

Supporting Information

Manganese(II) chloride catalyzed highly efficient one pot synthesis of propargylamines and fused triazoles *via* three component coupling reaction under solvent free condition.

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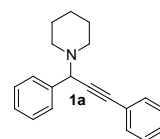
General

Ethanol was dried over magnesium cake. THF was distilled from sodium-benzophenone under argon. Dichloromethane (DCM), acetonitrile (ACN), diisopropylamine (DIPA) and dimethylformamide (DMF), dimethyl sulfoxide (DMSO) were distilled from CaH₂. The aldehydes, amine (piperidine, morpholine, aniline), and alkynes were used as purchased. The azidomethylpyrrolidine was prepared by reported procedure. All reactions were carried out in screw capped sealed tube at 90 °C. Reactions were monitored by thin-layer chromatography using pre-coated silica gel 60 glass plates with F254 indicator. Visualization was accomplished by UV light (254 nm) in combination with iodine, potassium permanganate staining solutions. The products were purified by neutral column chromatography on 70–230 mesh silica gels. Yields refer to chromatographically and spectrographically pure material, unless otherwise noted. ¹H NMR and ¹³C NMR spectra were obtained from 300 and 400 MHz NMR spectrometer, respectively. Chemical shifts (δ) are reported in parts per million (ppm) relative to CDCl₃ (7.26 and 77.0 ppm), the coupling constants are reported in Hertz (Hz) and the multiplicities are indicated as br = broad, s = singlet, d = doublet, dd = doublet of doublet, t = triplet, m = multiplet. Infrared spectra were recorded using Perkin Elmer FT/IR spectrometer. Mass spectra (EI-MS) and high resolution mass spectra (HRMS-EI) were determined on a Finnigan/Thermo Quest MAT 95XL mass spectrometer. Melting points are checked by the use of FGnFargo Instruments melting point apparatus. Melting point of the compounds might not be correct.

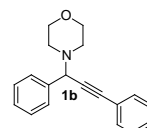
General experimental procedure for manganese(II) chloride catalyzed three component coupling reaction

A mixture of aldehyde (1.0 mmol), amine (1.2 mmol), alkyne (1.5 mmol) and MnCl₂ (10 mol%) in sealed tube was stirred without solvent for 12 h at 90 °C. The progress of reaction was monitored by TLC. After completion of reaction, the product was purified by column chromatography using *n*-hexane/EtOAc as eluent to give the desired product. The products were further identified by FT-IR, ¹H and ¹³C NMR spectroscopy, and HRMS, and all data were all in good agreement with assigned structures. The characterization data of all propargylamines are as follows.

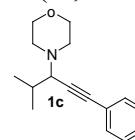
1-(1,3-diphenylprop-2-yn-1-yl)piperidine, 1a. *R*_f = 0.44 (EtOAc/hexane 1:9), Yield: 98%, Pale yellow solid; mp: 66–67 °C. ¹H NMR (300 MHz, CDCl₃, ppm δ): 7.64–7.62 (d, *J* = 6.0 Hz, 2H), 7.53–7.50 (m, 2H), 7.38–7.28 (m, 6H), 4.79 (s, 1H), 2.57–2.54 (m, 4H), 1.61–1.56 (m, 4H), 1.47–1.42 (m, 2H); ¹³C NMR (75 MHz, CDCl₃, δ): 138.52, 131.69, 128.38, 128.15, 127.93, 127.34, 123.27, 87.80, 85.97, 62.29, 50.61, 26.10, 24.36; IR (KBr, thin film, cm⁻¹): 3049, 2923, 2802 1596, 1486, 1445, 1270, 1152, 1094, 758, 691; LRMS-EI (*m/z*): 275 (12), 246 (3), 232 (4), 198 (50), 191 (100), 165 (7), 139 (2), 115 (9), 86 (5), 56 (6); HRMS-EI (*m/z*): M⁺ calcd for C₂₀H₂₁N, 275.1674; found 275.1669.



4-(1,3-diphenylprop-2-yn-1-yl)morpholine 1b. *R*_f = 0.19 (EtOAc/hexane 1:9), Yield: 90%, Pale yellow oil. ¹H NMR (CDCl₃, 300 MHz, ppm, δ): 7.64–7.62 (d, *J* = 6.0 Hz, 2H), 7.53–7.50 (m, 2H), 7.37–7.30 (m, 6H), 4.79 (s, 1H) 3.75–3.71 (m, 4H), 2.65–2.62 (m, 4H); ¹³C NMR (75 MHz, CDCl₃, δ): 137.70, 131.72, 128.51, 128.23, 128.15, 127.69, 122.91, 88.41, 84.96, 67.08, 61.97, 49.80; IR (KBr, thin film, cm⁻¹): 2950, 2857, 2818, 1599, 1316, 1228, 1110, 998, 864, 746, 699; LRMS-EI (*m/z*): 277 (27), 246 (7), 232 (2), 219 (4), 200 (4), 191 (100), 165 (5), 115 (4), 86 (15), 56 (11); HRMS-EI (*m/z*): M⁺ calcd for C₁₉H₁₉NO, 277.1467; found 277.1475.

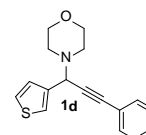


4-(4-methyl-1-phenylprop-1-yn-3-yl)morpholine 1c. $R_f = 0.19$ (EtOAc/hexane 1:9), Yield: 96%, Pale yellow solid; mp: 42–43 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.42 (m, 2H), 7.30–7.28 (m, 3H), 3.77–3.72 (m, 4H), 3.03–3.00 (m, 1H), 2.74–2.70 (m, 2H), 2.68–2.67 (m, 2H), 2.55–2.48 (m, 1H), 1.12–1.10 (d, $J = 6.7$ Hz, 3H), 1.04–1.02 (d, $J = 4.3$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3 , δ): 131.43, 127.95, 127.59, 123.15, 86.42, 66.88, 64.97, 49.75, 29.68, 20.12, 19.55; IR (KBr, thin film, cm^{-1}): 2961, 2802, 1593, 1484, 1319, 1253, 1111, 1009, 864, 760, 691; LRMS-EI (m/z): 242 (0.2), 228 (0.3), 200 (100), 169 (0.3), 141 (4), 128 (5), 115 (17), 91 (1), 77 (2), 54 (4); HRMS-EI (m/z): M^+ calcd for $\text{C}_{16}\text{H}_{21}\text{NO}$, 243.1623; found 243.1615.



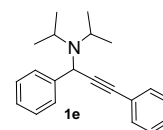
4-(3-phenyl-1-(thiophen-2-yl)prop-2-yn-1-yl)morpholine 1d.

$R_f = 0.19$ (EtOAc/hexane 1:9), Yield: 93%. Brown oil, ^1H NMR (CDCl_3 , 300 MHz, ppm, δ): 7.51–7.48 (m, 2H), 7.43–7.42 (m, 1H), 7.34–7.31 (m, 4H), 7.29–7.23 (m, 1H), 4.82 (s, 1H), 3.76–3.72 (m, 4H), 2.64–2.61 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3 , δ): 139.26, 131.49, 128.07, 127.38, 125.46, 123.37, 122.64, 87.02, 84.99, 66.79, 57.51, 53.22, 49.39. IR (KBr, thin film, cm^{-1}): 2956, 2851, 2736, 1596, 1486, 1451, 1316, 1281, 1113, 1004, 916, 754, 685; LRMS-EI (m/z): 283 (24), 252 (3), 198 (21), 197 (100), 165 (2), 152 (6), 139 (2), 115 (3), 86 (9), 56 (7); HRMS-EI (m/z): M^+ calcd for $\text{C}_{17}\text{H}_{17}\text{NOS}$, 283.1031; found 283.1022.



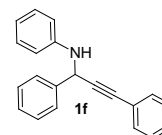
***N,N*-diisopropyl-1,3-diphenylprop-2-yn-1-amine 1e.**

$R_f = 0.19$ (EtOAc/hexane 1:9), Yield: 65%, Pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.77–7.74 (d, $J = 9.0$ Hz, 2H), 7.51–7.48 (m, 3H), 7.37–7.28 (m, 5H), 5.04 (s, 1H), 3.27–3.18 (m, 2H), 1.32–1.30 (d, $J = 6.0$ Hz, 6H), 1.08–1.06 (d, $J = 6.0$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 142.17, 131.31, 128.27, 127.80, 126.75, 91.59, 85.79, 50.55, 46.55, 23.76, 20.69; IR (KBr, thin film, cm^{-1}): 3428, 2956, 2917, 1633, 1486, 1445, 1270, 1182, 1113, 754, 688; LRMS-EI (m/z): 291 (3), 276 (11), 214 (7), 192 (15), 191 (100), 105 (4), 91 (6), 77 (3), 51 (1); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{25}\text{N}$, 291.1987; found 291.1992.



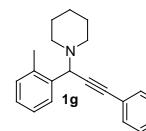
***N*-(1,3-diphenylprop-2-yn-1-yl)aniline 1f.**

$R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 69%, yellow solid, mp: 88–90 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.73–7.70 (d, $J = 9.0$ Hz, 2H), 7.48–7.39 (m, 5H), 7.33–7.29 (m, 5H), 6.87–6.82 (m, 2H), 5.56 (s, 1H), 4.33 (br, s 1H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 146.48, 139.65, 129.05, 131.65, 128.83, 128.70, 128.66, 128.18, 128.11, 127.96, 127.20, 122.68, 120.77, 118.45, 113.99, 88.47, 84.96, 50.51; IR (KBr, thin film, cm^{-1}): 3373, 3049, 1593, 1486, 754, 691; LRMS-EI (m/z): 283 (11), 206 (6), 191 (100), 189 (15), 165 (5), 77 (5), 65 (2); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{17}\text{N}$, 283.1361; found 283.1353.



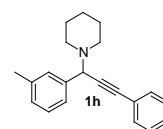
1-(3-phenyl-1-(*o*-tolyl)prop-2-yn-1-yl)piperidine 1g.

$R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 91%, Pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.70–7.68 (m, 1H), 7.53–7.49 (m, 2H), 7.33–7.31 (m, 3H), 7.19–7.17 (m, 3H), 4.84 (s, 1H), 2.57–2.53 (m, 4H), 2.46 (s, 3H), 1.56–1.51 (m, 4H), 1.49–1.40 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 137.59, 136.74, 131.74, 130.54, 128.90, 128.22, 127.90, 127.43, 125.13, 123.47, 88.07, 85.99, 60.19, 50.51, 26.28, 24.59, 19.01; IR (KBr, thin film, cm^{-1}): 2928, 2831, 2736, 1596, 1486, 1311, 1111, 1083, 847, 754, 688; LRMS-EI (m/z): 288 (9), 246 (3), 204 (100), 198 (67), 191 (10), 165 (4), 127 (7), 115 (9), 84 (11), 77 (5); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{23}\text{N}$, 289.1830; found 289.1822.



1-(3-phenyl-1-(*m*-tolyl)prop-2-yn-1-yl)piperidine 1h.

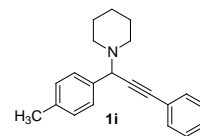
$R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 95%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.54–7.50 (m, 2H), 7.47–7.41 (m, 3H), 7.33–7.31 (m, 3H), 7.11–7.09 (m, 1H), 4.77 (s, 1H), 2.59–2.56 (m,



2H), 2.45–2.44 (m, 2H), 2.37 (s, 3H), 1.62–1.57 (m, 4H), 1.47–1.42 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 138.19, 137.58, 131.74, 129.22, 128.22, 128.18, 127.96, 127.87, 125.69, 123.29, 87.78, 86.15, 62.26, 50.61, 25.97, 24.35, 21.45 (KBr, thin film, cm^{-1}): 2928, 2851, 2727, 1604, 1486, 1314, 1157, 1083, 987, 754, 688; LRMS-EI (m/z): 289 (29), 246 (5), 221 (9), 205 (100), 198 (80), 189 (8), 178 (4), 119 (8), 91 (7), 65 (2); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{23}\text{N}$, 289.1830; found 289.1824.

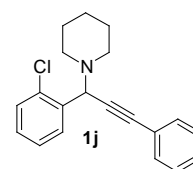
1-(3-phenyl-1-(*p*-tolyl)prop-2-yn-1-yl)piperidine 1i.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 97%; brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.52–7.49 (m, 4H), 7.33–7.30 (m, 3H), 7.17–7.15 (d, J = 6.0 Hz, 2H), 4.77 (s, 1H), 2.58–2.54 (m, 4H), 2.35 (s, 3H), 1.62–1.56 (m, 4H), 1.47–1.41 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 137.12, 135.32, 131.84, 128.72, 128.50, 128.21, 127.96, 123.43, 87.60, 86.27, 62.09, 50.61, 26.06, 24.40, 21.04; (KBr, thin film, cm^{-1}): 2928, 2851, 2802, 1596, 1440, 1314, 1270, 1091, 817, 751, 688; LRMS-EI (m/z): 289 (30), 274 (3), 246 (4), 207 (3), 205 (100), 198 (40), 189 (6), 115 (4), 105 (2), 84 (3); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{23}\text{N}$, 289.1830; found 289.1828.



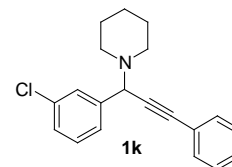
1-(1-(2-chlorophenyl)-3-phenylprop-2-yn-1-yl)piperidine 1j.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 93%, pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.77–7.76 (d, J = 3.0 Hz, 1H), 7.45–7.40, (m, 2H), 7.39–7.37 (m, 1H), 7.33–7.23, (m, 5H), 5.10 (s 1H), 2.63–2.59 (m, 4H), 1.59–1.56 (m, 4H), 1.42–1.41 (m, 2H), ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 136.29, 134.54, 131.62, 130.37, 129.62, 128.61, 128.11, 127.96, 126.00, 123.02, 87.65, 85.62, 59.19, 50.60, 26.03 24.35; IR (KBr, thin film, cm^{-1}): 3060, 2928, 2851, 2749, 1593, 1484 1314, 1156, 1086, 858, 746, 688; LRMS-EI (m/z): 309 (26), 266 (6), 232 (8), 227 (31), 225 (99), 198 (100), 189 (23), 115 (23), 84 (7); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{20}\text{ClN}$, 309.1284; found 309.1283.



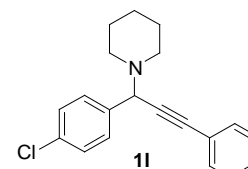
1-(1-(3-chlorophenyl)-3-phenylprop-2-yn-1-yl)piperidine 1k.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 92%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.65 (s, 1H), 7.65–7.64 (m, 3H), 7.53–7.50 (m, 3H), 7.35–7.27 (m, 2H), 4.77 (s, 1H), 2.56–2.53 (m, 4H), 1.64–1.55 (m, 4H) 1.48–1.42 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 140.82, 134.04, 131.78, 129.24, 128.48, 128.24, 128.18, 127.60, 126.59, 123.14, 88.36, 85.11, 61.92, 50.55, 26.20, 24.11; IR (KBr, thin film, cm^{-1}): 3060, 2928, 2846, 2741, 1593, 1489, 1314, 1152, 1086, 831, 791, 685; LRMS-EI (m/z): 309 (18), 266 (5), 232 (4), 227 (22), 225 (72), 198 (100), 189 (19), 115 (70), 84 (6); HRMS-EI (m/z): M^+ calcd for $\text{C}_{16}\text{H}_{20}\text{N}$, 309.1284; found 309.1279.



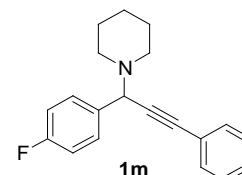
1-(1-(4-chlorophenyl)-3-phenylprop-2-yn-1-yl)piperidine 1l.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 96%, pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.59–7.52 (m, 2H), 7.51–7.49 (m, 2H), 7.34–7.30 (m, 5H), 4.77 (s, 1H), 2.56–2.52 (m, 4H), 1.64–1.56 (m, 4H), 1.48–1.42 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 140.78, 137.08, 134.62, 133.14, 131.70, 130.75, 129.75, 129.30, 128.21, 128.09, 122.99, 88.23, 85.20, 61.58, 50.49, 26.00, 24.27; IR (KBr, thin film, cm^{-1}): 3049, 2934, 2861, 2741, 1659, 1593, 1484, 1314, 1154, 1086, 852, 754, 688 ; LRMS-EI (m/z): 309 (20), 266 (4), 232 (3), 227 (31), 225 (100), 198 (48), 189 (18), 115 (5), 84 (3); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{20}\text{ClN}$, 309.1284; found 309.1287.



1-(1-(4-fluorophenyl)-3-phenylprop-2-yn-1-yl)piperidine 1m.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 94%, pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.44–7.36 (m, 5H), 7.34–7.29 (m, 4H), 4.79 (s, 1H), 2.57–2.53 (m, 4H), 1.62–1.59 (m, 4H), 1.48–1.42 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 ,



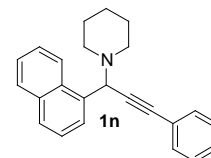
ppm, δ): 162.80 (d, $J = 244$ Hz), 141.44 (d, $J = 6.48$ Hz), 131.82, 129.39 (d, $J = 8.63$ Hz), 128.28, 128.18, 124.00, 123.97, 123.04, 115.34 (d, $J = 22.6$ Hz), 114.33 (d, $J = 21.6$ Hz), 88.24, 85.48, 61.98, 50.69, 26.03, 24.19; IR (KBr, thin film, cm^{-1}): 3049, 2934, 2918, 1593, 1484, 1314, 1201, 1086, 1012, 754, 688; LRMS-EI (m/z): 293 (24), 250 (6), 225 (9), 210 (19), 209 (100), 198 (95), 183 (4), 115 (6), 84 (5); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{20}\text{NF}$, 293.1580; found 293.1576.

1-(1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-yl)piperidine 1n.

$R_f = 0.48$ (EtOAc/hexane 1:9), Yield: 96%, pale yellow solid, mp: 126–128 °C.

^1H NMR (300 MHz, CDCl_3 , ppm, δ): 8.41–8.39 (d, $J = 9.0$ Hz, 1H), 7.93–7.79 (m, 3H), 7.56–7.50 (m, 5H), 7.44–7.33 (m, 3H), 5.42 (s, 1H), 2.67–2.58 (m, 4H), 1.59–1.52 (m, 4H), 1.50–1.44 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ):

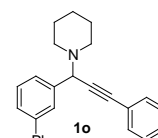
134.22, 133.98, 131.89, 131.78, 128.49, 128.33, 128.25, 127.97, 126.79, 125.67, 125.48, 124.98, 124.98, 124.70, 123.41, 88.34, 88.02, 60.59, 60.64, 26.20, 24.54, IR (KBr, thin film, cm^{-1}): 3054, 2928, 2802, 1593, 1488, 1437, 1281, 781, 751, 688; LRMS-EI (m/z): 325 (19), 242 (25), 241 (100), 239 (39), 198 (31), 115 (6), 84 (16); HRMS-EI (m/z): M^+ calcd for $\text{C}_{24}\text{H}_{23}\text{N}$, 325.1830; found 325.1822.



1-(1-(1,1'-biphenyl-3-yl)-3-phenylprop-2-yn-1-yl)piperidine 1o.

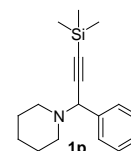
$R_f = 0.48$ (EtOAc/hexane 1:9), Yield: 94%, pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.83–7.80 (m, 1H), 7.57–7.55 (m, 2H), 7.48–7.43 (m, 2H), 7.42–7.35 (m, 5H), 7.34–7.29 (m, 4H), 4.63 (s, 1H), 2.58–2.54 (m, 2H), 2.38–2.32 (m, 2H), 1.50–1.48 (m, 4H), 1.42–1.39 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ):

142.77, 141.30, 136.55, 131.71, 129.73, 129.33, 128.19, 127.88, 127.60, 127.36, 126.92, 126.70, 123.44, 126.94, 87.54, 86.85, 59.19, 50.20, 26.20, 24.58. IR (KBr, thin film, cm^{-1}): 3043, 2928, 2796, 2747, 1432, 1390, 1196, 823, 746, 699; LRMS-EI (m/z): 351 (89), 350 (71), 308 (14), 274 (19), 266 (36), 265 (53), 252 (21), 198 (8), 165 (100), 115 (11), 84 (7); HRMS-EI (m/z): M^+ calcd for $\text{C}_{26}\text{H}_{25}\text{N}$, 351.1987; found 351.1989.



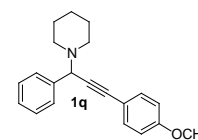
1-(1-phenyl-3-(trimethylsilyl)prop-2-yn-1-yl)piperidine 1p.

$R_f = 0.49$ (EtOAc/hexane 1:9), Yield: 89%, Yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.57–7.54 (m, 2H), 7.35–7.29 (m, 3H), 4.61 (s, 1H), 1.60–1.56 (m, 4H), 1.30–1.26 (m, 6H), 0.23 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 129.55, 128.82, 128.33, 127.84, 127.23, 102.27, 92.30, 62.61, 50.55, 26.20, 24.58, 0.2319; IR (KBr, thin film, cm^{-1}): 3308, 2934, 2802, 2159, 1448, 1251, 1103, 999, 839, 757; LRMS-EI (m/z): 271 (13), 198 (14), 195 (17), 194 (100), 187 (9), 159 (27), 145 (5), 105 (4), 84 (9), 73 (7); HRMS-EI (m/z): M^+ calcd for $\text{C}_{17}\text{H}_{25}\text{NSi}$, 271.1756; found 271.1750.



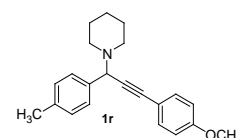
1-(3-(4-methoxyphenyl)-1-phenylprop-2-yn-1-yl)piperidine 1q.

$R_f = 0.42$ (EtOAc/hexane 1:9), Yield: 97%, Brown oil, ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.64–7.61 (m, 2H), 7.46–7.43 (m, 2H), 7.35–7.27 (m, 3H), 6.87–7.84 (m, 2H), 4.77 (s, 1H), 3.82 (s, 3H), 2.57–2.53 (m, 4H), 1.53–1.57 (m, 4H), 1.61–1.56 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , δ): 159.35, 138.70, 133.07, 128.43, 127.91, 127.29, 115.42, 113.79, 87.56, 84.41, 62.31, 55.13, 50.58, 26.10, 24.38; IR (KBr, thin film, cm^{-1}): 2934, 2840, 2791, 1602, 1508, 1286, 1245, 1171, 1028, 831, 705; LRMS-EI (m/z): 305 (26), 262 (3), 229 (5), 228 (41), 221 (100), 206 (6), 178 (10), 145 (3); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{23}\text{NO}$, 305.1780; found 305.1770.



1-(3-(4-methoxyphenyl)-1-(p-tolyl)prop-2-yn-1-yl)piperidine 1r.

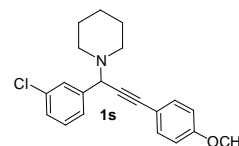
$R_f = 0.42$ (EtOAc/hexane 1:9), Yield: 96%, white solid. mp 81–82 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.50–7.42 (m, 4H), 7.17–7.14 (m, 2H), 6.86–6.83



(m, 2H), 4.72 (s, 1H), 3.81 (s, 3H), 2.55–2.53 (m, 4H), 2.35 (s, 3H), 1.60–1.55 (m, 4H), 1.46–1.41 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 159.34, 136.92, 135.68, 133.08, 128.65, 128.43, 115.52, 113.80, 87.32, 84.74, 62.09, 55.18, 50.59, 26.11, 24.41, 21.03; IR (KBr, thin film, cm^{-1}): 2928, 2796, 1602, 1508, 1289, 1245, 1166, 1028, 828, 653; LRMS-EI (m/z): 319 (17), 318 (6), 236 (18), 228 (13), 220 (5), 192 (7); HRMS-EI (m/z): M^+ calcd for $\text{C}_{22}\text{H}_{25}\text{NO}$, 319.1936; found 319.1930.

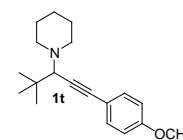
1-(1-(3-chlorophenyl)-3-(4-methoxyphenyl)prop-2-yn-1-yl)piperidine 1s.

R_f = 0.42 (EtOAc/hexane 1:9), Yield: 94%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.63 (s, 1H), 7.54–7.53 (m, 1H), 7.52–7.43 (m, 2H), 7.30–7.22 (m, 2H), 6.88–6.85 (m, 2H), 4.74 (s, 1H), 3.82 (s, 3H), 2.54–2.51 (m, 4H), 1.61–1.56 (m, 4H), 1.47–1.42 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 159.44, 141.09, 133.87, 129.09, 128.36, 127.40, 130.71, 126.48, 115.03, 88.07, 83.43, 61.77, 55.08, 50.55, 26.03, 24.26, IR (KBr, thin film, cm^{-1}): 2934, 2802, 1604, 1506, 1467, 1289, 1245, 1171, 1034, 828, 694; LRMS-EI (m/z): 339 (28), 257 (38), 255 (100), 228 (67), 212 (7), 176 (7), 145 (4), 84 (2); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{22}\text{ClNO}$, 339.1390; found 339.1386.



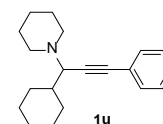
1-(1-(4-methoxyphenyl)-4,4-dimethylpent-1-yn-3-yl)piperidine 1t.

R_f = 0.42 (EtOAc/hexane 1:9), Yield: 98%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.38–7.36 (m, 2H), 6.84–6.81 (m, 2H), 3.80 (s, 3H), 3.05 (s, 1H), 2.68–2.74 (m, 2H), 2.50–2.42 (m, 2H), 1.59–1.55 (m, 4H), 1.43–1.37 (m, 2H), 1.01 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 159.06, 132.87, 116.10, 113.75, 86.81, 85.22, 68.47, 55.14, 54.14, 36.83, 27.19, 26.78, 24.44; IR (KBr, thin film, cm^{-1}): 2928, 2857, 2791, 1602, 1508, 1459, 1292, 1240, 1168, 1091, 1034, 995, 831, 803; LRMS-EI (m/z): 284 (0.1), 270 (2), 229 (25), 228 (100), 213 (1), 184 (1), 145 (17), 115 (30), 102 (2), 77 (0.5); HRMS-EI (m/z): M^+ calcd for $\text{C}_{19}\text{H}_{27}\text{NO}$, 285.2093; found 285.2101



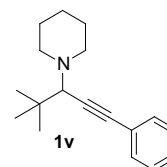
1-(1-(cyclohexyl-3-phenyl)prop-2-yn-1-yl)piperidine 1u:

R_f = 0.48 (EtOAc/hexane 1:9), Yield: 95%, Pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.42 (m, 2H), 7.31–7.27 (m, 3H), 3.12–3.09 (d, J = 9.0 Hz, 1H), 2.63–2.42 (m, 2H), 2.38–2.41 (m, 2H), 1.78–1.55 (m, 9H), 1.45–1.41 (m, 2H), 1.26–1.00 (m, 6H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 131.69, 128.16, 127.58, 123.81, 87.69, 86.15, 64.47, 50.78, 39.65, 31.27, 30.61, 26.78, 26.26, 26.09, 24.58; IR (KBr, thin film, cm^{-1}): 3055, 2928, 2852, 2750, 1598, 1489, 1443, 1318, 1156, 1103, 890, 755, 691; LRMS-EI (m/z): 280 (0.3), 200 (1), 199 (14), 198 (100), 167 (0.5), 115 (13), 83 (1); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{27}\text{N}$, 281.2143; found 281.2140.



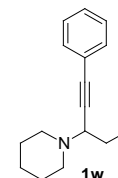
1-(4,4-dimethyl-1-phenylpent-1-yn-3-yl)piperidine 1v.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 97%, pale yellow oil; ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.46–7.42 (m, 2H), 7.30–7.27 (m, 3H), 3.07 (s, 1H), 2.75–2.68 (m, 2H), 2.49–2.44 (m, 2H), 1.60–1.55 (m, 4H), 1.43–1.38 (m, 2H), 1.02 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 159.08, 132.91, 116.16, 113.78, 86.79, 85.24, 68.53, 55.22, 54.19, 36.90, 27.20, 26.80, 24.43; IR (KBr, thin film, cm^{-1}): 2928, 2846, 2802, 2741, 1489, 1314, 1283, 1152, 1086, 990, 831, 751, 685; LRMS-EI (m/z): 254 (0.1), 200 (1), 199 (19), 198 (100), 156 (1), 115 (20), 91 (1); HRMS-EI (m/z): M^+ calcd for $\text{C}_{18}\text{H}_{25}\text{N}$, 255.1987; found 255.1980.



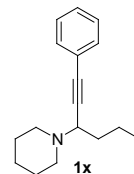
1-(1-ethyl-3-phenyl-prop-2-ynyl)-piperidine 1w.

R_f = 0.44 (EtOAc/hexane 1:9), Yield: 96%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.44–7.42 (m, 2H), 7.29–7.25 (m, 3H), 3.42–3.36 (dd, J_1 = 6.8 Hz, J_2 = 7.6 Hz, 1H), 2.70–2.64 (m, 2H), 2.51–2.43 (m, 2H), 1.78–1.47 (m, 8H), 1.08–1.03 (t, J = 6.8 Hz, 3H);

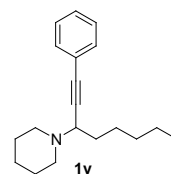


^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 131.64, 127.72, 123.57, 123.51, 87.81, 85.75, 60.31, 50.53, 26.51, 26.07, 24.55, 11.44; IR (KBr, thin film, cm^{-1}): 3043, 2925, 2851, 2796, 1596, 1486, 1440, 1325, 1116, 990, 754, 688; LRMS-EI (m/z): 226 (0.6), 199 (28), 198 (100), 166 (1), 141 (3), 128 (10), 115 (27), 91 (2); HRMS-EI (m/z): M^+ calcd for $\text{C}_{16}\text{H}_{21}\text{N}$, 227.1674; found 227.1667.

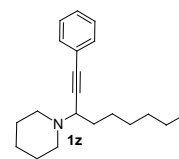
1-(1-phenylhex-1-yn-3-yl)piperidine 1x. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 95%, Pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.42 (m, 2H), 7.29–7.27 (m, 3H), 3.52–3.47 (dd, $J_1 = 10.2$ Hz, $J_2 = 9.0$ Hz, 1H), 3.71–2.65 (m, 2H), 2.52–2.45 (m, 2H), 1.72–1.52 (m, 10H), 0.98–0.93 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 131.56, 128.03, 127.56, 123.45, 87.90, 85.57, 58.14, 50.37, 35.42, 26.02, 24.45, 19.99, 13.75; IR (KBr, thin film, cm^{-1}): 3049, 2934, 2857, 2686, 1684, 1596, 1489, 1322, 1155, 1116, 1028, 905, 861, 751, 691; LRMS-EI (m/z): 241 (0.2), 221 (0.3), 199 (20), 198 (100), 169 (0.3), 128 (3), 115 (18), 91 (1); HRMS-EI (m/z): M^+ calcd for $\text{C}_{17}\text{H}_{23}\text{N}$, 241.1830; found 241.1827.



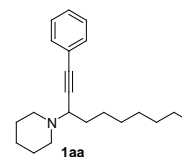
1-(1-phenyloct-1-yn-3-yl)piperidine 1y. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield 97%; brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.41 (m, 2H), 7.31–7.27 (m, 3H), 3.49–3.44 (dd, $J_1 = 9.2$ Hz, $J_2 = 8.8$ Hz, 1H), 2.70–2.66 (m, 2H), 2.65–2.48 (m, 2H), 1.73–1.42 (m, 8H), 1.34–1.30 (m, 6H), 0.91–0.87 (t, $J = 7.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3 , ppm, δ): 131.61, 128.12, 127.65, 123.50, 88.05, 85.51, 58.54, 50.53, 33.28, 31.48, 26.49, 26.02, 24.41, 22.53, 13.95; IR (KBr, thin film, cm^{-1}): 3060, 2923, 2857, 2747, 1761, 1687, 1598, 1443, 1322, 1094, 751, 688; LRMS-EI (m/z): 269 (0.3), 268 (0.4), 240 (0.6), 199 (21), 198 (100), 178 (0.8), 128 (3), 115 (16), 91 (2); HRMS-EI (m/z): M^+ calcd for $\text{C}_{19}\text{H}_{27}\text{N}$, 269.2143; found 269.2134.



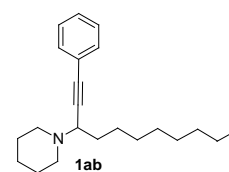
1-(1-phenylnon-1-yn-3-yl)piperidine 1z. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield 96%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.41 (m, 2H), 7.30–7.27 (m, 3H), 3.50–3.47 (dd, $J_1 = 9.0$ Hz, $J_2 = 8.6$ Hz, 1H), 2.72–2.65 (m, 2H), 2.52–2.46 (m, 2H), 1.73–1.60 (m, 10H), 1.36–1.30 (m, 6H), 0.90–0.86 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3 , ppm, δ): 131.56, 128.01, 127.56, 123.50, 87.97, 85.52, 58.48, 50.39, 33.32, 31.64, 28.96, 26.69, 26.05, 24.47, 22.49, 13.91; IR (KBr, thin film, cm^{-1}): 3054, 2938, 2864, 2796, 1593, 1486, 1440, 13.19, 1152, 1097, 861, 749, 685; LRMS-EI (m/z): 283 (0.1), 262 (0.5), 228 (5), 221 (16), 206 (1), 199 (15), 198 (100), 128 (3), 115 (13), 91 (3); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{29}\text{N}$, 283.2300; found 283.2295.



1-(1-phenylnon-1-yn-3-yl)piperidine 1aa. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield 97%, pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.42 (m, 2H), 7.30–7.27 (m, 3H), 3.50–3.45 (dd, $J_1 = 8.9$ Hz, $J_2 = 8.8$ Hz, 1H), 3.69–2.66 (m, 2H), 2.65–2.48 (m, 2H), 1.74–1.43 (m, 10H), 1.35–1.28 (m, 8H), 0.90–0.86 (t, $J = 6.7$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 131.53, 127.96, 127.51, 123.48, 87.93, 85.51, 58.43, 50.32, 33.28, 31.68, 29.23, 29.07, 26.71, 26.02, 24.45, 22.51, 13.93; IR (KBr, thin film, cm^{-1}): 3049, 2923, 2851, 2802, 1596, 1465, 1322, 1155, 1097, 754, 688; LRMS-EI (m/z): 297 (0.3), 276 (0.1), 228 (4), 221 (14), 206 (1), 199 (16), 198 (100), 178 (1), 115 (12), 84 (2); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{31}\text{N}$, 297.2457; found 297.2449.

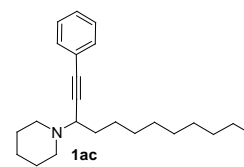


1-(1-phenylundec-1-yn-3-yl)piperidine 1ab. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 98%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.41 (m, 2H), 7.29–7.27 (m, 3H), 3.50–3.45 (dd, $J_1 = 9.1$ Hz, $J_2 = 8.3$ Hz, 1H), 2.72–2.66 (m, 2H), 2.64–2.48 (m, 2H), 1.73–1.54 (m, 10H), 1.35–1.24 (m, 10H), 0.90–0.85 (t, $J = 6.2$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 131.64, 128.08, 127.62, 123.59, 88.21, 85.60, 58.63, 50.45, 33.42, 31.82, 29.46, 29.38, 29.22, 26.88, 26.09, 24.53, 22.61,

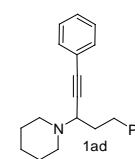


14.00; IR (KBr, thin film, cm^{-1}): 2923, 2851, 2890, 1593, 1462, 1322, 1097, 754, 688; LRMS-EI (m/z): 311 (0.2), 310 (0.3), 241 (6), 200 (1), 199 (14), 198 (100), 141 (1), 128 (2), 115 (9), 84 (1); HRMS-EI (m/z): M^+ calcd for $\text{C}_{22}\text{H}_{33}\text{N}$, 311.2613; found 311.2620.

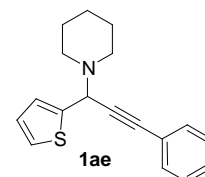
1-(1-phenyldodec-1-yn-3-yl)piperidine 1ac. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 96%, pale yellow oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.45–7.42 (m, 2H), 7.31–7.27 (m, 3H), 3.49–3.44, (dd, $J_1 = 9.3$ Hz, $J_2 = 8.7$ Hz, 1H), 2.70–2.67 (m, 2H), 1.66–1.50 (m, 2H), 1.71–1.43 (m, 8H), 1.29–1.23 (m, 14H), 0.89–0.85 (t, $J = 6.2$ Hz, 3H), ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 131.67, 128.10, 127.61, 123.55, 88.07, 85.57, 58.55, 50.10, 33.38, 31.85, 29.50, 29.35, 29.25, 26.11, 24.52, 22.64, 14.05; IR (KBr, thin film, cm^{-1}): 3049, 2928, 2791, 1684, 1593, 1486, 1462, 1316, 1155, 1097, 754, 688; LRMS-EI (m/z): 325 (0.4), 324 (0.5), 228 (2), 221 (7), 199 (26), 198 (100), 178 (0.7), 128 (3), 115 (13), 91 (3); HRMS-EI (m/z): M^+ calcd for $\text{C}_{23}\text{H}_{35}\text{N}$, 325.2770; found 325.2780



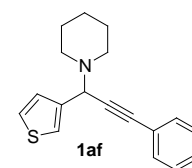
1-(1,5-diphenylpent-1-yn-3-yl)piperidine 1ad. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 97%, Brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.47–7.43 (m, 2H), 7.31–7.25 (m, 5H), 7.24–7.18 (m, 3H), 3.50–3.48 (dd, $J_1 = 8.0$ Hz, $J_2 = 7.6$ Hz, 1H), 2.87–2.67 (m, 4H), 2.51–2.47 (m, 2H), 2.08–2.03 (m, 2H), 1.65–1.63 (m, 4H), 1.47–1.44 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 141.47, 131.47, 128.34, 128.05, 127.95, 127.55, 125.56, 123.24, 87.47, 86.88, 57.25, 50.23, 34.78, 32.61, 25.96, 24.40, IR (KBr, thin film, cm^{-1}): 3021, 2923, 2851, 2802, 1696, 1489, 1454, 1322, 1152, 1100, 1031, 754, 691; LRMS-EI (m/z): 303 (0.9), 242 (0.1), 215 (0.5), 199 (20), 198 (100), 141 (1), 128 (3), 115 (15), 91 (9); HRMS-EI (m/z): M^+ calcd for $\text{C}_{22}\text{H}_{25}\text{N}$, 303.1987; found 303.1984.



1-(3-phenyl-1-(thiophen-2-yl)prop-2-yn-1-yl)piperidine 1ae. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 91%, pale yellow solid, mp: 75–77 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.27–7.23 (m, 3H), 7.22–7.17 (m, 5H), 6.97–6.94 (m, 1H), 4.98 (s, 1H), 2.52–2.48 (m, 4H), 1.59–1.51 (m, 4H), 1.40–1.36 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3 , ppm, δ): 143.94, 131.81, 128.25, 128.18, 126.15, 125.83, 125.34, 122.97, 86.85, 85.25, 58.18, 50.55, 26.09, 24.37; IR (KBr, thin film, cm^{-1}): 3060, 2928, 2802, 1593, 1485, 1437, 1316, 1275, 1155, 1094, 990, 951, 850, 760, 707; LRMS-EI (m/z): 281 (25), 204 (2), 198 (19), 197 (100), 165 (3), 152 (5), 115 (3), 97 (0.5), 84 (1); HRMS-EI (m/z): M^+ calcd for $\text{C}_{18}\text{H}_{19}\text{NS}$, 281.1238; found 281.1234.



1-(3-phenyl-1-(thiophen-3-yl)prop-2-yn-1-yl)piperidine 1af. $R_f = 0.44$ (EtOAc/hexane 1:9), Yield: 97%, brown oil. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.53–7.49 (m, 2H), 7.33–7.20 (m, 5H), 6.97–6.94 (m, 1H), 4.81 (s, 1H), 2.65–2.57 (m, 4H), 1.66–1.59 (m, 4H), 1.49–1.43 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 140.25, 131.72, 128.19, 128.01, 127.75, 125.23, 123.08, 86.56, 86.15, 58.21, 50.49, 26.11, 24.38; IR (KBr, thin film, cm^{-1}): 3058, 2846, 2802, 2741, 1593, 1489, 1440, 1314, 1283, 1152, 1086, 990, 909, 831, 751, 685; LRMS-EI (m/z): 281 (30), 238 (2), 204 (2), 198 (31), 197 (100), 165 (3), 152 (5), 115 (4), 84 (5); HRMS-EI (m/z): M^+ calcd for $\text{C}_{18}\text{H}_{19}\text{NS}$, 281.1238; found 281.1230.

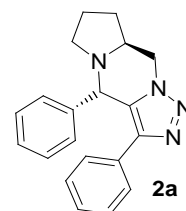


General experimental procedure for manganese(II) chloride catalyzed three component coupling followed by 1,3-dipolar cycloaddition.

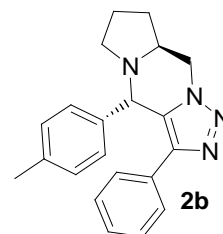
A mixture of aldehyde (1.0 mmol), (*S*)-azidomethylpyrrolidine (1.2 mmol), alkyne (1.5 mmol) and

MnCl₂ (10 mol%) in sealed tube was stirred without solvent for 12–14 h at 90 °C. The progress of reaction was monitored by TLC. After completion of reaction, the product was purified by column chromatography using *n*-hexane/EtOAc as eluent to give the desired product. The products were further identified by FT-IR, ¹H and ¹³C NMR spectroscopy, and HRMS, and all data were all in good agreement with assigned structures. The characterization data of all triazoles are as follows.

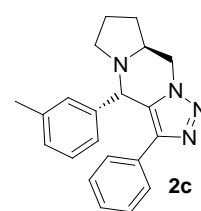
((4*S*,8*aS*)-3,4-diphenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2a. *R*_f = 0.31 (EtOAc/hexane 3:7), Yield: 84%. Diastereomeric ratio: >99, [α]²⁵_D –79.2° (*c* 1.0, CHCl₃), Brown solid, mp: 198–199 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.49–7.47 (d, *J* = 6.0 Hz, 2H), 7.32–7.30 (d, *J* = 6.0 Hz, 3H), 7.25–7.17 (m, 3H), 7.10–7.01 (m, 2H), 5.56 (s, 1H), 4.83–4.77 (m, 1H), 4.12–4.04 (t, *J* = 12.0 Hz, 1H), 3.25–3.22 (m, 1H), 2.96–2.92 (m, 1H), 2.38–2.25 (q, *J* = 9.0 Hz, 1H), 1.99–1.90 (m, 2H), 1.76–1.72 (m, 1H), 1.60–1.50 (m, 1H); ¹³C NMR (100 MHz, CDCl₃, ppm, δ): 141.92, 134.71, 130.83, 130.74, 129.23, 128.87, 128.33, 128.16, 127.9, 127.92, 127.41, 127.33, 126.20, 58.02, 51.67, 49.97, 48.63, 27.69, 21.92; IR (KBr, thin film, cm⁻¹): 3056, 3027, 2950, 2876, 2808, 1493, 1448, 1127, 1007, 722, 696; LRMS-EI (*m/z*): 317 (80), 287 (20), 277 (23), 191 (22), 138 (69), 106 (100), 65 (39); HRMS-EI (*m/z*) M⁺ calcd for C₂₀H₂₀N₄, 316.1688; found 316.1681.



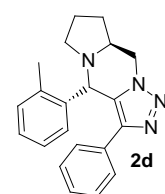
(4*S*,8*aS*)-3-phenyl-4-*p*-tolyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2b. *R*_f = 0.31 (EtOAc/hexane 3:7), Yield: 83%. Diastereomeric ratio: >99, [α]²⁵_D –78.3° (*c* 1.0, CHCl₃), Brown solid, mp: 121–122 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.51–7.49 (d, *J* = 6.0 Hz, 2H), 7.24–7.18 (m, 3H), 7.14–7.11 (m, 2H), 6.92–6.89 (d, *J* = 9.0 Hz, 2H), 5.53 (s, 1H), 4.83–4.77 (dd, *J*₁ = 6.0, *J*₂ = 12.0 Hz, 1H), 4.11–4.04 (t, *J* = 10.0 Hz, 1H), 3.27–3.17 (m, 1H), 2.97–2.91 (m, 1H), 2.41–2.35 (m, 1H), 2.31 (s, 3H), 2.04–1.89 (m, 2H), 1.64–1.56 (m, 2H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 141.91, 137.98, 131.70, 131.04, 130.98, 129.25, 129.08, 128.38, 127.34, 126.30, 57.84, 51.80, 50.04, 48.64, 27.79, 21.99, 21.05; IR (KBr, thin film, cm⁻¹): 3059, 2953, 285, 1607, 1449, 1358, 1161, 1007, 771, 696; LRMS-EI (*m/z*): 331 (70), 281 (38), 216 (40), 207 (45), 126 (100), 105 (24), 65 (15); HRMS-EI (*m/z*): M⁺ calcd for C₂₁H₂₂N₄, 330.1844; found 330.1848.



(4*S*,8*aS*)-3-phenyl-4-*m*-tolyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2c. *R*_f = 0.31 (EtOAc/hexane 3:7) Yield: 81%, Diastereomeric ratio: >99; [α]²⁵_D –75.2 °C (*c* 1.0, CHCl₃); Brown solid, mp: 218–219 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.50–7.47 (d, *J* = 9.0 Hz, 2H), 7.24–7.19 (m, 4H), 7.12–7.09 (d, *J* = 9.0 Hz, 1H), 6.85–6.79 (m, 2H), 5.52 (s, 1H), 4.83–4.77 (dd, *J*₁ = 6.0 Hz, *J*₂ = 12.0 Hz, 1H), 4.12–4.04 (t, *J* = 12.0 Hz, 1H), 3.29–3.20 (m, 1H), 2.96–2.90 (m, 1H), 2.43–2.34 (m, 1H), 2.30 (s, 3H), 2.04–1.88 (m, 2H), 1.65–1.56 (m, 2H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 141.93, 138.03, 130.92, 130.89, 129.72, 128.95, 128.32, 127.29, 126.49, 126.26, 58.02, 51.65, 50.02, 48.68, 27.77, 21.94, 21.40; IR (KBr, thin film, cm⁻¹): 3060, 2916, 2854, 1487, 1406, 1235, 1160, 1071, 1007, 800, 771, 692; LRMS-EI (*m/z*): 331 (79), 281 (29), 207 (29), 140 (38), 126 (93), 105 (100), 65 (26); HRMS-EI (*m/z*): M⁺ calcd for C₂₁H₂₂N₄, 330.1844; found 330.1849.



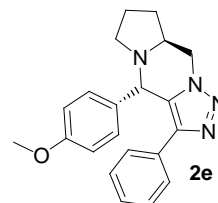
(4*S*,8*aS*)-3-phenyl-4-*o*-tolyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2d. *R*_f = 0.31 (EtOAc/hexane 3:7) Yield: 79%. Diastereomeric ratio: >99; [α]²⁵_D –73.4° (*c* 1.0, CHCl₃), Pale yellow gum. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.40–7.37 (d, *J* = 6.4 Hz, 2H), 7.25–7.15 (m, 5H), 7.04–6.99 (t, *J* = 7.8 Hz, 1H), 6.55–6.53 (d, *J* = 9.0 Hz, 1H), 5.72 (s, 1H), 4.73–4.68 (dd, *J*₁ = 6.0, *J*₂ = 12 Hz, 1H), 4.09–4.02 (t, *J* = 12 Hz, 1H), 3.46–3.42 (m, 1H), 2.92–2.89 (m, 1H), 2.63–2.58 (m,



1H), 2.55 (s, 3H), 2.02–1.83 (m, 2H), 1.68–1.59 (m, 2H); ¹³C NMR (100 MHz, CDCl₃, ppm, δ): 142.30, 136.97, 135.24, 131.01, 130.92, 130.42, 128.44, 128.29, 128.11, 127.40, 126.10, 125.93, 53.49, 49.89, 49.05, 48.29, 27.95, 21.75, 19.53; IR (KBr, thin film, cm⁻¹): 3059, 2953, 285, 1607, 1449, 1358, 1161, 1007, 771, 696; LRMS-EI (*m/z*): 331 (80), 281 (25), 207 (30), 140 (39), 126 (95), 105 (100), 65 (27); HRMS-EI (*m/z*): M⁺ calcd for C₂₁H₂₂N₄, 330.1844; found 330.1846.

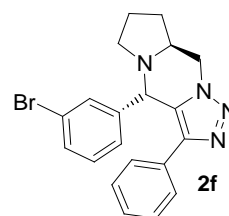
(4*S*,8*aS*)-4-(4-methoxyphenyl)-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2e.

*R*_f = 0.21 (EtOAc/hexane 3:7) Yield: 76%; Diastereomeric ratio: >99, [α]²⁵_D -73.6° (*c* 1.0, CHCl₃), Brown solid, mp: 204–205 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.50–7.48 (d, *J* = 6.0 Hz, 2H), 7.23–7.21 (m, 3H), 6.95–6.92 (m, 2H), 6.84–6.81 (m, 2H), 5.52 (s, 1H), 4.82–4.76 (dd, *J*₁ = 12.4 Hz, *J*₂ = 12 Hz, 1H), 4.09–4.02 (t, *J* = 12.0 Hz, 1H), 3.76 (s, 3H), 3.22–3.17 (m, 1H), 2.96–2.90 (m, 1H), 2.40–2.32 (q, *J* = 6.0 Hz, 1H), 1.75–1.71 (m, 2H), 1.64–1.59 (m, 2H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 159.31, 141.85, 131.14, 130.97, 130.51, 128.39, 127.35, 126.91, 126.30, 113.70, 57.48, 55.16, 51.81, 50.02, 48.60, 27.77, 21.99; IR (KBr, thin film, cm⁻¹): 2929, 2832, 1606, 1508, 1459, 1252, 1173, 1034, 807, 700; LRMS-EI (*m/z*): 347 (78), 317 (26), 281 (32), 221 (27), 207 (41), 140 (40), 126 (99), 105 (100), 65 (41); HRMS-EI (*m/z*): M⁺ calcd for C₂₁H₂₂N₄O, 346.1794; found 346.1797.



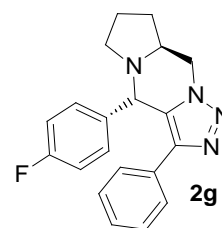
(4*S*,8*aS*)-4-(3-bromophenyl)-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2f.

*R*_f = 0.31 (EtOAc/hexane 3:7) Yield: 77%; Diastereomeric ratio: >99, [α]²⁵_D -74.4° (*c* 1.0, CHCl₃), Brown solid, mp: 206–207 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.50–7.41 (m, 3H), 7.30–7.17 (m, 5H), 6.95–6.92 (d, *J* = 9.0 Hz, 1H), 5.53 (s, 1H), 4.80–4.74 (dd, *J* = 12.0, 3.0 Hz, 1H), 4.12–4.04 (t, *J* = 12.0 Hz, 1H), 3.19–3.26 (m, 1H), 2.97–2.90 (m, 1H), 2.47–2.38 (m, 1H), 2.06–1.90 (m, 2H), 1.56 (m, 2H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 142.37, 137.54, 131.90, 131.47, 130.74, 129.98, 129.88, 128.55, 127.70, 127.64, 126.31, 122.86, 57.60, 51.29, 50.23, 48.86, 27.89, 22.04; IR (KBr, thin film, cm⁻¹): 3060, 2935, 2839, 1568, 1471, 1234, 1159, 1073, 1106, 791, 720; LRMS-EI (*m/z*): 395 (22), 341 (18), 325 (27), 227 (80), 207 (50), 166 (46), 126 (100), 105 (37), 95 (38), 65 (28); HRMS-EI (*m/z*): M⁺ calcd for C₂₀H₁₉BrN₄, 394.0793; found 394.0795.



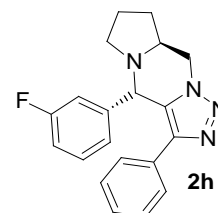
(4*S*,8*aS*)-4-(4-fluorophenyl)-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2g.

*R*_f = 0.31 (EtOAc/hexane 3:7) Yield: 79%. Diastereomeric ratio: >99, [α]²⁵_D -98.4° (*c* 1.0, CHCl₃), Brown solid, mp: 194–195 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.49–7.46 (d, *J* = 9.0 Hz, 2H), 7.24–7.21 (m, 3H), 7.19–6.98 (m, 4H), 5.56 (s, 1H), 4.80–4.74 (dd, *J*₁ = 11.4 Hz, *J*₂ = 12.0 Hz, 1H), 4.10–4.03 (t, *J* = 12.0 Hz, 1H), 3.21–3.14 (m, 1H), 2.96–2.89 (m, 1H), 2.41–2.33 (q, *J* = 6.0 Hz, 1H), 2.00–1.90 (m, 2H), 1.77–1.72 (m, 1H), 1.65–1.57 (m, 1H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 162.36 (d, *J* = 247 Hz), 142.05, 130.88 (d, *J* = 4.3 Hz), 130.78 (d, *J* = 4.3 Hz), 130.54, 128.44, 127.50, 126.23, 115.38 (d, *J* = 21.6 Hz), 57.33, 51.49, 50.07, 48.65, 27.78, 21.98; IR (KBr, thin film, cm⁻¹): 3054, 2950, 2806, 1611, 1588, 1441, 1239, 1133, 1006, 795, 694; LRMS-EI (*m/z*): 235 (46), 281 (36), 249 (40), 230 (88), 228 (100), 166 (40), 126 (98), 105 (61), 51 (69); HRMS-EI (*m/z*): M⁺ calcd for C₂₀H₁₉FN₄, 334.1594; found 334.1597.



(4*S*,8*aS*)-4-(3-fluorophenyl)-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2h.

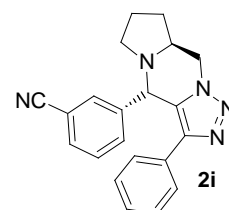
*R*_f = 0.31 (EtOAc/hexane 3:7) Yield: 77%; Diastereomeric ratio: >99, [α]²⁵_D -83.2° (*c* 1.0, CHCl₃). Brown solid, mp: 188–189 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.50–7.48 (d, *J* = 6.0 Hz, 2H),



7.33–7.18 (m, 4H), 7.21–7.00 (t, $J = 6.0$ Hz, 1H), 6.97–6.79 (t, $J = 6.0$ Hz, 2H), 5.56 (s, 1H), 4.80–4.74 (dd, $J_1 = 11.4$, $J_2 = 12.0$ Hz, 1H), 4.12–4.04 (t, $J = 12.0$ Hz, 1H), 3.26–3.23 (m, 1H), 2.95–2.94 (m, 1H), 2.44–2.41 (q, $J = 9.0$ Hz, 1H), 2.02–1.91 (m, 2H), 1.80–1.60 (m, 2H), ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 162.7, (d, $J = 246$ Hz), 142.27, 137.6 (d, $J = 23.76$ Hz), 130.3 (d, $J = 52.6$), 129.98, 128.46, 127.55, 126.25, 124.7 (d, $J = 2.9$ Hz), 116.0 (d, $J = 21.3$ Hz), 115.2 (d, $J = 21$ Hz), 57.64, 51.33, 50.24, 48.81, 27.85, 22.01 ; IR (KBr, thin film, cm^{-1}): 3054, 2950, 2806, 1611, 1588, 1441, 1239, 1133, 1006, 795, 694; LRMS-EI (m/z): 335 (51), 281 (31), 222 (25), 126 (100), 108 (30), 105 (70), 65 (22); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{19}\text{FN}_4$, 334.1594; found 334.1595.

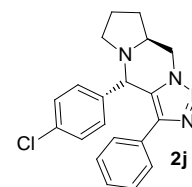
3-((4S,8aS)-3-phenyl-4,6,7,8,8a,9-hexahydropyrrolo[1,2-a][1,2,3]triazolo[1,5-d]pyrazin-4-yl)benzonitrile 2i.

$R_f = 0.21$ (EtOAc/hexane 3:7), Yield: 75%. Diastereomeric ratio: >99, $[\alpha]_D^{25} -73.2^\circ$ (c 1.0, CHCl_3), Brown solid, mp: 198–199 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.59–7.57 (d, $J = 6.0$ Hz, 1H), 7.48–7.45 (m, 2H), 7.42–7.39 (m, 2H), 7.29–7.20 (m, 4H), 5.62 (s, 1H), 4.78–4.72 (dd, $J = 15.0, 6.0$ Hz, 1H), 4.13–4.05 (t, $J = 12.0$ Hz, 1H), 3.24–3.14 (m, 1H), 2.98–2.91 (m, 1H), 2.47–2.41 (m, 1H), 2.07–1.92 (m, 2H), 1.69–1.56 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 142.54, 137.14, 133.00, 132.30, 130.50, 129.34, 129.09, 128.61, 127.80, 126.16, 118.27, 112.81, 57.37, 50.74, 50.36, 48.90, 27.85, 21.98; IR (KBr, thin film, cm^{-1}): 3054, 2954, 2834, 1606, 1496, 1448, 1234, 1157, 1007, 761, 695; LRMS-EI (m/z): 365 (100), 342 (23), 281 (20), 126 (45), 105 (30), 85 (20), 67 (48); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{19}\text{N}_5$, 341.1640; found 341.1636.



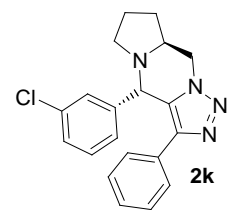
(4S,8aS)-4-(4-chlorophenyl)-3-phenyl-4,6,7,8,8a,9-hexahydropyrrolo[1,2-a][1,2,3]triazolo[1,5-d]pyrazine 2j.

$R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 82%; Distereomeric ratio: >99, $[\alpha]_D^{25} -79.2^\circ$ (c 1.0, CHCl_3). Pale yellow solid, mp: 189–190 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.49–7.48 (d, $J = 3.8$ Hz, 2H), 7.30–7.23 (m, 5H), 6.98–6.94 (m 2H), 5.56 (s, 1H), 4.80–4.73 (dd, $J_1 = 11.4$ Hz, $J_2 = 15.1$ Hz, 1H), 4.10–4.03 (t, $J = 15.0$ Hz, 1H), 3.21–3.15 (m, 1H), 2.92–2.90 (m, 1H) 2.42–2.35 (q, $J = 6.0$ Hz, 1H), 2.04–1.91 (m, 2H), 1.88–1.80 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 142.16 134.16, 133.55, 130.73, 130.35, 130.15, 128.63, 128.45, 128.05, 127.59, 126.24, 57.37, 51.38, 50.11, 48.73, 27.88, 22.06; IR(KBr, thin film, cm^{-1}): 3060, 2912, 2808, 1591, 1486, 1234, 1157, 1083, 1006, 801, 770, 691 ; LRMS-EI (m/z): 350 (0.8), 322 (39), 321 (100), 239 (16), 225 (18), 193 (35), 165 (16), 130 (22), 91 (22), 77 (12); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{19}\text{ClN}_4$, 350.1298; found 350.1300.



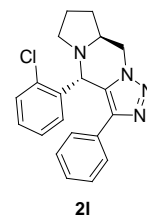
(4S,8aS)-4-(3-chlorophenyl)-3-phenyl-4,6,7,8,8a,9-hexahydropyrrolo[1,2-a][1,2,3]triazolo[1,5-d]pyrazine 2k.

$R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 79%; Distereomeric ratio: >99; $[\alpha]_D^{25} -74.2^\circ$ (c 1.0, CHCl_3); Pale yellow solid, mp: 193–194 °C. ^1H NMR (300 MHz, CDCl_3 , ppm, δ): 7.50–7.47 (m, 2H), 7.30–7.19 (m, 5H), 7.05 (s, 1H), 6.91–6.89 (d, $J = 6.0$ Hz, 1H), 5.54 (s, 1H), 4.81–4.74 (dd, $J_1 = 13.4$ Hz, $J_2 = 13.9$ Hz, 1H), 4.11–4.04 (t, $J = 12.0$ Hz, 1H), 3.23–3.21 (m, 1H), 2.43–2.41 (q, $J = 6.0$ Hz, 1H), (m, 1H), 2.04–1.97 (m, 2H), 1.80–1.62 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , ppm, δ): 142.25, 137.17, 134.54, 130.65, 129.87, 129.64, 128.94, 128.48, 127.52, 127.23, 126.52, 57.54, 51.25, 50.18, 48.76, 27.83, 21.97; IR(KBr, thin film, cm^{-1}): 3054, 2923, 2824, 1665, 1572, 1473, 1234, 1163, 1080, 1004, 770, 696; LRMS-EI (m/z): 350 (12), 323 (39), 321 (100), 225 (18), 193 (24), 192 (20), 138 (13), 130 (29), 125 (8), 91 (10); HRMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{19}\text{ClN}_4$, 350.1298; found 350.1293.

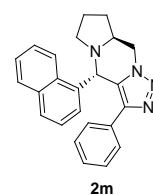


(4S,8aS)-4-(2-chlorophenyl)-3-phenyl-4,6,7,8,8a,9-hexahydropyrrolo[1,2-a][1,2,3]triazolo[1,5-d]

pyrazine 2l. $R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 76%. Distereomeric ratio: >99, $[\alpha]_D^{25} -72.2^\circ$ (c 1.0, CHCl_3), Pale yellow solid, mp: 187–188 °C. $^1\text{H NMR}$ (300 MHz, CDCl_3 , ppm, δ): 7.50–7.47 (m, 2H), 7.29–7.21 (m, 5H), 7.05 (s, 1H), 6.91–6.89 (d, $J = 6.0$ Hz, 1H), 5.54 (s, 1H), 4.81–4.75 (dd, $J = 11.0$ Hz, $J = 15.0$ Hz, 1H), 4.11–4.04 (t, $J = 9.0$ Hz, 1H), 3.25–3.21 (m, 1H), 2.94–2.91 (m, 1H), 2.43–2.40 (q, $J = 9.0$ Hz, 1H), 2.00–1.92 (m, 2H), 1.80–1.60 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3 , ppm, δ): 142.01, 135.08, 133.34, 130.07, 129.91, 129.62, 128.50, 127.61, 127.52, 126.85, 125.99, 54.00, 51.12, 50.36, 48.28, 27.59, 22.00; IR (KBr, thin film, cm^{-1}): 3060, 2912, 2857, 1588, 1487, 1234, 1160, 1083, 1001, 798, 688; H LRMS-EI (m/z): 350 (19), 321 (100), 287 (81), 239 (15), 225 (27), 193 (42), 165 (27), 130 (40), 91 (24); RMS-EI (m/z): M^+ calcd for $\text{C}_{20}\text{H}_{19}\text{ClN}_4$, 350.1298; found 350.1306.

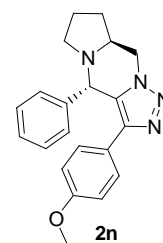


4*S*,8*aS*)-4-(naphthalen-1-yl)-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2m. $R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 81%. Distereomeric ratio: >99, $[\alpha]_D^{25} -62.2^\circ$ (c 1.0, CHCl_3), brown solid, mp: 116–117 °C. $^1\text{H NMR}$ (300 MHz, CDCl_3 , ppm, δ): 8.34–8.31 (d, $J = 9.0$ Hz, 1H), 7.94–7.91 (d, $J = 9.0$ Hz, 1H), 7.81–7.79 (d, $J = 6.0$ Hz, 1H), 7.67–7.55 (m, 3H), 7.42–7.39 (m, 2H), 7.29–7.09 (m, 1H), 7.09–7.07 (m, 2H), 6.76–6.73 (d, $J = 9.0$ Hz, 1H), 6.42 (s, 1H), 4.78–4.72 (dd, $J_1 = 12.0$ Hz, $J_2 = 15.0$ Hz, 1H), 4.72–4.13 (t, $J = 10.8$ Hz, 1H), 3.50–3.45 (m, 1H), 2.95–2.93 (m, 1H), 2.59–2.56 (q, $J = 6.0$ Hz, 1H), 1.94–1.61 (m, 4H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , ppm, δ): 142.38, 133.85, 132.71, 132.06, 130.84, 130.30, 129.12, 128.43, 127.91, 127.30, 126.68, 126.61, 124.85, 123.13, 53.22, 50.19, 49.31, 28.08, 22.01; IR (KBr, thin film, cm^{-1}): 3049, 2950, 2862, 1684, 1445, 1363, 1234, 1155, 1006, 776, 694; LRMS-EI (m/z): 366 (31), 337 (100), 268 (17), 239 (42), 208 (86), 180 (44), 115 (19), 91 (21); HRMS-EI (m/z): M^+ calcd for $\text{C}_{24}\text{H}_{22}\text{N}_4$ 366.1844; found 366.1850.

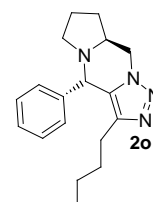


(4*S*,8*aS*)-3-(4-methoxyphenyl)-4-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2n.

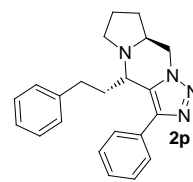
$R_f = 0.21$ (EtOAc/hexane 3:7), Yield: 83%. Distereomeric ratio: >99, $[\alpha]_D^{25} -74.2^\circ$ (c 1.0, CHCl_3), Pale yellow solid, mp: 207–208 °C. $^1\text{H NMR}$ (300 MHz, CDCl_3 , ppm, δ): 7.40–7.31 (m, 4H), 7.12 (s, 1H), 7.03–7.00 (d, $J = 9.0$ Hz, 2H), 6.77–6.75 (m, 2H), 5.52 (s, 1H), 4.80–4.75 (dd, $J_1 = 15.0$ Hz, $J_2 = 12.0$ Hz, 1H), 4.10–4.03 (t, $J = 12.0$ Hz, 1H), 3.74 (s, 3H), 3.25–3.21 (m, 1H), 2.97–2.94 (m, 1H), 2.38–2.31 (q, $J = 12.0$ Hz, 1H), 1.99–1.87 (m, 2H), 1.81–1.71 (m, 1H), 1.65–1.60 (m, 1H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , ppm, δ): 158.92, 141.91, 134.96, 129.94, 129.26, 128.35, 128.16, 127.56, 113.81, 58.04, 55.09, 51.64, 50.08, 48.67, 27.74, 21.97; IR (KBr, thin film, cm^{-1}): 3025, 2939, 2829, 1610, 1506, 1456, 1245, 1176, 1028, 836, 702, 606; LRMS-EI (m/z): 346 (4), 317 (100), 221 (8), 159 (16), 130 (7), 104 (12), 91 (8); HRMS-EI (m/z): M^+ calcd for $\text{C}_{21}\text{H}_{22}\text{N}_4\text{O}$, 346.1794; found 346.1786.



(4*S*,8*aS*)-3-butyl-4-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2o. Yield 74%. $R_f = 0.31$ (EtOAc/hexane 3:7), Diastereomeric ratio: >99, $[\alpha]_D^{25} -74.2^\circ$ (c 1.0, CHCl_3), Pale yellow gum. $^1\text{H NMR}$ (300 MHz, CDCl_3 , ppm, δ): 7.24–7.22 (m, 3H), 6.92–6.89 (m, 2H), 5.24 (s, 1H), 4.71–4.65 (dd, $J_1 = 6.0$ Hz, $J_2 = 15.0$ Hz, 1H), 3.86–3.94 (t, $J = 12.0$ Hz, 1H), 3.12–3.21 (m, 1H), 2.84–2.89 (m, 1H), 2.11–2.30 (m, 3H), 1.76–1.95 (m, 2H), 1.61–1.68 (m, 1H), 1.48–1.56 (m, 1H), 1.19–1.36 (m, 2H), 1.03–1.11 (m, 2H), 0.63–0.68 (t, $J = 9.0$ Hz, 3H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , ppm, δ): 143.15, 135.74, 130.95, 129.22, 128.26, 128.20, 57.44, 51.82, 51.14, 48.41, 30.44, 27.52, 24.40, 21.14, 22.01, 13.61; IR (KBr, thin film, cm^{-1}): 2955, 2871, 1453, 1228, 1157, 1080, 705; LRMS-EI (m/z): 297 (31), 138 (79), 126 (39), 105 (100), 65 (54); HRMS-EI (m/z): M^+ calcd for $\text{C}_{18}\text{H}_{24}\text{N}_4$, 296.2001; found 296.2007.

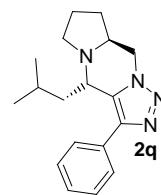


(4*S*,8*aS*)-4-phenethyl-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2p. $R_f = 0.31$ (EtOAc/hexane 3:7), Yield 77%. Diastereomeric ratio: >99, $[\alpha]^{25}_D -81.2^\circ$ (c 1.0, CHCl₃), Pale yellow solid, mp: 178–179 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.52–7.50 (m, 2H), 7.34–7.29 (m, 6H), 7.14–7.11 (m, 2H), 4.39–4.28 (m, 2H), 3.96–3.88 (t, $J = 9.0$ Hz, 1H), 3.76–3.69 (m, 1H), 3.13–3.07 (m, 1H), 2.83–2.69 (m, 3H), 2.25–2.18 (m, 1H), 2.09–2.03 (m, 1H), 1.89–1.87 (m, 2H), 1.58, (bs, 2H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 142.11, 141.04, 131.45, 130.93, 128.81, 128.64, 128.38, 127.45, 126.23, 126.09, 51.85, 50.11, 49.71, 44.81, 34.69, 32.43, 29.68, 28.49, 21.44; IR (KBr, thin film, cm⁻¹): 3024, 2923, 2823, 1604, 1495, 1428, 1345, 1130, 1006, 759, 709; LRMS-EI (m/z): 345 (39), 227 (25), 281 (36), 249 (25), 228 (66), 207 (40), 166 (38), 126 (100), 105 (94); HRMS-EI (m/z): M^+ calcd for C₂₂H₂₄N₄, 344.2001; found 344.2001.



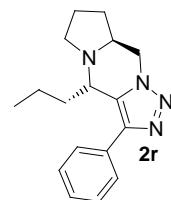
(4*S*,8*aS*)-4-isobutyl-3-phenyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2q.

$R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 76%. Brown gum, Diastereomeric ratio: 96:4, $[\alpha]^{25}_D -81.2^\circ$ (c 1.0, CHCl₃). ¹H NMR (CDCl₃, 300 MHz, ppm, δ): 7.69–7.67 (d, $J = 6.0$ Hz, 2H), 7.39–7.20 (m, 3H), 4.46–4.41 (m, 1H), 4.29–4.25 (m, 1H), 2.86–3.81 (t, $J = 9.0$ Hz, 1H), 3.45–3.20 (m, 1H), 3.10–3.02 (m, 1H), 2.70–2.62 (q, $J = 9.0$ Hz, 1H), 1.90–1.81 (m, 3H), 1.64–1.46 (m, 2H), 1.25–1.16 (m, 2H), 0.89–0.87 (d, $J = 6.0$ Hz, 3H), 0.78–0.75 (d, $J = 9.0$ Hz, 3H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 142.15, 131.68, 131.46, 128.59, 127.53, 126.49, 51.67, 49.81, 44.74, 42.44, 28.55, 24.87, 23.29, 21.37, 21.17; IR (KBr, thin film, cm⁻¹): 3054, 2950, 2862, 1687, 1443, 1336, 1259, 1138, 1006, 765, 696; LRMS-EI (m/z): 296 (0.2), 240 (17), 239 (100), 211 (6), 183 (4), 142 (38), 138 (12), 115 (6), 91 (19); HRMS-EI (m/z): M^+ calcd for C₁₈H₂₄N₄, 296.2001; found 296.1996



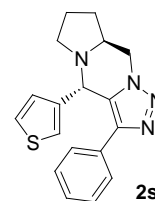
(4*S*,8*aS*)-3-phenyl-4-propyl-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine (2r).

$R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 75%. Pale yellow gum; Diastereomeric ratio: 94:6, $[\alpha]^{25}_D -69.4^\circ$ (c 1.0, CHCl₃). ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.74–7.71 (d, $J = 9.0$ Hz, 2H), 7.44–7.40 (t, $J = 6.0$ Hz, 2H), 7.27–7.32 (t, $J = 6.0$ Hz, 1H), 4.47–4.40 (m, 1H), 4.37–4.33 (dd, $J = 6.0, 9.0$ Hz, 1H), 3.95–3.87 (dd, $J_1 = 15, J_2 = 9.0$ Hz, 1H), 3.63–3.57 (m, 1H), 3.06–3.03 (m, 1H), 2.77–2.72 (q, $J = 6.0$ Hz, 1H), 2.21–2.16 (m, 1H), 1.96–1.92 (m, 3H), 1.69–1.64 (m, 1H), 1.52–1.38 (m, 3H), 0.86–0.82 (t, $J = 6.0$ Hz, 3H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 142.24, 131.81, 131.53, 128.68, 127.53, 53.35, 50.36, 49.89, 45.83, 35.30, 28.56, 21.60, 20.15, 13.61; IR (KBr, thin film, cm⁻¹): 3055, 2957, 2872, 2242, 1607, 149, 1237, 1141, 1008, 731; LRMS-EI (m/z): 283 (100), 239 (25), 138 (51), 106 (21), 67 (50); HRMS-EI (m/z): M^+ calcd for C₁₇H₂₂N₄, 282.1844; found 282.1840.



(4*R*,8*aS*)-3-phenyl-4-(thiophen-3-yl)-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine 2s.

$R_f = 0.31$ (EtOAc/hexane 3:7), Yield: 82%. Diastereomeric ratio >99, $[\alpha]^{25}_D -74.9^\circ$ (c 1.0, CHCl₃), Pale yellow solid, mp: 175–176 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.51–7.49 (d, $J = 6.0$ Hz, 2H), 7.48–7.21 (m, 4H), 6.88–6.85 (m, 2H), 5.65 (s, 1H), 4.80–4.75 (dd, $J_1 = 12.7$ Hz, $J_2 = 12.6$ Hz, 1H), 4.10–4.02 (t, $J = 10.5$ Hz, 1H), 3.23–3.21 (m, 1H), 2.97–2.95 (m, 1H), 2.50–2.47 (q, $J = 9.0$ Hz, 1H), 1.98–1.81 (m, 2H), 1.64–1.61 (m, 2H); ¹³C NMR (75 MHz, CDCl₃, ppm, δ): 141.65, 136.21, 131.13, 130.85, 128.33, 128.19, 127.33, 126.18, 125.90, 124.54, 53.28, 51.64, 50.67, 48.59, 27.70, 22.04; IR (KBr, thin film, cm⁻¹): 3060, 2972, 2846, 1607, 1448, 1226, 1157, 1001, 787, 691; LRMS-EI (m/z): 322 (22), 293 (100), 265 (13), 224 (11), 197 (29), 166 (18), 165 (57), 136 (16), 110 (26), 97 (2); HRMS-EI (m/z): M^+ calcd for C₁₈H₁₈N₄S, 322.1252; found 322.1250.



(4*R*,8*aS*)-3-phenyl-4-(thiophen-2-yl)-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine (2t).

$R_f = 0.31$ (EtOAc/Hexane 3:7), Yield: 78%. Distereomeric ratio >99, $[\alpha]_D^{25} -74.9^\circ$ (c 1.0, CHCl₃), brown solid, mp: 178–179 °C. ¹H NMR (300 MHz, CDCl₃, ppm, δ): 7.57–7.55 (m, 2H), 7.31–7.23 (m, 4H), 6.97–6.94 (m, 1H), 6.76–6.75 (d, $J = 3.8$ Hz, 1H), 5.82 (s, 1H), 4.79–4.73 (dd, $J_1 = 12.9$ Hz, $J_2 = 12.7$ Hz, 1H), 4.10–4.02 (t, $J = 12.0$ Hz, 1H), 3.39–3.37 (m, 1H) 2.96–2.92 (m, 1H), 2.62–2.53 (q, $J = 9.0$ Hz, 1H), 2.08–2.00 (m, 2H), 1.96–2.1.94 (m, 1H), 1.83–1.80 (m, 1H); ¹³C NMR (100 MHz, CDCl₃, ppm, δ): 142.22, 138.11, 130.96, 130.86, 128.53, 128.13, 127.66, 126.83, 126.50, 126.15, 53.44, 51.66, 50.97, 48.69, 28.10, 22.30; IR (KBr, thin film, cm⁻¹): 3054, 2934, 2851, 1610, 1492, 1355, 1220, 1080, 809, 760, 694; LRMS-EI (m/z): 322 (322 (13), 296 (71), 293 (84), 289 (96), 271 (37), 197 (24), 179 (12), 165 (100), 137 (15), 110 (30), 97 (20); HRMS-EI (m/z): M^+ calcd for C₁₈H₁₈N₄S, 322.1252; found 322.1257.

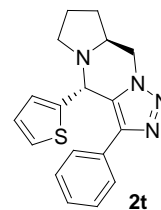


Figure 1. Crystal structure of (4*S*,8*aS*)-3-phenyl-4-(thien-3-yl)-4,6,7,8,8*a*,9-hexahydropyrrolo[1,2-*a*][1,2,3]triazolo[1,5-*d*]pyrazine (2s) (CCDC -956372)

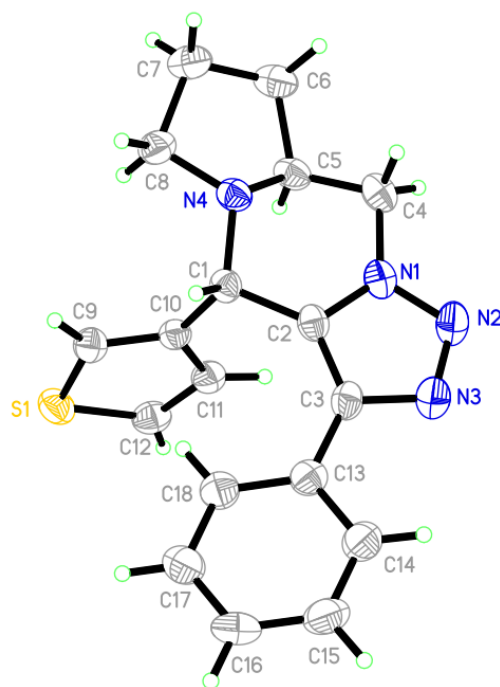


Fig. : The molecular structure of IC16202, thermal ellipsoids drawn at the 50% probability level.

Table 1. Crystal data and structure refinement for ic16202.

Identification code	ic16202
Empirical formula	C ₁₈ H ₁₈ N ₄ S
Formula weight	322.42
Temperature	150(2) K
Wavelength	0.71073 Å

Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 13.2080(2) Å $\alpha = 90^\circ$. b = 14.3890(2) Å $\beta = 90^\circ$. c = 16.8169(2) Å $\gamma = 90^\circ$.
Volume	3196.05(8) Å ³
Z	8
Density (calculated)	1.340 Mg/m ³
Absorption coefficient	0.207 mm ⁻¹
F(000)	1360
Crystal size	0.30 x 0.14 x 0.06 mm ³
Theta range for data collection	1.86 to 27.50°.
Index ranges	-16 ≤ h ≤ 17, -17 ≤ k ≤ 18, -20 ≤ l ≤ 21
Reflections collected	41328
Independent reflections	7320 [R(int) = 0.0652]
Completeness to theta = 27.50°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.990 and 0.932
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7320 / 0 / 416
Goodness-of-fit on F ²	1.023
Final R indices [I > 2σ(I)]	R1 = 0.0400, wR2 = 0.0905
R indices (all data)	R1 = 0.0718, wR2 = 0.1053
Absolute structure parameter	-0.01(7)
Largest diff. peak and hole	0.233 and -0.269 e.Å ⁻³

Table 2. A tomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² × 10³) for ic16202. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7668(1)	11443(1)	1979(1)	39(1)
N(1)	6118(2)	7662(1)	1288(1)	33(1)
N(2)	5427(2)	7186(1)	1712(1)	41(1)
N(3)	5633(2)	7331(1)	2469(1)	40(1)
N(4)	7695(1)	8473(1)	569(1)	31(1)
C(1)	7591(2)	8720(1)	1409(1)	28(1)
C(2)	6782(2)	8112(1)	1764(1)	29(1)
C(3)	6466(2)	7895(1)	2531(2)	32(1)

C(4)	6159(2)	7611(2)	420(1)	37(1)
C(5)	6736(2)	8445(2)	123(1)	33(1)
C(6)	7082(2)	8373(2)	-747(1)	44(1)
C(7)	8188(2)	8702(2)	-760(1)	44(1)
C(8)	8411(2)	9019(2)	96(1)	38(1)
C(9)	8135(2)	10384(2)	1705(1)	32(1)
C(10)	7380(2)	9745(1)	1594(1)	28(1)
C(11)	6406(2)	10144(2)	1728(1)	32(1)
C(12)	6450(2)	11061(2)	1940(1)	36(1)
C(13)	6870(2)	8134(2)	3315(1)	33(1)
C(14)	6552(2)	7635(2)	3984(2)	41(1)
C(15)	6959(2)	7822(2)	4728(2)	47(1)
C(16)	7669(2)	8513(2)	4825(1)	45(1)
C(17)	7975(2)	9022(2)	4171(2)	43(1)
C(18)	7590(2)	8833(2)	3421(1)	39(1)
S(2)	6180(1)	4882(1)	2218(1)	47(1)
S(2')	6646(1)	3794(1)	2211(1)	52(1)
N(5)	9563(1)	6846(1)	2890(1)	33(1)
N(6)	9756(2)	7586(1)	2421(1)	37(1)
N(7)	9687(1)	7294(1)	1678(1)	36(1)
N(8)	9281(1)	5254(1)	3710(1)	30(1)
C(19)	9099(2)	5162(2)	2848(1)	30(1)
C(20)	9379(2)	6070(1)	2458(1)	30(1)
C(21)	9450(2)	6365(2)	1678(1)	31(1)
C(22)	9526(2)	6914(2)	3758(1)	39(1)
C(23)	8893(2)	6113(2)	4063(1)	34(1)
C(24)	9015(2)	5937(2)	4957(2)	49(1)
C(25)	8916(2)	4885(2)	5050(2)	44(1)
C(26)	8900(2)	4491(2)	4204(1)	35(1)
C(27)	7226(2)	5441(2)	2455(1)	34(1)
C(28)	8049(2)	4860(1)	2597(1)	29(1)
C(29)	7780(2)	3929(2)	2487(2)	43(1)
C(30)	6646(1)	3794(1)	2211(1)	52(1)
C(30')	6180(1)	4882(1)	2218(1)	47(1)
C(31)	9297(2)	5859(2)	930(1)	32(1)
C(32)	9494(2)	4912(2)	861(2)	40(1)
C(33)	9376(2)	4463(2)	139(2)	44(1)
C(34)	9055(2)	4939(2)	-525(2)	44(1)

C(35)	8840(2)	5877(2)	-462(2)	43(1)
C(36)	8952(2)	6334(2)	256(1)	37(1)

Table 3. Bond

lengths [Å] and angles [°] for ic16202.

S(1)-C(12)	1.702(2)
S(1)-C(9)	1.706(2)
N(1)-N(2)	1.346(3)
N(1)-C(2)	1.352(3)
N(1)-C(4)	1.462(3)
N(2)-N(3)	1.318(3)
N(3)-C(3)	1.372(3)
N(4)-C(1)	1.463(3)
N(4)-C(8)	1.464(3)
N(4)-C(5)	1.472(3)
C(1)-C(2)	1.505(3)
C(1)-C(10)	1.534(3)
C(2)-C(3)	1.391(3)
C(3)-C(13)	1.463(3)
C(4)-C(5)	1.507(3)
C(5)-C(6)	1.538(3)
C(6)-C(7)	1.536(4)
C(7)-C(8)	1.538(3)
C(9)-C(10)	1.370(3)
C(10)-C(11)	1.426(3)
C(11)-C(12)	1.367(3)
C(13)-C(18)	1.395(3)
C(13)-C(14)	1.399(3)
C(14)-C(15)	1.387(4)
C(15)-C(16)	1.376(4)
C(16)-C(17)	1.381(4)
C(17)-C(18)	1.387(3)
S(2)-C(27)	1.647(3)
S(2')-C(29)	1.581(3)
N(5)-N(6)	1.350(3)
N(5)-C(20)	1.355(3)
N(5)-C(22)	1.464(3)
N(6)-N(7)	1.322(3)

N(7)-C(21)	1.373(3)
N(8)-C(23)	1.464(3)
N(8)-C(26)	1.466(3)
N(8)-C(19)	1.474(3)
C(19)-C(20)	1.507(3)
C(19)-C(28)	1.515(3)
C(20)-C(21)	1.382(3)
C(21)-C(31)	1.468(3)
C(22)-C(23)	1.514(3)
C(23)-C(24)	1.534(3)
C(24)-C(25)	1.528(3)
C(25)-C(26)	1.532(3)
C(27)-C(28)	1.391(3)
C(28)-C(29)	1.398(3)
C(31)-C(32)	1.393(3)
C(31)-C(36)	1.400(3)
C(32)-C(33)	1.383(3)
C(33)-C(34)	1.378(4)
C(34)-C(35)	1.383(4)
C(35)-C(36)	1.381(3)

C(12)-S(1)-C(9)	92.47(11)
N(2)-N(1)-C(2)	111.68(19)
N(2)-N(1)-C(4)	121.88(19)
C(2)-N(1)-C(4)	126.3(2)
N(3)-N(2)-N(1)	106.91(19)
N(2)-N(3)-C(3)	109.49(19)
C(1)-N(4)-C(8)	117.08(17)
C(1)-N(4)-C(5)	114.70(17)
C(8)-N(4)-C(5)	107.10(18)
N(4)-C(1)-C(2)	107.97(17)
N(4)-C(1)-C(10)	116.51(17)
C(2)-C(1)-C(10)	110.47(18)
N(1)-C(2)-C(3)	104.38(19)
N(1)-C(2)-C(1)	120.3(2)
C(3)-C(2)-C(1)	135.3(2)
N(3)-C(3)-C(2)	107.5(2)
N(3)-C(3)-C(13)	120.0(2)

C(2)-C(3)-C(13)	132.4(2)
N(1)-C(4)-C(5)	107.99(18)
N(4)-C(5)-C(4)	106.80(18)
N(4)-C(5)-C(6)	103.38(18)
C(4)-C(5)-C(6)	114.3(2)
C(7)-C(6)-C(5)	105.96(19)
C(6)-C(7)-C(8)	105.06(19)
N(4)-C(8)-C(7)	103.09(19)
C(10)-C(9)-S(1)	111.87(18)
C(9)-C(10)-C(11)	111.44(19)
C(9)-C(10)-C(1)	122.8(2)
C(11)-C(10)-C(1)	125.66(19)
C(12)-C(11)-C(10)	113.0(2)
C(11)-C(12)-S(1)	111.19(18)
C(18)-C(13)-C(14)	118.1(2)
C(18)-C(13)-C(3)	122.2(2)
C(14)-C(13)-C(3)	119.7(2)
C(15)-C(14)-C(13)	120.6(2)
C(16)-C(15)-C(14)	120.7(2)
C(15)-C(16)-C(17)	119.2(2)
C(16)-C(17)-C(18)	120.8(2)
C(17)-C(18)-C(13)	120.5(2)
N(6)-N(5)-C(20)	111.78(19)
N(6)-N(5)-C(22)	122.44(18)
C(20)-N(5)-C(22)	125.74(19)
N(7)-N(6)-N(5)	106.78(18)
N(6)-N(7)-C(21)	108.99(19)
C(23)-N(8)-C(26)	106.41(17)
C(23)-N(8)-C(19)	114.67(17)
C(26)-N(8)-C(19)	115.71(18)
N(8)-C(19)-C(20)	108.08(17)
N(8)-C(19)-C(28)	116.68(18)
C(20)-C(19)-C(28)	110.61(18)
N(5)-C(20)-C(21)	104.08(19)
N(5)-C(20)-C(19)	121.65(19)
C(21)-C(20)-C(19)	134.1(2)
N(7)-C(21)-C(20)	108.4(2)
N(7)-C(21)-C(31)	121.0(2)

C(20)-C(21)-C(31)	130.7(2)
N(5)-C(22)-C(23)	107.74(18)
N(8)-C(23)-C(22)	108.19(19)
N(8)-C(23)-C(24)	102.81(19)
C(22)-C(23)-C(24)	113.6(2)
C(25)-C(24)-C(23)	104.8(2)
C(24)-C(25)-C(26)	105.8(2)
N(8)-C(26)-C(25)	104.17(19)
C(28)-C(27)-S(2)	113.75(17)
C(27)-C(28)-C(29)	110.8(2)
C(27)-C(28)-C(19)	126.20(19)
C(29)-C(28)-C(19)	123.0(2)
C(28)-C(29)-S(2')	113.38(19)
C(32)-C(31)-C(36)	118.1(2)
C(32)-C(31)-C(21)	122.1(2)
C(36)-C(31)-C(21)	119.8(2)
C(33)-C(32)-C(31)	120.6(2)
C(34)-C(33)-C(32)	120.9(2)
C(33)-C(34)-C(35)	119.0(2)
C(36)-C(35)-C(34)	120.7(2)
C(35)-C(36)-C(31)	120.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ic16202. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
S(1)	50(1)	30(1)	37(1)	-5(1)	-1(1)	-4(1)
N(1)	31(1)	31(1)	39(1)	0(1)	-5(1)	-3(1)
N(2)	36(1)	40(1)	49(1)	4(1)	-1(1)	-11(1)
N(3)	38(1)	37(1)	45(1)	3(1)	0(1)	-7(1)
N(4)	29(1)	34(1)	29(1)	-4(1)	-3(1)	2(1)
C(1)	24(1)	30(1)	30(1)	-1(1)	-2(1)	0(1)
C(2)	28(1)	23(1)	36(1)	0(1)	-3(1)	1(1)
C(3)	31(1)	25(1)	39(1)	3(1)	2(1)	-2(1)
C(4)	36(1)	35(1)	39(1)	-5(1)	-8(1)	-1(1)

C(5)	30(1)	37(1)	30(1)	-7(1)	-4(1)	5(1)
C(6)	47(2)	51(2)	33(1)	-10(1)	-1(1)	6(1)
C(7)	43(2)	54(2)	34(1)	-3(1)	5(1)	6(1)
C(8)	32(1)	48(1)	34(1)	-4(1)	6(1)	-1(1)
C(9)	33(1)	31(1)	33(1)	1(1)	0(1)	0(1)
C(10)	31(1)	28(1)	24(1)	0(1)	1(1)	-1(1)
C(11)	32(1)	32(1)	31(1)	0(1)	3(1)	2(1)
C(12)	39(1)	35(1)	34(1)	0(1)	6(1)	7(1)
C(13)	36(1)	28(1)	35(1)	0(1)	4(1)	4(1)
C(14)	45(2)	37(1)	42(2)	0(1)	8(1)	-1(1)
C(15)	58(2)	47(2)	35(2)	2(1)	14(1)	1(1)
C(16)	56(2)	50(2)	29(1)	-8(1)	4(1)	9(1)
C(17)	48(2)	44(1)	37(2)	-6(1)	-2(1)	-1(1)
C(18)	44(2)	40(1)	32(1)	3(1)	-1(1)	-3(1)
S(2)	47(1)	57(1)	37(1)	1(1)	2(1)	1(1)
S(2')	53(1)	48(1)	54(1)	-1(1)	-2(1)	-15(1)
N(5)	35(1)	28(1)	36(1)	2(1)	1(1)	-1(1)
N(6)	39(1)	31(1)	42(1)	3(1)	0(1)	0(1)
N(7)	33(1)	34(1)	41(1)	2(1)	0(1)	0(1)
N(8)	33(1)	30(1)	28(1)	-2(1)	0(1)	3(1)
C(19)	33(1)	28(1)	29(1)	-2(1)	1(1)	2(1)
C(20)	29(1)	28(1)	33(1)	-1(1)	1(1)	1(1)
C(21)	29(1)	29(1)	36(1)	3(1)	4(1)	2(1)
C(22)	48(2)	34(1)	34(1)	-6(1)	-3(1)	3(1)
C(23)	37(1)	37(1)	29(1)	-4(1)	3(1)	5(1)
C(24)	69(2)	45(2)	34(1)	-3(1)	1(1)	2(1)
C(25)	49(2)	49(2)	34(1)	2(1)	2(1)	7(1)
C(26)	36(1)	39(1)	31(1)	6(1)	1(1)	3(1)
C(27)	35(1)	35(1)	31(1)	1(1)	1(1)	1(1)
C(28)	33(1)	31(1)	24(1)	-1(1)	2(1)	-2(1)
C(29)	54(2)	32(1)	42(1)	-1(1)	-8(1)	0(1)
C(30)	53(1)	48(1)	54(1)	-1(1)	-2(1)	-15(1)
C(30')	47(1)	57(1)	37(1)	1(1)	2(1)	1(1)
C(31)	27(1)	38(1)	30(1)	3(1)	4(1)	0(1)
C(32)	46(2)	42(1)	33(1)	3(1)	3(1)	2(1)
C(33)	49(2)	43(1)	40(2)	-5(1)	2(1)	-2(1)
C(34)	39(2)	59(2)	34(1)	-3(1)	-1(1)	-8(1)
C(35)	36(1)	59(2)	34(1)	7(1)	-4(1)	-2(1)

C(36) 30(1) 42(1) 40(1) 5(1) 2(1) -1(1)

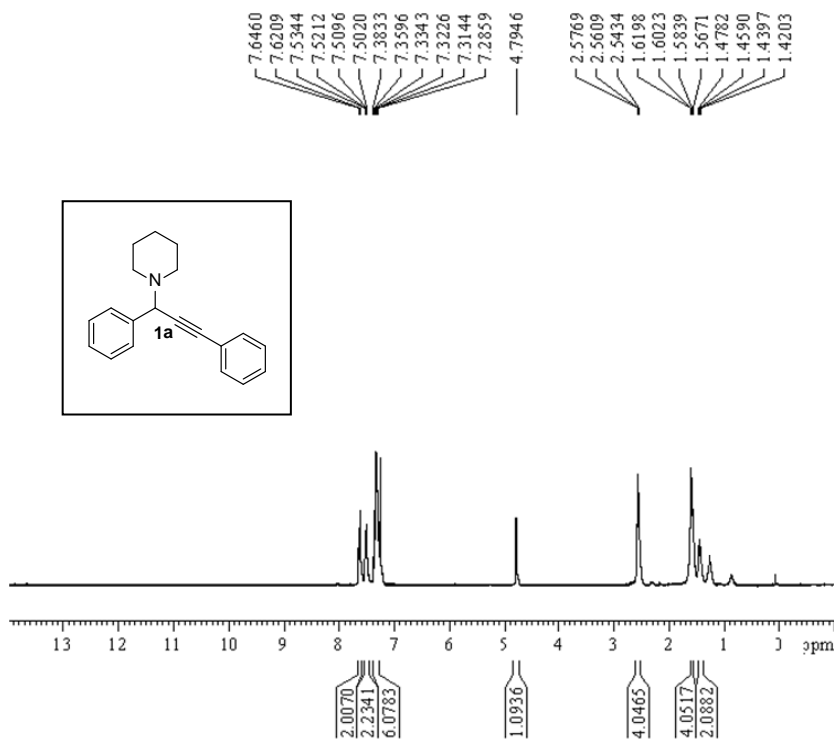
Table 5. H ydrogen

coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$)
for ic16202.

	x	y	z	U(eq)
H(1)	8243	8554	1676	33
H(4A)	5465	7610	197	44
H(4B)	6503	7032	253	44
H(5)	6339	9027	211	39
H(6A)	7031	7723	-937	52
H(6B)	6658	8772	-1092	52
H(7A)	8276	9224	-1138	52
H(7B)	8645	8189	-917	52
H(8A)	9118	8878	247	46
H(8B)	8288	9693	160	46
H(9)	8835	10254	1638	39
H(11)	5791	9807	1676	38
H(12)	5875	11435	2050	43
H(14)	6053	7164	3929	50
H(15)	6746	7470	5175	56
H(16)	7945	8639	5335	54
H(17)	8456	9507	4236	52
H(18)	7819	9181	2976	47
H(19)	9583	4683	2646	36
H(22A)	9220	7513	3919	46
H(22B)	10219	6880	3982	46
H(23)	8164	6204	3923	41
H(24A)	9685	6153	5145	59
H(24B)	8480	6263	5262	59
H(25A)	8283	4725	5334	53
H(25B)	9497	4631	5352	53
H(26A)	9343	3938	4160	42
H(26B)	8204	4316	4045	42
H(27)	7264	6099	2492	41

H(29)	8235	3427	2569	51
H(30)	6308	3233	2073	62
H(30')	5516	5106	2117	56
H(32)	9712	4571	1313	48
H(33)	9517	3817	102	53
H(34)	8983	4628	-1020	53
H(35)	8613	6210	-915	51
H(36)	8792	6976	292	44

^1H , ^{13}C , Spectra of propargyl amine [1a-1af]



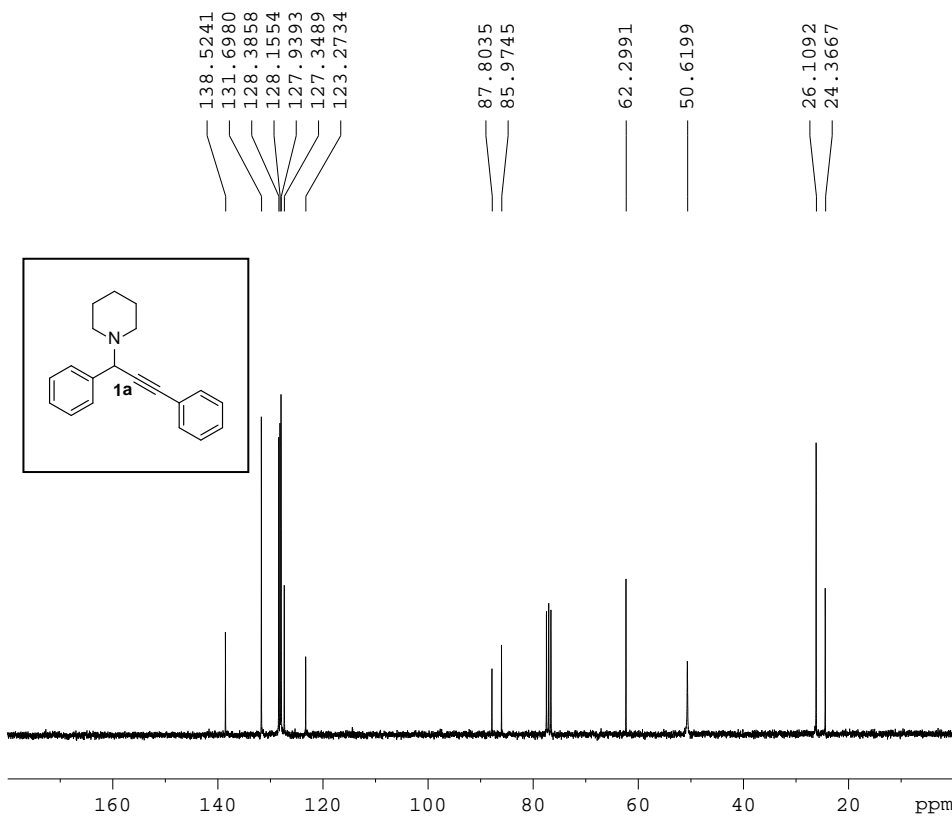
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PROCNO 1

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FIDRES 0.137219 Hz
AQ 3.6435515 sec
RG 1024
DW 111.260 usec
DE 6.50 usec
TE 299.2 K
D1 1.5000000 sec
MCREST 0.0000000 sec
MCWRK 0.01500000 sec

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F2 - Processing parameters
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SF 300.1300671 MHz
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SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
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F2P -1.014 ppm
F2 -364.45 Hz
PFMCM 0.74868 ppm/cm
HZCM 224.82013 Hz/cm



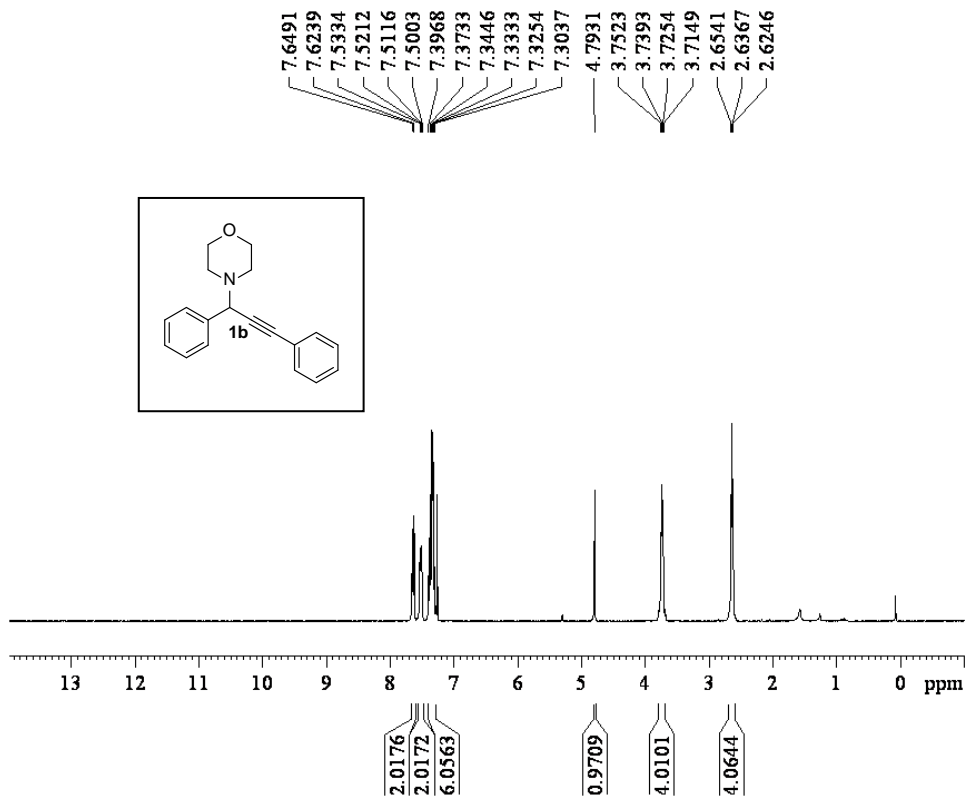
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RG 14596.5
DW 26.550 usec
DE 6.50 usec
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d11 0.03000000 sec
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MCWRK 0.01500000 sec

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NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
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F2 - Processing parameters
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SSB 0
LB 1.00 Hz
GB 0
PC 1.00



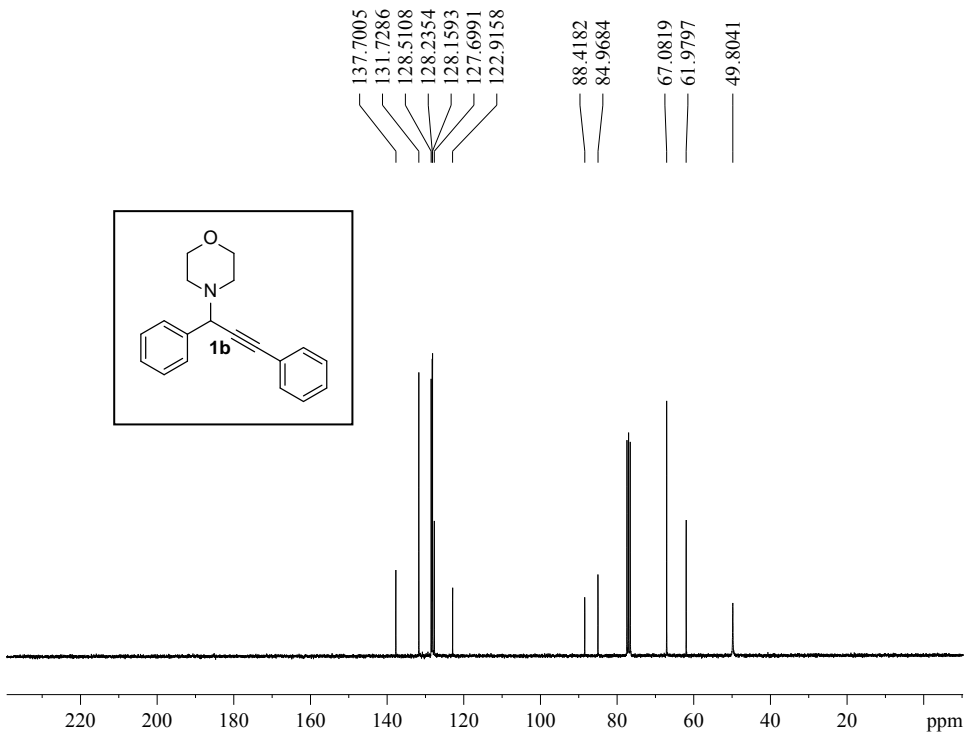
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 SOLVENT CDCl3
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 RG 1024
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 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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 PL1 0.00 dB
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ID NMR plot parameters
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 CY 0.00 cm
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 F2P -1.013 ppm
 F2 -303.90 Hz
 PPM CM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



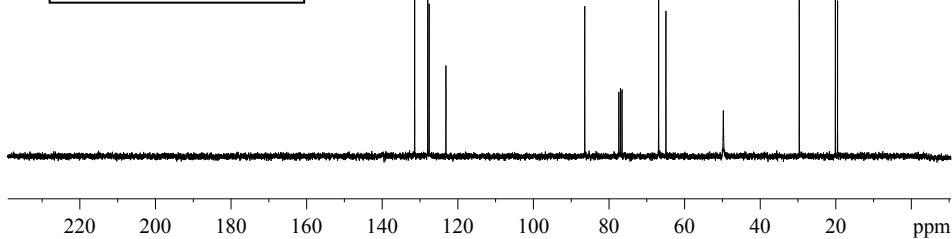
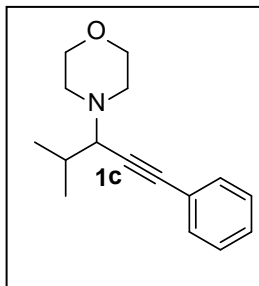
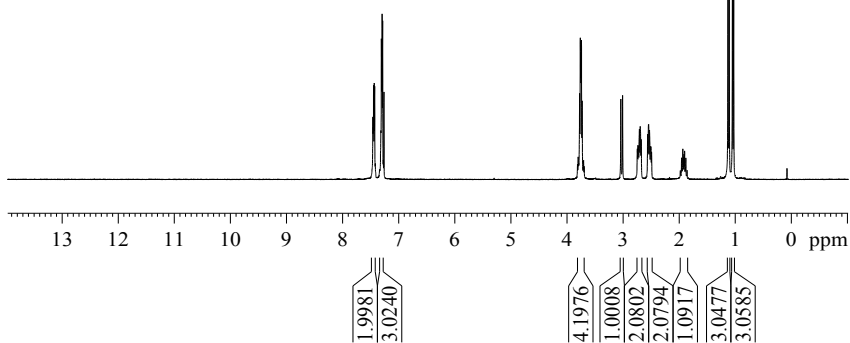
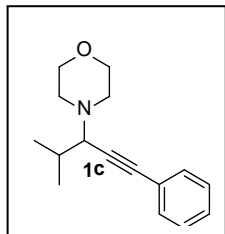
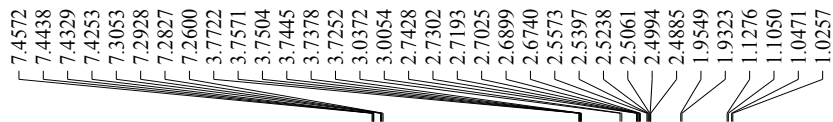
Current Data Parameters
 NAME SNA morpholine 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130519
 Time 19.30
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1855
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 A Q 1.7400308 sec
 RG 11585.2
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677500 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME SNA 44 proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130701
Time 17.35
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 322.5
DW 111.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 13.971 ppm
F1 4193.05 Hz
F2P -1.011 ppm
F2 -303.35 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm

Current Data Parameters
NAME SNA 44 13C
EXPNO 1
PROCNO 1

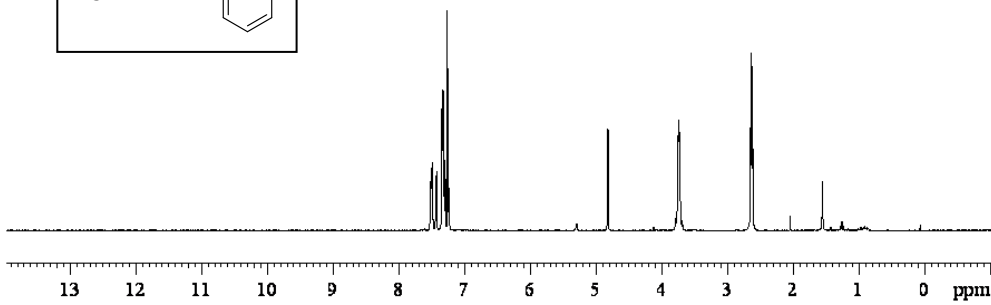
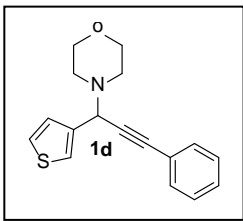
F2 - Acquisition Parameters
Date_ 20130701
Time 17.49
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 300.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

7.5186
7.5056
7.4995
7.4951
7.4855
7.4351
7.4307
7.4255
7.3476
7.3437
7.3326
7.3209
7.3100
7.3028
7.2932
7.2517
7.2475
7.2349
7.2306
4.8214
3.7619
3.7436
3.7297
3.7201
2.6489
2.6333
2.6185



2.0136
0.9952
4.1738
1.0163
0.9814
4.0188
4.0280

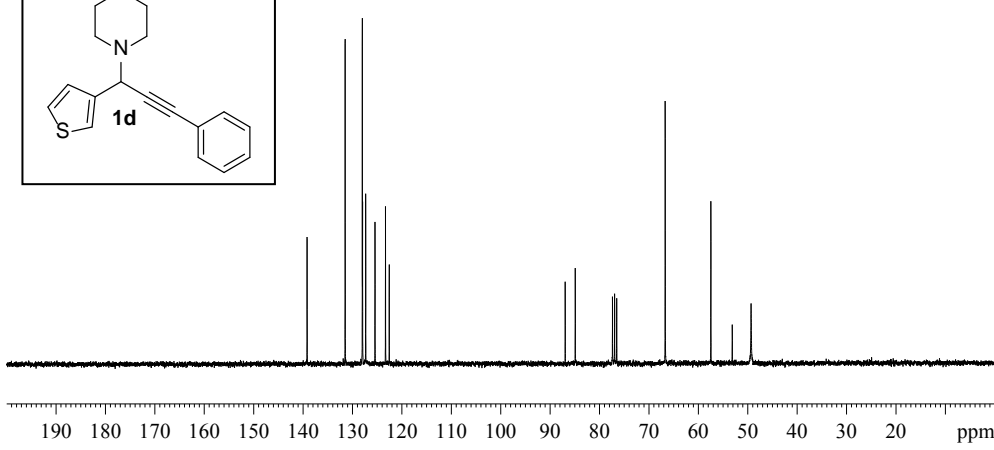
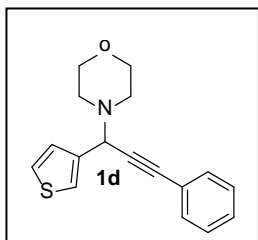
Current Data Parameters
NAME SNA 032 proton
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130621
Time 9.49
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 912.3
DW 111.200 usec
DE 6.50 usec
TE 300.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

139.2659
131.4967
128.0759
127.3801
125.4668
123.3796
122.5679
87.0267
84.9974
66.7920
57.5153
53.2248
49.3982



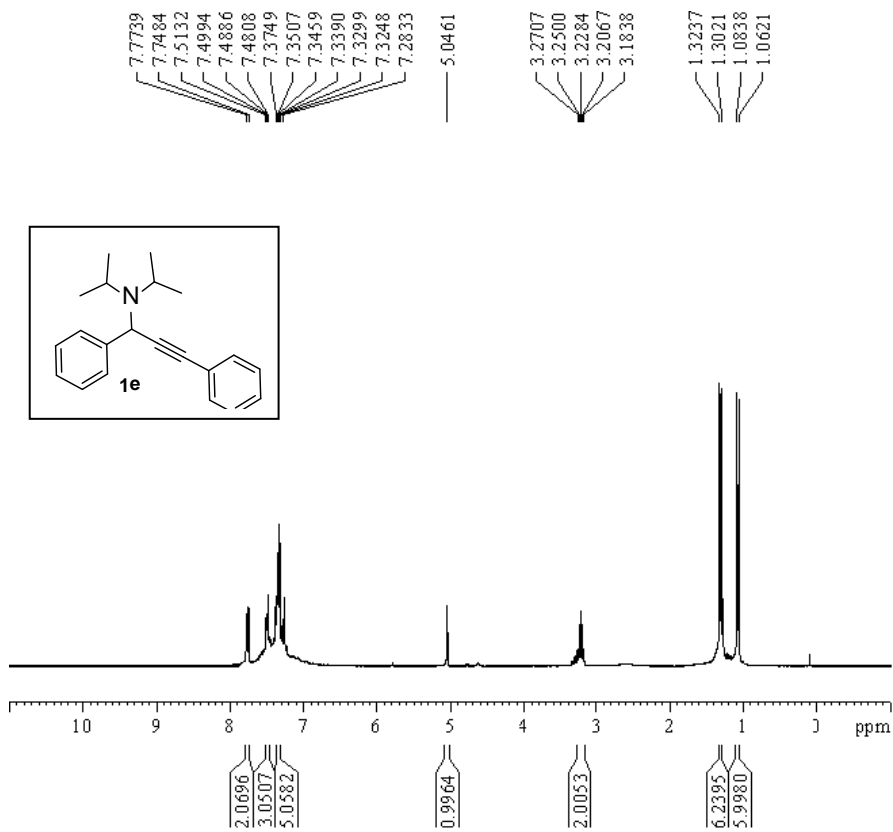
Current Data Parameters
NAME SNA 32 13c new
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130621
Time 10.32
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 10321.3
DW 26.550 usec
DE 6.50 usec
TE 300.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677752 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



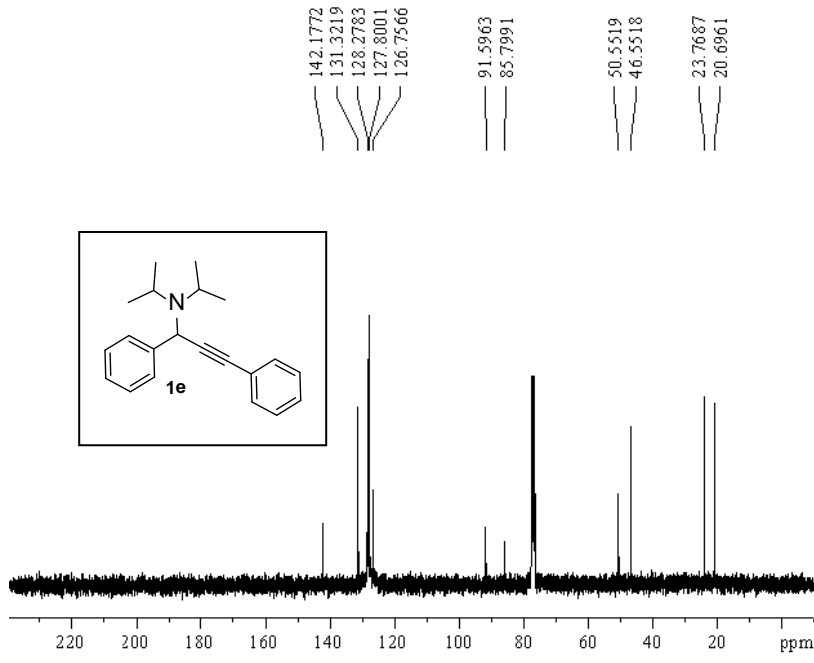
Current Data Parameters
 NAME shddiso t1f0
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131020
 Time 19.48
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 322.5
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 MCRE ST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SF O1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300052 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.974 ppm
 F1 4193.87 Hz
 F2P -1.008 ppm
 F2 -302.53 Hz
 PPM CM 0.74908 ppm/cm
 HZCM 2248.2013 Hz/cm



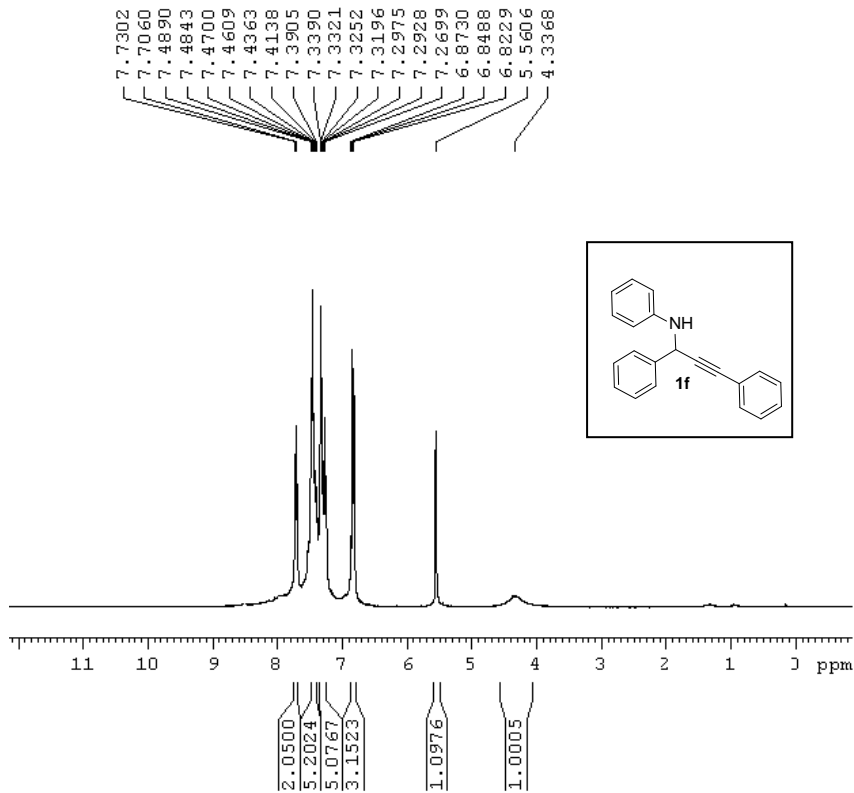
Current Data Parameters
 NAME SNA DIP 13C 4 agst
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20130805
 Time 9.56
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 12405
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCRE ST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SF O1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 walz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SF O2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677505 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



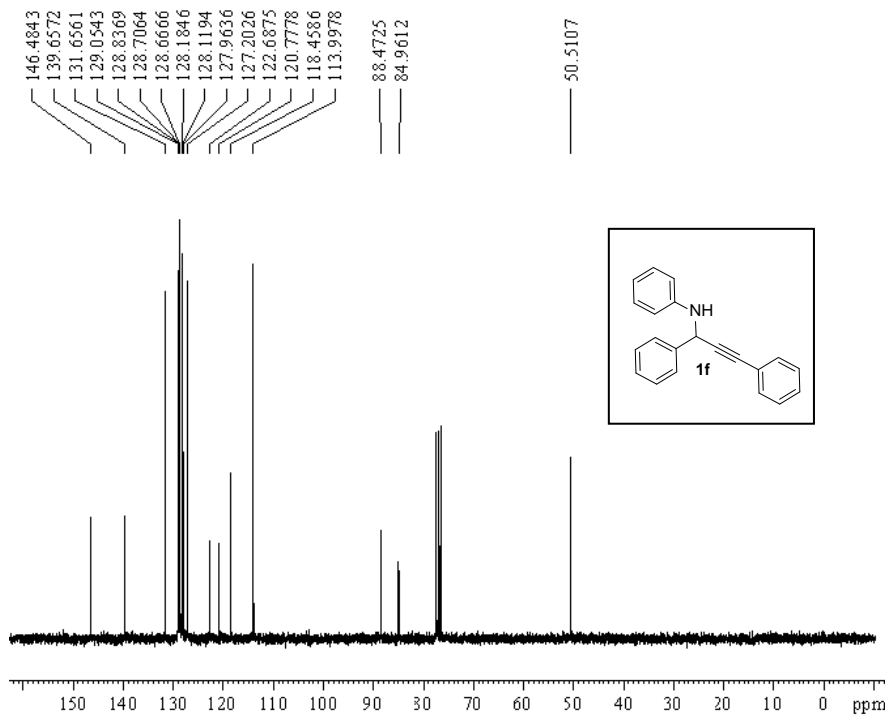
Current Data Parameters
 NAME sls aniline tafo
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131020
 Time 20.43
 INSTRUM spect
 PROBHD 5 mm Multima
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 181
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300054 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.973 ppm
 F1 4193.60 Hz
 F2 -1.009 ppm
 Fz -302.80 Hz
 DPMCM 0.7408 ppm/cm
 HZCM 22482013 Hz/cm



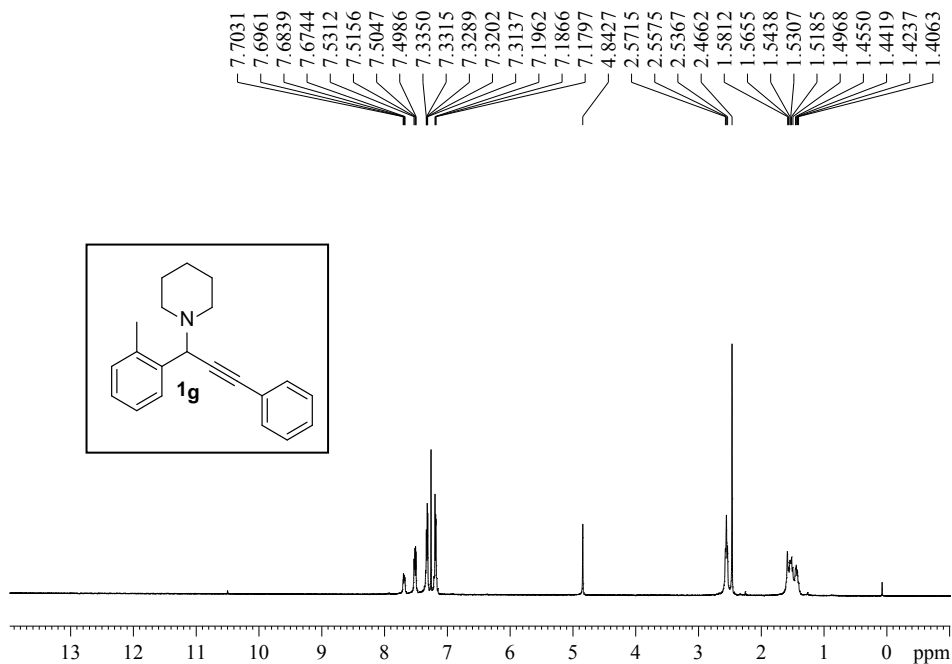
Current Data Parameters
 NAME SNA aniline 13C nev
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130621
 Time 10.55
 INSTRUM spect
 PROBHD 5 mm Multima
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313806 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677683 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

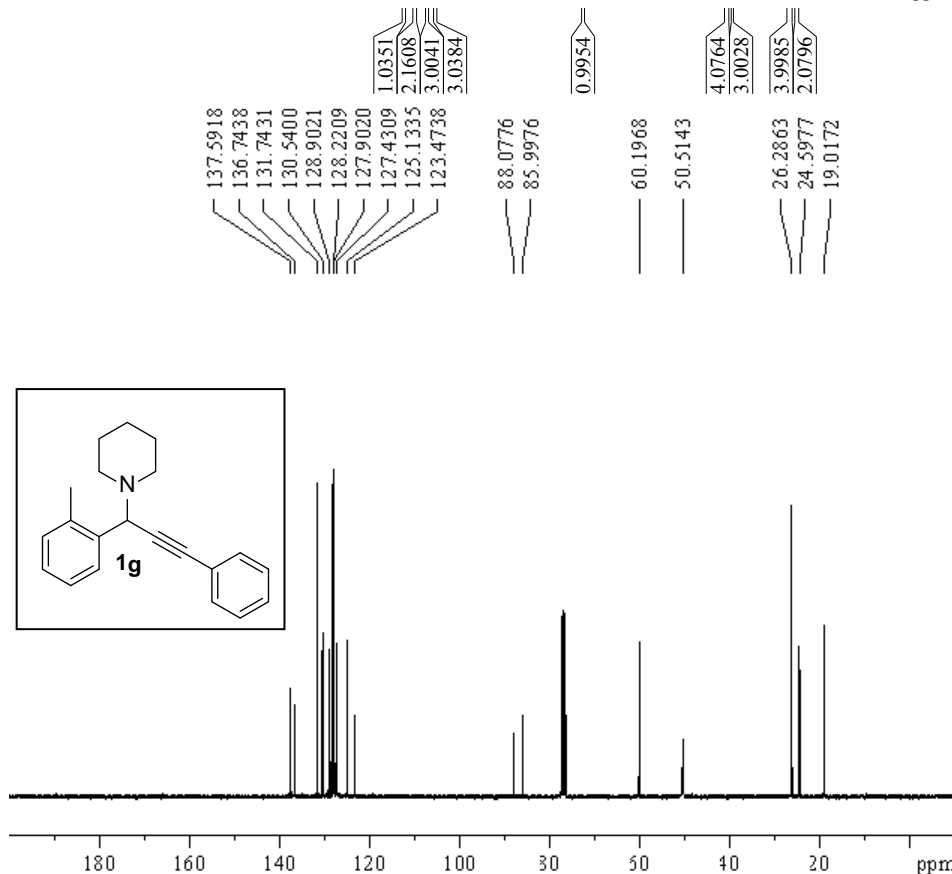


Current Data Parameters
 NAME SNA o toulaldehyde
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20130521
 Time 18.58
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 812.7
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 DI 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



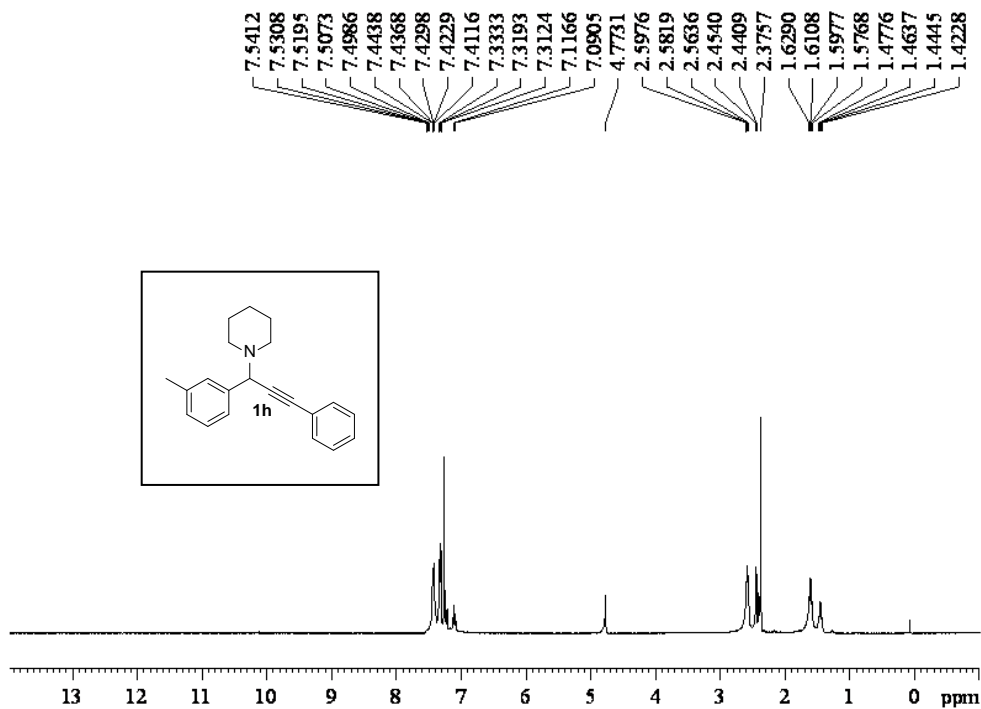
Current Data Parameters
 NAME SNA ortho ch3 EBC
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130519
 Time 17.44
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 3000
 DS 0
 SWH 18832.292 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.530 usec
 DE 6.50 usec
 TE 301.2 K
 DI 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.39999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763998 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313006 MHz

F2 - Processing parameters
 SI 32768
 SF 754677.923 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



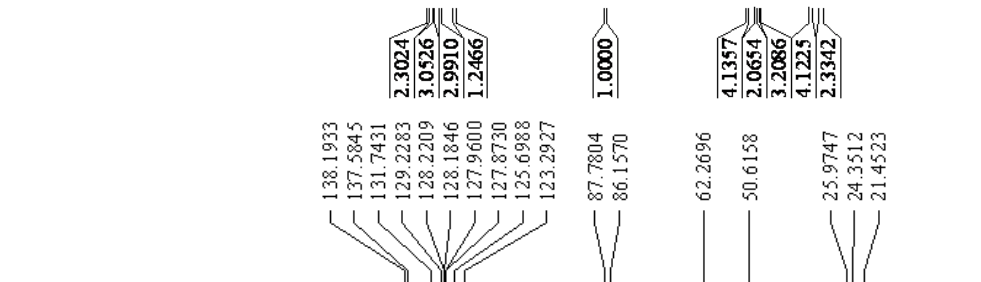
Current Data Parameters
 NAME SNA.m.ch3 new HSagst
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20130805
 Time 11.53
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 724.1
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16364
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.970 ppm
 F1 4192.77 Hz
 F2 -1.012 ppm
 F2 303.63 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



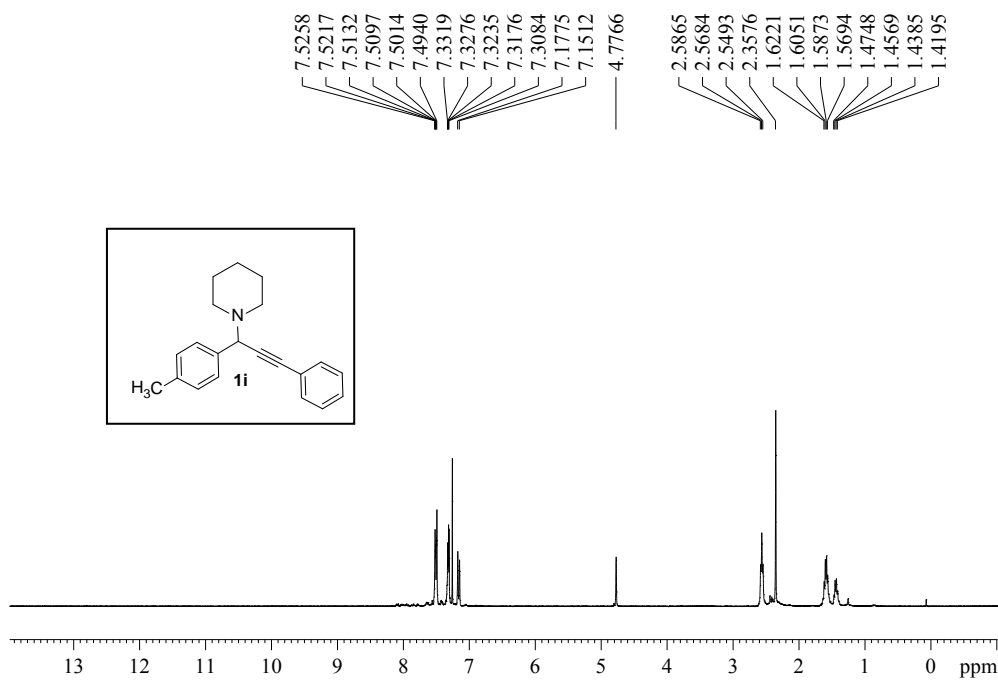
Current Data Parameters
 NAME SNA.meta CH3 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130519
 Time 23.32
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999999 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CFDP2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

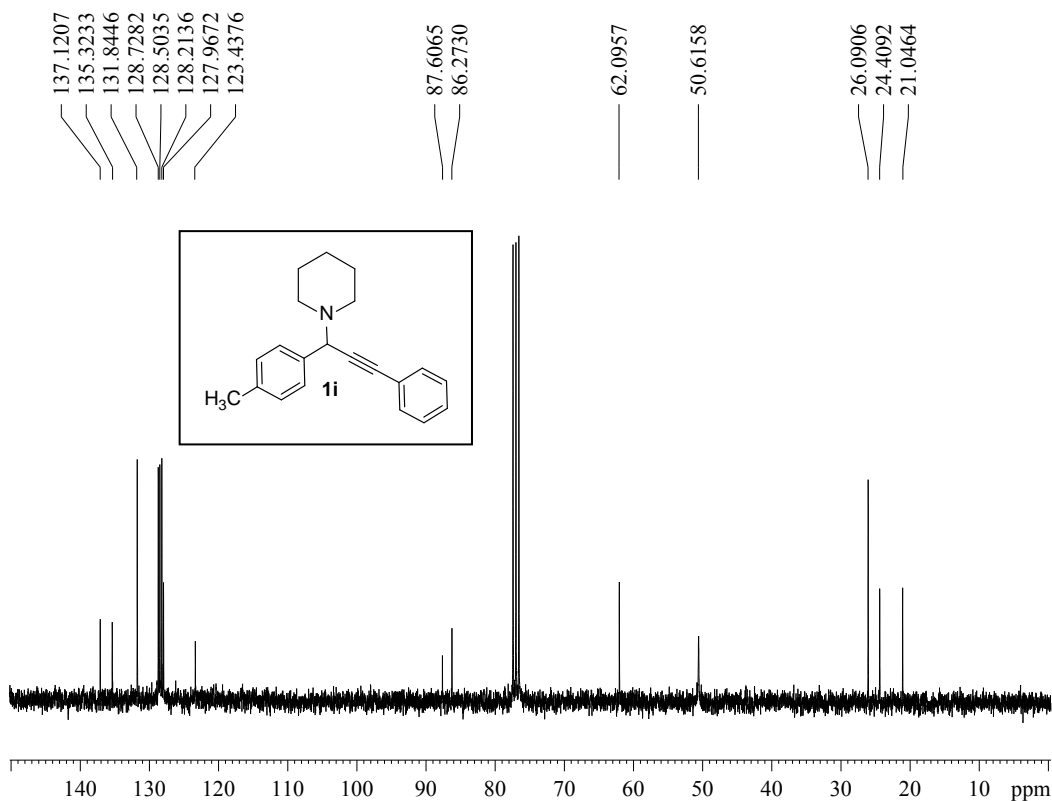
F2 - Processing parameters
 SI 32768
 SF 75.4677574 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME SNA p toulaldehyde
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20130521
 Time 19.07
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 724.1
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz
 F2 - Processing parameters
 SI 16384
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

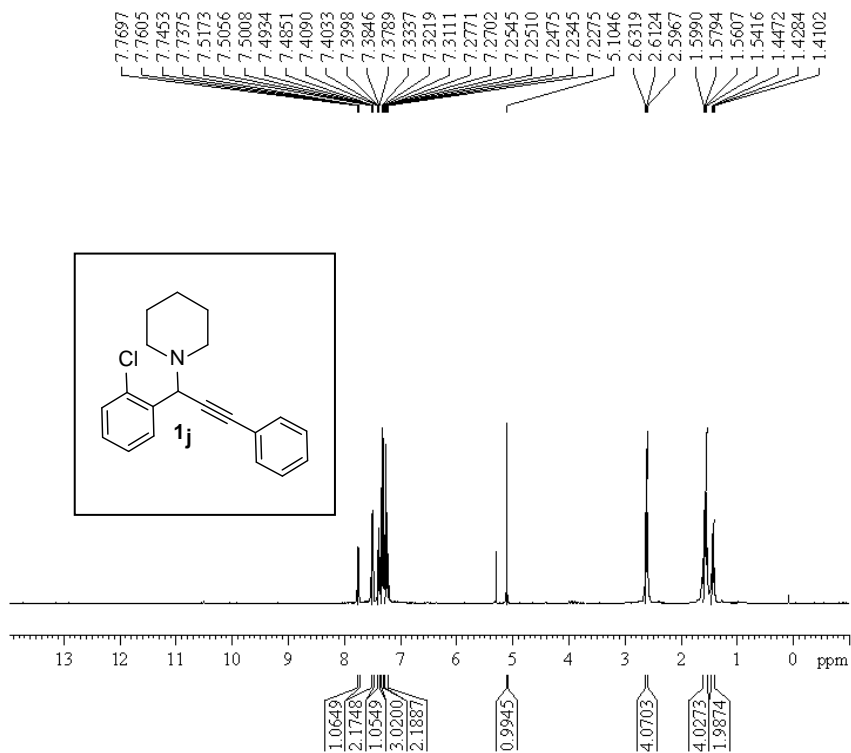


Current Data Parameters
 NAME SNA para ch3 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130520
 Time 15.40
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 520
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 8192
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz
 F2 - Processing parameters
 SI 32768
 SF 75.4677534 MHz
 WDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



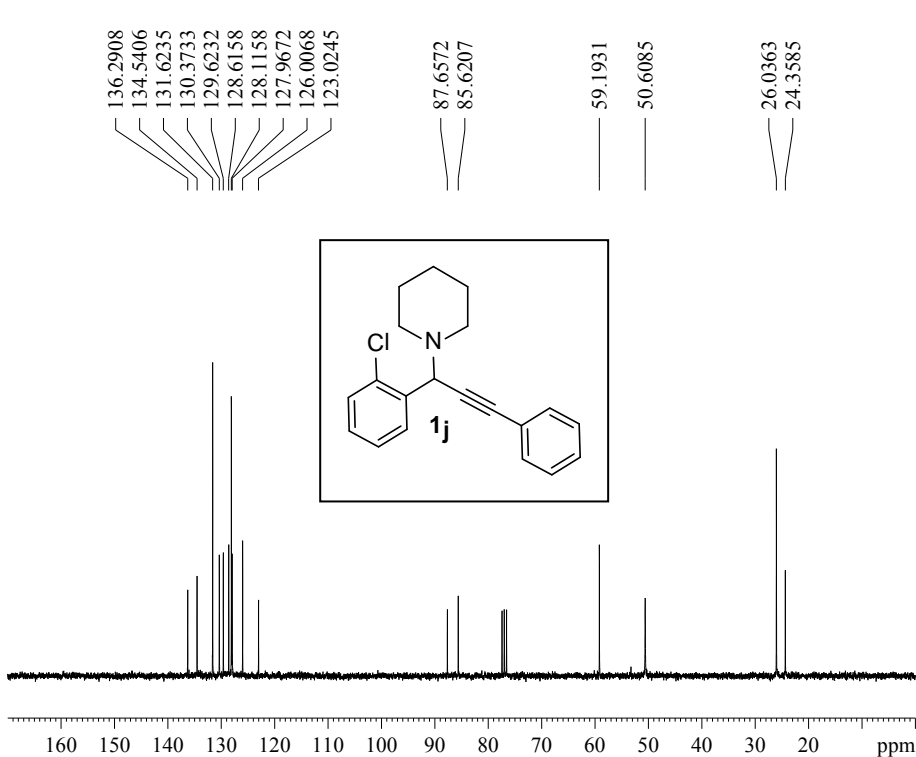
Current Data Parameters
 NAME SNA 2-clHNMR
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130621
 Time 9.40
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 362
 DW 111.200 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.130066 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

IDNMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1 13.989 ppm
 F2 4192.47 Hz
 F2P -1.013 ppm
 F2 -303.93 Hz
 PPMCM 0.7498 ppm/cm
 HZCM 224.82013 Hz/cm



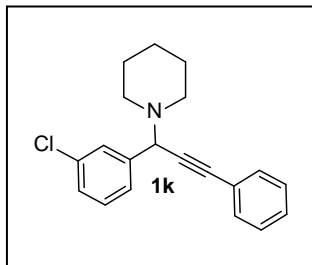
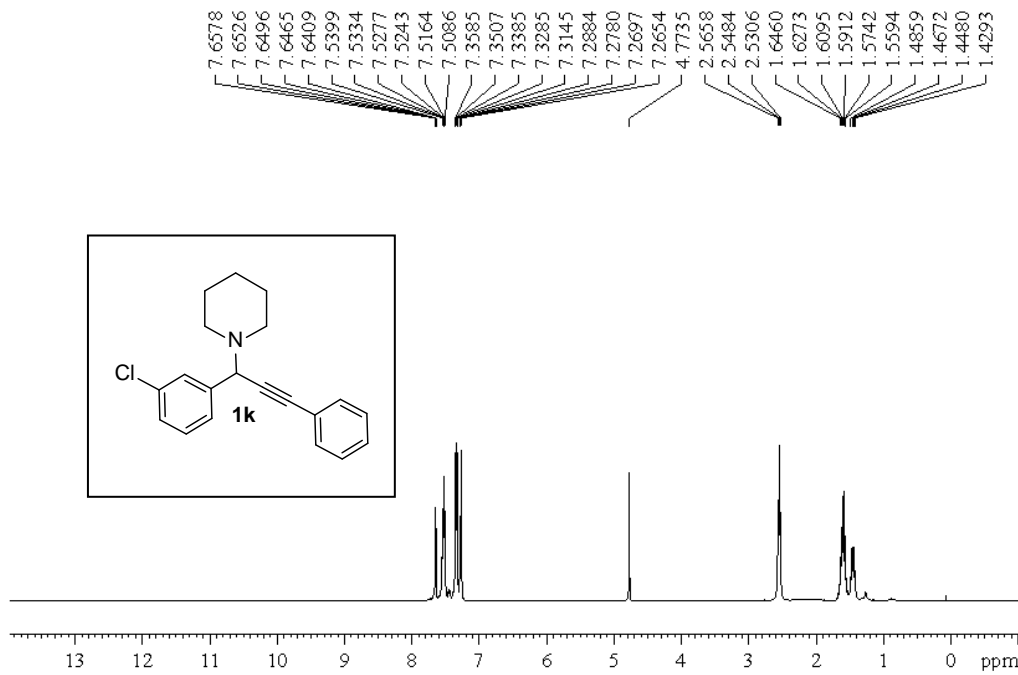
Current Data Parameters
 NAME 2-cl 13C n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130621
 Time 14.42
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 100
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 13004
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.39999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677701 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



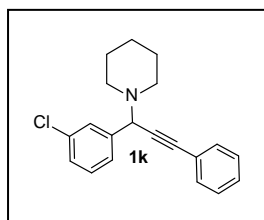
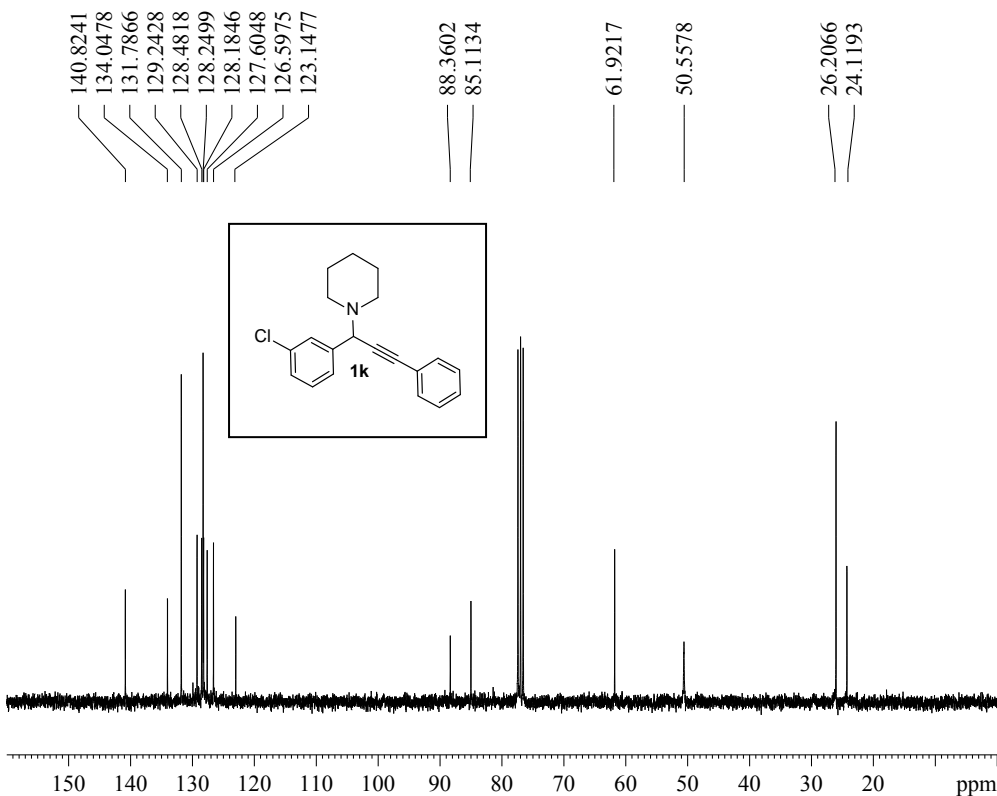
Current Data Parameters
NAME SNA 349 Iproton
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130403
Time 18.06
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 574.7
DW 111.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.5000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300063 MHz
WDW EM
SSB 0
LB 1.0 Hz
GB 0
PC 1.00

ID NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1 13.970 ppm
F2 4192.77 Hz
F3 -1.012 ppm
F4 -303.63 Hz
PPMCM 0.7408 ppm/cm
HZCM 22482014 Hz/cm



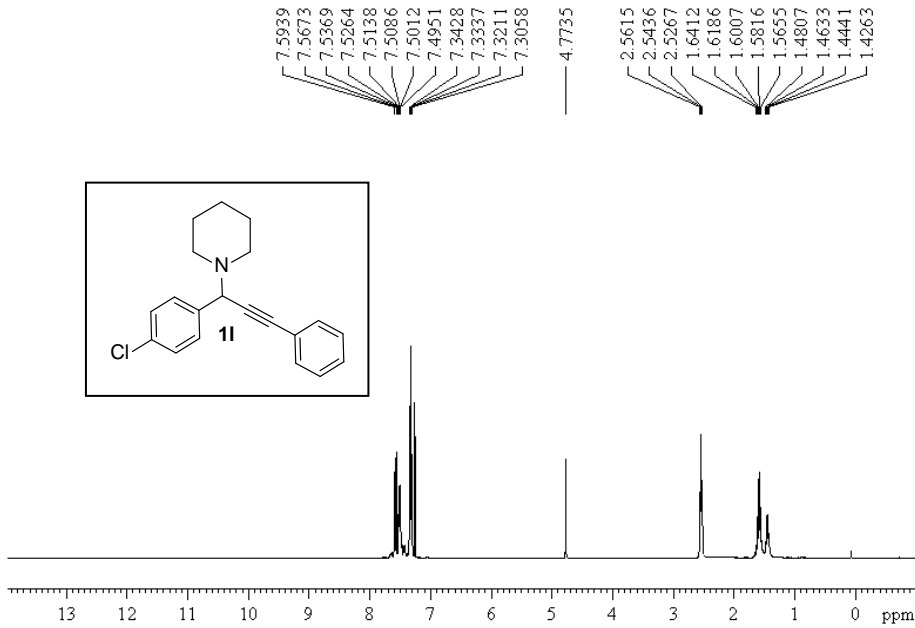
Current Data Parameters
NAME SNA 349 3c1 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130512
Time 18.59
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 300.2 K
D1 1.5000000 sec
dH 0.0300000 sec
DELTA 1.3999998 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677549 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

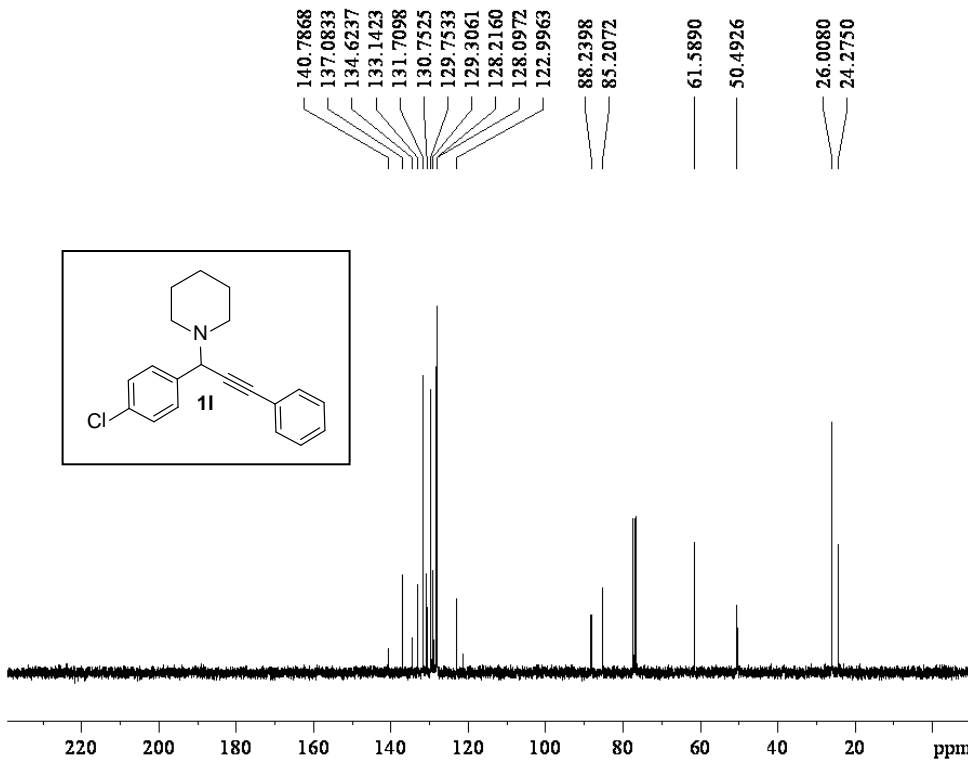


Current Data Parameters
 NAME SNA 4 CIH b
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20130521
 Time 19.43
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 724.1
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



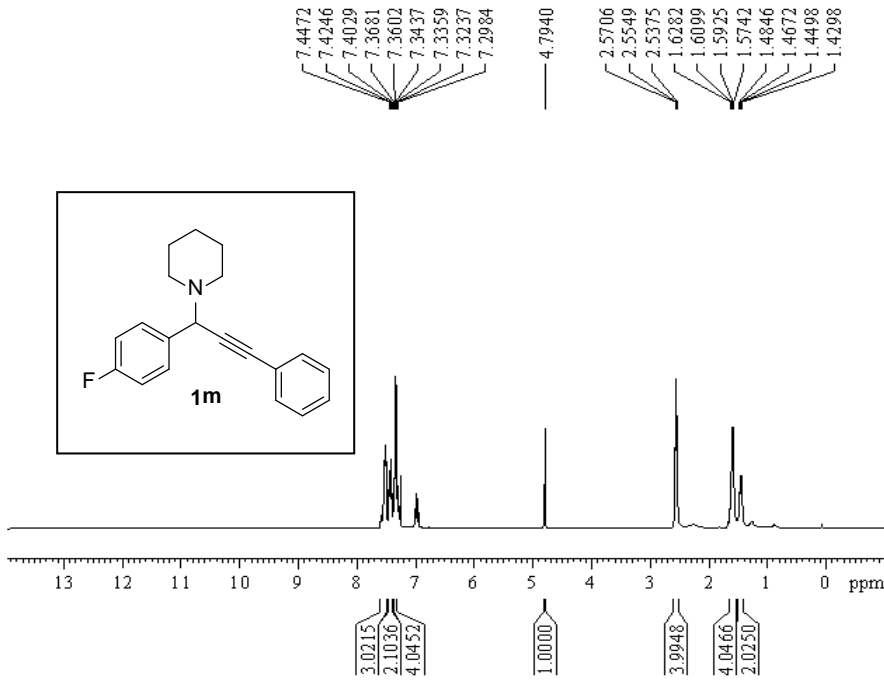
Current Data Parameters
 NAME SNA 347 13C p gla
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130517
 Time 19.56
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 276
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 14596.5
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

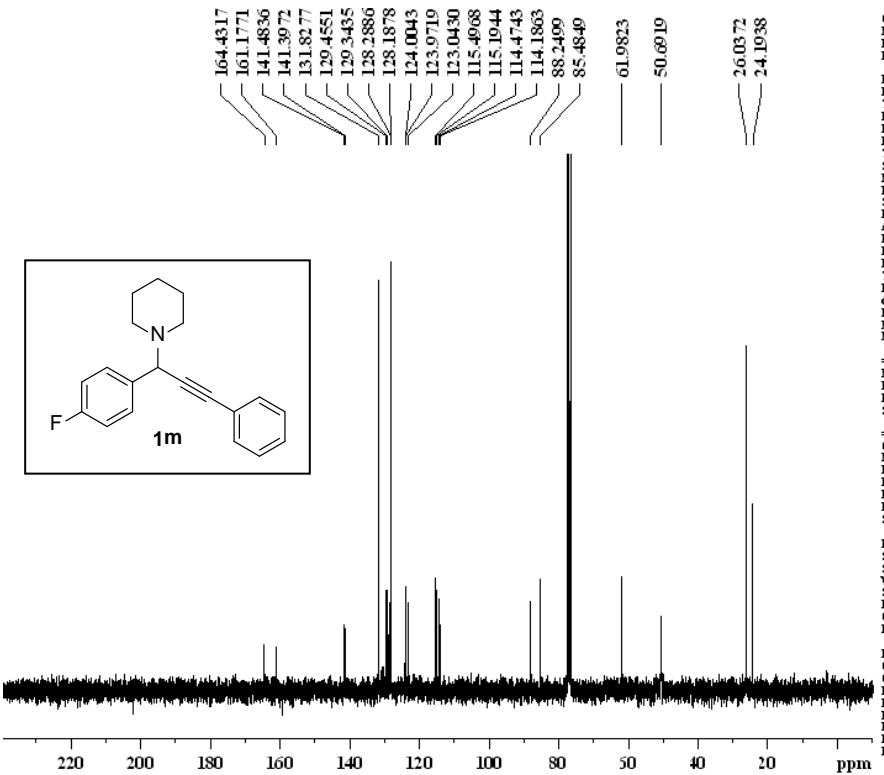
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677517 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



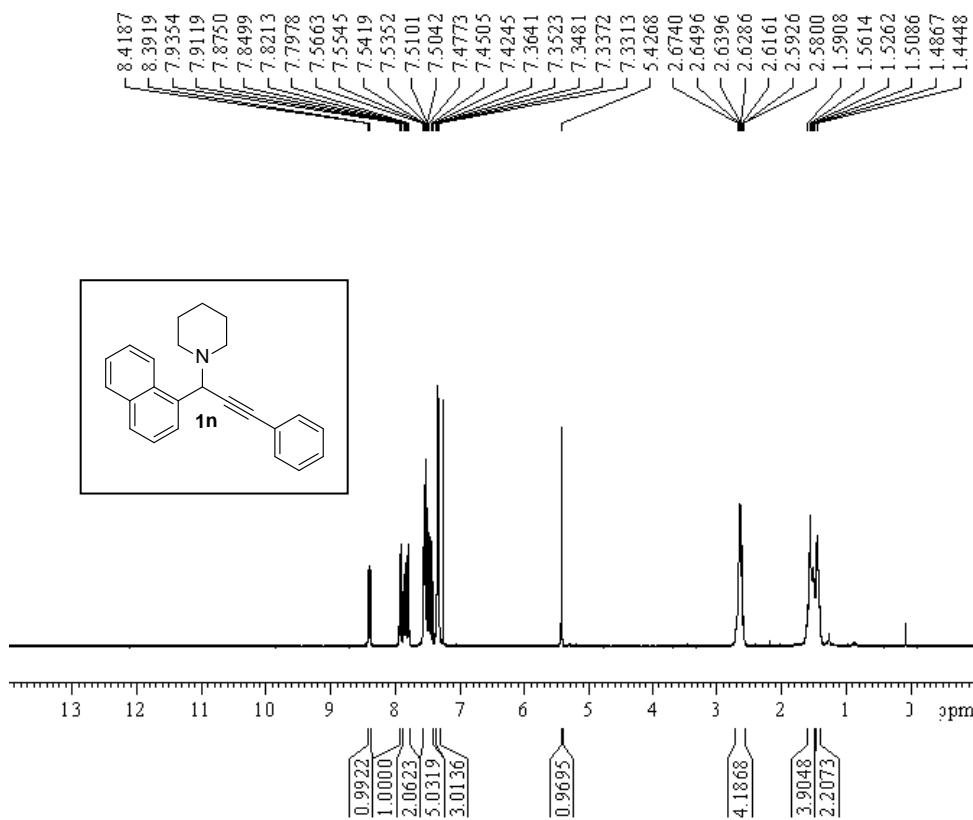
Current Data Parameters
 NAME SNA 354 proton
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130322
 Time 16.22
 INSTRUM spect
 PROBD 5 mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 4561
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz
 F2 - Processing parameters
 SI 16384
 SF 300.1300065 MHz
 WDWW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 13.969 ppm
 F1 4192.50 Hz
 F2P -1.013 ppm
 F2 -303.90 Hz
 FPMCM 0.74908 ppm/cm
 HZ CM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 344 13C 4F
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130511
 Time 11.04
 INSTRUM spect
 PROBD 5 mm Multinuc
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 913
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7460308 sec
 RG 18390.4
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz
 ==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz
 F2 - Processing parameters
 SI 32768
 SF 75.4677488 MHz
 WDWW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 239.276 ppm
 F1 18065.17 Hz
 F2P -10.166 ppm
 F2 -767.22 Hz
 FPMCM 12.47211 ppm/cm
 HZ CM 941.61957 Hz/cm



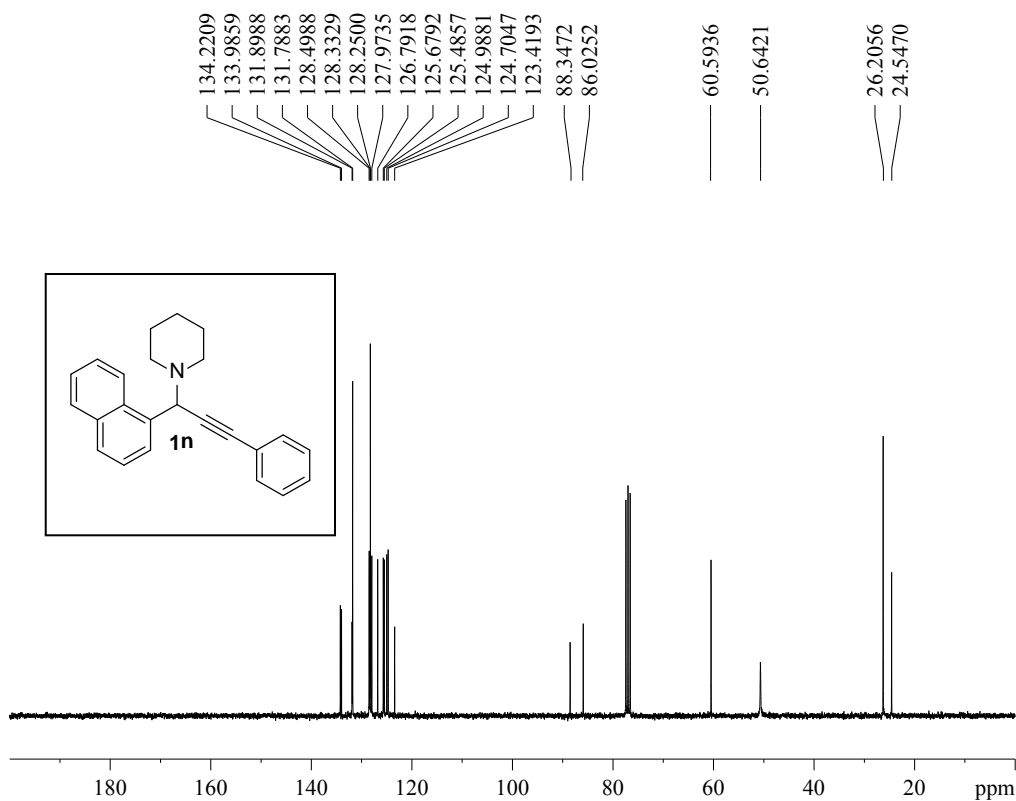
Current Data Parameters
 NAME SNA 360 proton.nmr
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130321
 Time 14.10
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 912.3
 DRY 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300076 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.965 ppm
 FI 4191.40 Hz
 F2P -1.016 ppm
 F2 -305.00 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 359 13C
 EXPNO 2
 PROCNO 1

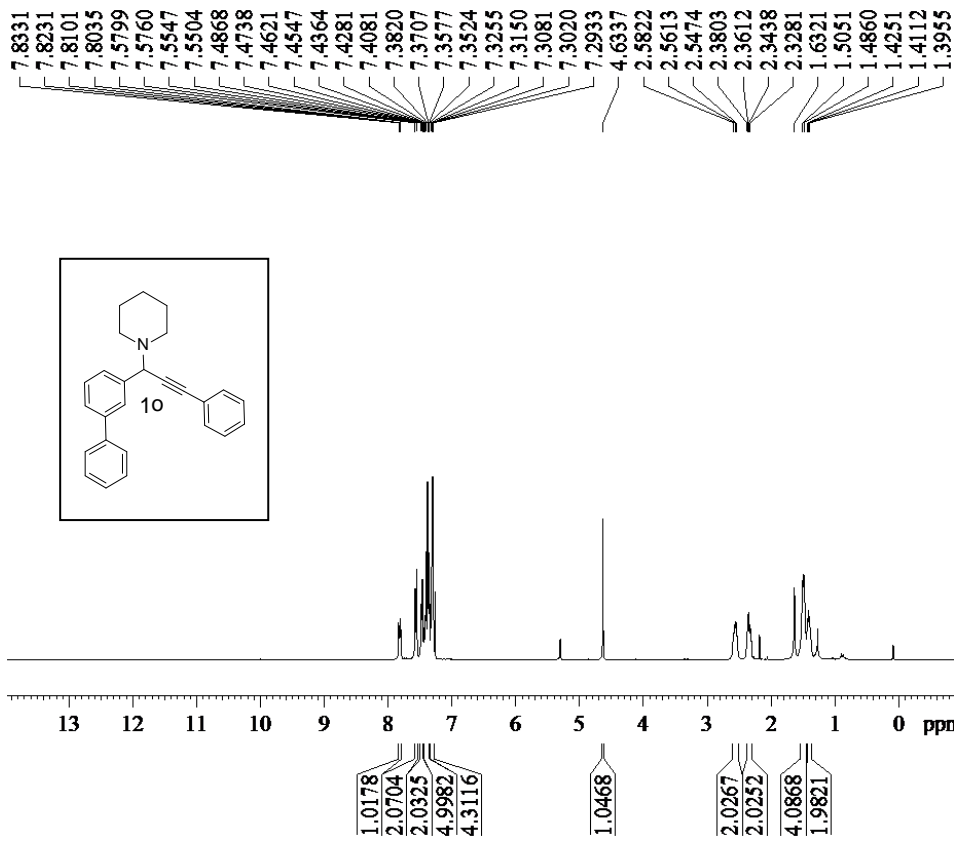
F2 - Acquisition Parameters
 Date_ 20130511
 Time 3.37
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 1883.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 18390.4
 DW 26.550 usec
 DE 6.50 usec
 TE 299.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677534 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 239.315 ppm
 FI 18060.58 Hz
 F2P -10.227 ppm
 F2 -771.81 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61951 Hz/cm



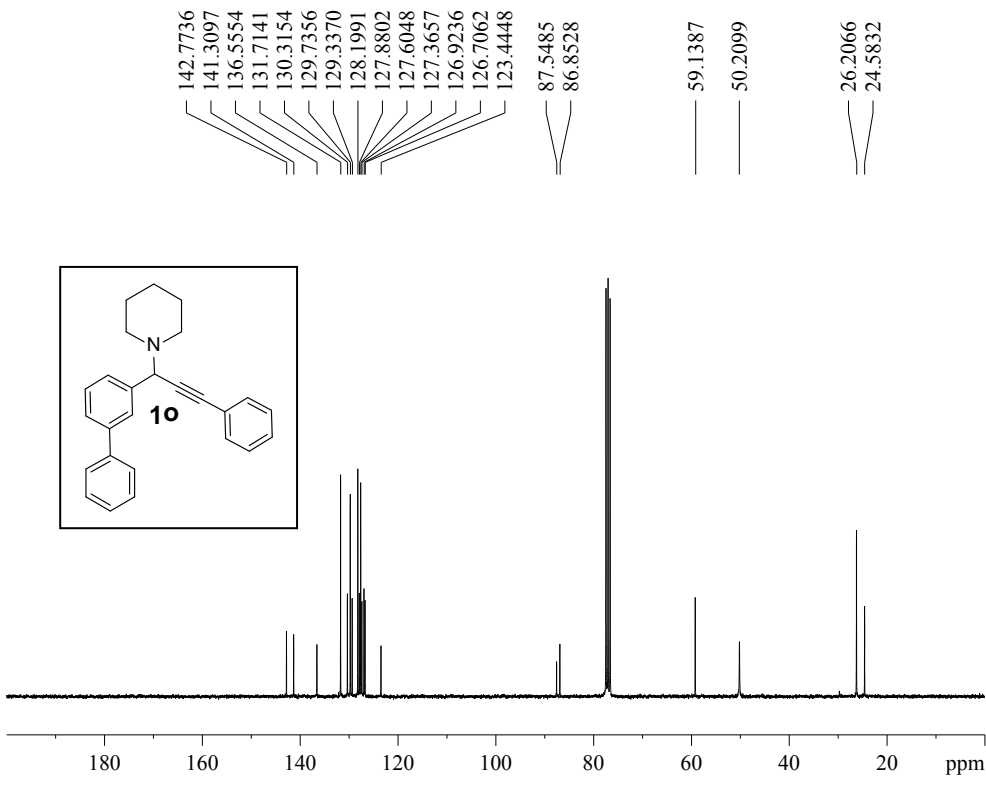
Current Data Parameters
 NAME SNA 380.1 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130403
 Time 14.27
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 406.4
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWKK 0.01500000 sec

CHANNEL f1
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300065 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 13.969 ppm
 F1 4192.50 Hz
 F2P -1.013 ppm
 F2 -303.90 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82015 Hz/cm



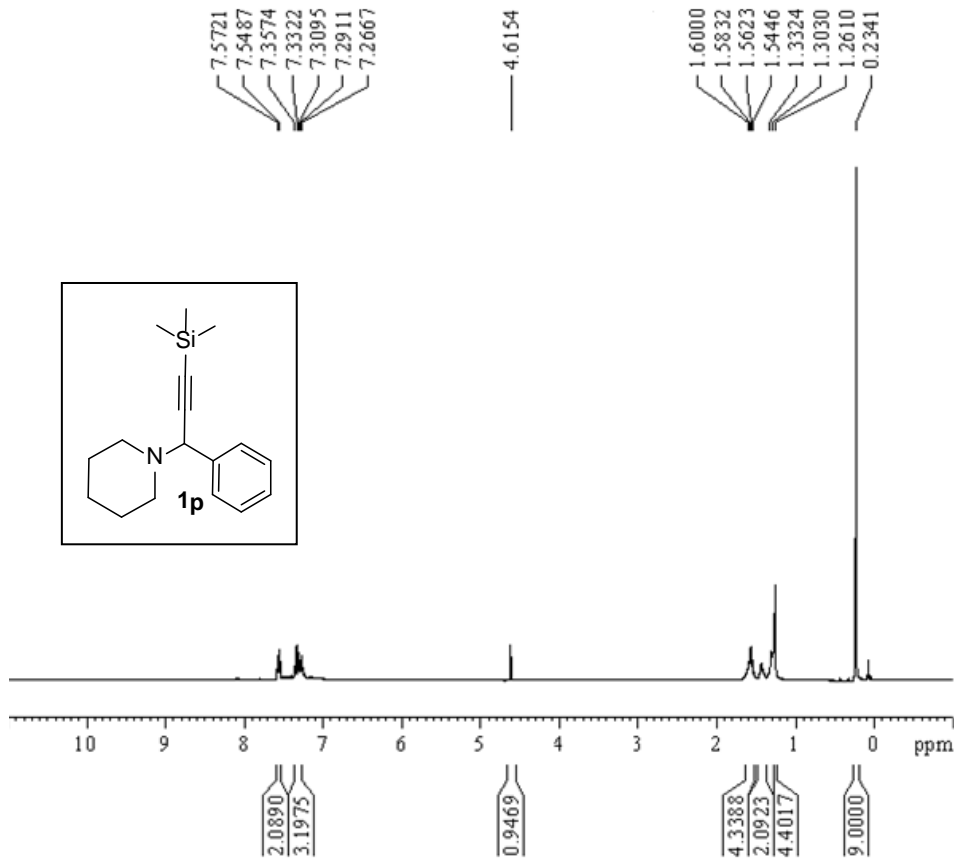
Current Data Parameters
 NAME SNA 380 biphenyl13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130519
 Time 10.24
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 11198
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999999 sec
 MCREST 0.00000000 sec
 MCWKK 0.01500000 sec

CHANNEL f1
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677511 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



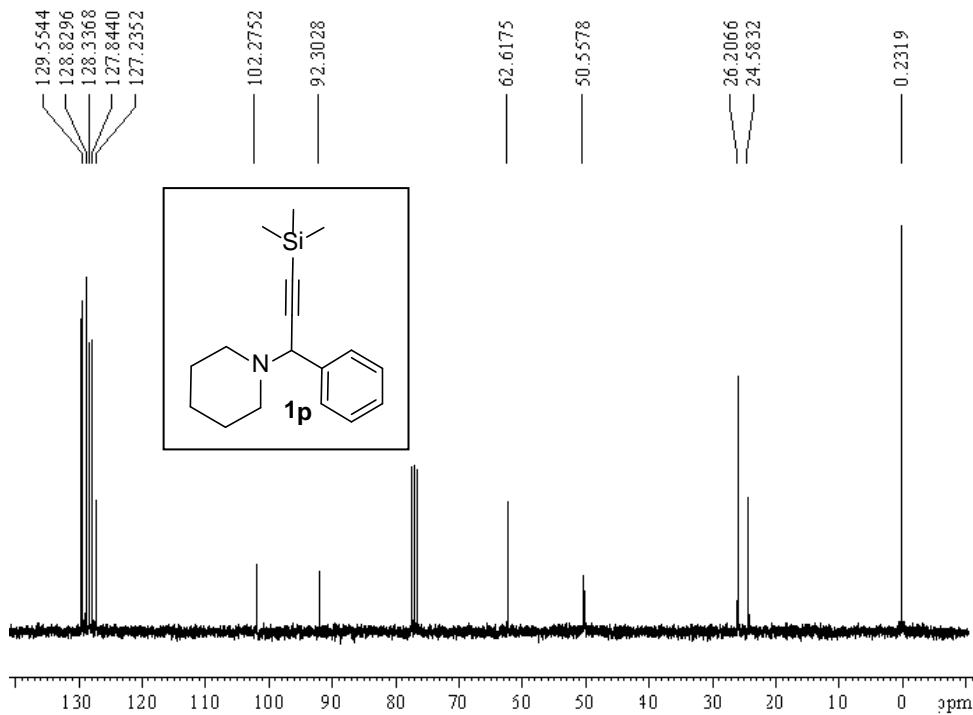
Current Data Parameters
 NAME SNA 372 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130320
 Time 22.00
 INSTRUM spect
 PROBHD 5mm Multinuc1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 267.4
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SF01 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300657 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 13.972 ppm
 F1 -0.9332 Hz
 F2P -1.610 ppm
 F2 -303.08 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



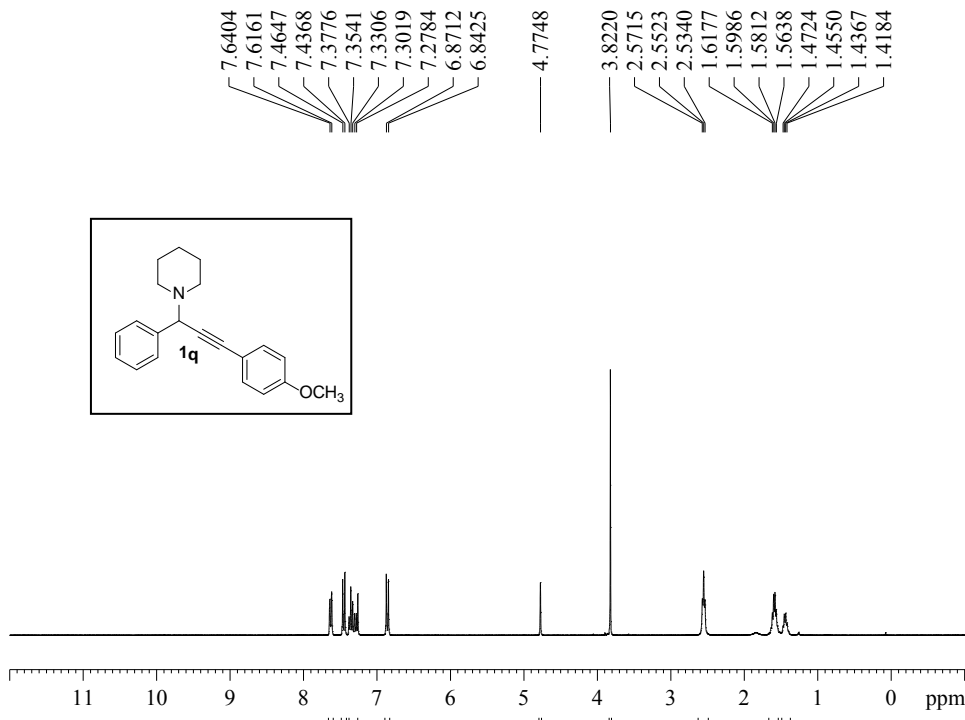
Current Data Parameters
 NAME SNA TMS 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130320
 Time 18.37
 INSTRUM spect
 PROBHD 5mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18432.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7409308 sec
 RG 13604
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SF01 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2PRG2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SF02 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677540 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



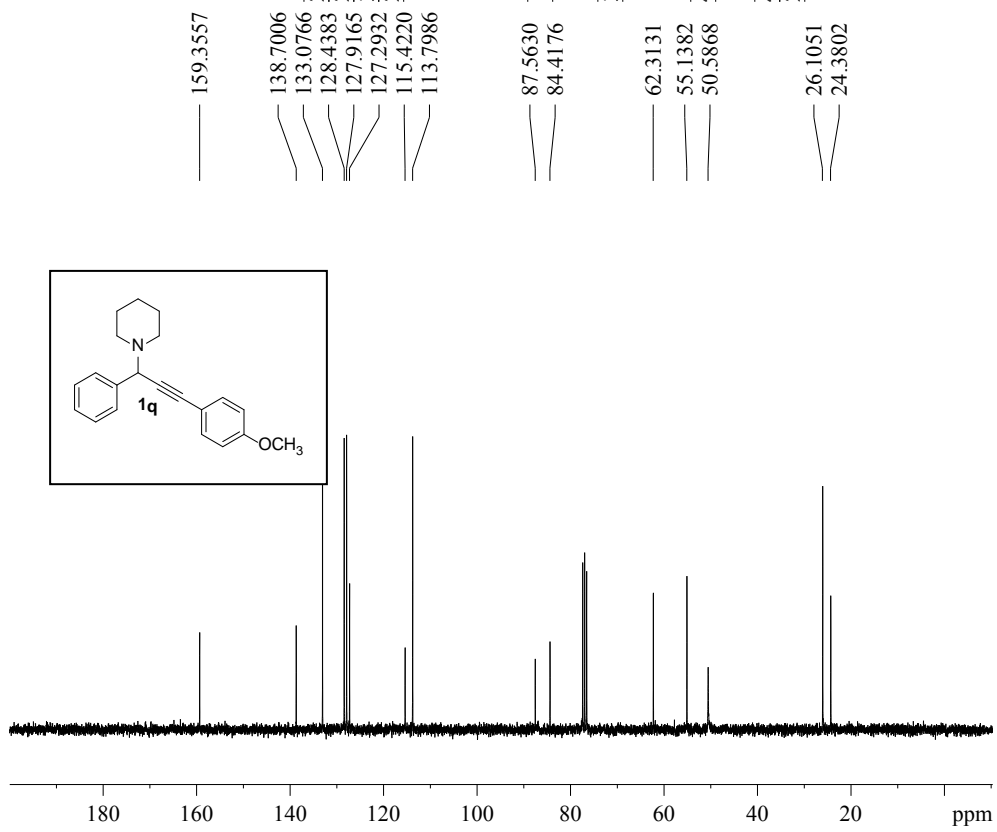
Current Data Parameters
 NAME SNA 367 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130322
 Time 19.39
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 15
 DS 0
 SWH 496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 574.7
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.970 ppm
 F1 4192.77 Hz
 F2P -1.012 ppm
 F2 -303.63 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 367 13C
 EXPNO 1
 PROCNO 1

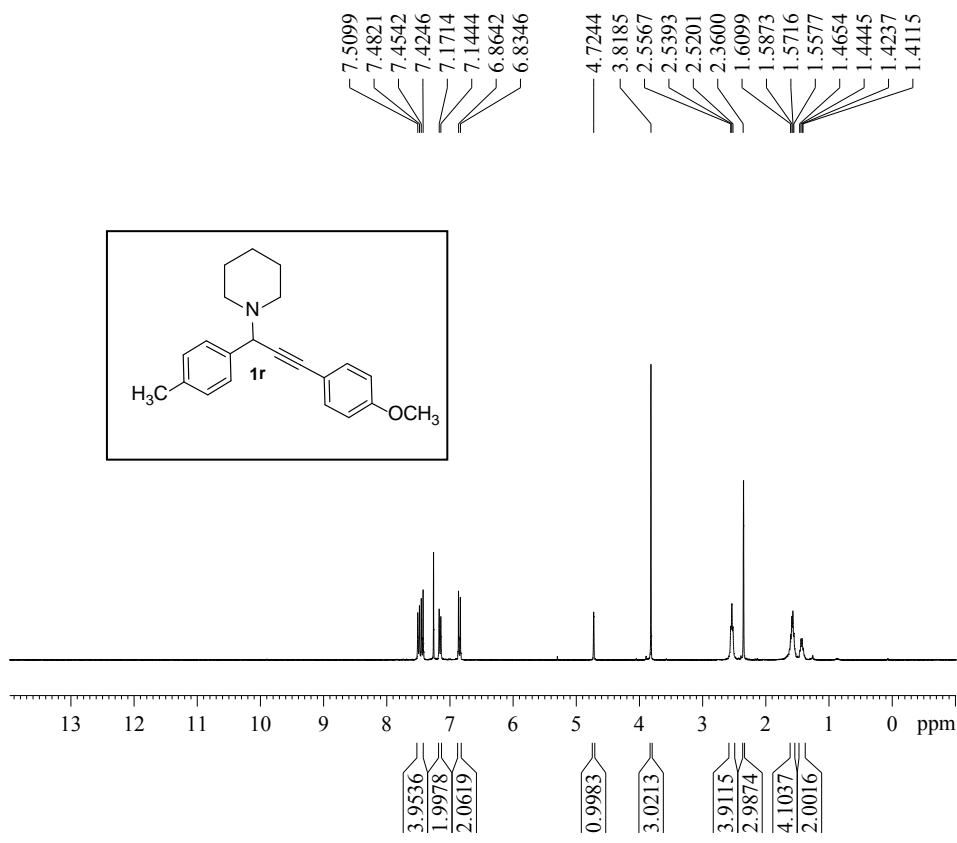
F2 - Acquisition Parameters
 Date 20130512
 Time 20.35
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 20642.5
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677523 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 239.330 ppm
 F1 18061.73 Hz
 F2P -10.212 ppm
 F2 -770.67 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61957 Hz/cm



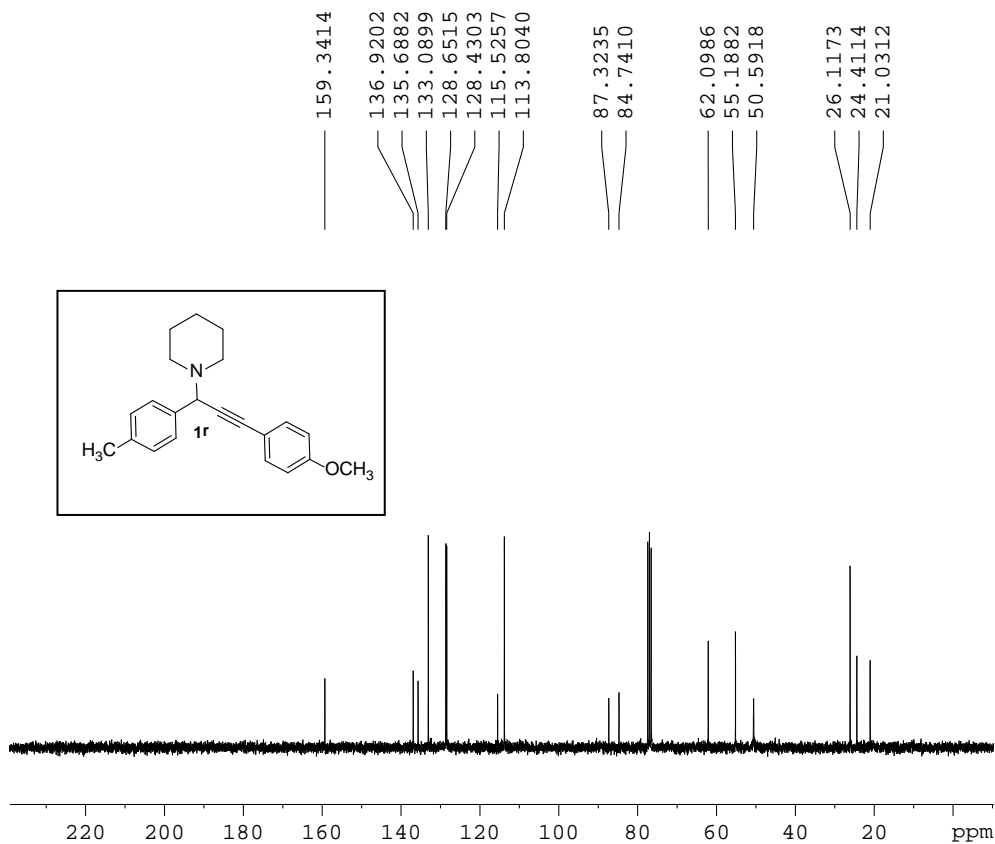
Current Data Parameters
 NAME SNA 384 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130403
 Time 14.58
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 1024
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 ¹H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300065 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.969 ppm
 F1 4192.50 Hz
 F2P -1.013 ppm
 F2 -303.90 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 384 AT 13C
 EXPNO 1
 PROCNO 1

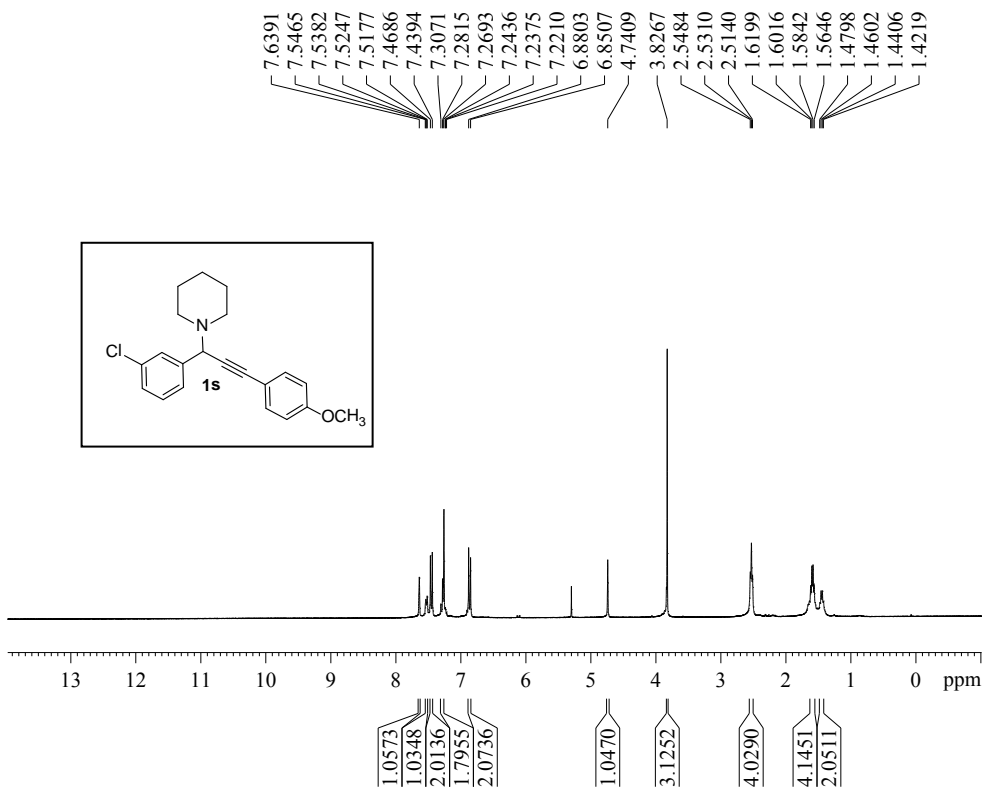
F2 - Acquisition Parameters
 Date_ 20130512
 Time 19.23
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 14596.5
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 ¹³C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677551 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 239.292 ppm
 F1 18058.85 Hz
 F2P -10.250 ppm
 F2 -773.54 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61957 Hz/cm



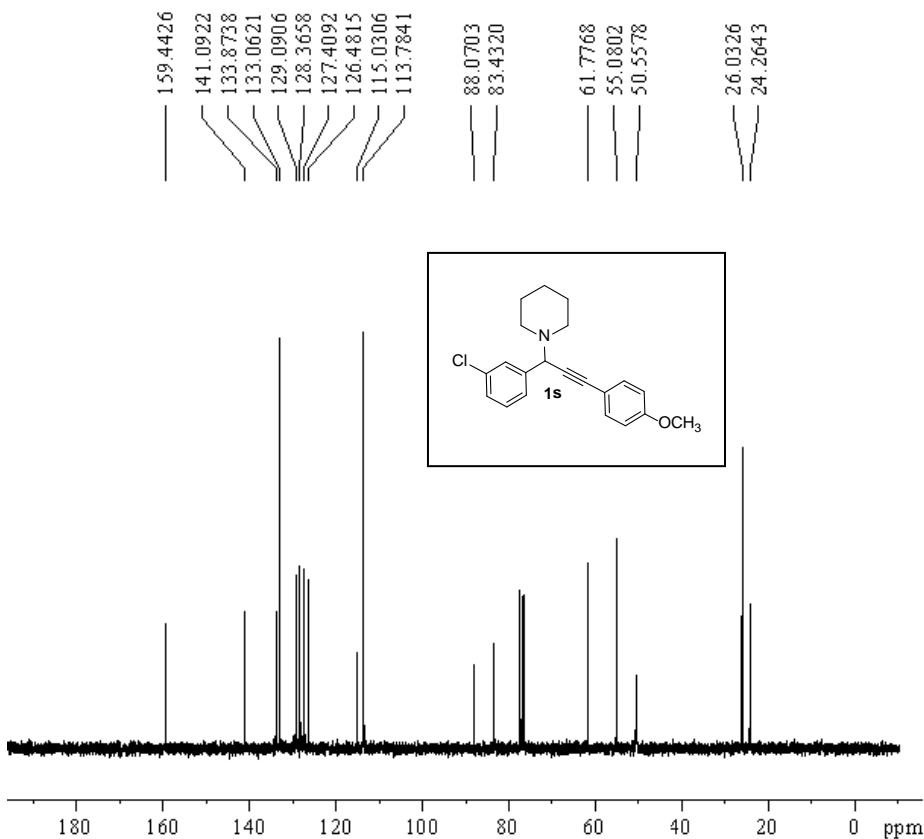
Current Data Parameters
 NAME SNA 385 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130403
 Time 14.45
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 645.1
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 13.970 ppm
 F1 4192.77 Hz
 F2P -1.012 ppm
 F2 -303.63 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



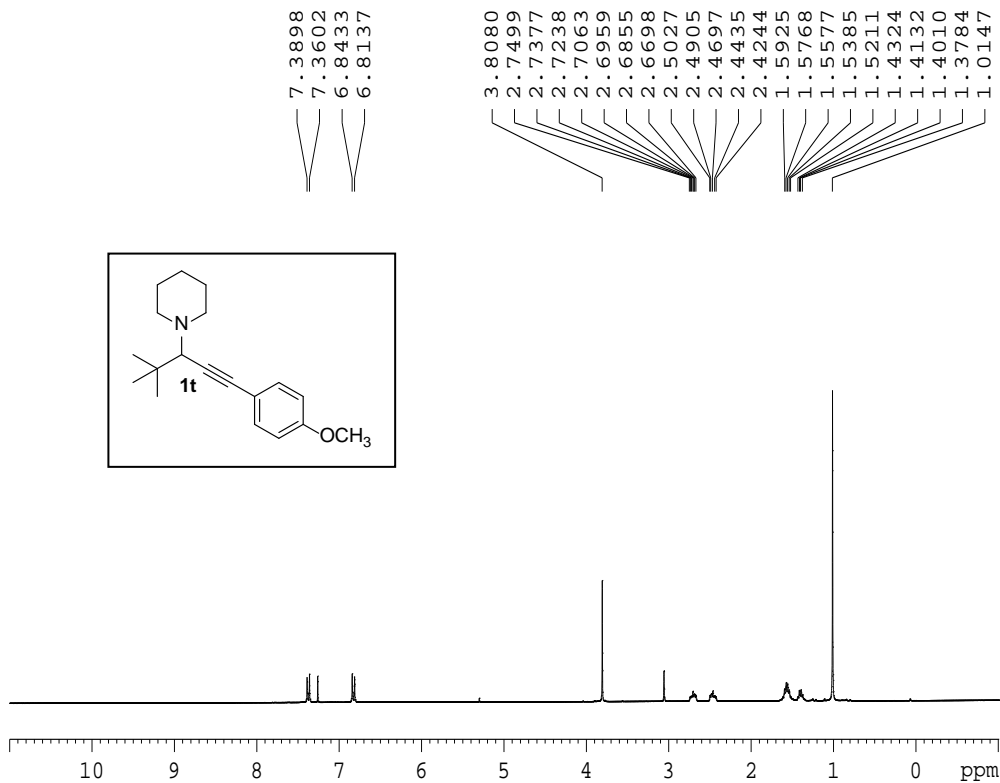
Current Data Parameters
 NAME SNA 385 13C c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130512
 Time 19.55
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 ID 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 ====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 ====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677523 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

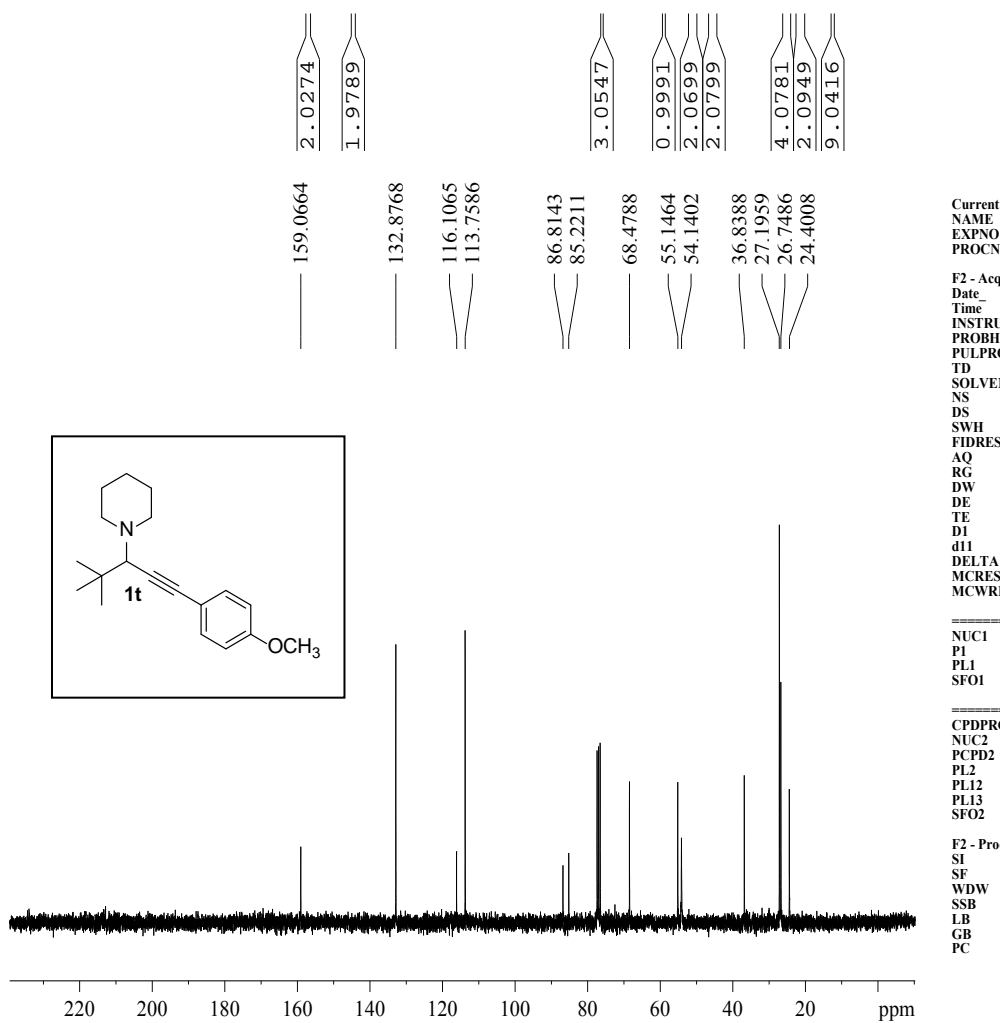


Current Data Parameters
 NAME SNA 387 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130403
 Time 14.37
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 724.1
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 DL 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300062 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



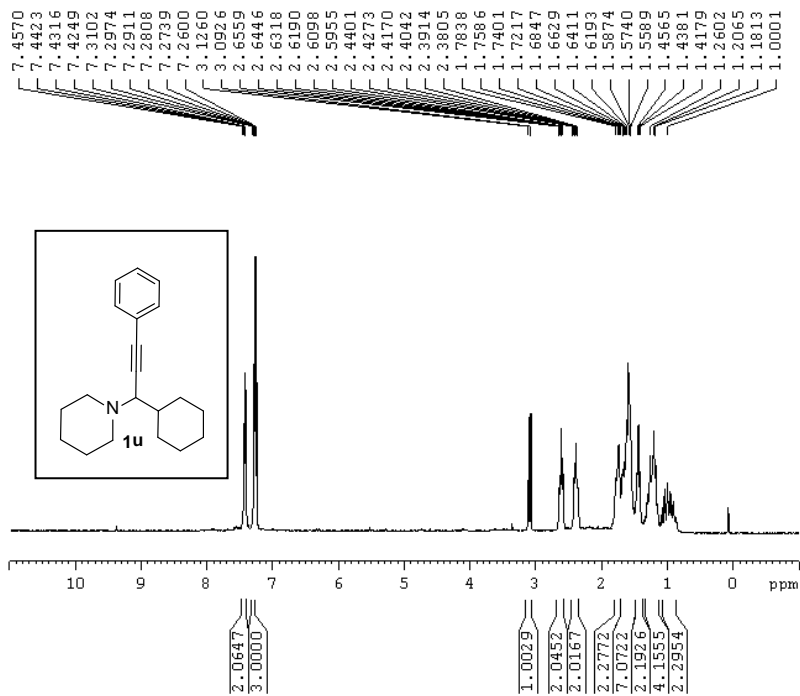
Current Data Parameters
 NAME (CH3)3CCH2Phacetylene
 EXPNO 130804
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130804
 Time 17.36
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 250
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 18390.4
 DW 26.550 usec
 DE 6.50 usec
 TE 302.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.39999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677540 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME SNA.339 H
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130321
Time 1418
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 4406.403 Hz
FIDRES 0.127219 Hz
AQ 3.6438515 sec
RG 456.1
DW 111.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.5000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319506 MHz

F2 - Processing parameters
SI 16384
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.969 ppm
FI 4192.50 Hz
FZF -1.013 ppm
FZ 303.90 Hz
FZCM 0.74068 ppm/cm
HZCM 224.82013 Hz/cm

131.6996
128.1629
127.5831
123.8145

87.6935
86.1570

64.4728

50.7897

39.6577

31.2797

30.6130

26.7864

26.2046

26.0906

24.5832

Current Data Parameters
NAME SNA cycloaldehyde 13C
EXPNO 2
PROCNO 1

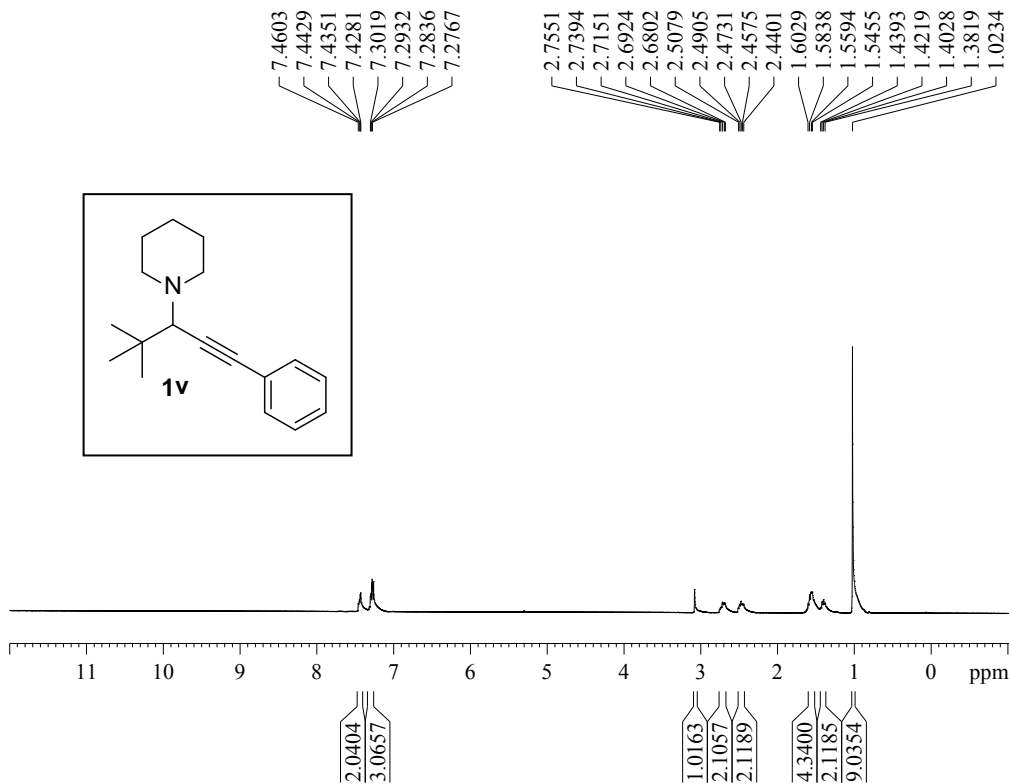
F2 - Acquisition Parameters
Date 20130511
Time 2.11
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.5000000 sec
d11 0.0300000 sec
DELTA 1.3999998 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677517 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
FIP 239.338 ppm
FI 18062.30 Hz
FZF 10.204 ppm
FZ -770.09 Hz
FZCM 12.47711 ppm/cm
HZCM 941.61957 Hz/cm



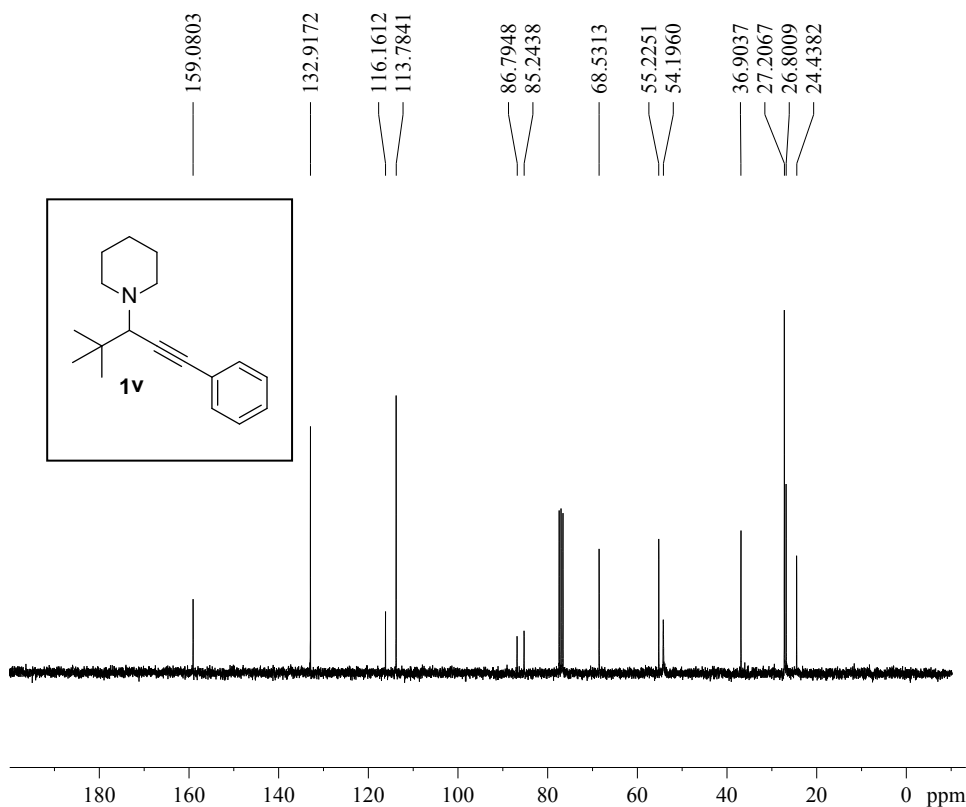
Current Data Parameters
 NAME SNA 382.1 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130326
 Time 21.46
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 645.1
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300071 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.967 ppm
 F1 4191.95 Hz
 F2P -1.014 ppm
 F2 -304.45 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 385 13C d
 EXPNO 1
 PROCNO 1

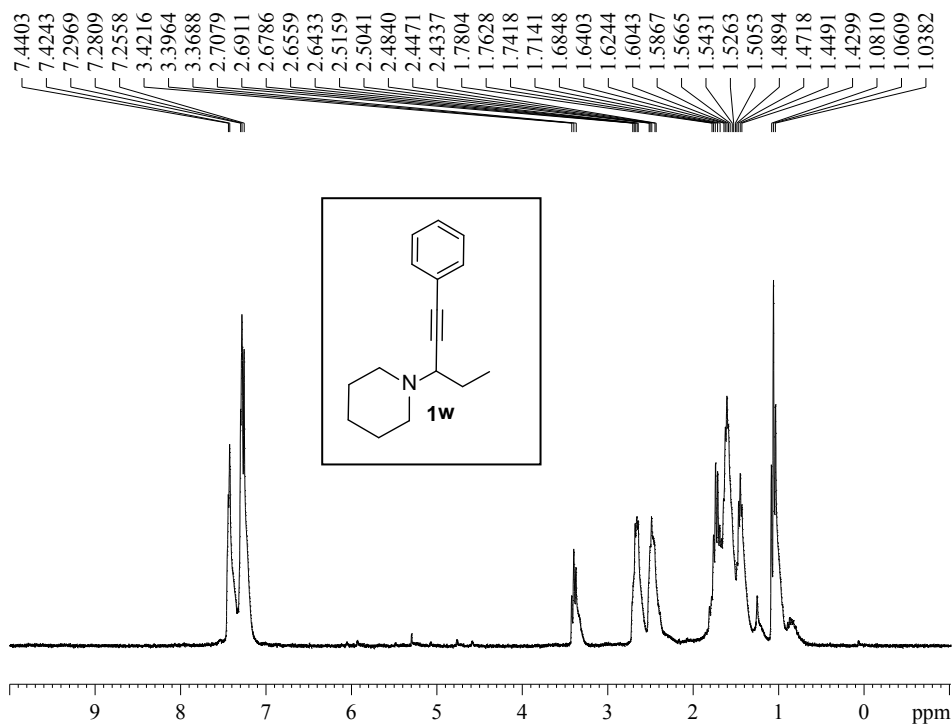
F2 - Acquisition Parameters
 Date_ 20130512
 Time 20.13
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677528 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 239.323 ppm
 F1 18061.15 Hz
 F2 -771.24 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61951 Hz/cm



Current Data Parameters
 NAME SNA 375 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130326
 Time 15.50
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 724.1
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 DI 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300082 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.963 ppm
 F1 4190.85 Hz
 F2P -1.018 ppm
 F2 -305.55 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm

2.0041
3.0578

1.0128
2.1605
2.3652

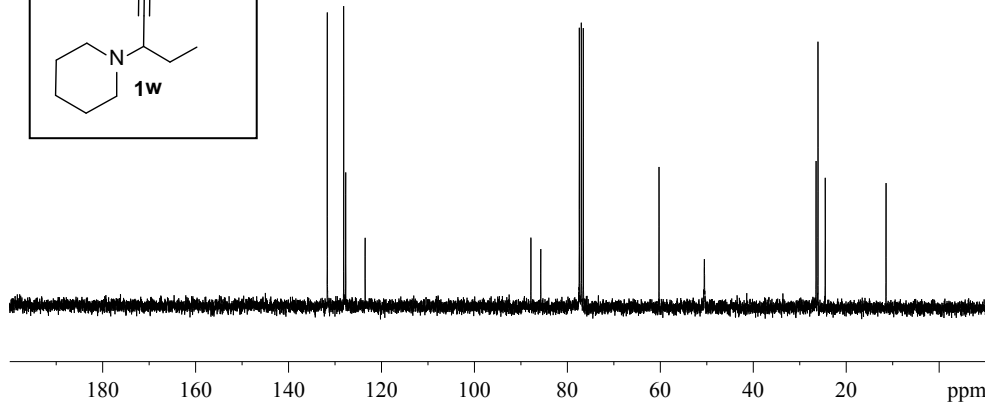
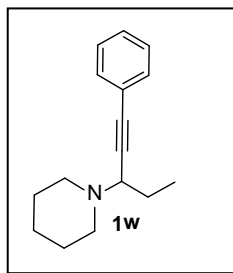
2.5388
4.4301
2.3038
3.0913

131.6435
128.1212
127.7299
123.5717

87.8112
85.7566

60.3182
50.5343

26.5146
26.0743
24.5578
11.4473



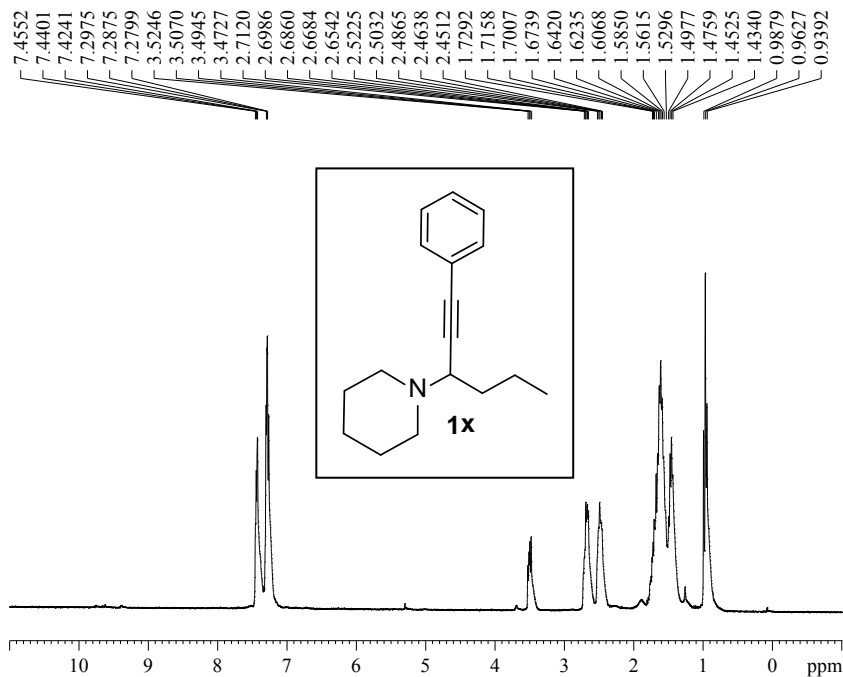
Current Data Parameters
 NAME SNA propanal 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130518
 Time 16.37
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 16384
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 DI 1.5000000 sec
 dI1 0.0300000 sec
 DELTA 1.39999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677540 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



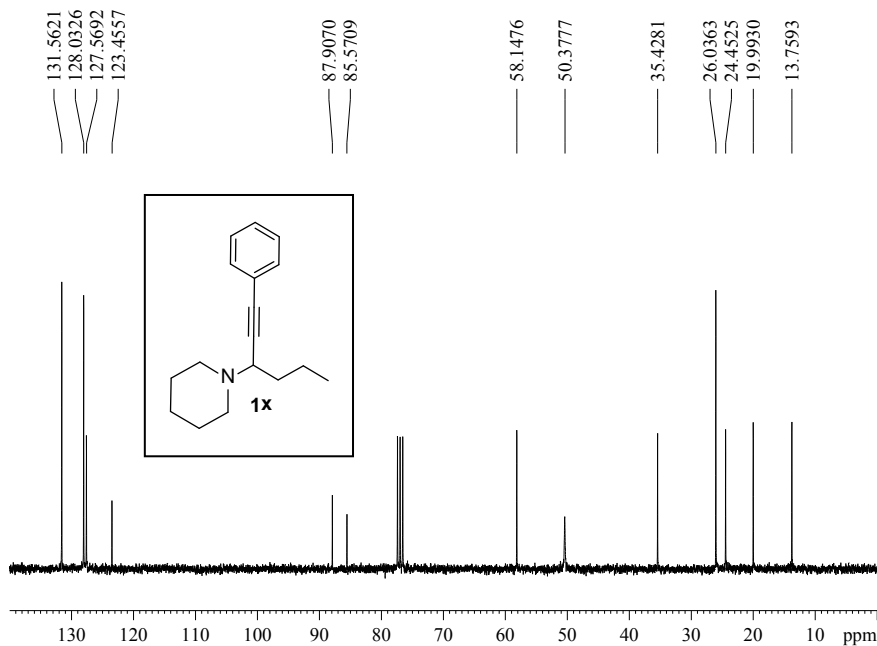
Current Data Parameters
NAME SNA 377
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130326
Time 15:34
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 456.1
DW 111.200 usec
DE 6.50 usec
TE 297.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300054 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 13.973 ppm
F1 4193.60 Hz
F2P -1.009 ppm
F2 -302.80 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm



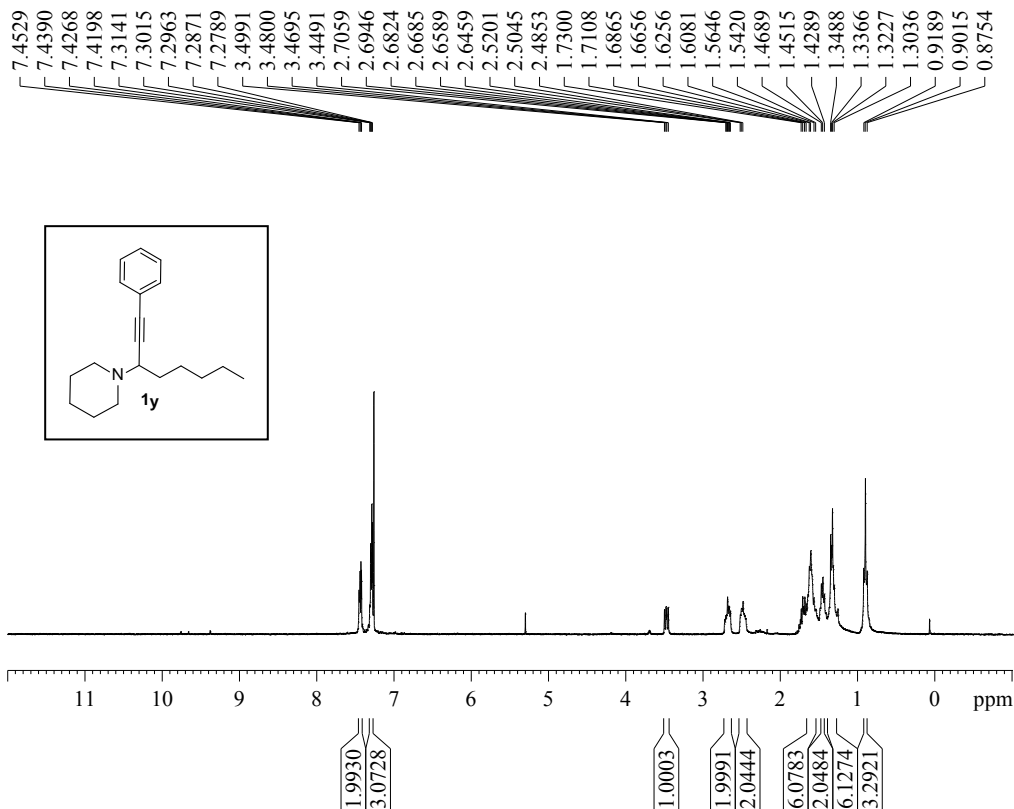
Current Data Parameters
NAME SNA butanal 13C 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130518
Time 16:18
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 18832.293 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677517 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



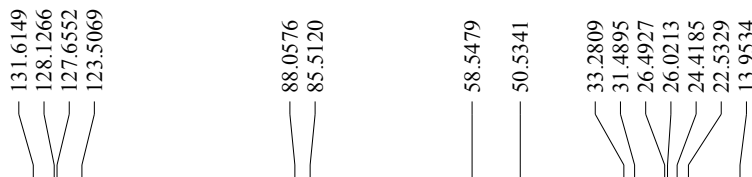
Current Data Parameters
 NAME SNA 374 proton
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130321
 Time 23.00
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 1024
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300065 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.969 ppm
 F1 4192.50 Hz
 F2P -1.013 ppm
 F2 -303.90 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



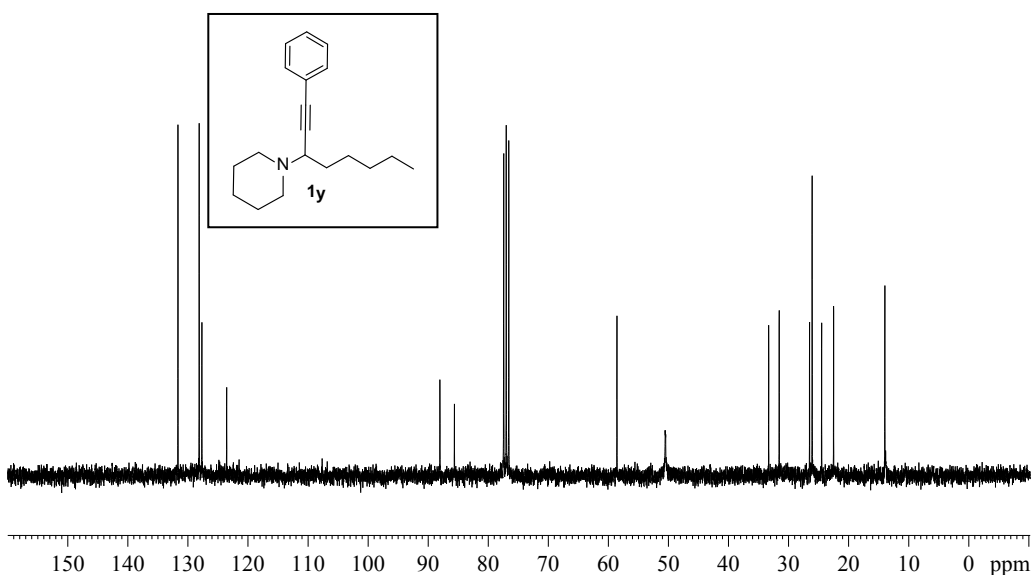
Current Data Parameters
 NAME SNA hexanal 13C 13C
 EXPNO 1
 PROCNO 1

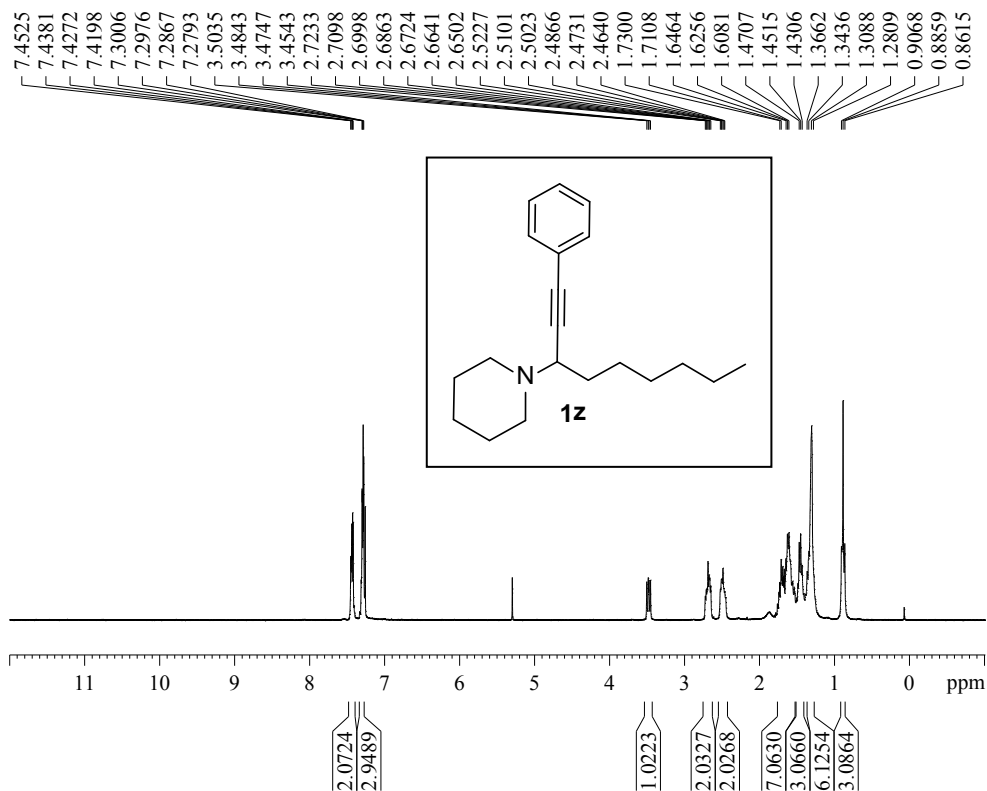
F2 - Acquisition Parameters
 Date_ 20130518
 Time 15.58
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677488 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00





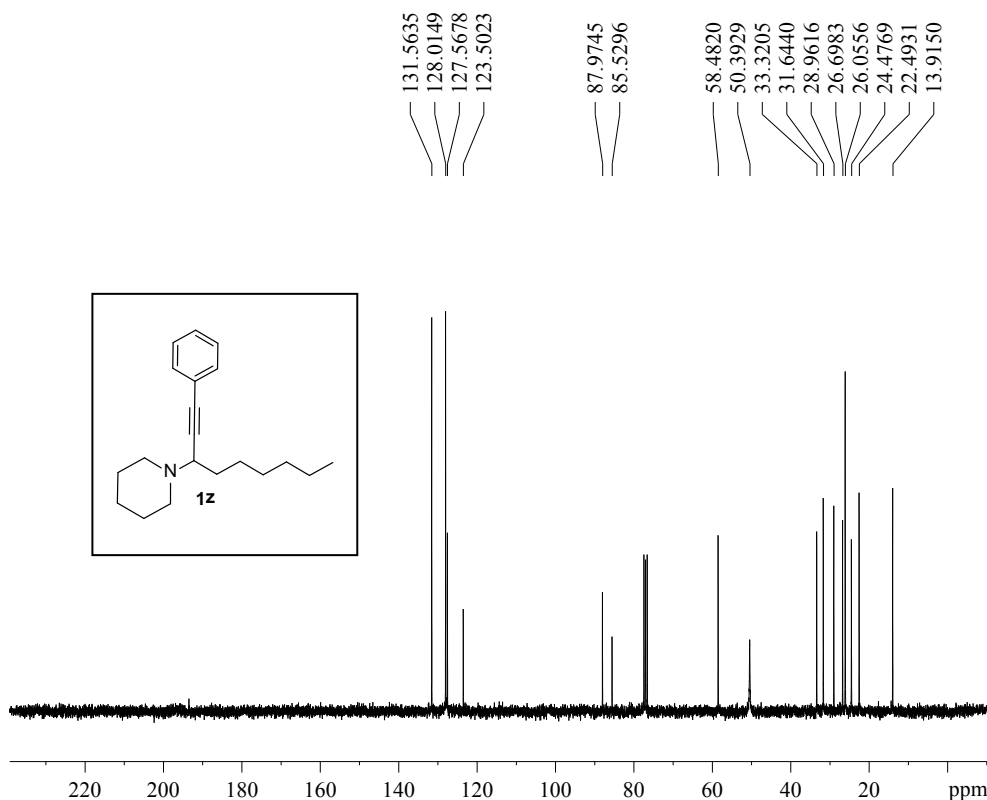
Current Data Parameters
NAME SNA 371.1 proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130320
Time 15.54
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 512
DW 111.200 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.966 ppm
F1 4191.68 Hz
F2P -4.015 ppm
F2 -304.73 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm



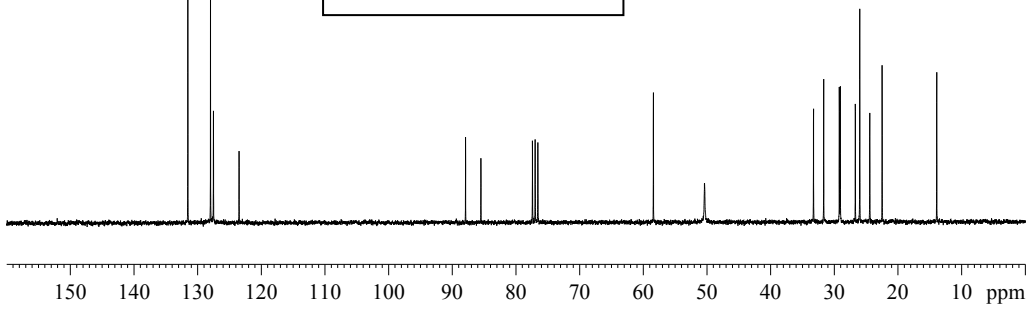
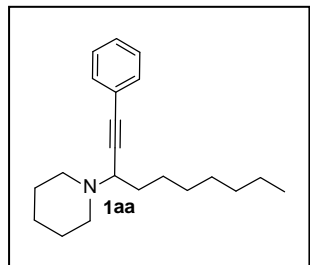
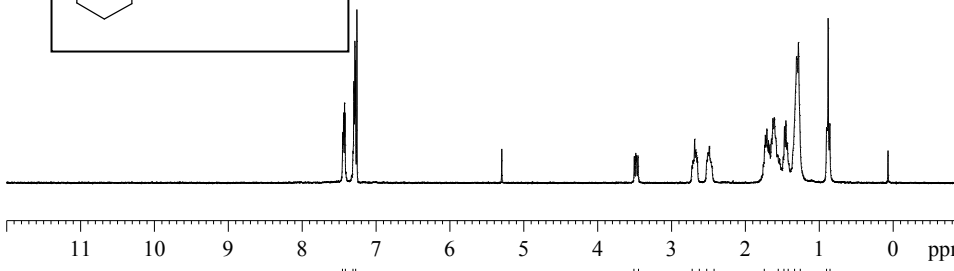
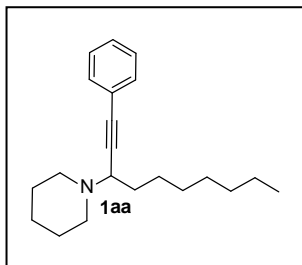
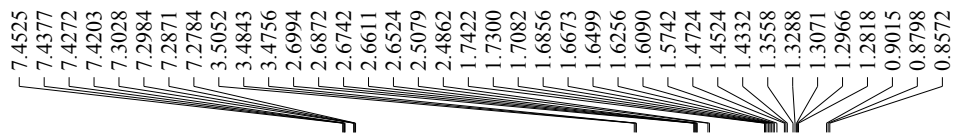
Current Data Parameters
NAME SNA heptaldehyde 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130517
Time 19.42
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 14596.5
DW 26.550 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME SNA 369 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130320
 Time 15.18
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 812.7
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300109 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.954 ppm
 F1 4188.11 Hz
 F2P -1.027 ppm
 F2 -308.29 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm

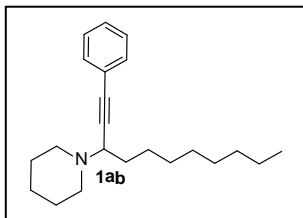
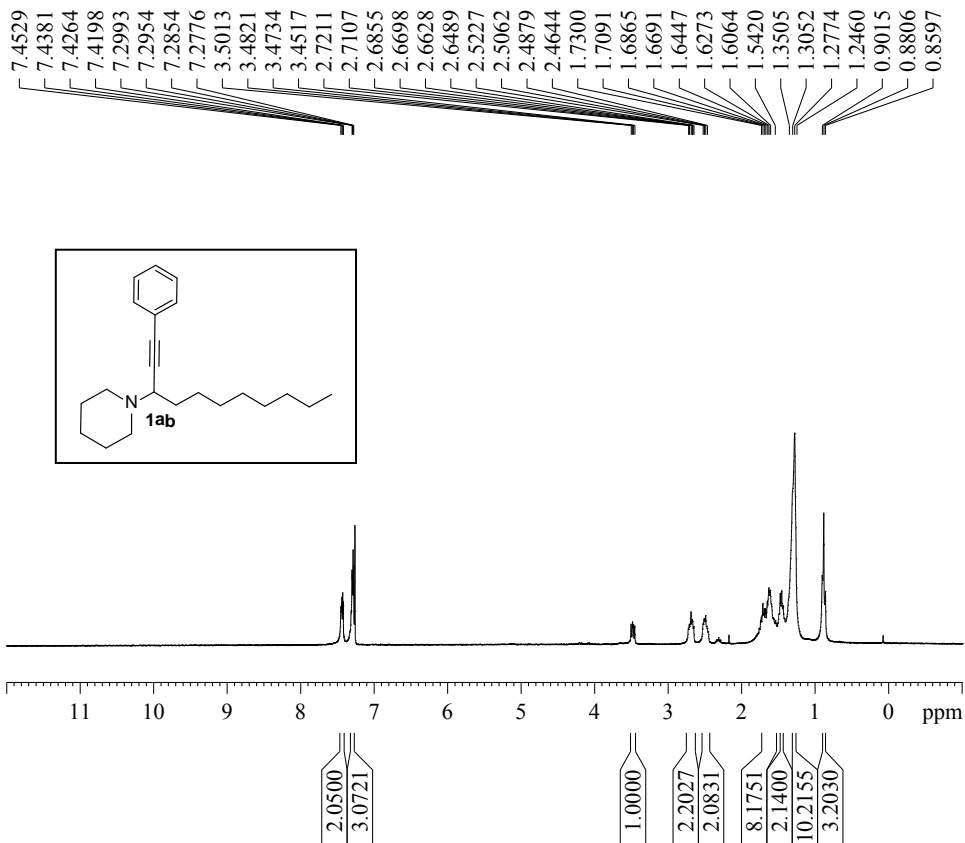
Current Data Parameters
 NAME SNA acetaldehyde 13C 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130518
 Time 15.26
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677534 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



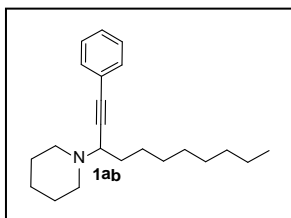
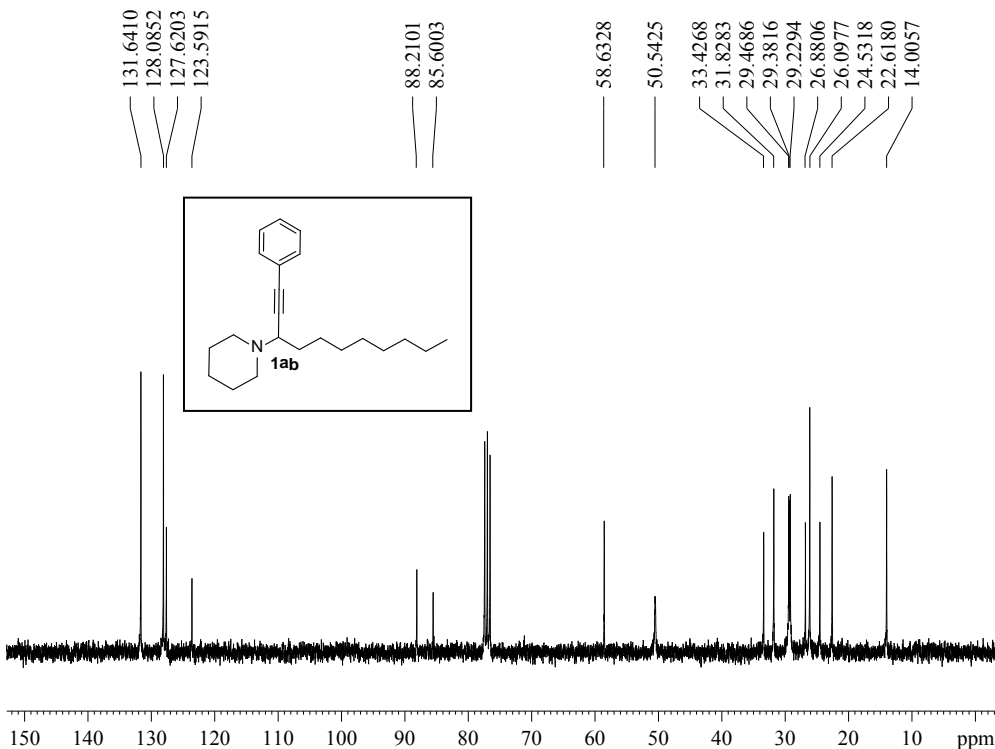
Current Data Parameters
NAME SNA (CH2)7n H5agst
EXPNO 1
PROCNO 2

F2 - Acquisition Parameters
Date_ 20130805
Time 11.22
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 574.7
DW 111.200 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 13.970 ppm
F1 4192.77 Hz
F2P -1.012 ppm
F2 -303.63 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm



Current Data Parameters
NAME SNA CH3(CH2)7 13C 13C
EXPNO 1
PROCNO 1

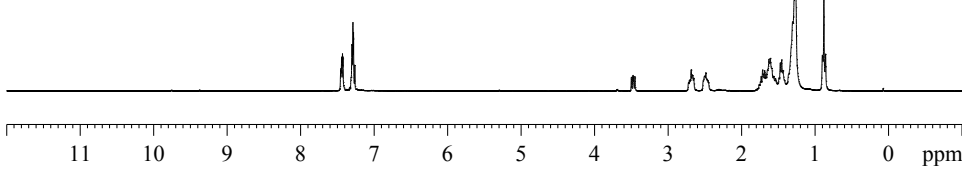
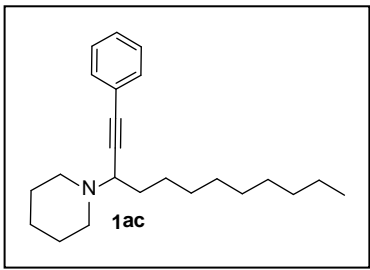
F2 - Acquisition Parameters
Date_ 20130518
Time 14.44
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677523 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

7.4538
7.4394
7.4294
7.4216
7.3132
7.3002
7.2967
7.2871
7.2793
3.4969
3.4782
3.4678
3.4469
2.7077
2.6972
2.6833
2.6702
2.6607
2.5193
2.5014
2.4836
1.7126
1.6847
1.6290
1.6116
1.5768
1.5525
1.4759
1.4550
1.4341
1.3610
1.2984
1.2670
1.2392
0.8981
0.8737
0.8528



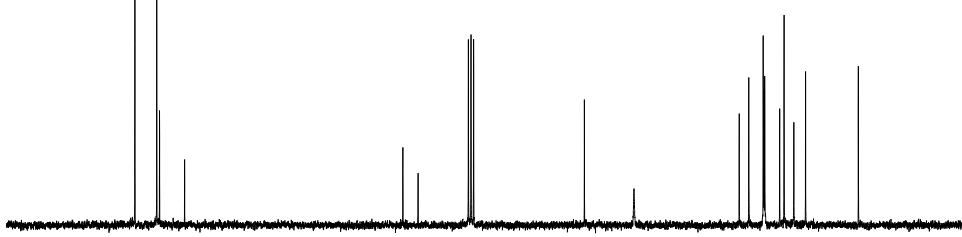
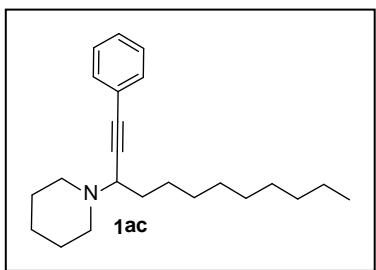
2.0557
3.0047
1.0003
2.0262
2.0364
6.2251
2.3438
14.4288
3.0228

131.6706
128.1049
127.6121
123.5536

88.0703
85.5772

58.5589

33.3815
31.8523
29.5078
29.3592
29.2577
26.8443
26.1196
24.5252
22.6409
14.0599



131.6706
128.1049
127.6121
123.5536
88.0703
85.5772
58.5589
33.3815
31.8523
29.5078
29.3592
29.2577
26.8443
26.1196
24.5252
22.6409
14.0599

Current Data Parameters
NAME SNA 373 proton
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130321
Time 22.48
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 20
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 287.4
DW 111.200 usec
DE 6.50 usec
TE 297.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13969 ppm
F1 4192.50 Hz
F2P -1.013 ppm
F2 -303.90 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm

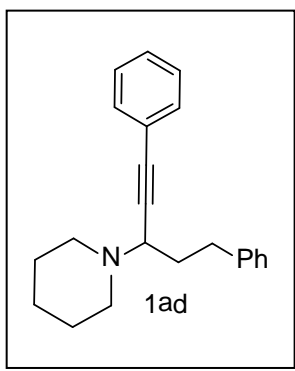
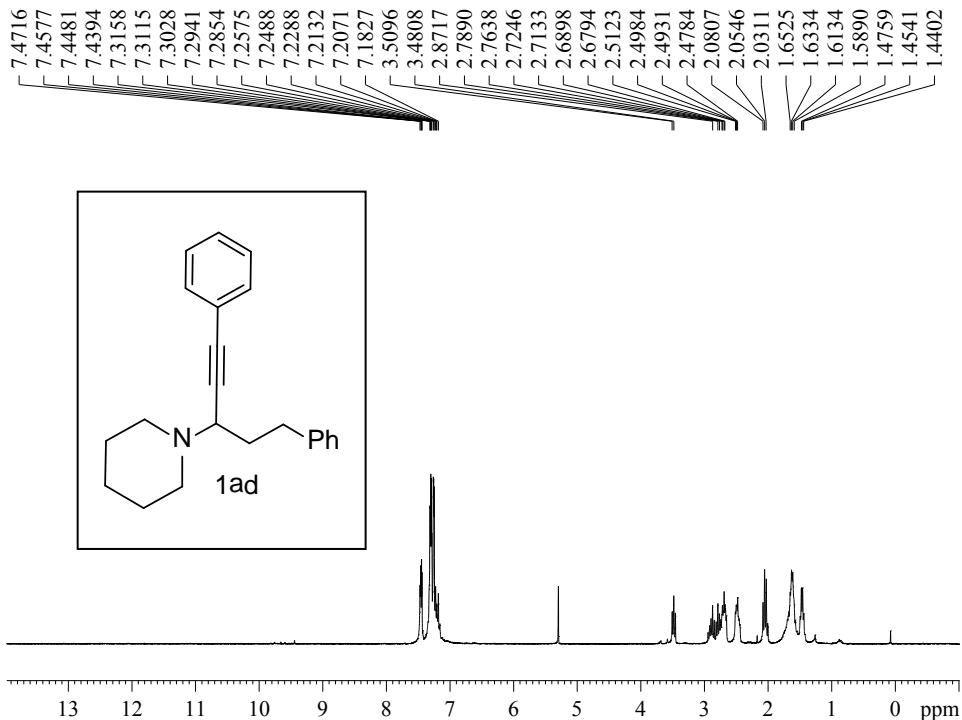
Current Data Parameters
NAME SNA decyl 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130518
Time 13.47
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677543 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

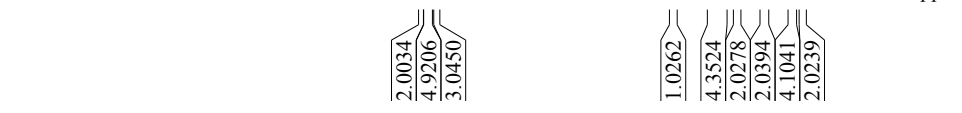


Current Data Parameters
 NAME SNA 371 proton new
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130320
 Time 16.03
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 574.7
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300067 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



141.4764
 131.4750
 128.3441
 128.0542
 127.9527
 127.5541
 125.5683
 123.2492

87.4760
 85.8816

57.2544

50.2389

34.7875

32.6133

25.9602

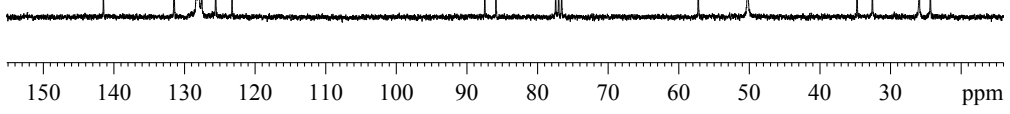
Current Data Parameters
 NAME SNA Ph(CH2)2 13C 13C
 EXPNO 1
 PROCNO 1

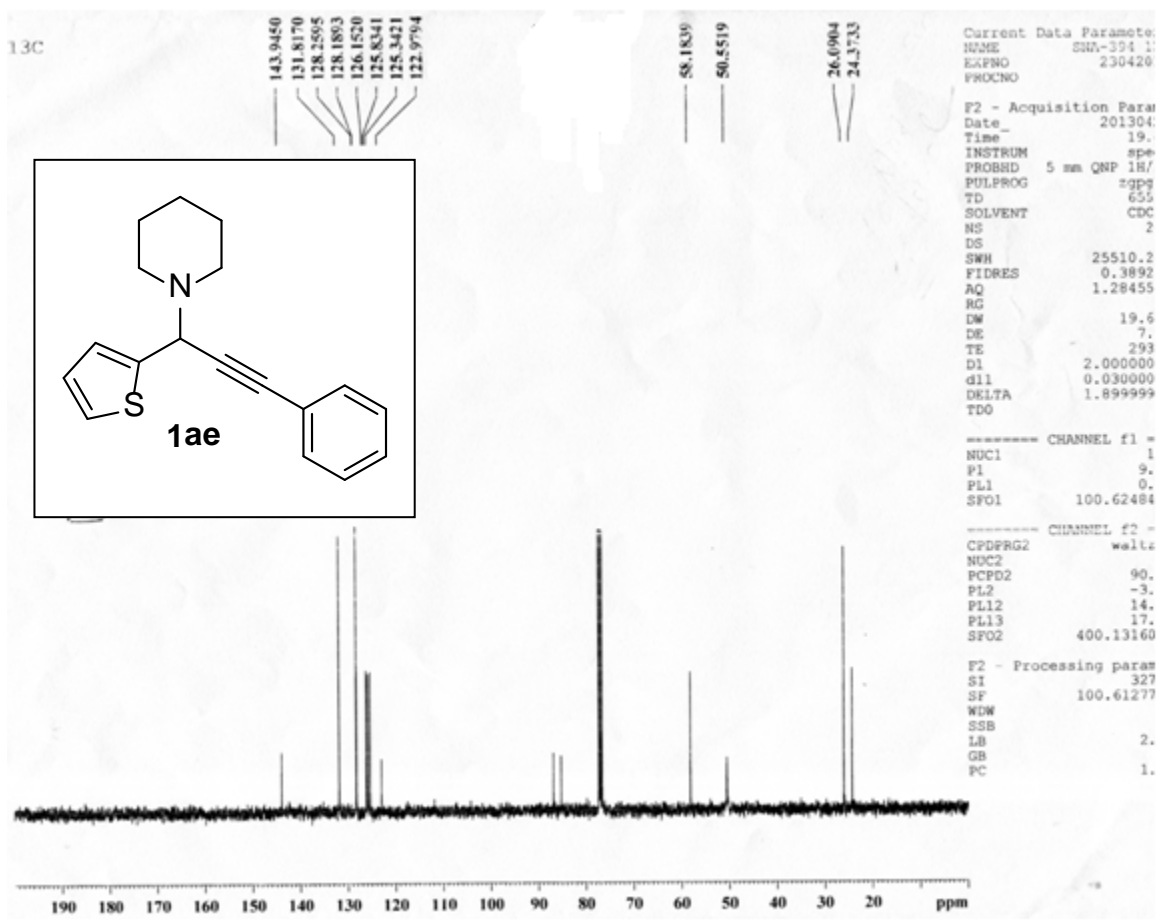
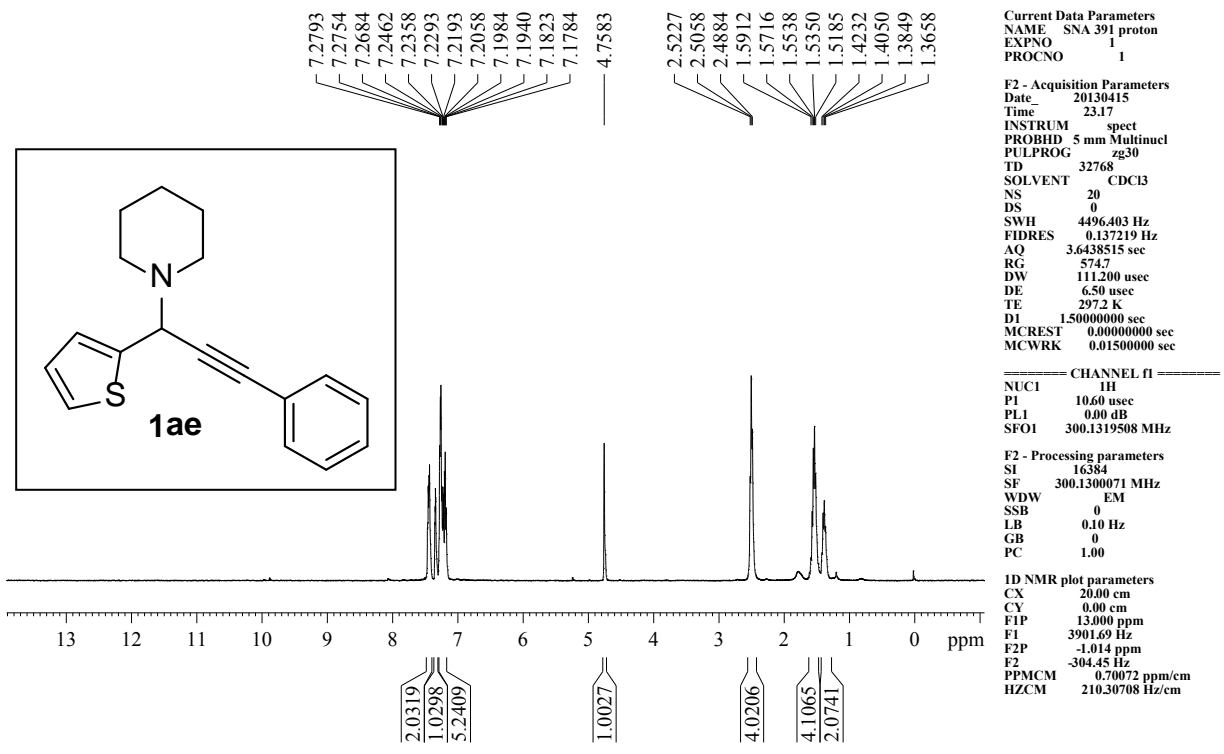
F2 - Acquisition Parameters
 Date 20130518
 Time 15.04
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

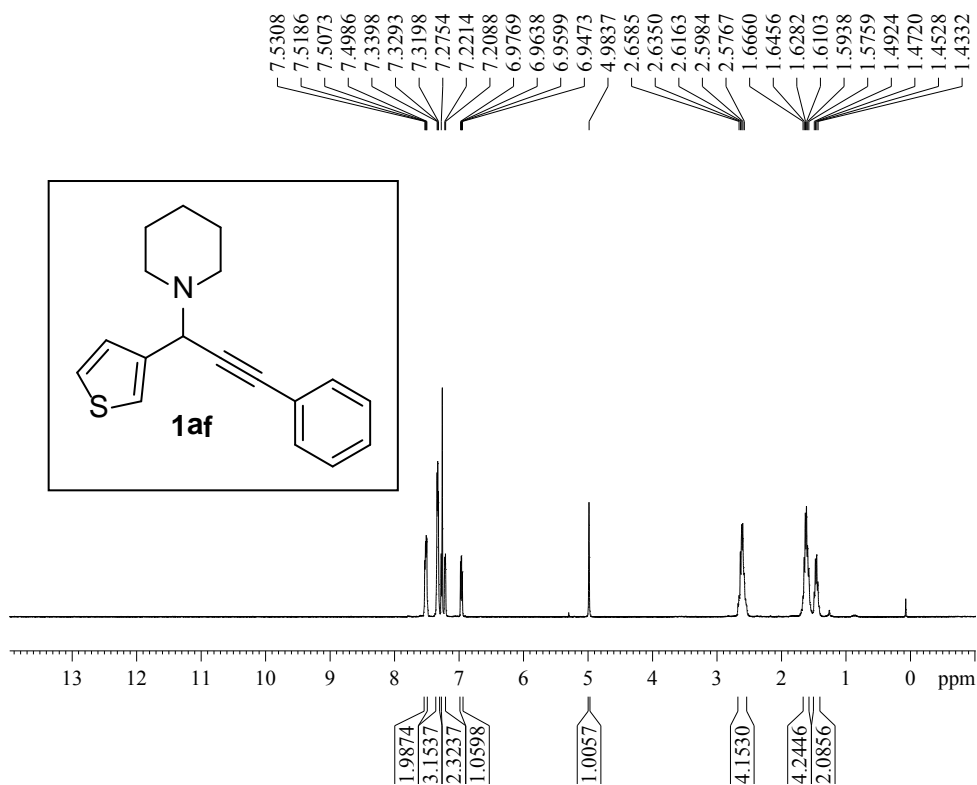
==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677500 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00







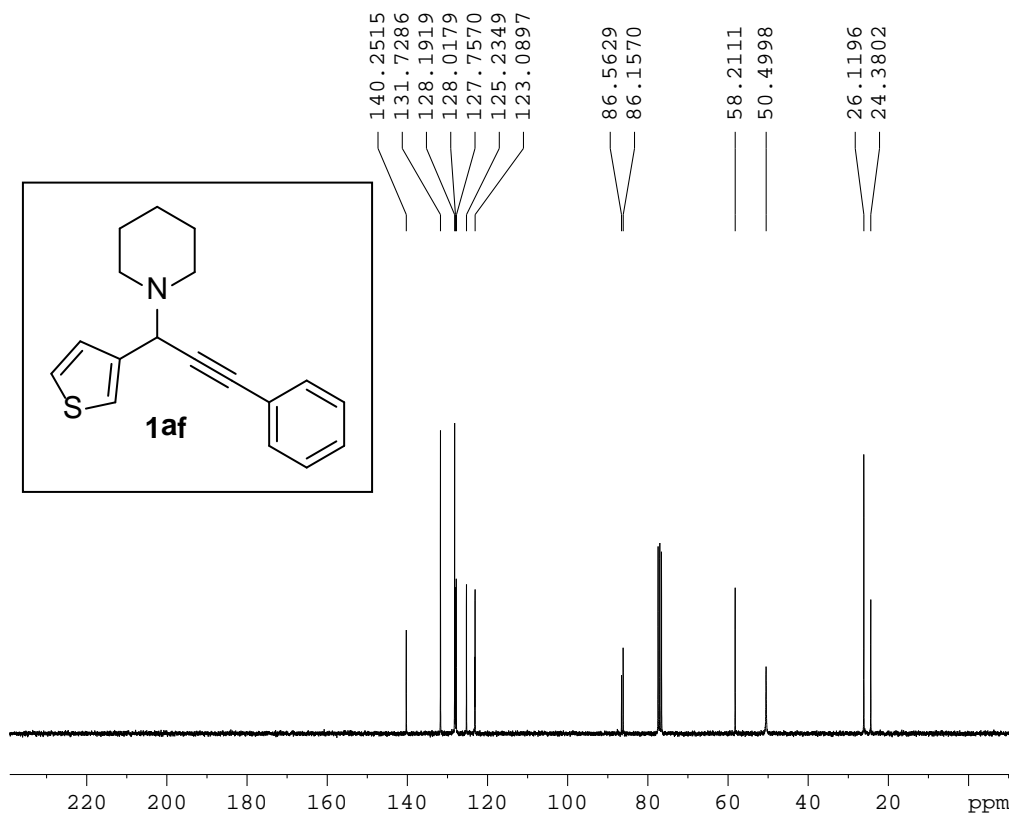
Current Data Parameters
 NAME SNA 394 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130423
 Time 12.25
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 812.7
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16364
 SF 300.1300065 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 13.969 ppm
 F1 4192.50 Hz
 F2P -1.013 ppm
 F2 -303.90 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 391 C13
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130416
 Time 0.19
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 14596.5
 DW 26.550 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

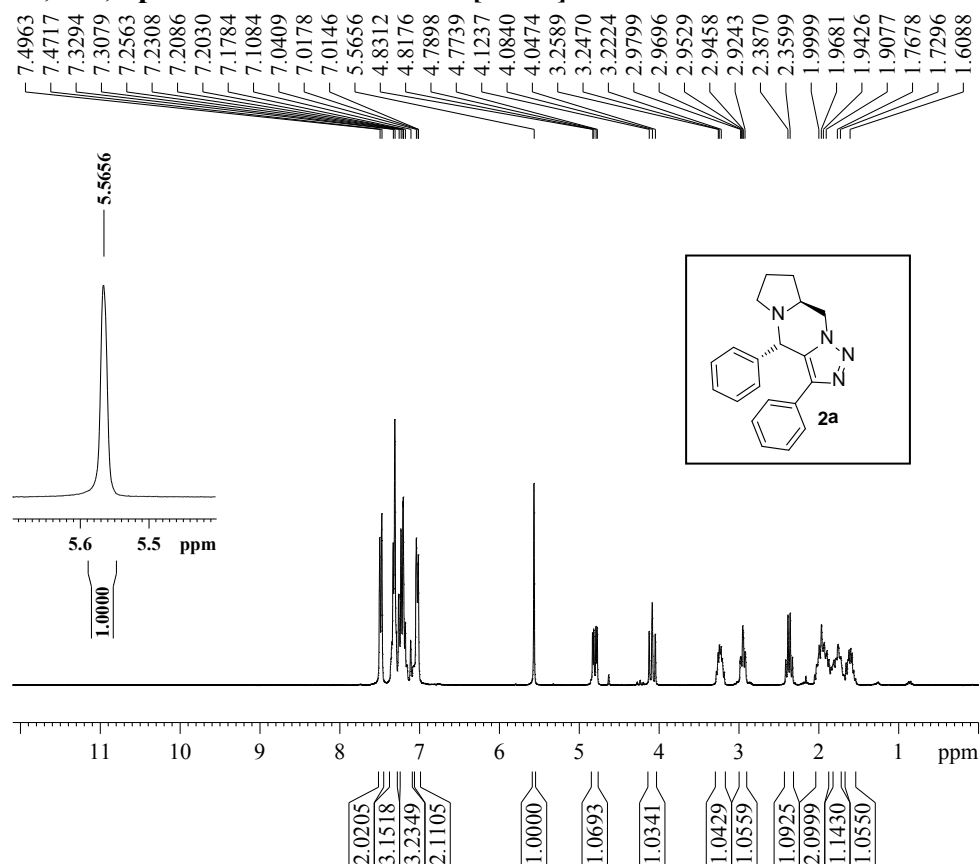
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677614 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 239.209 ppm
 F1 18052.53 Hz
 F2P -10.334 ppm
 F2 -779.86 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61951 Hz/cm

¹H, ¹³C, Spectra of fused triazoles [2a-2t]

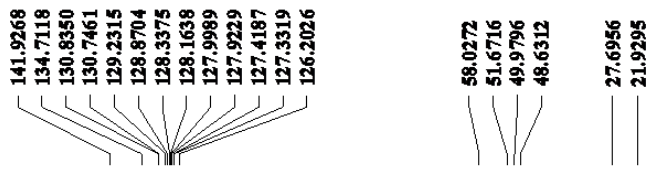


Current Data Parameters
 NAME SNA T
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20130510
 Time 23.31
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 256
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 DI 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.972 ppm
 F1 4193.32 Hz
 F2 -1.010 ppm
 F2 -303.08 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82014 Hz/cm



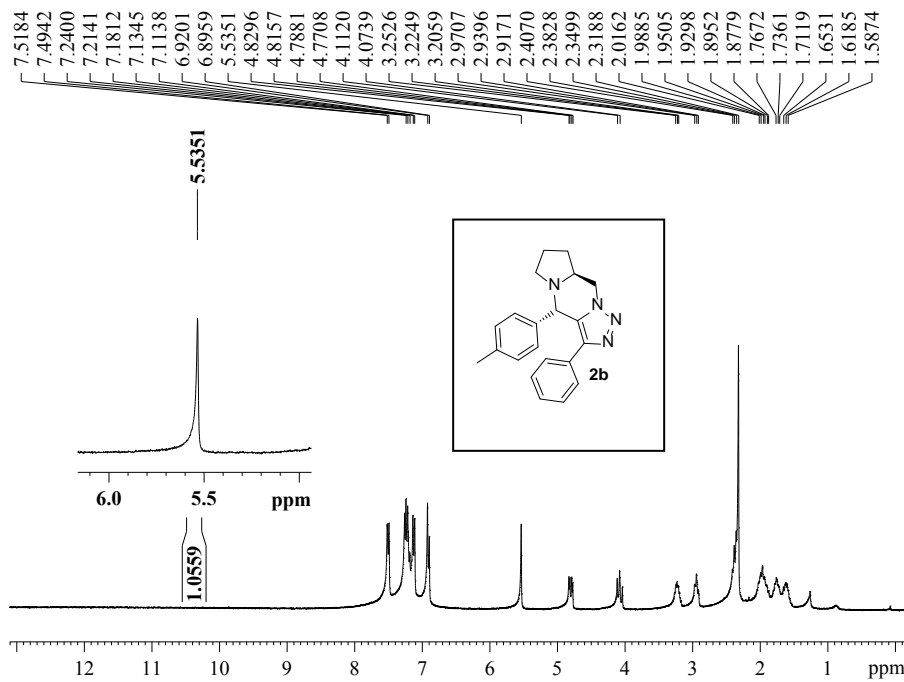
Current Data Parameters
 NAME sld ben T 13C ta1a
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20131020
 Time 23.07
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 192
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 302.2 K
 DI 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677614 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

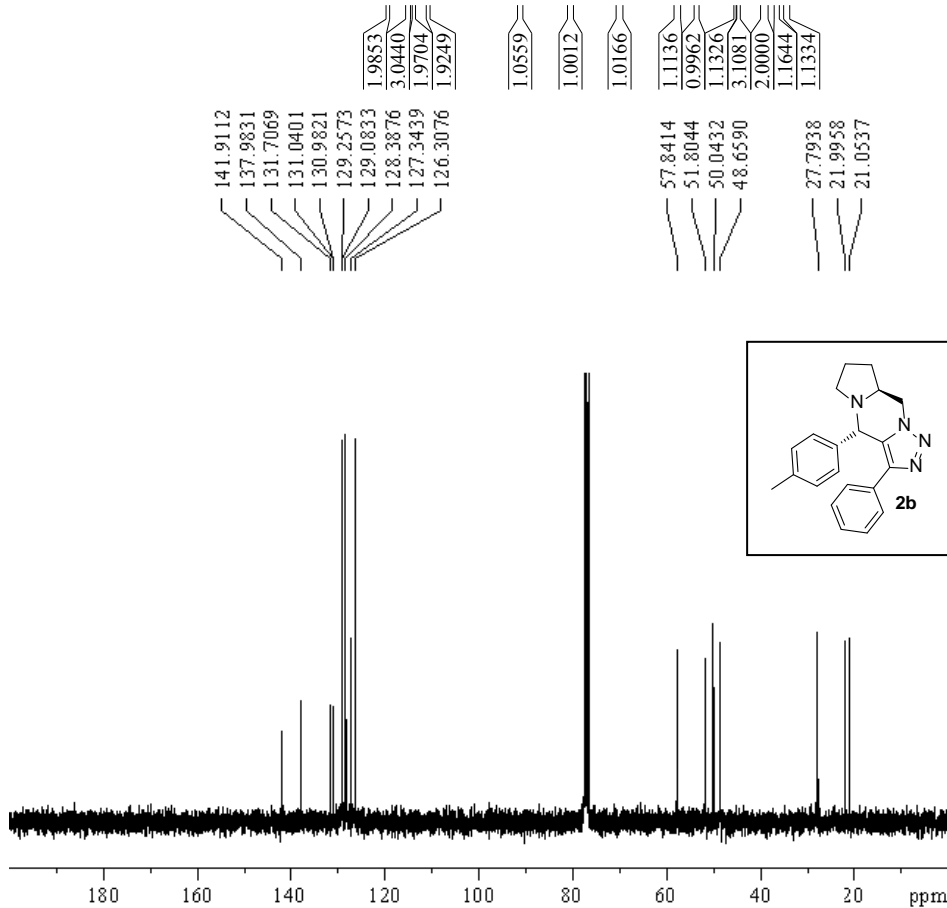


Current Data Parameters
 NAME skl p ch3 taflo
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20131020
 Time 22.31
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 512
 DW 111.200 usec
 DE 6.50 usec
 TE 302.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME SNA 18 13C
 EXPNO 2
 PROCNO 1

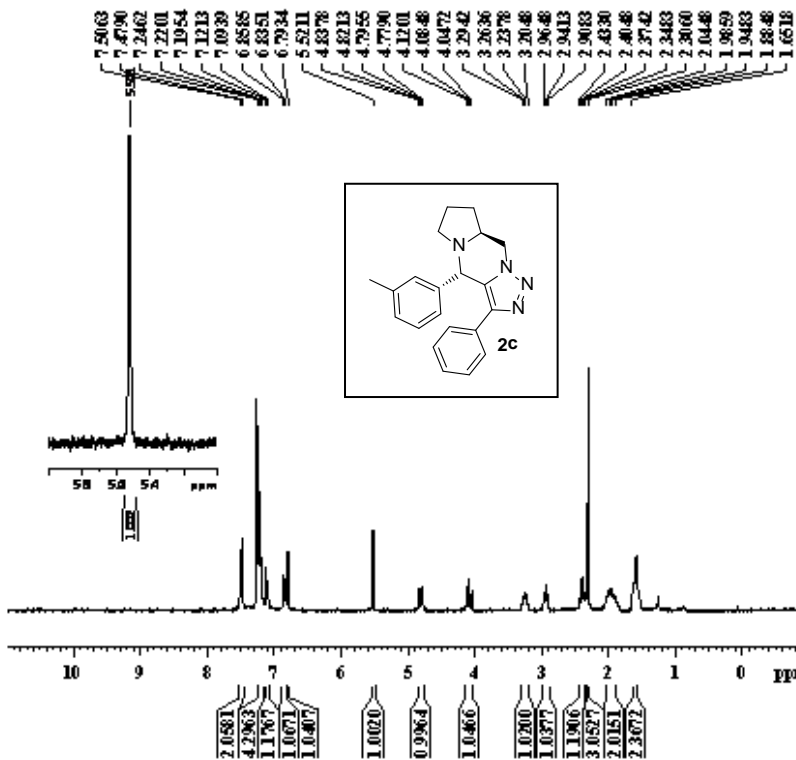
F2 - Acquisition Parameters
 Date 20130511
 Time 0.46
 INSTRUM spect
 PROBHD 5mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18832.203 Hz
 FIDRES 0.287560 Hz
 AQ 1.740308 sec
 RG 322.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763078 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313006 MHz

F2 - Processing parameters
 SI 32768
 SF 754677.222 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FID 239.323 ppm
 F1 1806.115 Hz
 F2 -10.219 ppm
 F2 -771.24 Hz
 FPMCM 124.771 ppm/cm
 HZCM 941.61931 Hz/cm

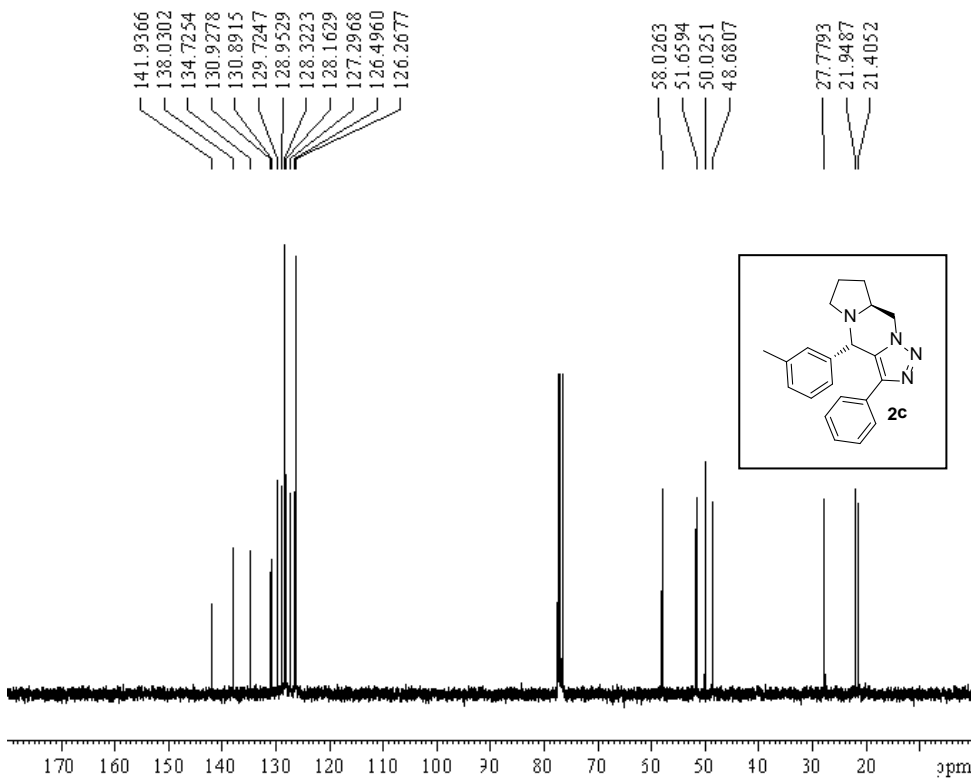


Current Data Parameters
 NAME sblmch3.taflo
 EXPN0 1
 PRO CNO 1

F2 - Acquisition Parameters
 Date 20131020
 Time 22.27
 INSTRUM spect
 PROBHD 5mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4486.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 72.41
 DW 111.200 usec
 DE 6.50 usec
 TE 302.2 K
 DI 150000000 sec
 MCREST 0.0000000 sec
 MCWREK 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SF01 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300059 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 FC 1.00



Current Data Parameters
 NAME SNAAL7 C13
 EXPN0 1
 PRO CNO 1

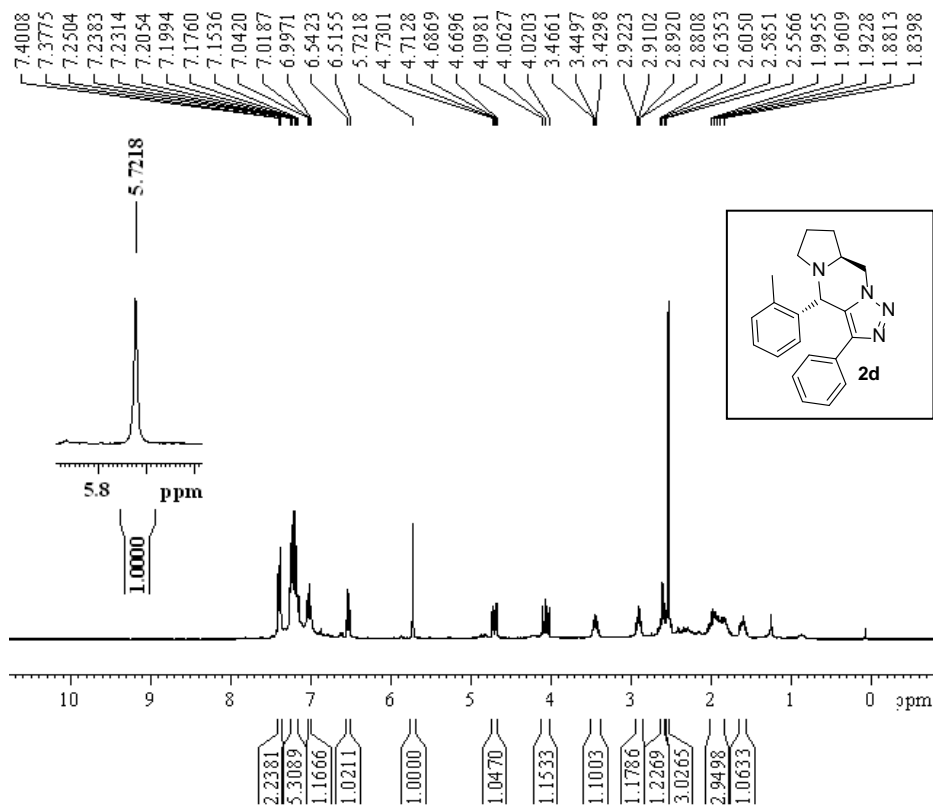
F2 - Acquisition Parameters
 Date 20130808
 Time 4.01
 INSTRUM spect
 PROBHD 5mm Multinuc
 PULPROG zgpg30
 TD 66536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18322.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 18396.4
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 DI 150000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWREK 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SF01 75.4763978 MHz

==== CHANNEL f2 =====
 CDFRC2 waltz16
 NUC2 1H
 P CDF2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SF02 300.131806 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4675551 MHz
 WDW BH
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FID 239.232 ppm
 F1 18458.85 Hz
 F2 -773.54 Hz
 F2CM 12.47711 ppm/cm
 WZ FM 8.0 619.0 15.5 cm

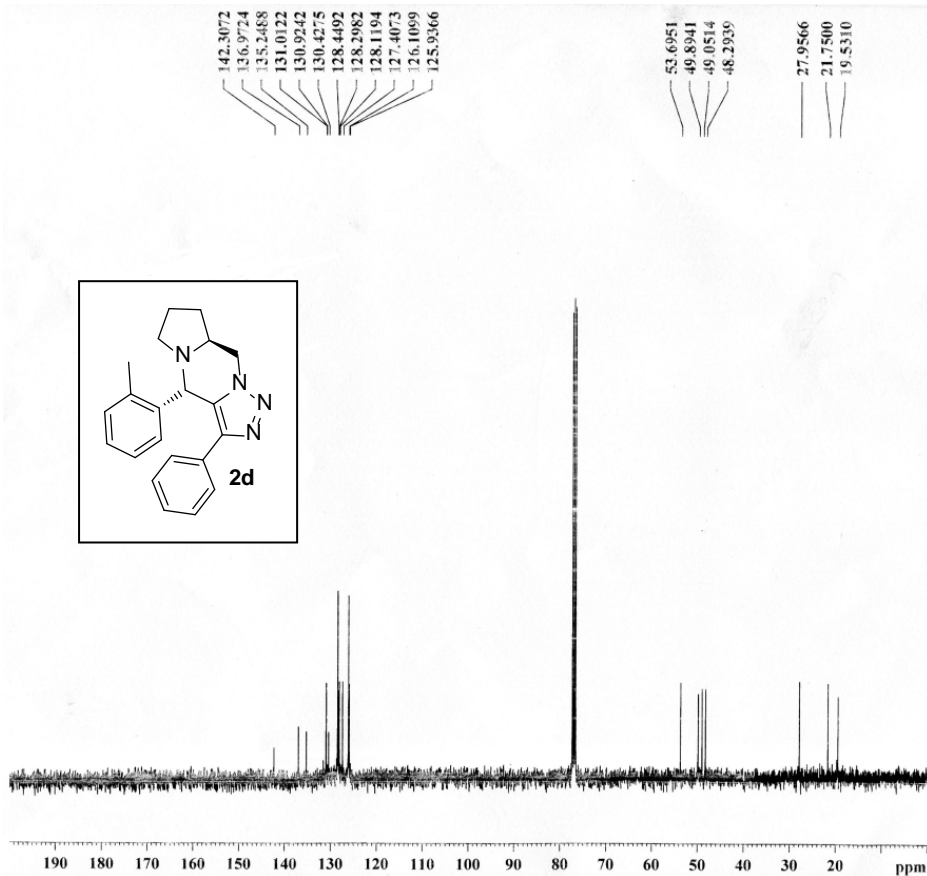


Current Data Parameters
 NAME SNA A.20.113C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130510
 Time 15.37
 INSTRUM spect
 PROBHD 5 mm Multiview1
 PULPROG zg30
 TD 32768
 SOLVENT CD CB
 NS 5
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 256
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRTK 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300089 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



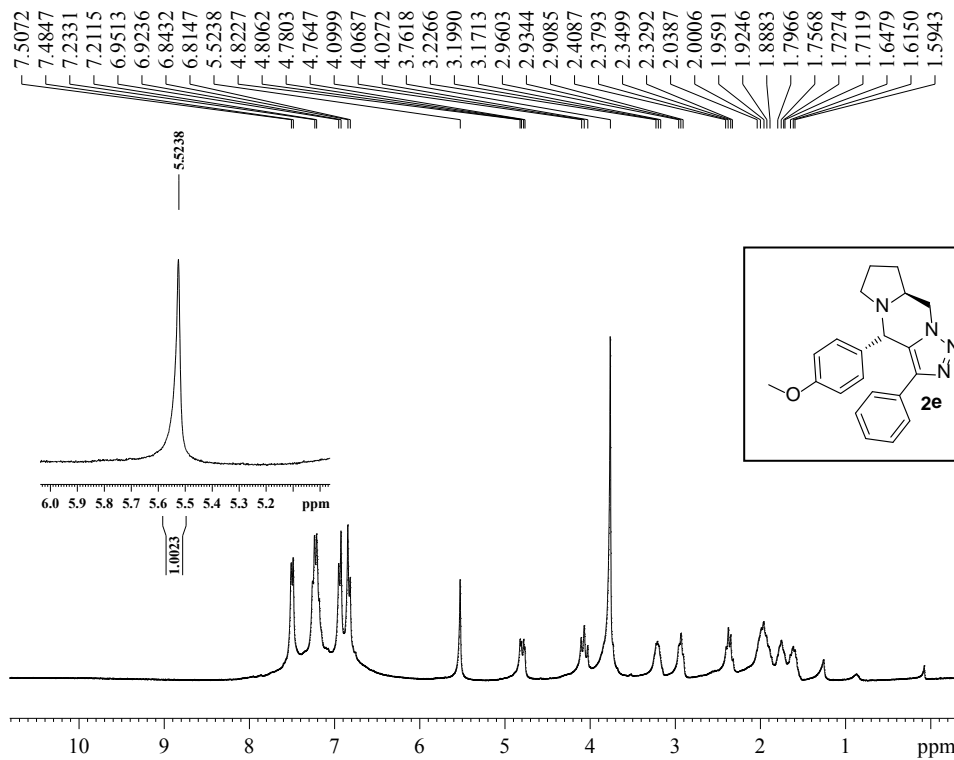
Current Data Parameters
 NAME SNA-20.13C
 EXPNO 10052013
 PROCNO 1

F2 - Acquisition Parame
 Date_ 20130510
 Time_ 19.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 250
 DS 0
 SWH 25510.203
 FIDRES 0.389255
 AQ 1.2845556
 RG 4
 DW 19.600
 DE 7.00
 TE 295.0
 D1 2.0000000
 d11 0.0300000
 DELTA 1.8999999
 TD0 1

==== CHANNEL f1 ===
 NUC1 13C
 P1 9.80
 PL1 0.00
 SFO1 100.6248425

==== CHANNEL f2 ===
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00
 PL2 -3.00
 PL12 14.00
 PL13 17.00
 SFO2 400.1316005

F2 - Processing paramet
 SI 32768
 SF 100.6127767
 WDW EM
 SSB 0
 LB 2.00
 GB 0
 PC 1.00

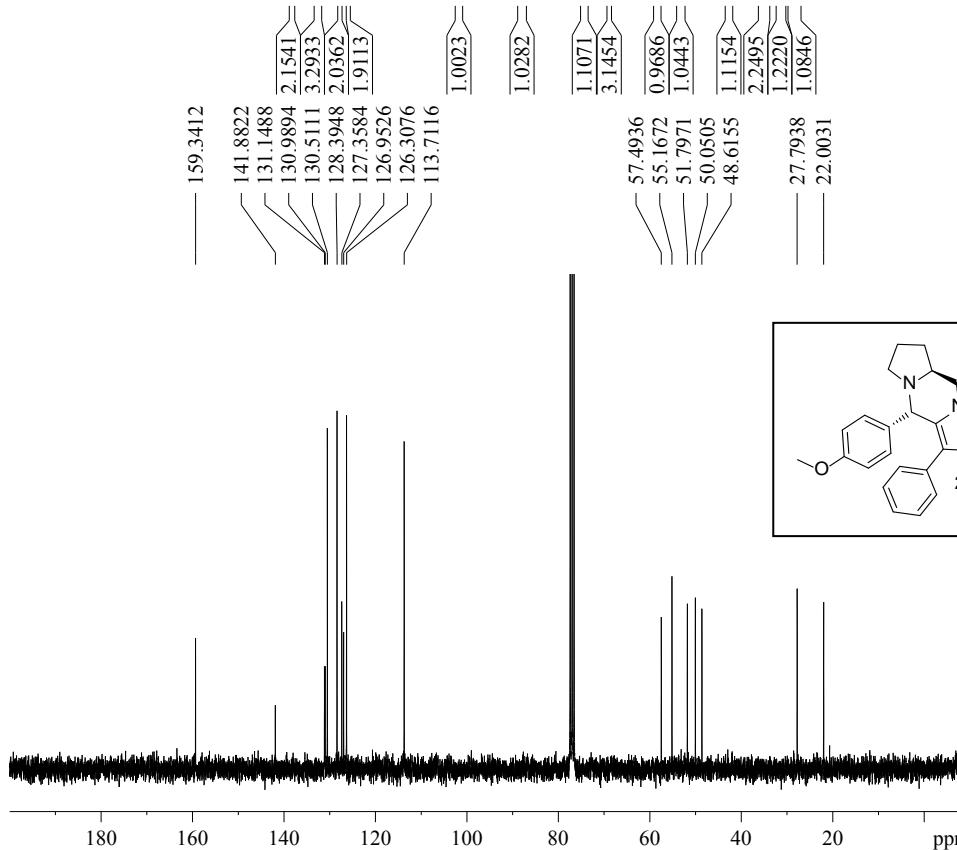


Current Data Parameters
 NAME skl p-0ch3 tafto
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20131020
 Time 22:37
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 228.1
 DW 111.200 usec
 DE 6.50 usec
 TE 302.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300046 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME SNA A24 C13
 EXPNO 1
 PROCNO 1

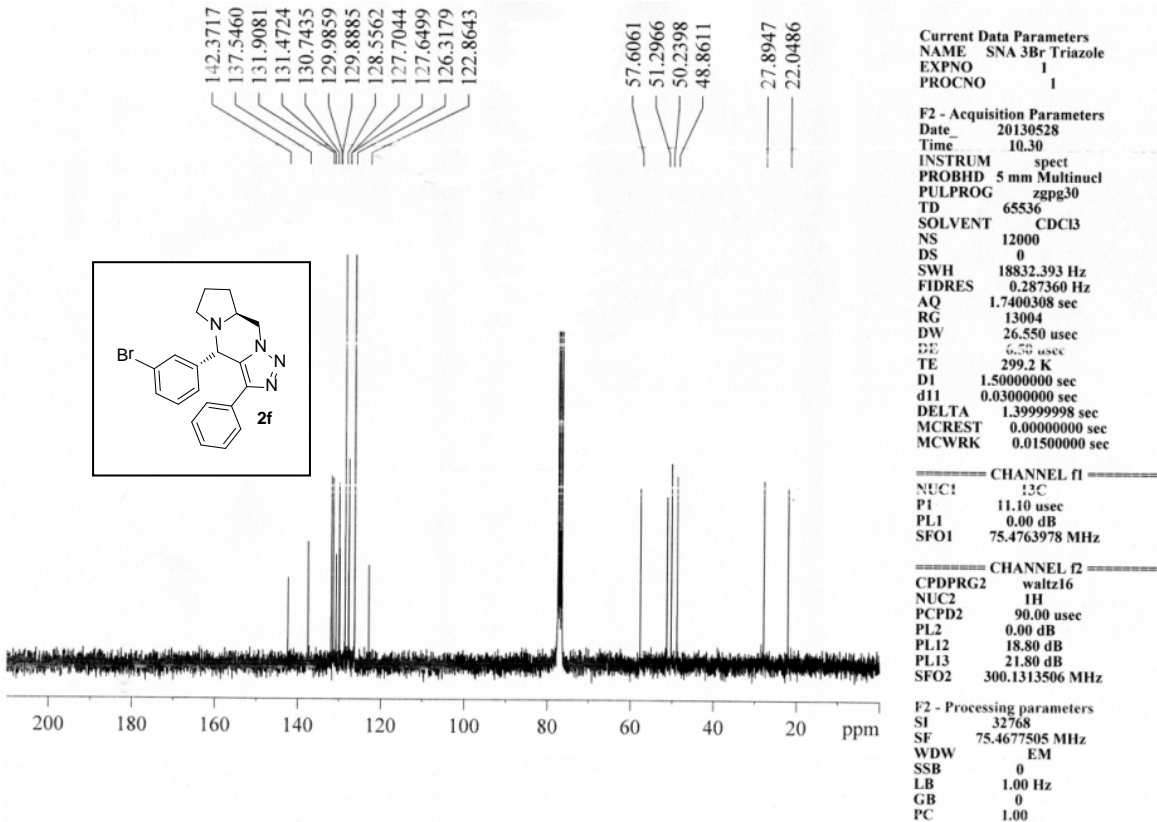
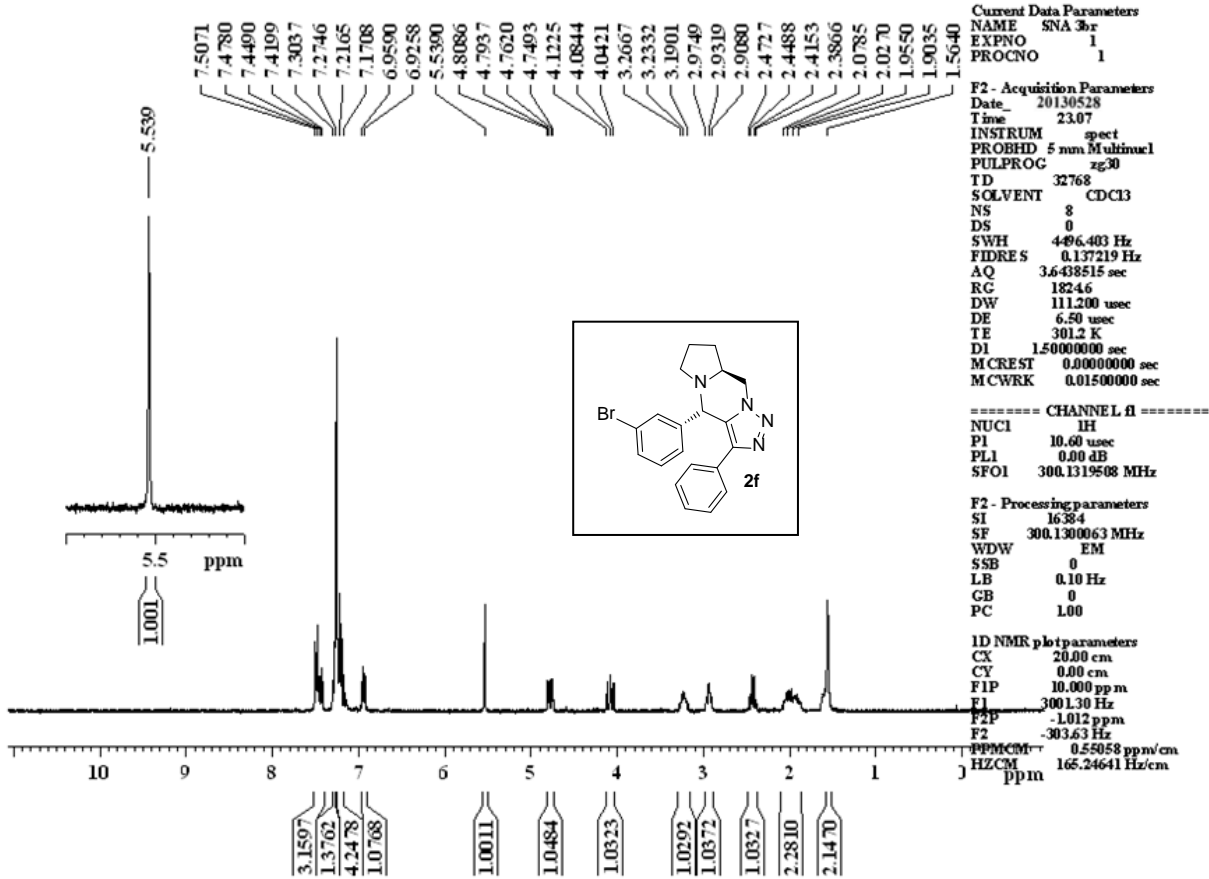
F2 - Acquisition Parameters
 Date 20130508
 Time 2:00
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

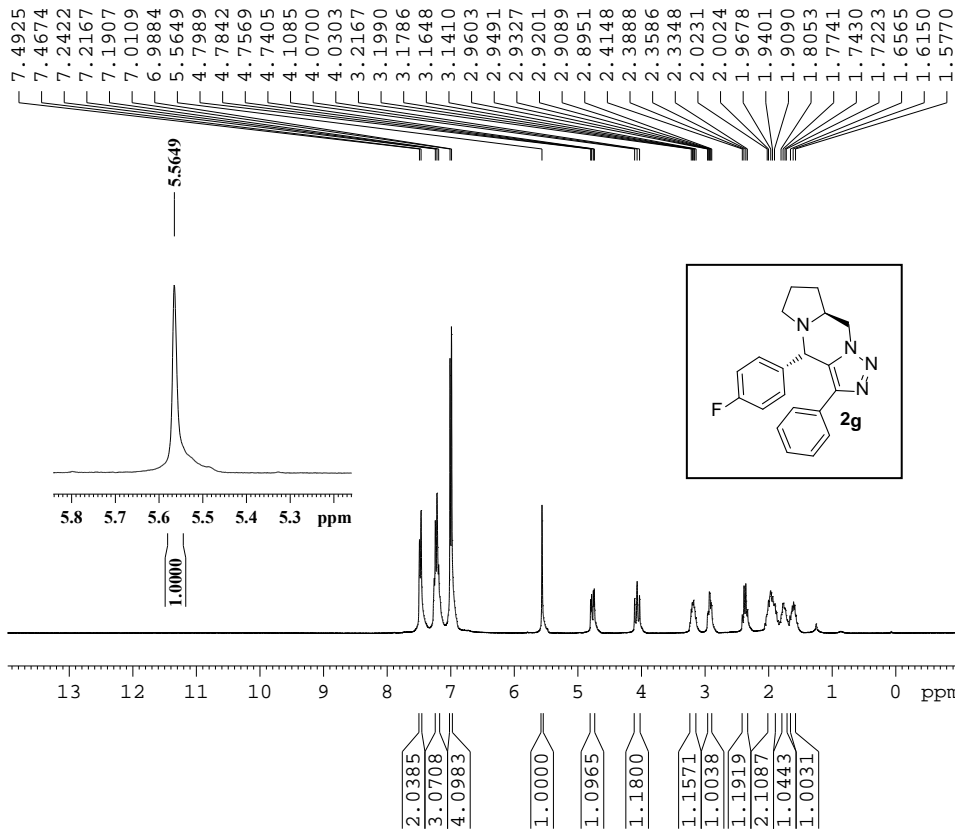
CHANNEL f1
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677523 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 220.000 ppm
 F1 16602.90 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 830.14520 Hz/cm





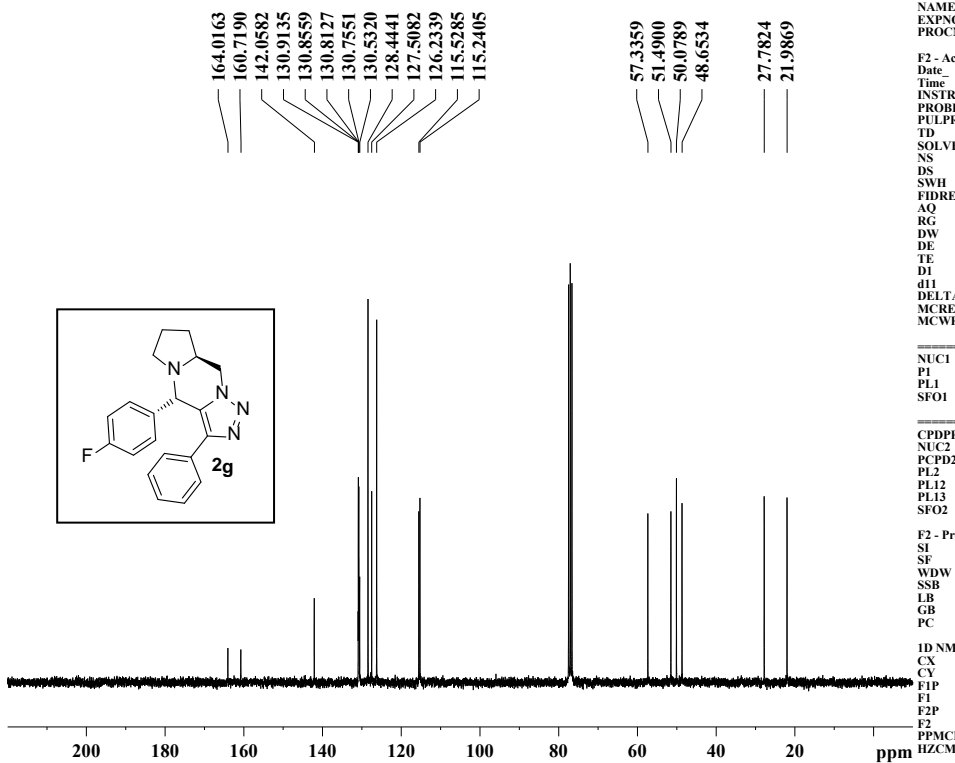
Current Data Parameters
 NAME skl 4 ftaflo
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131020
 Time 20.26
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 256
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300068 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 13.968 ppm
 F1 4192.23 Hz
 F2P -1.013 ppm
 F2 -304.18 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA A23 C13
 EXPNO 1
 PROCNO 1

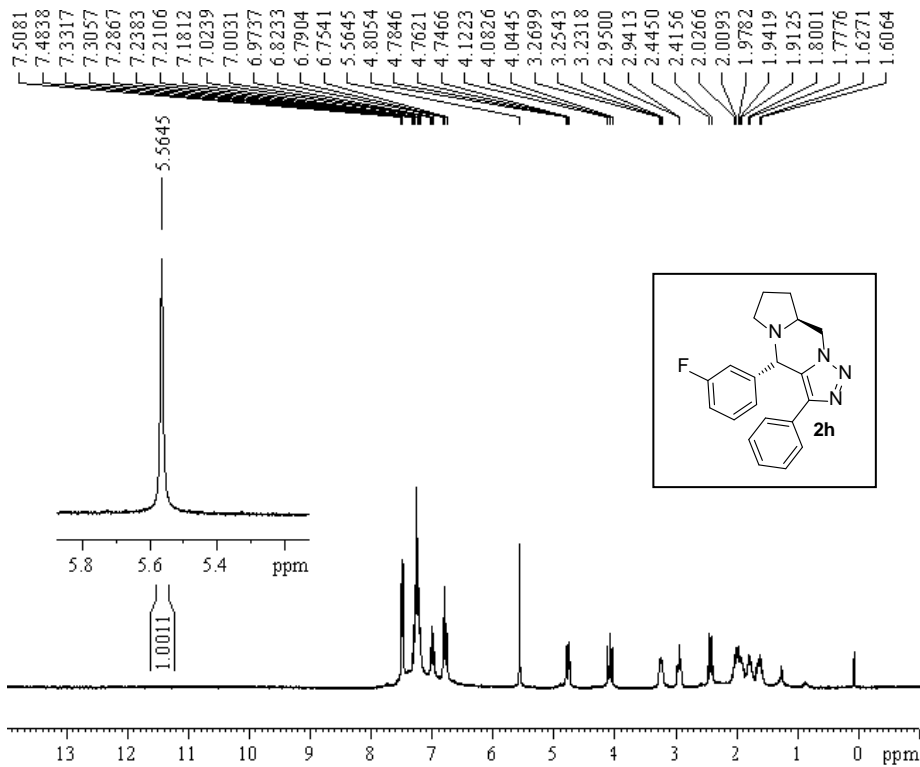
F2 - Acquisition Parameters
 Date_ 20130508
 Time 3.00
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677551 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 239.292 ppm
 F1 18058.85 Hz
 F2P -10.250 ppm
 F2 -773.54 Hz
 PPMCM 14.7711 ppm/cm
 HZCM 941.61969 Hz/cm

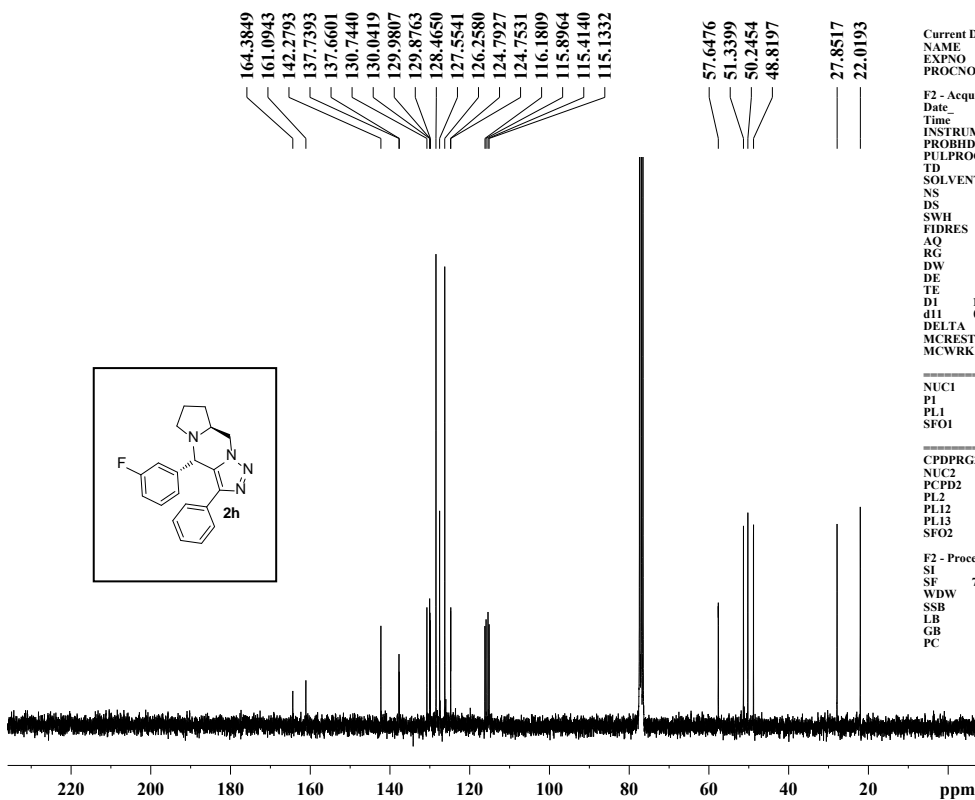


Current Data Parameters
NAME sld3 f infb
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131020
Time 18.59
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCB
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 574.7
DW 111.200 usec
DE 6.50 usec
TE 301.2 K
D1 1.5000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



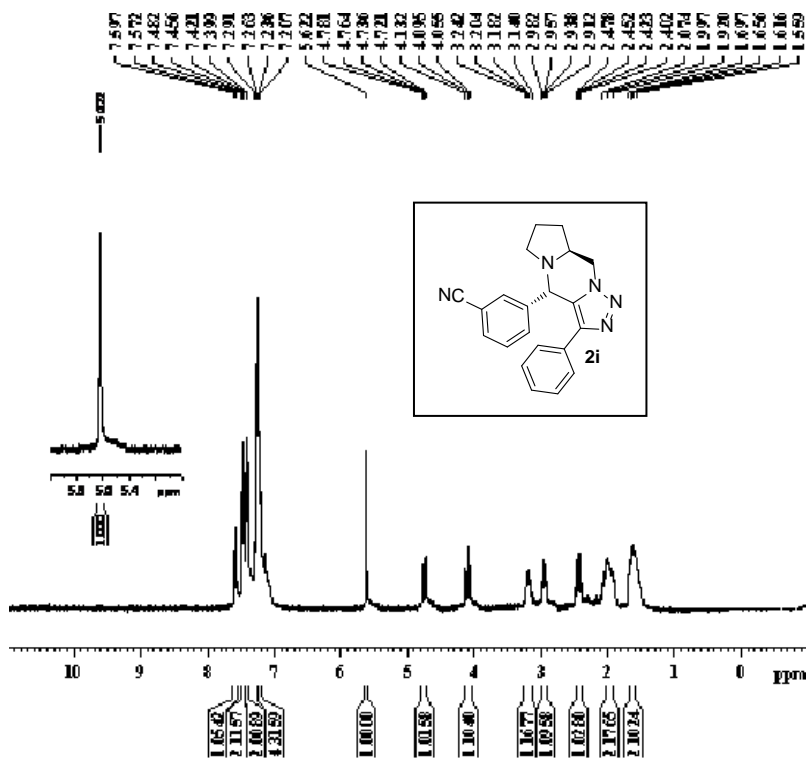
Current Data Parameters
NAME 3f triazole
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130708
Time 9.23
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10707
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 18390.4
DW 26.550 usec
DE 6.50 usec
TE 300.2 K
D1 1.5000000 sec
d11 0.0300000 sec
DELTA 1.3999999 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

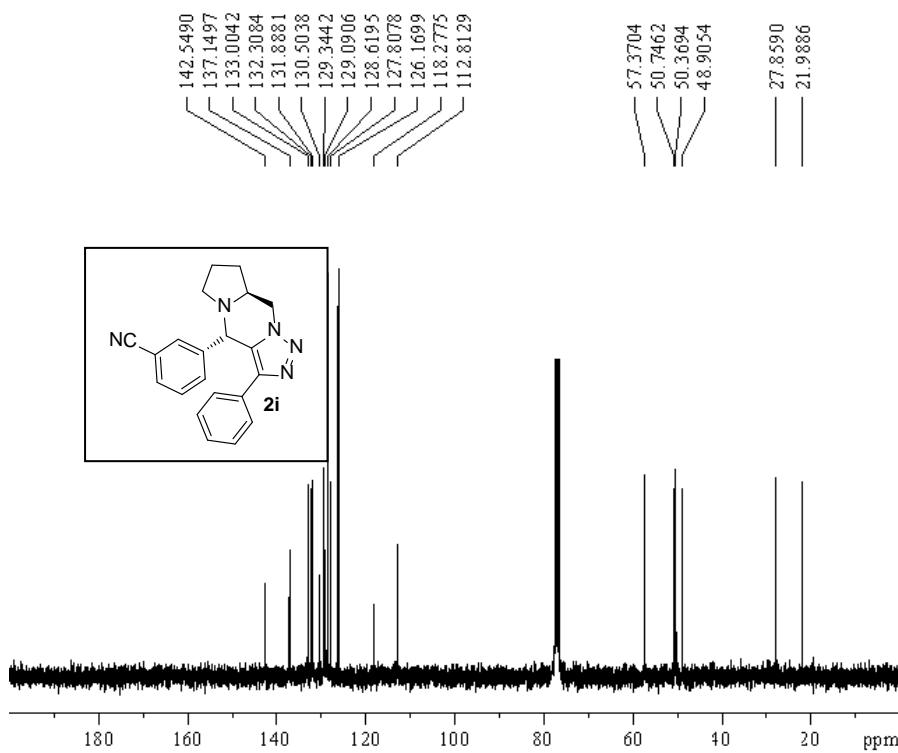


Current Data Parameters
 NAME sld3en.talks
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131020
 Time 22:41
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCB
 NS 8
 DS 0
 SWH 4496.003 Hz
 FIDRES 0.137219 Hz
 AQ 3.6419514 sec
 RG 574.7
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWVK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SF01 300.1319508 MHz

F2 - Processing parameters
 SI 16394
 SF 300.1300076 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



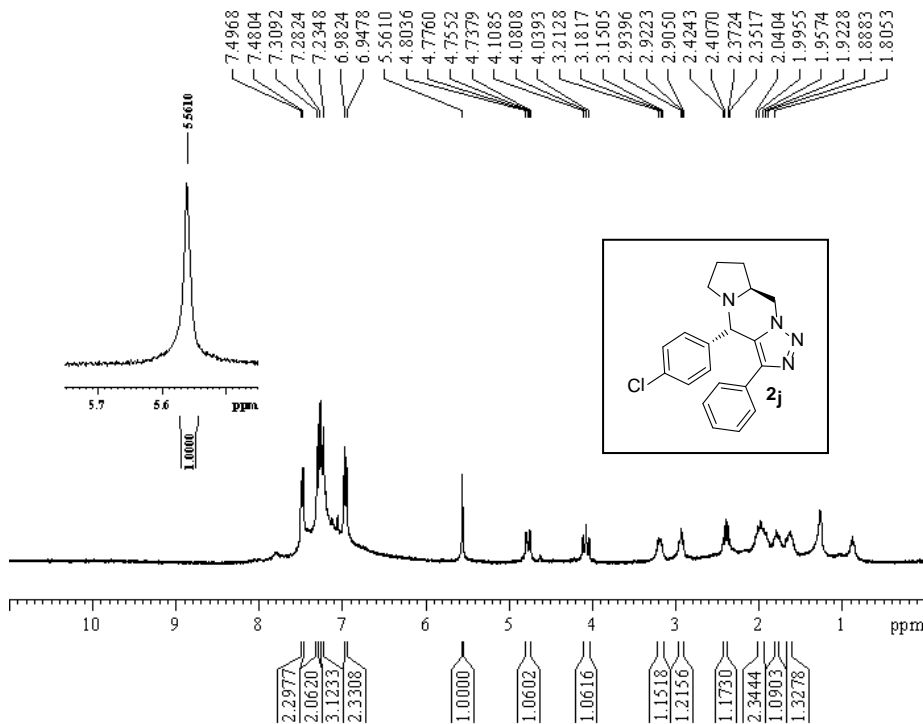
Current Data Parameters
 NAME 3 cynotriazole 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130716
 Time 9:34
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCB
 NS 11377
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWVK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SF01 75.4763978 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SF02 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677517 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



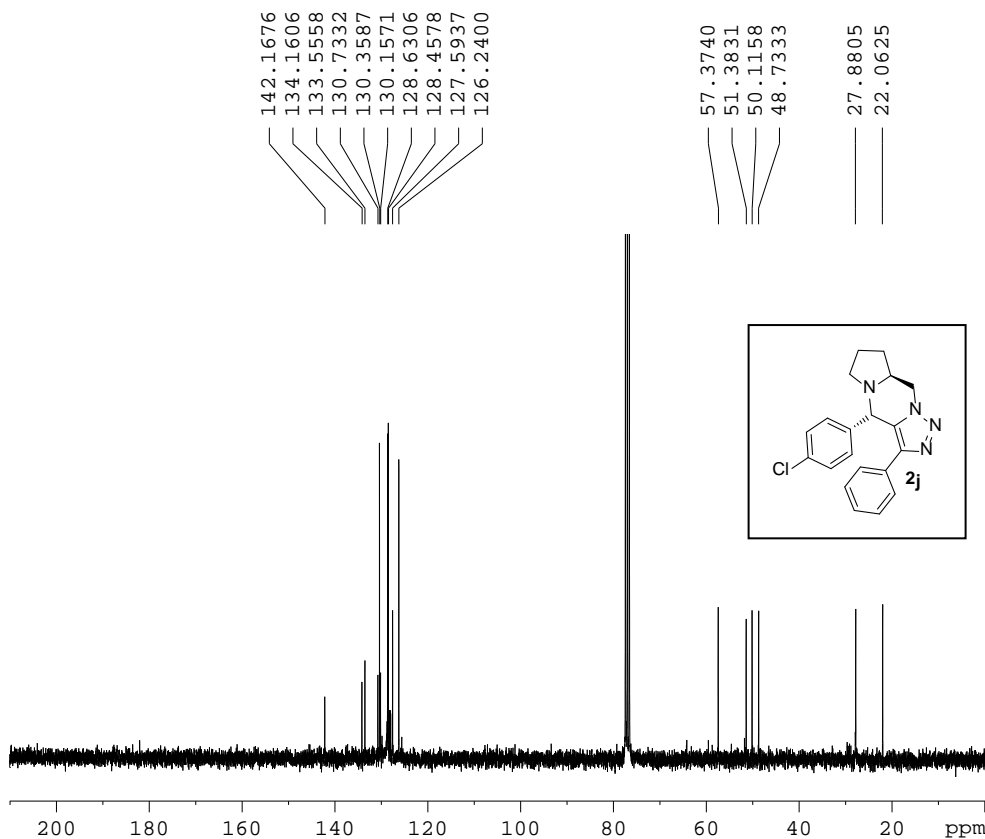
Current Data Parameters
 NAME s141414f6
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131020
 Time 20:33
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 512
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300657 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.972 ppm
 F1 4193.22 Hz
 F2 -1.010 ppm
 FZ -303.08 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 22482013 Hz/cm



Current Data Parameters
 NAME SNA del T C13
 EXPNO 1
 PROCNO 1

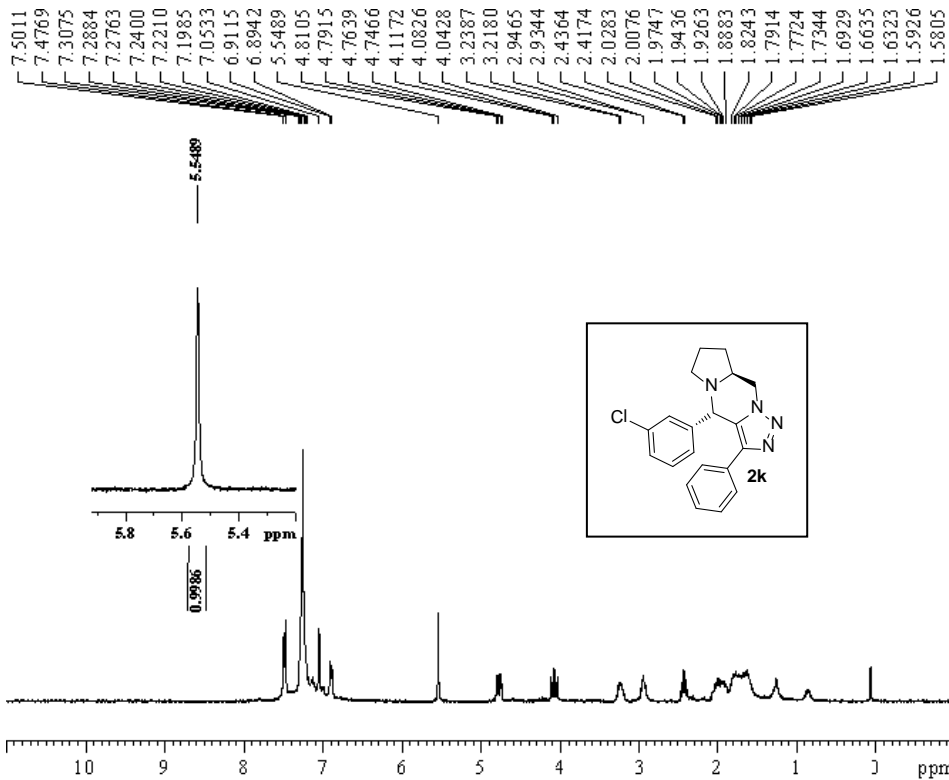
F2 - Acquisition Parameters
 Date_ 20130507
 Time 4:49
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 dH1 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677523 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 240.000 ppm
 F1 18112.26 Hz
 F2P 0.000 ppm
 FZ 0.00 Hz
 PPMCM 12.00000 ppm/cm
 HZCM 905.61298 Hz/cm

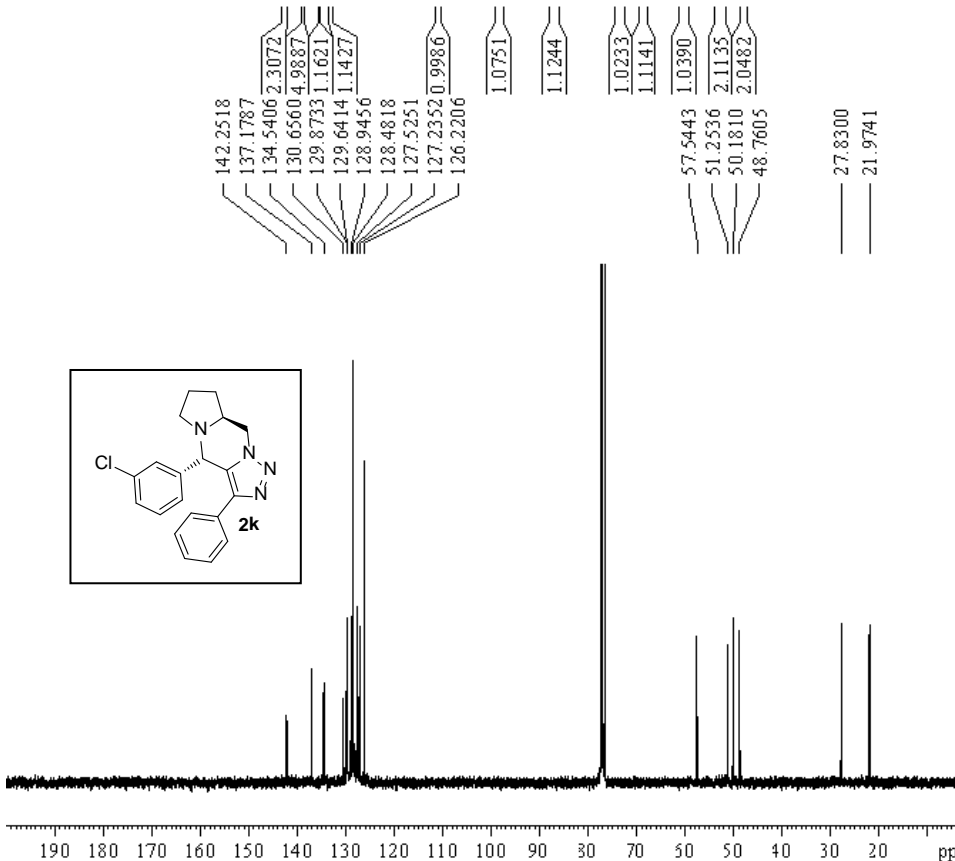


Current Data Parameters
 NAME SNA383-cl-triazole
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130531
 Time 16.48
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RC 724.1
 DW 111.200 usec
 DE 6.50 usec
 TE 300.2 K
 DI 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.130057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME SNA383-TCB
 EXPNO 1
 PROCNO 1

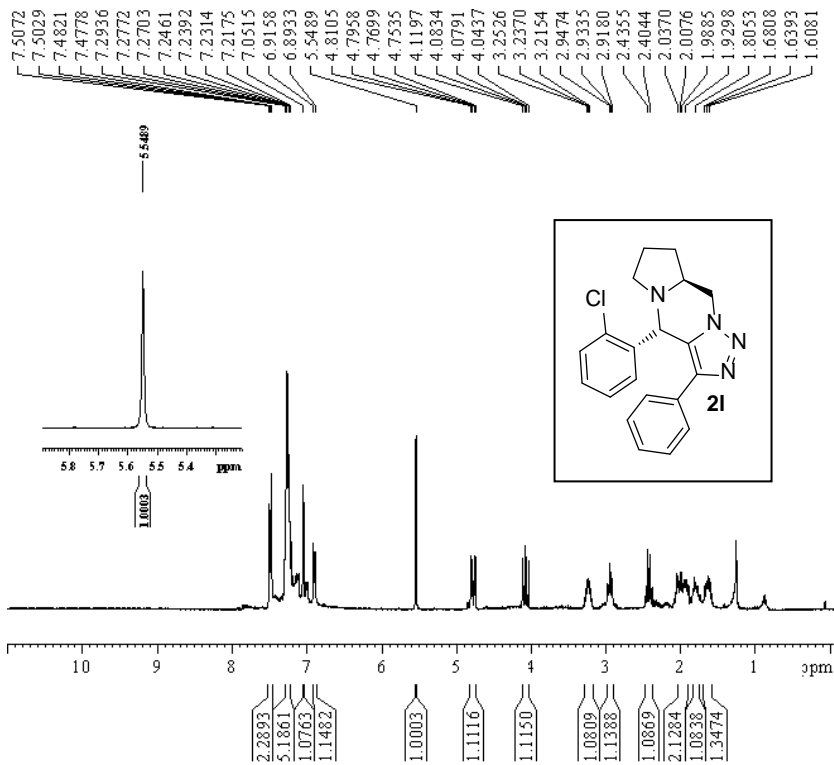
F2 - Acquisition Parameters
 Date_ 20130507
 Time 3.41
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400388 sec
 RC 16384
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 DI 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.2999998 sec
 MCREST 0.0000000 sec
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763976 MHz

===== CHANNEL f2 =====
 CENERG2 vsHz16
 NUC2 1H
 F CFB2 90.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 21.00 dB
 SFO2 300.1313806 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677534 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FID 240.000 ppm
 F1 16112.26 Hz
 F2 1.00 ppm
 F2 75.47 Hz
 FFCM 12.0500 ppm/cm
 HZ CM 909.38635 Hz/cm



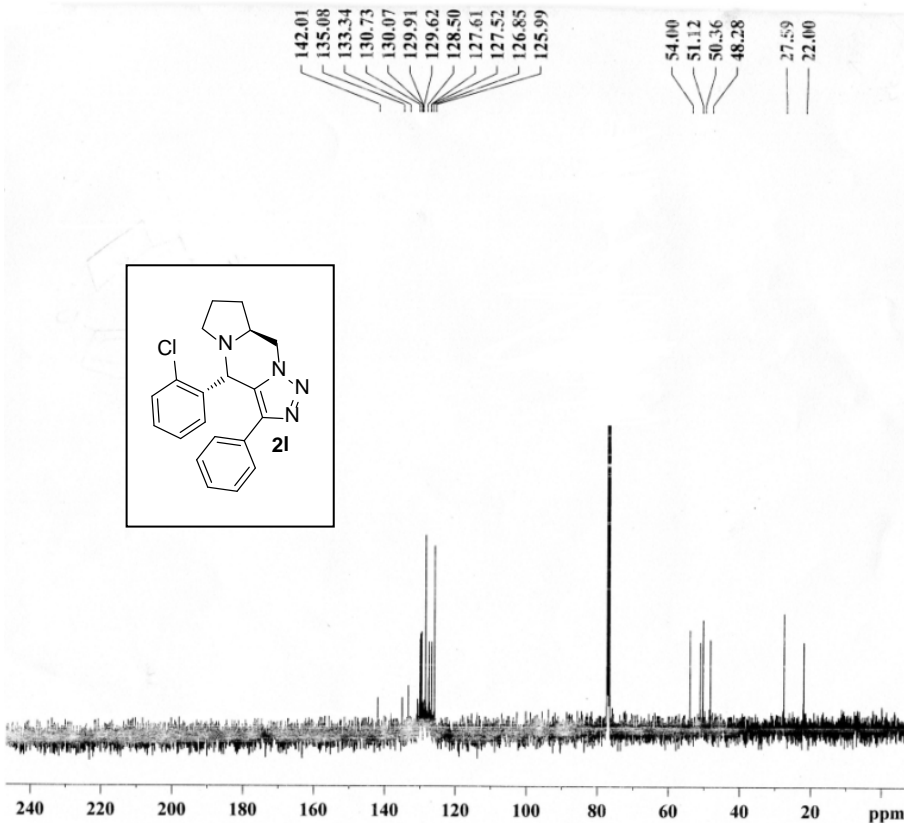
Current Data Parameters
 NAME SIA 389 proton
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130403
 Time 18.46
 INSTRUM spect
 PRORHD 5 mm Multinuc1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 645.1
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRE 0.00500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 CXP 13.970 ppm
 FL 4192.77 Hz
 F2P -1.012 ppm
 F2 -303.63 Hz
 PPM CM 0.74968 ppm/cm
 HZ CM 224.62014 Hz/cm



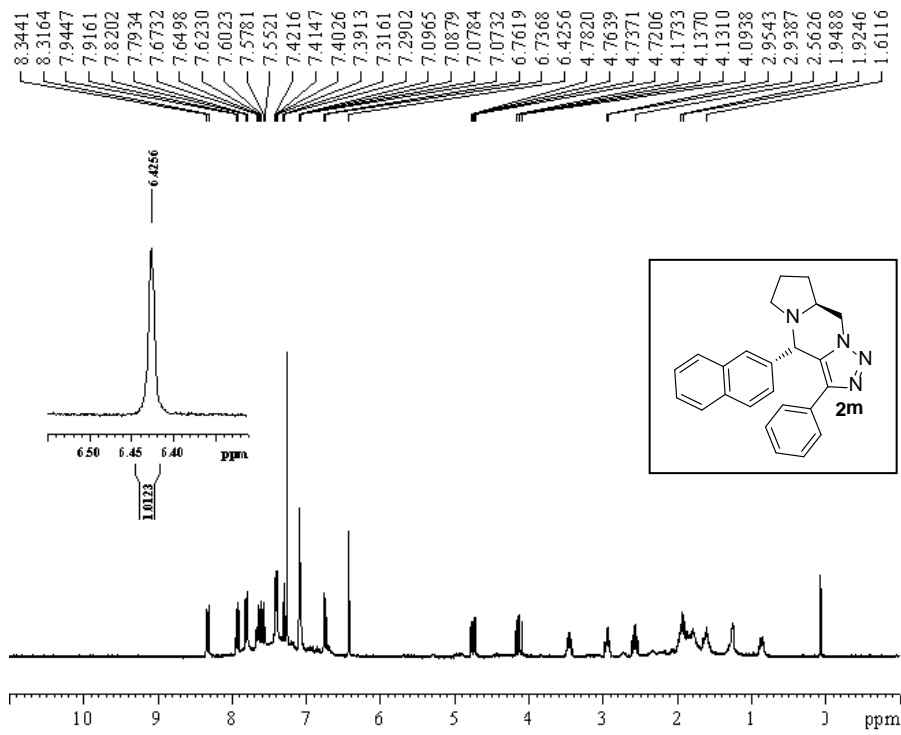
Current Data Parameters
 NAME 2Cl-triazole
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130507
 Time 21.11
 INSTRUM spect
 PRORHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 500
 DS 0
 SWH 25510.203 Hz
 FIDRES 0.389255 Hz
 AQ 1.2845556 sec
 RG 4
 DW 19.600 usec
 DE 7.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 100.6248425 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCTD2 90.00 usec
 PL2 -3.00 dB
 PL12 14.00 dB
 PL13 17.00 dB
 SFO2 400.1316003 MHz

F2 - Processing parameters
 SI 100.6127690 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



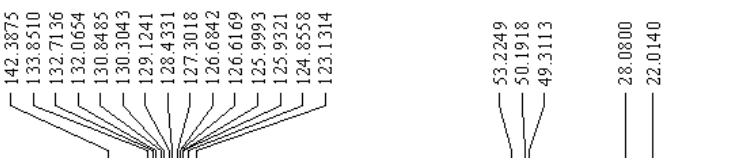
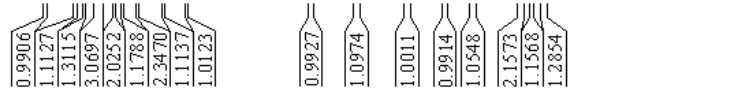
Current Data Parameters
 NAME SNA A3 5
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130426
 Time 20.26
 INSTRUM spect
 PROBHD 5mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 645.1
 DW 111.200 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWVK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 PL 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.972 ppm
 FI 4193.32 Hz
 F2P -1.010 ppm
 F2 -303.08 Hz
 F2MCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



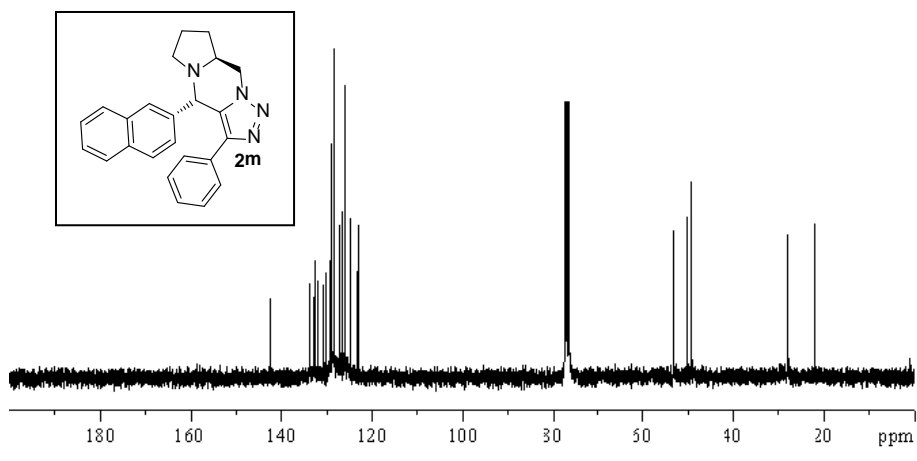
Current Data Parameters
 NAME SNA 3naphthiazole
 EXPNO 1
 PROCNO 1

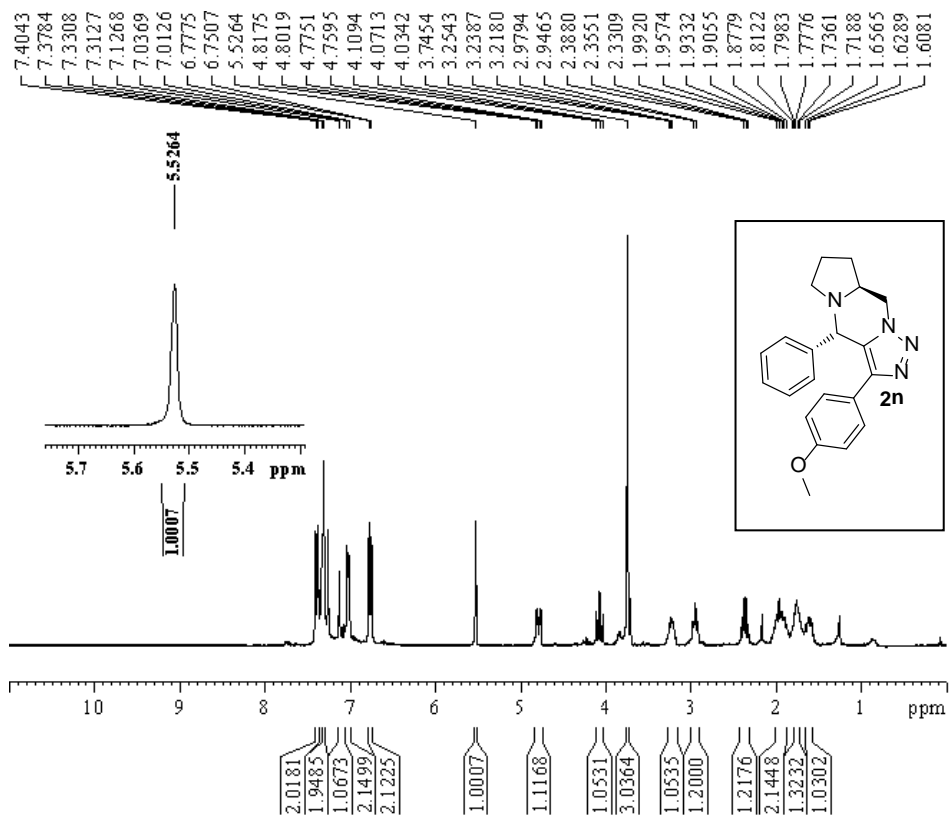
F2 - Acquisition Parameters
 Date_ 20130723
 Time 10.29
 INSTRUM spect
 PROBHD 5mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 11873
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWVK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 PL 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677528 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



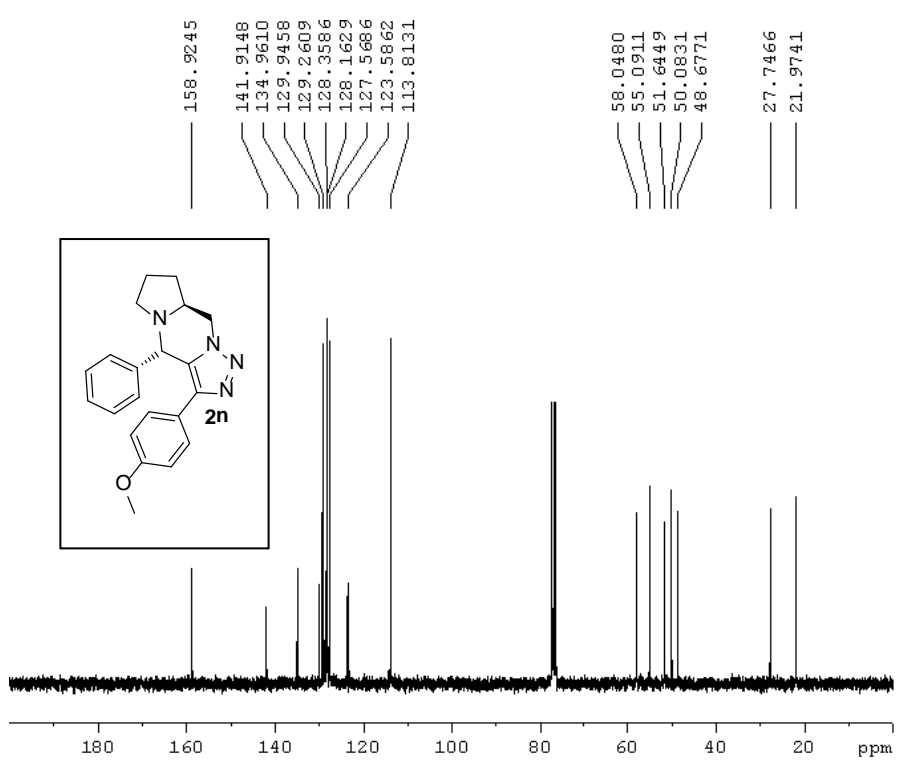


Current Data Parameters
 NAME SNA 399 O CH3 pyacety
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130529
 Time 21.45
 INSTRUM spect
 PROBHID 5mm Multinuc1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 512
 DW 111.200 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME SNA 378 CB
 EXPNO 1
 PROCNO 1

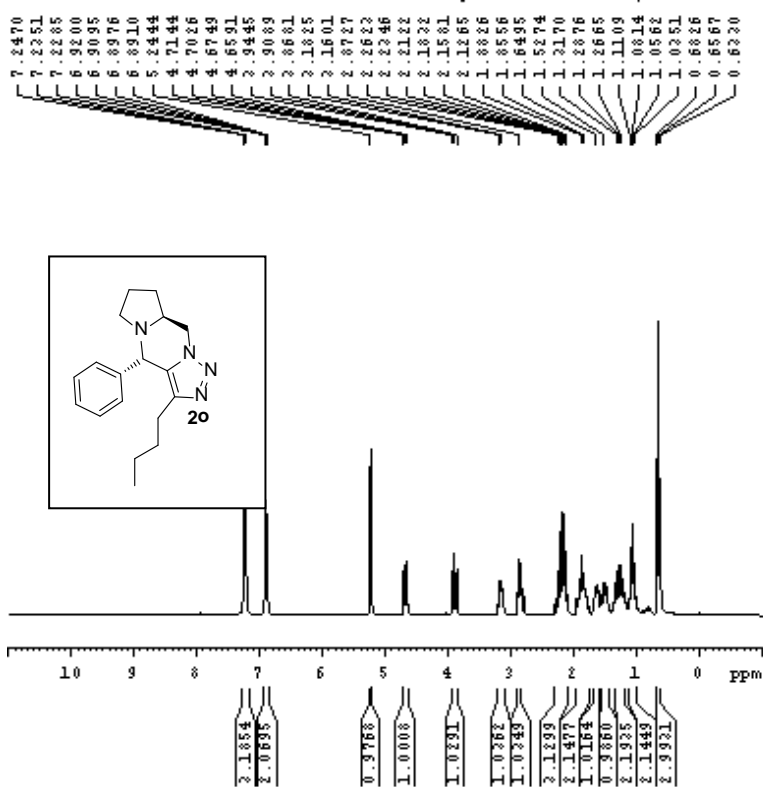
F2 - Acquisition Parameters
 Date_ 20130507
 Time 2.28
 INSTRUM spect
 PROBHID 5mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 18822.289 Hz
 FIDRES 0.237550 Hz
 AQ 1.7400208 sec
 RG 10321.3
 DW 265.30 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4762978 MHz

===== CHANNEL f2 =====
 CHDRG2 waLz16
 NUC2 1H
 PPRG2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1315306 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677328 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

ID NMR p1 parameters
 CX 20.00 cm
 CY 12.30 cm
 FID 240.000 ppm
 F1 18112.26 Hz
 F2 -1000 ppm
 F3 -75.47 Hz
 F4CM 12.05100 ppm/cm
 HEZCM 9093865 Hz/cm

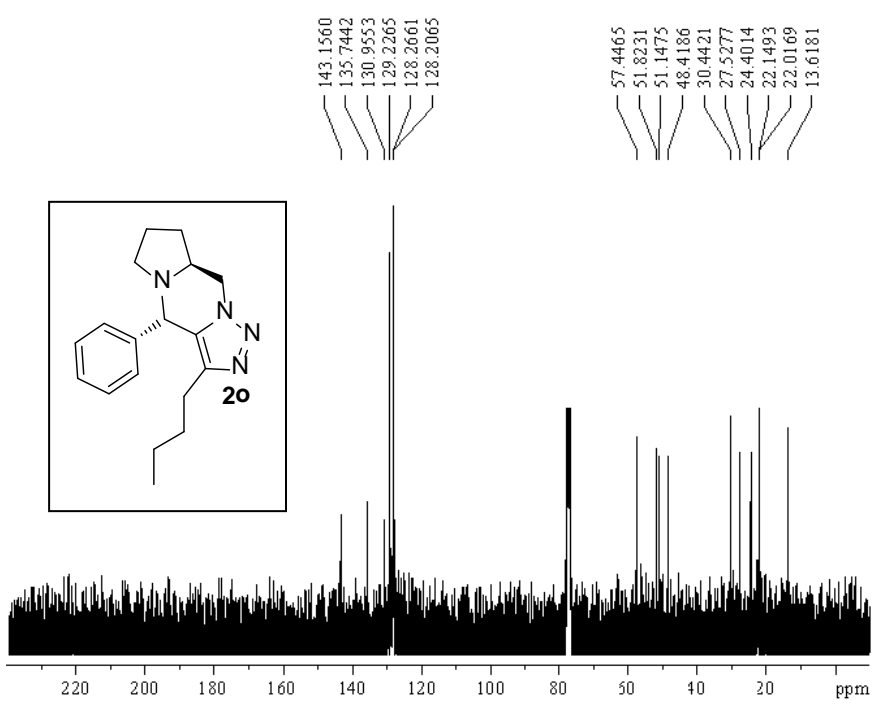


Current Data Parameters
 NAME SNA hexyne
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130612
 Time 15.25
 INSTRUM spect
 PROBHD 5mm Multisud
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 12
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 362
 DW 111.200 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300071 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



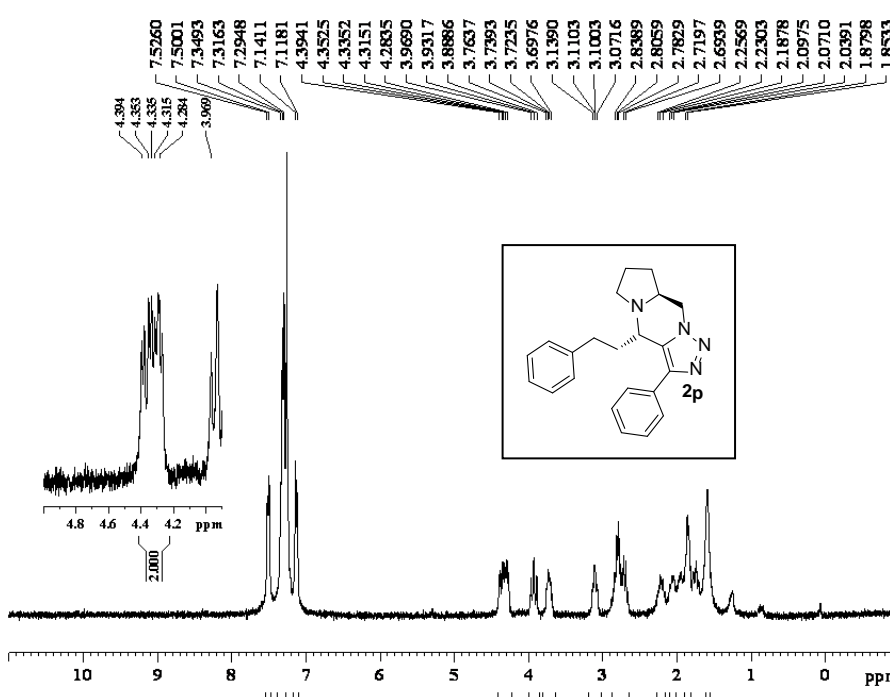
Current Data Parameters
 NAME SNA 26 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130618
 Time 10.18
 INSTRUM spect
 PROBHD 5mm Multisud
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 12000
 DS 0
 SWH 18832.399 Hz
 FIDRES 0.277860 Hz
 AQ 1.7408348 sec
 RG 10321.3
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

----- CHANNEL f2 -----
 CTDPRG2 vzbz16
 NUC2 1H
 PCTD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1312806 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677500 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



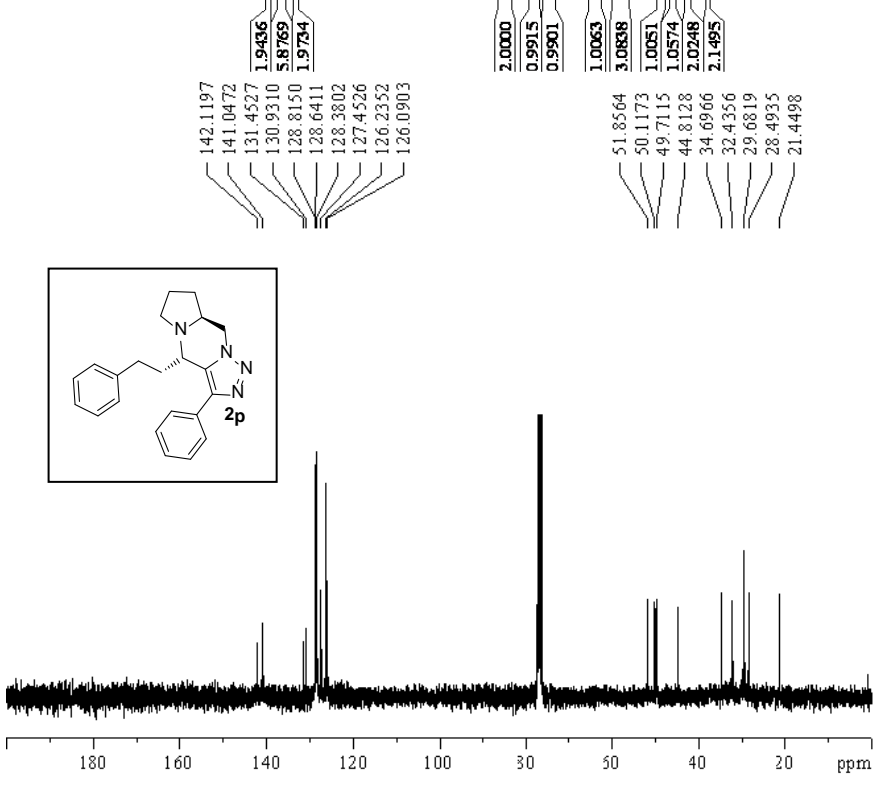
Current Data Parameters
 NAME SNA378
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130307
 Time 21.25
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 1448.2
 DW 111.200 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300076 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -1.016 ppm
 F2 -305.00 Hz
 PPMCM 0.55081 ppm/cm
 HZCM 165.31503 Hz/cm



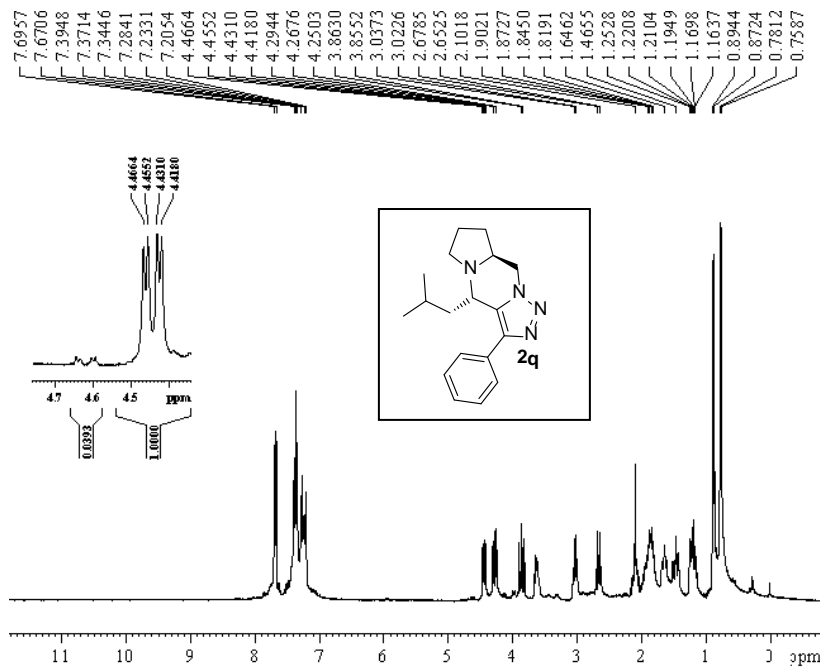
Current Data Parameters
 NAME SNA Decenam.13 C
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date 20130707
 Time 10.02
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8046
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287260 Hz
 AQ 1.7400308 sec
 RG 3792.6
 DW 26.500 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.39999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313806 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677546 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



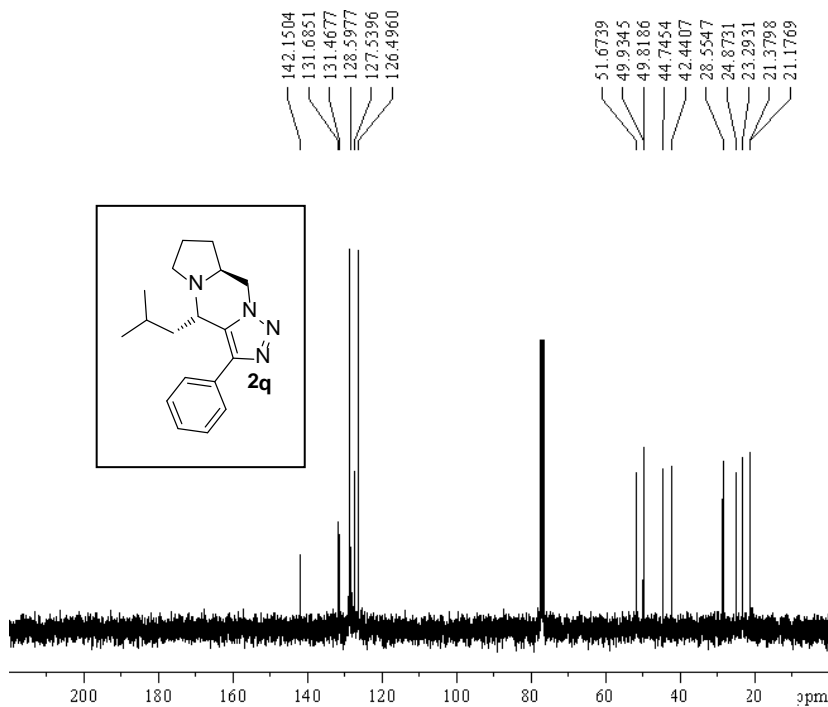
Current Data Parameters
 NAME SNA A07 2 proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130507
 Time 16.54
 INSTRUM spect
 PROBHD 5mm Multinuc1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 203.2
 DW 111.200 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRC 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1313508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300076 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FFP 13.965 ppm
 F1 4191.40 Hz
 F2 -1.016 ppm
 FZ -305.00 Hz
 PPMCM 0.74008 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA A071 C13
 EXPNO 1
 PROCNO 1

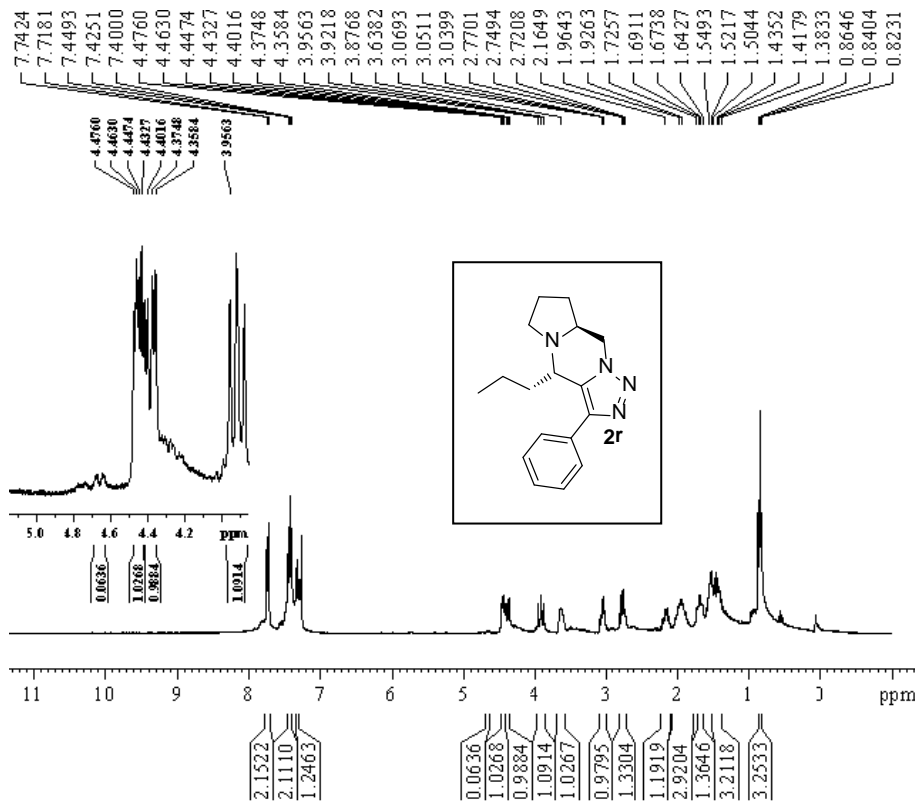
F2 - Acquisition Parameters
 Date_ 20130507
 Time 13.54
 INSTRUM spect
 PROBHD 5mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 945
 DS 0
 SWH 1832.303 Hz
 FIDRES 0.267360 Hz
 AQ 1.7500308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRC 0.0150000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763976 MHz

==== CHANNEL f2 =====
 NUC2 1H
 P2 90.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 21.00 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 22780
 SF 75.4675334 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FFP 233.315 ppm
 F1 18000.58 Hz
 F2 10.227 ppm
 FZ -711.82 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.63957 Hz/cm



Current Data Parameters
 NAME SNA.A.10 2 proton
 EXPNO 1
 PROCNO 1

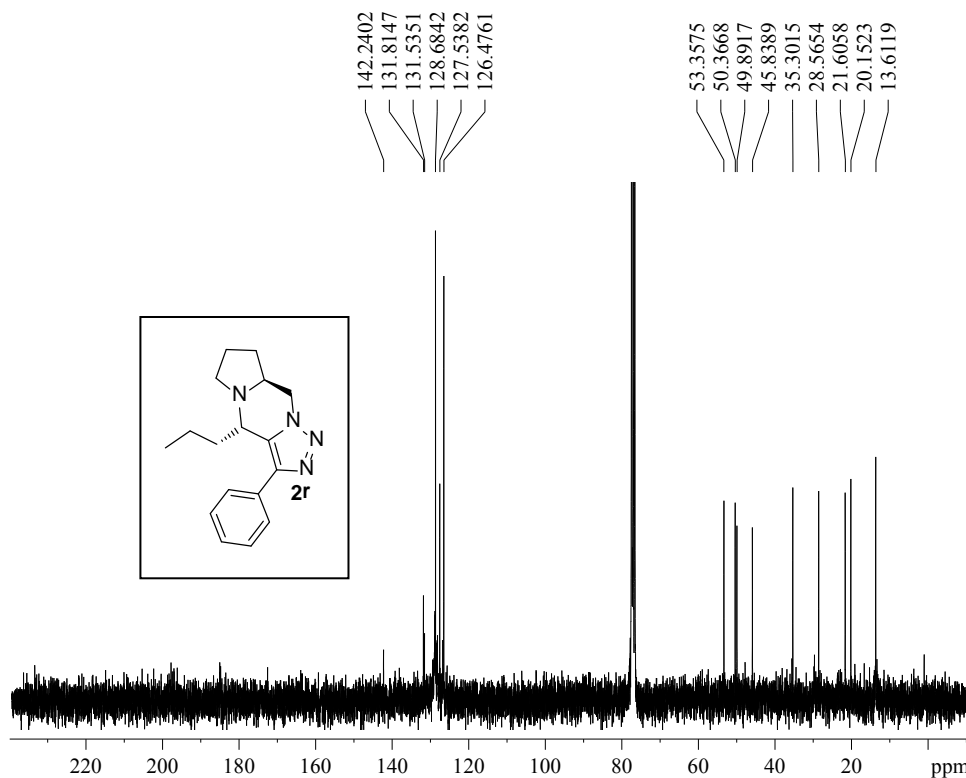
F2 - Acquisition Parameters
 Date_ 20130507
 Time 16.40
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 256
 DW 111.200 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====

NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 300.1319506 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300054 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.973 ppm
 FI 4193.60 Hz
 F2P -1.009 ppm
 F2 -302.80 Hz
 PPMCM 0.74908 ppm/cm
 HZ CM 224.82014 Hz/cm



Current Data Parameters
 NAME butarald triazole nw 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130702
 Time 10.48
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 12000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

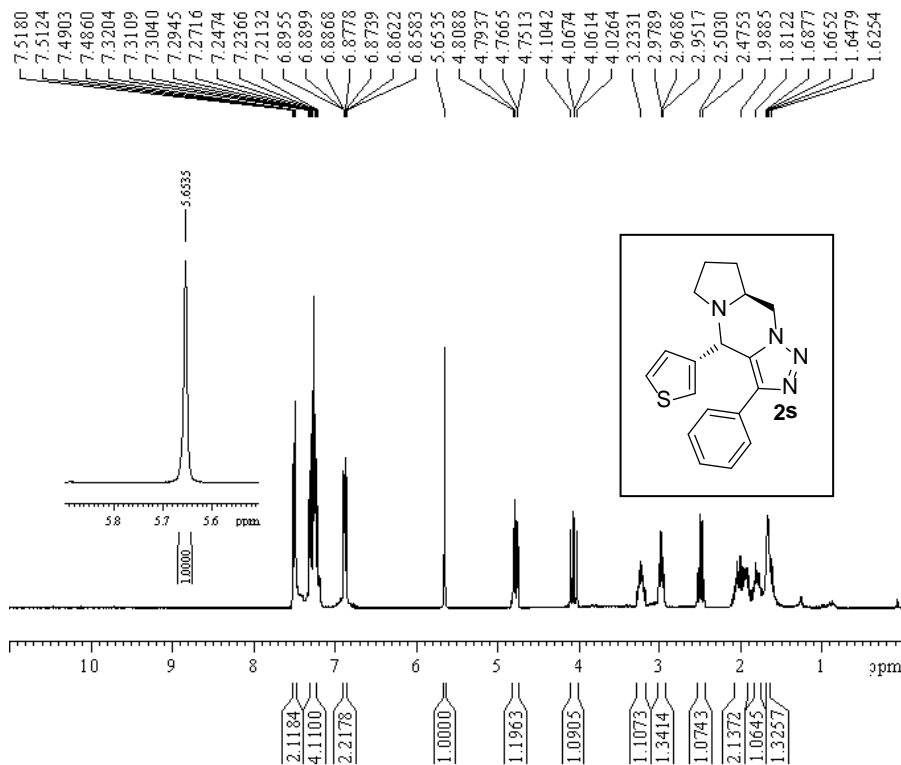
==== CHANNEL f1 =====

NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 18.80 dB
 PL13 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677517 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



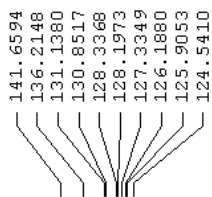
Current Data Parameters
 NAME SNA 397 A.ppten
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130417
 Time 23.30
 INSTRUM spect
 PROBHD 5mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 15
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 574.7
 DW 111.200 usec
 DE 6.50 usec
 TE 299.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319506 MHz

F2 - Processing parameters
 SI 16364
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.970 ppm
 FI 4192.77 Hz
 F2P -1.012 ppm
 F2 -363.63 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME SNA 397 C13
 EXTNO 1
 PROCNO 1

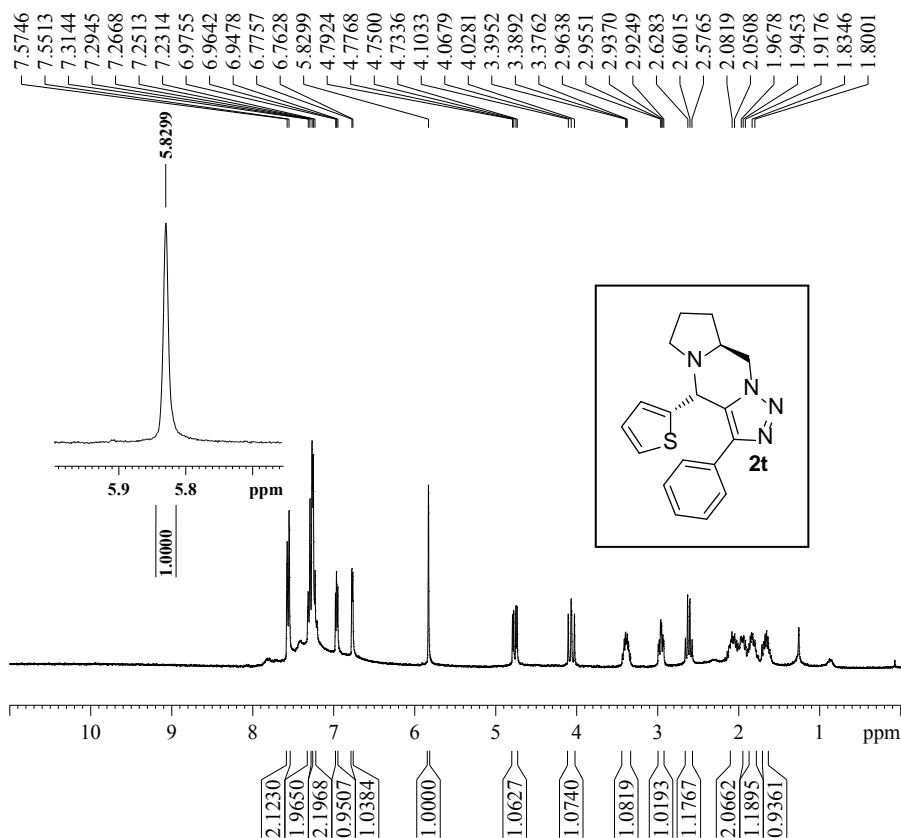
F2 - Acquisition Parameters
 Date_ 20130607
 Time 0.50
 INSTRUM spect
 PROBHD 5mm Multinuc
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 0
 SWH 16332.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400000 sec
 RG 5792.0
 DW 26.550 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.5000000 sec
 d11 0.0300000 sec
 DELTA 1.3999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CDFPRG2 waltz16
 NUC2 1H
 FCFB2 90.00 usec
 P12 0.00 dB
 P13 18.80 dB
 P15 21.80 dB
 SFO2 300.1313506 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677477 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.80 cm
 FIP 239.391 ppm
 FI 18066.29 Hz
 F2P -10.151 ppm
 F2 -766.10 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61957 Hz/cm



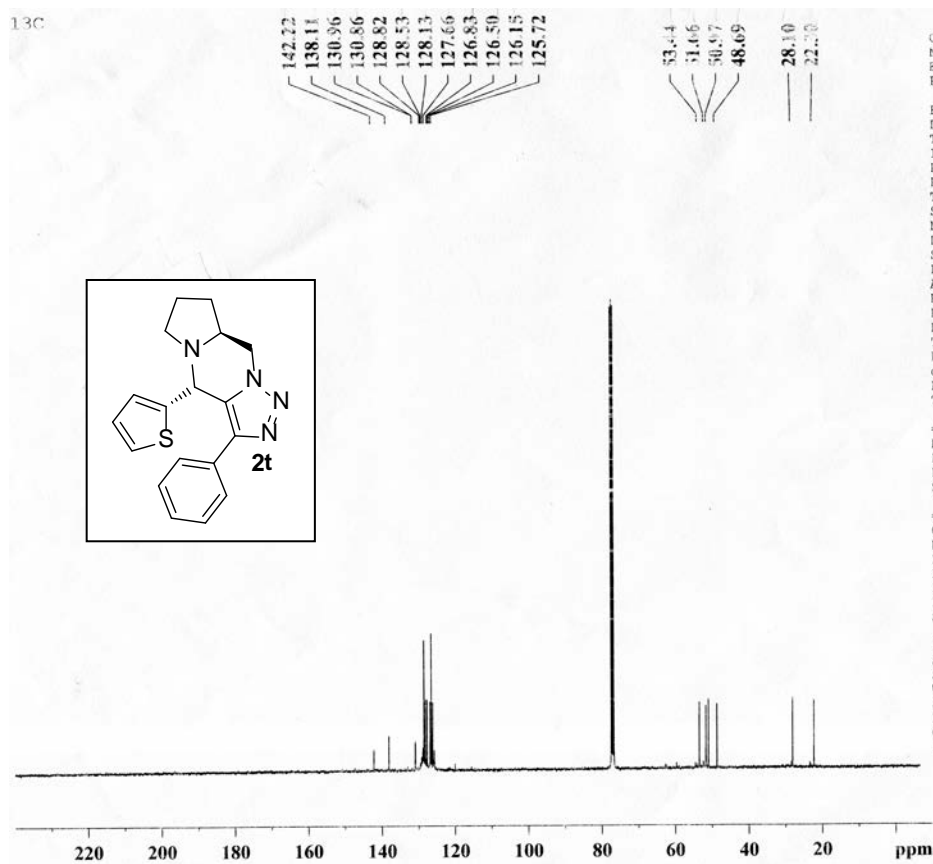
Current Data Parameters
 NAME skl 2 thio tafo
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131020
 Time 19.40
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 645.1
 DW 111.200 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1
 NUC1 1H
 P1 10.60 usec
 PL1 0.00 dB
 SFO1 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300057 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 FIP 13.972 ppm
 FI 4193.32 Hz
 F2P -1.010 ppm
 F2 -303.08 Hz
 PPMCM 0.74908 ppm/cm
 HZCM 224.82013 Hz/cm



Current Data Parameters
 NAME snaa513c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Paramet
 Date_ 20130508
 Time 10.54
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 9228
 DS 0
 SWH 25510.203
 FIDRES 0.389255
 AQ 1.2845556
 RG 4
 DW 19.600
 DE 7.00
 TE 300.0
 D1 2.00000000
 d11 0.03000000
 DELTA 1.89999996
 TD0 1

CHANNEL f1
 NUC1 13C
 P1 9.00
 PL1 0.00
 SFO1 100.6248425

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00
 PL2 -3.00
 PL12 14.00
 PL13 17.00
 SFO2 400.1316005

F2 - Processing paramet
 SI 32768
 SF 100.6127690
 WDW EM
 SSB 0
 LB 2.00
 GB 0
 PC 1.00

