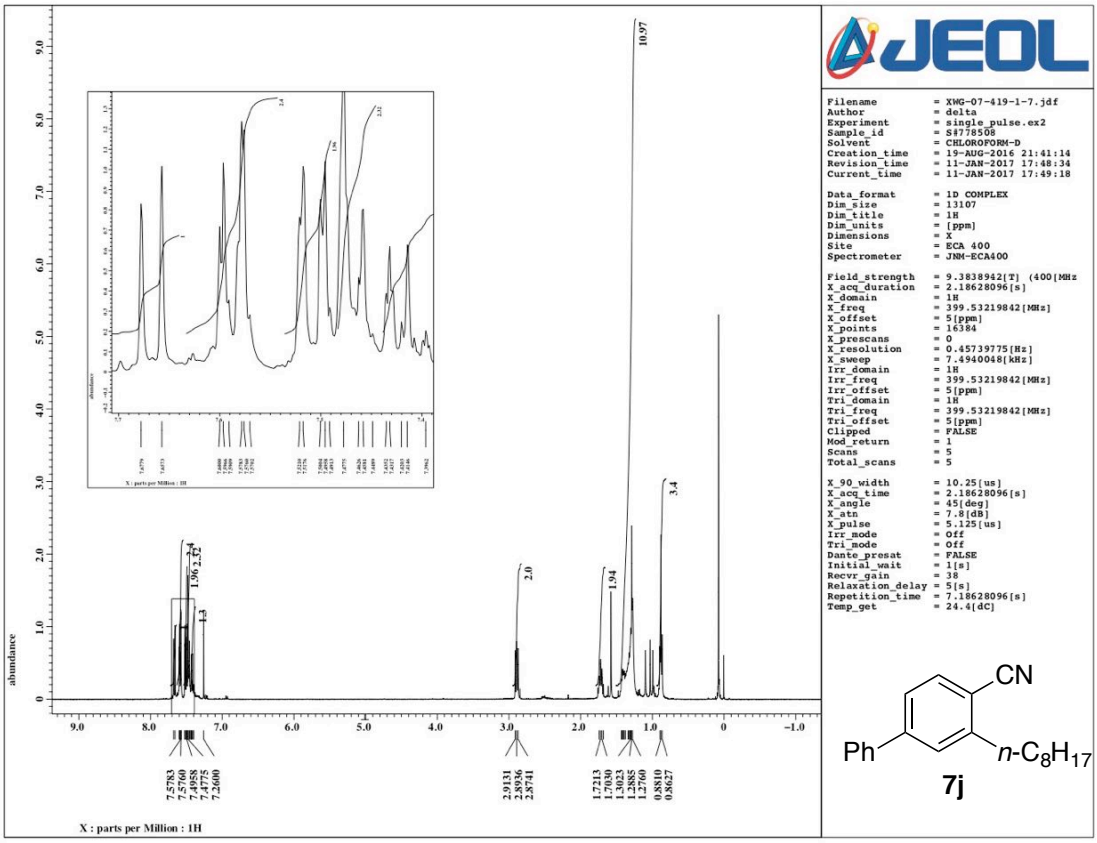

CN
7h
abundance
X : parts per Million : 13C

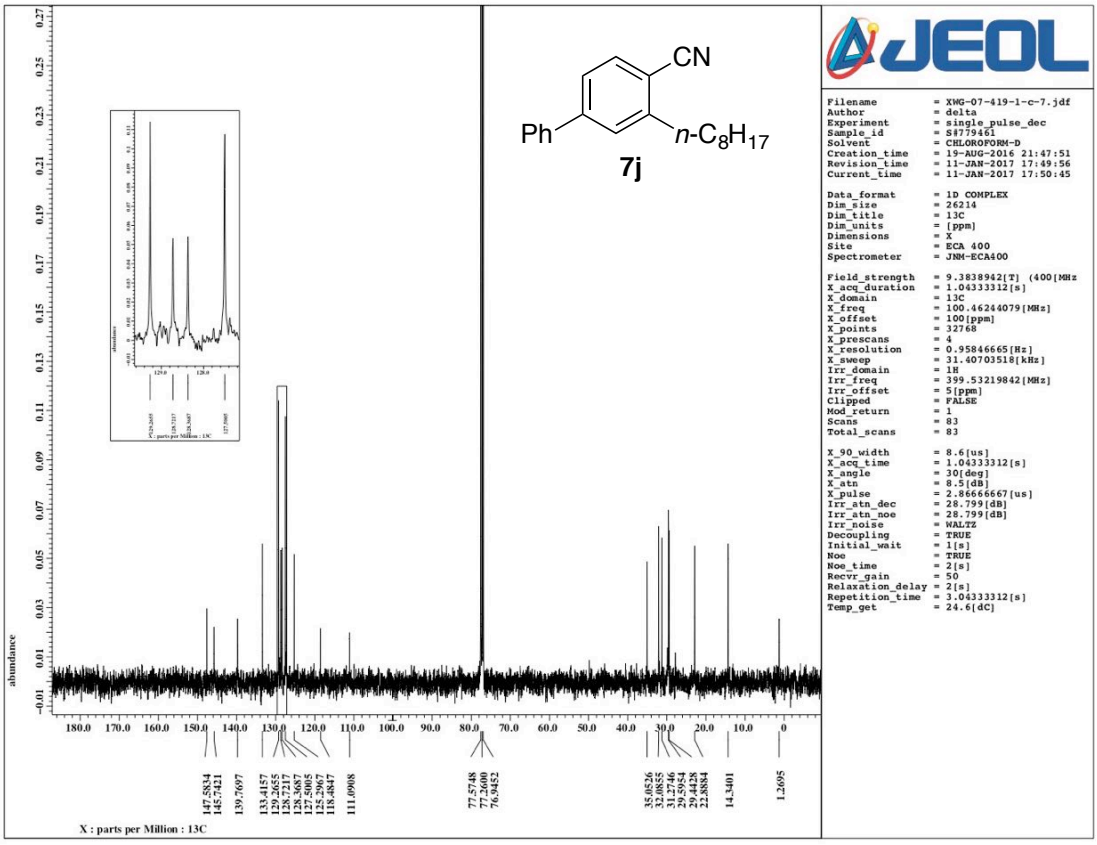


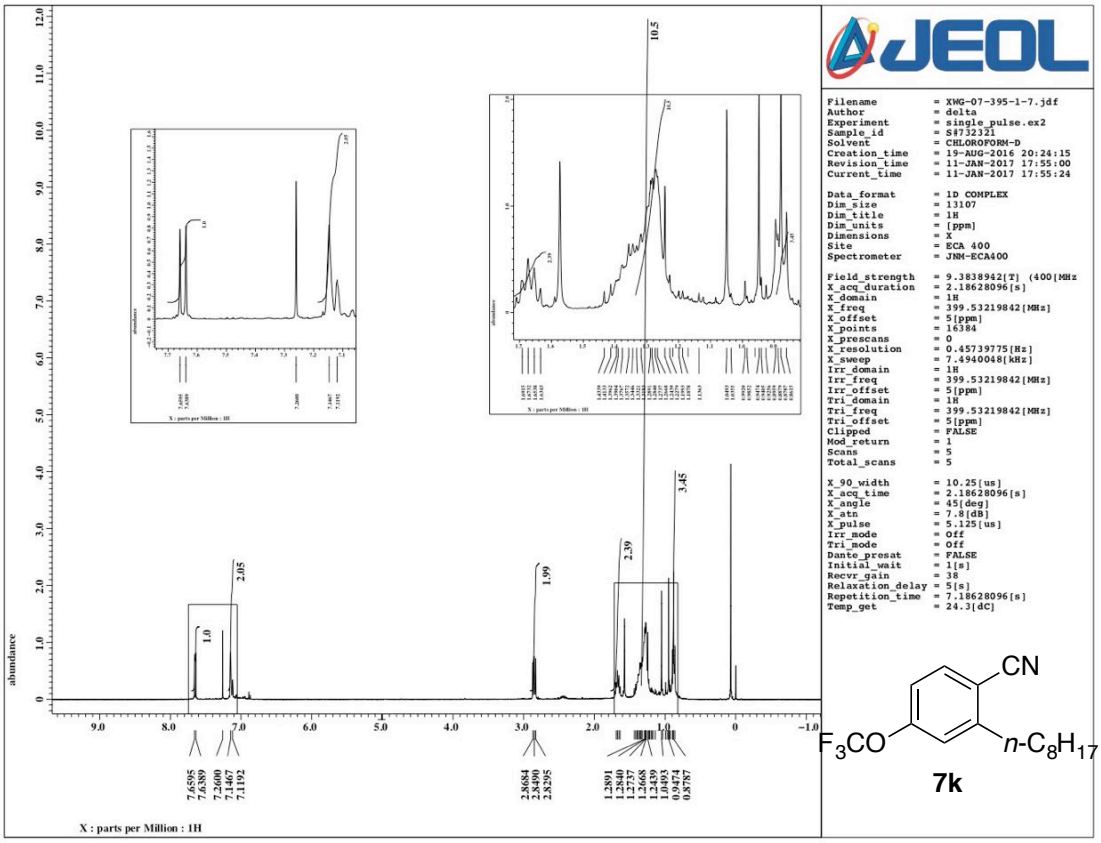

```
Filename        = XWG-07-393-1-7.jdf
Author          = delta
Experiment      = single_pulse.ex2
Sample_id       = S#721269
Solvent         = CHLOROFORM-D
Creation_time   = 19-AUG-2016 20:05:50
Revision_time   = 11-JAN-2017 17:43:27
Current_time    = 11-JAN-2017 17:44:29

Data_format     = 1D COMPLEX
Dim_size        = 13107
Dim_title       = 1H
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = JNM-ECA400

Field_strength  = 9.3838942[T] (400[MHz
X_acq_duration  = 2.18628096[s]
X_domain        = 1H
X_freq          = 399.53219842[MHz]
X_offset        = 5[ppm]
X_points        = 16384
X_prescans      = 0
X_resolution    = 0.45739775[Hz]
X_sweep         = 7.4940048[kHz]
Irr_domain      = 1H
Irr_freq        = 399.53219842[MHz]
Irr_offset      = 5[ppm]
Tri_domain      = 1H
Tri_freq        = 399.53219842[MHz]
Tri_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 5
Total_scans     = 5

X_90_width      = 10.25[us]
X_acq_time      = 2.18628096[s]
X_angle         = 45[deg]
X_atn           = 7.8[dB]
X_pulse         = 5.125[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get        = 24.2[dC]
```

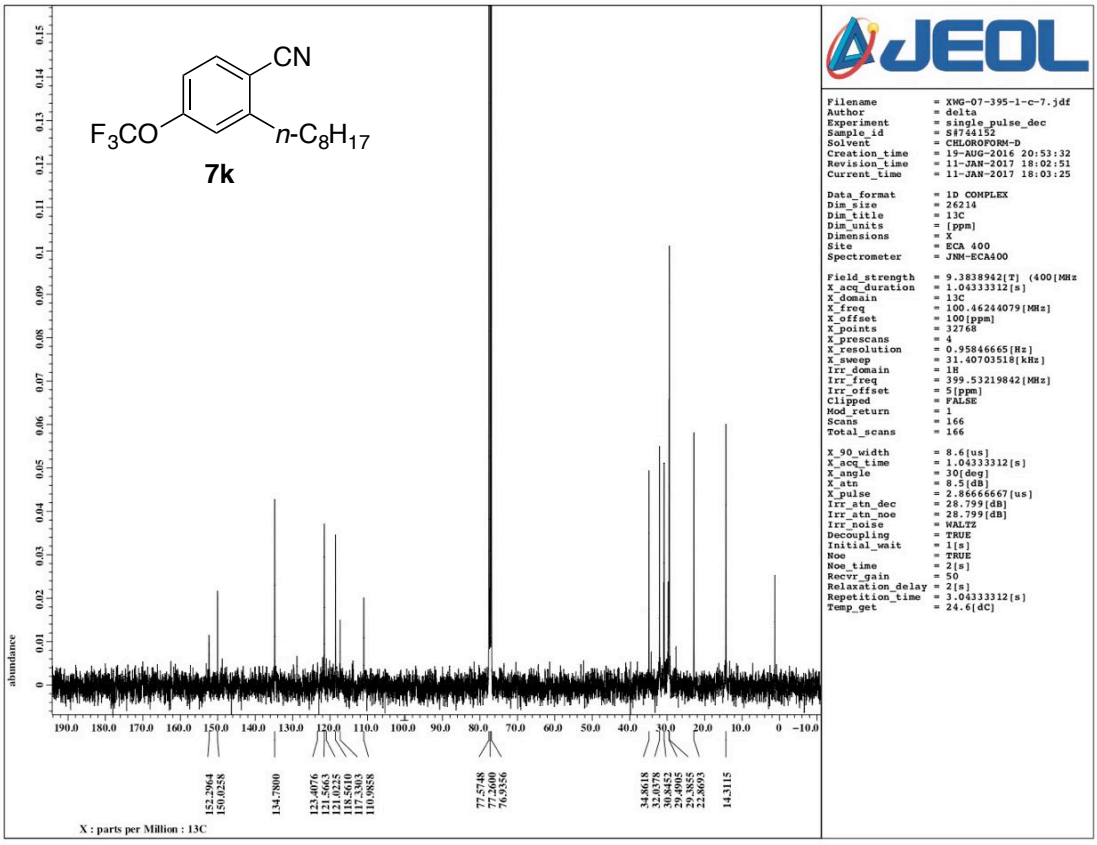


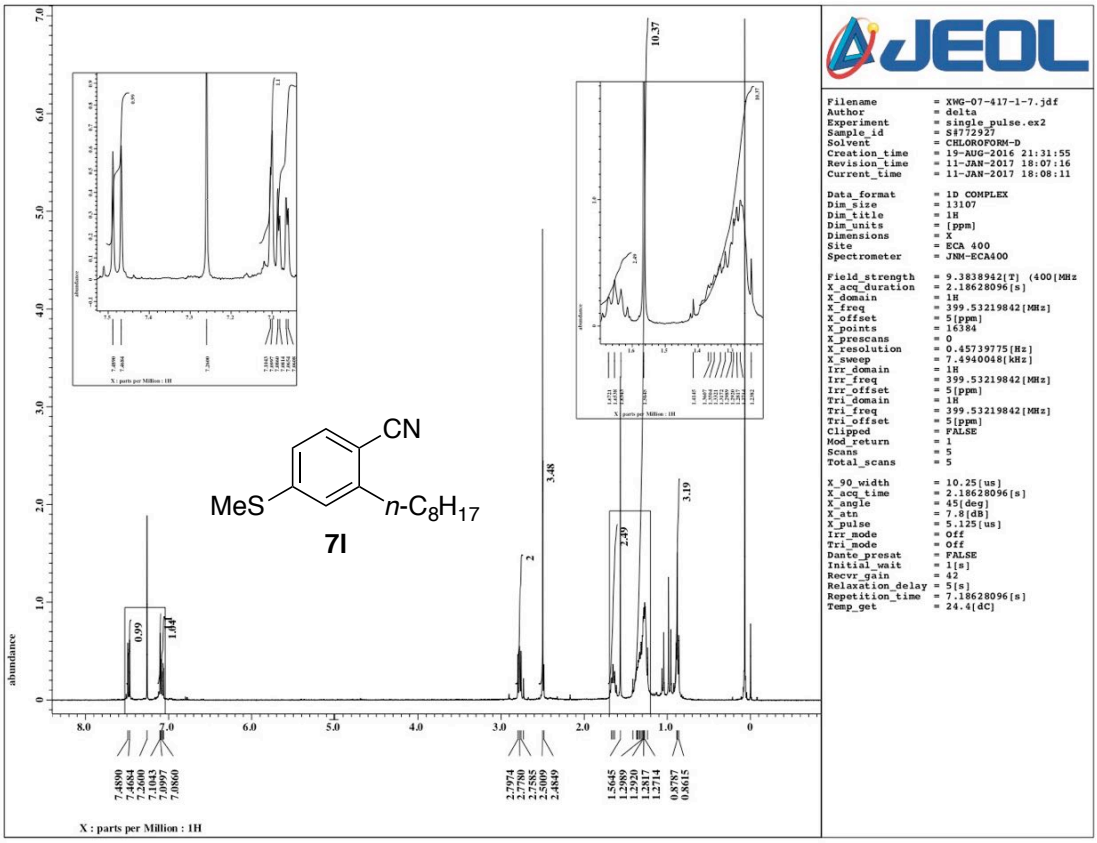

```
Filename        = XWG-07-393-1-c-6.jdf
Author          = delta
Experiment      = single_pulse_dec
Sample_id       = S#722061
Solvent         = CHLOROFORM-D
Creation_time   = 19-AUG-2016 20:11:05
Revision_time   = 11-JAN-2017 17:44:46
Current_time    = 11-JAN-2017 17:45:23

Data_format     = 1D COMPLEX
Dim_size        = 26214
Dim_title       = 13C
Dim_units       = [ppm]
Dimensions      = X
Site            = ECA 400
Spectrometer    = JNM-ECA400

Field_strength  = 9.3838942[T] (400[MHz
X_acq_duration  = 1.04333312[s]
X_domain        = 13C
X_freq          = 100.46244079[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        = 399.53219842[MHz]
Irr_offset      = 5[ppm]
Clipped         = FALSE
Mod_return      = 1
Scans           = 51
Total_scans     = 51

X_90_width      = 8.6[us]
X_acq_time      = 1.04333312[s]
X_angle         = 30[deg]
X_atn           = 8.5[dB]
X_pulse         = 2.86666667[us]
Irr_atn_dec     = 28.799[dB]
Irr_atn_noe     = 28.799[dB]
Irr_noise       = WALTZ
Decoupling      = TRUE
Initial_wait    = 1[s]
Noe             = TRUE
Noe_time        = 2[s]
Recvr_gain      = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get        = 24.4[dC]
```

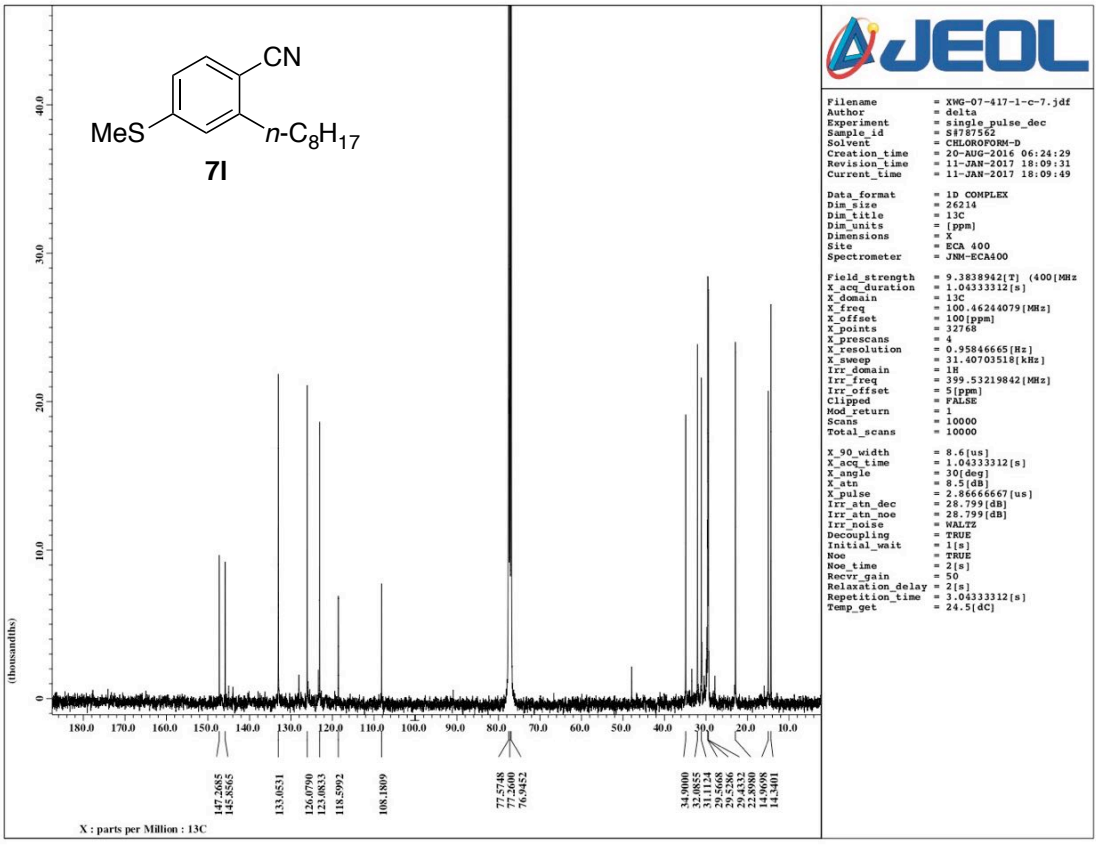

JEOL
Filename = XWG-07-419-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#778508
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 21:41:14
Revision_time = 11-JAN-2017 17:48:34
Current_time = 11-JAN-2017 17:49:18
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.4[dC]
abundance
X : parts per Million : 1H
10.97
3.4
2.0
1.94
1.96
2.72
1.3
7.5783
7.5760
7.4958
7.4775
7.2600
2.9131
2.8936
2.8741
1.7213
1.7030
1.3013
1.2885
1.2760
0.8810
0.8627
CN
Ph
n-C8H17
7j

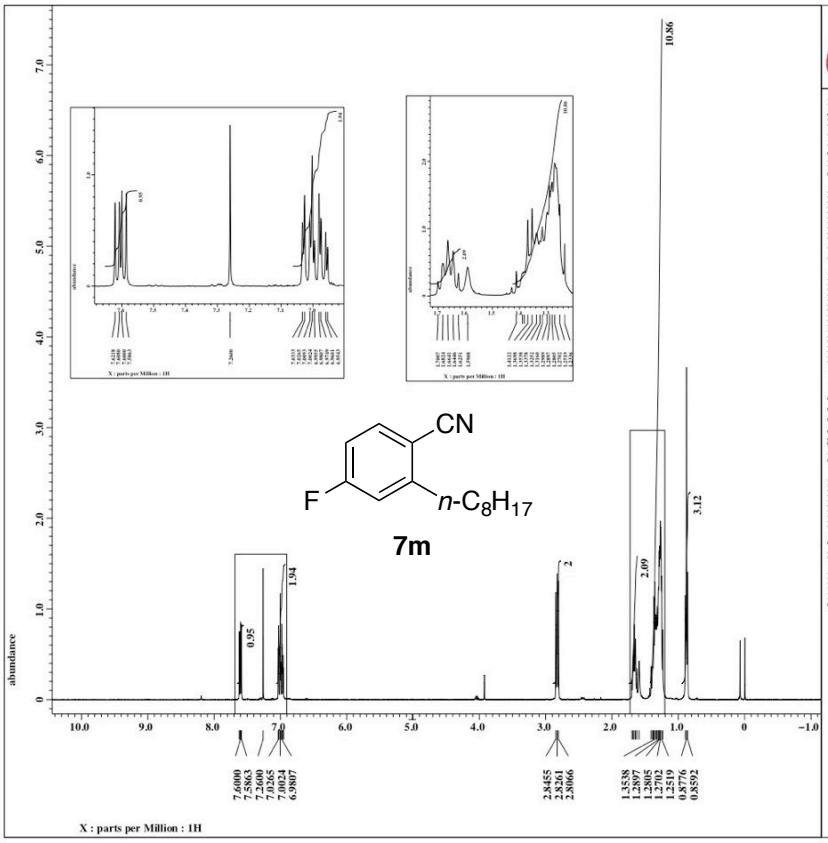

JEOL
CN
Ph
n-C8H17
7j
Filename = XWG-07-419-1-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#779461
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 21:47:51
Revision_time = 11-JAN-2017 17:49:56
Current_time = 11-JAN-2017 17:50:45
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 83
Total_scans = 83
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.6[dC]
abundance
X : parts per Million : 13C
147.5834
145.7421
139.7697
133.4157
129.2655
128.7217
128.3497
127.5005
125.2967
118.4847
111.0908
77.5748
77.2600
76.9452
35.0626
33.0855
31.2746
29.5954
29.4428
22.8884
14.3401
1.2695


Filename = XWG-07-395-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#732321
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 20:24:15
Revision_time = 11-JAN-2017 17:55:00
Current_time = 11-JAN-2017 17:55:24
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.3[dC]
abundance
X : parts per Million : 1H
CN
F3CO
n-C8H17
7k

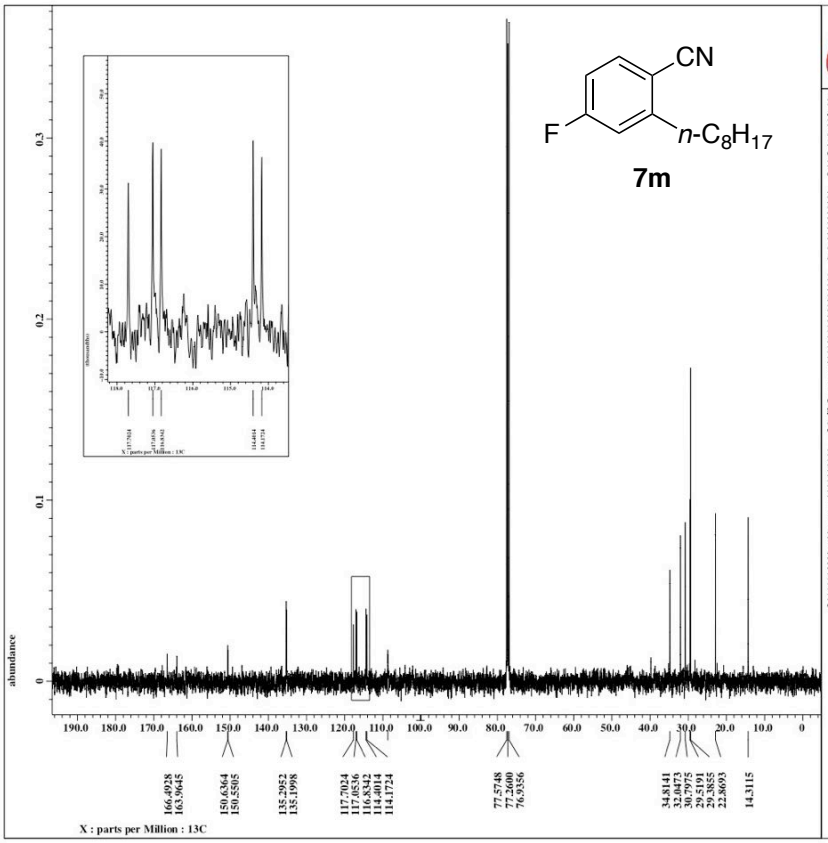

CN
F3CO
n-C8H17
7k
Filename = XWG-07-395-1-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#744152
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 20:53:32
Revision_time = 11-JAN-2017 18:02:51
Current_time = 11-JAN-2017 18:03:25
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 166
Total_scans = 166
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.6[dC]
abundance
X : parts per Million : 13C


CN
MeS
n-C8H17
7l
abundance
X : parts per Million : 1H
Filename = XWG-07-417-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#772927
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 21:31:55
Revision_time = 11-JAN-2017 18:07:16
Current_time = 11-JAN-2017 18:08:11
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 5
Total_scans = 5
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.4[dC]

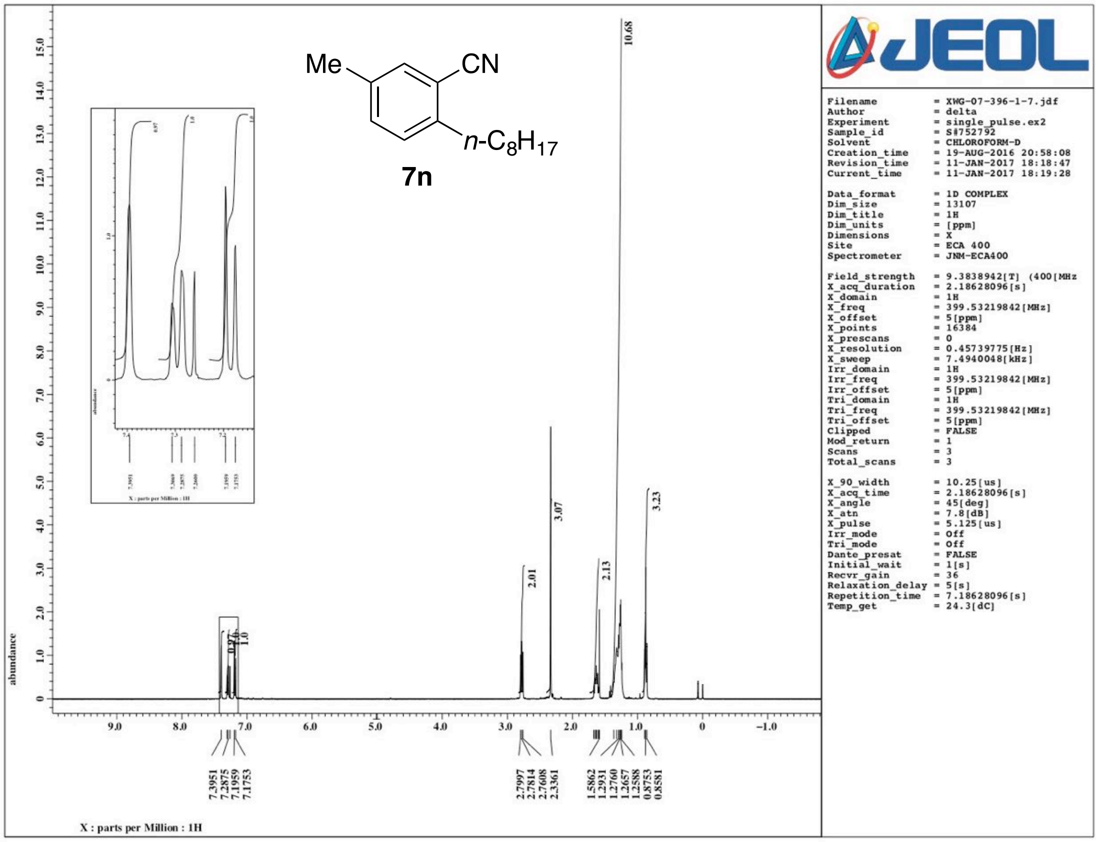

CN
MeS
n-C8H17
7l
(thousandths)
X : parts per Million : 13C
Filename = XWG-07-417-1-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#787562
Solvent = CHLOROFORM-D
Creation_time = 20-AUG-2016 06:24:29
Revision_time = 11-JAN-2017 18:09:31
Current_time = 11-JAN-2017 18:09:49
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.5[dC]

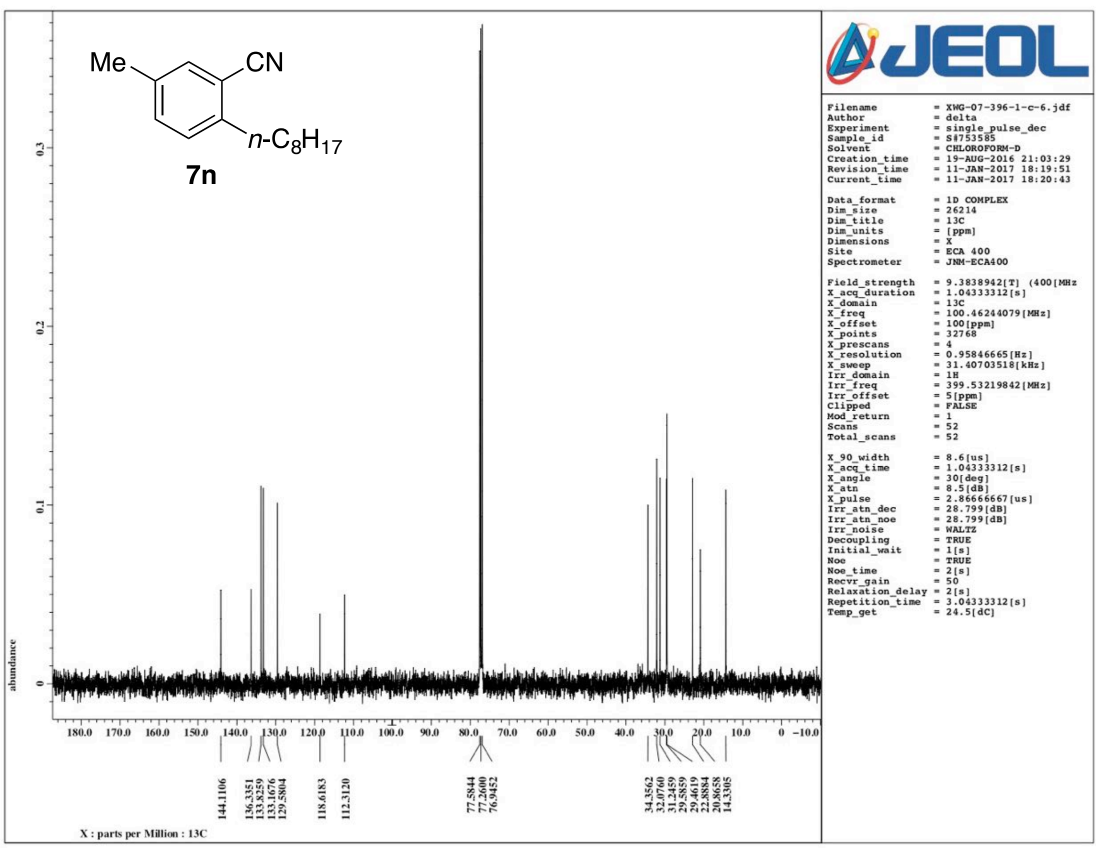


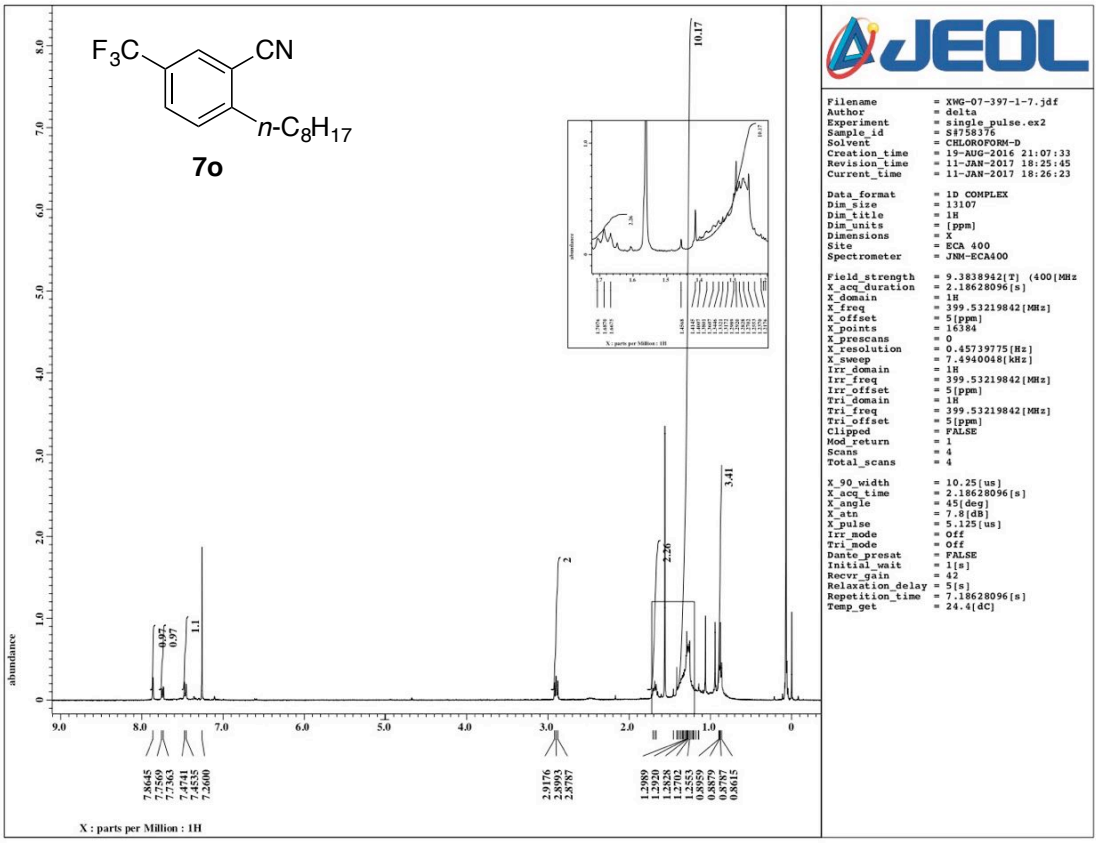

```
Filename          = XWG-07-392-1-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#726733
Solvent           = CHLOROFORM-D
Creation_time     = 19-AUG-2016 20:14:56
Revision_time     = 11-JAN-2017 18:12:05
Current_time      = 11-JAN-2017 18:13:00

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 2.18628096[s]
X_domain          = 1H
X_freq            = 399.53219842[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45739775[Hz]
X_sweep           = 7.4940048[kHz]
Irr_domain        = 1H
Irr_freq          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.53219842[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 5
Total_scans       = 5

X_90_width        = 10.25[us]
X_acq_time        = 2.18628096[s]
X_angle           = 45[deg]
X_atn             = 7.8[dB]
X_pulse           = 5.125[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18628096[s]
Temp_get          = 24.3[dC]
```

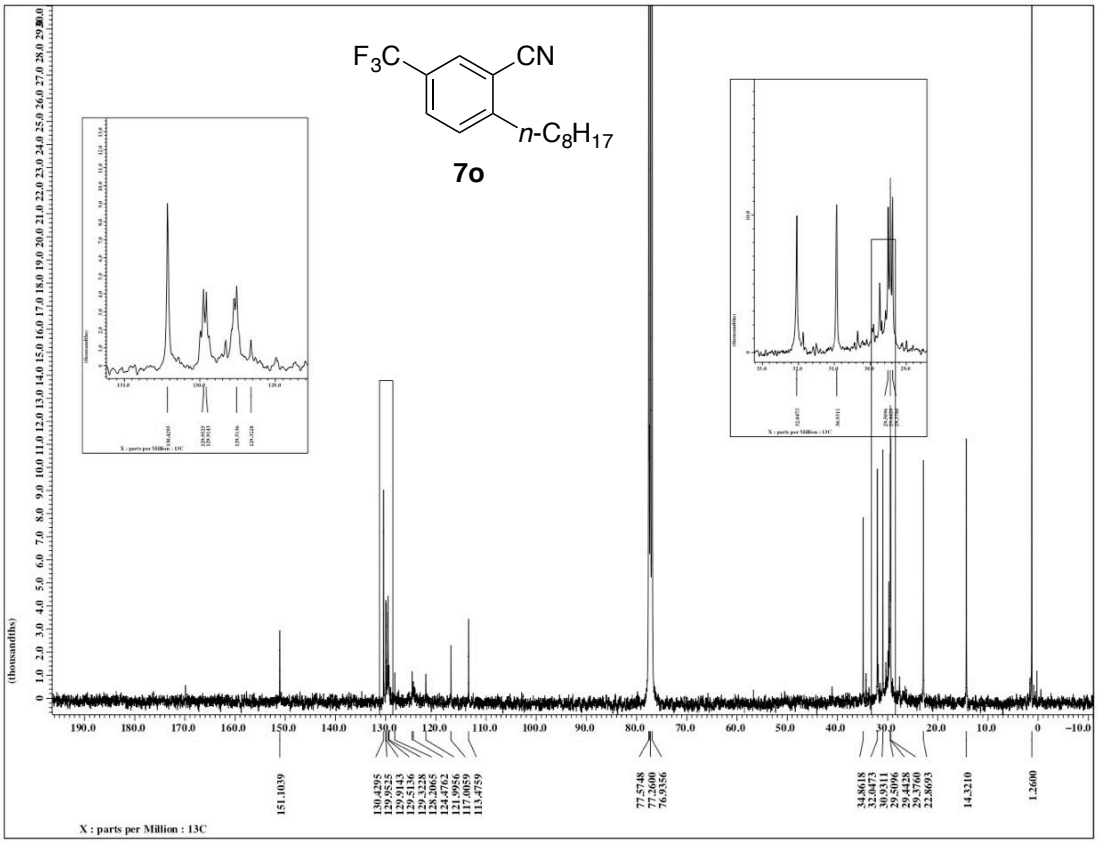


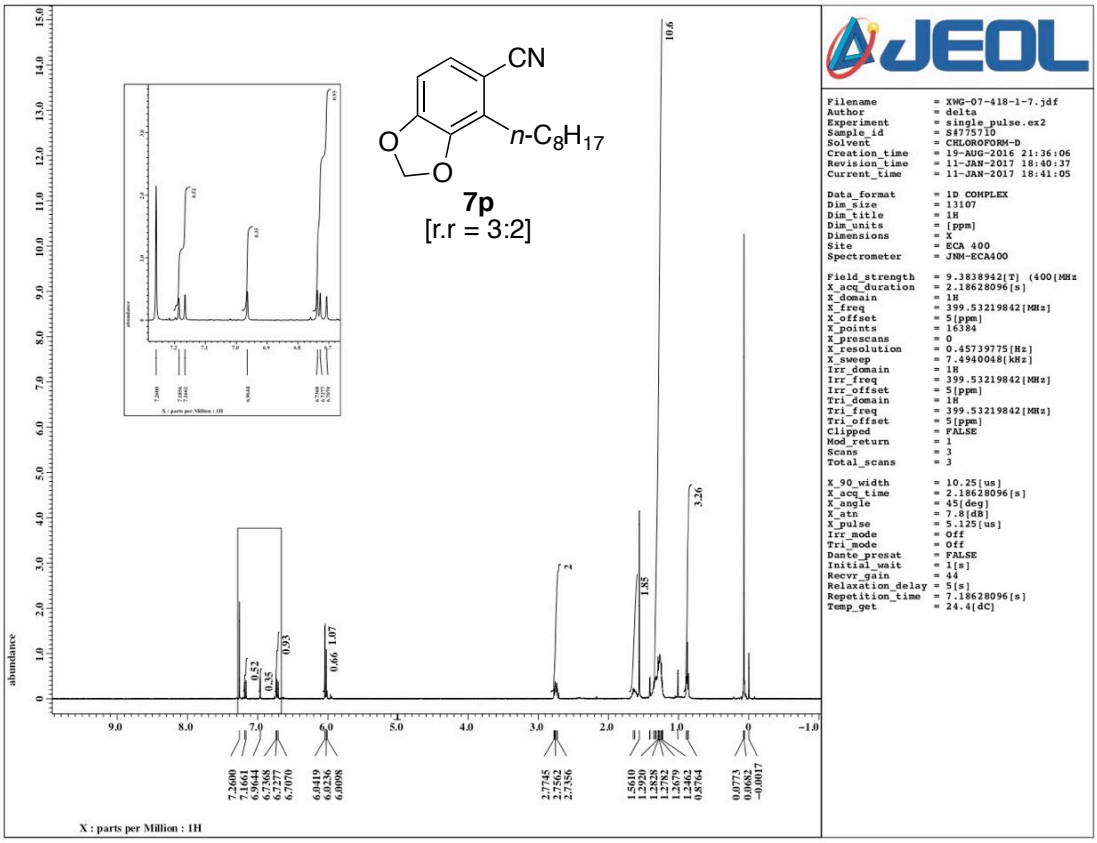

```
Filename          = XWG-07-392-1-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#727624
Solvent           = CHLOROFORM-D
Creation_time     = 19-AUG-2016 20:20:10
Revision_time     = 11-JAN-2017 18:15:24
Current_time      = 11-JAN-2017 18:16:19

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = JNM-ECA400

Field_strength    = 9.3838942[T] (400[MHz
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.46244079[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          = 399.53219842[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 57
Total_scans       = 57

X_90_width        = 8.6[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 8.5[dB]
X_pulse           = 2.86666667[us]
Irr_atn_dec       = 28.799[dB]
Irr_atn_noe       = 28.799[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 24.5[dC]
```

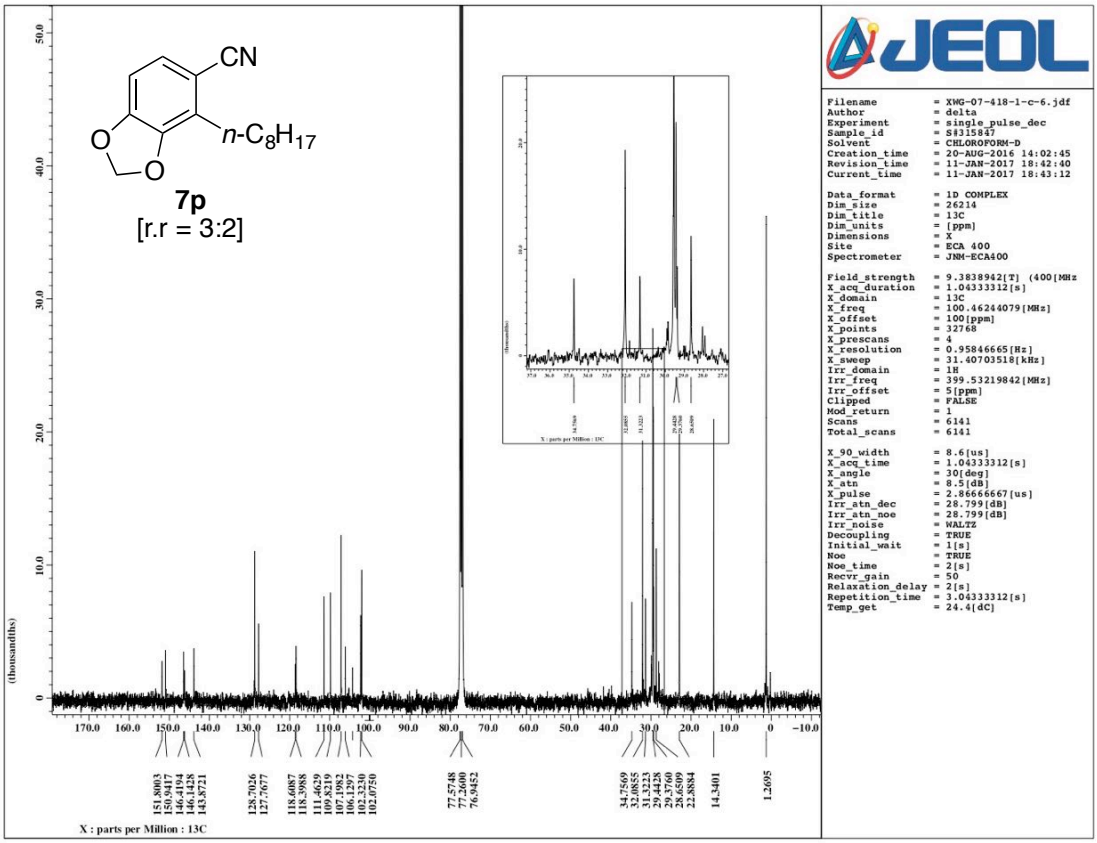

Me
CN
n-C8H17
7n
10.68
3.07
3.23
2.13
2.01
0.97
1.0
abundance
7.3951
7.2875
7.1959
7.1753
2.7997
2.7814
2.7608
2.3361
1.5862
1.2931
1.2760
1.2657
1.2588
0.8753
0.8581
X : parts per Million : 1H
JEOL
Filename = XWG-07-396-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#752792
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 20:58:08
Revision_time = 11-JAN-2017 18:18:47
Current_time = 11-JAN-2017 18:19:28
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3
Total_scans = 3
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.3[dC]

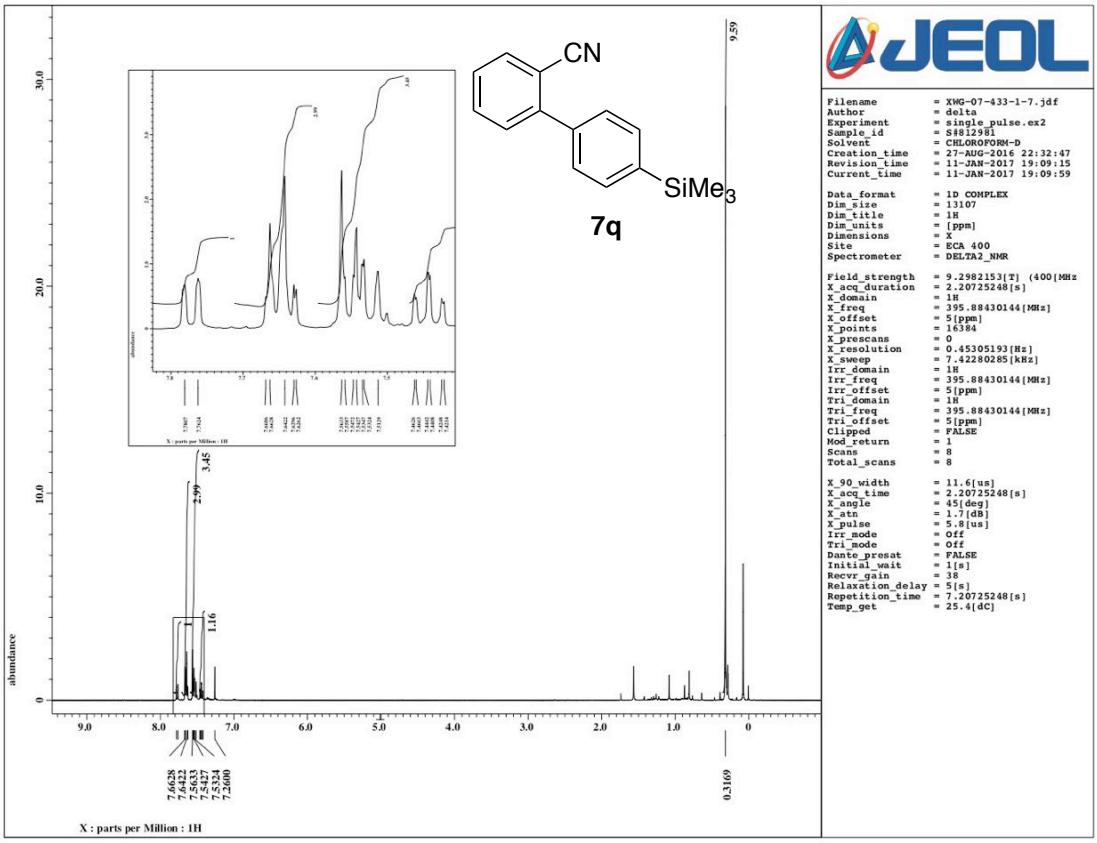

Me
CN
n-C8H17
7n
abundance
144.1106
136.3351
133.8259
133.1676
129.5804
118.6183
112.3120
77.5844
77.2600
76.9452
34.3562
32.0760
31.2459
29.5859
29.4619
22.8884
20.8658
14.3305
X : parts per Million : 13C
JEOL
Filename = XWG-07-396-1-c-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#753585
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 21:03:29
Revision_time = 11-JAN-2017 18:19:51
Current_time = 11-JAN-2017 18:20:43
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 52
Total_scans = 52
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.5[dC]


F3C
CN
n-C8H17
7o
10.17
3.41
2.26
2
1.1
0.97
0.97
abundance
X : parts per Million : 1H
Filename = XWG-07-397-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#758376
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 21:07:33
Revision_time = 11-JAN-2017 18:25:45
Current_time = 11-JAN-2017 18:26:23
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.4[dC]

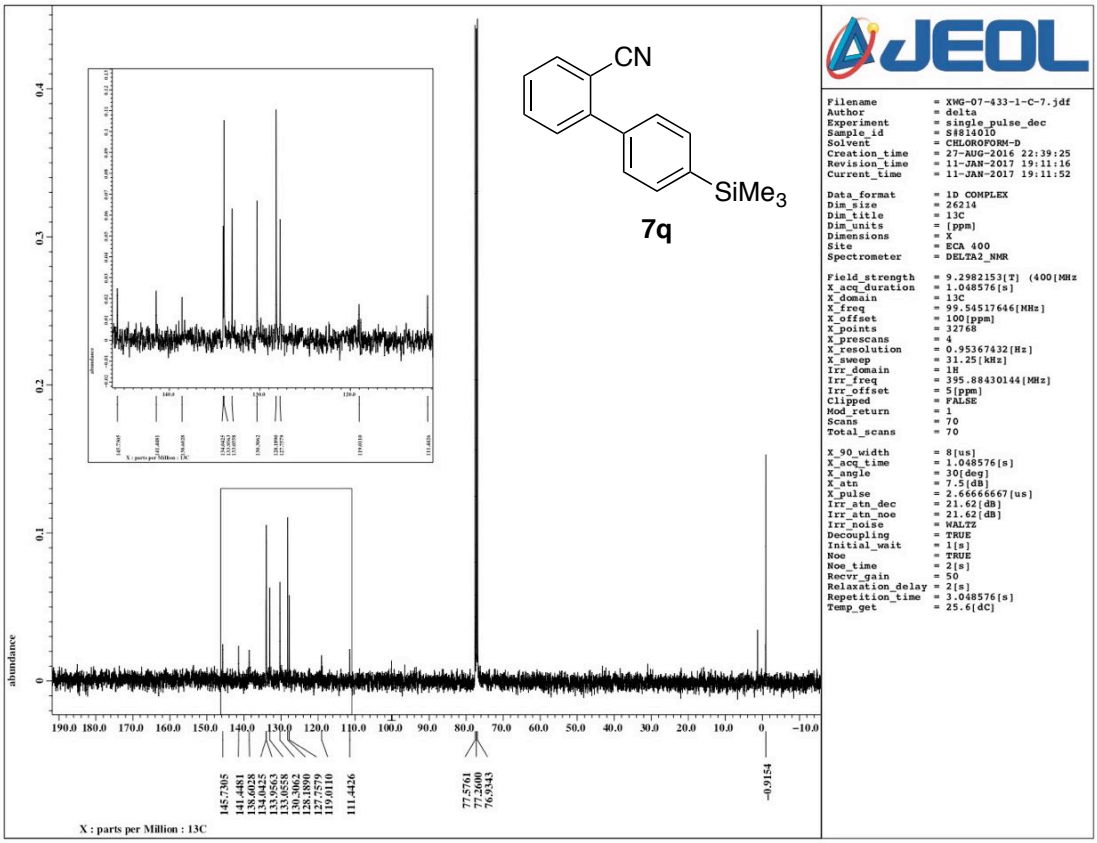

F3C
CN
n-C8H17
7o
(thousandths)
X : parts per Million : 13C


CN
n-C8H17
7p
[r.r = 3:2]
abundance
X : parts per Million : 1H
Filename = XWG-07-418-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#775710
Solvent = CHLOROFORM-D
Creation_time = 19-AUG-2016 21:36:06
Revision_time = 11-JAN-2017 18:40:37
Current_time = 11-JAN-2017 18:41:05
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 2.18628096[s]
X_domain = 1H
X_freq = 399.53219842[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45739775[Hz]
X_sweep = 7.4940048[kHz]
Irr_domain = 1H
Irr_freq = 399.53219842[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.53219842[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3
Total_scans = 3
X_90_width = 10.25[us]
X_acq_time = 2.18628096[s]
X_angle = 45[deg]
X_atn = 7.8[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.18628096[s]
Temp_get = 24.4[dC]

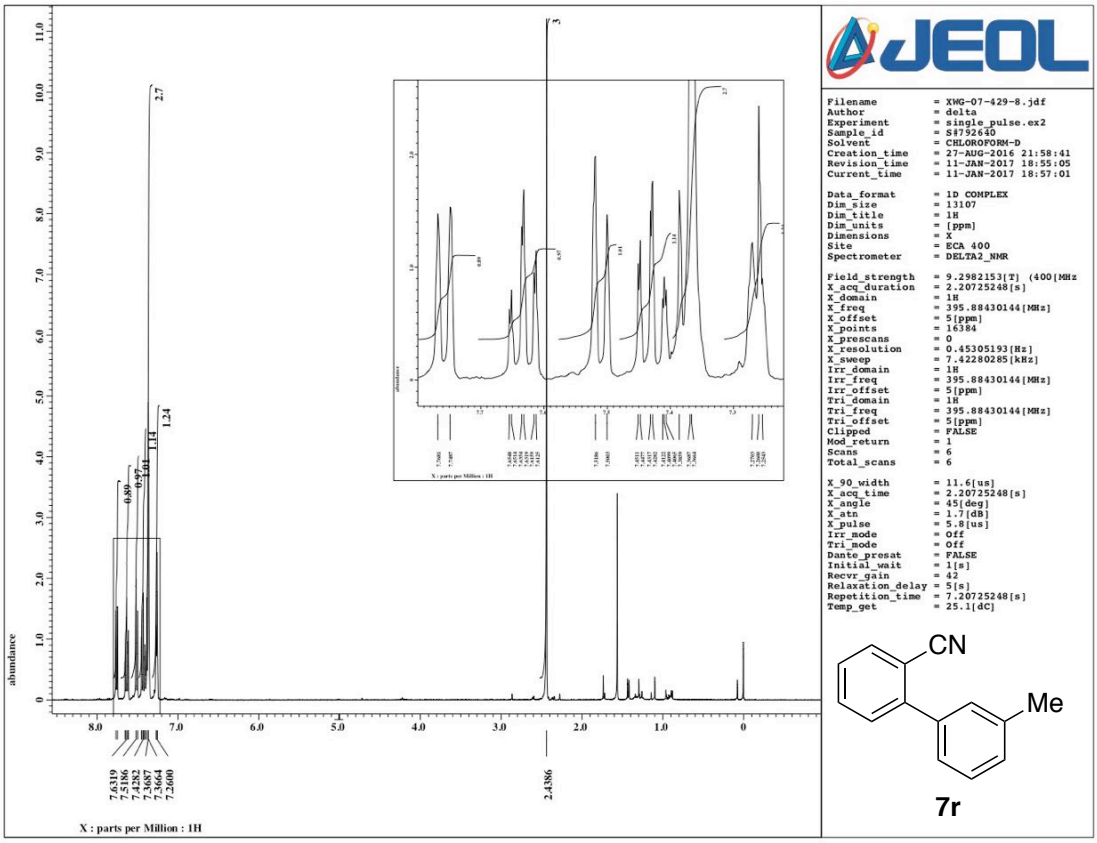

CN
n-C8H17
7p
[r.r = 3:2]
(thousandths)
X : parts per Million : 13C
Filename = XWG-07-418-1-c-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#315847
Solvent = CHLOROFORM-D
Creation_time = 20-AUG-2016 14:02:45
Revision_time = 11-JAN-2017 18:42:40
Current_time = 11-JAN-2017 18:43:12
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6141
Total_scans = 6141
X_90_width = 8.6[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.86666667[us]
Irr_atn_dec = 28.799[dB]
Irr_atn_noe = 28.799[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.4[dC]

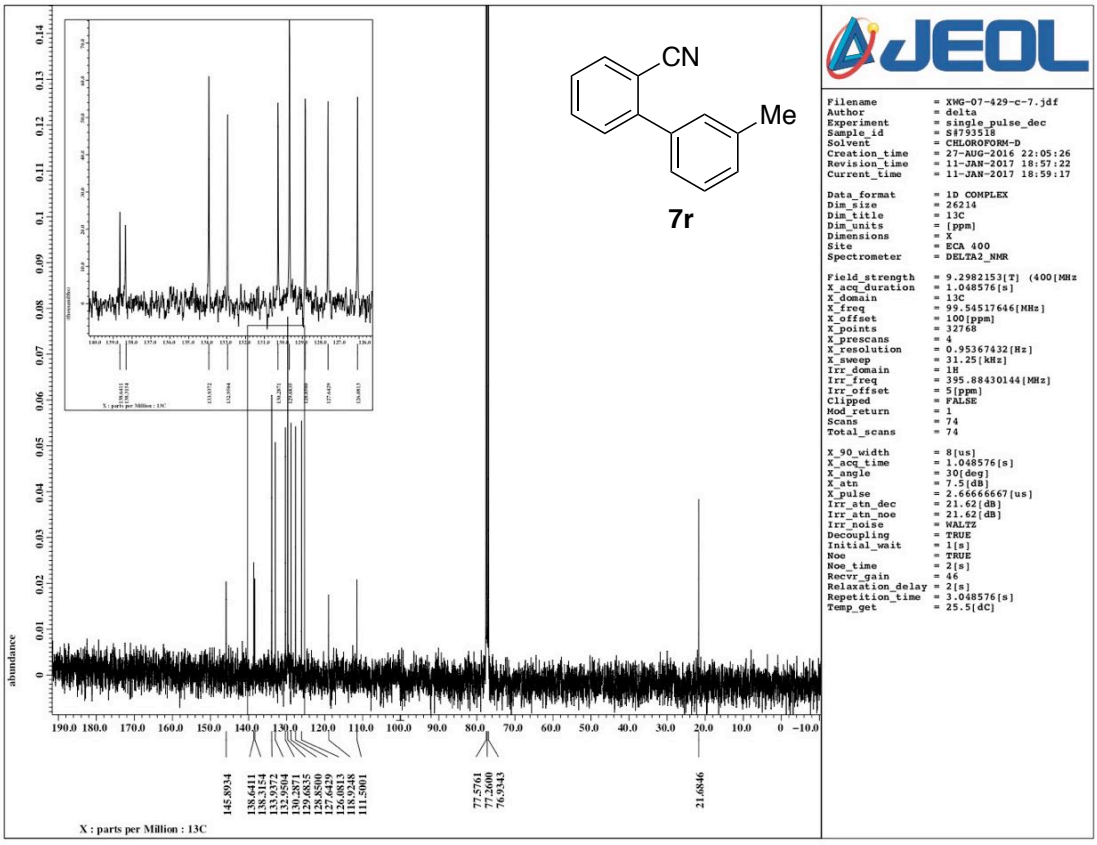


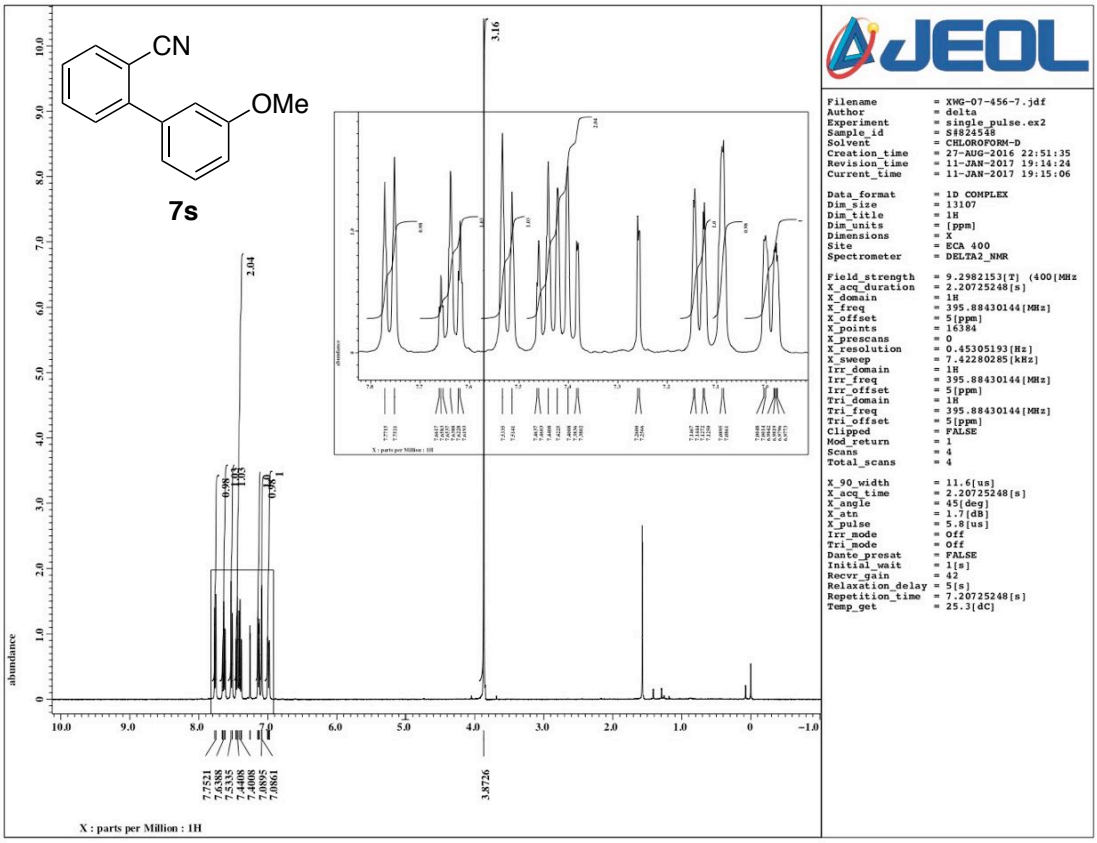

```
Filename          = XWG-07-433-1-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#812981
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 22:32:47
Revision_time     = 11-JAN-2017 19:09:15
Current_time      = 11-JAN-2017 19:09:59

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.4[dC]
```



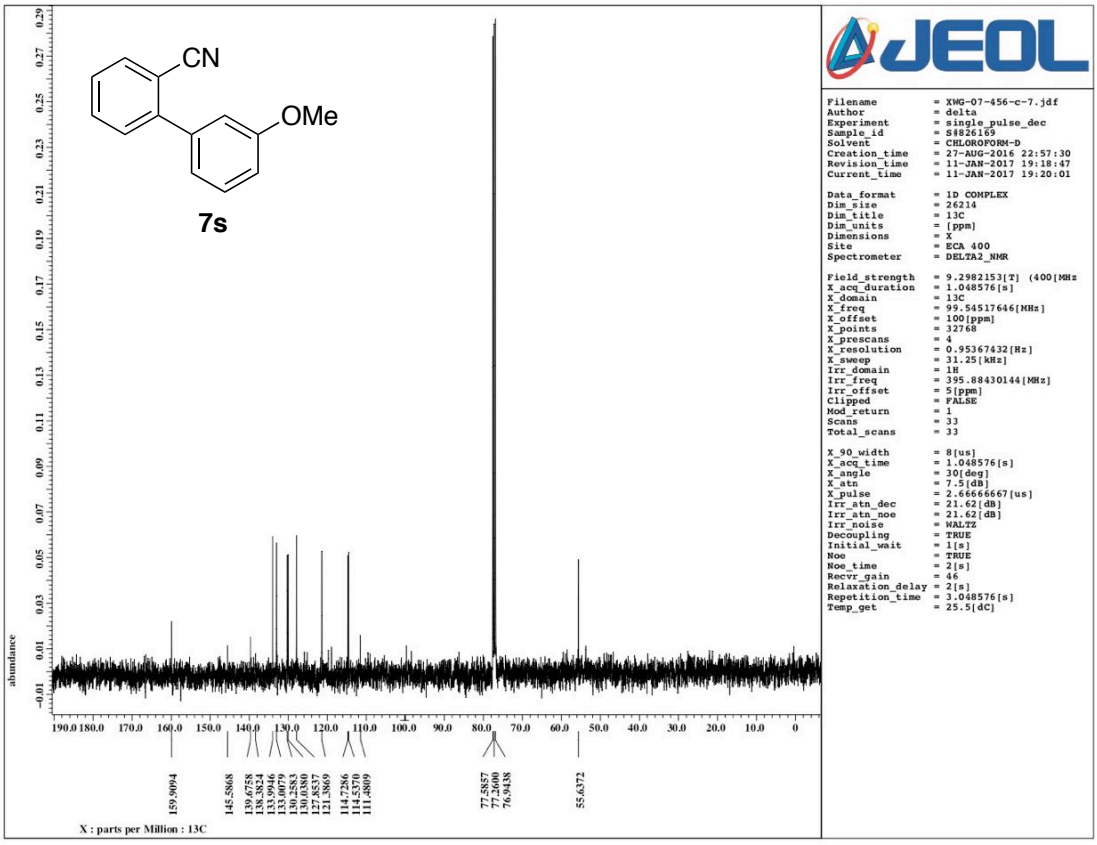

```
Filename          = XWG-07-433-1-C-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#814010
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 22:39:25
Revision_time     = 11-JAN-2017 19:11:16
Current_time      = 11-JAN-2017 19:11:52

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 70
Total_scans       = 70

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.6[dC]
```


abundance
X : parts per Million : 1H
7.6319
7.5186
7.4282
7.3687
7.3464
7.2600
2.4386
Filename = XWG-07-429-8.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#792640
Solvent = CHLOROFORM-D
Creation_time = 27-AUG-2016 21:58:41
Revision_time = 11-JAN-2017 18:55:05
Current_time = 11-JAN-2017 18:57:01
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6
Total_scans = 6
X_90_width = 11.6[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1.7[dB]
X_pulse = 5.8[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 25.1[dC]
CN
Me
7r

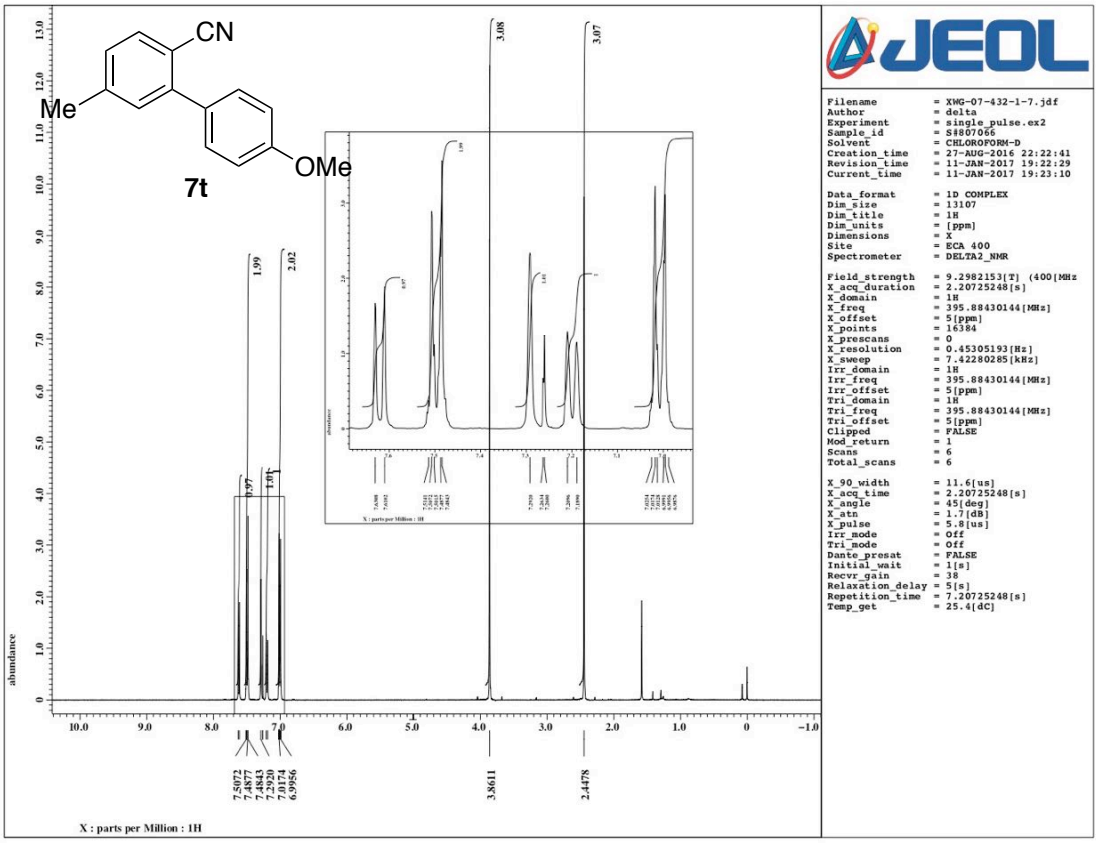

abundance
X : parts per Million : 13C
145.8934
138.6411
138.3154
133.9572
133.5774
130.2871
129.6835
128.8500
127.6429
118.9238
111.5001
77.5761
77.2609
76.9343
21.6846
CN
Me
7r
Filename = XWG-07-429-c-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#793518
Solvent = CHLOROFORM-D
Creation_time = 27-AUG-2016 22:05:26
Revision_time = 11-JAN-2017 18:57:22
Current_time = 11-JAN-2017 18:59:17
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 74
Total_scans = 74
X_90_width = 8[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 7.5[dB]
X_pulse = 2.66666667[us]
Irr_atn_dec = 21.62[dB]
Irr_atn_noe = 21.62[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 46
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 25.5[dC]



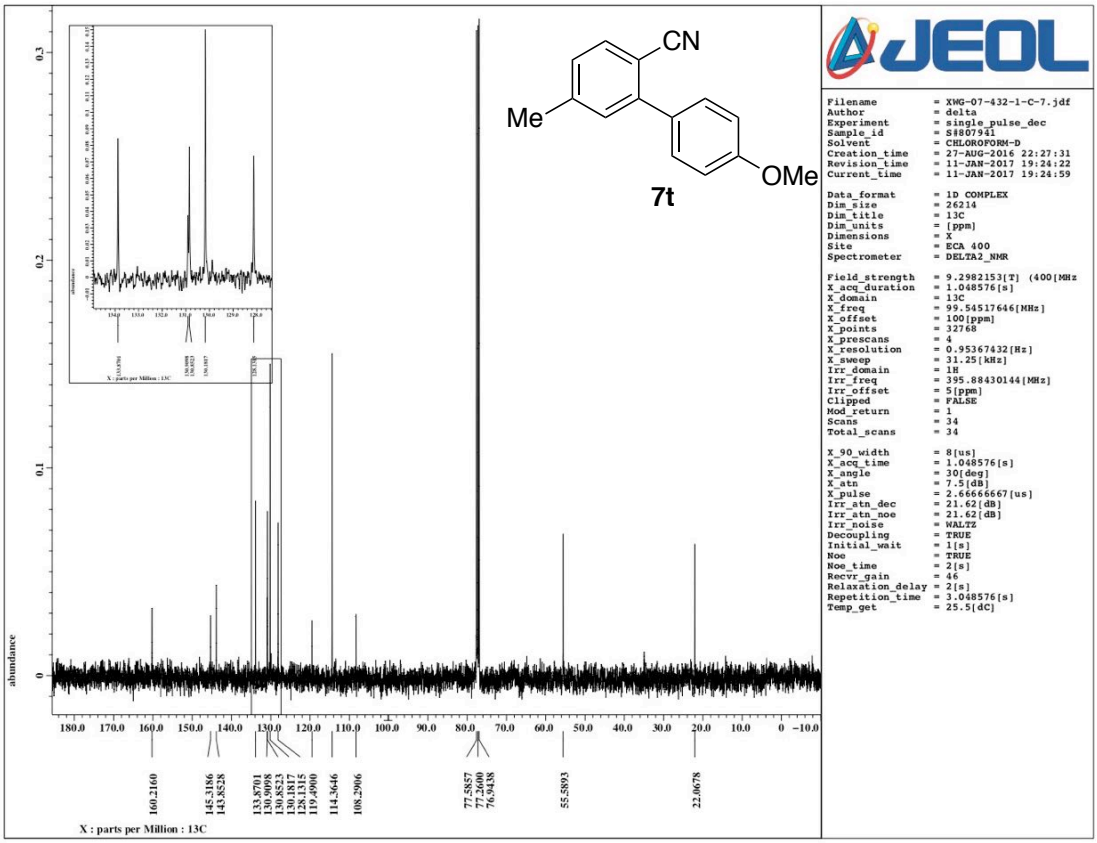

```
Filename          = XWG-07-456-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8824548
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 22:51:35
Revision_time     = 11-JAN-2017 19:14:24
Current_time      = 11-JAN-2017 19:15:06

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 4
Total_scans       = 4

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.3[dC]
```



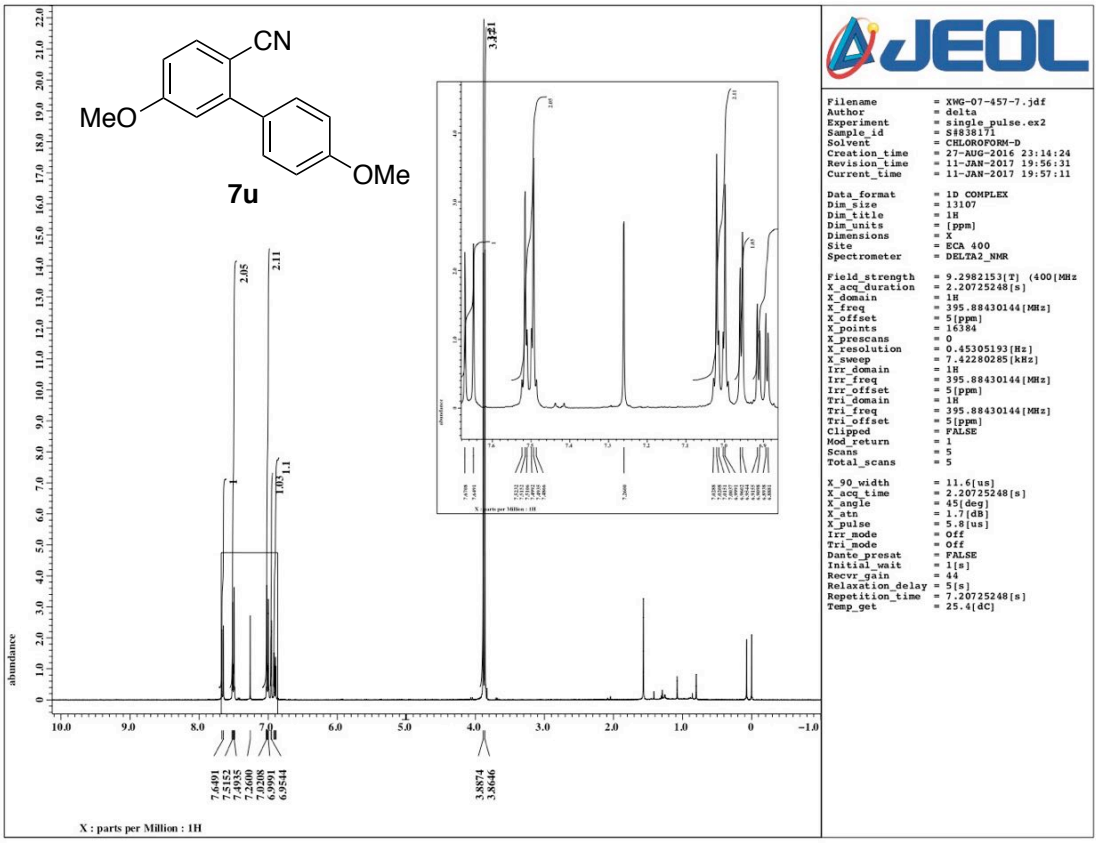

```
Filename          = XWG-07-456-c-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8826169
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 22:57:30
Revision_time     = 11-JAN-2017 19:18:47
Current_time      = 11-JAN-2017 19:20:01

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 33
Total_scans       = 33

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 46
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.5[dC]
```



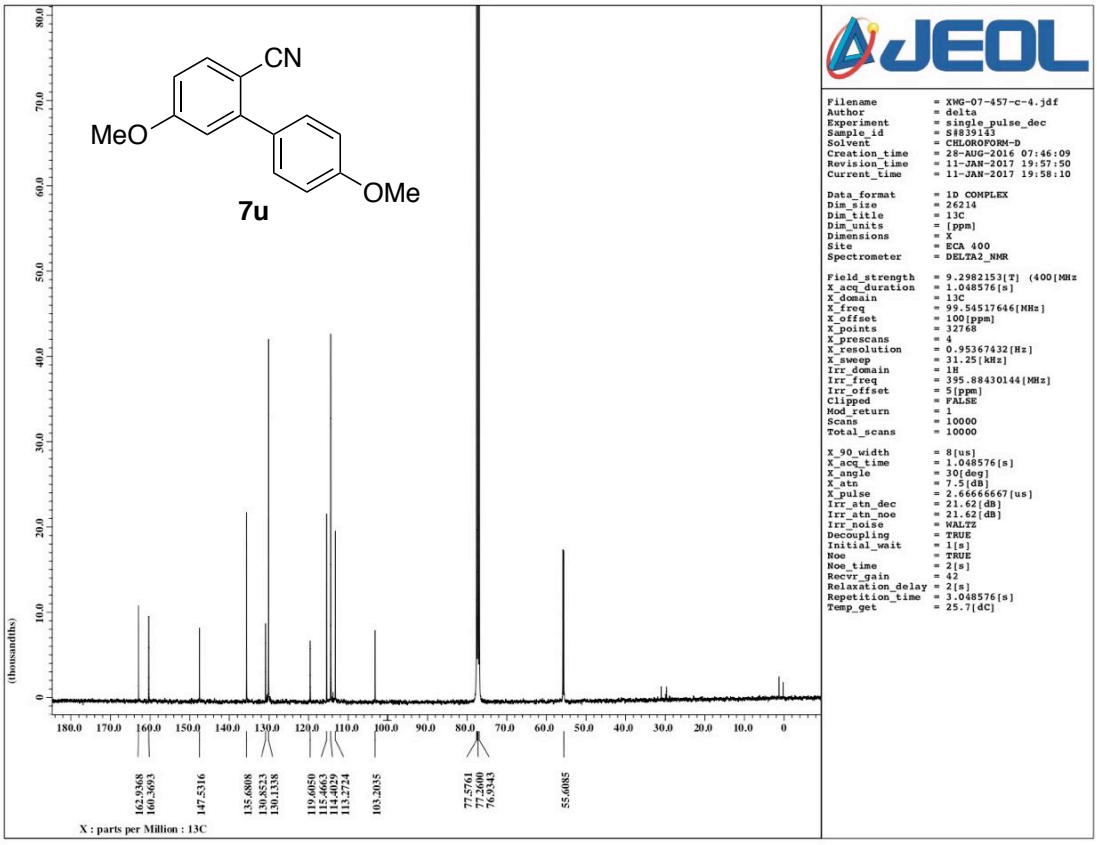

```
Filename          = XWG-07-432-1-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S8807066
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 22:22:41
Revision_time     = 11-JAN-2017 19:22:29
Current_time      = 11-JAN-2017 19:23:10

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 6
Total_scans       = 6

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.4[dC]
```



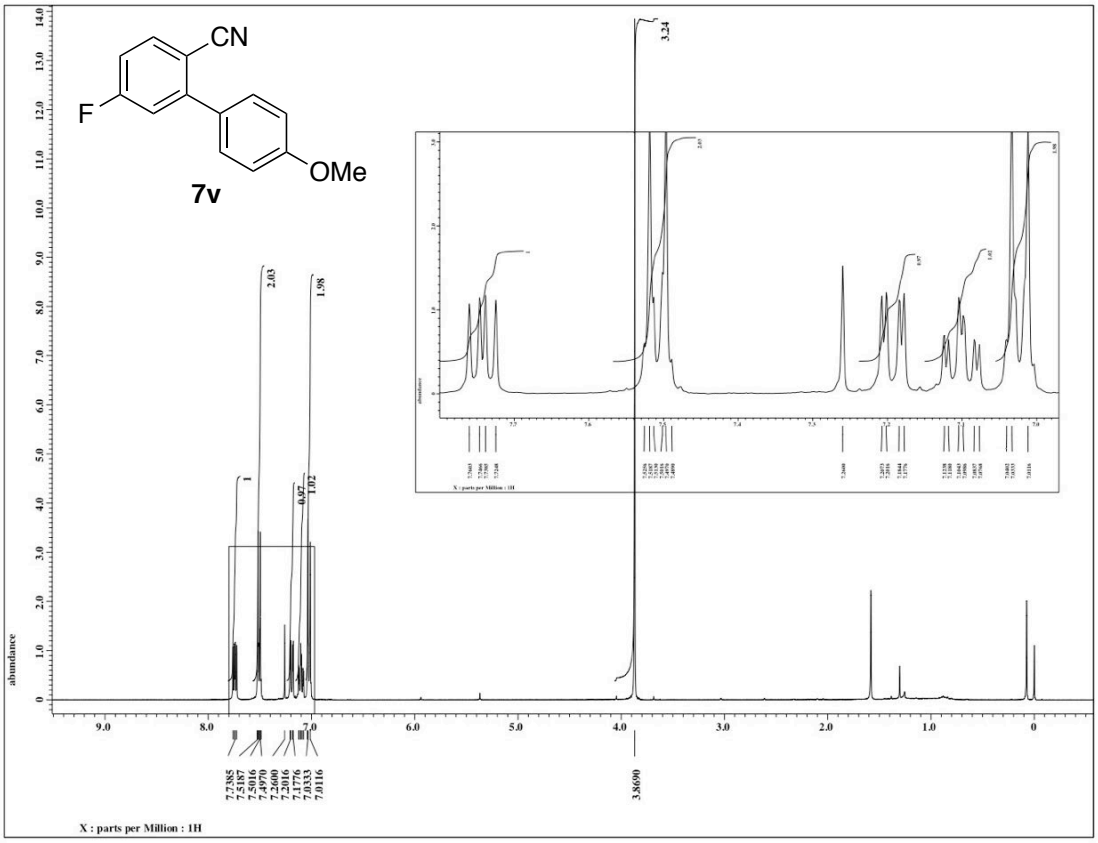

```
Filename          = XWG-07-432-1-C-7.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S8807941
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 22:27:31
Revision_time     = 11-JAN-2017 19:24:22
Current_time      = 11-JAN-2017 19:24:59

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 34
Total_scans       = 34

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 46
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.5[dC]
```

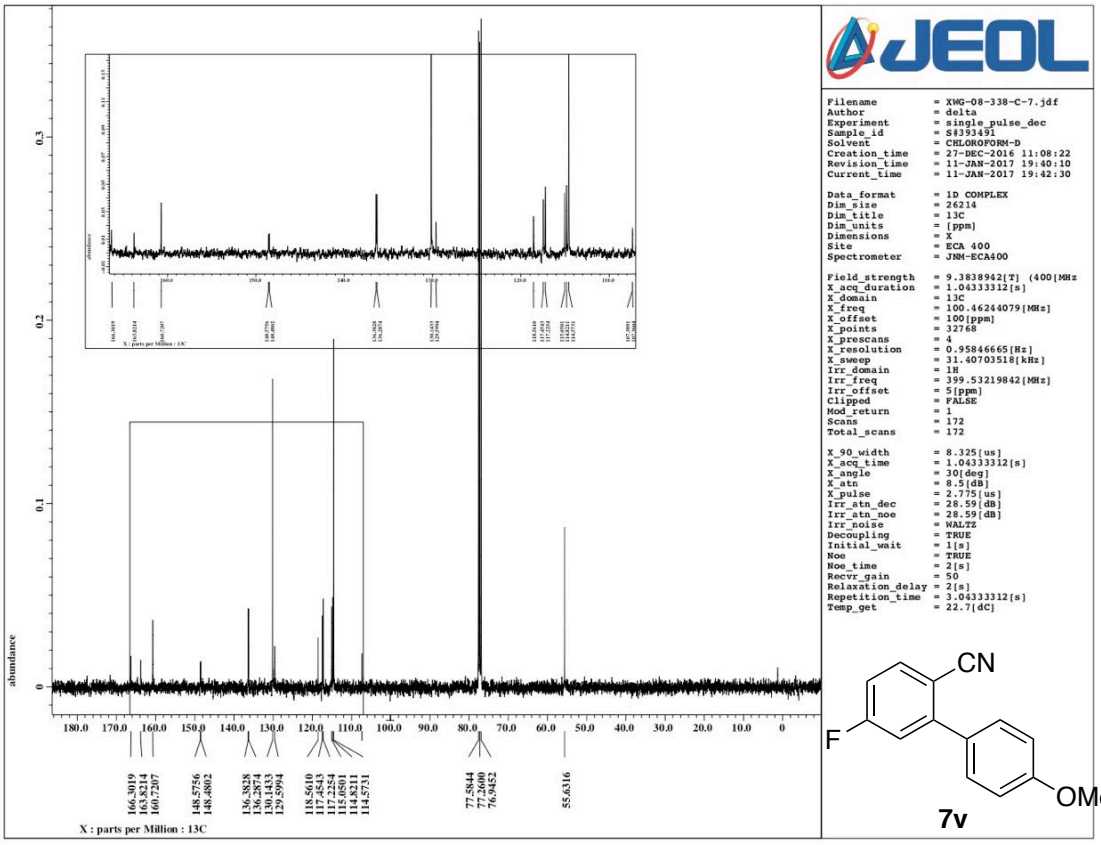


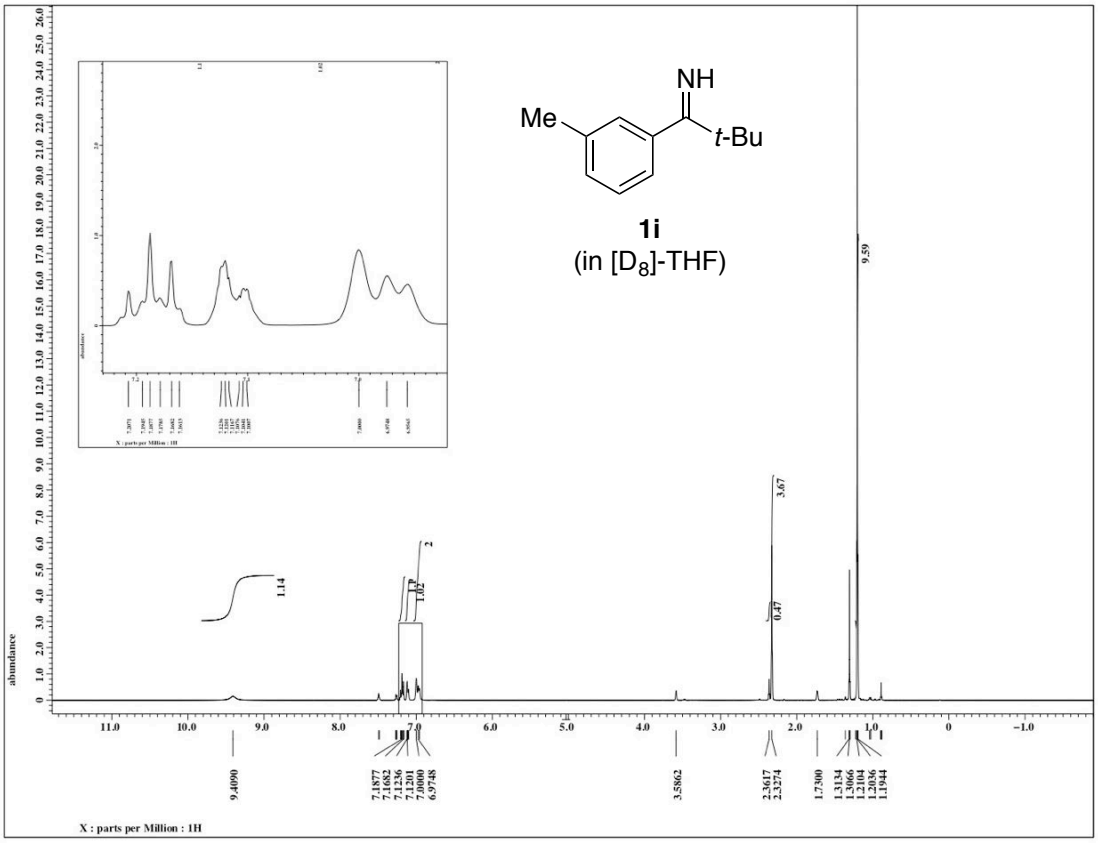

```
Filename          = XWG-07-457-7.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#838171
Solvent           = CHLOROFORM-D
Creation_time     = 27-AUG-2016 23:14:24
Revision_time     = 11-JAN-2017 19:56:31
Current_time      = 11-JAN-2017 19:57:11

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 5
Total_scans       = 5

X_90_width        = 11.6[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.7[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 25.4[dC]
```

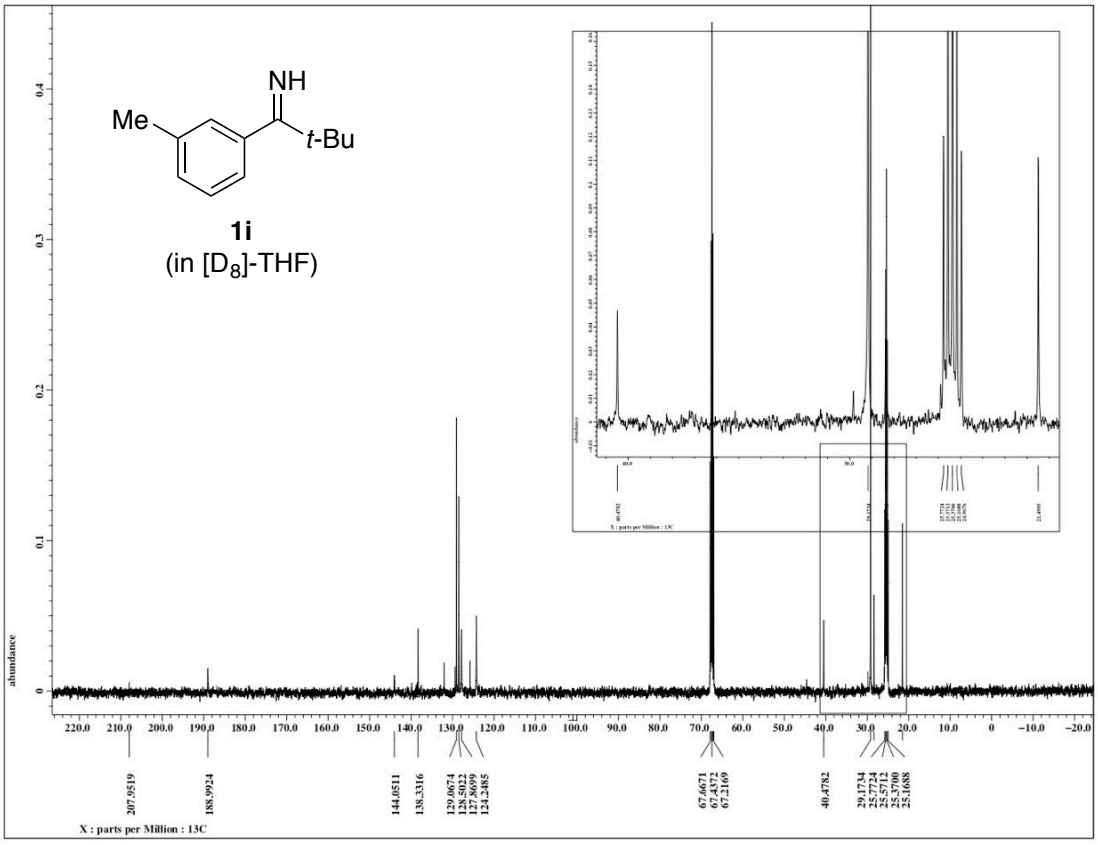


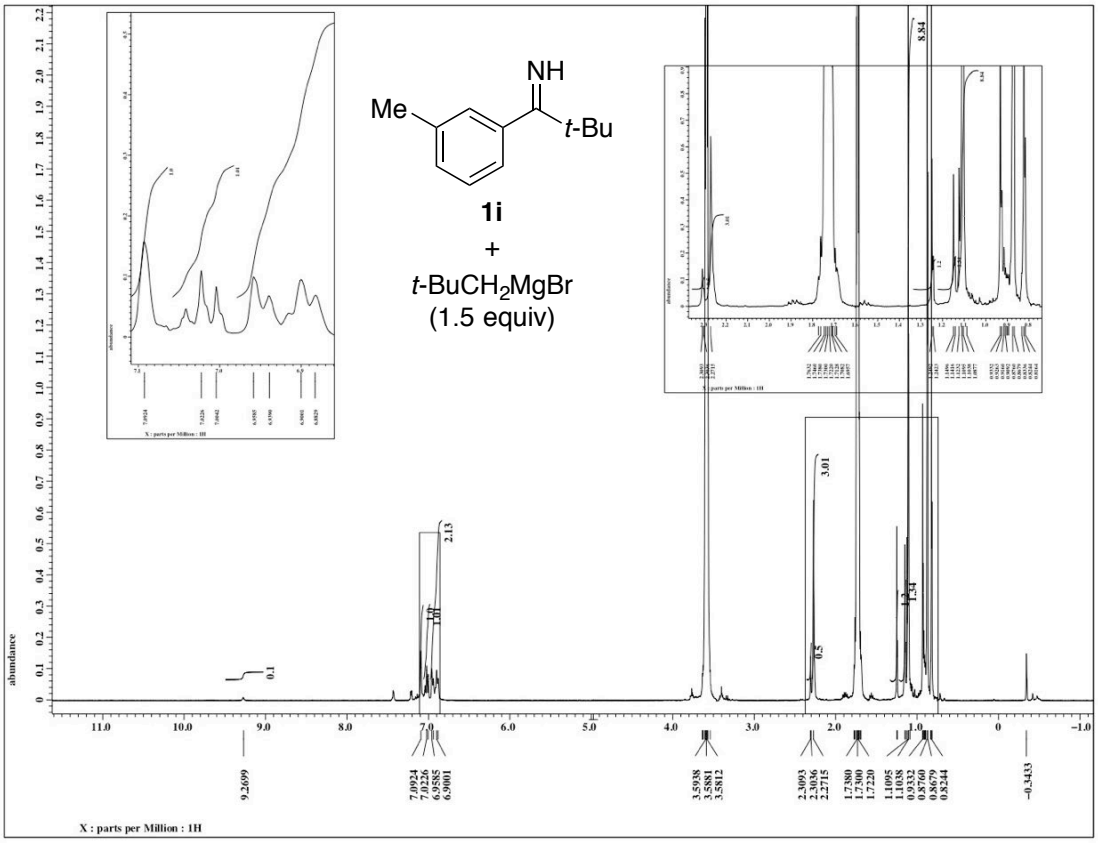

```
Filename          = XWG-07-457-c-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#839143
Solvent           = CHLOROFORM-D
Creation_time     = 28-AUG-2016 07:46:09
Revision_time     = 11-JAN-2017 19:57:50
Current_time      = 11-JAN-2017 19:58:10

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10000
Total_scans       = 10000

X_90_width        = 8[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 7.5[dB]
X_pulse           = 2.66666667[us]
Irr_atn_dec       = 21.62[dB]
Irr_atn_noe       = 21.62[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 42
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 25.7[dC]
```

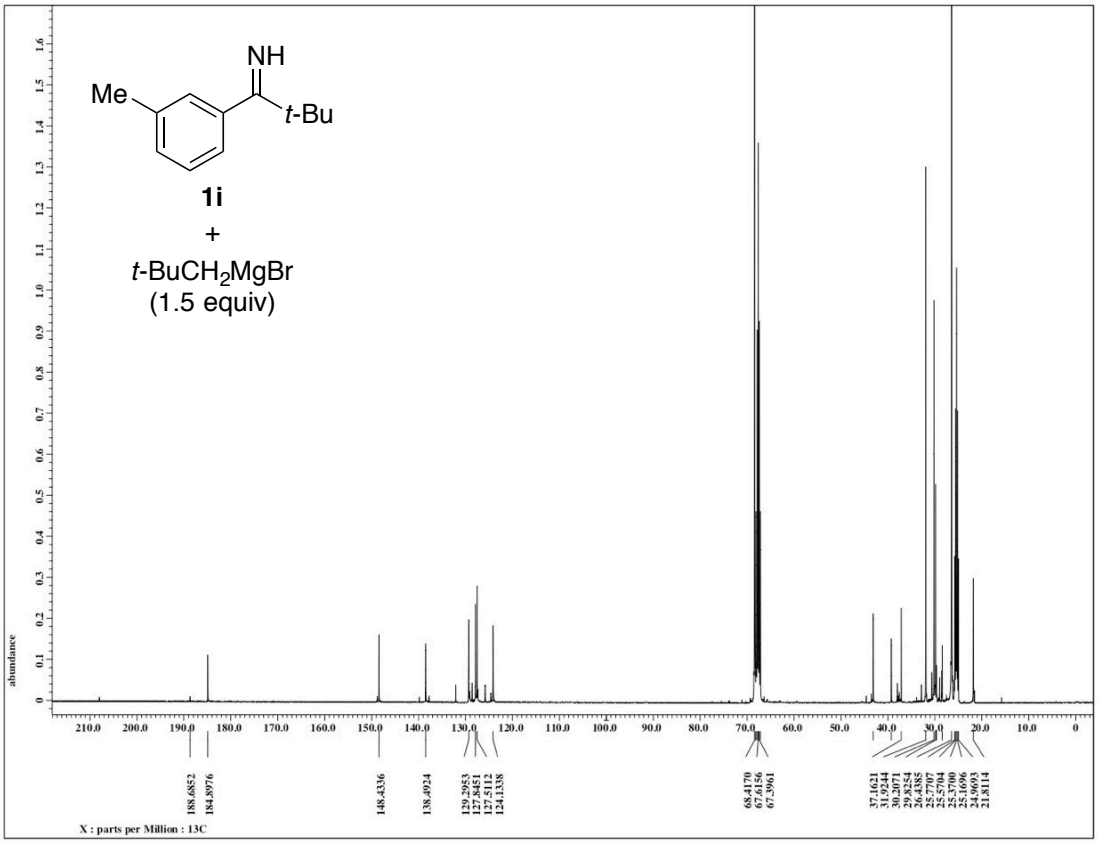

CN
F
OMe
7v
3.24
2.03
1.98
1.02
0.97
1
abundance
7.7385
7.5187
7.5016
7.4970
7.2600
7.2016
7.1776
7.0333
7.0116
3.8690
X : parts per Million : 1H


abundance
166.3019
165.5214
160.7207
148.5756
148.4802
136.3828
136.2874
130.1413
129.5994
118.5610
117.4543
117.2254
115.0501
114.8211
114.5731
77.5844
77.2600
76.9452
55.6316
X : parts per Million : 13C
Filename = XWG-08-338-C-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#393491
Solvent = CHLOROFORM-D
Creation_time = 27-DEC-2016 11:08:22
Revision_time = 11-JAN-2017 19:40:10
Current_time = 11-JAN-2017 19:42:30
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 400
Spectrometer = JNM-ECA400
Field_strength = 9.3838942[T] (400[MHz
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.46244079[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 = 399.53219842[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 172
Total_scans = 172
X_90_width = 8.325[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 8.5[dB]
X_pulse = 2.775[us]
Irr_atn_dec = 28.59[dB]
Irr_atn_noe = 28.59[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.7[dC]
CN
F
OMe
7v


NH
Me
t-Bu
1i
(in [D8]-THF)
abundance
X : parts per Million : 1H


NH
Me
t-Bu
1i
(in [D8]-THF)
abundance
X : parts per Million : 13C


NH
Me
t-Bu
1i
+
t-BuCH2MgBr
(1.5 equiv)
X : parts per Million : 1H


NH
Me
t-Bu
1i
+
t-BuCH2MgBr
(1.5 equiv)
X : parts per Million : 13C