

Ag-Catalyzed Thiocyanofunctionalization of Terminal Alkynes to Access Alkynylthiocyanates and α -Thiocyanoketones

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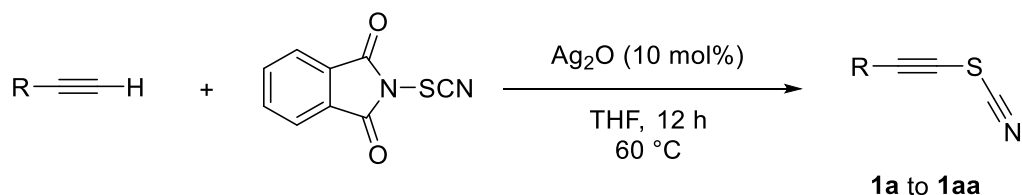
Supporting Information

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I. General information.

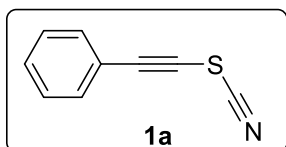
All reactions requiring anhydrous conditions were conducted by standard procedures under argon atmosphere. Commercially available reagents were used as received. The solvents were dried over a solvent purification system from Innovative Technology. Melting points (**MP**) were determined on a BÜCHI B-540b melting point apparatus. ^1H and ^{13}C NMR were recorded on a Bruker AMX500 (500 MHz) spectrometer. Proton and carbon chemical shifts are reported in parts per million (ppm) values downfield from TMS (δ 0.00) and referenced to residual protons in NMR solvents (CDCl_3 at δ 7.26, $\text{DMSO-}D_6$ at δ 2.50, CD_2Cl_2 at δ 5.31, CD_3OD at δ 3.31) or carbon signals in NMR solvent (CDCl_3 at δ 77.0, DMSO-CH_3 at δ 40.0, CD_2Cl_2 at δ 53.4, CD_3OD at δ 47.4). High resolution mass spectra (**HRMS**) were obtained on a Finnigan/MAT 95XL-T spectrometer. Analytical thin layer chromatography (**TLC**) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25 mm. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

General procedure for the preparation of thiocynoalkynes **1**



Into a small 1 mL vial were loaded Ag_2O (10 mol%), alkyne (0.19 mmol), anhydrous THF (0.3 mL) and *N*-thiocyanophthalimide (1.20 equiv.). The mixture was heated to 60 °C and allowed to stir overnight after which the product was purified directly through flash column chromatography using an ethyl acetate/hexanes eluent mixture (ratio of 1:10).

II. Characterization data for thiocynoalkynes **1**



(thiocyanatoethynyl)benzene

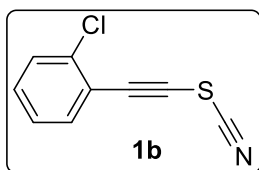
Physical appearance: Red oil

Yield: 27.5 mg, 90% (140.6 mg, 92% for 1 mmol scale)

^1H NMR (500 MHz, CDCl_3): δ 7.51 – 7.49 (m, 2H), 7.45 – 7.42 (m, 1H), 7.38 – 7.35 (m, 2H)

^{13}C NMR (125 MHz, CDCl_3): δ 132.6, 130.6, 128.8, 120.8, 106.6, 99.7, 62.3

HRMS (APCI): calcd for $\text{C}_9\text{H}_6\text{NS}$ m/z $[\text{M}+\text{H}]$: 160.0215; found: 160.0215.



1-chloro-2-(thiocyanatoethynyl)benzene

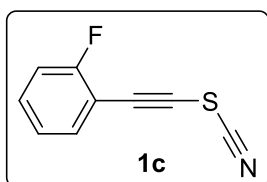
Physical appearance: Red liquid

Yield: 31.9 mg, 86%

^1H NMR (500 MHz, CDCl_3): δ 7.53 – 7.51 (m, 1H), 7.43 (d, J = 8.05 Hz, 1H), 7.37 – 7.34 (m, 1H), 7.28 – 7.25 (m, 1H)

^{13}C NMR (125 MHz, CDCl_3): δ 136.9, 133.9, 131.3, 129.6, 126.7, 120.7, 105.9, 96.0, 67.3

HRMS (ESI): calcd for $\text{C}_9\text{H}_5\text{ClNS}$ m/z $[\text{M}+\text{H}]$: 193.9826; found: 193.9831.



1-fluoro-2-(thiocyanatoethynyl)benzene

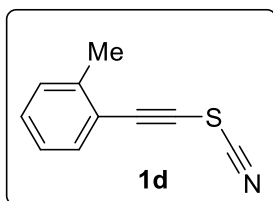
Physical appearance: Red oil

Yield: 21.3 mg, 62%

^1H NMR (500 MHz, CDCl_3): δ 7.50 – 7.47 (m, 1H), 7.44 – 7.40 (m, 1H), 7.17 – 7.09 (m, 2H)

^{13}C NMR (125 MHz, CDCl_3): δ 163.4 ($^1J_{\text{C-F}}$ = 254.90 Hz), 134.1, 132.4 ($^3J_{\text{C-F}}$ = 8.18 Hz), 124.3 ($^3J_{\text{C-F}}$ = 3.64 Hz), 115.9 ($^2J_{\text{C-F}}$ = 20.25 Hz), 109.4 ($^2J_{\text{C-F}}$ = 15.59 Hz), 105.9, 93.0, 67.4 ($^3J_{\text{C-F}}$ = 3.39 Hz)

HRMS (APCI): calcd for $\text{C}_9\text{H}_5\text{FNS}$ m/z $[\text{M}+\text{H}]$: 178.0121; found: 178.0120



1-methyl-2-(thiocyanatoethynyl)benzene

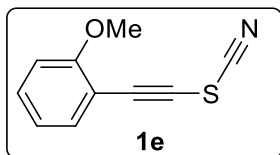
Physical appearance: Red oil

Yield: 28.4 mg, 85%

^1H NMR (500 MHz, CDCl_3): δ 7.46 (d, J = 7.70 Hz, 1H), 7.60 (t, J = 7.70 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.18 (t, J = 7.70 Hz, 1H), 2.45 (s, 3H)

^{13}C NMR (125 MHz, CDCl_3): δ 141.7, 132.8, 130.4, 129.7, 125.8, 120.5, 106.6, 98.6, 65.2, 20.5

HRMS (APCI): calcd for $\text{C}_{10}\text{H}_8\text{NS}$ m/z $[\text{M}+\text{H}]$: 174.0372; found: 174.0370.



1-methoxy-2-(thiocyanatoethynyl)benzene

Physical appearance: Orange solid

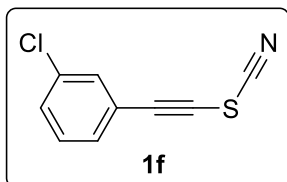
Yield: 27.2 mg, 74%

Melting Point: 69 °C

^1H NMR (500 MHz, CDCl_3): δ 7.45 – 7.44 (m, 1H), 7.41 – 7.37 (m, 1H), 6.95 – 6.89 (m, 2H), 3.89 (s, 3H)

^{13}C NMR (125 MHz, CDCl_3): δ 161.2, 134.5, 132.0, 120.6, 110.9, 109.9, 106.7, 96.3, 65.3, 55.8

HRMS (ESI): calcd for $\text{C}_{10}\text{H}_8\text{NOS}$ m/z $[\text{M}+\text{H}]$: 190.0318; found: 190.0321.



1-chloro-3-(thiocyanatoethynyl)benzene

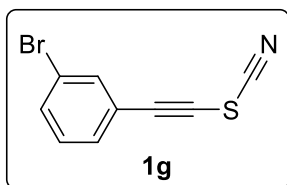
Physical appearance: Red oil

Yield: 18.6 mg, 50 %

^1H NMR (500 MHz, CDCl_3): δ 7.48 (t, J = 1.70 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.31 (t, J = 7.80 Hz, 1H)

^{13}C NMR (125 MHz, CDCl_3): δ 134.6, 132.1, 13.7, 130.4, 129.9, 122.2, 105.9, 97.8, 63.8

HRMS (APCI): calcd for $\text{C}_9\text{H}_4\text{ClNS}$ m/z $[\text{M}]$: 192.9747; found: 192.9748.



1-bromo-3-(thiocyanatoethynyl)benzene

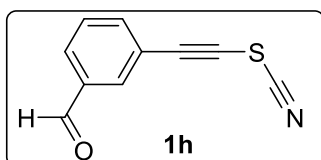
Physical appearance: Red oil

Yield: 15.7 mg, 34%

^1H NMR (500 MHz, CDCl_3): δ 7.68 (t, J = 1.55 Hz, 1H), 7.59 (d, J = 8.95 Hz, 1H), 7.46 (d, J = 7.90 Hz, 1H), 7.28 (t, J = 7.90 Hz, 1H)

^{13}C NMR (125 MHz, CDCl_3): δ 134.9, 133.5, 130.8, 130.1, 122.5, 122.4, 105.9, 97.7, 63.9

HRMS (APCI): calcd for $\text{C}_9\text{H}_4\text{BrNS}$ m/z [M]: 236.9242; found: 236.9238.



3-(thiocyanatoethynyl)benzaldehyde

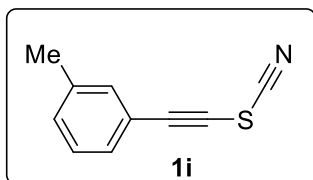
Physical appearance: Red oil

Yield: 35.5 mg, 85%

^1H NMR (500 MHz, CDCl_3): δ 9.99 (s, 1H), 7.99 (s, 1H), 7.93 (d, J = 7.60 Hz, 1H), 7.73 (d, J = 7.50 Hz, 1H), 7.56 (t, J = 7.70 Hz, 1H)

^{13}C NMR (125 MHz, CDCl_3): δ 190.8, 137.5, 136.6, 133.4, 130.9, 129.5, 121.8, 105.8, 97.8, 64.4

HRMS (ESI): calcd for $\text{C}_{10}\text{H}_4\text{NOS}$ m/z [M-H]: 186.0008; found: 186.0007.



1-methyl-3-(thiocyanatoethynyl)benzene

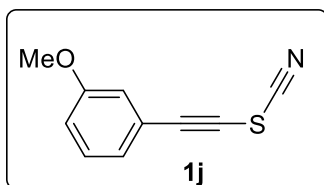
Physical appearance: Red oil

Yield: 22.4 mg, 67%

¹H NMR (500 MHz, CDCl₃): δ 7.33 – 7.31 (m, 2H), 7.26 – 7.25 (m, 2H), 2.36 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 138.5, 132.9, 131.3, 129.5, 128.5, 120.4, 106.4, 99.8, 61.6, 21.1

HRMS (APCI): calcd for C₁₀H₈NS *m/z* [M+H]: 174.0372; found: 174.0366.



1-methoxy-3-(thiocyanatoethynyl)benzene

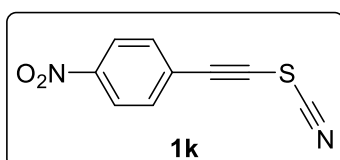
Physical appearance: Red oil

Yield: 28.3 mg, 78%

¹H NMR (500 MHz, CDCl₃): δ 7.28 (t, *J* = 8.15 Hz, 1H), 7.10 (d, *J* = 7.55 Hz, 1H), 7.01 – 6.97 (m, 2H), 3.82 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 159.4, 129.7, 124.9, 121.5, 117.1, 116.9, 106.4, 99.4, 61.9, 55.4

HRMS (APCI): calcd for C₁₀H₈NOS *m/z* [M+H]: 190.0316; found: 190.0321.



1-nitro-4-(thiocyanatoethynyl)benzene

Physical appearance: Red solid

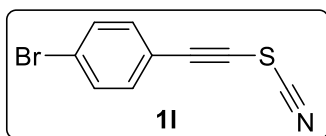
Yield: 23.4 mg, 60%

Melting Point: 92 °C

¹H NMR (500 MHz, CDCl₃): δ 8.24 (d, *J* = 8.75 Hz, 2H), 7.65 (d, *J* = 9.05 Hz, 2H)

¹³C NMR (125 MHz, CDCl₃): δ 148.2, 132.8, 126.9, 123.8, 105.2, 97.1, 68.3

HRMS (APCI): calcd for C₉H₅N₂O₂S *m/z* [M+H]: 205.0066; found: 205.0068.



1-bromo-4-(thiocyanatoethynyl)benzene

Physical appearance: Orange solid

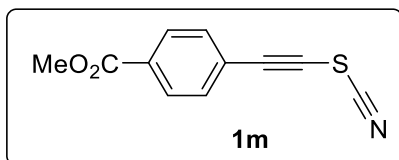
Yield: 41.1 mg, 92%

Melting Point: 66 °C

¹H NMR (500 MHz, CDCl₃): δ 7.52 (d, *J* = 8.30 Hz, 2H), 7.36 (d, *J* = 8.30 Hz, 2H)

¹³C NMR (125 MHz, CDCl₃): δ 133.8, 132.2, 125.2, 119.6, 106.1, 98.5, 63.7

HRMS (APCI): calcd for C₉H₄BrNS *m/z* [M]: 236.9242; found: 236.9235.



Methyl-4-(thiocyanatoethynyl)benzoate

Physical appearance: Yellow solid

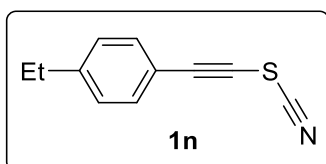
Yield: 28.3 mg, 70 %

Melting Point: 80 °C

¹H NMR (500 MHz, CDCl₃): δ 8.03 (d, *J* = 8.20 Hz, 2H), 7.55 (d, *J* = 8.20 Hz, 2H), 3.93 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 166.2, 132.1, 131.5, 129.8, 125.1, 105.9, 98.6, 65.4, 52.6

HRMS (APCI): calcd for C₁₁H₈NO₂S *m/z* [M+H]: 218.0270; found: 218.0271.



1-ethyl-4-(thiocyanatoethynyl)benzene

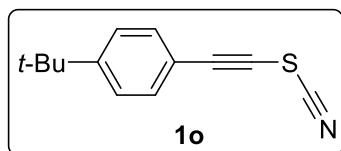
Physical appearance: Red oil

Yield: 32.8 mg, 91%

¹H NMR (500 MHz, CDCl₃): δ 7.42 (d, *J* = 8.05 Hz, 2H), 7.20 (d, *J* = 8.05 Hz, 2H), 2.67 (q, *J* = 7.60 Hz, 2H), 0.63 (t, *J* = 7.60 Hz, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 147.2, 132.5, 128.2, 117.7, 106.6, 99.8, 61.1, 28.9, 15.1

HRMS (APCI): calcd for C₁₁H₁₀NS *m/z* [M+H]: 188.0528; found:188.0530.



1-(*tert*-butyl)-4-(thiocyanatoethynyl)benzene

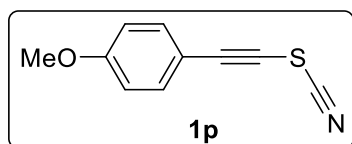
Physical appearance: Red oil

Yield: 34.9 mg, 84% (137.9 mg, 83% yield for 1 mmol scale)

¹H NMR (500 MHz, CDCl₃): δ 7.43 (d, *J* = 8.50 Hz, 2H), 7.39 (d, *J* = 8.50 Hz, 2H), 1.32 (s, 9H)

¹³C NMR (125 MHz, CDCl₃): δ 154.0, 132.3, 125.6, 117.5, 106.6, 99.9, 61.1, 35.0, 31.0

HRMS (APCI): calcd for C₁₃H₁₃NS *m/z* [M+H]: 216.0841; found: 216.0834.



1-methoxy-4-(thiocyanatoethynyl)benzene

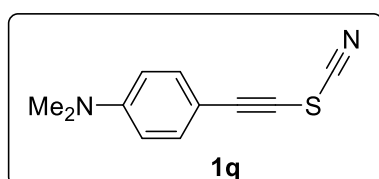
Physical appearance: Red oil

Yield: 23.6 mg, 65%

¹H NMR (500 MHz, CDCl₃): δ 7.45 (d, *J* = 8.75 Hz, 2H), 6.87 (d, *J* = 8.75 Hz, 2H), 3.83 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 161.5, 134.7, 114.4, 112.7, 106.9, 100.0, 60.6, 55.5

HRMS (APCI): calcd for C₁₀H₈NOS *m/z* [M+H]: 190.0321; found:190.0321.



N,N-dimethyl-4-(thiocyanatoethynyl)aniline

Physical appearance: Black solid

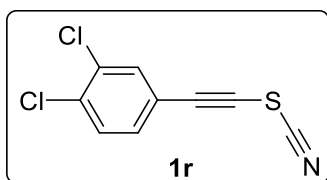
Yield: 13.8 mg, 36%

Melting Point: 121 °C

¹H NMR (500 MHz, CDCl₃): δ 7.38 (d, *J* = 8.75 Hz, 2H), 6.60 (d, *J* = 8.75 Hz, 2H), 3.01 (s, 6H)

¹³C NMR (125 MHz, CDCl₃): δ 151.4, 134.5, 111.4, 107.5, 106.6, 101.9, 59.0, 40.0

HRMS (APCI): calcd for C₁₁H₁₁N₂S *m/z* [M+H]: 203.0637; found: 203.0640.



1,2-dichloro-4-(thiocyanatoethynyl)benzene

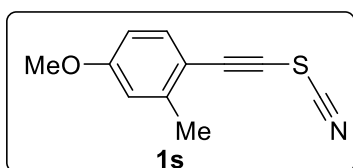
Physical appearance: Red oil

Yield: 31 mg, 70%

¹H NMR (500 MHz, CDCl₃): δ 7.58 (d, *J* = 1.90 Hz, 1H), 7.45 (d, *J* = 8.40 Hz, 1H), 7.32 (dd, *J* = 1.90 Hz, *J* = 8.40 Hz, 1H)

¹³C NMR (125 MHz, CDCl₃): δ 135.2, 133.8, 133.1, 131.3, 130.8, 120.4, 105.6, 96.9, 64.9

HRMS (APCI): calcd for C₉H₃Cl₂NS *m/z* [M]: 226.9358; found: 226.9350.



4-methoxy-2-methyl-1-(thiocyanatoethynyl)benzene

Physical appearance: Red oil

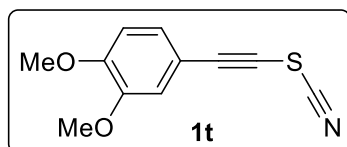
Yield: 35.3 mg, 90%

¹H NMR (500 MHz, CDCl₃): δ 7.40 (d, *J* = 8.50 Hz, 1H), 6.75 (d, *J* = 2.50 Hz, 1H), 6.70 (dd, *J* = 2.50 Hz, *J* = 8.50 Hz, 1H), 3.81 (s, 3H), 2.42 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 161.3, 144.2, 134.9, 115.4, 112.6, 111.7, 107.0, 99.1, 63.5,

55.3, 20.8

HRMS (APCI): calcd for C₁₁H₁₀NOS *m/z* [M+H]: 204.0478; found: 204.0480.



1,2-dimethoxy-4-(thiocyanatoethynyl)benzene

Physical appearance: Red solid

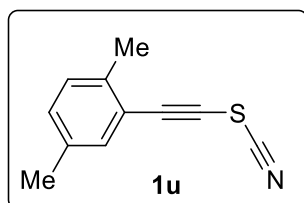
Yield: 28.0 mg, 66%

Melting Point: 65 °C

¹H NMR (500 MHz, CDCl₃): δ 7.13 (dd, *J* = 1.50 Hz, *J* = 8.15 Hz, 1H), 6.98 (s, 1H), 6.82 (d, *J* = 8.40 Hz, 1H), 3.89 (s, 3H), 3.87 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 151.3, 148.8, 126.7, 114.9, 112.5, 111.0, 106.8, 99.9, 60.4, 56.0, 55.9

HRMS (APCI): calcd for C₁₁H₁₀NO₂S *m/z* [M+H]: 220.0427; found: 220.0429.



1,4-dimethyl-2-(thiocyanatoethynyl)benzene

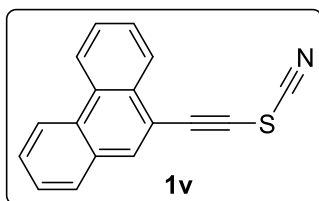
Physical appearance: Orange oil

Yield: 26.0 mg, 72%

¹H NMR (500 MHz, CDCl₃): δ 7.28 (s, 1H), 7.12 – 7.11 (m, 2H), 2.39 (s, 3H), 2.30 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 138.6, 135.4, 133.2, 131.3, 129.7, 120.2, 106.7, 98.9, 64.7, 20.7, 20.0

HRMS (APCI): calcd for C₁₁H₁₀NS *m/z* [M+H]: 188.0528; found: 188.0529.



9-(thiocyanatoethynyl)phenanthrene

Physical appearance: Yellow solid

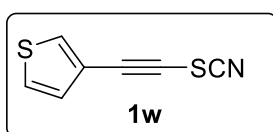
Yield: 12.9 mg, 25%

Melting Point: 121 °C

¹H NMR (500 MHz, CDCl₃): δ 8.75 – 8.61 (m, 2H), 8.28 – 8.27 (m, 1H), 8.08 (s, 1H), 7.86 (d, *J* = 7.40 Hz, 1H), 7.74 – 7.69 (m, 3H), 7.63 (t, *J* = 7.20 Hz, 1H)

¹³C NMR (125 MHz, CDCl₃): δ 134.6, 131.1, 130.6, 130.5, 130.1, 129.0, 128.7, 127.6, 127.5, 127.3, 126.3, 122.9, 122.7, 117.1, 106.4, 98.3, 65.9

HRMS (APCI): calcd for C₁₇H₁₀NS *m/z* [M+H]: 260.0528; found: 260.0519.



3-(thiocyanatoethynyl)thiophene

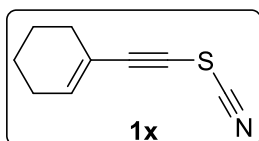
Physical appearance: Black oil

Yield: 24.9 mg, 79%

¹H NMR (500 MHz, CDCl₃): δ 7.67 (d, *J* = 3.00 Hz, 1H), 7.32 (dd, *J* = 3.10 Hz, *J* = 5.0 Hz, 1H), 7.17 (d, *J* = 5.00 Hz, 1H)

¹³C NMR (125 MHz, CDCl₃): δ 133.0, 129.9, 126.1, 119.8, 106.4, 94.8, 62.0

HRMS (APCI): calcd for C₇H₄NS₂ *m/z* [M+H]: 165.9780; found: 165.9777.



1-(thiocyanatoethynyl)cyclohex-1-ene

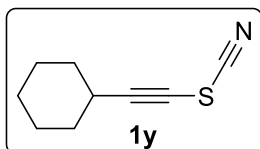
Physical appearance: Red oil

Yield: 30.0 mg, 96%

¹H NMR (500 MHz, CDCl₃): δ 6.34 – 6.32 (m, 1H), 2.15 – 2.11 (m, 4H), 1.67 – 1.59 (m, 4H)

¹³C NMR (125 MHz, CDCl₃): δ 140.9, 119.7, 107.1, 101.6, 58.9, 28.4, 26.0, 22.1, 21.2

HRMS (ESI): calcd for C₉H₁₀NS *m/z* [M+H]: 164.0521; found 164.0511;



(thiocyanatoethynyl)cyclohexane

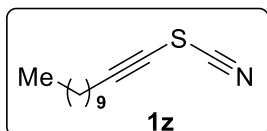
Physical appearance: Yellow oil

Yield: 11.4 mg, 36%

¹H NMR (500 MHz, CDCl₃): δ 2.56 – 2.52 (m, 1H), 1.82 – 1.79 (m, 2H), 1.72 – 1.67 (m, 2H), 1.66 – 1.44 (m, 3H), 1.37 – 1.29 (m, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 107.5, 105.9, 52.4, 31.6, 30.4, 25.6, 24.6

HRMS (APCI): calcd for C₉H₁₂NS *m/z* [M+H]: 166.0685; found: 166.0682.



1-thiocyanatododec-1-yne

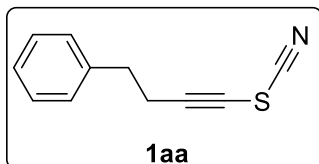
Physical appearance: Yellow oil

Yield: 26.5 mg, 62%

¹H NMR (500 MHz, CDCl₃): δ 2.35 (t, *J* = 7.10 Hz, 2H), 1.57 – 1.51 (m, 2H), 1.37 – 1.35 (m, 2H), 1.27 (s, 12H), 0.87 (t, *J* = 7.10 Hz, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 107.4, 102.5, 52.3, 31.8, 29.5, 29.4, 29.3, 29.0, 28.8, 27.8, 22.7, 20.1, 14.1

HRMS (APCI): calcd for C₁₃H₂₂NS *m/z* [M+H]: 224.1467; found: 224.1468.



(4-thiocyanatobut-3-yn-1-yl)benzene

Physical appearance: Yellow oil

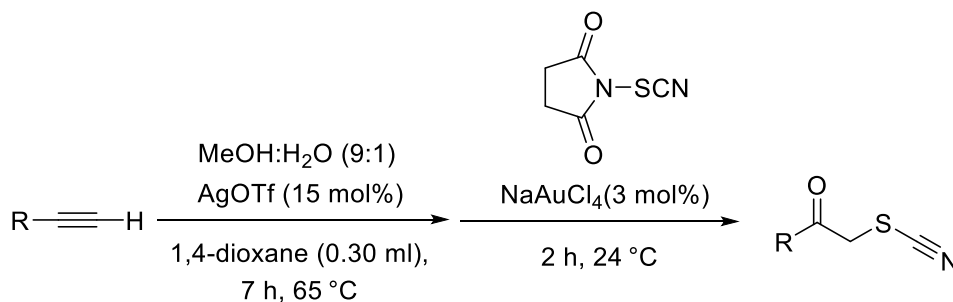
Yield: 17.6 mg, 49%

¹H NMR (500 MHz, CDCl₃): δ 7.34 – 7.31 (t, *J* = 7.40 Hz, 2H), 7.24 (d, *J* = 7.40 Hz, 1H)
7.20 (d, *J* = 7.40 Hz, 2H), 2.87 (t, *J* = 7.35 Hz, 2H), 2.66 (t, *J* = 7.35 Hz, 2H)

¹³C NMR (125 MHz, CDCl₃): δ 139.5, 128.6, 128.3, 126.7, 106.9, 101.4, 53.6, 34.0, 22.2

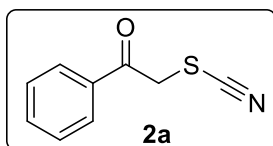
HRMS (APCI): calcd for C₁₁H₁₀NS *m/z* [M+H]: 188.0526; found: 188.0528.

III. General procedure for preparation of thiocyanoketones 2



In a 1.0 mL vial were loaded the reagents in the following sequence: silver triflate (7.0 mg, 15.0 mol%), 1,4-dioxane (0.30 mL), alkyne (0.19 mmol) and 20 μL of a methanol:water mixture prepared in 9:1 ratio. The mixture was heated to $65\text{ }^\circ\text{C}$ for 7 h and then cooled to room temperature. Sodium gold tetrachloride dehydrate (3.0 mol%) was added and the mixture was allowed to stir at room temperature for 10 mins. Finally, *N*-thiocyanosuccinimide (2.0 equiv.) was added and the mixture continued to stir for 2 hours during which reaction completion was monitored through TLC. The product was purified by flash column chromatography using ethyl acetate/ hexanes as the eluent (ratio of 1:5).

IV. Characterization data for thiocyanoketones 2 & 4



1-phenyl-2-thiocyanatoethan-1-one

Physical appearance: Red solid

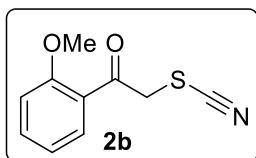
Yield: 25.5 mg, 75% yield

Melting Point: $66.3\text{ }^\circ\text{C}$

^1H NMR (500 MHz, CDCl_3): δ 7.94 (d, $J = 7.40\text{ Hz}$, 2H), 7.67 (t, $J = 7.55\text{ Hz}$, 1H), 7.53 (t, $J = 7.75\text{ Hz}$, 2H), 4.74 (s, 2H)

^{13}C NMR (125 MHz, CDCl_3): δ 190.8, 134.8, 134.0, 129.2, 128.5, 111.8, 42.9

HRMS (APCI): calcd for $\text{C}_6\text{H}_8\text{NOS}$ m/z $[\text{M}+\text{H}]$: 178.0321; found: 178.0323.



1-(2-methoxyphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

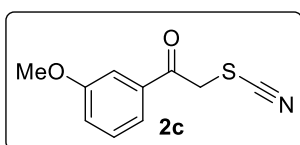
Yield: 23.1 mg, 58% yield

Melting Point: 90.3 °C

¹H NMR (500 MHz, CDCl₃): δ 7.94-7.92 (m, 1H), 7.60 – 7.57 (m, 1H), 7.08 – 7.02 (m, 2H), 4.71 (s, 2H), 3.98 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 191.3, 159.6, 136.0, 131.4, 123.7, 121.3, 112.8, 111.8, 55.8, 47.6

HRMS (APCI): calcd for C₁₀H₁₀NO₂S *m/z* [M+H]: 208.0427; found: 208.0424.



1-(3-methoxyphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

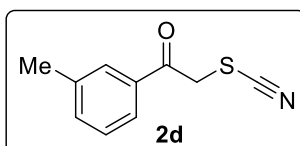
Yield: 29.5 mg, 74% yield

Melting Point: 81.6 °C

¹H NMR (500 MHz, CDCl₃): δ 7.49 – 7.41 (m, 3H), 7.21 – 7.19 (m, 1H), 4.72 (s, 2H), 3.87 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 190.7, 160.2, 135.2, 130.2, 121.3, 121.0, 112.6, 111.8, 55.6, 43.0

HRMS (APCI): calcd for C₁₀H₁₀NO₂S *m/z* [M+H]: 208.0427; found: 208.0426.



2-thiocyanato-1-(m-tolyl)ethan-1-one

Physical appearance: Yellow solid

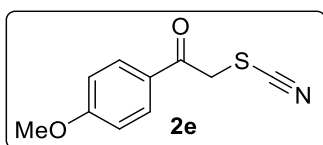
Yield: 28.6 mg, 78% yield

Melting Point: 78.4 °C

¹H NMR (500 MHz, CDCl₃): δ 7.75 – 7.72 (m, 2H), 7.48 (d, *J* = 7.70 Hz, 1H), 7.41 (t, *J* = 7.70 Hz, 1H), 4.73 (s, 2H), 2.43 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 190.9, 139.2, 135.6, 133.9, 129.0, 128.9, 125.7, 111.9, 43.1, 21.3

HRMS (APCI): calcd for C₁₀H₁₀NOS *m/z* [M+H]: 192.0478; found: 192.0483.



1-(4-methoxyphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

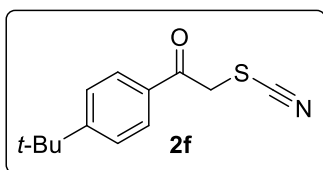
Yield: 17.5 mg, 44% yield

Melting Point: 118.3 °C

¹H NMR (500 MHz, CDCl₃): δ 7.91 (d, *J* = 8.35 Hz, 2H), 6.98 (d, *J* = 8.35 Hz, 2H), 4.70 (s, 2H), 3.89 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 189.2, 164.8, 130.9, 127.0, 114.3, 112.1, 55.7, 42.9

HRMS (APCI): calcd for C₁₀H₁₀NO₂S *m/z* [M+H]: 208.0427; found: 208.0427.



1-(4-(tert-butyl)phenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

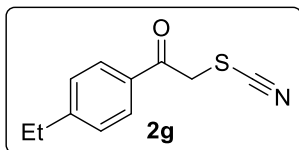
Yield: 35.4 mg, 79% yield

Melting Point: 80.3 °C

¹H NMR (500 MHz, CDCl₃): δ 7.87 (d, *J* = 8.40 Hz, 2H), 7.52 (d, *J* = 8.40 Hz, 2H), 4.73 (s, 2H), 1.35 (s, 9H)

¹³C NMR (125 MHz, CDCl₃): δ 190.4, 158.9, 131.4, 128.5, 126.2, 112.0, 43.0, 35.4, 30.9

HRMS (APCI): calcd for C₁₃H₁₆NOS *m/z* [M+H]: 234.0947 ; found: 234.0946



1-(4-ethylphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

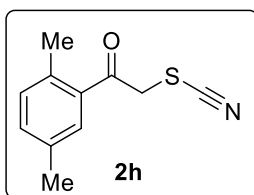
Yield: 30.7 mg, 78 % yield

Melting Point: 56.3 °C

¹H NMR (500 MHz, CDCl₃): δ 7.85 (d, *J* = 7.85 Hz, 2H), 7.34 (d, *J* = 7.85 Hz, 2H), 4.72 (s, 2H), 2.73 (q, *J* = 7.60 Hz, 2H), 1.27 (t, *J* = 7.55 Hz, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 190.5, 152.2, 131.7, 128.7, 128.6, 112.0, 43.0, 29.0, 15.0

HRMS (APCI): calcd for C₁₁H₁₂NOS *m/z* [M+H]: 206.0634; found: 206.0627.



1-(2,5-dimethylphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Light brown solid

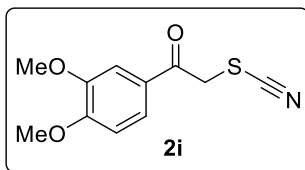
Yield: 29.2 mg, 74% yield

Melting Point: 111.9 °C

¹H NMR (500 MHz, CDCl₃): 7.49 (s, 1H), 7.30 (d, *J* = 7.70 Hz, 1H), 7.20 (d, *J* = 7.70 Hz, 1H), 4.72 (s, 2H), 2.51 (s, 3H), 2.39 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): 193.2, 137.3, 135.9, 134.3, 133.3, 132.7, 130.1, 112.1, 45.1, 21.4, 20.9

HRMS (APCI): calcd for C₁₁H₁₂NOS *m/z* [M+H]: 206.0634; found: 206.0632.



1-(3,4-dimethoxyphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

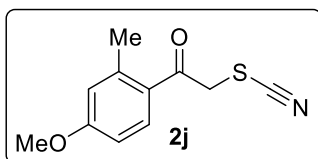
Yield: 27.3 mg, 60% yield

Melting Point: 136.0 °C

¹H NMR (500 MHz, CDCl₃): δ 7.53 (dd, *J* = 8.35 Hz, *J* = 1.79 Hz, 1H), 7.48 (d, *J* = 1.75 Hz, 1H), 6.92 (d, *J* = 8.40 Hz, 1H), 4.71 (s, 2H), 3.97 (s, 3H), 3.94 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 189.3, 154.8, 149.6, 127.2, 123.5, 112.1, 110.4, 110.2, 56.3, 56.1, 42.7

HRMS (APCI): calcd for C₁₁H₁₃NO₃S *m/z* [M+H]: 238.0532; found: 238.0537.



1-(4-methoxy-2-methylphenyl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

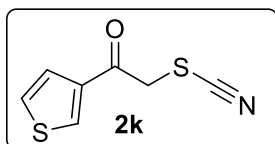
Yield: 20.4 mg, 48% yield

Melting Point: 120 °C

¹H NMR (500 MHz, CDCl₃): δ 7.71 (d, *J* = 9.30 Hz, 1H), 6.80 (s, 2H), 4.74 (s, 2H), 3.88 (s, 3H), 2.59 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 190.8, 163.5, 144.3, 132.7, 125.9, 118.2, 112.4, 111.3, 55.5, 45.2, 22.8

HRMS (APCI): calcd for C₁₁H₁₂NO₂S *m/z* [M+H]: 222.0583; found: 222.0581.



2-thiocyanato-1-(thiophen-3-yl)ethan-1-one

Physical appearance: White solid

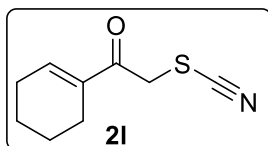
Yield: 25.3 mg, 72% yield

Melting Point: 81.2 °C

¹H NMR (500 MHz, CDCl₃): δ 8.17 – 8.15 (m, 1H), 7.56 – 7.54 (m, 1H), 7.41 – 7.40 (m, 1H), 4.58 (s, 2H)

¹³C NMR (125 MHz, CDCl₃): δ 184.7, 138.8, 134.0, 127.6, 126.7, 111.7, 42.7

HRMS (APCI): calcd for C₇H₆NOS₂ *m/z* [M+H]: 183.9885; found: 183.9881.



1-(cyclohex-1-en-1-yl)-2-thiocyanatoethan-1-one

Physical appearance: Pale yellow solid

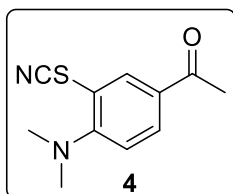
Yield: 24.3 mg, 70% yield

Melting Point: 53.5 °C

¹H NMR (500 MHz, CDCl₃): δ 6.97 – 6.96 (m, 1H), 4.44 (s, 2H), 2.33 – 2.31 (m, 2H), 2.25 – 2.22 (m, 2H), 1.68 – 1.62 (m, 4H)

¹³C NMR (125 MHz, CDCl₃): δ 191.4, 144.2, 137.8, 112.3, 42.1, 26.3, 23.0, 21.5, 21.2

HRMS (APCI): calcd for C₉H₁₂NOS *m/z* [M+H]: 182.0634; found: 182.0633.



1-(4-(dimethylamino)-3-thiocyanatophenyl)ethan-1-one

Physical appearance: White crystal

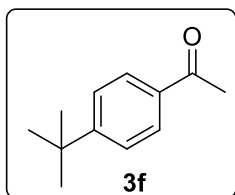
Yield: 37.1 mg, 88% yield

Melting Point: 76.0 °C

¹H NMR (500 MHz, CDCl₃): δ 8.16 (s, 1H), 7.89 (d, *J* = 8.50 Hz, 1H), 7.19 (d, *J* = 8.50 Hz, 1H), 2.79 (s, 6H), 2.58 (s, 3H)

¹³C NMR (125 MHz, CDCl₃): δ 195.7, 155.5, 133.8, 129.7, 129.5, 122.2, 120.5, 110.8, 44.1, 26.4

HRMS (ESI): calcd for C₁₁H₁₃N₂OS *m/z* [M+H]: 221.0743; found: 221.0743.



4-t-butylacetophenone

Physical appearance: Clear oil

Yield: 30.1 mg, 89% yield

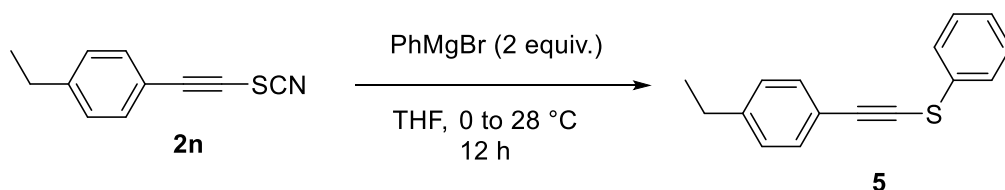
¹H NMR (500 MHz, CDCl₃): δ 7.90 (d, *J* = 8.35 Hz, 2H), 7.48 (d, *J* = 8.35 Hz, 2H), 2.59 (s, 3H), 1.34 (s, 9H)

¹³C NMR (125 MHz, CDCl₃): δ 198.9, 156.8, 134.7, 128.3, 125.5, 35.1, 31.0, 26.5

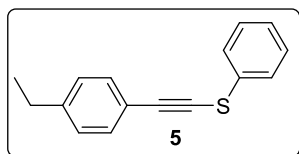
HRMS (ESI): calcd for C₁₂H₁₇O *m/z* [M+H]: 177.1274; found: 177.1273.

V. General procedure for preparation of 5 to 8 & corresponding characterization data

a) General procedure for the preparation of 5



Into a degassed 10 mL schlenk flask was loaded a magnetic stirrer and 30 mg (0.16 mmol) of **2n**, after which 2 mL of anhydrous THF was added under argon atmosphere. The flask was lowered into an ice bath after which 0.10 mL of 1M PhMgBr in THF was added slowly. The reaction was allowed to proceed overnight after which solids were noticed to form. THF was removed under reduced pressure and the residue was purified by column chromatography directly to afford the product as a clear oil in 67% yield (25.7 mg).^[1]



((4-ethylphenyl)ethynyl)(phenyl)sulfane

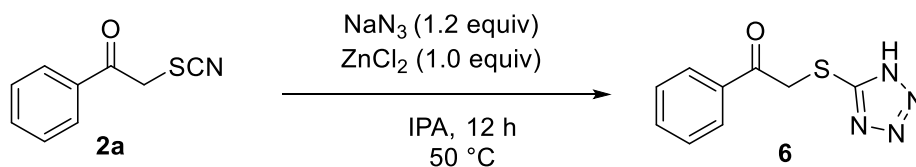
Physical appearance: Clear oil

¹H NMR (500 MHz, CDCl₃): δ 7.50 (d, *J* = 8.10 Hz, 2H), 7.46 (d, *J* = 8.10 Hz, 2H), 7.36 (t, *J* = 7.60 Hz, 2H), 7.25- 7.22 (m, 1H), 7.19 (d, *J* = 8.10 Hz, 2H), 2.68 (q, *J* = 7.60 Hz, 2H), 1.26 (t, *J* = 7.70 Hz, 3H)

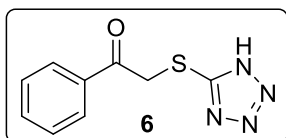
¹³C NMR (125 MHz, CDCl₃): δ 145.3, 133.3, 131.9, 129.2, 128.0, 126.4, 126.1, 120.1, 98.2, 74.4, 28.9, 15.4

HRMS (ESI): calcd for C₁₆H₁₅S *m/z* [M+H]: 239.0889; found: 239.0891.

b) General procedure for the preparation of 6



Into a 10 mL vial were loaded 50 mg (0.28 mmol) of **2a**, 0.40 mL of isopropyl alcohol, 22 mg (0.34 mmol, 1.20 equiv.) of NaN_3 and 38 mg of ZnCl_2 (0.28 mmol). After the starting material was consumed as judged by TLC, the solvent was removed under reduced pressure. 5% NaOH solution was then added and the mixture was allowed to stir for two minutes until a suspension of $\text{Zn}(\text{OH})_2$ had formed. The residue was washed several times with 5% NaOH solution and the filtrate was combined. The filtrate was acidified to pH 1.0 using concentrated HCl, causing the tetrazole product to precipitated, which was collected through filtration, dried. The product was obtained in a pure form in 78% yield (48.4 mg).^[2]



2-((1H-tetrazol-5-yl)thio)-1-phenylethan-1-one

Physical appearance: Yellow solid

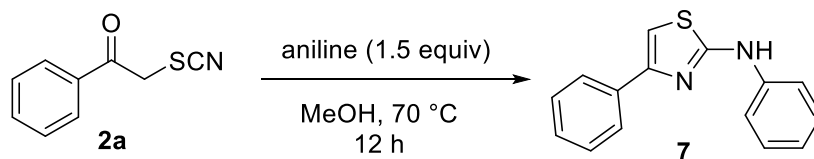
Melting Point: 140 °C

¹H NMR (500 MHz, DMSO): δ 8.04 (d, J = 7.95 Hz, 2H), 7.70 (t, J = 7.75 Hz, 1H), 7.58 (t, J = 7.75 Hz, 2H), 5.06 (s, 2H)

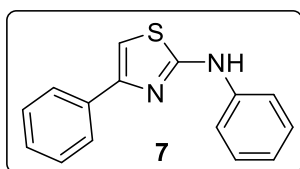
¹³C NMR (125 MHz, DMSO): δ 193.3, 154.6, 135.7, 134.3, 129.3, 128.9, 40.8

HRMS (ESI): calcd for $\text{C}_9\text{H}_8\text{N}_4\text{NaOS}$ m/z $[\text{M}+\text{Na}]$: 243.0311; found: 243.0310.

c) General procedure for the preparation of 7



Into a small 10 mL vial was placed 30 mg of **2a** (0.17 mmol) and 30 μ L of aniline (0.32 mmol, 1.9 eq.) in 0.30 mL methanol. The mixture was refluxed overnight after which the solvent was removed under reduced pressure and the residue columned directly using hexanes/ethyl acetate in 10:1 ratio to afford the product in 64% yield (42.7 mg).^[3]



N-4-diphenylthiazol-2-amine

Physical appearance: Yellow solid

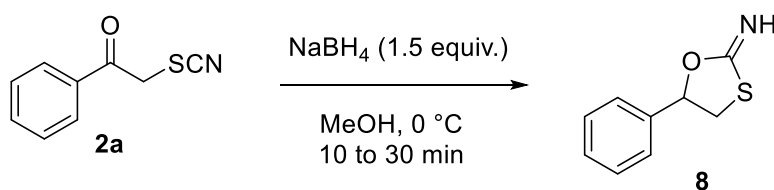
Melting Point: 109 °C

¹H NMR (500 MHz, CDCl₃): δ 7.84 (d, J = 7.55 Hz, 2H), 7.43 – 7.31 (m, 8H), 7.09 (t, J = 7.00 Hz, 1H), 6.79 (s, 1H)

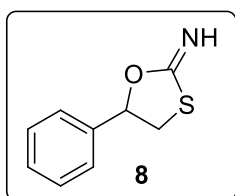
¹³C NMR (125 MHz, CDCl₃): δ 164.9, 150.2, 139.9, 133.8, 129.5, 128.7, 128.2, 126.1, 123.5, 118.5, 101.4

HRMS (ESI): calcd for C₁₅H₁₃N₂S m/z [M+H]: 253.0794; found: 253.0800.

d) General procedure for the preparation of 8



Into a 10 mL schlenk flask was loaded 80 mg of **2a** (0.45 mmol). The vessel was then degassed and loaded with 0.30 mL of anhydrous methanol and the vessel was lowered into an ice bath. Sodium borohydride (1.2 equiv., 21 mg) was then added portionwise. The reaction was monitored until the starting materials were completely reacted. Methanol was then removed under reduced pressure. Solvent extraction of the residue with dichlormethane and distilled water was carried out. The organic extracts were combined, dried with sodium sulfate and solvent subsequently removed under reduced pressure to directly afford the pure product in 79.3 mg (98% yield). ^[4]



5-phenyl-1,3-oxathiolan-2-imine

Physical appearance: Pale yellow solid

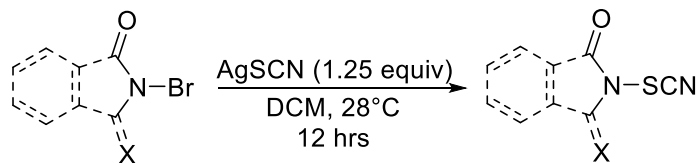
Melting Point: 90.6 °C

¹H NMR (500 MHz, CDCl₃): δ 7.37 – 7.33 (m, 5H), 5.57 – 5.53 (m, 1H), 3.61 – 3.57 (m, 1H), 3.44 – 3.40 (m, 1H)

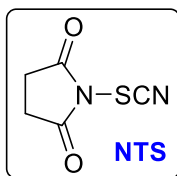
¹³C NMR (125 MHz, CDCl₃): δ 169.2, 137.1, 129.1, 128.9, 125.8, 84.4, 39.8

HRMS (ESI): calcd for C₉H₁₀NOS *m/z* [M+H]: 180.0478; found: 180.0480.

VI. General procedure for the preparation of NTS, NTP and NTSc & corresponding characterization data



Into a 50 mL flask was added 1 equiv. of *N*-bromosuccinimide, *N*-bromophthalimide or *N*-bromosuccinimide along with a magnetic stirrer. The solids were then dissolved in 25 mL of anhydrous dichloromethane after which silver thiocyanate (1.25 equiv.) was then added and the reaction allowed to stir overnight. Formation of light green to yellow precipitate (silver bromide) was observed after overnight stirring. The residue was filtered off and washed several times with DCM. The organic filtrate was consolidated and the dichloromethane removed under reduced pressure to yield the products as solids (near quantitative yield). Residual dichloromethane was removed under absolute vacuum (for approximately 10 mins) after which the products were packed into a glass vial, saturated with argon atmosphere and stored at 0 °C to -20 °C.



N-thiocyanosuccinimide

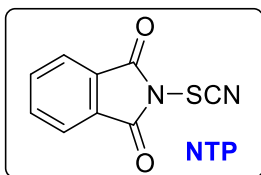
Physical appearance: White solid

Melting point: 85.6 °C

¹H NMR (500 MHz, CDCl₃): δ 2.72 (s, 4H)

¹³C NMR (125 MHz, CDCl₃): δ 178.0, 107.6, 29.6

HRMS (APCI): calcd for C₄H₅N₂S *m/z* [M+H]: 157.0066; found: 157.0065.



N-thiocyanophthalimide

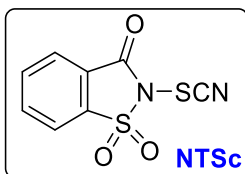
Physical appearance: Yellow powder

Melting point: 122.4 °C

¹H NMR (500 MHz, CDCl₃): δ 7.85 – 7.81 (m, 4H)

¹³C NMR (125 MHz, CDCl₃): δ 168.7, 134.3, 132.9, 122.9, 102.4

HRMS (APCI): calcd for C₉H₅N₂O₂S *m/z* [M+H]: 205.0066; found: 205.0070.



N-thiocyanosaccharin

Physical appearance: While solid

Melting point: 136.0 °C

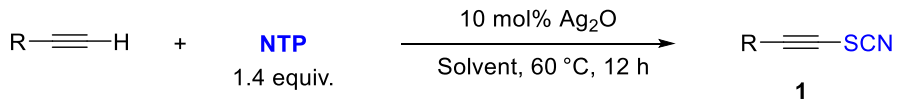
¹H NMR (500 MHz, CDCl₃): δ 8.04 – 7.99 (m, 2H), 7.98 – 7.96 (m, 1H), 7.94 – 7.91 (m, 1H)

¹³C NMR (125 MHz, CDCl₃): δ 159.9, 139.4, 135.6, 134.7, 127.5, 125.1, 120.9, 102.4

HRMS (APCI): calcd for C₁₂H₄N₂O₂S *m/z* [M]: 239.9988; found: 239.9989.

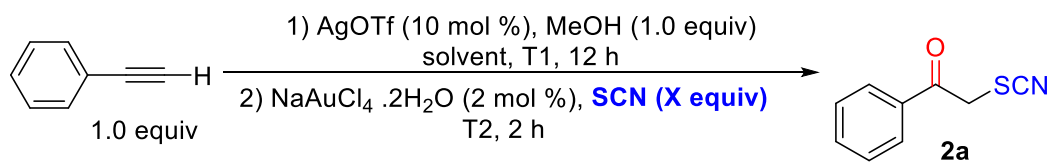
VII. Screening Tables

Table S1: Finetuning solvents, yield and SCN source for thiocyanation of alkynes



Entry ^[a]	R	SCN source (eq.)	Solvent	Yield ^[b]
1	2-Cl-Ph	NTS (1.20)	THF	43
2	4-Ethyl-Ph	NTS (1.20)	THF	58
3	2-Cl-Ph	NTS (1.20)	1,2 DCE	<2
4	2-Cl-Ph	NTS (1.20)	1,4 dioxane	Unidentified product
5	2-Cl-Ph	NTS (1.20)	Acetone	messy
6	2-Cl-Ph	NTS (1.20)	DCM	Unidentified product
7	2-Cl-Ph	NTS (1.20)	Methanol	Unidentified product
8	2-Cl-Ph	NTS (1.40)	THF	71
9	2-Cl-Ph	NTSc (1.40)	THF	Unidentified product
10	2-Cl-Ph	NTP (1.40)	THF	86

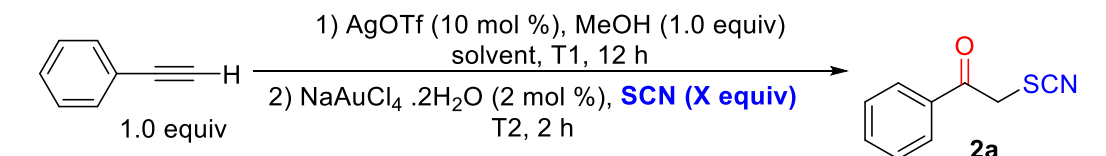
[a] Unless otherwise stated, reaction is conducted using 0.2 mmol of substrate, SCN source (1.20 eq.) and catalyst (10 mol %) in 0.30 ml of solvent under specified conditions. **[b]** Isolated yield.

Table S2: Finetuning solvents for hydrothiocyanation of alkynes

Index	[Ag]	Co-catalyst	additive	NTS	Yield 2a (%) ^a	Yield 3a (%) ^a
1	AgOTf	\	\	1.2 equiv.	26	\
2	AgOTf	\	H ₂ O (0.1 mL)	1.2 equiv.	<2	\
3	AgOTf	\	MeOH (6.5 equiv.)	1.2 equiv.	<2	\
4	AgOTf	\	AgClO ₄ (1.0 equiv.)	1.2 equiv.	<2	\
5	AgOTf	\	MeOH (6.5 equiv.)	\	\	62
6	AgOTf	NaAuCl ₄	MeOH (6.5 equiv.)	1.2 equiv.	42	\
7	AgOTf	LiAuCl ₄	MeOH (6.5 equiv.)	1.2 equiv.	38	\
8	AgOTf	JohnPhos AuCl	MeOH (6.5 equiv.)	1.2 equiv.	<2	\
9	AgOTf	AuBr ₃	MeOH (6.5 equiv.)	1.2 equiv.	30	\
10	\	NaAuCl ₄	MeOH (6.5 equiv.)	1.2 equiv.	<2	\
11 ^b	AgOTf	NaAuCl ₄	MeOH (6.5 equiv.)	1.2 equiv.	50	\

[a] Isolated yield. [b] AgOTf & MeOH were allowed to react with alkyne for 12 h before the addition of NaAuCl₄ and NTS.

Table S3: Finetuning solvents for hydrothiocyanation of alkynes



1) AgOTf (10 mol %), MeOH (1.0 equiv)
solvent, T1, 12 h
2) NaAuCl₄ · 2H₂O (2 mol %), SCN (X equiv)
T2, 2 h

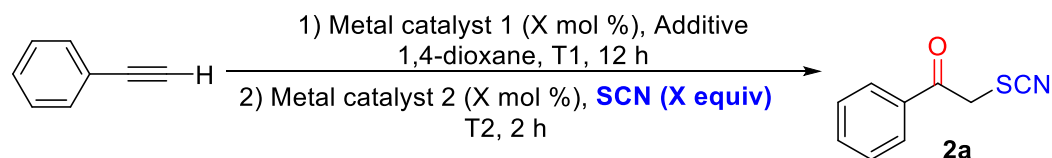
1.0 equiv

2a

Index ^[a]	Additive (equiv)	Solvent	Reagent (eq)	T1 (°C)	T2 (°C)	% Yield ^[b]
1	MeOH (1.5)	1,4 dioxane	NTS (2.00)	65	RT	63.5
2	MeOH (1.0)	THF	NTS (1.00)	65	80	33.5
3	MeOH (1.0)	ACN	NTS (1.00)	65	80	21
4	MeOH (1.0)	DMSO	NTS (1.00)	65	80	NR
5	MeOH (1.0)	DMF	NTS (1.00)	65	80	NR
6	MeOH (1.0)	ethylene glycol	NTS (1.00)	65	80	NR

[a] Unless otherwise stated, reaction is conducted using 0.2 mmol of substrate, SCN source (1.20 eq.) and catalyst (10 mol %) in 0.30 ml of THF under specified conditions. **[b]** Isolated yield.

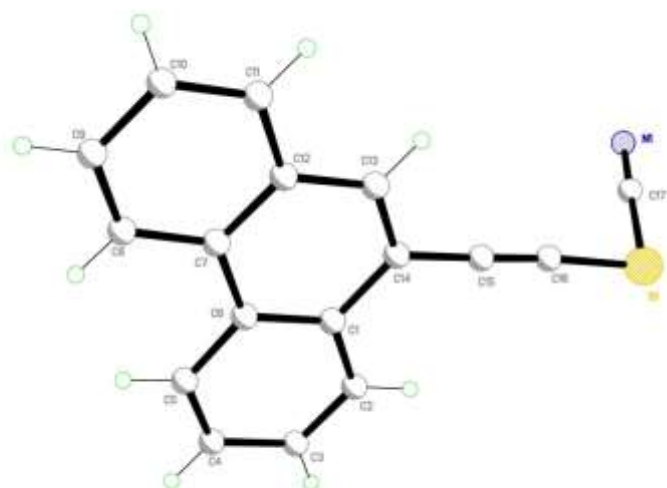
Table S4: Finetuning catalyst and additive ratio for hydrothiocyanation of alkynes



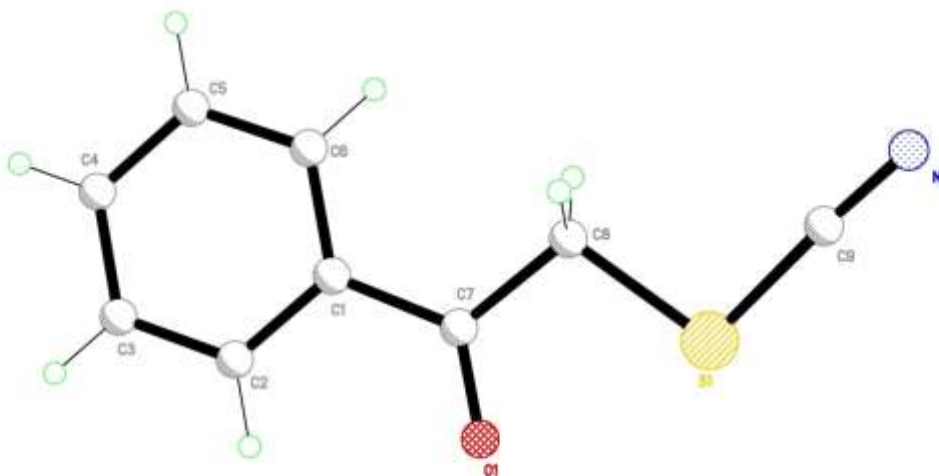
Index ^[a]	Metal Catalyst 1 (mol %)	Metal Catalyst 2 (mol %)	Additive (equiv)	Phenylace(eq)	Reagent (eq)	T1 (°C)	T2 (°C)	% Yield ^[b]
1	AgOTf (10)		MeOH (1.0)	2.0	NTS (1.00)	60	60	side products
2	NaAuCl ₄ .2H ₂ O(2)		MeOH (1.0)	2.0	NTS (1.00)	60	60	side products
3	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	MeOH (1.0): H ₂ O (0.3)	1.0	NTS (1.50)	60	RT	48.2
4	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	MeOH (1.2): H ₂ O (0.3)	1.0	NTS (1.50)	60	RT	41.4
5	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	MeOH (2.0): H ₂ O (0.6)	1.0	NTS (1.50)	60	RT	66.7
6	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	MeOH (2.5): H ₂ O (0.6)	1.0	NTS (1.50)	60	RT	75.0
7	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	MeOH (7.0)	1.0	NTS (1.50)	60	RT	33.2
8	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	H ₂ O (7.0)	1.0	NTS (1.50)	60	RT	NR
9	AgOTf (15)	NaAuCl ₄ .2H ₂ O(2)	MeOH (2.0): H ₂ O (0.6)	1.0	NBS (1.50)	60	RT	Messy
10	AgOTf (15)	N/A	MeOH (2.0): H ₂ O (0.6)	1.0	NBS (1.50)	60	RT	N.R.
11	N/A	N/A	N/A	1.0	NBS (1.50)	N/A	RT	N.R.
12	N/A	NaAuCl ₄ .2H ₂ O(2)	N/A	1.0	NBS (1.50)	N/A	RT	N.R.

[a] Unless otherwise stated, reaction is conducted using 0.2 mmol of substrate, SCN source (1.20 eq.) and catalyst (10 mol %) in 0.30 ml of THF under specified conditions. **[b]** Isolated yield.

VIII. Crystal Data

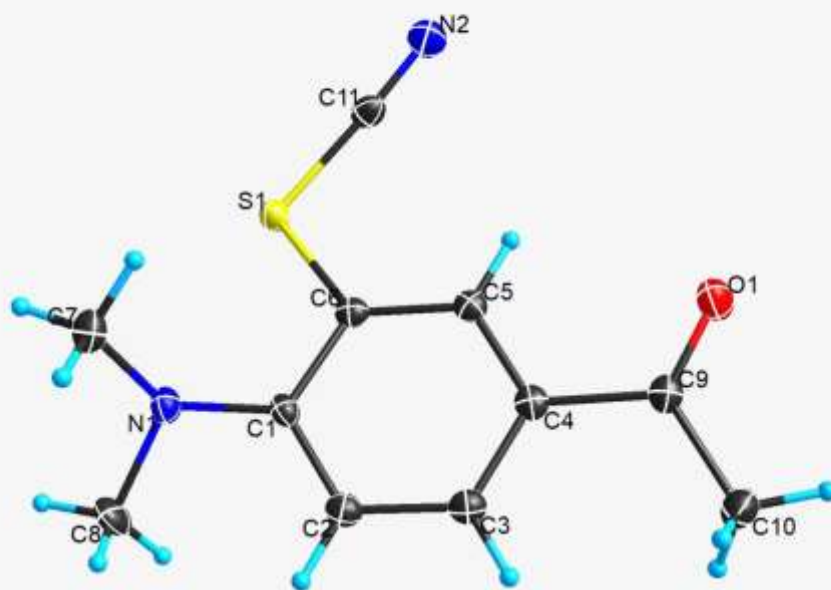


Crystal data	
CCDC number	1866145
Chemical formula	C ₁₇ H ₉ NS
M _r	259.31
Crystal system	Monoclinic
Crystal system, space group	P2 ₁ /n
Temperature (K)	100(2)
a, b, c (Å)	a = 12.9956(8)
	b = 5.4342(4)
	c = 17.9421(10)
V (Å ³)	1219.99(14)
Z	4
Analytical Wavelength	0.71073
Crystal size (mm)	0.554 x 0.209 x 0.206
Absorption coefficient (mm ⁻¹)	0.247



Crystal data

CCDC number	1866142
Chemical formula	C ₉ H ₇ NOS
M _r	177.22
Crystal system	Monoclinic
Crystal system, space group	P2 ₁ /c
Temperature (K)	100(2)
a, b, c (Å)	a = 10.6135(4)
	b = 5.5409(2)
	c = 14.9229(5)
V (Å ³)	845.23(5)
Z	4
Analytical Wavelength	1.54178
Crystal size (mm)	0.589 x 0.117 x 0.056
Absorption coefficient (mm ⁻¹)	2.963



Crystal data

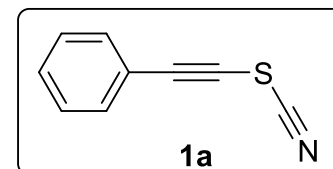
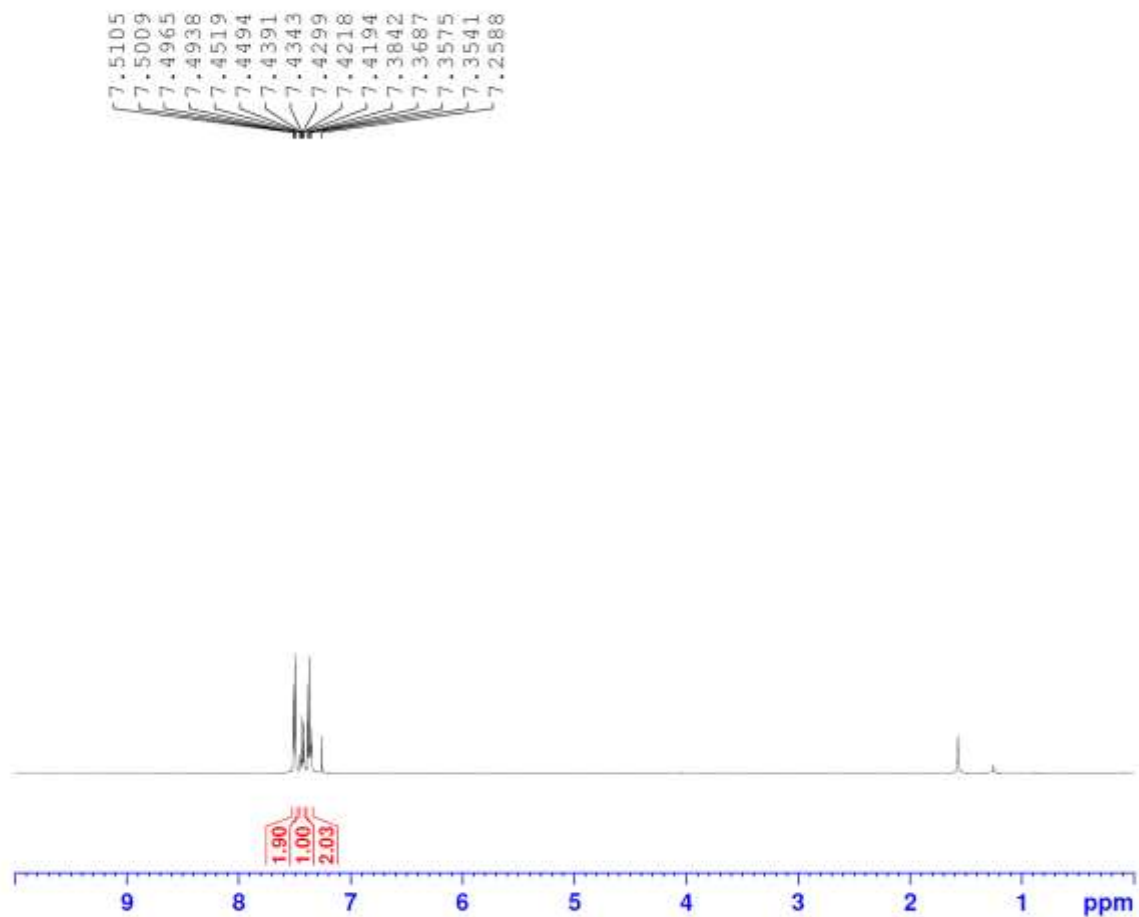
CCDC number	1866144
Chemical formula	C ₁₁ H ₁₂ N ₂ OS
M _r	220.29
Crystal system	Orthorhombic
Crystal system, space group	Pbca
Temperature (K)	100(2)
a, b, c (Å)	a = 7.1790(2)
	b = 17.3113(4)
	c = 17.4130(4)
V (Å ³)	2164.05(9)
Z	8
Analytical Wavelength	1.54178
Crystal size (mm)	0.294 x 0.266 x 0.108
Absorption coefficient (mm ⁻¹)	2.446

IX. References

- [1] R. Adams, H. B. Bramlet, F. H. Tendick, *Journal of the American Chemical Society* **1920**, *42*, 2369-2374.
- [2] S. Vorona, T. Artamonova, Y. Zevatskii, L. Myznikov, *Synthesis* **2014**, *46*, 781-786.
- [3] I. Lagoja, C. Pannecouque, G. Griffioen, S. Wera, V. M. Rojasdelaparra, A. Van Aerschot, *European Journal of Pharmaceutical Sciences* **2011**, *43*, 386-392.
- [4] F. R. Bisogno, A. Cuetos, I. Lavandera, V. Gotor, *Green Chemistry* **2009**, *11*, 452-454.

X. NMR spectra

P192-1-55



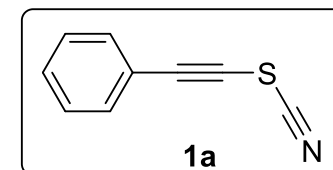
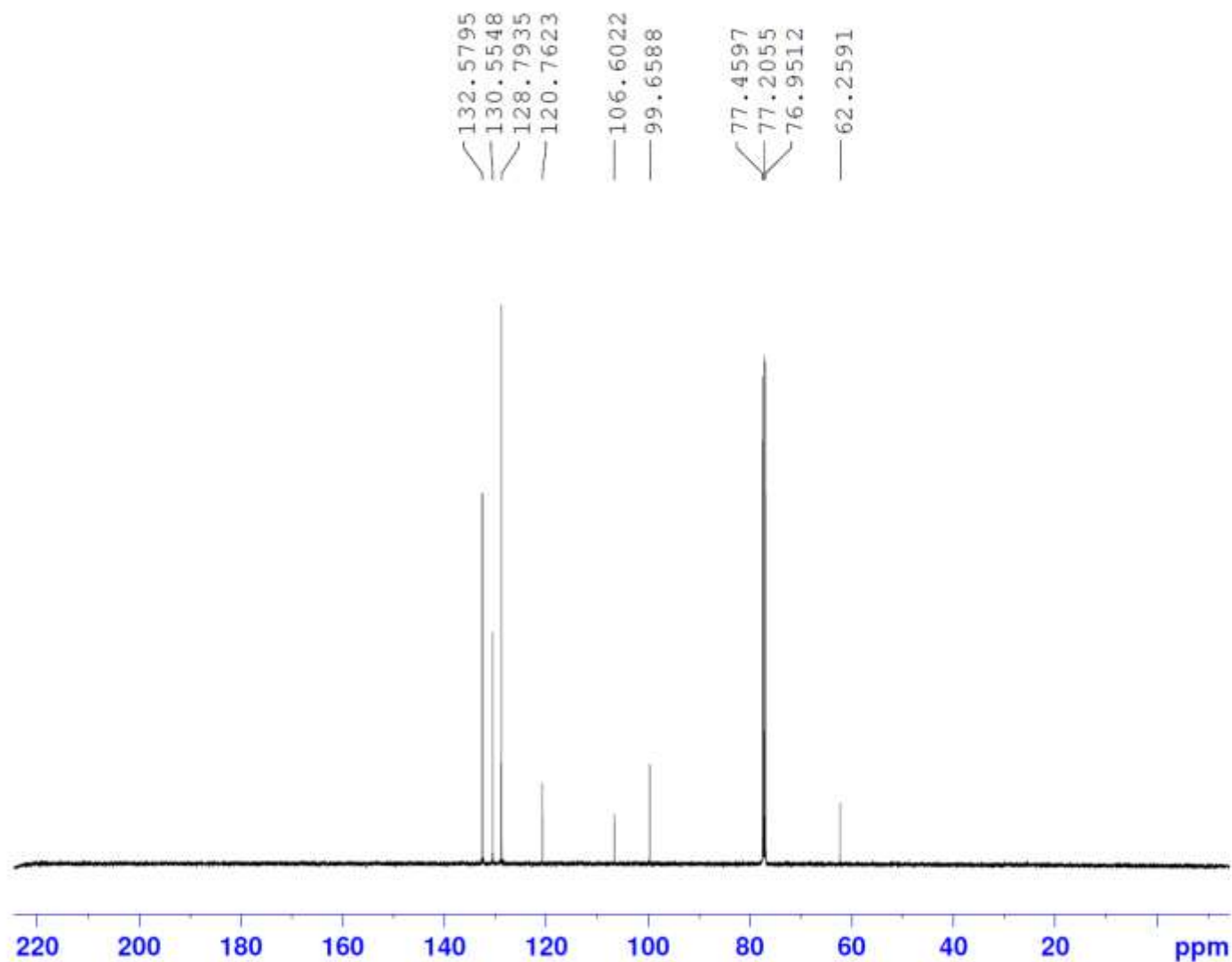
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PULPROG   zg30
TD        32768
SOLVENT   CDCl3
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SWH       10330.578 Hz
FIDRES    0.315264 Hz
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RG         228.1
DW        46.400 usec
DE         6.00 usec
TE        296.7 K
D1        1.00000000 sec
TD0        1

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PL1        0.25 dB
SFO1       500.1330885 MHz

F2 - Processing parameters
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P192-1-55



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EXPNO 2
PROCNO 1

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FIDRES 0.458222 Hz
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D1 2.00000000 sec
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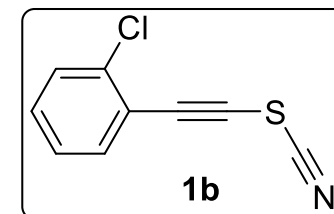
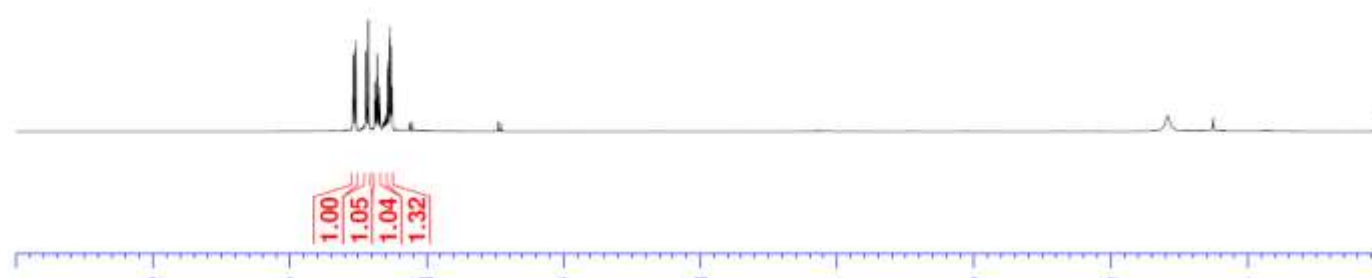
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NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

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WDW EM
SSB 0
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P146-11

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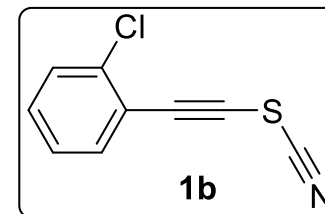
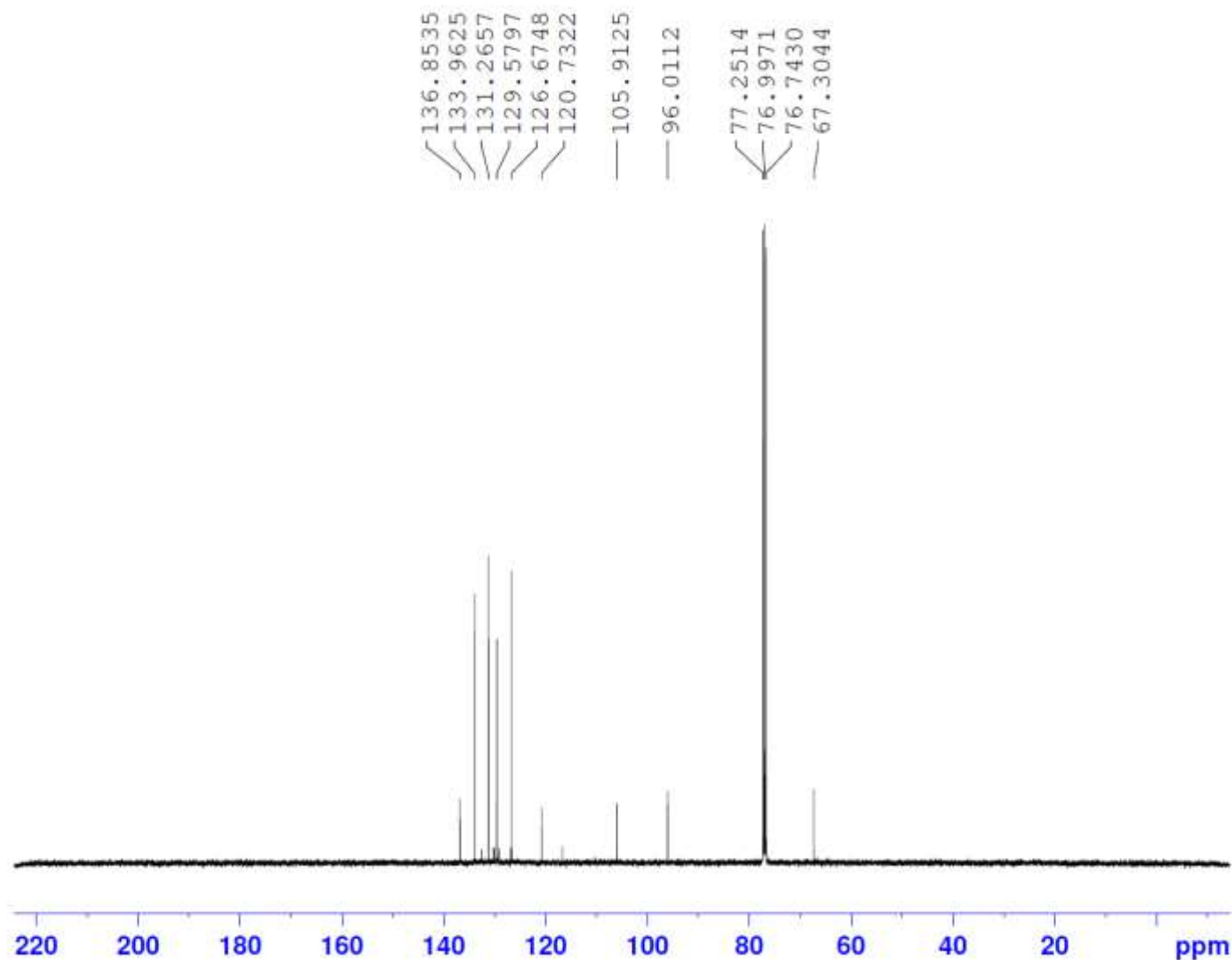
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FIDRES 0.315264 Hz
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TE 296.5 K
D1 1.00000000 sec
TD0 1

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P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

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P146-11



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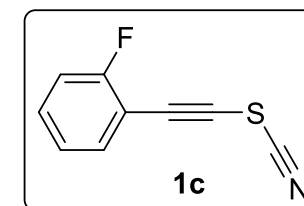
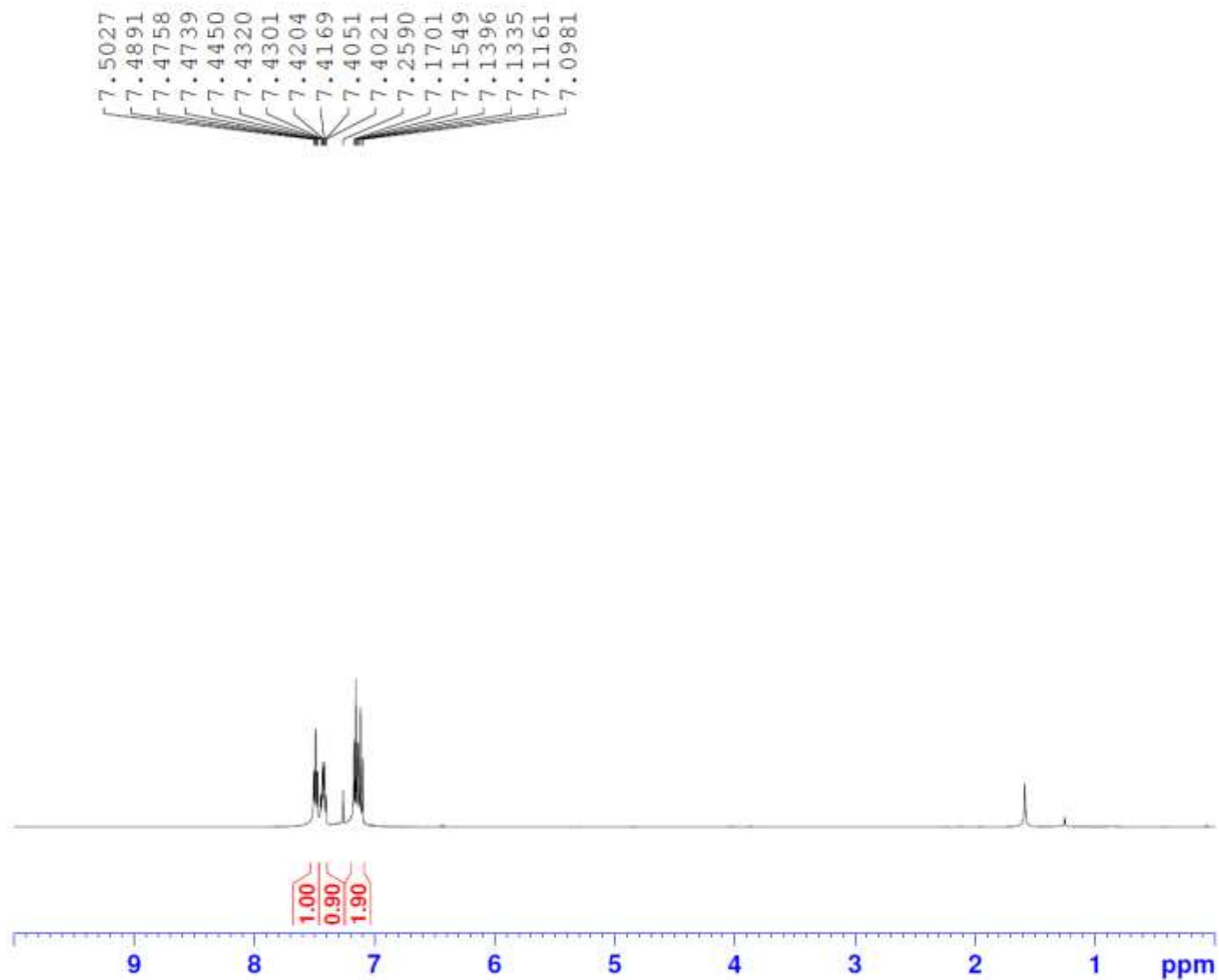
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 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 296.8 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
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P186-6



Current Data Parameters

NAME sjy3011
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

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Time 15.47
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PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
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TE 298.0 K
D1 1.00000000 sec
TD0 1

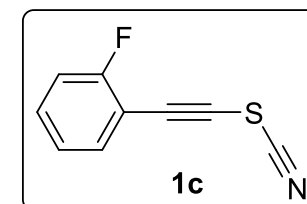
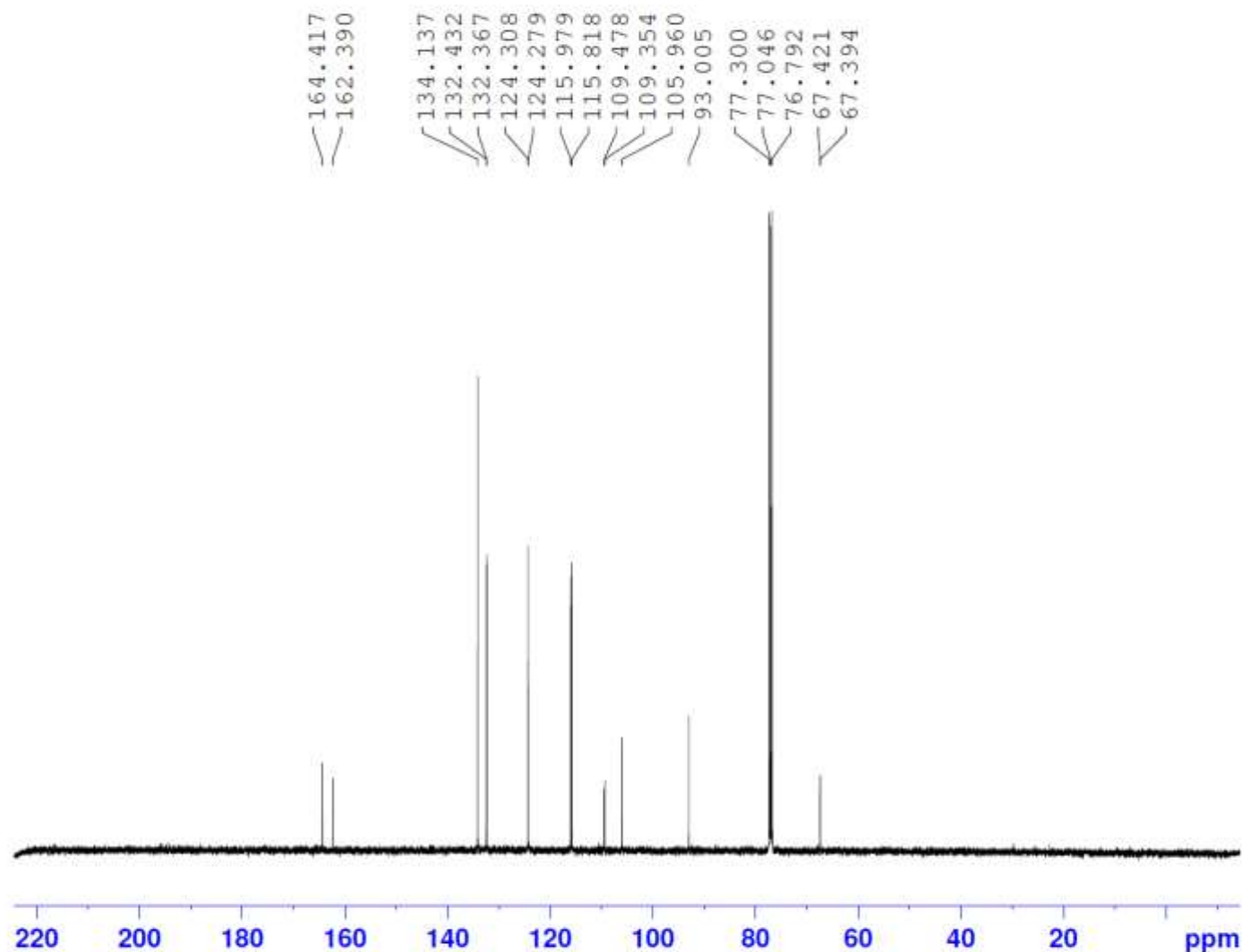
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PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

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LB 0.30 Hz
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P185-6



Current Data Parameters
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PROCNO 1

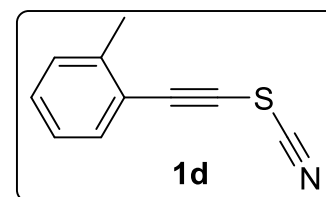
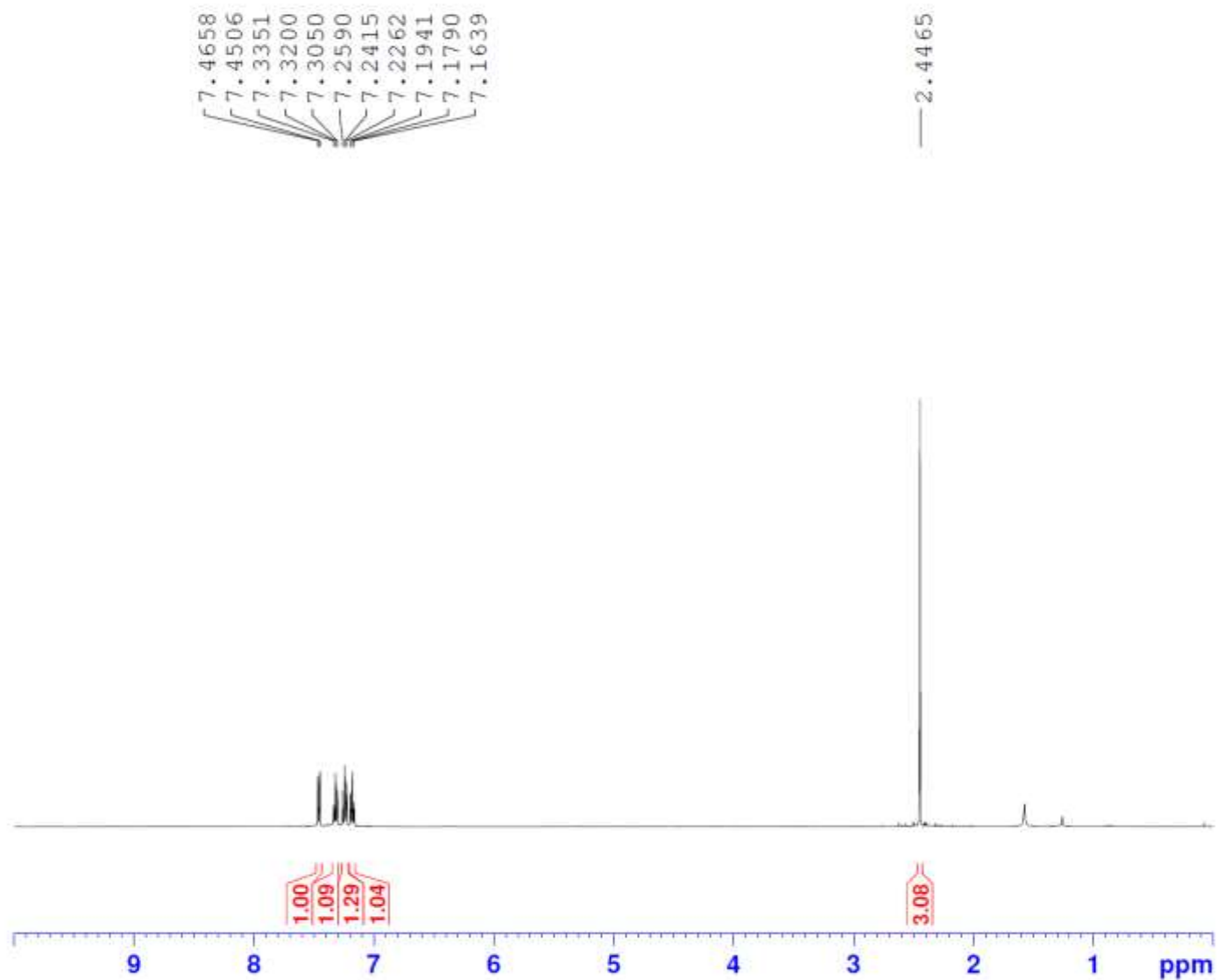
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SOLVENT CDC13
NS 803
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SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
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LB 1.00 Hz
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P192-8



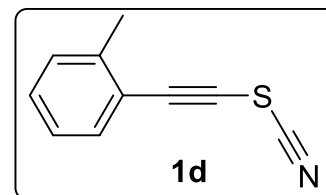
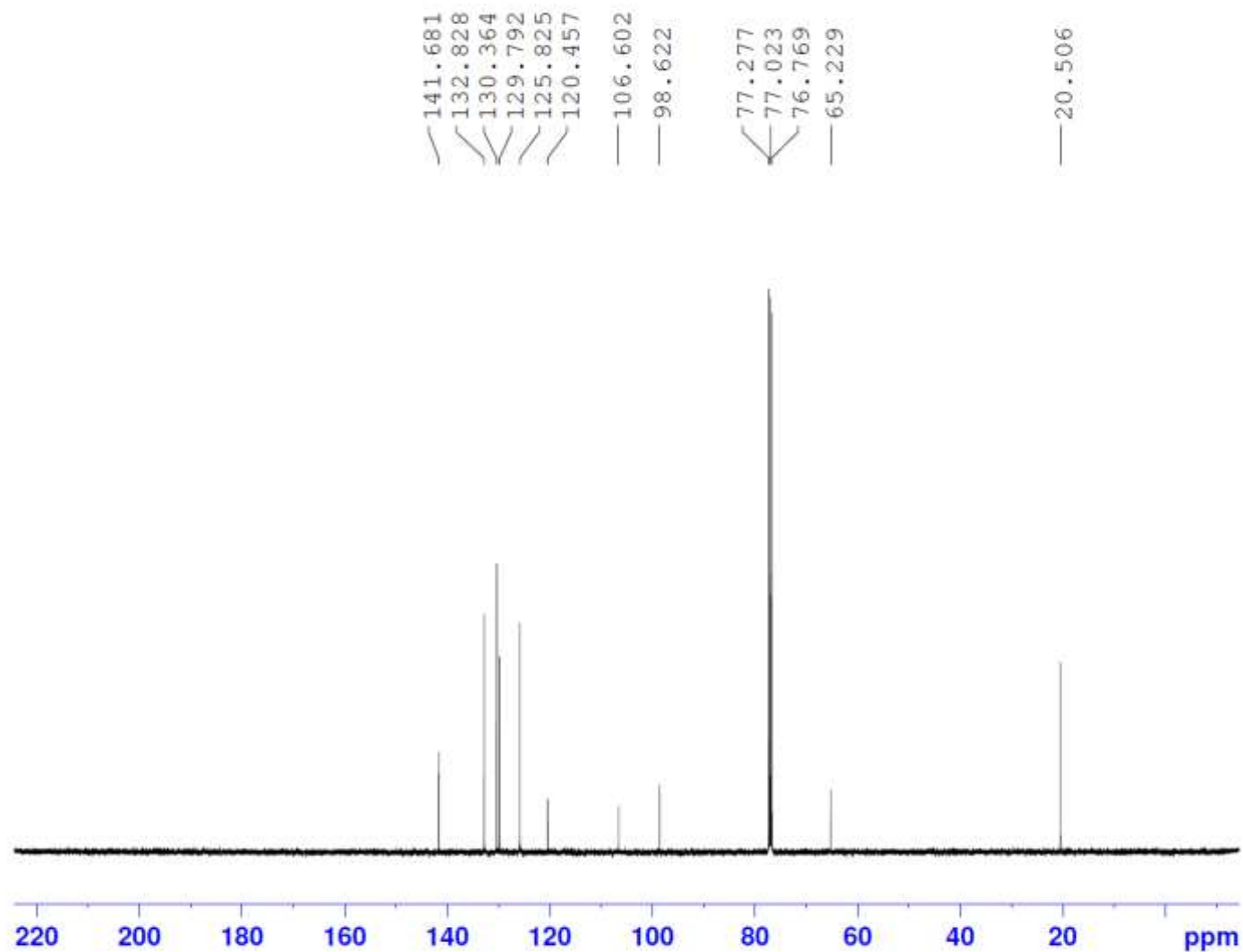
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PROCNO 1

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FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
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P192-8



Current Data Parameters
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PROCNO 1

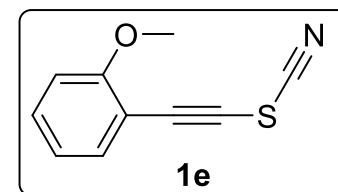
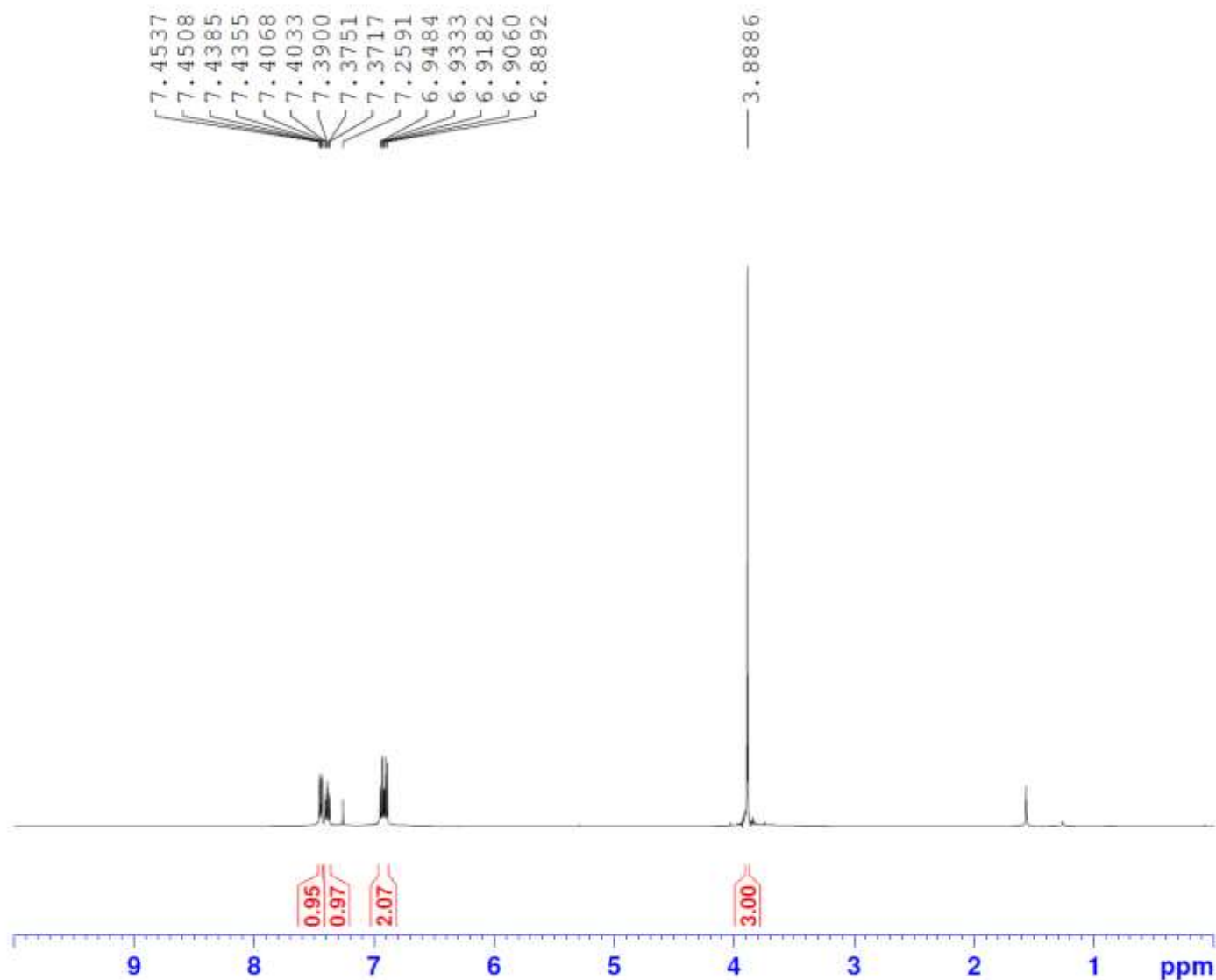
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SOLVENT CDC13
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DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 300.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
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P185-9



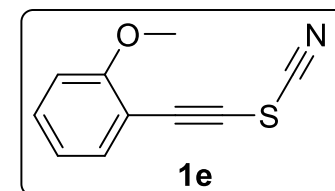
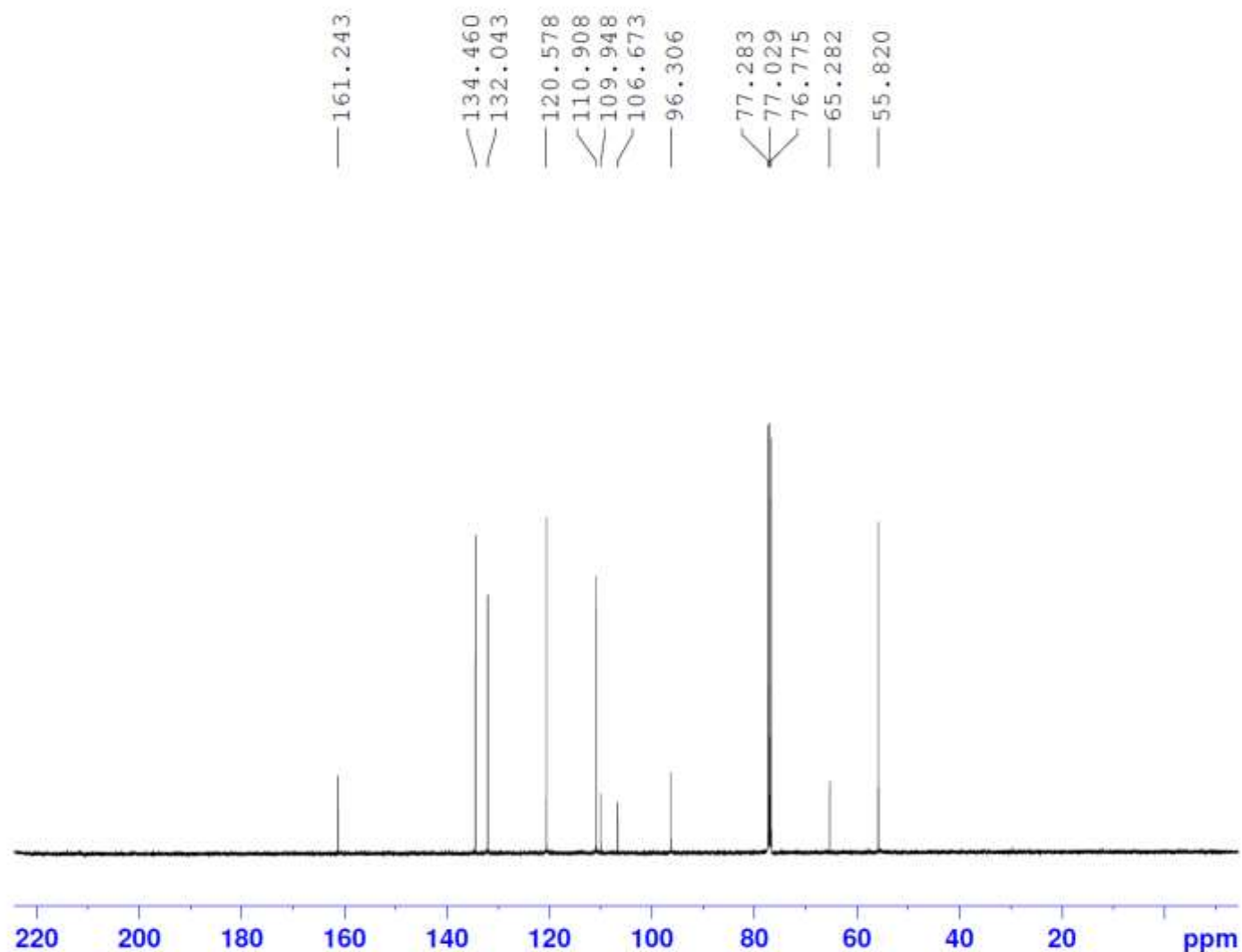
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 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 303.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

P185-9



Current Data Parameters
NAME sjy0112
EXPNO 2
PROCNO 1

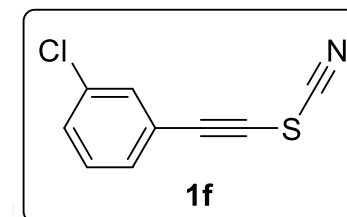
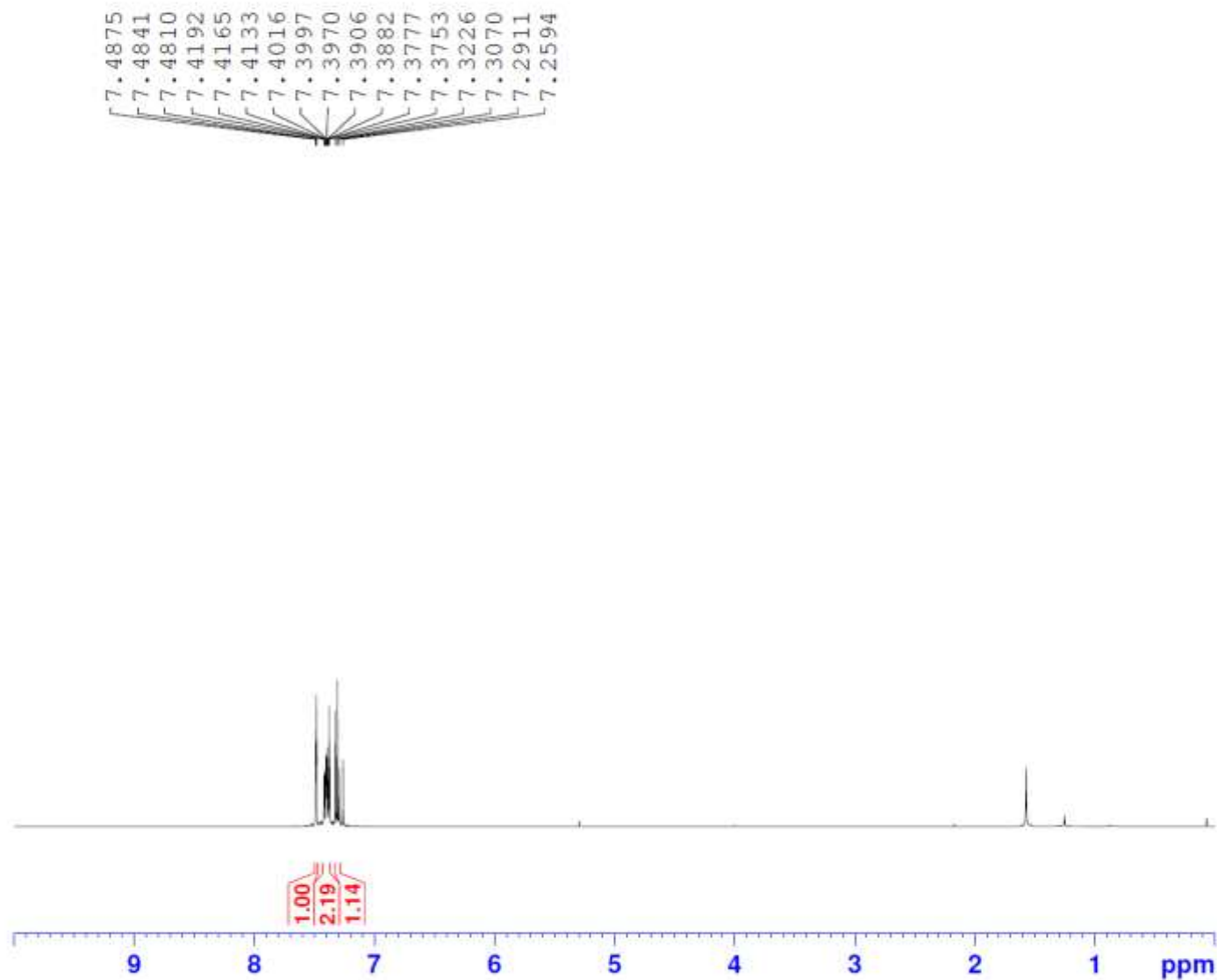
F2 - Acquisition Parameters
Date_ 20171201
Time 14.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1066
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 303.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P183-5



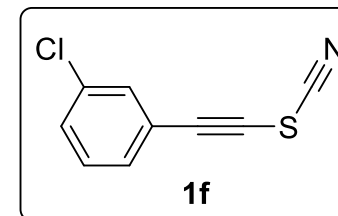
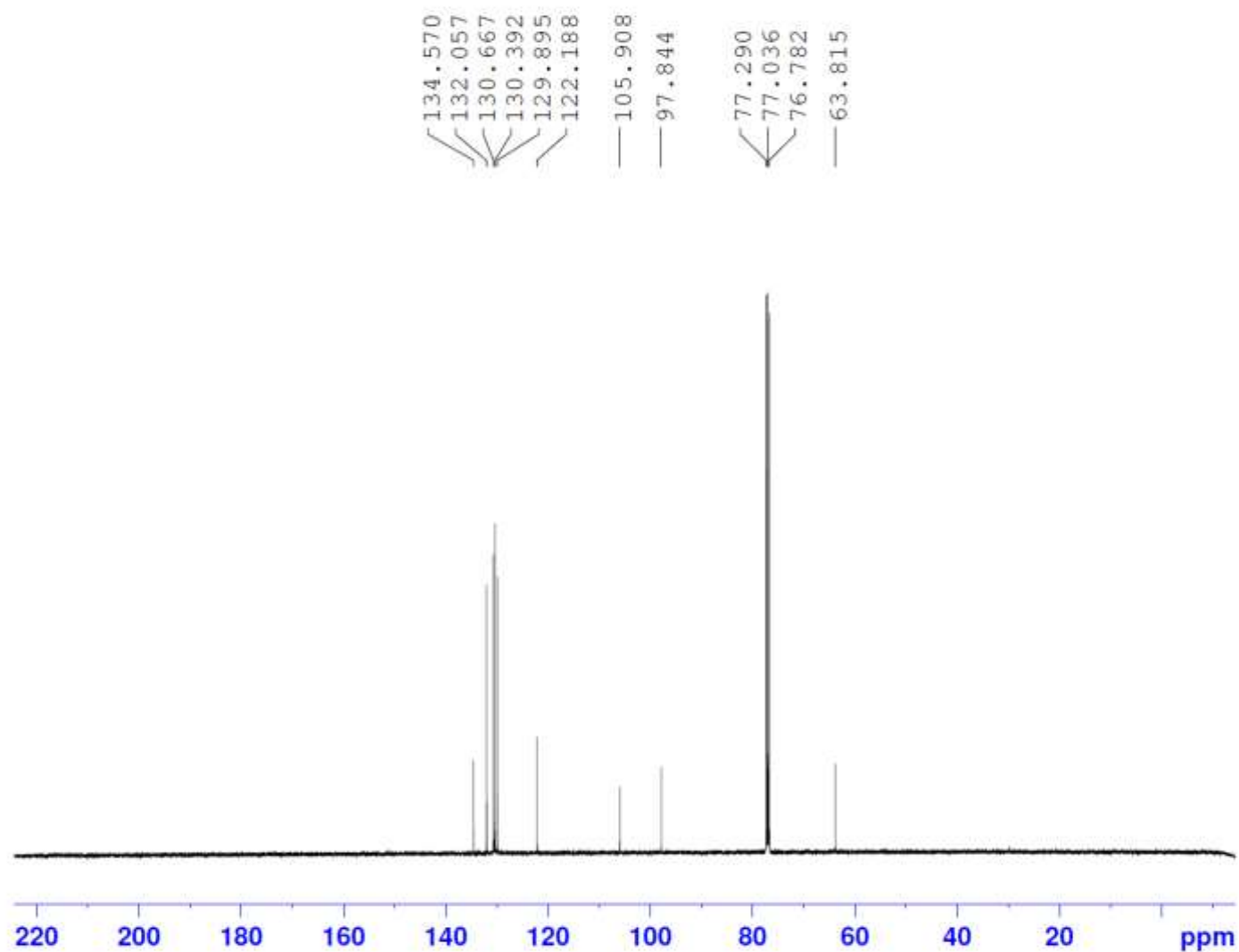
NAME sjy1912
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171219
Time 15.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P183-5



Current Data Parameters
NAME sjy1912
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171219
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1356
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

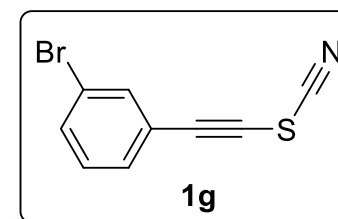
===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P183-4

7.6500
7.6469
7.6440
7.5719
7.5555
7.5524
7.4370
7.4212
7.2599
7.2445
7.2288

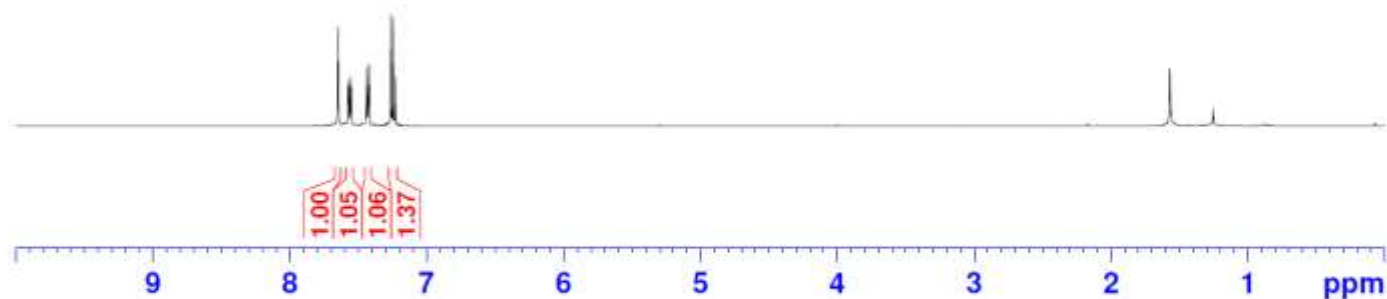


NAME sjy1412
EXPNO 4
PROCNO 1

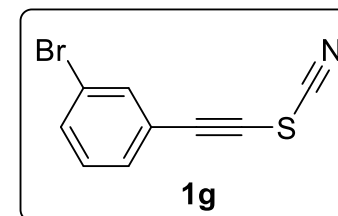
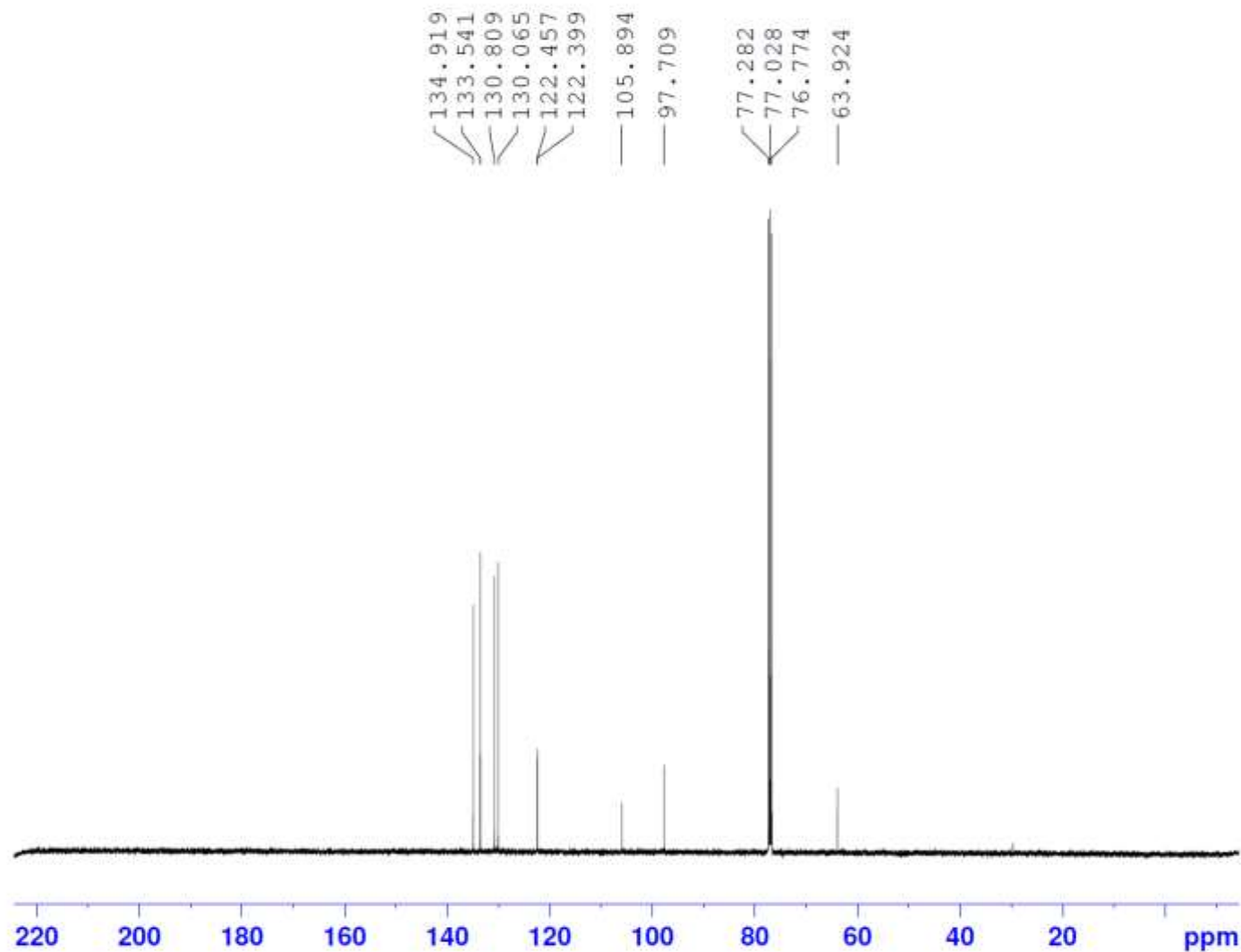
F2 - Acquisition Parameters
Date_ 20171214
Time 15.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 362
DW 48.400 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



P183-4



Current Data Parameters

NAME sjy1412
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171214
Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1029
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

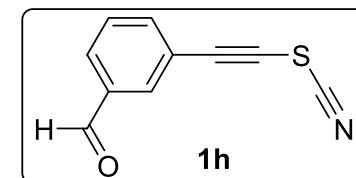
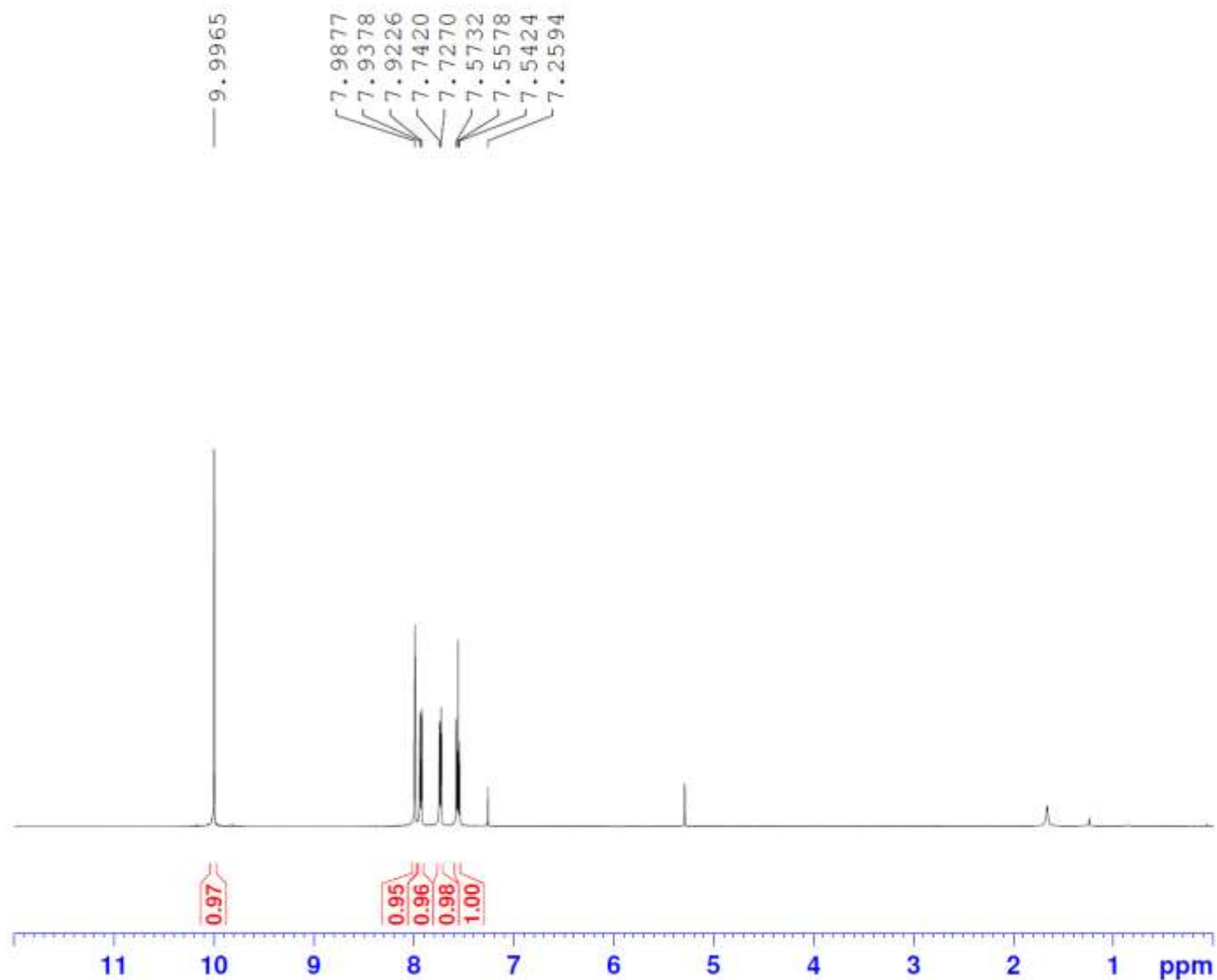
===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P191-11



Current Data Parameters

NAME sjy2710
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171027
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 143.7
DW 48.400 usec
DE 6.00 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

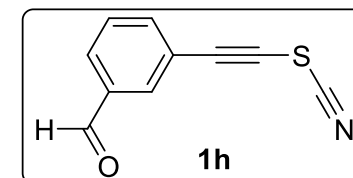
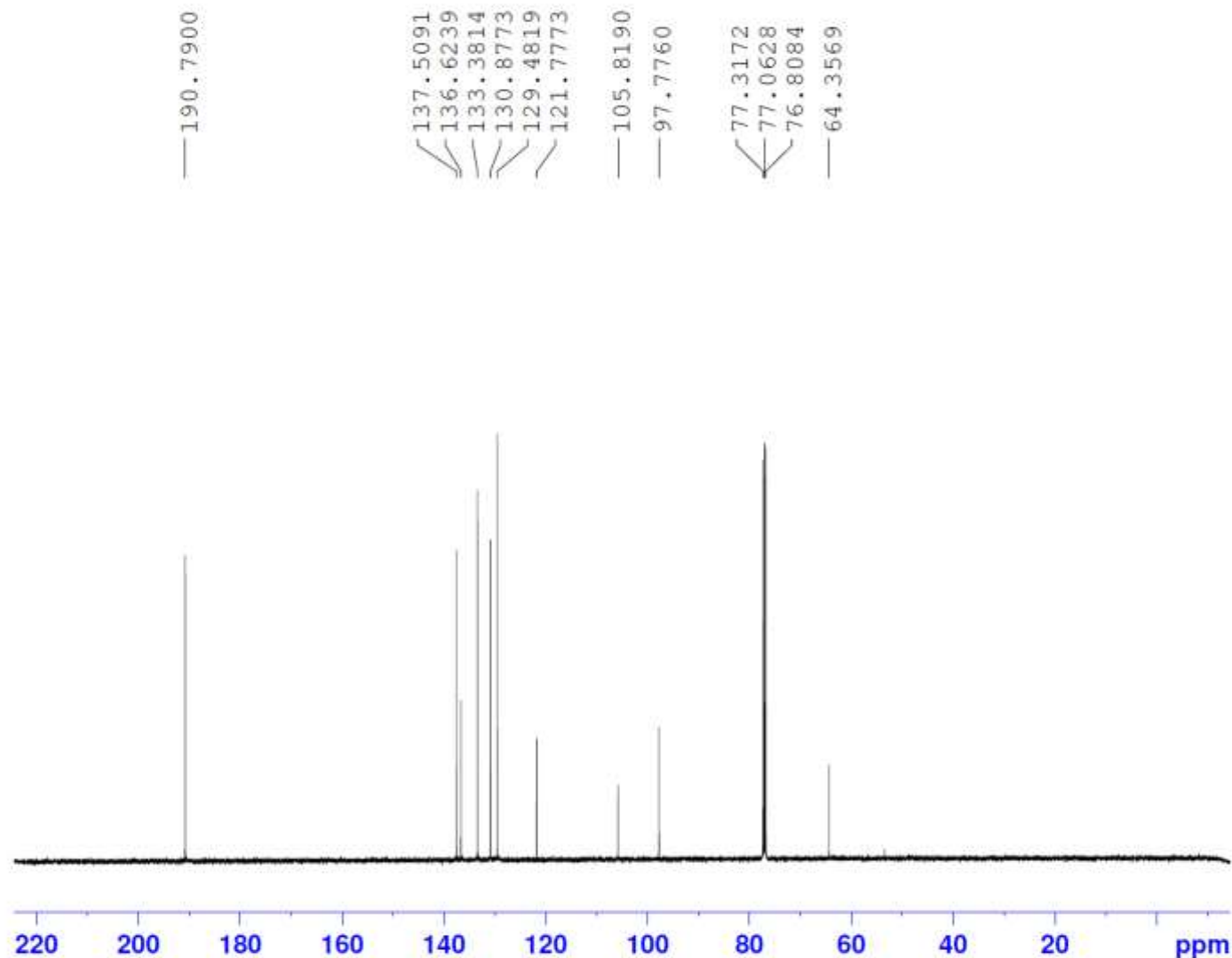
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P191-11



Current Data Parameters
NAME sjy2710
EXPNO 2
PROCNO 1

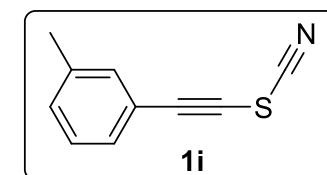
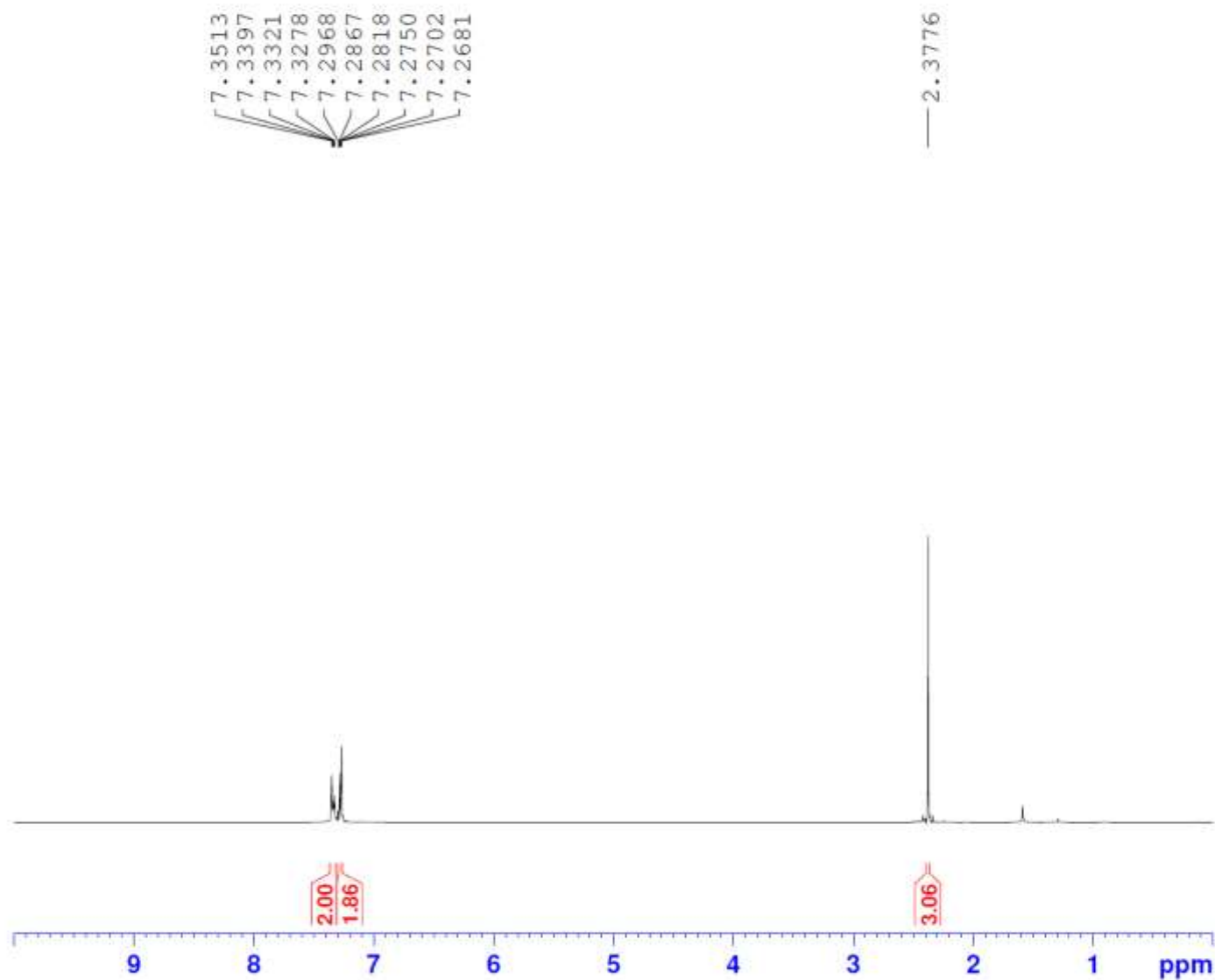
F2 - Acquisition Parameters
Date_ 20171027
Time 16.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 543
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P185-8



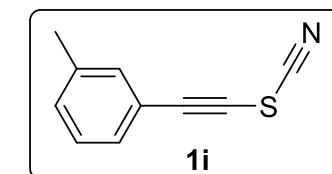
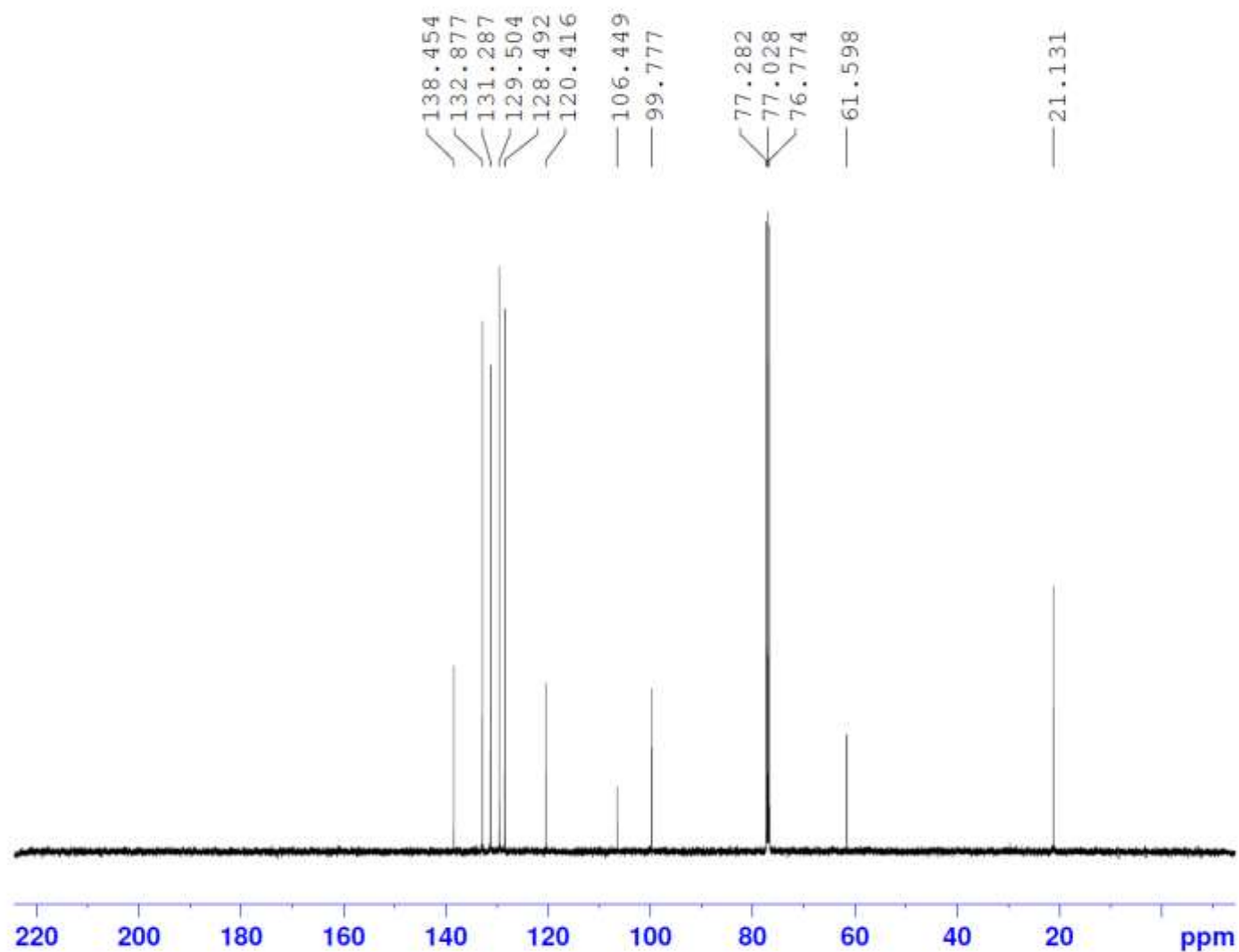
Current Data Parameters
 NAME sjy3011
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171130
 Time 14.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 304.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

P185-8



Current Data Parameters
 NAME sjy3011
 EXPNO 2
 PROCNO 1

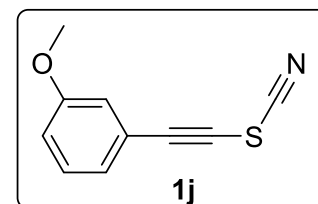
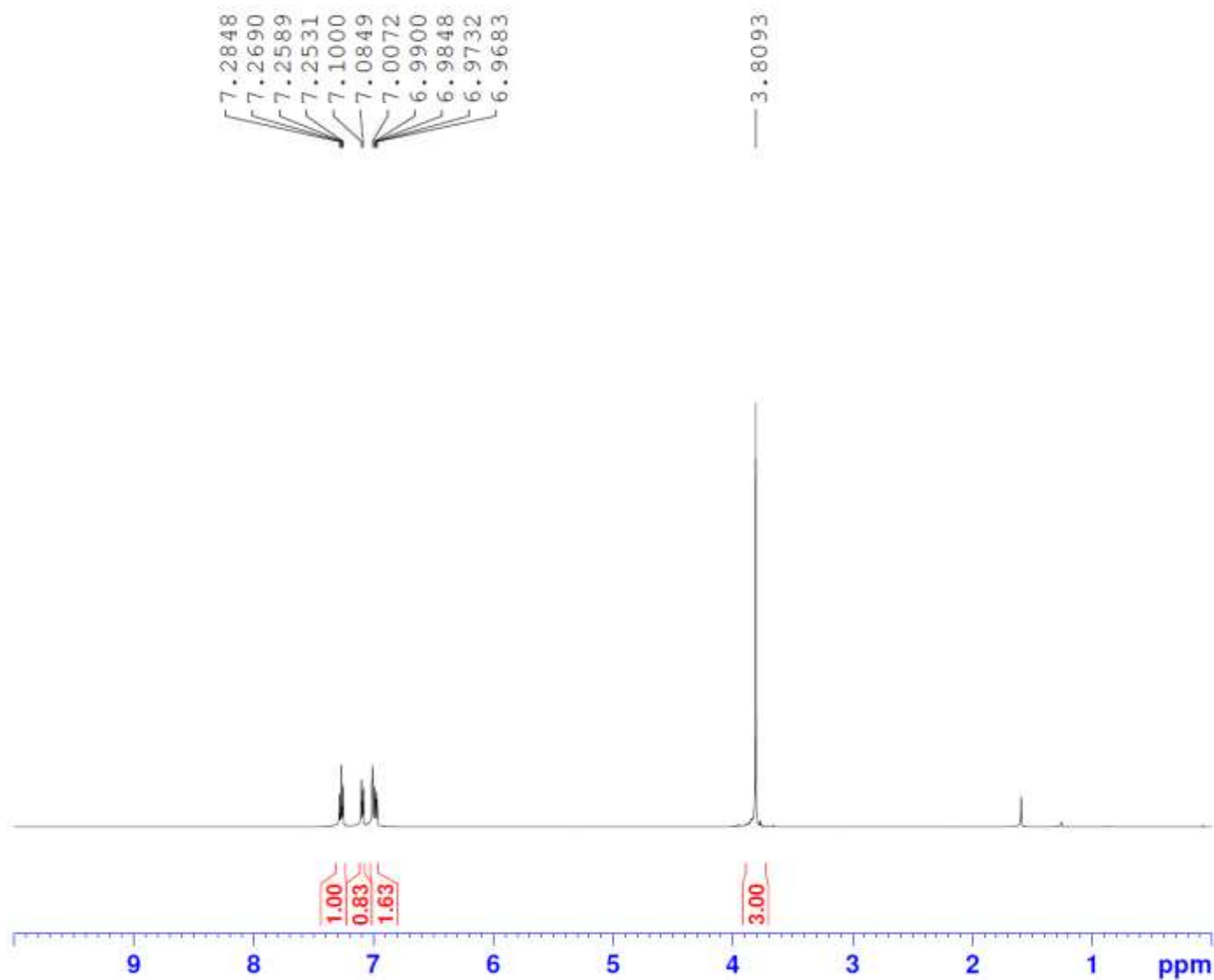
F2 - Acquisition Parameters
 Date_ 20171130
 Time 14.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 641
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 305.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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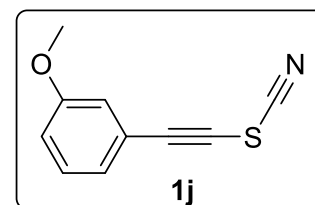
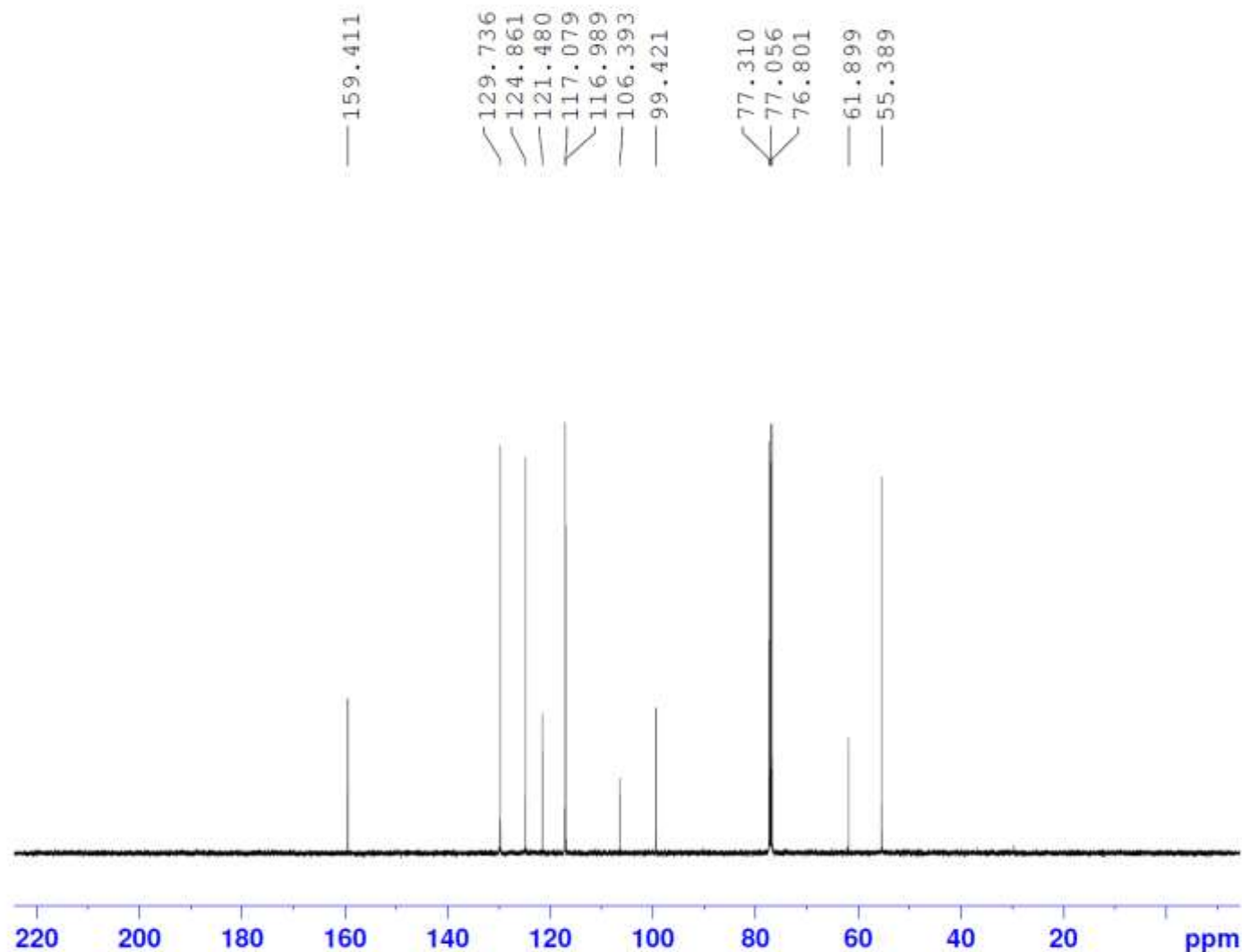
Current Data Parameters
 NAME sjy1412
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171214
 Time 14.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

P183-2



Current Data Parameters
NAME sjyl412
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171214
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 604
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

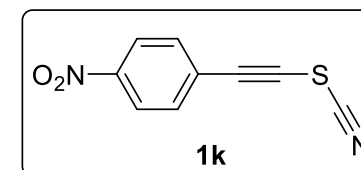
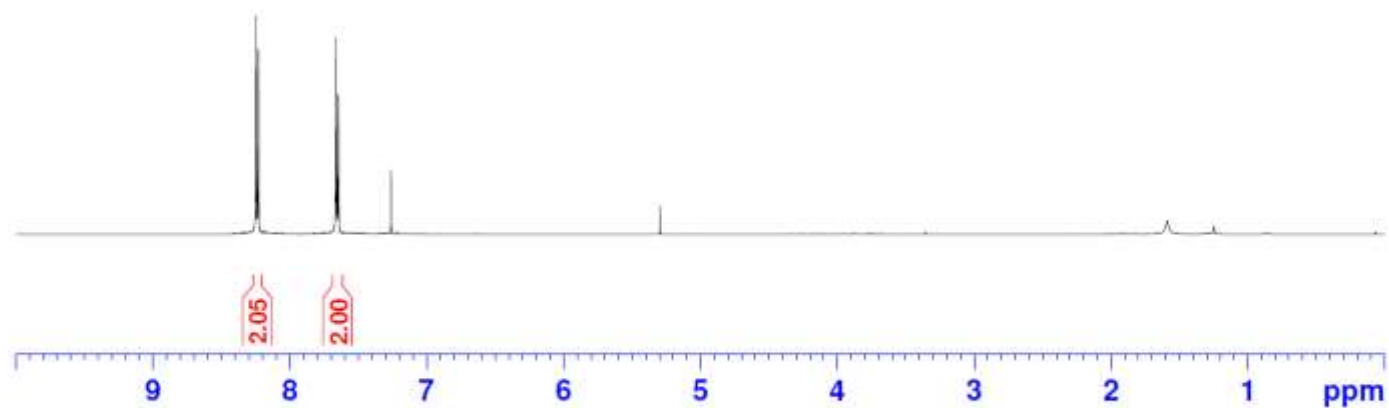
===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P191-16

8.2464
8.2289
7.6626
7.6445
7.2594



Current Data Parameters

NAME sjy3010
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171030
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

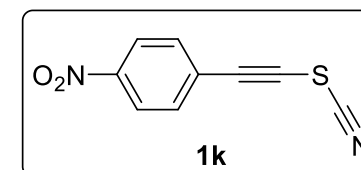
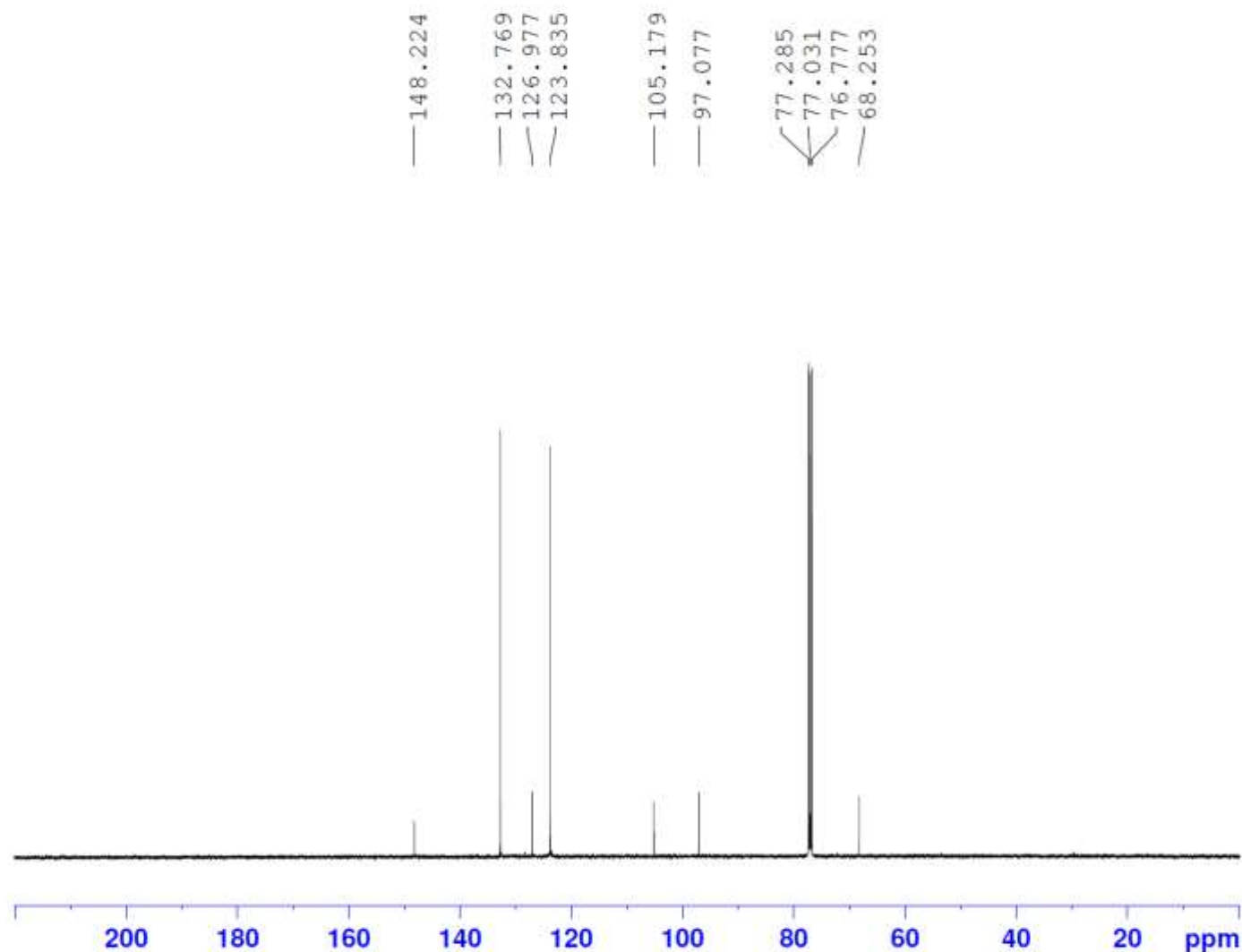
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Current Data Parameters

NAME sjy3010
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171030
Time 15.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 798
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 301.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

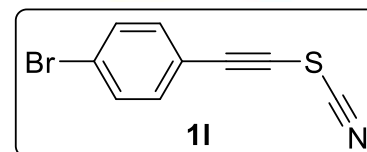
===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P199-4 4-Br

7.5231
7.5065
7.3681
7.3514
7.2595



Current Data Parameters

NAME sjy0310
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

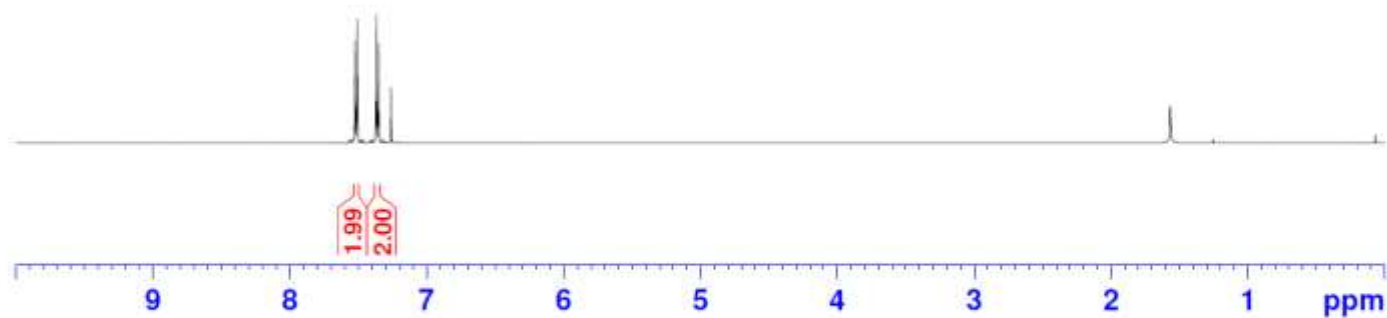
Date_ 20171003
Time 14.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

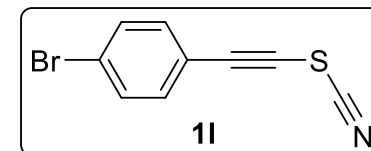
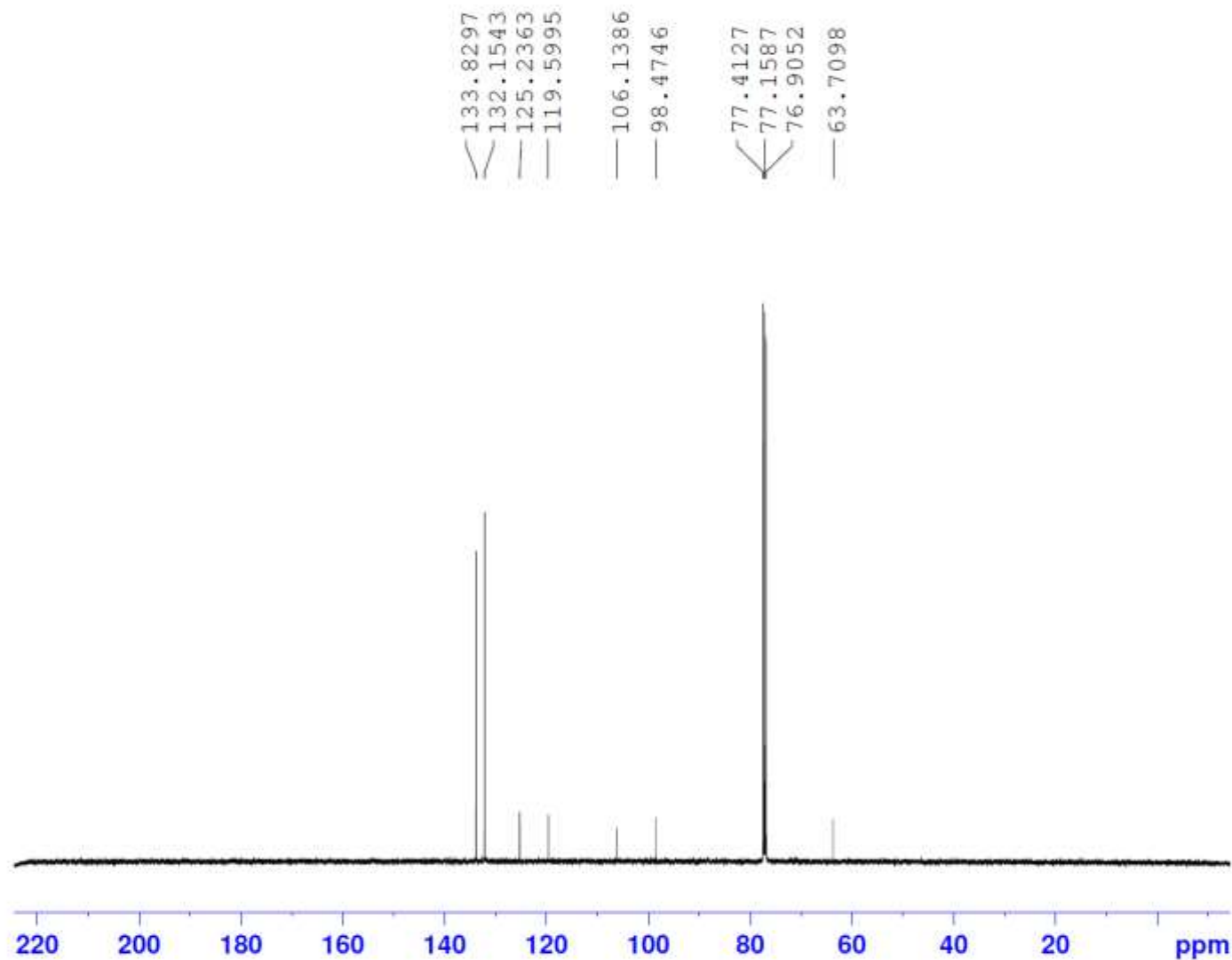
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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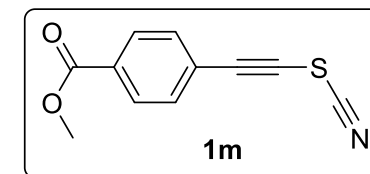
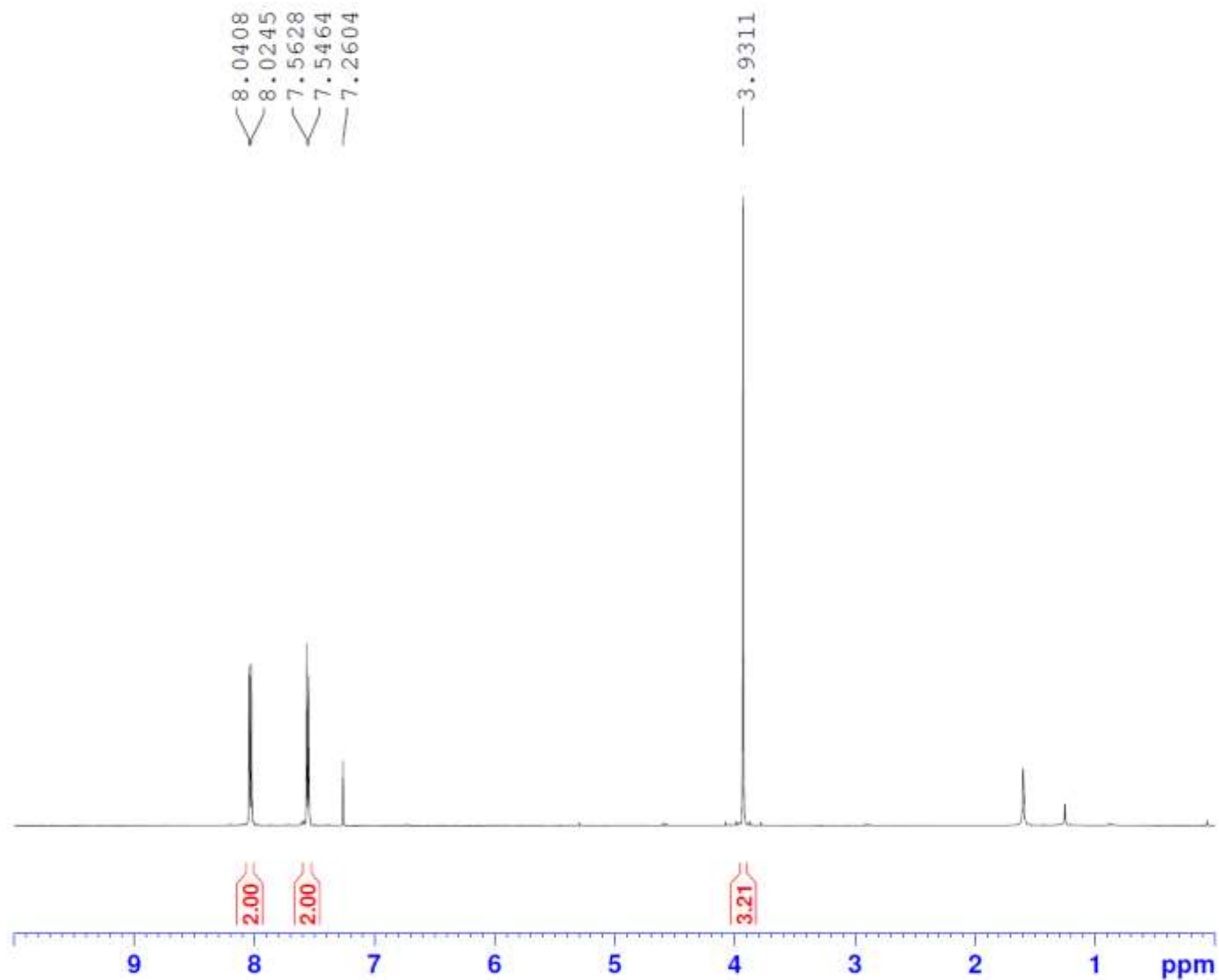
Current Data Parameters
 NAME sjy0310
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171003
 Time 14.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 778
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 297.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577719 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters

NAME sjy1810
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

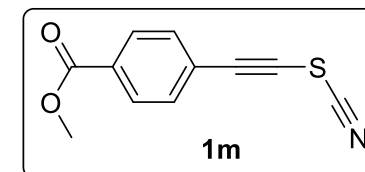
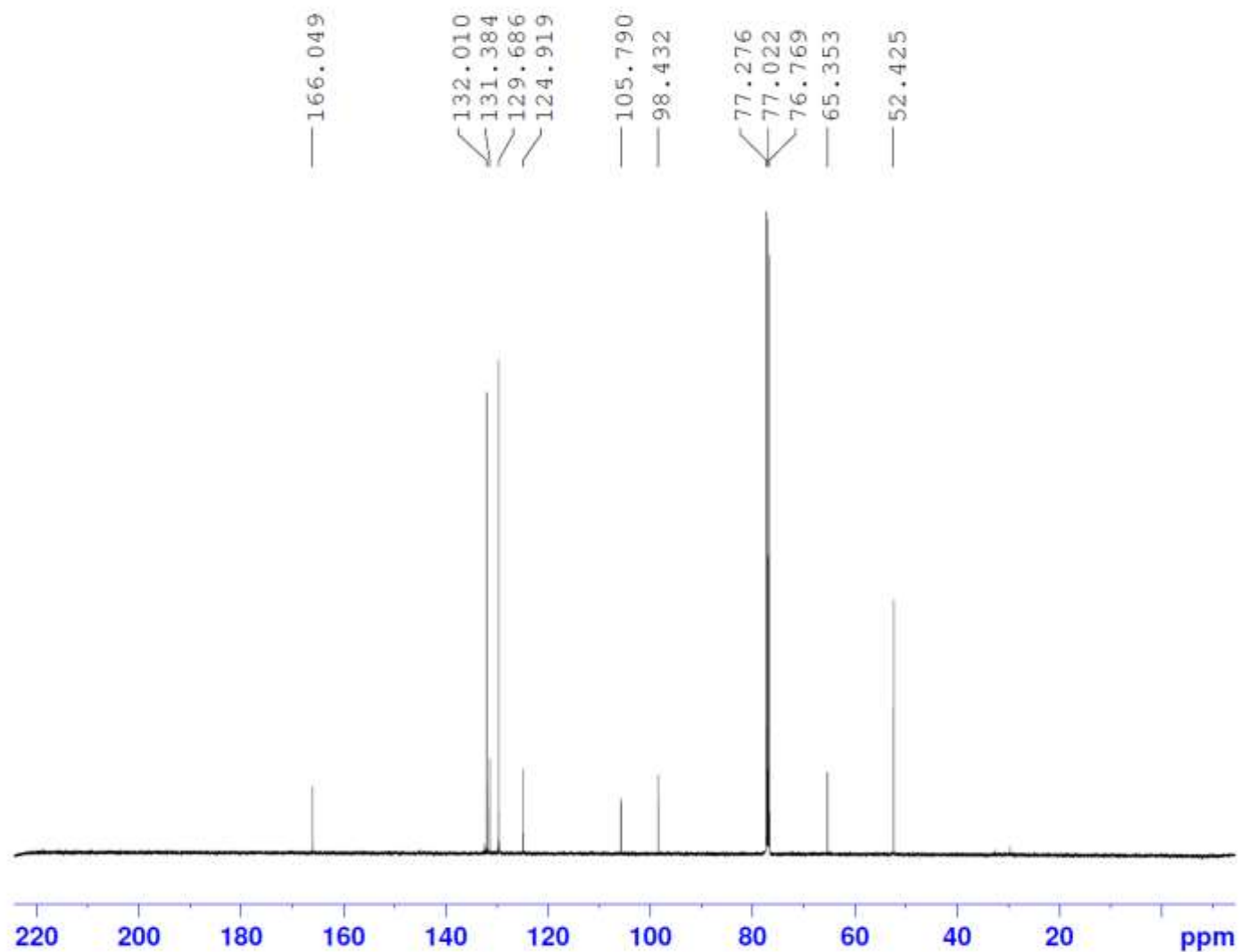
Date_ 20171018
Time 8.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters

NAME sjy1810
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171018
Time 8.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2500
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

===== CHANNEL f1 =====

NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

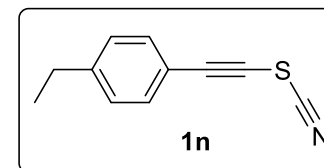
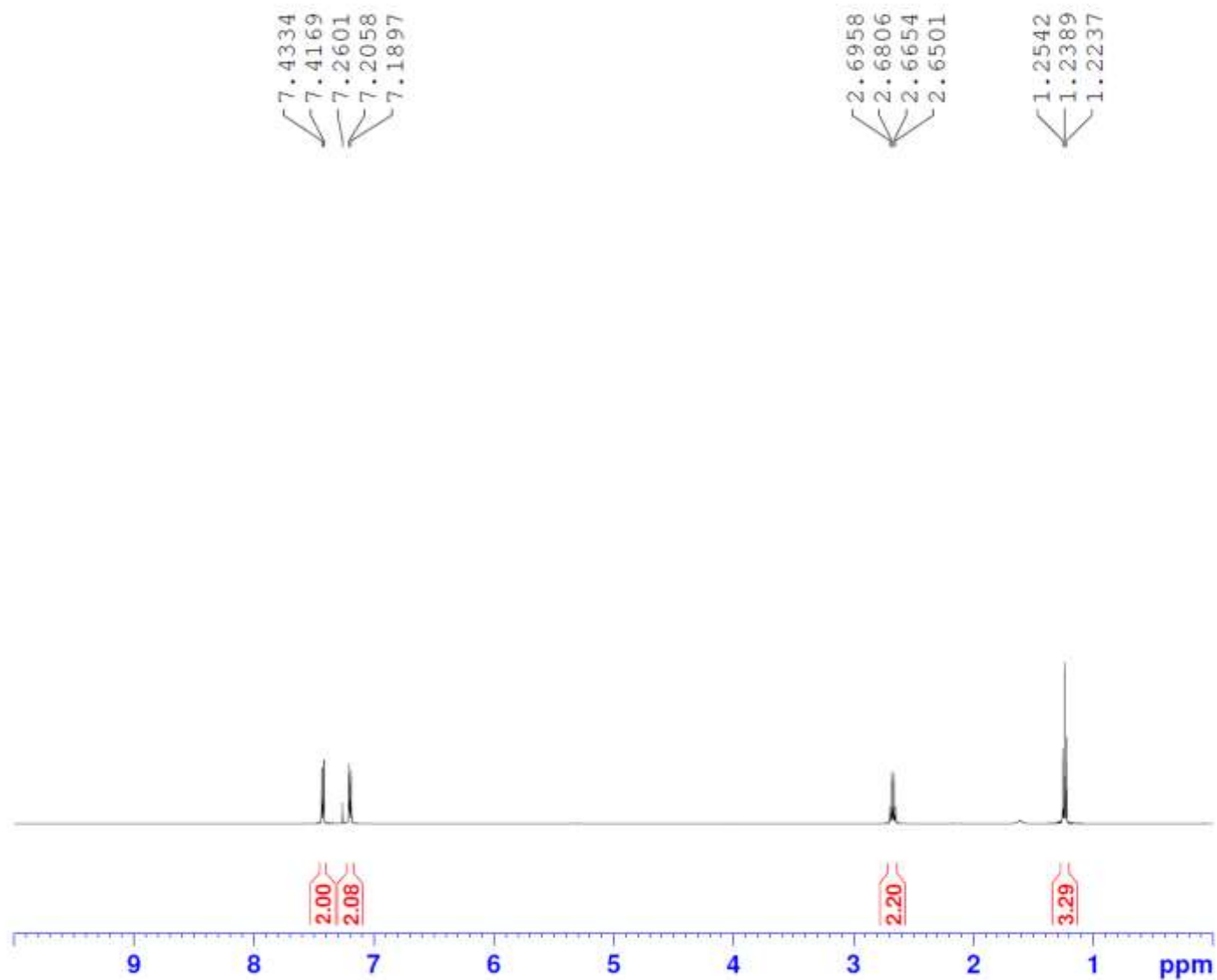
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P146-10



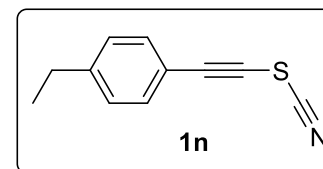
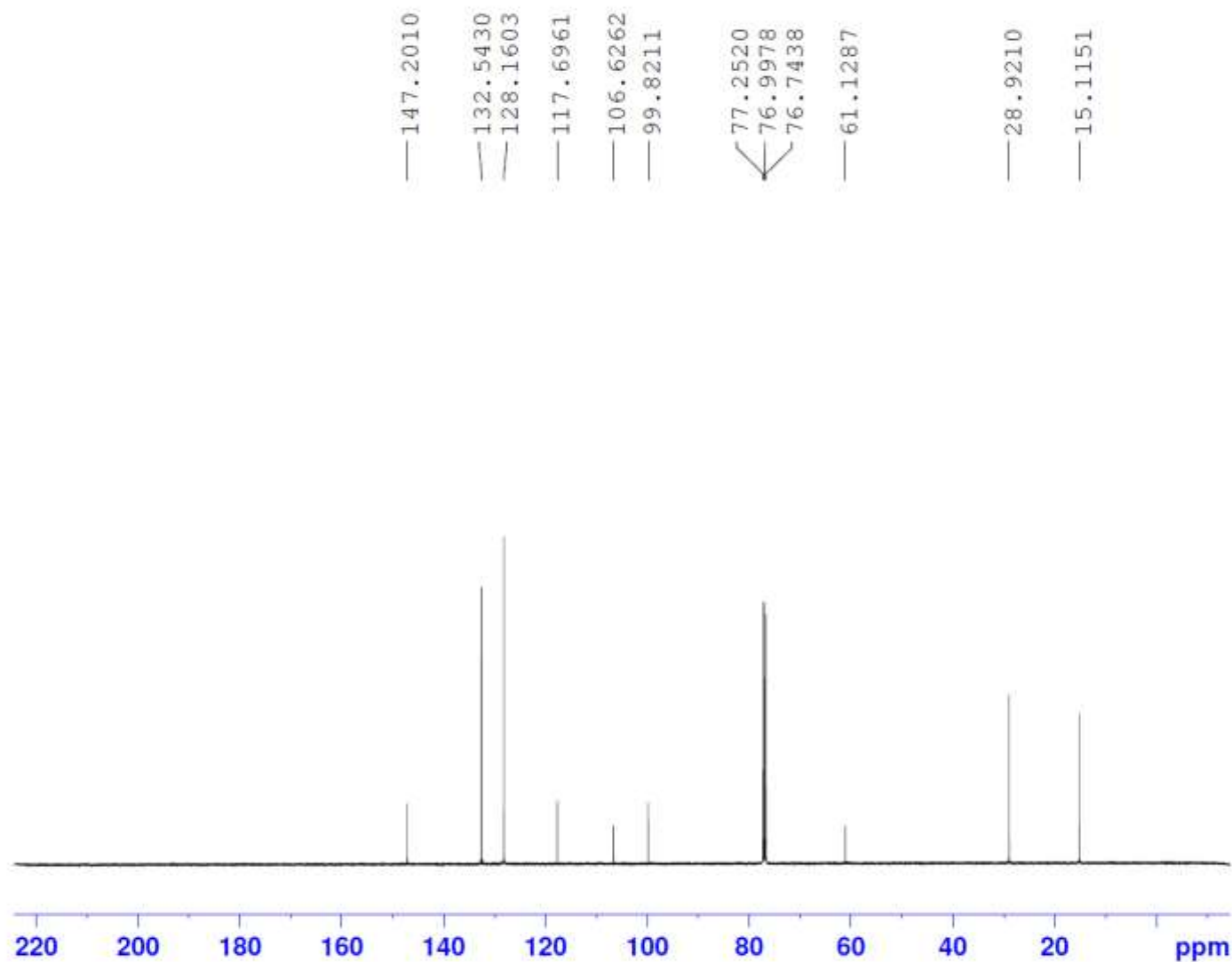
Current Data Parameters
NAME sjy2808
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170828
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

146-10



Current Data Parameters
 NAME sjy3108
 EXPNO 4
 PROCNO 1

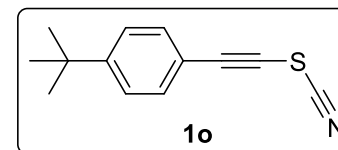
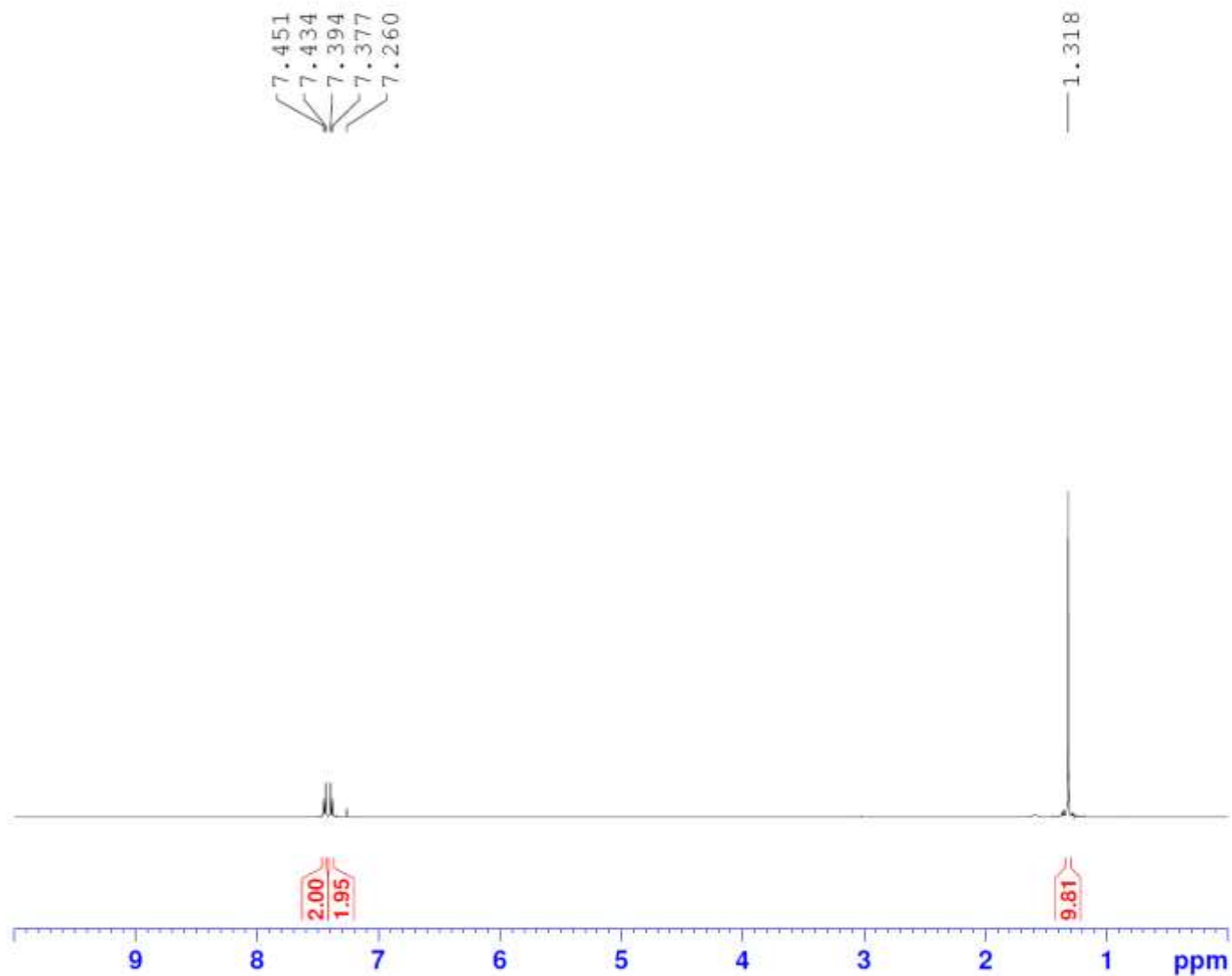
F2 - Acquisition Parameters
 Date_ 20170831
 Time 14.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 895
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 296.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577947 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P146-9



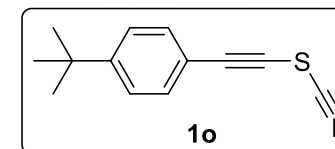
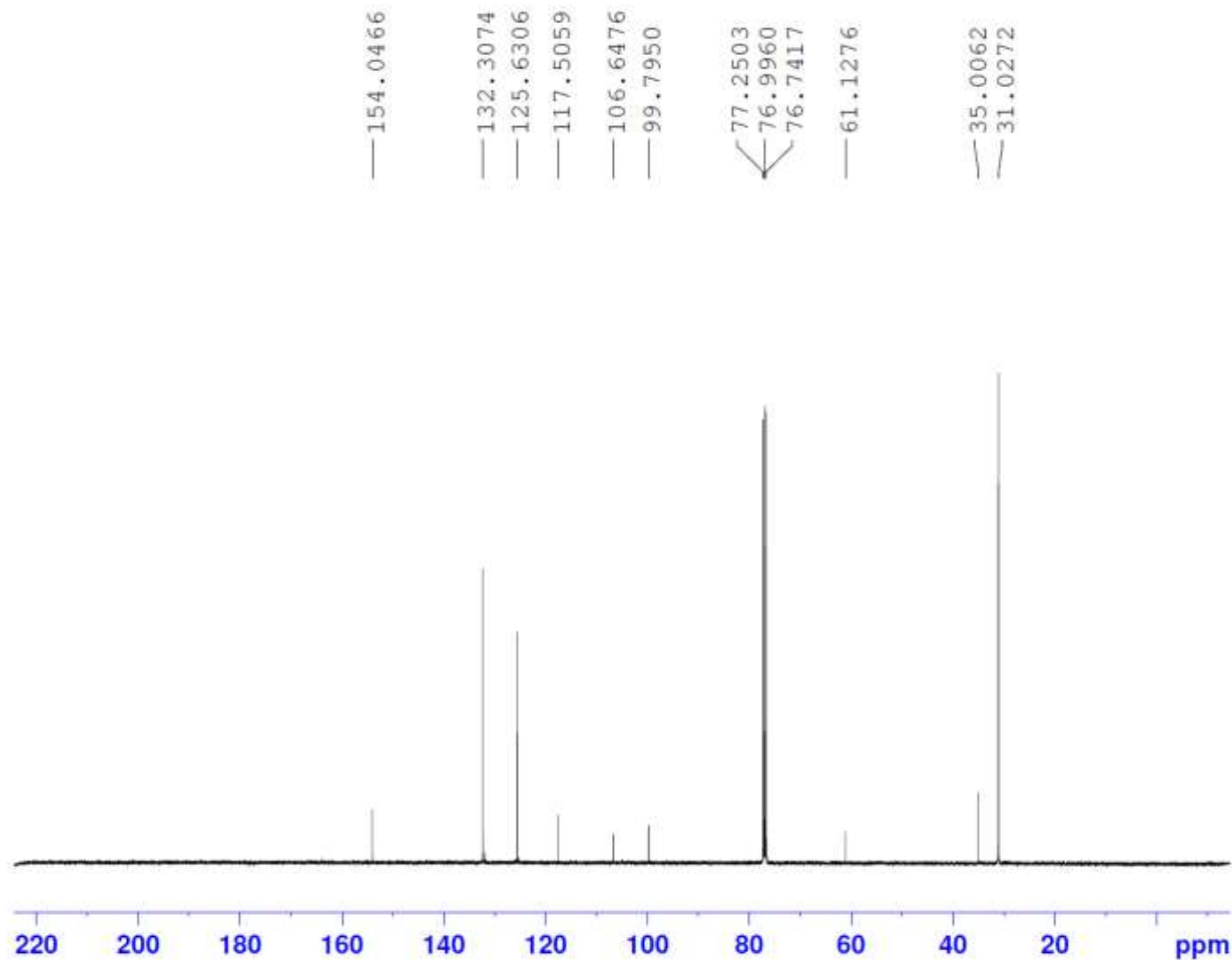
Current Data Parameters
NAME sjy2808
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170828
Time 14.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P146-9



Current Data Parameters
 NAME sjy3108
 EXPNO 2
 PROCNO 1

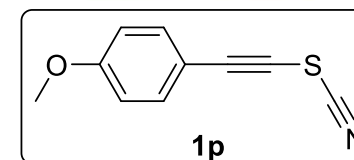
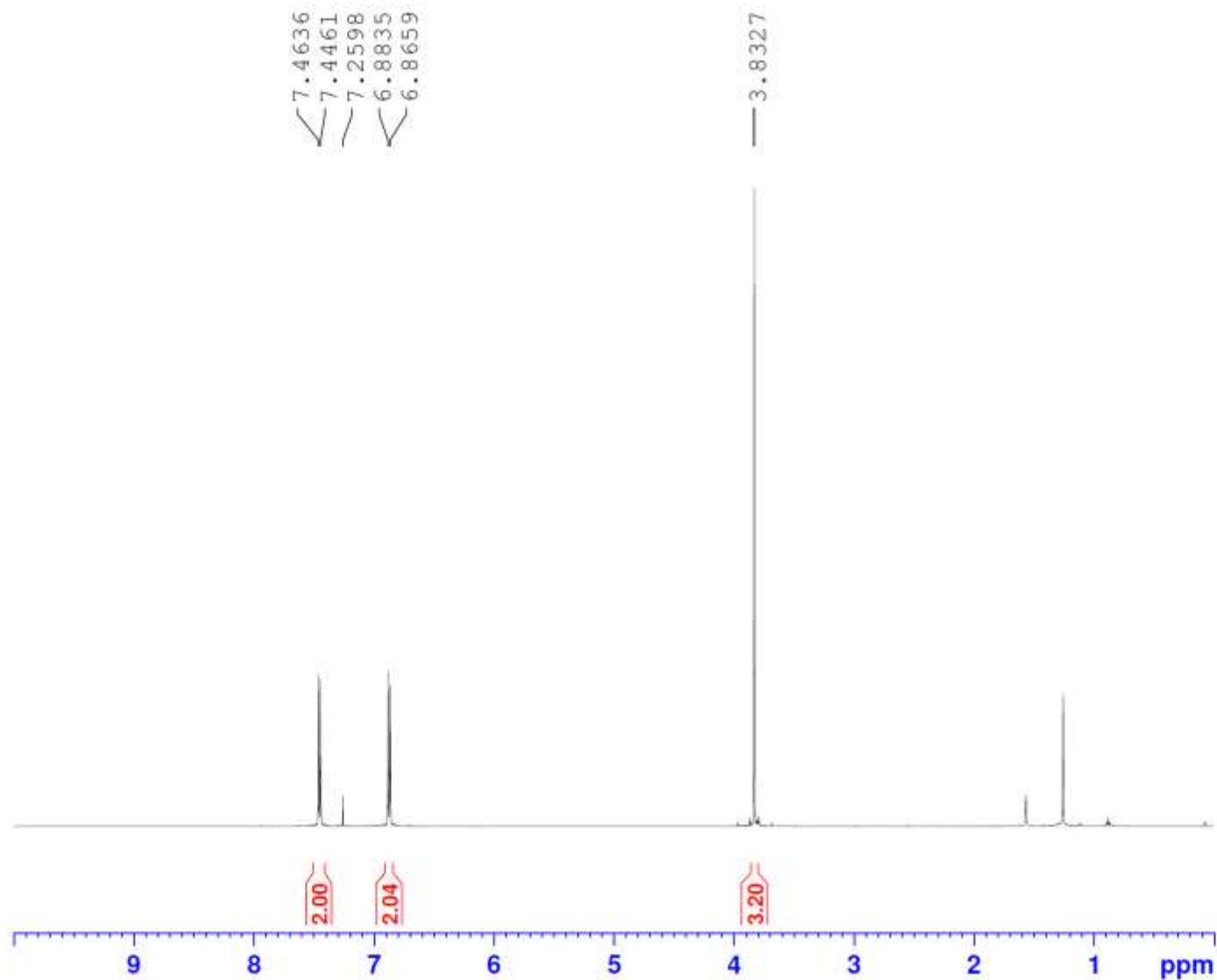
F2 - Acquisition Parameters
 Date_ 20170831
 Time 12.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1189
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 295.8 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577929 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P194-7



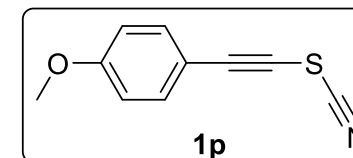
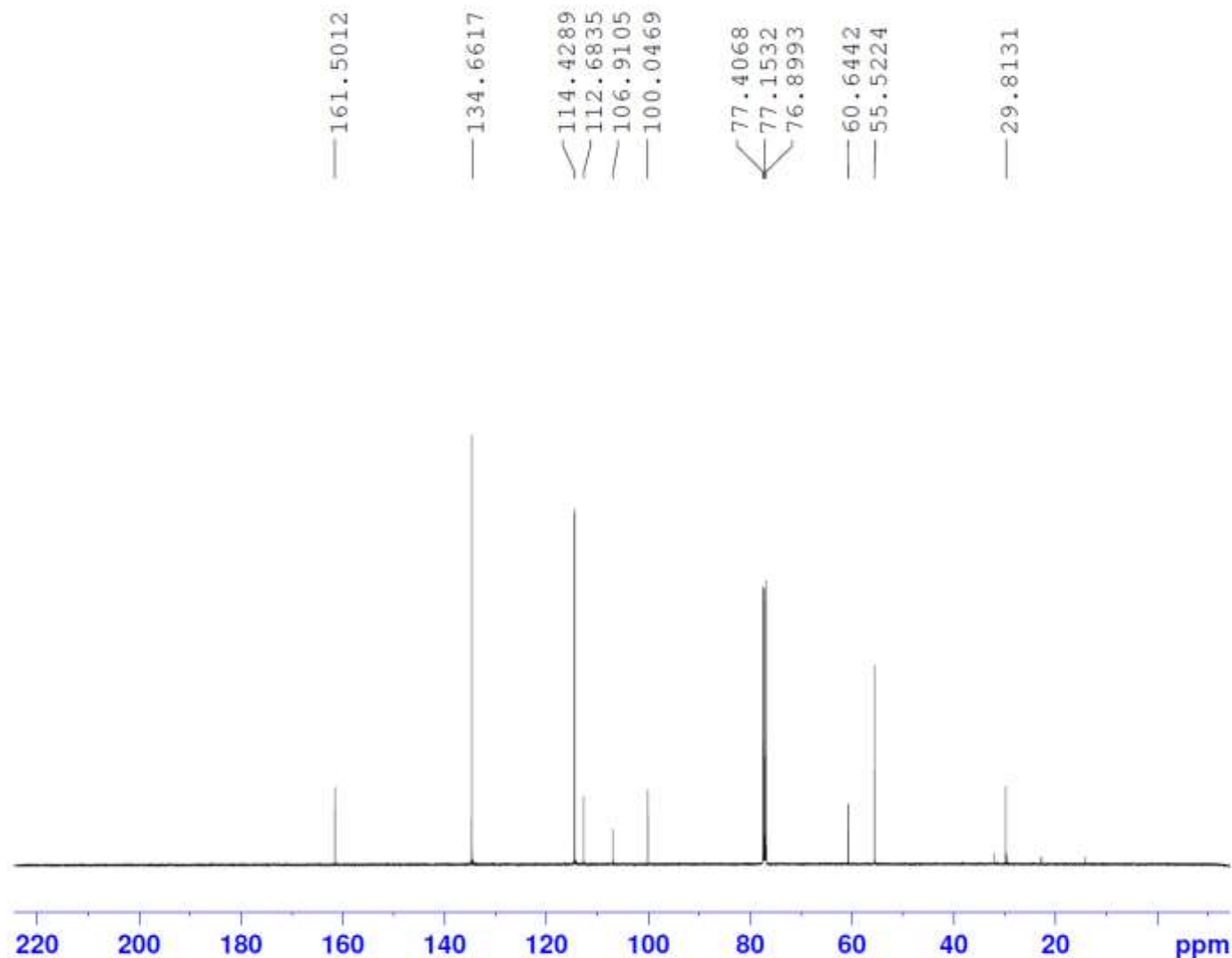
Current Data Parameters
NAME sjy2909-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170929
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 301.9 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P194-7



Current Data Parameters

NAME sjy3009
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20170930
Time 10.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1707
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 304.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 200

===== CHANNEL f1 =====

NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

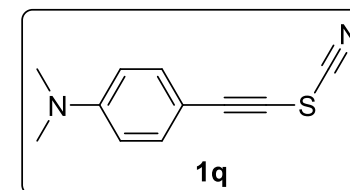
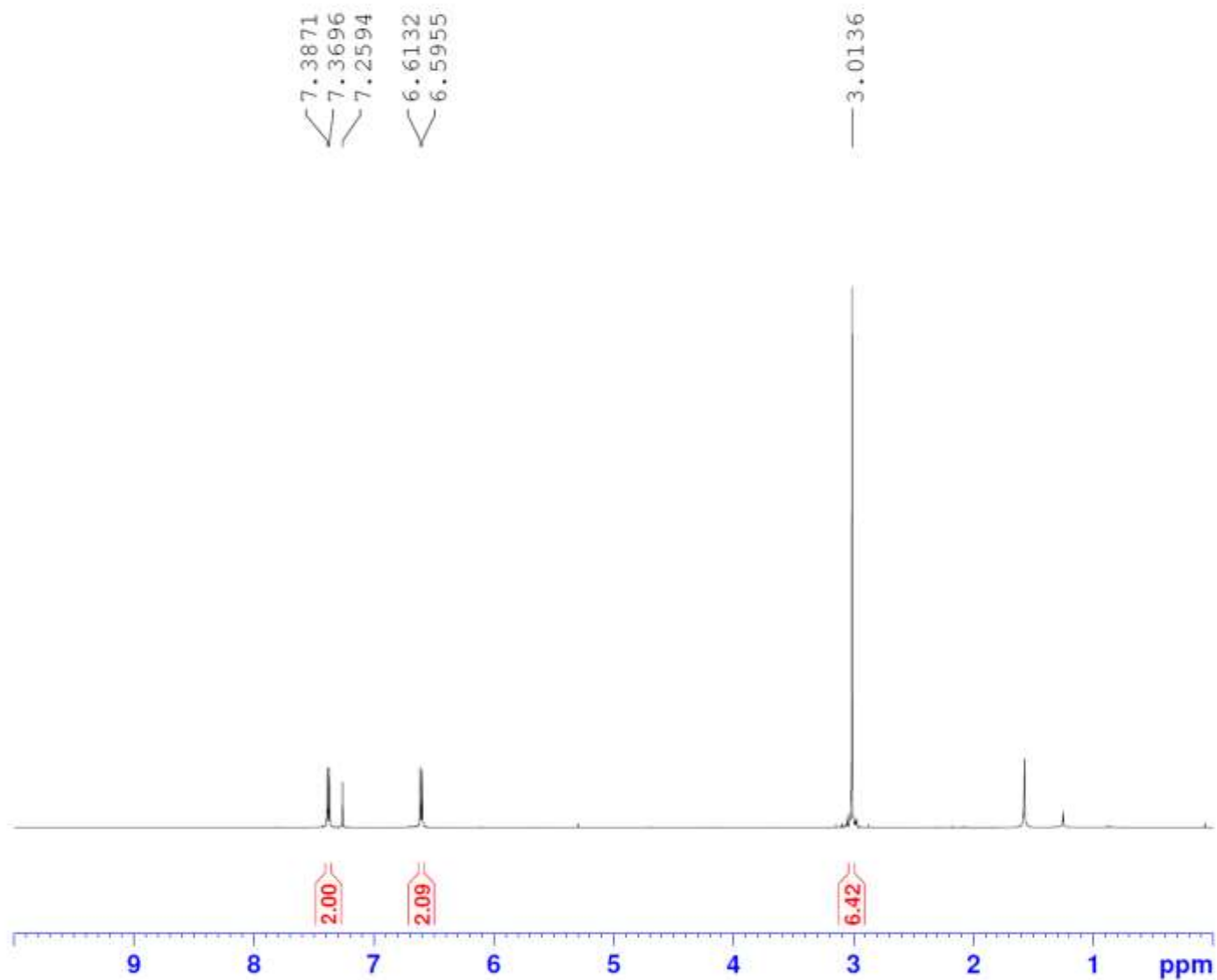
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P180-4



Current Data Parameters

NAME sjy0901
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180109
Time 15.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

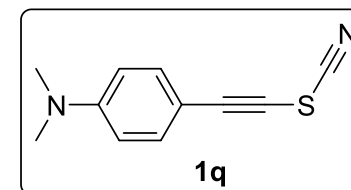
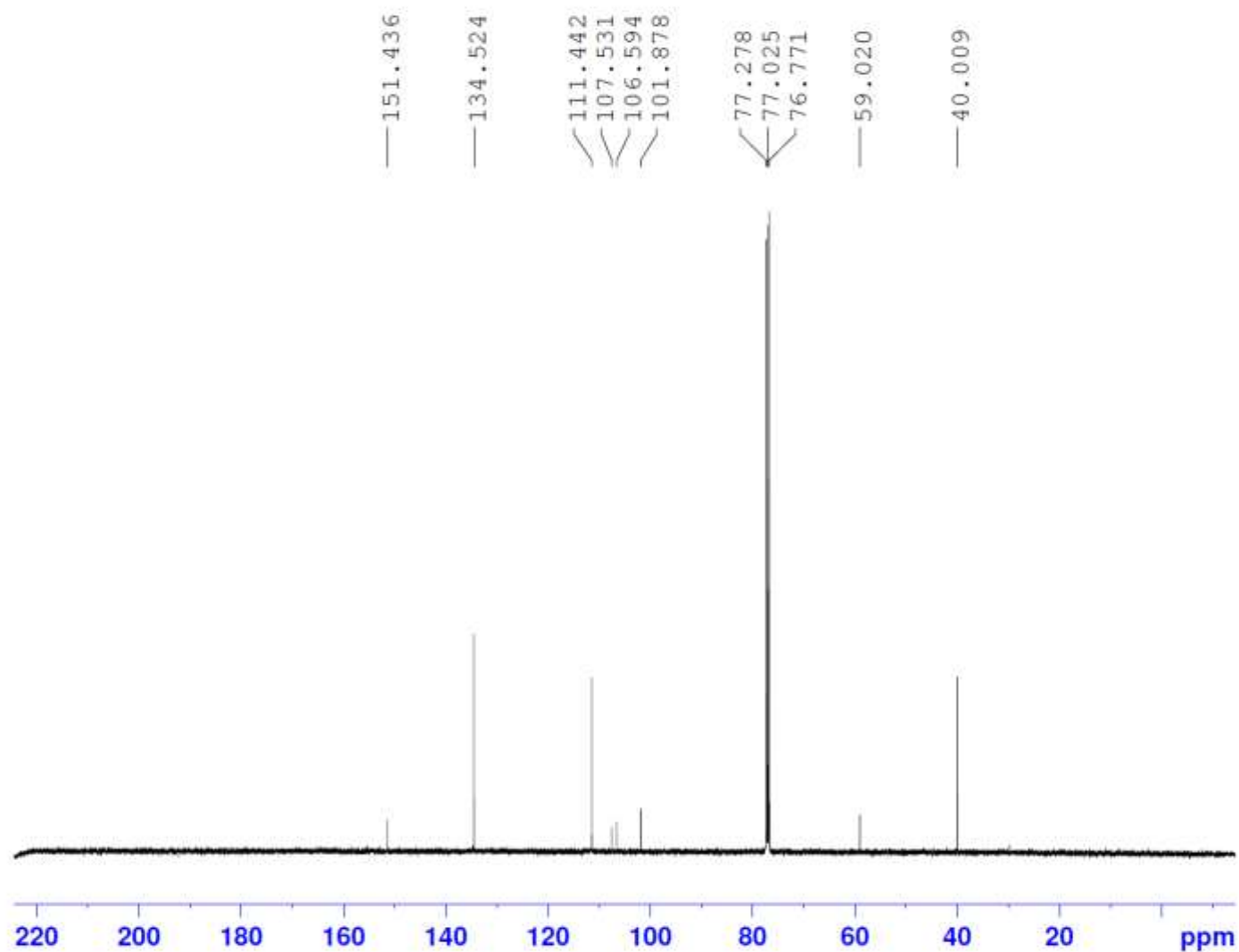
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P180-4



Current Data Parameters
 NAME sjy0901
 EXPNO 2
 PROCNO 1

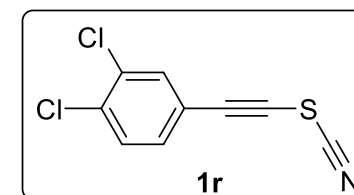
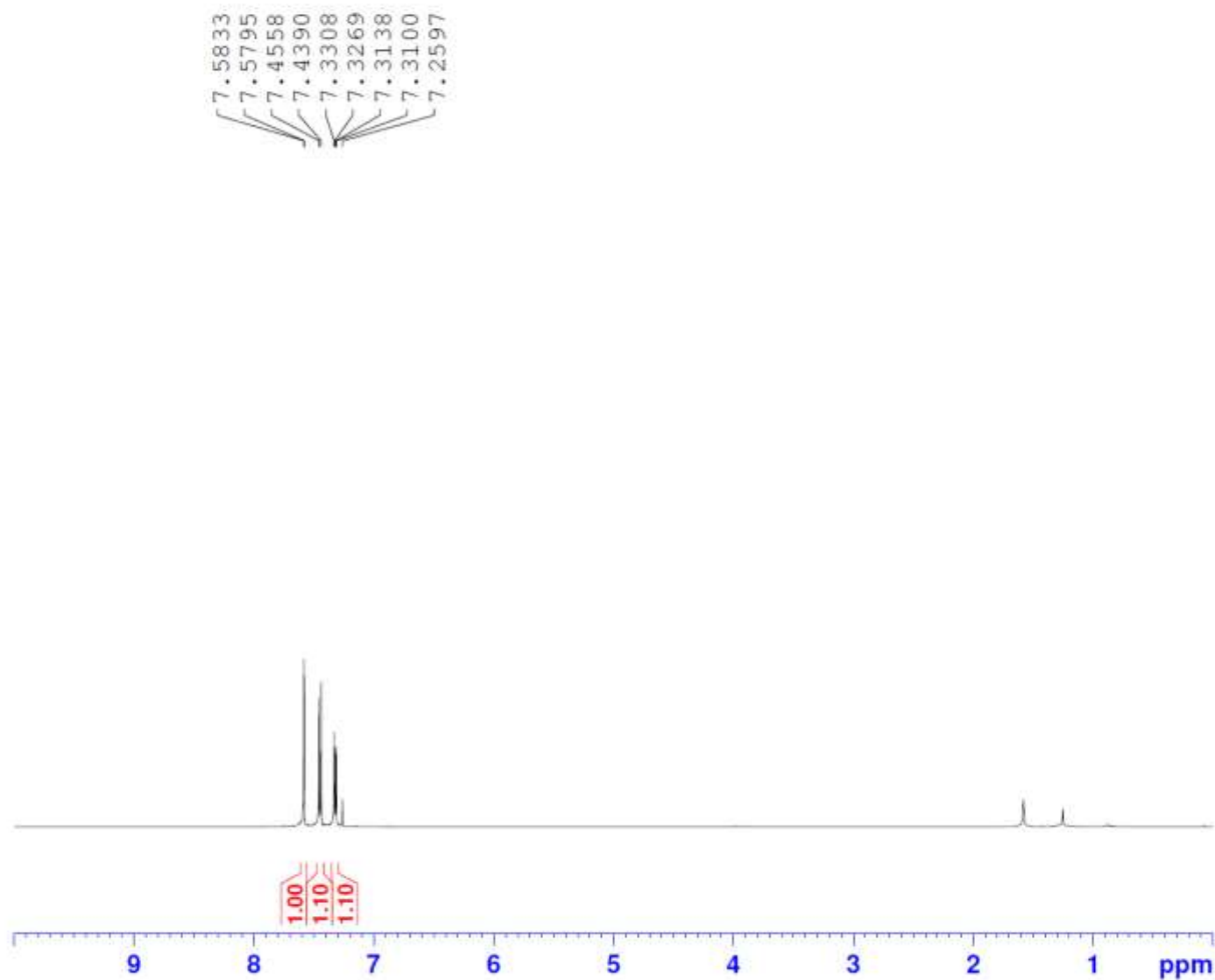
F2 - Acquisition Parameters
 Date_ 20180109
 Time 15.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 997
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P185-1



Current Data Parameters

NAME sjy2111
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171121
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1

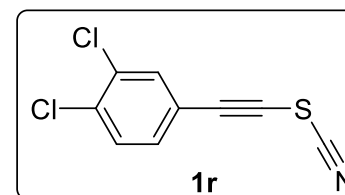
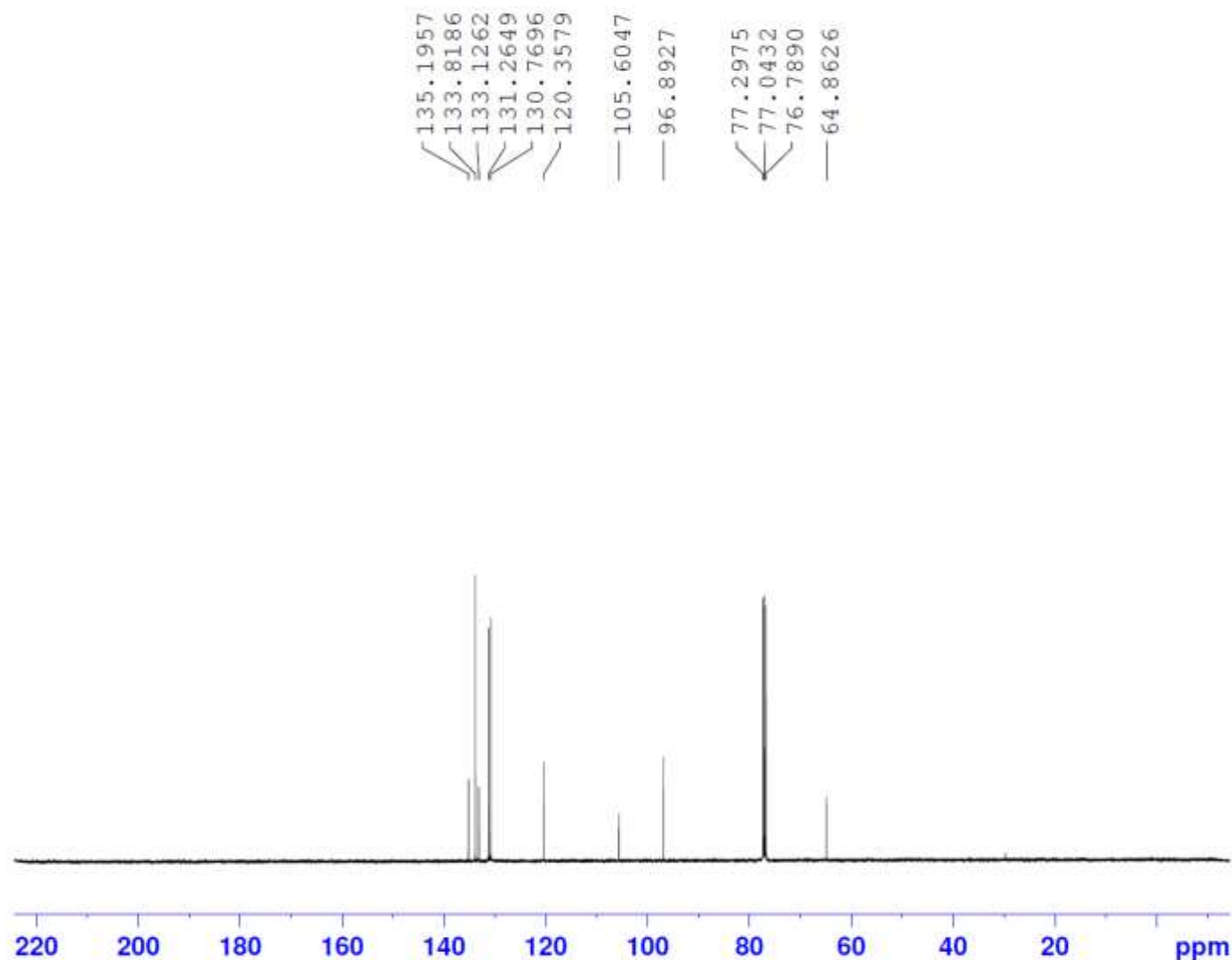
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P185-2



Current Data Parameters

NAME sjy2111
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

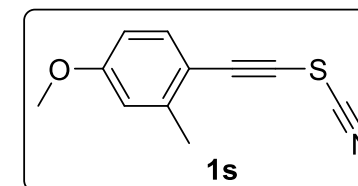
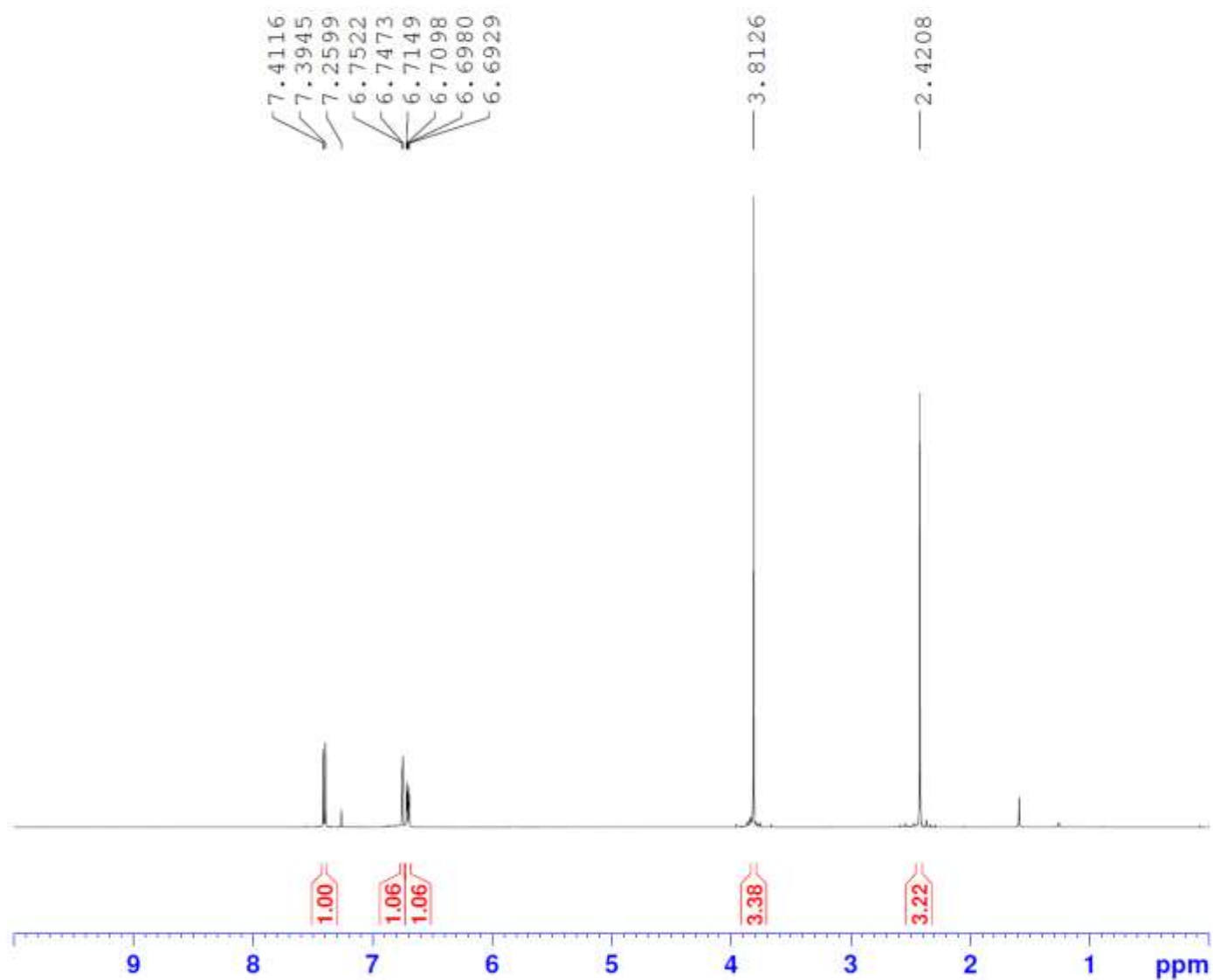
Date_ 20171121
Time 15.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 687
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-Me 4-Ome



Current Data Parameters

NAME sjy3110

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20171031

Time 14.28

INSTRUM spect

PROBHD 5 mm PABBO BB/

PULPROG zg30

TD 32768

SOLVENT CDC13

NS 8

DS 0

SWH 10330.578 Hz

FIDRES 0.315264 Hz

AQ 1.5859712 sec

RG 101.6

DW 48.400 usec

DE 6.00 usec

TE 298.8 K

D1 1.00000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 1H

P1 10.50 usec

PL1 0.25 dB

SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384

SF 500.1300131 MHz

WDW EM

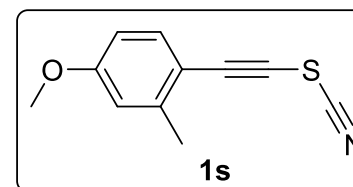
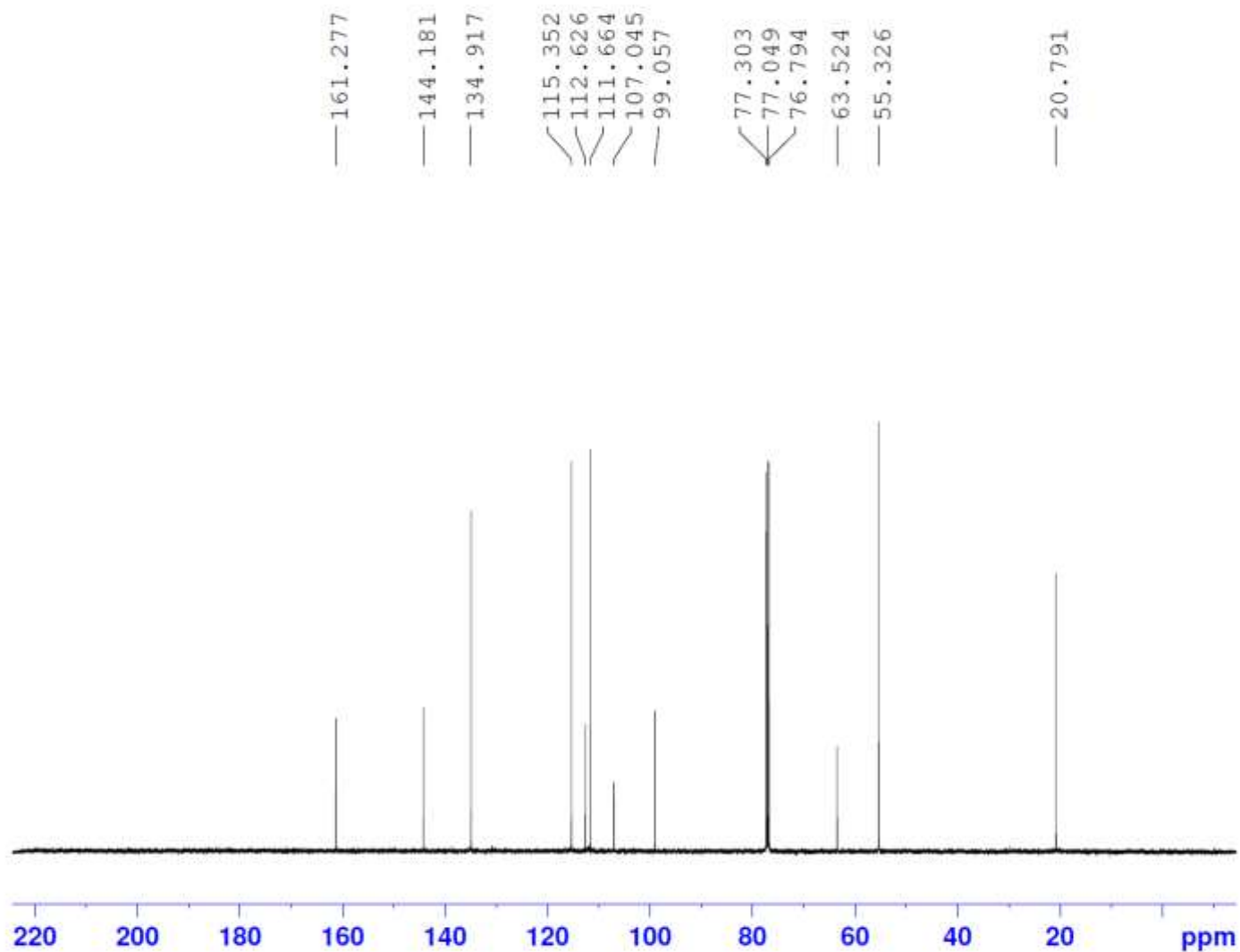
SSB 0

LB 0.30 Hz

GB 0

PC 1.00

2ME 4-OMe



Current Data Parameters
NAME sjy3110
EXPNO 2
PROCNO 1

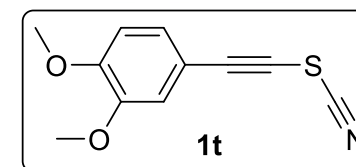
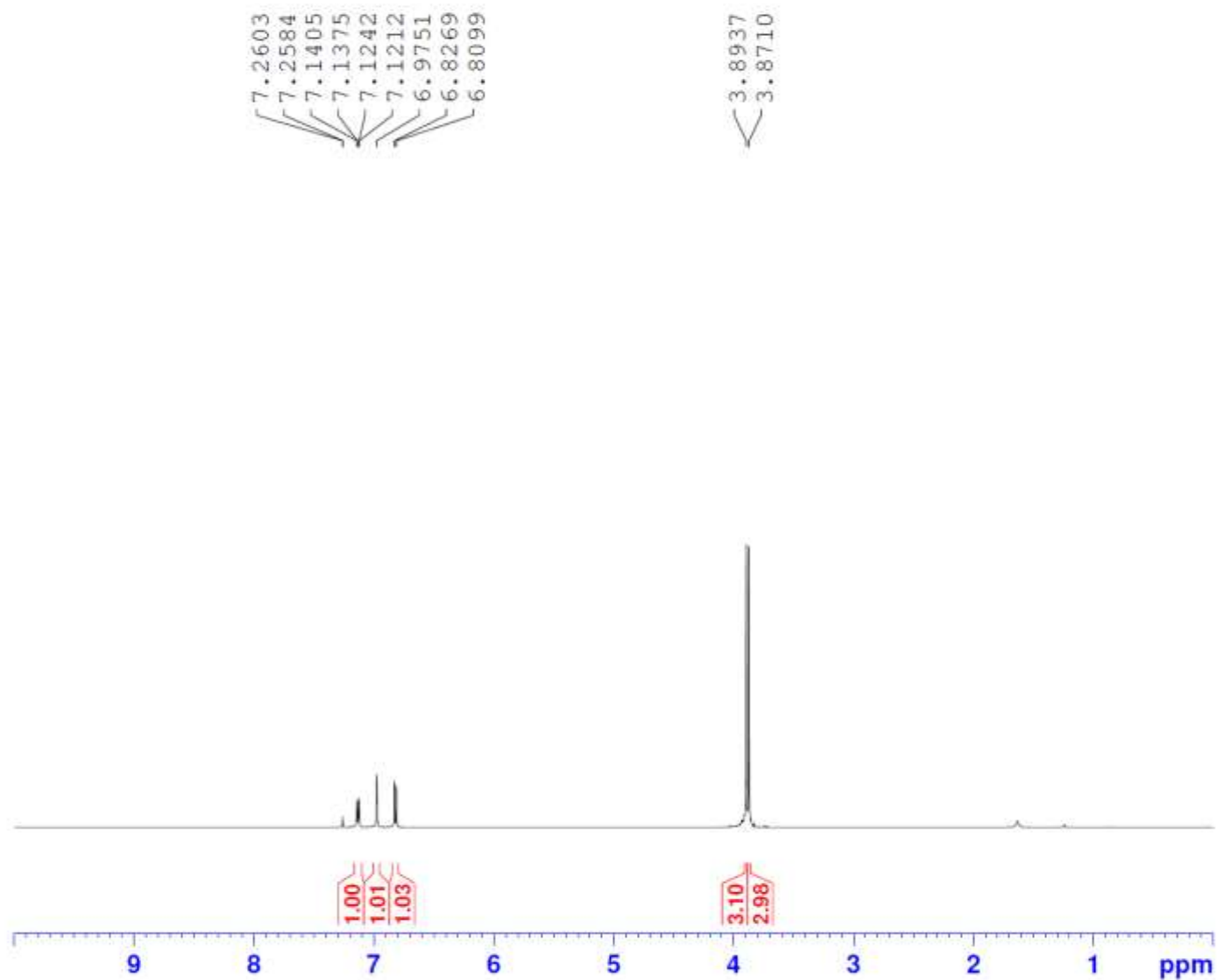
F2 - Acquisition Parameters
Date_ 20171031
Time 14.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 546
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 299.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P185-4



Current Data Parameters

NAME sjy2411
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171124
Time 15.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

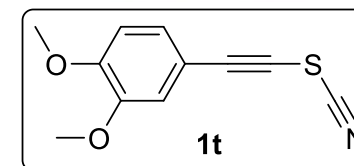
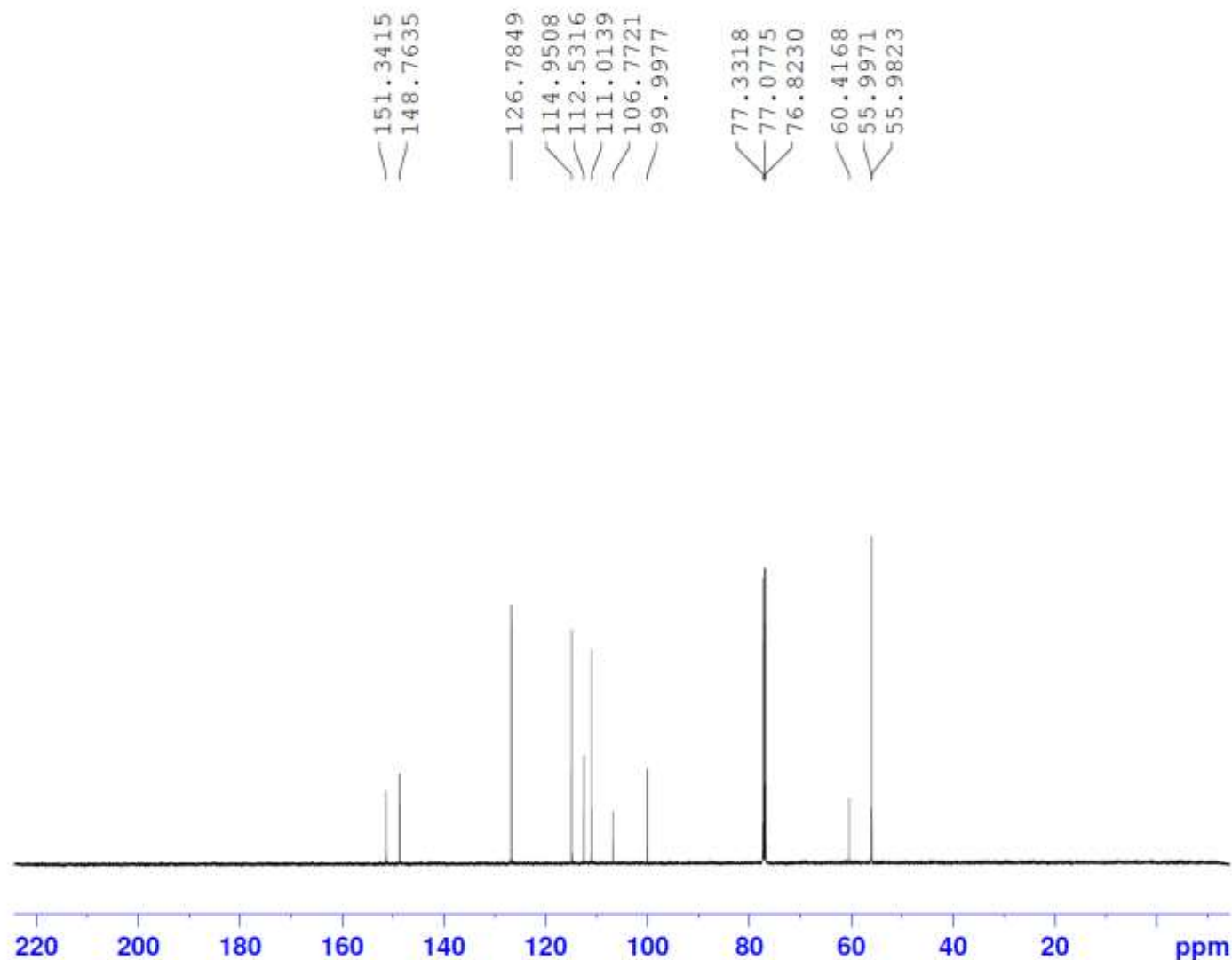
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P185-4



Current Data Parameters

NAME sjy2411
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

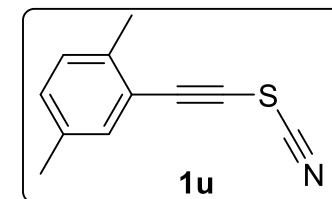
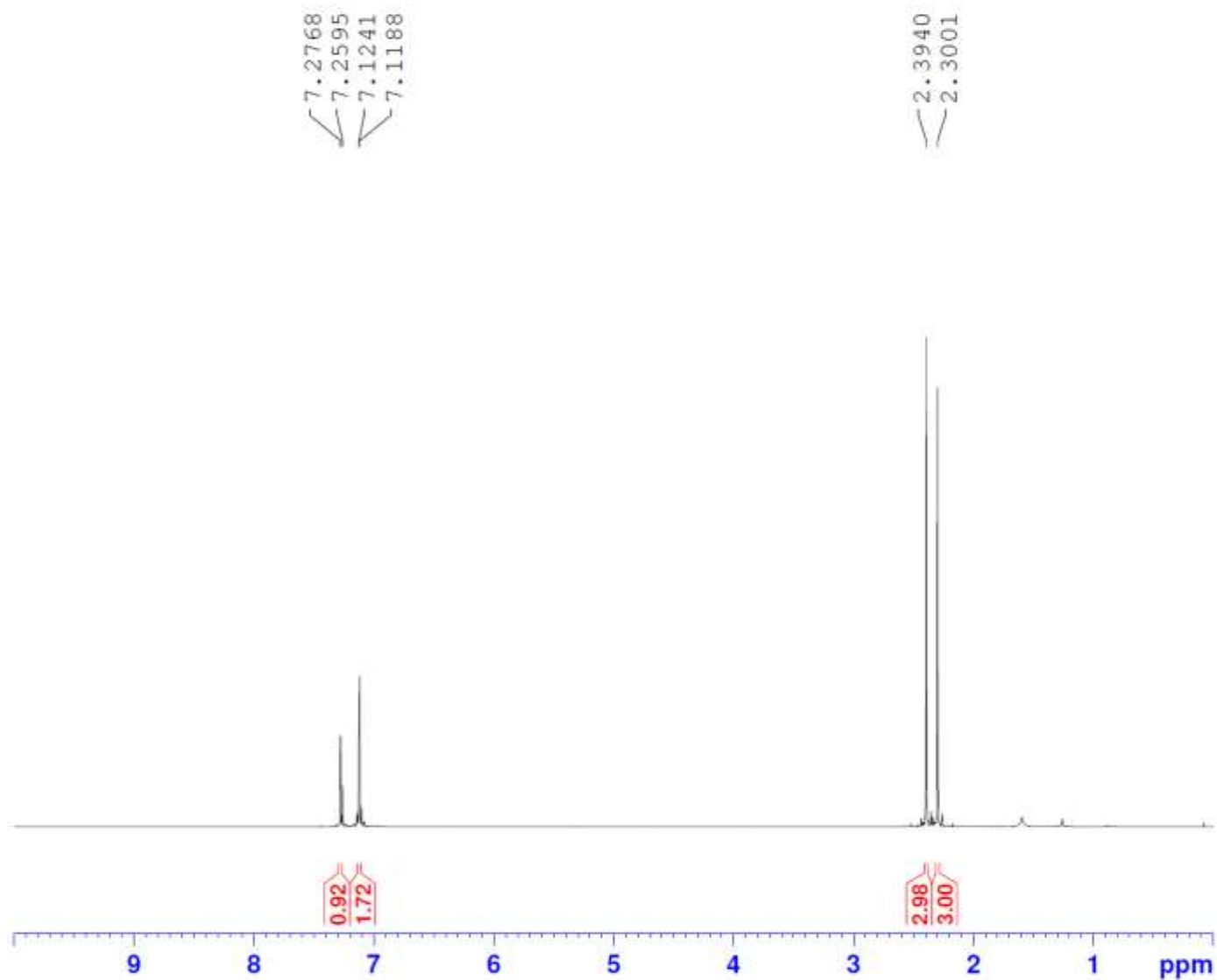
Date_ 20171124
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 571
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P185-3



Current Data Parameters

NAME sjy2911
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171129
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

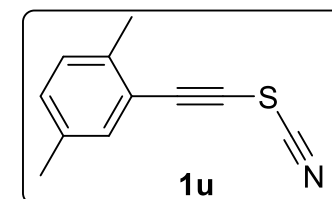
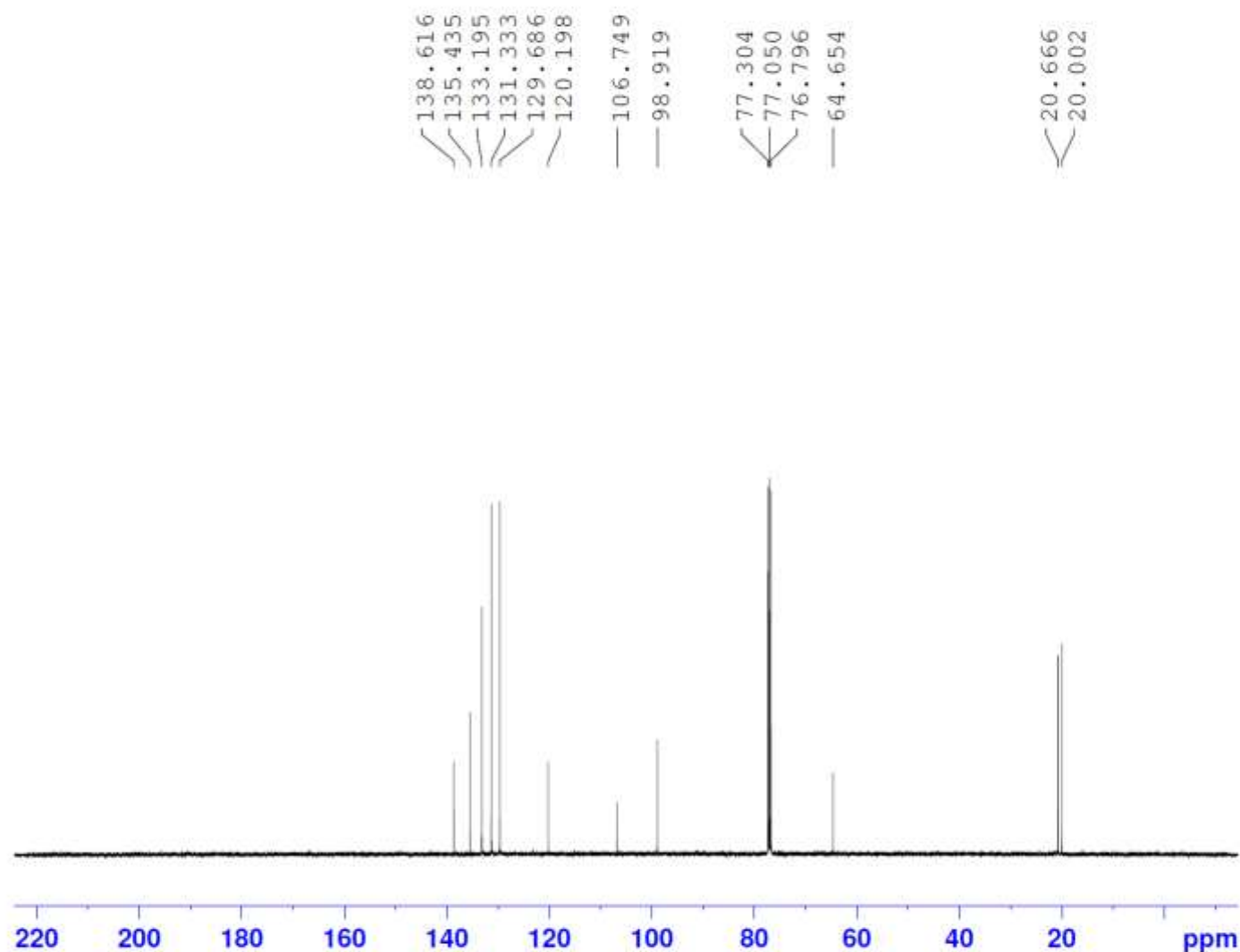
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P185-3



Current Data Parameters
 NAME sjy2911
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171129
 Time 16.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 656
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 296.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

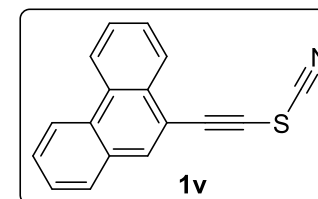
===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P180-2

8.688
8.684
8.676
8.670
8.657
8.640
8.288
8.285
8.281
8.274
8.269
8.078
7.870
7.855
7.735
7.724
7.720
7.712
7.705
7.700
7.689
7.641
7.626
7.612
7.260

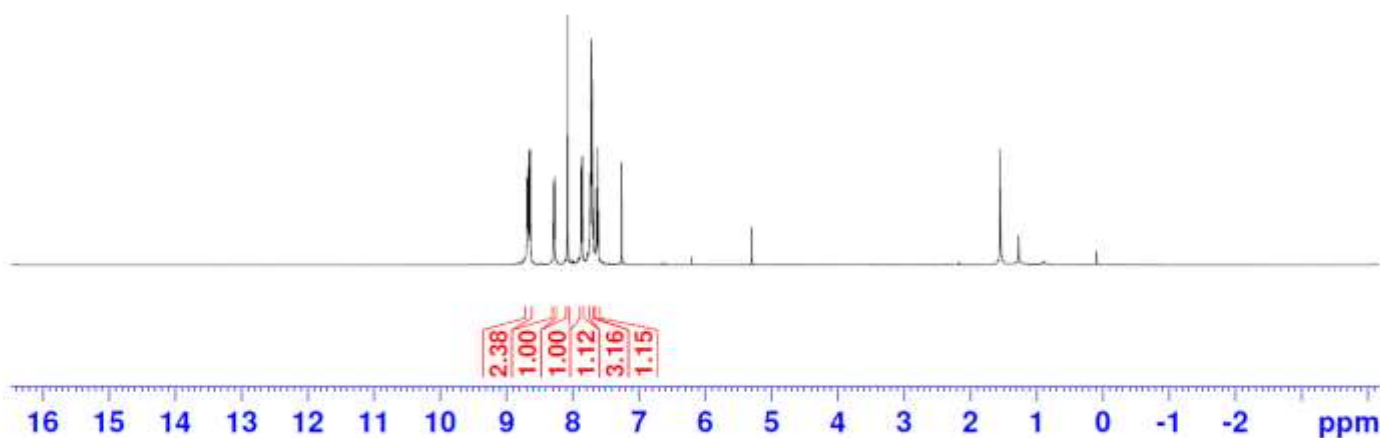


Current Data Parameters
NAME sjy2612
EXPNO 1
PROCNO 1

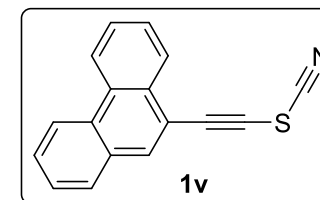
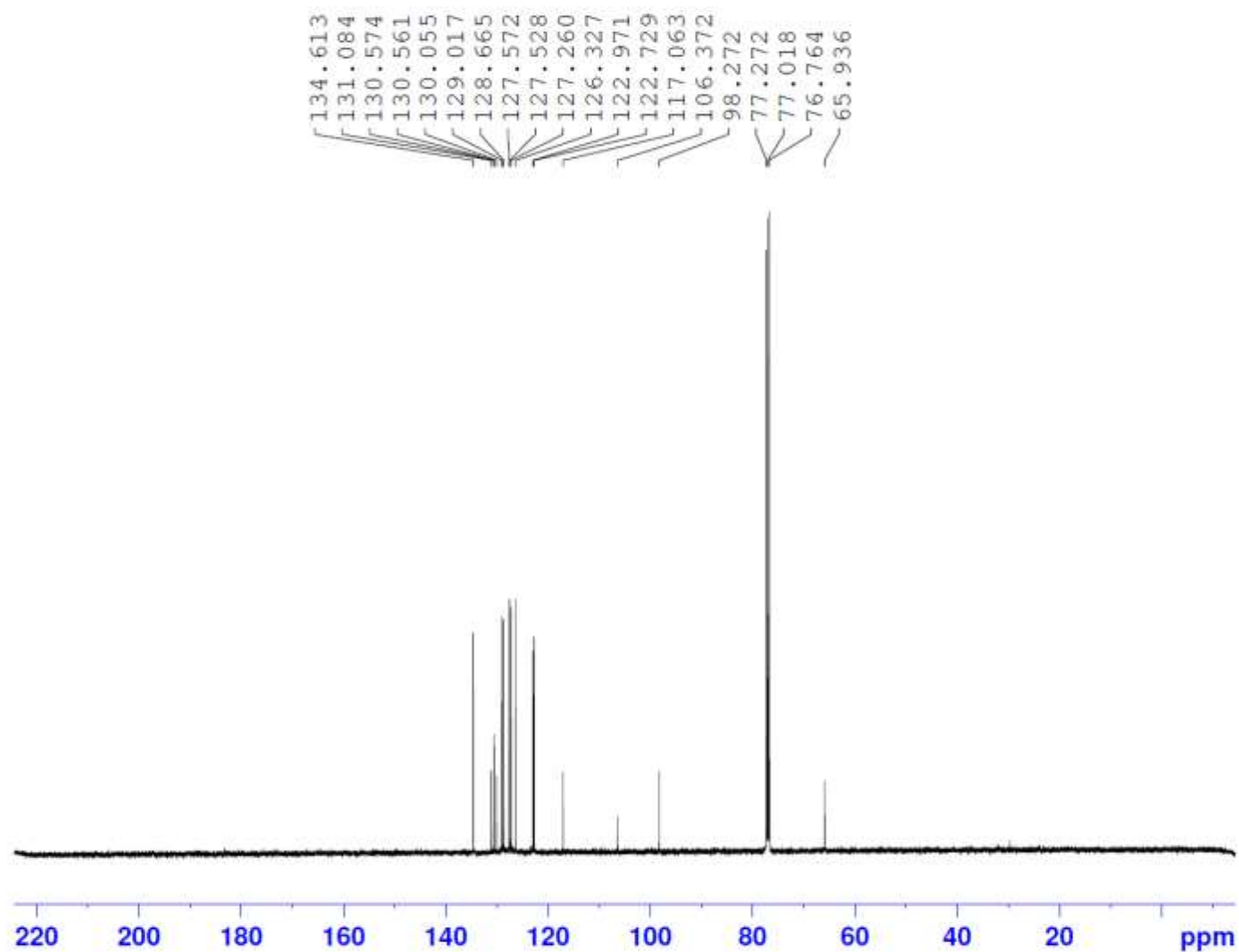
F2 - Acquisition Parameters
Date_ 20171226
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 305.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



P180-2



Current Data Parameters
 NAME sjy2612
 EXPNO 2
 PROCNO 1

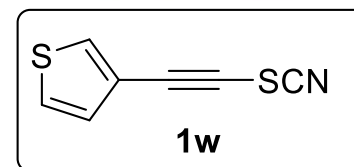
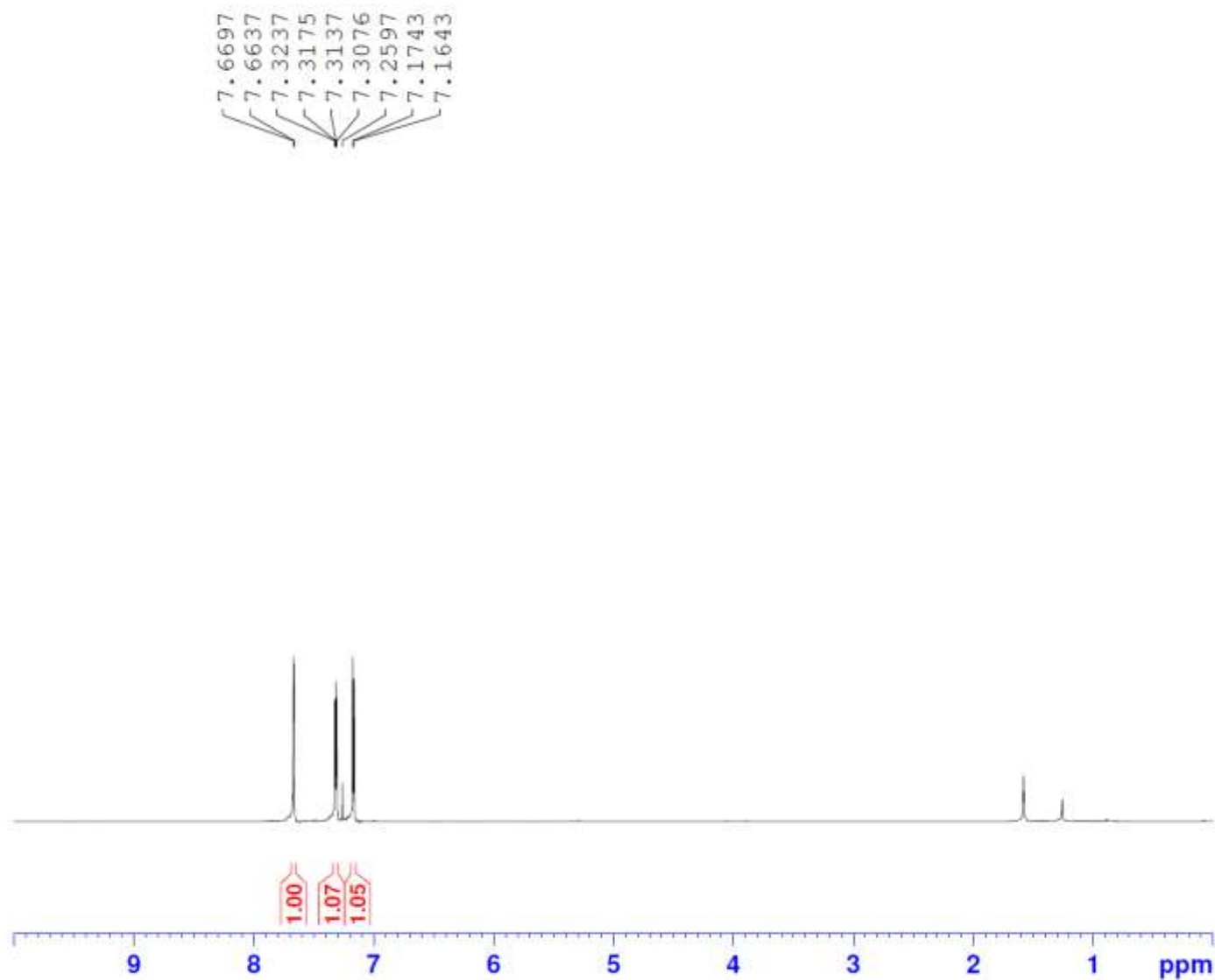
F2 - Acquisition Parameters
 Date_ 20171226
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1559
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 306.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P186-2



Current Data Parameters

NAME sjy2211
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171122
Time 15.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 300.4 K
D1 1.00000000 sec
TD0 1

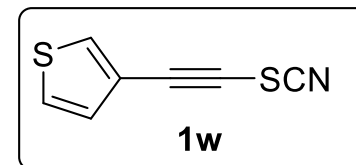
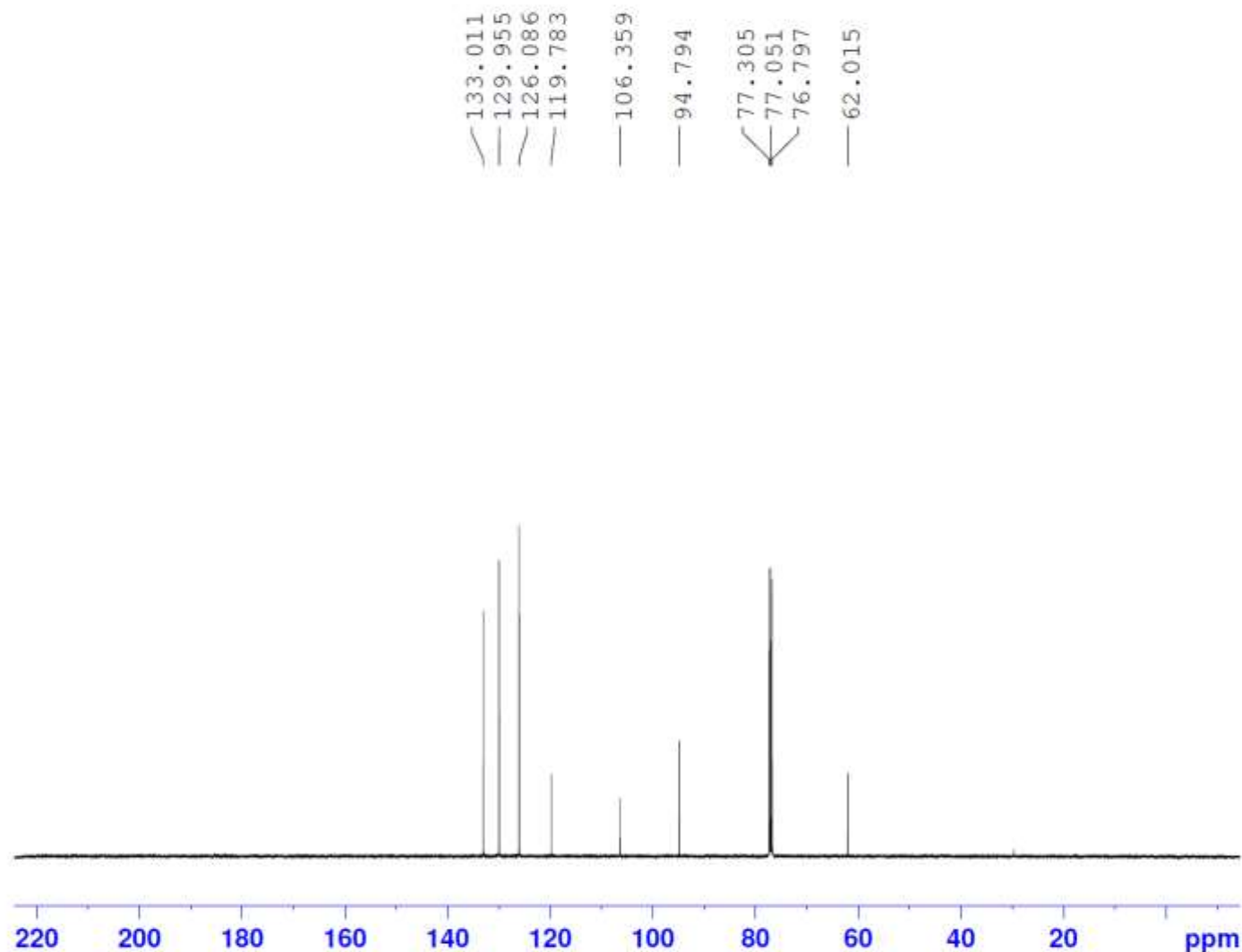
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P186-2



Current Data Parameters
 NAME sjy2211
 EXPNO 2
 PROCNO 1

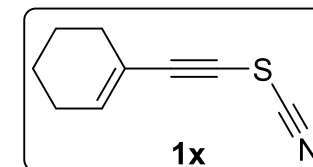
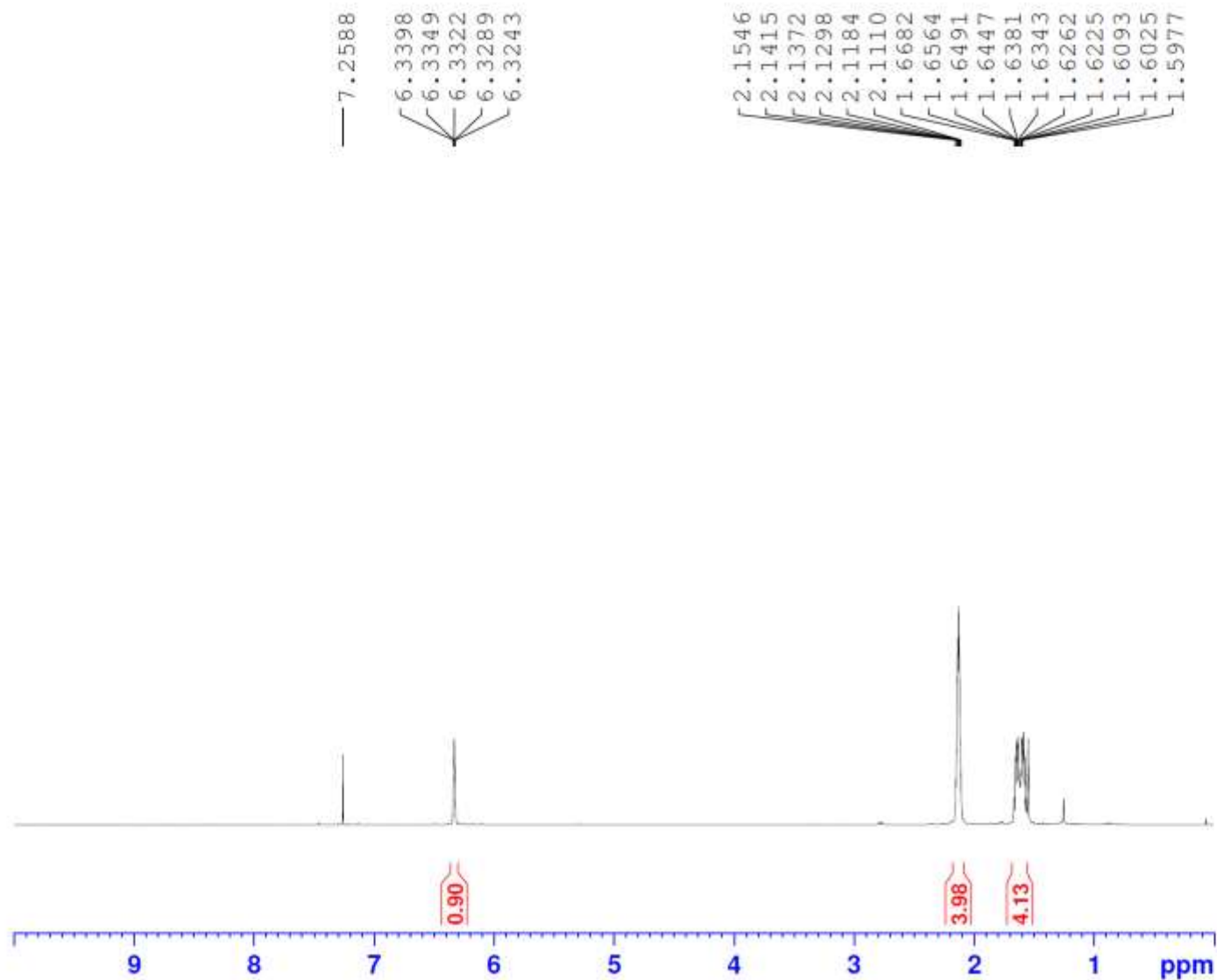
F2 - Acquisition Parameters
 Date_ 20171122
 Time 15.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 825
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 301.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P194-5



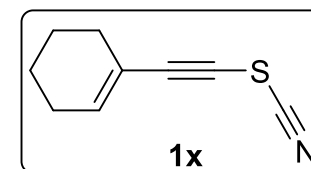
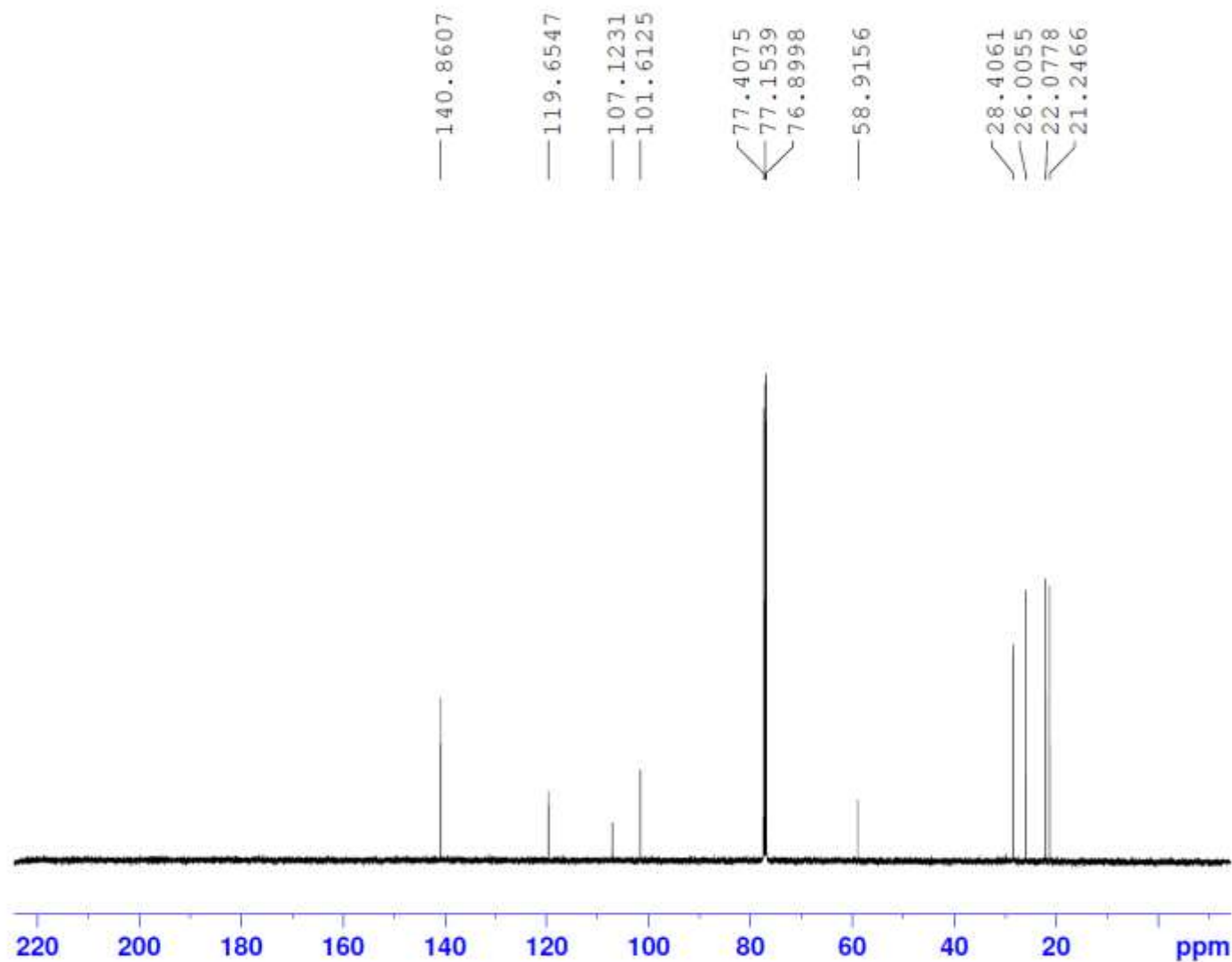
Current Data Parameters
 NAME sjy2909-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170929
 Time 16.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 301.9 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

P194-5



Current Data Parameters
NAME sjy3009
EXPNO 2
PROCNO 1

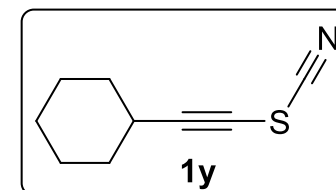
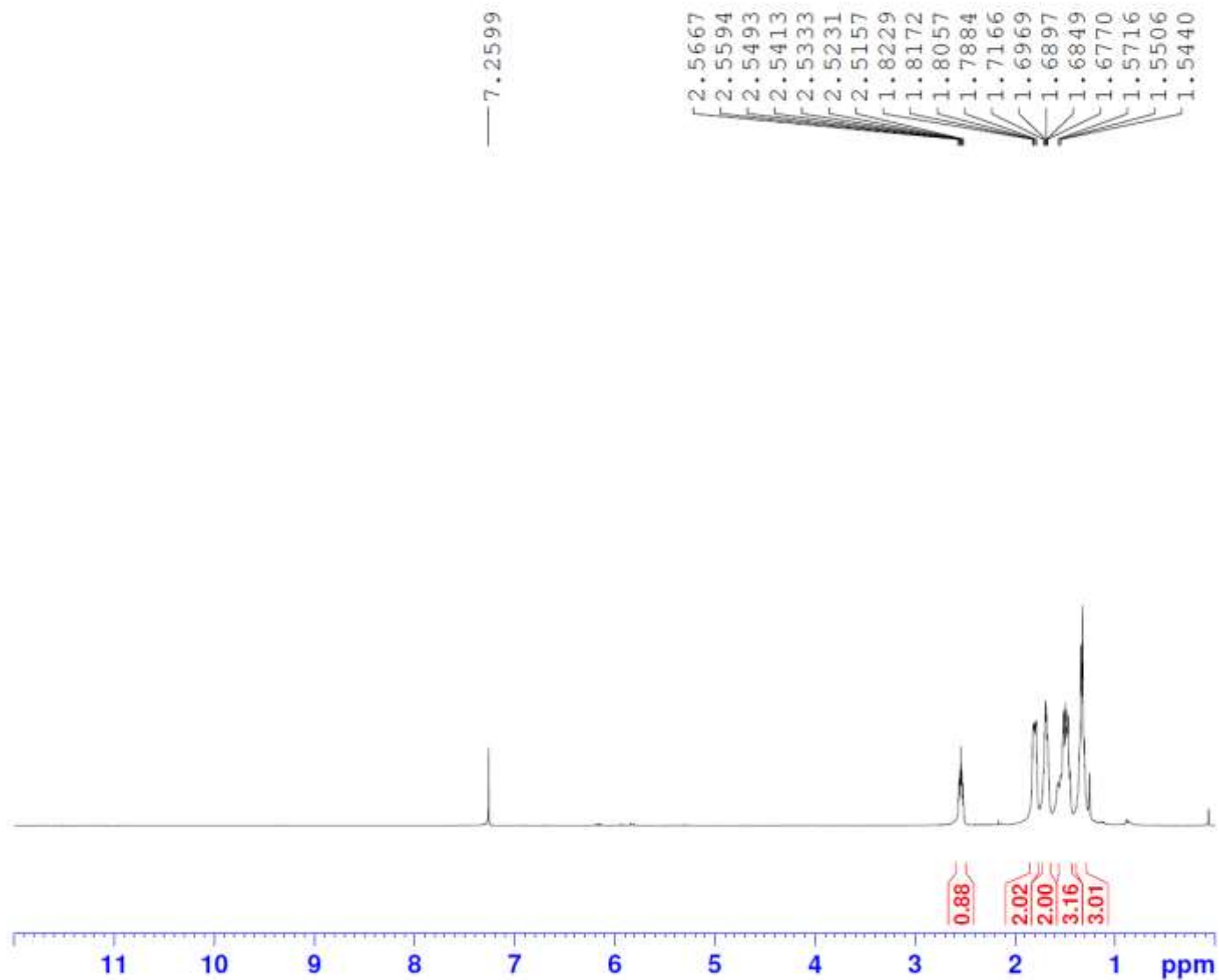
F2 - Acquisition Parameters
Date_ 20170930
Time 9.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 485
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 303.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 200

----- CHANNEL f1 -----
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P180-1



Current Data Parameters

NAME sjy2001
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180120
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 304.2 K
D1 1.00000000 sec
TD0 1

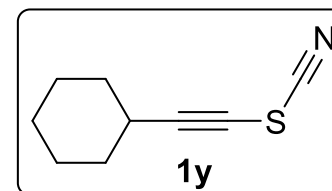
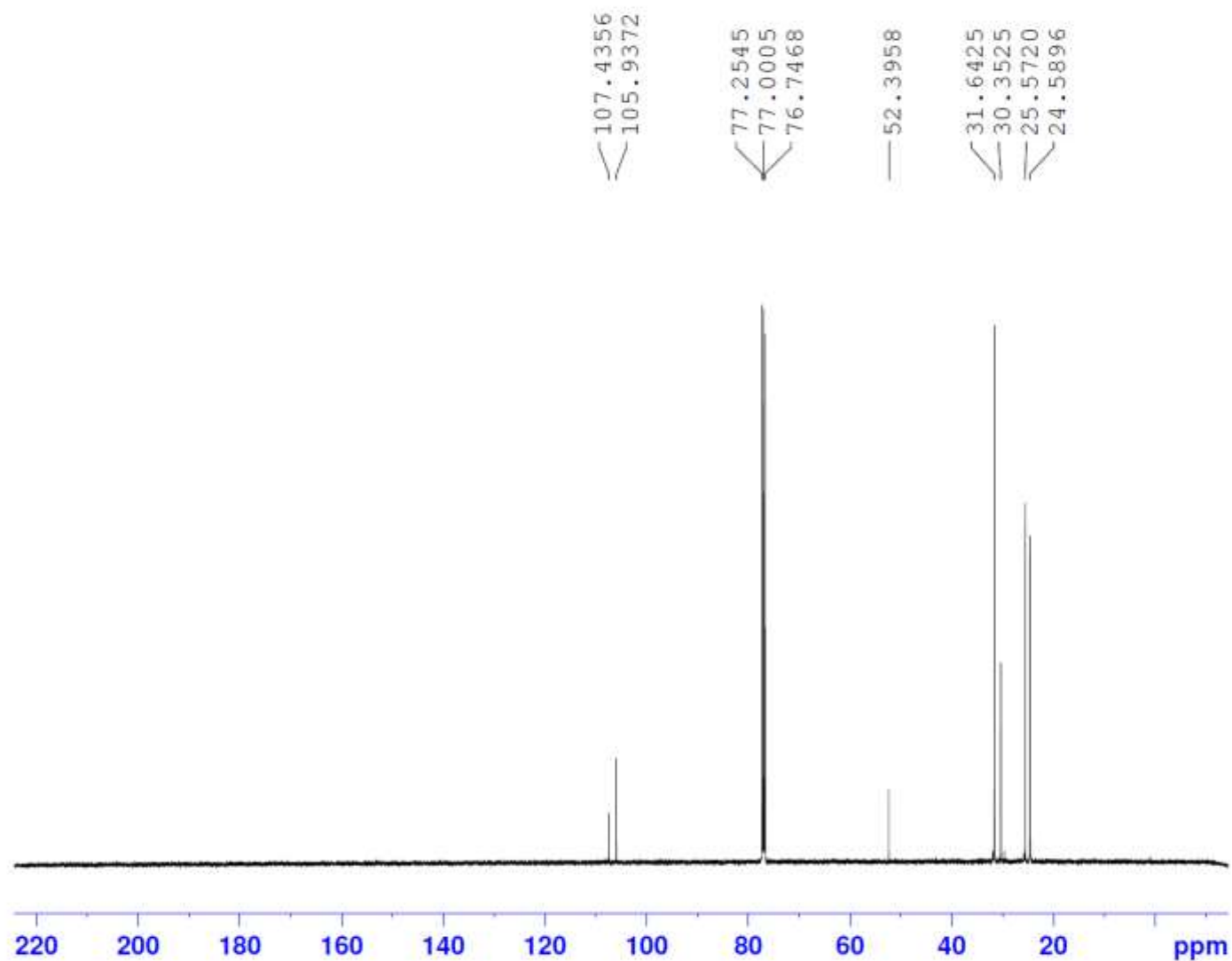
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

p180-1



Current Data Parameters
NAME sjy2001
EXPNO 4
PROCNO 1

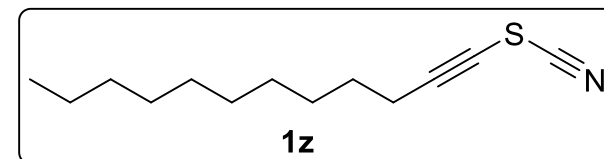
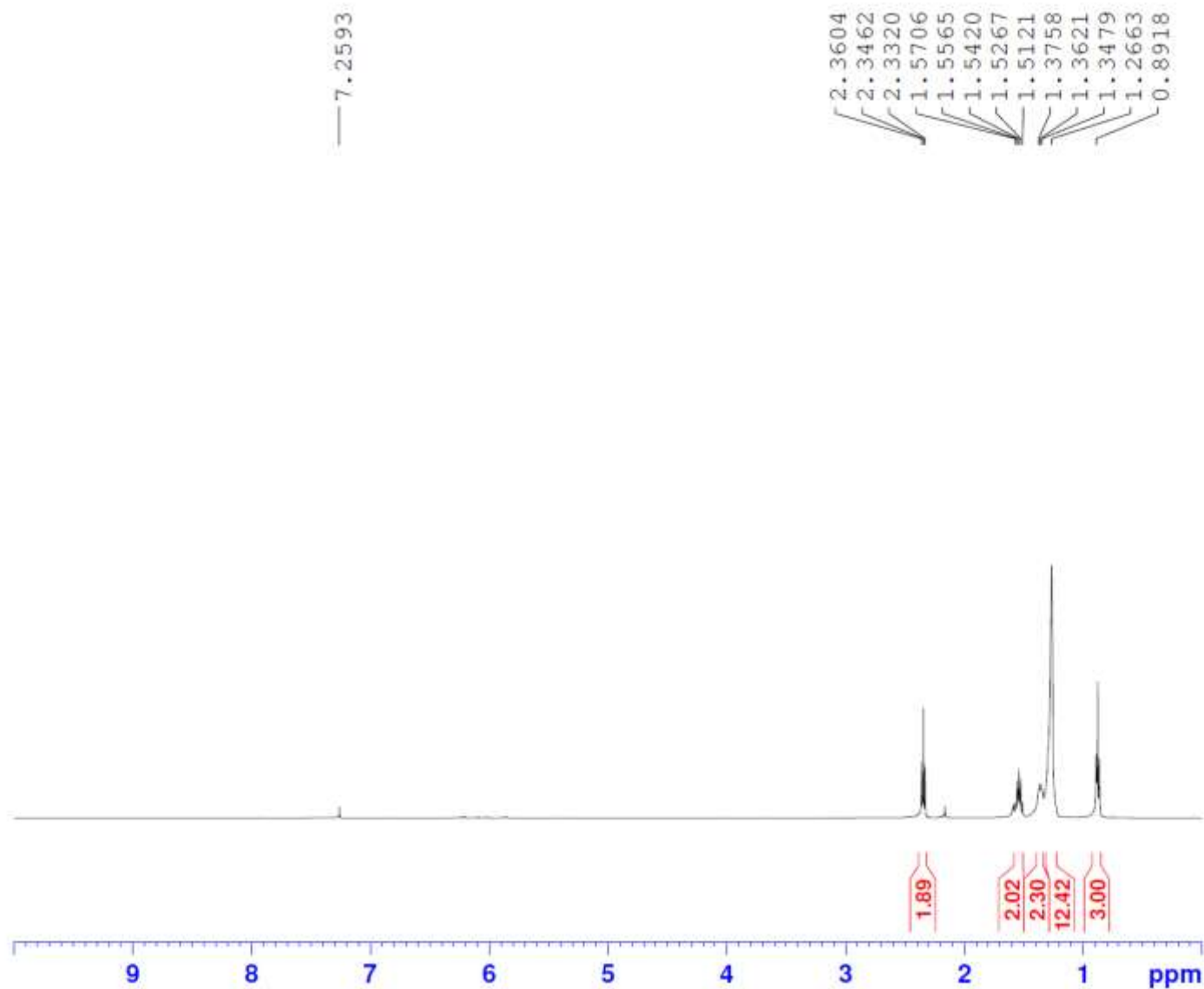
F2 - Acquisition Parameters
Date_ 20180120
Time 10.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1874
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 304.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 750

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P185-13



Current Data Parameters

NAME sjy0712
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171207
Time 13.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 35.9
DW 48.400 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

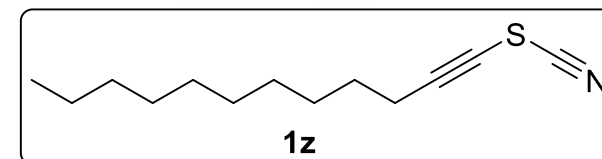
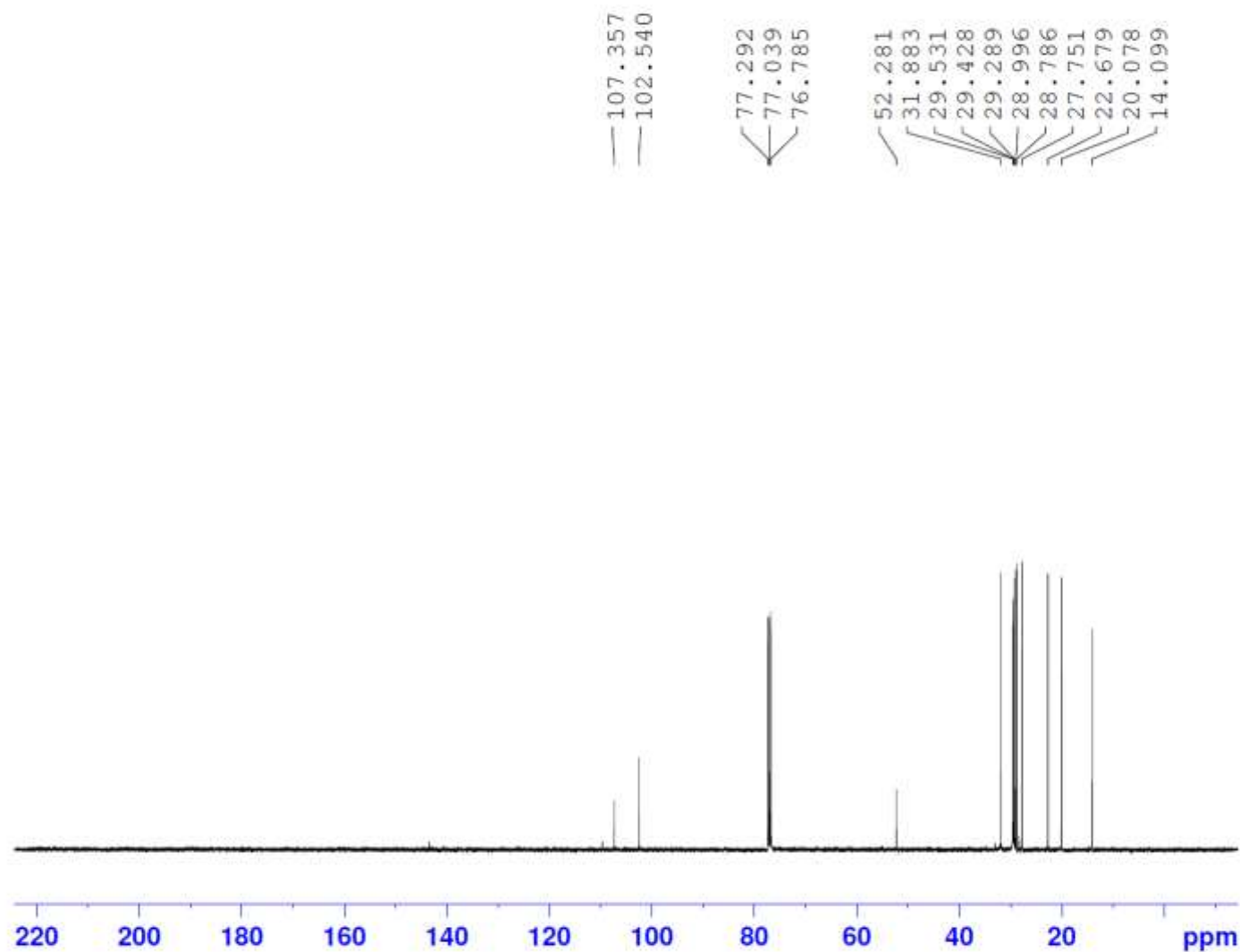
----- CHANNEL f1 -----

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P185-13



Current Data Parameters

NAME sjy0712
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

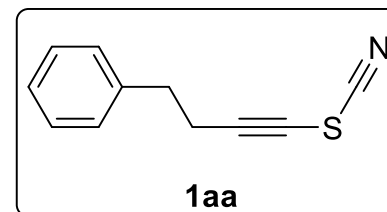
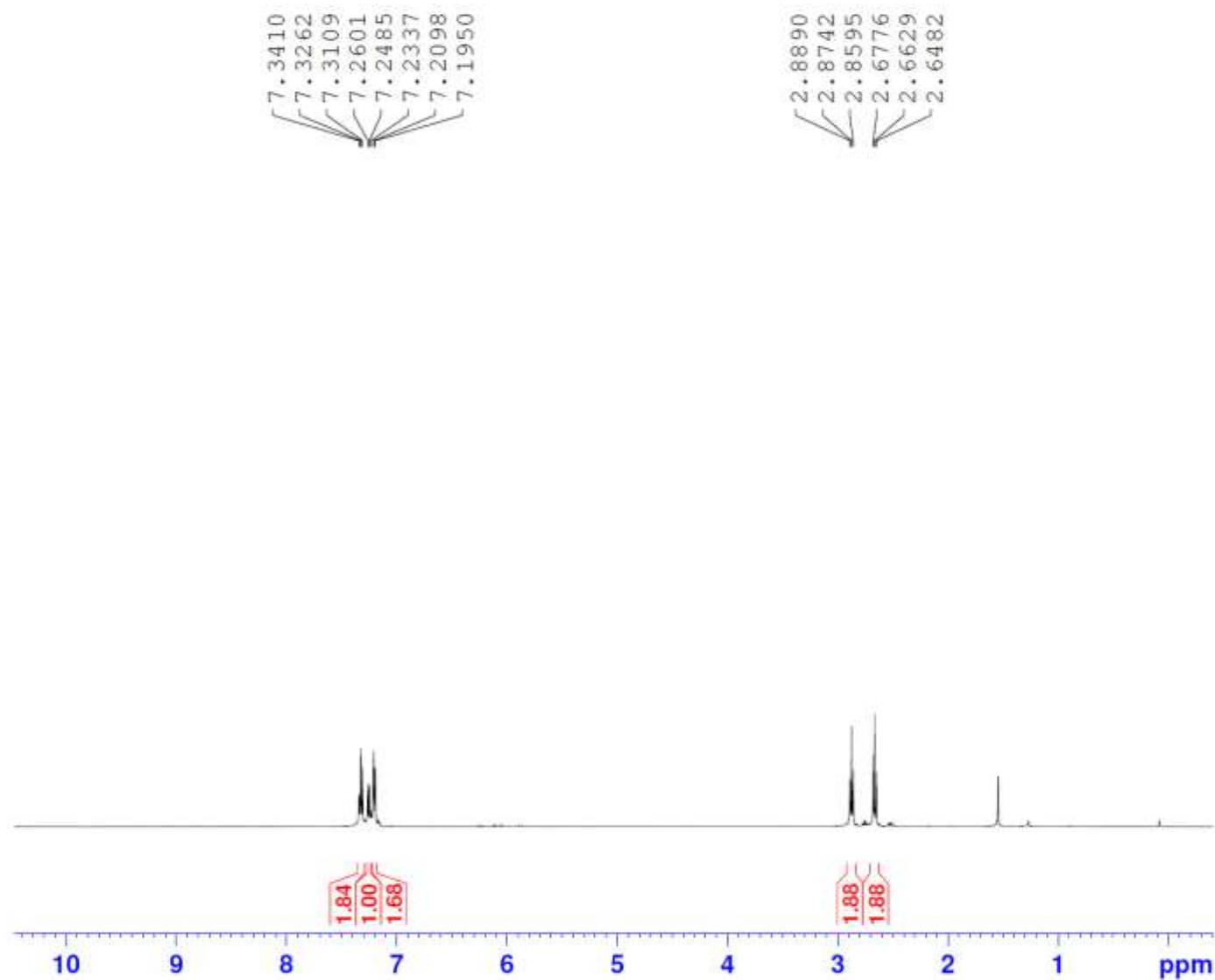
Date_ 20171207
Time 14.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 365
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P180-7



Current Data Parameters

NAME sjy2601
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180126
Time 15.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 305.2 K
D1 1.00000000 sec
TD0 1

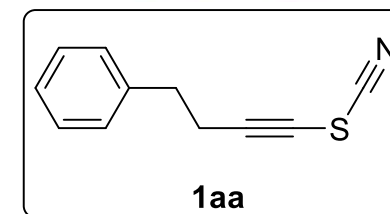
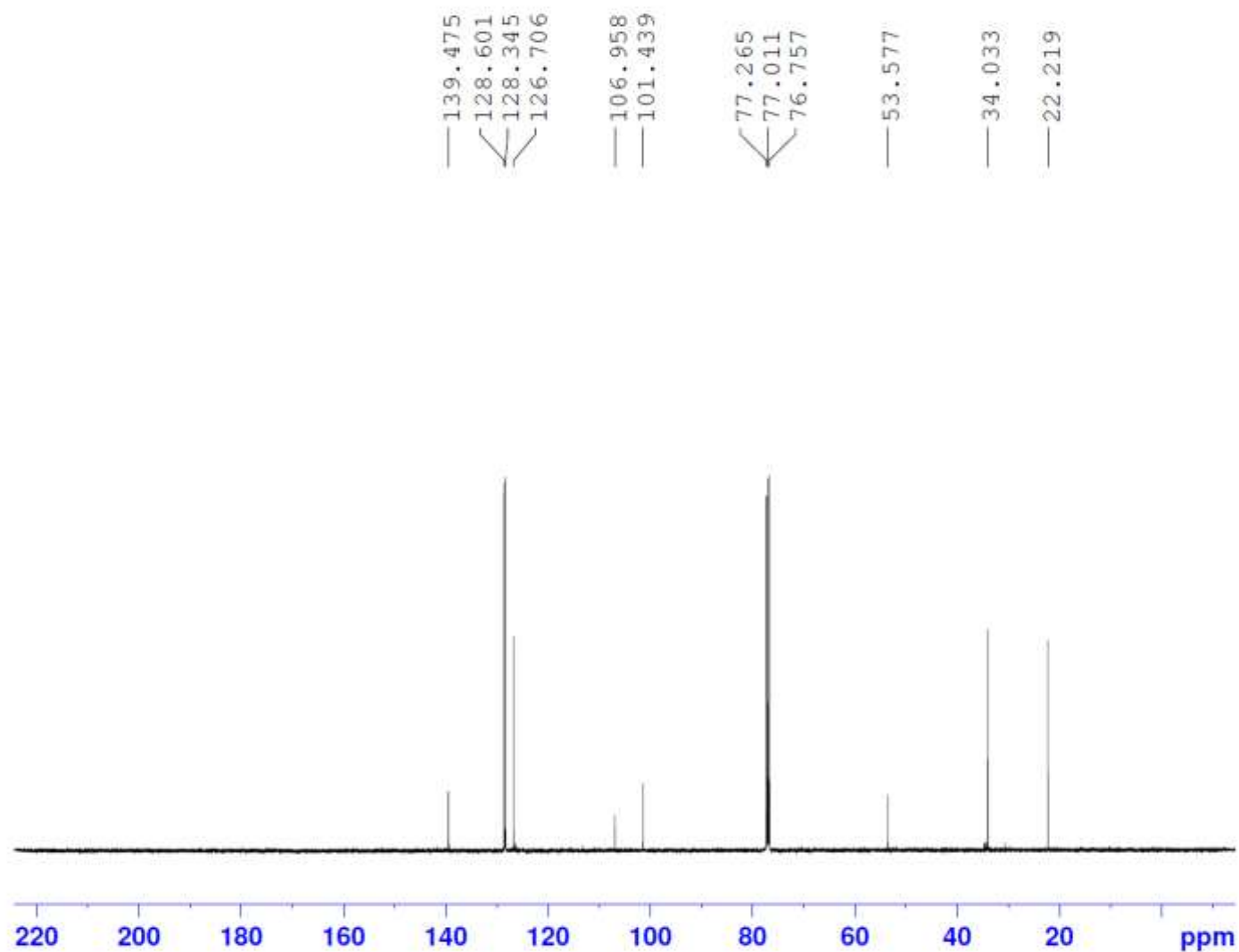
===== CHANNEL f1 =====

NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P180-7



```

EXPNO      2
PROCNO     1

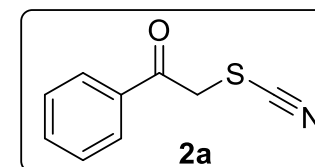
F2 - Acquisition Parameters
Date_      20180126
Time       15.12
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         967
DS         0
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0911744 sec
RG         16384
DW         16.650 usec
DE         6.00 usec
TE         306.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        250

===== CHANNEL f1 =====
NUC1       13C
P1         8.90 usec
PL1        0 dB
SFO1       125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2]  waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.25 dB
PL12       17.89 dB
PL13       15.83 dB
SFO2       500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

P188-7

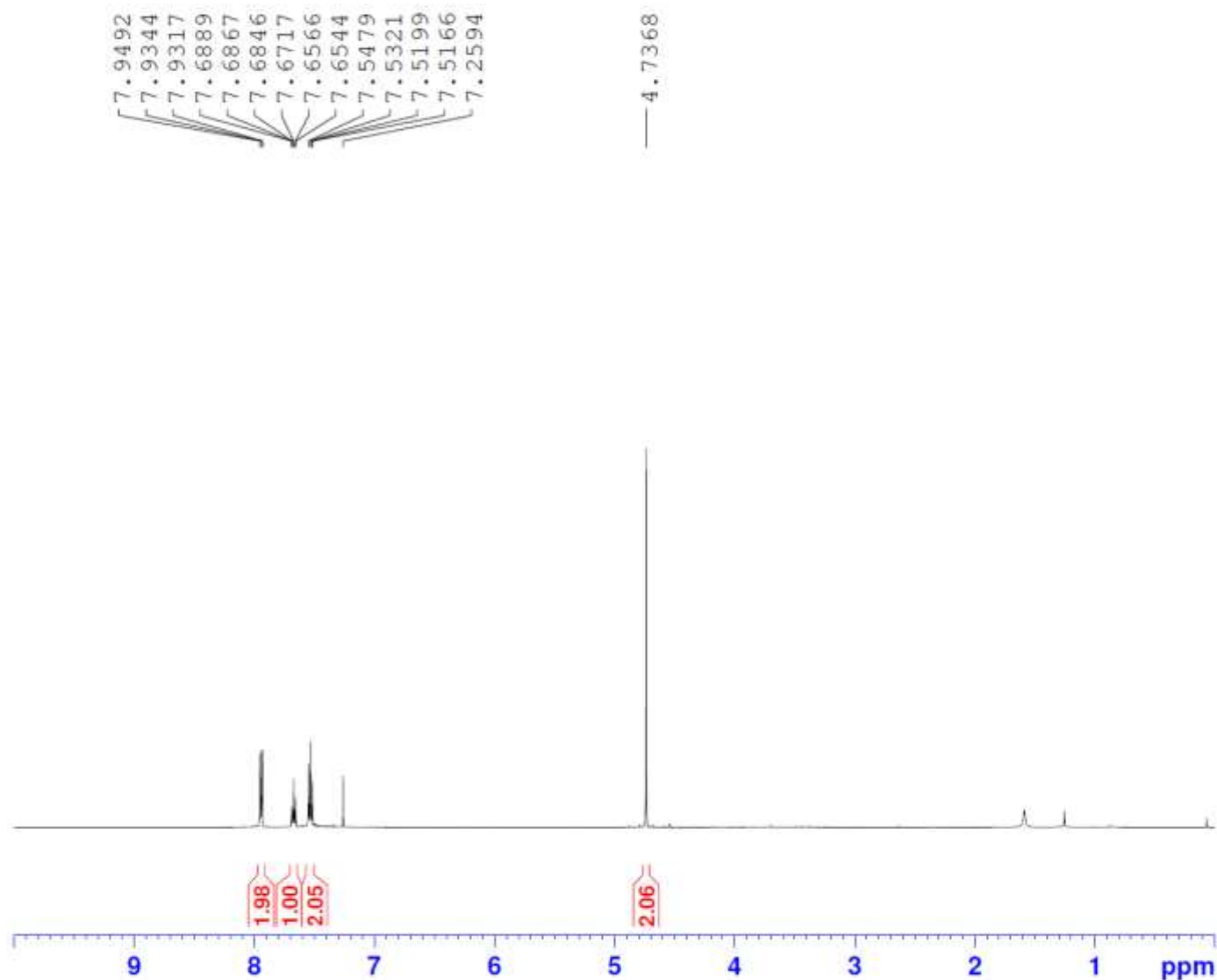


Current Data Parameters
 NAME sjy0311
 EXPNO 1
 PROCNO 1

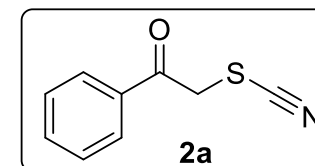
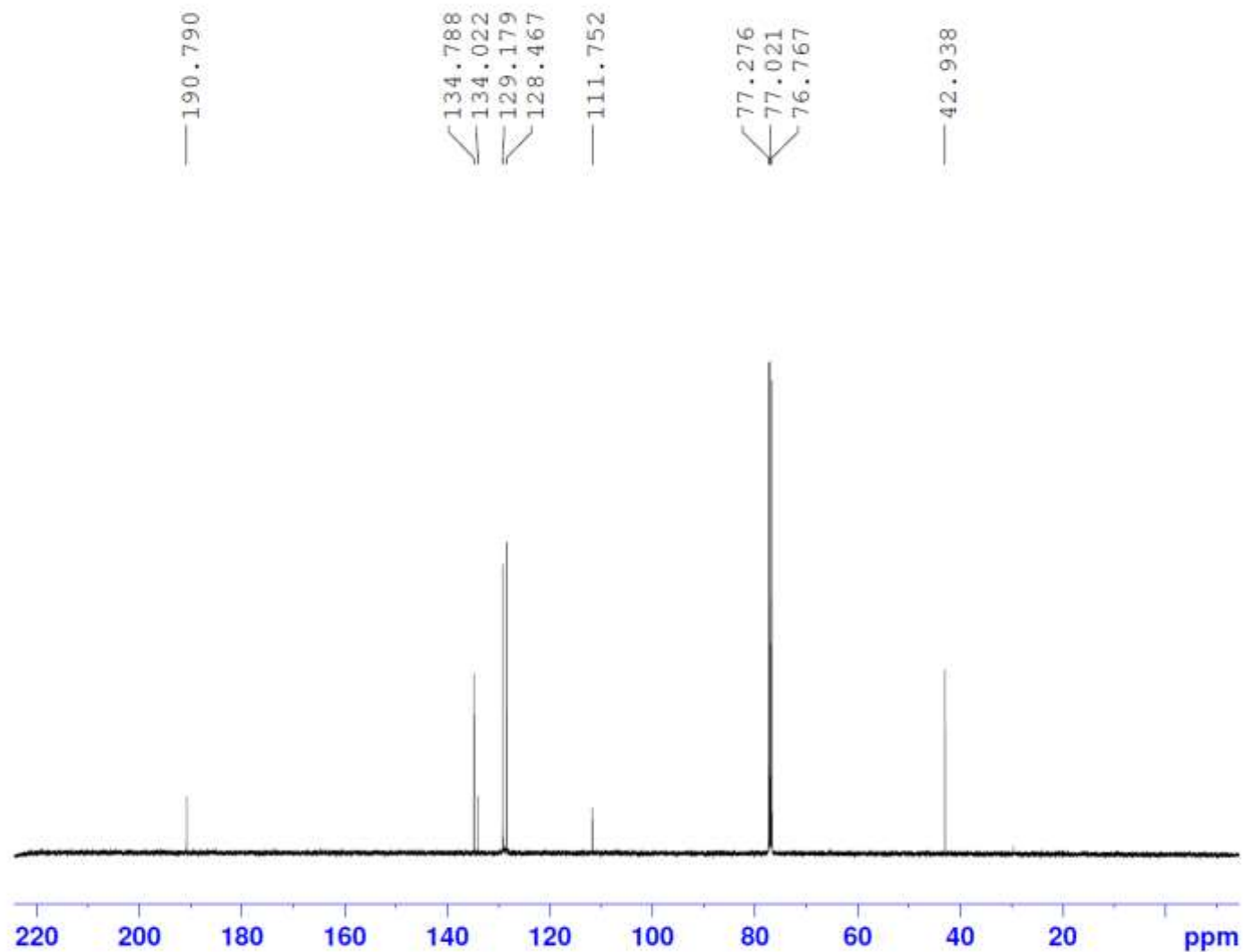
F2 - Acquisition Parameters
 Date_ 20171103
 Time 14.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 300.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



P188-7



Current Data Parameters
 NAME sjy0311
 EXPNO 2
 PROCNO 1

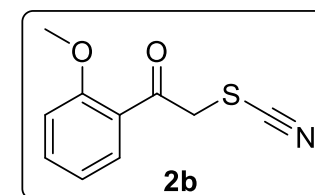
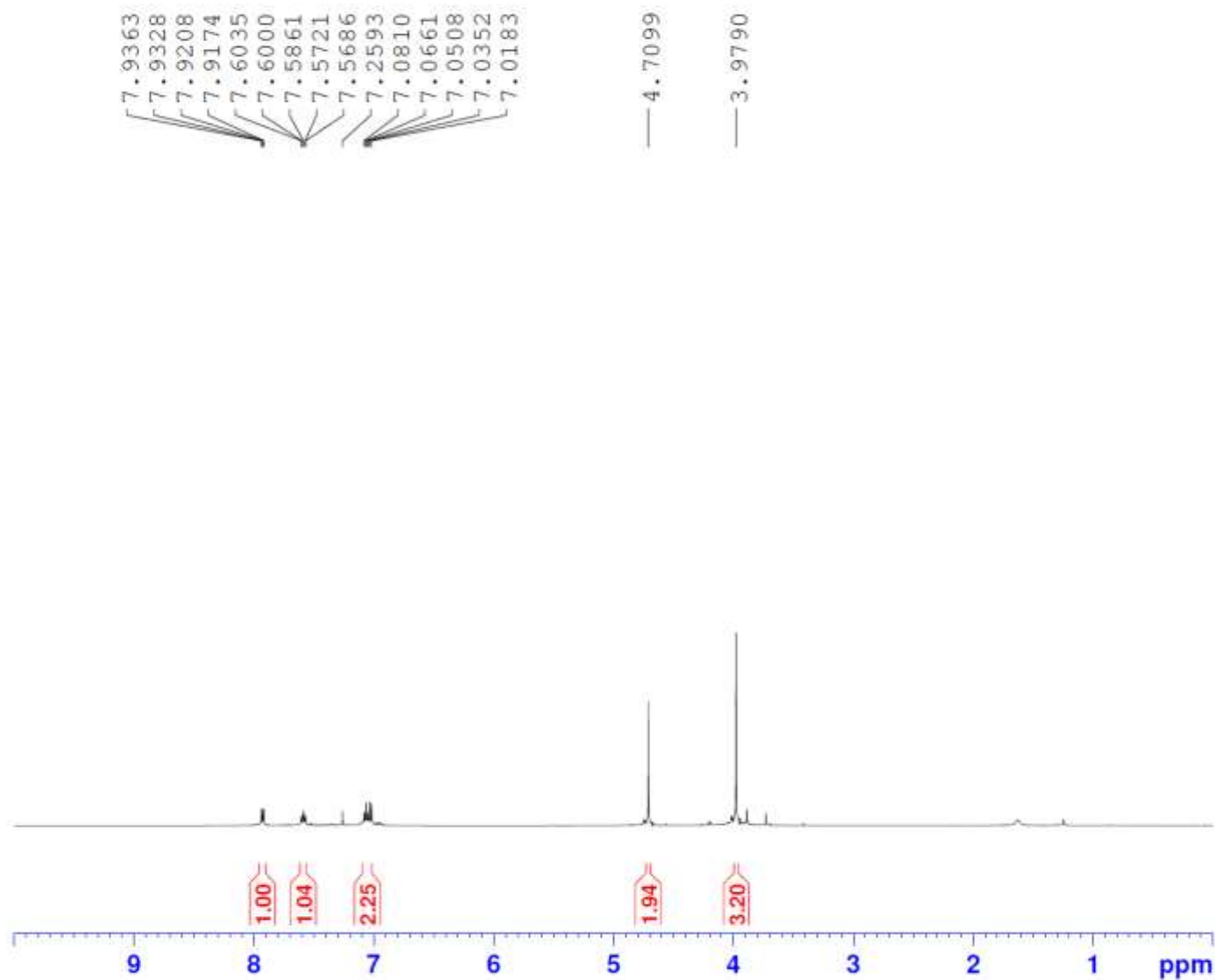
F2 - Acquisition Parameters
 Date_ 20171103
 Time 14.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 735
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 301.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P164-3



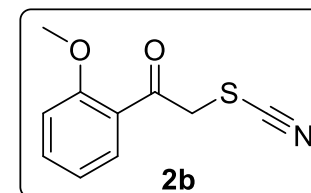
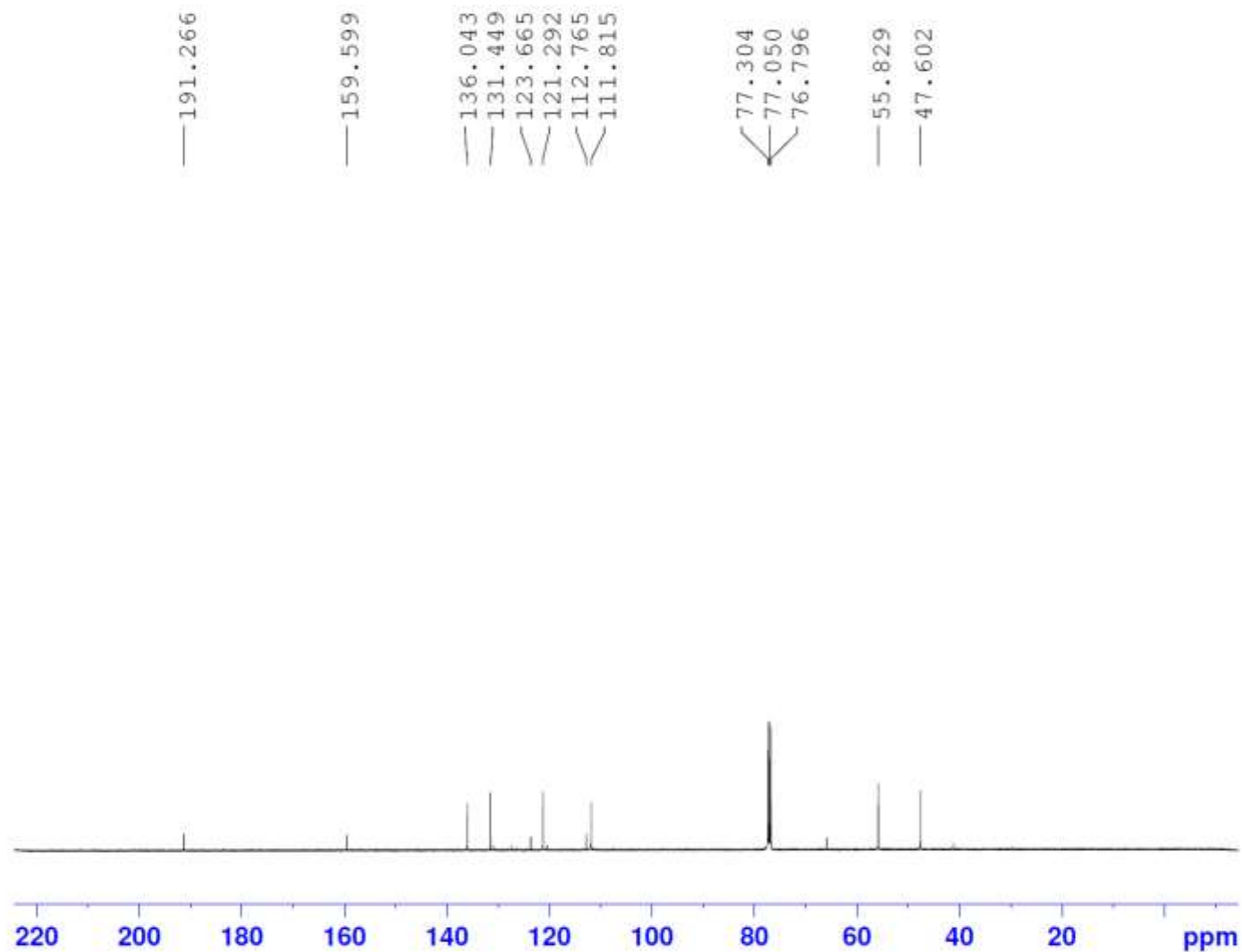
Current Data Parameters
NAME sjy2005
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180520
Time 9.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P164-3



Current Data Parameters
 NAME sjy2005
 EXPNO 5
 PROCNO 1

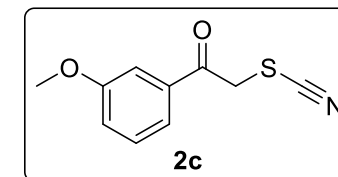
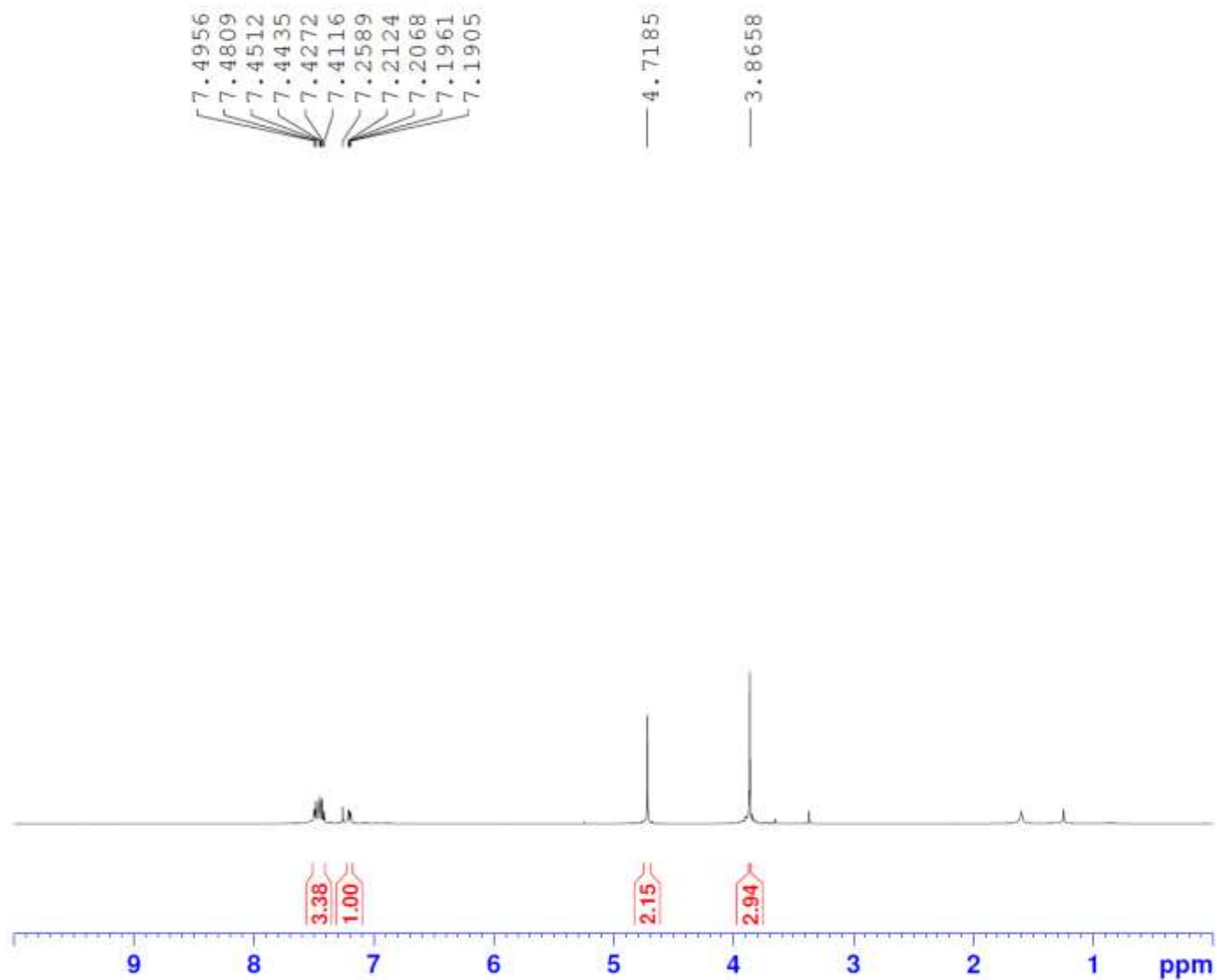
F2 - Acquisition Parameters
 Date_ 20180520
 Time 10.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1218
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P164-2



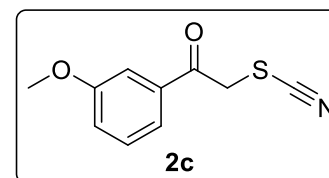
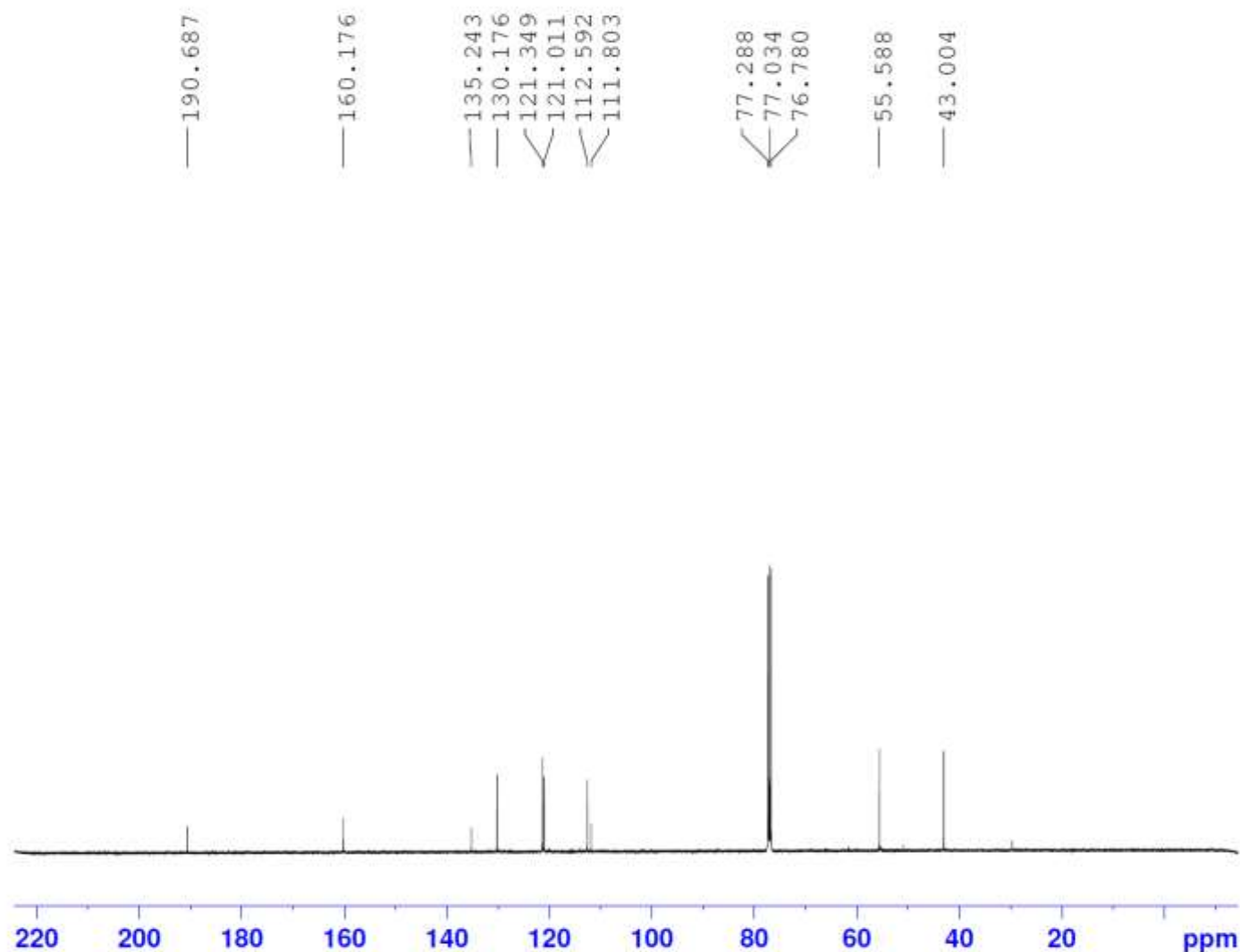
Current Data Parameters
NAME sjy2005
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180520
Time 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P164-2



Current Data Parameters
 NAME sjy2005
 EXPNO 6
 PROCNO 1

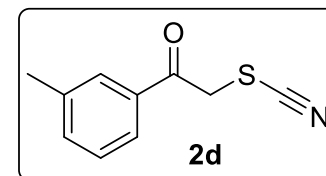
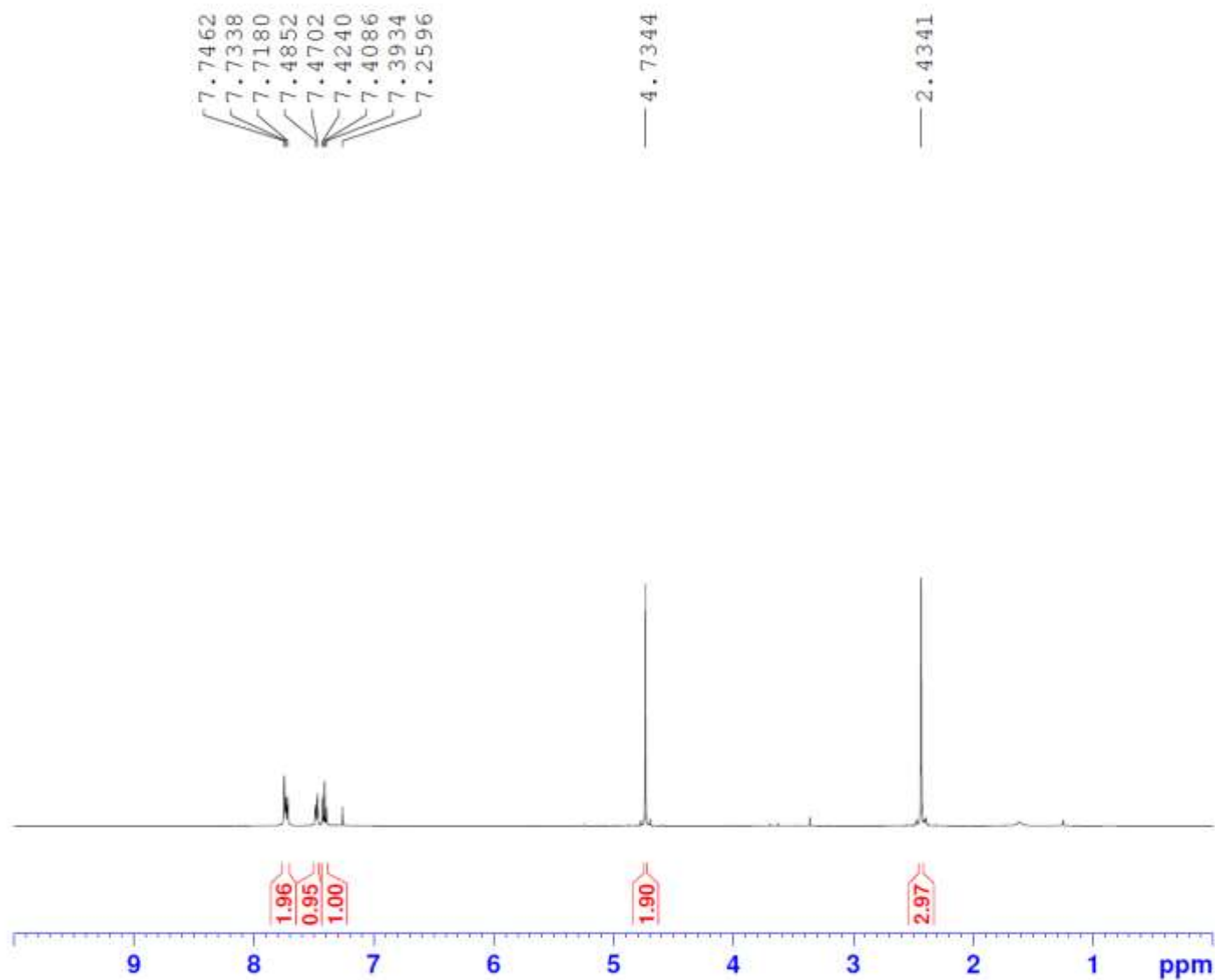
F2 - Acquisition Parameters
 Date_ 20180520
 Time 11.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1568
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 570.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P164-9



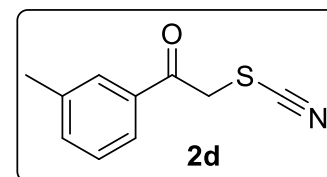
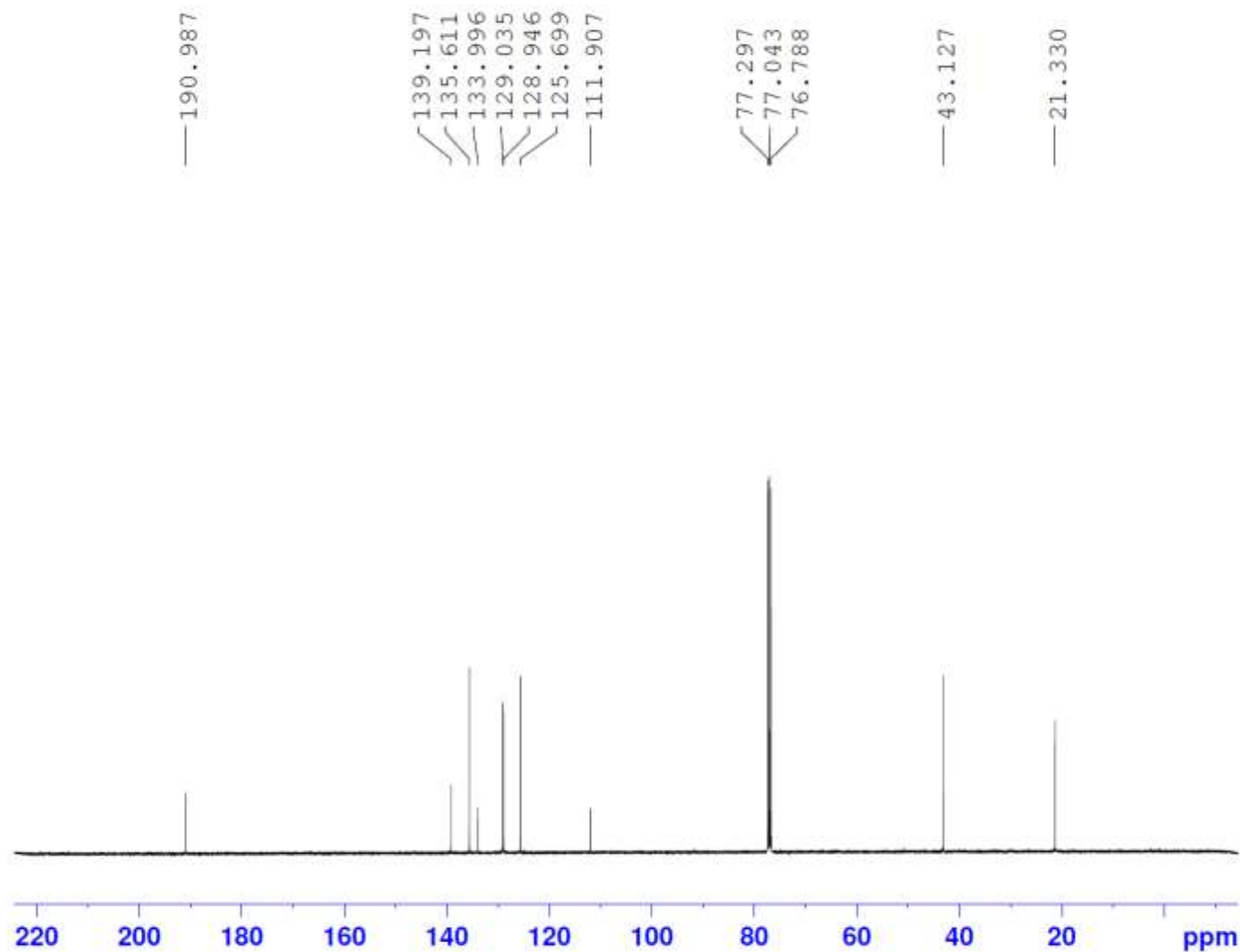
Current Data Parameters
 NAME sjy2305
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180523
 Time 9.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 296.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

P164-9



Current Data Parameters
 NAME sjy2305
 EXPNO 2
 PROCNO 1

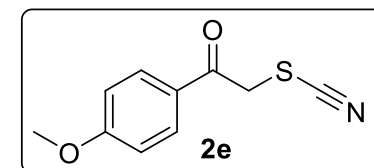
F2 - Acquisition Parameters
 Date_ 20180523
 Time 9.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1281
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 296.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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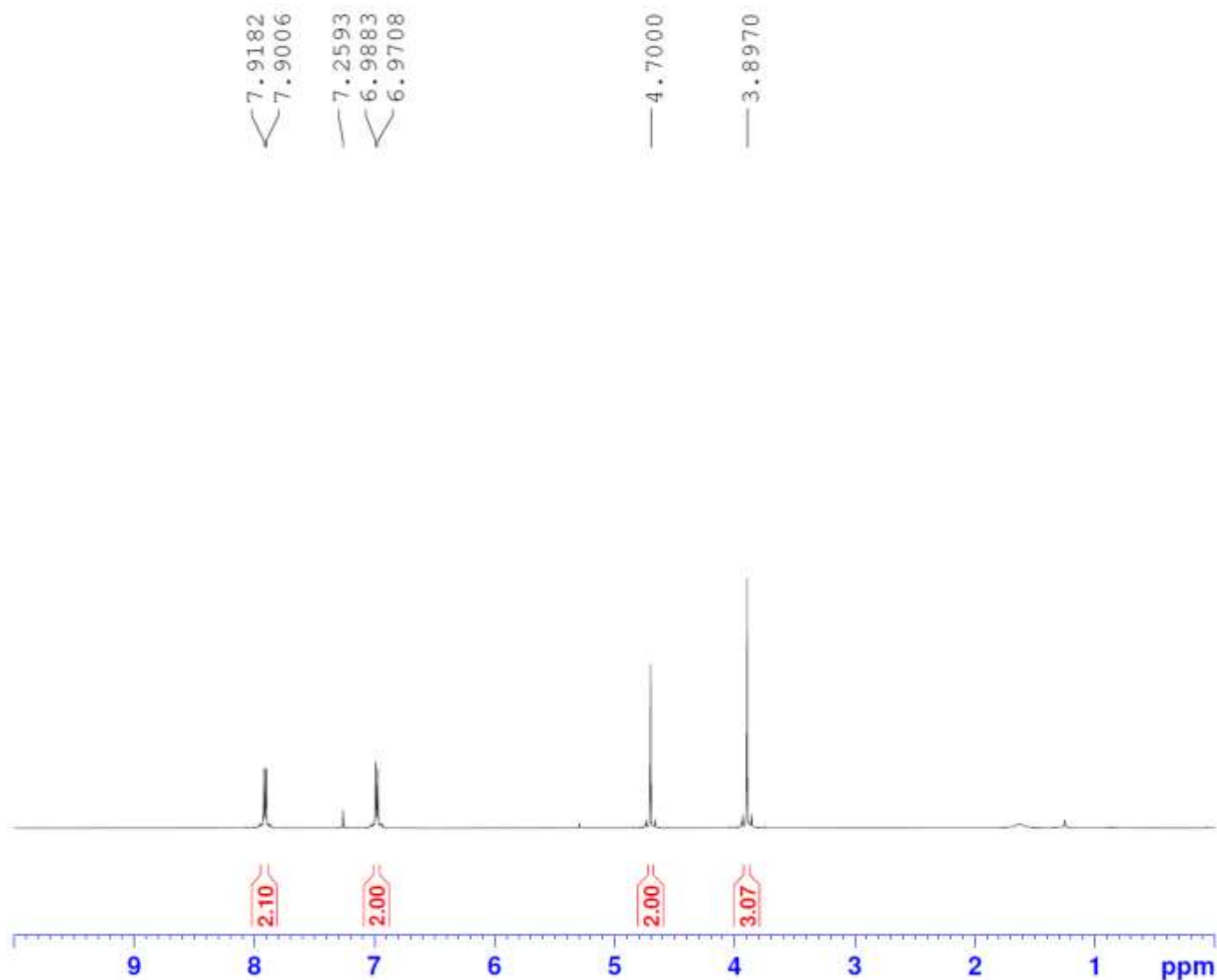


Current Data Parameters
 NAME sjy2006
 EXPNO 1
 PROCNO 1

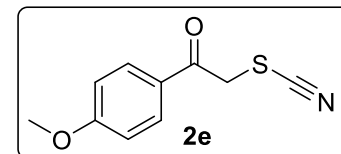
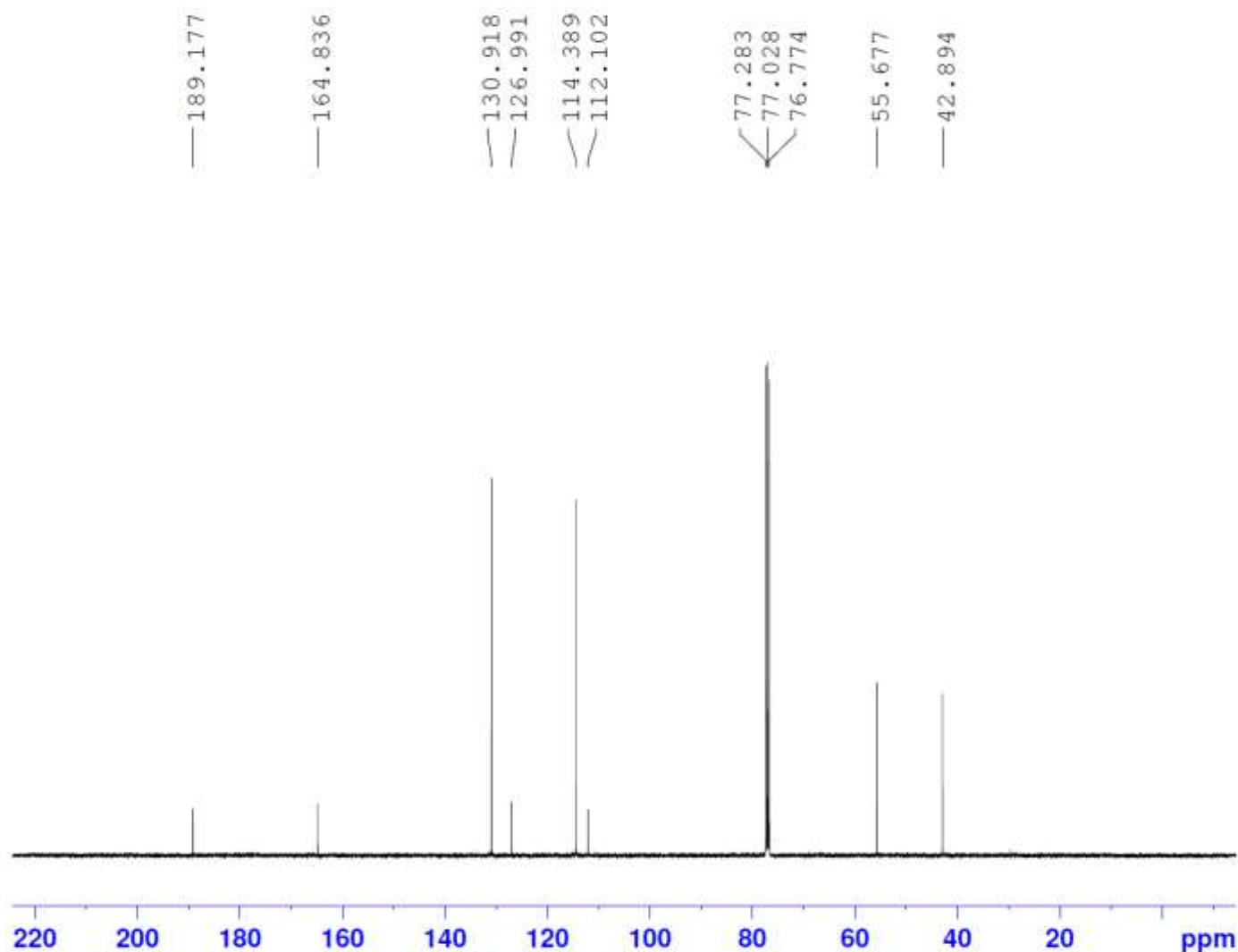
F2 - Acquisition Parameters
 Date_ 20180620
 Time 8.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 299.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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Current Data Parameters
NAME sjy2006
EXPNO 2
PROCNO 1

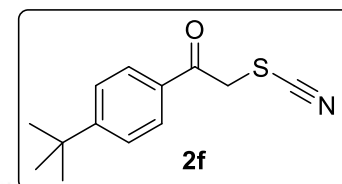
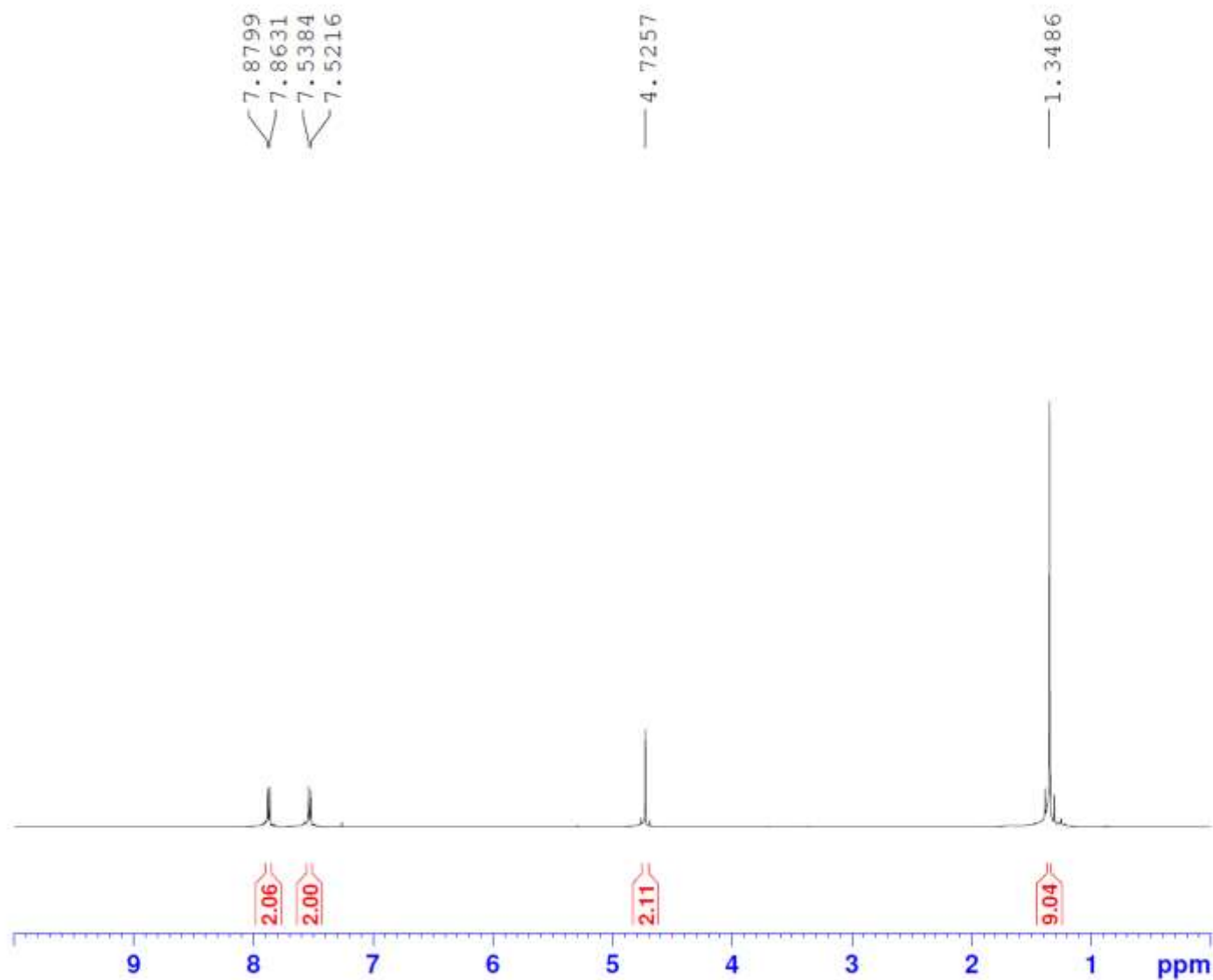
F2 - Acquisition Parameters
Date_ 20180620
Time 8.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 919
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 299.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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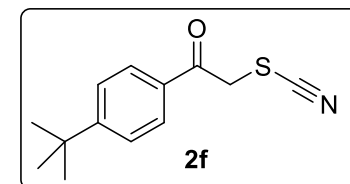
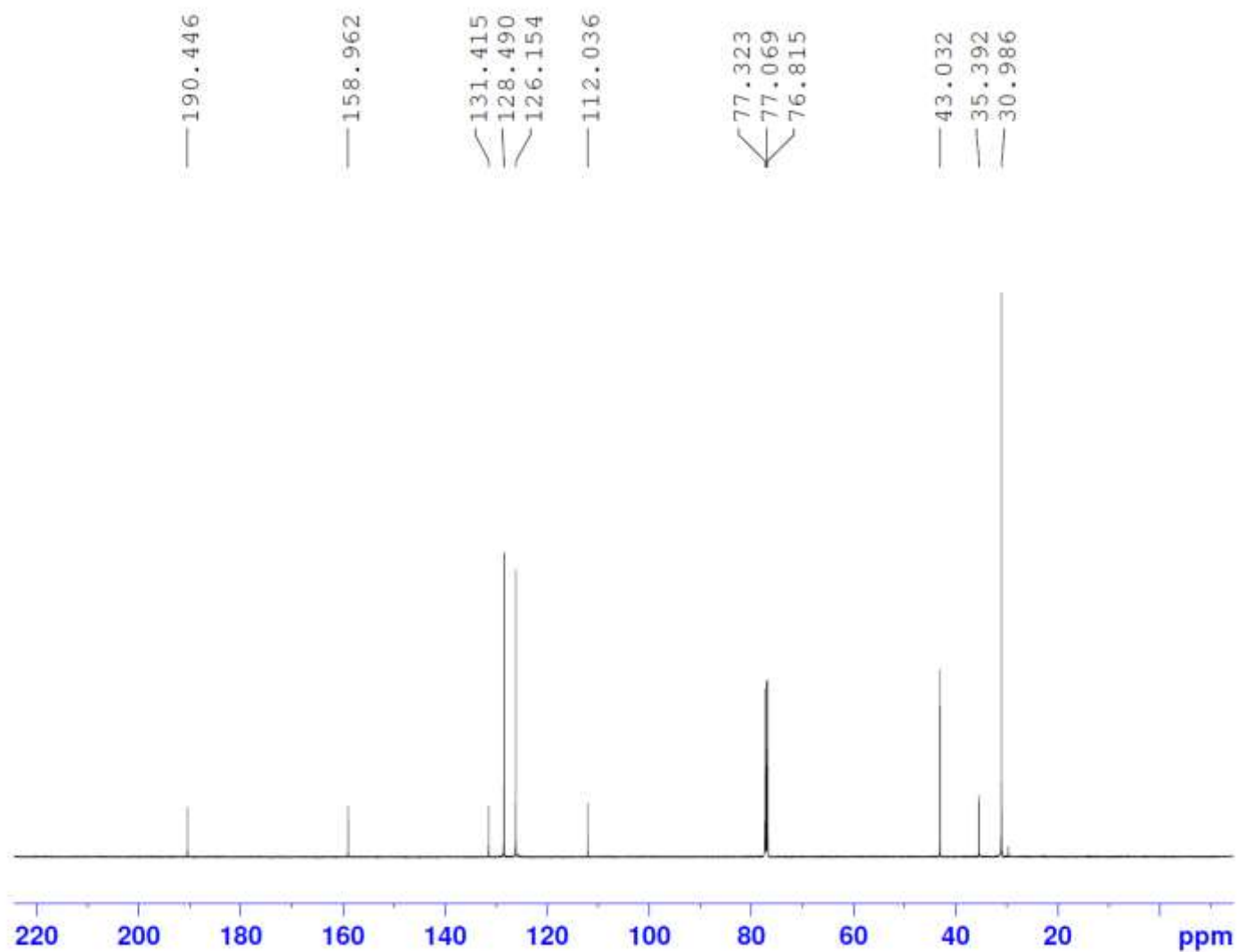
Current data parameters
 NAME sjy2905
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180529
 Time 9.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 57
 DW 48.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

P164-17



Current Data Parameters
 NAME sjy2905
 EXPNO 2
 PROCNO 1

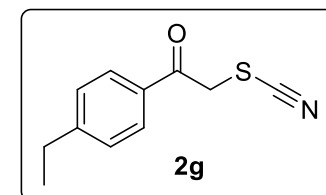
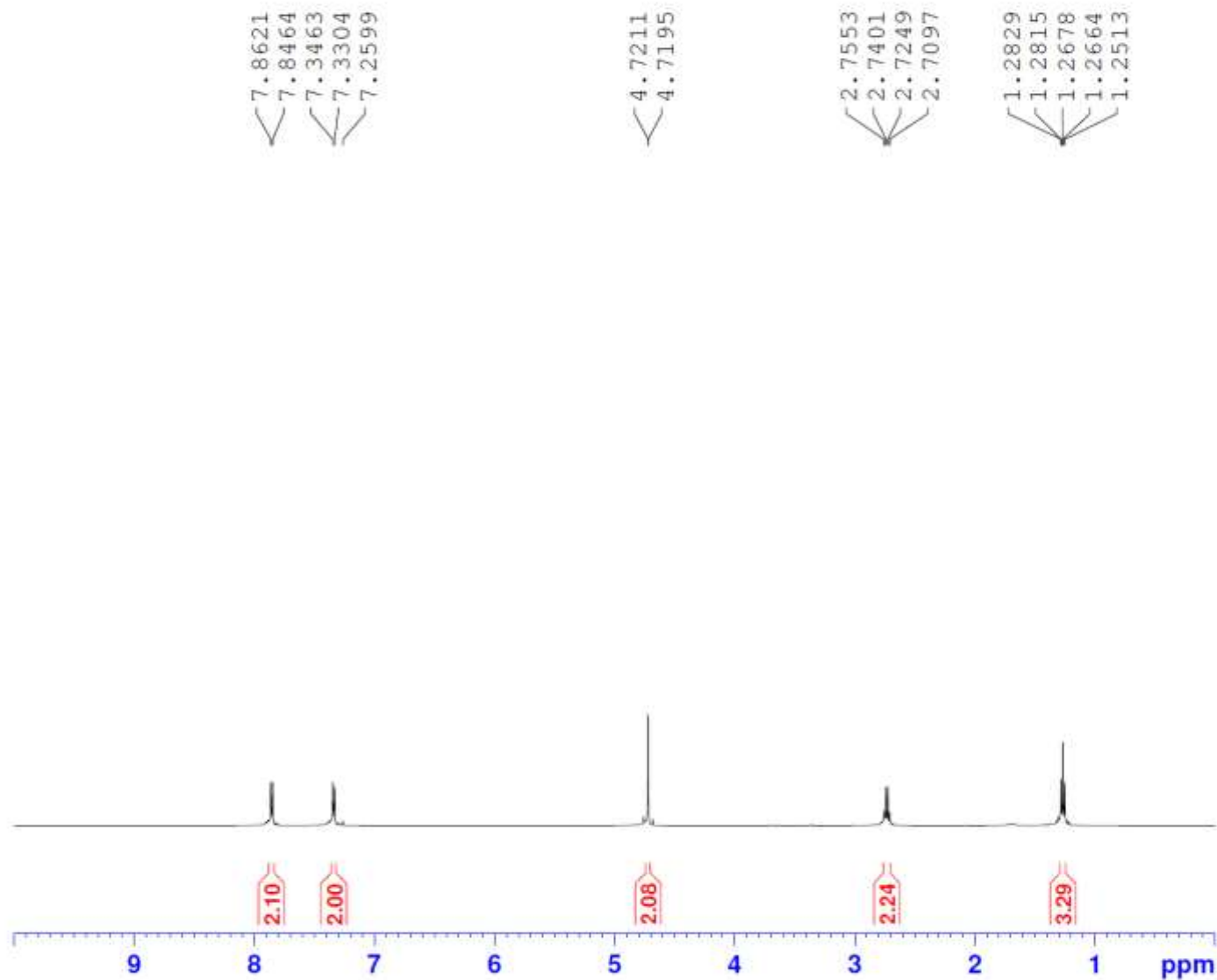
F2 - Acquisition Parameters
 Date_ 20180529
 Time 9.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2392
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 298.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P163-3



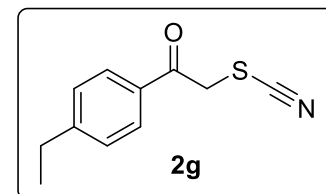
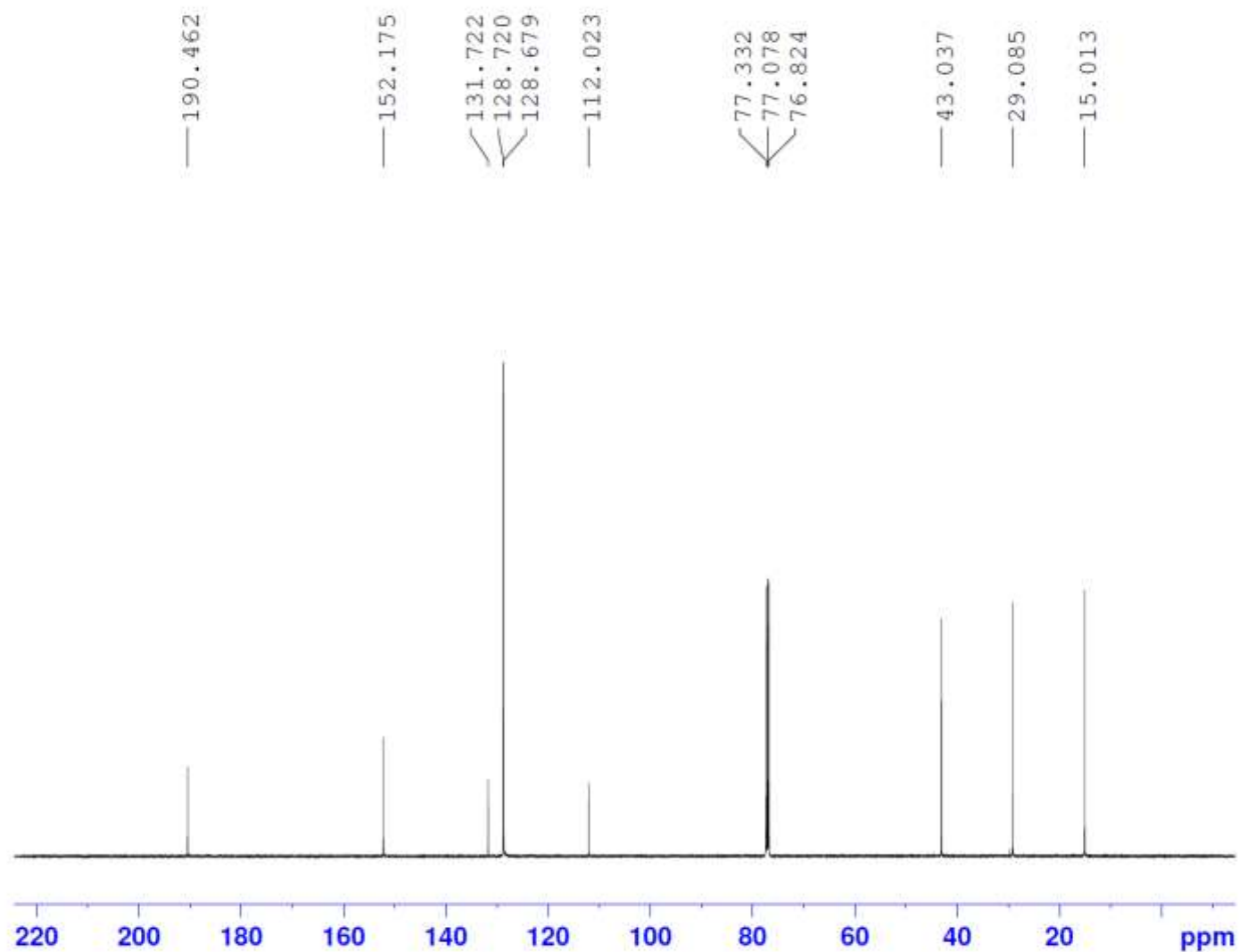
Current Data Parameters
 NAME sjy0306
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180603
 Time 8.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 64
 DW 48.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300131 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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Current Data Parameters
 NAME sjy0306
 EXPNO 3
 PROCNO 1

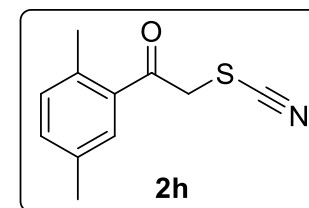
F2 - Acquisition Parameters
 Date_ 20180603
 Time 8.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1314
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 298.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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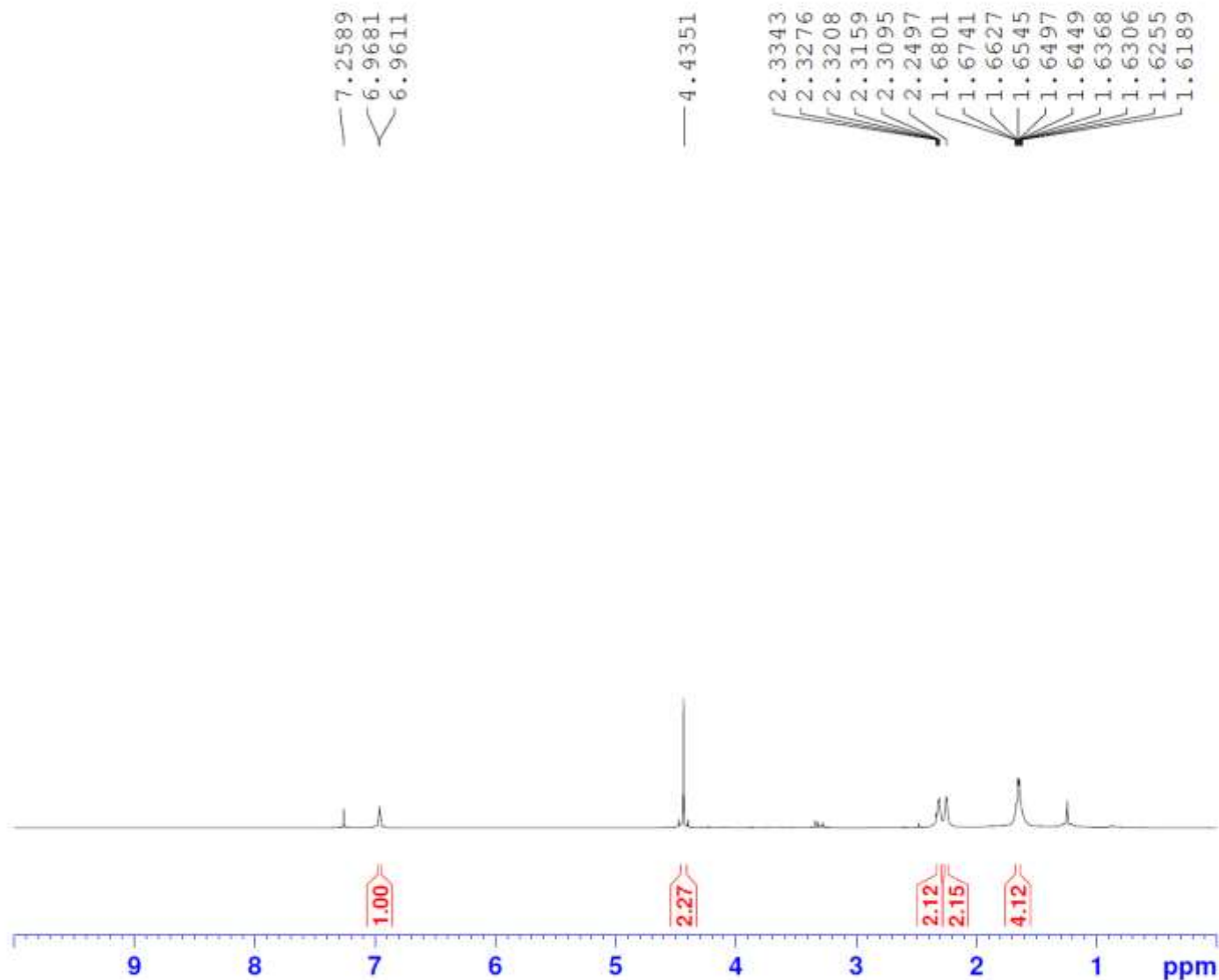


Current Data Parameters
 NAME sjy2605
 EXPNO 7
 PROCNO 1

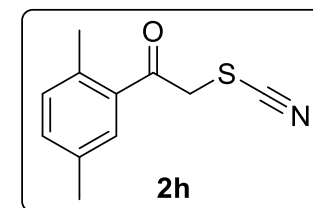
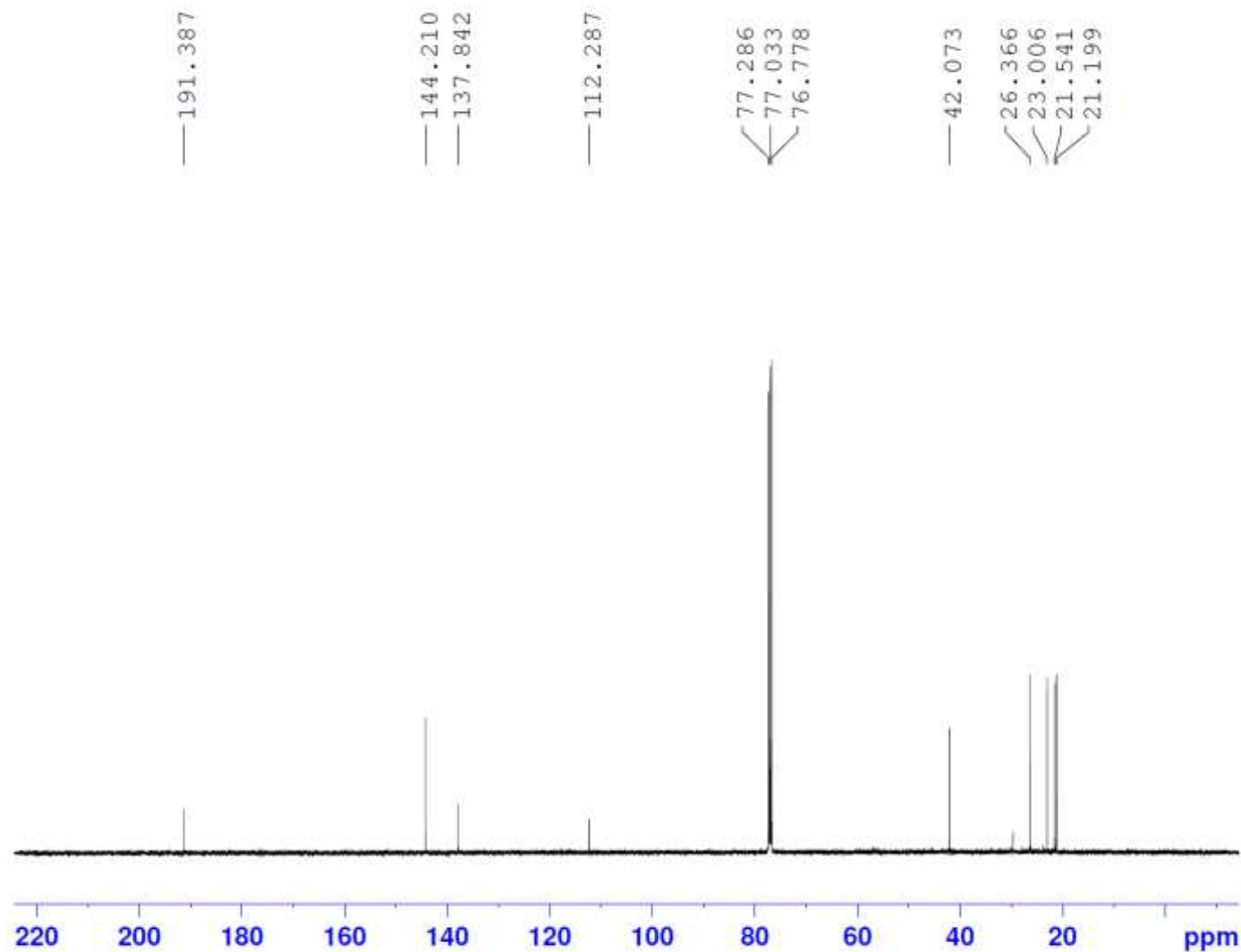
F2 - Acquisition Parameters
 Date_ 20180526
 Time 11.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 296.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300143 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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Current Data Parameters
 NAME sjy2605
 EXPNO 6
 PROCNO 1

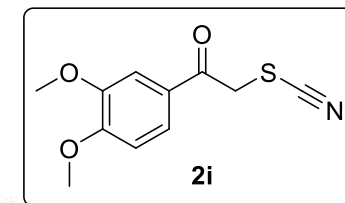
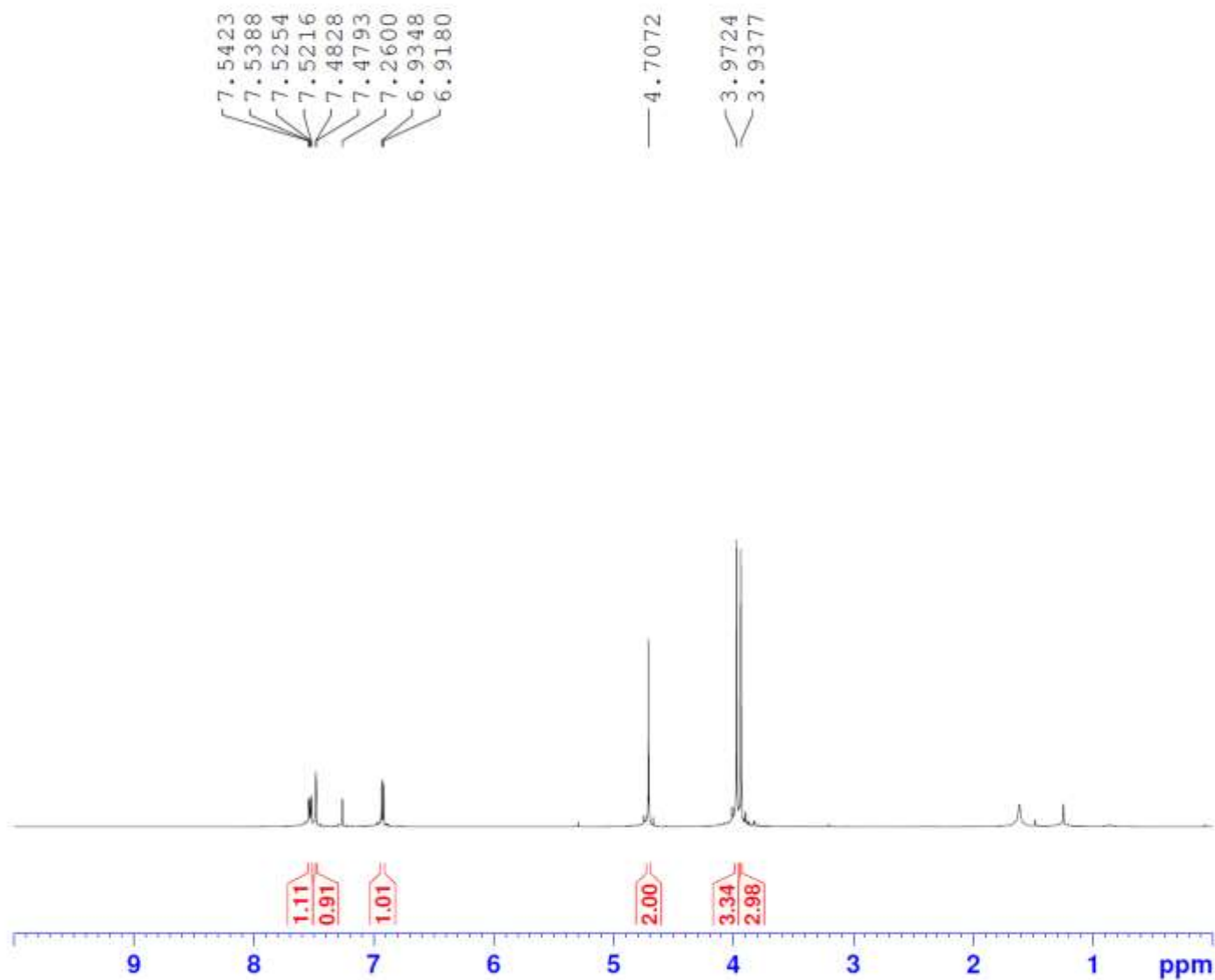
F2 - Acquisition Parameters
 Date_ 20180526
 Time 11.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 998
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.899999998 sec
 TD0 150

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P163-2



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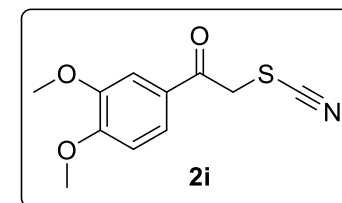
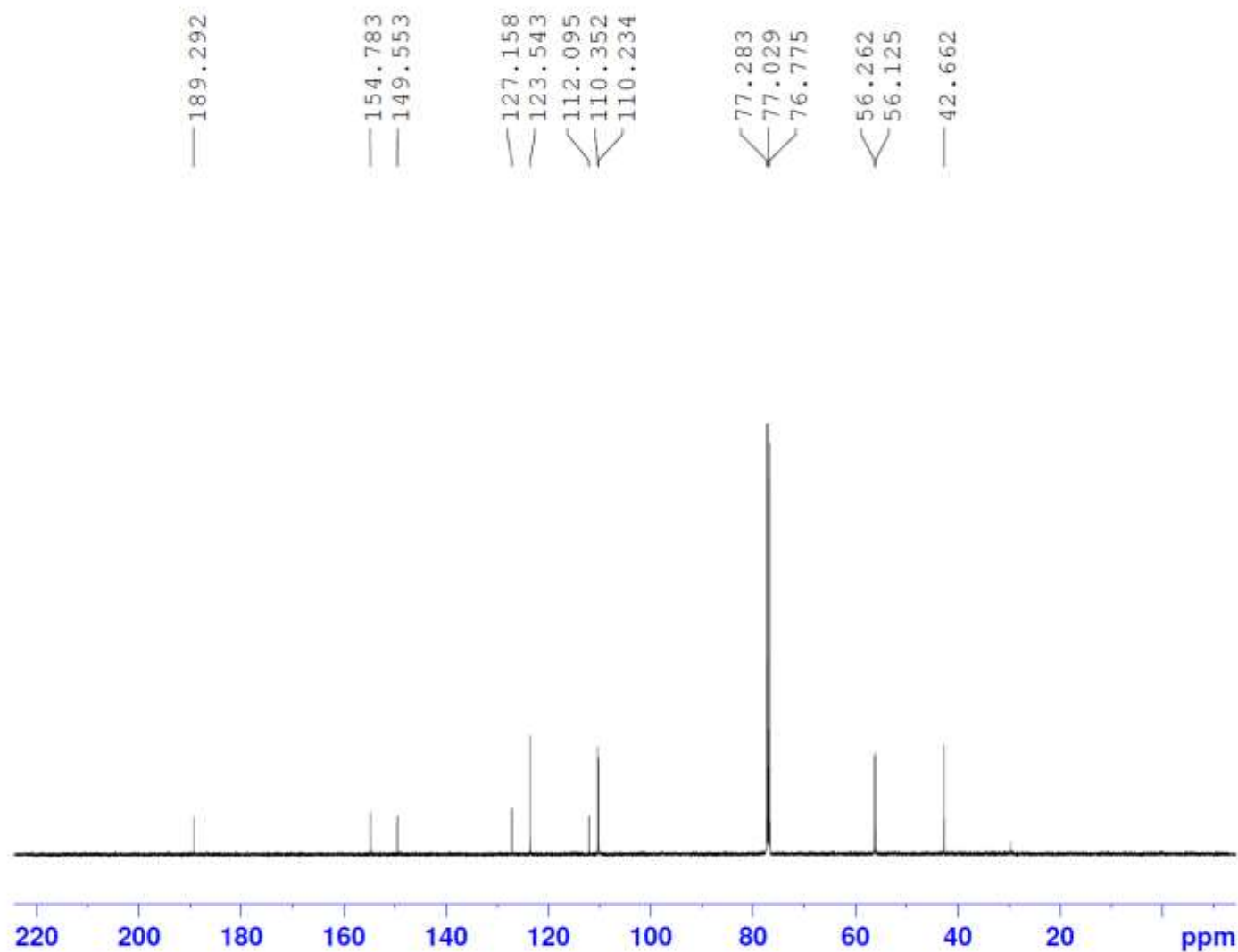
=====
NAME      sjy0306
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20180603
Time      8.39
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        32768
SOLVENT   CDC13
NS        8
DS        0
SWH       10330.578 Hz
FIDRES    0.315264 Hz
AQ        1.5859712 sec
RG        228.1
DW        48.400 usec
DE        6.00 usec
TE        298.0 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        10.50 usec
PL1       0.25 dB
SFO1      500.1330885 MHz

F2 - Processing parameters
SI        16384
SF        500.1300131 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

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Current Data Parameters
 NAME sjy0306
 EXPNO 4
 PROCNO 1

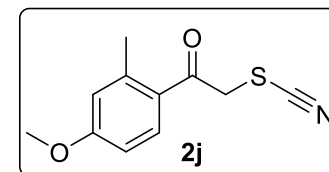
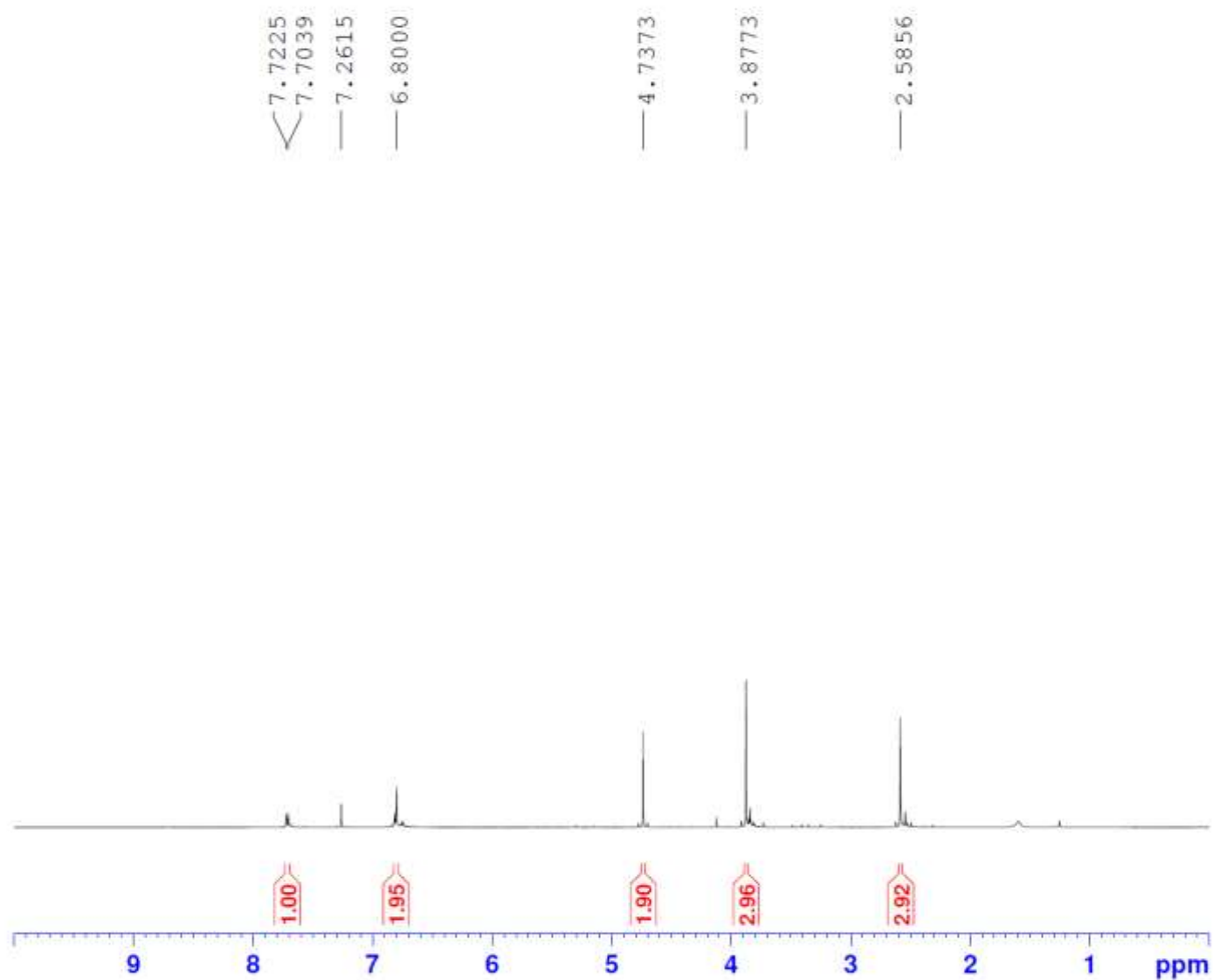
F2 - Acquisition Parameters
 Date_ 20180603
 Time 9.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1559
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 298.9 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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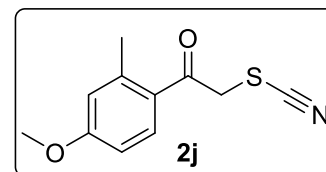
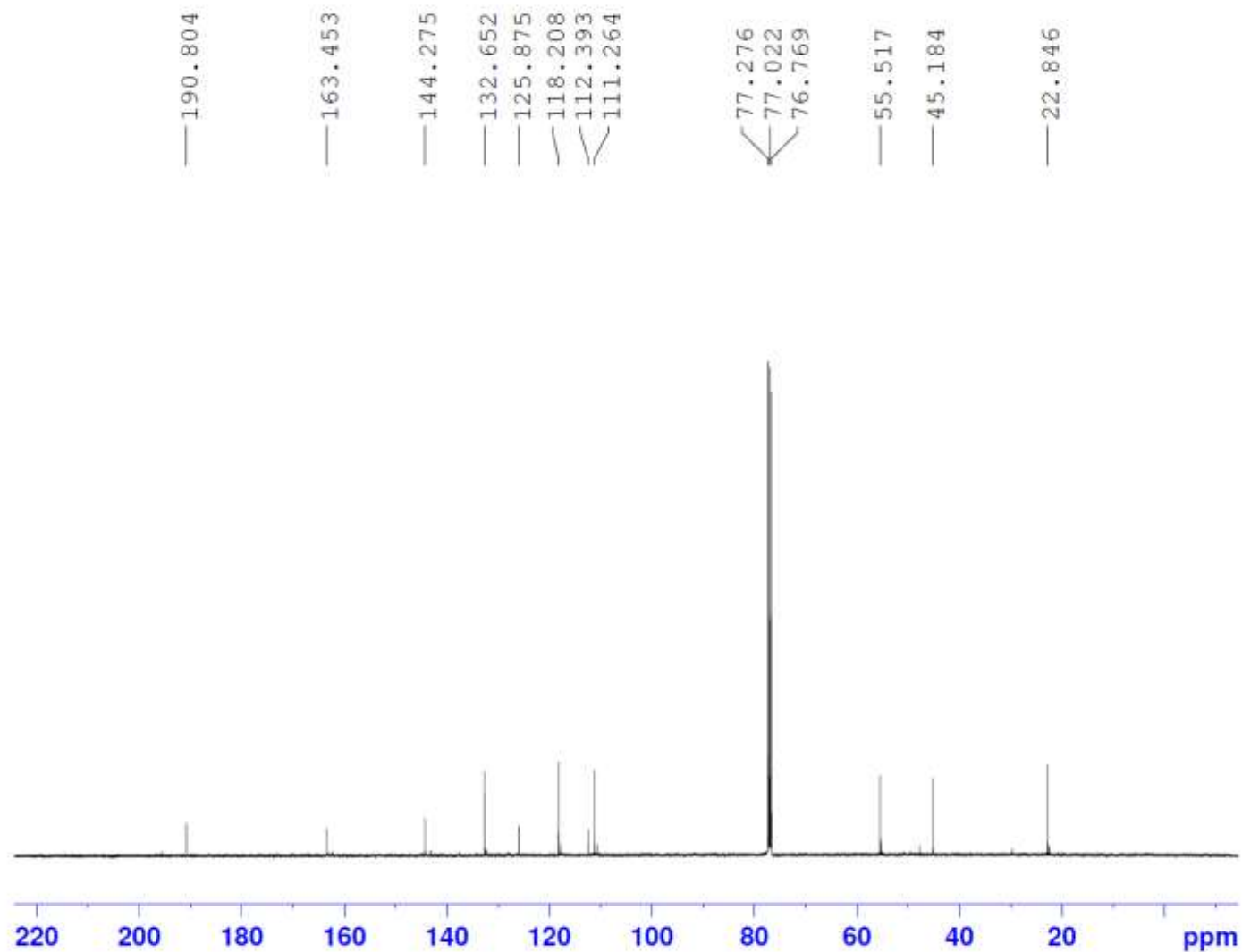
Current Data Parameters
NAME sjy0806
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180608
Time 9.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Current Data Parameters
 NAME sjy0806
 EXPNO 5
 PROCNO 1

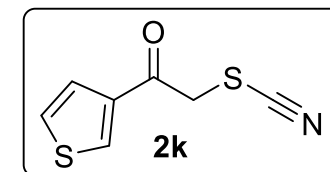
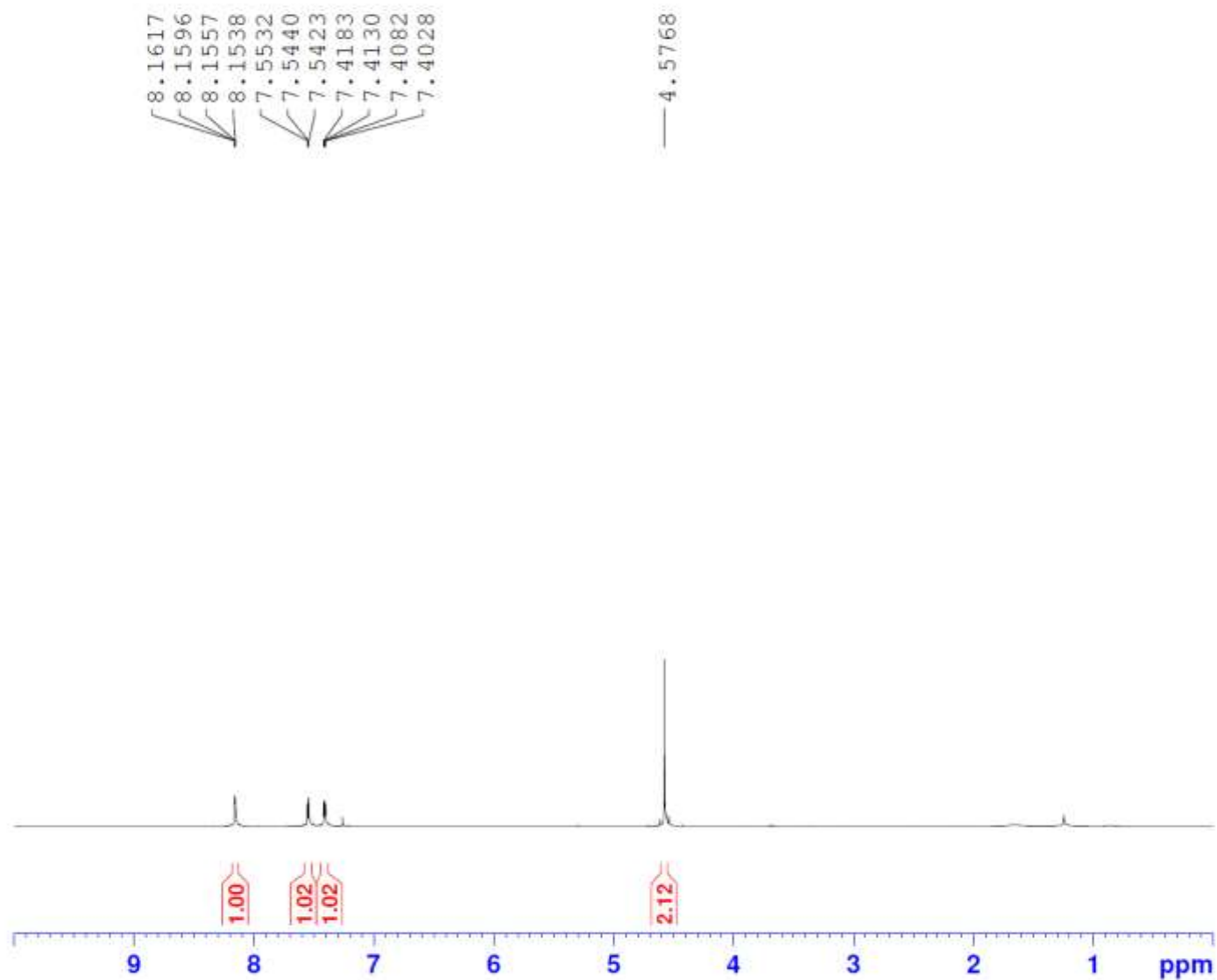
F2 - Acquisition Parameters
 Date_ 20180608
 Time 9.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2382
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 298.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P163-12



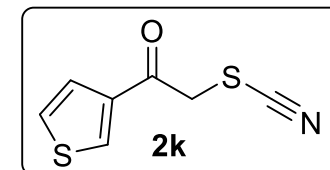
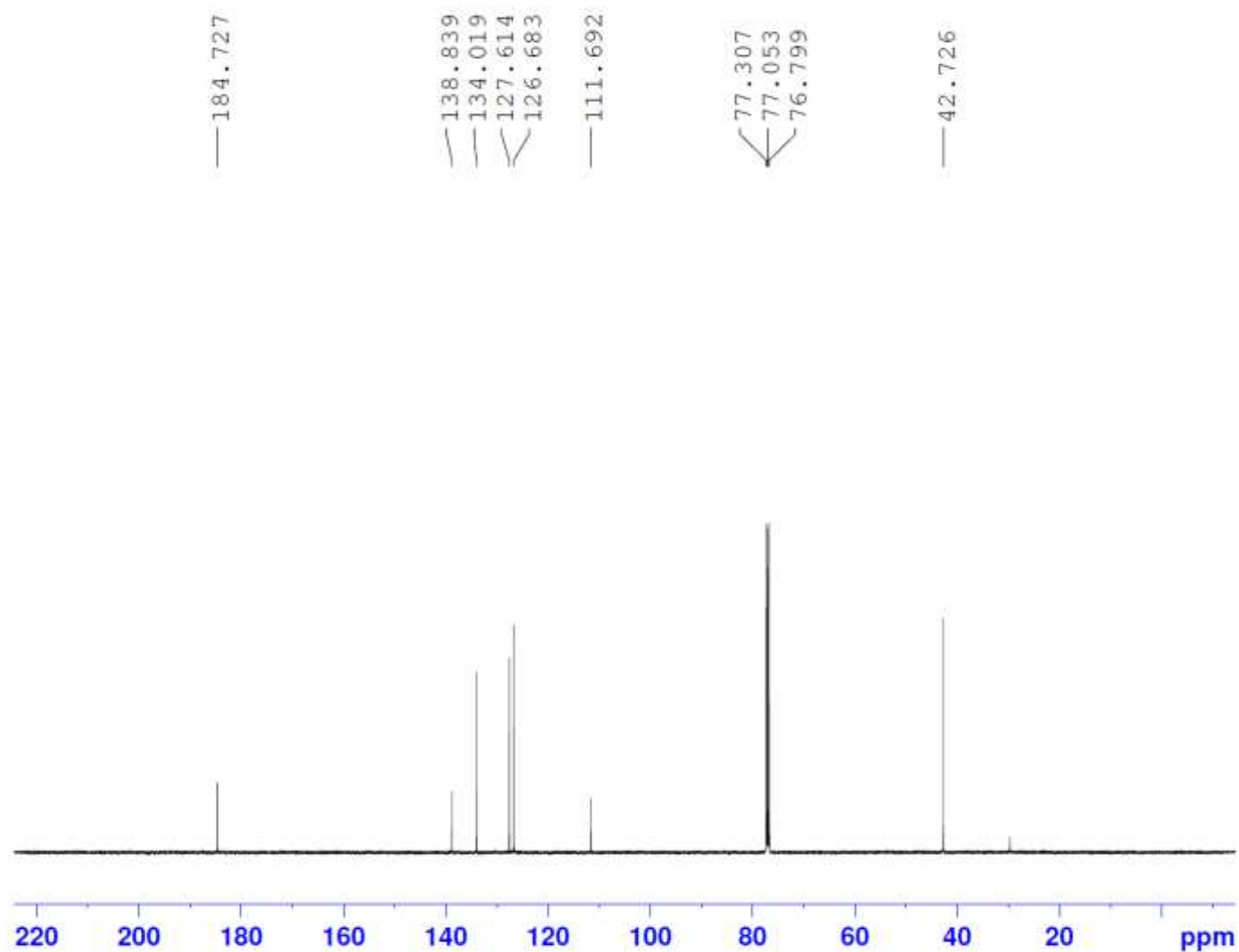
Current Data Parameters
NAME sjy0306-2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180603
Time 11.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Current Data Parameters
NAME sjy0306-2
EXPNO 4
PROCNO 1

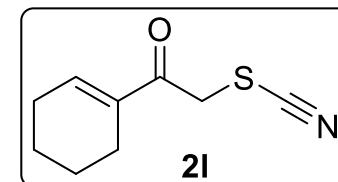
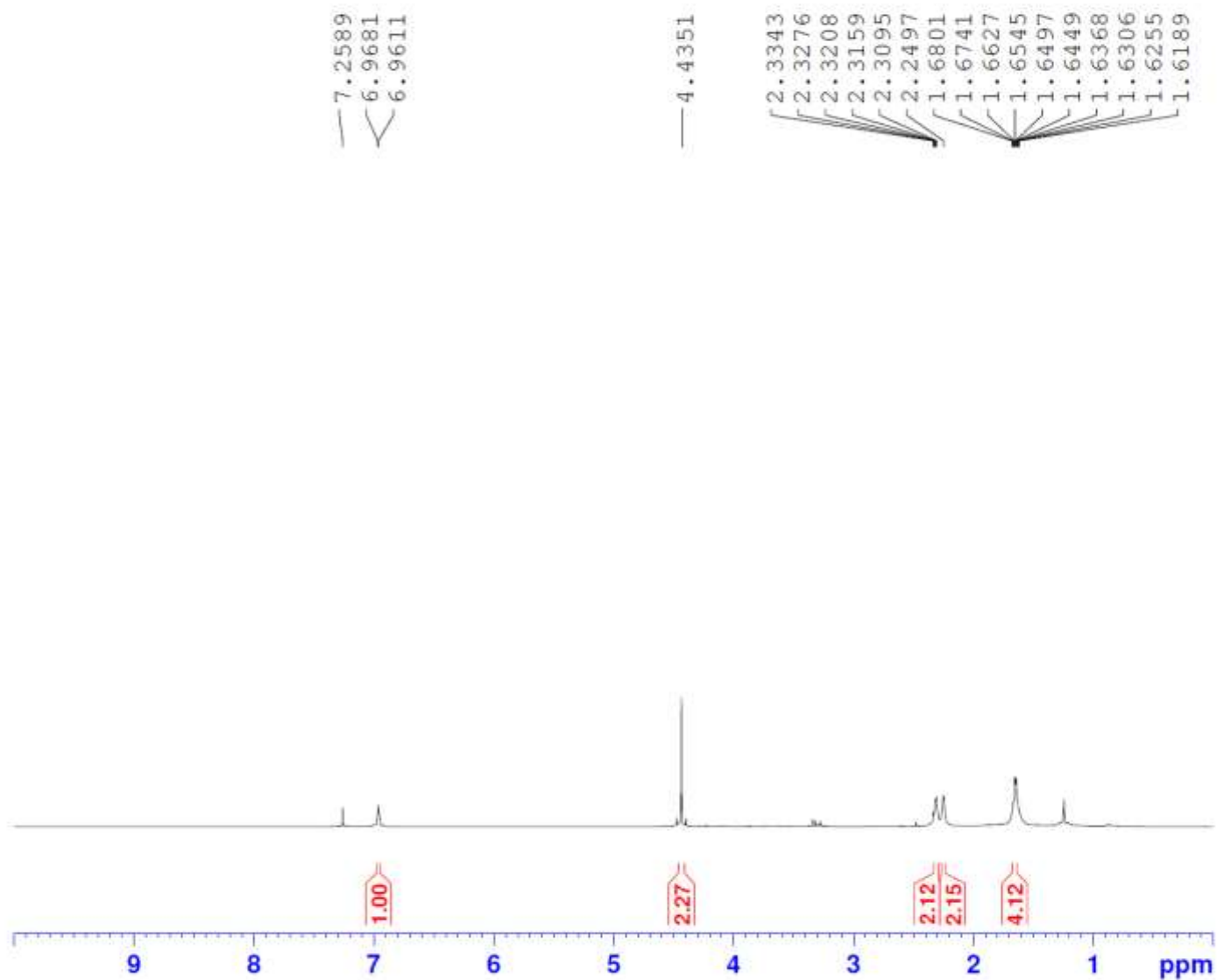
F2 - Acquisition Parameters
Date_ 20180603
Time 11.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1455
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 298.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P164-14



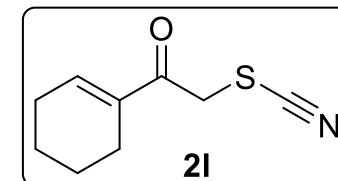
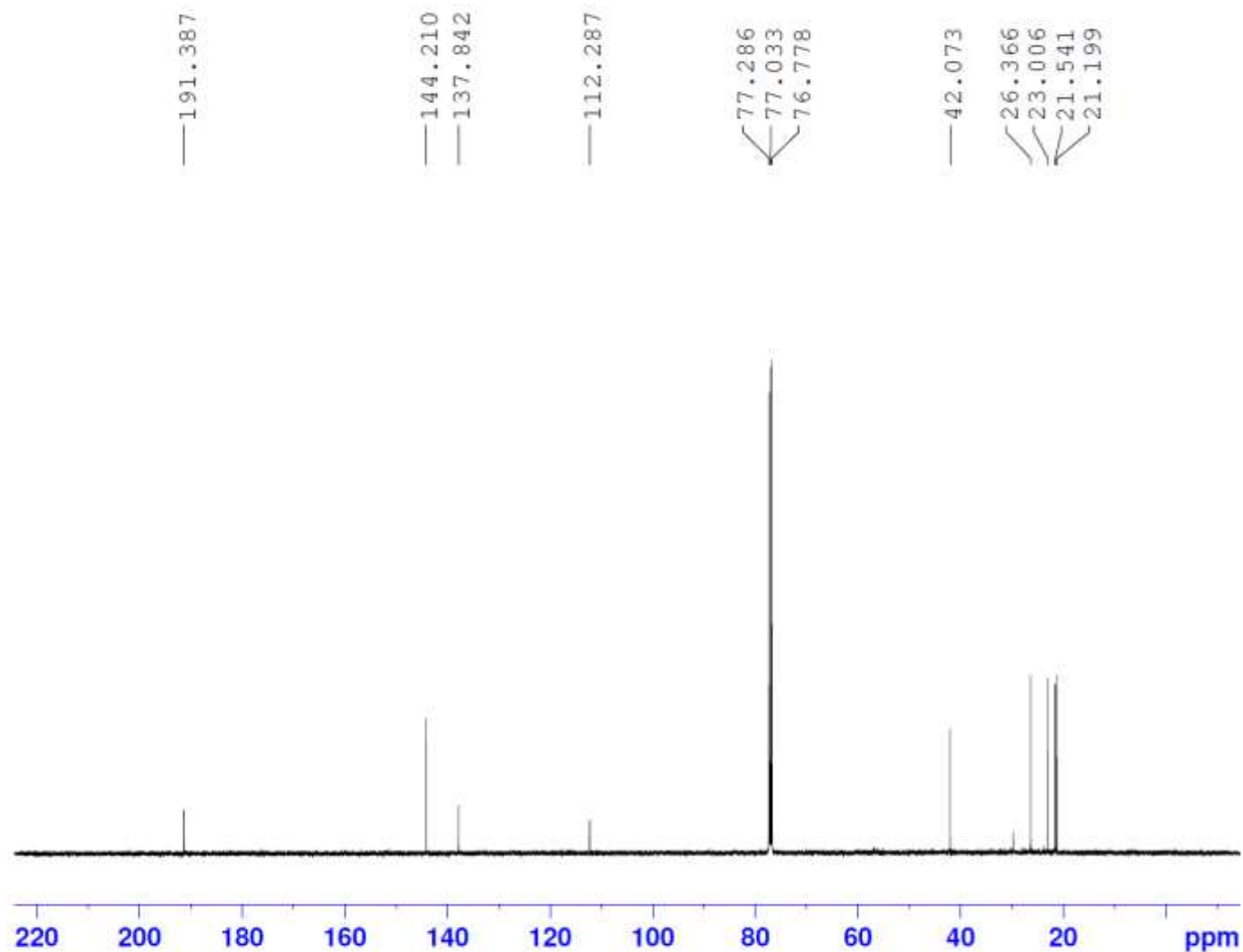
Current Data Parameters
 NAME sjy2605
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180526
 Time 11.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 296.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300143 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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Current Data Parameters
 NAME sjy2605
 EXPNO 6
 PROCNO 1

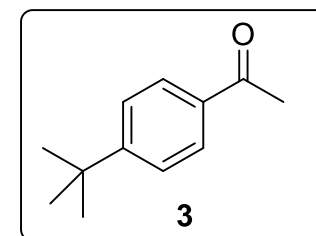
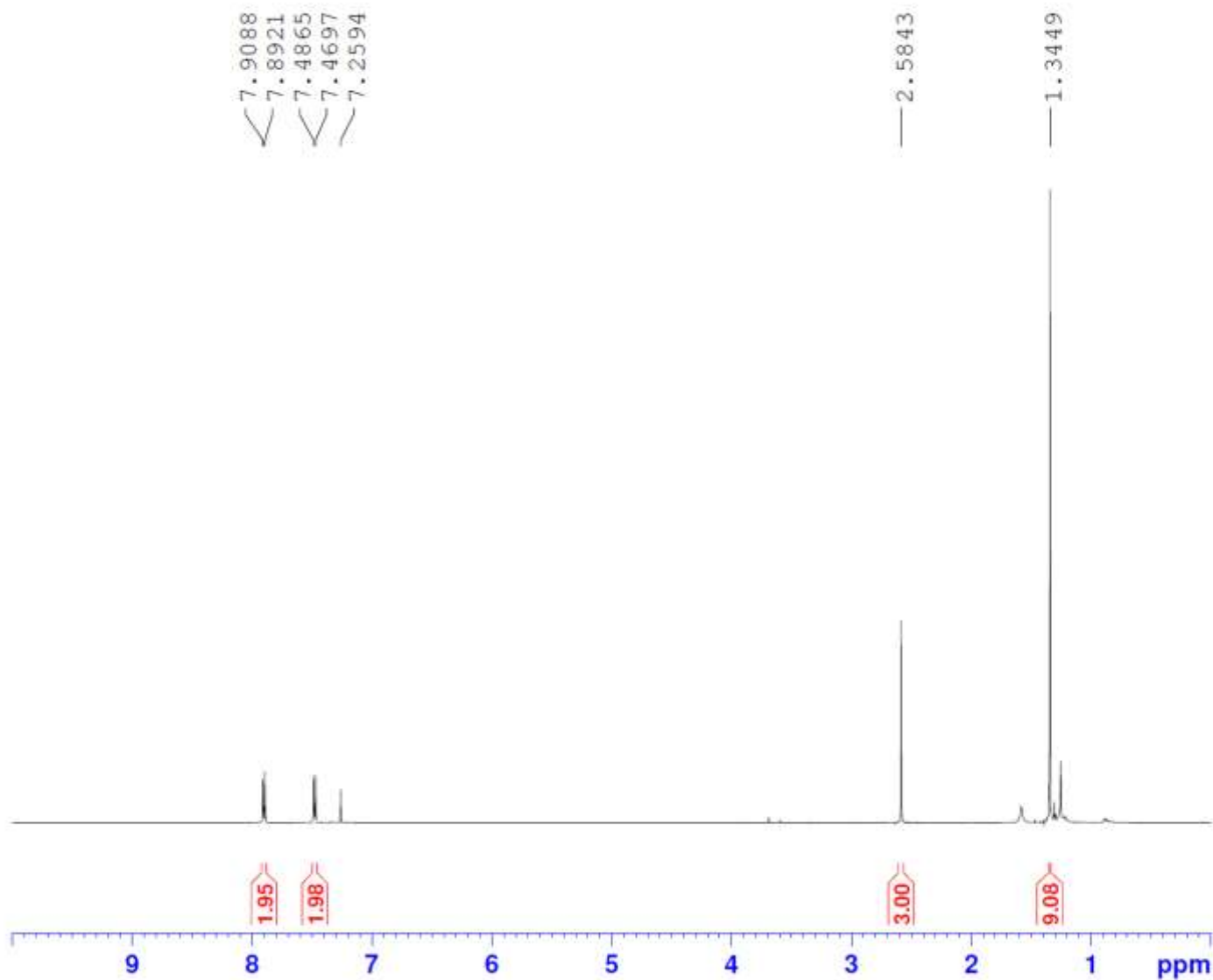
F2 - Acquisition Parameters
 Date_ 20180526
 Time 11.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 998
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.899999998 sec
 TD0 150

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

----- CHANNEL f2 -----
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

intermediate t-bu substrate



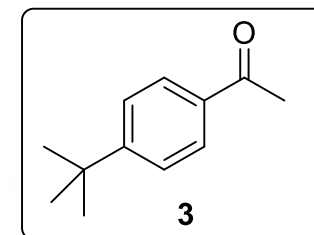
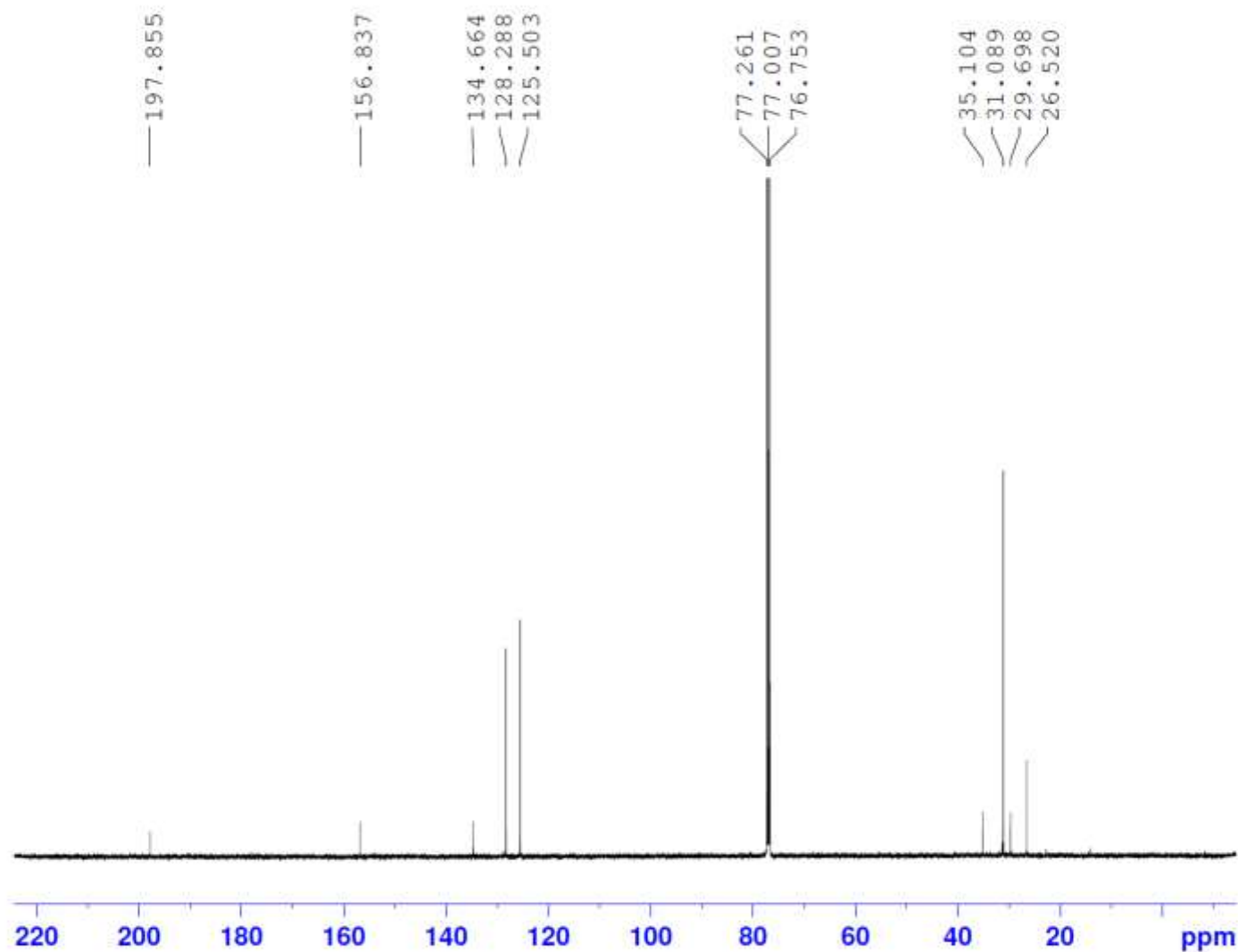
Current Data Parameters
NAME sjy2406
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180624
Time 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

t bu intermediate



Current Data Parameters
NAME sjy2406
EXPNO 2
PROCNO 1

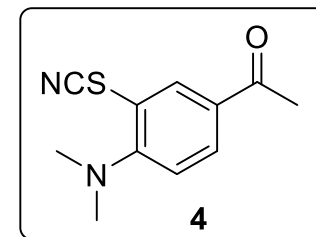
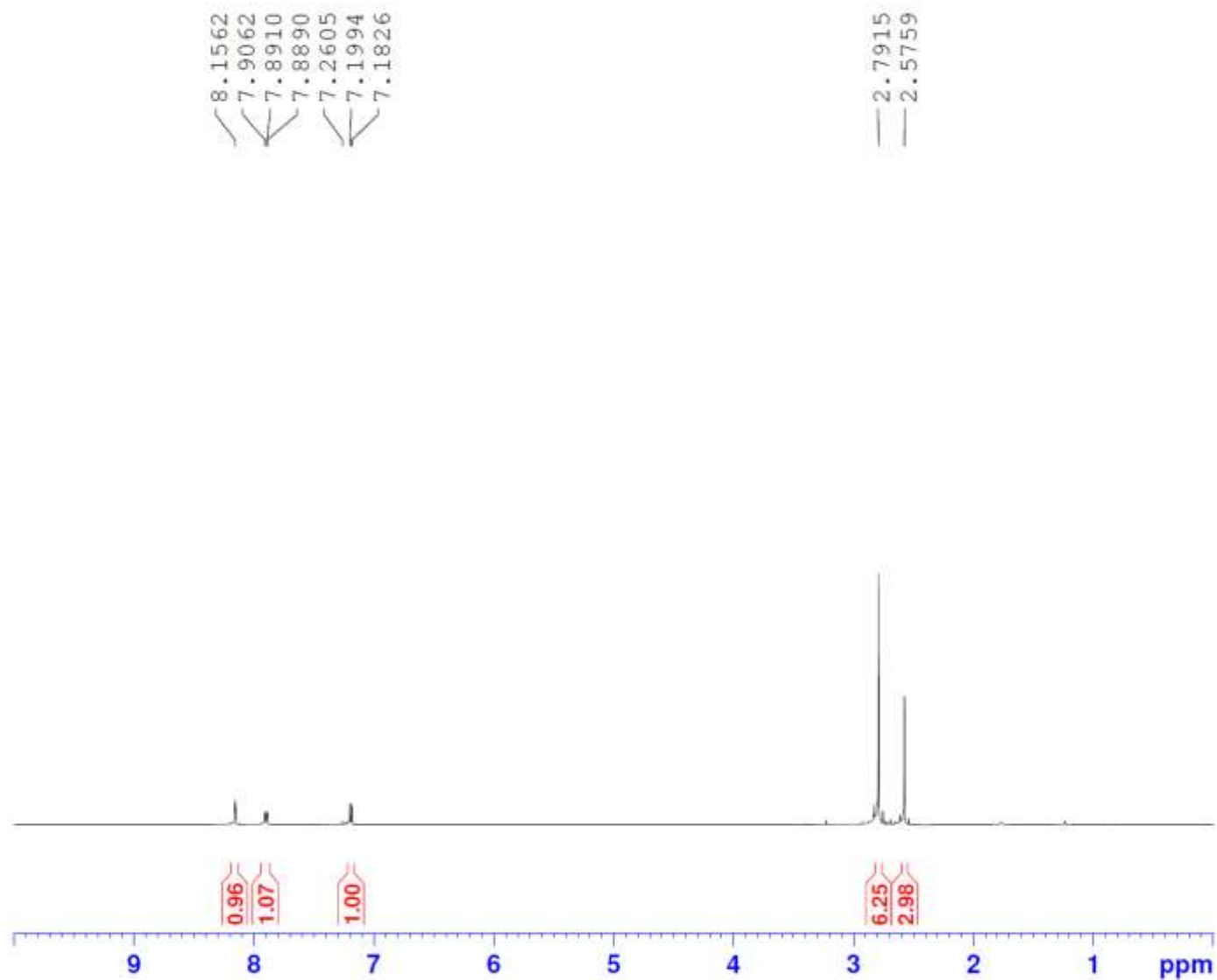
F2 - Acquisition Parameters
Date_ 20180624
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2088
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 299.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P162-1



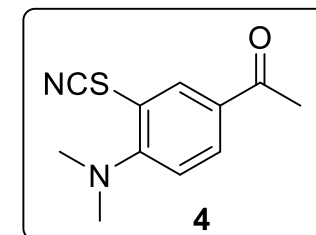
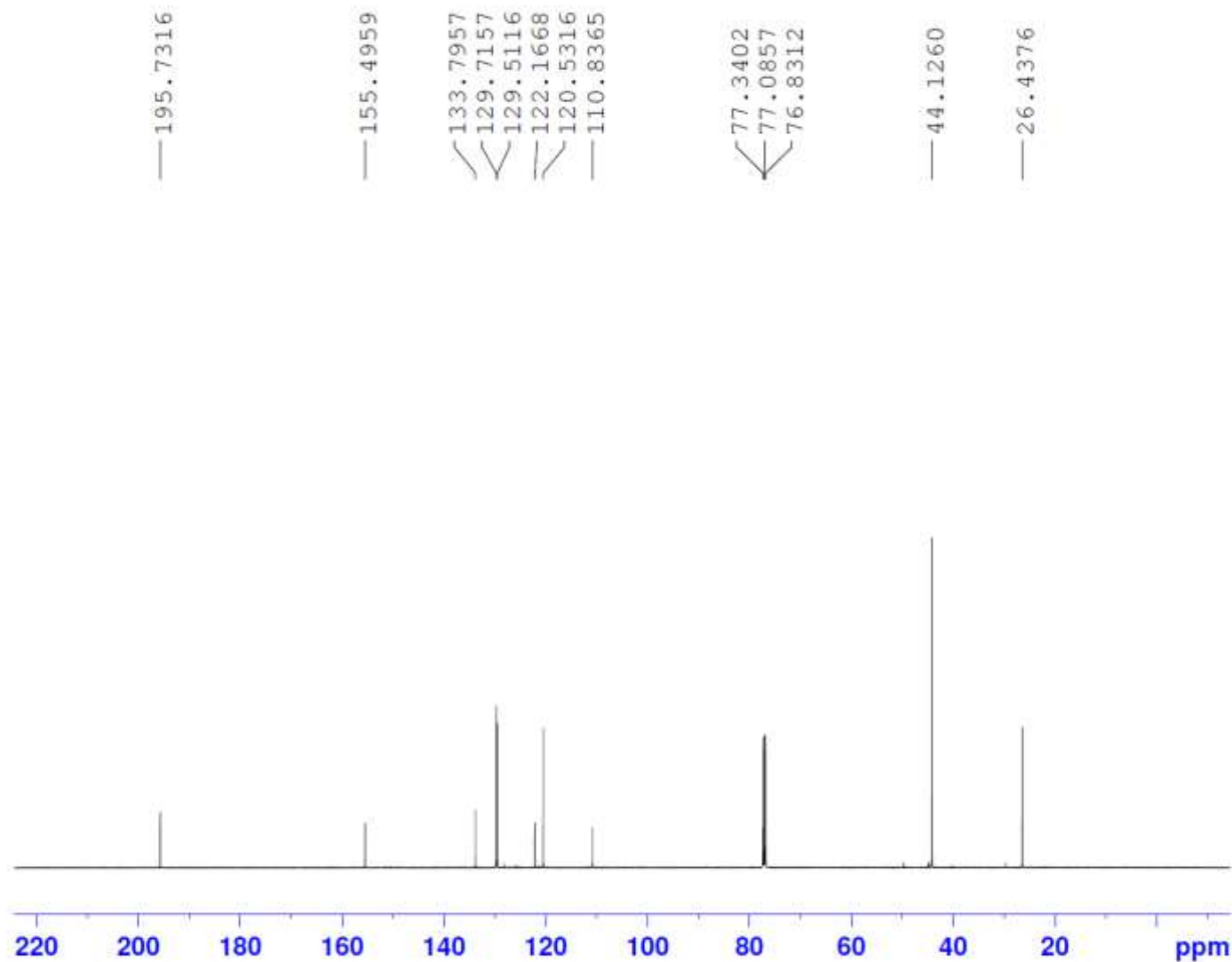
Current Data Parameters
NAME sjy0506
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180605
Time 10.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 57
DW 48.400 usec
DE 6.00 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P162-1



Current Data Parameters
 NAME sjy0506
 EXPNO 5
 PROCNO 1

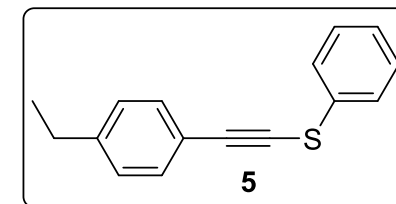
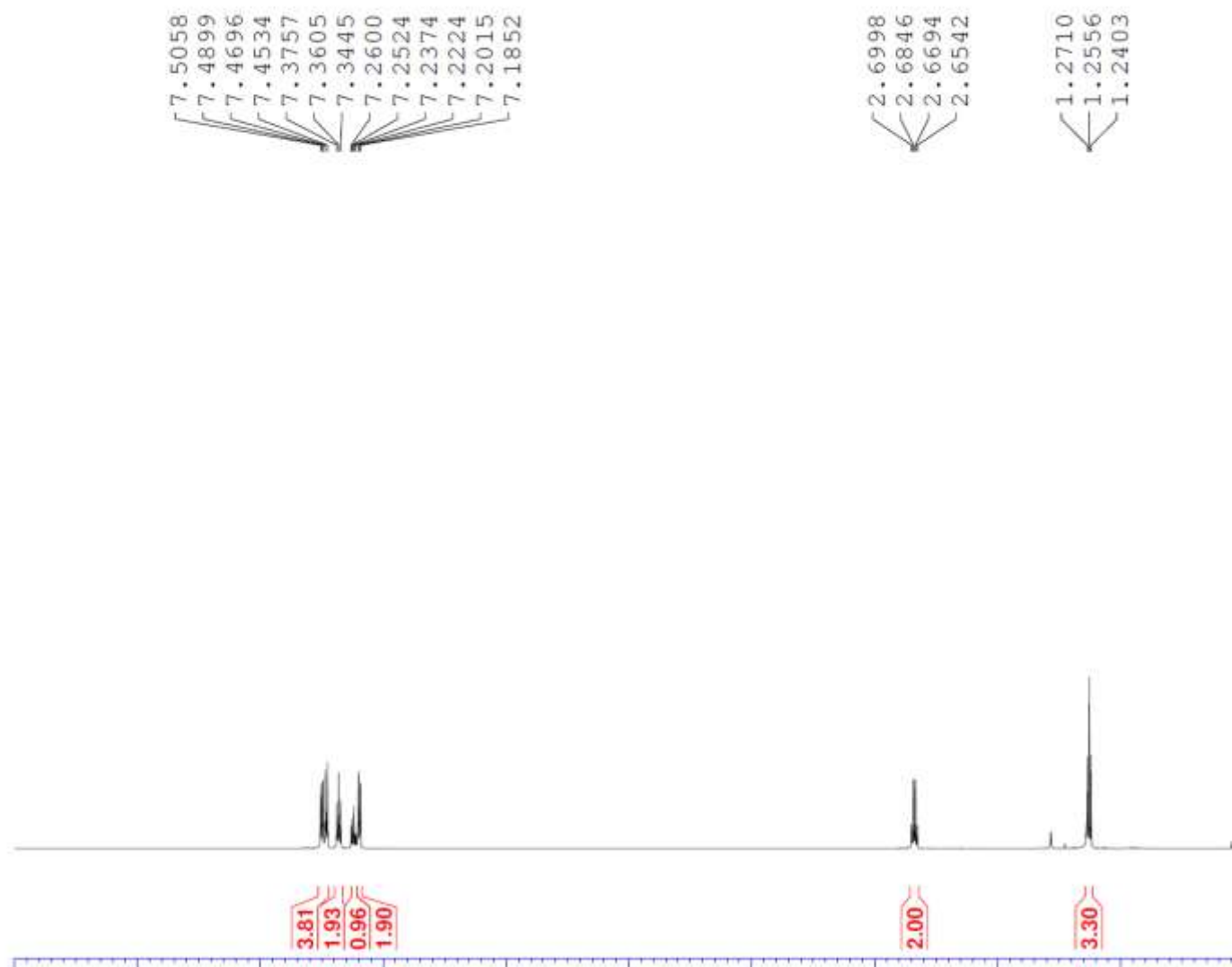
F2 - Acquisition Parameters
 Date_ 20180605
 Time 10.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1971
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 298.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

grignard alkyne SCN



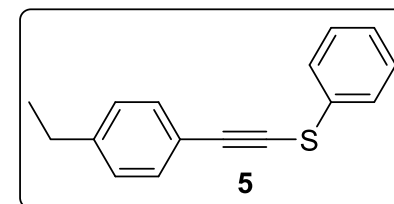
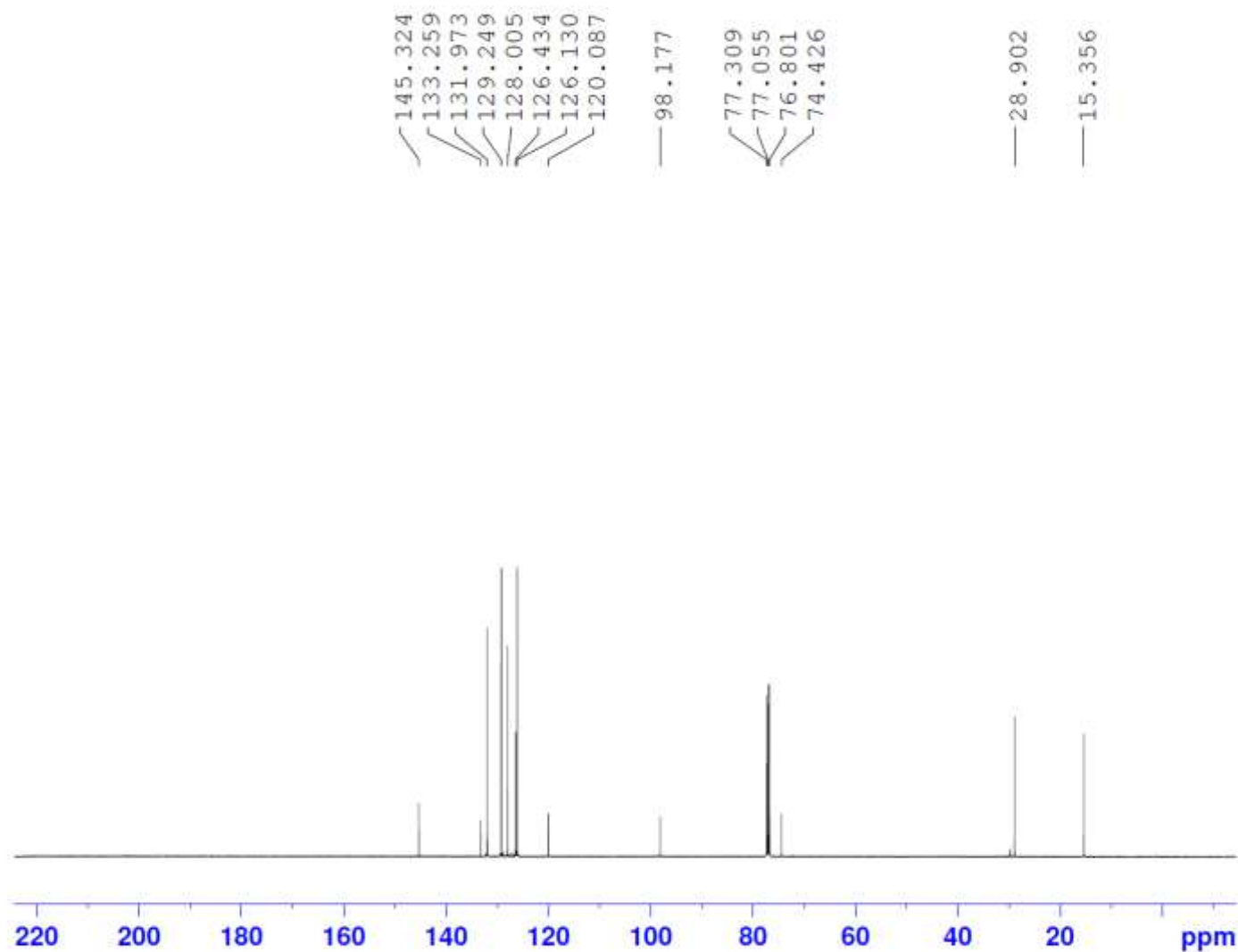
Current Data Parameters
 NAME sjy1307
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180713
 Time 10.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 64
 DW 48.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300134 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

grignard. alkyne SCN



Current Data Parameters
 NAME sjy1307
 EXPNO 2
 PROCNO 1

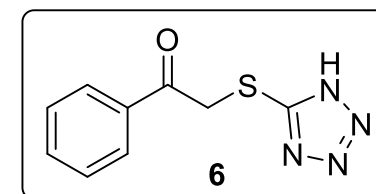
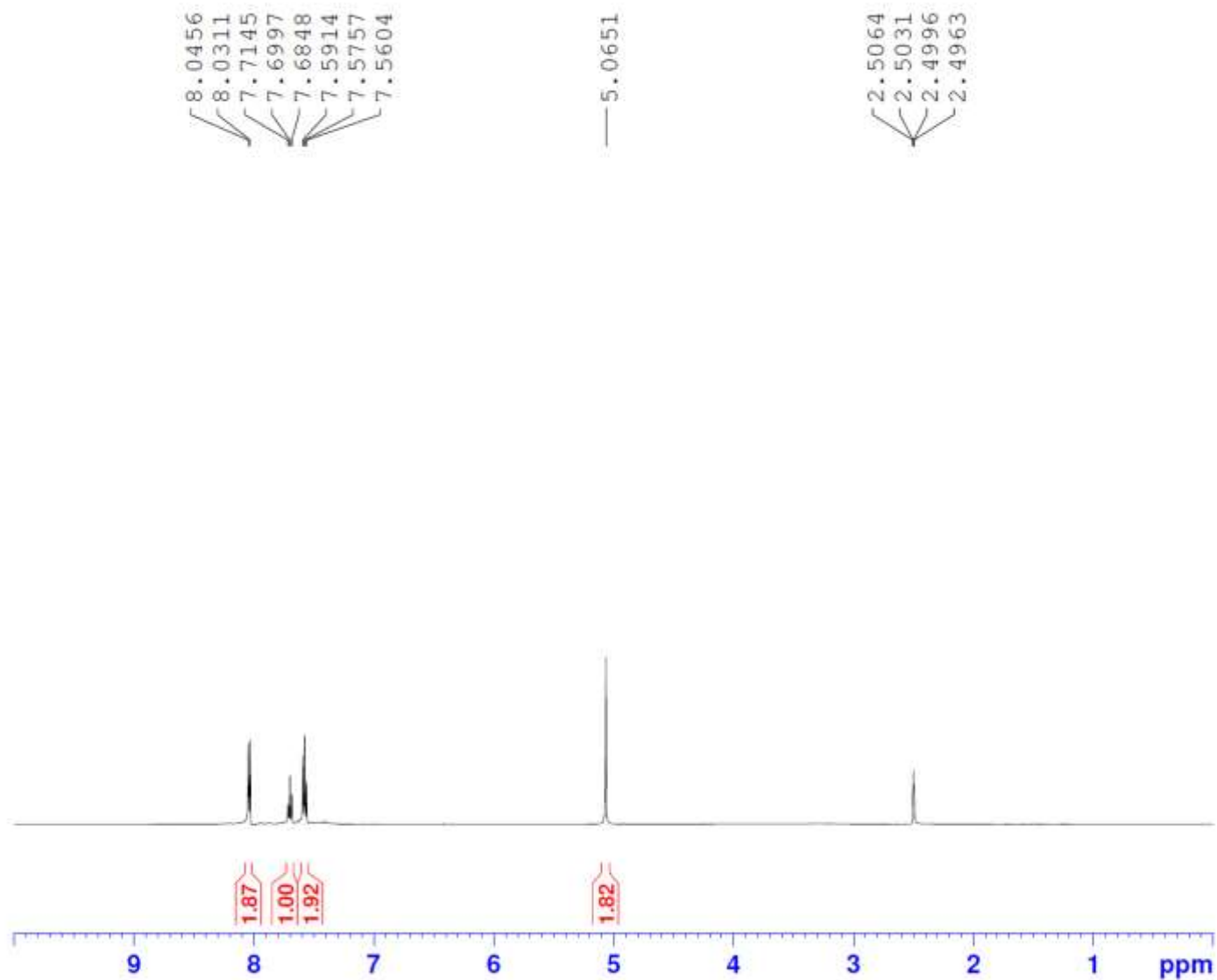
F2 - Acquisition Parameters
 Date_ 20180713
 Time 10.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2500
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 295.9 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 250

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P140 tetrazole



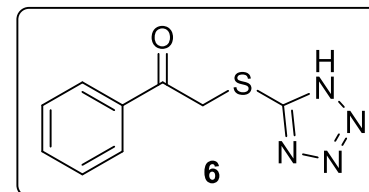
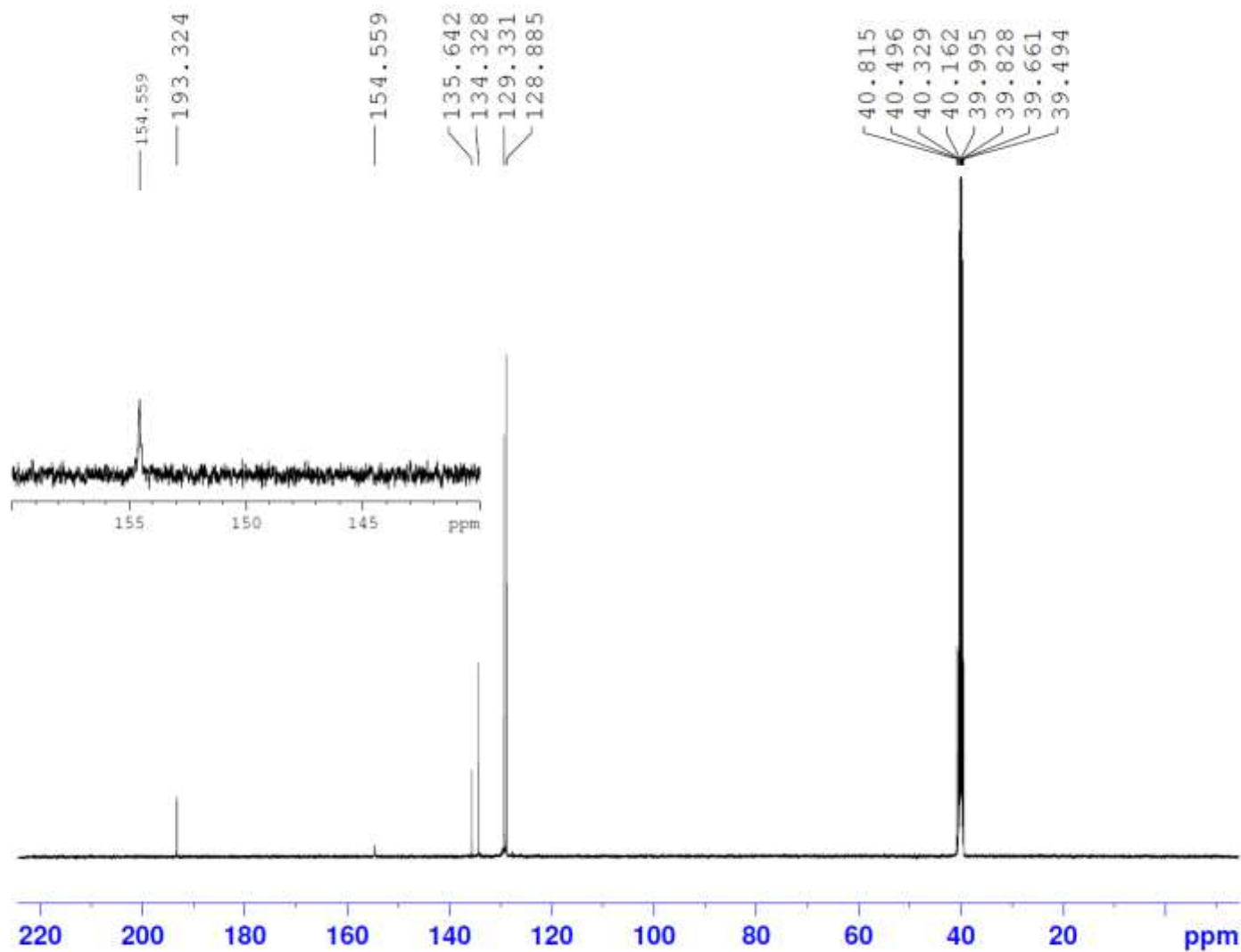
Current Data Parameters
 NAME sjy0209
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180902
 Time 7.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5859712 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.50 usec
 PL1 0.25 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C AMX500



Current Data Parameters
 NAME sjy0209
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180902
 Time 7.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 3616
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 16384
 DW 16.650 usec
 DE 6.00 usec
 TE 296.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 500

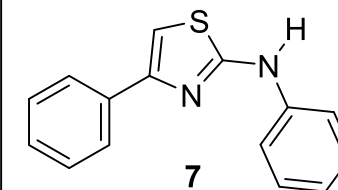
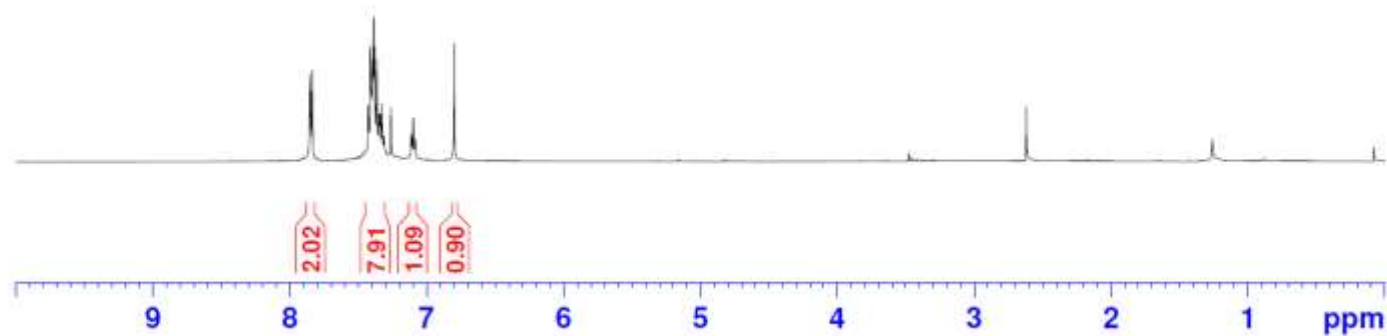
===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 0 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.25 dB
 PL12 17.89 dB
 PL13 15.83 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

P12

7.8514
7.8363
7.4255
7.4105
7.4027
7.3947
7.3874
7.3802
7.3658
7.3490
7.3418
7.3270
7.3125
7.2604
7.1123
7.0986
7.0846
6.7992



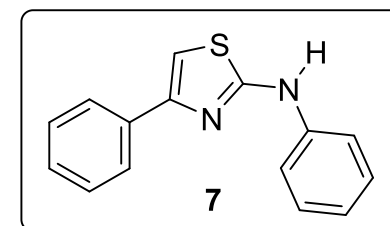
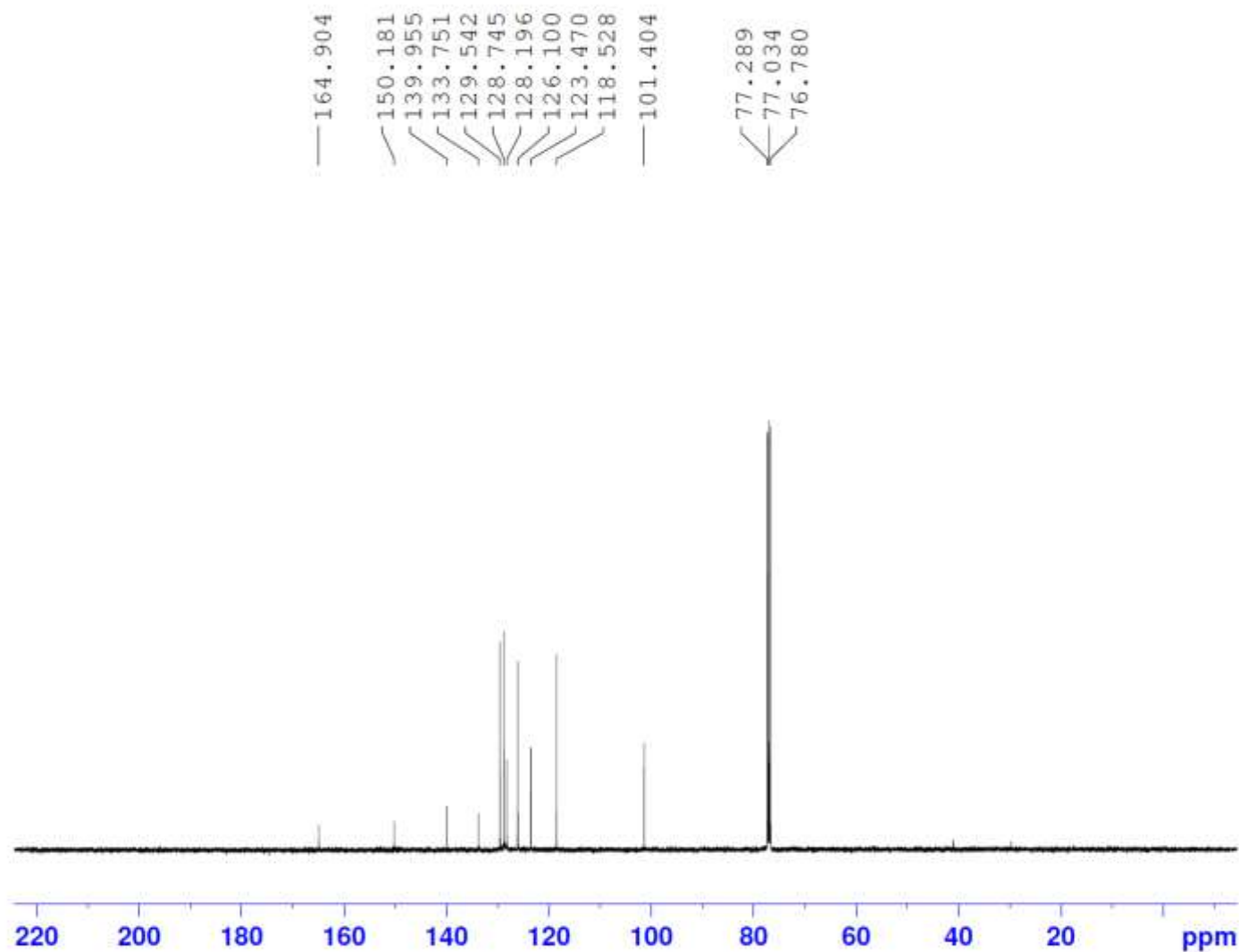
NAME SJY1303
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180313
Time 14.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P12-1



Current Data Parameters
NAME sjy1303
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180313
Time 14.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 842
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 299.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

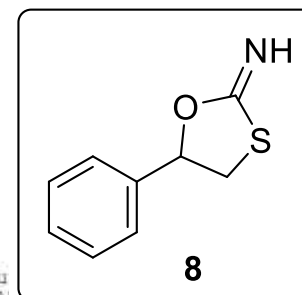
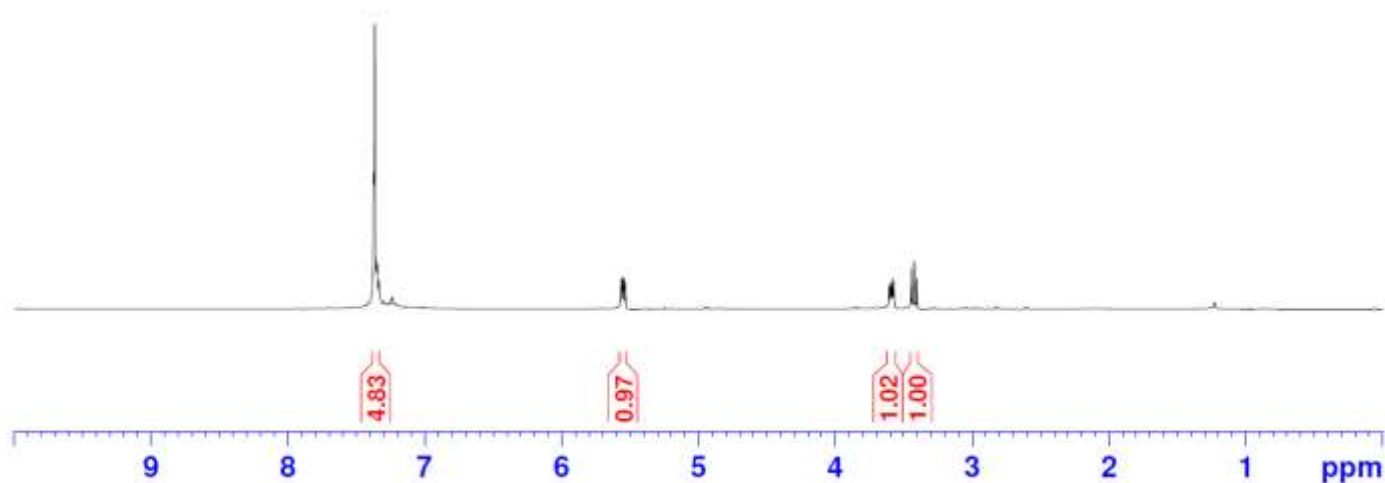
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

reduction of ph SCN Ketone with NaBH₄

7.3721
7.3637
7.3512
7.3449
7.3346

5.5651
5.5534
5.5465
5.5348

3.6065
3.5948
3.5844
3.5728
3.4440
3.4248
3.4031



Cu
NA
EXPNO
PROCNO

3
1

F2 - Acquisition Parameters

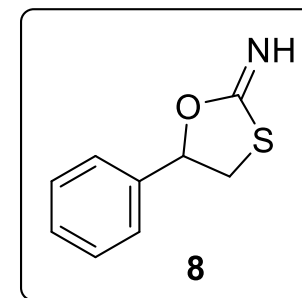
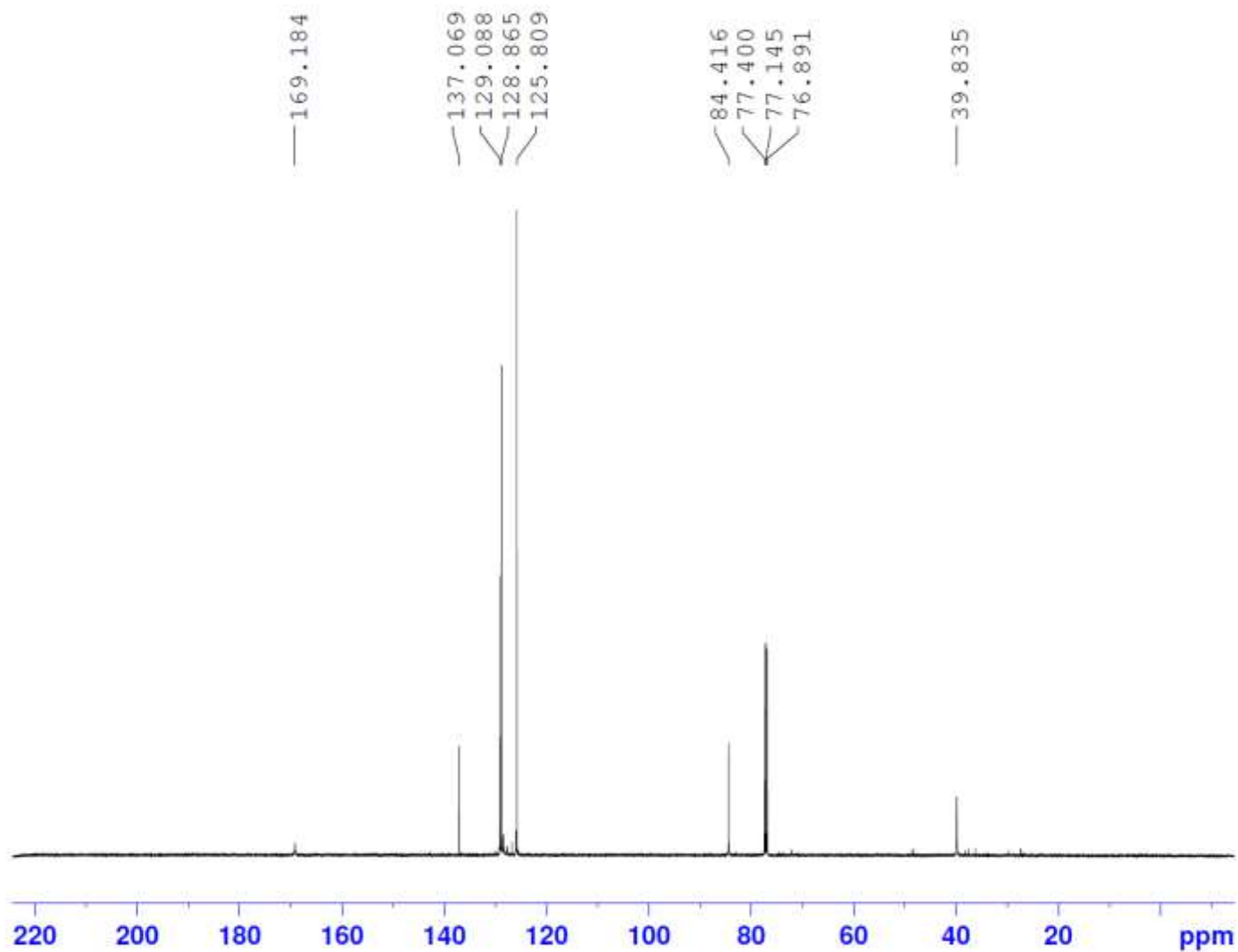
Date_ 20180626
Time 8.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 45.3
DW 48.400 usec
DE 6.00 usec
TE 299.4 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 16384
SF 500.1300248 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C AMX500



Current Data Parameters
NAME sjy2606
EXPNO 4
PROCNO 1

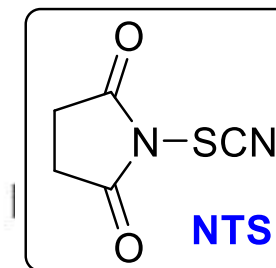
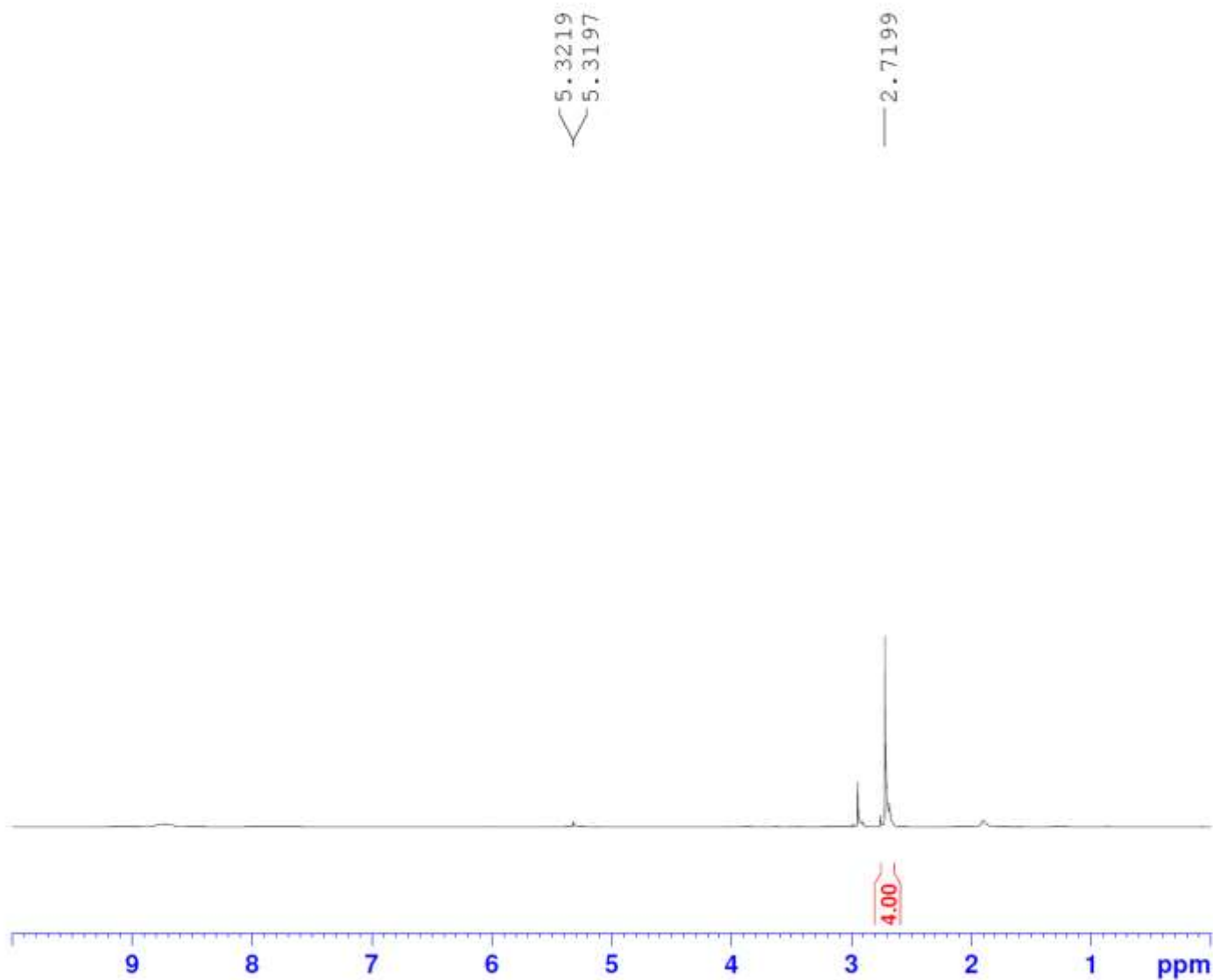
F2 - Acquisition Parameters
Date_ 20180626
Time 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 442
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 150

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NBS



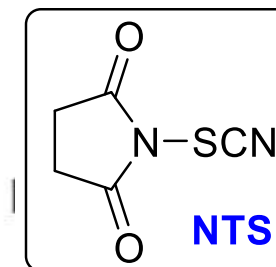
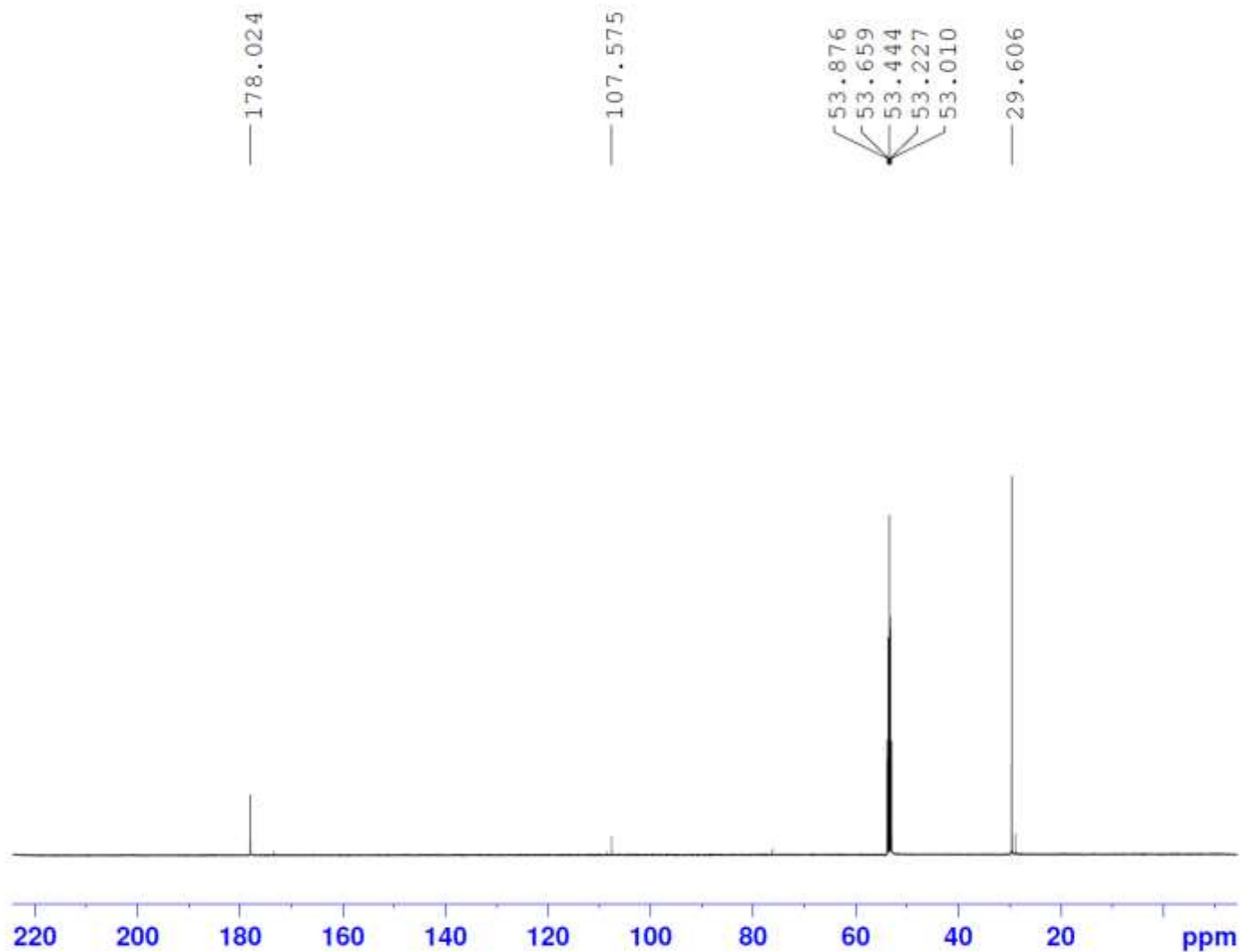
Current Data Parameters
NAME sjy1506
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180615
Time 10.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1309806 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NBS



Current Data Parameters
NAME sjy1506
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180615
Time 11.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 2500
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 298.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

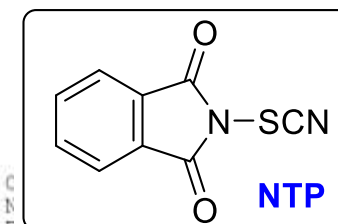
===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.852
7.846
7.844
7.839
7.834
7.832
7.827
7.825
7.820
7.816
7.807

1.980
1.975
1.970
1.965
1.960



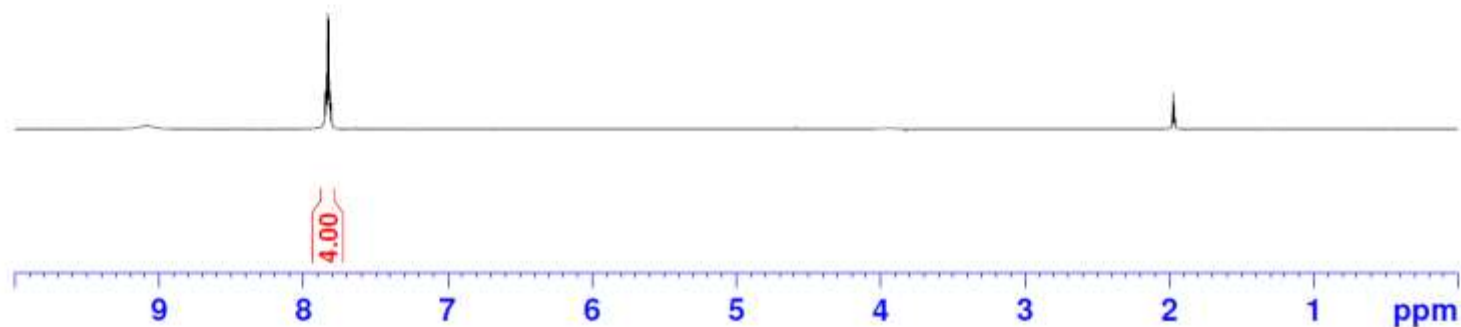
C
N
E

PROCNO 1

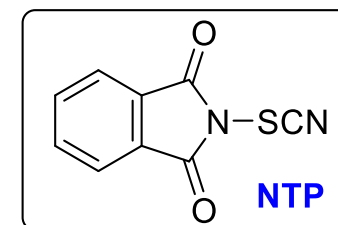
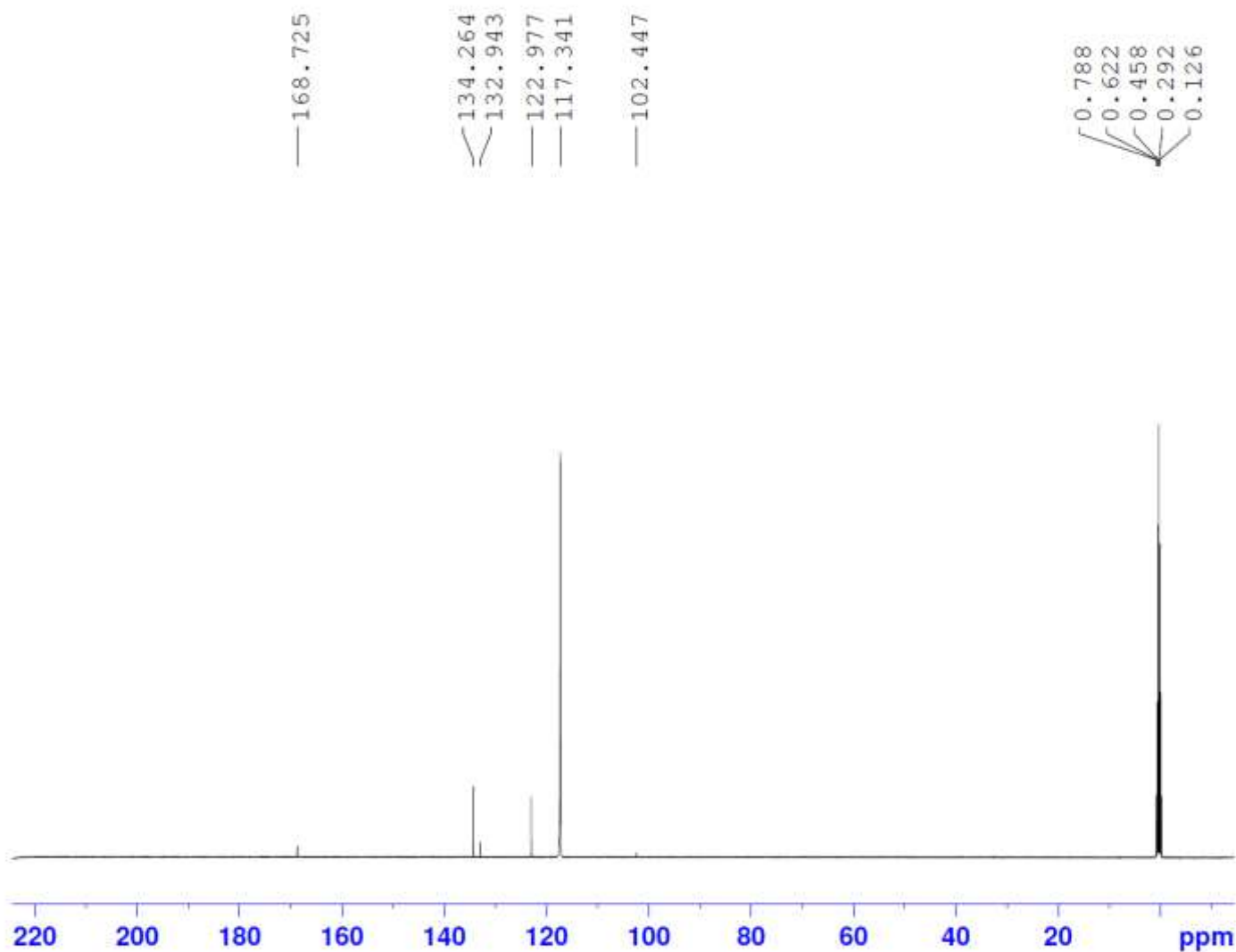
F2 - Acquisition Parameters
Date_ 20180723
Time 10.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpr
TD 32768
SOLVENT CD3CN
NS 2
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 300.6 K
D1 2.00000000 sec
d12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 0.25 dB
PL9 53.81 dB
SFO1 500.1319132 MHz

F2 - Processing parameters
SI 16384
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C AMX500



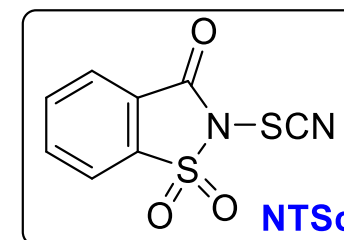
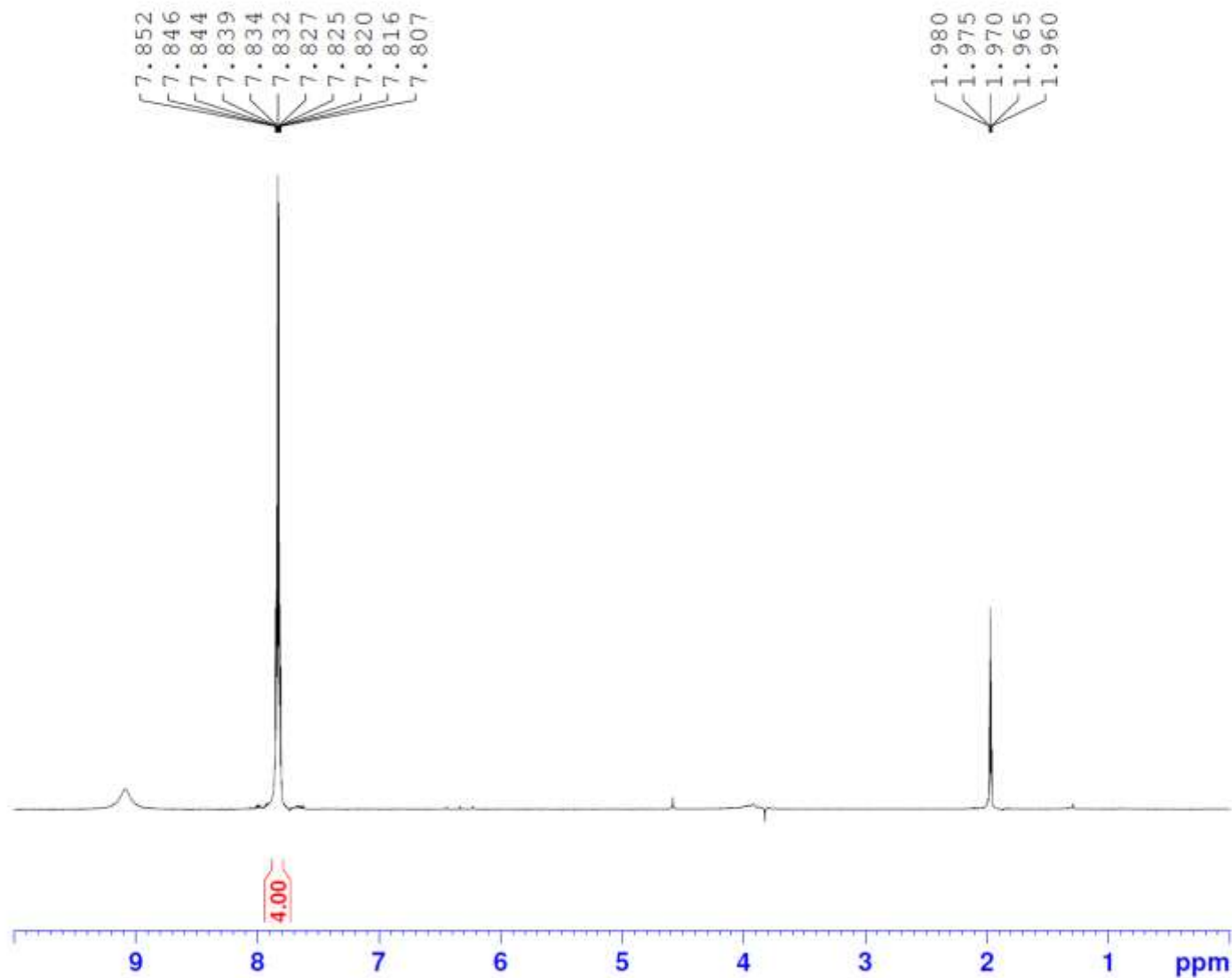
Current Data Parameters
NAME sjy2307
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180723
Time 9.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 1603
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 301.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 250

===== CHANNEL f1 =====
NUC1 ¹³C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



```

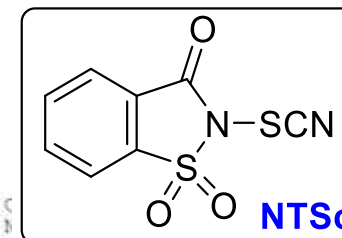
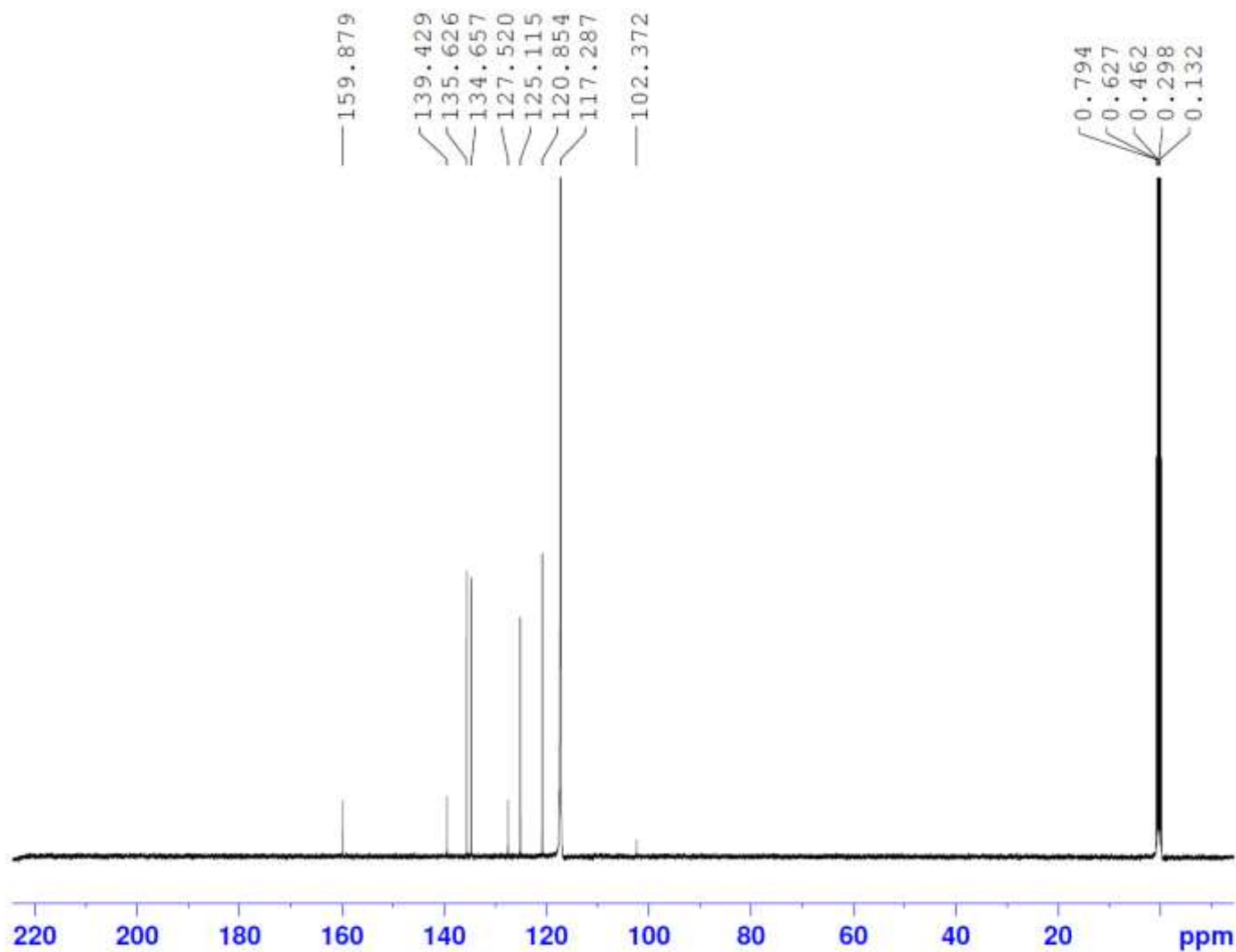
PROCNO      1

F2 - Acquisition Parameters
Date_       20180723
Time        10.35
INSTRUM     spect
PROBHD      5 mm PABBO BB/
PULPROG     zgpr
TD          32768
SOLVENT      CD3CN
NS           2
DS           2
SWH         10330.578 Hz
FIDRES      0.315264 Hz
AQ          1.5859712 sec
RG           228.1
DW          48.400 usec
DE           6.00 usec
TE           300.6 K
D1          2.00000000 sec
d12         0.00002000 sec
TD0          1

===== CHANNEL f1 =====
NUC1        1H
P1           9.00 usec
PL1          0.25 dB
PL9          53.81 dB
SFO1        500.1319132 MHz

F2 - Processing parameters
SI           16384
SF          500.1300000 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

Sacc SCN



```

===== CHANNEL f1 =====
NUC1      13C
P1        8.90 usec
PL1       0 dB
SFO1      125.7709936 MHz

===== CHANNEL F2 =====
CPDPRG[2]  waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.25 dB
PL12       17.89 dB
PL13       15.83 dB
SFO2      500.1320005 MHz

F2 - Acquisition Parameters
Date_      20180719
Time       8.50
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zgpg30
TD         65536
SOLVENT    CD3CN
NS         2320
DS         0
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0911744 sec
RG         16384
DW         16.650 usec
DE         6.00 usec
TE         301.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        250
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        8.90 usec
PL1       0 dB
SFO1      125.7709936 MHz
  
```

```

===== CHANNEL F2 =====
CPDPRG[2]  waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.25 dB
PL12       17.89 dB
PL13       15.83 dB
SFO2      500.1320005 MHz
  
```

```

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```