

Supporting Information

Direct Access to Benzofuro[2,3-*b*]quinoline and 6*H*-Chromeno[3,4-*b*]quinoline Cores through Gold-Catalyzed Annulation of Anthranils with Arenoxyethynes and Aryl propargyl ethers

Manoj D. Patil and Rai-Shung Liu*

Frontier Research Center for Matter Science and Technology, Department of Chemistry,
National Tsing-Hua University, Hsinchu, Taiwan, ROC.

E-mail: rsliu@mx.nthu.edu.tw

TABLE OF CONTENTS

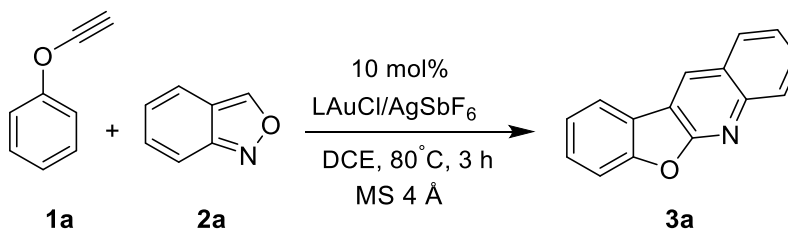
1. Representative synthetic procedures-----	03
2. Spectral Data of Key Compounds-----	05
3. Crystallographic data -----	21
4. ^1H & ^{13}C Spectra of Key Compounds-----	34

1. Representative synthetic procedures.

1.1 General Procedure.

Unless otherwise noted, all reactions were carried out under a nitrogen atmosphere in oven-dried glassware using the standard syringe, cannula and septa apparatus. Tetrahydrofuran was dried with sodium, benzophenone and distilled before use. Dichloromethane, Toluene, and DCE were dried over CaH₂ and distilled. Reagents were purchased from commercial sources and used without purification unless otherwise stated. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker 400 MHz, Varian 500 MHz and Bruker 600 MHz, spectrometers using chloroform-*d* (CDCl₃) as the internal standard. Chemical shifts are reported in parts per million (ppm). Multiplicities are indicated by s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), dt (doublet of triplet), td (triplet of doublet). Coupling constants *J* are reported in Hertz (Hz). The Alkynyl Aryl ethers substrates (**1a–1j**, **7b**, **7c**)^[s1], benzoisoxazole (**2a–2m**)^[s2], and (ethynyloxy)benzene substrates (**5a–5h**)^[s3] were prepared according to literature methods.

1.2 Standard procedure for the benzofuro[2,3-*b*]quinoline (**3a**):



A two-neck tube was charged with P(*t*-Bu)₂(*o*-biphenyl)gold(I)-chloride (0.022 g, 0.042 mmol) and AgSb₆ (0.014 g, 0.042 mmol) and to this mixture was added dry DCE (0.5 mL); the resulting mixture was stirred at room temperature for 5 min. To this suspension was added a DCE (1.5 mL) solution of compound **1a** (0.05 g, 0.42 mmol) and compound **2a** (0.05 g, 0.42 mmol) at room temperature. The resulting mixture was stirred for 3 h at 80 °C before filtration over a short celite bed. The solvent was evaporated under reduced pressure and eluted through a silica column with (ethyl acetate/hexane = 1:20) to afford the resulting product, which was then triturated or recrystallized in pentane to get pure compound **3a** as a white solid in (0.057 g, 0.26 mmol, 61%) yield.

1.3 Standard procedure for the 6H-chromeno[3,4-*b*]quinoline (6a):



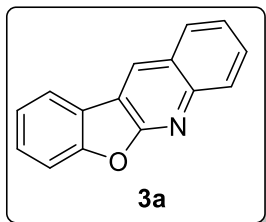
A two-neck tube was charged with P(*t*-Bu)₂(*o*-biphenyl)gold(I)-chloride (0.019 g, 0.037 mmol) and AgSb₆ (0.012 g, 0.037 mmol) and to this mixture was added dry DCE (0.5 mL); the resulting mixture was stirred at room temperature for 5 min. To this suspension was added a DCE (1.5 mL) solution of compound **1a** (0.05 g, 0.37 mmol) and compound **2a** (0.04 g, 0.37 mmol) at room temperature. The resulting mixture was stirred for 35 h at 80 °C then add Zinc triflate (0.027 g, 0.075 mmol) and again stirred for 3 h at 80 °C before filtration over a short celite bed. The solvent was evaporated under reduced pressure and eluted through a silica column with (ethyl acetate/hexane = 1:20) to afford the resulting product, which was then triturated or recrystallized in pentane to get pure compound **3a** as a white solid in (0.056 g, 0.24 mmol, 64%) yield.

1.4 References.

- [S1] a) K. Graf, C. L. Ruhl, M. Rudolph, F. Rominger, A. S. K. Hashmi, *Angew. Chem. Int. Ed.* 2013, **52**, 12727. b) B. Alcaide, P. Almendros, C. Lazaro-Milla, *Adv.Synth.Catal.*, 2017, **359**, 2630. c) X.-Q. Zhu, H. Yuan, Q. Sun, B. Zhou, X.-Q. Han, Z.-X. Zhang, X. Lu, L.-W. Ye, *Green Chem.*, 2018, **20**, 4287.
- [S2] a) R. L. Sahani, R.-S. Liu, *Angew. Chem. Int. Ed.* 2017, **56**, 1026; b) J. Chauhana, S. Fletcher, *Tetrahedron Lett.* 2012, **53**, 4951.
- [S3] V. S. P. R. Lingam, R. Vinodkumar, K. Mukkanti, A. Thomas and B. Gopalan, *Tetrahedron Lett.*, 2008, **49**, 4260.

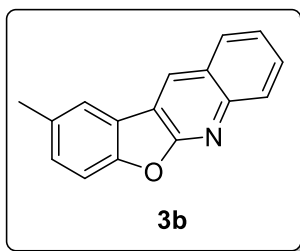
2. Spectral Data of Key Compounds:

Spectral data for benzofuro[2,3-*b*]quinoline (3a):



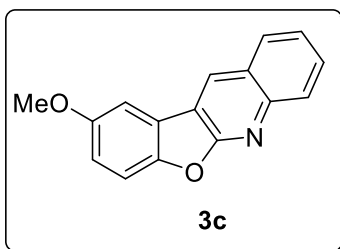
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.64 (s, 1H), 8.13 (d, $J = 8.5$ Hz, 1H), 7.99 (td, $J = 8.2, 0.6$ Hz, 2H), 7.74 (td, $J = 8.4, 1.3$ Hz, 1H), 7.61 (dd, $J = 8.2, 0.6$ Hz, 1H), 7.55-7.52 (m, 2H), 7.38 (td, $J = 8.4, 0.8$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.5, 155.8, 145.9, 129.6, 129.3, 129.0, 128.4, 128.1, 126.0, 125.0, 123.4, 122.2, 121.6, 117.7, 112.0; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{NO}$ ($\text{M}+\text{H}$): 220.0762, found: 220.0757.

Spectral data for 2-methylbenzofuro[2,3-*b*]quinoline (3b):



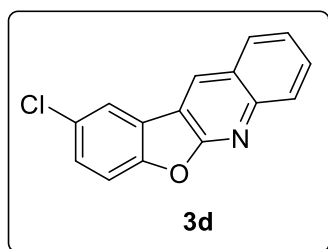
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.57 (s, 1H), 8.11 (d, $J = 8.4$ Hz, 1H), 7.96 (d, $J = 8.1$ Hz, 1H), 7.77 (s, 1H), 7.72 (td, $J = 6.8, 1.3$ Hz, 1H), 7.52 (td, $J = 7.9, 1.0$ Hz, 1H), 7.47 (d, $J = 8.3$ Hz, 1H), 7.32 (d, $J = 8.3$ Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.8, 154.1, 145.9, 133.0, 130.2, 129.4, 128.7, 128.4, 128.1, 126.0, 124.9, 122.0, 121.7, 117.8, 111.5, 21.3; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{12}\text{NO}$ ($\text{M}+\text{H}$): 234.0919, found: 234.0913.

Spectral data for 2-methoxybenzofuro[2,3-*b*]quinoline (3c):



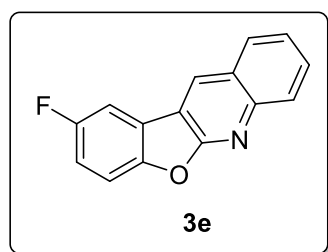
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.62 (s, 1H), 8.12 (dt, $J = 8.4, 0.4$ Hz, 1H), 7.98 (dt, $J = 8.2, 0.7$ Hz, 1H), 7.74 (td, $J = 8.4, 1.4$ Hz, 1H), 7.54 (td, $J = 8.1, 1.2$ Hz, 1H), 7.51 (d, $J = 8.8$ Hz, 1H), 7.48 (d, $J = 2.6$ Hz, 1H), 7.11 (dd, $J = 8.8, 2.6$ Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 163.1, 156.2, 150.4, 146.0, 129.6, 128.9, 128.4, 128.1, 125.9, 125.0, 122.6, 118.1, 116.8, 112.6, 105.2, 56.0; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{12}\text{NO}_2$ (M+H): 250.0868, found: 250.0870.

Spectral data for 2-chlorobenzofuro[2,3-*b*]quinoline (3d):



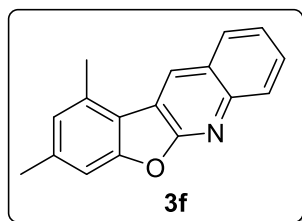
White solid; ^1H NMR (400 MHz, CDCl_3): δ 8.65 (s, 1H), 8.14 (d, $J = 8.8$ Hz, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.98 (d, $J = 2.0$ Hz, 1H), 7.77 (td, $J = 8.4, 1.4$ Hz, 1H), 7.58-7.54 (m, 2H), 7.50 (dd, $J = 8.7, 2.0$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.6, 154.1, 146.3, 130.1, 129.7, 129.3, 129.0, 128.5, 128.3, 126.0, 125.3, 123.6, 121.5, 116.8, 113.1; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{ClNO}$ (M+H): 254.0373, found: 254.0373.

Spectral data for 2-fluorobenzofuro[2,3-*b*]quinoline (3e):



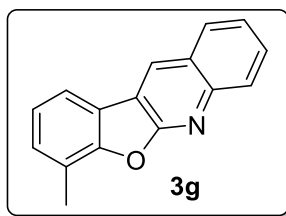
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.65 (s, 1H), 8.14 (d, $J = 8.5$ Hz, 1H), 8.01 (dd, $J = 8.1, 0.6$ Hz, 1H), 7.77 (td, $J = 8.3, 1.4$ Hz, 1H), 7.68 (dd, $J = 7.6, 2.6$ Hz, 1H), 7.58-7.55 (m, 2H), 7.26 (td, $J = 8.9, 2.7$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): 163.0, 159.9 ($J_{\text{C-F}} = 240.6$ Hz), 151.8, 146.2, 130.1 ($J_{\text{C-F}} = 12.1$ Hz), 129.6, 128.5, 128.2, 125.9, 125.3, 123.1 ($J_{\text{C-F}} = 10.2$ Hz), 117.4, 116.5, ($J_{\text{C-F}} = 25.4$ Hz), 112.9 ($J_{\text{C-F}} = 8.9$ Hz), 108.0 ($J_{\text{C-F}} = 11.1$ Hz); HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{FNO}$ (M+H): 238.0668, found: 238.0671.

Spectral data for 1,3-dimethylbenzofuro[2,3-*b*]quinoline (3f):



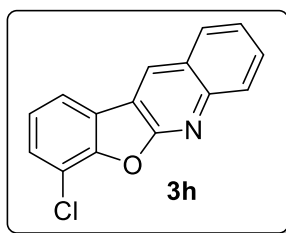
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.45 (s, 1H), 8.07 (dd, $J = 8.4, 0.4$ Hz, 1H), 7.90 (d, $J = 8.1$ Hz, 1H), 7.68 (td, $J = 8.3, 1.4$ Hz, 1H), 7.48 (td, $J = 8.0, 1.0$ Hz, 1H), 7.19 (s, 1H), 6.91 (s, 1H), 2.72 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.5, 156.0, 145.0, 139.9, 134.1, 129.3, 129.0, 128.1, 128.0, 126.0, 125.7, 124.8, 118.3, 118.2, 109.5, 21.9, 19.6; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ (M+H): 248.1075, found: 248.1078.

Spectral data for 4-methylbenzofuro[2,3-*b*]quinoline (3g):



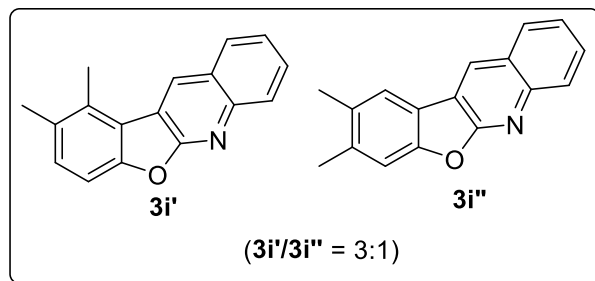
White solid; ^1H NMR (400 MHz, CDCl_3): δ 8.62 (s, 1H), 8.12 (d, $J = 8.0$ Hz, 1H), 7.98 (dd, $J = 8.2, 0.7$ Hz, 1H), 7.82 (dd, $J = 7.4, 0.4$ Hz, 1H), 7.73 (td, $J = 8.3, 1.3$ Hz, 1H), 7.53 (td, $J = 8.1, 1.1$ Hz, 1H), 7.35 (dd, $J = 6.3, 0.8$ Hz, 1H), 7.28 (t, $J = 7.7$ Hz, 1H), 2.61 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.5, 154.6, 145.9, 130.4, 129.4, 129.0, 128.4, 128.1, 126.0, 124.9, 123.3, 122.4, 121.6, 119.0, 118.2, 15.1; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{12}\text{NO}$ (M+H): 234.0919, found: 234.0909.

Spectral data for 4-chlorobenzofuro[2,3-*b*]quinoline (3h):



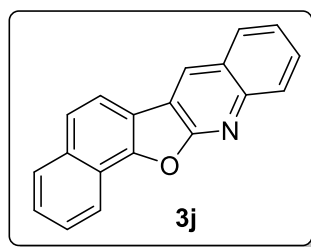
White solid; ^1H NMR (400 MHz, CDCl_3): δ 8.68 (s, 1H), 8.14 (d, $J = 8.6$ Hz, 1H), 8.01 (d, $J = 8.2$ Hz, 1H), 7.90 (dd, $J = 7.5, 0.9$ Hz, 1H), 7.78 (td, $J = 8.3, 1.3$ Hz, 1H), 7.58 (td, $J = 8.1, 1.1$ Hz, 1H), 7.54 (dd, $J = 7.9, 1.0$ Hz, 1H), 7.33 (t, $J = 7.8$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.1, 151.9, 146.3, 130.0, 129.8, 129.4, 128.7, 128.2, 126.1, 125.4, 124.2, 123.9, 119.8, 117.7, 117.4; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{NO}$ (M+H): 254.0373, found: 254.0372.

Spectral data for 1,2-dimethylbenzofuro[2,3-*b*]quinoline (3i') (major isomer):



White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.61 (s, 1H), 8.47 (s, 1H), 8.09 (d, $J = 8.4$ Hz, 1H), 7.94-7.91 (m, 2H), 7.70-7.67 (m, 3H), 7.51-7.48 (m, 2H), 7.34 (s, 1H), 7.30 (s, 1H), 7.29-7.25 (m, 2H), 2.69 (s, 6H), 3.35 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.7, 162.5, 154.6, 154.1, 145.5, 145.2, 138.9, 132.9, 131.9, 131.3, 130.7, 130.2, 129.3, 129.1, 128.3, 128.2, 128.1, 128.0, 127.9, 126.0, 125.9, 124.8, 121.9, 120.9, 119.6, 118.6, 118.0, 112.5, 108.7, 20.8, 19.8, 19.2, 16.2, one carbon is merged with others; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ (M+H): 248.1075, found: 248.1078.

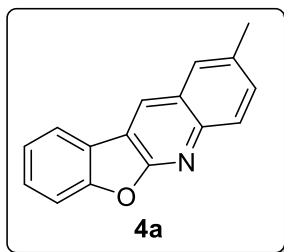
Spectral data for naphtho[2',1':4,5]furo[2,3-*b*]quinoline (3j):



Pale yellow solid; ^1H NMR (600 MHz, CDCl_3): δ 8.64 (s, 1H), 8.46 (d, $J = 8.2$ Hz, 1H), 8.16 (d, $J = 8.4$ Hz, 1H), 7.99 (t, $J = 6.6$ Hz, 2H), 7.95 (d, $J = 8.2$ Hz, 1H), 7.79 (d, $J = 8.4$ Hz, 1H), 7.74 (td, $J = 8.2, 1.3$ Hz, 1H), 7.65 (td, $J = 7.9, 0.9$ Hz, 1H), 7.59 (td, $J = 8.1, 1.4$ Hz, 1H), 7.55 (td, $J = 7.9, 1.0$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.2, 152.3, 145.4, 134.0, 129.3, 128.5,

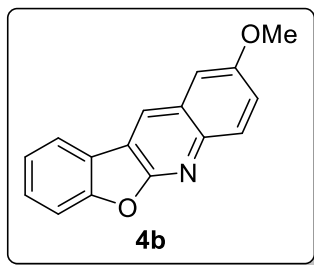
128.4, 128.3, 128.0, 127.1, 127.0, 126.2, 125.1, 123.9, 121.5, 120.9, 118.5, 118.4, 116.9; HRMS-ESI+ calcd for C₁₉H₁₂NO (M+H): 270.1919, found: 270.0917.

Spectral data for 9-methylbenzofuro[2,3-*b*]quinoline (4a):



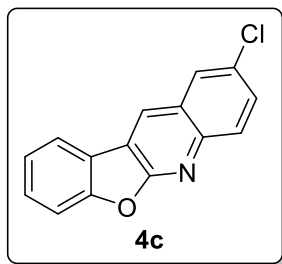
White solid; ¹H NMR (600 MHz, CDCl₃): δ 8.56 (s, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.75 (s, 1H), 7.59 (m, 2H), 7.53 (td, *J* = 7.3, 1.1 Hz, 1H), 7.37 (td, *J* = 7.2, 0.7 Hz, 1H), 2.56 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 162.2, 155.8, 144.5, 134.8, 131.9, 129.1, 128.3, 128.1, 127.0, 126.1, 123.3, 122.3, 121.6, 117.6, 112.0, 21.4; HRMS-ESI+ calcd for C₁₆H₁₂NO (M+H): 234.0919, found: 234.0913.

Spectral data for 9-methoxybenzofuro[2,3-*b*]quinoline (4b):



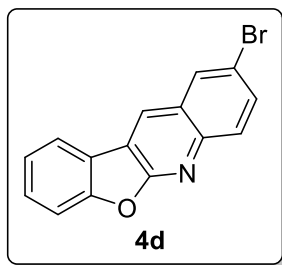
White solid; ¹H NMR (600 MHz, CDCl₃): δ 8.58 (s, 1H), 8.13 (d, *J* = 9.1 Hz, 1H), 7.99 (d, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 2.5 Hz, 1H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.57-7.53 (m, 2H), 7.38 (td, *J* = 7.6, 0.8 Hz, 1H), 3.95 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 162.6, 156.0, 154.2, 147.8, 143.9, 129.9, 129.7, 128.5, 126.0, 124.0, 123.5, 121.8, 118.4, 118.2, 112.1, 55.5; HRMS-ESI+ calcd for C₁₆H₁₂NO₂ (M+H): 250.0868, found: 250.0869.

Spectral data for 9-chlorobenzofuro[2,3-*b*]quinoline (4c):



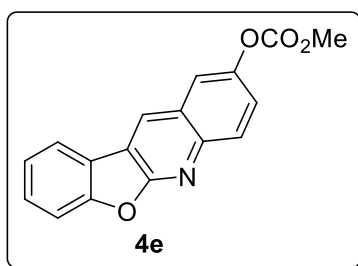
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.54 (s, 1H), 8.06 (d, $J = 9.0$ Hz, 1H), 8.00 (d, $J = 7.7$ Hz, 1H), 7.90 (d, $J = 1.8$ Hz, 1H), 7.67 (d, $J = 9.0$ Hz, 1H), 7.61 (d, $J = 8.2$ Hz, 1H), 7.56 (dd, $J = \text{td}, 8.2, 0.9$ Hz, 1H), 7.39 (d, $J = 7.2$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.6, 156.0, 144.3, 130.7, 130.3, 129.9, 129.8, 127.9, 126.7, 126.6, 123.6, 121.9, 121.8, 118.6, 112.1; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{ClNO}$ ($\text{M}+\text{H}$): 254.0373, found: 254.0361.

Spectral data for 9-bromobenzofuro[2,3-*b*]quinoline (4d):



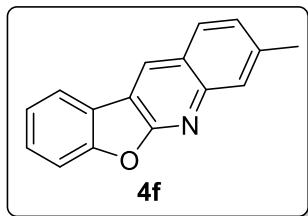
Pale yellow solid; ^1H NMR (600 MHz, CDCl_3): δ 8.52 (s, 1H), 8.12 (d, $J = 2.0$ Hz, 1H), 7.99 (m, 2H), 7.78 (dd, $J = 9.0, 2.1$ Hz, 1H), 7.60 (d, $J = 8.1$ Hz, 1H), 7.55 (td, $J = 8.2, 0.9$ Hz, 1H), 7.39 (t, $J = 7.2$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.6, 156.0, 144.5, 132.8, 130.0, 129.9, 129.8, 127.8, 127.1, 123.6, 121.9, 121.7, 118.5, 112.1, one carbon is merged with others; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{BrNO}$ ($\text{M}+\text{H}$): 297.9868, found: 297.9863.

Spectral data for benzofuro[2,3-*b*]quinolin-9-yl methyl carbonate (4e):



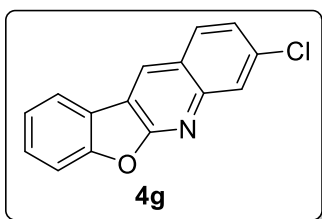
White solid; ^1H NMR (400 MHz, CDCl_3): δ 8.61 (s, 1H), 8.14 (d, $J = 9.4$ Hz, 1H), 8.01 (d, $J = 8.0$ Hz, 1H), 7.82 (d, $J = 2.7$ Hz, 1H), 7.61 (d, $J = 8.1$ Hz, 1H), 7.58-7.54 (m, 2H), 7.39 (td, $J = 7.4, 1.1$ Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.6, 156.0, 154.3, 147.8, 143.9, 129.9, 129.7, 129.2, 128.6, 126.1, 124.0, 123.6, 121.9, 118.4, 118.2, 112.1, 55.6; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{12}\text{NO}_4$ (M+H): 294.0766, found: 294.0714.

Spectral Data of 8-methylbenzofuro[2,3-*b*]quinoline (4f):



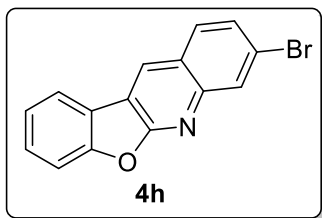
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.60 (s, 1H), 7.99 (dt, $J = 7.6, 0.5$ Hz, 1H), 7.91-7.87 (m, 2H), 7.60 (dd, $J = 8.2, 0.6$ Hz, 1H), 7.52 (td, $J = 8.1, 1.2$ Hz, 1H), 7.39-7.36 (m, 2H), 2.59 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.7, 155.7, 146.3, 140.1, 129.0, 128.8, 127.7, 127.5, 127.3, 124.1, 123.3, 122.4, 121.4, 116.8, 112.0, 21.9; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{12}\text{NO}$ (M+H): 234.0919, found: 234.0913.

Spectral Data of 8-chlorobenzofuro[2,3-*b*]quinoline (4g):



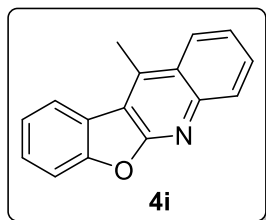
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.58 (s, 1H), 8.12 (t, $J = 0.4$ Hz, 1H), 7.98 (d, $J = 7.6$ Hz, 1H), 7.89 (d, $J = 8.7$ Hz, 1H), 7.60 (d, $J = 8.2$ Hz, 1H), 7.54 (t, $J = 7.9$ Hz, 1H), 7.48 (dd, $J = 8.7, 1.0$ Hz, 1H), 7.38 (td, $J = 7.9, 0.4$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 163.2, 156.1, 146.6, 135.6, 129.6, 129.1, 128.6, 127.6, 126.2, 124.5, 123.6, 122.0, 121.7, 118.1, 112.1; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{ClNO}$ (M+H): 254.0373, found: 254.0374.

Spectral Data of 8-bromobenzofuro[2,3-*b*]quinoline (4h):



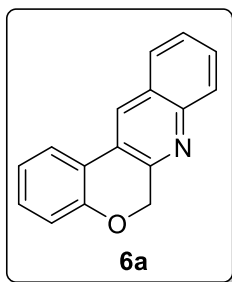
Pale yellow solid; ^1H NMR (600 MHz, CDCl_3): δ 8.61 (s, 1H), 8.31 (d, $J = 1.9$ Hz, 1H), 8.0 (dt, $J = 7.6, 0.6$ Hz, 1H), 7.85 (d, $J = 8.7$ Hz, 1H), 7.62 (m, 2H), 7.56 (td, $J = 7.3, 1.2$ Hz, 1H), 7.39 (td, $J = 7.6, 0.9$ Hz, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ 163.0, 156.0, 146.6, 132.9, 130.8, 129.6, 129.2, 128.8, 128.7, 124.7, 123.8, 123.7, 121.8, 118.1, 112.1; HRMS-ESI+ calcd for $\text{C}_{15}\text{H}_9\text{BrNO}$ ($\text{M}+\text{H}$): 297.9868, found: 297.9868.

Spectral Data of 11-methylbenzofuro[2,3-*b*]quinoline (4i):



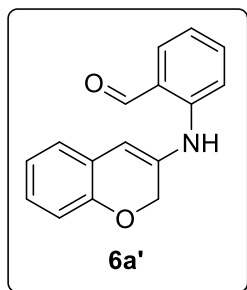
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.17 (d, $J = 0.7$ Hz, 1H), 8.12-8.00 (m, 1H), 7.72 (td, $J = 8.2, 1.3$ Hz, 1H), 7.60 (dd, $J = 8.1, 0.6$ Hz, 1H), 7.55 (td, $J = 8.2, 1.2$ Hz, 1H), 7.51 (td, $J = 8.5, 1.2$ Hz, 1H), 7.38 (td, $J = 7.6, 1.0$ Hz, 1H), 3.10 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.0, 155.5, 145.8, 140.6, 129.3, 129.0, 128.5, 125.9, 124.7, 123.7, 123.2, 123.1, 115.9, 111.9, 15.1, one carbon is merged with others; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{12}\text{NO}$ ($\text{M}+\text{H}$): 234.0919, found: 234.0920.

Spectral Data of 6H-chromeno[3,4-*b*]quinoline (6a):



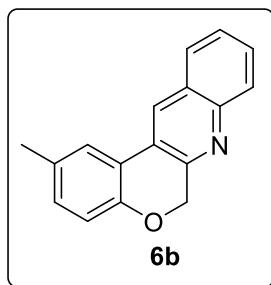
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.35 (s, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.85-7.83 (m, 2H), 7.67 (td, $J = 8.4, 1.4$ Hz, 1H), 7.52 (td, $J = 8.1, 1.1$ Hz, 1H), 7.30 (td, $J = 8.1, 1.5$ Hz, 1H), 7.11 (td, $J = 8.8, 1.2$ Hz, 1H), 7.05 (dd, $J = 8.1, 1.0$ Hz, 1H), 5.36 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 154.8, 153.3, 147.1, 130.4, 129.5, 128.8, 128.4, 127.9, 127.7, 126.8, 123.8, 123.7, 122.6, 121.0, 117.9, 70.5; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{12}\text{NO}$ (M+H): 234.0919, found: 234.0914.

Spectral Data of 2-((2H-chromen-3-yl)amino)benzaldehyde (6a'):



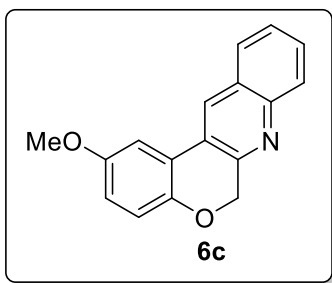
White solid; ^1H NMR (600 MHz, CDCl_3): δ 10.23 (s, 1H), 10.09 (s, 1H), 7.87 (dd, $J = 7.8, 0.7$ Hz, 1H), 7.63 (dd, $J = 7.3, 0.9$ Hz, 1H), 7.30-7.28 (m, 2H), 7.25-7.23 (m, 1H), 7.01-7.00 (m, 2H), 6.61-6.60 (m, 1H), 5.23 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 193.3, 158.2, 135.9, 134.2, 129.5, 129.2, 128.9, 127.9, 121.4, 120.3, 119.6, 114.8, 101.9, 63.3, two carbons are merged with other; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{14}\text{NO}_2$ (M+H): 252.1025, found: 252.1024.

Spectral Data of 2-methyl-6H-chromeno[3,4-b]quinoline (6b):



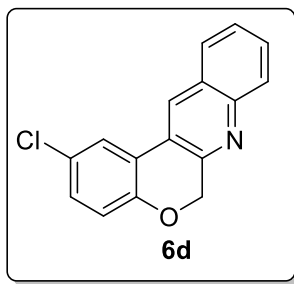
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.34 (s, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.84 (d, $J = 8.1$ Hz, 1H), 7.67-7.64 (m, 2H), 7.52 (t, $J = 7.2$ Hz, 1H), 7.11-7.09 (m, 1H), 6.95 (d, $J = 8.2$ Hz, 1H), 5.36 (s, 2H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 153.5, 152.7, 146.9, 131.9, 131.2, 129.5, 128.7, 128.4, 127.9, 127.6, 126.8, 124.0, 123.8, 120.6, 117.6, 70.5, 20.8; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ (M+H): 248.1075, found: 248.1080.

Spectral Data of 2-methoxy-6H-chromeno[3,4-*b*]quinoline (6c):



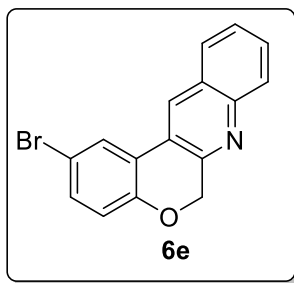
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.23 (s, 1H), 7.98 (d, $J = 8.4$ Hz, 1H), 7.81 (d, $J = 8.1$ Hz, 1H), 7.74 (d, $J = 8.4$ Hz, 1H), 7.63 (td, $J = 7.8, 1.2$ Hz, 1H), 7.50 (t, $J = 7.2$ Hz, 1H), 7.69 (d, $J = 6.0$ Hz, 1H), 6.59 (d, $J = 3$ Hz, 1H), 5.34 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 161.7, 156.1, 152.7, 146.6, 129.0, 128.7, 125.6, 127.7, 126.7, 126.3, 124.8, 123.4, 113.7, 109.8, 102.4, 77.7, 55.5; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_2$ ($\text{M}+\text{H}$): 264.1025, found: 264.1022.

Spectral Data of 2-chloro-6H-chromeno[3,4-*b*]quinoline (6d):



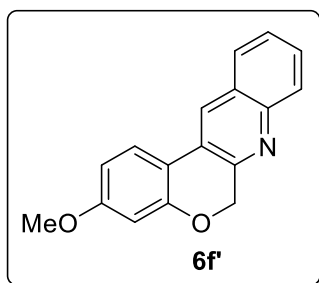
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.31 (s, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.86 (d, $J = 8.1$ Hz, 1H), 7.79 (d, $J = 2.4$ Hz, 1H), 7.69 (td, $J = 8.3, 1.3$ Hz, 1H), 7.54 (td, $J = 7.9, 0.7$ Hz, 1H), 7.24-7.22 (m, 1H), 6.99 (d, $J = 8.6$ Hz, 1H), 5.34 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 153.3, 152.7, 147.3, 130.1, 129.9, 128.8, 128.2, 128.1, 128.0, 127.7, 127.0, 123.5, 122.5, 122.4, 119.3, 70.5; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{11}\text{ClNO}$ ($\text{M}+\text{H}$): 268.0529, found: 268.0531.

Spectral Data of 2-bromo-6H-chromeno[3,4-*b*]quinolone (6e):



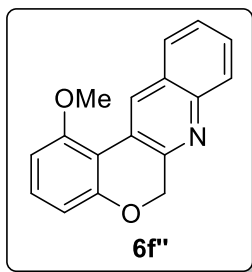
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.27 (s, 1H), 7.99 (d, $J = 8.4$ Hz, 1H), 7.90 (d, $J = 2.2$ Hz, 1H), 7.82 (d, $J = 8.1$ Hz, 1H), 7.67 (td, $J = 8.2, 1.3$ Hz, 1H), 7.52 (td, $J = 7.0, 1.0$ Hz, 1H), 7.35 (dd, $J = 8.6, 2.2$ Hz, 1H), 6.92 (d, $J = 8.7$ Hz, 1H), 5.32 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 153.7, 152.6, 147.2, 132.9, 129.9, 128.7, 128.2, 128.1, 128.0, 127.0, 126.4, 122.9, 122.3, 129.7, 114.9, 70.4; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{11}\text{BrNO}$ ($\text{M}+\text{H}$): 312.0024, found: 312.0021.

Spectral Data of 3-methoxy-6H-chromeno[3,4-*b*]quinoline (6f') (major):



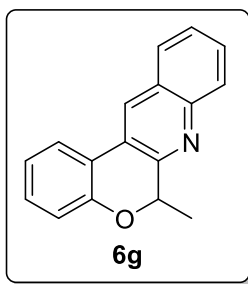
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.22 (s, 1H), 7.98 (d, $J = 8.4$ Hz, 1H), 7.81 (d, $J = 8.1$ Hz, 1H), 7.73 (d, $J = 8.4$ Hz, 1H), 7.63 (td, $J = 8.3, 1.3$ Hz, 1H), 7.50 (t, $J = 7.3$ Hz, 1H), 7.69 (dd, $J = 8.6, 2.5$ Hz, 1H), 6.59 (d, $J = 2.5$ Hz, 1H), 5.34 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 161.7, 156.1, 152.7, 146.5, 129.0, 128.7, 125.6, 127.7, 126.7, 126.2, 124.7, 123.8, 113.7, 109.8, 102.4, 77.7, 55.5; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_2$ ($\text{M}+\text{H}$): 264.1025, found: 264.1022.

Spectral Data of 1-methoxy-6H-chromeno[3,4-*b*]quinoline (6f'') (minor):



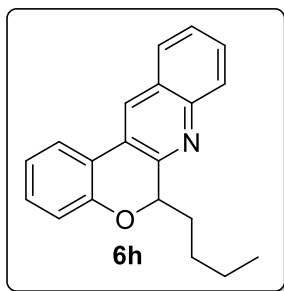
White solid; ^1H NMR (600 MHz, CDCl_3): δ 9.06 (s, 1H), 7.99 (d, $J = 8.3$ Hz, 1H), 7.85 (d, $J = 8.1$ Hz, 1H), 7.65 (t, $J = 7.2$ Hz, 1H), 7.50 (t, $J = 7.3$ Hz, 1H), 7.29 (t, $J = 8.2$ Hz, 1H), 6.73 (d, $J = 8.1$ Hz, 1H), 6.69 (d, $J = 8.3$ Hz, 1H), 5.27 (s, 2H), 4.01 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 158.6, 156.7, 153.5, 146.1, 132.9, 129.9, 129.3, 128.5, 128.4, 126.4, 122.3, 110.9, 110.6, 105.6, 105.1, 70.8, 55.7, one carbon is merge with other; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_2$ (M+H): 264.1025, found: 264.1021.

Spectral Data of 6-methyl-6H-chromeno[3,4-*b*]quinoline (6g):



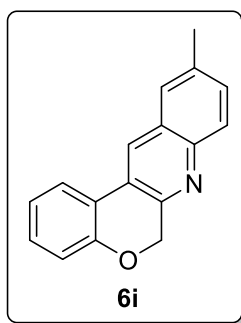
White solid; ^1H NMR (400 MHz, CDCl_3): δ 8.36 (s, 1H), 8.03 (d, $J = 8.0$ Hz, 1H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.66 (t, $J = 8.2, 1.2$ Hz, 1H), 7.52 (t, $J = 6.8$ Hz, 1H), 7.31 (t, $J = 7.2$ Hz, 1H), 7.12-7.04 (m, 2H), 5.50 (q, $J = 6.8$ Hz, 1H), 1.73 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 156.5, 153.4, 147.2, 130.4, 129.3, 129.0, 128.2, 127.9, 126.7, 123.5, 122.8, 122.3, 120.8, 118.4, 76.0, 19.2; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ (M+H): 248.1075, found: 248.1090.

Spectral Data of 6-butyl-6H-chromeno[3,4-*b*]quinoline (6h):



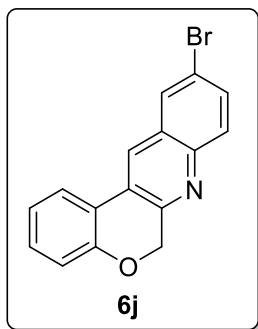
White semi-solid; ^1H NMR (600 MHz, CDCl_3): δ 8.36 (s, 1H), 8.02 (d, $J = 8.4$ Hz, 1H), 7.85-7.83 (m, 2H), 7.66 (td, $J = 8.4, 1.4$ Hz, 1H), 7.51 (td, $J = 8.0, 1.1$ Hz, 1H), 7.30 (td, $J = 8.1, 1.6$ Hz, 1H), 7.09 (td, $J = 7.5, 1.1$ Hz, 1H), 7.05 (dd, $J = 8.1, 1.0$ Hz, 1H), 5.50 (q, $J = 5.4$ Hz, 1H), 1.98-1.88 (m, 2H), 1.63-1.52 (m, 2H), 136-1.27 (m, 2H), 0.88 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 156.3, 152.9, 147.1, 130.4, 129.3, 128.9, 128.1, 127.8, 126.6, 123.4, 122.8, 122.1, 120.8, 118.5, 79.8, 33.2, 29.6, 27.7, 22.4, 14.0; HRMS-ESI+ calcd for $\text{C}_{20}\text{H}_{20}\text{NO}$ ($\text{M}+\text{H}$): 290.1545, found: 290.1550.

Spectral Data of 10-methyl-6H-chromeno[3,4-*b*]quinoline (6d):



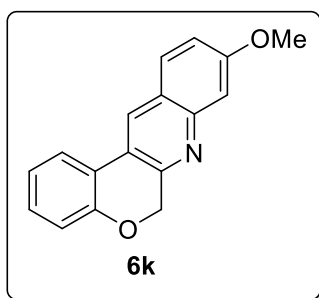
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.25 (s, 1H), 7.89 (d, $J = 8.5$ Hz, 1H), 7.82 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.60 (s, 1H), 7.49 (dd, $J = 8.5, 1.8$ Hz, 1H), 7.29 (td, $J = 8.3, 1.5$ Hz, 1H), 7.10 (td, $J = 7.6, 1.1$ Hz, 1H), 7.04 (dd, $J = 8.1, 1.0$ Hz, 1H), 5.33 (s, 2H), 2.52 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 154.7, 152.3, 145.6, 136.6, 131.8, 130.3, 128.4, 128.3, 127.1, 126.8, 123.7, 123.5, 122.5, 121.1, 117.9, 70.5, 21.5; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ ($\text{M}+\text{H}$): 248.1075, found: 248.1087.

Spectral Data of 10-bromo-6H-chromeno[3,4-*b*]quinoline (6j):



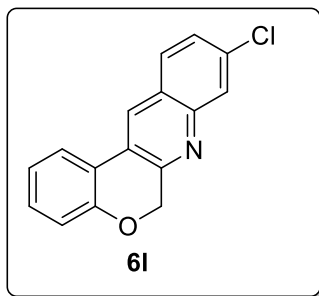
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.31 (s, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.86 (d, $J = 8.1$ Hz, 1H), 7.79 (d, $J = 2.4$ Hz, 1H), 7.69 (td, $J = 8.3, 1.3$ Hz, 1H), 7.54 (td, $J = 7.9, 0.7$ Hz, 1H), 7.24-7.22 (m, 1H), 6.99 (d, $J = 8.6$ Hz, 1H), 5.34 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 153.3, 152.7, 147.3, 130.1, 129.9, 128.8, 128.2, 128.1, 128.0, 127.7, 127.0, 123.5, 122.5, 122.4, 119.3, 70.5; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{11}\text{BrNO}$ ($\text{M}+\text{H}$): 312.0024, found: 312.0049.

Spectral Data of 9-methoxy-6H-chromeno[3,4-*b*]quinoline (6k):



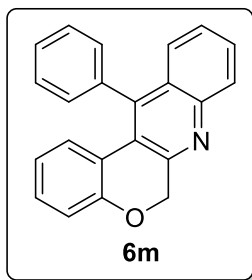
Pale yellow solid; ^1H NMR (600 MHz, CDCl_3): δ 8.26 (s, 1H), 7.78 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.71 (d, $J = 8.9$ Hz, 1H), 7.38 (d, $J = 2.3$ Hz, 1H), 7.26 (td, $J = 8.1, 1.5$ Hz, 1H), 7.17 (dd, $J = 9.0, 2.5$ Hz, 1H), 7.09 (t, $J = 7.6$ Hz, 1H), 7.03 (d, $J = 8.1$ Hz, 1H), 5.32 (s, 2H), 3.93 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 160.9, 154.4, 153.3, 148.7, 129.8, 129.0, 127.6, 123.5, 123.4, 122.5, 121.6, 121.2, 119.9, 117.8, 106.8, 70.4, 55.5; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_2$ ($\text{M}+\text{H}$): 264.1025, found: 264.1034.

Spectral Data of 9-chloro-6H-chromeno[3,4-*b*]quinoline (6l):



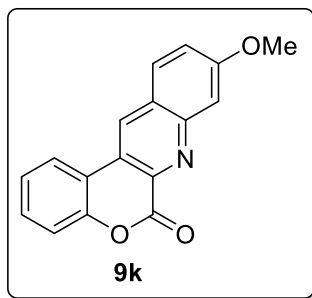
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.21 (s, 1H), 7.95 (d, $J = 1.5$ Hz, 1H), 7.74 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.70 (d, $J = 8.7$ Hz, 1H), 7.42 (dd, $J = 8.7, 1.9$ Hz, 1H), 7.28 (t, $J = 8.2$ Hz, 1H), 7.08 (t, $J = 7.7$ Hz, 1H), 7.02 (t, $J = 8.1$ Hz, 1H) 5.28 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 154.6, 154.2, 147.1, 135.1, 130.6, 129.0, 127.7, 127.2, 126.6, 123.8, 123.7, 122.6, 120.4, 117.9, 70.2, one carbon is merged with other; HRMS-ESI+ calcd for $\text{C}_{16}\text{H}_{11}\text{ClNO}$ (M+H): 268.0529, found: 268.0531.

Spectral Data of 12-phenyl-6H-chromeno[3,4-*b*]quinoline (6m):



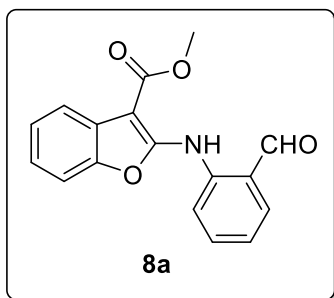
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.06 (d, $J = 8.3$ Hz, 1H), 7.66 (td, $J = 8.2, 1.3$ Hz, 1H), 7.54-7.51 (m, 2H), 7.40 (td, $J = 8.2, 1.1$ Hz, 1H), 7.31-7.30 (m, 2H), 7.24-7.20 (m, 1H), 7.13-7.10 (m, 1H), 7.03 (dd, $J = 8.1, 1.1$ Hz, 1H), 7.64 (dd, $J = 8.5, 0.9$ Hz, 1H), 6.66 (dd, $J = 8.1, 1.5$ Hz, 1H), 6.60 (t, $J = 8.3$ Hz, 1H), 5.30 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 156.5, 155.2, 146.2, 143.2, 137.1, 126.6, 129.4, 129.2, 128.8, 128.5, 128.3, 126.6, 121.9, 121.6, 121.4, 120.4, 117.8, 115.3, 71.5; HRMS-ESI+ calcd for $\text{C}_{22}\text{H}_{16}\text{NO}$ (M+H): 310.1232, found: 310.1241.

Spectral Data of 9-methoxy-6H-chromeno[3,4-*b*]quinolin-6-one (9k):



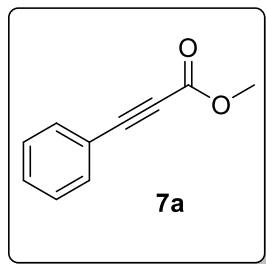
White solid; ^1H NMR (600 MHz, CDCl_3): δ 8.80 (s, 1H), 8.11 (d, $J = 7.9$ Hz, 1H), 7.88 (d, $J = 9.0$ Hz, 1H), 7.68 (d, $J = 2.2$ Hz, 1H), 7.48 (td, $J = 8.5, 1.3$ Hz, 1H), 7.39-7.36 (m, 3H), 3.97 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 162.0, 159.1, 150.6, 150.1, 138.5, 130.4, 129.4, 128.6, 125.7, 125.4, 124.8, 124.5, 122.6, 117.9, 117.4, 107.7, 55.8; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{12}\text{NO}_3$ (M+H): 278.0817, found: 278.0812.

Spectral Data of methyl 2-((2-formylphenyl)amino)benzofuran-3-carboxylate (8a):



Yellow solid; ^1H NMR (600 MHz, CDCl_3): δ 12.3 (s, 1H), 9.99 (s, 1H), 8.26 (d, $J = 8.5$ Hz, 1H), 7.84 (d, $J = 7.74$ Hz, 1H), 7.69 (dd, $J = 8.5, 2.3$ Hz, 1H), 7.63 (td, $J = 7.26, 1.4$ Hz, 1H), 7.41 (d, $J = 8.1$ Hz, 1H), 7.27 (t, $J = 7.5$ Hz, 1H), 7.18-7.15 (m, 2H), 4.01 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 193.8, 165.0, 158.4, 149.6, 140.0, 136.4, 135.7, 125.9, 124.5, 122.4, 121.8, 121.6, 120.3, 117.9, 110.1, 51.3, one carbon is merged with others; HRMS-ESI+ calcd for $\text{C}_{17}\text{H}_{13}\text{NO}_4$ (M+Na): 318.0742, found: 318.0746.

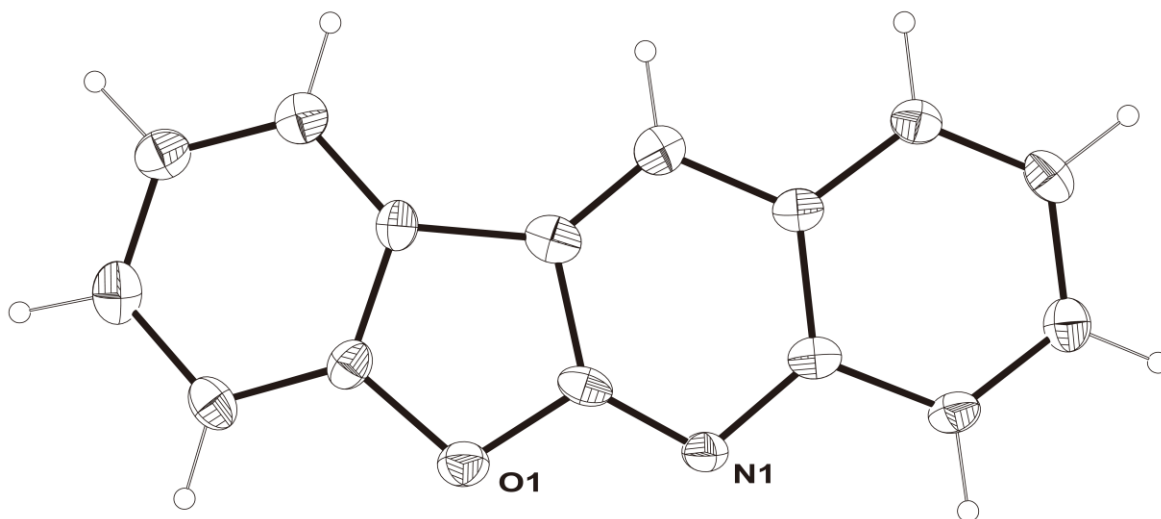
Spectral Data of methyl 3-phenylpropiolate (7a):



Yellow liquid; ^1H NMR (400 MHz, CDCl_3): δ 7.45-7.43 (m, 2H), 7.38-7.34 (m, 2H), 7.30-7.26 (m, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 153.2, 129.7, 129.3, 127.9, 127.4, 91.3, 80.4, 52.6.

3. X-Ray crystallographic Data:

X-Ray Data of Compound 3a:



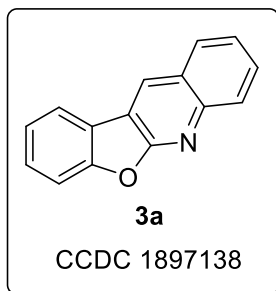


Table 1. Crystal data and structure refinement for d20681.

Identification code	d20681	
Empirical formula	C ₁₅ H ₉ N O	
Formula weight	219.23	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 23.736(4) Å	α = 90°.
	b = 5.9771(6) Å	β = 90°.
	c = 21.990(3) Å	γ = 90°.
Volume	3119.7(7) Å ³	
Z	12	
Density (calculated)	1.400 Mg/m ³	
Absorption coefficient	0.089 mm ⁻¹	
F(000)	1368	
Crystal size	0.10 x 0.05 x 0.02 mm ³	
Theta range for data collection	2.53 to 25.06°.	
Index ranges	-28 ≤ h ≤ 22, -5 ≤ k ≤ 7, -26 ≤ l ≤ 25	
Reflections collected	12552	
Independent reflections	5380 [R(int) = 0.0949]	
Completeness to theta = 25.06°	99.4 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9982 and 0.9912	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5380 / 0 / 440	
Goodness-of-fit on F ²	1.013	

Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0820$, $wR2 = 0.1809$
R indices (all data)	$R1 = 0.2074$, $wR2 = 0.2602$
Absolute structure parameter	0(4)
Largest diff. peak and hole	0.506 and -0.762 e. $\text{\AA}^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d20681. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	3942(4)	3085(14)	5192(4)	47(2)
C(2)	3640(4)	2399(15)	5684(5)	56(3)
C(3)	3605(4)	3942(16)	6155(5)	62(3)
C(4)	3853(4)	6035(15)	6103(5)	59(3)
C(5)	4144(4)	6694(15)	5599(5)	53(2)
C(6)	4193(4)	5184(14)	5134(4)	43(2)
C(7)	4435(4)	5157(14)	4511(5)	51(2)
C(8)	4328(4)	2997(13)	4259(5)	46(2)
C(9)	4729(4)	6573(15)	4178(5)	51(2)
C(10)	4890(4)	5843(12)	3583(4)	45(2)
C(11)	5202(4)	7263(14)	3205(5)	50(2)
C(12)	5352(4)	6611(15)	2632(5)	56(2)
C(13)	5189(4)	4467(15)	2413(5)	54(2)
C(14)	4897(4)	3038(13)	2780(4)	49(2)
C(15)	4741(3)	3675(13)	3384(4)	45(2)
C(16)	2735(4)	6303(14)	4885(4)	48(2)
C(17)	3043(4)	7037(14)	4379(5)	54(3)
C(18)	3094(4)	5544(16)	3899(5)	56(3)
C(19)	2840(4)	3506(15)	3907(5)	55(2)
C(20)	2531(4)	2781(14)	4393(5)	51(2)
C(21)	2476(4)	4213(14)	4897(4)	41(2)
C(22)	2203(4)	4195(16)	5494(6)	69(3)
C(23)	2336(4)	6375(12)	5802(5)	43(2)
C(24)	1939(4)	2876(18)	5833(5)	69(3)
C(25)	1750(4)	3558(14)	6447(4)	44(2)

C(26)	1442(4)	2057(14)	6797(5)	54(2)
C(27)	1263(4)	2700(15)	7349(5)	53(2)
C(28)	1400(4)	4789(17)	7582(5)	58(3)
C(29)	1715(4)	6265(14)	7257(4)	49(2)
C(30)	1890(3)	5625(13)	6667(4)	45(2)
C(31)	1702(4)	6892(17)	3471(6)	69(3)
C(32)	2042(4)	7565(18)	2980(7)	86(4)
C(33)	2124(5)	6090(20)	2519(6)	85(4)
C(34)	1882(4)	4030(20)	2493(5)	72(3)
C(35)	1540(4)	3308(14)	2964(4)	51(2)
C(36)	1454(3)	4730(14)	3477(4)	45(2)
C(37)	1102(8)	3640(30)	3948(9)	45(5)
C(38)	1038(8)	4830(30)	4450(9)	37(4)
C(46)	909(7)	3520(30)	4409(8)	44(4)
C(47)	1195(6)	4940(30)	4069(8)	36(3)
C(39)	1301(4)	7082(14)	4375(5)	58(3)
C(40)	729(3)	4378(13)	5002(4)	42(2)
C(41)	427(4)	2868(14)	5366(5)	52(2)
C(42)	261(4)	3432(17)	5914(5)	59(3)
C(43)	379(5)	5540(20)	6168(5)	79(4)
C(44)	673(5)	7052(17)	5816(6)	71(3)
C(45)	844(4)	6469(15)	5256(5)	55(2)
N(1)	4441(3)	2168(10)	3727(4)	48(2)
N(2)	2202(3)	7189(10)	6335(4)	42(2)
O(1)	4026(2)	1721(9)	4663(3)	54(2)
O(2)	2646(2)	7627(9)	5396(3)	54(2)
O(3)	1616	8191	3963	42
N(3)	1167	7935	4911	40
O(3A)	1167	7935	4911	41
N(3A)	1616	8191	3963	41

Table 3. Bond lengths [Å] and angles [°] for d20681.

C(1)-C(2)	1.362(12)
C(1)-C(6)	1.395(11)

C(1)-O(1)	1.435(9)
C(2)-C(3)	1.389(12)
C(2)-H(2)	0.9500
C(3)-C(4)	1.387(12)
C(3)-H(3)	0.9500
C(4)-C(5)	1.366(12)
C(4)-H(4)	0.9500
C(5)-C(6)	1.368(11)
C(5)-H(5)	0.9500
C(6)-C(7)	1.486(12)
C(7)-C(9)	1.319(12)
C(7)-C(8)	1.427(11)
C(8)-N(1)	1.300(11)
C(8)-O(1)	1.372(10)
C(9)-C(10)	1.431(12)
C(9)-H(9)	0.9500
C(10)-C(11)	1.400(11)
C(10)-C(15)	1.413(11)
C(11)-C(12)	1.365(12)
C(11)-H(11)	0.9500
C(12)-C(13)	1.422(12)
C(12)-H(12)	0.9500
C(13)-C(14)	1.363(11)
C(13)-H(13)	0.9500
C(14)-C(15)	1.432(11)
C(14)-H(14)	0.9500
C(15)-N(1)	1.373(10)
C(16)-O(2)	1.391(10)
C(16)-C(21)	1.392(12)
C(16)-C(17)	1.402(12)
C(17)-C(18)	1.388(12)
C(17)-H(17)	0.9500
C(18)-C(19)	1.359(12)
C(18)-H(18)	0.9500
C(19)-C(20)	1.367(12)
C(19)-H(19)	0.9500

C(20)-C(21)	1.406(11)
C(20)-H(20)	0.9500
C(21)-C(22)	1.465(14)
C(22)-C(24)	1.252(13)
C(22)-C(23)	1.501(12)
C(23)-N(2)	1.310(10)
C(23)-O(2)	1.377(10)
C(24)-C(25)	1.480(13)
C(24)-H(24)	0.9500
C(25)-C(30)	1.368(11)
C(25)-C(26)	1.390(12)
C(26)-C(27)	1.343(12)
C(26)-H(26)	0.9500
C(27)-C(28)	1.389(12)
C(27)-H(27)	0.9500
C(28)-C(29)	1.359(12)
C(28)-H(28)	0.9500
C(29)-C(30)	1.415(11)
C(29)-H(29)	0.9500
C(30)-N(2)	1.398(10)
C(31)-O(3)	1.349(11)
C(31)-N(3A)	1.349(11)
C(31)-C(32)	1.406(15)
C(31)-C(36)	1.420(12)
C(32)-C(33)	1.355(16)
C(32)-H(32)	0.9500
C(33)-C(34)	1.362(16)
C(33)-H(33)	0.9500
C(34)-C(35)	1.384(13)
C(34)-H(34)	0.9500
C(35)-C(36)	1.427(11)
C(35)-H(35)	0.9500
C(36)-C(47)	1.446(18)
C(36)-C(37)	1.48(2)
C(37)-C(38)	1.32(3)
C(37)-H(37)	0.9500

C(38)-C(40)	1.44(2)
C(38)-C(39)	1.49(2)
C(46)-C(47)	1.32(2)
C(46)-C(40)	1.465(18)
C(46)-H(46)	0.9500
C(47)-C(39)	1.470(18)
C(39)-N(3)	1.322(10)
C(39)-O(3A)	1.322(10)
C(39)-N(3A)	1.348(10)
C(39)-O(3)	1.348(10)
C(40)-C(45)	1.396(12)
C(40)-C(41)	1.403(11)
C(41)-C(42)	1.313(11)
C(41)-H(41)	0.9500
C(42)-C(43)	1.406(14)
C(42)-H(42)	0.9500
C(43)-C(44)	1.379(14)
C(43)-H(43)	0.9500
C(44)-C(45)	1.344(13)
C(44)-H(44)	0.9500
C(45)-O(3A)	1.390(9)
C(45)-N(3)	1.390(9)
C(2)-C(1)-C(6)	124.6(8)
C(2)-C(1)-O(1)	123.1(8)
C(6)-C(1)-O(1)	112.2(7)
C(1)-C(2)-C(3)	115.1(8)
C(1)-C(2)-H(2)	122.5
C(3)-C(2)-H(2)	122.5
C(4)-C(3)-C(2)	120.8(9)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	122.8(9)
C(5)-C(4)-H(4)	118.6
C(3)-C(4)-H(4)	118.6
C(4)-C(5)-C(6)	117.3(8)

C(4)-C(5)-H(5)	121.3
C(6)-C(5)-H(5)	121.3
C(5)-C(6)-C(1)	119.3(8)
C(5)-C(6)-C(7)	136.8(8)
C(1)-C(6)-C(7)	103.8(7)
C(9)-C(7)-C(8)	117.4(9)
C(9)-C(7)-C(6)	135.2(9)
C(8)-C(7)-C(6)	107.3(8)
N(1)-C(8)-O(1)	118.6(7)
N(1)-C(8)-C(7)	131.1(9)
O(1)-C(8)-C(7)	110.2(8)
C(7)-C(9)-C(10)	116.9(8)
C(7)-C(9)-H(9)	121.5
C(10)-C(9)-H(9)	121.5
C(11)-C(10)-C(15)	120.3(8)
C(11)-C(10)-C(9)	120.0(8)
C(15)-C(10)-C(9)	119.7(8)
C(12)-C(11)-C(10)	120.9(8)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	119.9(8)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	120.2(9)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(15)	120.9(8)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6
N(1)-C(15)-C(10)	124.2(8)
N(1)-C(15)-C(14)	118.0(7)
C(10)-C(15)-C(14)	117.8(8)
O(2)-C(16)-C(21)	115.3(8)
O(2)-C(16)-C(17)	122.9(8)
C(21)-C(16)-C(17)	121.7(8)
C(18)-C(17)-C(16)	116.6(8)

C(18)-C(17)-H(17)	121.7
C(16)-C(17)-H(17)	121.7
C(19)-C(18)-C(17)	121.9(9)
C(19)-C(18)-H(18)	119.0
C(17)-C(18)-H(18)	119.0
C(18)-C(19)-C(20)	122.1(9)
C(18)-C(19)-H(19)	118.9
C(20)-C(19)-H(19)	118.9
C(19)-C(20)-C(21)	118.2(8)
C(19)-C(20)-H(20)	120.9
C(21)-C(20)-H(20)	120.9
C(16)-C(21)-C(20)	119.4(8)
C(16)-C(21)-C(22)	102.7(8)
C(20)-C(21)-C(22)	138.0(8)
C(24)-C(22)-C(21)	139.4(11)
C(24)-C(22)-C(23)	112.5(11)
C(21)-C(22)-C(23)	107.7(8)
N(2)-C(23)-O(2)	120.5(6)
N(2)-C(23)-C(22)	132.4(9)
O(2)-C(23)-C(22)	107.0(8)
C(22)-C(24)-C(25)	121.4(11)
C(22)-C(24)-H(24)	119.3
C(25)-C(24)-H(24)	119.3
C(30)-C(25)-C(26)	121.0(8)
C(30)-C(25)-C(24)	119.8(8)
C(26)-C(25)-C(24)	119.1(9)
C(27)-C(26)-C(25)	118.8(8)
C(27)-C(26)-H(26)	120.6
C(25)-C(26)-H(26)	120.6
C(26)-C(27)-C(28)	121.1(9)
C(26)-C(27)-H(27)	119.4
C(28)-C(27)-H(27)	119.4
C(29)-C(28)-C(27)	121.2(9)
C(29)-C(28)-H(28)	119.4
C(27)-C(28)-H(28)	119.4
C(28)-C(29)-C(30)	118.0(8)

C(28)-C(29)-H(29)	121.0
C(30)-C(29)-H(29)	121.0
C(25)-C(30)-N(2)	123.2(8)
C(25)-C(30)-C(29)	119.8(8)
N(2)-C(30)-C(29)	117.0(7)
O(3)-C(31)-N(3A)	0.0
O(3)-C(31)-C(32)	122.6(11)
N(3A)-C(31)-C(32)	122.6(11)
O(3)-C(31)-C(36)	116.9(10)
N(3A)-C(31)-C(36)	116.9(10)
C(32)-C(31)-C(36)	120.3(10)
C(33)-C(32)-C(31)	118.1(11)
C(33)-C(32)-H(32)	120.9
C(31)-C(32)-H(32)	120.9
C(32)-C(33)-C(34)	123.9(12)
C(32)-C(33)-H(33)	118.1
C(34)-C(33)-H(33)	118.1
C(33)-C(34)-C(35)	119.9(11)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	119.3(9)
C(34)-C(35)-H(35)	120.4
C(36)-C(35)-H(35)	120.4
C(31)-C(36)-C(35)	118.4(8)
C(31)-C(36)-C(47)	96.2(10)
C(35)-C(36)-C(47)	145.4(10)
C(31)-C(36)-C(37)	129.8(11)
C(35)-C(36)-C(37)	111.8(11)
C(47)-C(36)-C(37)	33.7(8)
C(38)-C(37)-C(36)	114.3(19)
C(38)-C(37)-H(37)	122.8
C(36)-C(37)-H(37)	122.8
C(37)-C(38)-C(40)	131.3(19)
C(37)-C(38)-C(39)	110.1(19)
C(40)-C(38)-C(39)	118.4(13)
C(47)-C(46)-C(40)	115.4(16)

C(47)-C(46)-H(46)	122.3
C(40)-C(46)-H(46)	122.3
C(46)-C(47)-C(36)	132.5(16)
C(46)-C(47)-C(39)	112.9(16)
C(36)-C(47)-C(39)	114.5(12)
N(3)-C(39)-O(3A)	0.0
N(3)-C(39)-N(3A)	122.8(6)
O(3A)-C(39)-N(3A)	122.8(6)
N(3)-C(39)-O(3)	122.8(6)
O(3A)-C(39)-O(3)	122.8(6)
N(3A)-C(39)-O(3)	0.0
N(3)-C(39)-C(47)	134.7(10)
O(3A)-C(39)-C(47)	134.7(10)
N(3A)-C(39)-C(47)	102.5(9)
O(3)-C(39)-C(47)	102.5(9)
N(3)-C(39)-C(38)	98.5(10)
O(3A)-C(39)-C(38)	98.5(10)
N(3A)-C(39)-C(38)	138.6(10)
O(3)-C(39)-C(38)	138.6(10)
C(47)-C(39)-C(38)	36.2(8)
C(45)-C(40)-C(41)	116.6(8)
C(45)-C(40)-C(38)	93.9(10)
C(41)-C(40)-C(38)	149.3(10)
C(45)-C(40)-C(46)	127.8(10)
C(41)-C(40)-C(46)	115.5(9)
C(38)-C(40)-C(46)	33.9(8)
C(42)-C(41)-C(40)	120.8(9)
C(42)-C(41)-H(41)	119.6
C(40)-C(41)-H(41)	119.6
C(41)-C(42)-C(43)	122.3(10)
C(41)-C(42)-H(42)	118.8
C(43)-C(42)-H(42)	118.8
C(44)-C(43)-C(42)	117.7(10)
C(44)-C(43)-H(43)	121.1
C(42)-C(43)-H(43)	121.1
C(45)-C(44)-C(43)	119.8(9)

C(45)-C(44)-H(44)	120.1
C(43)-C(44)-H(44)	120.1
C(44)-C(45)-O(3A)	120.3(9)
C(44)-C(45)-N(3)	120.3(9)
O(3A)-C(45)-N(3)	0.0
C(44)-C(45)-C(40)	122.6(9)
O(3A)-C(45)-C(40)	117.0(8)
N(3)-C(45)-C(40)	117.0(8)
C(8)-N(1)-C(15)	110.6(7)
C(23)-N(2)-C(30)	110.4(7)
C(8)-O(1)-C(1)	106.3(6)
C(23)-O(2)-C(16)	107.2(6)
C(31)-O(3)-C(39)	109.9(6)
C(39)-N(3)-C(45)	112.1(6)
C(39)-O(3A)-C(45)	112.1(6)
C(31)-N(3A)-C(39)	109.9(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d20681. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	49(6)	52(5)	40(5)	-3(4)	-6(4)	9(5)
C(2)	57(7)	57(6)	54(6)	19(5)	-3(5)	1(5)
C(3)	55(6)	76(7)	56(7)	9(6)	6(5)	23(5)
C(4)	58(7)	54(6)	65(7)	-4(5)	-5(6)	9(5)
C(5)	45(6)	58(6)	55(6)	2(5)	-15(5)	6(4)
C(6)	40(5)	54(6)	36(5)	5(4)	-4(4)	7(4)
C(7)	42(5)	48(5)	64(7)	10(5)	-17(5)	4(4)
C(8)	39(5)	33(4)	65(7)	9(5)	-11(5)	-2(4)
C(9)	41(5)	55(5)	58(6)	-3(5)	-6(5)	5(4)
C(10)	43(5)	39(5)	52(6)	1(4)	-10(4)	5(4)
C(11)	47(6)	43(5)	58(6)	2(4)	-4(5)	-1(4)
C(12)	50(6)	56(6)	62(7)	19(5)	2(5)	-4(5)

C(13)	52(6)	65(6)	44(6)	5(5)	-3(5)	3(5)
C(14)	60(6)	36(5)	51(6)	-4(4)	-8(5)	5(4)
C(15)	38(5)	40(5)	55(6)	-2(4)	-15(4)	3(4)
C(16)	49(6)	49(5)	47(6)	-9(5)	-17(5)	10(4)
C(17)	49(6)	45(5)	68(7)	13(5)	-5(5)	3(4)
C(18)	56(6)	70(6)	42(6)	18(5)	-3(5)	14(5)
C(19)	57(6)	64(6)	44(6)	3(5)	-1(5)	13(5)
C(20)	46(6)	49(5)	58(6)	-1(5)	-13(5)	7(4)
C(21)	36(5)	57(5)	31(5)	7(4)	-1(4)	2(4)
C(22)	43(6)	60(6)	103(9)	29(6)	-28(6)	5(5)
C(23)	35(5)	36(5)	58(6)	-2(4)	-13(4)	-3(4)
C(24)	52(7)	63(6)	93(9)	14(6)	-20(6)	14(5)
C(25)	46(5)	41(5)	44(5)	-5(4)	1(4)	13(4)
C(26)	43(6)	42(5)	79(7)	3(5)	-12(5)	4(4)
C(27)	45(6)	58(6)	55(6)	5(5)	4(5)	9(5)
C(28)	43(6)	85(7)	46(6)	-2(5)	5(5)	17(5)
C(29)	56(6)	44(5)	45(6)	-8(4)	-7(5)	9(4)
C(30)	35(5)	44(5)	57(6)	12(5)	-12(4)	9(4)
C(31)	46(6)	68(7)	93(8)	3(6)	-14(6)	18(5)
C(32)	44(7)	56(7)	158(13)	40(8)	-12(8)	11(5)
C(33)	67(8)	108(10)	82(9)	56(8)	1(7)	15(8)
C(34)	50(7)	117(9)	50(7)	0(7)	-13(5)	29(6)
C(35)	53(6)	55(5)	46(5)	7(5)	0(5)	5(4)
C(36)	33(5)	49(5)	53(6)	5(4)	-7(4)	8(4)
C(39)	46(6)	35(5)	92(8)	-8(5)	-28(5)	10(4)
C(40)	37(5)	41(5)	49(6)	-1(4)	-4(4)	1(4)
C(41)	55(6)	48(5)	53(6)	-3(4)	-7(5)	0(4)
C(42)	42(6)	90(7)	43(6)	19(5)	10(4)	16(5)
C(43)	85(9)	107(9)	44(7)	-19(7)	-26(6)	59(8)
C(44)	78(8)	52(6)	84(9)	-18(6)	-45(7)	12(6)
C(45)	46(6)	62(6)	56(7)	7(5)	-17(5)	6(5)
N(1)	59(5)	39(4)	44(5)	-3(3)	-1(4)	-10(3)
N(2)	44(4)	39(4)	42(4)	6(3)	-6(3)	2(3)
O(1)	61(4)	43(3)	59(4)	-1(3)	-2(3)	2(3)
O(2)	56(4)	46(3)	60(4)	-4(3)	-11(3)	3(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d20681.

	x	y	z	U(eq)
H(2)	3465	971	5704	67
H(3)	3409	3559	6517	75
H(4)	3818	7054	6433	71
H(5)	4307	8143	5572	63
H(9)	4830	8011	4327	61
H(11)	5310	8698	3348	59
H(12)	5564	7587	2381	67
H(13)	5284	4030	2011	64
H(14)	4796	1600	2631	59
H(17)	3210	8482	4366	65
H(18)	3311	5958	3555	67
H(19)	2878	2554	3563	66
H(20)	2359	1347	4391	62
H(24)	1859	1407	5693	83
H(26)	1359	601	6647	65
H(27)	1038	1708	7584	63
H(28)	1272	5194	7977	70
H(29)	1814	7683	7420	58
H(32)	2209	9009	2971	103
H(33)	2366	6528	2195	102
H(34)	1946	3091	2152	87
H(35)	1365	1880	2946	61
H(37)	936	2208	3893	54
H(46)	826	2037	4279	53
H(41)	342	1419	5214	62
H(42)	53	2379	6148	70
H(43)	261	5907	6569	94

H(44)

753

8504

5970

86

4. ^1H & ^{13}C Spectra of Key Compounds:

8.011
8.010
7.998
7.997
7.994
7.983
7.960
7.957
7.948
7.945
7.943
7.934
7.932
7.919
7.918
7.905
7.904
7.859
7.858
7.855
7.853
7.848
7.846
7.844
7.843
7.841
7.840
7.834
7.833
7.829
7.827
7.826
7.825
7.824
7.823
7.822
7.821
7.820
7.819



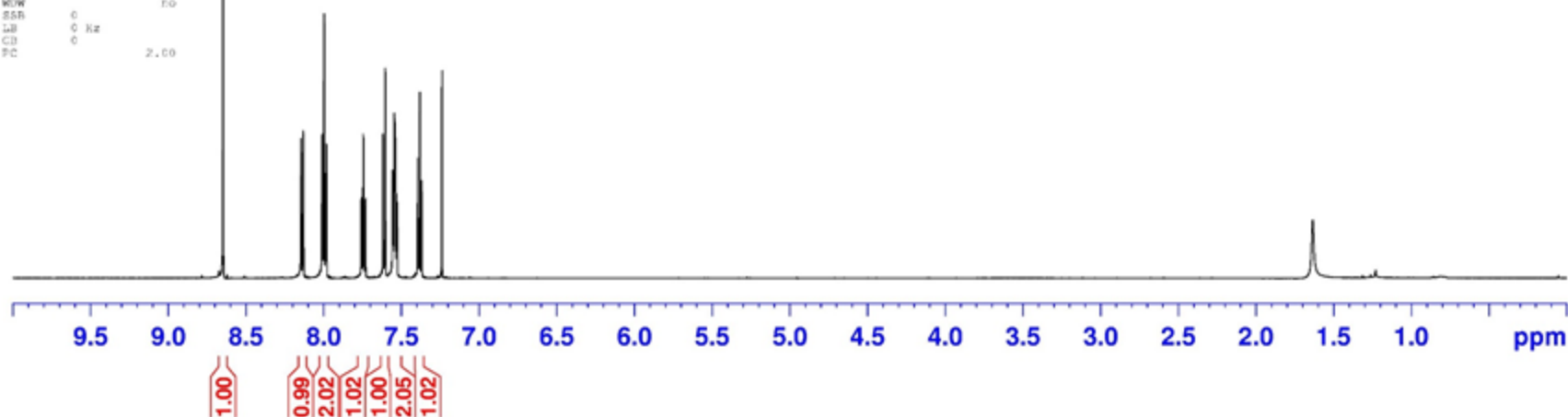
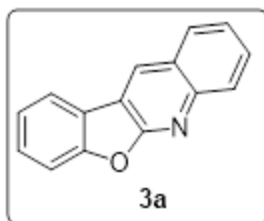
Current Data Parameters
NAME MDP-2-18
EXFNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190130
Time 13.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8375.209 Hz
FIDRES 0.255591 Hz
AQ 1.9562395 sec
RG 512
SW 59.700 usec
SE 6.50 usec
TE 295.2 K
D1 2.0000000 sec
d12 0.0000000 sec
MCLEST 0 sec
MCW3K 0.0130000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
PL9 23.00 dB
SFO1 500.2029910 MHz

F2 - Processing parameters
ST 32768
SF 500.2030277 MHz
WDW no
SSB 0
LB 0 Hz
CB 0
PC 2.00





Current Data Parameters
NAME MDP-2-18
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190130
Time 16.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3672
DS 0

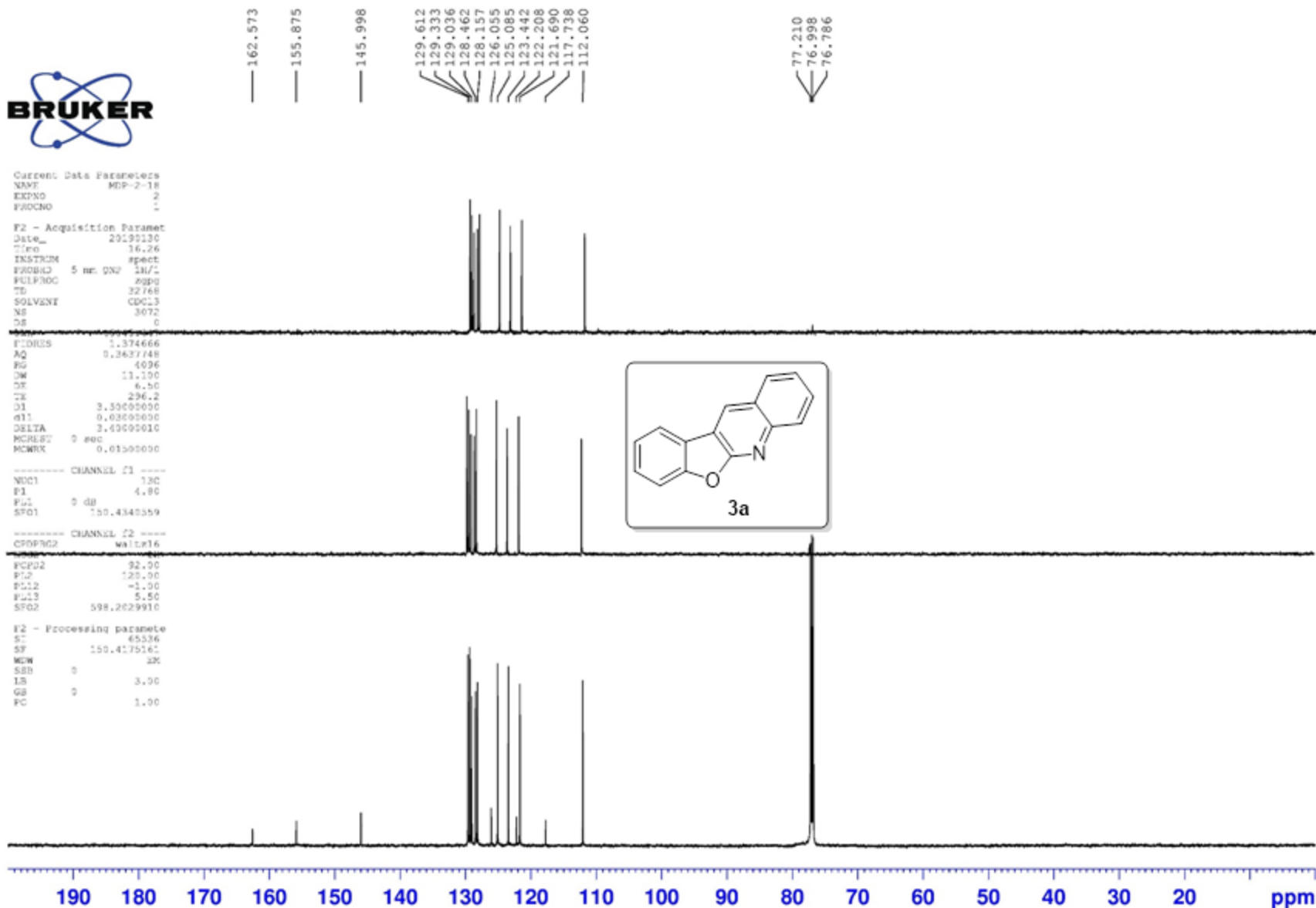
FIDRES 1.374666
AQ 0.3637748
RG 4096
DM 11.100
DE 6.50
TE 296.2
D1 3.3000000
d11 0.0300000
DELTA 2.4000000
MCREST 0 sec
MCMRK 0.0100000

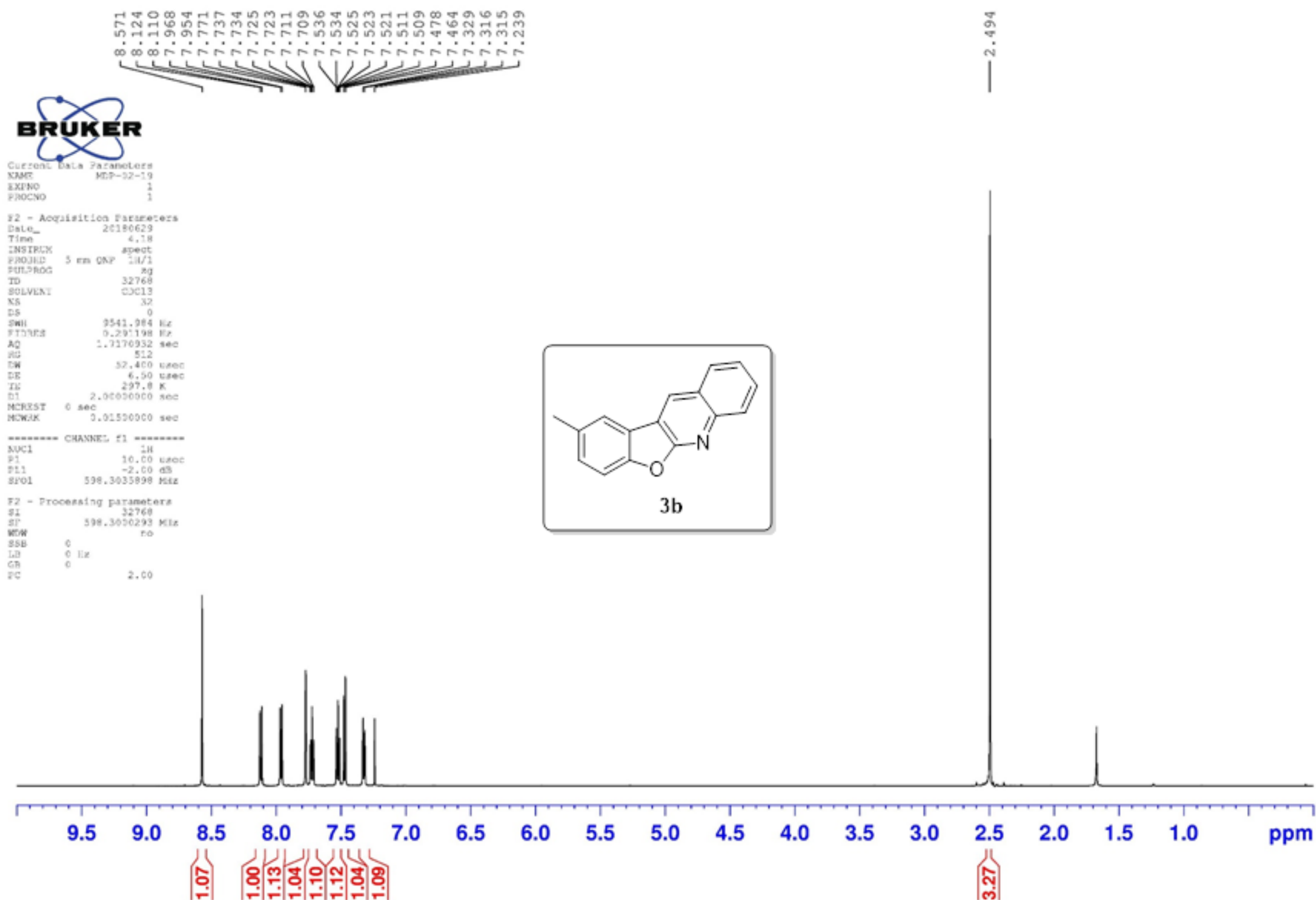
----- CHANNEL f1 -----
NUC1 13C
P1 120
PL1 0 dB
SFO1 100.628159

----- CHANNEL f2 -----
CPDPRG2 waltz16

PCPD2 92.00
PL2 120.00
PL12 -1.00
PL13 5.50
SFO2 598.2629910

F2 - Processing parameters
SI 65536
SF 150.4175161
WDW 300
SSB 0
LB 3.00
GB 0
PC 1.00







Current Data Parameters
NAME MCP-02-19
EXPNO 2
PROCNO 1

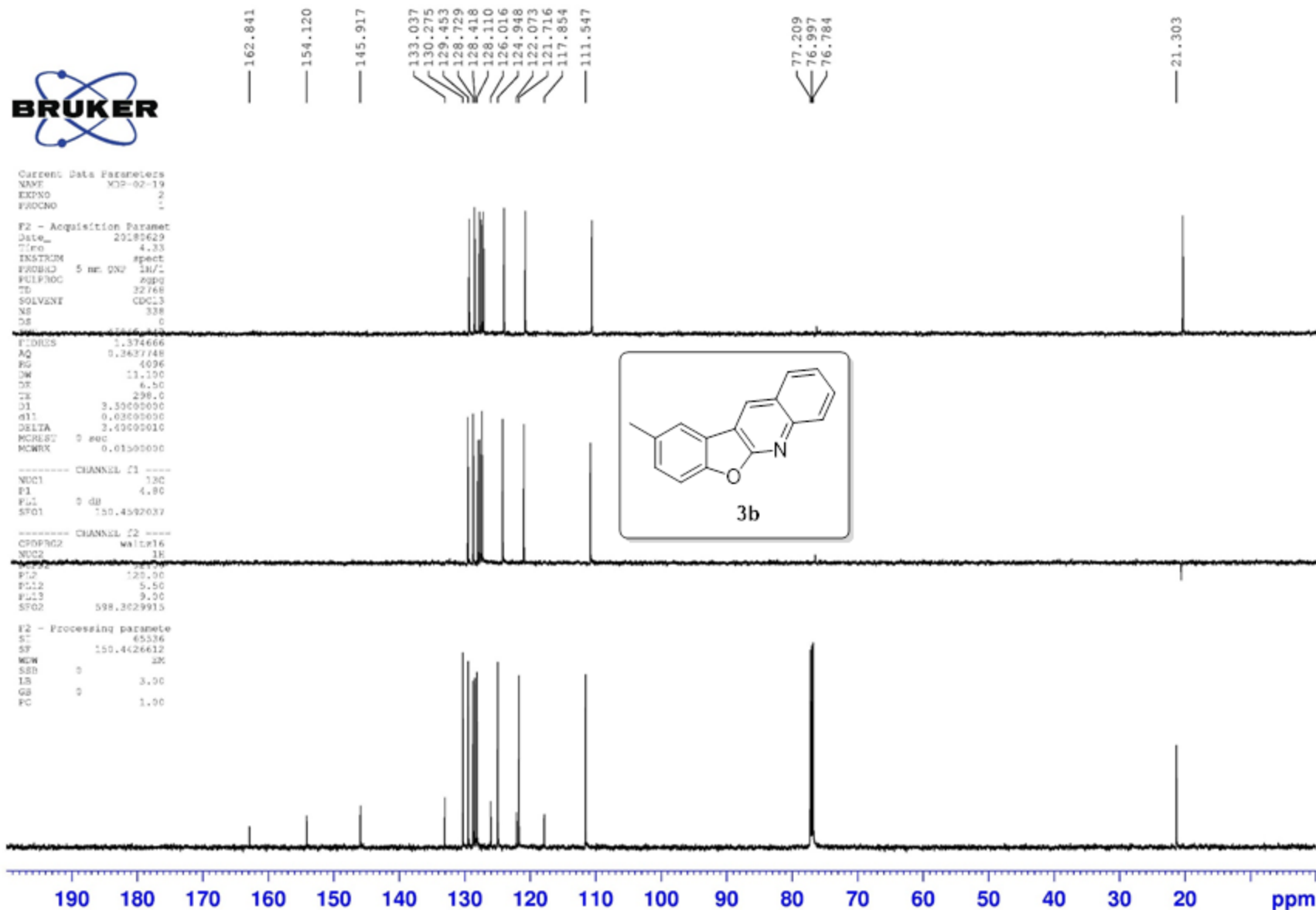
F2 - Acquisition Parameters
Date_ 20180629
Time 4.33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 338
DS 0

FIDRES 1.374666
AQ 0.3637748
RG 4096
DM 11.130
DE 6.50
TE 298.0
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCHRSZ 0 sec
MCHRX 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 100.626127

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P2 12.00
PL2 0.00
PL12 5.50
PL13 9.00
SFO2 500.13629915

F2 - Processing parameters
SI 65536
SF 150.4426612
WDW 20
SSB 0
LB 3.00
GB 0
PC 1.00



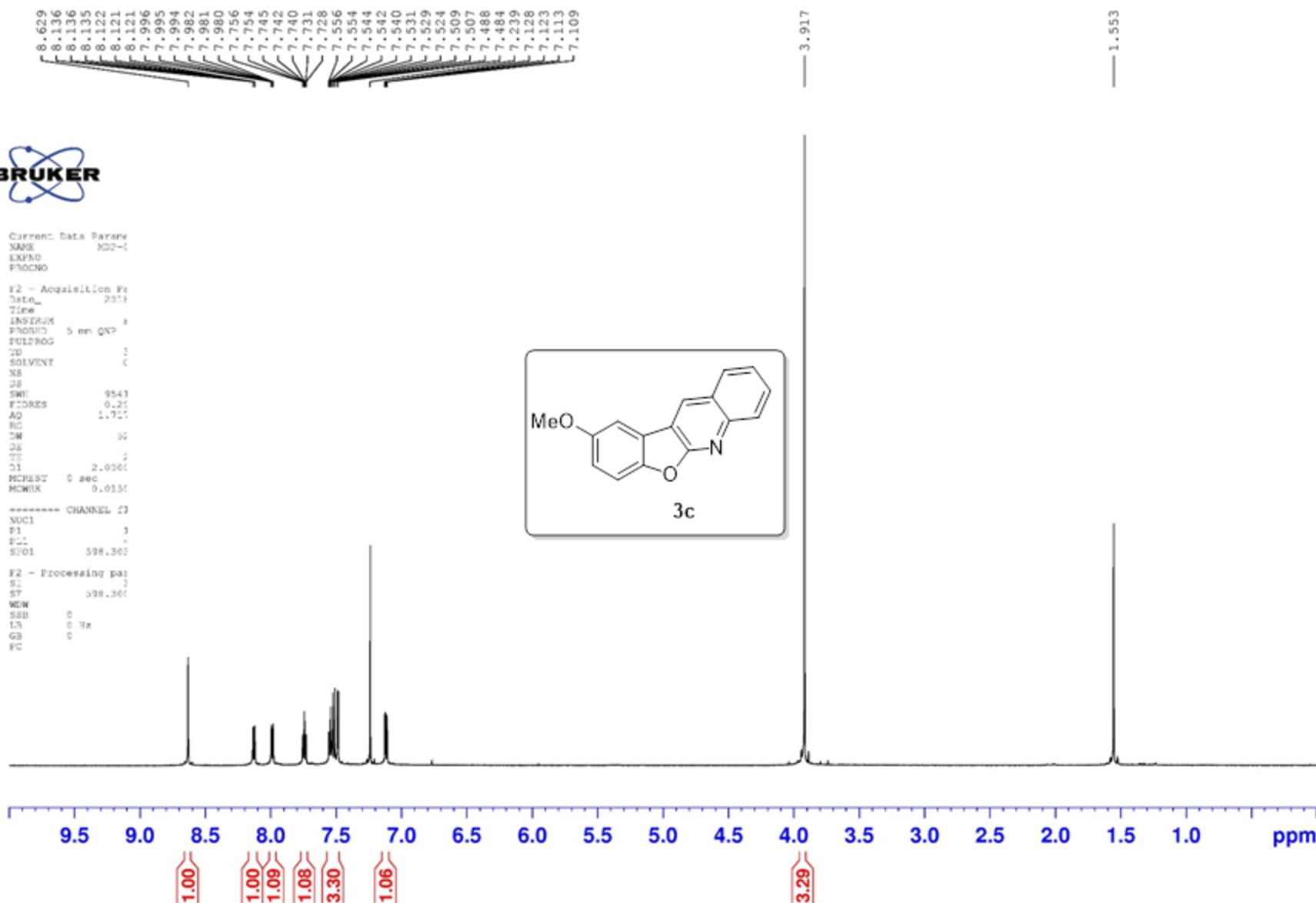
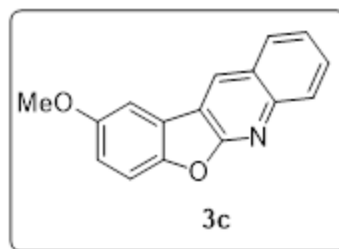


Current Data Params
NAME: M02-1
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_ 2011
Time 10:10:10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT c
NS 2048
DS 4
SWH 9541
FIDRES 0.21
AQ 1.71
RG 327.68
CW 36
ZS 2
TE 300.2
D1 2.0000
MCPRST 0 sec
MCWIR 0.0131

----- CHANNEL f2
NUC1 13C
P1 12.00
PC 0.00
SFO1 598.301

F2 - Processing parameters
SI 32768
SF 598.301
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00





Current Data Parameters
NAME MDP-02-20
EXPNO 2
PROCNO 1

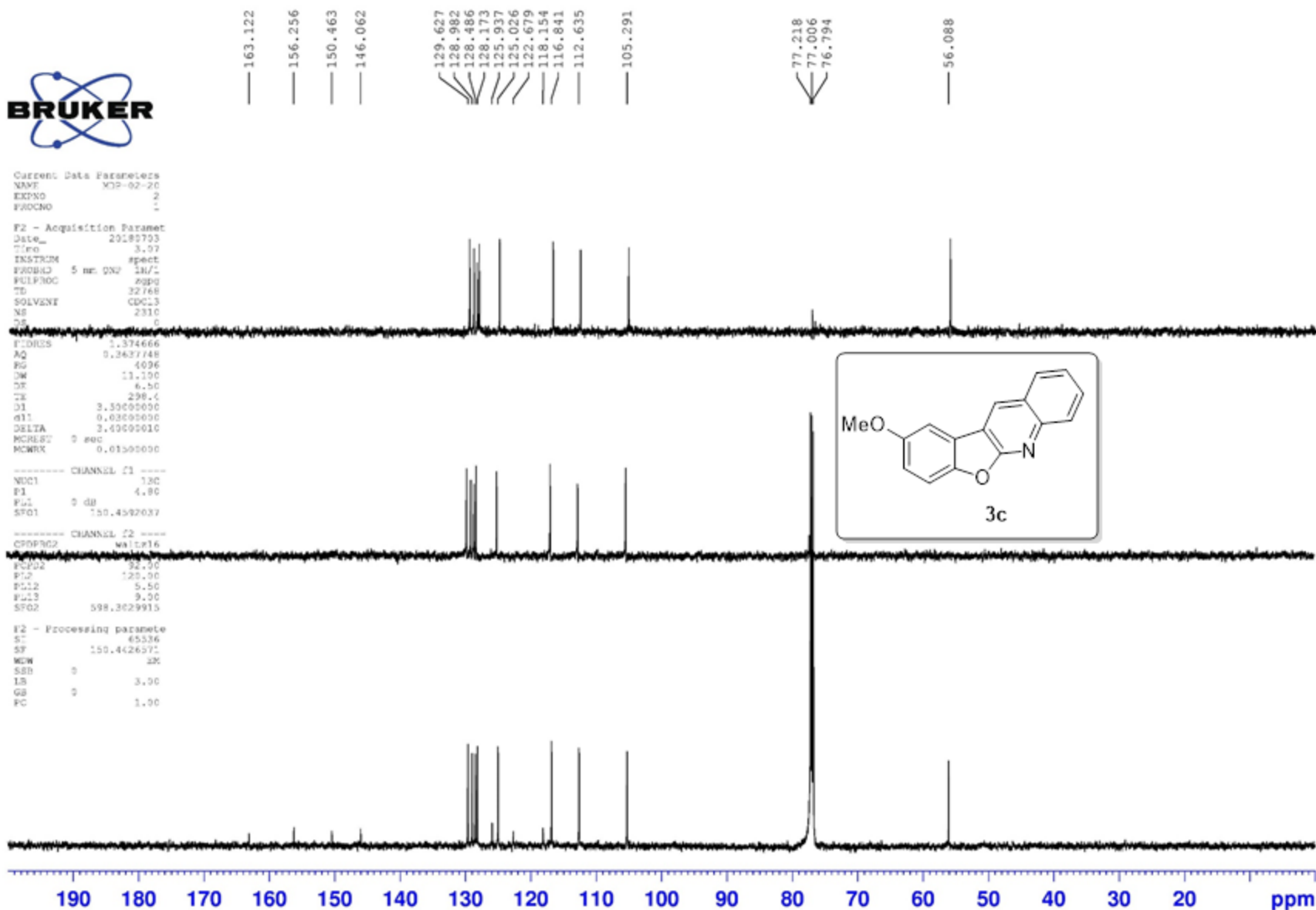
F2 - Acquisition Parameters
Date_ 20180703
Time 3.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2310
DS 0

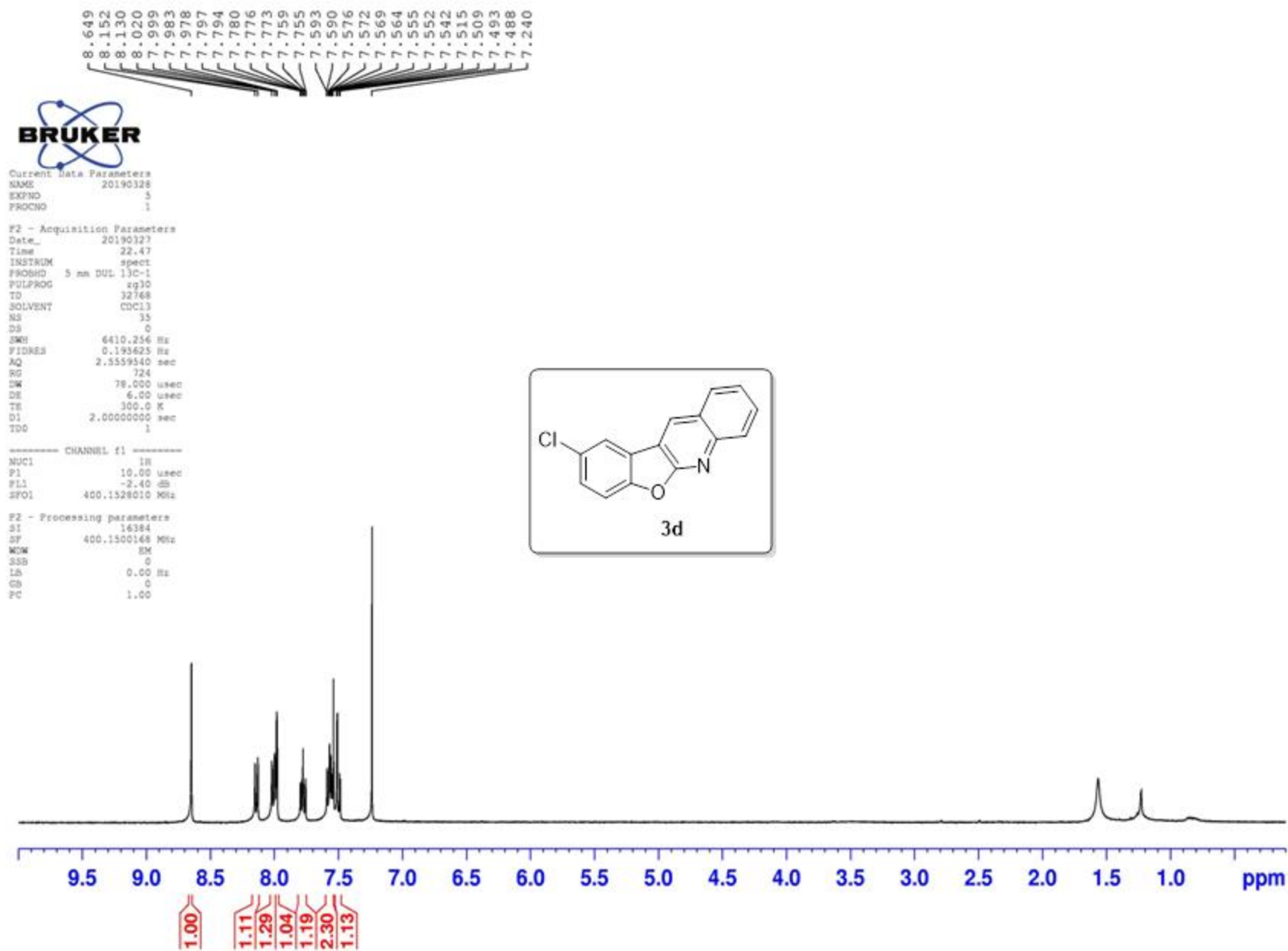
FIDRES 1.374666
AQ 0.2637748
RG 4096
DM 11.100
DE 6.50
TE 298.4
D1 3.3000000
d11 0.0300000
DELTA 2.4000000
MCHRG 0 sec
MCHRG 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 120
PL1 0 dB
SFO1 100.626137

----- CHANNEL f2 -----
CPDPRG2 waltz16
PCPD2 32.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 508.3029915

F2 - Processing parameters
SI 65536
SF 150.4426571
WDW 300
SSB 0
LB 3.00
GB 0
PC 1.00





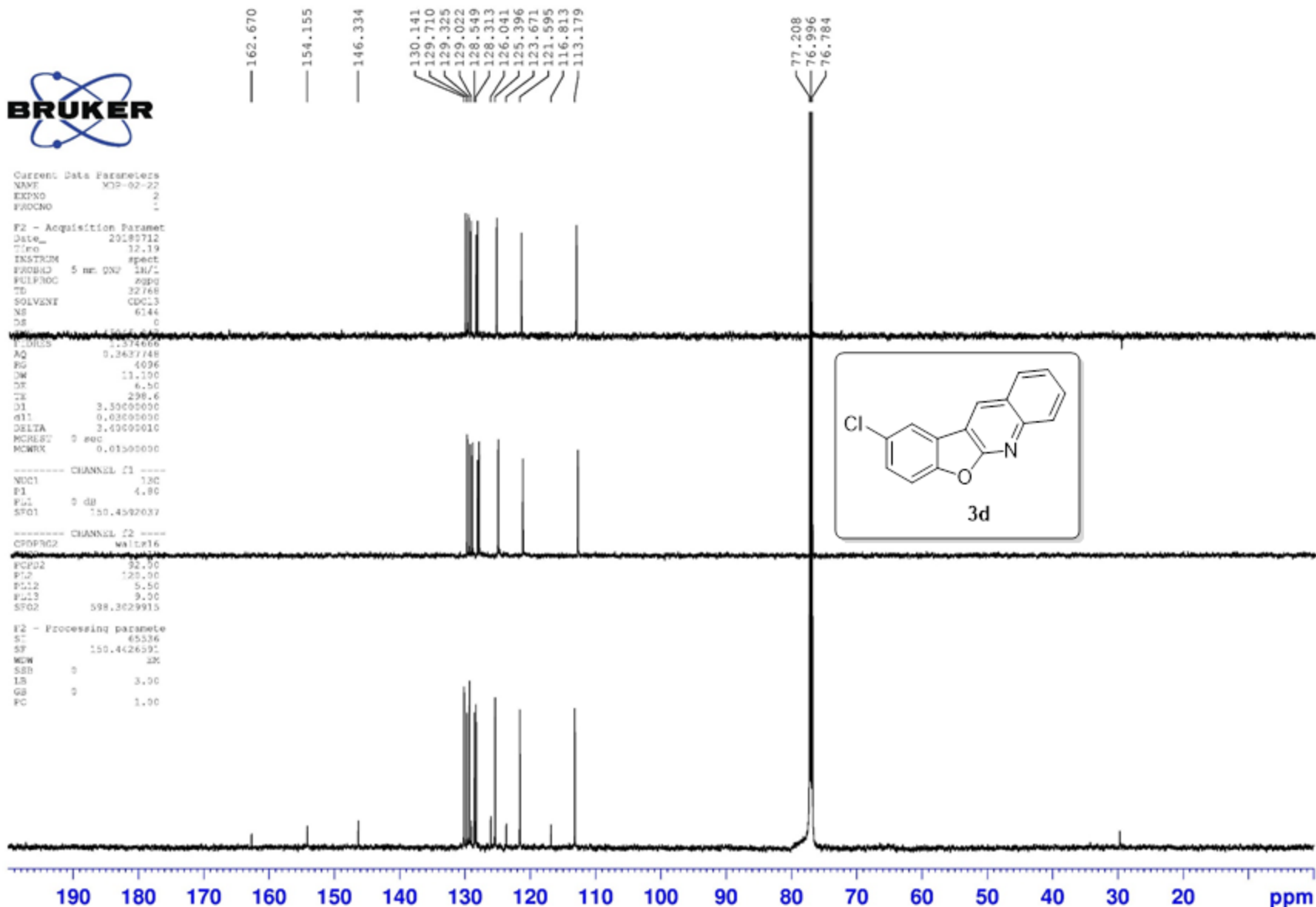


Current Data Parameters
NAME MCP-02-22
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180712
Time 12.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0

===== CHANNEL f1 =====
NUC1 13C
P1 120
PL1 0 dB
SFO1 100.626127
===== CHANNEL f2 =====
CPDPRG2 waltz16
PCPD2 92.50
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3629915

F2 - Processing parameters
SI 65536
SF 150.4426591
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00



8.58
8.50
8.36
8.19
8.08
8.05
8.003
7.90
7.87
7.778
7.776
7.773
7.764
7.762
7.694
7.690
7.682
7.677
7.585
7.583
7.577
7.573
7.571
7.562
7.560
7.558
7.555
7.279
7.274
7.264
7.260
7.249
7.245
7.244
7.240



Current Data Parameters
NAME: MDP-2-44-F
EXFNO: 1
PROCNO: 1

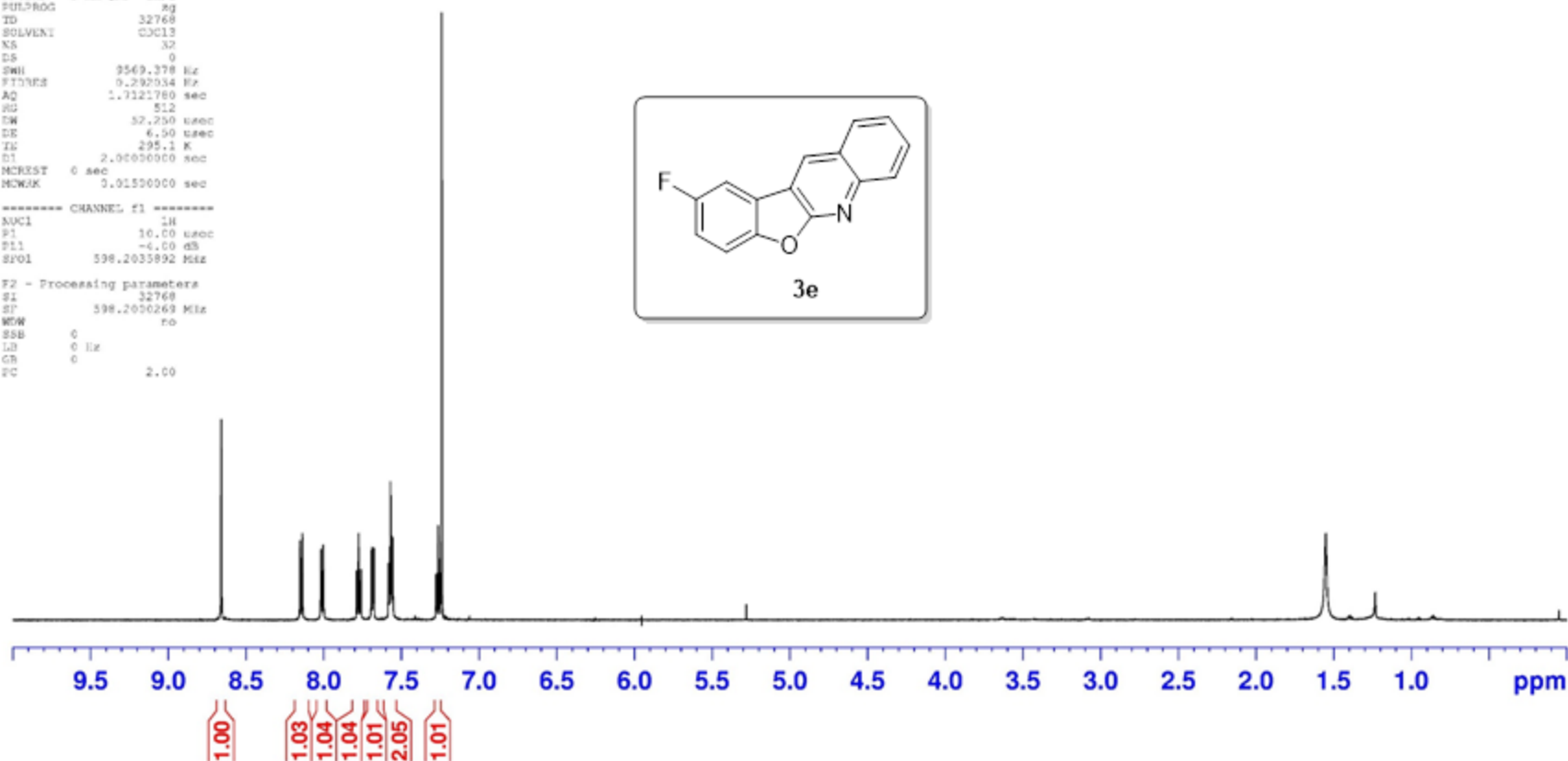
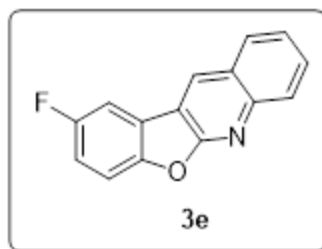
F2 - Acquisition Parameters

Date_: 20181220
Time: 17.30
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zg
TD: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 9569.378 Hz
FIDRES: 0.292034 Hz
AQ: 1.7121780 sec
RG: 512
CW: 52.250 usec
DE: 6.50 usec
TE: 295.1 K
D1: 2.0000000 sec
MCREST: 0 sec
MCHWAX: 0.0150000 sec

----- CHANNEL f1 -----
NUC1: 1H
P1: 10.00 usec
PL1: -4.00 dB
SFO1: 500.2035992 MHz

F2 - Processing parameters

SI: 32768
SF: 500.2030269 MHz
WDW: no
SSB: 0
LB: 0 Hz
GB: 0
PC: 2.00





Current Data Parameters
NAME MDP-2-44-F
EXPNO 2
PROCNO 1

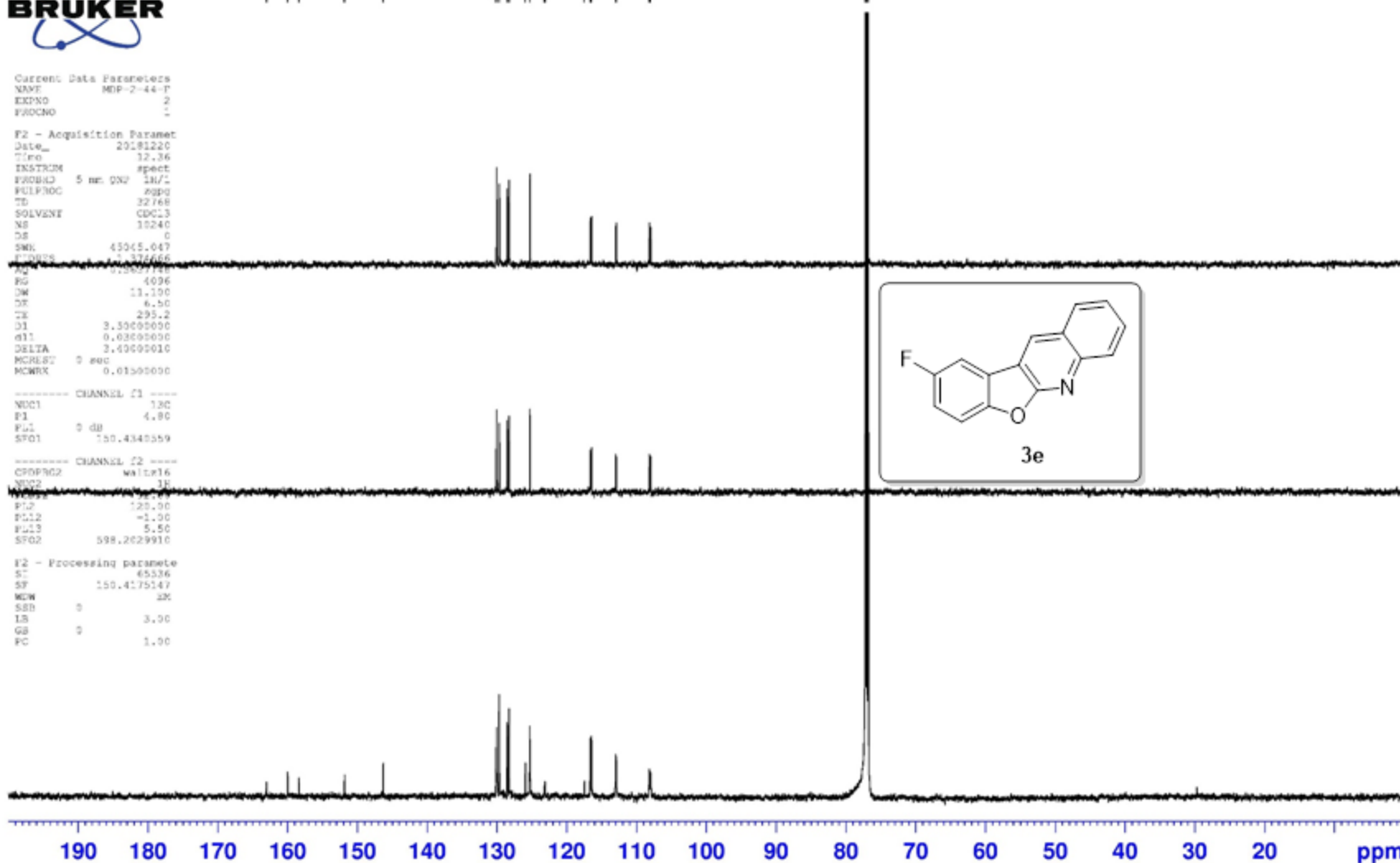
F2 - Acquisition Parameters
Date_ 20181220
Time 12.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 13240
DS 0
SWH 45045.047
FIDRES 0.376666
AQ 0.0007148
RG 4096
DM 11.100
DE 6.50
TE 295.2
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCHS2 0 sec
MCHRX 0.0100000

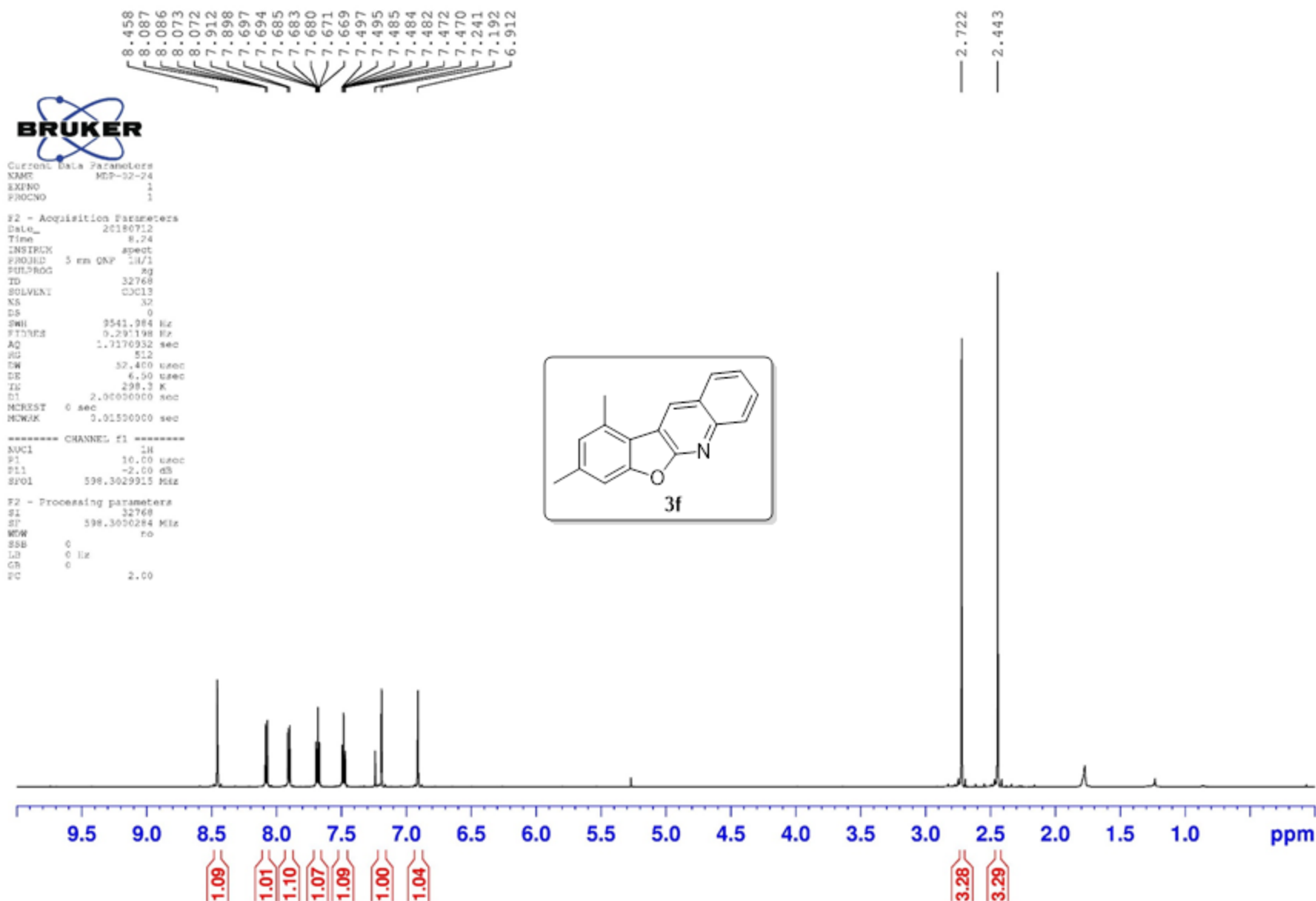
----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 100.626125

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 -1.00
PL12 5.50
SFO2 500.136099

F2 - Processing parameters
SI 65536
SF 150.4175147
WDW 20
SSB 0
LB 3.00
GB 0
PC 1.00

163.025
159.986
158.382
151.831
146.295
130.151
130.070
129.698
128.524
128.289
125.922
125.307
123.177
123.109
117.474
116.635
116.465
112.971
112.912
108.163
108.089
107.994
77.210
76.997
76.785







Current Data Parameters
NAME MDP-02-24
EXPNO 2
PROCNO 1

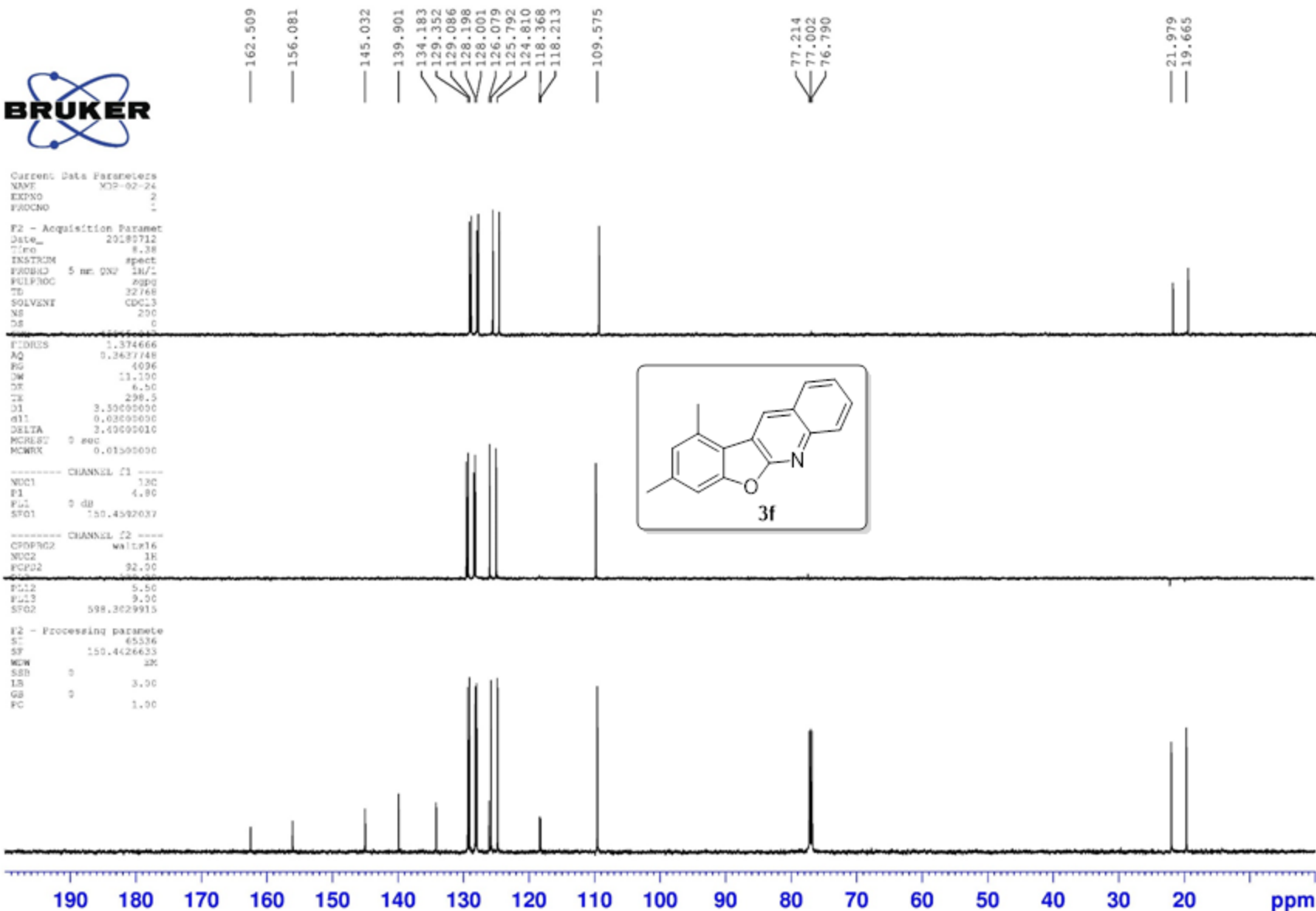
F2 - Acquisition Parameters
Date_ 20180712
Time 8.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 230
DS 0

----- CHANNEL f1 -----
NUC1 13C
P1 12.00
PL1 0 dB
SFO1 100.626137
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00

F2 - Processing parameters
SI 65536
SF 150.4426633
WDW 230
SSB 0
LB 3.00
GB 0
PC 1.00



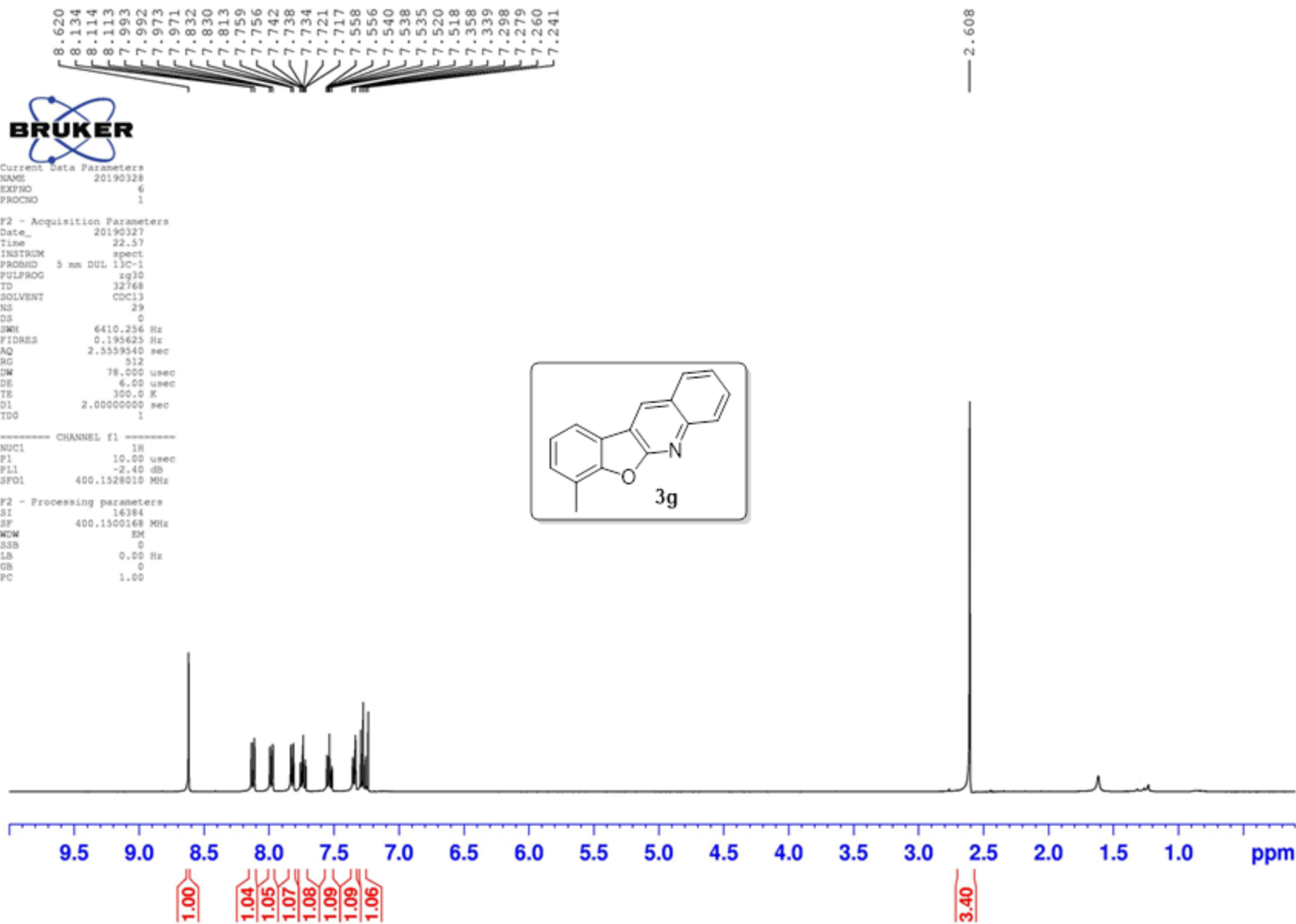


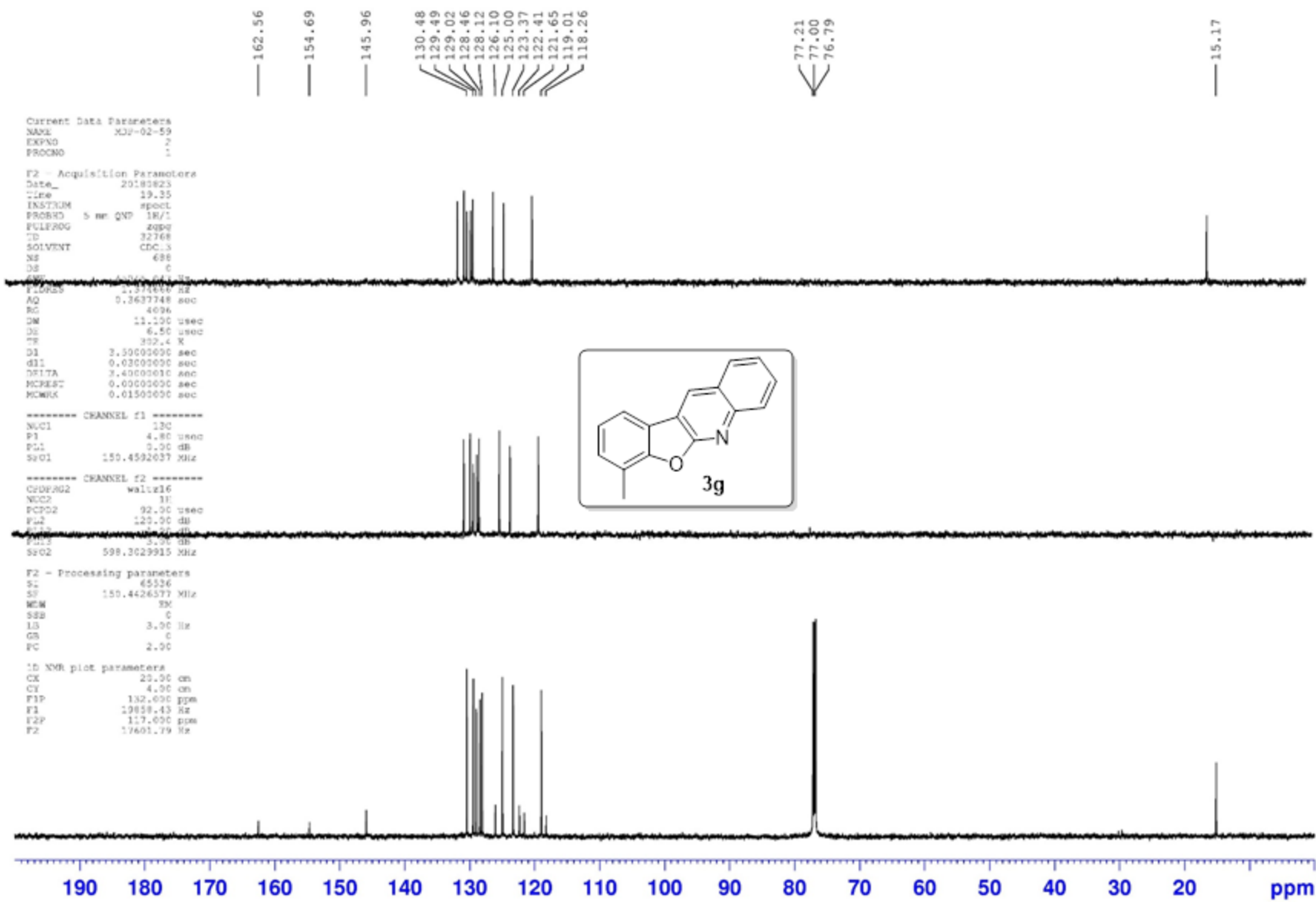
Current Data Parameters
NAME 20190328
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190327
Time 22.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 29
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00





8.683
8.18
8.147
8.06
8.05
7.98
7.915
7.899
7.897
7.803
7.800
7.786
7.782
7.778
7.765
7.761
7.600
7.598
7.583
7.580
7.577
7.562
7.559
7.556
7.554
7.537
7.534
7.350
7.311
7.240

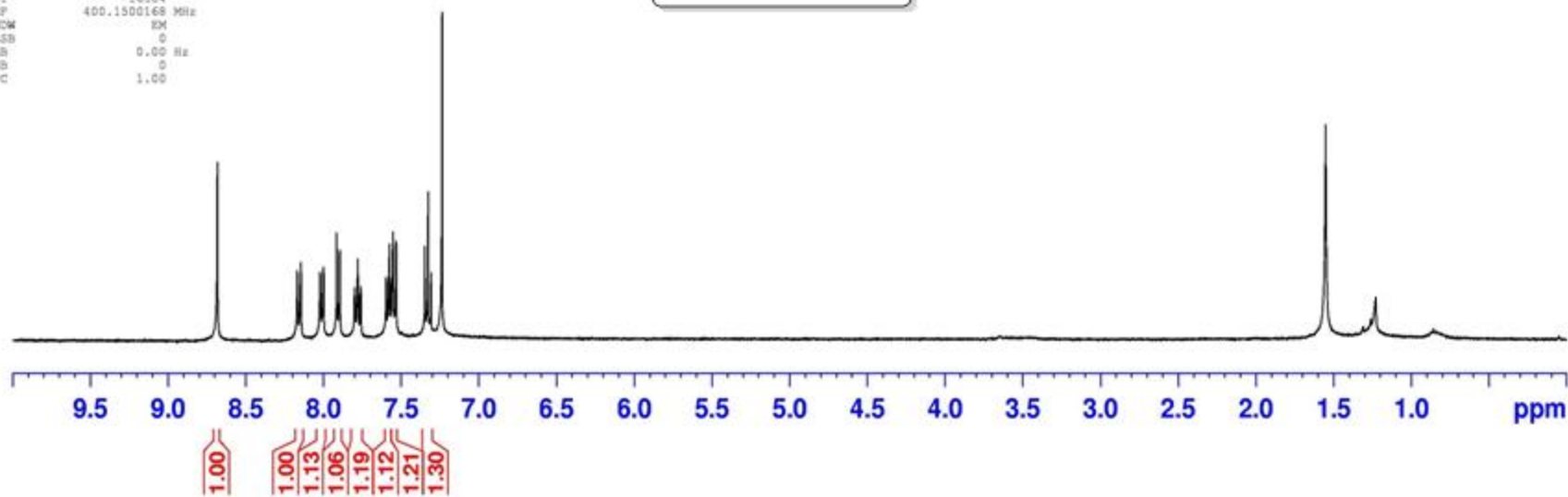
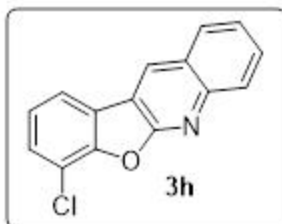


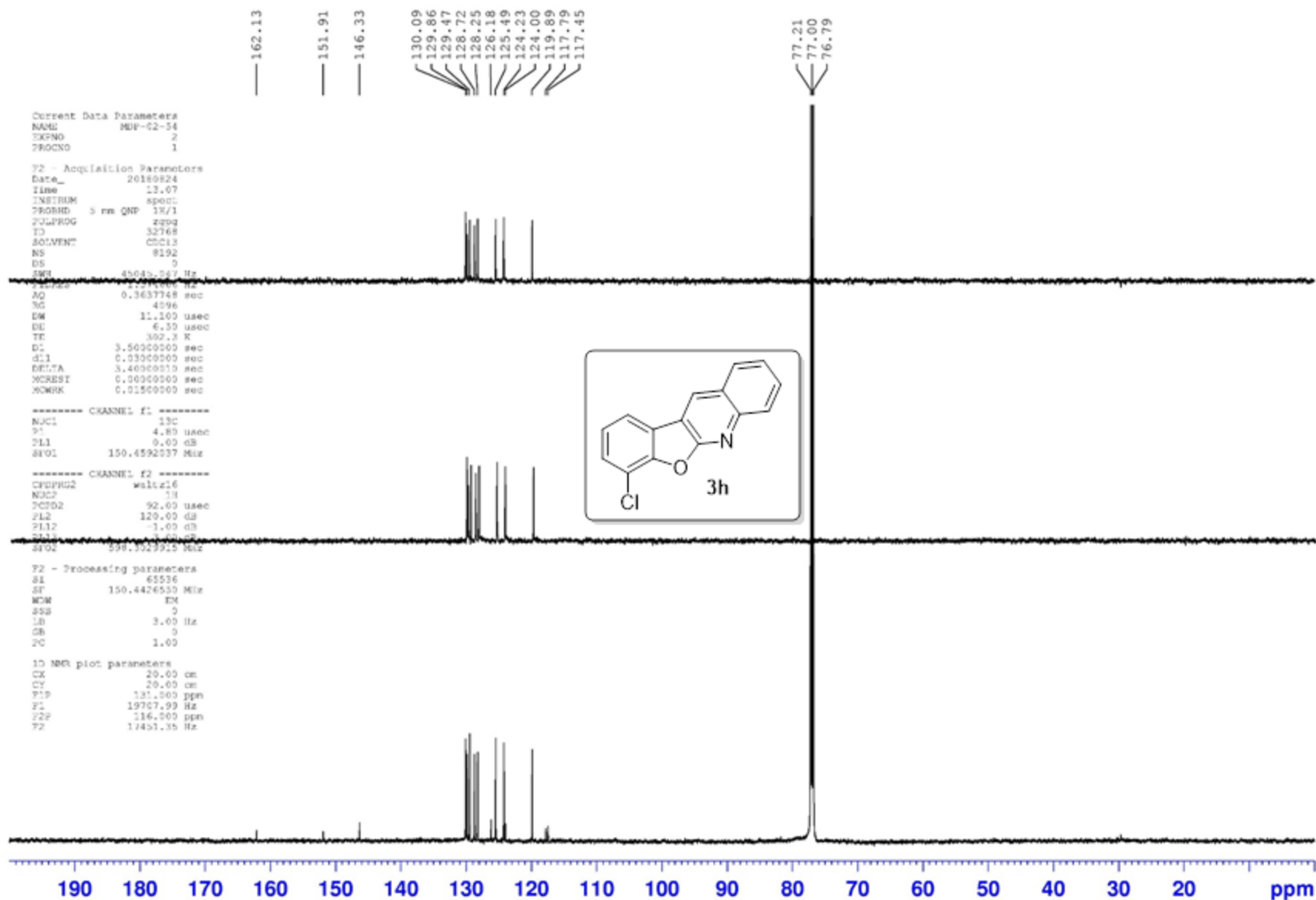
Current Data Parameters
NAME 20190328
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190327
Time 23.16
INSTRUM spect
PROBHD 5 mm DUL 1JC-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559340 sec
RG 724
DM 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW RM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00







Current Data Parameters
NAME MDP-02-16
EXFNO 1
PROCNO 1

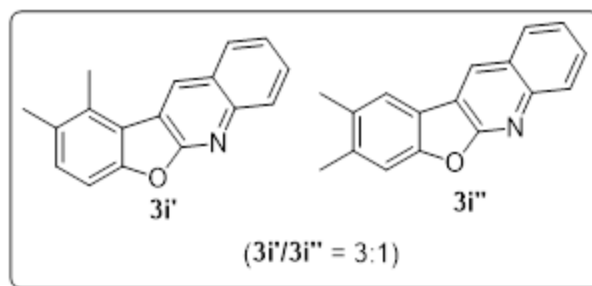
F2 - Acquisition Parameters

Date_ 20180726
Time 6.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256070 Hz
AQ 1.9536228 sec
RG 512
SW 59.600 usec
SE 6.50 usec
TE 299.0 K
D1 2.0000000 sec
MCREST 6 sec
MCWAK 0.01500000 sec

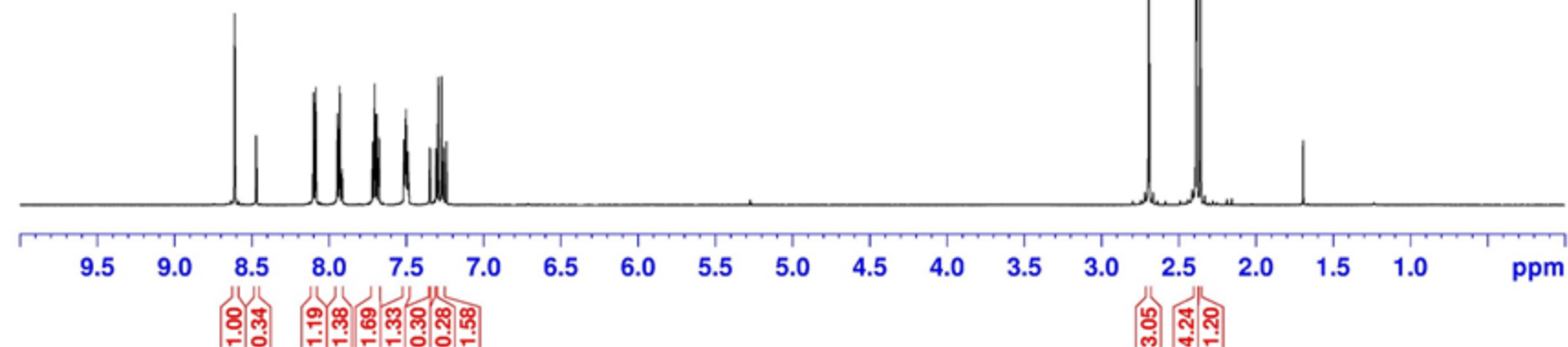
----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 500.13035998 MHz

F2 - Processing parameters

SI 32768
SF 500.13030284 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00



2.694
2.387
2.360





Current Data Parameters
NAME MCP-02-36
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180726
Time 6.58
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 430
DS 0
SWH 40061.843

FIDRES 1.374666
AQ 0.2637748
RG 4096
DM 11.130
DE 6.50
TE 299.2
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCHRG 0 sec
MCHRG 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 120
PL1 0 dB
SFO1 100.626137

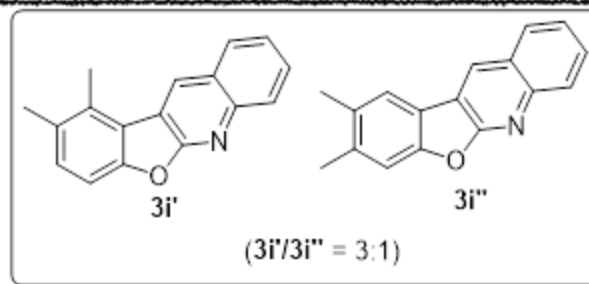
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 5.50
PL12 9.00
SFO2 500.1362932

F2 - Processing parameters
SI 65536
SF 150.4426612
WDW 20
SSB 0
LB 1.00
GB 0
PC 1.00

162.766
162.572
154.627
154.177
145.563
145.223
138.922
132.905
131.937
131.302
130.760
130.262
129.327
129.120
128.351
128.196
128.157
127.987
127.963
126.047
125.975
124.819
121.936
120.962
119.616
118.603
118.004
112.552
108.704

77.210
76.998
76.786

20.819
19.838
19.273
16.297



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

8.161
8.005
7.994
7.980
7.961
7.948
7.797
7.783
7.760
7.758
7.748
7.746
7.744
7.734
7.732
7.671
7.670
7.658
7.646
7.645
7.604
7.602
7.593
7.591
7.589
7.579
7.577
7.565
7.563
7.553
7.551
7.550
7.540
7.538
7.240

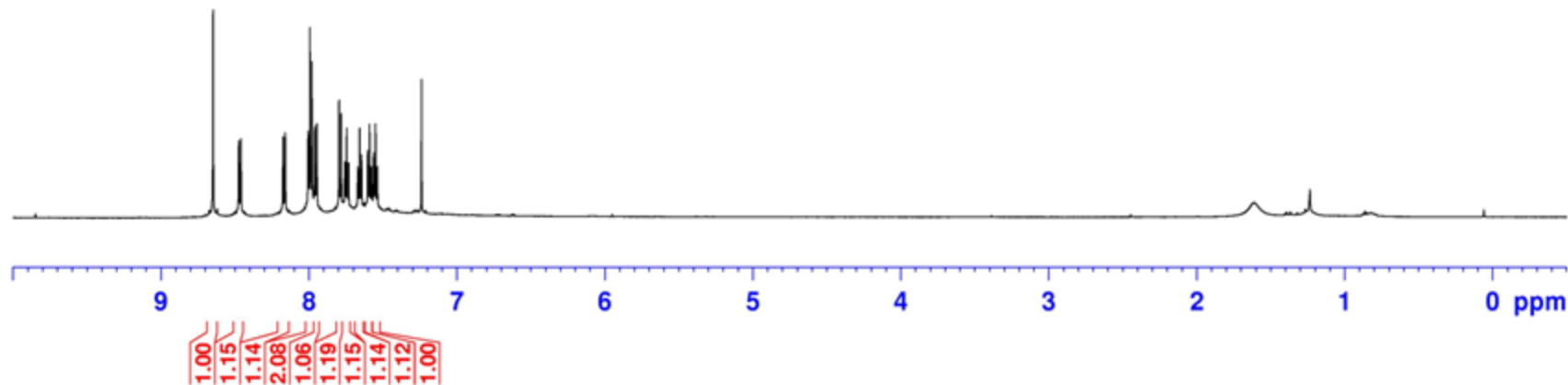
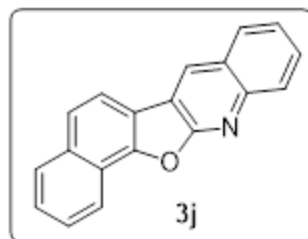


Current Data Parameter
NAME MDP-02-
EXPNO
PROCNO

F2 - Acquisition Param
Date_ 2019032
Time 12.4
INSTRUM spec
PROBHD 5 mm QNP 1H/
PULPROG z
TD 3276
SOLVENT CDCl₃
NS 3
DS
SWH 12531.32
FIDRES 0.38242
AQ 1.307493
RG 51
DM 39.90
DE 6.5
TE 303.
D1 2.0000000
MCREST 0 sec
MCMRK 0.0150000

----- CHANNEL f1 --
NUC1 1
P1 10.0
PL1 -9.0
SFO1 598.305085

F2 - Processing param
--





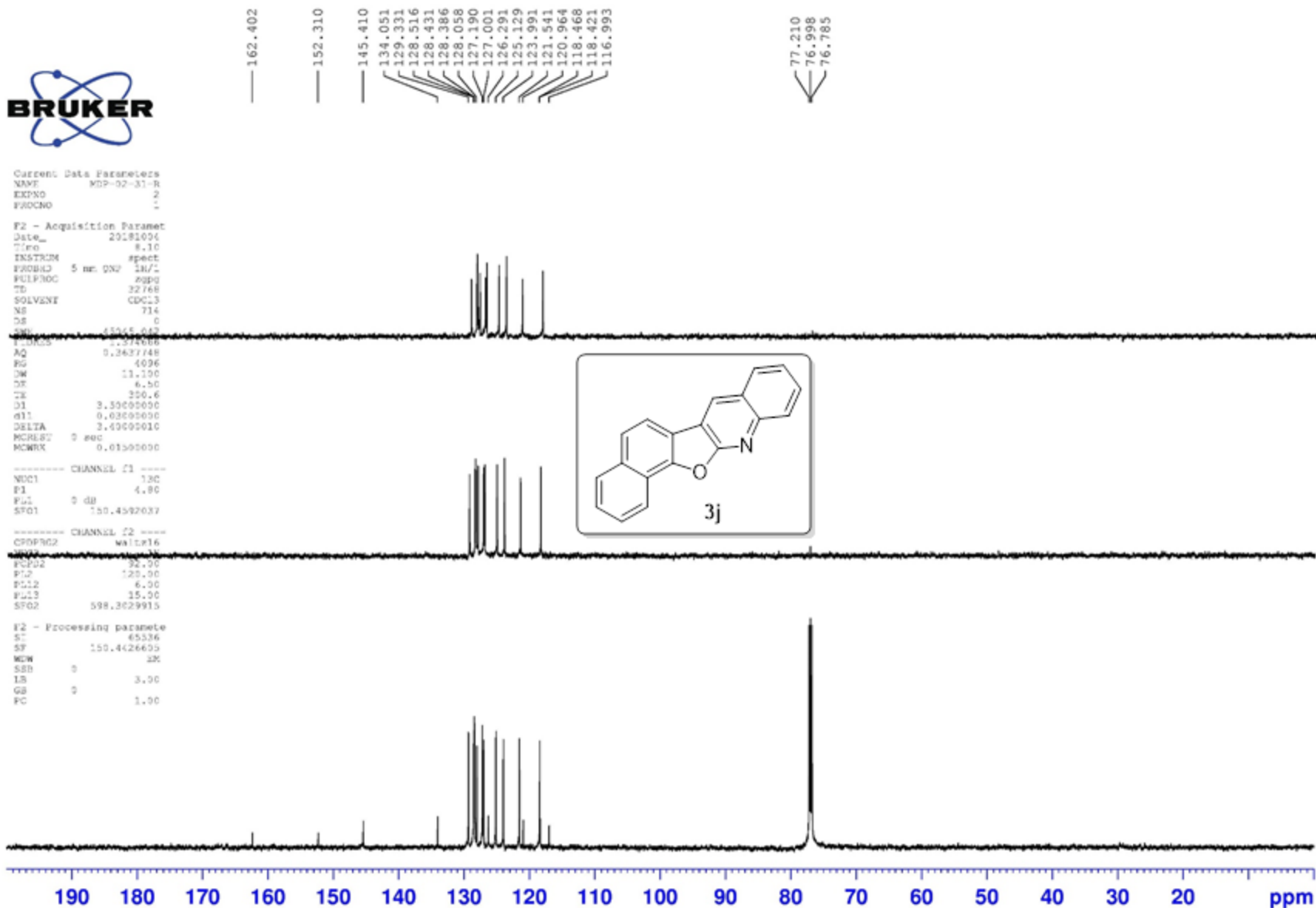
Current Data Parameters
NAME MDP-02-31-R
EXPNO 2
PROCNO 1

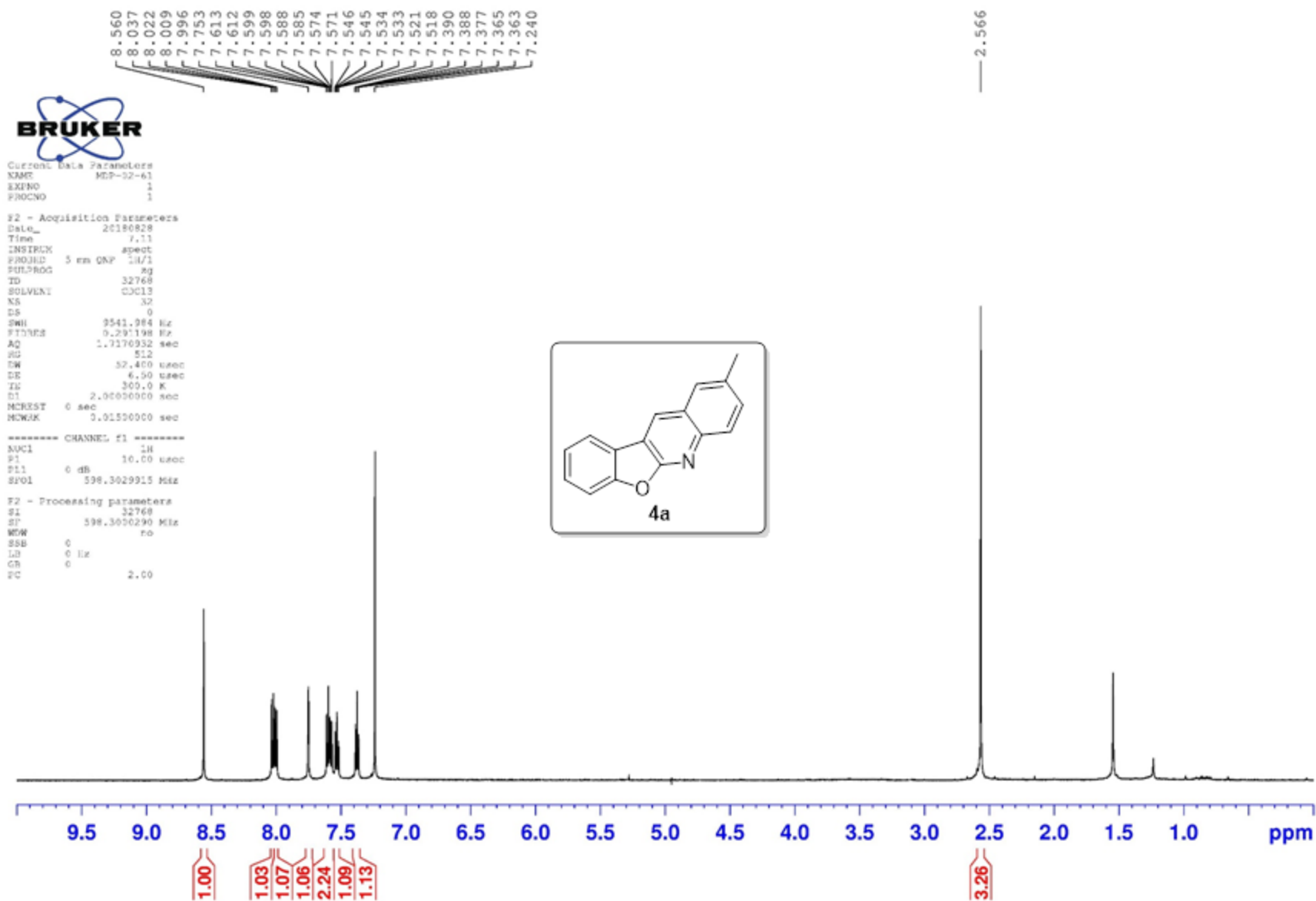
F2 - Acquisition Parameters
Date_ 20181004
Time 8.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 714
DS 0
SWH 15045.032
FIDRES 0.074668
AQ 0.2637748
RG 4096
DM 11.130
DE 6.50
TE 300.6
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCHRG 0 sec
MCHRG 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 100.626137

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 13C
PCPD2 32.00
PL2 120.00
PL3 6.00
PL13 15.00
SFO2 508.3029915

F2 - Processing parameters
SI 65536
SF 150.4426605
WDW 20
SSB 0
LB 3.00
GB 0
PC 1.00







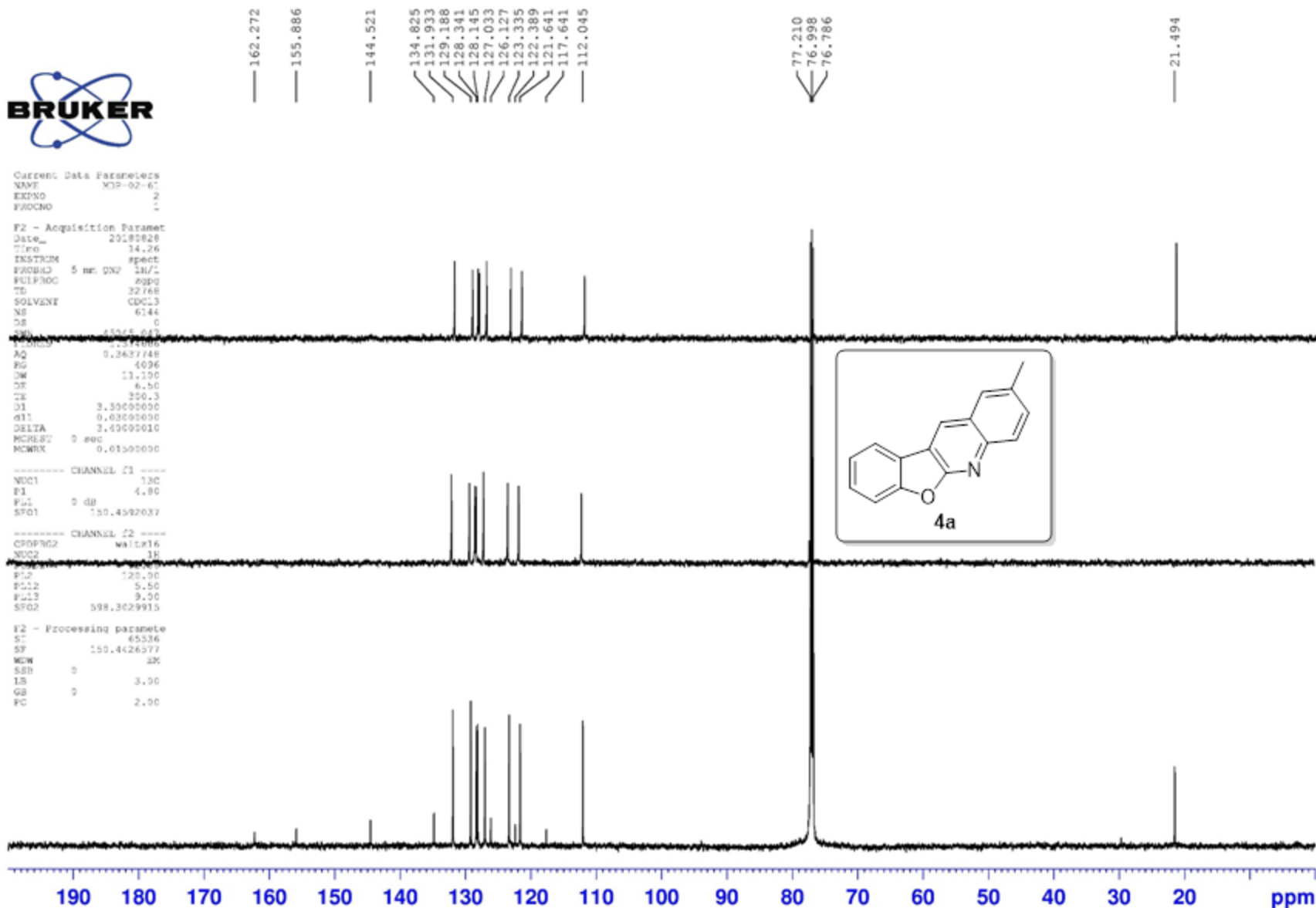
Current Data Parameters
NAME MCP-02-61
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180828
Time 14.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 15065.843
F2FREQ 101.625000
AQ 0.2637748
RG 4096
DM 11.130
DE 6.50
TE 300.3
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCRST 0 sec
MCRM 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 101.625000

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 5.50
PL12 9.00
SFO2 500.13629915

F2 - Processing parameters
SI 65536
SF 150.4426577
WDW 20
SSB 0
LB 3.00
GB 0
PC 2.00





Current Data Parameters
NAME: M07-02-56
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters

Acq_ 20180820
Time: 9.44
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 9541.984 Hz
FIDRES: 0.291198 Hz
AQ: 1.7170932 sec
RG: 512
DM: 32.400 usec
DE: 6.50 usec
TE: 300.2 K
SI: 2.0360000 sec
MCREST: 0 sec
MCMRK: 0.0150000 sec

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

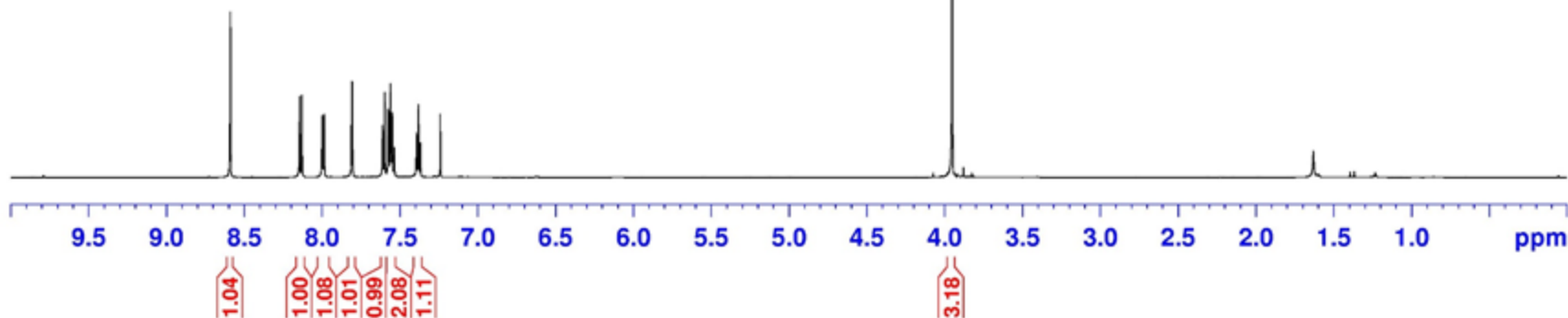
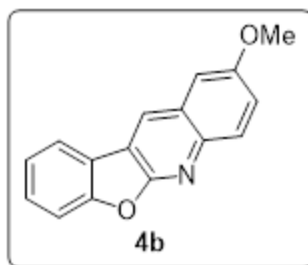
NUC1: 1H
P1: 10.00 usec
PL1: -4.50 dB
SFO1: 500.136290 MHz

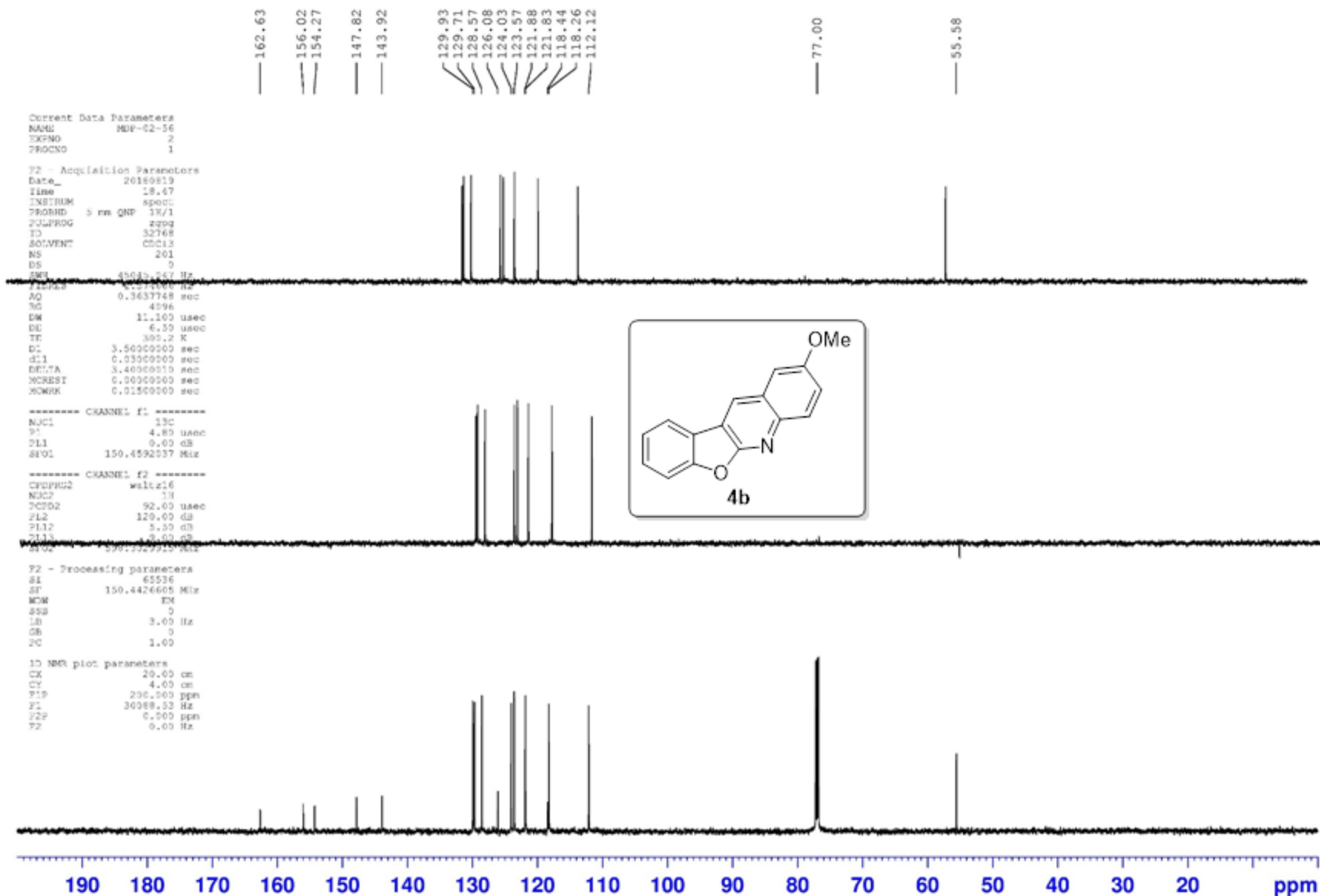
F2 - Processing parameters

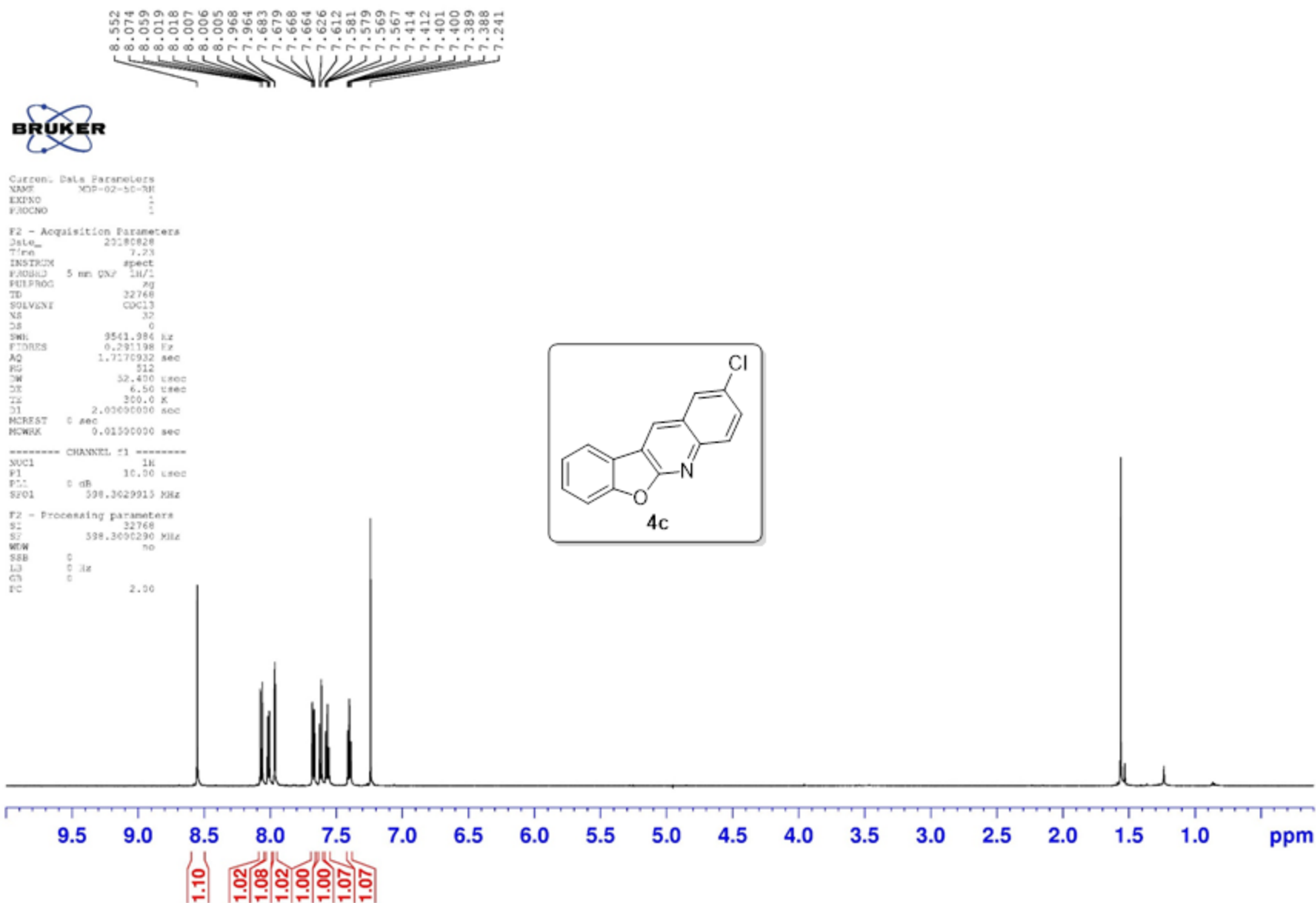
SI: 32768
SF: 500.136291 MHz
WDW: EM
SSB: 0
LB: 0.20 Hz
GB: 0
PC: 2.00

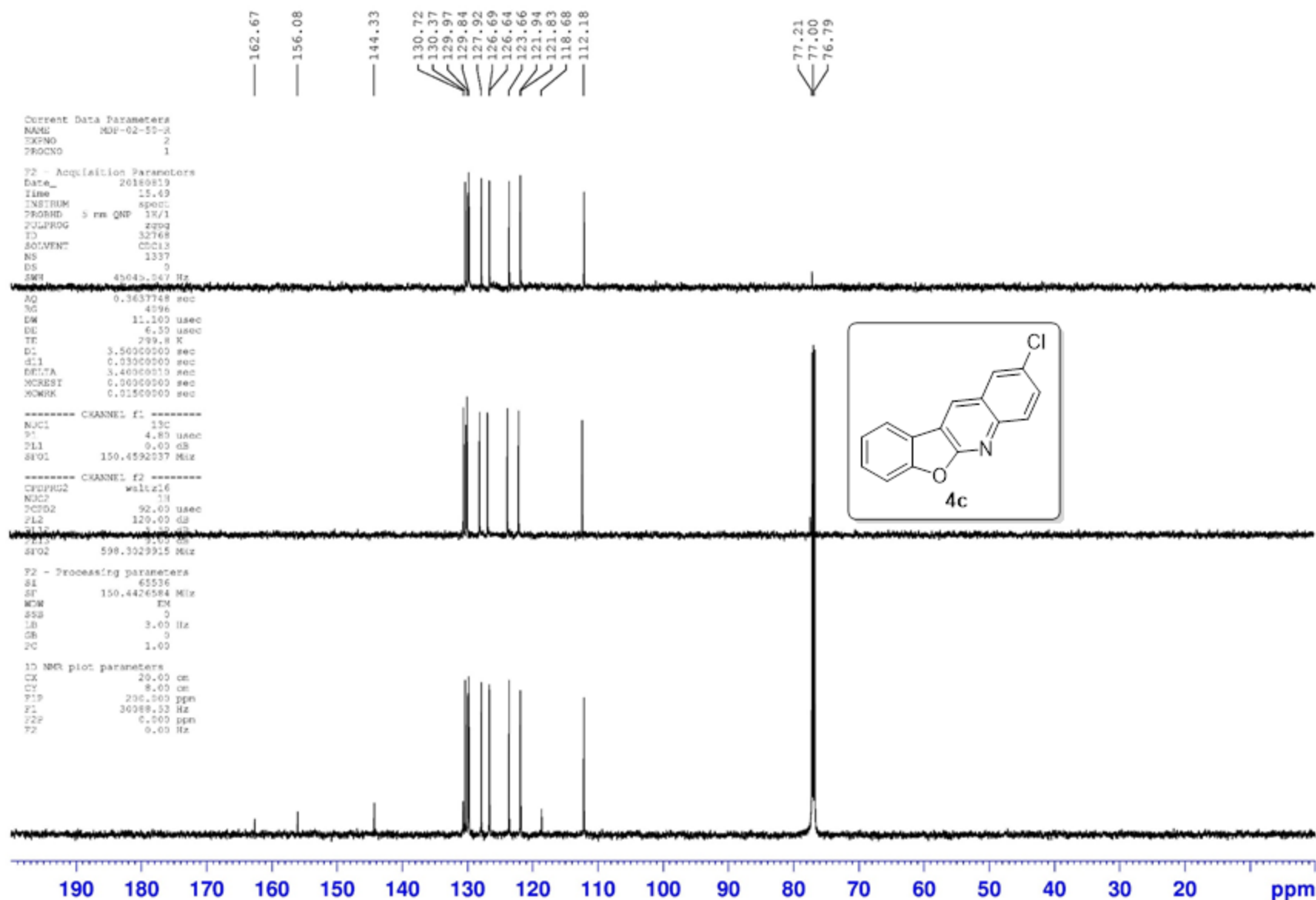
8.589
8.145
8.130
7.999
7.986
7.809
7.805
7.611
7.597
7.576
7.572
7.561
7.556
7.550
7.548
7.393
7.392
7.381
7.380
7.240

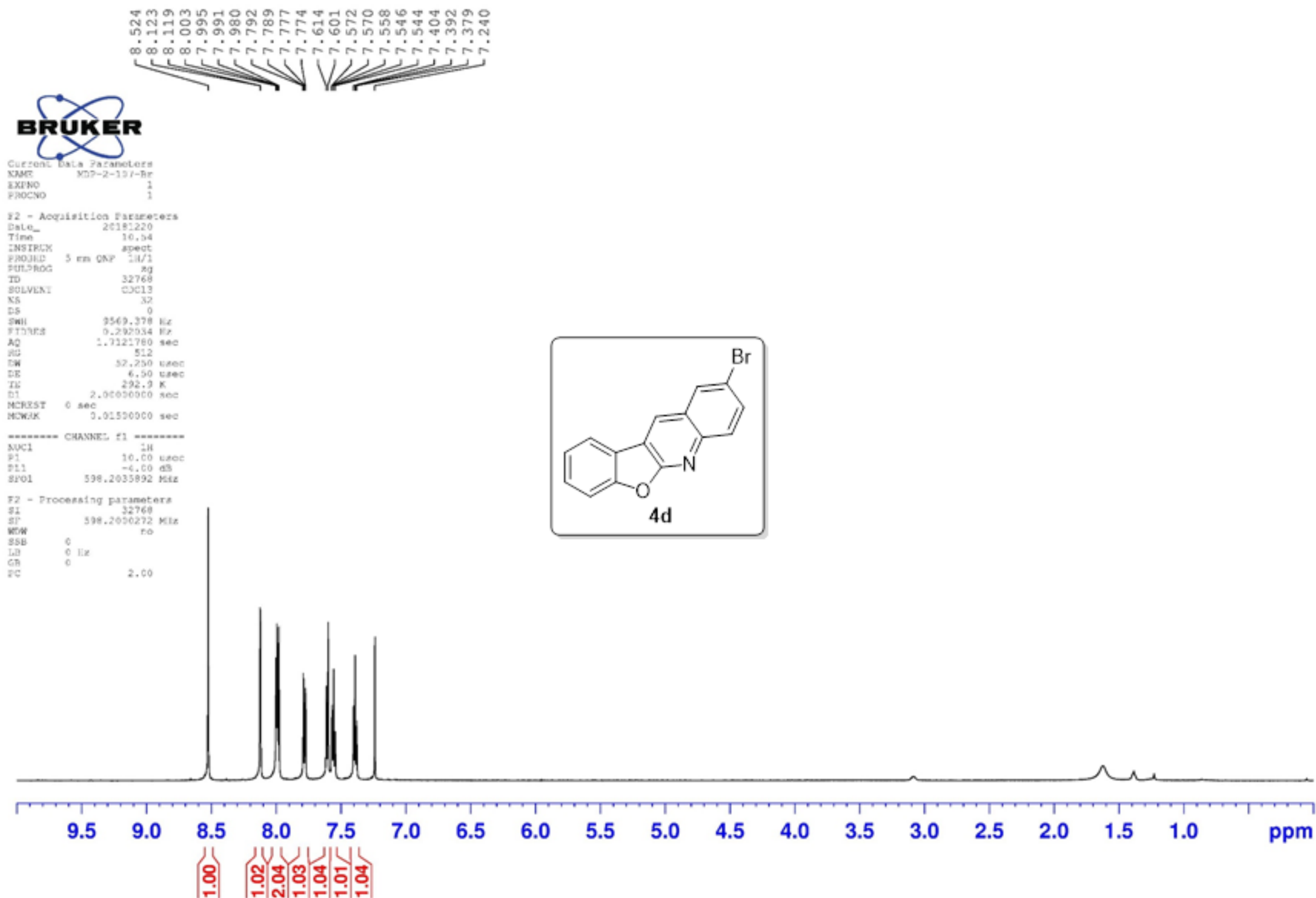
3.951













Current Data Parameters
NAME MDP-2-107-Br
EXPNO 2
PROCNO 1

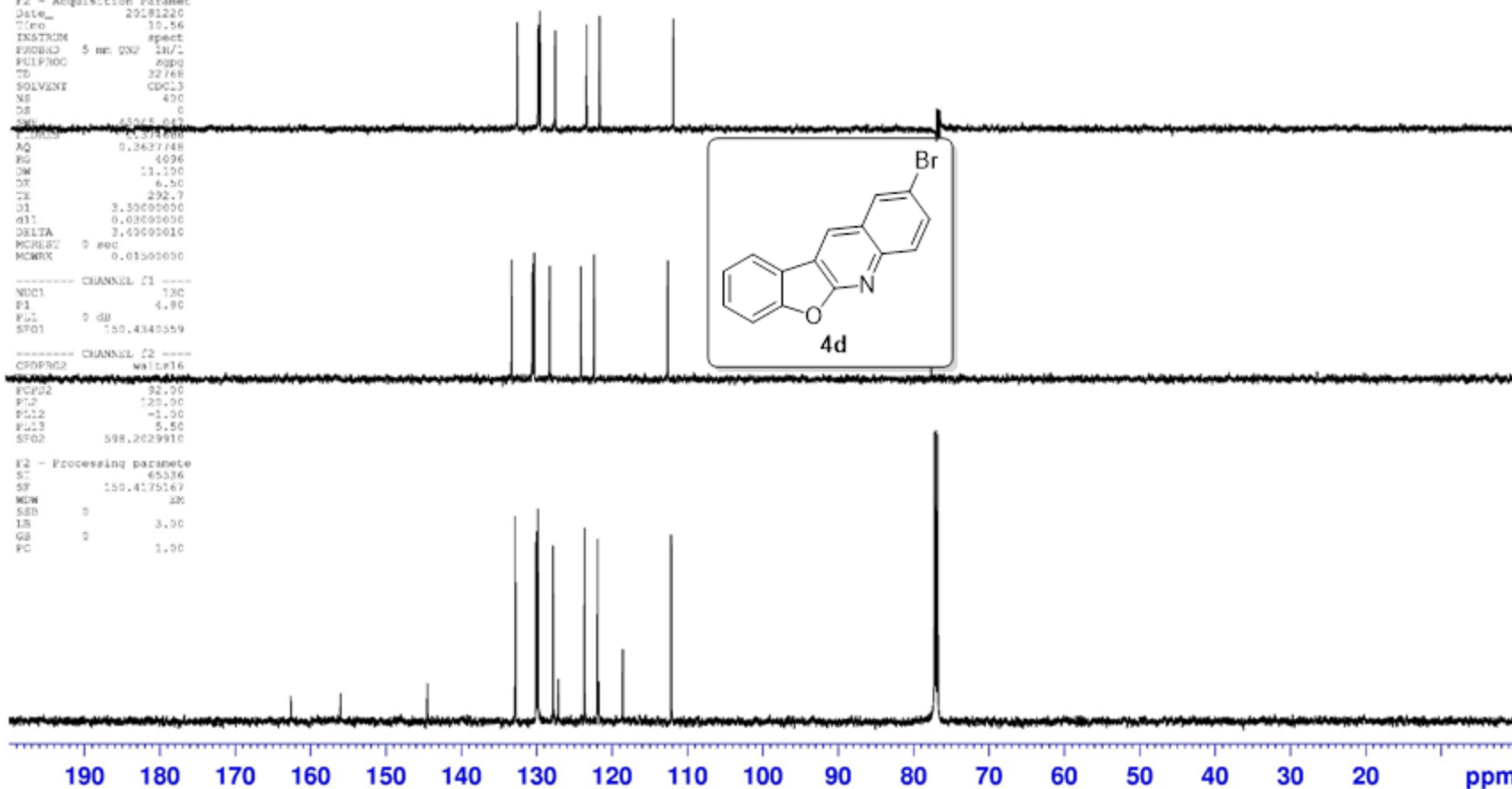
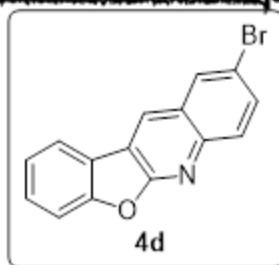
F2 - Acquisition Parameters
Date_ 20181220
Time 10.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 430
DS 0
SWH 5565.047
FIDRES 0.131488
AQ 0.3637748
RG 4096
DM 11.130
DE 6.50
TE 292.7
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCHRG 0 sec
MCHRG 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 100.626125

----- CHANNEL f2 -----
CPDPRG2 waltz16
PCPD2 92.00
PL2 120.00
PL12 -1.00
PL13 5.50
SFO2 598.2629910

F2 - Processing parameters
SI 65536
SF 150.4175167
WDW 300
SSB 0
LB 3.00
GB 0
PC 1.00

162.630
156.023
144.500
132.855
130.084
129.992
129.836
127.839
127.149
123.656
121.933
121.770
118.598
112.152
77.209
76.997
76.784





Current Data Parameters
NAME 20190328
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190327
Time 23.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 25
DS 0

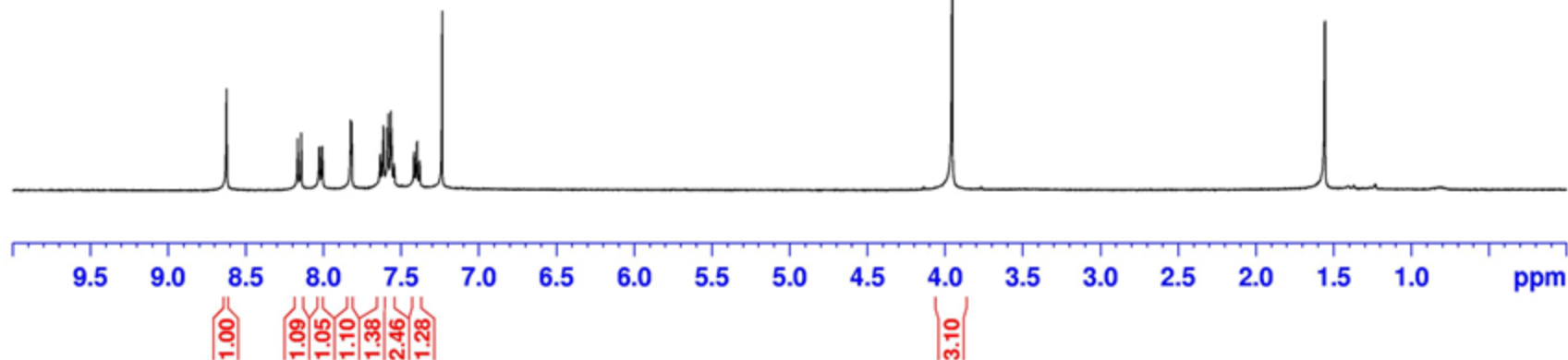
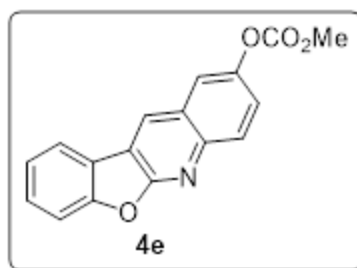
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 724
DM 76.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

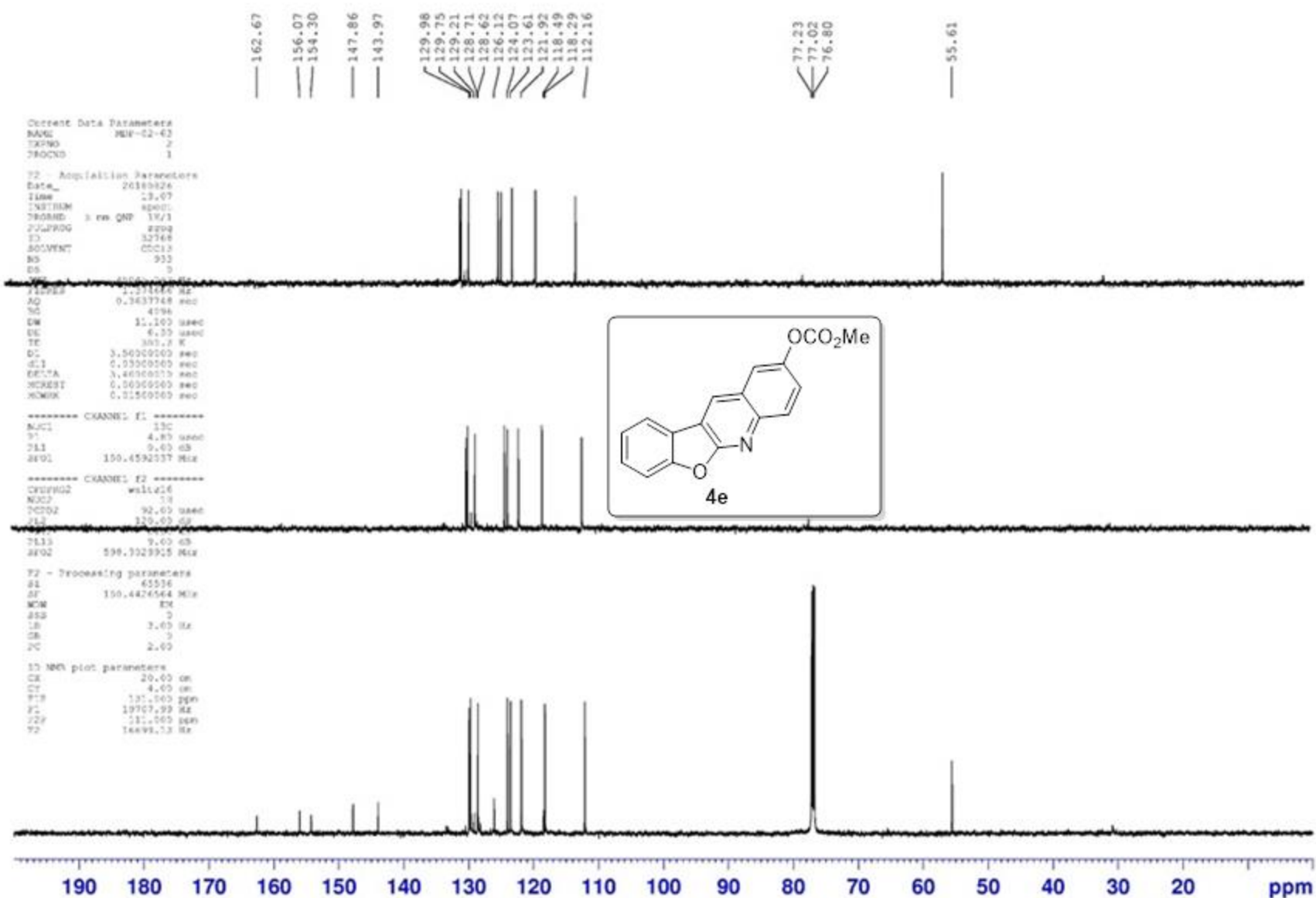
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

8.624
8.166
8.142
8.031
8.011
7.828
7.822
7.637
7.617
7.591
7.588
7.585
7.569
7.562
7.549
7.546
7.420
7.418
7.402
7.383
7.380
7.240

3.955







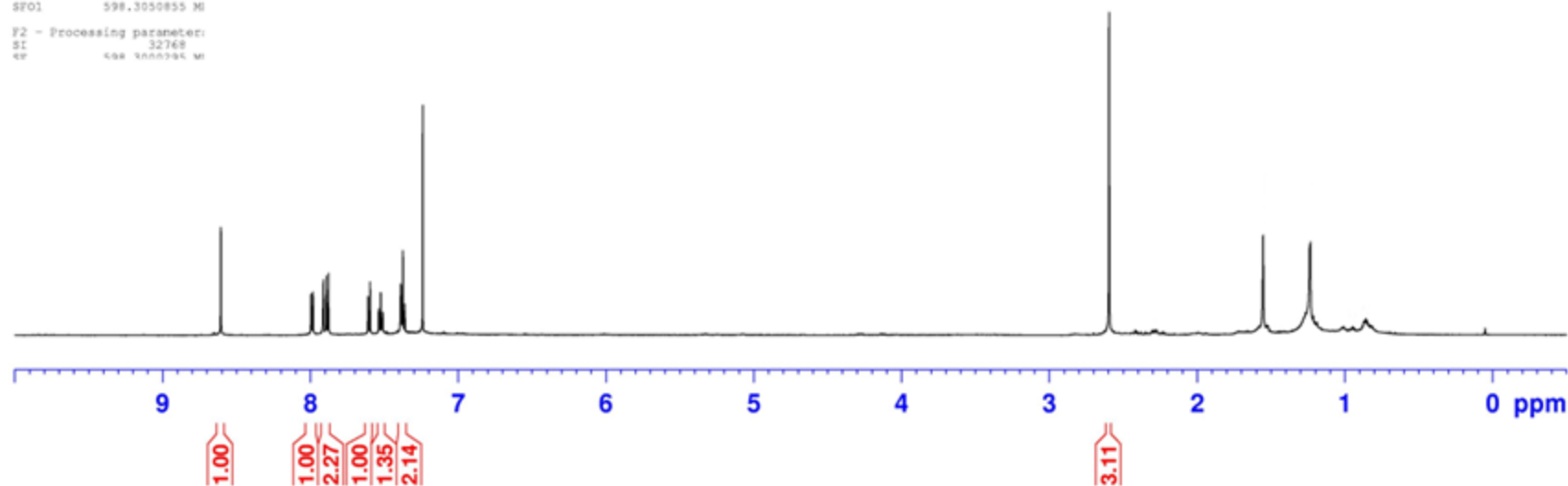
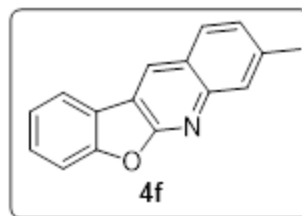
Current Data Parameters
NAME: MDP-02-51-1
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20190325
Time: 12.48
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 12531.328 Hz
FIDRES: 0.382426 Hz
AQ: 1.3074932 s
RG: 512
DM: 39.900 us
DE: 6.50 us
TE: 301.1 K
D1: 2.00000000 s
MCREST: 0 sec
MCMRG: 0.01500000 s

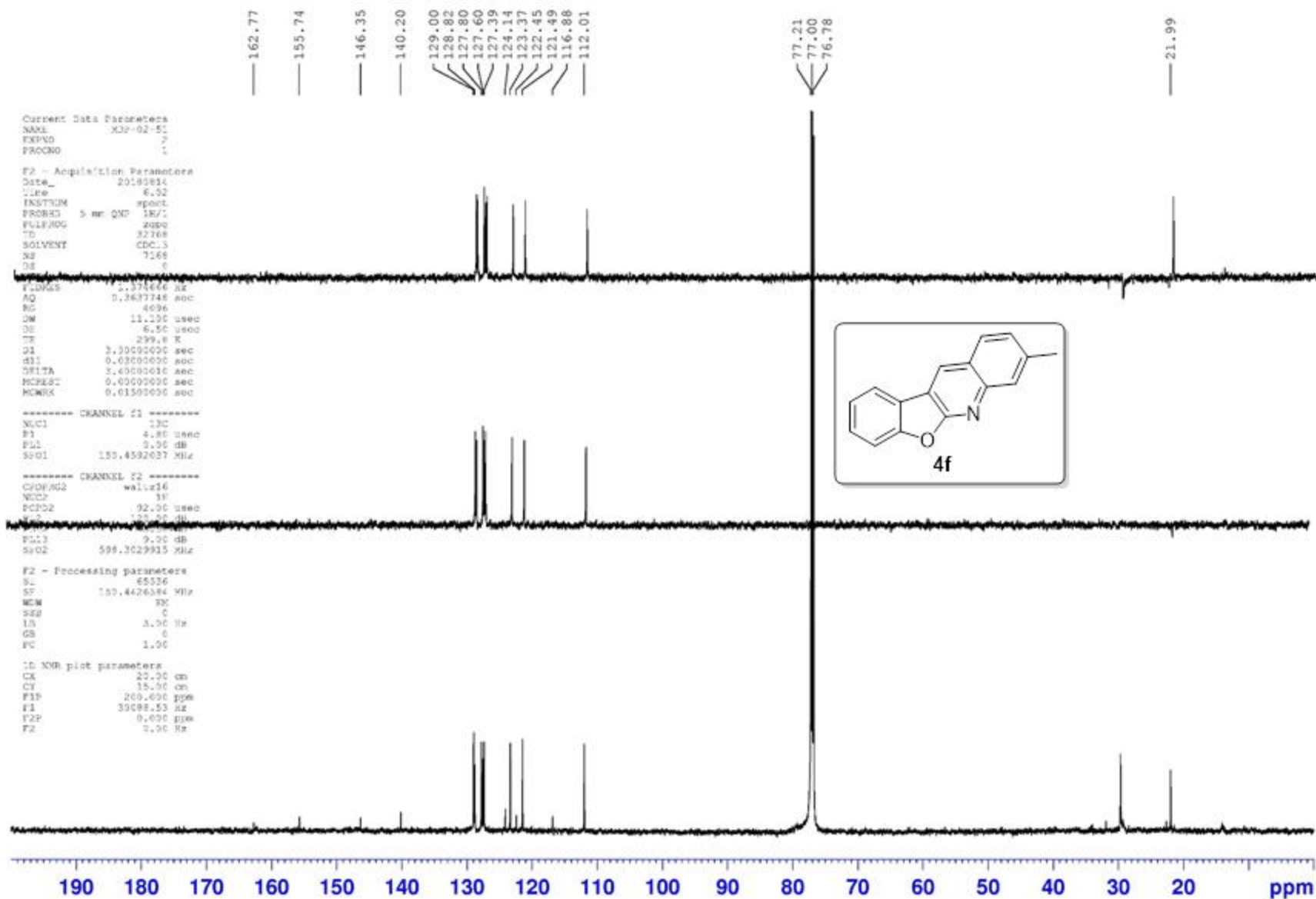
***** CHANNEL f1 *****
NUC1: 1H
P1: 10.00 us
PL1: -5.00 dB
SFO1: 500.1300000 MHz

F2 - Processing parameters:
SI: 32768
SF: 500.1300000 MHz

8.607
7.996
7.995
7.984
7.983
7.982
7.912
7.912
7.892
7.878
7.611
7.610
7.597
7.596
7.538
7.536
7.525
7.524
7.524
7.513
7.512
7.510
7.392
7.389
7.387
7.386
7.375
7.363
7.362
7.240



— 2.596



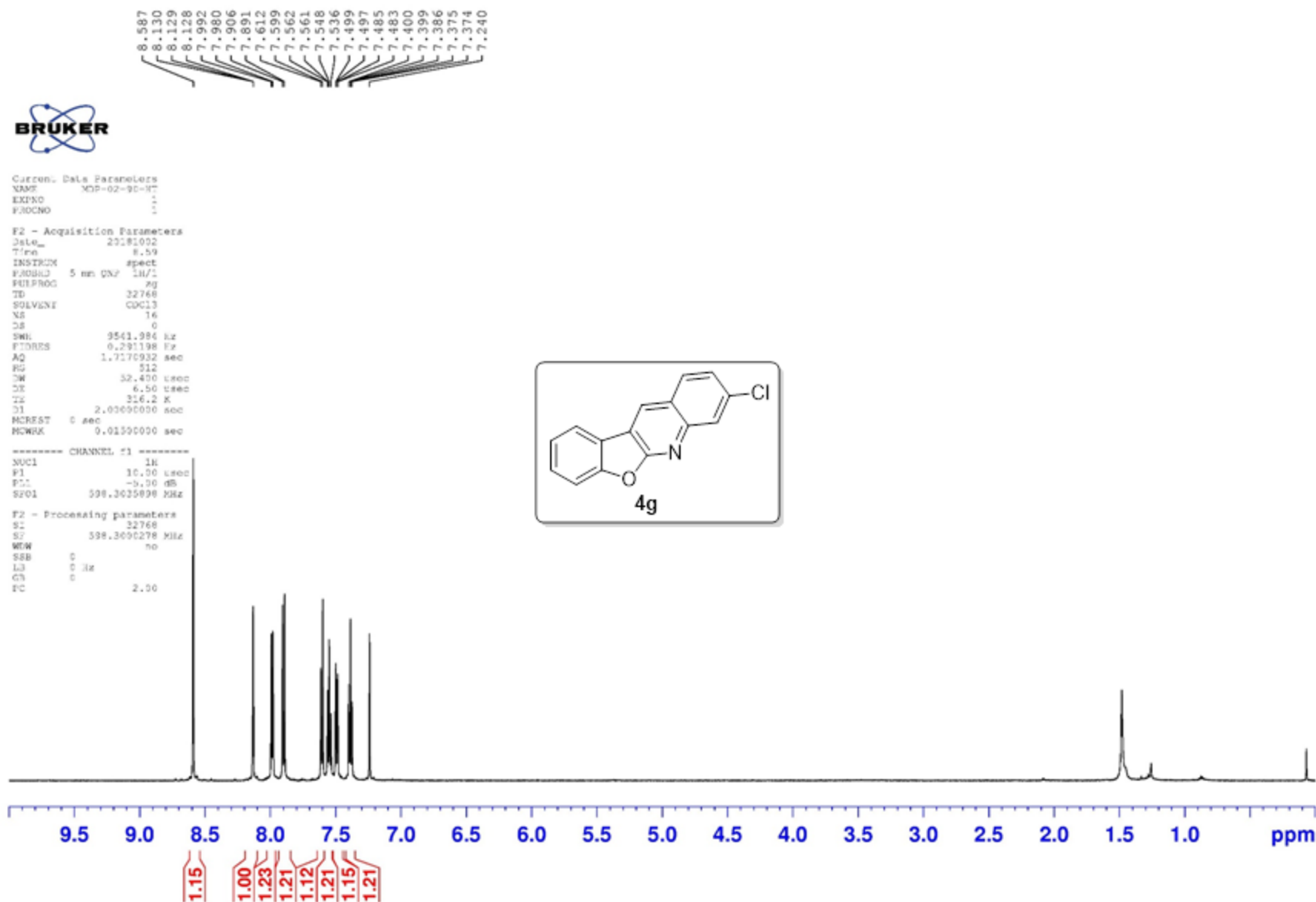
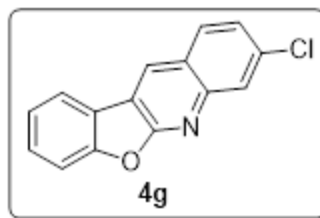


Current Data Parameters
NAME: MDP-02-90-H7
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_ 20181002
Time 8.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DM 32.400 usec
DE 6.50 usec
TE 316.2 K
SI 2.0360000 sec
MCREST 0 sec
MORPH 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -0.50 dB
SFO1 500.1362598 MHz

F2 - Processing parameters
SI 32768
SF 500.1362598 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00



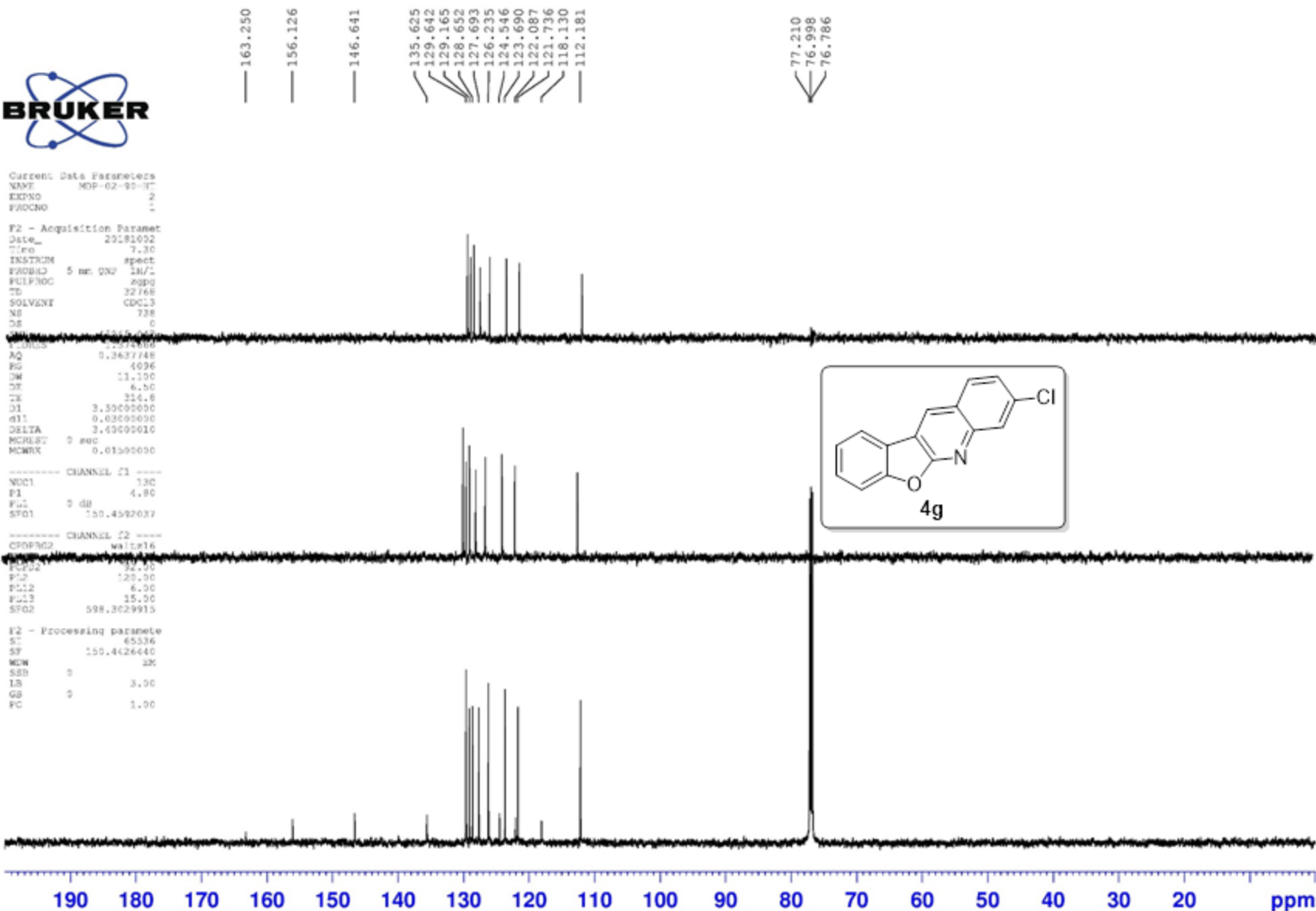


Current Data Parameters
NAME MDP-02-05-07
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181002
Time 7.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 738
DS 0

===== CHANNEL f1 =====
NUC1 13C
P1 12.00
PL1 0 dB
SFO1 100.626127
===== CHANNEL f2 =====
CPDPRG2 waltz16
PCPD2 32.00
PL2 120.00
PL12 6.00
PL13 15.00
SFO2 508.3629915

F2 - Processing parameters
SI 65536
SF 150.4426440
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00





Current Data Parameters
NAME: M07-02-63
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters

Date_ 20180927
Time 3.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9330228 sec
RG 512
DM 39.600 usec
DE 6.50 usec
TE 301.3 K
SI 2.0360000 sec
MCREST 0 sec
MCWRR 0.0150000 sec

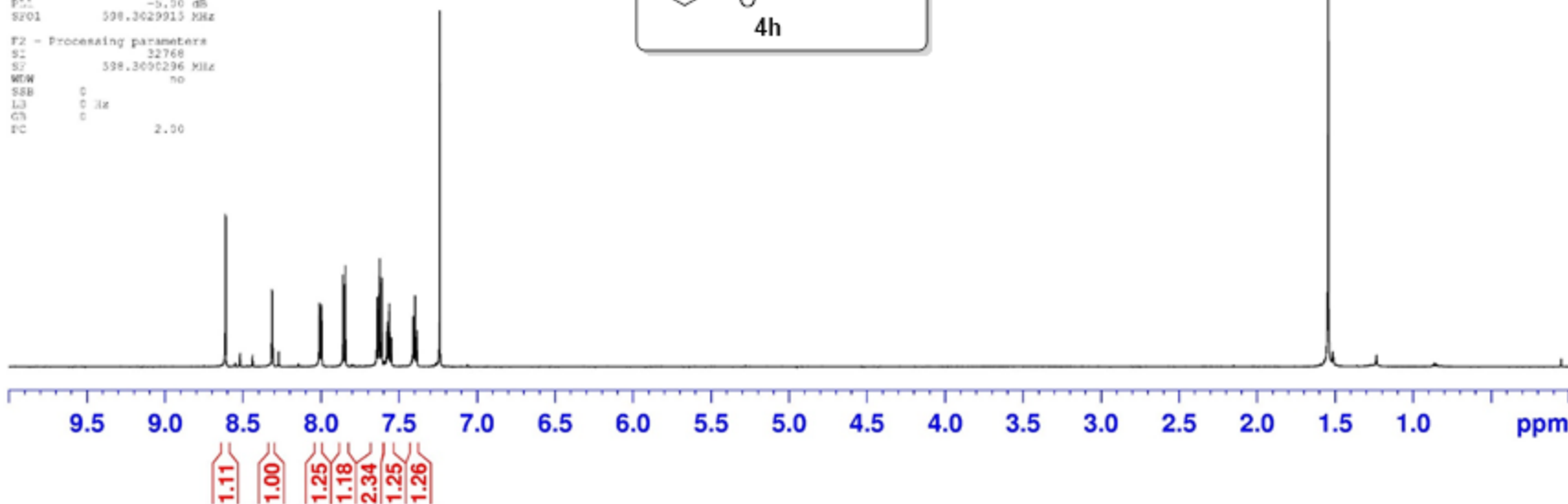
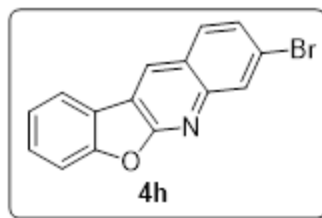
----- CHANNEL f1 -----

NUC1 1H
P1 10.00 usec
PL1 -0.00 dB
SFO1 500.13629915 MHz

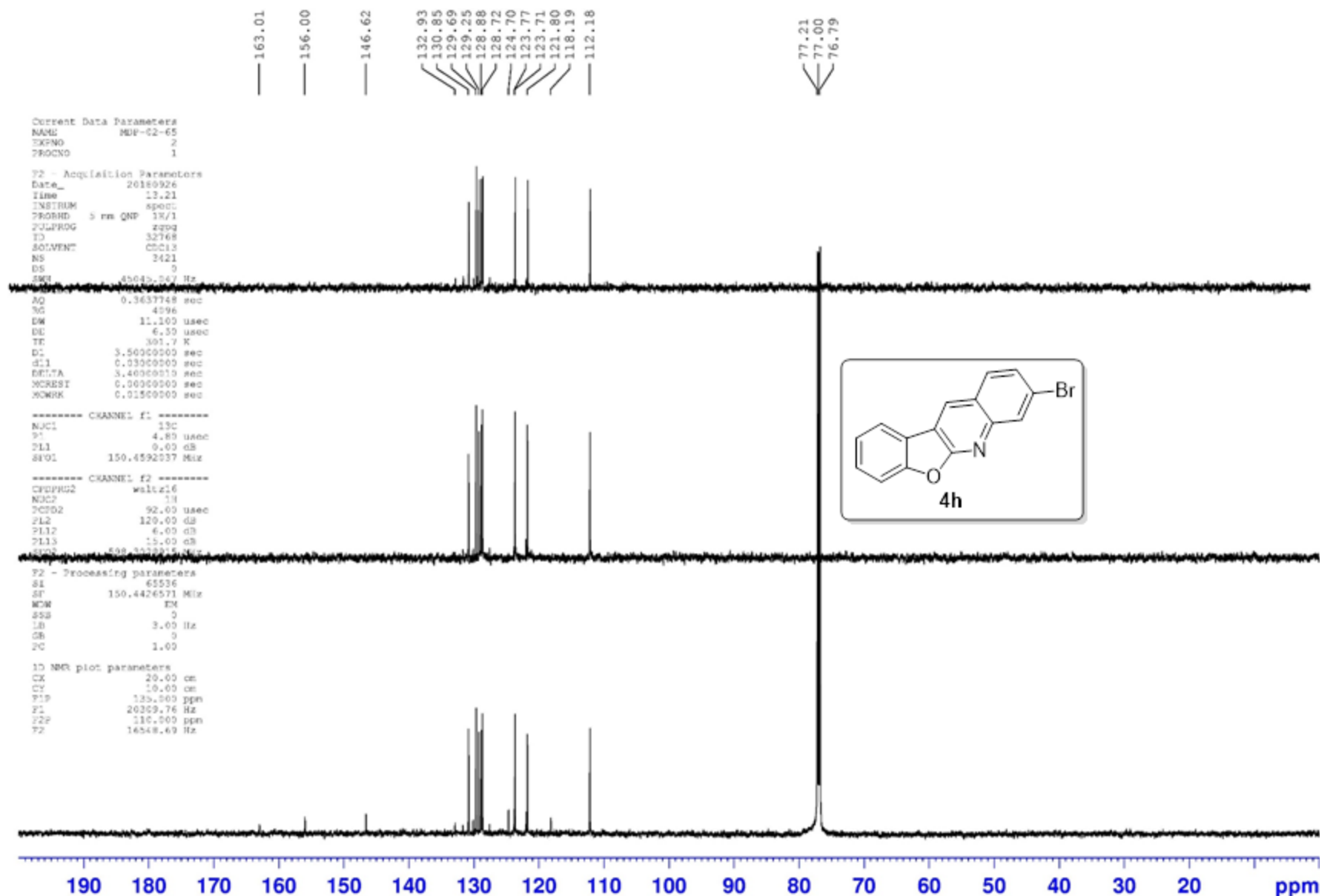
F2 - Processing parameters

SI 32768
SF 500.13629915 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00

8.613
8.316
8.312
8.011
8.010
7.999
7.998
7.997
7.860
7.845
7.643
7.640
7.628
7.625
7.612
7.577
7.575
7.565
7.563
7.551
7.549
7.412
7.410
7.399
7.398
7.387
7.385
7.240



1.544



8.163
8.161
8.122
8.121
8.120
8.119
8.108
8.107
8.105
8.090
7.739
7.737
7.727
7.725
7.723
7.713
7.711
7.608
7.607
7.594
7.593
7.566
7.564
7.555
7.552
7.550
7.540
7.538
7.530
7.528
7.518
7.516
7.515
7.504
7.502
7.394
7.393
7.382
7.380
7.369
7.367
7.240



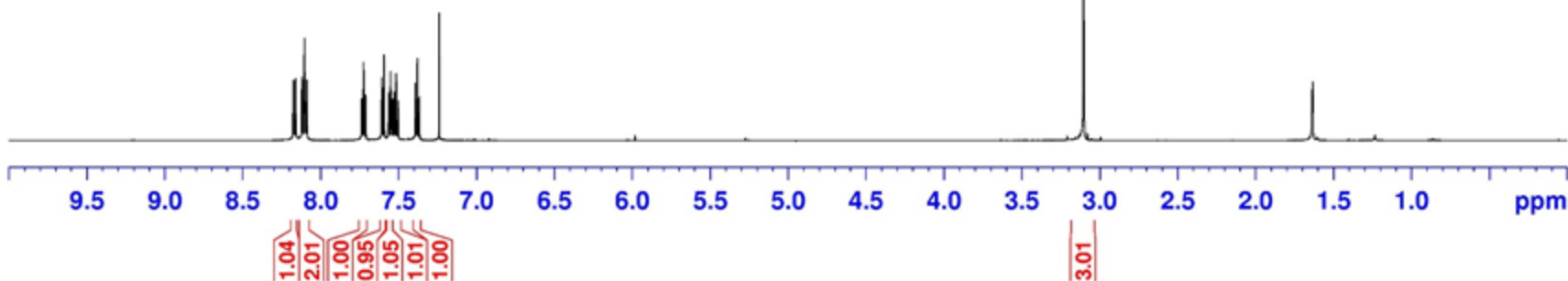
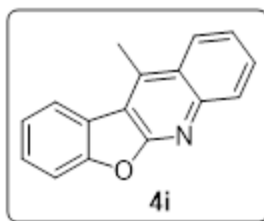
Current Data Parameters
NAME: M07-02-64
EXPNO: 1
PROCNO: 1

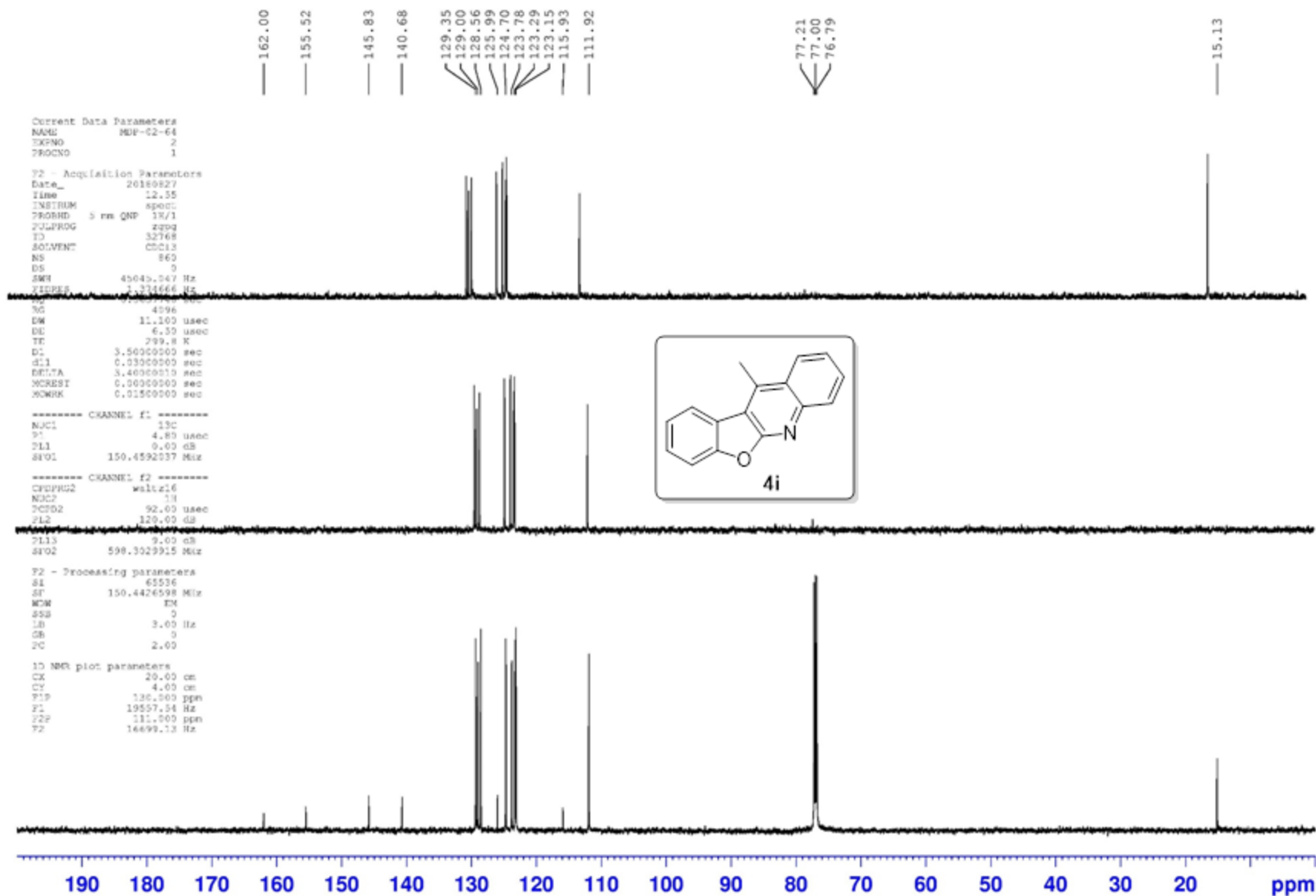
F2 - Acquisition Parameters

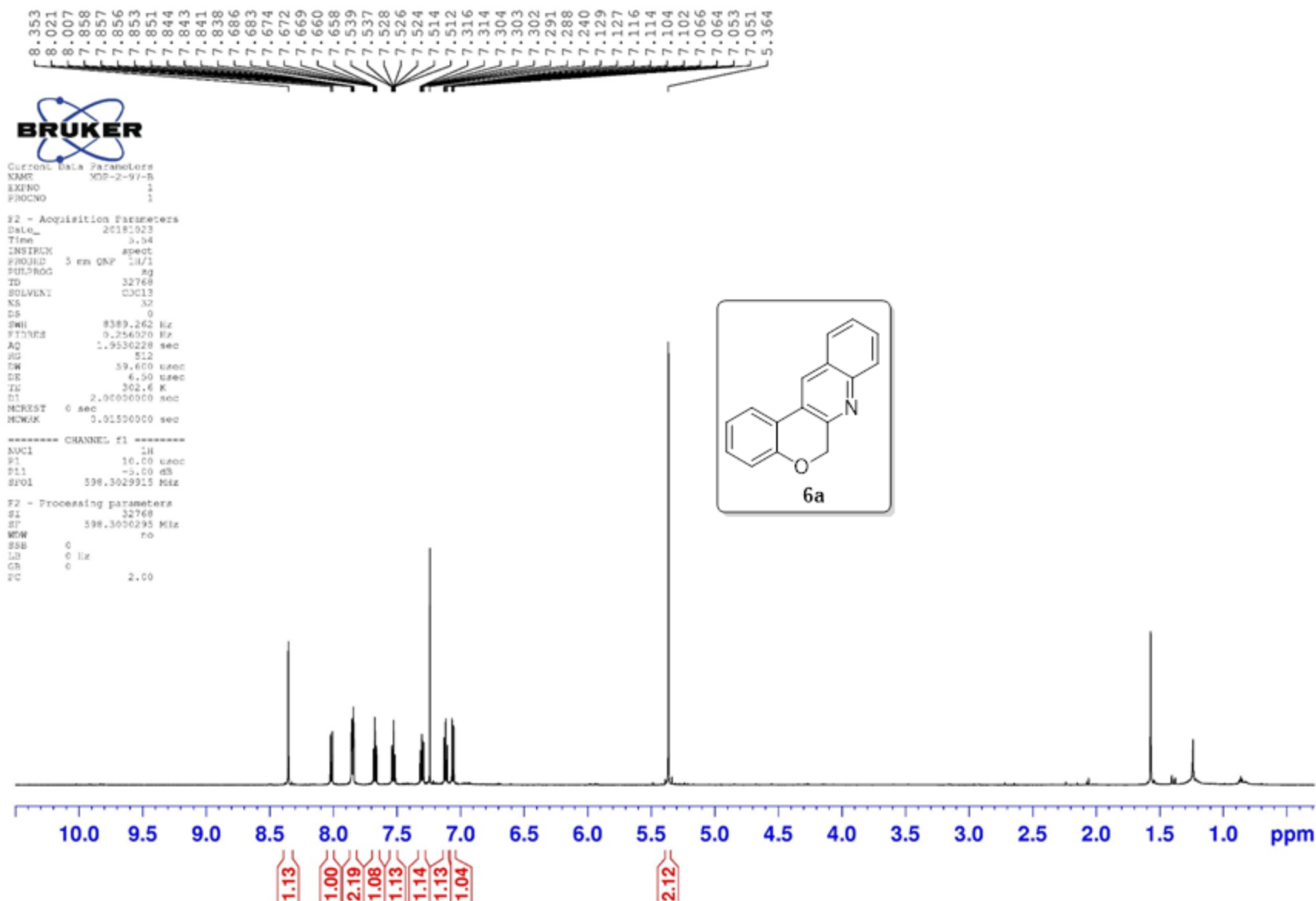
Acq_ 20180828
Time: 3.35
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 9541.984 Hz
FIDRES: 0.291198 Hz
AQ: 1.7170932 sec
RG: 512
DM: 32.400 usec
DE: 6.50 usec
TE: 299.7 K
SI: 2.0369000 sec
MCREST: 0 sec
MCWRR: 0.0150000 sec

----- CHANNEL f1 -----
NUC1: 1H
P1: 10.00 usec
PL1: 0 dB
SFO1: 500.13629915 MHz

F2 - Processing parameters
SI: 32768
SF: 500.1362990 MHz
WDW: no
SSB: 0
LB: 0 Hz
GB: 0
PC: 2.00









Current Data Parameters
NAME MDP-2-97-B
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181023
Time 5.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl₃
NS 1566

SWH 43945.047
FIDRES 1.374666
AQ 0.2677748
RG 4096
DM 11.230
DE 6.50
TE 302.6
D1 3.5000000
d11 0.0300000
DELTA 2.6000000
PCORE2 0.0000000
MCORE 0.0100000

----- CHANNEL f1 -----
NUC1 13C
P1 12.00
PL1 0 dB
SFO1 125.76037

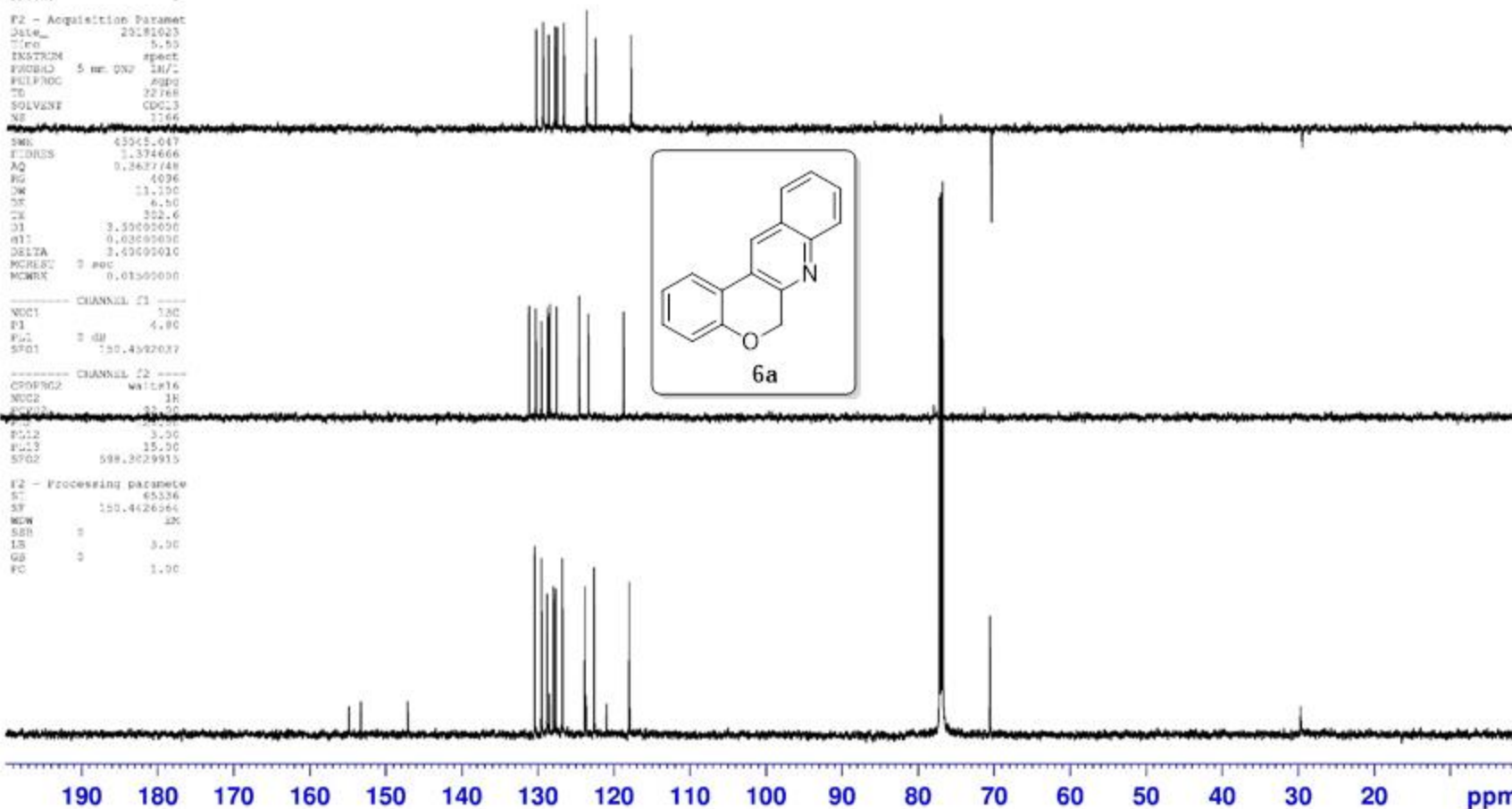
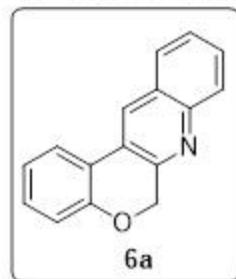
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 12.00
PL2 0 dB
SFO2 500.13629915

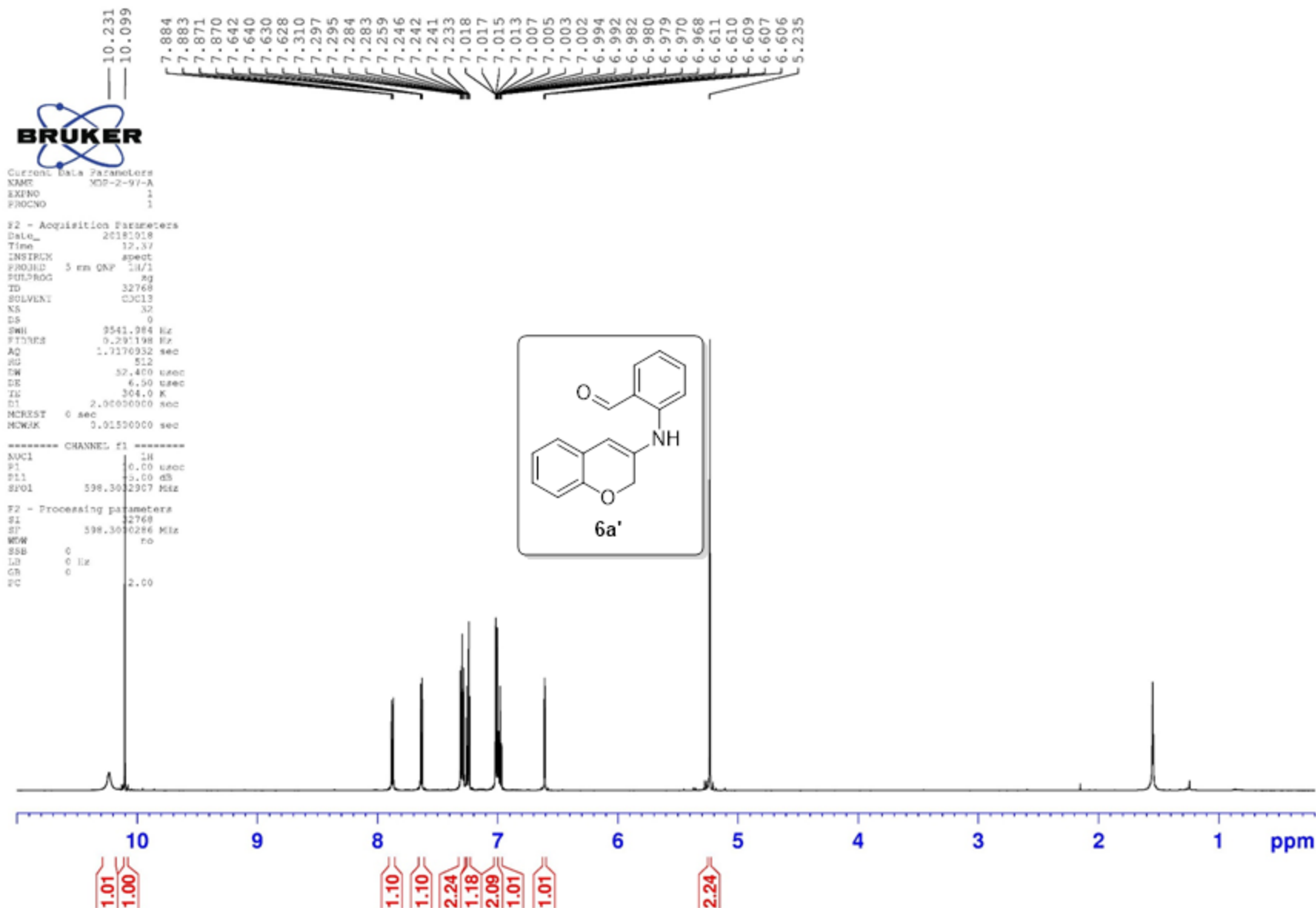
F2 - Processing parameters
SI 65536
SF 150.4426064
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

154.879
153.325
147.140
130.453
129.564
128.809
128.487
127.992
127.721
126.827
123.839
123.719
122.639
121.013
117.999

77.213
77.001
76.788
70.572

29.694







Current Data Parameters
NAME MDP-2-97-A
EXPNO 2
PROCNO 1

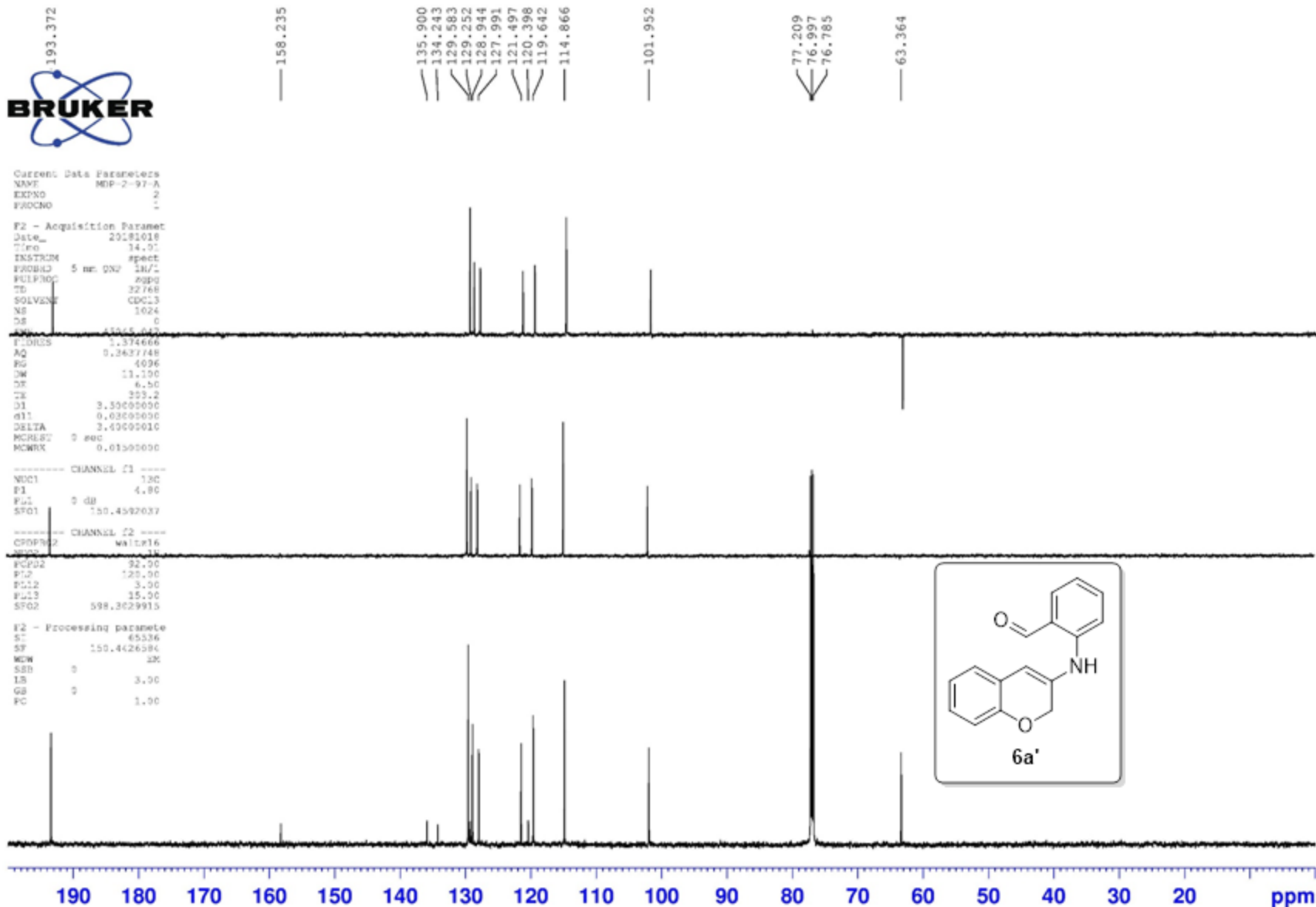
F2 - Acquisition Parameters
Date_ 20181018
Time 14.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1024
DS 0

NUC1 13C
FIDRES 1.374666
AQ 0.2637748
RG 4096
DM 11.100
DE 6.50
TE 303.2
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCRST 0 sec
MCRM 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 100.626137

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 3.00
PL13 15.00
SFO2 500.13629915

F2 - Processing parameters
SI 65536
SF 150.4426584
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00



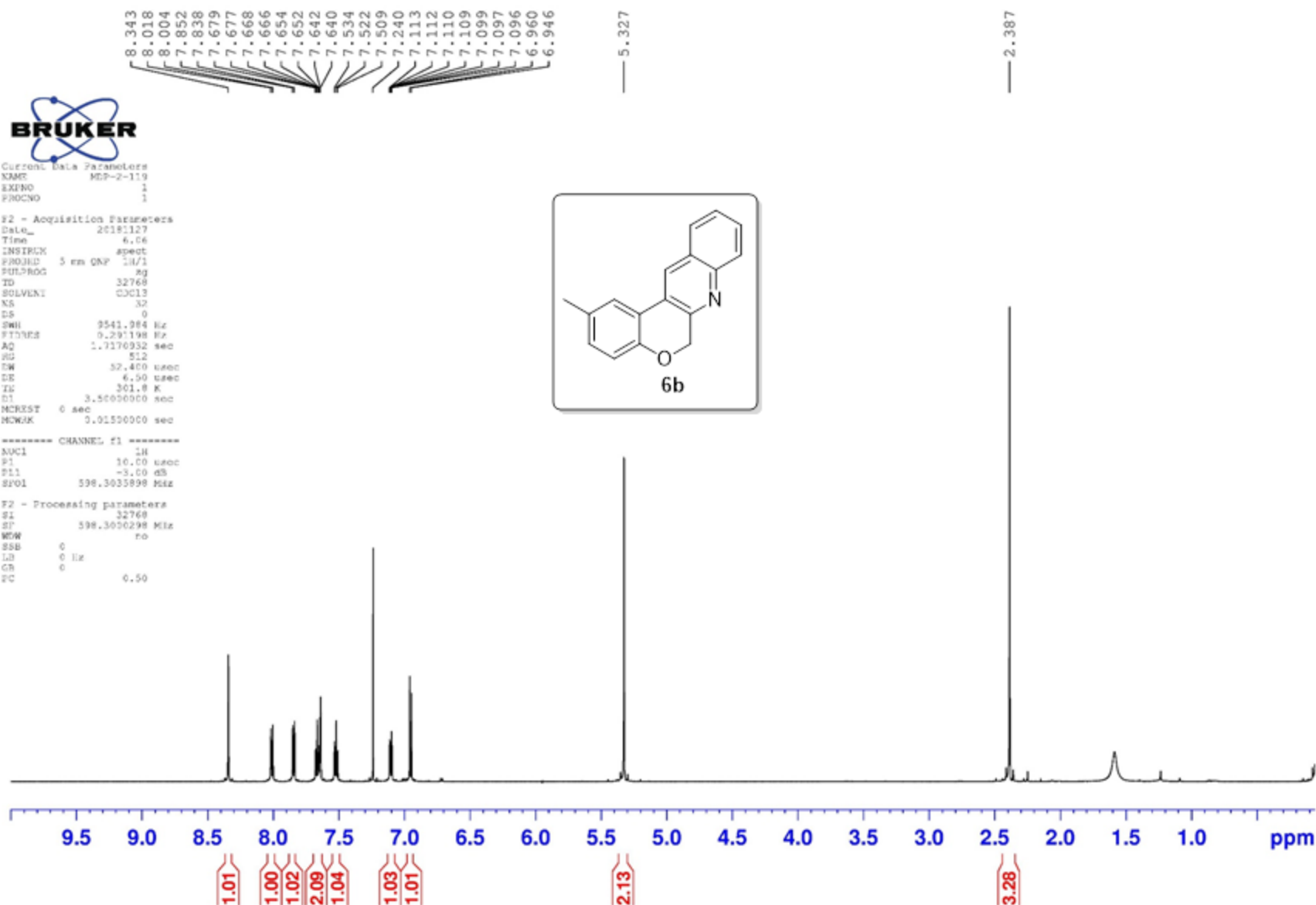
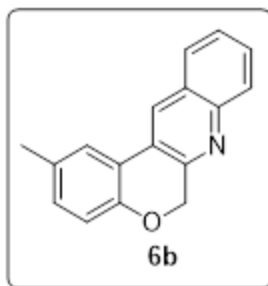


Current Data Parameters
NAME MDP-2-119
EXFNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181127
Time 6.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170332 sec
RG 512
CW 52.400 usec
DE 6.50 usec
TE 301.8 K
D1 3.5000000 sec
MCREST 0 sec
MCWAK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.3035998 MHz

F2 - Processing parameters
SI 32768
SF 500.3030298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.50





Current Data Parameters
NAME MCP-2-119
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181127
Time 6.58
INSTRUM spect
PULPROG 5 ms. DNP 1M/2
PCPD/OC 200
TD 32768
SOLVENT Acetone
NS 1320

SWH 43345.047
FIDRES 1.374666
AQ 0.2677748
RG 4096
DM 11.230
DE 6.50
TE 301.8
D1 3.5000000
d11 0.0300000
DELTA 2.6000000
PCPD 0.0000000
PCPD 0.0100000

CHANNEL F1
NUC1 13C
P1 12.00
PL1 0 dB
SFO1 125.4302037

CHANNEL F2
CPDPRG2 waltz16

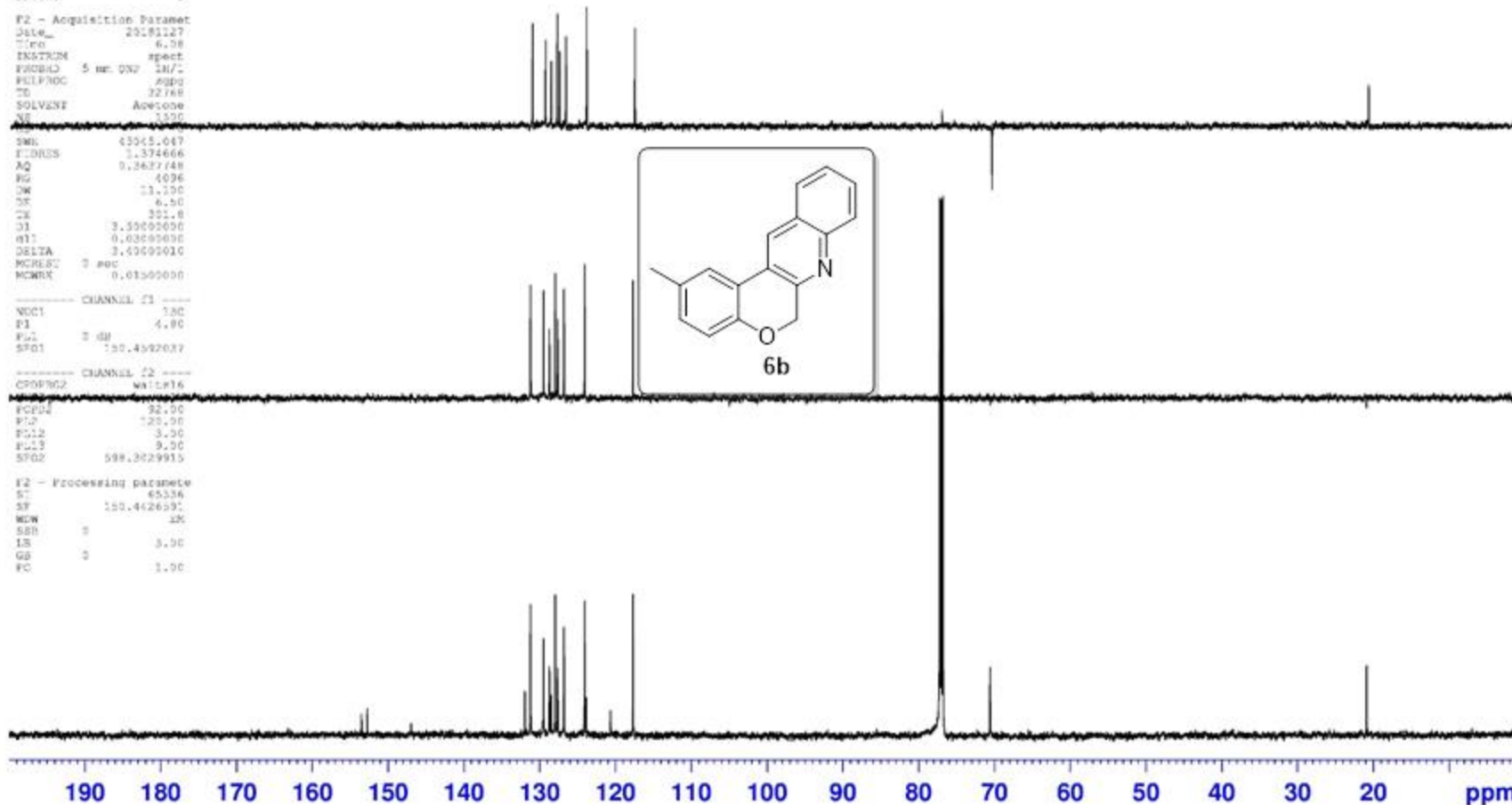
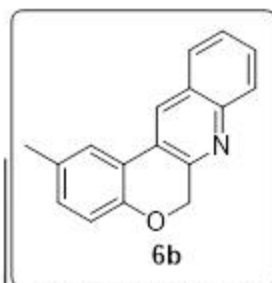
PCPD 32.00
PL2 120.00
PL3 3.00
PL4 9.00
SFO2 598.3029915

F2 - Processing parameters
SI 65536
SF 150.4426591
WDW 20
SSB 0
LB 3.00
GB 0
PC 1.00

153.530
152.746
146.944
131.973
131.211
129.503
128.715
128.481
127.951
127.615
126.803
124.067
123.865
120.643
117.692

77.208
76.996
76.783
70.551

20.868





Current Data Params
NAME: ME8-2-1
EXPTNO:
PROCNO:

F2 - Acquisition Pa
Date_: 2019
Time:
INSTRUM: A
PROBHD: 5 mm QNP
PULPROG:
TD: 3
SOLVENT: C
NS:
DS:
SWH: 9569
FIDRES: 0.29
AQ: 1.712
RG:
DM: 52
DE:
TE: 2
D1: 2.0000
MCREST: 0 sec
MCMRK: 0.0150

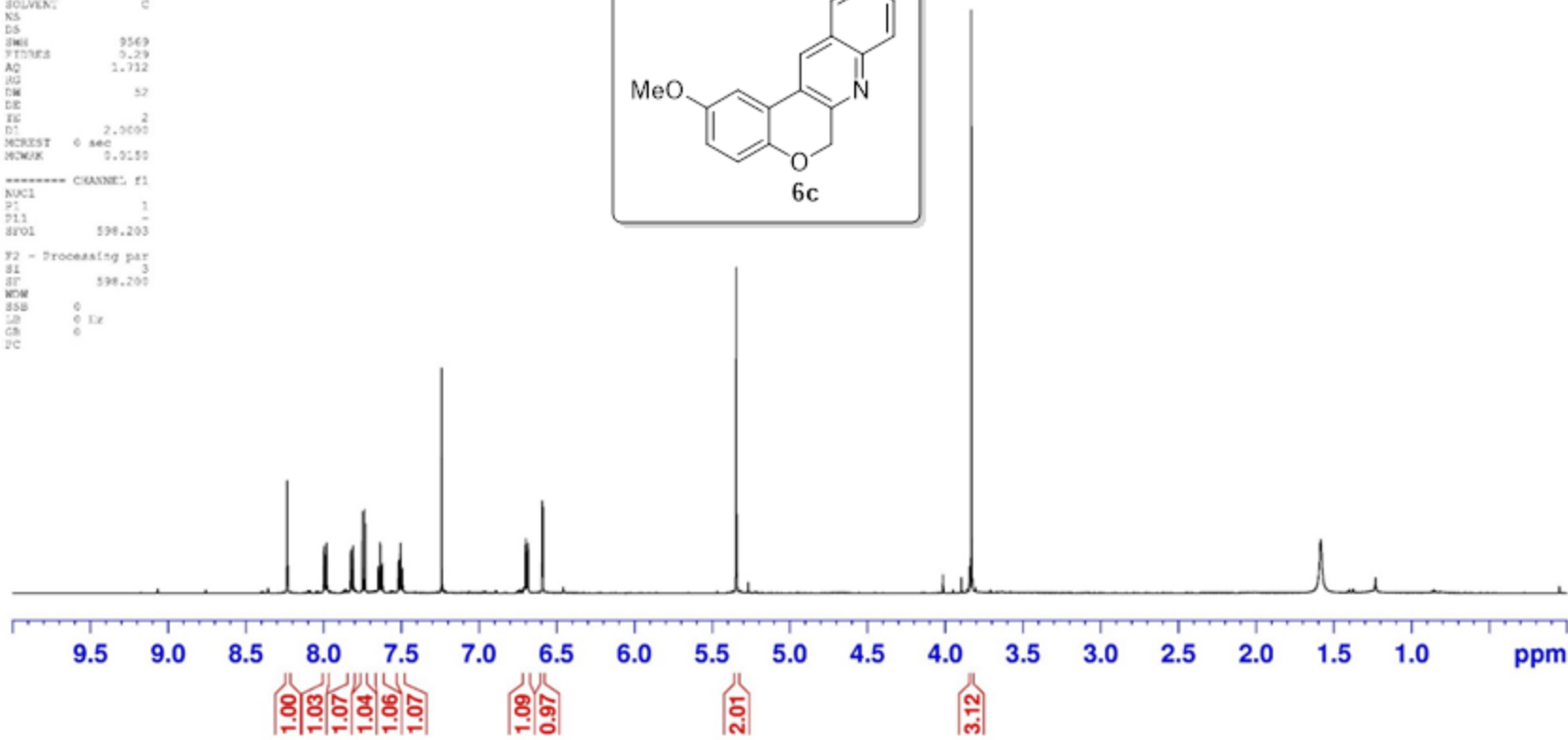
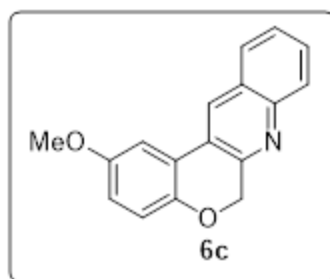
----- CHANNEL f1
NUC1:
P1: 1
P13:
SFO1: 598.203

F2 - Processing par
S1: 3
SF: 598.203
WDW:
SSB: 0
LB: 0 Hz
GB: 0
PC:

8.229
7.993
7.979
7.823
7.809
7.747
7.733
7.648
7.646
7.637
7.635
7.632
7.623
7.621
7.516
7.504
7.491
7.240
6.698
6.688
6.593
6.588

5.344

3.831

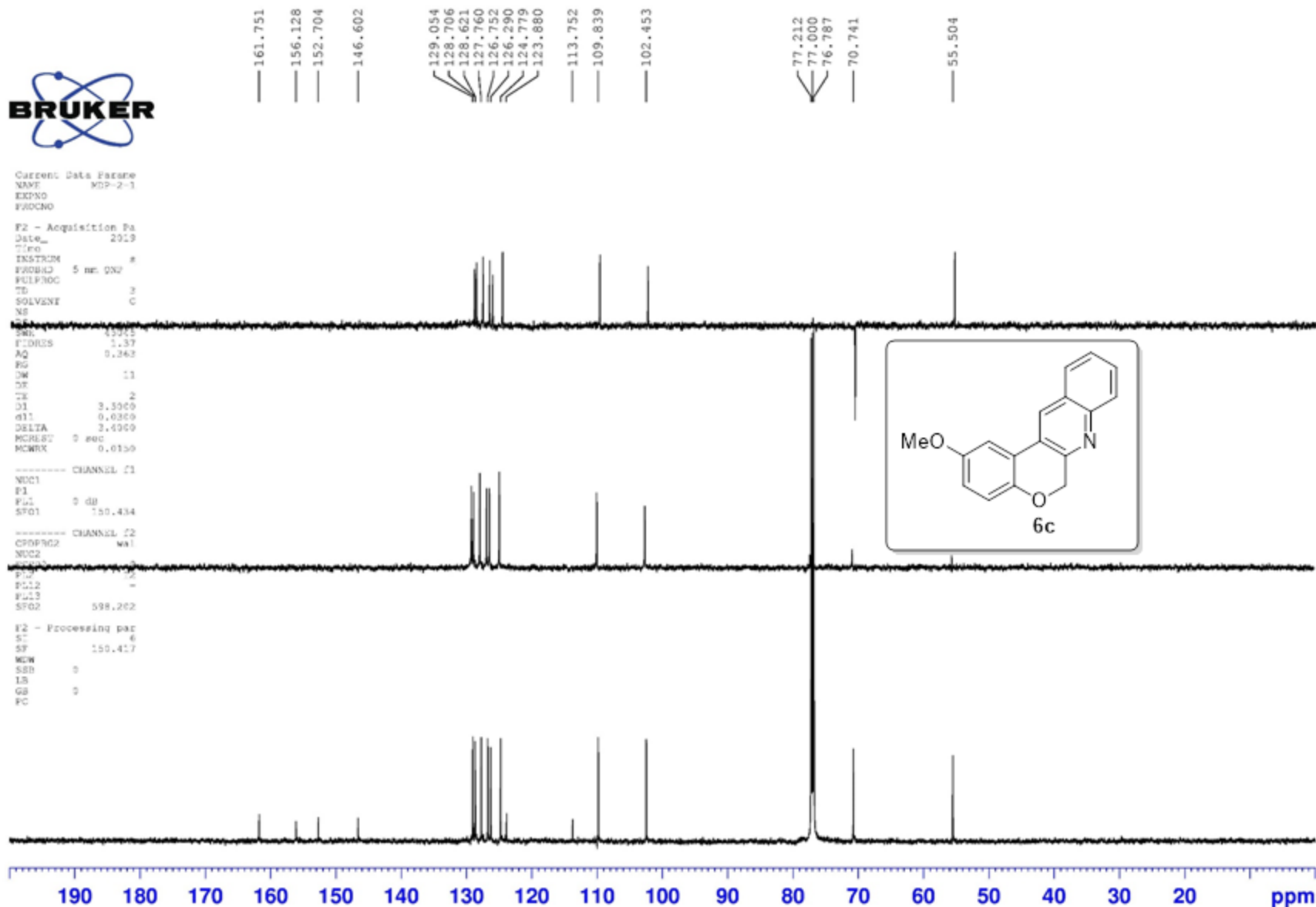




Current Data Parameters
NAME MDP-2-1
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_ 2019
Time
INSTRUM
PULPROG 5 ms. DNP
TE 3
SOLVENT C
NS

===== CHANNEL f1
NUC1
P1
PL1 0 dB
SFO1 150.434
===== CHANNEL f2
CPDPRG2 waltz
NUC2
P2
PL2
PL12
SFO2 598.262
F2 - Processing parameters
SI 6
SF 150.417
WDW
SSB 0
LB 0
GB 0
PC





Current Data Parameters
NAME MDP-2-117
EXPNO 1
PROCNO 1

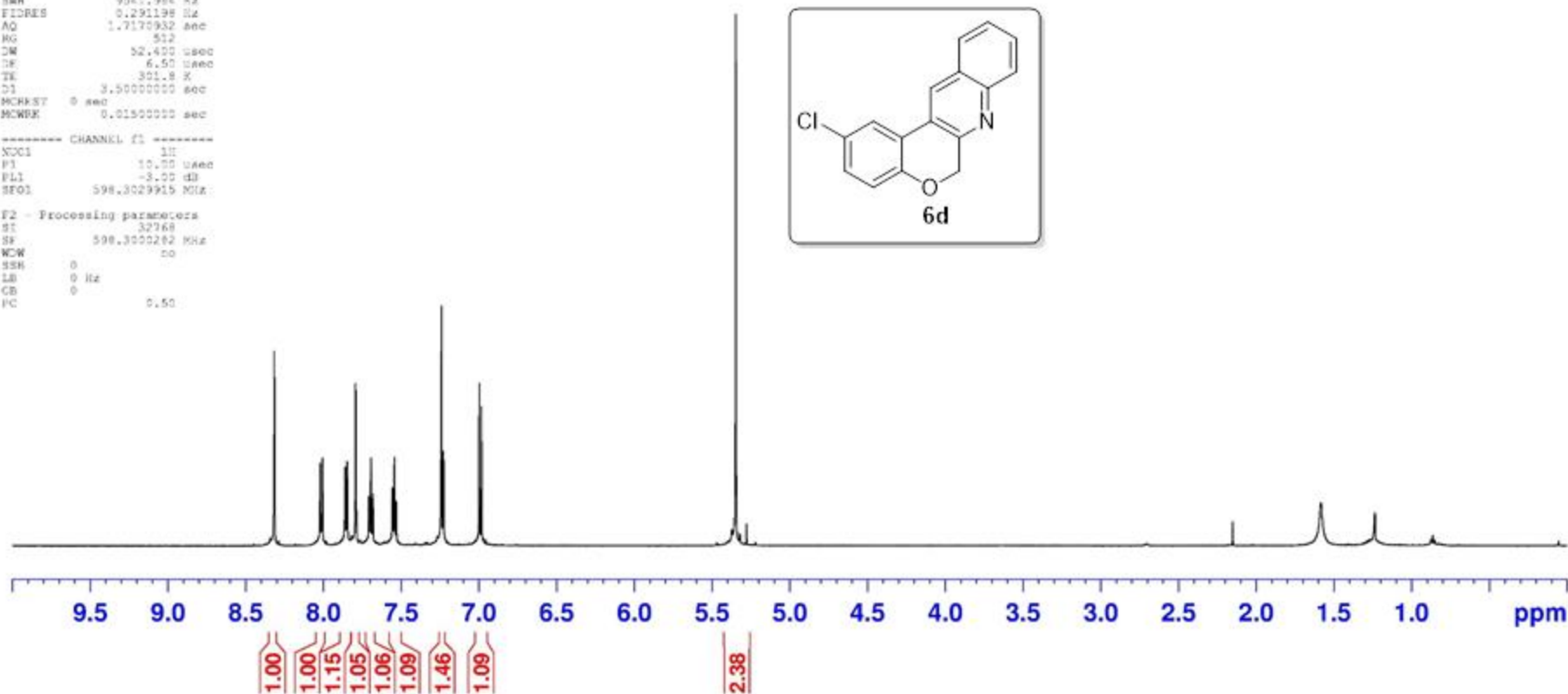
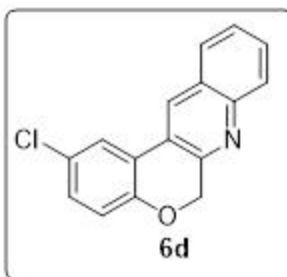
F2 - Acquisition Parameters
Date_ 20181123
Time 6.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Kz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DM 52.400 usec
DE 6.50 usec
TE 301.2 K
D1 3.50000000 sec
MCKEY 0 sec
MCWDE 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
RF01 598.3029915 MHz

F2 - Processing parameters
SI 32768
SF 598.3000242 MHz
WDW do
SSB 0
LB 0 Hz
GB 0
PC 0.50

8.317
8.021
8.007
7.862
7.861
7.848
7.795
7.791
7.709
7.707
7.697
7.695
7.692
7.683
7.681
7.558
7.557
7.545
7.533
7.531
7.245
7.241
7.231
7.226
6.998
6.984

5.348





Current Data Parameters
NAME MDP-2-117
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181123
Time 7.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 704
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 301.9
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCPST 0 sec
MCWK 0.01500000

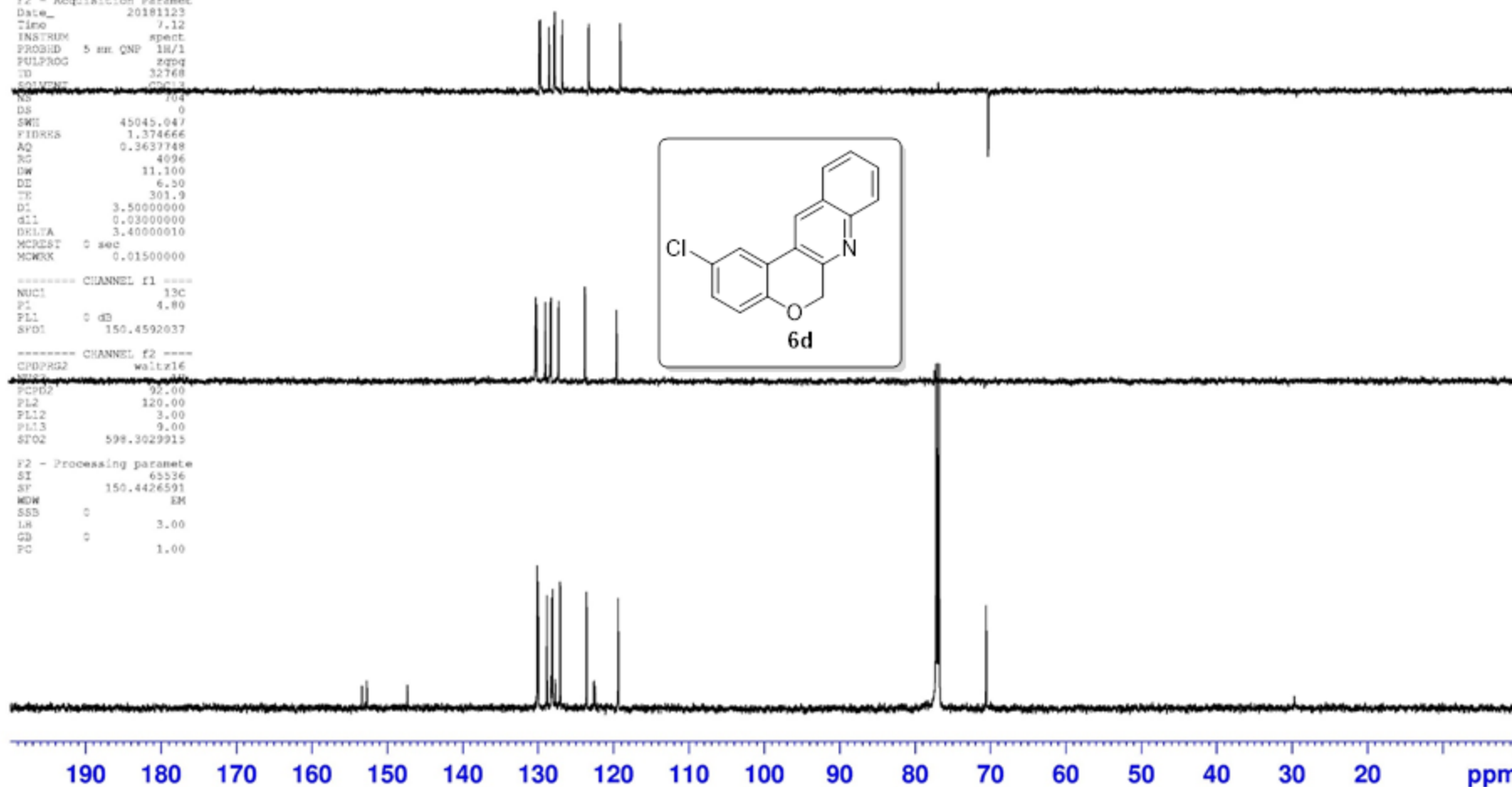
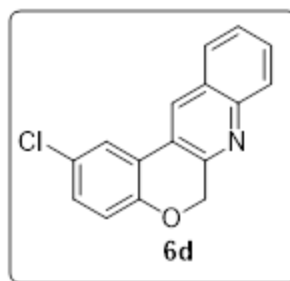
----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4592037

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 3.00
PL13 9.00
SFO2 598.3029915

F2 - Processing parameters
SI 65536
SF 150.4426591
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

153.359
152.725
147.347
130.122
129.999
128.817
128.288
128.163
128.079
127.727
127.071
123.576
122.593
122.452
119.386

77.208
76.996
76.784
70.578





Current Data Parameters
NAME MDP-2-135-3
EXPNO 1
PROCNO 1

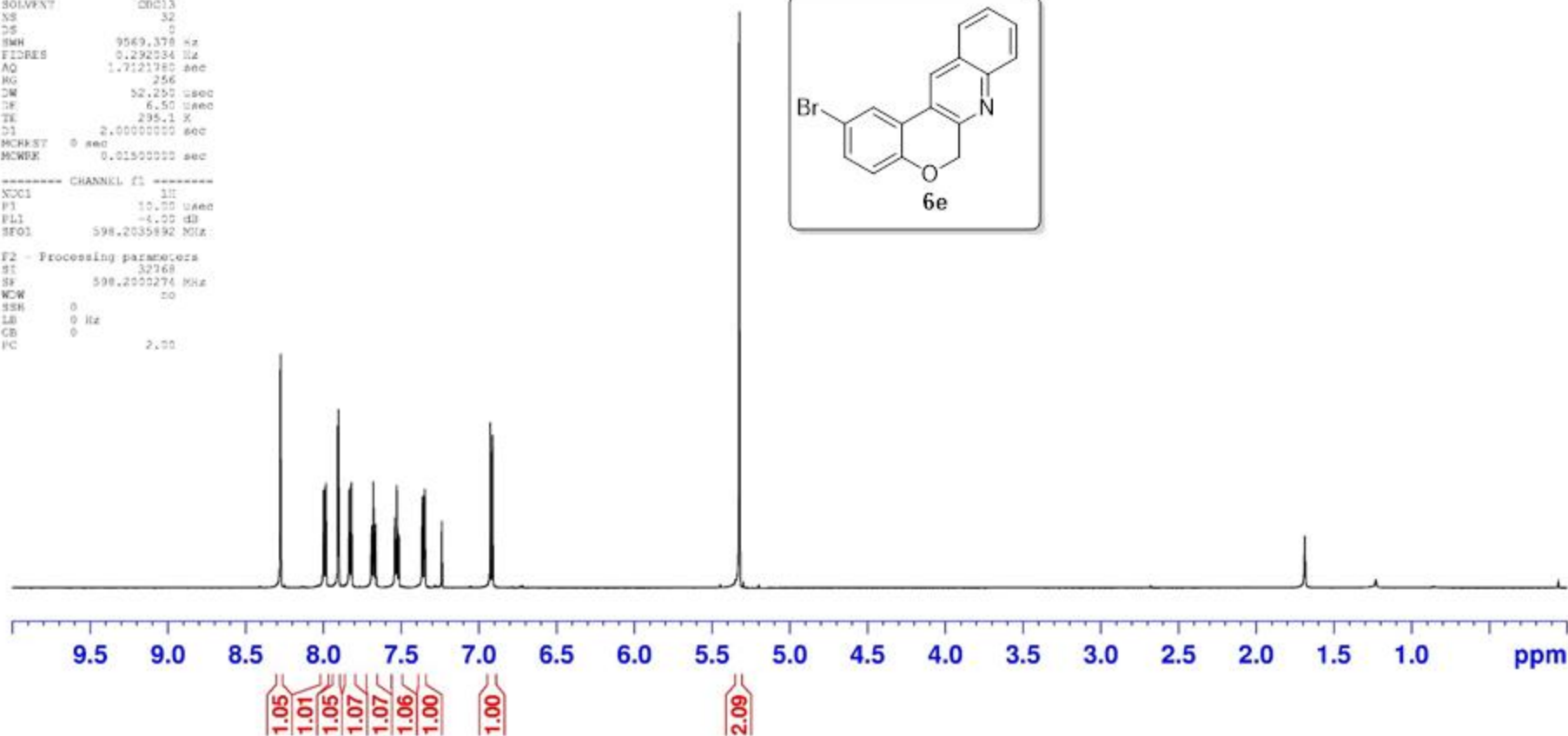
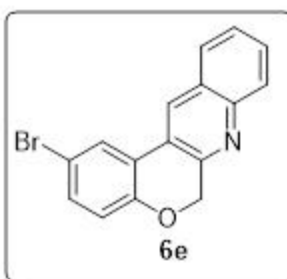
F2 - Acquisition Parameters
Date_ 20190110
Time 10.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT DMSO
NS 32
DS 2
SWH 9569.378 Kz
FIDRES 0.292534 Hz
AQ 1.7121780 sec
RG 256
DM 52.250 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCKEY 0 sec
MCWPR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
SFO1 500.2035992 MHz

F2 - Processing parameters
SI 32768
SF 500.2035992 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 2.00

8.275
8.000
7.986
7.908
7.904
7.834
7.821
7.693
7.691
7.682
7.680
7.677
7.668
7.665
7.541
7.530
7.528
7.518
7.516
7.366
7.363
7.352
7.348
7.240
7.238
6.928
6.913

5.326





Current Data Parameters
NAME MDP-2-135-R
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190110
Time 10.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.940

F1 FIDRES 1.1574460
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 295.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCPRST 0 sec
MCWRR 0.01500000

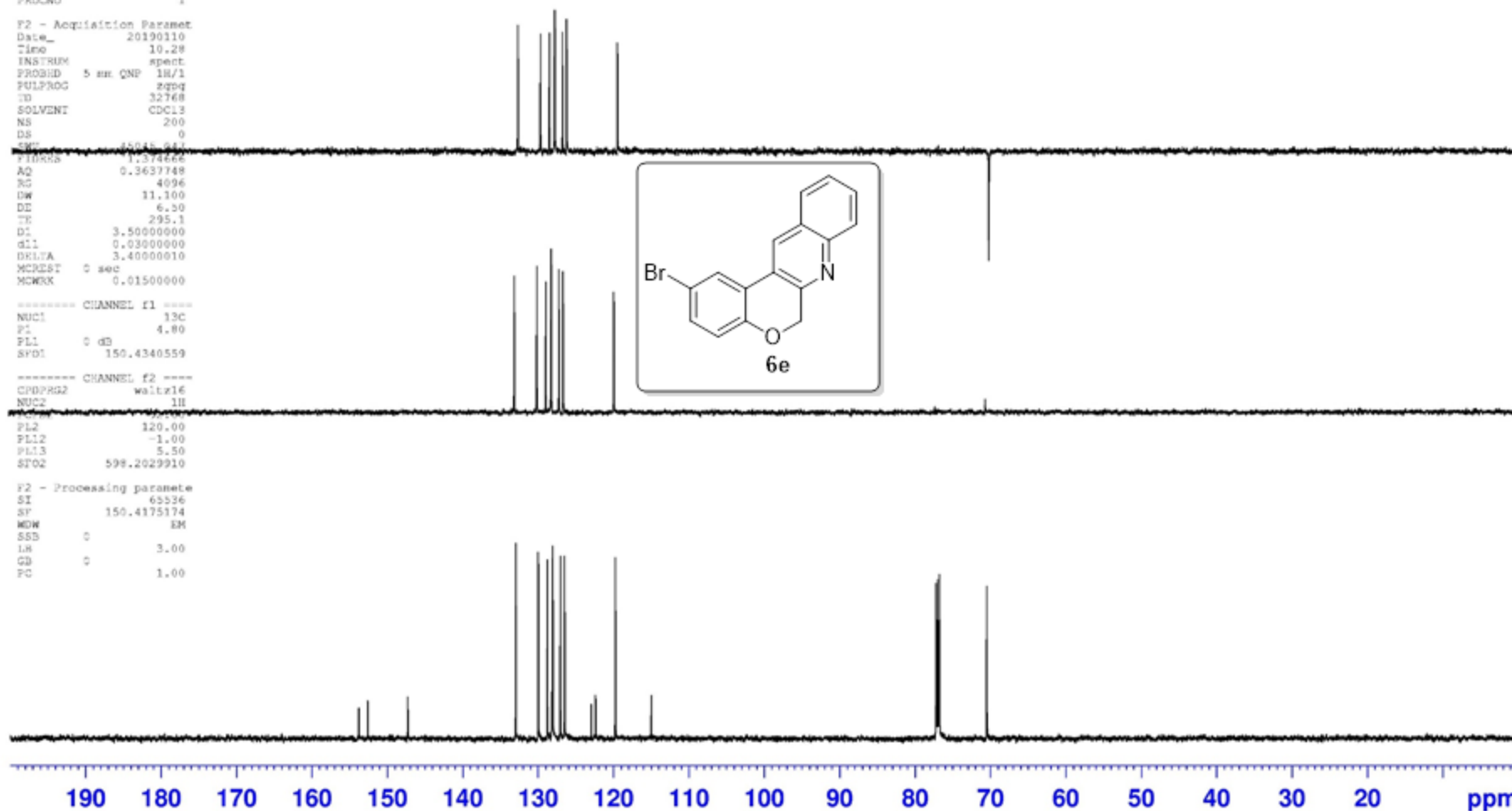
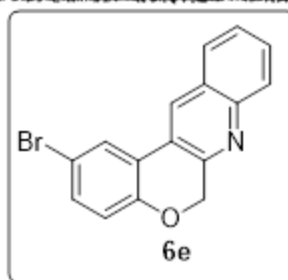
----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 -1.00
PL3 5.50
SFO2 598.2629910

F2 - Processing parameters
SI 65536
SF 150.4175174
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

153.786
152.604
147.290
132.964
129.982
128.766
128.224
128.109
128.055
127.044
126.495
122.921
122.384
119.762
114.980

77.207
76.994
76.782
70.496





Current Data Parameters
NAME MDP-2-142-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190115
Time 5.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 9569.378 Kz
FIDRES 0.292534 Hz
AQ 1.7121785 sec
RG 512
DM 52.255 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
MCHKEST 0 sec
MCWDE 0.01500000 sec

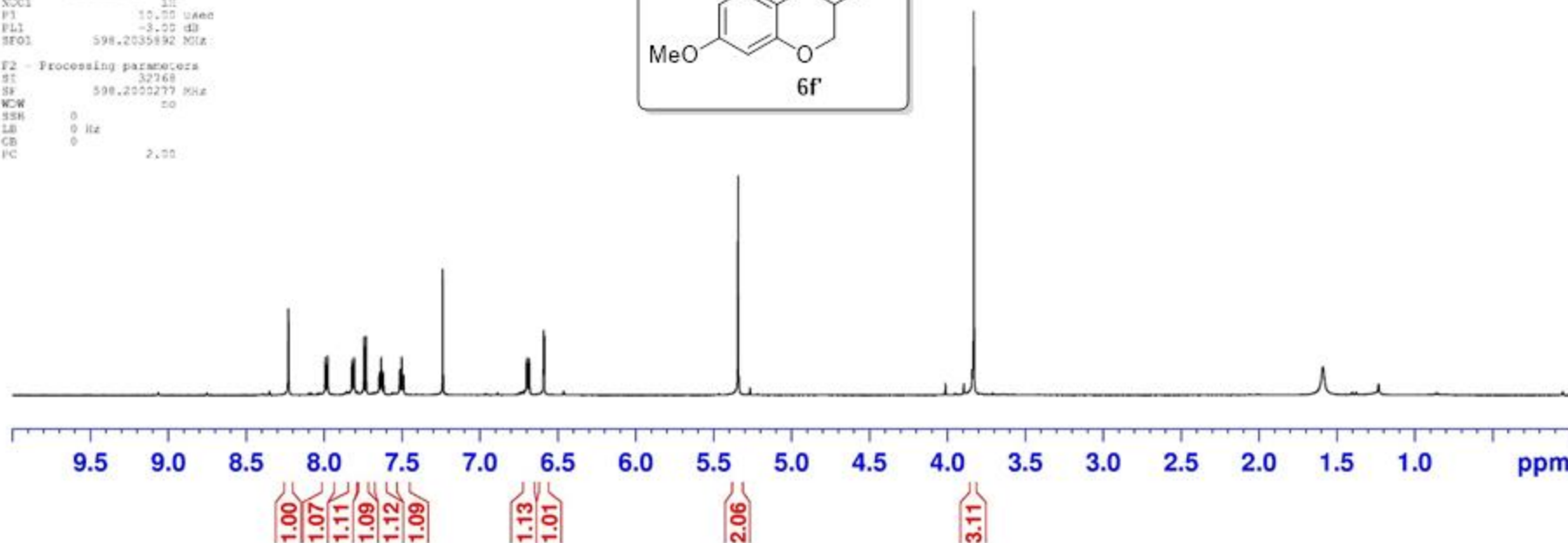
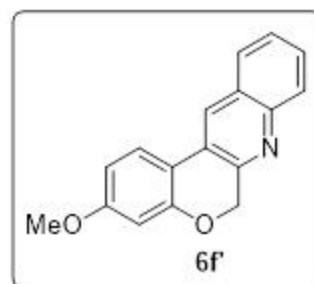
----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
RF01 598.2035892 MHz

F2 - Processing parameters
SI 32768
SF 598.2000277 MHz
WDW 20
SSB 0
LB 0 Hz
GB 0
PC 2.00

8.228
7.993
7.979
7.822
7.808
7.747
7.732
7.648
7.646
7.637
7.634
7.632
7.623
7.620
7.517
7.515
7.504
7.502
7.492
7.490
7.240
6.702
6.698
6.688
6.683
6.593
6.588

5.344

3.831





Current Data Parameters
NAME MDP-2-142-B
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190115
Time 6.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2296
DS 4
SWH 40013.747
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 296.0
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MPCREST 0 sec
MPCWEX 0.01500000

----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

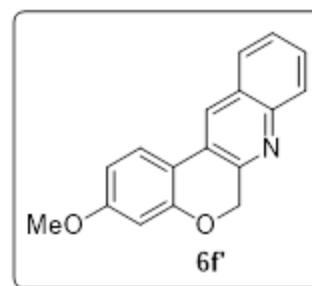
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL12 -1.00
PL13 5.50
STO2 598.2029210

F2 - Processing parameters
SI 65536
SF 150.4175147
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

161.747
156.124
152.700
146.598

129.051
128.702
128.617
127.757
126.749
126.287
124.775
123.876
113.748
109.835
102.450

77.208
76.996
76.784
70.737
55.500



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

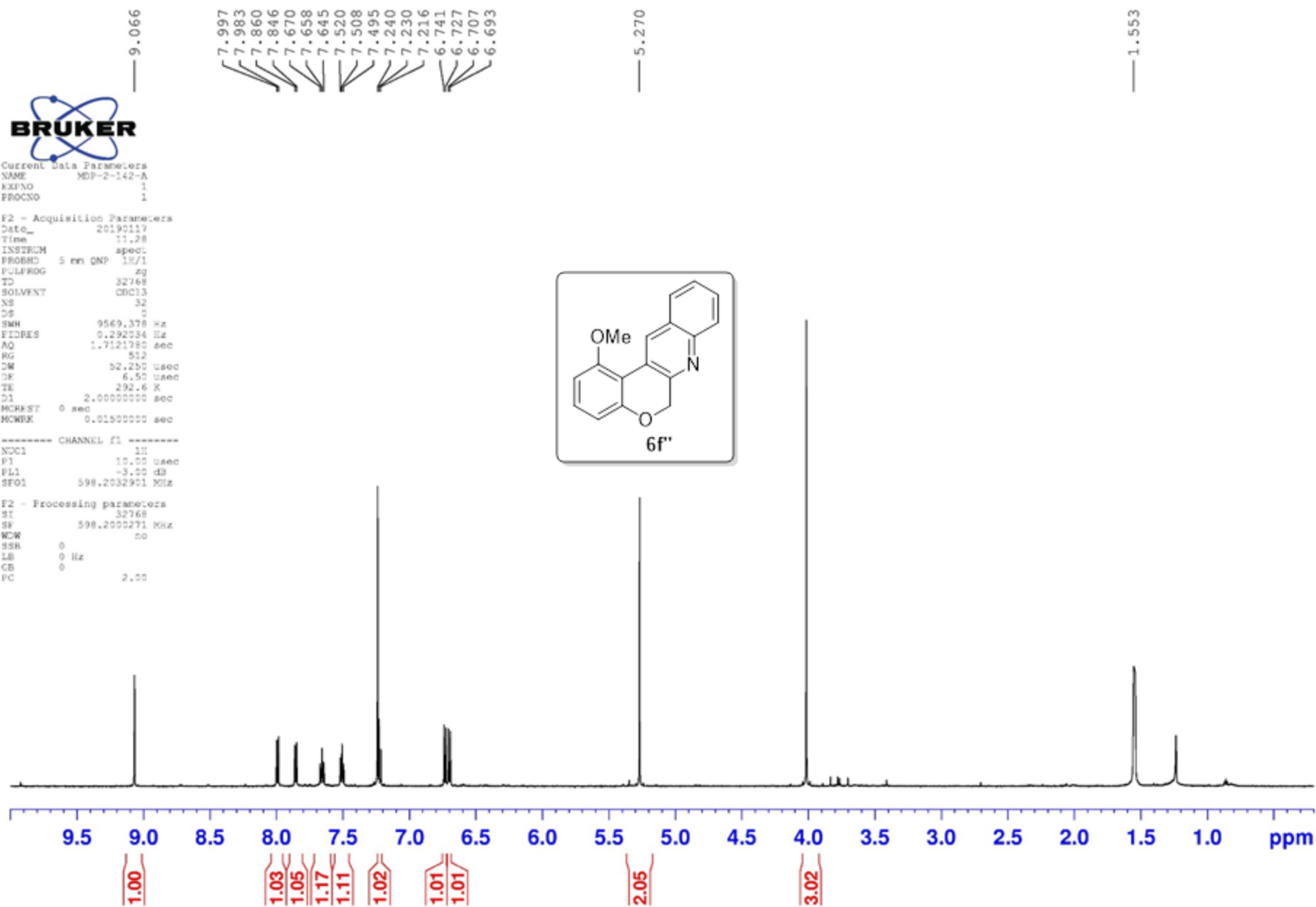


Current Data Parameters
NAME MDP-2-142-A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190117
Time 11.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 9569.378 Hz
FIDRES 0.292034 Hz
AQ 1.7121780 sec
RG 512
DM 52.250 usec
DE 6.50 usec
TE 292.6 K
D1 2.00000000 sec
MCHKEST 0 sec
MCWPRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.2032901 MHz

F2 - Processing parameters
SI 32768
SF 500.2032901 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00





Current Data Parameters
NAME MDP-2-142-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190117
Time 12.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 16045.242
FIDRES 1.074664
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 292.3
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MPCST 0 sec
MCWRR 0.01500000

----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
P12 1.00
PL12 -1.00
PL13 5.50
STO2 598.2029210

F2 - Processing parameters
SI 65536
SF 150.4175154
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

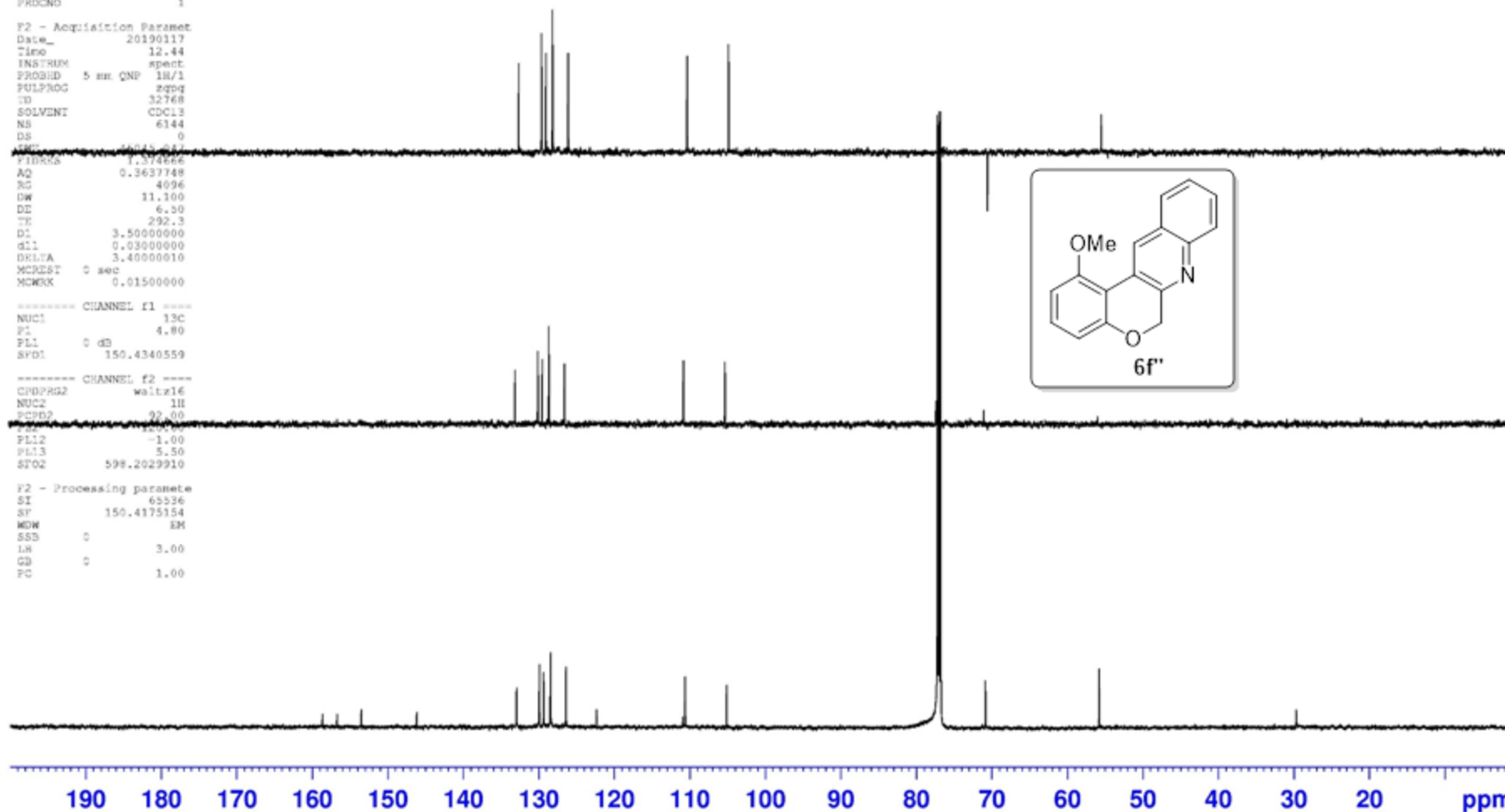
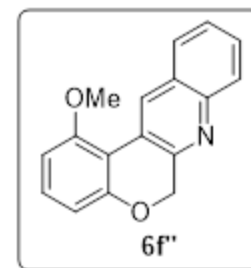
158.661
156.727
153.528
146.184

132.947
129.926
129.373
128.487
128.446
126.412
122.359

110.946
110.628
105.126

77.212
76.999
76.787
70.848

55.793



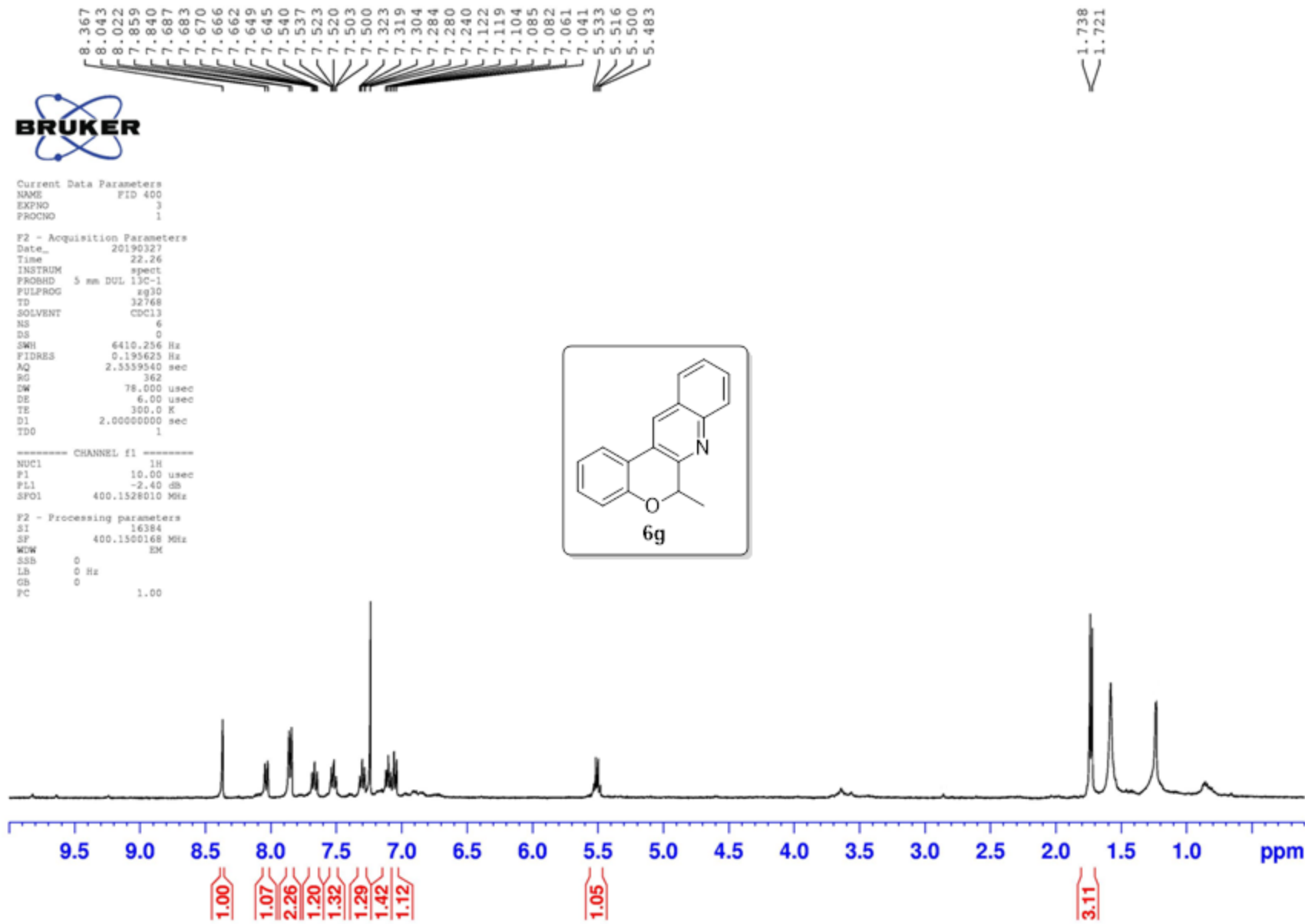
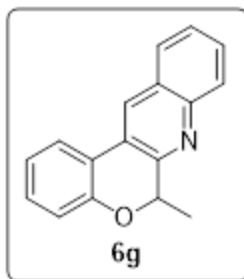


Current Data Parameters
 NAME FID 400
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190327
 Time 22.26
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 6
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5359540 sec
 RG 362
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 10.00 usec
 PL1 -2.40 dB
 SFO1 400.1528010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1500168 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





EXPNO 2
PROCNO 1

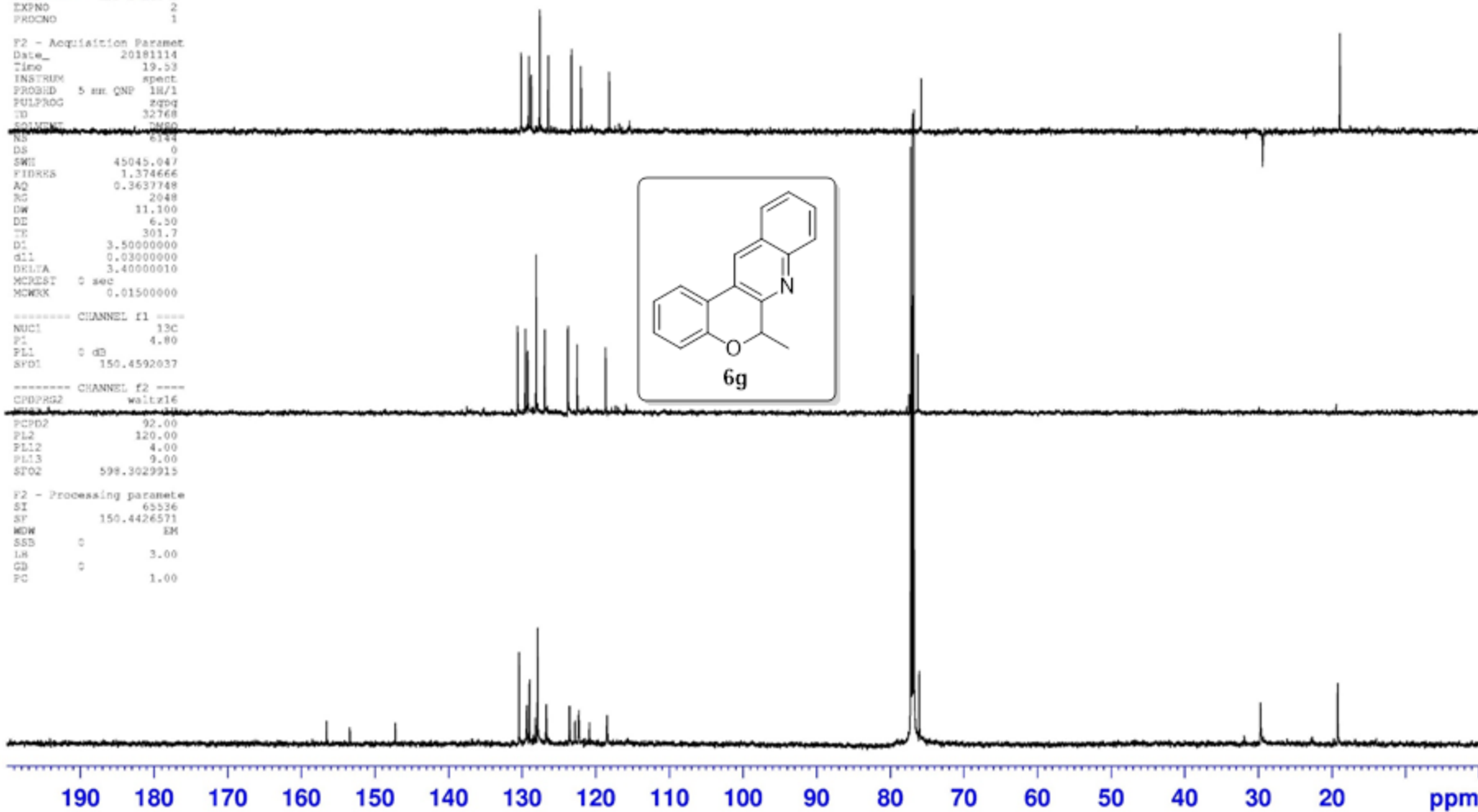
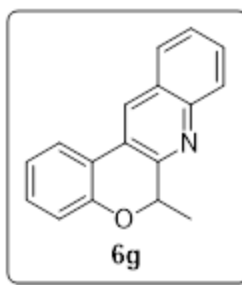
F2 - Acquisition Parameters
Date_ 20181114
Time 19.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CHLORO
NS 6144
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 2048
DW 11.100
DE 6.50
TE 301.7
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCPRST 0 sec
MCWRR 0.01500000

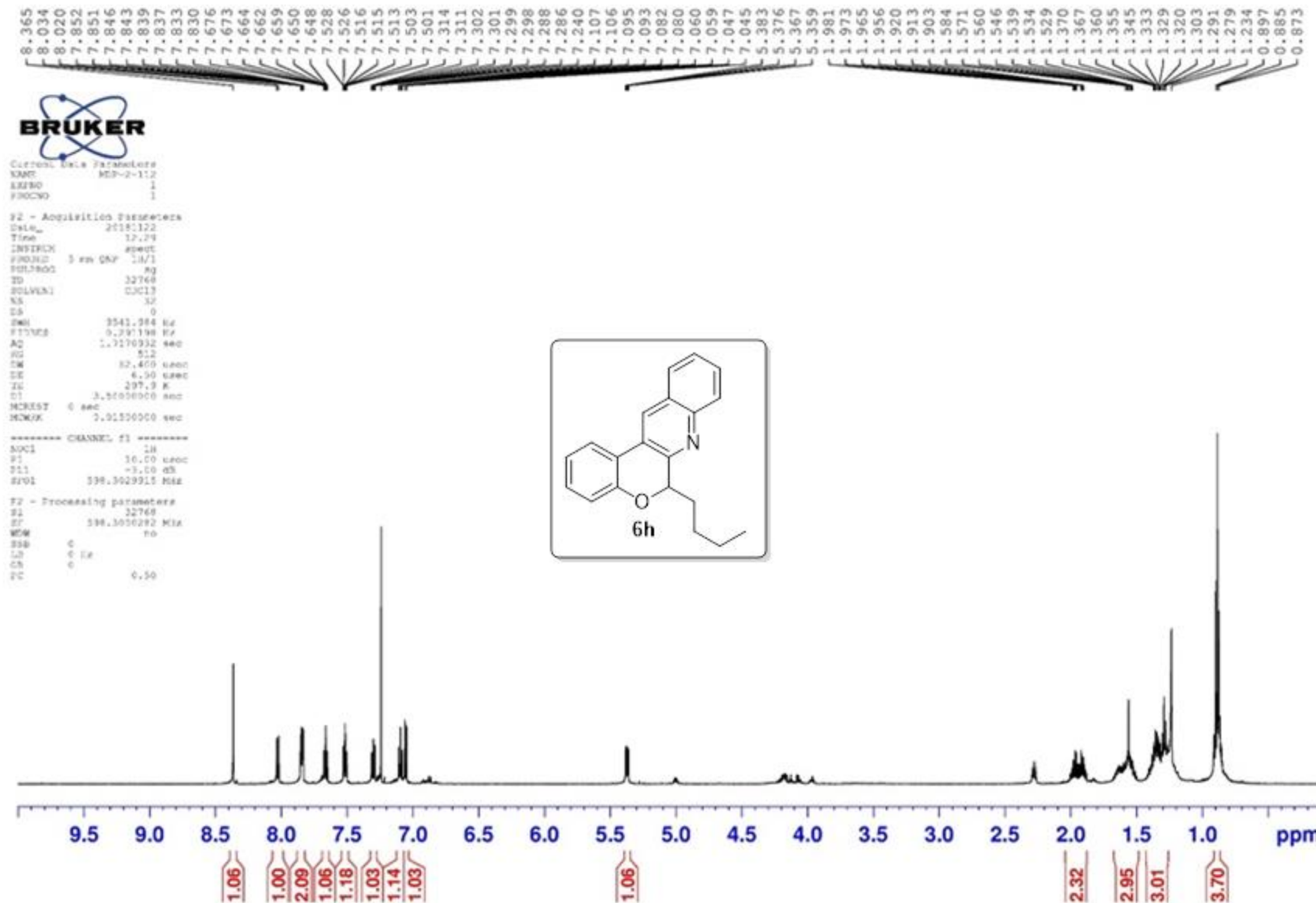
----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4592037

----- CHANNEL f2 -----
CPDPRG2 waltz16
PCPD2 92.00
PL2 120.00
PL12 4.00
PL13 9.00
STO2 598.3029915

F2 - Processing parameters
SI 65536
SF 150.4426571
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

156.564
153.418
147.245
130.418
129.363
129.006
128.226
127.910
126.721
123.573
122.813
122.307
120.863
118.464
77.211
76.999
76.787
76.057
19.211







Current Data Parameters
NAME KDP-2-112
EXPNO 2
PROCNO 1

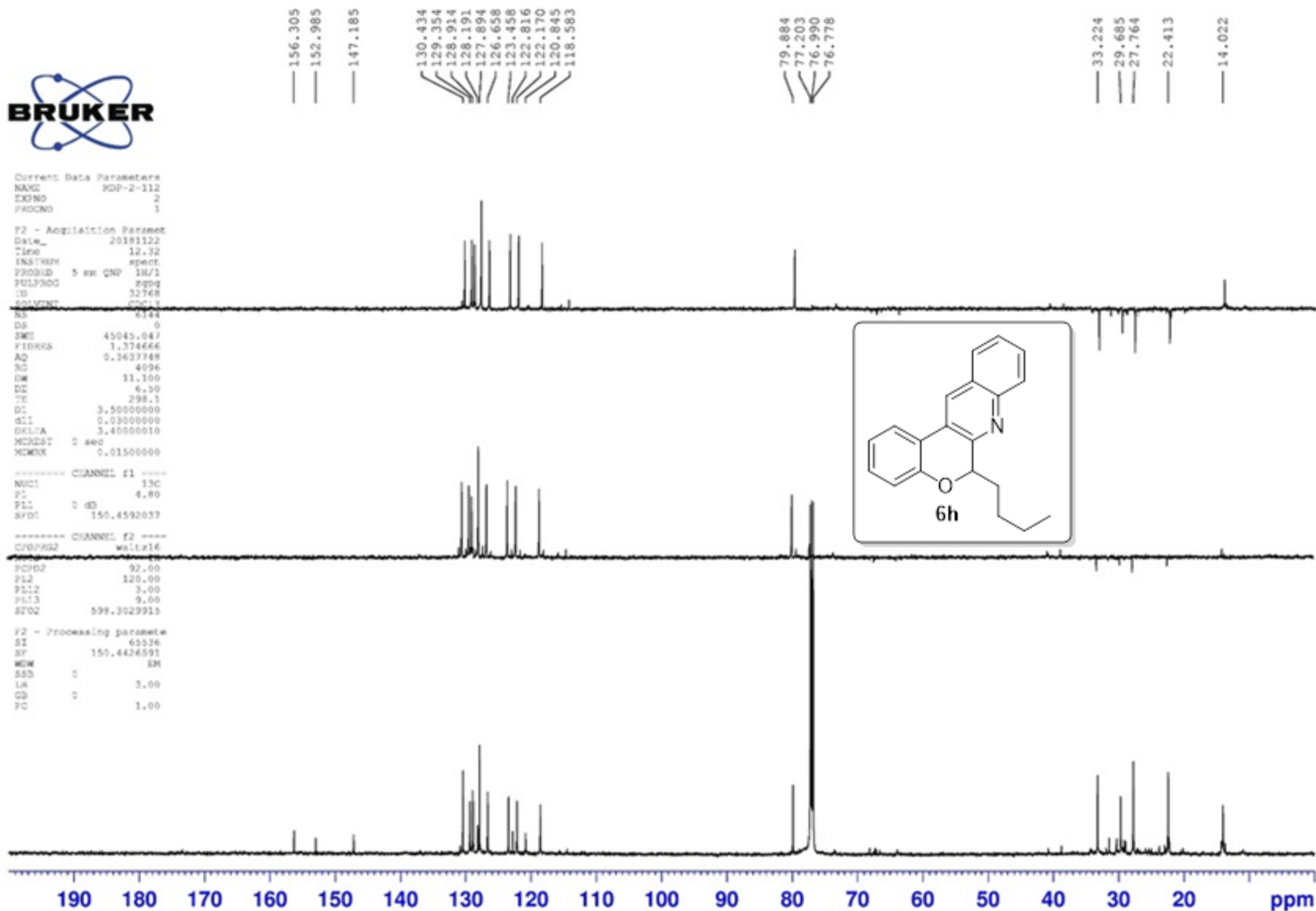
F2 - Acquisition Parameters
Date_ 20181122
Time 12.32
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zgpg30
TD 32768
SOLVENT CDCl3

NS 6144
DS 0
SWH 45045.047
FIDRES 1.374466
AQ 0.3637748
RG 4096
OW 11.100
DE 6.50
TE 298.1
D1 3.50000000
d11 0.00000000
DELTA 3.40000010
MCHGAT 0 sec
MCHW 0.01500000

===== CHANNEL f1 =====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4592037

===== CHANNEL f2 =====
CPDPRG2 waltz16
PCPD2 92.00
P12 320.00
PL12 3.00
PL13 9.00
SFO2 598.3029913

F2 - Processing parameters
SI 65536
SF 150.4426591
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00





Current Data Parameters
NAME MDP-2-129
EXPNO 1
PROCNO 1

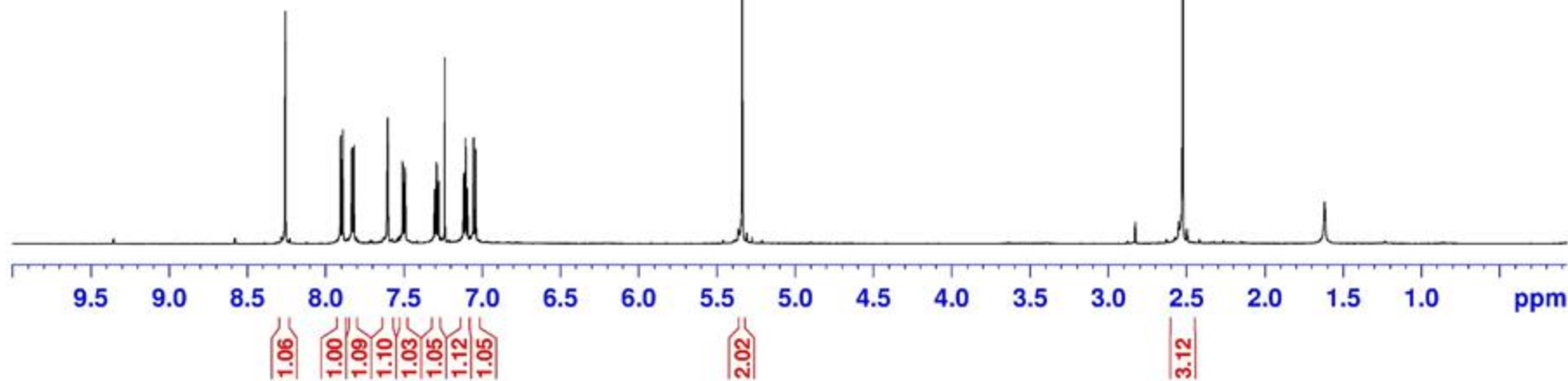
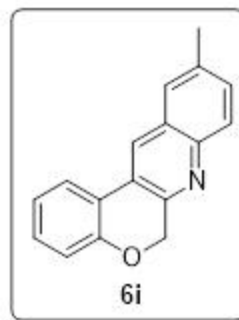
F2 - Acquisition Parameters
Date_ 20181218
Time 6.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 9569.378 Kz
FIDRES 0.292534 Hz
AQ 1.7121785 sec
RG 512
DM 52.250 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCHKST 0 sec
MCWPR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
RF01 598.2038893 MHz

F2 - Processing parameters
SI 32768
SF 598.2000272 MHz
WDW so
SSB 0
LB 0 Hz
GB 0
PC 2.00

8.257
7.903
7.889
7.832
7.830
7.819
7.817
7.602
7.506
7.503
7.492
7.489
7.306
7.304
7.294
7.292
7.292
7.281
7.278
7.240
7.121
7.119
7.108
7.107
7.096
7.094
7.057
7.055
7.043
7.042
5.339

2.526





Current Data Parameters
NAME MDP-2-129
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181218
Time 6.58
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 488
DS 8
SWH 12013.041
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 295.2
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MPCST 0 sec
MCWK 0.01500000

----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

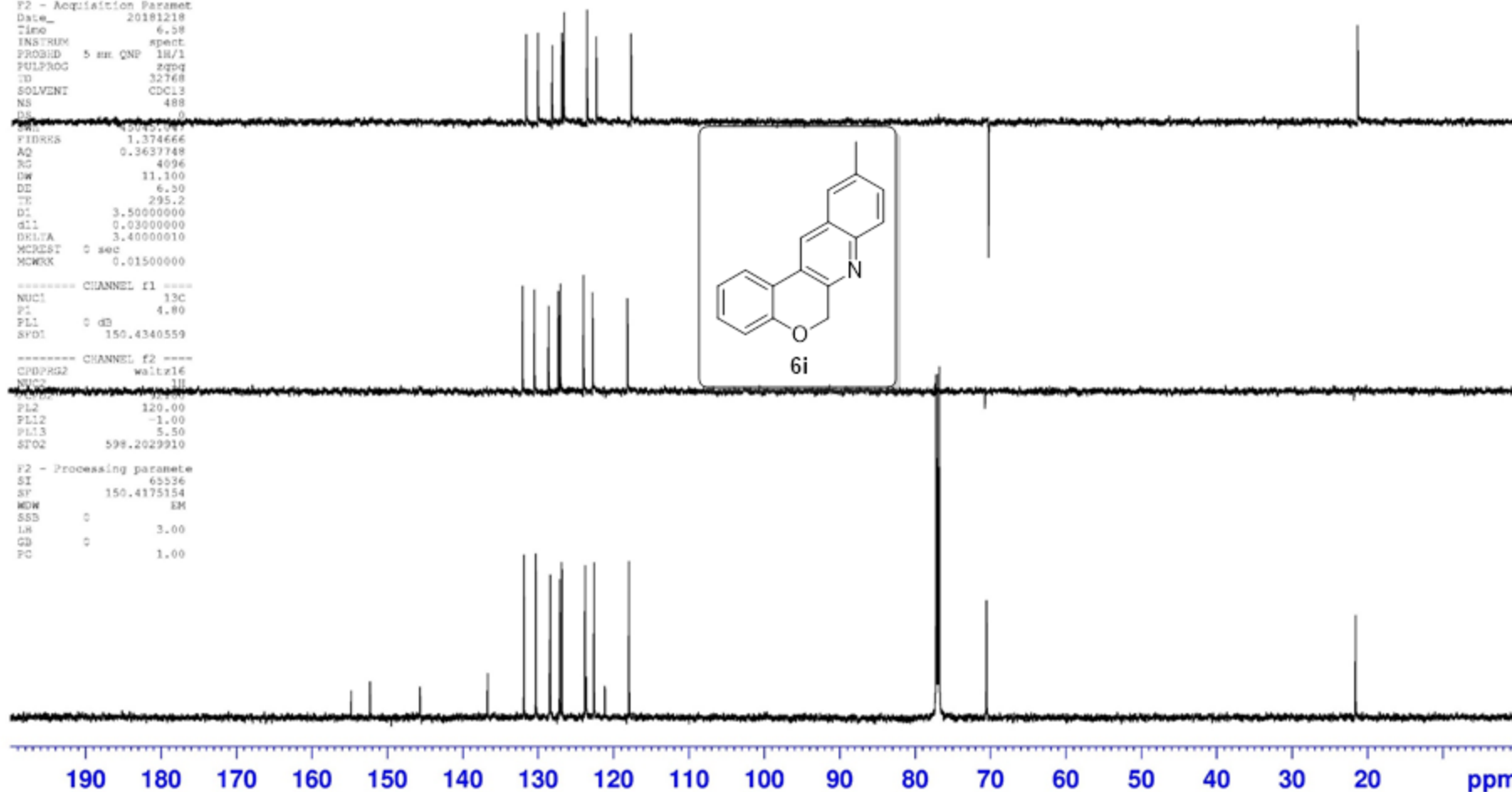
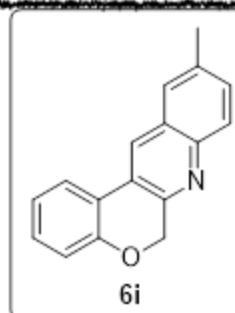
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P2 12.00
PL2 -1.00
PL13 5.50
SFO2 598.2029210

F2 - Processing parameters
SI 65536
SF 150.4175154
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

154.794
152.303
145.670
136.695
131.876
130.305
128.473
128.392
127.138
126.856
123.772
123.593
122.575
121.146
117.939

77.208
76.996
76.783
70.527

21.578





Current Data Parameters
NAME MDP-2-120
EXPNO 1
PROCNO 1

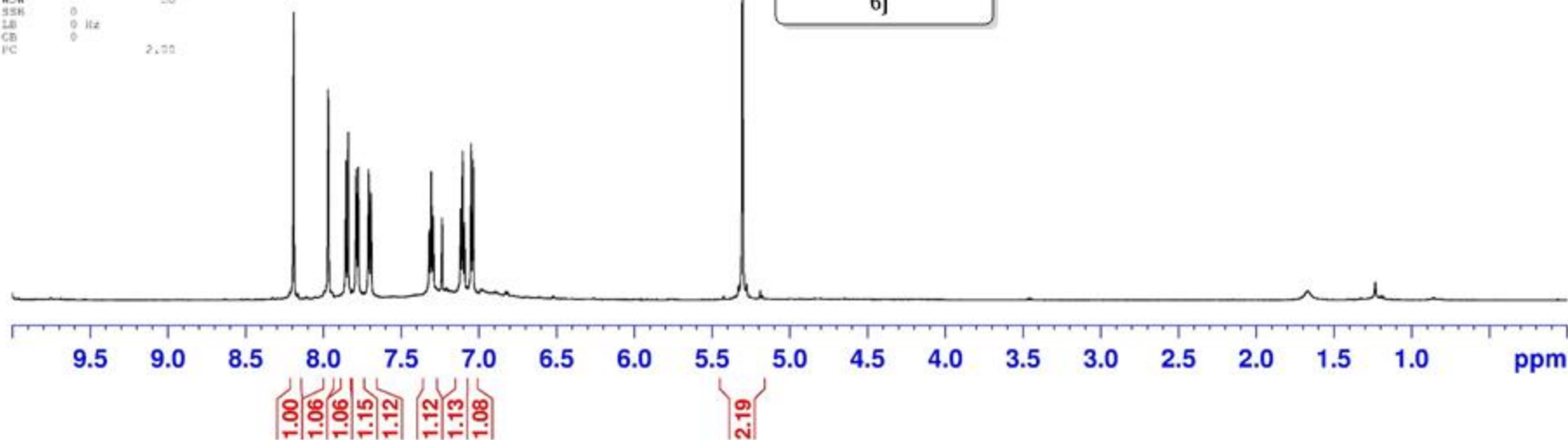
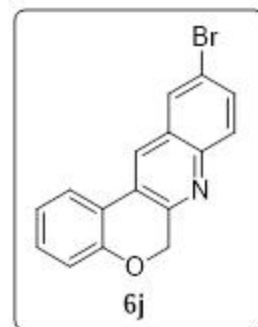
F2 - Acquisition Parameters
Date_ 20181204
Time 7.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 9569.378 Kz
FIDRES 0.292534 Hz
AQ 1.7121780 sec
RG 512
DM 52.250 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
MCHKST 0 sec
MCWPR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
RF01 598.2035892 MHz

F2 - Processing parameters
SI 32768
SF 598.200280 MHz
WDW 20
SSB 0
LB 0 Hz
GB 0
PC 2.00

8.190
7.968
7.965
7.854
7.839
7.788
7.775
7.708
7.705
7.693
7.690
7.321
7.307
7.295
7.238
7.119
7.106
7.093
7.051
7.038

5.304





Current Data Parameters
NAME MDP-2-120
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191204
Time 7.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 324
DS 0
SWH 100.625000

FIDRES 1.374466
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 296.8
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
PCREST 0 sec
PCWCK 0.01500000

----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL13 5.50
SFO2 598.2629910

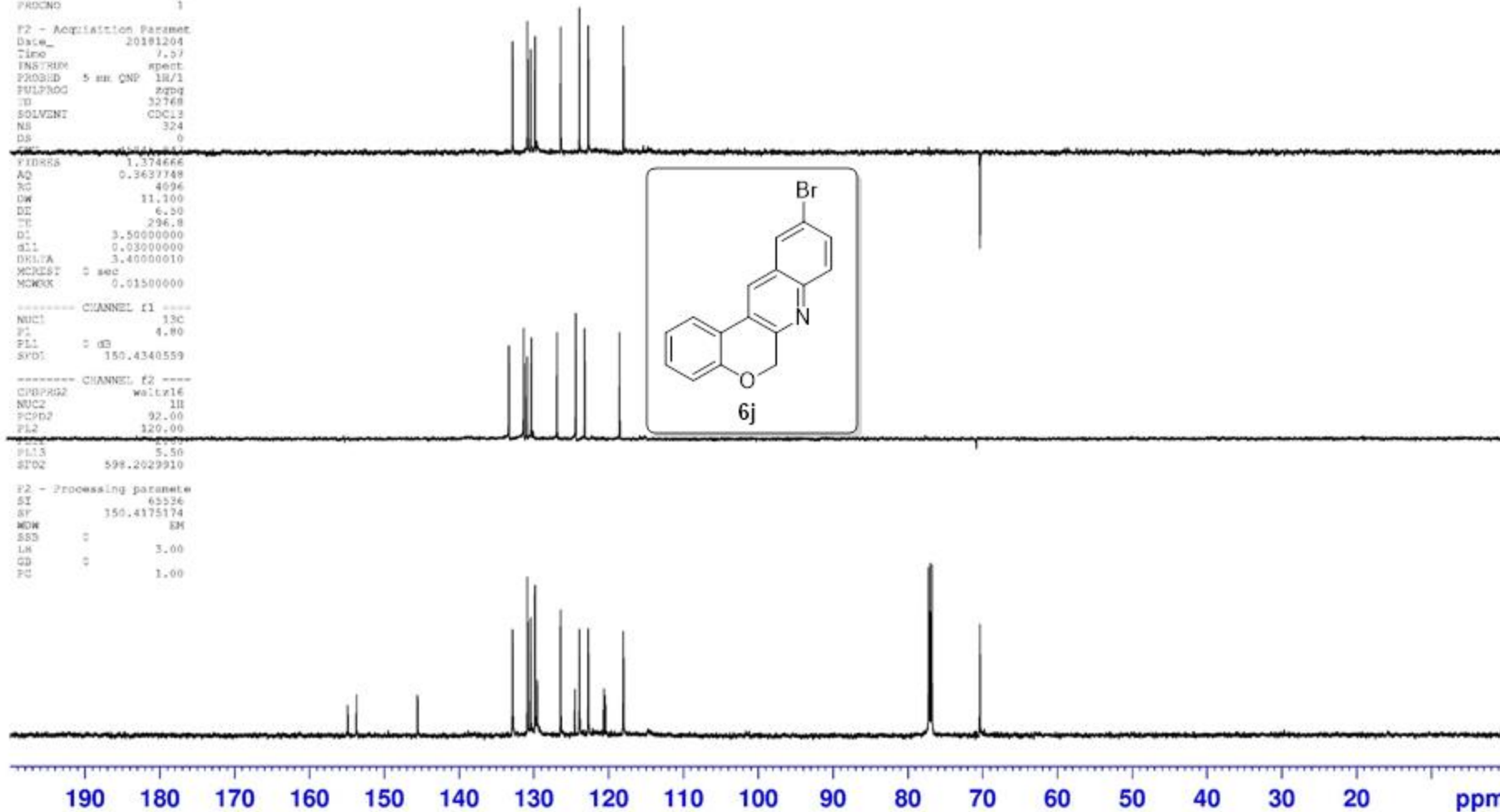
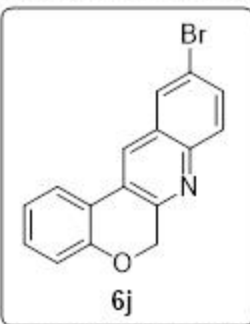
F2 - Processing parameters
SI 65526
SF 350.4175174
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

154.889
153.709

145.548

132.842
130.860
130.439
129.867
129.550
126.417
124.512
123.911
122.725
120.636
120.457
118.045

77.210
76.998
76.786
70.370



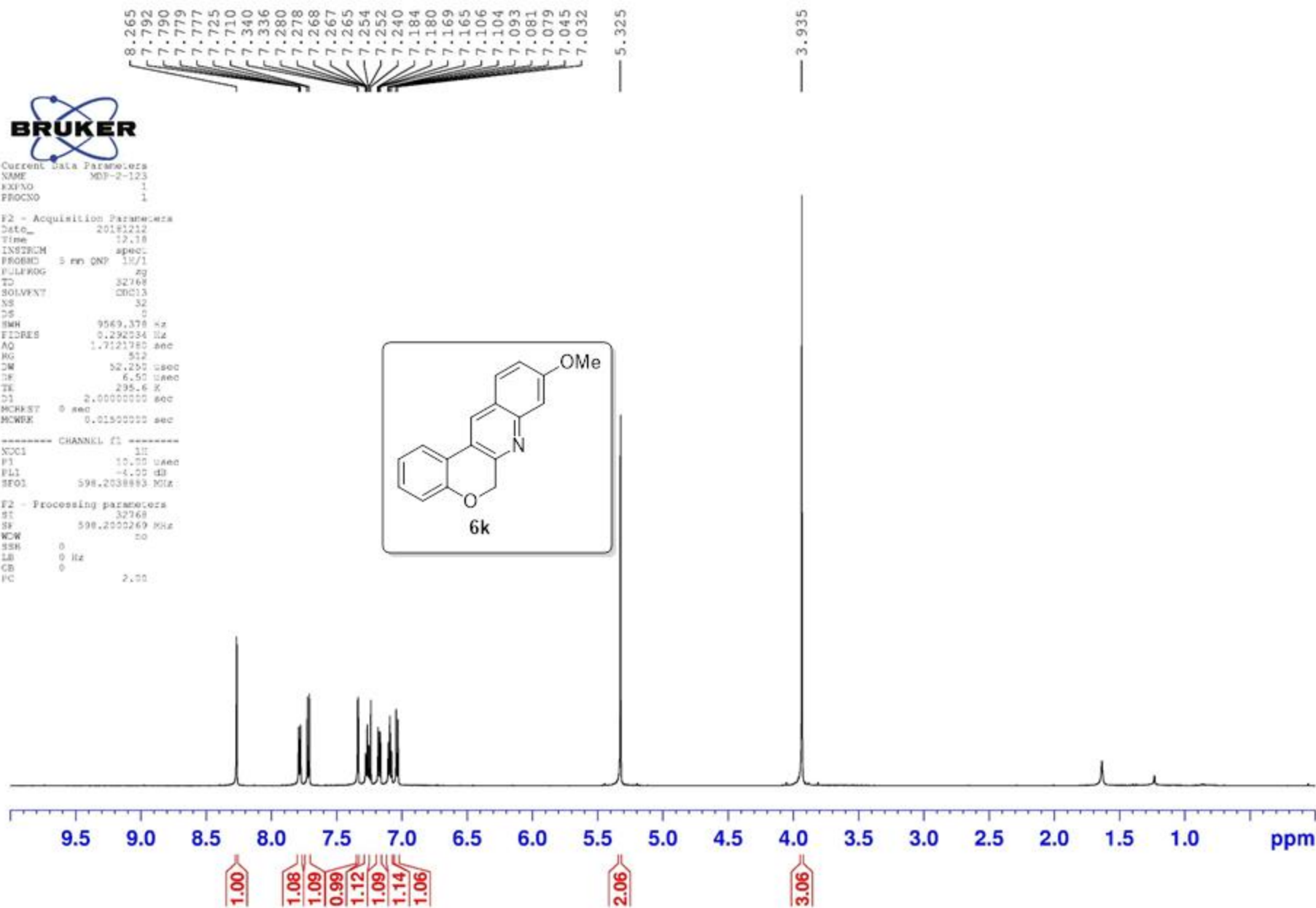
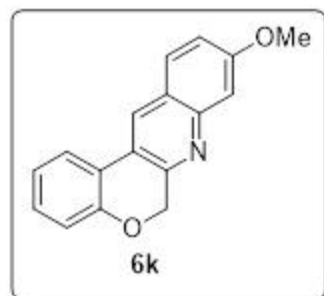


Current Data Parameters
NAME MDP-2-123
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181212
Time 12.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 9569.378 Kz
FIDRES 0.292534 Hz
AQ 1.7121785 sec
RG 512
DM 52.250 used
DE 6.50 used
TE 295.6 K
D1 2.00000000 sec
WCHKST 0 sec
MCWPR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 used
PL1 -4.00 dB
SFO1 500.2000000 MHz

F2 - Processing parameters
SI 32768
SF 500.2000000 MHz
WDW 20
SSB 0
LB 0 Hz
GB 0
PC 2.00





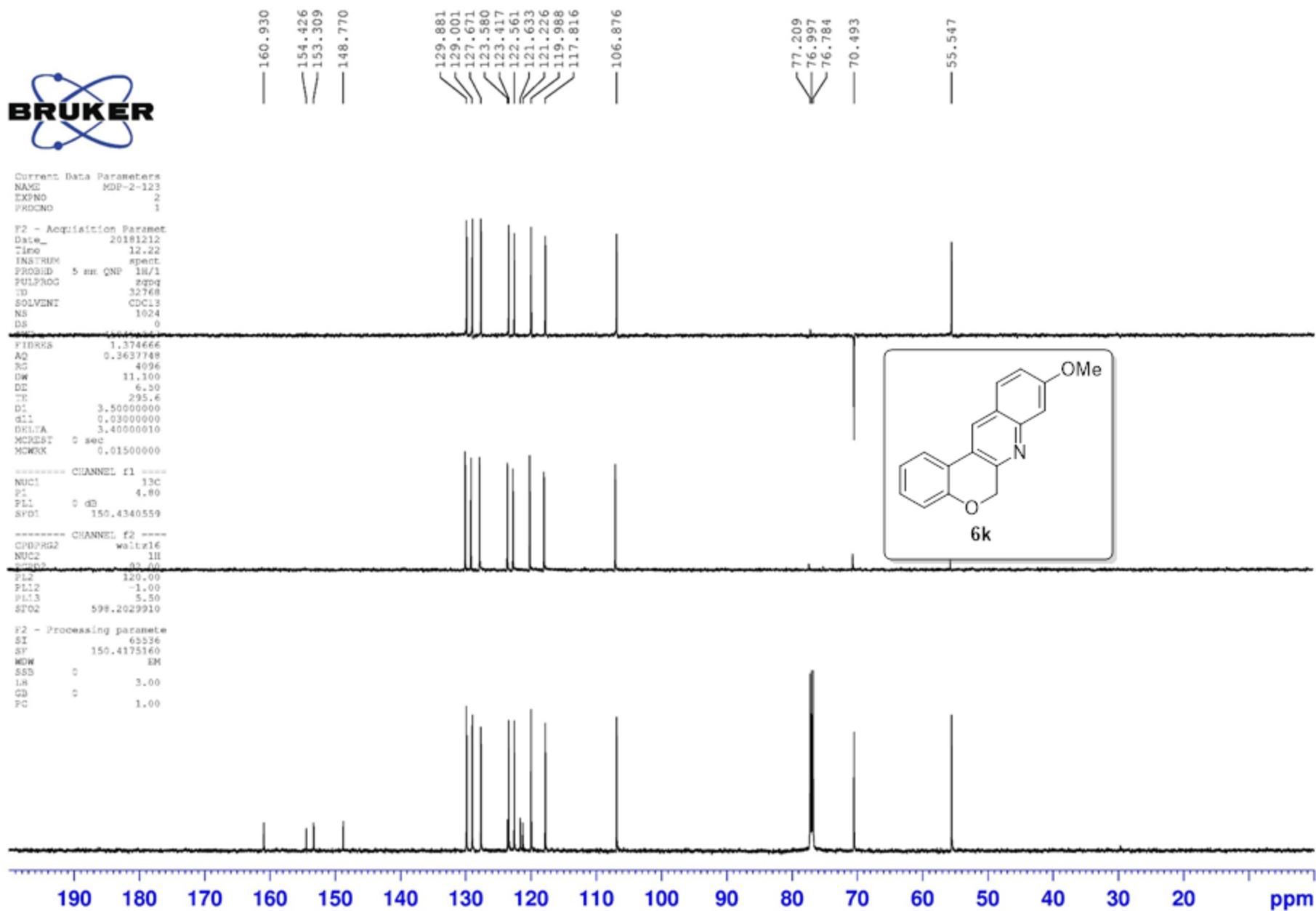
Current Data Parameters
NAME MDP-2-123
EXPNO 2
PROCNO 1

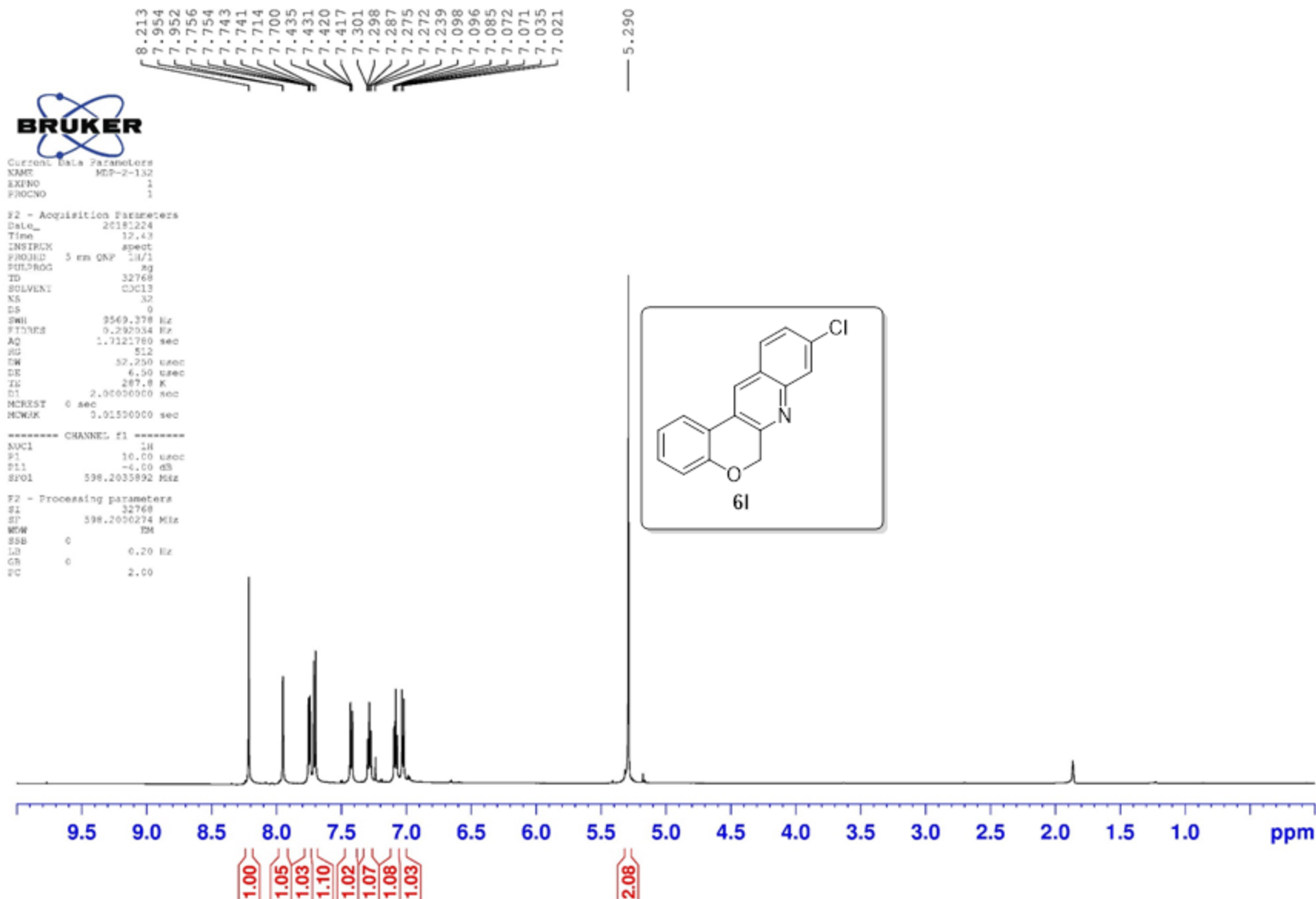
F2 - Acquisition Parameters
Date_ 20181212
Time 12.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 0

===== CHANNEL f1 =====
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 12.00
PL2 -1.00
PL3 5.50
SFO2 598.2629210

F2 - Processing parameters
SI 65536
SF 150.4175160
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00







Current Data Parameters
NAME MOP-2-132
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181224
Time 12.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 130
DS 0

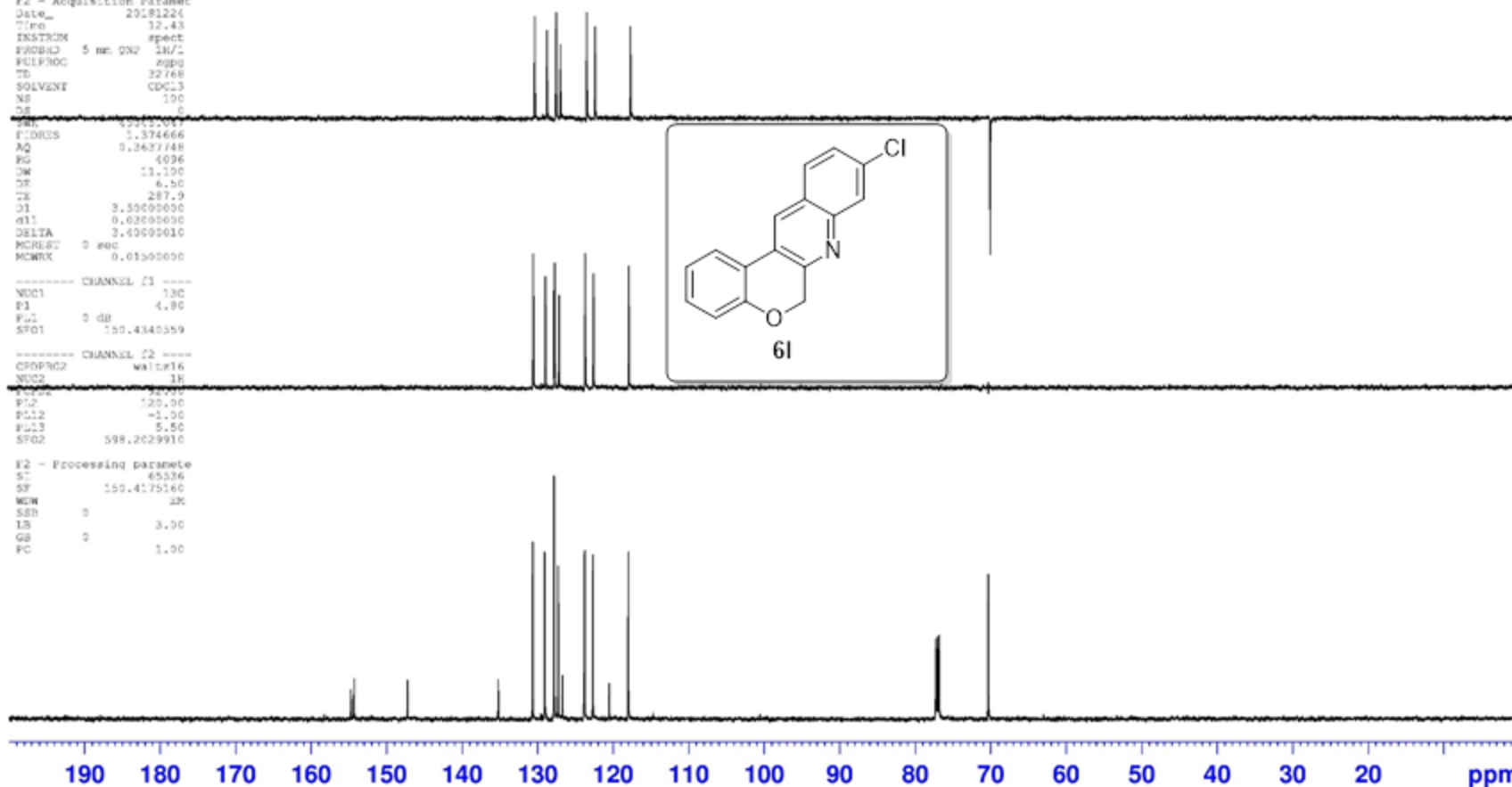
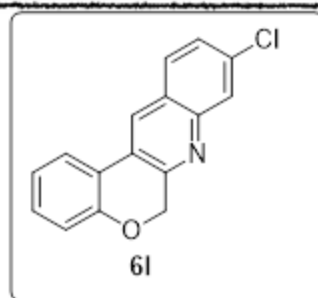
===== CHANNEL f1 =====
NUC1 13C
P1 120.00
PL1 0 dB
SFO1 125.7603559
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 -1.00
PL12 5.50
SFO2 500.1364910

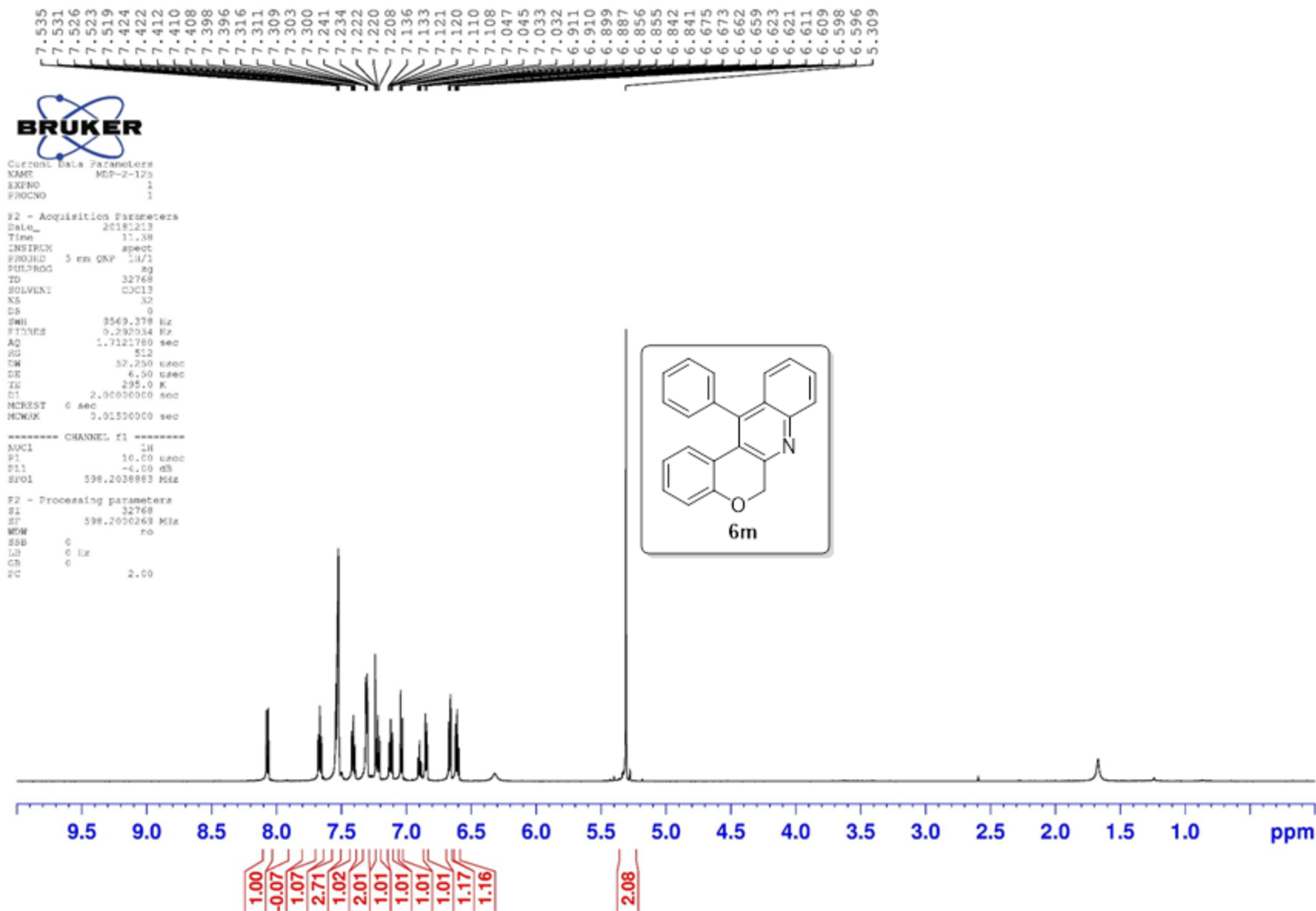
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 -1.00
PL12 5.50
SFO2 500.1364910

F2 - Processing parameters
SI 65536
SF 150.4175160
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

154.723
154.303
147.239
135.223
130.670
129.061
127.824
127.300
126.720
123.864
123.781
122.699
120.539
118.001

77.254
77.041
76.829
70.336







Current Data Parameters
NAME MDP-2-123
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181213
Time 11.52
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 211
DS 0
SWH 45045.000
FIDRES 1.574666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.30
TE 295.0
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MPCST 0 sec
MCWK 0.01500000

----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SFO1 150.4340559

----- CHANNEL f2 -----
CPDPRG2 waltz16
SFO2 92.00
PL2 120.00
PL12 -1.00
PL13 5.50
SFO2 598.2029910

F2 - Processing parameters
SI 65536
SF 150.4175167
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00

156.587
155.202

146.246
143.272

137.161
129.628

129.481
129.229

128.886
128.598

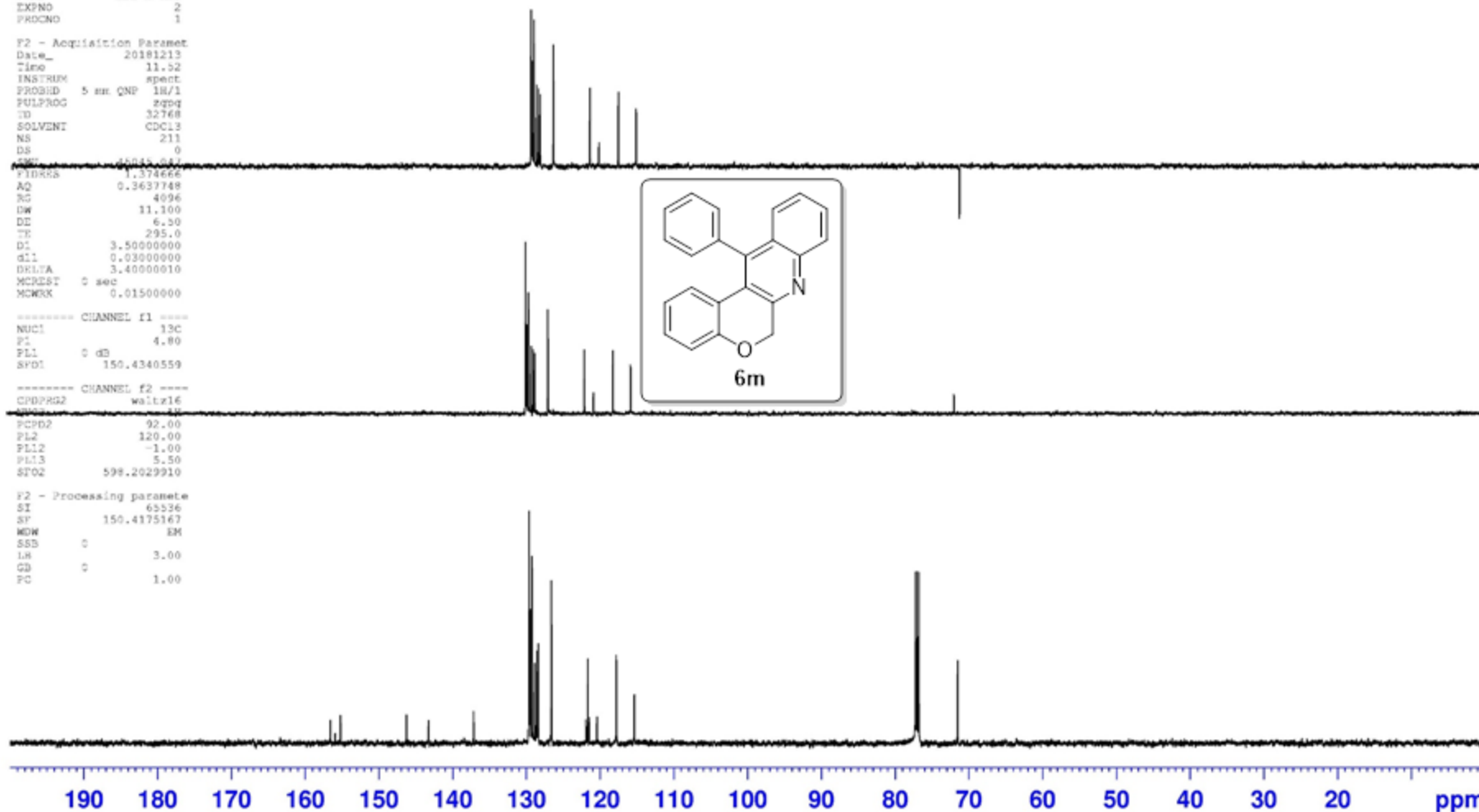
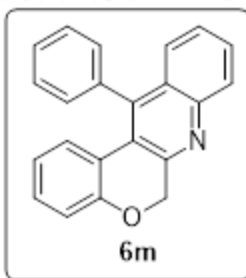
128.395
126.606

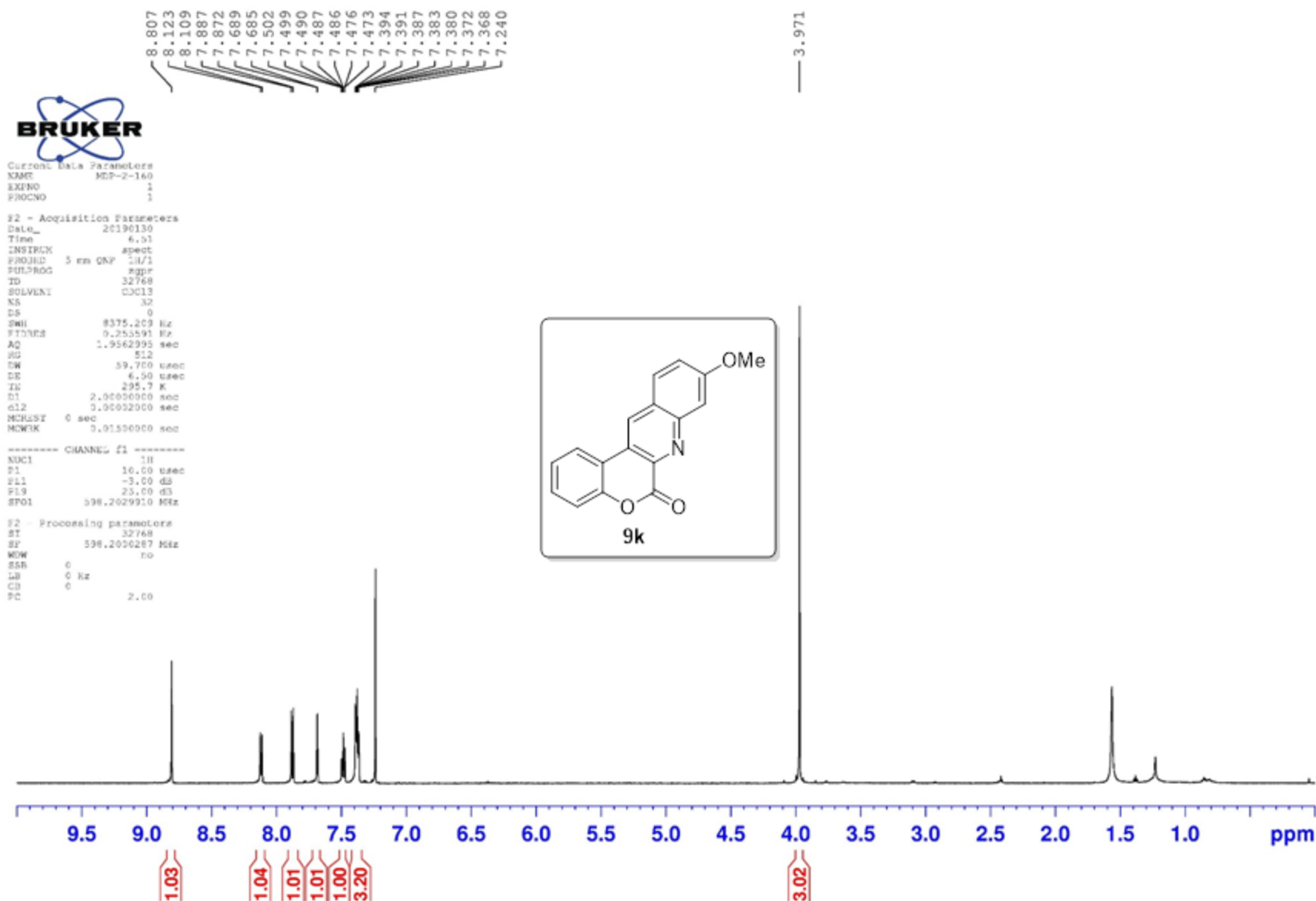
121.910
121.668

121.460
120.433

117.804
115.378

77.213
77.001
76.788
71.528







Current Data Parameters
NAME MDP-2-160
EXPNO 2
PROCNO 1

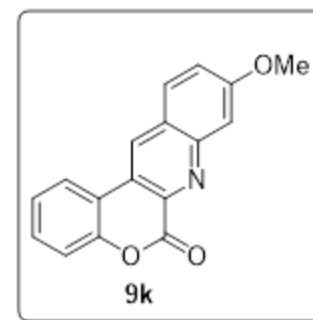
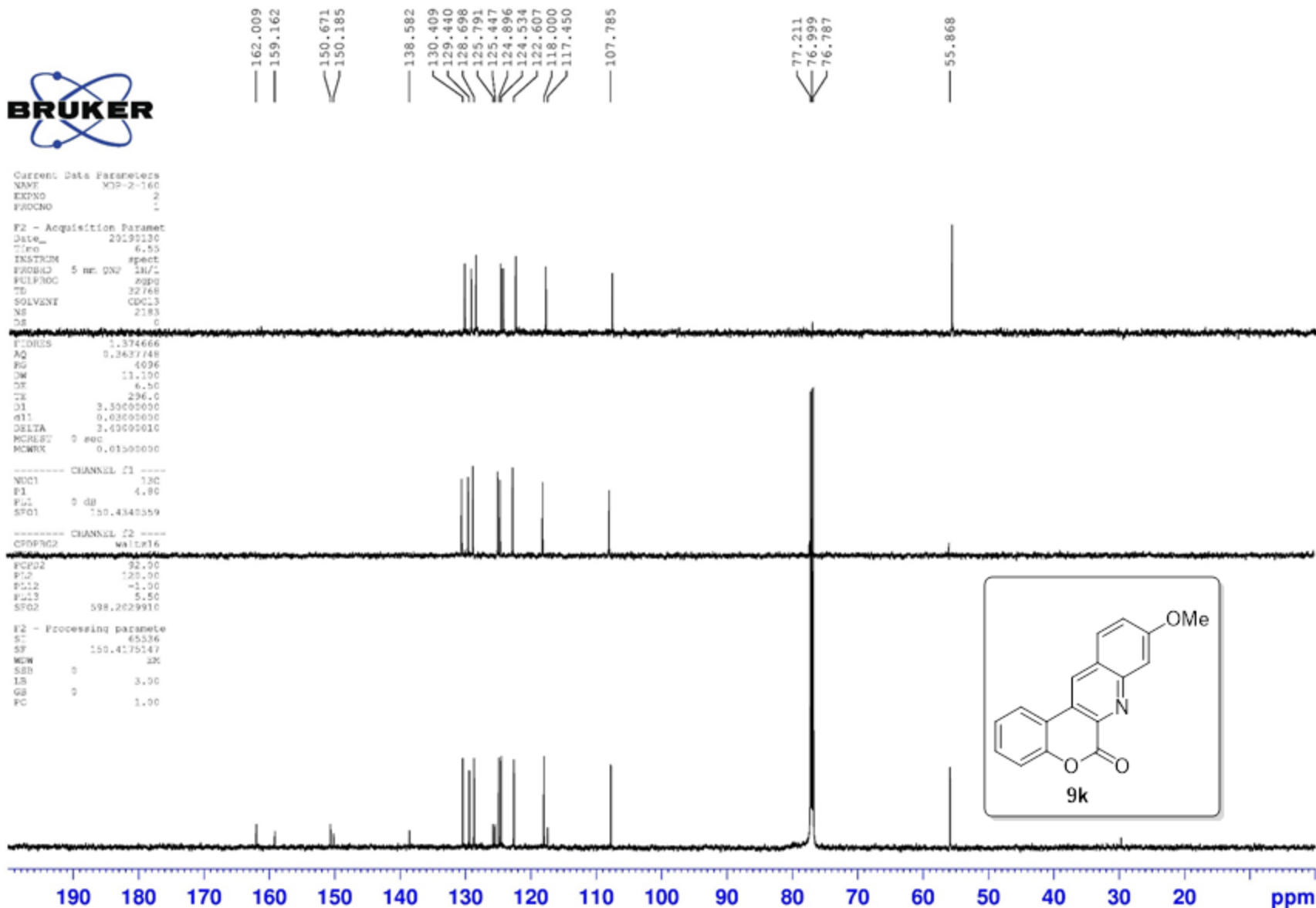
F2 - Acquisition Parameters
Date_ 20190130
Time 6.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2183
DS 0

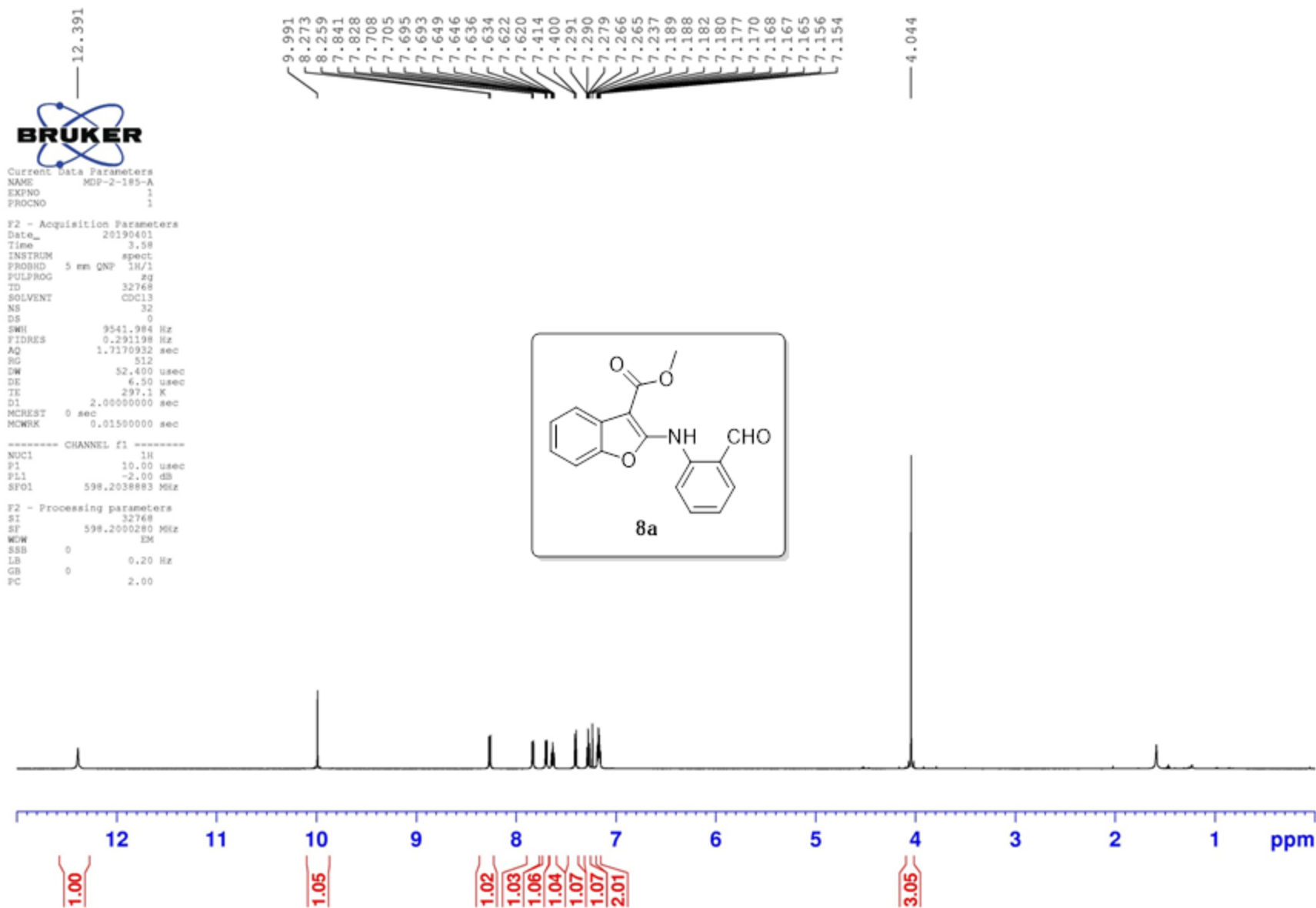
FIDRES 1.374666
AQ 0.3637748
RG 4096
DM 11.100
DE 6.50
TE 296.0
D1 3.3000000
d11 0.0300000
DELTA 2.4000010
MCREST 0 sec
MCMRK 0.0130000

----- CHANNEL f1 -----
NUC1 13C
P1 4.00
PL1 0 dB
SF01 100.6261259

----- CHANNEL f2 -----
CPDPRG2 waltz16
PCPD2 92.00
PL2 120.00
PL12 -1.00
PL13 5.50
SF02 508.2029910

F2 - Processing parameters
SI 65536
SF 150.4175147
WDW 200
SSB 0
LB 3.00
GB 0
PC 1.00







Current Data Parameters
NAME MDP-2-185-A
EXPNO 2
PROCNO 1

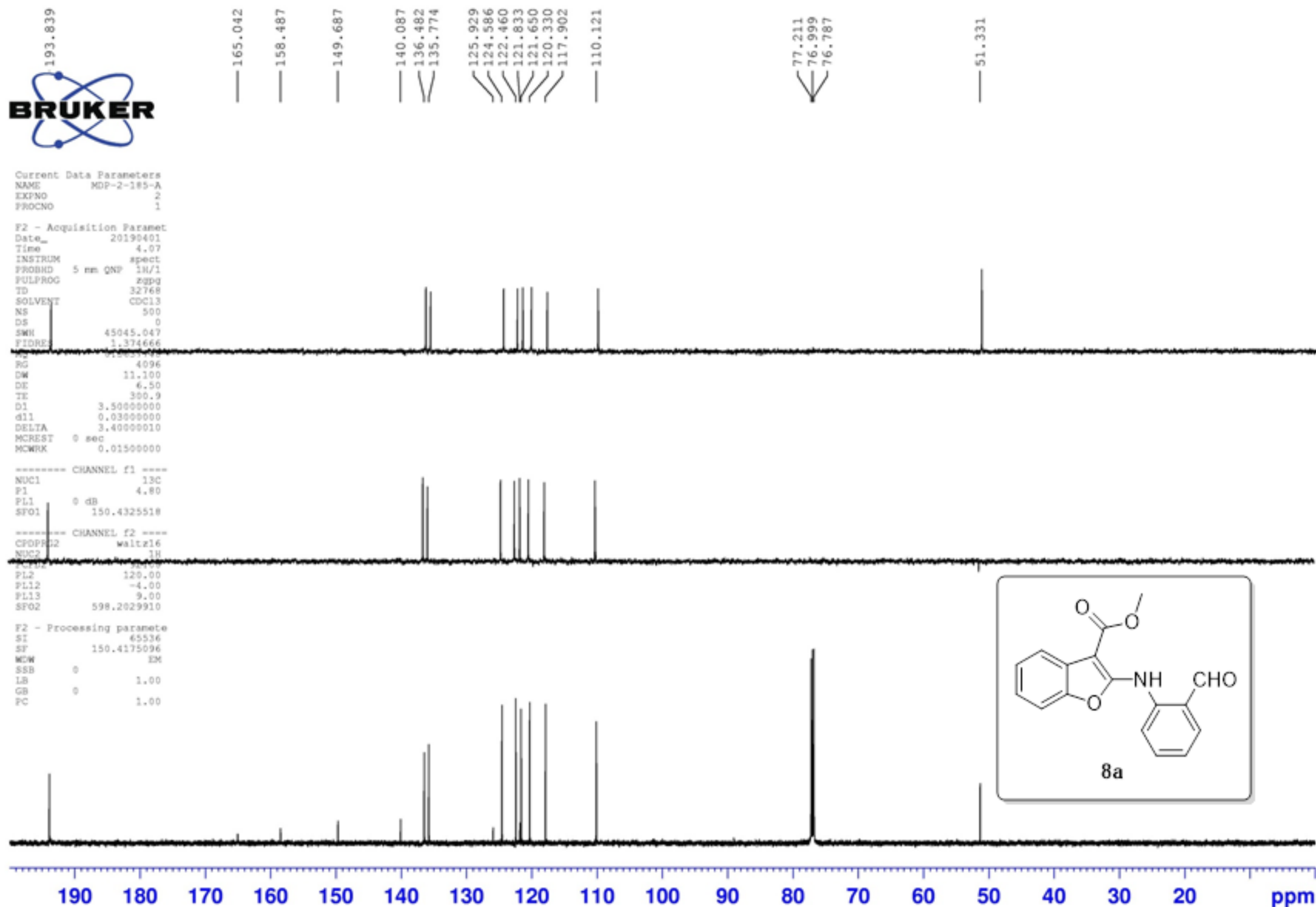
F2 - Acquisition Parameters
Date_ 20190401
Time 4.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 45045.047
FIDRES 1.374666

RG 4096
DM 11.100
DE 6.50
TE 300.9
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRR 0.01500000

===== CHANNEL f1 =====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4325518

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 120.00
PL2 -4.00
PL13 9.00
SFO2 598.2029910

F2 - Processing parameters
SI 65536
SF 150.4175096
WDW EM
SSB 0
LB 1.00
GB 0
PC 1.00





MDP-2-184

Current Data Parameters
NAME 20190402
EXPNO 2
PROCNO 1

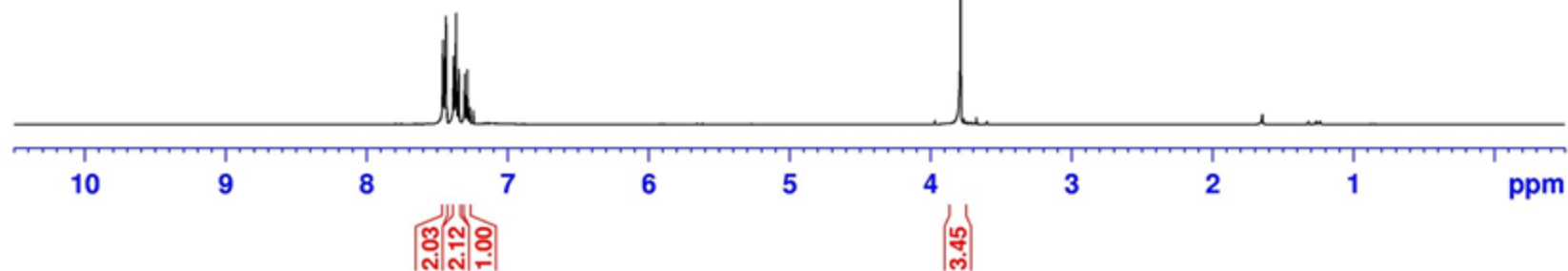
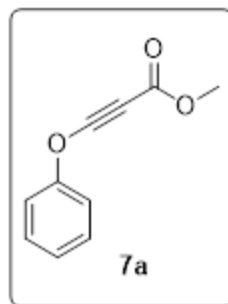
F2 - Acquisition Parameters
Date_ 20190402
Time 16.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

7.4575
7.4539
7.4389
7.4358
7.4335
7.3829
7.3813
7.3764
7.3630
7.3592
7.3472
7.3437
7.3049
7.3019
7.2986
7.2887
7.2836
7.2652
7.2404

3.7862





MDP-02-184

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Current Data Parameters
NAME      20190402
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20190402
Time      12.08
INSTRUM   spect
PROBHD    5 mm QNP 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         694
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4418420 sec
RG         57
RW         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
  
```

153.296

129.717
129.357
127.957
127.438

91.368

80.409
77.407
77.089
76.771

52.672

