

Visible Light Promoted Coupling of Alkynyl Bromides and Hantzsch Esters for the Synthesis of Internal Alkynes

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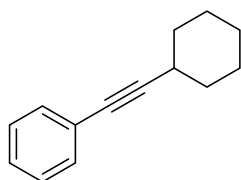
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Part I Experimental Part

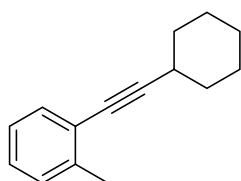
1. Characterization data of product 3



3aa

1-(2-cyclohexylethynyl)benzene¹

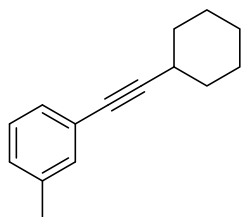
Yield: 27.6 mg, 75% yield; colorless oil; ¹H NMR (500 MHz, Chloroform-*d*) δ 7.40 – 7.39 (m, 2H), 7.27 (d, J = 5.6 Hz, 2H), 2.58 (tt, J = 9.3, 3.9 Hz, 1H), 1.88 (dt, J = 9.6, 3.8 Hz, 2H), 1.81 – 1.69 (m, 2H), 1.54 (dt, J = 9.6, 3.8 Hz, 3H), 1.35 (p, J = 6.9, 5.6 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 131.6, 128.1, 127.4, 124.1, 94.5, 80.5, 32.7, 29.7, 25.9, 24.9.



3ba

1-(cyclohexylethynyl)-2-methylbenzene

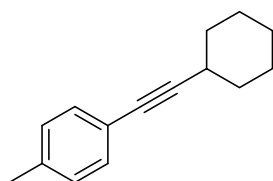
Yield: 34.5 mg, 87% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, J = 7.5 Hz, 1H), 7.21 – 7.03 (m, 3H), 2.65 (tt, J = 8.6, 3.8 Hz, 1H), 2.41 (s, 3H), 1.98 – 1.83 (m, 2H), 1.83 – 1.66 (m, 2H), 1.56 (dt, J = 14.3, 4.9 Hz, 3H), 1.37 (q, J = 8.3, 6.1 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 139.9, 131.7, 129.2, 127.4, 125.4, 123.9, 98.6, 79.4, 32.8, 29.8, 26.0, 24.8, 20.8; HRMS (ESI) calcd for C₁₅H₁₉ [M+H]⁺ 199.1481, found 199.1480.



3ca

1-(cyclohexylethynyl)-3-methylbenzene

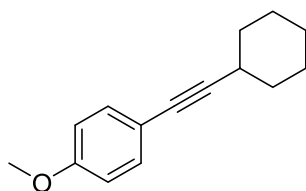
Yield: 30.5 mg, 77% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.11 (m, 3H), 7.05 (d, J = 7.4 Hz, 1H), 2.57 (dt, J = 9.3, 5.0 Hz, 1H), 2.30 (s, 3H), 1.97 – 1.82 (m, 2H), 1.75 (q, J = 5.4, 4.8 Hz, 2H), 1.53 (tq, J = 9.7, 6.0, 4.8 Hz, 3H), 1.35 (d, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 137.8, 132.2, 128.6, 128.3, 128.0, 123.9, 94.1, 80.6, 32.8, 29.7, 26.0, 24.9, 21.2; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{19}$ $[\text{M}+\text{H}]^+$ 199.1481, found 199.1482.



3da

1-(cyclohexylethynyl)-4-methylbenzene²

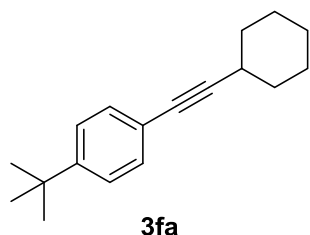
Yield: 33.3 mg, 84% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.28 (d, J = 7.8 Hz, 2H), 7.07 (d, J = 7.8 Hz, 2H), 2.57 (tt, J = 8.9, 3.8 Hz, 1H), 2.32 (s, 3H), 1.87 (dq, J = 12.5, 3.3 Hz, 2H), 1.75 (h, J = 5.9, 5.2 Hz, 2H), 1.52 (dq, J = 12.4, 6.2, 3.5 Hz, 3H), 1.34 (tq, J = 6.4, 3.0 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 137.3, 131.4, 128.9, 121.1, 93.6, 80.5, 32.8, 29.7, 26.0, 24.9, 21.4; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{19}$ $[\text{M}+\text{H}]^+$ 199.1481, found 199.1482.



3ea

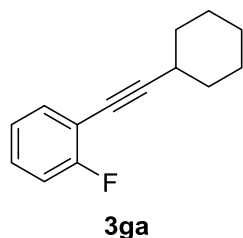
1-(cyclohexylethynyl)-4-methoxybenzene³

Yield: 36.4 mg, 85% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, J = 8.5 Hz, 2H), 6.80 (d, J = 8.5 Hz, 2H), 3.79 (s, 3H), 2.56 (tt, J = 9.0, 3.8 Hz, 1H), 2.02 – 1.82 (m, 2H), 1.82 – 1.66 (m, 2H), 1.53 (dq, J = 13.5, 4.3, 3.6 Hz, 3H), 1.34 (p, J = 7.1, 6.0 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.0, 132.9, 116.4, 113.8, 92.9, 80.2, 55.3, 32.9, 29.7, 26.0, 25.0; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{19}\text{O}$ $[\text{M}+\text{H}]^+$ 215.1430, found 215.1430.



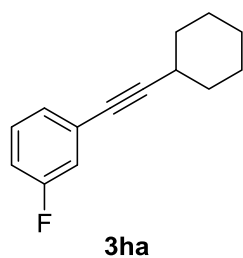
1-(tert-butyl)-4-(cyclohexylethynyl)benzene

Yield: 31 mg, 64% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.31 (q, J = 8.4 Hz, 4H), 2.57 (tt, J = 8.9, 3.8 Hz, 1H), 1.86 (dt, J = 12.4, 3.6 Hz, 2H), 1.75 (q, J = 5.7, 4.8 Hz, 2H), 1.54 (ddd, J = 13.3, 8.8, 3.9 Hz, 3H), 1.40 – 1.26 (m, 12H); ^{13}C NMR (101 MHz, CDCl_3) δ 150.5, 131.3, 125.1, 121.1, 93.7, 80.5, 34.7, 32.8, 31.2, 29.7, 26.0, 24.9; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{25}$ $[\text{M}+\text{H}]^+$ 241.1951, found 241.1951.



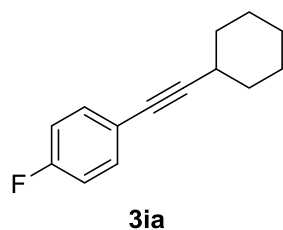
1-(cyclohexylethynyl)-2-fluorobenzene

Yield: 30.7 mg, 76% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.39 (td, J = 7.6, 1.9 Hz, 1H), 7.22 (dtd, J = 7.3, 5.6, 5.1, 2.5 Hz, 1H), 7.09 – 6.98 (m, 2H), 2.64 (tt, J = 8.7, 3.8 Hz, 1H), 1.89 (ddd, J = 12.6, 6.8, 3.4 Hz, 2H), 1.76 (dtt, J = 8.8, 6.6, 3.3 Hz, 2H), 1.57 (ddd, J = 18.3, 9.3, 4.7 Hz, 3H), 1.44 – 1.29 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.0 (d, $J_{\text{C-F}}$ = 148.5 Hz, 2C), 133.6 (d, $J_{\text{C-F}}$ = 1.46 Hz, 2C), 129.0 (d, $J_{\text{C-F}}$ = 7.8 Hz, 2C), 123.7 (d, $J_{\text{C-F}}$ = 3.8 Hz, 2C), 115.4 (d, $J_{\text{C-F}}$ = 210 Hz, 2C), 112.5 (d, $J_{\text{C-F}}$ = 15.6 Hz, 2C), 99.9, 73.9, 32.6, 29.8, 25.9, 24.8. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{F}$ $[\text{M}+\text{H}]^+$ 203.1231, found 203.1230.



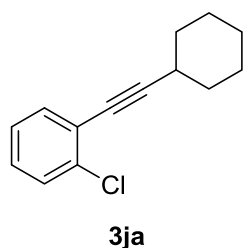
1-(cyclohexylethynyl)-3-fluorobenzene

Yield: 22.3 mg, 55% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.20 – 7.11 (m, 1H), 7.09 (d, J = 7.6 Hz, 1H), 7.01 (dt, J = 9.6, 1.8 Hz, 1H), 6.88 (td, J = 8.5, 2.6 Hz, 1H), 2.50 (tt, J = 8.9, 3.8 Hz, 1H), 1.87 – 1.74 (m, 2H), 1.68 (q, J = 6.0, 5.1 Hz, 2H), 1.53 – 1.39 (m, 3H), 1.28 (dt, J = 6.6, 3.1 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 163.6 (d, $J_{\text{C-F}}$ = 246.5 Hz, 2C), 129.7 (d, $J_{\text{C-F}}$ = 8.8 Hz, 2C), 127.4 (d, $J_{\text{C-F}}$ = 3.0 Hz, 2C), 126.1 (d, $J_{\text{C-F}}$ = 9.6 Hz, 2C), 118.5 (d, $J_{\text{C-F}}$ = 22.6 Hz, 2C), 114.8 (d, $J_{\text{C-F}}$ = 21.1 Hz, 2C), 95.6, 79.5, 32.6, 29.6, 25.9, 24.9; HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{F}$ $[\text{M}+\text{H}]^+$ 203.1231, found 203.1228.



1-(cyclohexylethynyl)-4-fluorobenzene

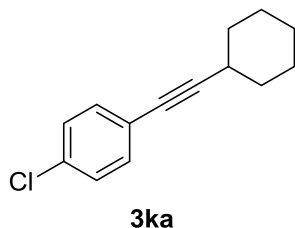
Yield: 29 mg, 69% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 (dd, J = 8.4, 5.5 Hz, 2H), 6.96 (t, J = 8.6 Hz, 2H), 2.56 (tt, J = 8.9, 3.8 Hz, 1H), 1.95 – 1.82 (m, 2H), 1.75 (q, J = 5.0, 4.6 Hz, 2H), 1.53 (dq, J = 13.0, 3.8 Hz, 3H), 1.34 (qd, J = 7.4, 4.8, 3.4 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 163.2 (d, $J_{\text{C-F}}$ = 248.8 Hz, 2C), 133.4 (d, $J_{\text{C-F}}$ = 8.2 Hz, 2C), 120.2 (d, $J_{\text{C-F}}$ = 3.7 Hz, 2C), 115.4 (d, $J_{\text{C-F}}$ = 22.0 Hz, 2C), 94.1, 79.4, 32.7, 29.6, 25.9, 24.9; HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{F}$ $[\text{M}+\text{H}]^+$ 203.1231, found 203.1230.



1-chloro-2-(cyclohexylethynyl)benzene³

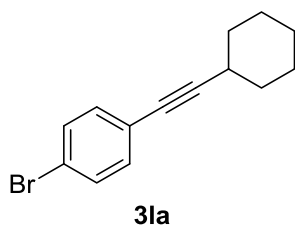
Yield: 35.3 mg, 81% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.39 (m, 1H), 7.39 – 7.33 (m, 1H), 7.22 – 7.12 (m, 2H), 2.68 (tt, J = 8.5, 3.8 Hz, 1H), 1.87 (dq, J = 9.1, 3.2 Hz, 2H), 1.83 – 1.72 (m, 2H), 1.65 – 1.49 (m, 3H), 1.45 – 1.31 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 135.8, 133.2, 129.1, 128.4, 126.3, 123.9,

100.1, 77.6, 32.5, 29.7, 26.0, 24.7; HRMS (ESI) calcd for C₁₄H₁₆Cl [M+H]⁺ 219.0935, found 219.0935.



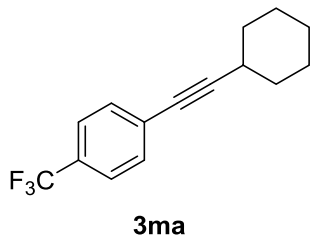
1-chloro-4-(cyclohexylethynyl)benzene⁴

Yield: 32.3 mg, 74% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.31 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 2.57 (tt, *J* = 8.9, 3.8 Hz, 1H), 1.86 (dt, *J* = 12.6, 3.6 Hz, 2H), 1.74 (ddd, *J* = 10.2, 6.7, 3.5 Hz, 2H), 1.52 (ddt, *J* = 13.0, 9.5, 5.7 Hz, 3H), 1.34 (qd, *J* = 7.2, 6.5, 2.7 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 133.3, 132.8, 128.4, 122.7, 95.5, 79.5, 32.6, 29.7, 25.9, 24.9; HRMS (ESI) calcd for C₁₄H₁₆Cl [M+H]⁺ 219.0935, found 219.0931.



1-bromo-4-(cyclohexylethynyl)benzene⁵

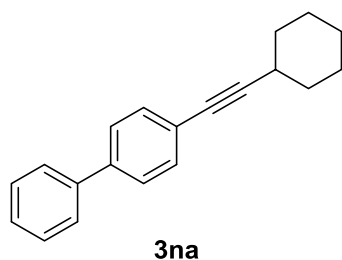
Yield: 49 mg, 93% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 2.49 (tt, *J* = 9.3, 3.8 Hz, 1H), 1.88 – 1.73 (m, 2H), 1.73 – 1.61 (m, 2H), 1.53 – 1.38 (m, 3H), 1.27 (dt, *J* = 6.8, 2.6 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 133.1, 131.4, 123.1, 121.5, 95.7, 79.5, 32.6, 29.7, 25.9, 24.9; HRMS (ESI) calcd for C₁₄H₁₆Br [M+H]⁺ 263.0430, found 263.0428.



1-(cyclohexylethynyl)-4-(trifluoromethyl)benzene⁶

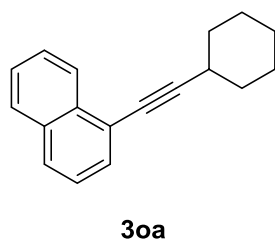
Yield: 35.3 mg, 70% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.51 (q, *J* = 8.3 Hz, 4H), 2.60 (dq, *J* = 8.9, 4.4, 3.9 Hz, 1H), 1.97 – 1.83 (m, 2H), 1.76

(tt, $J = 5.8, 3.2$ Hz, 2H), 1.56 (tt, $J = 9.2, 3.4$ Hz, 3H), 1.37 (qd, $J = 6.9, 4.4, 3.2$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 131.8, 129.4, 129.0, 128.1, 125.4, 125.12, 125.09, 125.05, 125.01, 122.7, 97.3, 79.5, 32.5, 29.7, 25.9, 24.9; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{F}_3$ $[\text{M}+\text{H}]^+$ 253.1199, found 253.1195.



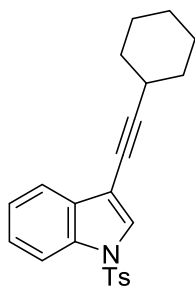
4-(cyclohexylethynyl)-1,1'-biphenyl⁷

Yield: 41.1 mg, 79% yield; colorless oil; ^1H NMR (400 MHz, Chloroform- d) δ 7.50 (dd, $J = 7.6, 1.7$ Hz, 2H), 7.43 (d, $J = 8.3$ Hz, 2H), 7.36 (dd, $J = 18.2, 8.0$ Hz, 4H), 7.30 – 7.21 (m, 1H), 2.53 (tt, $J = 9.0, 3.8$ Hz, 1H), 1.82 (dt, $J = 9.2, 3.7$ Hz, 2H), 1.75 – 1.63 (m, 2H), 1.52 – 1.42 (m, 3H), 1.28 (tt, $J = 6.9, 3.4$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 140.6, 140.1, 132.0, 128.8, 127.4, 127.0, 126.8, 123.1, 95.2, 80.4, 32.8, 29.8, 26.0, 24.9; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{21}$ $[\text{M}+\text{H}]^+$ 261.1638, found 261.1637.



1-(cyclohexylethynyl)naphthalene⁸

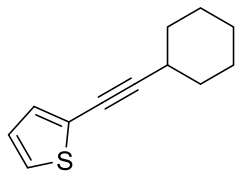
Yield: 24.81 mg, 53% yield; colorless oil; ^1H NMR (400 MHz, Chloroform- d) δ 8.27 (d, $J = 8.2$ Hz, 1H), 7.74 (d, $J = 8.0$ Hz, 1H), 7.68 (d, $J = 8.2$ Hz, 1H), 7.54 (d, $J = 7.1$ Hz, 1H), 7.51 – 7.36 (m, 2H), 7.31 (t, $J = 7.7$ Hz, 1H), 2.68 (tt, $J = 8.8, 3.9$ Hz, 1H), 1.90 (dt, $J = 12.4, 3.9$ Hz, 2H), 1.75 (q, $J = 6.3, 5.2$ Hz, 2H), 1.65 – 1.53 (m, 3H), 1.33 (dp, $J = 6.8, 4.1, 3.6$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 133.5, 133.2, 129.9, 128.2, 127.8, 126.5, 126.3, 126.2, 125.2, 121.8, 99.6, 78.5, 32.9, 30.0, 26.0, 25.0; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{19}$ $[\text{M}+\text{H}]^+$ 235.1481, found 235.1480.



3pa

3-(cyclohexylethynyl)-1-tosyl-1H-indole

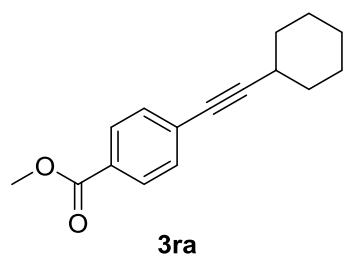
Yield: 46.8 mg, 62% yield; white solid, mp 122-124 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 8.2 Hz, 1H), 7.75 (d, J = 8.1 Hz, 2H), 7.64 (s, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.33 (t, J = 7.7 Hz, 1H), 7.29 – 7.23 (m, 1H), 7.19 (d, J = 8.0 Hz, 2H), 2.65 (dt, J = 9.1, 4.9 Hz, 1H), 2.31 (s, 3H), 1.97 – 1.85 (m, 2H), 1.77 (q, J = 4.5 Hz, 2H), 1.57 (d, J = 10.3 Hz, 3H), 1.37 (qd, J = 6.9, 4.3, 3.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.1, 135.0, 134.2, 131.3, 129.9, 127.9, 126.9, 125.2, 123.5, 120.5, 113.5, 106.0, 99.0, 71.1, 32.7, 29.9, 25.9, 24.9, 21.5; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{24}\text{O}_2\text{NS}$ $[\text{M}+\text{H}]^+$ 378.1522, found 378.1527



3qa

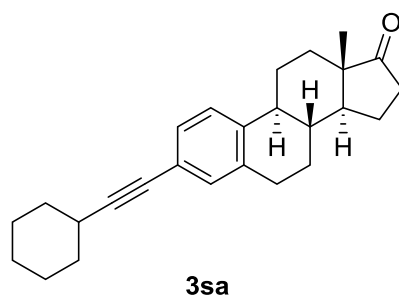
2-(cyclohexylethynyl)thiophene³

Yield: 17.1 mg, 45% yield; colorless oil; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.12 (d, J = 5.2 Hz, 1H), 7.09 (d, J = 3.6 Hz, 1H), 6.89 (dd, J = 5.1, 3.7 Hz, 1H), 2.58 (tt, J = 8.9, 3.8 Hz, 1H), 1.85 (dt, J = 12.7, 3.6 Hz, 2H), 1.73 (q, J = 9.9, 7.0 Hz, 2H), 1.52 (qd, J = 9.7, 4.8 Hz, 3H), 1.40 – 1.24 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 130.8, 126.6, 125.7, 124.2, 98.3, 73.6, 32.5, 29.9, 25.8, 24.9; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{15}\text{S}$ $[\text{M}+\text{H}]^+$ 191.0889, found 191.0894.



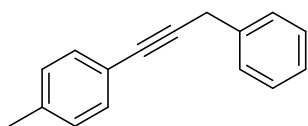
methyl 4-(cyclohexylethynyl)benzoate⁹

Yield: 32 mg, 66% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.83 (m, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 3.83 (s, 3H), 2.53 (td, *J* = 9.1, 4.4 Hz, 1H), 1.89 – 1.75 (m, 2H), 1.68 (dd, *J* = 9.8, 4.5 Hz, 2H), 1.53 – 1.40 (m, 3H), 1.28 (q, *J* = 4.2, 3.5 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 166.7, 131.5, 129.4, 129.0, 128.7, 97.9, 80.1, 52.1, 32.5, 29.7, 25.9, 24.9; HRMS (ESI) calcd for C₁₆H₁₉O₂ [M+H]⁺ 243.1380, found 243.1379.



(8R,9S,13S,14S)-3-(cyclohexylethynyl)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one

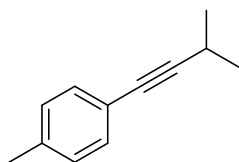
Yield: 40.3 mg, 56% yield; white solid, mp 173-175 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 2.5 Hz, 2H), 7.15 (s, 1H), 2.87 (dd, *J* = 9.0, 4.3 Hz, 2H), 2.65 – 2.45 (m, 2H), 2.40 (dt, *J* = 9.2, 2.8 Hz, 1H), 2.28 (td, *J* = 10.6, 4.3 Hz, 1H), 2.18 – 1.93 (m, 4H), 1.92 – 1.81 (m, 2H), 1.75 (q, *J* = 5.9, 5.2 Hz, 2H), 1.66 – 1.44 (m, 8H), 1.35 (d, *J* = 7.1 Hz, 3H), 0.91 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 220.8, 139.2, 136.3, 132.0, 128.9, 125.2, 121.5, 93.8, 80.4, 50.5, 48.0, 44.4, 38.0, 35.9, 32.8, 31.6, 29.7, 29.1, 26.4, 26.0, 25.6, 24.9, 21.6, 13.9; HRMS (ESI) calcd for C₂₆H₃₃O [M+H]⁺ 361.2526, found 361.2520.



3db

1-methyl-4-(3-phenylprop-1-yn-1-yl)benzene¹⁰

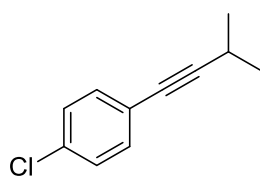
Yield: 37.9 mg, 92% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 7.6 Hz, 2H), 7.33 (dd, *J* = 8.0, 6.6 Hz, 4H), 7.25 (d, *J* = 7.1 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 3.82 (s, 2H), 2.33 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 137.8, 136.9, 131.5, 129.0, 128.5, 128.0, 126.6, 120.6, 86.7, 82.7, 25.8, 21.4; HRMS (ESI) calcd for C₁₆H₁₅ [M+H]⁺ 207.1168, found 203.1167.



3dc

1-methyl-4-(3-methylbut-1-yn-1-yl)benzene

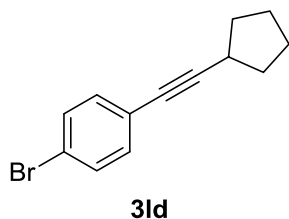
Yield: 28.1 mg, 89% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.28 (d, *J* = 7.8 Hz, 2H), 7.07 (d, *J* = 7.8 Hz, 2H), 2.76 (hept, *J* = 6.9 Hz, 1H), 2.32 (s, 3H), 1.25 (d, *J* = 6.7 Hz, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 137.4, 131.4, 128.9, 120.9, 95.0, 79.7, 23.1, 21.4, 21.1; HRMS (ESI) calcd for C₁₂H₁₅ [M+H]⁺ 159.1168, found 159.1168.



3kc

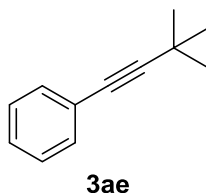
1-chloro-4-(3-methylbut-1-yn-1-yl)benzene

Yield: 25.5 mg, 72% yield; colorless oil; ¹H NMR (500 MHz, Chloroform-*d*) δ 7.31 (d, *J* = 8.4 Hz, 2H), 7.23 (s, 2H), 2.76 (hept, *J* = 6.9 Hz, 1H), 1.25 (d, *J* = 7.0 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 133.4, 132.8, 128.5, 122.6, 96.8, 78.7, 22.9, 21.1; HRMS (ESI) calcd for C₁₁H₁₂Cl [M+H]⁺ 179.0622, found 179.0620



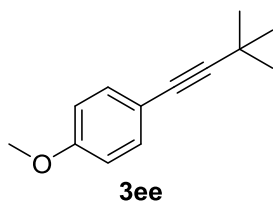
1-bromo-4-(cyclopentylethynyl)benzene⁵

Yield: 45.3 mg, 91% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 8.5 Hz, 2H), 2.80 (p, *J* = 7.5 Hz, 1H), 2.07 – 1.89 (m, 2H), 1.81 – 1.54 (m, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 133.0, 131.4, 123.2, 121.4, 95.9, 79.1, 33.8, 30.8, 25.1; HRMS (ESI) calcd for C₁₃H₁₄Br [M+H]⁺ 249.0273, found 249.0271.



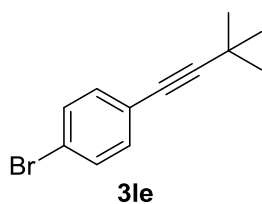
(3,3-dimethylbut-1-ynyl)benzene¹¹

Yield: 29.5 mg, 91% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.38 (dd, *J* = 7.8, 2.0 Hz, 2H), 7.28 – 7.22 (m, 3H), 1.32 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 131.6, 128.1, 127.4, 124.1, 98.5, 79.0, 31.1, 27.9; HRMS (ESI) calcd for C₁₂H₁₅ [M+H]⁺ 159.1168, found 159.1168



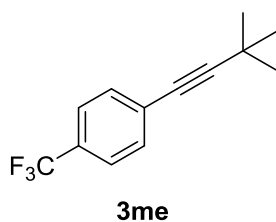
(3,3-dimethylbut-1-yn-1-yl)-4-methoxybenzene¹²

Yield: 33.5 mg, 89% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.31 (dd, *J* = 8.7, 1.7 Hz, 2H), 6.80 (dd, *J* = 8.7, 1.6 Hz, 2H), 3.79 (d, *J* = 1.6 Hz, 3H), 1.30 (d, *J* = 1.5 Hz, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 158.9, 132.9, 116.3, 113.7, 96.9, 78.7, 55.2, 31.2, 27.9; HRMS (ESI) calcd for C₁₃H₁₇O [M+H]⁺ 189.1274, found 189.1272



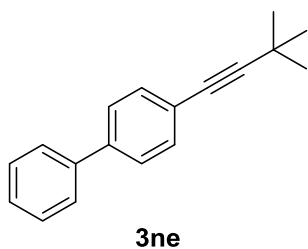
1-bromo-4-(3,3-dimethylbut-1-yn-1-yl)benzene⁵

Yield: 43.1 mg, 91% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H), 1.30 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 133.0, 131.3, 123.1, 121.4, 99.7, 78.1, 30.9, 28.0; HRMS (ESI) calcd for C₁₂H₁₄Br [M+H]⁺ 237.0273, found 237.0272



1-(3,3-dimethylbut-1-yn-1-yl)-4-(trifluoromethyl)benzene¹³

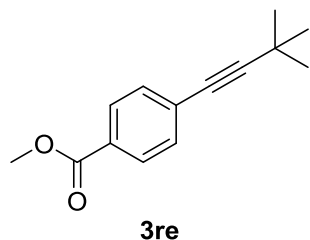
Yield: 28.5 mg, 63% yield; pale yellow solid, mp 78-80 °C; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 1.32 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 131.8, 129.4 (s, q: ²*J*_{C-F} = 32.6 Hz, 1C), 129.0 (s, 1C), 128.0 (d, q: ³*J*_{C-F} = 3.8 Hz, 2C), 125.0 (s, q: ¹*J*_{C-F} = 272.0 Hz, 1C), 101.3 (s, 1C), 78.0 (s, 1C), 30.9 (q, 3C), 28.0 (s, 1C); IR (KBr): 3362, 2974, 2933, 2907, 2871, 2236, 1924, 1613, 1459, 1401, 1362, 1326, 1292, 1204, 1167, 1104, 1065, 1015, 916, 841, 738, 675 cm⁻¹; HRMS (ESI) calcd for C₁₃H₁₄F₃ [M+H]⁺ 227.1042, found 227.1039.



4-(3,3-dimethylbut-1-yn-1-yl)-1,1'-biphenyl

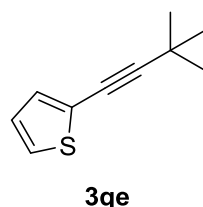
Yield: 41.5 mg, 89% yield; colorless oil; ¹H NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.43 (dd, *J* = 12.5, 7.8 Hz, 4H), 7.37 – 7.30 (m, 1H), 1.33 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 140.6, 140.1, 132.0,

128.8, 127.4, 127.0, 126.8, 123.1, 99.3, 78.9, 31.1, 28.0; HRMS (ESI) calcd for $C_{18}H_{19}$ $[M+H]^+$ 235.1481, found 235.1480.



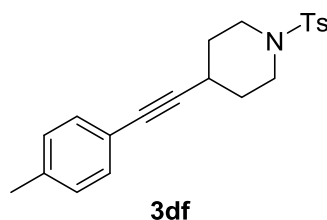
methyl 4-(3,3-dimethylbut-1-yn-1-yl)benzoate

Yield: 45 mg, 99% yield; colorless oil; 1H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.82 (m, 2H), 7.40 – 7.31 (m, 2H), 3.82 (s, 3H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 131.5, 129.3, 128.9, 128.7, 101.9, 78.6, 52.1, 30.9, 28.1; HRMS (ESI) calcd for $C_{14}H_{17}O_2$ $[M+H]^+$ 271.1223, found 217.1221.



2-(3,3-dimethylbut-1-yn-1-yl)thiophene

Yield: 16.7 mg, 51% yield; colorless oil; 1H NMR (400 MHz, Chloroform-*d*) δ 7.11 (dd, J = 5.2, 1.2 Hz, 1H), 7.08 (dd, J = 3.6, 1.1 Hz, 1H), 6.88 (dd, J = 5.2, 3.6 Hz, 1H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 130.8, 126.7, 125.8, 124.2, 102.2, 72.3, 30.8, 28.2; HRMS (ESI) calcd for $C_{10}H_{13}S$ $[M+H]^+$ 165.0733, found 165.0736.



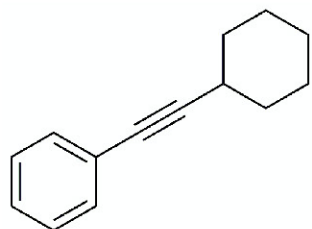
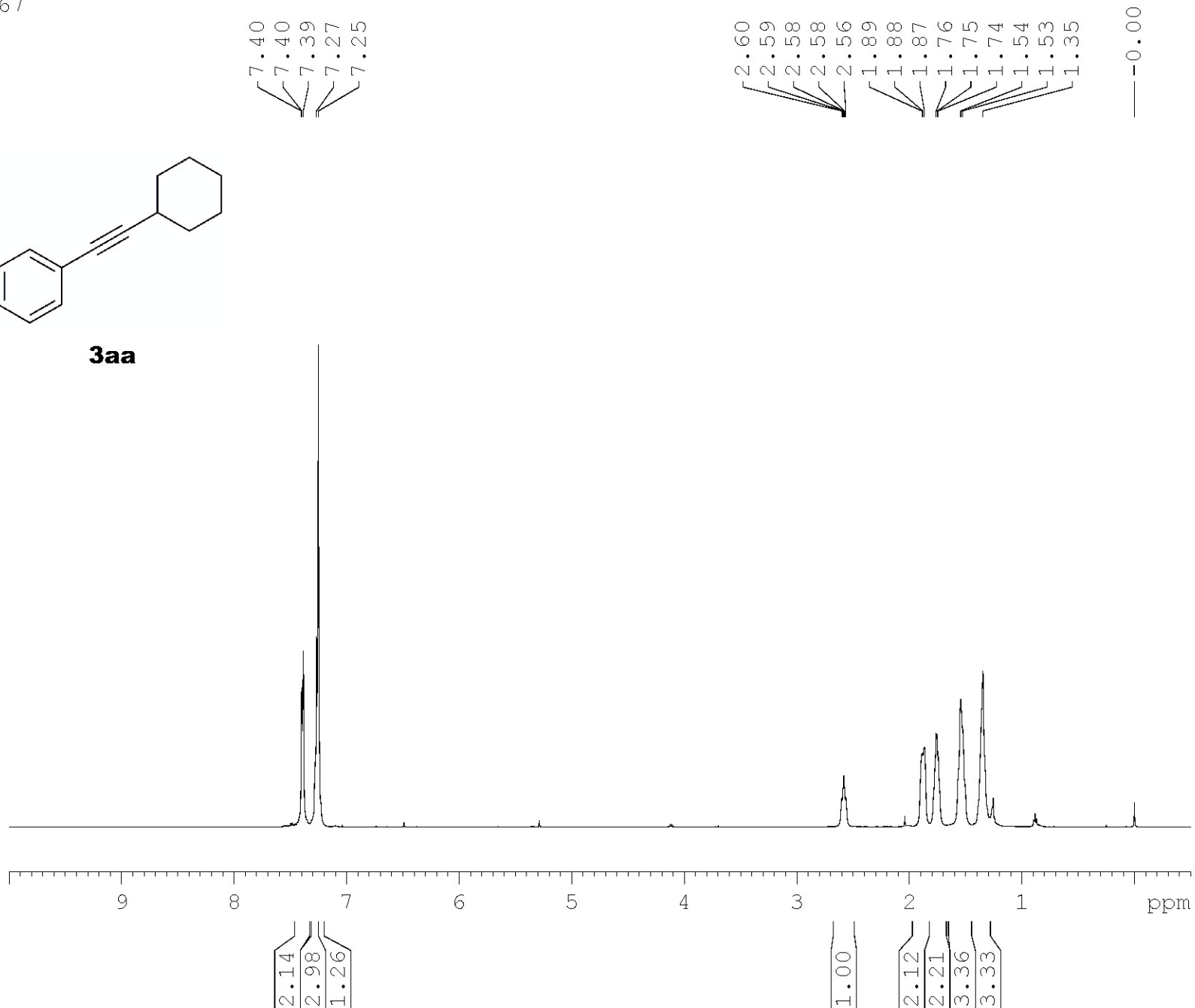
4-(p-tolyethynyl)-1-tosylpiperidine¹⁴

Yield: 45.9 mg, 65% yield; colorless oil; 1H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 7.9 Hz, 2H), 6.98 (d, J = 7.9 Hz, 2H), 3.24 (ddd, J = 11.3, 7.4, 3.5 Hz, 2H), 2.84 (ddd, J = 11.6, 7.8, 3.4 Hz, 2H), 2.57 (tt, J = 7.8, 4.0 Hz, 1H), 2.36 (s, 3H), 2.25 (s, 3H), 1.88 (ddt, J = 14.5, 7.4, 3.7 Hz, 2H), 1.73 (dtd, J = 11.6, 7.7, 3.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ

143.5, 137.9, 133.2, 131.3, 129.6, 128.9, 127.7, 120.1, 90.0, 82.7, 44.4, 30.9, 26.6, 21.5, 21.4; HRMS (ESI) calcd for C₂₁H₂₄O₂NS [M+H]⁺ 354.1522, found 354.1520.

2. References

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**3aa**

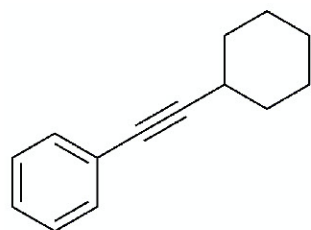
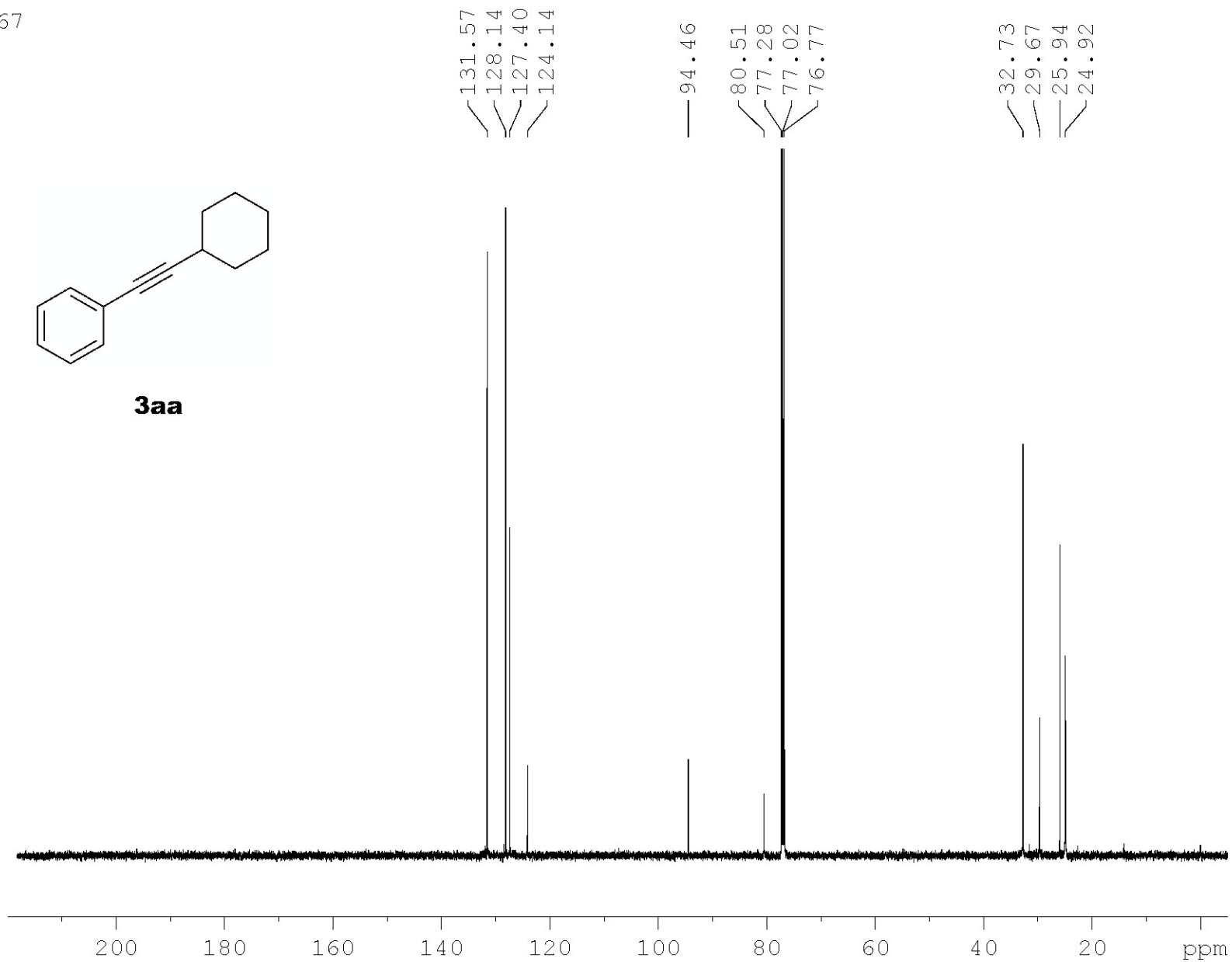
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TDO 1

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 NUC1 1H
 P1 11.50 usec
 PLW1 20.00000000 W

===== CHANNEL f2 =====
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 NUC2 off
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 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

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 WDW EM
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 GB 0
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**3aa**

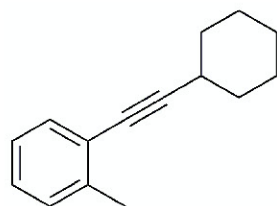
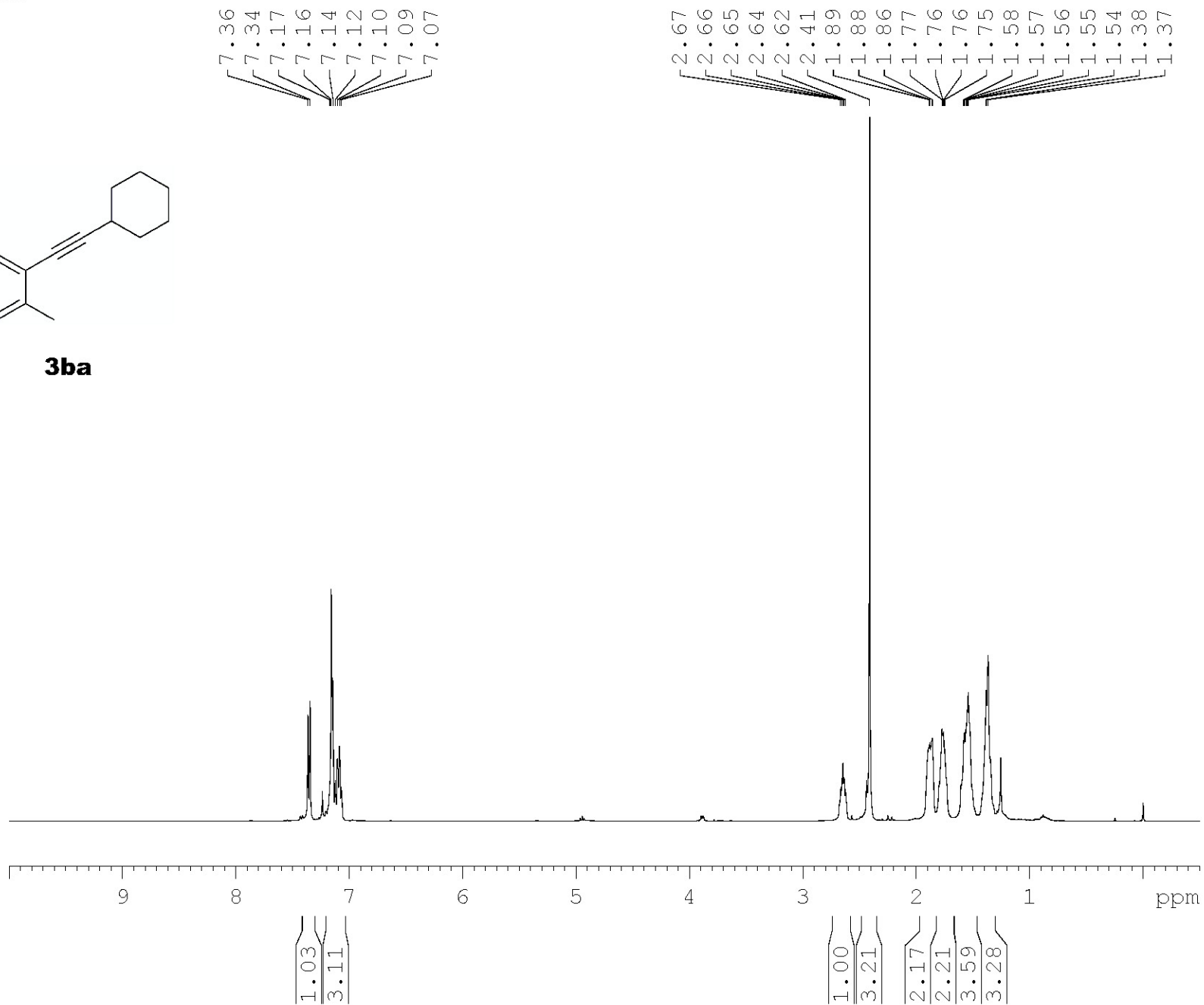
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 NS 47
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

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 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

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 NUC2 1H
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 PCPD2 80.00 usec
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**3ba**

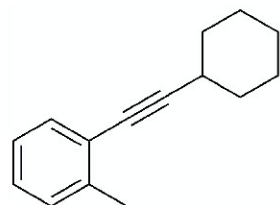
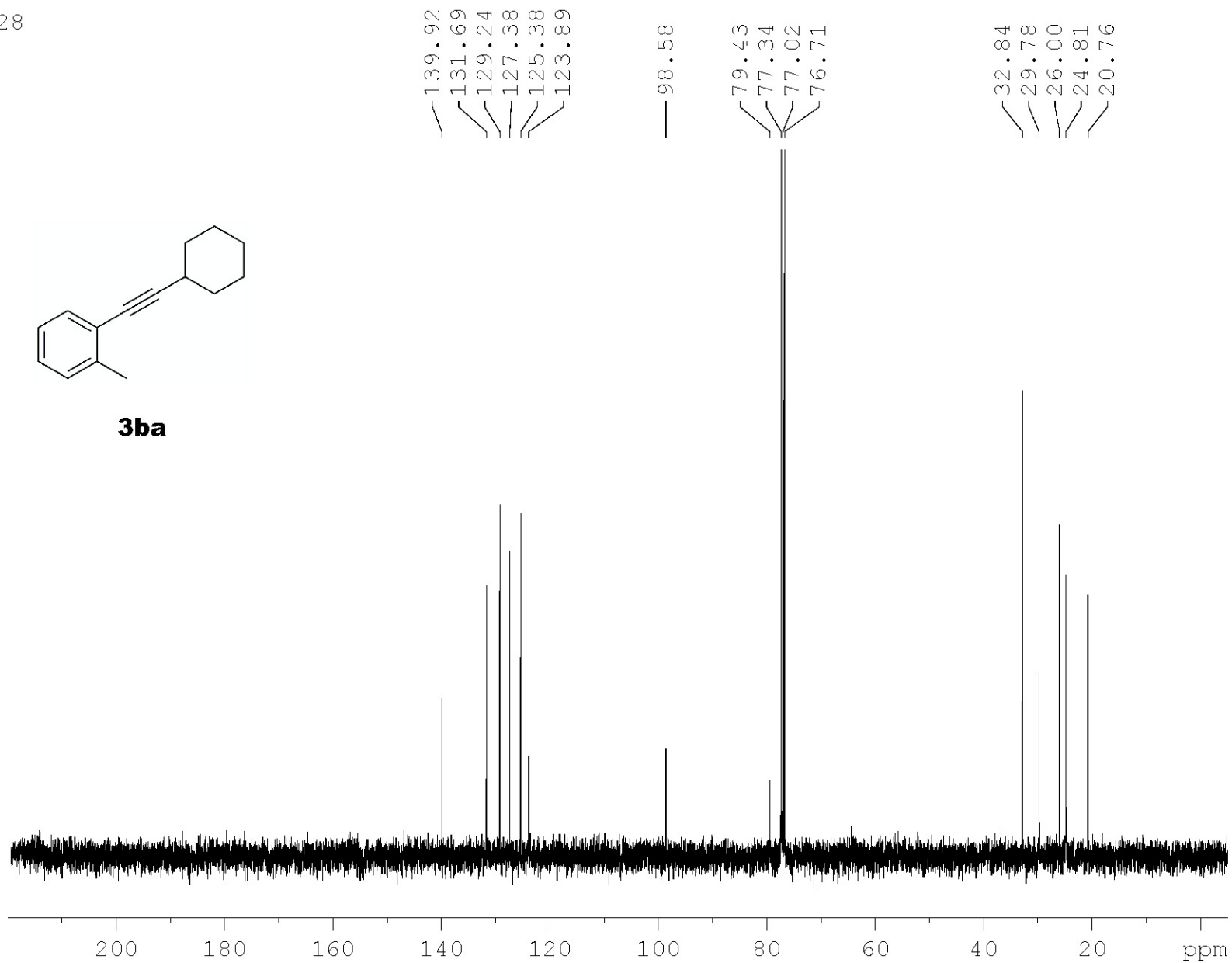
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 55.55
 DW 62.400 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
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 SF 400.2400187 MHz
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**3ba**

Current Data Parameters
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 EXPNO 95
 PROCNO 1

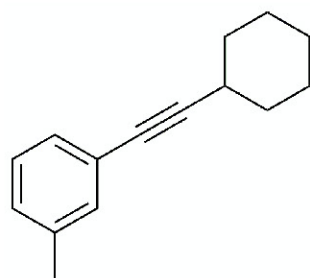
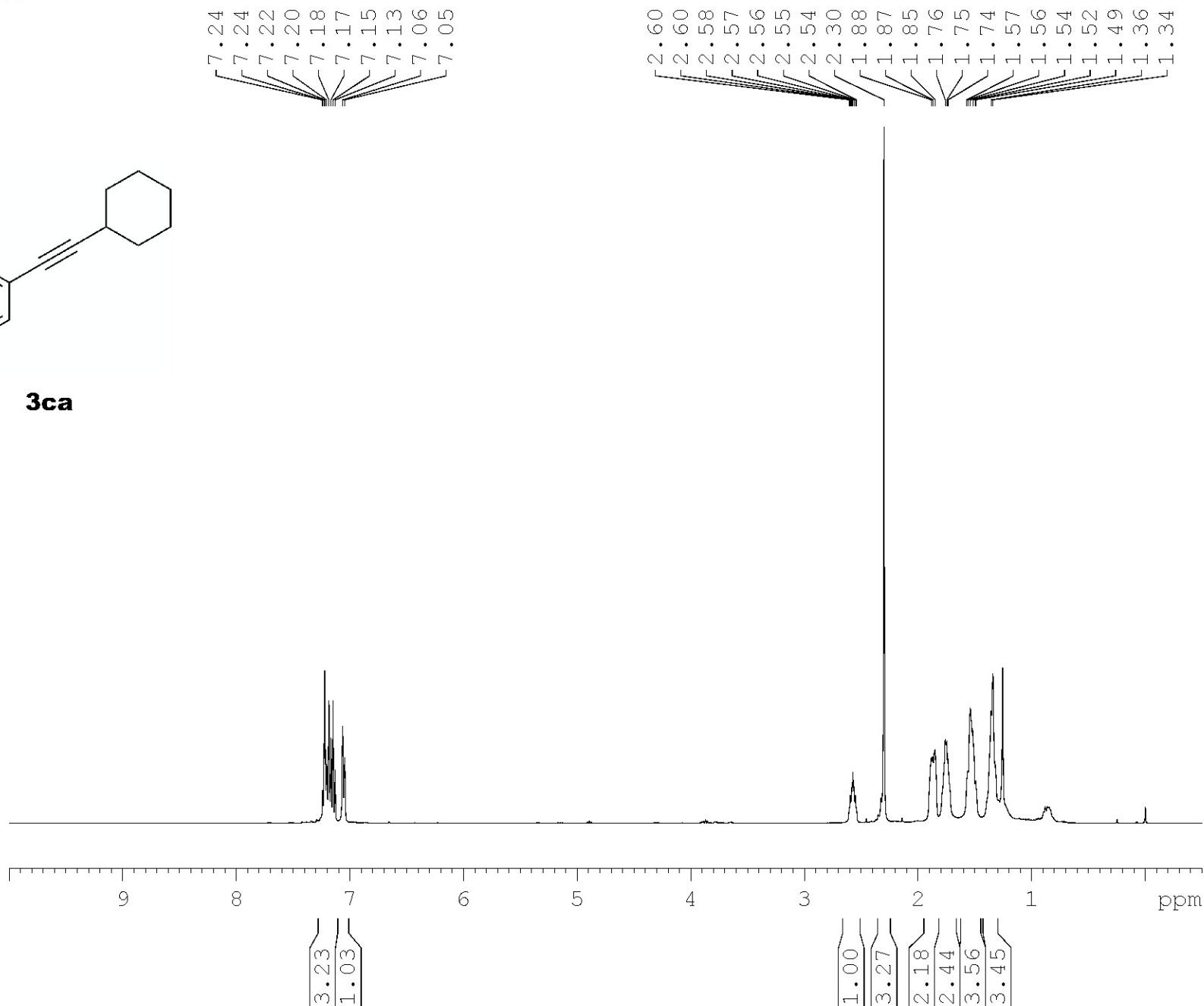
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 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
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 DW 20.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

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729

**3ca**

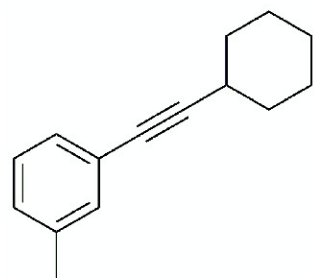
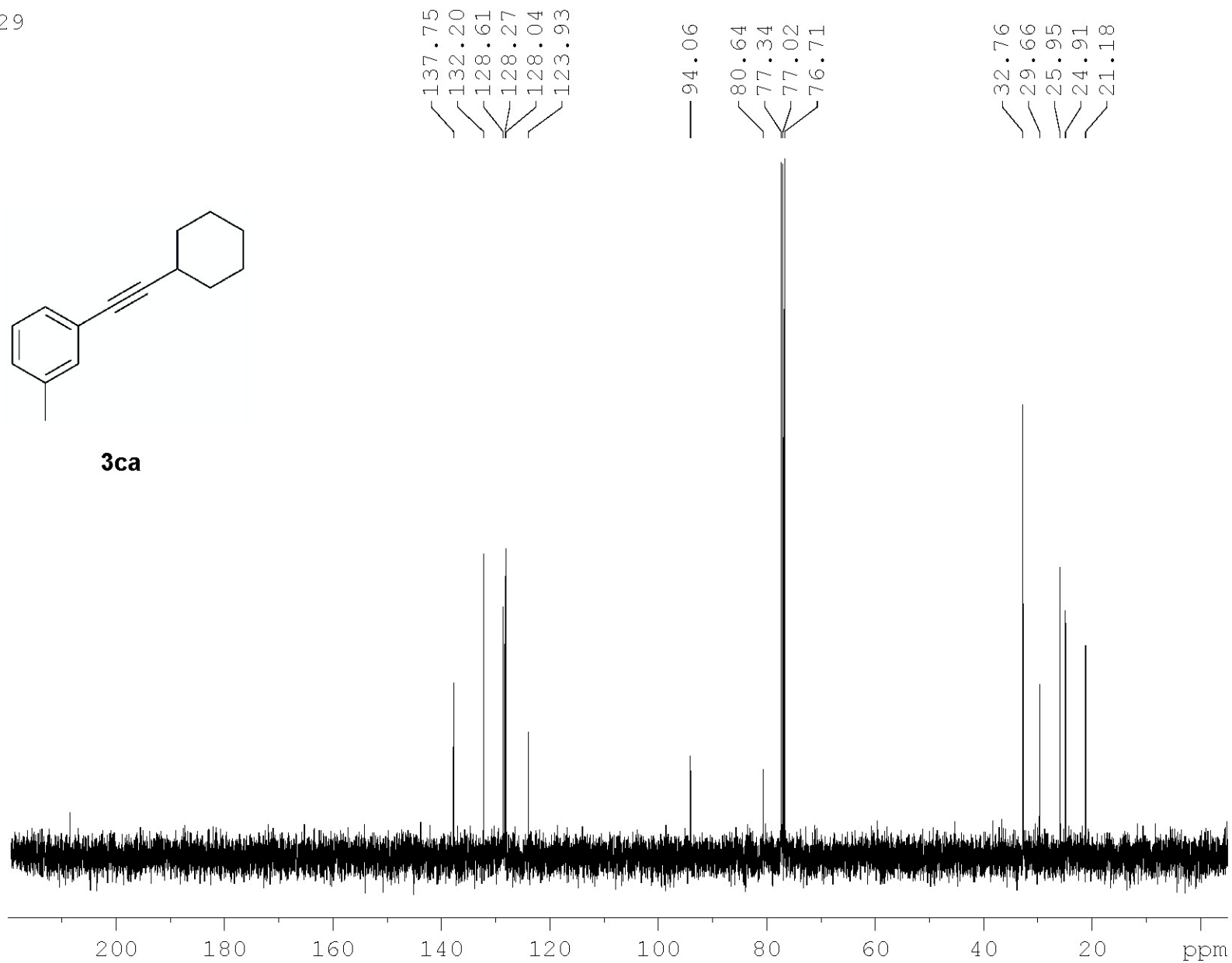
Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zg30
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 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 55.55
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
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 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
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 SF 400.2400173 MHz
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**3ca**

Current Data Parameters
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 PROCNO 1

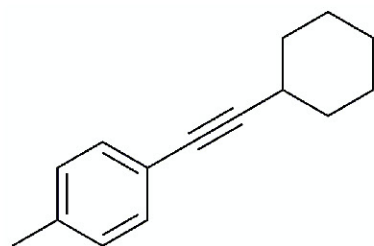
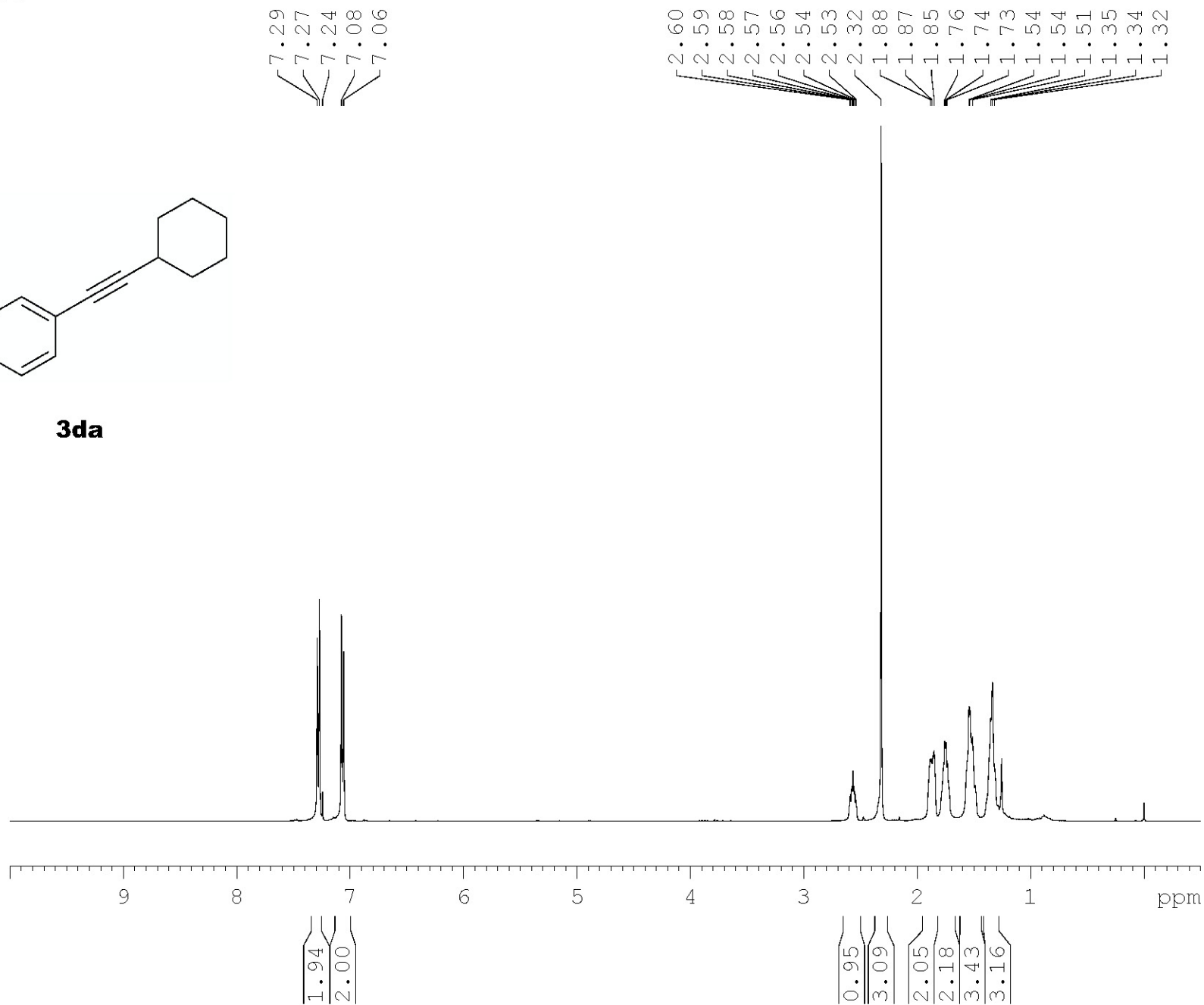
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 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
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===== CHANNEL f1 =====
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===== CHANNEL f2 =====
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730

**3da**

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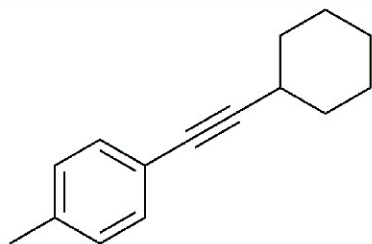
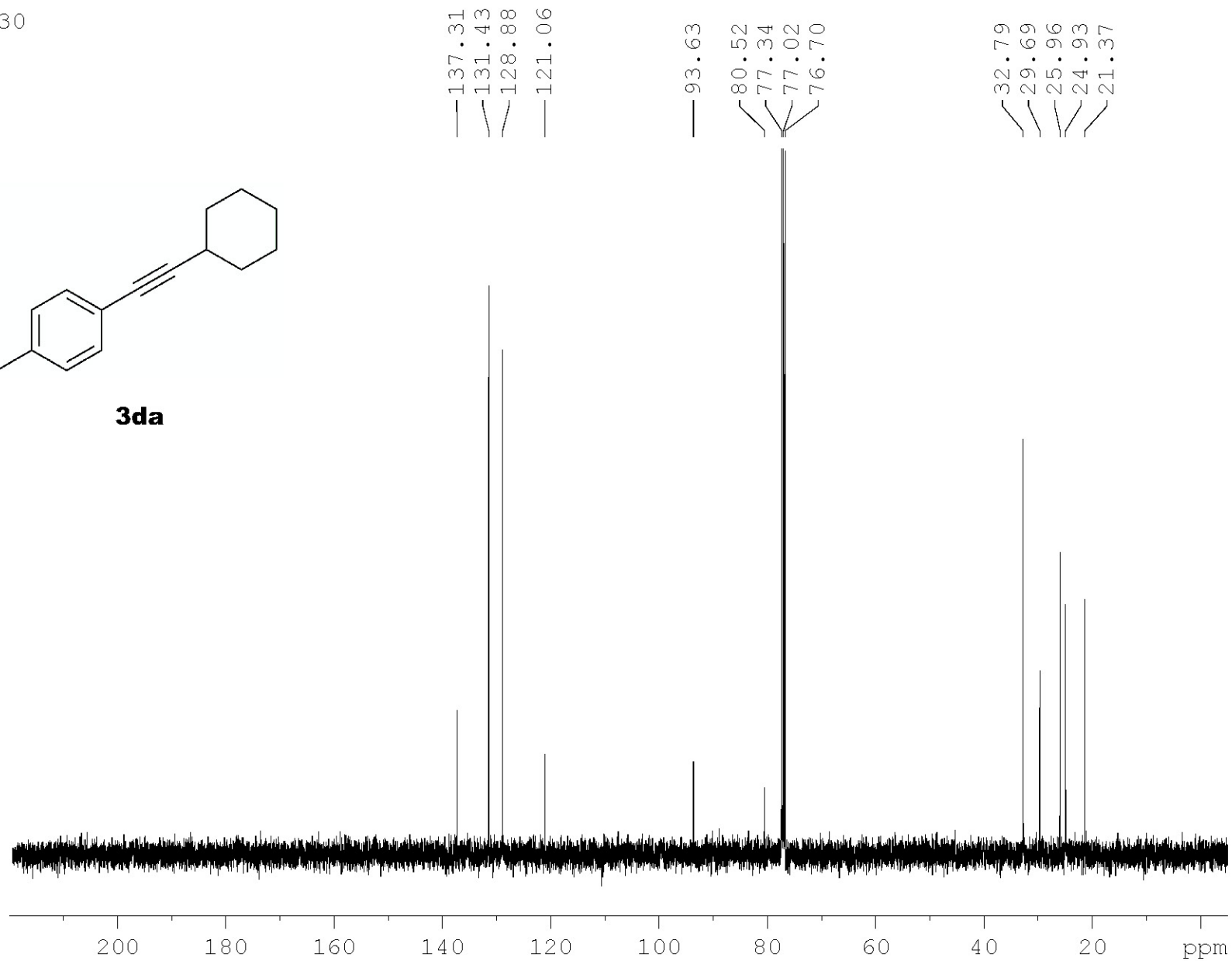
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 D11 0 sec
 TDO 1

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 CPDPRG[2]
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 LB 0.30 Hz
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 PC 1.00

730

**3da**

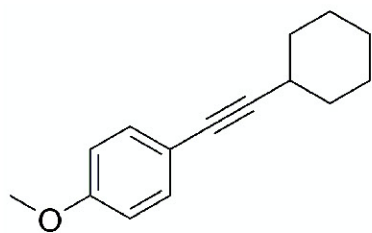
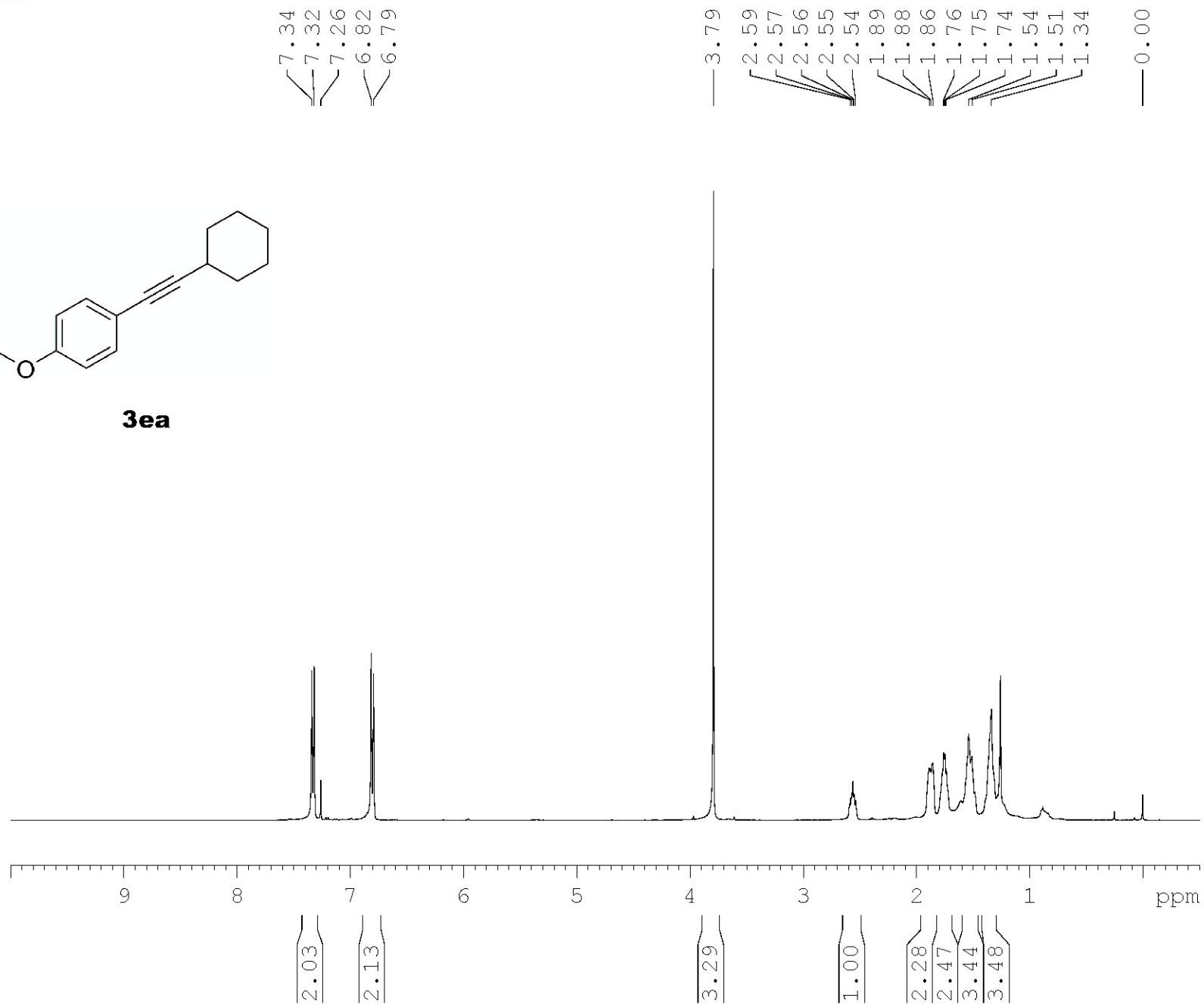
Current Data Parameters
 NAME szy-400
 EXPNO 99
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180813
 Time_ 16.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 46
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404296 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3ea**

Current Data Parameters
 NAME szy-400
 EXPNO 86
 PROCNO 1

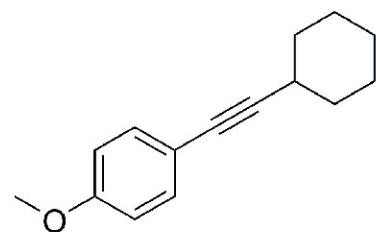
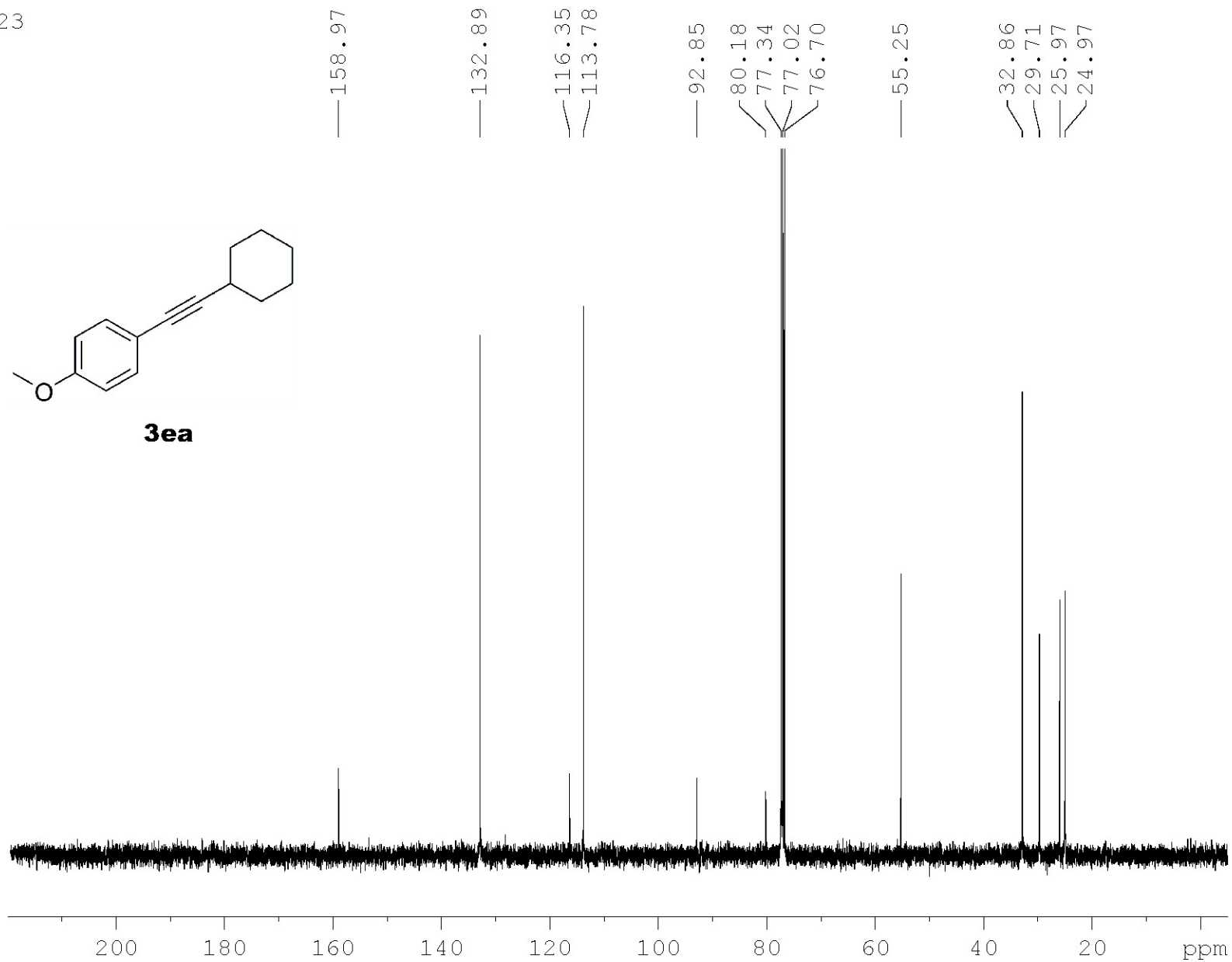
F2 - Acquisition Parameters
 Date_ 20180810
 Time_ 14.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 73.9
 DW 62.400 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

723

**3ea**

Current Data Parameters
 NAME szy-400
 EXPNO 87
 PROCNO 1

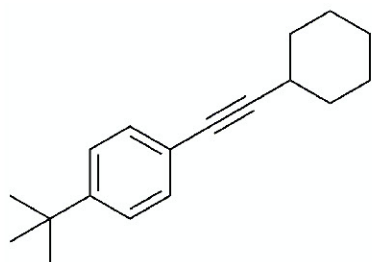
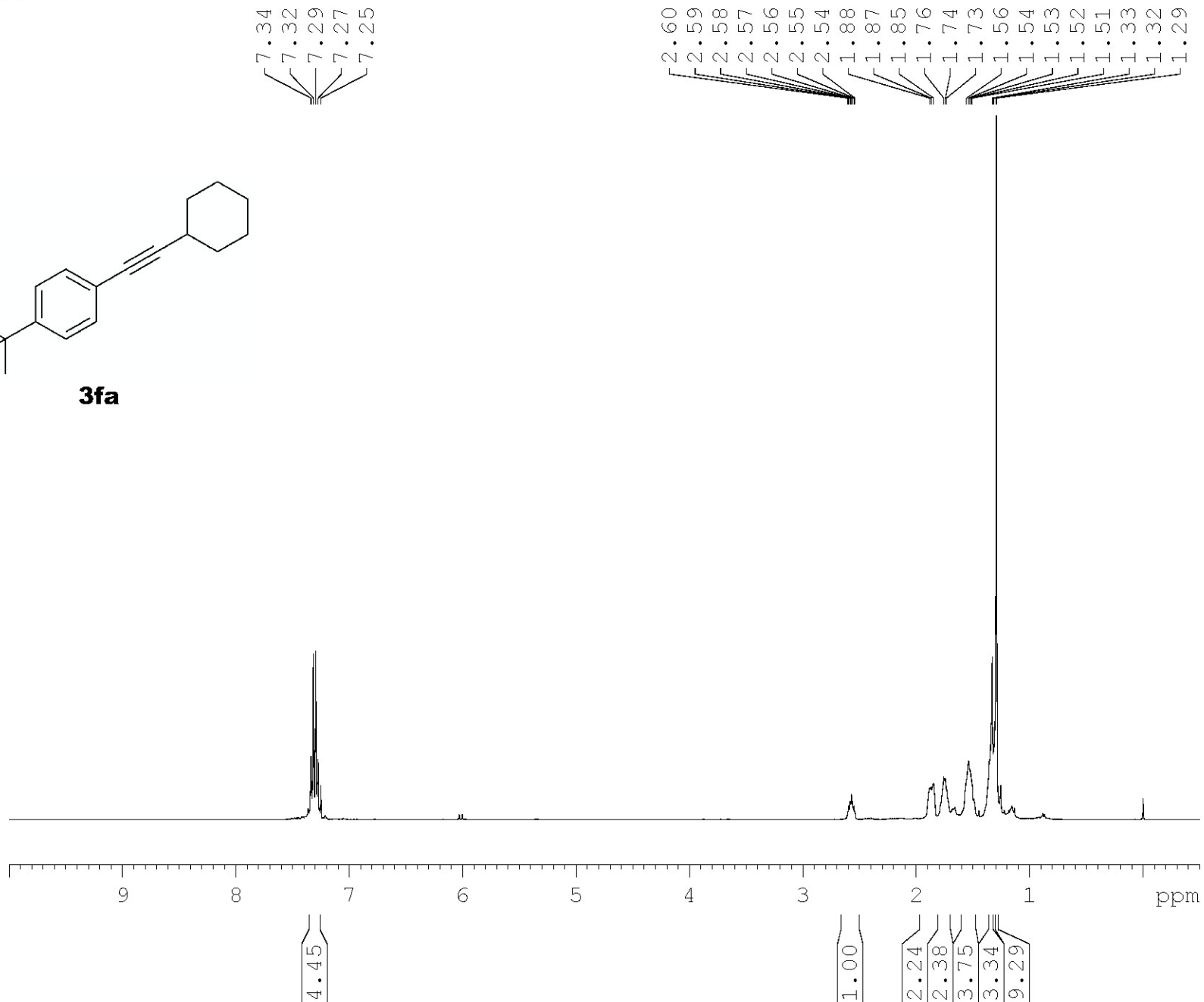
F2 - Acquisition Parameters
 Date_ 20180810
 Time_ 14.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 120
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404274 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

726

**3fa**

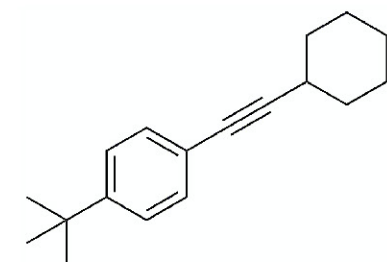
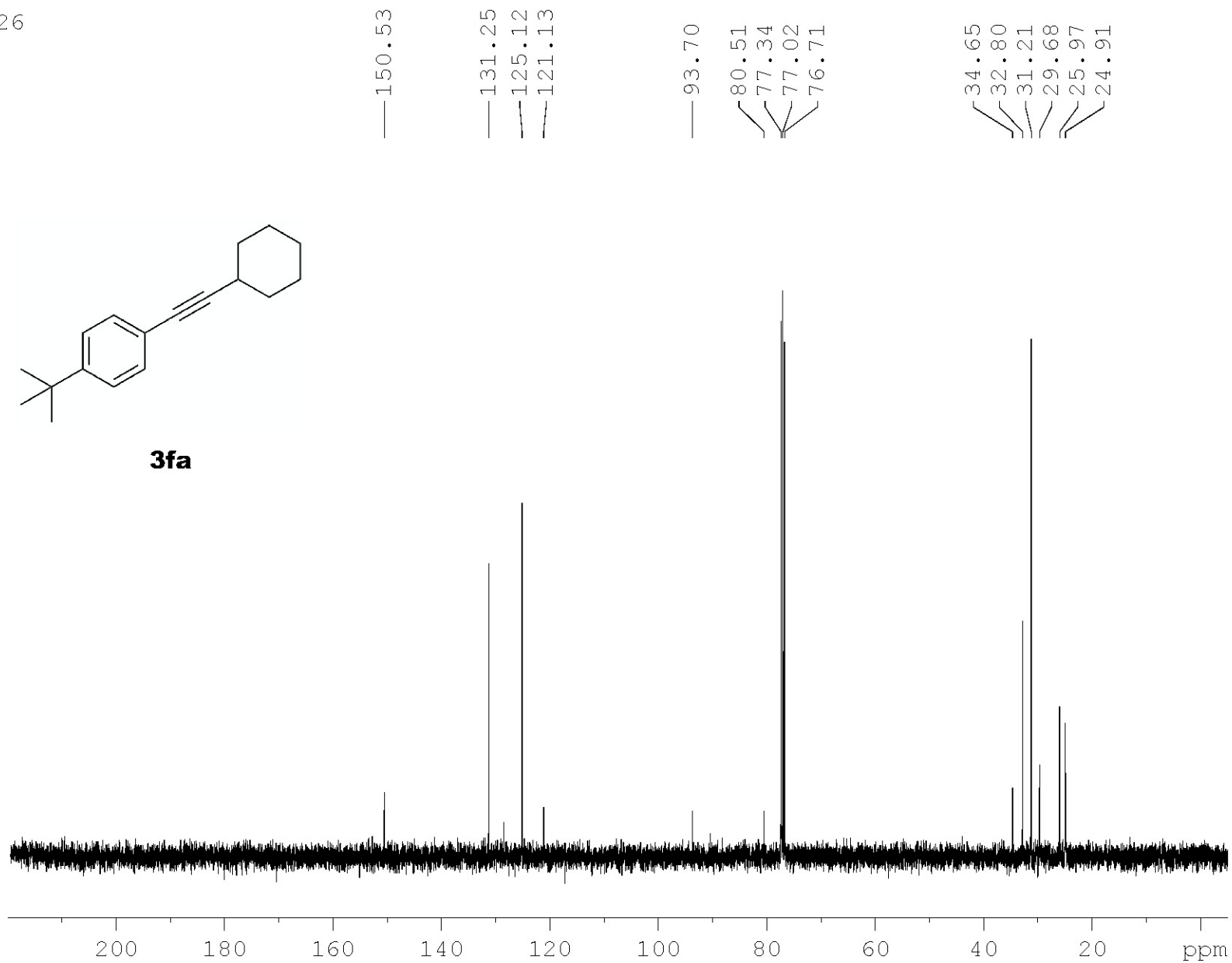
Current Data Parameters
 NAME szy-400
 EXPNO 141
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180824
 Time_ 15.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 65.71
 DW 62.400 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400138 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**3fa**

Current Data Parameters
 NAME szy-400
 EXPNO 142
 PROCNO 1

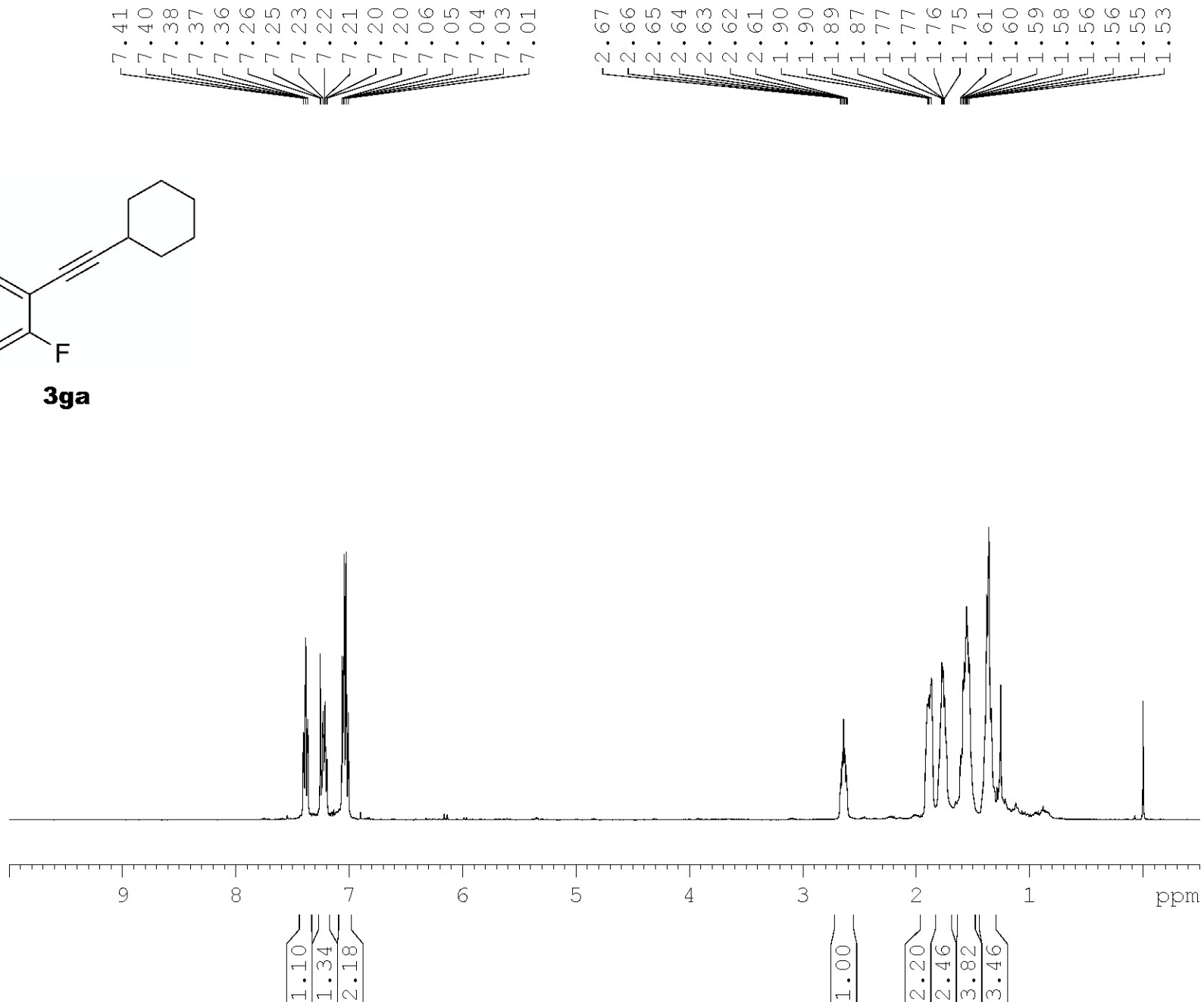
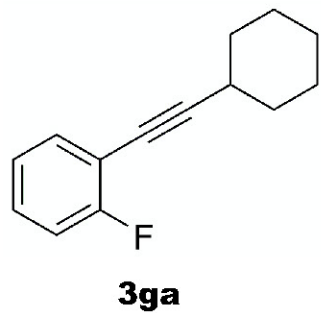
F2 - Acquisition Parameters
 Date_ 20180824
 Time_ 15.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 27
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

747



Current Data Parameters
 NAME szy-400
 EXPNO 148
 PROCNO 1

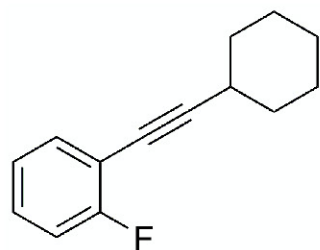
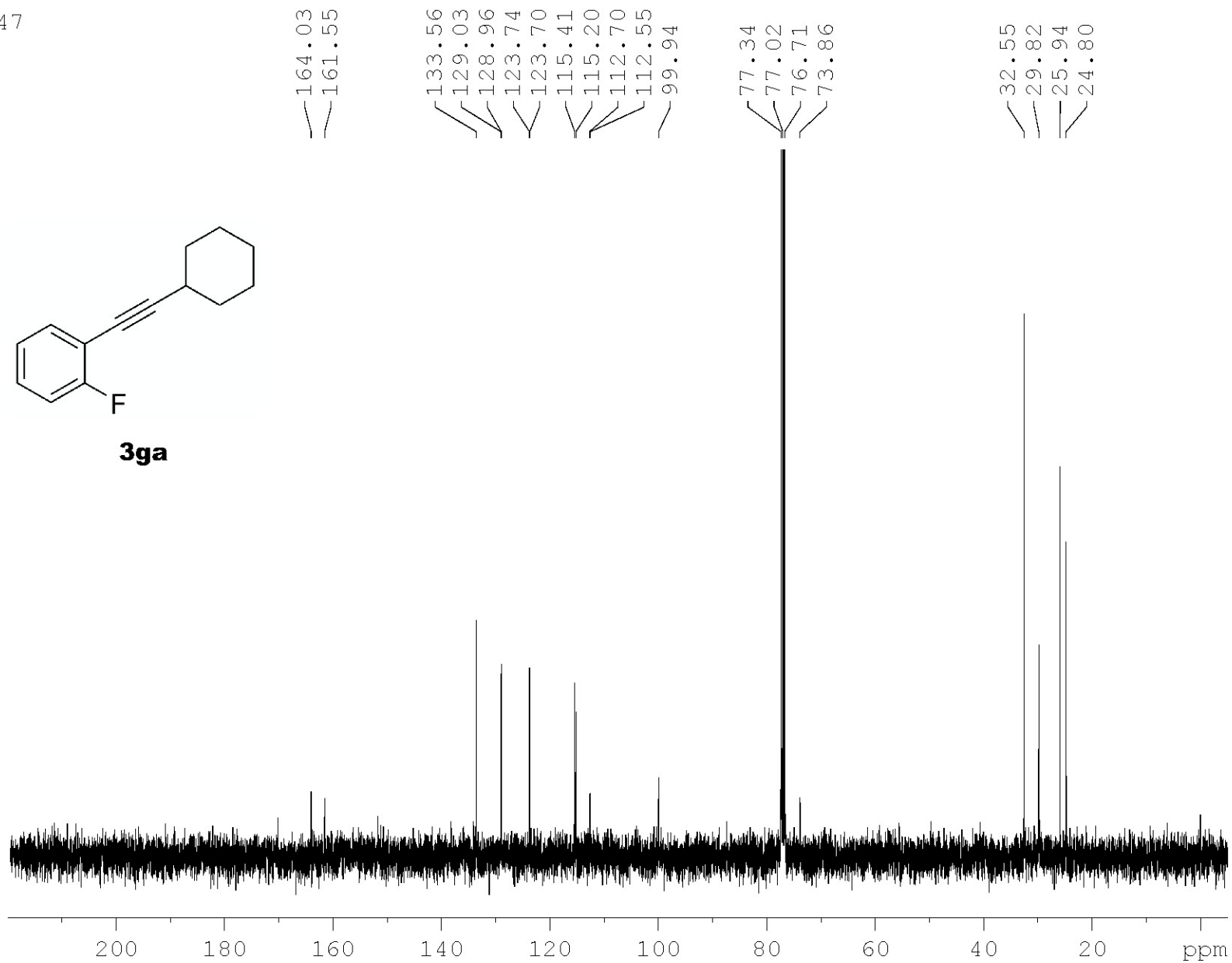
F2 - Acquisition Parameters
 Date_ 20180830
 Time_ 10.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 206.33
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400114 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

747

**3ga**

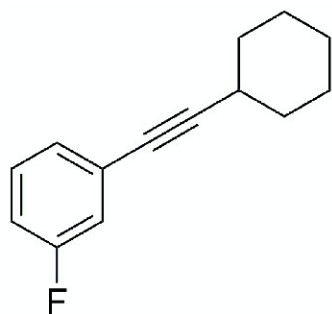
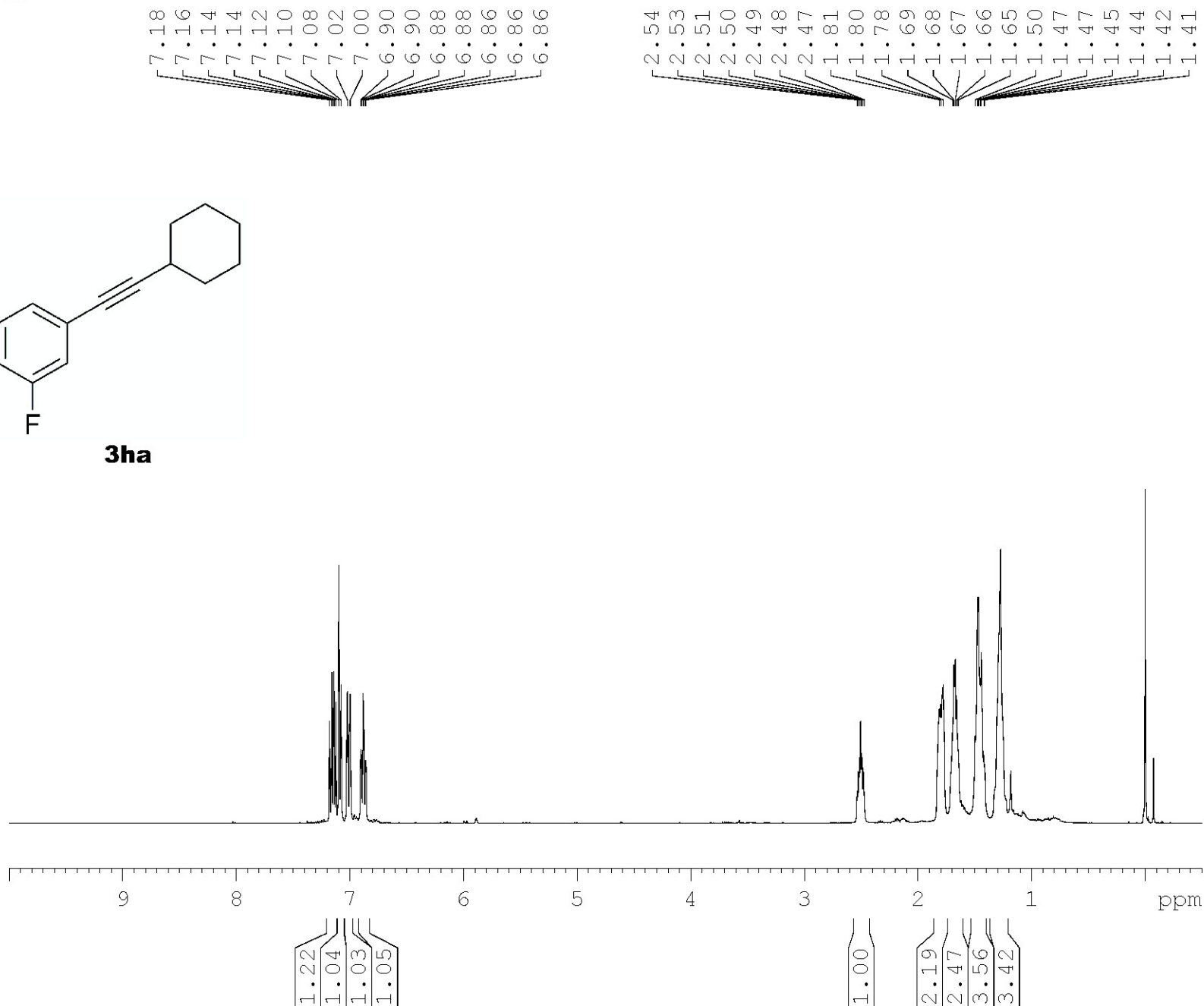
Current Data Parameters
 NAME szy-400
 EXPNO 149
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180830
 Time_ 10.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 153
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404270 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3ha**

Current Data Parameters
 NAME szy-400
 EXPNO 135
 PROCNO 1

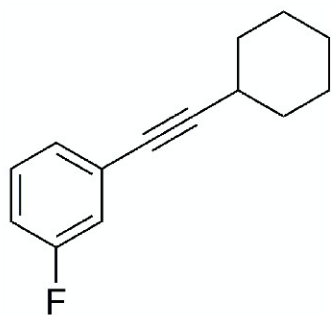
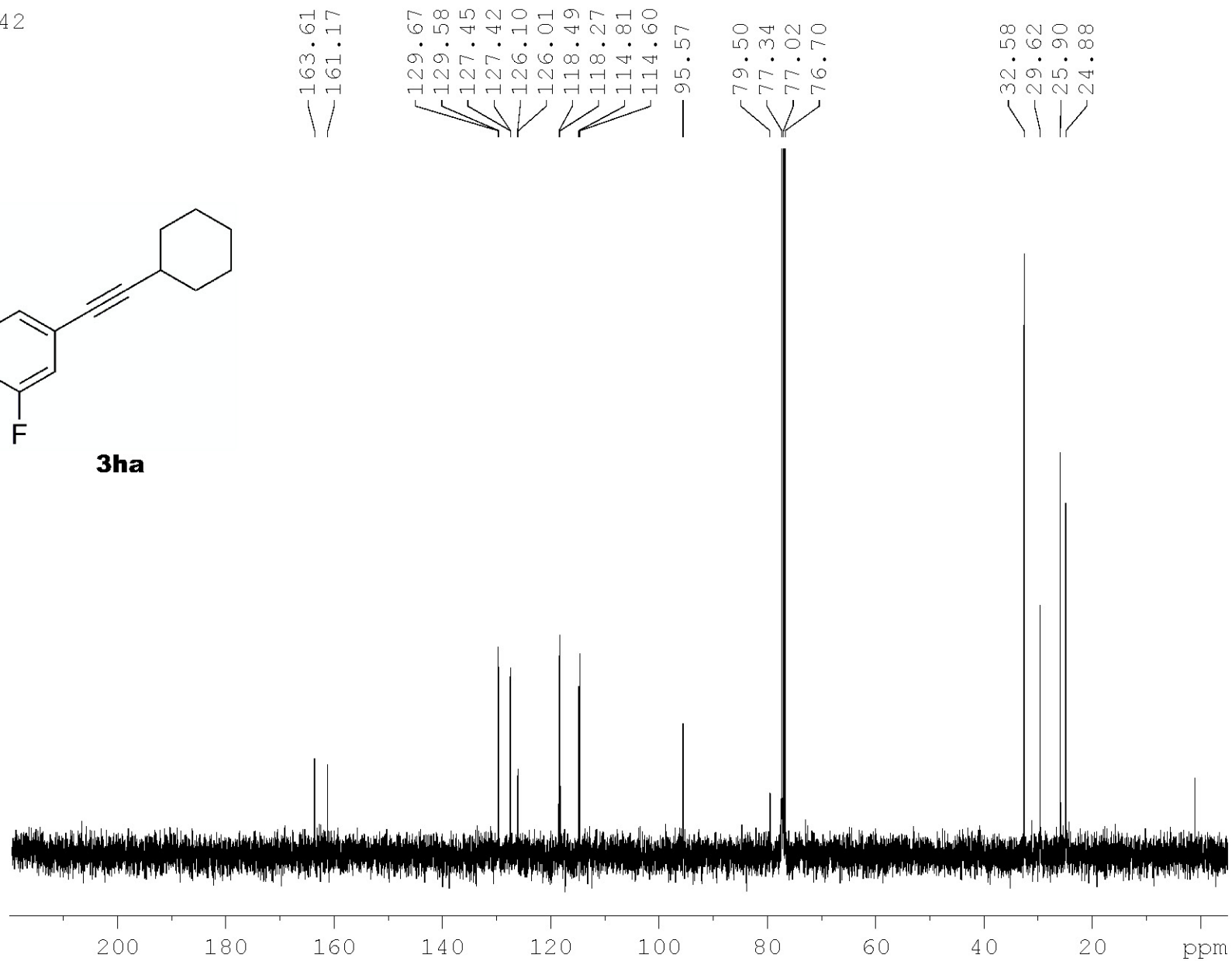
F2 - Acquisition Parameters
 Date_ 20180821
 Time_ 12.37
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 73.9
 DW 62.400 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400414 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

742

**3ha**

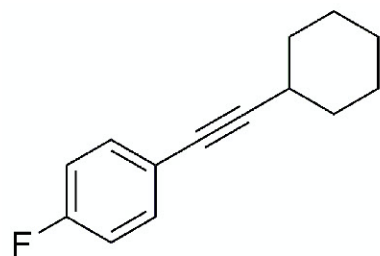
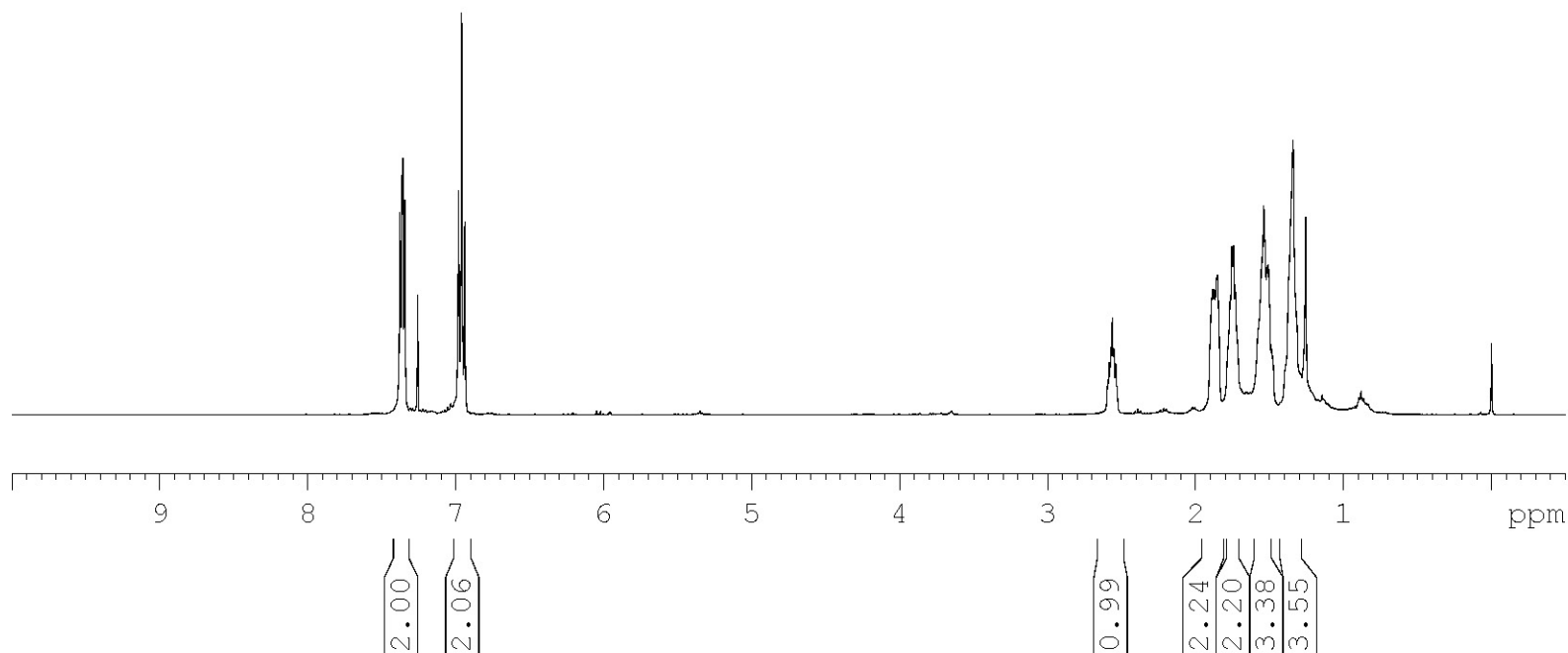
Current Data Parameters
 NAME szy-400
 EXPNO 136
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180821
 Time_ 12.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 61
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404278 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3ia**

Current Data Parameters
 NAME szy-400
 EXPNO 143
 PROCNO 1

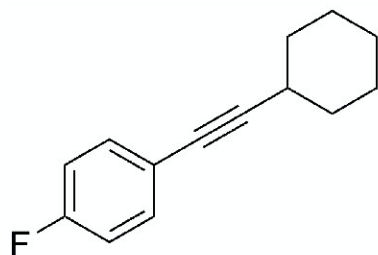
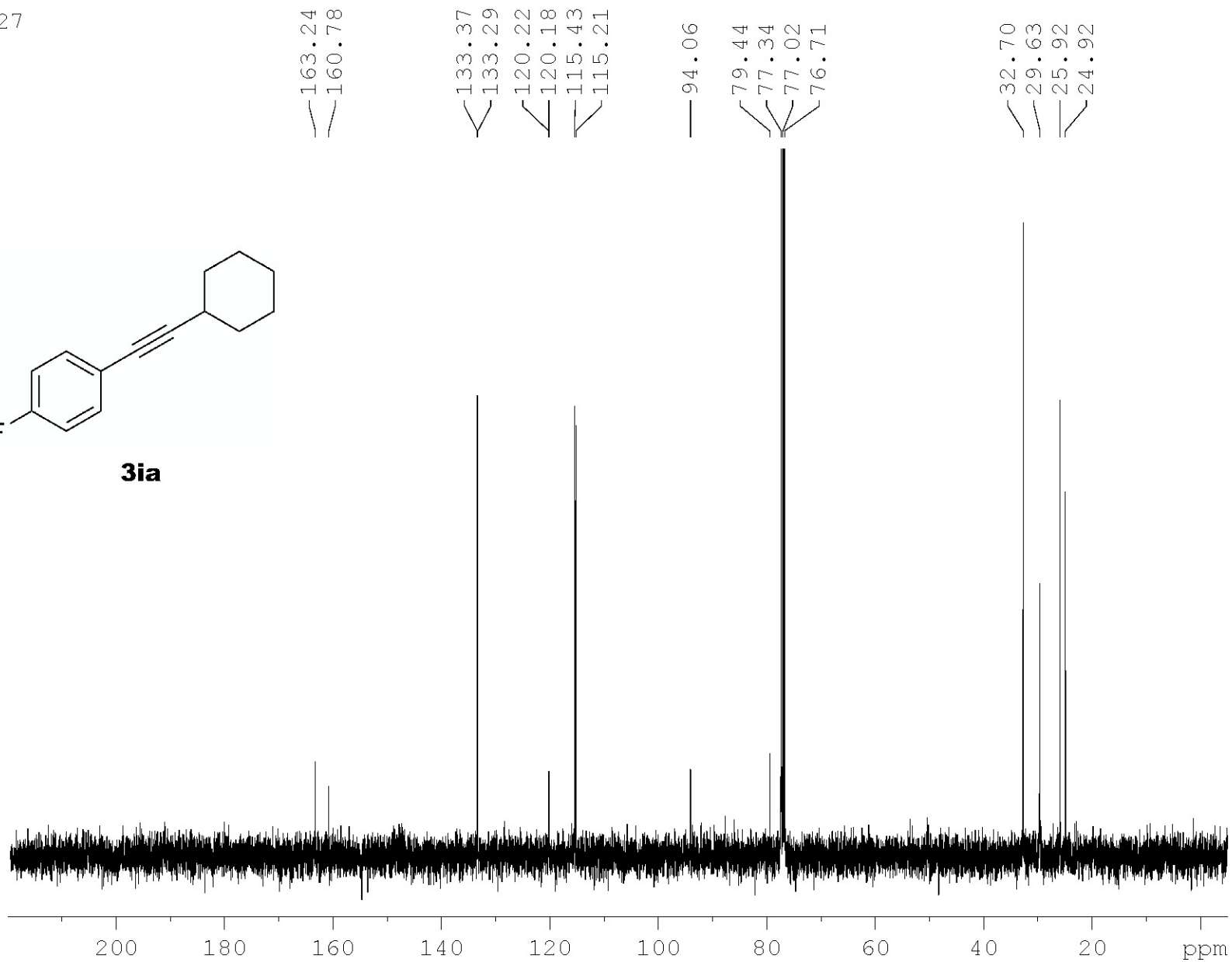
F2 - Acquisition Parameters
 Date_ 20180824
 Time_ 15.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 140.59
 DW 62.400 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400112 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

727

**3ia**

Current Data Parameters
 NAME szy-400
 EXPNO 144
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180824
 Time_ 15.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 73
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

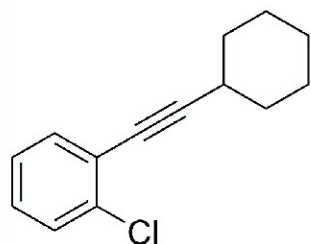
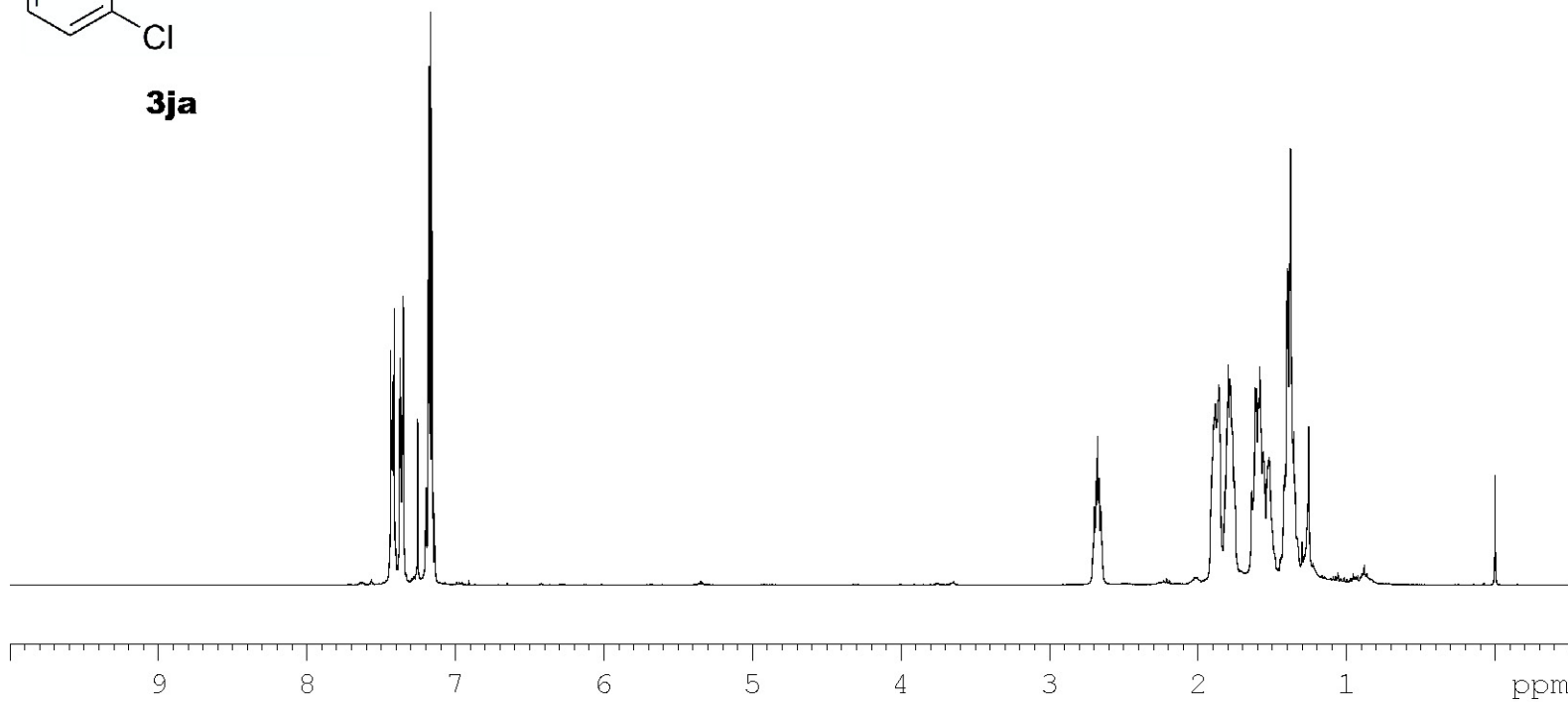
===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404274 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

746

7.44
7.43
7.43
7.42
7.41
7.37
7.37
7.37
7.36
7.35
7.35
7.25
7.20
7.18
7.18
7.17
7.16
7.15
2.69
2.68
2.67
1.90
1.90
1.88
1.86
1.80
1.80
1.79
1.78
1.77
1.77
1.76
1.64
1.62
1.61
1.59
1.58
1.56
1.53
1.52
1.41
1.40
1.39
1.38
1.36
1.35

**3ja**

1.06
1.06
2.14

1.00

2.19
2.28
3.58
3.35

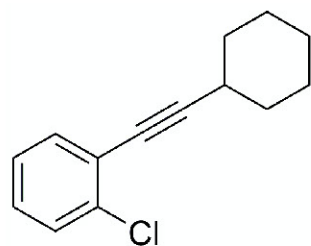
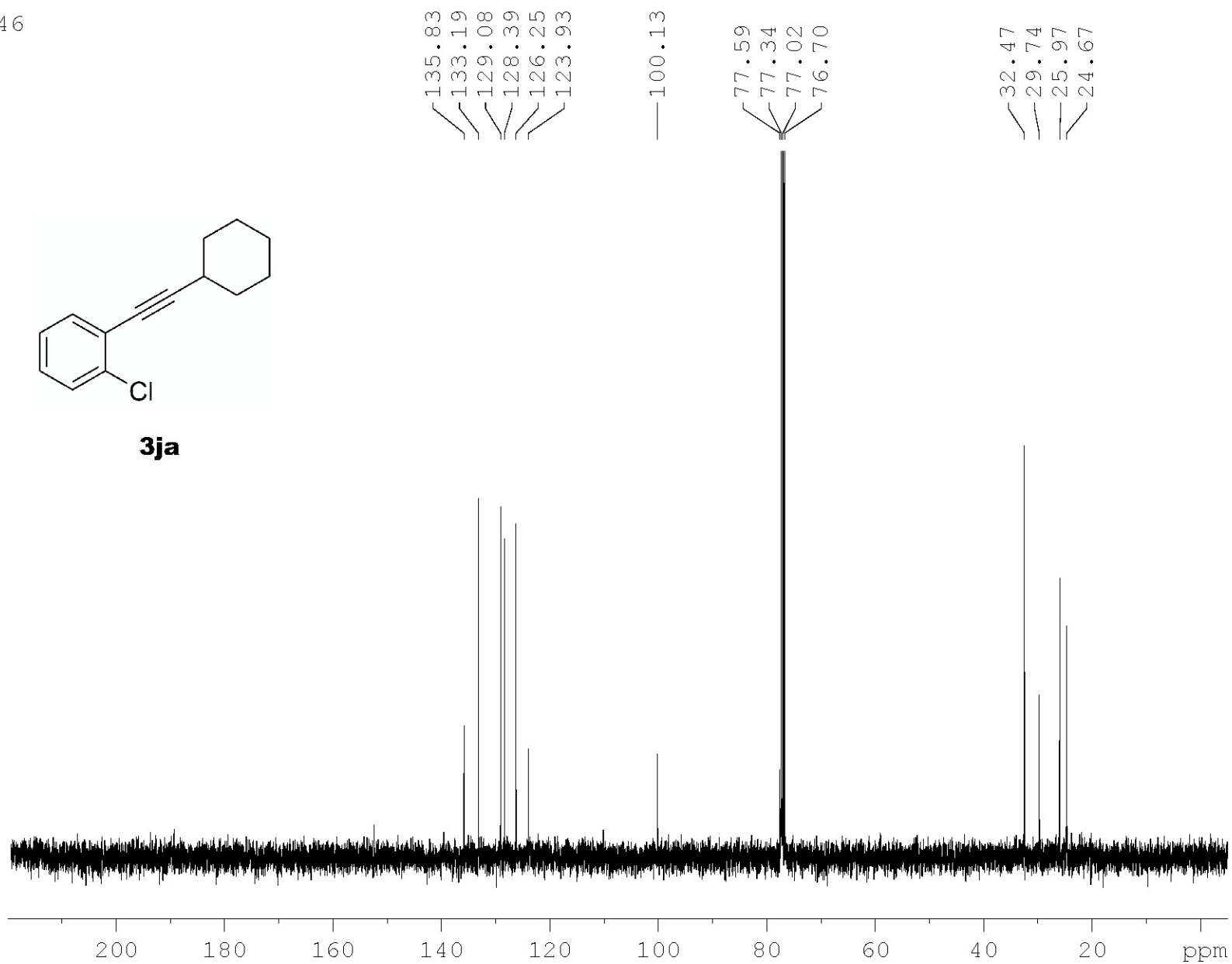
Current Data Parameters
NAME szy-400
EXPNO 146
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180829
Time_ 14.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 102.73
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

**3ja**

Current Data Parameters
 NAME szy-400
 EXPNO 147
 PROCNO 1

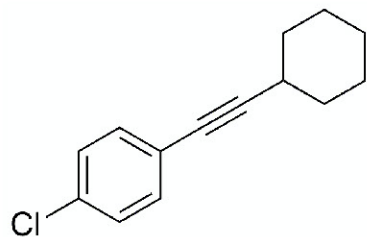
F2 - Acquisition Parameters
 Date_ 20180829
 Time_ 14.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 48
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404288 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

731

**3ka**

7.32
7.30
7.25
7.23

2.60
2.59
2.58
2.57
2.56
2.54
2.54
1.88
1.87
1.85
1.76
1.75
1.74
1.73
1.56
1.55
1.54
1.51
1.48
1.34

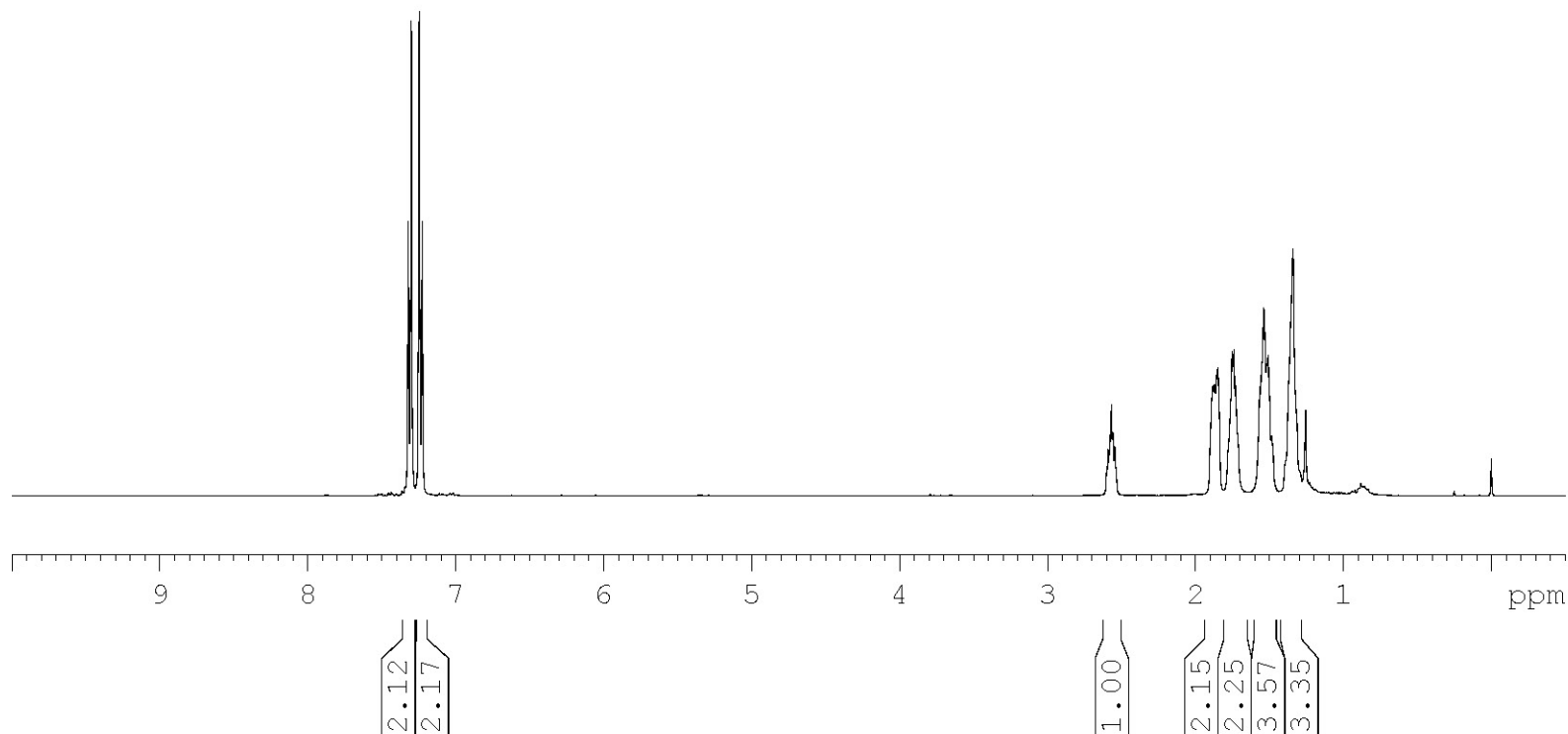
Current Data Parameters
NAME szy-400
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180813
Time_ 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0 sec
TDO 1

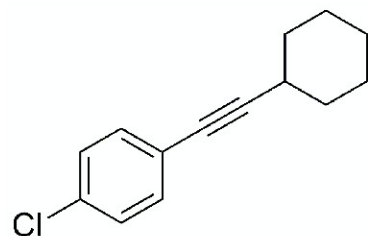
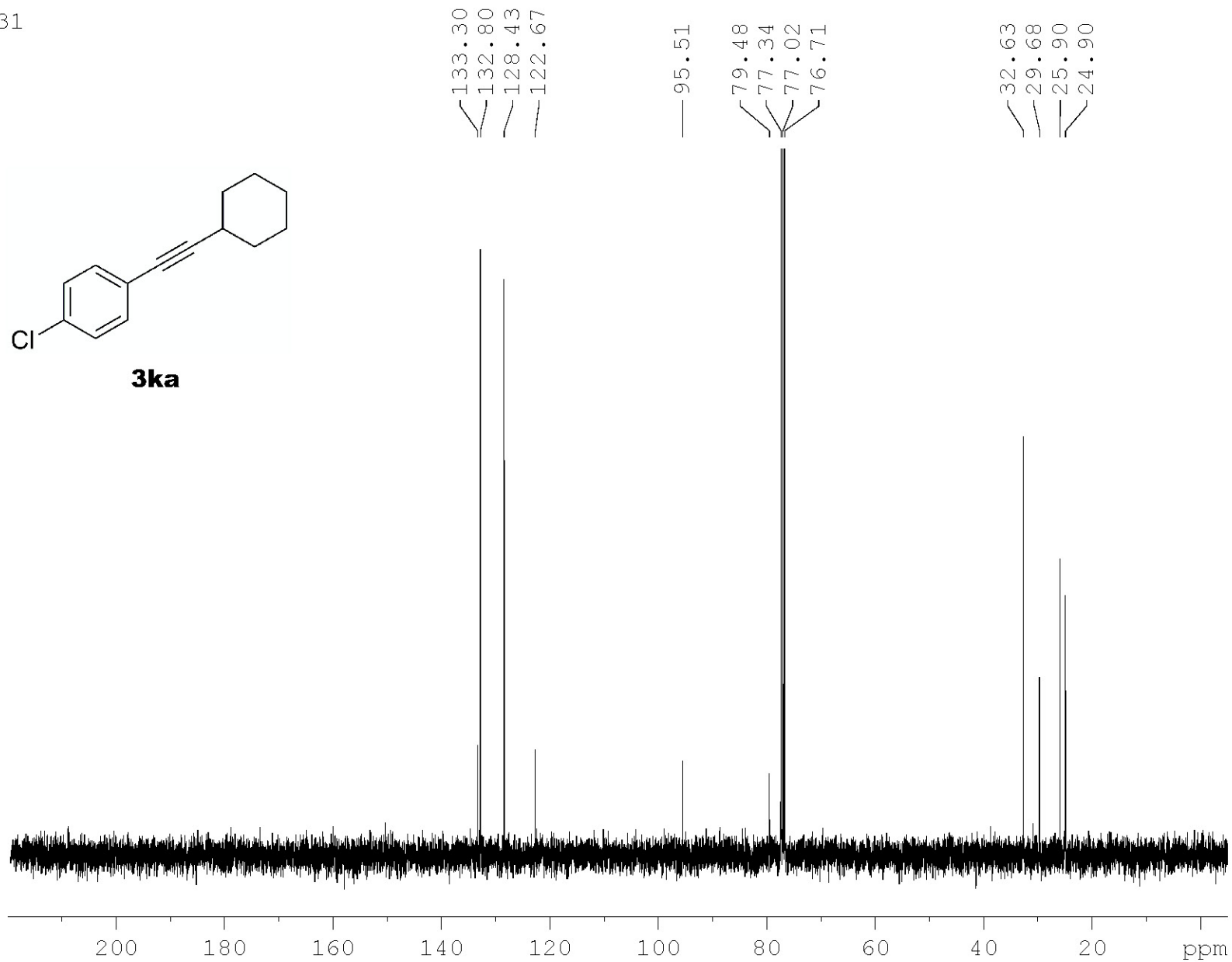
===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



731

**3ka**

Current Data Parameters
 NAME szy-400
 EXPNO 101
 PROCNO 1

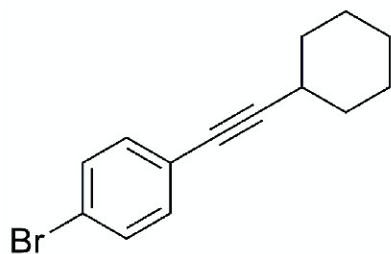
F2 - Acquisition Parameters
 Date_ 20180813
 Time_ 16.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 39
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404281 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

743

**3la**

7.33
7.31
7.18
7.16

2.52
2.51
2.50
2.49
2.48
2.47
2.46
1.81
1.80
1.78
1.77
1.69
1.68
1.67
1.66
1.64
1.48
1.47
1.44
1.43
1.41
1.40

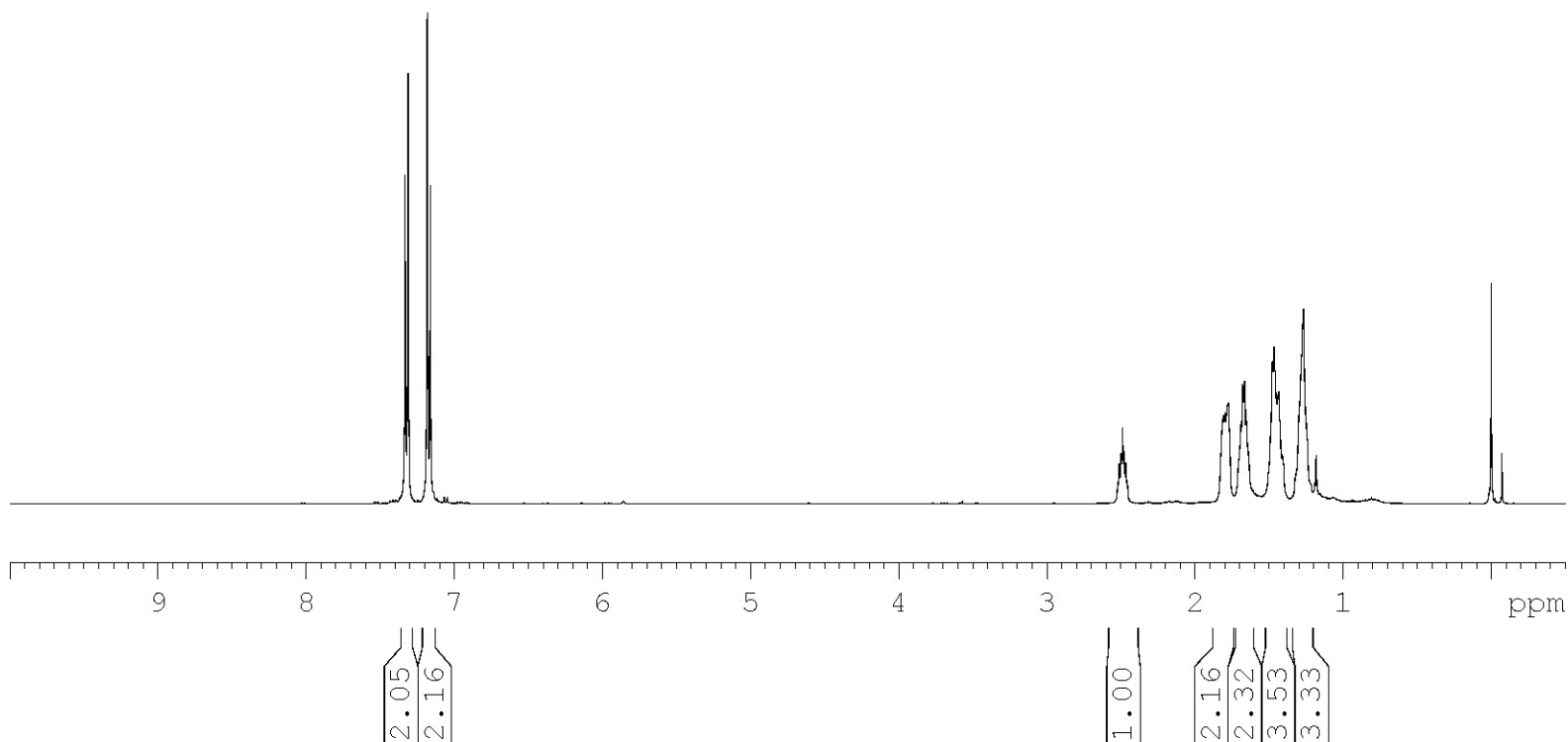
Current Data Parameters
NAME szy-400
EXPNO 137
PROCNO 1

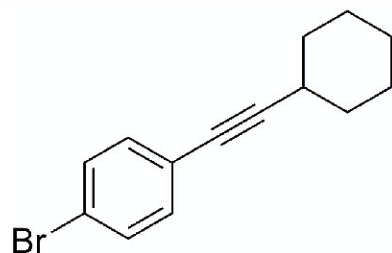
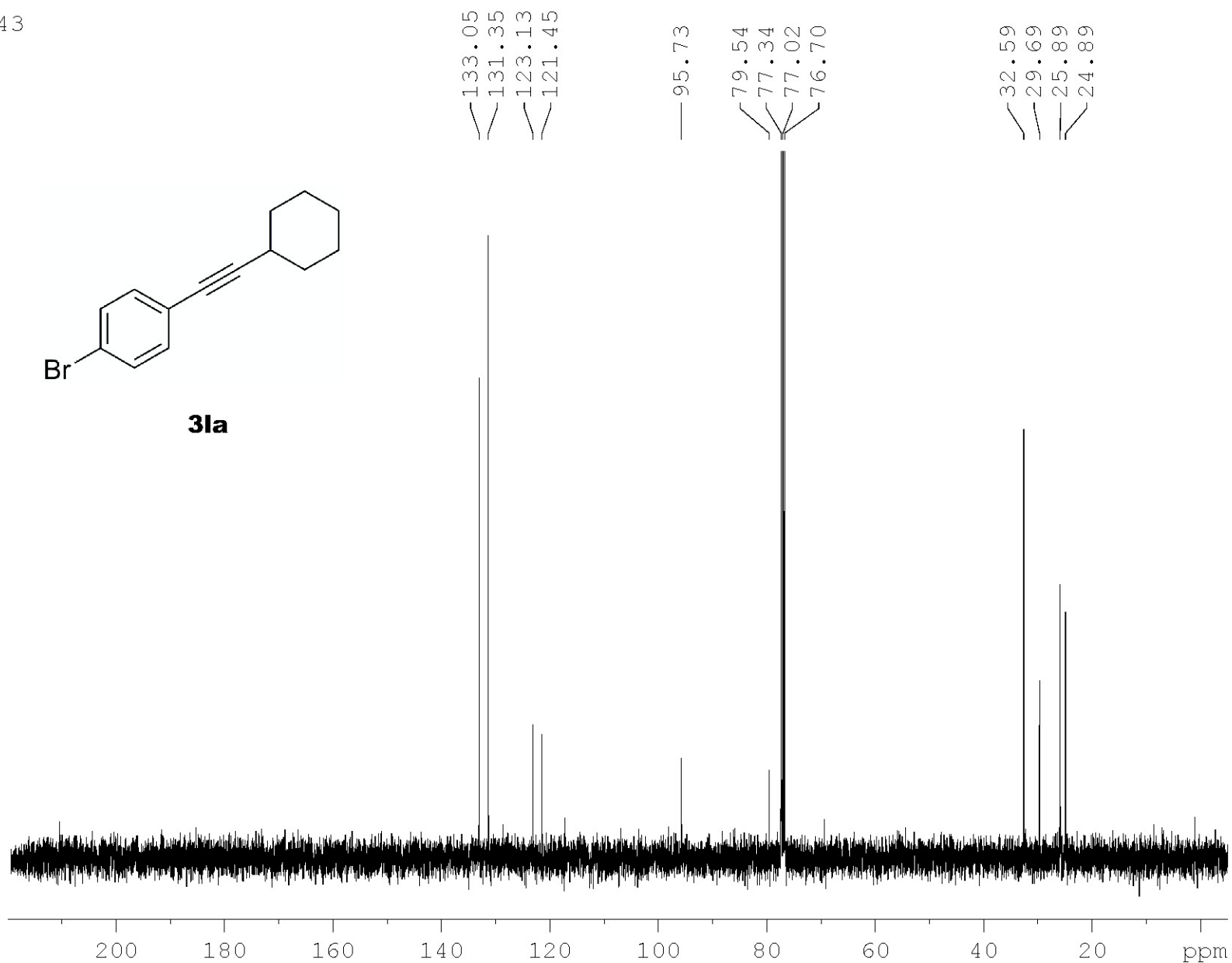
F2 - Acquisition Parameters
Date_ 20180821
Time_ 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 80.72
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400407 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



**3la**

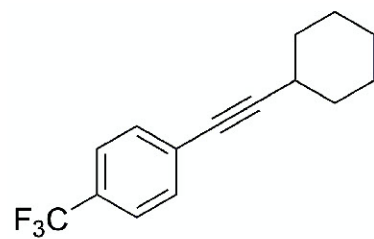
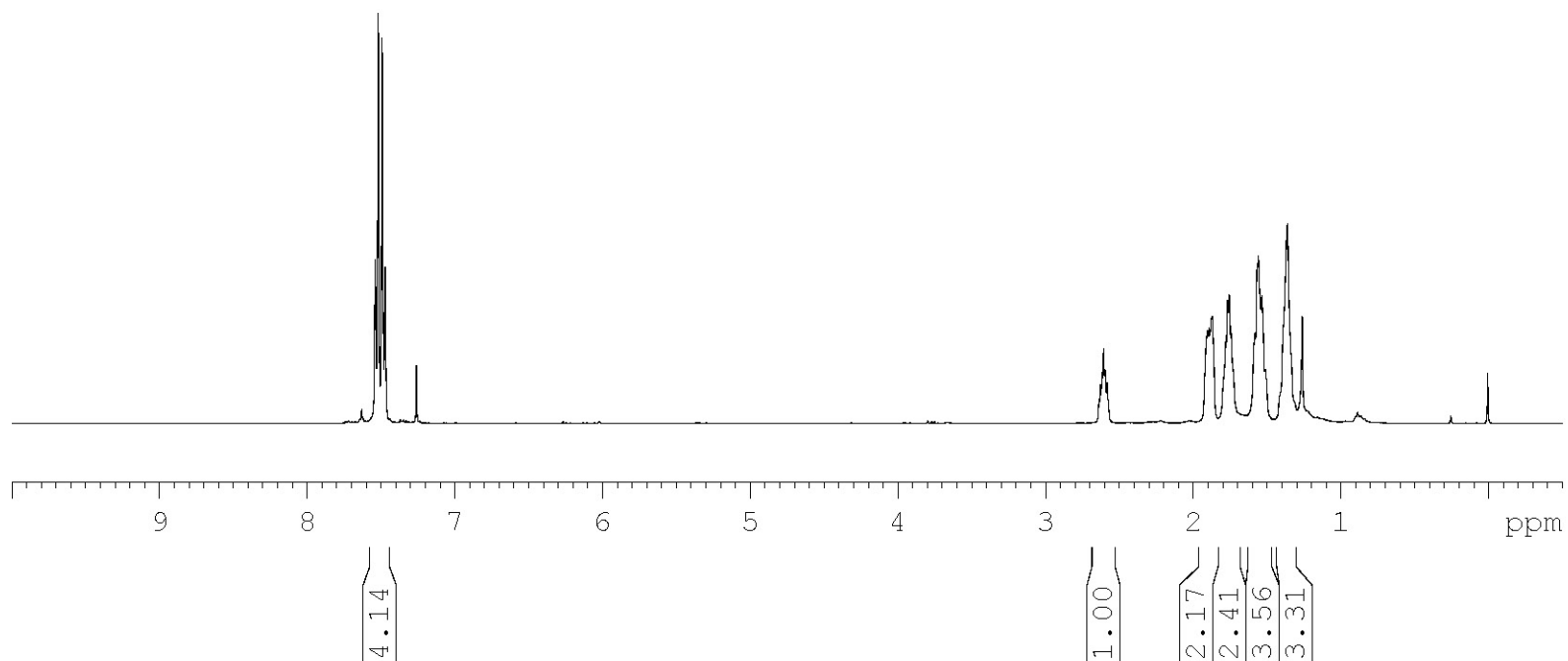
Current Data Parameters
 NAME szy-400
 EXPNO 138
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180821
 Time_ 12.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 45
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404288 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3ma**

7.54
7.52
7.49
7.47
7.26
2.64
2.63
2.62
2.61
2.60
2.58
2.58
1.90
1.89
1.87
1.78
1.77
1.76
1.75
1.58
1.57
1.56
1.53
1.51
1.36

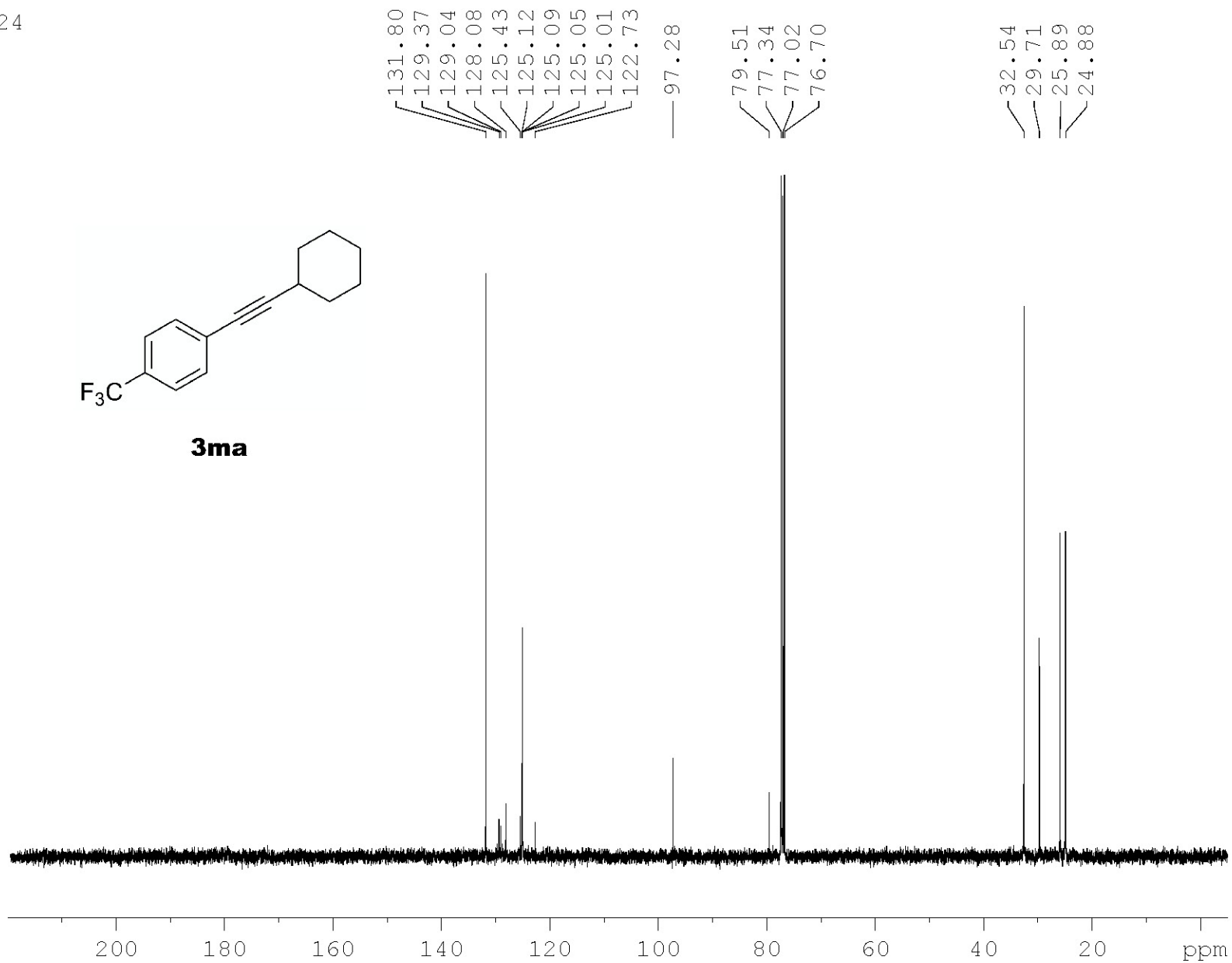
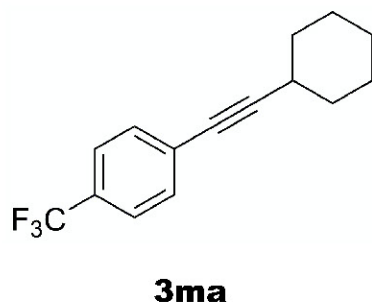
Current Data Parameters
NAME szy-400
EXPNO 88
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180810
Time_ 16.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME szy-400
 EXPNO 89
 PROCNO 1

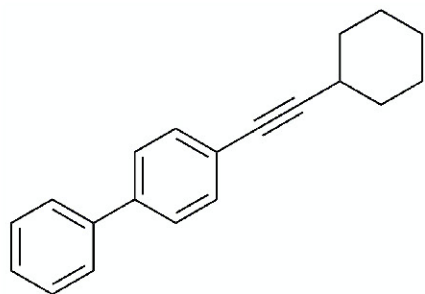
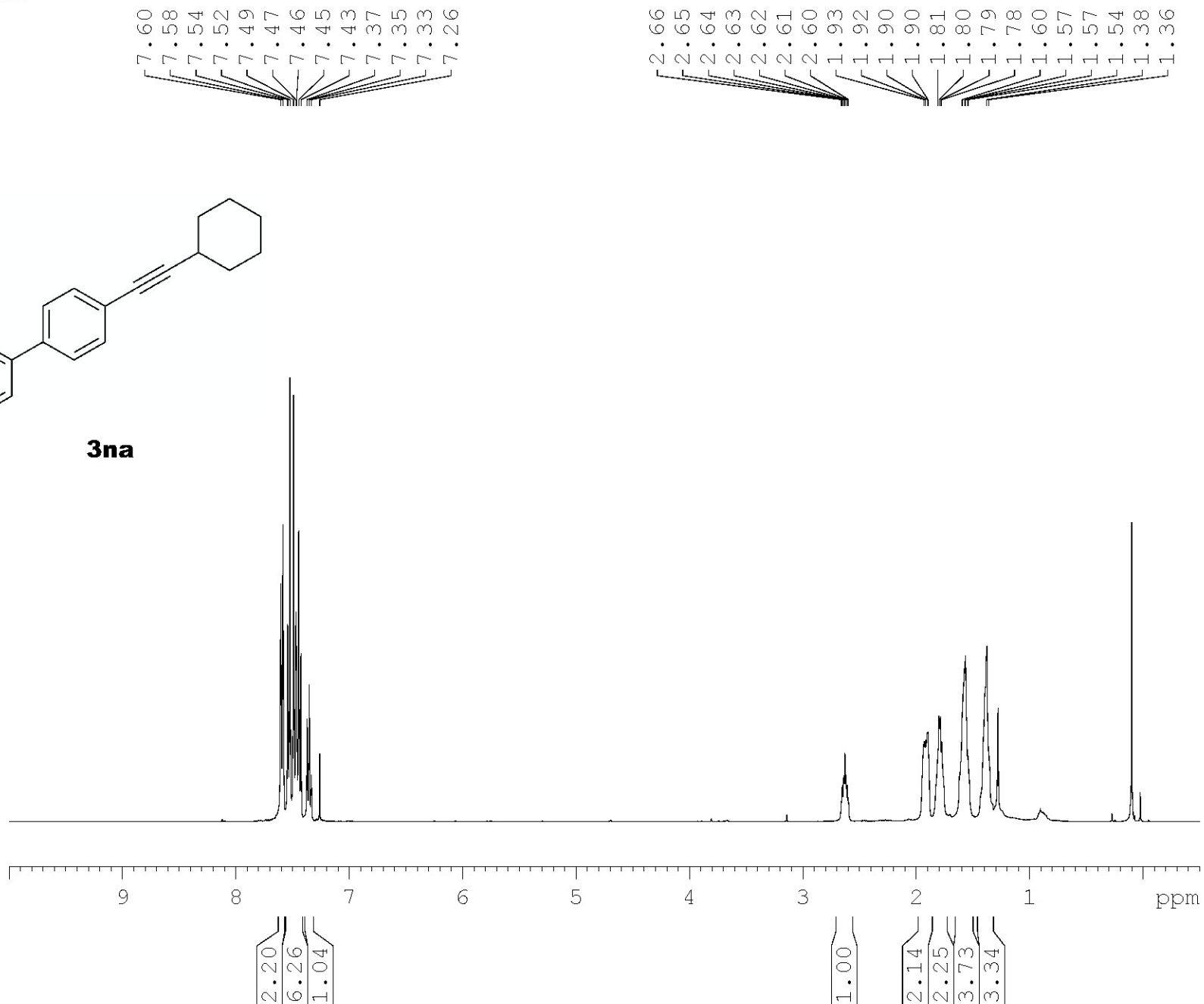
F2 - Acquisition Parameters
 Date_ 20180810
 Time_ 16.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 143
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404259 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

722

**3na**

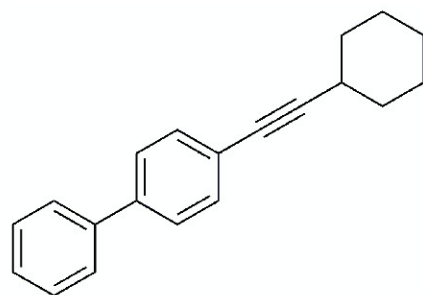
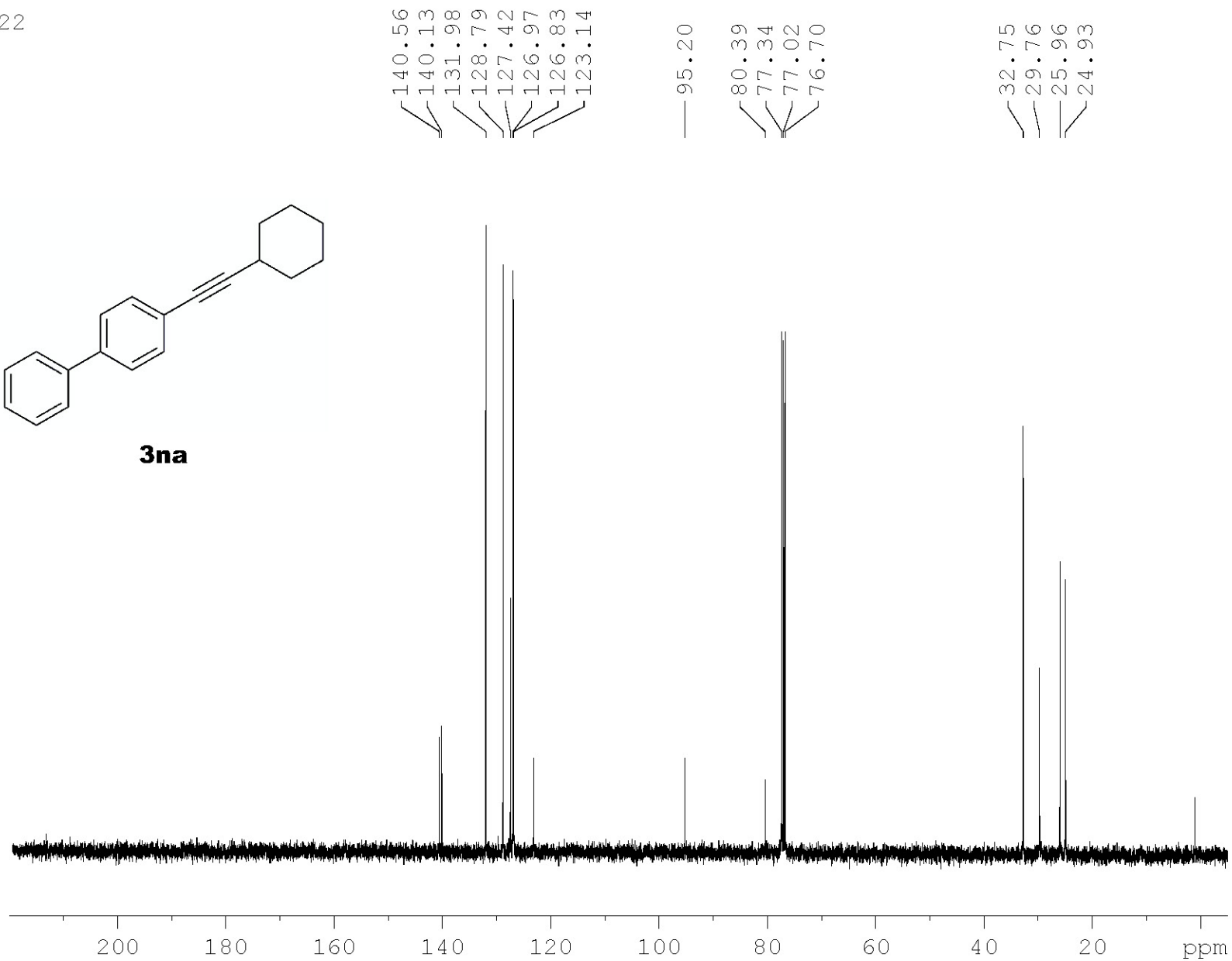
Current Data Parameters
 NAME szy-400
 EXPNO 84
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180809
 Time_ 20.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 55.55
 DW 62.400 usec
 DE 6.50 usec
 TE 299.6 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**3na**

Current Data Parameters
 NAME szy-400
 EXPNO 85
 PROCNO 1

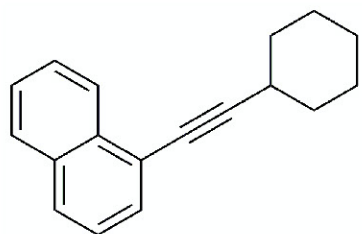
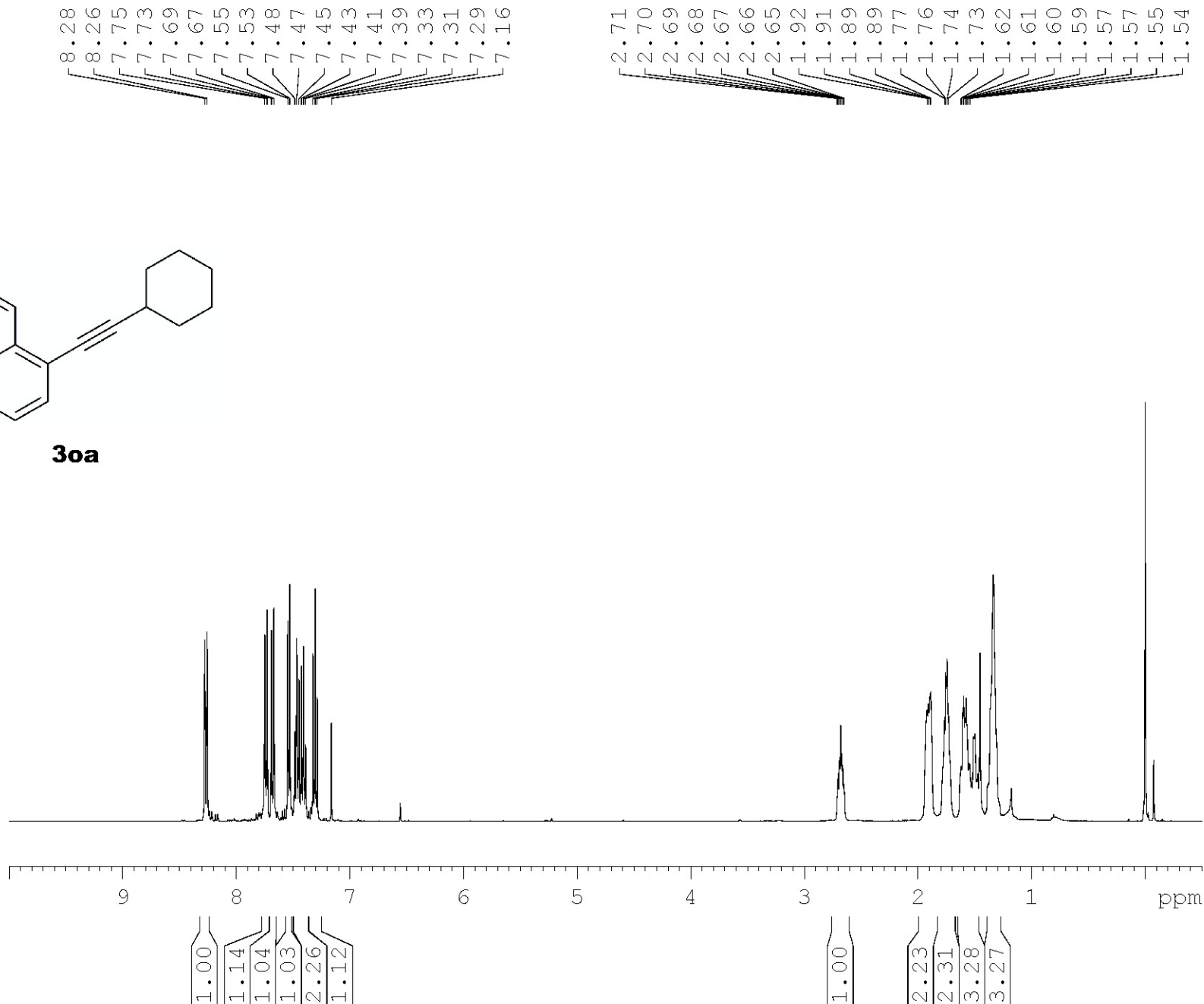
F2 - Acquisition Parameters
 Date_ 20180809
 Time_ 21.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 72
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404301 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

732

**30a**

Current Data Parameters
 NAME szy-400
 EXPNO 131
 PROCNO 1

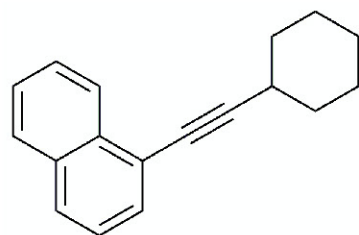
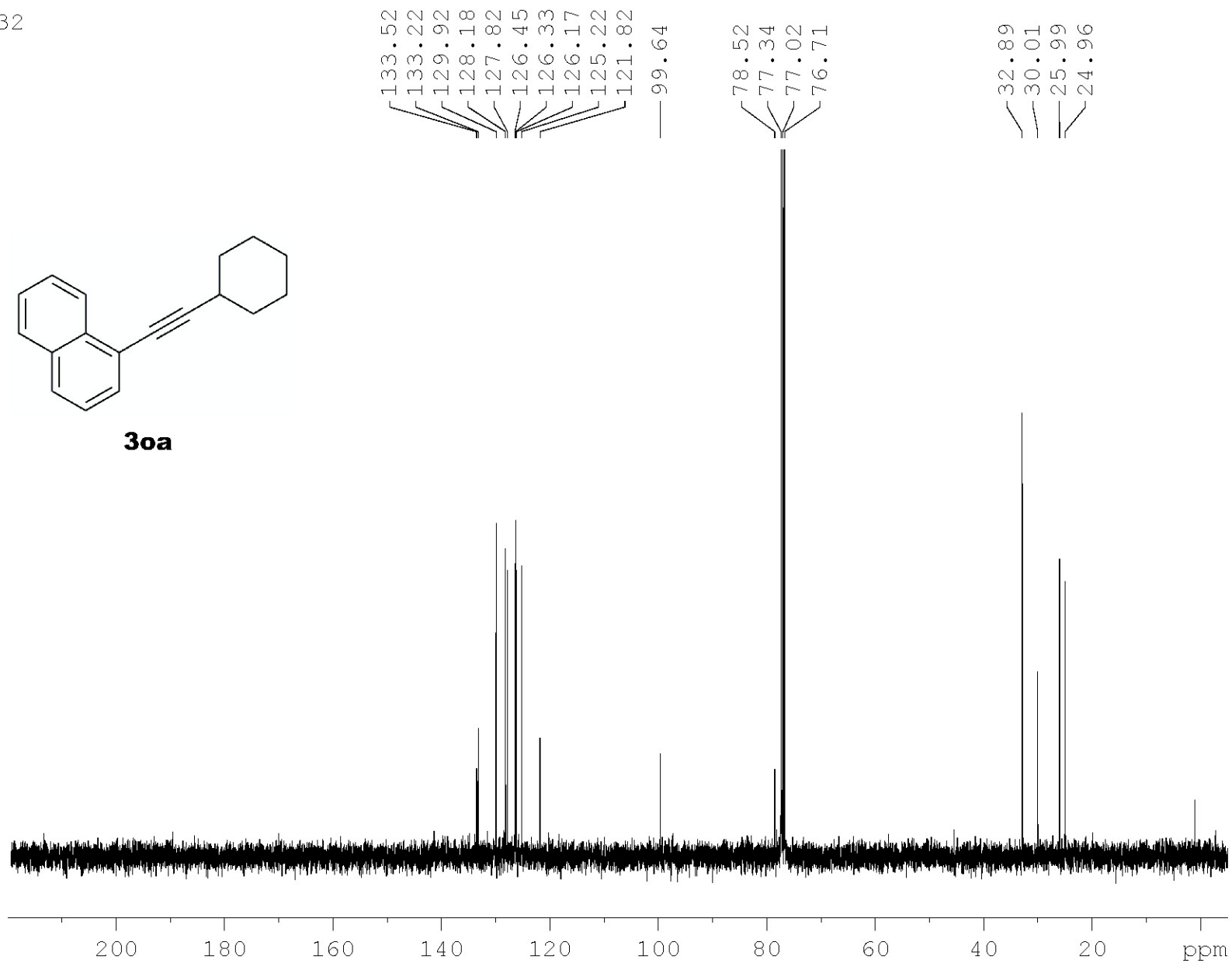
F2 - Acquisition Parameters
 Date_ 20180817
 Time_ 16.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 73.9
 DW 62.400 usec
 DE 6.50 usec
 TE 299.5 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400484 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

732

**30a**

Current Data Parameters
 NAME szy-400
 EXPNO 132
 PROCNO 1

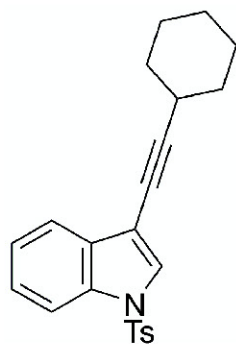
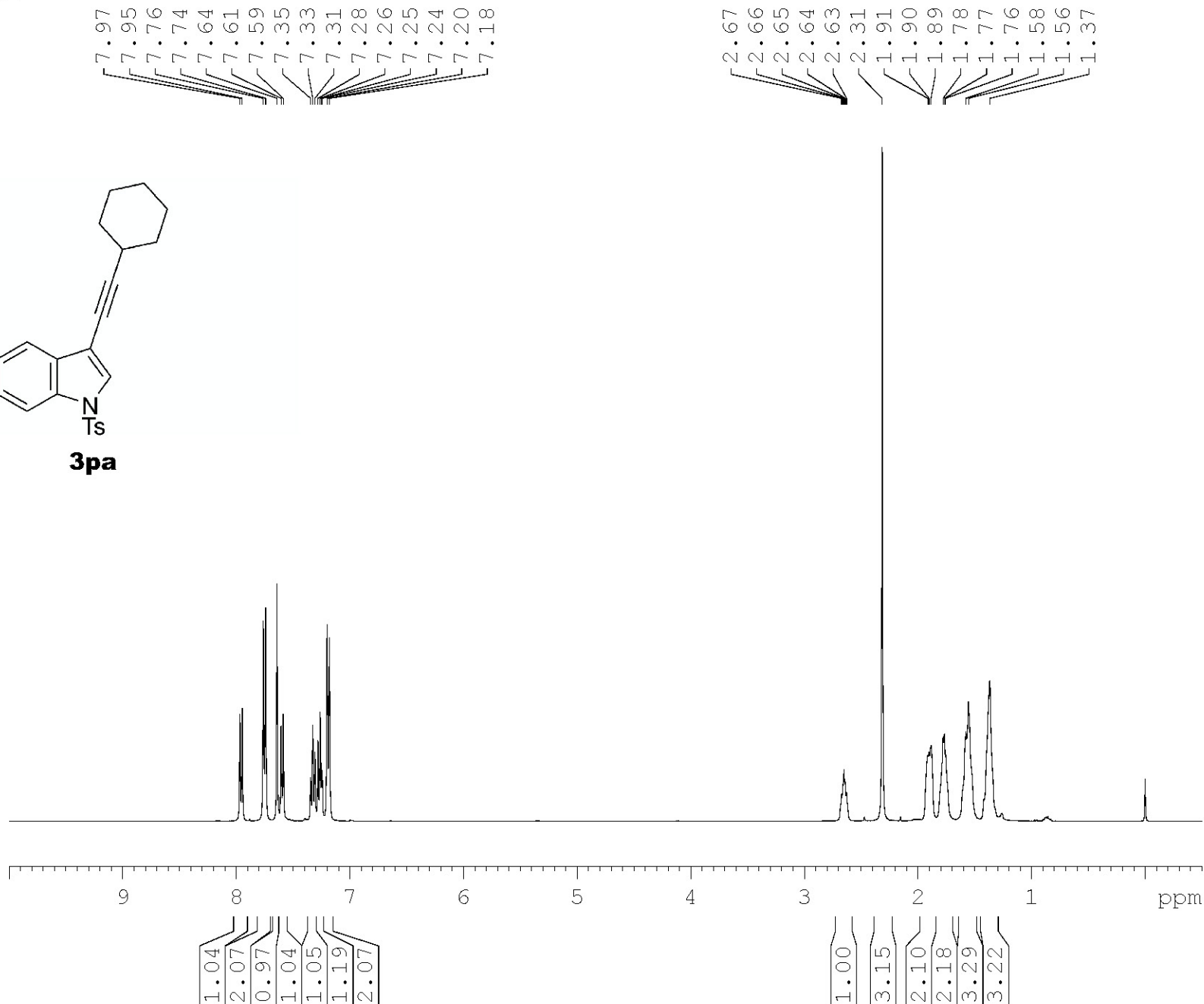
F2 - Acquisition Parameters
 Date_ 20180817
 Time_ 16.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 43
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404296 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

757

**3pa**

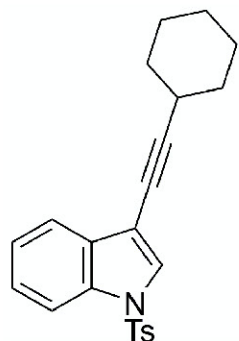
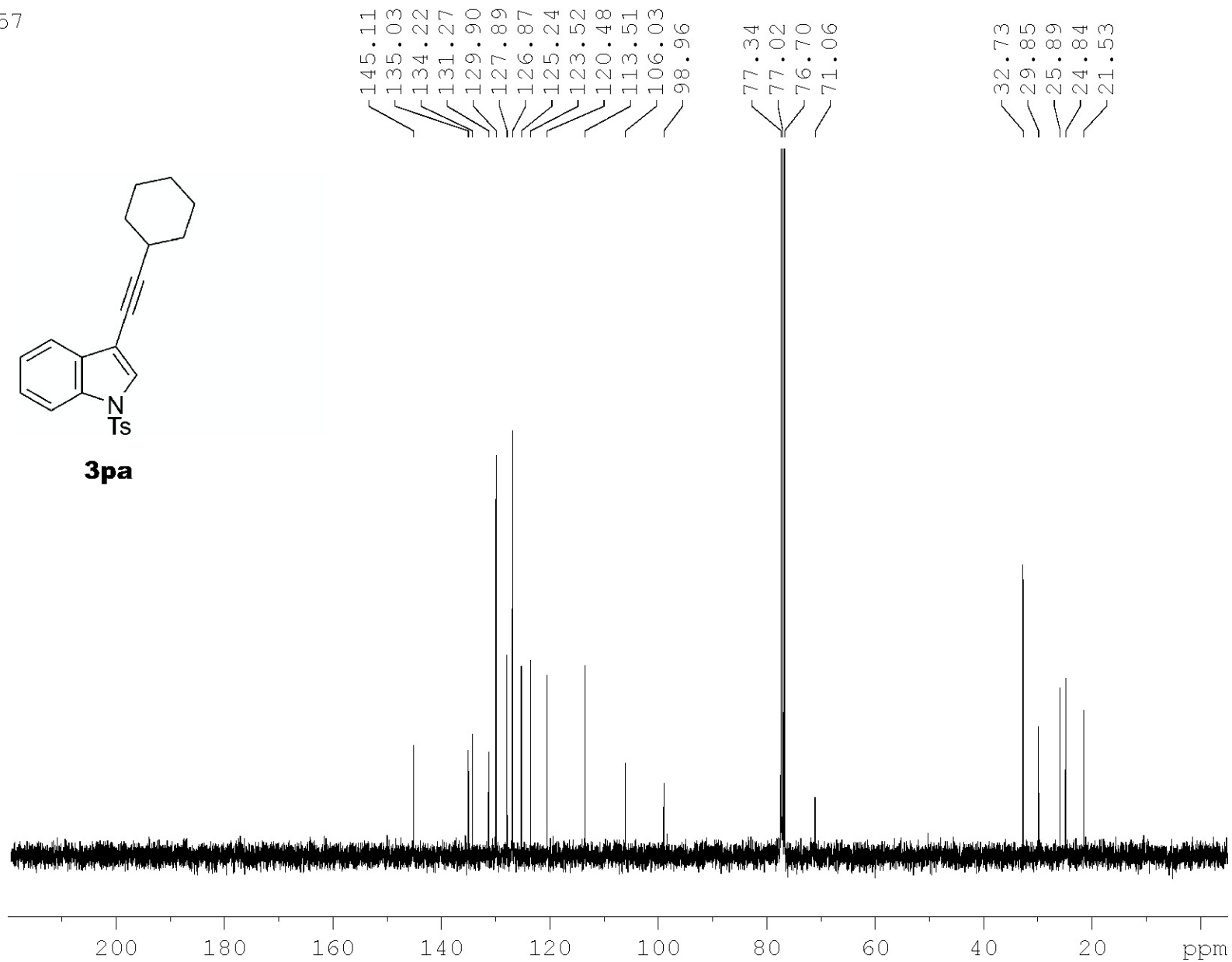
Current Data Parameters
 NAME szy-400
 EXPNO 195
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181029
 Time_ 14.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 73.9
 DW 62.400 usec
 DE 6.50 usec
 TE 298.7 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 ¹H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400138 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**3pa**

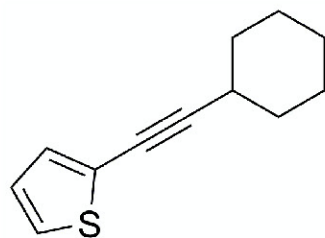
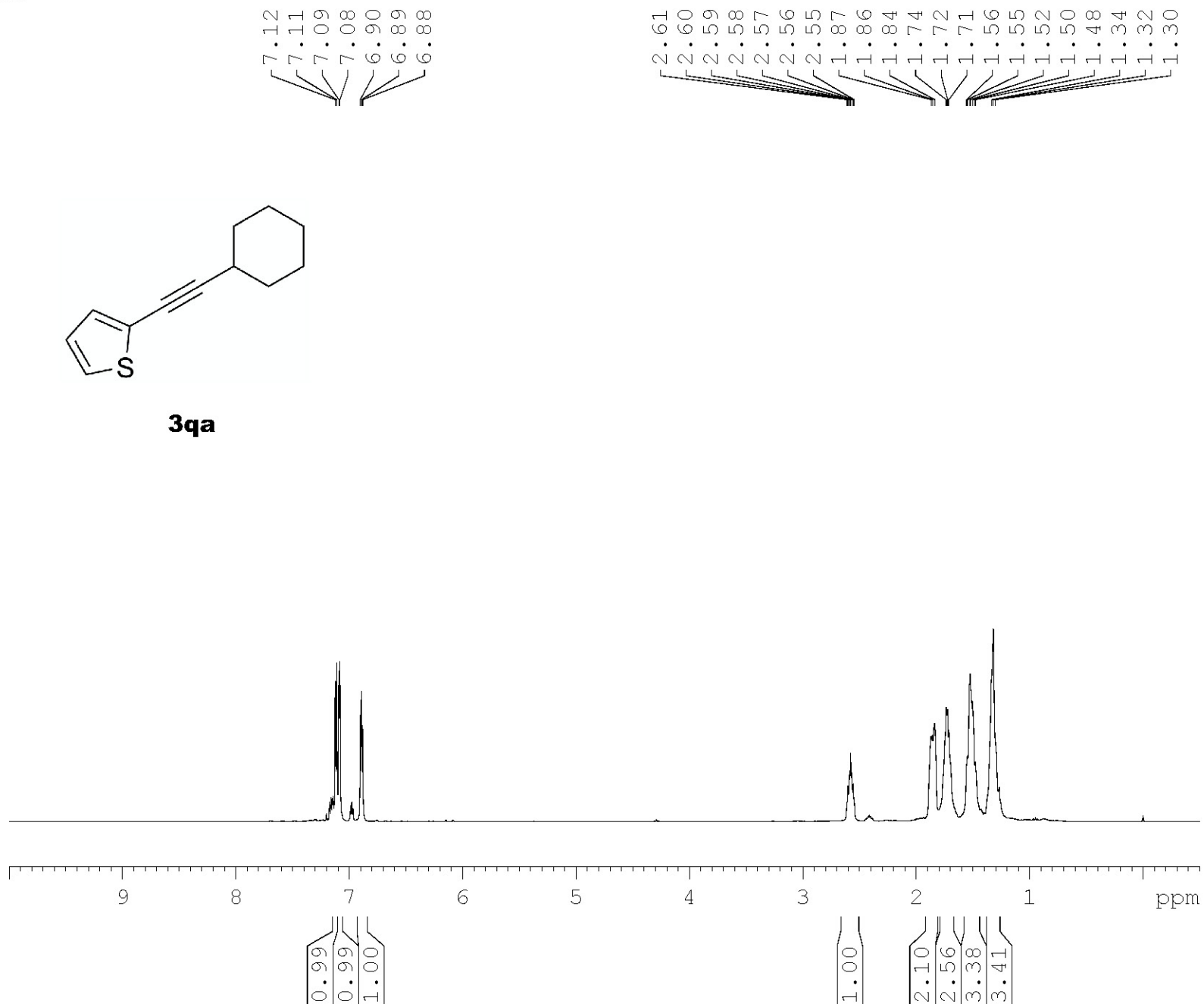
Current Data Parameters
 NAME szy-400
 EXPNO 196
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181029
 Time_ 14.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 100
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404310 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3qa**

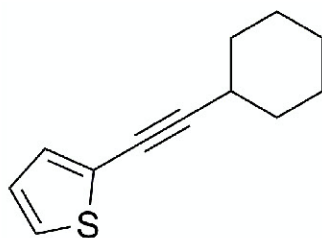
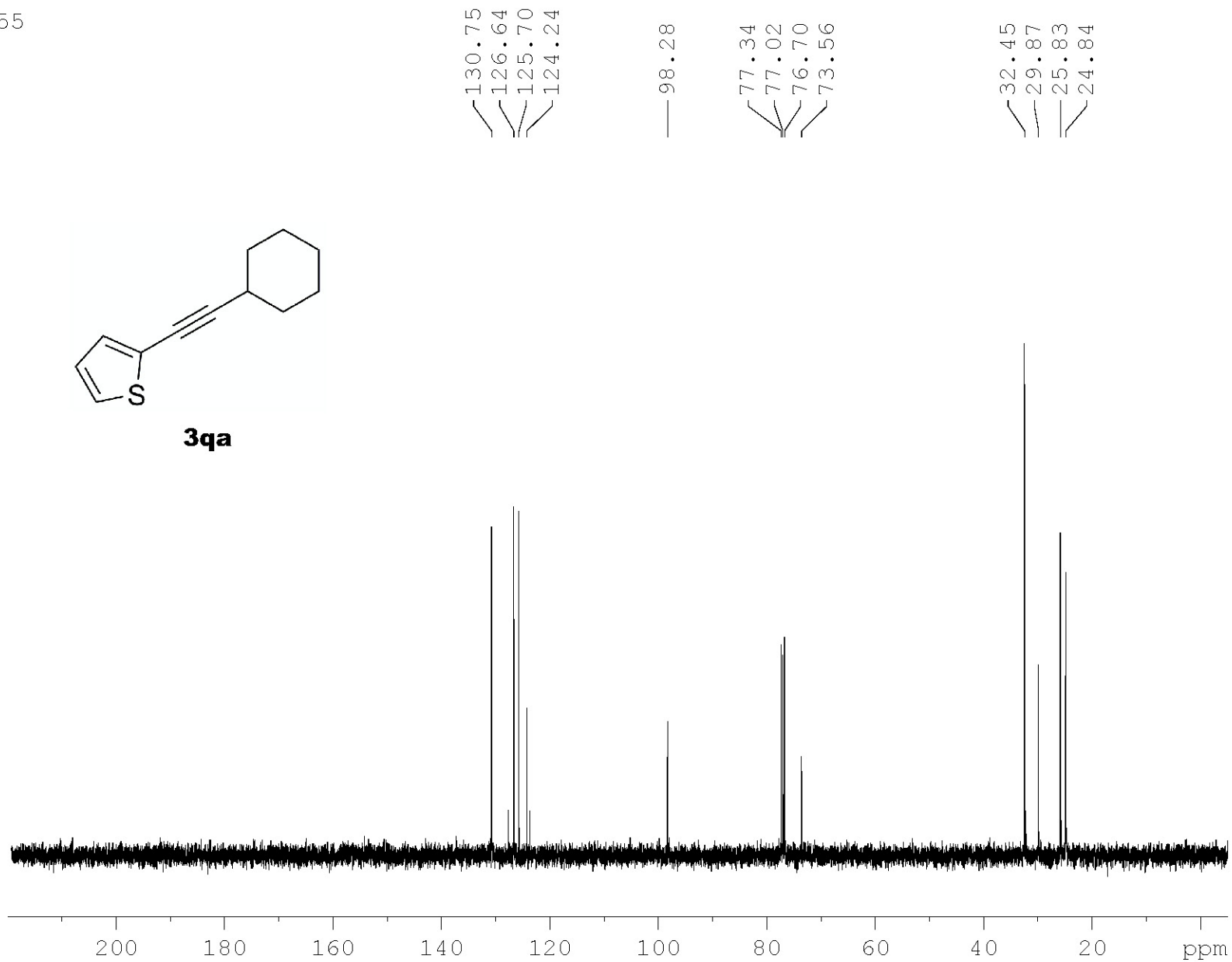
Current Data Parameters
 NAME szy-400
 EXPNO 191
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181029
 Time_ 14.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 19.61
 DW 62.400 usec
 DE 6.50 usec
 TE 298.4 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400334 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**3qa**

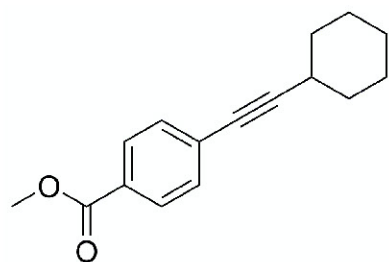
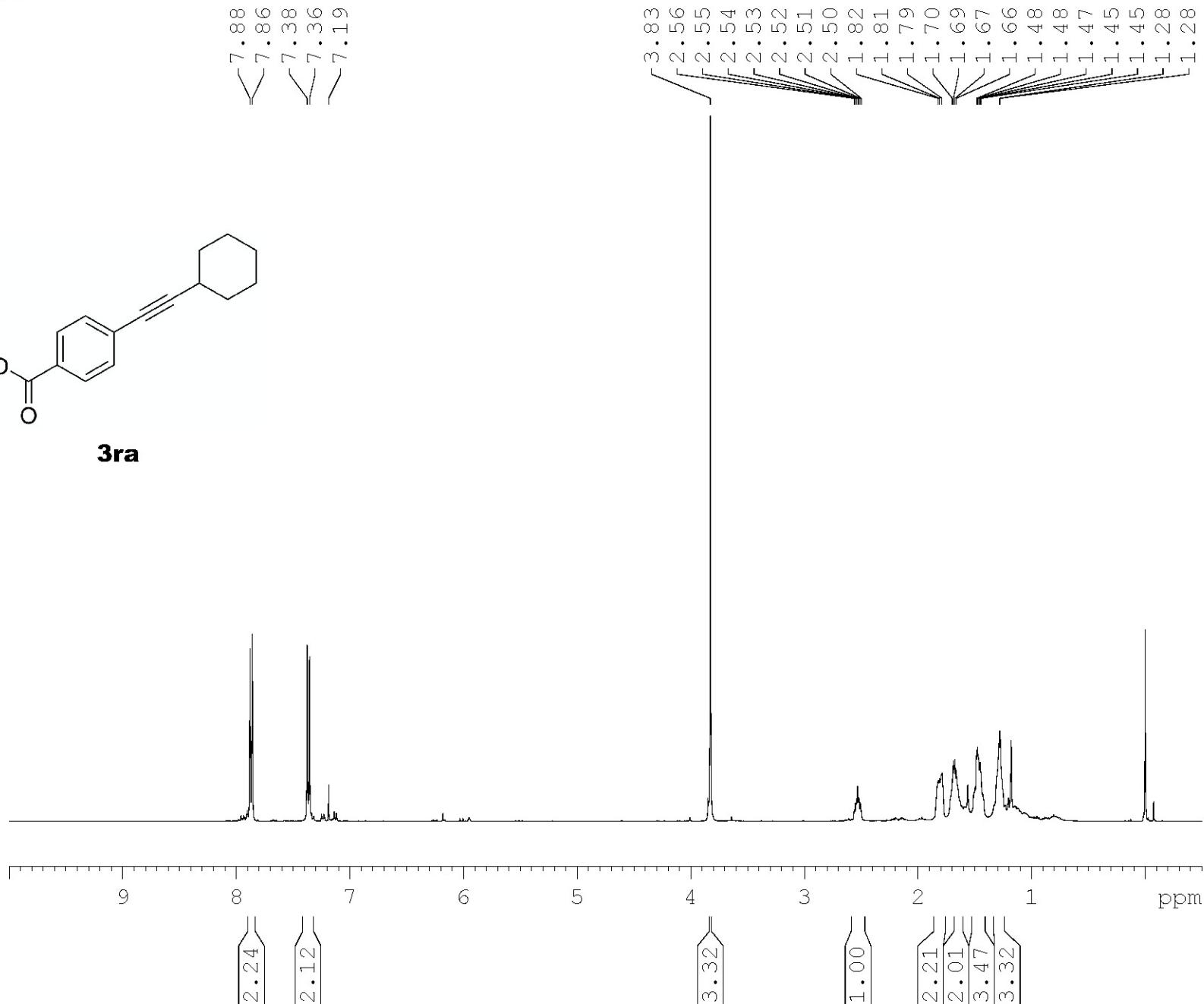
Current Data Parameters
 NAME szy-400
 EXPNO 192
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181029
 Time_ 14.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 7
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404421 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3ra**

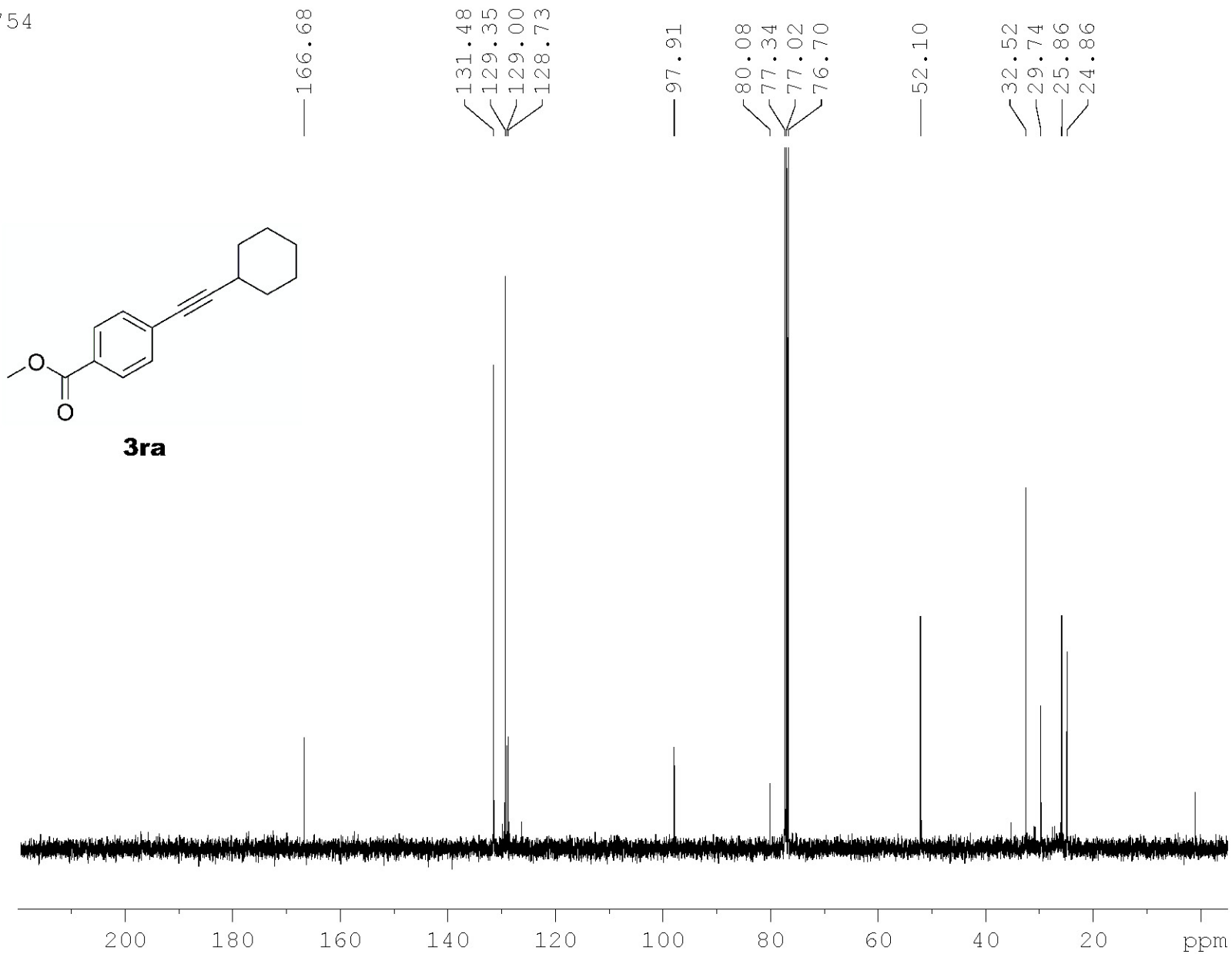
Current Data Parameters
 NAME szy-400
 EXPNO 158
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180918
 Time_ 14.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 49.81
 DW 62.400 usec
 DE 6.50 usec
 TE 298.7 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400388 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



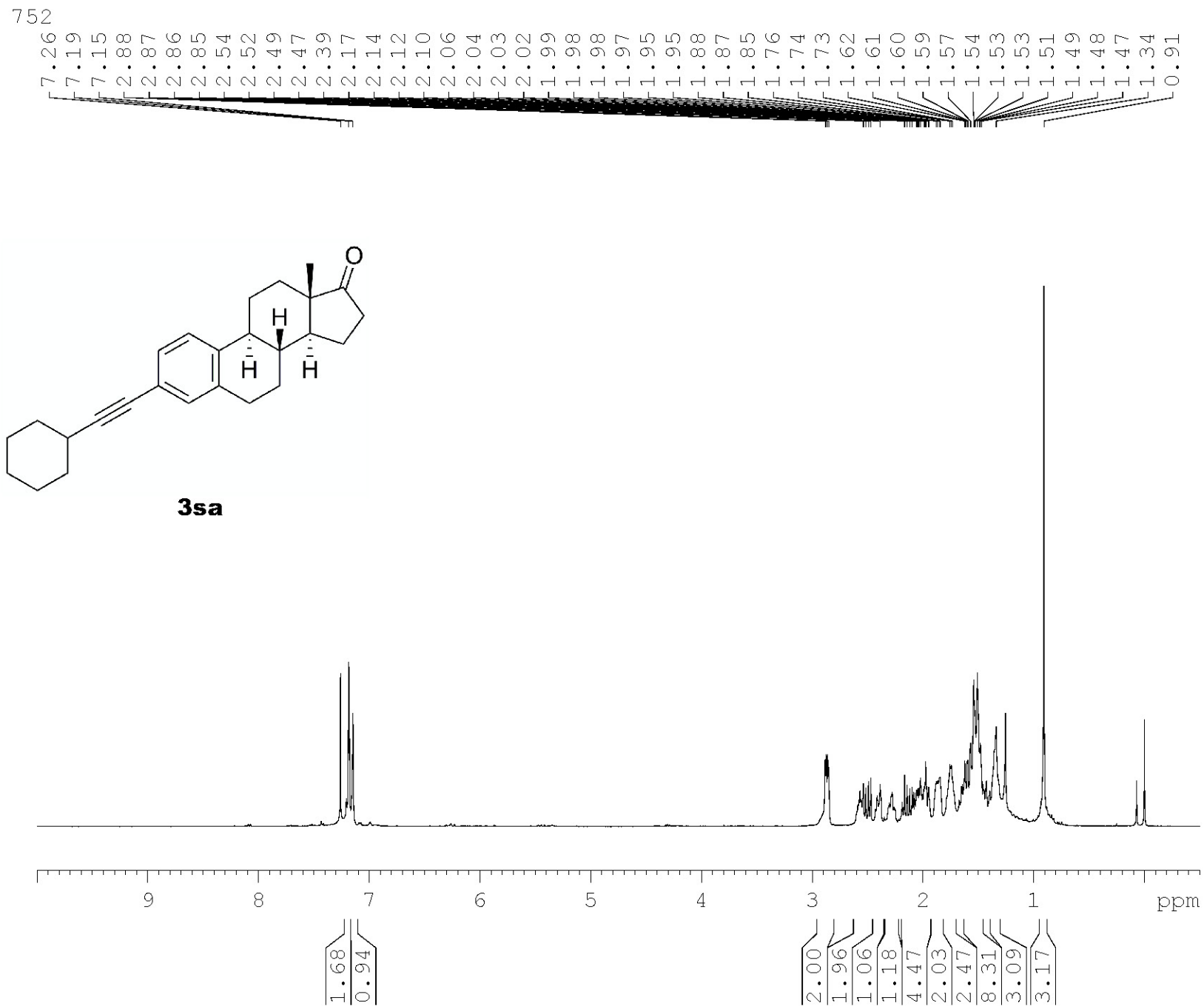
Current Data Parameters
 NAME szy-400
 EXPNO 159
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180918
 Time_ 15.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 88
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404295 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME szy-400
EXPNO 199
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181106
Time_ 14.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 162.77
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0 sec
TDO 1

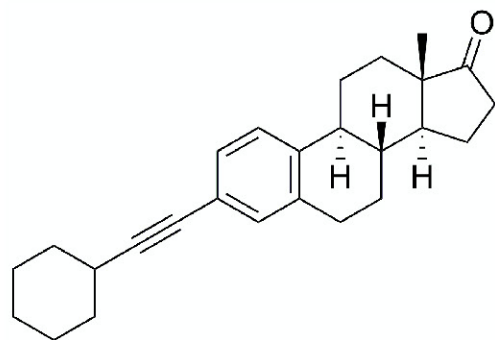
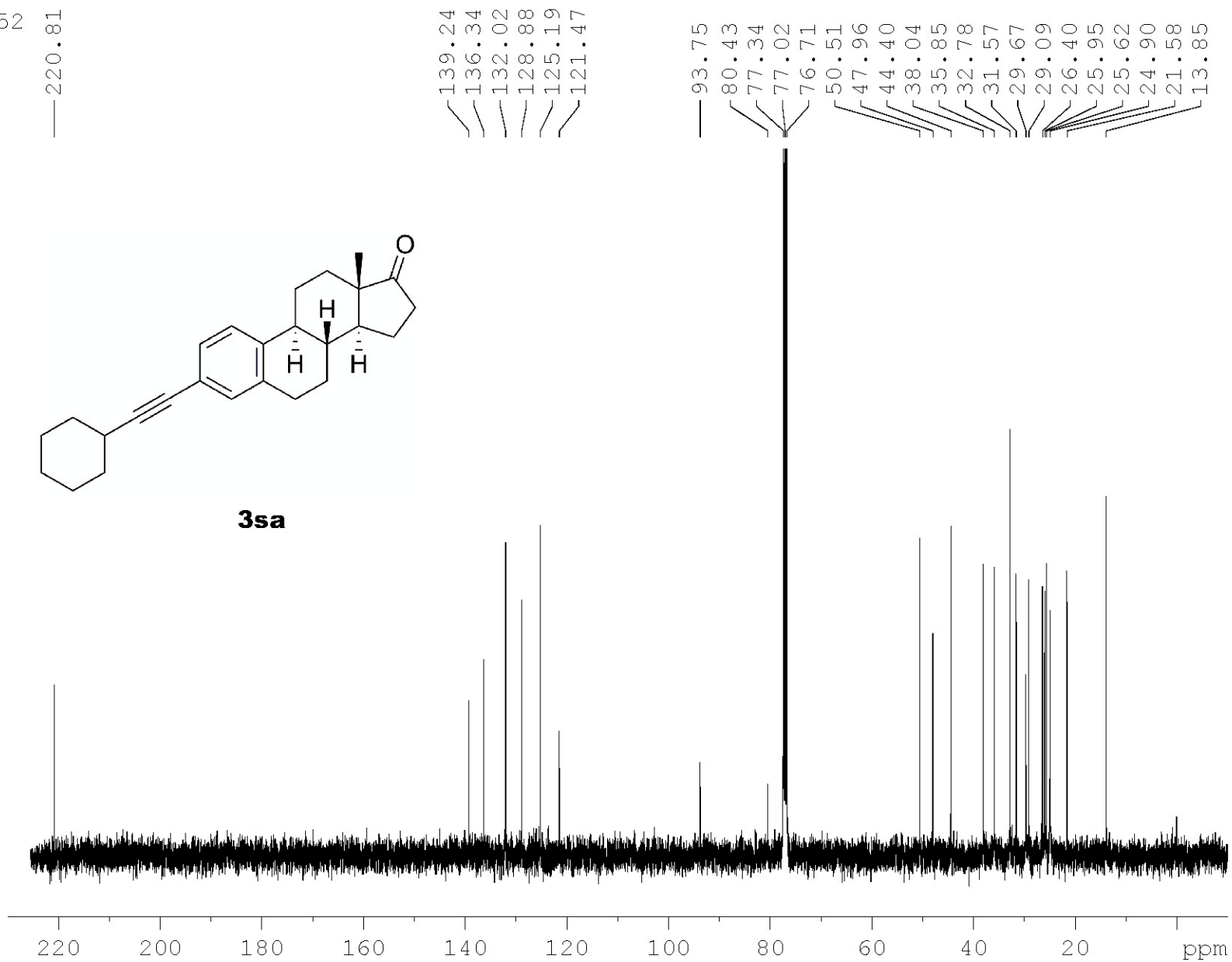
===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

752

—220.81

**3sa**

Current Data Parameters
 NAME szy-400
 EXPNO 201
 PROCNO 1

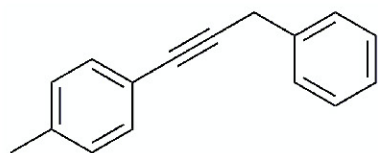
F2 - Acquisition Parameters
 Date_ 20181106
 Time_ 15.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 448
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976128 sec
 RG 206.33
 DW 19.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404286 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

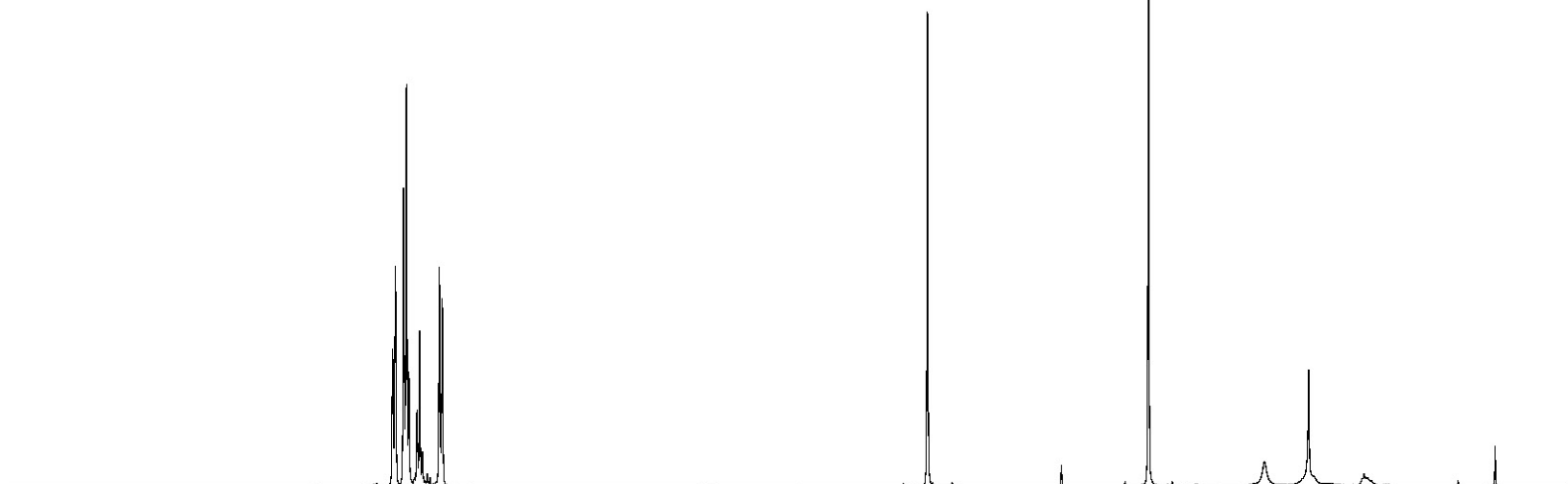
735

**3db**

7.42
7.40
7.35
7.33
7.31
7.26
7.24
7.22
7.11
7.09

— 3.82

— 2.33



1.87
3.80
1.23
1.97

2.00

3.04

Current Data Parameters
NAME szy-400
EXPNO 106
PROCNO 1

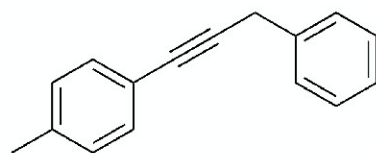
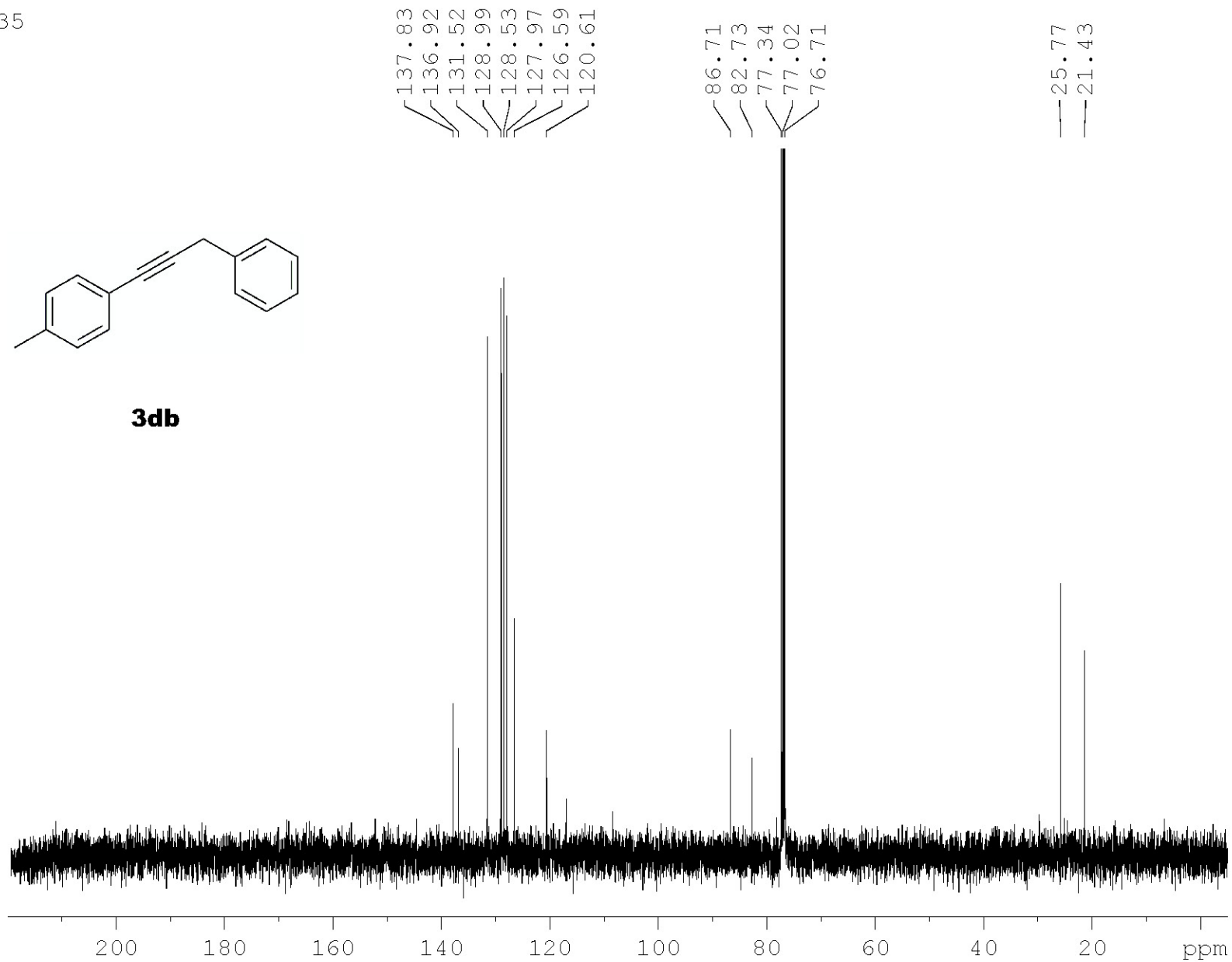
F2 - Acquisition Parameters
Date_ 20180814
Time_ 20.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 140.59
DW 62.400 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400174 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

735

**3db**

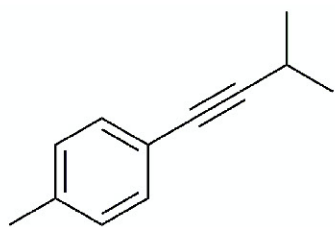
Current Data Parameters
 NAME szy-400
 EXPNO 107
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180814
 Time_ 20.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 61
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

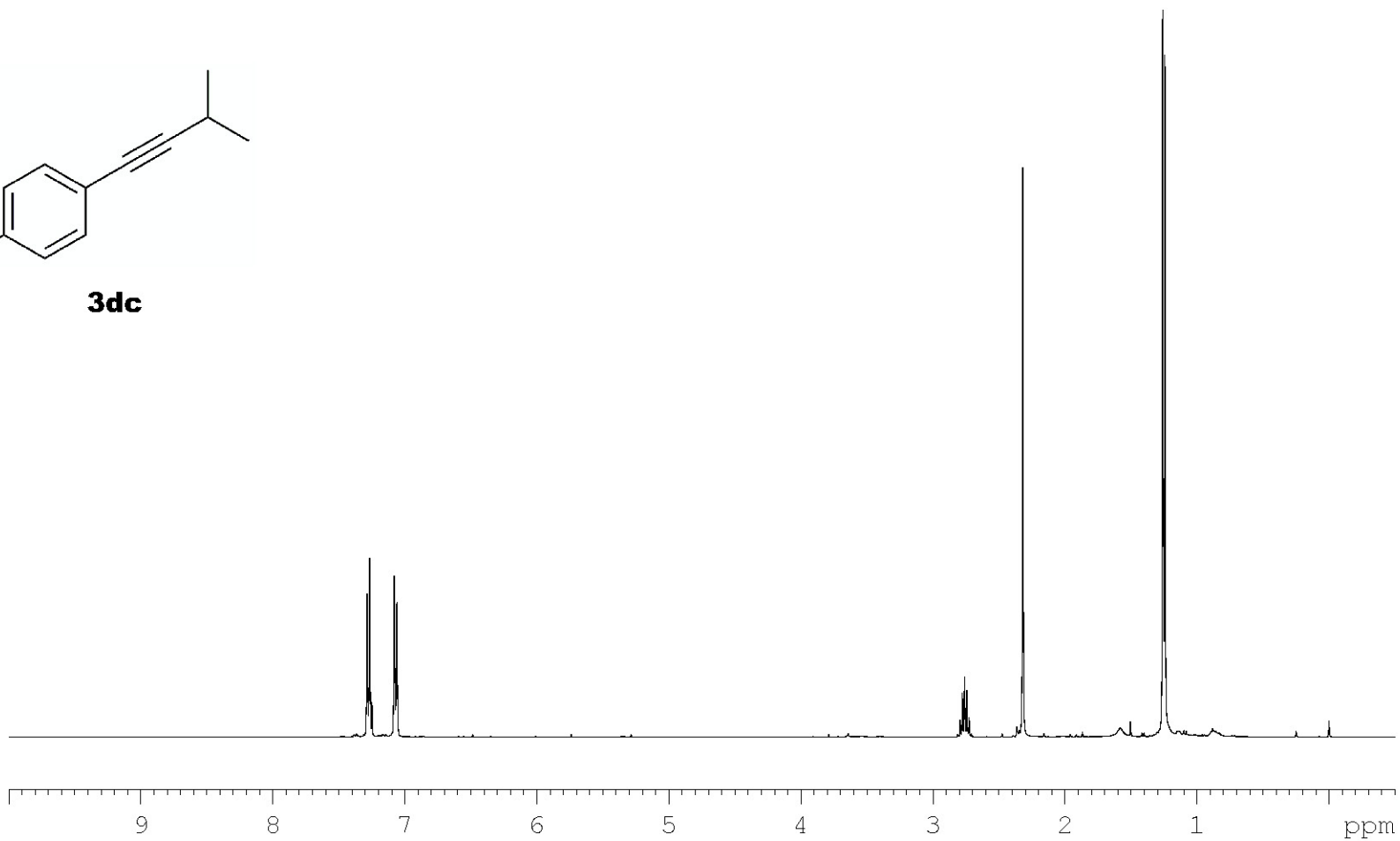
F2 - Processing parameters
 SI 32768
 SF 100.6404289 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3dc**

7.29
7.27
7.25
7.08
7.06

2.81
2.79
2.78
2.76
2.74
2.73
2.71
2.32

1.26
1.24



2.08
2.00

0.93

3.17

6.47

Current Data Parameters
NAME szy-400
EXPNO 118
PROCNO 1

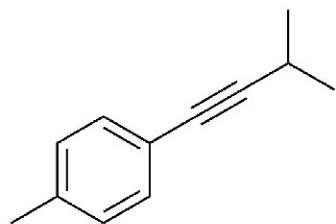
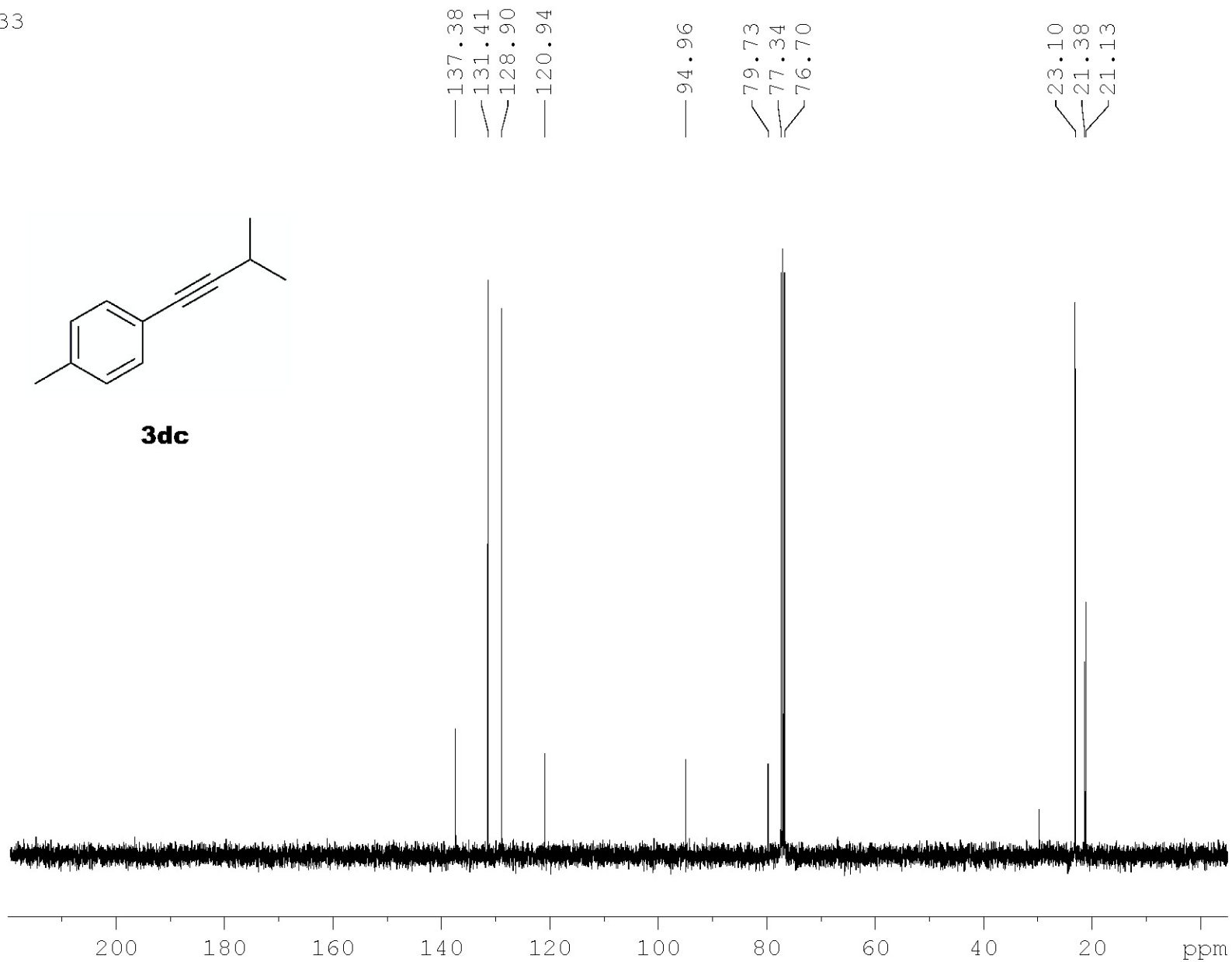
F2 - Acquisition Parameters
Date_ 20180816
Time_ 17.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

733

**3dc**

Current Data Parameters
 NAME szy-400
 EXPNO 119
 PROCNO 1

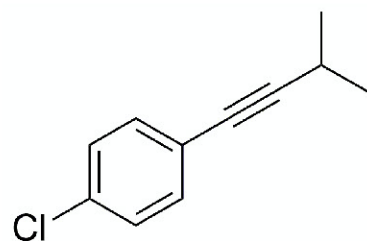
F2 - Acquisition Parameters
 Date_ 20180816
 Time_ 17.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 42
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404282 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

671

**3kc**

7.31
7.30
7.25
7.23

2.80
2.79
2.77
2.76
2.74
2.73
2.72

1.26
1.24

— 0.00

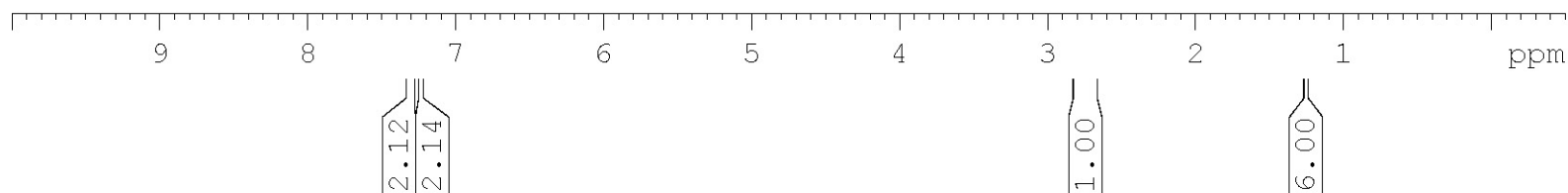
Current Data Parameters
NAME szy-2-500
EXPNO 185
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171210
Time_ 9.30
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TDO 1

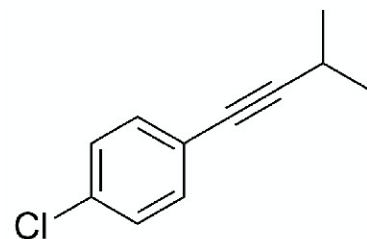
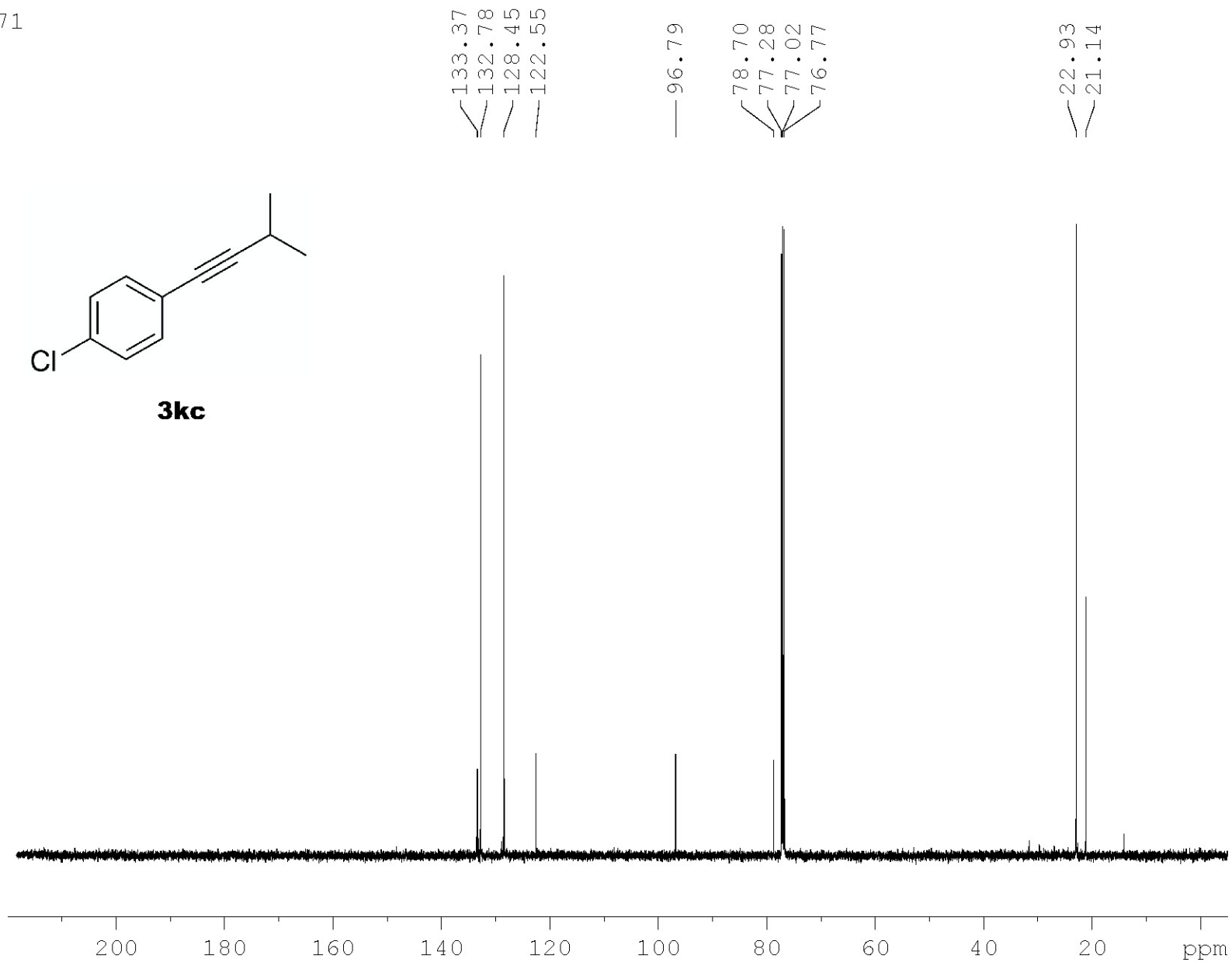
===== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

===== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300152 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



671

**3kc**

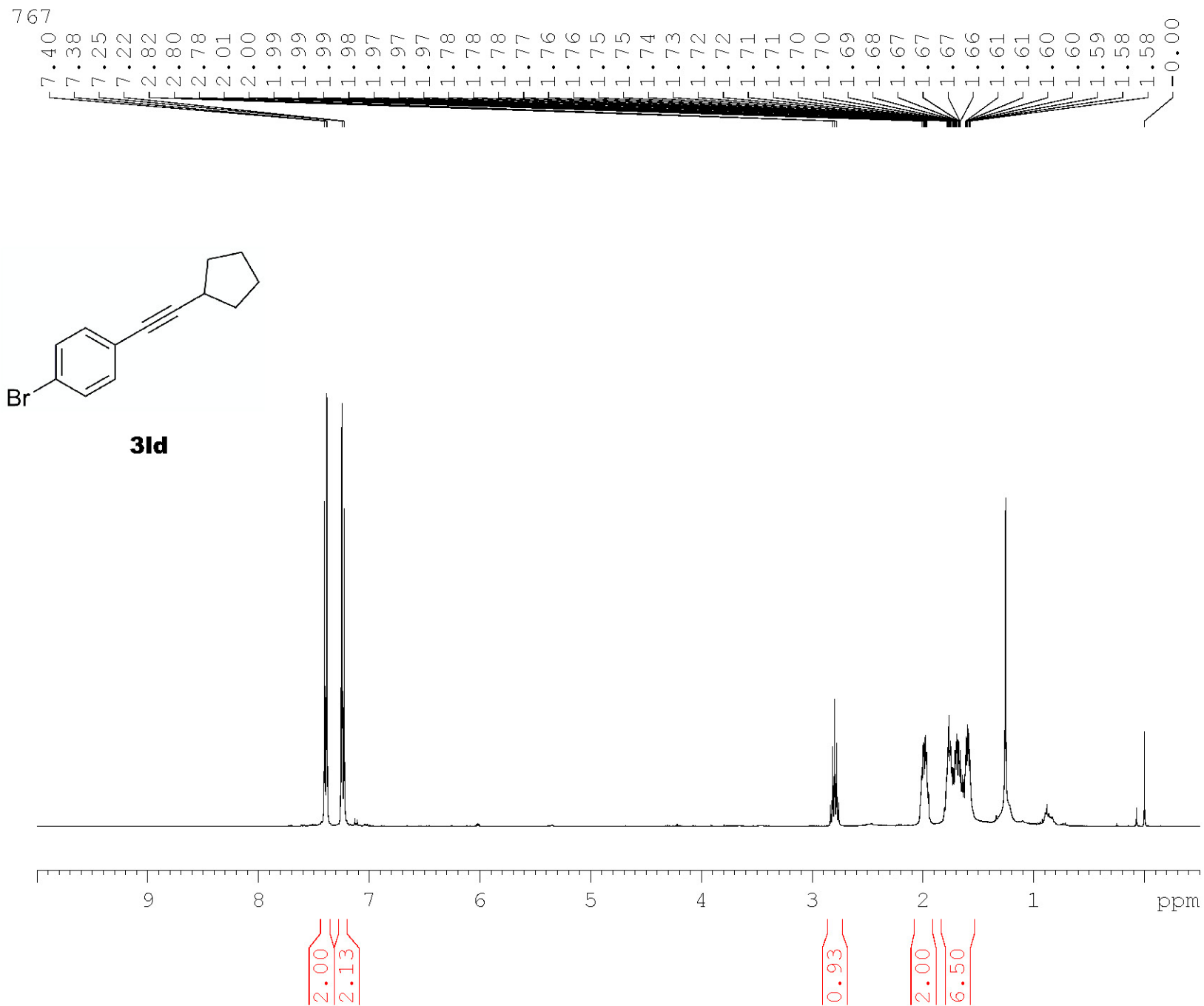
Current Data Parameters
 NAME szy-2-500
 EXPNO 186
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171210
 Time_ 9.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 22
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577888 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



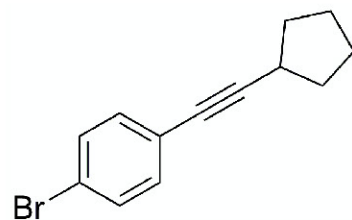
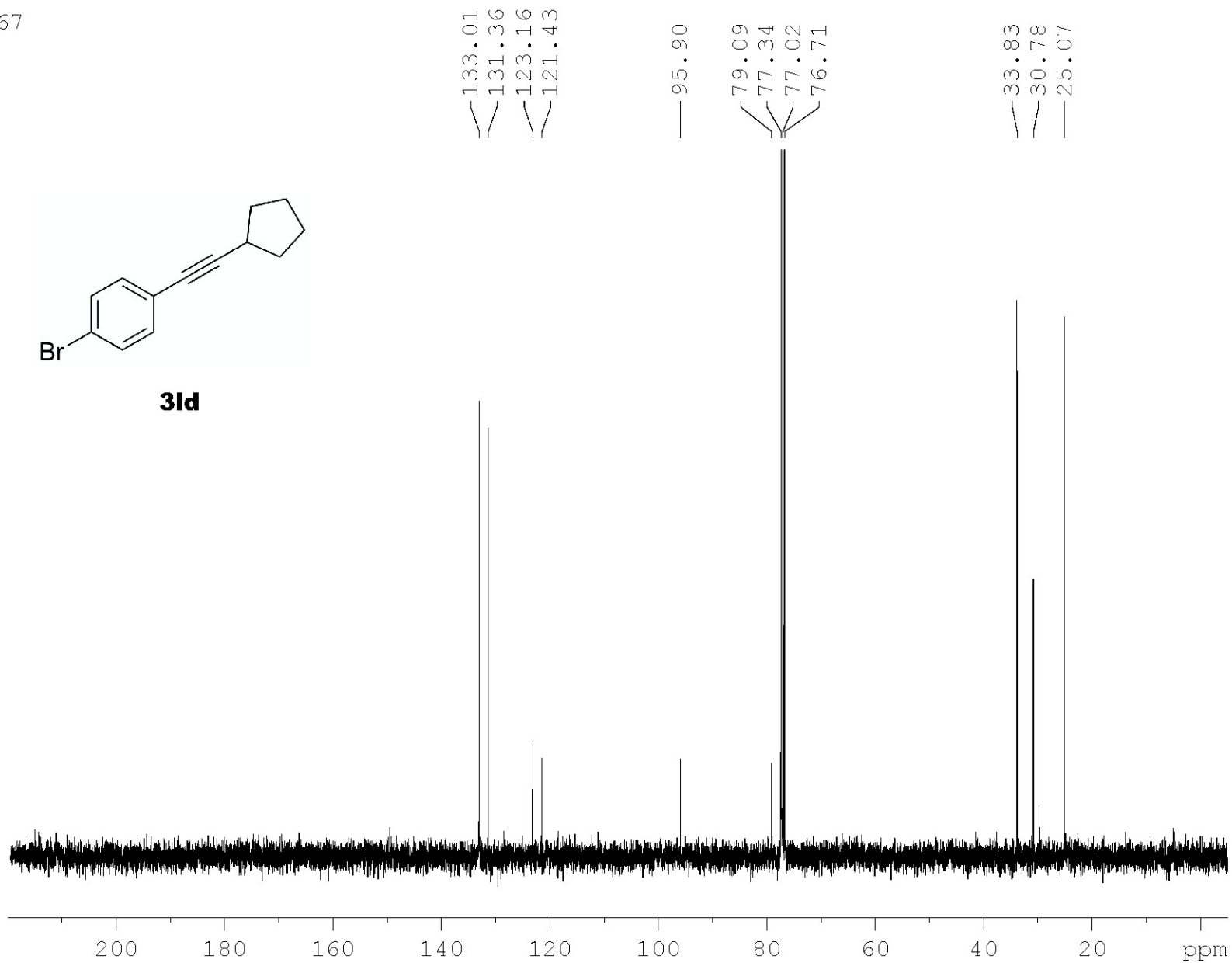
Current Data Parameters
NAME szy-400
EXPNO 178
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181009
Time_ 15.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 140.59
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

**3ld**

Current Data Parameters
 NAME szy-400
 EXPNO 179
 PROCNO 1

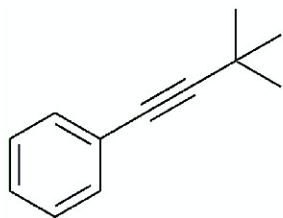
F2 - Acquisition Parameters
 Date_ 20181009
 Time_ 15.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 99
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 298.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

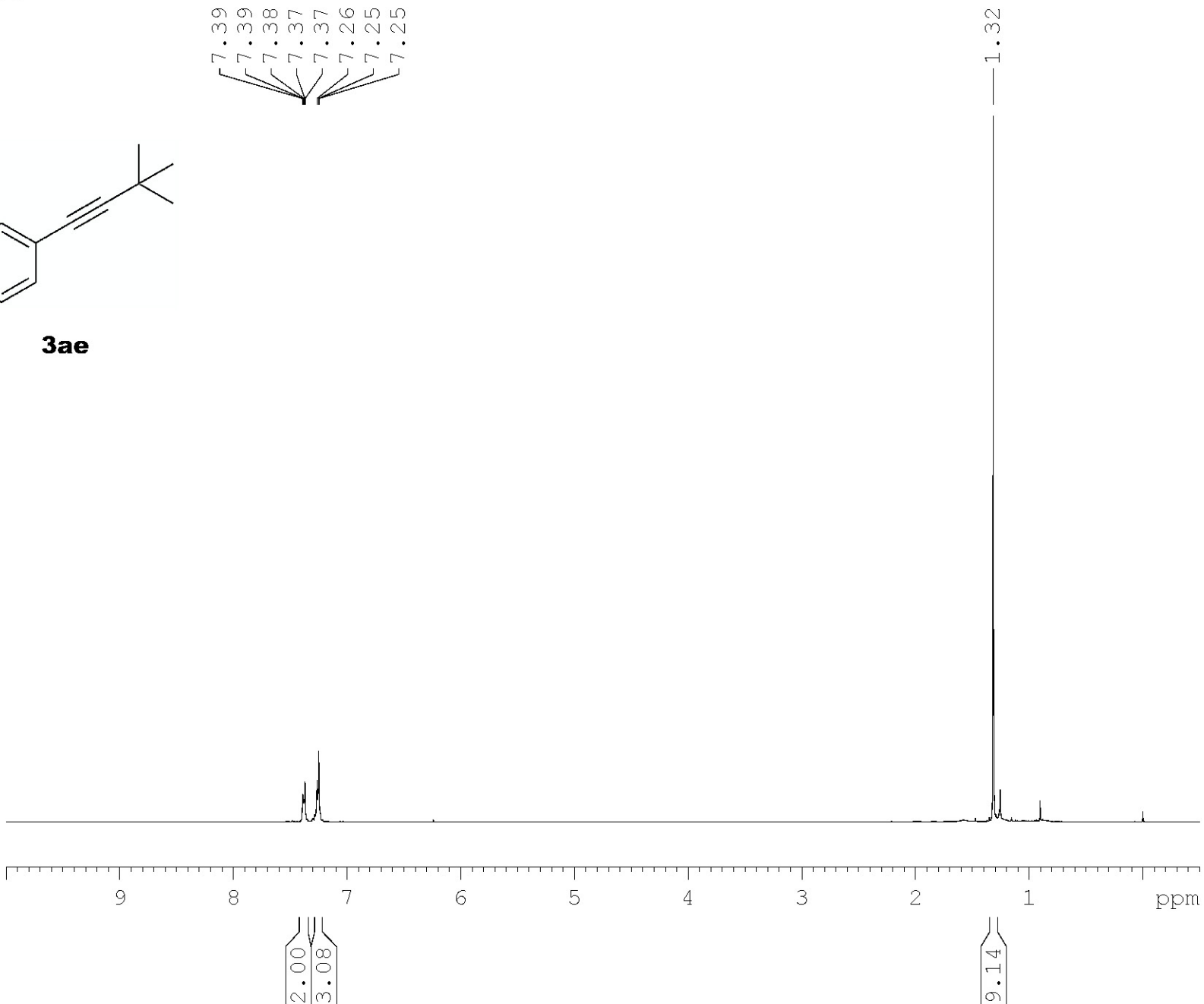
===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404281 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

759

**3ae**

7.39
7.39
7.38
7.37
7.37
7.26
7.25
7.25



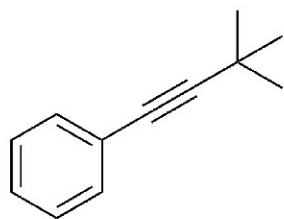
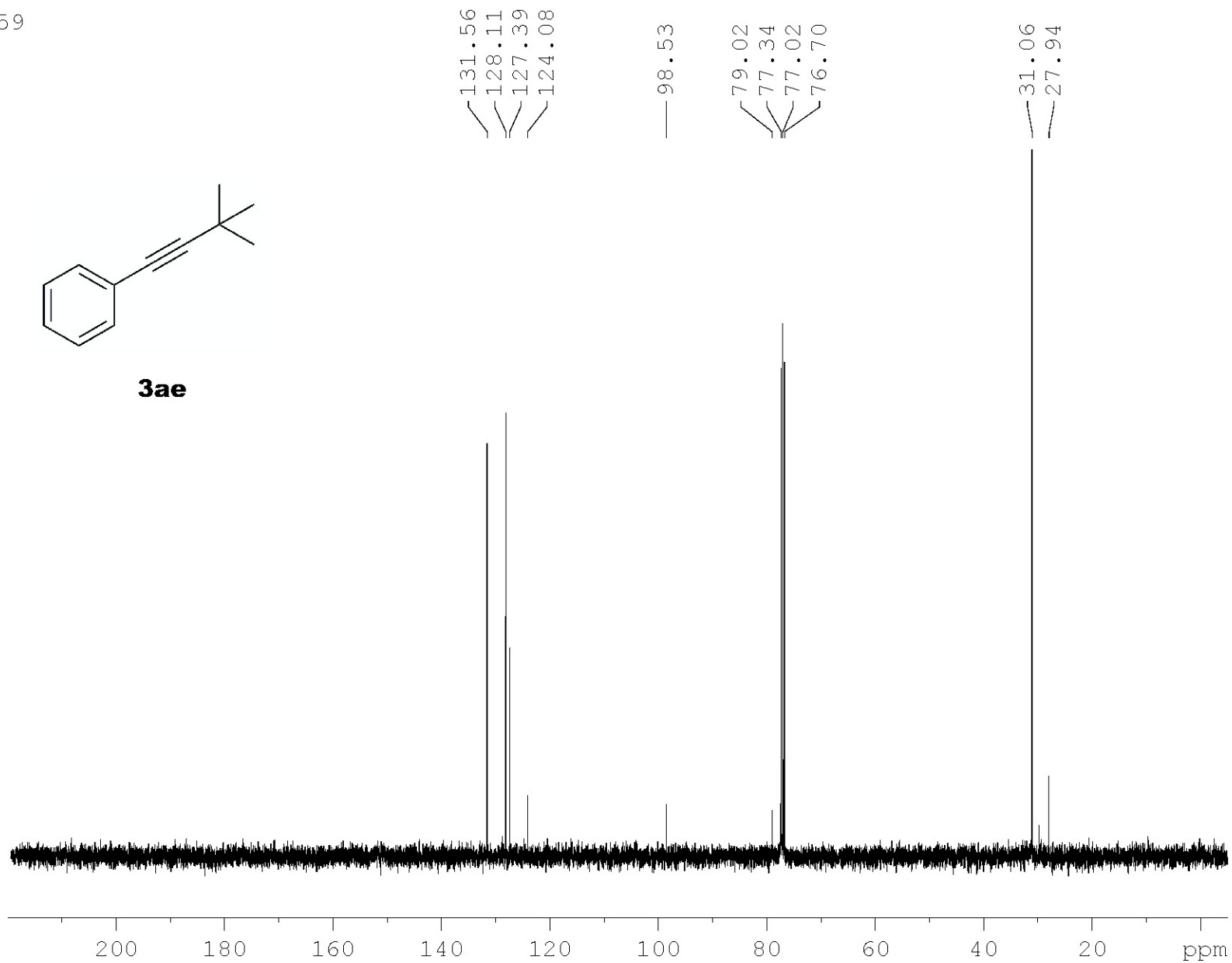
Current Data Parameters
NAME szy-400
EXPNO 160
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180920
Time_ 20.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 140.59
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

**3ae**

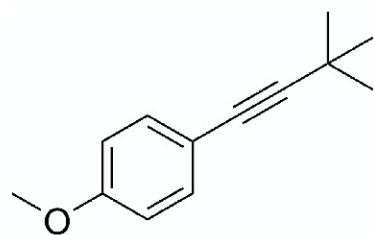
Current Data Parameters
 NAME szy-400
 EXPNO 162
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180920
 Time_ 21.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

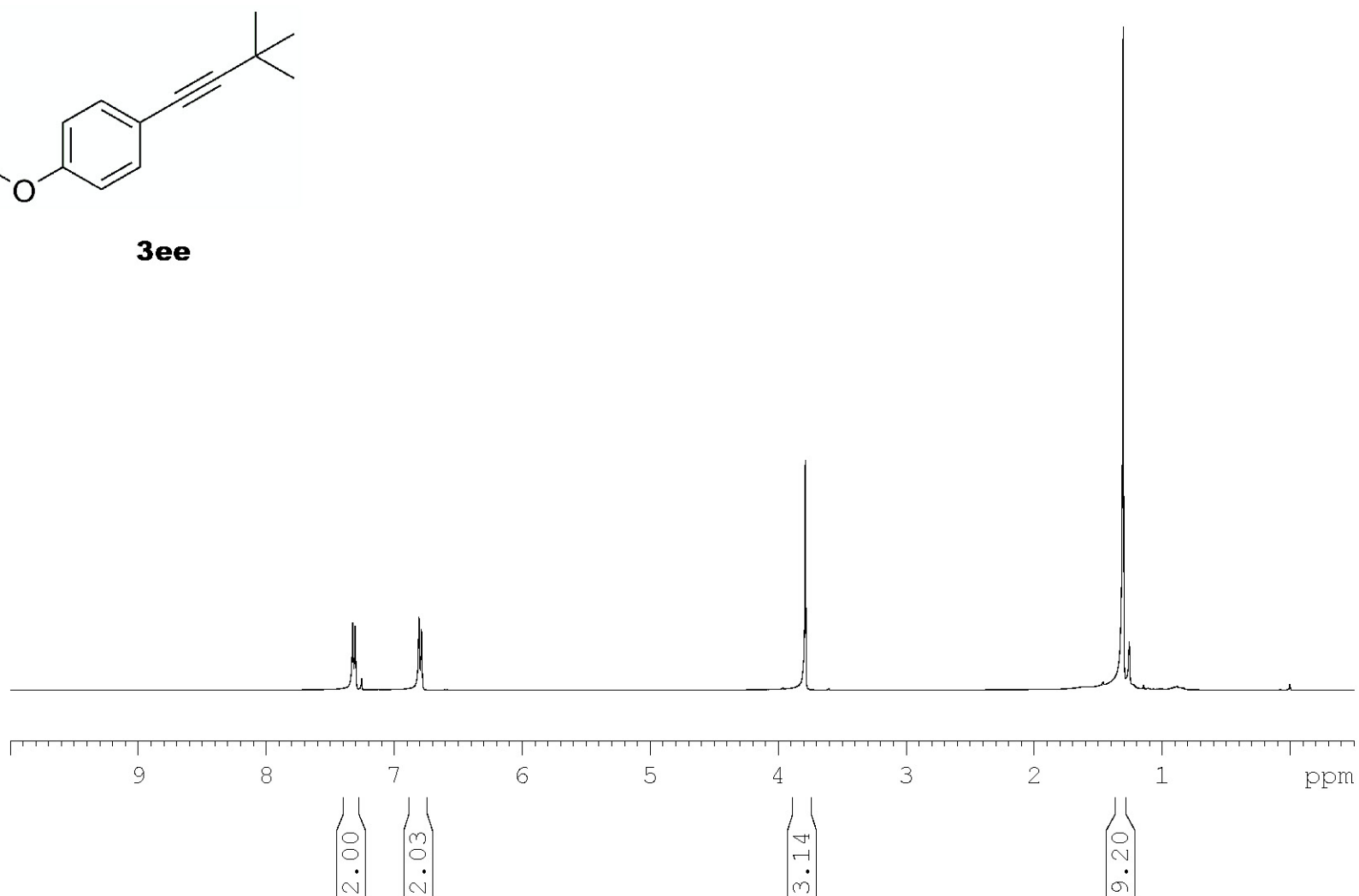
F2 - Processing parameters
 SI 32768
 SF 100.6404281 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

**3ee**

7.32
7.30
7.26
7.25
6.81
6.79

— 3.79

— 1.30



Current Data Parameters
NAME szy-400
EXPNO 163
PROCNO 1

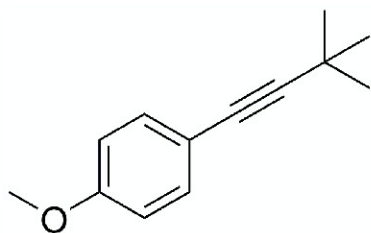
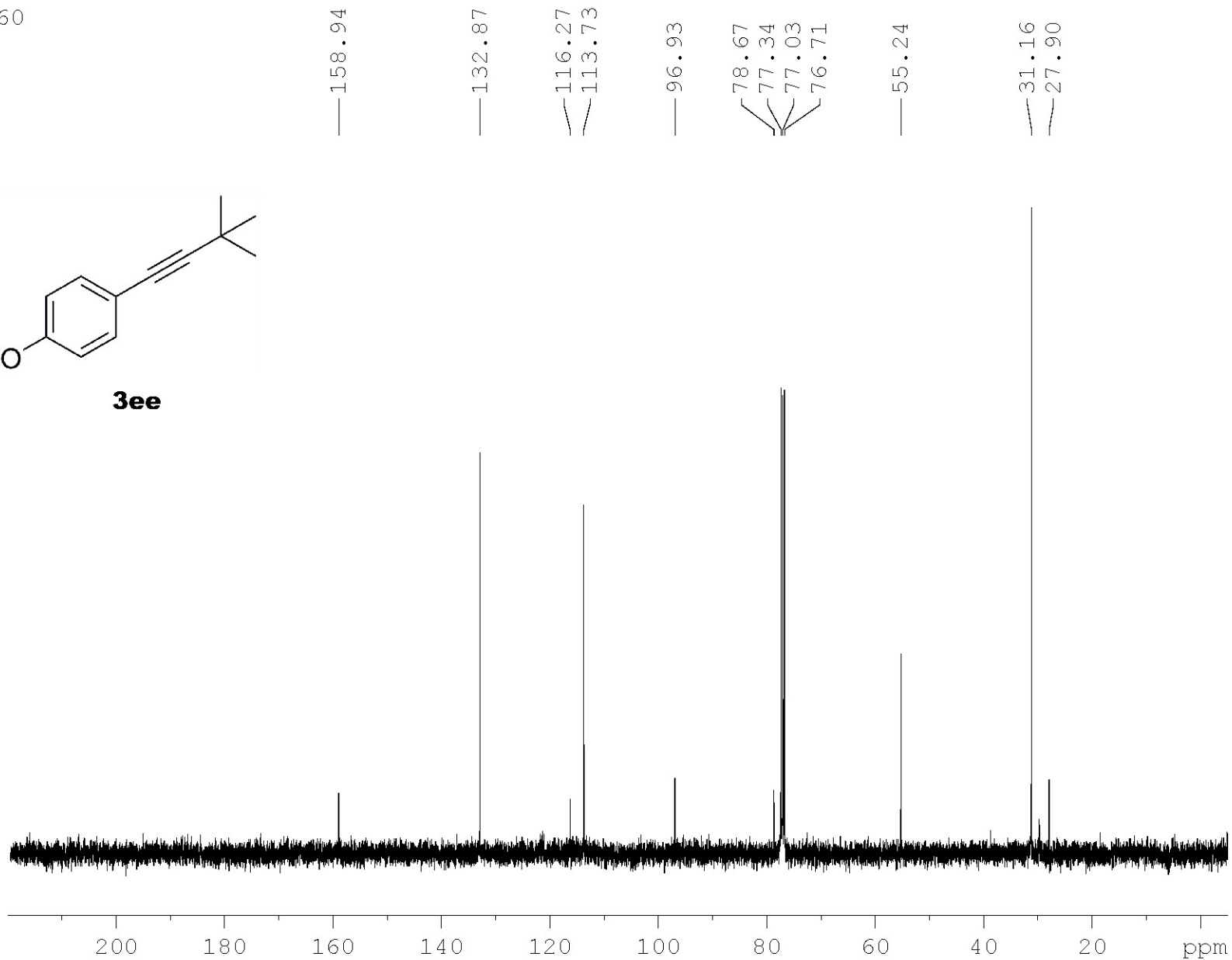
F2 - Acquisition Parameters
Date_ 20180921
Time_ 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

760

**3ee**

Current Data Parameters
 NAME szy-400
 EXPNO 164
 PROCNO 1

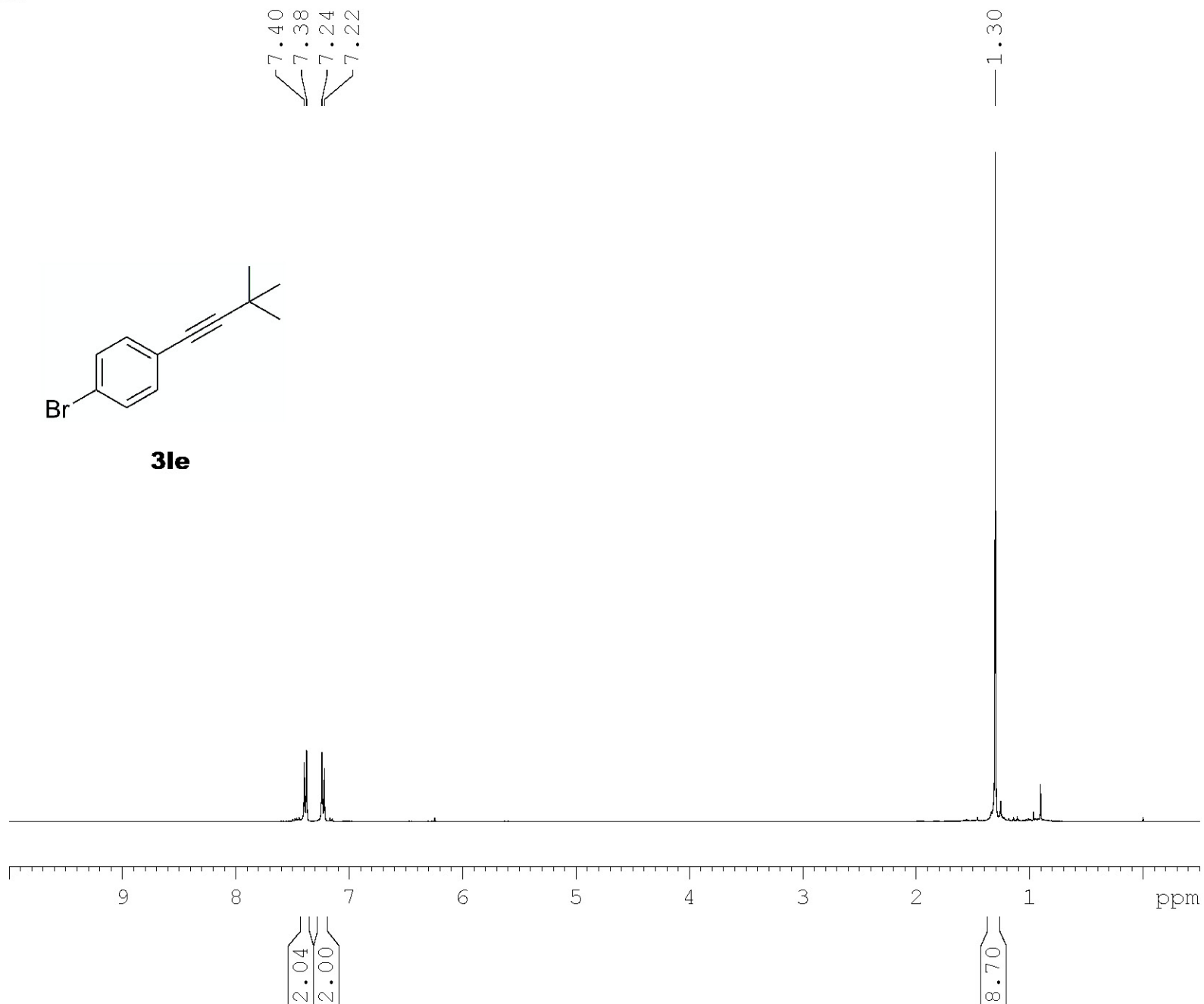
F2 - Acquisition Parameters
 Date_ 20180921
 Time_ 14.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 30
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

761



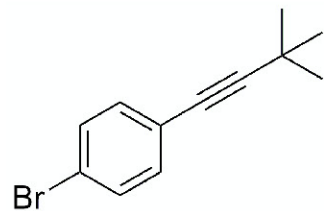
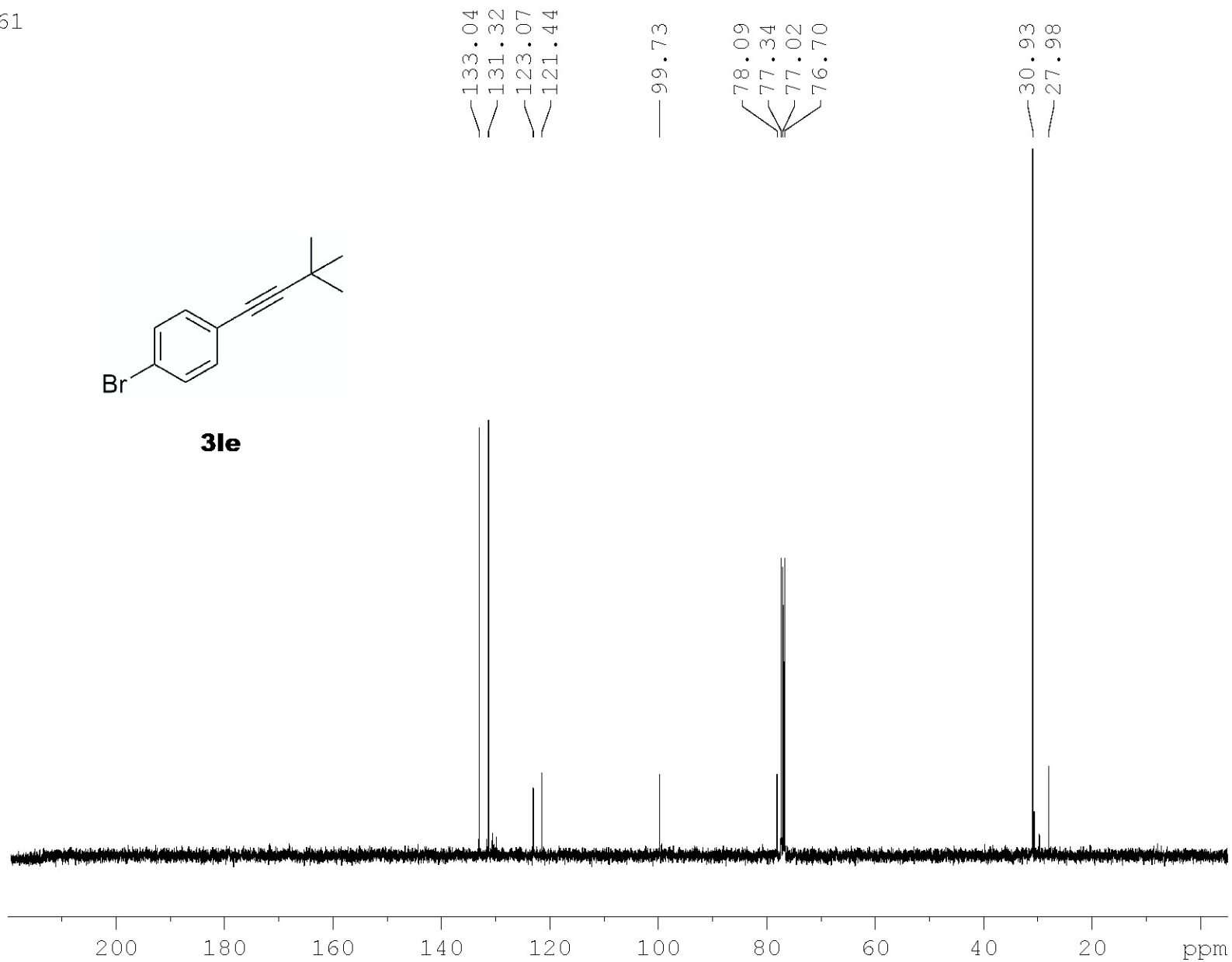
Current Data Parameters
NAME szy-400
EXPNO 165
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180921
Time_ 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 55.55
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

**3le**

Current Data Parameters
 NAME szy-400
 EXPNO 166
 PROCNO 1

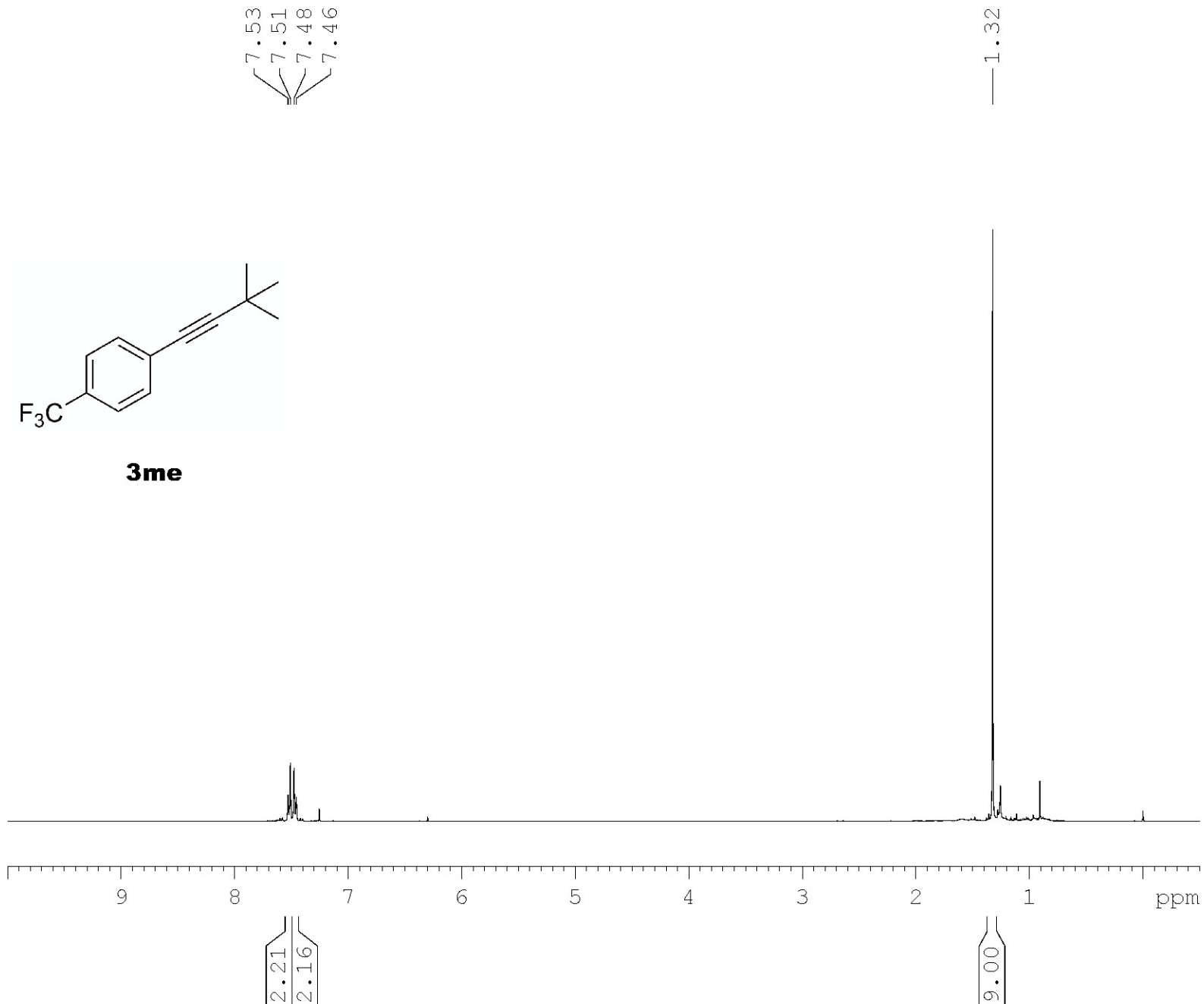
F2 - Acquisition Parameters
 Date_ 20180921
 Time_ 14.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 25
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404295 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

765



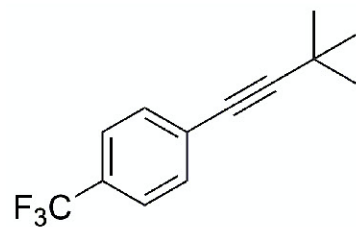
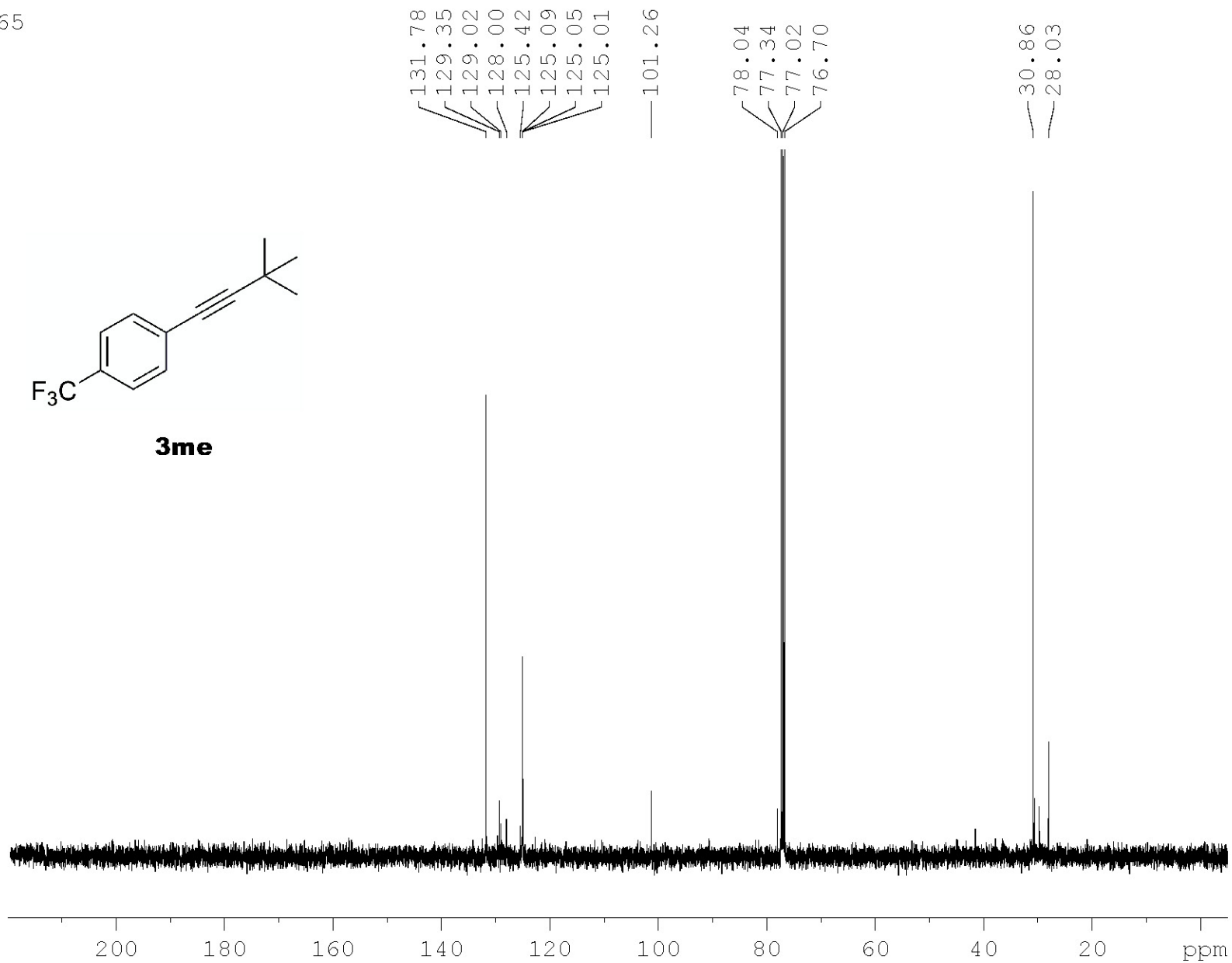
Current Data Parameters
NAME szy-400
EXPNO 173
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180928
Time_ 14.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.80 usec
PLW1 12.00000000 W

===== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

**3me**

Current Data Parameters
 NAME szy-400
 EXPNO 174
 PROCNO 1

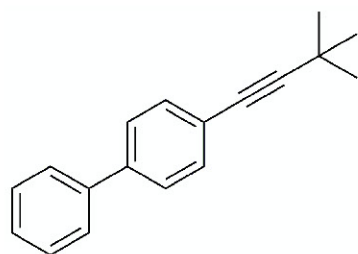
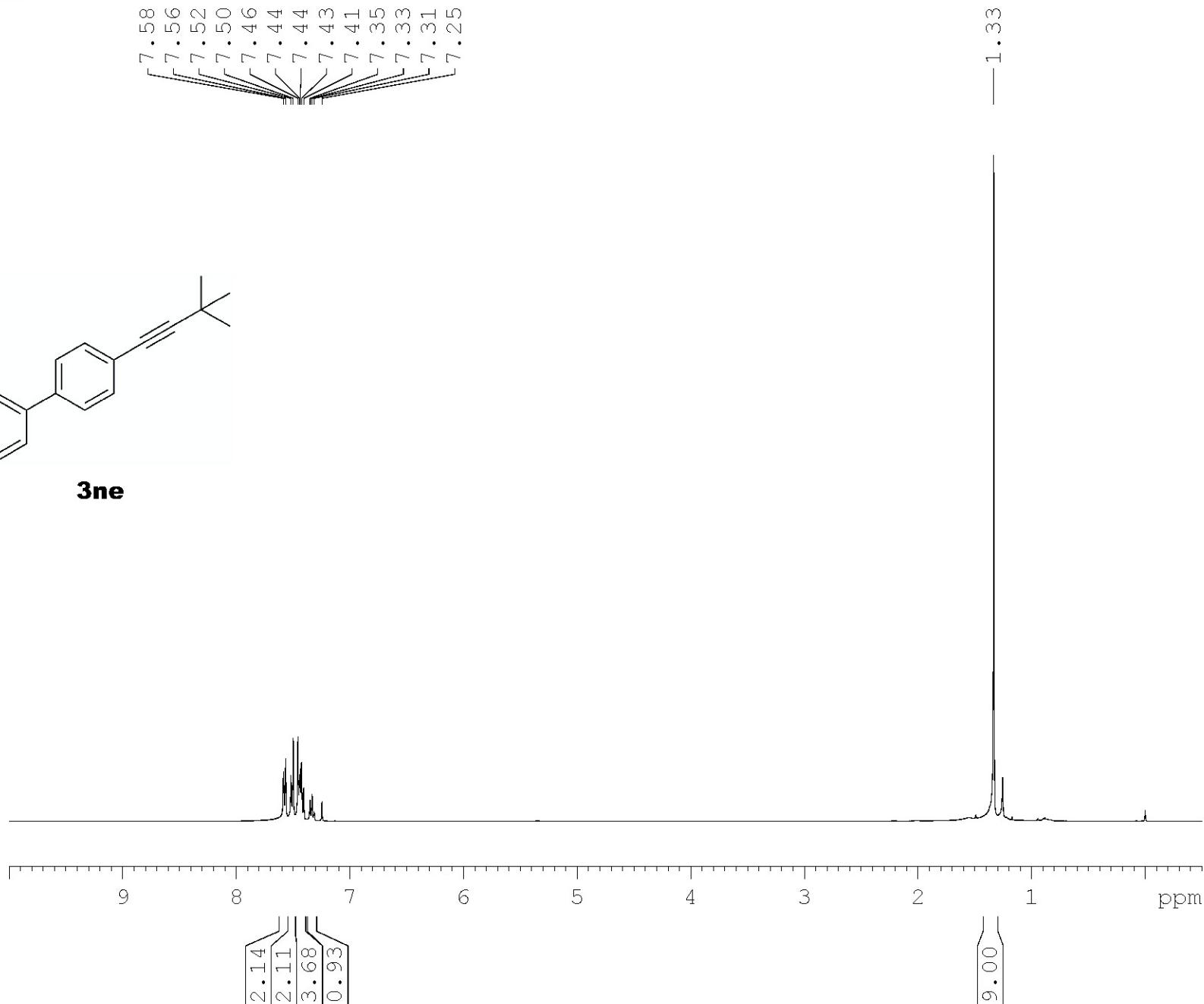
F2 - Acquisition Parameters
 Date_ 20180928
 Time_ 14.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 39
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404267 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

762

**3ne**

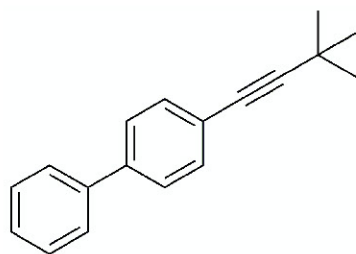
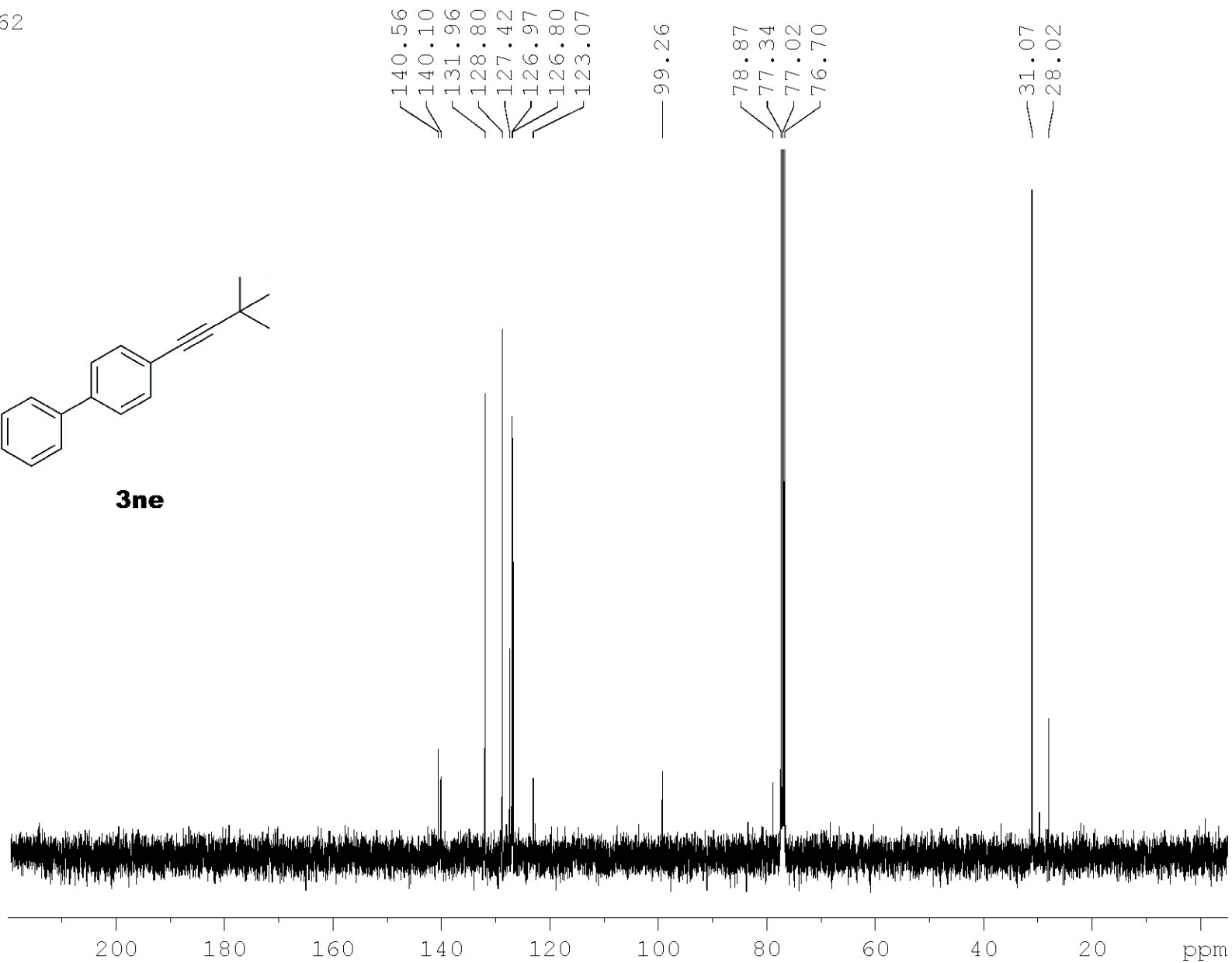
Current Data Parameters
 NAME szy-400
 EXPNO 167
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180921
 Time_ 21.37
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 140.59
 DW 62.400 usec
 DE 6.50 usec
 TE 299.0 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400156 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**3ne**

Current Data Parameters
 NAME szy-400
 EXPNO 168
 PROCNO 1

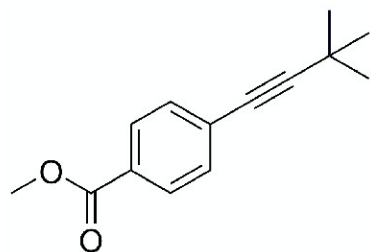
F2 - Acquisition Parameters
 Date_ 20180921
 Time_ 21.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 40
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404289 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

763

**3re**

7.87
7.85
7.36
7.34

3.82

1.25

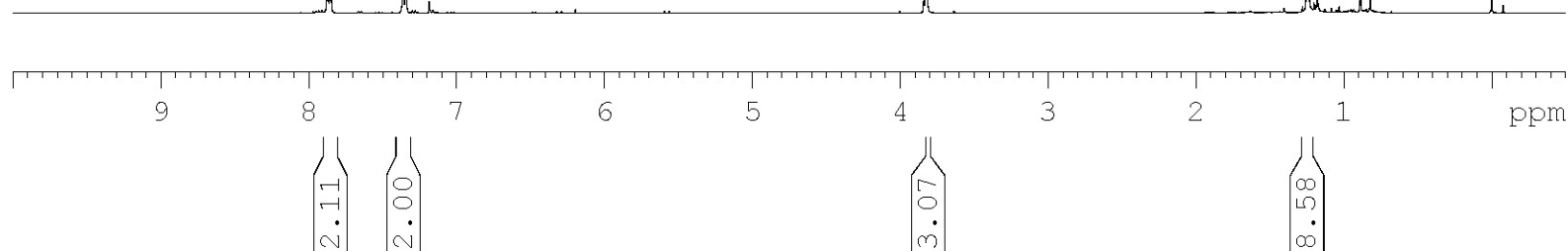
Current Data Parameters
 NAME szy-400
 EXPNO 169
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180921
 Time_ 21.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 49.81
 DW 62.400 usec
 DE 6.50 usec
 TE 299.1 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

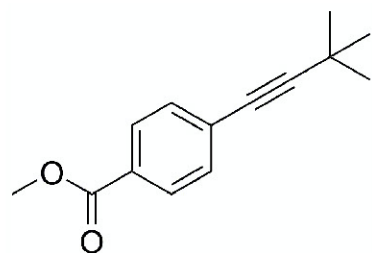
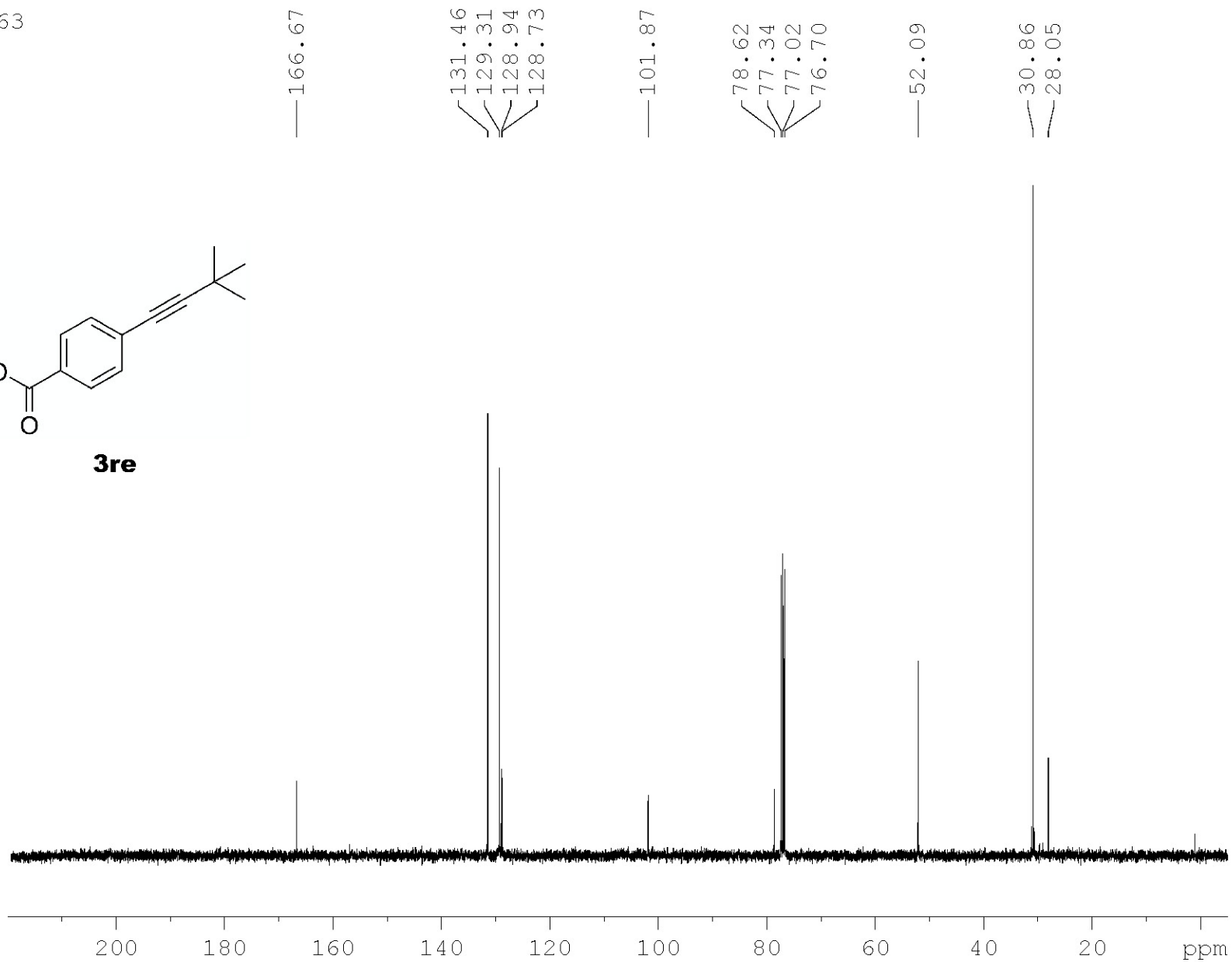
===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400397 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



763

**3re**

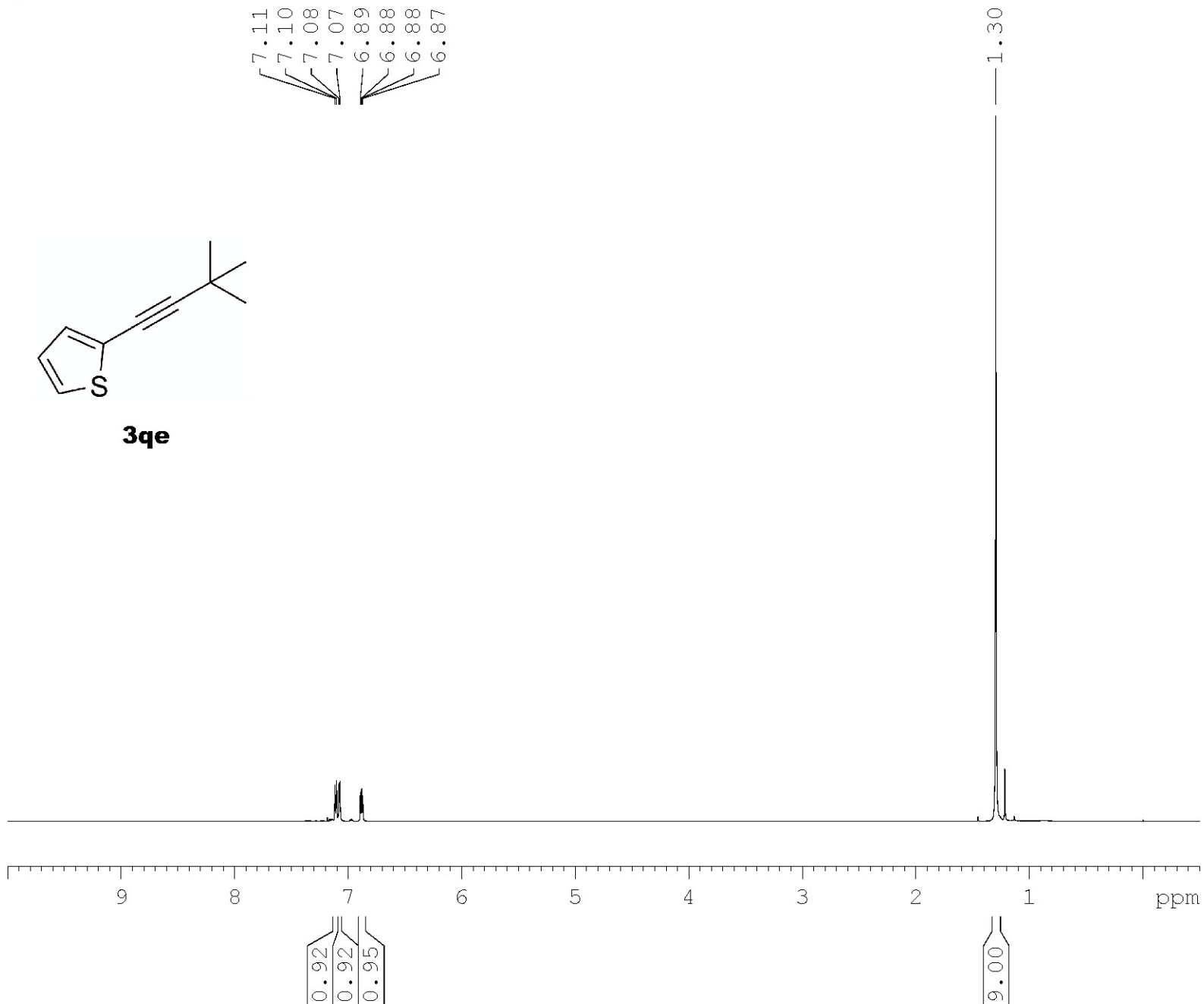
Current Data Parameters
 NAME szy-400
 EXPNO 170
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180921
 Time_ 21.46
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 30
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404296 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



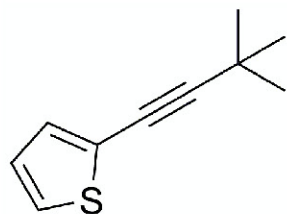
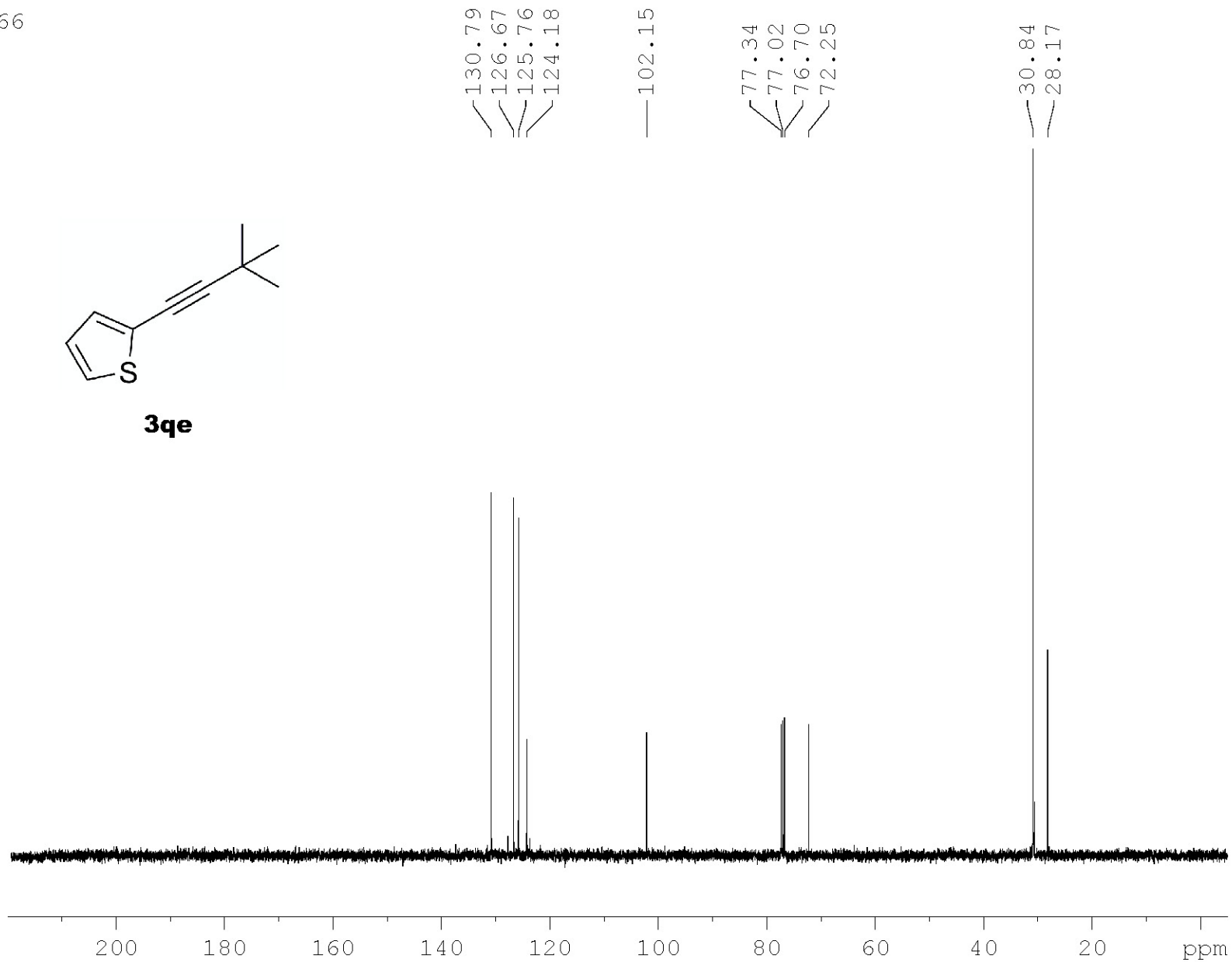
Current Data Parameters
 NAME szy-400
 EXPNO 193
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181029
 Time_ 14.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 19.61
 DW 62.400 usec
 DE 6.50 usec
 TE 298.5 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400401 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

**3qe**

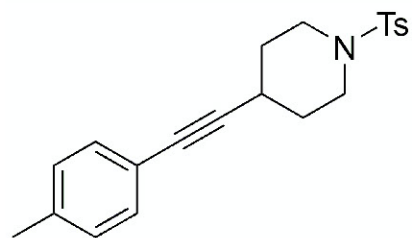
Current Data Parameters
 NAME szy-400
 EXPNO 194
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181029
 Time_ 14.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 15
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 299.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

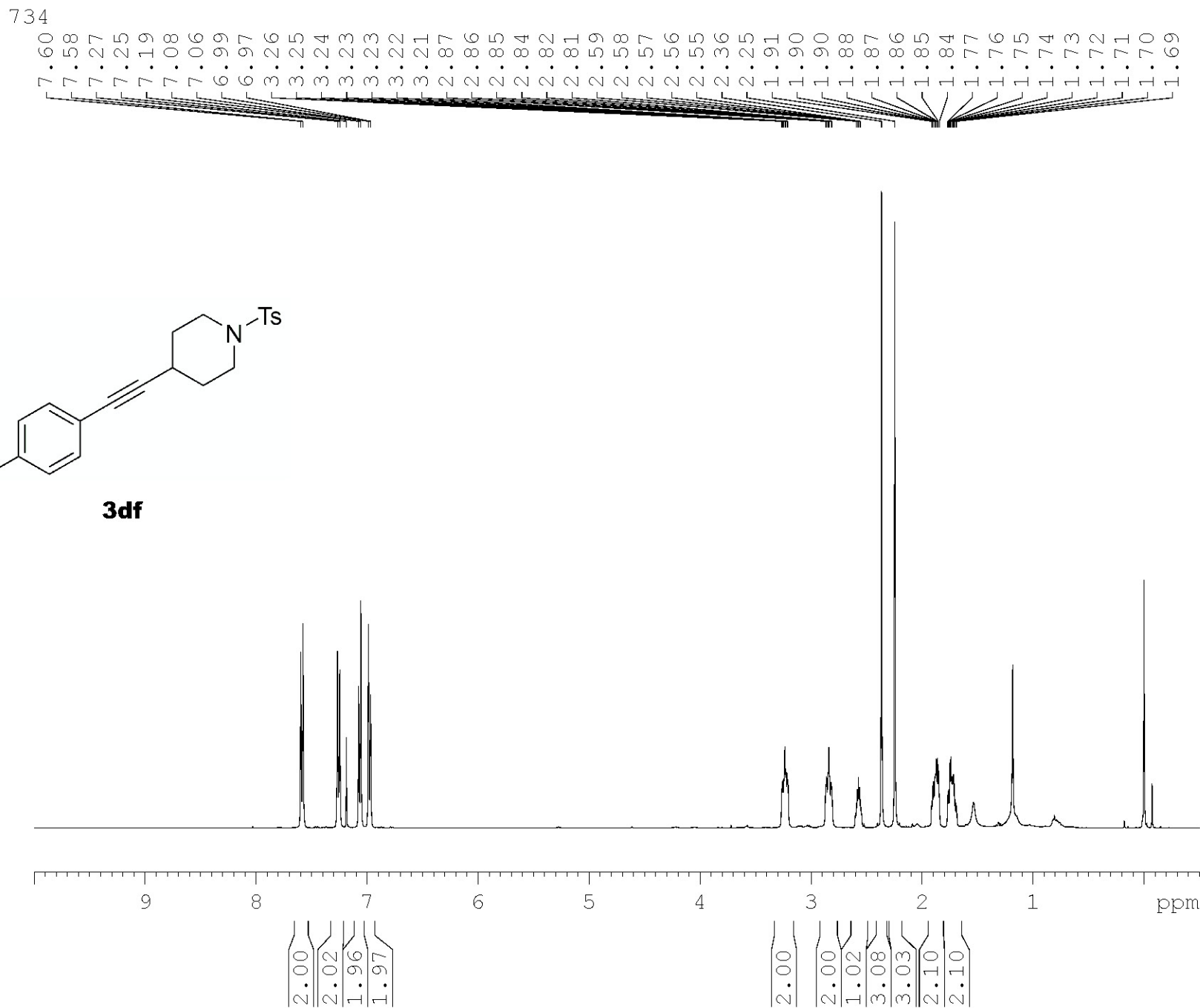
===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404398 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



3df



Current Data Parameters
 NAME szy-400
 EXPNO 133
 PROCNO 1

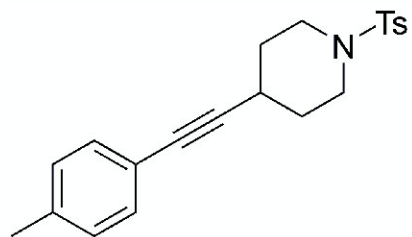
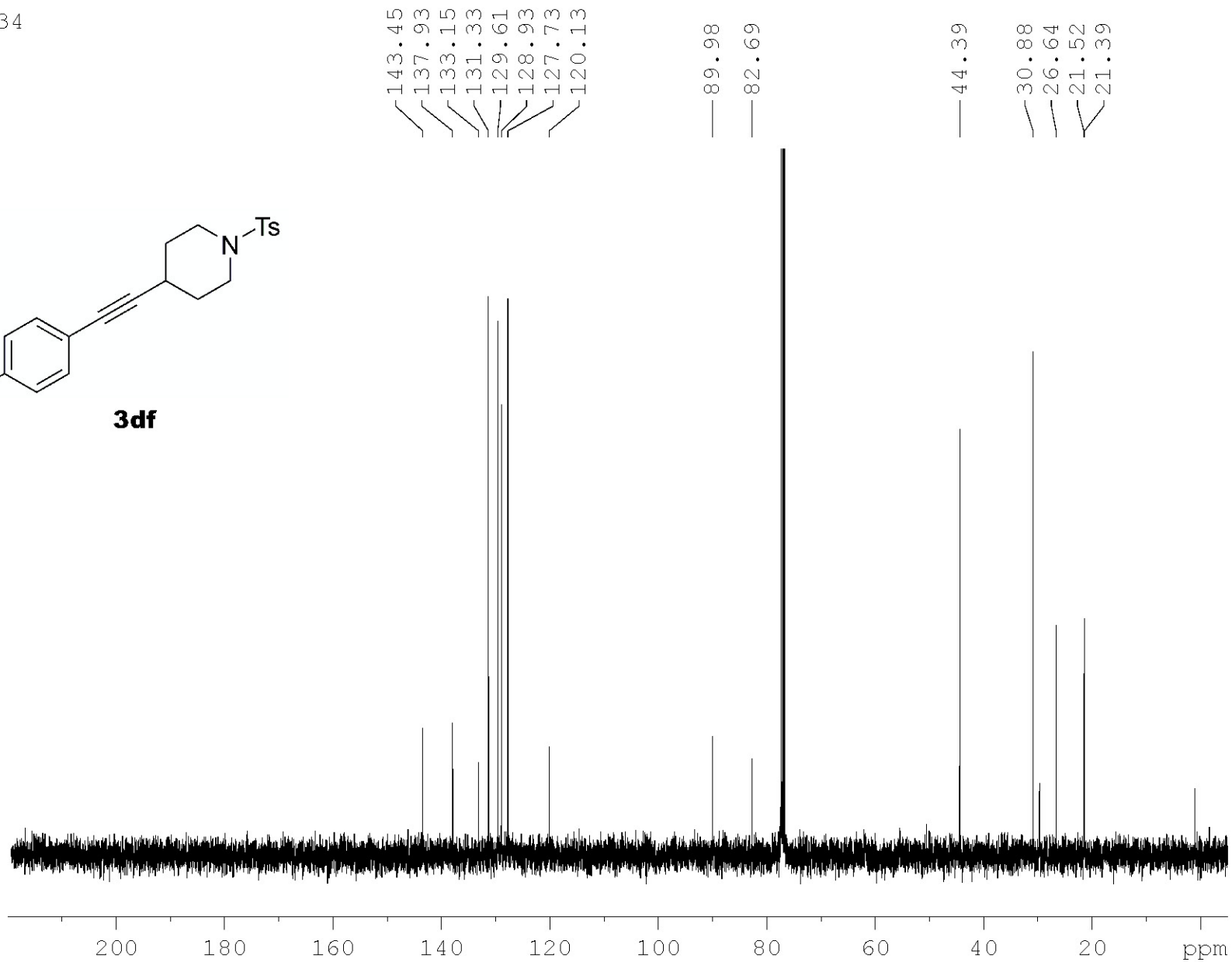
F2 - Acquisition Parameters
 Date_ 20180817
 Time_ 16.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 116.67
 DW 62.400 usec
 DE 6.50 usec
 TE 299.7 K
 D1 2.00000000 sec
 D11 0 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.80 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400392 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

734

**3df**

Current Data Parameters
 NAME szy-400
 EXPNO 134
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180817
 Time_ 16.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 59
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.34680000 W
 PLW13 0.28090999 W

F2 - Processing parameters
 SI 32768
 SF 100.6404296 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40