Supporting Information

Gold-catalyzed Bicyclic Annulations of 4-Methoxy-1,2-dienyl-5-ynes with Isoxazoles to Form Indolizine Derivatives *via* Au-π-Allene Intermediate

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Contents:

(1) Representative Synthetic Procedures:

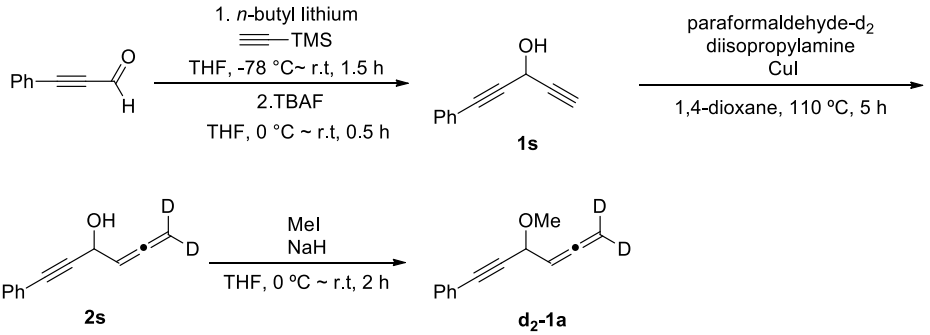
(a) General procedure:

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under Nitrogen atmosphere. DCE, DCM and Ether were distilled from CaH_2 under nitrogen. THF were distilled from Na metal under nitrogen. All other commercial reagents were used without further purification, unless otherwise indicated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz, Varian 400 MHz and 600 MHz spectrometers using chloroform-*d* ($CDCl_3$) and *d*-Acetone as the internal standards.

(b) Preparation of 4-Methoxy-1,2-dienyl-5-ynes.

All 4-Methoxy-1,2-dienyl-5-ynes **1a, 1b, 1c, 1d, 1e, 1f, 1g, 1h, 1k, ^{13}C-1a, 6** and 3-disustituted-4-Methoxy-1,2-dienyl-5-ynes **4e** were prepared from the reported procedure in the literature. [S1]

(c) Preparation of (3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (d_2-1a).

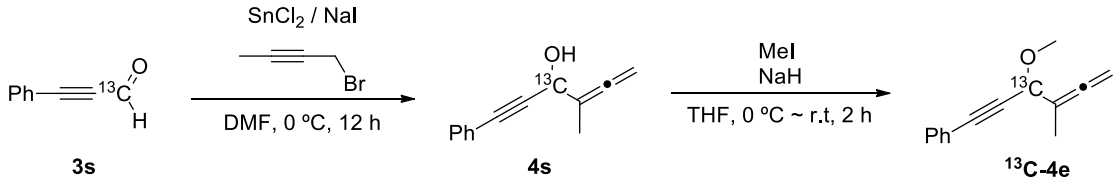


Compound **1s** was prepared from 3-phenylpropiolaldehyde according to a literature procedure. [S2]

To a dried flask was added CuI (0.3 g, 1.6 mmol), paraformaldehyde-d_2 (0.82 g, 25.6 mmol) and 1,4-dioxane (10 mL). The resulting mixture was stirred at room temperature before subsequent addition of iPr_2NH (2.3 g, 22.4 mmol), **1s** (2.5 g, 16 mmol) and 1,4-dioxane (5 mL). The mixture was stirred at 110 °C without protection of an inert atmosphere. After 5 h, the crude reaction mixture was cooled to room temperature, filtered through a celite bed (Et_2O), and concentrated in vacuo. The residue was purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford 1-phenylhexa-4,5-dien-1-yn-3-ol (**2s**) as brown oil (1.9 g, 11.2 mmol, 72%).

The compound **2s** (1.9 g, 11.03 mmol) was added to a stirred solution of NaH (0.318 g, 13.24 mmol) in THF (30 mL) at 0 °C, and the resulting mixture was stirred at 0 °C for 30 min. MeI (3.13 g, 22.1 mmol) was added, and the resulting mixture was stirred at rt for 2 h. The reaction was quenched with water and extracted with Et_2O. The organic layer was washed with water and brine, dried over MgSO4, and concentrated. The residue was purified by silica gel chromatography (SiO2, eluent: EtOAc/hexane) to afford (3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (**d_2-1a**) as brown oil (1.29 g, 6.95 mmol, 63%).

(d) Preparation of (3-methoxy-4-methylhexa-4,5-dien-1-yn-1-yl)benzene (^{13}C-4e).



3s was prepared according to literature procedure[S1] and **4s** was prepared form the corresponding **3s** according to literature procedure. [S3]

The compound **4s** (2 g, 10.8mmol) was added to a stirred solution of NaH (0.310 g, 13.0 mmol) in THF (30 mL) at 0 °C and the resulting mixture was stirred at 0 °C for 30 min. MeI (3.06 g, 21.6 mmol) was added and the resulting mixture was stirred at rt for 2 h. The reaction was quenched with water and extracted with Et_2O. The organic layer was washed with water and brine, dried over MgSO4 and concentrated. The residue was purified by silica gel chromatography (SiO2, eluent: EtOAc/hexane) to afford (3-methoxy-4-methylhexa-4,5-dien-1-yn-1-yl)benzene (**^{13}C-4e**) as yellow oil (1.61 g, 8.12 mmol, 75%).

(e) Preparation of isoxazoles.

3-methyl isoxazole **2c** was prepared according to literature procedure.[S4] and Isoxazoles (**2d-2e**) were prepared according to literature procedure.[S5]

[S1] : H-C. Hsieh, K-C. Tan, A.S.K. Raj and R-S. Liu, *Chem. Commun.*, 2019, **55**, 1979.

[S2] : R. D. Kardile, B. S. Kale, P. Sharma and R.-S. Liu, *Org.Lett.*, 2018, **20**, 3806.

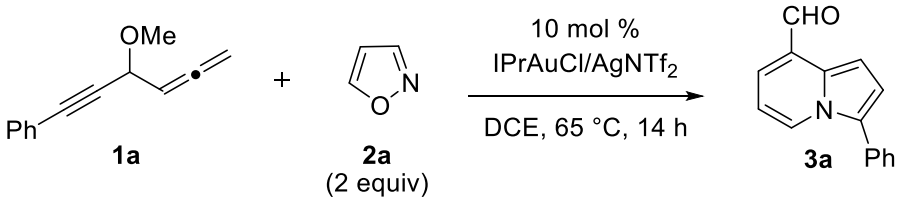
[S3] : D. Xu, Z. Li and S. Ma, *Tetrahedron Asymmetry* 2003, **14**, 3657.

[S4] : A. G. Griesbeck, M. Franke, J. Neudörfl and H. Kotaka, *Beilstein J. Org. Chem.*, 2011, **7**, 127.

[S5] : Y. He, Y.-Y. Xie, Y.-C. Wang, X.-M. Bin, D.-C. Hu, H.-S. Wang and Y.-M. Pan, *RSC. Adv*., 2016, **6**, 58988.

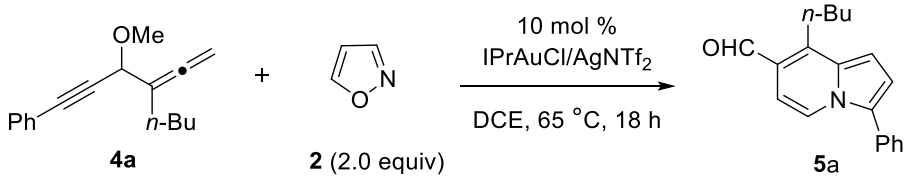
(2) Standard procedures for catalytic operations.

(a) Typical procedure for the synthesis of 3-phenylindolizine-8-carbaldehyde (3a):



A suspension of IPrAuCl (33.7 mg, 0.054 mmol) and $AgNTf_2$ (21 mg, 0.054 mmol) in dry DCE (1 mL) was fitted with N_2 balloon and the mixture was stirred at 25 °C for 5 min. To this solution was added DCE (1 mL) solution of (3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene **1a** (100 mg, 0.54 mmol) and isoxazole **2a** (75 mg, 1.08 mmol) at 25 °C. The resulting mixture was stirred for 14 h at 65 °C. The solution was filtered over a short celite bed and evaporated under reduced pressure. The residue was purified on a silica gel column using ethyl acetate/hexane (10:90) as eluent to give compound **3a** as yellow solid (106 mg, 0.48 mmol, 88%).

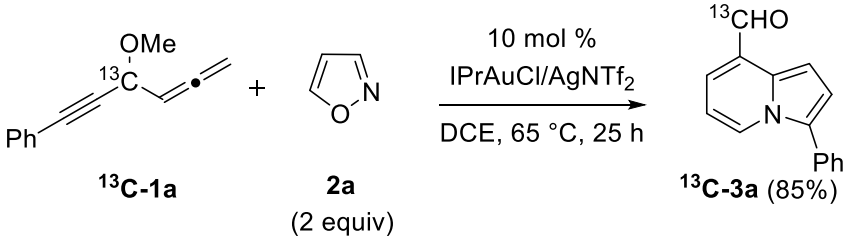
(b) Typical procedure for the synthesis of 8-butyl-3-phenylindolizine-7-carbaldehyde (5a):



A suspension of IPrAuCl (25.8 mg, 0.042 mmol) and $AgNTf_2$ (16.1 mg, 0.042 mmol) in dry DCE (1 mL) was fitted with N_2 balloon and the mixture was stirred at 25 °C for 5 min. To this solution was added DCE (1 mL) solution of (3-methoxy-4-vinylideneoct-1-yn-1-yl)benzene **4a** (100 mg, 0.416 mmol) and isoxazole **2a** (57.4 mg, 0.832 mmol) at 25 °C. The resulting mixture was stirred for 18 h at 65 °C. The solution was filtered over a short celite bed and evaporated under reduced pressure. The residue was purified on a silica gel column using ethyl acetate/hexane (10:90) as eluent to give compound **5a** as yellow oil (87 mg, 0.313 mmol, 75%).

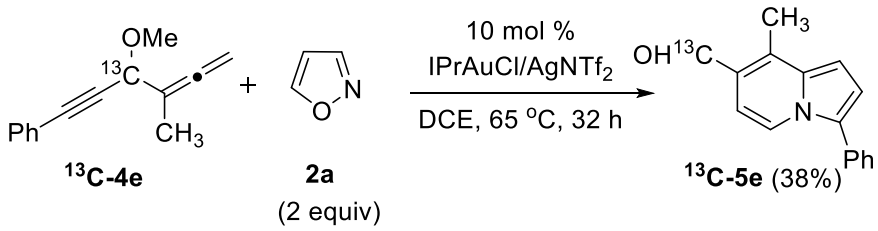
(3) Mechanistic Investigation

(a) Typical procedure for the synthesis of 3-phenylindolizine-8-carbaldehyde (^{13}C-3a):



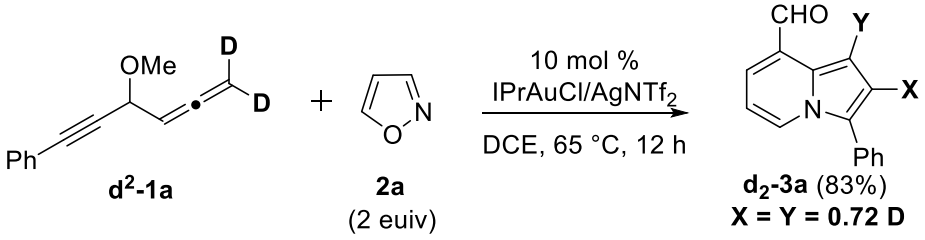
Experimental procedure according to standard procedure for catalytic opreration (**2-a**). Yields are reported after purification from silica column.

(b) Typical procedure for the synthesis of 8-methyl-3-phenylindolizine-7-carbaldehyde (^{13}C-5e):



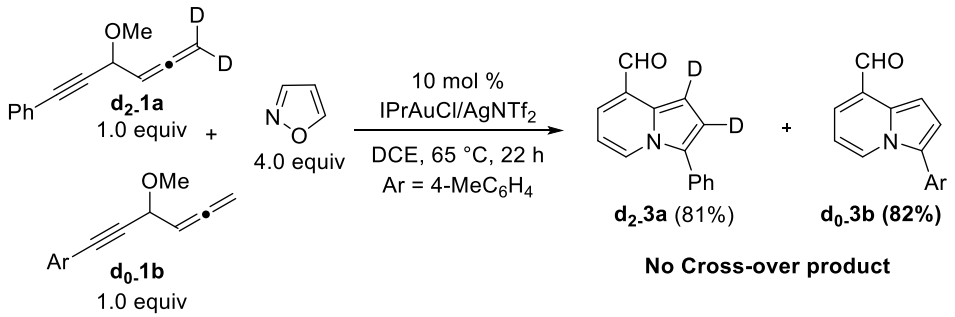
Experimental procedure according to standard procedure for catalytic opreration (**2-a**). Yields are reported after purification from silica column.

(c) Typical procedure for the synthesis of 3-phenylindolizine-8-carbaldehyde (d_2-3a):



Experimental procedure according to standard procedure for catalytic opreration (**2-a**). Yields are reported after purification from silica column.

(d) Cross-Over experiment



Experimental procedure according to standard procedure for catalytic opreration (**2-a**). Yields are reported after purification from silica column.

(4) Computational details:

The B3LYP functional [S6-S8] combined with the LACVP** basis set (LanL2DZ for Au and 6-31G** for the others) was used for the geometry optimizations and zero-point vibrational energy (ZPVE). To obtain more accurate electronic energies, single point energy calculations using a larger basis set (LACV3P++**, LanL2TZ for Au, and 6-311++G** for the others) were performed on the B3LYP/LACVP** optimized structures. All calculations were performed under the influence of implicit solvent, which was simulated using the Poisson-Boltzmann self-consistent polarizable continuum method implemented in Jaguar to represent dichloroethane (dielectric constant = 10.65 and effective radius = 2.51 Å).[S9-S10] Enthalpies were calculated as

$$H_{298K} = E_{elec} + ZPVE + \sum_{v} \frac{hv}{e^{hv/kT} - 1} + 4kT$$

with T = 298K.

[S6] A. D. Becke, *Phys. Rev. A* 1988, **38**, 3098-3100.

[S7] A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.

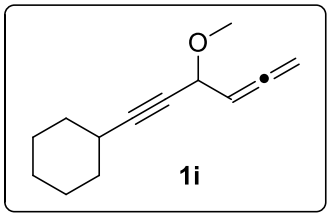
[S8] C. T. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789.

[S9] D. J. Tannor, B. Marten, R. Murphy, R. A. Friesner, D. Sitkoff, A. Nicholls, M. Ringnalda, W. A. Goddard, B. Honig, *J. Am. Chem. Soc*., 1994, **116**, 11875-11882.

[S10] B. Marten, K. Kim, C. Cortis, R. A. Friesner, R. B. Murphy, M. N. Ringnalda, D. Sitkoff, B. Honig, *J. Phys. Chem.*, 1996, **100**, 11775-11788.

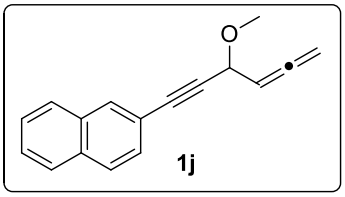
(5) Spectral data for compounds:

(3-methoxyhexa-4,5-dien-1-yn-1-yl)cyclohexane (1i):



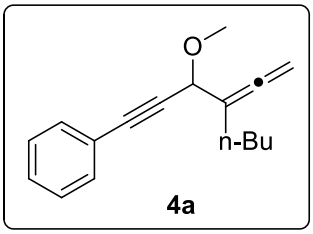
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.26 ~ 5.21 (m, 1H), 4.88 ~ 4.86 (m, 2H), 4.55 ~ 4.53 (m, 1H), 3.34 (s, 3H), 2.42 ~ 2.38 (m, 1H), 1.78 ~ 1.74 (m, 2H), 1.70 ~ 1.66 (m, 2H), 1.50 ~ 1.39 (m, 3H), 1.34 ~ 1.23 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 208.8, 91.6, 90.8, 77.3, 76.8, 69.4, 55.1, 32.5, 28.9, 25.8, 24.7; FI-MS calcd for $C_{13}H_{18}O[M^+]$: 190.1358; found : 190.1352.

2-(3-methoxyhexa-4,5-dien-1-yn-1-yl)naphthalene (1j):



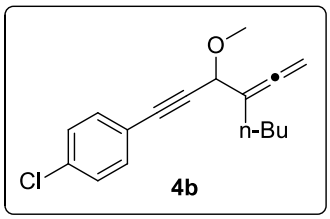
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (s, 1H), 7.80 ~ 7.75 (m, 3H), 7.49 ~ 7.45 (m, 3H), 5.39 (q, *J* = 6.8 Hz, 1H), 4.97 (dd, *J* = 6.8, 2.0 Hz, 2H), 4.85 ~ 4.82 (m, 1H), 3.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 132.9, 132.8, 131.8, 128.4, 127.9, 127.7, 126.7, 126.5, 119.7, 90.4, 87.0, 86.3, 77.7, 69.8, 55.5, one CH carbon merged with other peaks; FI-MS calcd for $C_{17}H_{14}O[M^+]$: 234.1045; found : 234.1039.

(3-methoxy-4-vinylideneoct-1-yn-1-yl)benzene (4a):



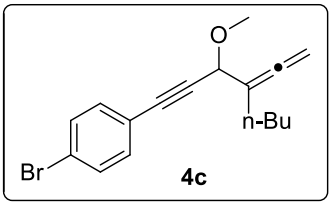
Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.44 ~ 7.43 (m, 2H), 7.29 ~ 7.27 (m, 3H), 4.89 ~ 4.88 (m, 2H), 4.73 (s, 1H), 3.40 (s, 3H), 2.18 ~ 2.09 (m, 2H), 1.50 ~ 1.46 (m, 2H), 1.40 ~ 1.35 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 206.9, 131.8, 128.4, 128.2, 122.6, 102.6, 86.7, 86.1, 77.6, 73.1, 55.5, 29.7, 27.0, 22.4, 13.9; FI-MS calcd for $C_{17}H_{20}O[M^+]$: 240.1514; found : 240.1509.

1-chloro-4-(3-methoxy-4-vinylideneoct-1-yn-1-yl)benzene (4b):



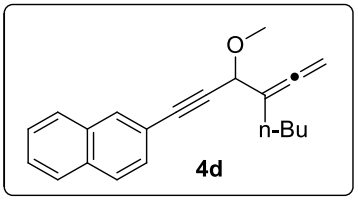
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 ~ 7.34 (m, 2H), 7.27 ~ 7.25 (m, 2H), 4.89 ~ 4.87 (m, 2H), 4.71 (t, *J* = 1.6 Hz, 1H), 3.39 (s, 3H), 2.19 ~ 2.04 (m, 2H), 1.50 ~ 1.43 (m, 2H), 1.40 ~ 1.30 (m, 2H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.8, 134.5, 132.9, 128.6, 121.1, 102.4, 87.1, 85.5, 77.7, 73.0, 55.6, 29.7, 26.9, 22.4, 13.9; FI-MS calcd for $C_{17}H_{19}ClO[M^+]$: 274.1124; found : 274.1119.

1-bromo-4-(3-methoxy-4-vinylideneoct-1-yn-1-yl)benzene (4c):



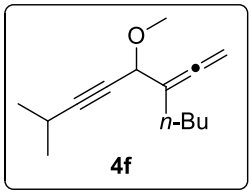
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 ~ 7.40 (m, 2H), 7.30 ~ 7.28 (m, 2H), 4.89 ~ 4.87 (m, 2H), 4.70 (s, 1H), 3.38 (s, 3H), 2.18 ~ 2.03 (m, 2H), 1.63 ~ 1.43 (m, 2H), 1.33 ~ 1.26 (m, 2H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.9, 133.2, 131.5, 131.2, 122.7, 121.6, 102.4, 87.3, 85.6, 77.7, 73.0, 55.6, 29.7, 27.0, 22.4, 13.9; FI-MS calcd for $C_{17}H_{19}BrO[M^+]$: 318.0619; found : 318.0614.

2-(3-methoxy-4-vinylideneoct-1-yn-1-yl)naphthalene (4d):



Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (s, 1H), 7.81 ~ 7.75 (m, 3H),7.49 ~ 7.46 (m, 3H), 4.93 ~ 4.91 (m, 2H), 4.79 (t, *J* = 1.6 Hz, 1H), 3.44 (s, 3H), 2.26 ~ 2.09 (m, 2H), 1.55 ~ 1.47 (m, 2H), 1.44 ~ 1.35 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.9, 132.9, 131.7, 128.5, 127.9, 127.7, 126.7, 126.5, 119.9, 102.6, 86.9, 86.4, 77.7, 73.2, 55.6, 29.7, 27.0, 22.4, 13.9, One quaternary carbon and one CH carbon merged with other peaks; FI-MS calcd for $C_{21}H_{22}O[M^+]$: 290.1671; found : 290.1665.

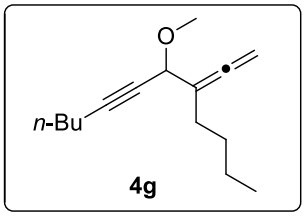
5-methoxy-2-methyl-6-vinylidenedec-3-yne (4f):



4f

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.83 ~ 4.80 (m, 2H), 4.47 (q, *J* = 1.6 Hz, 1H), 3.29 (s, 3H), 2.62 ~ 2.55 (m, 1H), 2.14 ~ 1.94 (m, 2H), 1.47 ~1.43 (m, 2H), 1.42 ~ 1.40 (m, 2H), 1.40 (d, *J* = 7.2 Hz, 6H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.7, 102.8, 92.9, 77.3, 76.0, 72.8, 55.3, 29.7, 26.7, 22.9, 22.4, 20.6, 13.9; FI-MS calcd for $C_{14}H_{22}O[M^+]$: 206.1671; found : 206.1665.

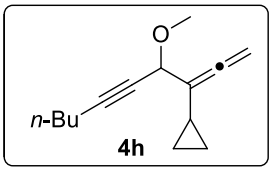
7-methoxy-8-vinylidenedodec-5-yne (4g):



4g

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.83 ~ 4.80 (m, 2H), 4.47 (t, *J* = 1.6 Hz, 1H), 3.30 (s, 3H), 2.24 ~ 2.20 (m, 2H), 2.13 ~ 1.95 (m, 2H), 1.52 ~ 1.28 (m, 8H), 0.90 ~ 0.86 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.6, 102.8, 87.4, 77.3, 72.9, 55.3, 30.6, 29.6, 26.7, 22.4, 21.8, 18.4, 13.9, 13.5, One quaternary carbon merged with other peaks; FI-MS calcd for $C_{15}H_{24}O[M^+]$: 220.1827; found : 220.1822.

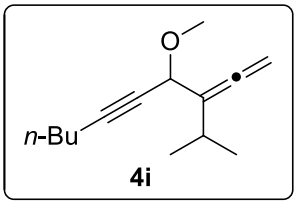
(4-methoxydeca-1,2-dien-5-yn-3-yl)cyclopropane (4h):



4h

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.85 (t, *J* = 1.8 Hz, 2H), 4.58 ~ 4.56 (m, 1H), 3.34 (s, 3H), 2.25 ~ 2.21 (m, 2H), 1.49 ~ 1.44 (m, 2H), 1.43 ~ 1.37 (m, 2H), 1.33 ~ 1.29 (m, 1H), 0.89 (t, *J* = 7.2 Hz, 3H), 0.72 ~ 0.67 (m, 2H), 0.47 ~ 0.38 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 205.1, 106.4, 87.5, 78.6, 76.9, 72.6, 55.3, 30.6, 21.8, 18.4, 13.5, 8.1, 6.8, 6.7; FI-MS calcd for $C_{14}H_{20}O[M^+]$: 204.1514; found : 204.1509.

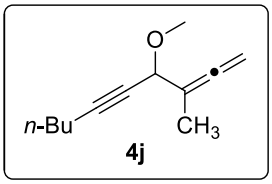
3-isopropyl-4-methoxydeca-1,2-dien-5-yne (4i):



4i

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.86 (t, *J* = 1.6 Hz, 2H), 4.54 ~ 4.52 (m, 1H), 3.31 (s, 3H), 2.39 ~ 2.31 (m, 1H), 2.23 ~ 2.19 (m, 2H), 1.49 ~ 1.43 (m, 2H), 1.42 ~ 1.36 (m, 2H), 1.05 (t, *J* = 6.8 Hz, 6H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.0, 109.2, 87.5, 78.5, 71.9, 55.2, 30.7, 27.0, 22.4, 22.3, 21.9, 18.4, 13.5, One quaternary carbon merged with other peaks; FI-MS calcd for $C_{14}H_{22}O[M^+]$: 206.1671; found : 206.1665.

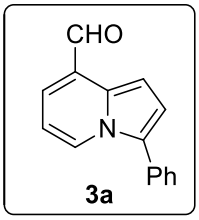
4-methoxy-3-methyldeca-1,2-dien-5-yne (4j):



4j

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.71 (t, *J* = 2.0 Hz, 2H), 4.42 (d, *J* = 0.8 Hz, 1H), 3.28 (s, 3H), 2.22 ~ 2.18 (m, 2H), 1.70 (t, *J* = 3.2 Hz, 3H), 1.49 ~ 1.44 (m, 2H), 1.42 ~ 1.34 (m, 2H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.9, 97.5, 87.3, 76.7, 75.5, 73.1, 55.3, 30.6, 21.8, 18.3, 13.6, 13.5, One quaternary carbon merged with other peaks; FI-MS calcd for $C_{12}H_{18}O[M+]$: 178.1358; found : 178.1352.

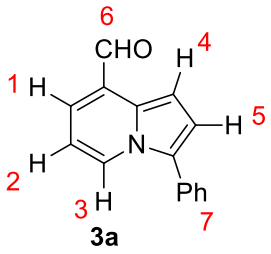
3-phenylindolizine-8-carbaldehyde (3a):



3a

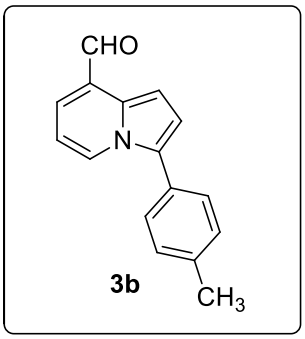
Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.03 (s, 1H), 8.44 (d, *J* = 7.2 Hz, 1H), 7.53 ~ 7.51 (m, 2H), 7.49 ~ 7.47 (m, 2H), 7.41 (dd, *J* = 4.2, 1.2 Hz, 1H), 7.39 ~ 7.36 (m, 1H), 7.31 (dd, *J* = 6.6, 0.6 Hz, 1H), 6.99 (d, *J* = 4.2 Hz, 1H), 6.64 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.4, 131.7, 129.5, 129.1, 128.6, 128.4, 128.1, 127.8, 127.7, 126.6, 116.5, 109.2, 102.2; HRMS calcd for $C_{15}H_{11}NO$: 221.0841; found : 221.0845.

^{1}H-NOE map of compound (3a).



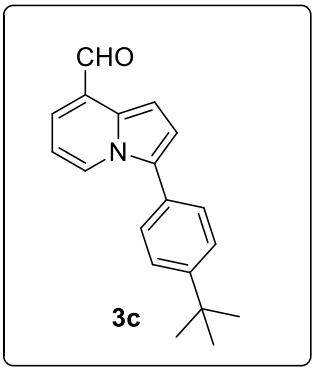
Irradiation	Enhancement (%)
H^2 (δ 6.64)	H^1 (δ 7.31, 6.66%), H^3 (δ 8.44, 8.27%)
H^1 (δ 7.31)	H^2 (δ 6.64, 7.51%), H^6 (δ 10.03, 11.68%)
H^4 (δ 7.41)	H^5 (δ 6.99, 2.52%), H^6 (δ 10.03, 1.08%)
H^7 (δ 7.49 ~ 7.47)	H^3 (δ 8.44, 1.66%), H^5 (δ 6.99, 0.56%)
H^6 (δ 10.03)	H^1 (δ 7.31, 10.61%)

3-(*p*-tolyl)indolizine-8-carbaldehyde (3b):



Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.02 (s, 1H), 8.41 (d, *J* = 7.1 Hz, 1H), 7.41 ~ 7.38 (m, 3H), 7.30 ~ 7.28 (m, 3H), 6.96 (d, *J* = 3.9 Hz, 1H), 6.62 (t, *J* = 6.9 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.5, 137.7, 129.8, 129.4, 128.8, 128.5, 128.2, 127.6, 126.6, 116.2, 109.1, 102.1, 21.3, One quaternary carbon merged with other peaks; HRMS calcd for $C_{16}H_{13}NO$: 235.0997; found : 235.0992.

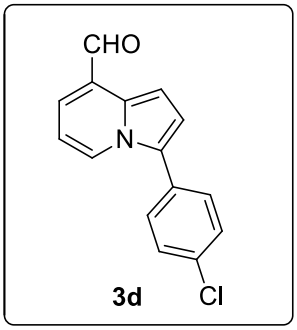
3-(4-(*tert*-butyl)phenyl)indolizine-8-carbaldehyde (3c):



Brown solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.02 (s, 1H), 8.45 (d, *J* = 6.8 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 4.0 Hz, 1H), 7.29 (d, *J* = 6.8 Hz, 1H), 6.98 (d,

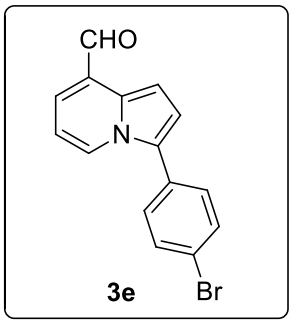
J = 3.6 Hz, 1H), 6.62 (t, *J* = 6.8 Hz, 1H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 150.9, 129.3, 128.7, 128.3, 127.6, 126.6, 125.9, 116.2, 109.0, 102.1, 34.7, 31.3, One quaternary carbon and CH carbon merged with other peaks; HRMS calcd for $C_{19}H_{19}NO$: 277.1467; found : 277.01472.

3-(4-chlorophenyl)indolizine-8-carbaldehyde (3d):



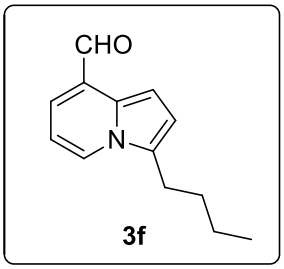
Brown solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.03 (s, 1H), 8.37 (d, *J* = 7.2 Hz, 1H), 7.45 (s, 4H), 7.40 (d, *J* = 4.2 Hz, 1H), 7.33 (d, *J* = 6.6 Hz, 1H), 6.97 (d, *J* = 3.6 Hz, 1H), 6.67 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.4, 133.6, 130.2, 129.7, 129.5, 129.3, 128.7, 127.9, 127.7, 125.3, 116.7, 109.5, 102.4; HRMS calcd for $C_{15}H_{10}ClNO$: 255.0451; found : 255.0453.

3-(4-bromophenyl)indolizine-8-carbaldehyde (3e):



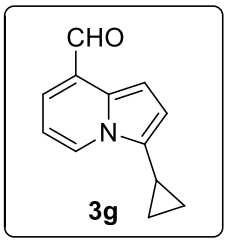
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.02 (s, 1H), 8.44 (d, *J* = 7.2 Hz, 1H), 7.54 ~ 7.46 (m, 3H), 7.41 ~ 7.35 (m, 2H), 7.31 (d, *J* = 6.8 Hz, 1H), 6.99 (d, *J* = 4.0 Hz, 1H), 6.64 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 131.7, 129.5, 129.1, 128.5, 128.4, 128.1, 127.8, 127.7, 126.6, 116.4, 109.2, 102.2; HRMS calcd for $C_{15}H_{10}BrNO$: 298.9946; found : 298.9949.

3-butylindolizine-8-carbaldehyde (3f):



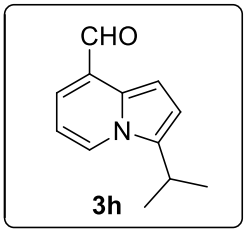
Brown oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.99 (s, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.25 ~ 7.24 (m, 2H), 6.72 (d, *J* = 4.2 Hz, 1H), 6.66 (t, *J* = 6.6 Hz, 1H), 2.83 (t, *J* = 7.8 Hz, 2H), 1.76 ~ 1.71 (m, 2H), 1.47 ~ 1.41 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.6, 128.2, 127.4, 127.1, 125.7, 114.1, 108.4, 100.7, 29.5, 25.5, 22.6, 13.9, One quaternary carbon merged with other peaks; HRMS calcd for $C_{13}H_{15}NO$: 201.1154; found : 201.1152.

3-cyclopropylindolizine-8-carbaldehyde (3g):



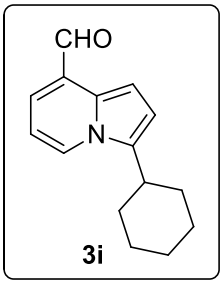
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.99 (s, 1H), 8.32 (d, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 6.8 Hz, 1H), 7.19 (d, *J* = 4.0 Hz, 1H), 6.70 (t, *J* = 6.8 Hz, 1H), 6.66 (d, *J* = 3.6 Hz, 1H), 1.90 ~ 1.84 (m, 1H), 1.03 ~ 0.98 (m, 2H), 0.71 ~ 0.67 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.6, 128.9, 128.1, 127.3, 114.1, 108.5, 100.4, 6.1, 5.5, Two quaternary carbon merged with other peaks; HRMS calcd for $C_{12}H_{11}NO$: 185.0841; found : 185.0821.

3-isopropylindolizine-8-carbaldehyde (3h):



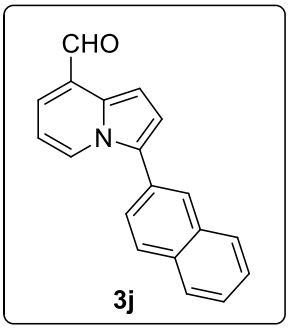
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.96 (s, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.24 ~ 7.21 (m, 2H), 6.71 (d, *J* = 3.6 Hz, 1H), 6.64 (t, *J* = 6.7 Hz, 1H), 3.20 ~ 3.14 (m, 1H), 1.33 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.6, 131.8, 128.2, 127.5, 127.3, 111.8, 108.4, 100.7, 25.2, 21.3, One quaternary carbon merged with other peaks; HRMS calcd for $C_{12}H_{13}NO$: 187.0997; found : 187.0995.

3-cyclohexylindolizine-8-carbaldehyde (3i):



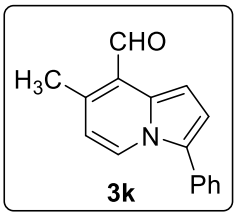
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.99 (s, 1H), 8.04 (d, *J* = 6.8 Hz, 1H), 7.28 ~ 7.24 (m, 2H), 6.72 (d, *J* = 4.0 Hz, 1H), 6.66 (t, *J* = 7.2 Hz, 1H), 2.87 ~ 2.81 (m, 1H), 2.08 ~ 2.03 (m, 2H), 1.90 ~ 1.79 (m, 2H), 1.79 (d, *J* = 1.6 Hz, 1H), 1.49 ~ 1.44 (m, 4H), 1.41 ~ 1.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.6, 131.1, 128.3, 127.5, 127.1, 111.9, 108.3, 100.8, 35.2, 31.9, 26.5, 26.2, One quaternary carbon merged with other peaks; HRMS calcd for $C_{15}H_{17}NO$: 227.1310; found : 227.1314.

3-(naphthalen-2-yl)indolizine-8-carbaldehyde (3j):



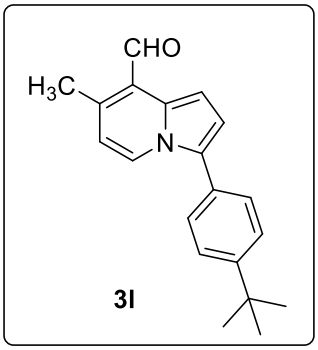
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.04 (s, 1H), 8.53 (d, *J* = 7.2 Hz,1H), 7.97 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.87 (q, *J* = 3.6 Hz, 2H), 7.63 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.55 ~ 7.48 (m, 2H), 7.46 (d, *J* = 4.0 Hz 1H), 7.33 (d, *J* = 6.4 Hz, 1H), 7.10 (d, *J* = 4.0 Hz, 1H), 6.66 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.4, 133.6, 132.6, 129.5, 129.0, 128.8, 128.6, 128.1, 127.9, 127.8, 127.7, 127.1, 126.6, 126.5, 126.4, 126.3, 116.9, 109.3, 102.4; HRMS calcd for $C_{19}H_{13}NO$: 271.0997; found : 271.0996.

7-methyl-3-phenylindolizine-8-carbaldehyde (3k):



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.60 (s, 1H), 8.32 (d, *J* = 7.0 Hz, 1H), 7.50 ~ 7.45 (m, 4H), 7.36 ~ 7.34 (m, 2H), 6.93 (d, *J* = 4.0 Hz, 1H), 6.36 (d, *J* = 7.0 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 189.0, 138.1, 131.9, 129.6, 129.0, 128.4, 127.7, 127.5, 125.7, 123.1, 116.3, 114.2, 101.2, 17.4; HRMS calcd for $C_{16}H_{13}NO$: 235.0997; found : 235.0999.

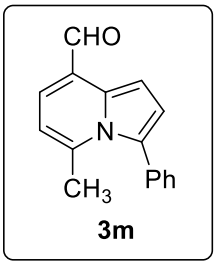
3-(4-(*tert*-butyl)phenyl)-7-methylindolizine-8-carbaldehyde (3l):



3l

Brown solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.6 (s, 1H), 8.32 (d, *J* = 7.3 Hz, 1H), 7.49 ~ 7.47 (m, 2H), 7.44 ~ 7.42 (m, 2H), 7.33 (dd, *J* = 3.8 , 0.5 Hz , 1H), 6.91 (d, *J* = 3.6 Hz, 1H), 6.34 (d, *J* = 7.2 Hz, 1H), 2.65 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 188.9, 150.6, 137.8, 129.4, 129.3, 128.9, 128.2, 127.8, 125.9, 123.1, 116.1, 113.9, 101.0, 34.7, 31.3, 17.4; HRMS calcd for $C_{20}H_{21}NO$: 291.1623; found : 291.1628.

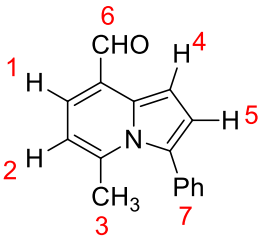
5-methyl-3-phenylindolizine-8-carbaldehyde (3m):



3m

Brown oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.99 (s, 1H), 7.48 (d, *J* = 3.6 Hz, 1H), 7.40 ~ 7.35 (m, 5H), 7.26 (d, *J* = 6.6 Hz, 1H), 6.87 (d, *J* = 3.9 Hz, 1H), 6.42 (dd, *J* = 6.8 , 0.8 Hz , 1H), 2.17 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.1, 142.0, 135.2, 131.2, 129.8, 127.9, 127.5, 127.2, 125.7, 119.3, 111.1, 101.7, 23.6, One quaternary carbon merged with other peaks; ESI-MS calcd for $C_{16}H_{14}NO$[M+H]: 236.1075; found : 236.1079.

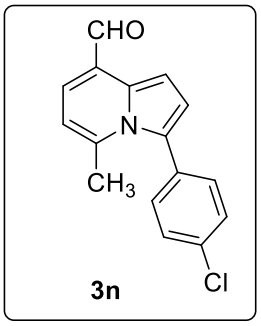
^{1}H-NOE map of compound (3m).



3m

Irradiation	Enhancement (%)
H^3 (δ 2.17)	H^2 (δ 6.42, 3.53%), H^7 (δ 7.40 ~ 7.35, 2.19%), H^5 (δ 6.97, 0.76%)
H^2 (δ 6.42)	H^3 (δ 2.17, 5.12%), H^1 (δ 7.26, 10.59%)
H^1 (δ 7.26)	H^2 (δ 6.42, 8.82%), H^6 (δ 9.99, 12.36%))
H^6 (δ 9.99)	H^1 (δ 7.26, 12.37%)

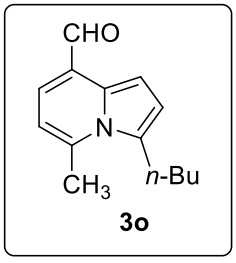
3-(4-chlorophenyl)-5-methylindolizine-8-carbaldehyde (3n):



3n

Orange oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.99 (s, 1H), 7.48 (d, *J* = 4.0 Hz, 1H), 7.35 ~ 7.31 (m, 4H), 7.27 (d, *J* = 4.0 Hz, 1H), 6.85 (d, *J* = 4.0 Hz, 1H), 6.44 (dd, *J* = 6.8, 0.8 Hz, 1H), 2.19 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.0, 141.7, 134.1, 133.8, 132.2, 130.3, 129.7, 127.5, 126.0, 125.9, 119.6, 111.4, 101.9, 23.7; ESI-MS calcd. for $C_{16}H_{13}ClNO$[M+H]: 270.0686; found: 270.0684.

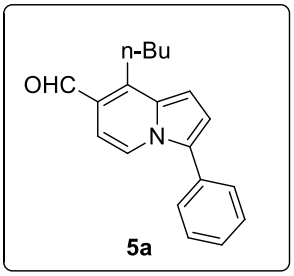
3-butyl-5-methylindolizine-8-carbaldehyde (3o):



3o

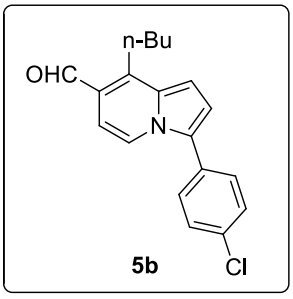
Orange oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.90 (s, 1H), 7.32 (d, *J* = 4.0 Hz, 1H), 7.11 (d, *J* = 6.8 Hz, 1H), 6.70 (d, *J* = 4.0 Hz, 1H), 6.35 (dd, *J* = 6.8, 0.8 Hz, 1H), 3.20 (t, *J* = 7.4 Hz, 2H), 2.88 (s, 3H), 1.71 ~ 1.66 (m, 2H), 1.46 ~ 1.41 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 190.0, 141.6, 129.9, 129.1, 128.5, 125.9, 116.6, 111.0, 101.3, 33.2, 29.6, 22.4, 22.3, 13.9; ESI-MS calcd. for $C_{14}H_{18}NO$[M+H]: 216.1388; found: 216.1382.

8-butyl-3-phenylindolizine-7-carbaldehyde (5a):



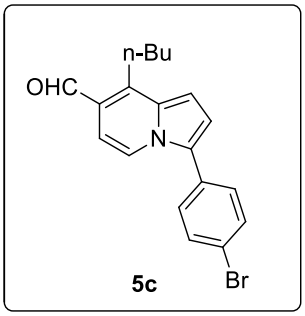
Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.28 (s, 1H), 8.07 (d, *J* = 7.4 Hz, 1H), 7.56 ~ 7.54 (m, 2H), 7.48 (t, *J* = 7.9 Hz, 2H), 7.39 (q, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 4.3 Hz, 1H), 6.92 (d, *J* = 4.3 Hz, 1H), 3.23 (t, *J* = 7.9 Hz, 2H), 1.81 ~ 1.76 (m, 2H), 1.52 ~ 1.39 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.9, 141.8, 133.0, 131.5, 130.0, 129.1, 128.4, 128.1, 122.1, 120.3, 115.7, 108.0, 105.7, 33.9, 27.0, 23.1, 13.9; HRMS calcd for $C_{19}H_{19}NO$: 277.1467; found : 277.1492.

8-butyl-3-(4-chlorophenyl)indolizine-7-carbaldehyde (5b):



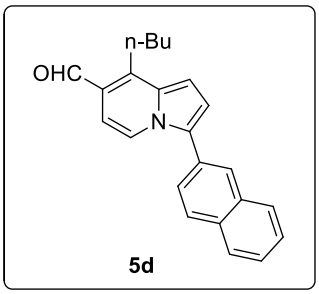
Brown solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.27 (s, 1H), 7.99 (d, *J* = 7.6 Hz, 1H), 7.48 ~ 7.43 (m, 4H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 4.4 Hz, 1H), 6.89 (d, *J* = 4.4 Hz, 1H), 3.21 (t, *J* = 7.6 Hz, 2H), 1.81 ~ 1.73 (m, 2H), 1.52 ~ 1.43 (m, 2H), 0.96 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.8, 141.6, 133.8, 133.2, 129.8, 129.4, 129.3, 128.5, 122.2, 119.9, 115.8, 108.2, 105.7, 33.8, 26.9, 23.0, 13.8; HRMS calcd for $C_{19}H_{18}ClNO$: 311.1077; found : 311.1074.

3-(4-bromophenyl)-8-butylindolizine-7-carbaldehyde (5c):



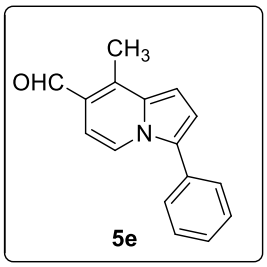
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.28 (s, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.62 ~ 7.59 (m, 2H), 7.43 ~ 7.39 (m, 2H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 4.0 Hz, 1H), 6.90 (d, *J* = 4.0 Hz, 1H), 3.22 (t, *J* = 7.6 Hz, 2H), 1.81 ~ 1.73 (m, 2H), 1.51 ~ 1.45 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.9, 141.7, 133.3, 132.3, 130.3, 129.7, 128.6, 122.3, 121.9, 120.1, 115.8, 108.3, 105.7, 33.8, 26.9, 23.1, 13.8; HRMS calcd for $C_{19}H_{18}BrNO$: 355.0572; found : 355.0578.

8-butyl-3-(naphthalen-2-yl)indolizine-7-carbaldehyde (5d):



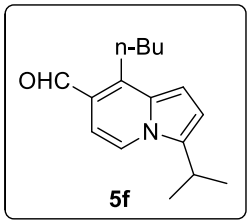
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.29 (s, 1H), 8.17 (d, *J* = 7.2 Hz, 1H), 8.01 (s, 1H), 7.95 (d, *J* = 8.8 Hz, 1H), 7.89 ~ 7.86 (m, 2H), 7.65 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.53 ~ 7.50 (m, 2H), 7.07 ~ 7.03 (m, 3H), 3.26 (t, *J* = 8.0 Hz, 2H), 1.84 ~ 1.76 (m, 2H), 1.58 ~ 1.47 (m, 2H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.9, 141.8, 133.5, 133.2, 132.8, 130.0, 128.8, 128.0, 127.8, 127.1, 126.7, 126.5, 126.1, 122.3, 120.3, 116.1, 108.2, 105.9, 33.9, 27.0, 23.1, 13.9, One quaternary carbon merged with other peaks; HRMS calcd for $C_{23}H_{21}NO$: 327.1623; found : 327.1624.

8-methyl-3-phenylindolizine-7-carbaldehyde (5e):



Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.30 (s, 1H), 8.08 (d, *J* = 7.2 Hz, 1H), 7.56 ~ 7.50 (m, 2H), 7.50 ~ 7.46 (m, 2H), 7.41 ~ 7.36 (m, 1H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.99 (dd, *J* = 4.4, 0.8 Hz, 1H), 6.93 (d, *J* = 4.4 Hz, 1H), 2.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.1, 136.4, 133.4, 131.4, 130.1, 129.1, 128.3, 128.1, 122.6, 120.2, 115.7, 107.9, 105.9, 12.7; HRMS calcd for $C_{16}H_{13}NO$: 235.0997; found : 235.0996.

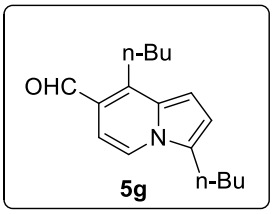
8-butyl-3-isopropylindolizine-7-carbaldehyde (5f):



5f

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.25 (s, 1H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 7.2 Hz, 1H), 6.88 (d, *J* = 4.4 Hz, 1H), 6.67 (d, *J* = 4.0 Hz, 1H), 3.22 ~ 3.15 (m, 3H), 1.78 ~ 1.70 (m, 2H), 1.49 ~ 1.40 (m, 2H), 1.34 (d, *J* = 6.8 Hz, 6H), 0.94 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.0, 141.7, 135.8, 131.8, 120.8, 119.5, 111.2, 107.2, 104.7, 33.9, 26.9, 25.3, 23.0, 21.0, 13.8; HRMS calcd for $C_{16}H_{21}NO$: 243.1623; found : 243.1621.

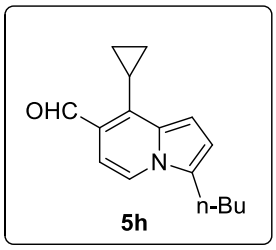
3,8-dibutylindolizine-7-carbaldehyde (5g):



5g

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.26 (s, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 4.4 Hz, 1H), 6.66 (d, *J* = 4 Hz, 1H), 3.18 (t, *J* = 8.0 Hz, 2H), 2.80 (t, *J* = 7.6 Hz, 2H), 1.78 ~ 1.64 (m, 4H), 1.49 ~ 1.39 (m, 4H), 0.95 (q, *J* = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.1, 141.6, 131.8, 129.9, 120.8, 119.5, 113.7, 107.4, 104.6, 33.9, 29.3, 26.9, 25.7, 23.1, 22.6, 13.8; HRMS calcd for $C_{17}H_{23}NO$: 257.1780; found : 257.1785.

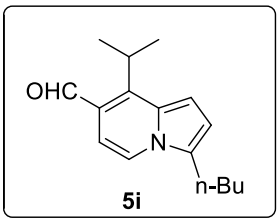
3-butyl-8-cyclopropylindolizine-7-carbaldehyde (5h):



5h

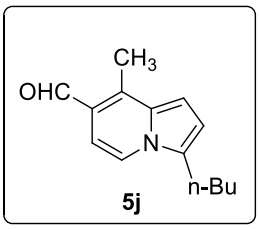
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.69 (s, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.05 (t, *J* = 7.2 Hz, 2H), 6.66 (d, *J* = 4.0 Hz, 1H), 2.80 (t, *J* = 7.6 Hz, 2H), 2.22 ~ 2.15 (m, 1H), 1.75 ~ 1.68 (m, 2H), 1.47 ~ 1.38 (m, 2H), 1.21 ~ 1.17 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H), 0.88 ~ 0.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.5, 140.6, 132.1, 129.6, 123.5, 120.0, 113.8, 106.7, 106.0, 29.3, 25.7, 22.5, 13.8, 8.9, 7.2; HRMS calcd for $C_{16}H_{19}NO$: 241.1467; found : 241.1470.

3-butyl-8-isopropylindolizine-7-carbaldehyde (5i):



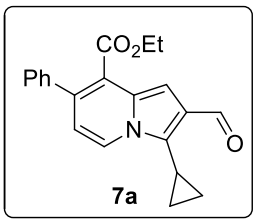
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.45 (s, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 4.4 Hz, 1H), 6.66 (d, *J* = 4.0 Hz, 1H), 4.05 (bs, 1H), 2.79 (t, *J* = 7.6 Hz, 2H), 1.76 ~ 1.68 (m, 2H), 1.57 (d, *J* = 7.2 Hz, 6H), 1.48 ~ 1.39 (m, 2H), 0.96 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.1, 146.8, 130.0, 129.4, 121.1, 119.5, 113.5, 107.7, 106.4, 29.2, 28.0, 25.8, 23.0, 22.6, 13.8; HRMS calcd for $C_{16}H_{21}NO$: 243.1623; found : 243.1622.

3-butyl-8-methylindolizine-7-carbaldehyde (5j):



Brown solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.27 (s, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.86 (d, *J* = 4.0 Hz, 1H), 6.66 (d, *J* = 4.0 Hz, 1H), 2.81 (t, *J* = 7.2 Hz, 2H), 2.74 (s, 3H), 1.76 ~ 1.67 (m, 2H), 1.47 ~ 1.38 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3, 136.2, 132.1, 130.0, 121.3, 119.4, 113.7, 107.3, 104.9, 29.3, 25.7, 22.5, 13.8, 12.6; HRMS calcd for $C_{14}H_{17}NO$: 215.1310; found : 215.1315.

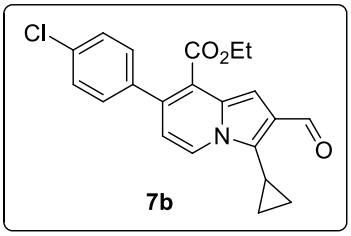
ethyl 3-cyclopropyl-8-formyl-7-phenylindolizine-1-carboxylate (7a):



Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.42 (s, 1H), 8.22 (dd, *J* = 7.4, 0.9 Hz, 1H), 7.41 ~ 7.34 (m, 5H), 7.01 (d, *J* = 0.7 Hz, 1H), 6.71 (d, *J* =7.4 Hz, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 2.00 ~ 1.96 (m, 1H), 1.26 ~1.21 (m, 2H), 1.04 (t, *J* = 7.1 Hz, 3H), 0.83 ~ 0.81 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.5, 166.6, 139.3, 133.1, 131.0, 129.6, 128.4, 128.0, 127.9, 127.1, 124.5,

122.9, 114.9, 99.1, 61.4, 13.7, 6.4, 4.4; ESI-MS calcd. for $C_{21}H_{20}NO_3$[M+H]: 334.1443; found: 334.1451.

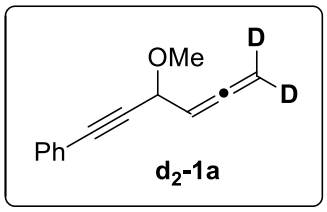
ethyl 7-(4-chlorophenyl)-3-cyclopropyl-8-formylindolizine-1-carboxylate (7b):



7b

Yellow solid; mp: 34.1 ~ 35.3 ºC; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.41 (s, 1H), 8.23 ~ 8.22 (m, 1H), 7.37 (dd, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 8.6 Hz, 2H), 7.02 (s, 1H), 6.65 (d, *J* =7.4 Hz, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 2.00 ~ 1.95 (m, 1H), 1.27 ~1.24 (m, 2H), 1.10 (t, *J* = 7.1 Hz, 3H), 0.83 ~ 0.80 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.4, 166.3, 137.8, 134.0, 131.8, 131.1, 129.4, 128.6, 127.2, 124.7, 124.2, 123.0, 114.5, 99.6, 61.6, 13.8, 6.4, 4.5; ESI-MS calcd. for $C_{21}H_{20}NO_3$[M+H]: 368.1054; found: 368.1048.

(3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (d_2-1a):

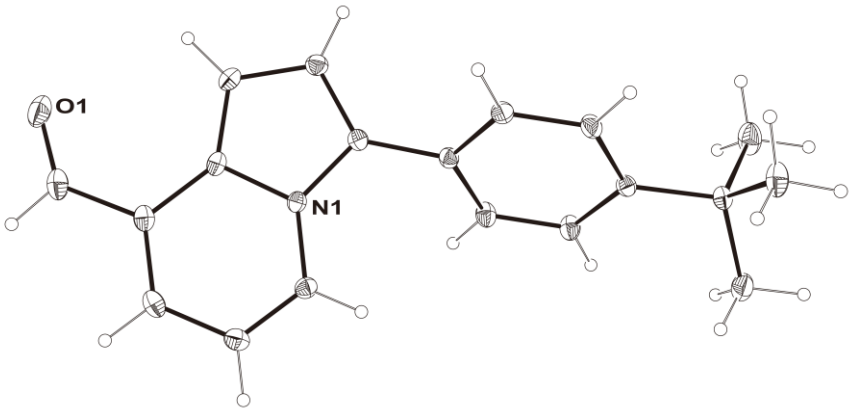


d_2-1a

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 ~ 7.43 (m, 2H), 7.31 ~ 7.27 (m, 3H), 5.36 (d, *J* = 6.8 Hz, 1H), 4.79 (d, *J* = 7.2 Hz, 1H), 3.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 131.8, 128.5, 128.2, 122.4, 90.5, 86.7, 85.9, 69.7, 55.5; ESI-MS calcd for $C_{13}H_{11}D_2O$[M+H]: 187.1092; found : 187.1086.

(6) X-ray crystallographic structure and data for compound 3c, 3d, 3l, 5b, 5j and 7b:

(A) X-ray crystallographic data of compound (3c).



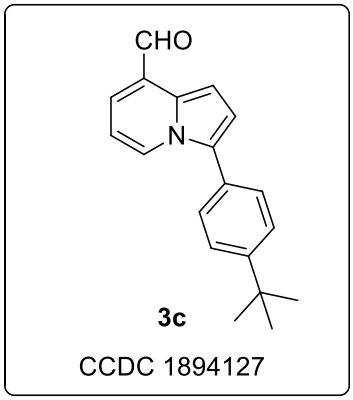


Table S1. Crystal data and structure refinement for d19599.

Identification code	d19599	
Empirical formula	C19 H19 N O	
Formula weight	277.35	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.2570(3) Å	α= 90°.
	b = 14.9320(3) Å	β= 109.5890(10)°.

	c = 11.4194(3) Å γ = 90°.
Volume	1487.09(7) $Å^3$
Z	4
Density (calculated)	1.239 Mg/m^3
Absorption coefficient	0.076 mm^{-1}
F(000)	592
Crystal size	0.58 x 0.52 x 0.38 mm^3
Theta range for data collection	2.46 to 25.06°.
Index ranges	-11<=h<=10, -17<=k<=17, -13<=l<=13
Reflections collected	16035
Independent reflections	2600 [R(int) = 0.0458]
Completeness to theta = 25.06°	98.5 %
Absorption correction	multi-scan
Max. and min. transmission	0.9717 and 0.9573
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2600 / 0 / 194
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.0977
R indices (all data)	R1 = 0.0460, wR2 = 0.1028
Extinction coefficient	0.035(10)
Largest diff. peak and hole	0.215 and -0.182 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d19599. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5490(2)	1571(1)	3302(2)	42(1)
C(2)	5656(2)	2528(1)	3604(1)	31(1)
C(3)	6160(2)	2782(1)	4823(1)	36(1)
C(4)	6313(2)	3697(1)	5159(1)	35(1)
C(5)	5952(2)	4331(1)	4264(1)	29(1)
C(6)	5265(1)	3190(1)	2645(1)	27(1)
C(7)	4688(2)	3187(1)	1371(1)	31(1)
C(8)	4472(2)	4082(1)	974(1)	31(1)
C(9)	4934(1)	4638(1)	1989(1)	26(1)
C(10)	4911(2)	5623(1)	2063(1)	26(1)
C(11)	6206(2)	6125(1)	2689(1)	33(1)
C(12)	6149(2)	7051(1)	2706(1)	33(1)
C(13)	4805(1)	7522(1)	2102(1)	26(1)
C(14)	4776(2)	8549(1)	2073(1)	28(1)
C(15)	5902(2)	8940(1)	3266(2)	51(1)
C(16)	5237(2)	8857(1)	975(2)	51(1)
C(17)	3188(2)	8918(1)	1921(2)	46(1)
C(18)	3520(2)	7013(1)	1475(1)	34(1)
C(19)	3568(2)	6087(1)	1459(1)	33(1)
N(1)	5438(1)	4095(1)	3030(1)	24(1)
O(1)	5024(1)	1252(1)	2273(1)	53(1)

Table S3. Bond lengths [Å] and angles [°] for d19599.

C(1)-O(1)	1.205(2)
C(1)-C(2)	1.466(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.365(2)
C(2)-C(6)	1.4287(19)
C(3)-C(4)	1.413(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3495(19)
C(4)-H(4)	0.9500
C(5)-N(1)	1.3738(17)
C(5)-H(5)	0.9500
C(6)-C(7)	1.371(2)
C(6)-N(1)	1.4133(16)
C(7)-C(8)	1.4045(19)
C(7)-H(7)	0.9500
C(8)-C(9)	1.3715(19)
C(8)-H(8)	0.9500
C(9)-N(1)	1.3849(16)
C(9)-C(10)	1.4733(18)
C(10)-C(19)	1.3879(19)
C(10)-C(11)	1.3917(19)
C(11)-C(12)	1.3840(19)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3940(19)
C(12)-H(12)	0.9500
C(13)-C(18)	1.3906(19)
C(13)-C(14)	1.5345(18)
C(14)-C(16)	1.524(2)
C(14)-C(17)	1.5242(19)
C(14)-C(15)	1.526(2)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800

C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.3844(19)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

O(1)-C(1)-C(2)	126.15(15)
O(1)-C(1)-H(1)	116.9
C(2)-C(1)-H(1)	116.9
C(3)-C(2)-C(6)	120.05(12)
C(3)-C(2)-C(1)	119.00(13)
C(6)-C(2)-C(1)	120.93(13)
C(2)-C(3)-C(4)	120.97(13)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	119.70(13)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-N(1)	120.65(12)
C(4)-C(5)-H(5)	119.7
N(1)-C(5)-H(5)	119.7
C(7)-C(6)-N(1)	107.20(11)
C(7)-C(6)-C(2)	135.99(12)
N(1)-C(6)-C(2)	116.77(12)
C(6)-C(7)-C(8)	107.58(12)
C(6)-C(7)-H(7)	126.2
C(8)-C(7)-H(7)	126.2
C(9)-C(8)-C(7)	109.47(12)
C(9)-C(8)-H(8)	125.3
C(7)-C(8)-H(8)	125.3
C(8)-C(9)-N(1)	106.87(11)
C(8)-C(9)-C(10)	130.26(12)
N(1)-C(9)-C(10)	122.86(11)

C(19)-C(10)-C(11)	117.40(12)
C(19)-C(10)-C(9)	119.82(12)
C(11)-C(10)-C(9)	122.75(12)
C(12)-C(11)-C(10)	121.03(12)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(11)-C(12)-C(13)	121.91(12)
C(11)-C(12)-H(12)	119.0
C(13)-C(12)-H(12)	119.0
C(18)-C(13)-C(12)	116.56(12)
C(18)-C(13)-C(14)	121.95(11)
C(12)-C(13)-C(14)	121.40(11)
C(16)-C(14)-C(17)	108.82(13)
C(16)-C(14)-C(15)	108.88(14)
C(17)-C(14)-C(15)	107.90(13)
C(16)-C(14)-C(13)	108.16(11)
C(17)-C(14)-C(13)	111.88(11)
C(15)-C(14)-C(13)	111.15(11)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

C(19)-C(18)-C(13)	121.79(13)
C(19)-C(18)-H(18)	119.1
C(13)-C(18)-H(18)	119.1
C(18)-C(19)-C(10)	121.31(13)
C(18)-C(19)-H(19)	119.3
C(10)-C(19)-H(19)	119.3
C(5)-N(1)-C(9)	129.18(11)
C(5)-N(1)-C(6)	121.85(11)
C(9)-N(1)-C(6)	108.86(11)

Symmetry transformations used to generate equivalent atoms:

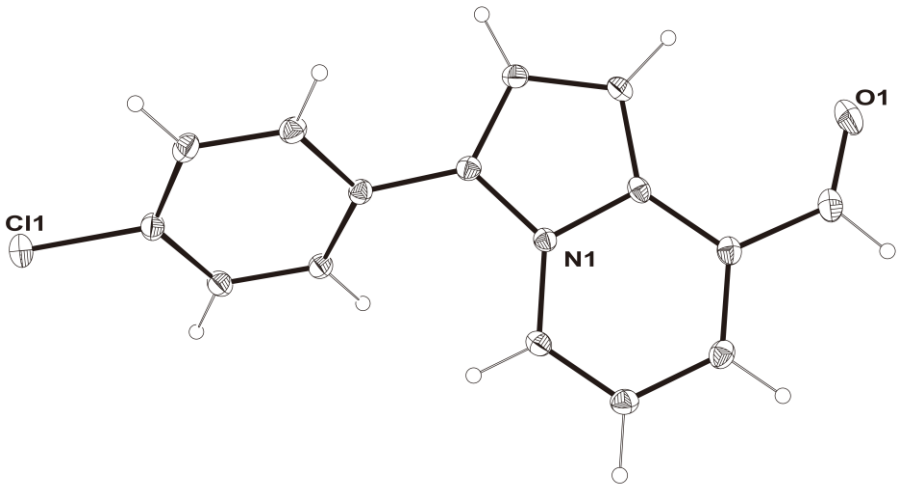
Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for d19599. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(1)	28(1)	60(1)	7(1)	19(1)	4(1)
C(2)	26(1)	27(1)	42(1)	4(1)	14(1)	3(1)
C(3)	34(1)	35(1)	42(1)	12(1)	14(1)	7(1)
C(4)	36(1)	41(1)	28(1)	2(1)	11(1)	4(1)
C(5)	29(1)	30(1)	28(1)	-3(1)	11(1)	2(1)
C(6)	23(1)	22(1)	37(1)	-3(1)	13(1)	-1(1)
C(7)	31(1)	28(1)	35(1)	-8(1)	12(1)	-3(1)
C(8)	33(1)	33(1)	27(1)	0(1)	10(1)	-2(1)
C(9)	25(1)	27(1)	28(1)	2(1)	11(1)	0(1)
C(10)	30(1)	25(1)	26(1)	2(1)	12(1)	0(1)
C(11)	24(1)	28(1)	44(1)	4(1)	8(1)	2(1)
C(12)	24(1)	27(1)	44(1)	2(1)	7(1)	-3(1)
C(13)	27(1)	26(1)	27(1)	3(1)	11(1)	0(1)
C(14)	28(1)	24(1)	33(1)	4(1)	11(1)	1(1)
C(15)	57(1)	29(1)	55(1)	-5(1)	1(1)	2(1)
C(16)	70(1)	35(1)	62(1)	10(1)	40(1)	1(1)
C(17)	39(1)	30(1)	72(1)	4(1)	23(1)	6(1)
C(18)	28(1)	29(1)	37(1)	4(1)	2(1)	3(1)
C(19)	29(1)	30(1)	33(1)	1(1)	2(1)	-4(1)
N(1)	24(1)	23(1)	28(1)	-1(1)	10(1)	0(1)
O(1)	60(1)	29(1)	68(1)	-7(1)	19(1)	-2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d19599.

	x	y	z	U(eq)
H(1)	5776	1164	3980	51
H(3)	6411	2338	5455	44
H(4)	6669	3865	6010	42
H(5)	6053	4946	4490	35
H(7)	4474	2672	852	37
H(8)	4069	4273	133	37
H(11)	7144	5828	3112	39
H(12)	7053	7375	3143	39
H(15A)	6950	8770	3334	77
H(15B)	5666	8707	3983	77
H(15C)	5813	9594	3246	77
H(16A)	4486	8638	200	77
H(16B)	6252	8617	1059	77
H(16C)	5268	9513	961	77
H(17A)	3227	9574	1948	69
H(17B)	2855	8695	2596	69
H(17C)	2461	8723	1121	69
H(18)	2584	7310	1045	40
H(19)	2664	5762	1026	39

(B) X-ray crystallographic data of compound (3d).



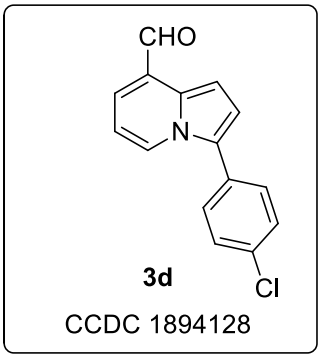


Table S6. Crystal data and structure refinement for d19220.

Identification code	d19220	
Empirical formula	C15 H10 Cl N O	
Formula weight	255.69	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 3.9037(4) Å	α= 90°.

	b = 39.676(5) Å	β= 98.326(3)°.
	c = 7.6371(9) Å	γ = 90°.
Volume	1170.4(2) $Å^3$	
Z	4	
Density (calculated)	1.451 Mg/m^3	
Absorption coefficient	0.311 mm^{-1}	
F(000)	528	
Crystal size	0.66 x 0.09 x 0.03 mm^3	
Theta range for data collection	2.74 to 25.06°.	
Index ranges	-4<=h<=4, -47<=k<=47, -9<=l<=8	
Reflections collected	15094	
Independent reflections	2058 [R(int) = 0.0283]	
Completeness to theta = 25.06°	99.0 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9907 and 0.8212	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2058 / 0 / 163	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1100	
R indices (all data)	R1 = 0.0452, wR2 = 0.1129	
Largest diff. peak and hole	0.502 and -0.224 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d19220. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3383(5)	4488(1)	3551(2)	30(1)
C(2)	3168(5)	4590(1)	5257(3)	33(1)
C(3)	4165(5)	4370(1)	6641(2)	30(1)
C(4)	5355(4)	4047(1)	6331(2)	26(1)
C(5)	5586(4)	3954(1)	4594(2)	28(1)
C(6)	4609(5)	4173(1)	3199(2)	31(1)
C(7)	6468(4)	3827(1)	7849(2)	26(1)
C(8)	8546(5)	3901(1)	9422(2)	29(1)
C(9)	8846(5)	3617(1)	10520(2)	29(1)
C(10)	6904(4)	3365(1)	9632(2)	25(1)
C(11)	6050(5)	3027(1)	10035(2)	28(1)
C(12)	7403(5)	2872(1)	11730(3)	38(1)
C(13)	3896(5)	2843(1)	8829(2)	31(1)
C(14)	2488(5)	2985(1)	7178(2)	31(1)
C(15)	3273(4)	3305(1)	6786(2)	28(1)
Cl(1)	2084(2)	4761(1)	1793(1)	47(1)
N(1)	5446(4)	3494(1)	7967(2)	24(1)
O(1)	9268(5)	3002(1)	12932(2)	58(1)

Table S8. Bond lengths [Å] and angles [°] for d19220.

C(1)-C(2)	1.379(3)
C(1)-C(6)	1.380(3)
C(1)-Cl(1)	1.7432(18)
C(2)-C(3)	1.384(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.393(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.392(3)
C(4)-C(7)	1.466(2)
C(5)-C(6)	1.385(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.380(3)
C(7)-N(1)	1.386(2)
C(8)-C(9)	1.401(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.372(3)
C(9)-H(9)	0.9500
C(10)-N(1)	1.412(2)
C(10)-C(11)	1.428(3)
C(11)-C(13)	1.363(3)
C(11)-C(12)	1.460(3)
C(12)-O(1)	1.202(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.417(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.349(3)
C(14)-H(14)	0.9500
C(15)-N(1)	1.370(2)
C(15)-H(15)	0.9500
C(2)-C(1)-C(6)	121.42(17)
C(2)-C(1)-Cl(1)	119.61(14)
C(6)-C(1)-Cl(1)	118.97(15)

C(1)-C(2)-C(3)	119.10(17)
C(1)-C(2)-H(2)	120.4
C(3)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	121.00(17)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	118.43(16)
C(5)-C(4)-C(7)	122.79(15)
C(3)-C(4)-C(7)	118.71(16)
C(6)-C(5)-C(4)	121.11(16)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(1)-C(6)-C(5)	118.93(17)
C(1)-C(6)-H(6)	120.5
C(5)-C(6)-H(6)	120.5
C(8)-C(7)-N(1)	106.54(15)
C(8)-C(7)-C(4)	129.13(16)
N(1)-C(7)-C(4)	124.30(15)
C(7)-C(8)-C(9)	109.71(16)
C(7)-C(8)-H(8)	125.1
C(9)-C(8)-H(8)	125.1
C(10)-C(9)-C(8)	107.33(16)
C(10)-C(9)-H(9)	126.3
C(8)-C(9)-H(9)	126.3
C(9)-C(10)-N(1)	107.61(15)
C(9)-C(10)-C(11)	135.00(16)
N(1)-C(10)-C(11)	117.36(15)
C(13)-C(11)-C(10)	119.73(16)
C(13)-C(11)-C(12)	118.93(17)
C(10)-C(11)-C(12)	121.33(17)
O(1)-C(12)-C(11)	126.81(19)
O(1)-C(12)-H(12)	116.6
C(11)-C(12)-H(12)	116.6
C(11)-C(13)-C(14)	120.78(17)
C(11)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6

C(15)-C(14)-C(13)	119.93(17)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-N(1)	120.62(16)
C(14)-C(15)-H(15)	119.7
N(1)-C(15)-H(15)	119.7
C(15)-N(1)-C(7)	129.56(15)
C(15)-N(1)-C(10)	121.57(15)
C(7)-N(1)-C(10)	108.81(14)

Symmetry transformations used to generate equivalent atoms:

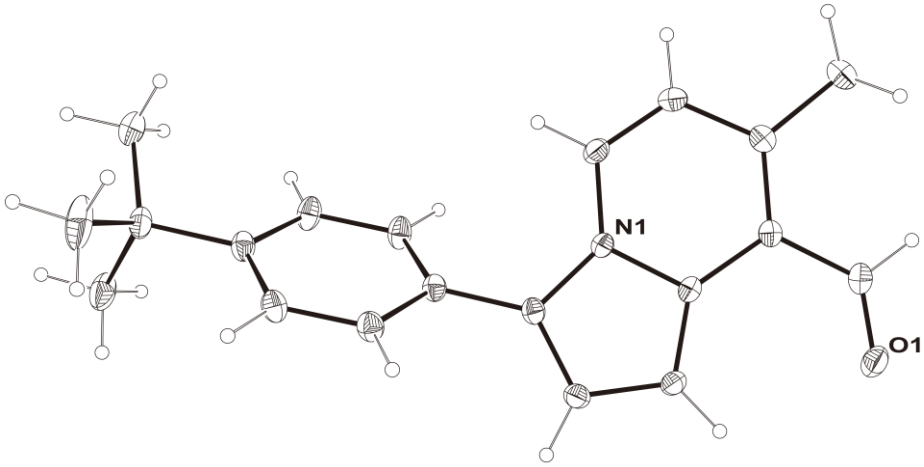
Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for d19220. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(1)	28(1)	33(1)	7(1)	0(1)	-2(1)
C(2)	35(1)	23(1)	40(1)	1(1)	5(1)	3(1)
C(3)	35(1)	26(1)	30(1)	-2(1)	8(1)	0(1)
C(4)	24(1)	25(1)	29(1)	2(1)	4(1)	-1(1)
C(5)	30(1)	24(1)	29(1)	-1(1)	5(1)	3(1)
C(6)	31(1)	34(1)	26(1)	1(1)	2(1)	-2(1)
C(7)	27(1)	25(1)	26(1)	-2(1)	6(1)	1(1)
C(8)	33(1)	28(1)	26(1)	-4(1)	4(1)	-3(1)
C(9)	32(1)	34(1)	20(1)	-1(1)	1(1)	0(1)
C(10)	27(1)	30(1)	19(1)	1(1)	6(1)	5(1)
C(11)	31(1)	29(1)	26(1)	2(1)	8(1)	5(1)
C(12)	46(1)	38(1)	33(1)	10(1)	7(1)	3(1)
C(13)	37(1)	25(1)	32(1)	0(1)	11(1)	1(1)
C(14)	33(1)	29(1)	30(1)	-5(1)	5(1)	-2(1)
C(15)	29(1)	30(1)	24(1)	-2(1)	2(1)	2(1)
Cl(1)	61(1)	36(1)	40(1)	13(1)	-7(1)	3(1)
N(1)	25(1)	24(1)	22(1)	-1(1)	3(1)	3(1)
O(1)	71(1)	65(1)	33(1)	15(1)	-9(1)	-8(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d19220.

	x	y	z	U(eq)
H(2)	2346	4809	5480	40
H(3)	4036	4439	7820	36
H(5)	6429	3736	4363	33
H(6)	4779	4107	2018	37
H(8)	9611	4113	9716	35
H(9)	10153	3601	11668	35
H(12)	6741	2645	11899	46
H(13)	3334	2618	9099	37
H(14)	992	2855	6347	37
H(15)	2309	3400	5682	33

(C) X-ray crystallographic data of compound (3l).



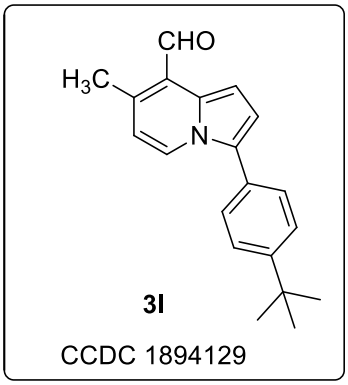


Table S11. Crystal data and structure refinement for d19746.

Identification code	d19746	
Empirical formula	C20 H21 N O	
Formula weight	291.38	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.7561(3) Å	α= 90.518(2)°.
	b = 8.5826(5) Å	β= 90.543(2)°.
	c = 14.0541(8) Å	γ = 103.168(2)°.
Volume	793.41(7) $Å^3$	

Z	2
Density (calculated)	1.220 Mg/m^3
Absorption coefficient	0.074 mm^{-1}
F(000)	312
Crystal size	0.75 x 0.72 x 0.23 mm^3
Theta range for data collection	2.44 to 25.06°.
Index ranges	-8<=h<=8, -10<=k<=10, -16<=l<=16
Reflections collected	17180
Independent reflections	2745 [R(int) = 0.0527]
Completeness to theta = 25.06°	97.7 %
Absorption correction	multi-scan
Max. and min. transmission	0.9831 and 0.9463
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2745 / 0 / 204
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1205
R indices (all data)	R1 = 0.0506, wR2 = 0.1247
Extinction coefficient	0.24(5)
Largest diff. peak and hole	0.201 and -0.180 $e.Å^{-3}$

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d19746. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4951(2)	12984(2)	9784(1)	39(1)
C(2)	5501(2)	11844(2)	9114(1)	30(1)
C(3)	7424(2)	12123(2)	8735(1)	34(1)
C(4)	9089(3)	13583(2)	8941(1)	48(1)
C(5)	7883(2)	10941(2)	8110(1)	39(1)
C(6)	6535(2)	9567(2)	7906(1)	36(1)
C(7)	4024(2)	10416(2)	8873(1)	29(1)
C(8)	2009(2)	9822(2)	9072(1)	33(1)
C(9)	1379(2)	8333(2)	8615(1)	35(1)
C(10)	2990(2)	7983(2)	8134(1)	32(1)
C(11)	3099(2)	6579(2)	7546(1)	33(1)
C(12)	4634(3)	5754(2)	7658(1)	41(1)
C(13)	4686(3)	4433(2)	7095(1)	43(1)
C(14)	3229(2)	3864(2)	6399(1)	37(1)
C(15)	1660(2)	4664(2)	6315(1)	43(1)
C(16)	1604(2)	5996(2)	6866(1)	40(1)
C(17)	3327(3)	2402(2)	5782(1)	42(1)
C(18)	5533(4)	2309(3)	5621(2)	83(1)
C(19)	2342(5)	2472(3)	4808(1)	82(1)
C(20)	2241(4)	902(2)	6290(1)	64(1)
N(1)	4627(2)	9265(1)	8285(1)	29(1)
O(1)	3298(2)	12855(1)	10145(1)	48(1)

Table S13. Bond lengths [Å] and angles [°] for d19746.

C(1)-O(1)	1.2137(19)
C(1)-C(2)	1.462(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.380(2)
C(2)-C(7)	1.429(2)
C(3)-C(5)	1.423(2)
C(3)-C(4)	1.505(2)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.342(2)
C(5)-H(5)	0.9500
C(6)-N(1)	1.3697(18)
C(6)-H(6)	0.9500
C(7)-C(8)	1.373(2)
C(7)-N(1)	1.4138(17)
C(8)-C(9)	1.400(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.375(2)
C(9)-H(9)	0.9500
C(10)-N(1)	1.3842(18)
C(10)-C(11)	1.4711(19)
C(11)-C(16)	1.388(2)
C(11)-C(12)	1.391(2)
C(12)-C(13)	1.384(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.385(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.393(2)
C(14)-C(17)	1.533(2)
C(15)-C(16)	1.383(2)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(20)	1.517(2)

C(17)-C(19)	1.524(3)
C(17)-C(18)	1.529(3)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

O(1)-C(1)-C(2)	125.55(14)
O(1)-C(1)-H(1)	117.2
C(2)-C(1)-H(1)	117.2
C(3)-C(2)-C(7)	120.42(13)
C(3)-C(2)-C(1)	120.71(13)
C(7)-C(2)-C(1)	118.86(13)
C(2)-C(3)-C(5)	117.93(13)
C(2)-C(3)-C(4)	124.71(14)
C(5)-C(3)-C(4)	117.36(14)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(3)	122.28(14)
C(6)-C(5)-H(5)	118.9
C(3)-C(5)-H(5)	118.9
C(5)-C(6)-N(1)	120.45(13)
C(5)-C(6)-H(6)	119.8
N(1)-C(6)-H(6)	119.8
C(8)-C(7)-N(1)	106.59(12)
C(8)-C(7)-C(2)	135.20(13)
N(1)-C(7)-C(2)	118.21(12)

C(7)-C(8)-C(9)	108.16(12)
C(7)-C(8)-H(8)	125.9
C(9)-C(8)-H(8)	125.9
C(10)-C(9)-C(8)	109.31(13)
C(10)-C(9)-H(9)	125.3
C(8)-C(9)-H(9)	125.3
C(9)-C(10)-N(1)	106.63(12)
C(9)-C(10)-C(11)	130.14(13)
N(1)-C(10)-C(11)	123.22(12)
C(16)-C(11)-C(12)	117.23(13)
C(16)-C(11)-C(10)	120.23(13)
C(12)-C(11)-C(10)	122.51(13)
C(13)-C(12)-C(11)	121.01(14)
C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5
C(12)-C(13)-C(14)	122.21(14)
C(12)-C(13)-H(13)	118.9
C(14)-C(13)-H(13)	118.9
C(13)-C(14)-C(15)	116.33(13)
C(13)-C(14)-C(17)	121.18(14)
C(15)-C(14)-C(17)	122.46(14)
C(16)-C(15)-C(14)	121.92(14)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(15)-C(16)-C(11)	121.23(14)
C(15)-C(16)-H(16)	119.4
C(11)-C(16)-H(16)	119.4
C(20)-C(17)-C(19)	109.54(17)
C(20)-C(17)-C(18)	108.64(17)
C(19)-C(17)-C(18)	107.52(18)
C(20)-C(17)-C(14)	108.78(13)
C(19)-C(17)-C(14)	111.55(14)
C(18)-C(17)-C(14)	110.77(14)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5

C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(6)-N(1)-C(10)	129.94(12)
C(6)-N(1)-C(7)	120.56(12)
C(10)-N(1)-C(7)	109.32(11)

Symmetry transformations used to generate equivalent atoms:

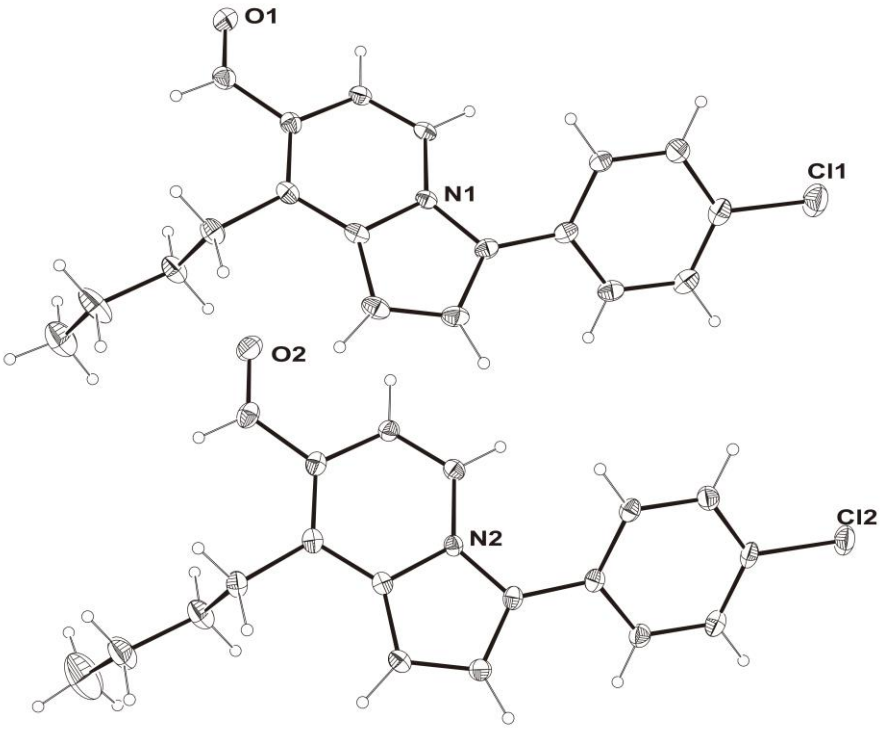
Table S14. Anisotropic displacement parameters ($Å^2$x 10^3)for d19746. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	47(1)	32(1)	40(1)	-5(1)	-6(1)	12(1)
C(2)	36(1)	28(1)	28(1)	2(1)	-4(1)	9(1)
C(3)	36(1)	33(1)	33(1)	5(1)	-4(1)	7(1)
C(4)	44(1)	42(1)	53(1)	2(1)	-2(1)	-1(1)
C(5)	31(1)	46(1)	39(1)	2(1)	6(1)	8(1)
C(6)	34(1)	41(1)	36(1)	-4(1)	5(1)	13(1)
C(7)	36(1)	29(1)	24(1)	1(1)	0(1)	13(1)
C(8)	33(1)	35(1)	34(1)	0(1)	6(1)	11(1)
C(9)	30(1)	34(1)	40(1)	2(1)	2(1)	5(1)
C(10)	35(1)	27(1)	34(1)	0(1)	-3(1)	7(1)
C(11)	40(1)	29(1)	31(1)	0(1)	-1(1)	8(1)
C(12)	50(1)	40(1)	37(1)	-9(1)	-15(1)	18(1)
C(13)	59(1)	38(1)	38(1)	-6(1)	-9(1)	24(1)
C(14)	52(1)	29(1)	28(1)	0(1)	0(1)	6(1)
C(15)	46(1)	41(1)	39(1)	-7(1)	-10(1)	5(1)
C(16)	40(1)	37(1)	43(1)	-3(1)	-6(1)	11(1)
C(17)	61(1)	30(1)	32(1)	-4(1)	4(1)	6(1)
C(18)	76(2)	69(1)	97(2)	-45(1)	26(1)	4(1)
C(19)	151(2)	60(1)	38(1)	-16(1)	-17(1)	30(1)
C(20)	104(2)	33(1)	51(1)	-4(1)	24(1)	6(1)
N(1)	31(1)	29(1)	29(1)	-1(1)	0(1)	11(1)
O(1)	51(1)	49(1)	46(1)	-13(1)	2(1)	19(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d19746.

	x	y	z	U(eq)
H(1)	5975	13905	9950	47
H(4A)	10040	13763	8410	72
H(4B)	9815	13420	9525	72
H(4C)	8496	14516	9022	72
H(5)	9187	11132	7829	46
H(6)	6908	8798	7497	44
H(8)	1186	10332	9455	40
H(9)	47	7668	8634	42
H(12)	5663	6104	8129	49
H(13)	5757	3898	7190	52
H(15)	597	4284	5865	51
H(16)	521	6520	6779	48
H(18A)	5564	1396	5202	124
H(18B)	6176	2172	6233	124
H(18C)	6272	3298	5325	124
H(19A)	2981	3478	4499	123
H(19B)	887	2414	4884	123
H(19C)	2527	1568	4414	123
H(20A)	795	897	6343	96
H(20B)	2834	883	6928	96
H(20C)	2394	-44	5928	96

(D) X-ray crystallographic data of compound (5b).



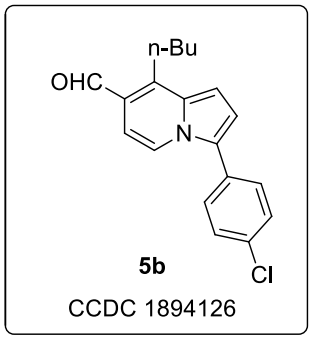


Table S16. Crystal data and structure refinement for d19628.

Identification code	d19628
Empirical formula	C19 H18 Cl N O
Formula weight	311.79
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1

Unit cell dimensions	a = 8.3841(9) Å	α= 90.770(3)°.
	b = 13.7451(15) Å	β= 97.215(3)°.
	c = 14.1044(15) Å	γ = 94.980(3)°.
Volume	1606.0(3) $Å^3$	
Z	4	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	0.239 mm^{-1}	
F(000)	656	
Crystal size	0.32 x 0.05 x 0.01 mm^3	
Theta range for data collection	2.46 to 25.07°.	
Index ranges	-9<=h<=9, -16<=k<=16, -16<=l<=16	
Reflections collected	39950	
Independent reflections	5665 [R(int) = 0.1459]	
Completeness to theta = 25.07°	99.5 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9976 and 0.9274	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5665 / 0 / 400	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.1312	
R indices (all data)	R1 = 0.1365, wR2 = 0.1607	
Extinction coefficient	0.0125(16)	
Largest diff. peak and hole	0.652 and -0.251 $e.Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d19628. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8502(4)	8849(3)	7803(3)	46(1)
C(2)	8401(4)	7860(3)	7561(3)	43(1)
C(3)	8250(4)	7577(3)	6613(3)	36(1)
C(4)	8183(4)	8265(3)	5889(3)	35(1)
C(5)	8252(4)	9248(3)	6158(3)	42(1)
C(6)	8420(4)	9547(3)	7100(3)	47(1)
C(7)	8174(4)	8011(3)	4884(3)	35(1)
C(8)	8991(4)	8510(3)	4217(3)	45(1)
C(9)	8743(4)	8001(3)	3357(3)	44(1)
C(10)	7733(4)	7162(3)	3458(3)	35(1)
C(11)	7097(4)	6373(3)	2842(2)	35(1)
C(12)	7571(4)	6366(3)	1842(2)	42(1)
C(13)	6326(4)	6771(3)	1113(3)	49(1)
C(14)	6759(5)	6712(4)	87(3)	76(2)
C(15)	5580(6)	7088(4)	-630(3)	83(2)
C(16)	6029(4)	5674(3)	3167(2)	35(1)
C(17)	5307(5)	4828(3)	2585(3)	43(1)
C(18)	5600(4)	5766(3)	4106(3)	36(1)
C(19)	6262(4)	6495(3)	4711(3)	33(1)
C(20)	8377(4)	3422(3)	9383(2)	39(1)
C(21)	8246(4)	4075(3)	8655(3)	42(1)
C(22)	7831(4)	3744(3)	7715(3)	36(1)
C(23)	7532(4)	2745(3)	7498(2)	33(1)
C(24)	7652(4)	2103(3)	8256(3)	41(1)
C(25)	8071(4)	2432(3)	9191(3)	45(1)
C(26)	7033(4)	2351(3)	6524(2)	33(1)
C(27)	5957(4)	1544(3)	6242(3)	37(1)
C(28)	5798(4)	1434(3)	5255(3)	38(1)
C(29)	6768(4)	2175(3)	4907(2)	32(1)
C(30)	7042(4)	2448(3)	3978(2)	34(1)
C(31)	6120(4)	1844(3)	3153(3)	41(1)

C(32)	7011(5)	1028(3)	2799(3)	58(1)
C(33)	6054(6)	490(4)	1923(4)	76(2)
C(34)	6807(8)	-247(5)	1472(5)	128(3)
C(35)	8133(4)	3238(3)	3871(2)	35(1)
C(36)	8475(5)	3588(3)	2944(3)	42(1)
C(37)	8970(4)	3748(3)	4709(2)	35(1)
C(38)	8687(4)	3501(3)	5592(3)	34(1)
Cl(1)	8719(2)	9226(1)	8998(1)	72(1)
Cl(2)	8896(1)	3834(1)	10558(1)	57(1)
N(1)	7378(3)	7190(2)	4411(2)	30(1)
N(2)	7542(3)	2736(2)	5706(2)	30(1)
O(1)	4350(3)	4203(2)	2841(2)	57(1)
O(2)	9409(3)	4293(2)	2820(2)	53(1)

Table S18. Bond lengths [Å] and angles [°] for d19628.

C(1)-C(2)	1.389(5)
C(1)-C(6)	1.389(6)
C(1)-Cl(1)	1.739(4)
C(2)-C(3)	1.375(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.400(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(5)
C(4)-C(7)	1.454(5)
C(5)-C(6)	1.373(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(1)	1.378(4)
C(7)-C(8)	1.387(5)
C(8)-C(9)	1.376(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.390(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.405(5)
C(10)-N(1)	1.412(4)
C(11)-C(16)	1.379(5)
C(11)-C(12)	1.513(5)
C(12)-C(13)	1.518(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.538(5)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.456(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800

C(16)-C(18)	1.423(5)
C(16)-C(17)	1.456(5)
C(17)-O(1)	1.214(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.342(5)
C(18)-H(18)	0.9500
C(19)-N(1)	1.386(4)
C(19)-H(19)	0.9500
C(20)-C(21)	1.373(5)
C(20)-C(25)	1.379(5)
C(20)-Cl(2)	1.734(4)
C(21)-C(22)	1.387(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.397(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.395(5)
C(23)-C(26)	1.467(5)
C(24)-C(25)	1.381(5)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-N(2)	1.375(4)
C(26)-C(27)	1.388(5)
C(27)-C(28)	1.387(5)
C(27)-H(27)	0.9500
C(28)-C(29)	1.382(5)
C(28)-H(28)	0.9500
C(29)-C(30)	1.409(5)
C(29)-N(2)	1.412(4)
C(30)-C(35)	1.381(5)
C(30)-C(31)	1.508(5)
C(31)-C(32)	1.513(5)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.530(6)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900

C(33)-C(34)	1.423(7)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(37)	1.437(5)
C(35)-C(36)	1.453(5)
C(36)-O(2)	1.221(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.339(5)
C(37)-H(37)	0.9500
C(38)-N(2)	1.386(4)
C(38)-H(38)	0.9500

C(2)-C(1)-C(6)	120.7(4)
C(2)-C(1)-Cl(1)	120.1(3)
C(6)-C(1)-Cl(1)	119.1(3)
C(3)-C(2)-C(1)	119.3(4)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	121.3(4)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	117.9(4)
C(5)-C(4)-C(7)	118.6(3)
C(3)-C(4)-C(7)	123.4(3)
C(6)-C(5)-C(4)	121.8(4)
C(6)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
C(5)-C(6)-C(1)	119.1(4)
C(5)-C(6)-H(6)	120.5
C(1)-C(6)-H(6)	120.5
N(1)-C(7)-C(8)	106.0(3)
N(1)-C(7)-C(4)	126.1(3)
C(8)-C(7)-C(4)	127.9(3)

C(9)-C(8)-C(7)	110.0(3)
C(9)-C(8)-H(8)	125.0
C(7)-C(8)-H(8)	125.0
C(8)-C(9)-C(10)	108.1(3)
C(8)-C(9)-H(9)	125.9
C(10)-C(9)-H(9)	125.9
C(9)-C(10)-C(11)	133.8(4)
C(9)-C(10)-N(1)	106.0(3)
C(11)-C(10)-N(1)	120.2(3)
C(16)-C(11)-C(10)	118.4(3)
C(16)-C(11)-C(12)	123.8(3)
C(10)-C(11)-C(12)	117.7(3)
C(11)-C(12)-C(13)	112.7(3)
C(11)-C(12)-H(12A)	109.1
C(13)-C(12)-H(12A)	109.1
C(11)-C(12)-H(12B)	109.1
C(13)-C(12)-H(12B)	109.1
H(12A)-C(12)-H(12B)	107.8
C(12)-C(13)-C(14)	112.8(3)
C(12)-C(13)-H(13A)	109.0
C(14)-C(13)-H(13A)	109.0
C(12)-C(13)-H(13B)	109.0
C(14)-C(13)-H(13B)	109.0
H(13A)-C(13)-H(13B)	107.8
C(15)-C(14)-C(13)	114.1(4)
C(15)-C(14)-H(14A)	108.7
C(13)-C(14)-H(14A)	108.7
C(15)-C(14)-H(14B)	108.7
C(13)-C(14)-H(14B)	108.7
H(14A)-C(14)-H(14B)	107.6
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

C(11)-C(16)-C(18)	119.7(3)
C(11)-C(16)-C(17)	122.6(3)
C(18)-C(16)-C(17)	117.7(3)
O(1)-C(17)-C(16)	124.5(4)
O(1)-C(17)-H(17)	117.7
C(16)-C(17)-H(17)	117.7
C(19)-C(18)-C(16)	121.9(3)
C(19)-C(18)-H(18)	119.1
C(16)-C(18)-H(18)	119.1
C(18)-C(19)-N(1)	119.4(3)
C(18)-C(19)-H(19)	120.3
N(1)-C(19)-H(19)	120.3
C(21)-C(20)-C(25)	120.4(3)
C(21)-C(20)-Cl(2)	120.4(3)
C(25)-C(20)-Cl(2)	119.2(3)
C(20)-C(21)-C(22)	120.3(4)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(21)-C(22)-C(23)	120.5(3)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	117.7(3)
C(24)-C(23)-C(26)	119.1(3)
C(22)-C(23)-C(26)	123.1(3)
C(25)-C(24)-C(23)	121.7(4)
C(25)-C(24)-H(24)	119.1
C(23)-C(24)-H(24)	119.1
C(20)-C(25)-C(24)	119.3(4)
C(20)-C(25)-H(25)	120.3
C(24)-C(25)-H(25)	120.3
N(2)-C(26)-C(27)	106.9(3)
N(2)-C(26)-C(23)	125.6(3)
C(27)-C(26)-C(23)	127.6(3)
C(28)-C(27)-C(26)	109.1(3)
C(28)-C(27)-H(27)	125.4
C(26)-C(27)-H(27)	125.4

C(29)-C(28)-C(27)	108.1(3)
C(29)-C(28)-H(28)	126.0
C(27)-C(28)-H(28)	126.0
C(28)-C(29)-C(30)	133.3(3)
C(28)-C(29)-N(2)	106.7(3)
C(30)-C(29)-N(2)	120.0(3)
C(35)-C(30)-C(29)	118.8(3)
C(35)-C(30)-C(31)	123.9(3)
C(29)-C(30)-C(31)	117.3(3)
C(30)-C(31)-C(32)	114.6(3)
C(30)-C(31)-H(31A)	108.6
C(32)-C(31)-H(31A)	108.6
C(30)-C(31)-H(31B)	108.6
C(32)-C(31)-H(31B)	108.6
H(31A)-C(31)-H(31B)	107.6
C(31)-C(32)-C(33)	111.8(4)
C(31)-C(32)-H(32A)	109.3
C(33)-C(32)-H(32A)	109.3
C(31)-C(32)-H(32B)	109.3
C(33)-C(32)-H(32B)	109.3
H(32A)-C(32)-H(32B)	107.9
C(34)-C(33)-C(32)	117.6(5)
C(34)-C(33)-H(33A)	107.9
C(32)-C(33)-H(33A)	107.9
C(34)-C(33)-H(33B)	107.9
C(32)-C(33)-H(33B)	107.9
H(33A)-C(33)-H(33B)	107.2
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(30)-C(35)-C(37)	119.1(3)
C(30)-C(35)-C(36)	122.9(3)
C(37)-C(35)-C(36)	117.9(3)

O(2)-C(36)-C(35)	124.9(4)
O(2)-C(36)-H(36)	117.6
C(35)-C(36)-H(36)	117.6
C(38)-C(37)-C(35)	122.1(3)
C(38)-C(37)-H(37)	119.0
C(35)-C(37)-H(37)	119.0
C(37)-C(38)-N(2)	119.3(3)
C(37)-C(38)-H(38)	120.3
N(2)-C(38)-H(38)	120.3
C(7)-N(1)-C(19)	129.9(3)
C(7)-N(1)-C(10)	109.8(3)
C(19)-N(1)-C(10)	120.0(3)
C(26)-N(2)-C(38)	130.3(3)
C(26)-N(2)-C(29)	109.1(3)
C(38)-N(2)-C(29)	120.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S19. Anisotropic displacement parameters ($Å^2$x 10^3)for d19628. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	39(2)	51(3)	49(3)	-12(2)	8(2)	-2(2)
C(2)	37(2)	46(3)	46(3)	2(2)	5(2)	1(2)
C(3)	32(2)	32(2)	43(2)	0(2)	6(2)	1(2)
C(4)	24(2)	33(2)	48(2)	0(2)	7(2)	0(2)
C(5)	34(2)	37(2)	55(3)	6(2)	7(2)	-1(2)
C(6)	40(2)	40(2)	60(3)	-8(2)	10(2)	-1(2)
C(7)	29(2)	31(2)	45(2)	2(2)	4(2)	0(2)
C(8)	38(2)	43(2)	54(3)	10(2)	12(2)	-7(2)
C(9)	32(2)	54(3)	48(3)	16(2)	12(2)	1(2)
C(10)	28(2)	40(2)	39(2)	12(2)	7(2)	7(2)
C(11)	30(2)	42(2)	33(2)	8(2)	6(2)	12(2)
C(12)	34(2)	57(3)	37(2)	5(2)	8(2)	7(2)
C(13)	39(2)	73(3)	37(2)	10(2)	6(2)	1(2)
C(14)	49(3)	136(5)	47(3)	33(3)	18(2)	13(3)
C(15)	67(3)	126(5)	57(3)	16(3)	6(3)	5(3)
C(16)	36(2)	38(2)	33(2)	4(2)	2(2)	10(2)
C(17)	47(2)	43(3)	39(2)	6(2)	3(2)	11(2)
C(18)	36(2)	36(2)	36(2)	9(2)	4(2)	-1(2)
C(19)	30(2)	37(2)	34(2)	11(2)	9(2)	4(2)
C(20)	36(2)	59(3)	25(2)	-1(2)	9(2)	2(2)
C(21)	40(2)	45(2)	39(2)	-6(2)	8(2)	-1(2)
C(22)	31(2)	44(2)	33(2)	3(2)	8(2)	4(2)
C(23)	30(2)	41(2)	30(2)	2(2)	5(2)	7(2)
C(24)	49(2)	39(2)	37(2)	2(2)	11(2)	8(2)
C(25)	51(2)	54(3)	32(2)	6(2)	10(2)	11(2)
C(26)	32(2)	39(2)	30(2)	-1(2)	7(2)	10(2)
C(27)	38(2)	35(2)	38(2)	1(2)	7(2)	2(2)
C(28)	35(2)	36(2)	40(2)	-5(2)	0(2)	-1(2)
C(29)	29(2)	33(2)	32(2)	-3(2)	1(2)	7(2)
C(30)	31(2)	39(2)	33(2)	-3(2)	3(2)	11(2)
C(31)	40(2)	50(3)	32(2)	-4(2)	2(2)	4(2)

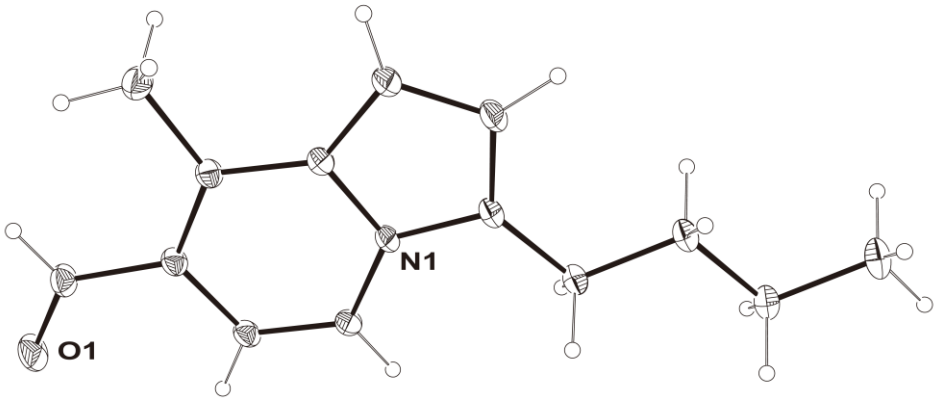
C(32)	50(3)	61(3)	62(3)	-22(2)	6(2)	1(2)
C(33)	81(3)	71(4)	71(3)	-33(3)	8(3)	-6(3)
C(34)	110(5)	138(6)	135(6)	-70(5)	4(4)	26(4)
C(35)	37(2)	37(2)	32(2)	1(2)	7(2)	14(2)
C(36)	48(2)	46(3)	35(2)	8(2)	6(2)	18(2)
C(37)	37(2)	33(2)	35(2)	1(2)	8(2)	3(2)
C(38)	31(2)	35(2)	36(2)	-1(2)	0(2)	2(2)
Cl(1)	79(1)	79(1)	56(1)	-22(1)	13(1)	-8(1)
Cl(2)	58(1)	80(1)	31(1)	-8(1)	7(1)	-7(1)
N(1)	27(2)	32(2)	31(2)	7(1)	7(1)	2(1)
N(2)	28(2)	34(2)	28(2)	-2(1)	3(1)	3(1)
O(1)	73(2)	42(2)	53(2)	-3(1)	11(2)	-5(2)
O(2)	66(2)	49(2)	46(2)	11(1)	16(1)	8(2)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d19628.

	x	y	z	U(eq)
H(2)	8436	7386	8044	52
H(3)	8189	6902	6446	43
H(5)	8181	9724	5676	51
H(6)	8479	10221	7269	56
H(8)	9629	9115	4336	54
H(9)	9185	8190	2792	53
H(12A)	7717	5687	1651	51
H(12B)	8619	6758	1844	51
H(13A)	6226	7462	1285	59
H(13B)	5265	6402	1138	59
H(14A)	7819	7083	65	91
H(14B)	6871	6021	-79	91
H(15A)	5910	7000	-1266	125
H(15B)	5516	7785	-500	125
H(15C)	4520	6734	-607	125
H(17)	5606	4761	1961	51
H(18)	4822	5298	4312	43
H(19)	5968	6536	5338	39
H(21)	8441	4756	8795	50
H(22)	7749	4201	7215	43
H(24)	7439	1421	8126	49
H(25)	8149	1982	9696	54
H(27)	5415	1133	6659	44
H(28)	5138	935	4883	45
H(31A)	5848	2281	2616	49
H(31B)	5093	1557	3352	49
H(32A)	7215	558	3317	69
H(32B)	8069	1303	2633	69
H(33A)	5033	187	2116	91
H(33B)	5765	983	1440	91

H(34A)	6020	-597	985	192
H(34B)	7210	-706	1951	192
H(34C)	7710	56	1168	192
H(36)	7931	3242	2392	51
H(37)	9750	4276	4635	42
H(38)	9264	3847	6134	41

(E) X-ray crystallographic data of compound (5j).



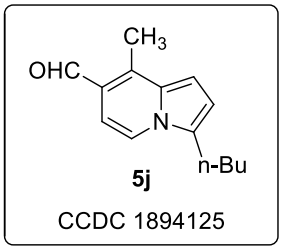


Table S21. Crystal data and structure refinement for d19548.

Identification code	d19548	
Empirical formula	C14 H17 N O	
Formula weight	215.29	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.469(3) Å	α= 90°.
	b = 7.941(4) Å	β= 90.051(14)°.
	c = 19.929(8) Å	γ = 90°.
Volume	1182.0(8) $Å^3$	
Z	4	
Density (calculated)	1.210 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	464	

Crystal size	0.65 x 0.30 x 0.11 mm^3
Theta range for data collection	2.73 to 25.13°.
Index ranges	-8<=h<=8, -9<=k<=9, -23<=l<=23
Reflections collected	17667
Independent reflections	2070 [R(int) = 0.0855]
Completeness to theta = 25.13°	98.3 %
Absorption correction	multi-scan
Max. and min. transmission	0.9917 and 0.9524
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2070 / 0 / 147
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.1648
R indices (all data)	R1 = 0.0836, wR2 = 0.1940
Largest diff. peak and hole	0.225 and -0.269 $e.Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d19548. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5870(3)	2093(3)	2850(1)	39(1)
C(2)	6346(3)	2710(3)	3519(1)	31(1)
C(3)	6810(3)	1620(3)	4034(1)	32(1)
C(4)	6822(3)	-272(3)	3983(1)	44(1)
C(5)	7295(3)	2312(3)	4664(1)	31(1)
C(6)	6799(3)	5138(3)	4237(1)	32(1)
C(7)	6338(3)	4485(3)	3637(1)	33(1)
C(8)	7839(3)	1617(3)	5271(1)	40(1)
C(9)	8165(3)	2952(3)	5714(1)	40(1)
C(10)	7833(3)	4463(3)	5393(1)	32(1)
C(11)	7957(3)	6232(3)	5624(1)	34(1)
C(12)	8493(3)	6408(3)	6360(1)	37(1)
C(13)	8604(3)	8219(3)	6595(1)	39(1)
C(14)	9153(4)	8377(4)	7328(1)	52(1)
N(1)	7302(2)	4059(2)	4750(1)	29(1)
O(1)	5463(3)	2991(2)	2382(1)	54(1)

Table S23. Bond lengths [Å] and angles [°] for d19548.

C(1)-O(1)	1.212(3)
C(1)-C(2)	1.465(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.386(3)
C(2)-C(7)	1.429(3)
C(3)-C(5)	1.417(3)
C(3)-C(4)	1.505(3)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(8)	1.391(3)
C(5)-N(1)	1.397(3)
C(6)-C(7)	1.349(3)
C(6)-N(1)	1.385(3)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.400(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.382(3)
C(9)-H(9)	0.9500
C(10)-N(1)	1.378(3)
C(10)-C(11)	1.481(3)
C(11)-C(12)	1.528(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.514(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.523(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

O(1)-C(1)-C(2)	124.3(2)
O(1)-C(1)-H(1)	117.8
C(2)-C(1)-H(1)	117.8
C(3)-C(2)-C(7)	119.75(19)
C(3)-C(2)-C(1)	121.7(2)
C(7)-C(2)-C(1)	118.53(19)
C(2)-C(3)-C(5)	118.5(2)
C(2)-C(3)-C(4)	125.1(2)
C(5)-C(3)-C(4)	116.44(19)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(8)-C(5)-N(1)	106.63(18)
C(8)-C(5)-C(3)	133.7(2)
N(1)-C(5)-C(3)	119.66(18)
C(7)-C(6)-N(1)	119.1(2)
C(7)-C(6)-H(6)	120.5
N(1)-C(6)-H(6)	120.5
C(6)-C(7)-C(2)	121.5(2)
C(6)-C(7)-H(7)	119.2
C(2)-C(7)-H(7)	119.2
C(5)-C(8)-C(9)	107.3(2)
C(5)-C(8)-H(8)	126.3
C(9)-C(8)-H(8)	126.3
C(10)-C(9)-C(8)	109.5(2)
C(10)-C(9)-H(9)	125.2
C(8)-C(9)-H(9)	125.2
N(1)-C(10)-C(9)	106.2(2)
N(1)-C(10)-C(11)	121.81(19)
C(9)-C(10)-C(11)	131.9(2)
C(10)-C(11)-C(12)	113.65(19)
C(10)-C(11)-H(11A)	108.8

C(12)-C(11)-H(11A)	108.8
C(10)-C(11)-H(11B)	108.8
C(12)-C(11)-H(11B)	108.8
H(11A)-C(11)-H(11B)	107.7
C(13)-C(12)-C(11)	113.42(19)
C(13)-C(12)-H(12A)	108.9
C(11)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12B)	108.9
C(11)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
C(12)-C(13)-C(14)	112.9(2)
C(12)-C(13)-H(13A)	109.0
C(14)-C(13)-H(13A)	109.0
C(12)-C(13)-H(13B)	109.0
C(14)-C(13)-H(13B)	109.0
H(13A)-C(13)-H(13B)	107.8
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(10)-N(1)-C(6)	128.2(2)
C(10)-N(1)-C(5)	110.25(17)
C(6)-N(1)-C(5)	121.50(18)

Symmetry transformations used to generate equivalent atoms:

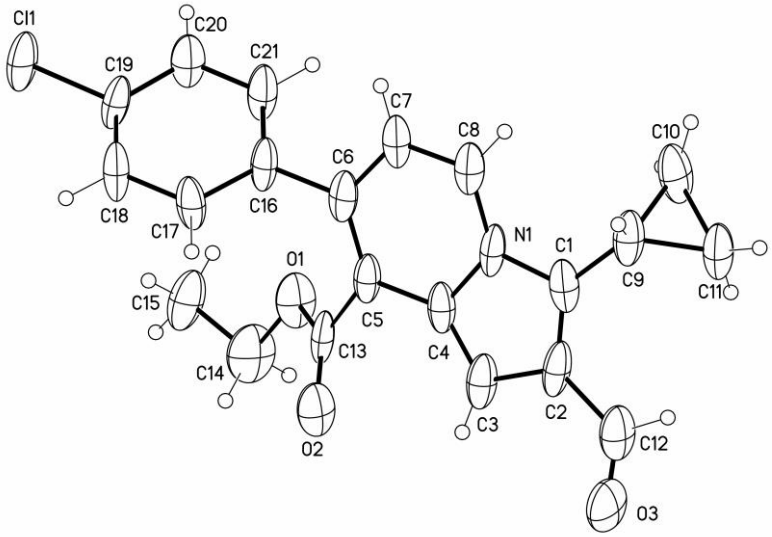
Table S24. Anisotropic displacement parameters ($Å^2$x 10^3)for d19548. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	45(1)	43(1)	30(1)	-4(1)	-9(1)	-1(1)
C(2)	32(1)	36(1)	26(1)	1(1)	-6(1)	-1(1)
C(3)	32(1)	35(1)	28(1)	1(1)	-6(1)	0(1)
C(4)	55(1)	37(1)	41(1)	-2(1)	-11(1)	-2(1)
C(5)	35(1)	33(1)	26(1)	2(1)	-3(1)	0(1)
C(6)	38(1)	29(1)	28(1)	5(1)	-6(1)	2(1)
C(7)	34(1)	38(1)	26(1)	5(1)	-5(1)	-1(1)
C(8)	56(1)	35(1)	29(1)	5(1)	-8(1)	1(1)
C(9)	51(1)	43(1)	25(1)	2(1)	-9(1)	2(1)
C(10)	35(1)	41(1)	21(1)	0(1)	-3(1)	1(1)
C(11)	37(1)	39(1)	25(1)	-2(1)	-4(1)	2(1)
C(12)	37(1)	47(1)	26(1)	-2(1)	-6(1)	2(1)
C(13)	39(1)	48(1)	31(1)	-8(1)	-5(1)	0(1)
C(14)	59(2)	65(2)	33(1)	-14(1)	-9(1)	1(1)
N(1)	34(1)	33(1)	21(1)	3(1)	-6(1)	1(1)
O(1)	77(1)	56(1)	30(1)	2(1)	-19(1)	5(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d19548.

	x	y	z	U(eq)
H(1)	5880	911	2777	47
H(4A)	5915	-740	4285	66
H(4B)	8006	-699	4111	66
H(4C)	6555	-607	3521	66
H(6)	6779	6321	4308	38
H(7)	6000	5223	3283	39
H(8)	7966	451	5368	48
H(9)	8554	2837	6166	48
H(11A)	6782	6785	5555	40
H(11B)	8845	6832	5343	40
H(12A)	7609	5802	6641	44
H(12B)	9672	5864	6428	44
H(13A)	7422	8762	6531	47
H(13B)	9482	8829	6313	47
H(14A)	10333	7861	7393	78
H(14B)	8273	7800	7611	78
H(14C)	9208	9570	7453	78

(F) X-ray crystallographic data of compound (7b).



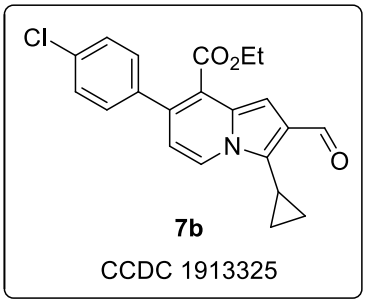


Table S26. Crystal data and structure refinement for 190231lt_0m_a.

Identification code	190231lt_0m_a	
Empirical formula	C21 H18 Cl N O3	
Formula weight	367.81	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.421(2) Å	a= 90°.
	b = 9.1933(15) Å	b= 91.484(4)°.
	c = 14.5321(18) Å	g = 90°.
Volume	1792.4(5) Å^3	
Z	4	

Density (calculated)	1.363 Mg/m^3
Absorption coefficient	0.234 mm^{-1}
F(000)	768
Crystal size	0.12 x 0.10 x 0.03 mm^3
Theta range for data collection	1.518 to 26.446°.
Index ranges	-16<=h<=16, -11<=k<=11, -18<=l<=10
Reflections collected	9874
Independent reflections	3700 [R(int) = 0.0336]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6583
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3700 / 0 / 237
Goodness-of-fit on F^2	2.432
Final R indices [I>2sigma(I)]	R1 = 0.1746, wR2 = 0.4876
R indices (all data)	R1 = 0.1943, wR2 = 0.5549
Extinction coefficient	0.06(2)
Largest diff. peak and hole	1.805 and -2.806 $e.Å^{-3}$

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 190231lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8515(4)	6420(7)	2817(5)	46(2)
C(2)	8424(4)	6637(7)	3763(5)	49(2)
C(3)	7419(4)	6835(7)	3969(5)	48(2)
C(4)	6876(4)	6749(6)	3163(4)	40(1)
C(5)	5845(4)	6772(6)	2911(4)	39(1)
C(6)	5546(4)	6686(6)	1984(4)	41(1)
C(7)	6286(4)	6509(7)	1301(4)	45(2)
C(8)	7269(4)	6421(7)	1546(4)	46(2)
C(9)	9360(4)	6126(7)	2230(5)	49(2)
C(10)	9450(4)	4665(8)	1768(5)	58(2)
C(11)	10162(5)	5060(8)	2539(5)	55(2)
C(12)	9245(5)	6672(8)	4438(5)	56(2)
C(13)	5138(4)	6748(6)	3685(4)	42(2)
C(14)	3639(5)	5723(11)	4242(6)	70(2)
C(15)	2656(5)	5481(10)	3755(5)	63(2)
C(16)	4488(4)	6797(6)	1683(5)	44(2)
C(17)	3912(5)	7961(6)	1952(5)	46(2)
C(18)	2921(5)	8080(7)	1649(5)	49(2)
C(19)	2522(4)	7027(7)	1089(5)	45(2)
C(20)	3082(5)	5859(7)	793(4)	50(2)
C(21)	4073(5)	5752(7)	1093(5)	55(2)
Cl(1)	1292(1)	7196(2)	686(1)	58(1)
N(1)	7566(3)	6523(5)	2465(4)	44(1)
O(1)	4384(3)	5836(5)	3514(3)	54(1)
O(2)	5265(3)	7413(5)	4388(3)	54(1)
O(3)	9137(4)	6938(7)	5250(4)	64(2)

Table S28. Bond lengths [Å] and angles [°] for 190231lt_0m_a.

C(1)-N(1)	1.363(8)
C(1)-C(2)	1.398(10)
C(1)-C(9)	1.461(8)
C(2)-C(3)	1.401(9)
C(2)-C(12)	1.456(9)
C(3)-C(4)	1.365(9)
C(3)-H(3)	0.9500
C(4)-N(1)	1.406(8)
C(4)-C(5)	1.422(8)
C(5)-C(6)	1.399(8)
C(5)-C(13)	1.490(8)
C(6)-C(7)	1.432(8)
C(6)-C(16)	1.479(8)
C(7)-C(8)	1.360(8)
C(7)-H(7)	0.9500
C(8)-N(1)	1.388(8)
C(8)-H(8)	0.9500
C(9)-C(10)	1.508(10)
C(9)-C(11)	1.516(9)
C(9)-H(9)	1.0000
C(10)-C(11)	1.497(9)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-O(3)	1.218(9)
C(12)-H(12)	0.9500
C(13)-O(2)	1.199(8)
C(13)-O(1)	1.333(7)
C(14)-O(1)	1.478(8)
C(14)-C(15)	1.497(10)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.382(8)
C(16)-C(21)	1.393(9)
C(17)-C(18)	1.394(9)
C(17)-H(17)	0.9500
C(18)-C(19)	1.365(10)
C(18)-H(18)	0.9500
C(19)-C(20)	1.385(9)
C(19)-Cl(1)	1.744(6)
C(20)-C(21)	1.392(9)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500

N(1)-C(1)-C(2)	104.7(5)
N(1)-C(1)-C(9)	121.7(6)
C(2)-C(1)-C(9)	133.5(6)
C(1)-C(2)-C(3)	109.7(6)
C(1)-C(2)-C(12)	125.6(6)
C(3)-C(2)-C(12)	124.7(7)
C(4)-C(3)-C(2)	107.8(6)
C(4)-C(3)-H(3)	126.1
C(2)-C(3)-H(3)	126.1
C(3)-C(4)-N(1)	106.3(5)
C(3)-C(4)-C(5)	135.6(6)
N(1)-C(4)-C(5)	118.1(5)
C(6)-C(5)-C(4)	120.1(5)
C(6)-C(5)-C(13)	123.6(5)
C(4)-C(5)-C(13)	116.1(5)
C(5)-C(6)-C(7)	119.1(6)
C(5)-C(6)-C(16)	122.1(6)
C(7)-C(6)-C(16)	118.8(5)
C(8)-C(7)-C(6)	120.8(6)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(7)-C(8)-N(1)	120.0(5)

C(7)-C(8)-H(8)	120.0
N(1)-C(8)-H(8)	120.0
C(1)-C(9)-C(10)	119.8(5)
C(1)-C(9)-C(11)	120.2(6)
C(10)-C(9)-C(11)	59.3(4)
C(1)-C(9)-H(9)	115.3
C(10)-C(9)-H(9)	115.3
C(11)-C(9)-H(9)	115.3
C(11)-C(10)-C(9)	60.6(4)
C(11)-C(10)-H(10A)	117.7
C(9)-C(10)-H(10A)	117.7
C(11)-C(10)-H(10B)	117.7
C(9)-C(10)-H(10B)	117.7
H(10A)-C(10)-H(10B)	114.8
C(10)-C(11)-C(9)	60.1(4)
C(10)-C(11)-H(11A)	117.8
C(9)-C(11)-H(11A)	117.8
C(10)-C(11)-H(11B)	117.8
C(9)-C(11)-H(11B)	117.8
H(11A)-C(11)-H(11B)	114.9
O(3)-C(12)-C(2)	123.4(7)
O(3)-C(12)-H(12)	118.3
C(2)-C(12)-H(12)	118.3
O(2)-C(13)-O(1)	124.7(6)
O(2)-C(13)-C(5)	123.8(5)
O(1)-C(13)-C(5)	111.4(5)
O(1)-C(14)-C(15)	106.0(6)
O(1)-C(14)-H(14A)	110.5
C(15)-C(14)-H(14A)	110.5
O(1)-C(14)-H(14B)	110.5
C(15)-C(14)-H(14B)	110.5
H(14A)-C(14)-H(14B)	108.7
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5

H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	119.3(6)
C(17)-C(16)-C(6)	120.6(6)
C(21)-C(16)-C(6)	120.0(5)
C(16)-C(17)-C(18)	120.5(6)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	119.3(6)
C(19)-C(18)-H(18)	120.4
C(17)-C(18)-H(18)	120.4
C(18)-C(19)-C(20)	121.8(6)
C(18)-C(19)-Cl(1)	119.4(5)
C(20)-C(19)-Cl(1)	118.8(5)
C(19)-C(20)-C(21)	118.6(6)
C(19)-C(20)-H(20)	120.7
C(21)-C(20)-H(20)	120.7
C(20)-C(21)-C(16)	120.5(6)
C(20)-C(21)-H(21)	119.8
C(16)-C(21)-H(21)	119.8
C(1)-N(1)-C(8)	126.7(5)
C(1)-N(1)-C(4)	111.5(5)
C(8)-N(1)-C(4)	121.8(5)
C(13)-O(1)-C(14)	115.8(5)

Symmetry transformations used to generate equivalent atoms:

Table S29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 190231lt_0m_a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(3)	23(3)	92(4)	-9(3)	-2(3)	0(2)
C(2)	23(3)	23(3)	100(4)	-1(3)	-21(3)	-2(2)
C(3)	24(3)	27(3)	92(4)	4(3)	-9(3)	-3(2)
C(4)	22(3)	20(3)	77(3)	2(2)	0(2)	1(2)
C(5)	21(3)	19(3)	75(3)	-1(2)	-7(2)	0(2)
C(6)	27(3)	16(3)	78(3)	5(2)	-7(2)	0(2)
C(7)	24(3)	27(3)	83(3)	1(3)	-1(2)	3(2)
C(8)	26(3)	30(3)	81(3)	1(3)	-4(2)	2(2)
C(9)	25(3)	29(3)	93(4)	4(3)	-6(3)	-2(2)
C(10)	26(3)	39(4)	110(5)	-9(4)	7(3)	-3(3)
C(11)	27(3)	39(4)	99(4)	-5(3)	-7(3)	6(3)
C(12)	29(4)	38(4)	100(5)	-11(3)	-12(3)	-4(3)
C(13)	17(3)	23(3)	87(4)	2(3)	-13(2)	2(2)
C(14)	38(4)	73(6)	98(5)	1(4)	0(3)	-20(4)
C(15)	30(4)	58(5)	101(4)	13(4)	-17(3)	-5(3)
C(16)	24(3)	20(3)	87(3)	4(3)	-9(3)	2(2)
C(17)	29(3)	20(3)	90(4)	-6(3)	-1(3)	3(2)
C(18)	21(3)	24(3)	102(4)	8(3)	0(3)	4(2)
C(19)	21(3)	34(3)	80(3)	9(3)	-15(2)	0(2)
C(20)	32(3)	30(3)	89(4)	-5(3)	-8(3)	-1(3)
C(21)	32(3)	29(3)	103(4)	-9(3)	-17(3)	6(3)
Cl(1)	20(1)	49(1)	103(1)	7(1)	-12(1)	0(1)
N(1)	20(2)	24(3)	87(3)	-2(2)	-14(2)	2(2)
O(1)	32(2)	37(3)	92(3)	0(2)	1(2)	-12(2)
O(2)	31(3)	38(3)	94(3)	-10(2)	-6(2)	-7(2)
O(3)	29(3)	74(4)	89(3)	-9(3)	-13(2)	-4(2)

Table S30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 190231lt_0m_a.

	x	y	z	U(eq)
H(3)	7161	7000	4562	57
H(7)	6088	6452	670	53
H(8)	7753	6291	1087	55
H(9)	9597	6975	1865	59
H(10A)	8935	3926	1893	70
H(10B)	9710	4643	1137	70
H(11A)	10859	5283	2382	66
H(11B)	10083	4565	3138	66
H(12)	9899	6477	4234	67
H(14A)	3625	6628	4610	84
H(14B)	3800	4898	4659	84
H(15A)	2501	6317	3359	95
H(15B)	2135	5369	4210	95
H(15C)	2690	4599	3379	95
H(17)	4193	8685	2346	56
H(18)	2527	8884	1831	59
H(20)	2795	5145	395	61
H(21)	4469	4961	894	66

7. Cartesian Coordinates for Optimized Structures

A

C1	2.8651898575	0.8815578228	0.5226673070
C2	2.2773073053	1.2849595545	-0.6192363583
C3	1.6031370236	1.5369007244	-1.7079764976
C4	0.4242174207	0.6723039790	-2.1960347307
H5	3.6270301734	0.1033375407	0.5059824235
H6	2.4175997014	1.1215311090	1.4861371170
H7	1.8444244762	2.4038132724	-2.3184219791
H8	0.7246883646	0.2522519480	-3.1721543820
C9	0.1128219228	-0.4222044146	-1.2835104341
C10	-0.1261229272	-1.3357857040	-0.5263559446
C11	-0.4051601532	-2.4124370223	0.3707231202
C12	-0.0836002746	-3.7359965254	0.0173988421
C13	-0.9981055037	-2.1586686421	1.6213223444
C14	-0.3466380457	-4.7789452037	0.9006254569
H15	0.3690882690	-3.9344633425	-0.9487515826
C16	-1.2593765774	-3.2080894470	2.4970432196
H17	-1.2541422496	-1.1391530710	1.8914718954
C18	-0.9331660965	-4.5185563043	2.1410339027
H19	-0.0959544288	-5.7976479188	0.6196195059
H20	-1.7205614019	-3.0040298942	3.4589498066
H21	-1.1385713290	-5.3353104128	2.8268753810
O22	-0.7161236049	1.5021135632	-2.3585584399
C23	-0.7795550461	2.1749391471	-3.6087140733
H24	-1.7336923905	2.7046052014	-3.6260502420
H25	0.0301684367	2.9099042540	-3.7334909435

H26	-0.7468913769	1.4667808545	-4.4488759768
Au27	4.0362122049	2.7933495115	-0.0137722677
C28	6.2561043013	6.3057564813	-0.8886698417
C29	6.9460214759	5.8745781962	0.1984508569
H30	6.3906553408	7.1651910666	-1.5258207435
H31	7.8064804857	6.2804057315	0.7058838892
C32	5.2758715007	4.4065696849	-0.1711676768
N33	5.2321970877	5.3935846452	-1.1012030276
N34	6.3293731361	4.7083275385	0.6271504213
C35	6.7499363513	3.9400324900	1.7801173415
C36	7.7268768749	2.9403716102	1.6003141359
C37	6.1741290155	4.2468831619	3.0288397937
C38	8.1084245639	2.2154768731	2.7352770914
C39	6.5954580391	3.4866709664	4.1258285178
C40	7.5477731750	2.4815725836	3.9814235401
H41	8.8581591406	1.4356020618	2.6424555572
H42	6.1764944495	3.6891556679	5.1069281197
H43	7.8614152070	1.9068093766	4.8481833834
C44	4.2549380209	5.5085969566	-2.1626260610
C45	4.5380741563	4.9028047811	-3.4030537537
C46	3.0832828073	6.2508189538	-1.9125227594
C47	3.5806912170	5.0494020204	-4.4141730809
C48	2.1646468839	6.3630045624	-2.9628021630
C49	2.4084638208	5.7690983317	-4.1980813977
H50	3.7609736270	4.6032332350	-5.3872487845
H51	1.2503668127	6.9291865301	-2.8126998784
H52	1.6854111165	5.8777427619	-5.0017162100
C53	2.7937177809	6.9261626126	-0.5738796876
H54	3.6386071080	6.7385041412	0.0960215969

C55	5.8234767306	4.1244956242	-3.6768448150
H56	6.4357709280	4.1431711071	-2.7699855576
C57	2.6677931439	8.4547963828	-0.7307943599
H58	1.8128096003	8.7268060575	-1.3582757009
H59	2.5224793442	8.9259189018	0.2467916884
H60	3.5647857744	8.8875968215	-1.1852872153
C61	1.5404954475	6.3310595965	0.0972366529
H62	0.6422058160	6.5025088539	-0.5050516694
H63	1.6429252397	5.2509258636	0.2468311416
H64	1.3755687604	6.7953864072	1.0750971405
C65	5.5309441139	2.6449372375	-3.9956521227
H66	4.9838686229	2.1617328785	-3.1784252555
H67	4.9349533500	2.5401135001	-4.9084680955
H68	6.4660753179	2.0954363473	-4.1471036676
C69	6.6512182446	4.7821495649	-4.7992760576
H70	7.5960078458	4.2464832193	-4.9383320784
H71	6.1185684135	4.7660750300	-5.7558626933
H72	6.8851349536	5.8259426866	-4.5667041204
C73	8.3706104637	2.6374139963	0.2482826421
H74	7.9584503376	3.3305740982	-0.4918072911
C75	5.1437042161	5.3583437684	3.2194430529
H76	4.9775463746	5.8428409704	2.2520568958
C77	3.7859103505	4.7973353958	3.6848326682
H78	3.3950840114	4.0611246226	2.9738993768
H79	3.8660386285	4.3104911008	4.6623114723
H80	3.0509838380	5.6039258262	3.7761407078
C81	5.6571483718	6.4432177011	4.1870384286
H82	6.6083935914	6.8657619519	3.8481050584
H83	4.9311889796	7.2595282595	4.2613862097

H84	5.8102903035	6.0449667414	5.1952924814
C85	9.8947145287	2.8679412854	0.2839701203
H86	10.3917253717	2.1770889310	0.9726536514
H87	10.3260979450	2.7101972178	-0.7100393904
H88	10.1393692490	3.8867156919	0.6013303221
C89	8.0352068089	1.2107302496	-0.2295122872
H90	8.4358818201	0.4536285225	0.4526428698
H91	6.9524247805	1.0593986015	-0.2999094125
H92	8.4686633568	1.0277097804	-1.2184409335

AB-TS

C1	2.7158356927	0.4793390408	0.1989515751
C2	2.8240438109	1.5339912226	-0.7212136851
C3	1.8641923302	2.0191497169	-1.4985126637
C4	0.4666610465	1.4243091674	-1.3237382099
H5	3.0572293210	-0.5187499752	-0.0708655296
H6	2.6798824867	0.6845251249	1.2673690566
H7	1.9748820481	2.8310766041	-2.2081224411
H8	0.1017361511	1.0268496759	-2.2876607066
C9	0.5417195217	0.3014270586	-0.3539122764
C10	0.3413820847	-0.6291643050	0.4199505721
C11	0.1893293265	-1.6932118635	1.3483671226
C12	0.3765149287	-3.0302558378	0.9390743125
C13	-0.1367032652	-1.4132277393	2.6924299062
C14	0.2455821503	-4.0613668271	1.8623619351
H15	0.6200759427	-3.2434631342	-0.0970336603
C16	-0.2648810006	-2.4534936571	3.6053924921

H17	-0.2872930201	-0.3835029307	3.0012518088
C18	-0.0724027263	-3.7752480904	3.1931680989
H19	0.3899587308	-5.0899814048	1.5467405875
H20	-0.5158639220	-2.2366847971	4.6391522028
H21	-0.1728900896	-4.5845747881	3.9104286811
O22	-0.3842746556	2.4614515210	-0.8800966589
C23	-1.7726623930	2.1617012961	-0.9846126813
H24	-2.3085490644	3.0627733016	-0.6821306468
H25	-2.0503414517	1.9040971033	-2.0168025122
H26	-2.0584413557	1.3331750364	-0.3222226339
Au27	4.8180315499	2.1359219653	-0.4226621709
C28	8.7243763759	3.3982705495	0.7613344625
C29	8.5686436720	4.1630733505	-0.3495655911
H30	9.5331417185	3.3259938268	1.4707105575
H31	9.2124965374	4.8966390869	-0.8077828236
C32	6.7112649753	2.8945937901	-0.1329583622
N33	7.5768576060	2.6254891872	0.8788767184
N34	7.3299309497	3.8400224661	-0.8852058636
C35	6.7862758573	4.4124209573	-2.0975098438
C36	5.9837159201	5.5654832864	-1.9963583708
C37	7.0914860531	3.7886661173	-3.3238188611
C38	5.4646383915	6.0858731425	-3.1875412990
C39	6.5460001105	4.3563232851	-4.4806938977
C40	5.7398255092	5.4889925121	-4.4143682745
H41	4.8392216235	6.9729480893	-3.1532864235
H42	6.7561377959	3.9051903767	-5.4459052619
H43	5.3273194169	5.9122677428	-5.3258580626
C44	7.3686468228	1.6379402944	1.9151532474
C45	6.7312533981	2.0322716699	3.1074698526

C46	7.8381900436	0.3282443298	1.6894199411
C47	6.5599792630	1.0529479953	4.0932130867
C48	7.6390606988	-0.6069665482	2.7113162715
C49	7.0069512452	-0.2506703772	3.8990974284
H50	6.0765954856	1.3183175815	5.0288390570
H51	7.9889334709	-1.6262079583	2.5764097513
H52	6.8688864946	-0.9919049084	4.6813618854
C53	6.2413323019	3.4558625402	3.3596460468
H54	6.4718556868	4.0582756208	2.4762029930
C55	4.7125695654	3.4986094479	3.5519444319
H56	4.1930467052	3.0943068029	2.6762972945
H57	4.4009732677	2.9198377594	4.4282256598
H58	4.3747971021	4.5299298920	3.6990731834
C59	6.9715923624	4.0986593061	4.5558316802
H60	8.0567584164	4.0969001870	4.4109071359
H61	6.6493154369	5.1371475855	4.6856659550
H62	6.7604811517	3.5676176538	5.4900673843
C63	8.5410439282	-0.0937849215	0.4007184172
H64	8.6191959752	0.7812416956	-0.2513420570
C65	7.7238482779	-1.1554644604	-0.3617537162
H66	7.6155263918	-2.0749703490	0.2235196721
H67	6.7206517623	-0.7862005367	-0.6004156439
H68	8.2217165414	-1.4177260316	-1.3015279360
C69	9.9762052723	-0.5859878433	0.6738565864
H70	10.4819588977	-0.8243911289	-0.2677328464
H71	10.5690522948	0.1739484990	1.1930023051
H72	9.9829001553	-1.4909904846	1.2902572703
C73	5.6732757230	6.2497505847	-0.6671642433
H74	6.1867648397	5.7015644273	0.1289567963

C75	6.2062070692	7.6958837786	-0.6409513550
H76	5.7087627898	8.3220027309	-1.3889340789
H77	6.0285189187	8.1488269133	0.3400710483
H78	7.2820594498	7.7307840732	-0.8405186396
C79	4.1654350365	6.2067524825	-0.3507896682
H80	3.5826791347	6.7541575209	-1.0991142675
H81	3.7939857175	5.1767459800	-0.3233381718
H82	3.9670883437	6.6658383844	0.6236344432
C83	7.9715541113	2.5448720742	-3.4285508386
H84	8.3137235903	2.2797266418	-2.4234630517
C85	7.1771103744	1.3401038804	-3.9698228376
H86	6.3082609280	1.1227140079	-3.3395859247
H87	6.8168875539	1.5219810656	-4.9877940676
H88	7.8109609957	0.4471260146	-3.9974087040
C89	9.2285335755	2.8102597367	-4.2803366466
H90	9.8118164061	3.6480938263	-3.8849591524
H91	9.8731468067	1.9250289101	-4.2926598611
H92	8.9707141262	3.0448825252	-5.3182462446

B

C1	4.0128649356	0.6392856083	-0.6431596473
C2	4.7619797343	1.5804568952	-1.5590312444
C3	4.1890247261	1.6483878385	-2.7645087721
C4	2.9337724260	0.8079991683	-2.9471401444
H5	4.6293338645	-0.1811736233	-0.2624429001
H6	3.5714642196	1.1483288650	0.2211791038
H7	4.5208795025	2.2638220054	-3.5962527491
H8	3.0217249901	0.0693572387	-3.7603072407

C9	2.8872305918	0.0775294768	-1.5672519473
C10	2.0557753330	-0.8444975256	-1.2803027283
C11	1.1051915740	-1.7995547772	-0.9808917550
C12	1.3769717067	-3.1826182966	-1.1962239511
C13	-0.1685302264	-1.3985052210	-0.4789065137
C14	0.4021381509	-4.1242863558	-0.9211017695
H15	2.3485872746	-3.4756325659	-1.5789600075
C16	-1.1313388002	-2.3557747585	-0.2105132633
H17	-0.3636291998	-0.3423646513	-0.3248960485
C18	-0.8464392508	-3.7112687520	-0.4320213351
H19	0.5994168144	-5.1785721644	-1.0847446027
H20	-2.1044574420	-2.0599104807	0.1672909484
H21	-1.6080207602	-4.4565397660	-0.2208186260
O22	1.7528126557	1.5567450983	-3.1189658169
C23	1.4107615354	1.8016053920	-4.4795702344
H24	0.4498642804	2.3191501917	-4.4713834018
H25	2.1526396729	2.4382466905	-4.9788795337
H26	1.3117595295	0.8629154230	-5.0445526422
Au27	6.4101854470	2.6267771841	-0.9241981048
C28	9.7327851375	4.5885783977	0.9369832796
C29	9.7416644197	5.2380312904	-0.2546567333
H30	10.3599278193	4.6876546090	1.8084499829
H31	10.3785587976	6.0198766120	-0.6366476933
C32	8.0473129009	3.7345650984	-0.3140654424
N33	8.6900806794	3.6726471922	0.8827810777
N34	8.7050164452	4.7019126179	-1.0076113060
C35	8.3483415299	2.7657424976	1.9544655266
C36	7.4014141272	3.1776998731	2.9118603598
C37	8.9772030325	1.5056065336	1.9893866488

C38	7.0930235961	2.2751768091	3.9363784920
C39	8.6301233604	0.6451906993	3.0372053076
C40	7.7004903065	1.0246800362	4.0009573731
H41	6.3696354483	2.5579466646	4.6955773518
H42	9.0955470694	-0.3342233873	3.0990007017
H43	7.4490371893	0.3421150309	4.8081556759
C44	8.3815775411	5.1149301268	-2.3543595433
C45	9.0123119623	4.4538181908	-3.4264963515
C46	7.4589531670	6.1638668953	-2.5338684880
C47	8.6867432997	4.8774659365	-4.7198377237
C48	7.1738677815	6.5463284461	-3.8499327252
C49	7.7787720872	5.9109511492	-4.9305199252
H50	9.1537622587	4.3939890675	-5.5728620888
H51	6.4689859807	7.3528350678	-4.0298960301
H52	7.5441712846	6.2264949167	-5.9434644393
C53	6.7188891625	4.5425618896	2.8698177432
H54	7.1000091940	5.0895781229	2.0026940623
C55	5.1954797247	4.3998379791	2.6812230547
H56	4.9638524153	3.8560529898	1.7592387560
H57	4.7355214385	3.8635350667	3.5184532573
H58	4.7246350702	5.3871958627	2.6212062889
C59	7.0504566609	5.3786101377	4.1213632559
H60	8.1306903387	5.5111201039	4.2400083540
H61	6.5938528063	6.3713826133	4.0477987653
H62	6.6707404983	4.9068961273	5.0338655326
C63	6.7762086971	6.8773764848	-1.3695686307
H64	7.1279413595	6.4250538946	-0.4375968260
C65	5.2470529401	6.6860655061	-1.4146985625
H66	4.8118325861	7.1346945357	-2.3142212459

H67	4.9817733177	5.6238935190	-1.4036678266
H68	4.7785300639	7.1645258951	-0.5475708738
C69	7.1516466644	8.3718420516	-1.3258451210
H70	6.6942533735	8.8550202940	-0.4558728889
H71	8.2356202046	8.5115980848	-1.2595469080
H72	6.8027064470	8.9006828805	-2.2192280809
C73	10.0220810196	3.3261341586	-3.2263527181
H74	10.1138592654	3.1352120210	-2.1531279298
C75	9.5388866382	2.0151184755	-3.8770045156
H76	8.5694708381	1.7087234465	-3.4705720865
H77	9.4341494137	2.1178611123	-4.9623409656
H78	10.2578341268	1.2099807791	-3.6894193558
C79	11.4190129050	3.7254544628	-3.7429976085
H80	12.1409420717	2.9246342108	-3.5501954484
H81	11.4106611863	3.9104895928	-4.8224070942
H82	11.7836099889	4.6344318774	-3.2533943763
C83	9.9913033578	1.0563209452	0.9400291922
H84	10.1395498283	1.8779656278	0.2331574931
C85	9.4607322591	-0.1445544633	0.1319073585
H86	9.3020404983	-1.0191185818	0.7723396574
H87	8.5102781064	0.0975275228	-0.3551044432
H88	10.1795633493	-0.4283917110	-0.6446612658
C89	11.3623750373	0.7437029834	1.5700197802
H90	12.0867075453	0.4802046654	0.7919801219
H91	11.7556924666	1.6039984091	2.1211484475
H92	11.3050848923	-0.0994478006	2.2664896893

BC-TS

C1	3.3801190947	0.1007305773	1.0324121060
C2	3.6153214680	0.9891696445	-0.1757760315
C3	2.5676644633	0.9816045406	-1.0241829354
C4	1.4654039942	0.0159642824	-0.8651735689
H5	4.1024175496	-0.7269678662	1.0671533784
H6	3.5245972221	0.6644467032	1.9614371459
H7	2.4588524626	1.6602845413	-1.8676162737
H8	1.6147219655	-1.0231614873	-1.1774321432
C9	1.9761320642	-0.4292353884	1.0173107496
C10	1.0290519776	-0.9845853765	1.5989897952
C11	-0.1232738320	-1.5793169124	2.1459757414
C12	-0.3387207156	-2.9729645130	2.0170025067
C13	-1.0753442332	-0.7831543089	2.8279536811
C14	-1.4853996085	-3.5466299336	2.5475223270
H15	0.3984238315	-3.5797476173	1.5006132202
C16	-2.2171583289	-1.3714893694	3.3538801455
H17	-0.9004926736	0.2831931252	2.9285088466
C18	-2.4235911470	-2.7484016338	3.2123195670
H19	-1.6540268213	-4.6141599017	2.4465690197
H20	-2.9493166972	-0.7626167669	3.8747844019
H21	-3.3199196988	-3.2028914858	3.6242781714
O22	0.2537334658	0.4923587022	-1.1205719096
C23	-0.7952779108	-0.4421044965	-1.4396745430
H24	-1.5662924695	0.1294592473	-1.9558647070
H25	-0.4194788256	-1.2366837330	-2.0922876434
H26	-1.2012549436	-0.8683338181	-0.5193665625
Au27	5.3118430827	2.1175641080	-0.3630516761

C28	8.9802708951	4.2594746766	0.1063234034
C29	8.5798647697	4.8161013676	-1.0650614338
H30	9.8523949818	4.4308576125	0.7167044409
H31	9.0307093239	5.5731980640	-1.6864040122
C32	7.0106486005	3.2948151810	-0.4678070638
N33	8.0087341814	3.3315800553	0.4562619793
N34	7.3734373450	4.2148319296	-1.4009102759
C35	8.0566309594	2.5035352778	1.6397022518
C36	8.7245583209	1.2655626176	1.5636444661
C37	7.4298655695	2.9674613799	2.8129275811
C38	8.7508974469	0.4802699520	2.7219750188
C39	7.4870615363	2.1384436973	3.9393776947
C40	8.1396546240	0.9098336874	3.8962733426
H41	9.2565327524	-0.4807230985	2.7029092438
H42	7.0162053848	2.4616068930	4.8631866713
H43	8.1753935166	0.2846034198	4.7842008992
C44	6.6184639926	4.5325405545	-2.5921107776
C45	6.8829751149	3.8032465770	-3.7677529682
C46	5.6684319315	5.5704692519	-2.5295403264
C47	6.1456534211	4.1392974597	-4.9089592474
C48	4.9618389970	5.8624216461	-3.7019959244
C49	5.1956353358	5.1557892279	-4.8779001992
H50	6.3206942919	3.5990113519	-5.8346540469
H51	4.2206394975	6.6561689099	-3.6937825871
H52	4.6377276932	5.4023133636	-5.7770301728
C53	5.3898984079	6.3655816680	-1.2562780842
H54	6.0638928929	6.0053125680	-0.4732572009
C55	3.9498124285	6.1341840935	-0.7577654194
H56	3.2124025994	6.4857763622	-1.4874772049

H57	3.7628604038	5.0711794176	-0.5730636922
H58	3.7775078449	6.6793276062	0.1768271514
C59	5.6792906568	7.8668907646	-1.4508840416
H60	5.5323042994	8.4080532763	-0.5101156639
H61	6.7089406754	8.0370602275	-1.7817922998
H62	5.0127648546	8.3138112977	-2.1960198197
C63	7.9192420804	2.6840222638	-3.8339603194
H64	8.4020668947	2.6058213955	-2.8552935439
C65	7.2531246112	1.3240797704	-4.1210342278
H66	6.5023567199	1.0850795326	-3.3605817370
H67	6.7583581786	1.3196340545	-5.0982782142
H68	8.0028775385	0.5252585627	-4.1249134358
C69	9.0241706945	2.9938702644	-4.8627262441
H70	9.7868196305	2.2079565493	-4.8500895459
H71	8.6250345628	3.0494972093	-5.8809208611
H72	9.5172477601	3.9471638535	-4.6464414786
C73	9.3892900289	0.7592088588	0.2854624832
H74	9.2931401443	1.5342103034	-0.4807539467
C75	8.6780543392	-0.4991086404	-0.2511122670
H76	8.7457224229	-1.3302977333	0.4593106362
H77	7.6179036453	-0.3015268574	-0.4420678985
H78	9.1385561036	-0.8262967758	-1.1898262706
C79	10.8955396093	0.5054352262	0.4885071997
H80	11.3606483827	0.2036234944	-0.4558958466
H81	11.4084299514	1.4040650071	0.8461507068
H82	11.0776161799	-0.2930327570	1.2154006870
C83	6.7012081365	4.3072210154	2.8901430012
H84	6.8077727827	4.8103335449	1.9244910188
C85	5.1915527559	4.1097568572	3.1341057422

H86	4.7426125825	3.5002324432	2.3425458506
H87	5.0031169628	3.6160680100	4.0940302130
H88	4.6779620657	5.0772384517	3.1513715311
C89	7.3217226627	5.2309599854	3.9559981659
H90	8.3884027186	5.3944227187	3.7720081688
H91	6.8236549881	6.2062605289	3.9497124260
H92	7.2178772934	4.8141087506	4.9633206436

C

C1	2.5746975099	0.2475397579	-0.2240175585
C2	2.8090551353	1.6974782973	0.1217531648
C3	1.8372323445	2.6187159171	0.5254858684
C4	0.4798665623	2.3532162443	0.6742660392
H5	3.0067354354	0.1194491148	-1.2301918241
H6	3.2788748168	-0.3160058653	0.4098513524
H7	2.1778663561	3.6272472234	0.7381544082
H8	0.0635124865	1.3701106032	0.4792731274
C9	1.2662047444	-0.4024156154	-0.1784082486
C10	0.2309630561	-1.0348459999	-0.1731162051
C11	-1.0019501261	-1.7591855291	-0.1589267809
C12	-1.8397272066	-1.7592501672	-1.2902608115
C13	-1.3888559049	-2.4817939818	0.9855146595
C14	-3.0384408276	-2.4664679306	-1.2717931479
H15	-1.5403459801	-1.2071569710	-2.1758402253
C16	-2.5892208310	-3.1861025214	0.9939931909
H17	-0.7416092330	-2.4870930036	1.8570658812
C18	-3.4162506231	-3.1794199337	-0.1316313765

H19	-3.6788830855	-2.4631542441	-2.1489380132
H20	-2.8801792286	-3.7428292649	1.8799077218
H21	-4.3520020085	-3.7308322447	-0.1211656177
O22	-0.4351223979	3.2034458170	1.0487095434
C23	-0.0969927035	4.5772870412	1.3607242523
H24	-1.0398412585	5.0450466470	1.6377162080
H25	0.6049061568	4.6092181191	2.1975352031
H26	0.3278314834	5.0672147340	0.4812409658
Au27	4.7587034656	2.3056891129	-0.0379673961
C28	8.9598586816	2.8203785395	-0.5802117839
C29	8.6400435058	4.0886893509	-0.2110142137
H30	9.9044253881	2.3718436731	-0.8439190981
H31	9.2493341659	4.9696755961	-0.0876358448
C32	6.7313474212	2.8789102151	-0.2102845502
N33	7.7785383933	2.0933309996	-0.5744559321
N34	7.2703355898	4.1061184367	0.0111304696
C35	7.6708822698	0.6906392172	-0.9209997268
C36	7.4214956603	0.3486676091	-2.2649782554
C37	7.8192146375	-0.2669572431	0.1015873980
C38	7.3098009779	-1.0134842902	-2.5671748850
C39	7.6993328536	-1.6134544436	-0.2615687959
C40	7.4463066377	-1.9839692407	-1.5789762980
H41	7.1173440604	-1.3182589821	-3.5915905629
H42	7.8078421078	-2.3819559700	0.4981057214
H43	7.3591313444	-3.0355453723	-1.8378612315
C44	6.5175356498	5.2740704392	0.4195399017
C45	5.9801103780	6.1096305588	-0.5798717844
C46	6.3637114272	5.5240292479	1.7975887158
C47	5.2610211127	7.2338056385	-0.1546210130

C48	5.6354275600	6.6629966815	2.1638178863
C49	5.0911636450	7.5077051009	1.2000477126
H50	4.8342787021	7.9043255863	-0.8946200228
H51	5.4983443614	6.8921663739	3.2163879718
H52	4.5361218850	8.3899718355	1.5069765587
C53	6.9466615715	4.6132137444	2.8755436325
H54	7.4781765605	3.7956511674	2.3803957962
C55	5.8357609276	3.9752691329	3.7330542692
H56	5.2656788556	4.7331754587	4.2811662243
H57	5.1348976959	3.4064804969	3.1122970270
H58	6.2695593658	3.2905592908	4.4697931779
C59	7.9723870890	5.3575404501	3.7522883428
H60	8.4198496024	4.6717869362	4.4794180727
H61	8.7798177830	5.7841497810	3.1485717519
H62	7.5072920338	6.1756413887	4.3121090865
C63	6.1480085411	5.8322646571	-2.0721102565
H64	6.7492223666	4.9256955332	-2.1849386932
C65	4.7895129326	5.5603626710	-2.7483133410
H66	4.2746174673	4.7169879102	-2.2754201877
H67	4.1310852093	6.4339896691	-2.6922076258
H68	4.9320628724	5.3206286594	-3.8075776241
C69	6.9063549178	6.9717710081	-2.7799768550
H70	7.0648954296	6.7246472760	-3.8349500160
H71	6.3489555385	7.9134801234	-2.7415275284
H72	7.8855290365	7.1456247974	-2.3225215968
C73	7.2710581636	1.3853600939	-3.3758875805
H74	7.4227789737	2.3786499804	-2.9425538918
C75	8.3391948616	1.1984177622	-4.4716020224
H76	8.2262676799	0.2384509551	-4.9861051671

H77	8.2535079347	1.9880791451	-5.2253261655
H78	9.3512021445	1.2355150673	-4.0559491294
C79	5.8509785093	1.3617921940	-3.9751689994
H80	5.6286821326	0.3957454746	-4.4409387244
H81	5.0940656874	1.5482282648	-3.2055695081
H82	5.7488387941	2.1329623178	-4.7463244457
C83	8.0966645208	0.1035578104	1.5562761691
H84	8.1826249977	1.1921121914	1.6216273330
C85	9.4320610868	-0.4900573501	2.0461786078
H86	9.6416878359	-0.1625315218	3.0698241674
H87	9.4108778252	-1.5848775182	2.0482396389
H88	10.2670556350	-0.1752680058	1.4121780356
C89	6.9298334811	-0.3151387985	2.4727519287
H90	5.9901923617	0.1486775269	2.1533725105
H91	6.7882659386	-1.4012665590	2.4710000600
H92	7.1266629713	-0.0086054375	3.5057255355

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C1	1.9687074814	-0.3108368697	0.7939088149
C2	2.9494829315	0.8436819733	1.0393853997
C3	2.8012452704	1.7067331086	2.1828325802
C4	1.7604288540	1.6403174407	3.0603502334
H5	2.2494869441	-0.8116211969	-0.1384367197
H6	2.2008405256	-1.0409258275	1.5862666448
H7	3.6008997263	2.4178174235	2.3611286734
H8	0.9313722941	0.9541195166	2.9214597759
C9	0.5330630613	-0.0364468469	0.7484782579

C10	-0.6539237046	0.1684491078	0.6123449213
C11	-2.0492003005	0.4164044313	0.4176839322
C12	-2.6530378640	0.0962757533	-0.8134886862
C13	-2.8347442590	0.9871570718	1.4362039622
C14	-4.0072088539	0.3442404780	-1.0176430332
H15	-2.0505989082	-0.3484555679	-1.5997586936
C16	-4.1887191991	1.2323863488	1.2231986449
H17	-2.3764949751	1.2331127884	2.3893240179
C18	-4.7782066992	0.9132065758	-0.0017658302
H19	-4.4630457283	0.0915021168	-1.9707306860
H20	-4.7868949389	1.6720427080	2.0160586687
H21	-5.8350234071	1.1048098300	-0.1634560046
O22	1.6055092145	2.3379262564	4.1792960160
C23	2.5817017984	3.3313554147	4.5235177855
H24	2.2331312280	3.7781520045	5.4539935636
H25	3.5632319218	2.8702481874	4.6746203465
H26	2.6463067323	4.0958158885	3.7424215287
Au27	4.8714310059	0.4646275569	0.3397431997
C28	8.5537405415	-1.2853337000	-0.9364149992
C29	9.0039890158	-0.0309864668	-0.6782455294
H30	9.0662371307	-2.1720938547	-1.2734861632
H31	9.9895430082	0.4013881889	-0.7446224730
C32	6.7782469554	-0.0515571378	-0.2647468593
N33	7.1902086693	-1.2800046445	-0.6783480852
N34	7.9039140132	0.7103854745	-0.2680959733
N35	2.2369803290	2.0756283094	-0.4463072349
C36	2.3421585785	2.1614685534	-1.7525770300
C37	1.5421596520	3.2211218969	-2.2516204725
H38	2.9822570295	1.4688218890	-2.2822484255

C39	0.9691609401	3.7423433602	-1.1320199394
H40	1.4195153219	3.5385578504	-3.2753287224
H41	0.2831150771	4.5570396255	-0.9516440049
O42	1.3740825403	3.0709202516	-0.0390326966
C43	7.9613144049	2.1053790398	0.1070629012
C44	8.1226691596	2.4308182095	1.4682530530
C45	7.8722902038	3.0766068660	-0.9095392577
C46	8.1863384619	3.7899917243	1.7965445137
C47	7.9470215712	4.4190985120	-0.5213938251
C48	8.1007560655	4.7733573858	0.8155912213
H49	8.3133614659	4.0814856867	2.8350013003
H50	7.8851421760	5.1968560510	-1.2769139100
H51	8.1593716755	5.8218776977	1.0939382525
C52	6.3312314358	-2.4341739384	-0.8266305744
C53	6.1105673324	-3.2590210934	0.2941786878
C54	5.7627120187	-2.6880494759	-2.0904328074
C55	5.2736385161	-4.3673387226	0.1167957075
C56	4.9388740806	-3.8132554207	-2.2084929460
C57	4.6937694222	-4.6425824190	-1.1179412093
H58	5.0776201678	-5.0266368724	0.9572461467
H59	4.4842576627	-4.0436810805	-3.1675967559
H60	4.0510563532	-5.5109705044	-1.2324431735
C61	7.6948636586	2.7210116409	-2.3837786668
H62	7.6505265806	1.6315273224	-2.4698939876
C63	6.3656054107	3.2725500520	-2.9348630952
H64	6.2236329085	2.9564014161	-3.9742246112
H65	5.5164039381	2.9116473742	-2.3448877109
H66	6.3457017955	4.3673497607	-2.9168925912
C67	8.8897944443	3.1997509058	-3.2317219645

H68	9.8338033080	2.7837984702	-2.8651475134
H69	8.7665034577	2.8901315422	-4.2750415720
H70	8.9810594787	4.2909998774	-3.2190314094
C71	6.0087665920	-1.7967236783	-3.3057194553
H72	6.6564447832	-0.9699035314	-2.9992305569
C73	4.6954932843	-1.1747238209	-3.8191714998
H74	4.0015906007	-1.9380813433	-4.1868541296
H75	4.1905586992	-0.6203675636	-3.0200559704
H76	4.8964296493	-0.4845032883	-4.6459123198
C77	6.7383638612	-2.5602040016	-4.4289533865
H78	6.9468202460	-1.8935951535	-5.2726065051
H79	7.6909725265	-2.9714563223	-4.0798976540
H80	6.1359407276	-3.3933223706	-4.8061158409
C81	6.7423927290	-2.9982256851	1.6600183204
H82	7.3578210539	-2.0965176325	1.5866449844
C83	5.6715379648	-2.7314509472	2.7363522991
H84	5.0434156298	-1.8765153966	2.4638342300
H85	5.0191848615	-3.5996953893	2.8789875971
H86	6.1454464379	-2.5122855988	3.6994642811
C87	7.6733430701	-4.1539159853	2.0767857788
H88	8.1638471204	-3.9232985133	3.0283374314
H89	7.1196525725	-5.0893988188	2.2085143320
H90	8.4523728169	-4.3308538628	1.3283432563
C91	8.2419387878	1.3785973788	2.5683186873
H92	8.1588417551	0.3897603220	2.1078333495
C93	7.0956981054	1.4982774009	3.5921755790
H94	7.1198942412	2.4628403222	4.1113047071
H95	6.1203212540	1.3974951643	3.1040209919
H96	7.1794001720	0.7122636625	4.3505321567

C97	9.6168763240	1.4468460843	3.2621458189
H98	9.7073817341	0.6507922115	4.0087829964
H99	10.4340443057	1.3308816786	2.5430429359
H100	9.7605497697	2.4021841519	3.7778535809

C’

C1	1.9102217775	-0.0152032257	0.6837285986
C2	2.8023493780	1.2507523727	0.4891833689
C3	2.8653566814	2.1981262044	1.6535199162
C4	2.2507959954	2.0129775751	2.8347234673
H5	2.0992311562	-0.7005173926	-0.1505724820
H6	2.2935478013	-0.5231522744	1.5771153512
H7	3.5123368913	3.0583256374	1.5082044683
H8	1.5877256299	1.1760200502	3.0267054795
C9	0.4666699922	0.1935862035	0.7941621934
C10	-0.7390638708	0.3151702335	0.8212203594
C11	-2.1629316422	0.4486852569	0.8449799977
C12	-2.9416285449	-0.0934410769	-0.1960025961
C13	-2.8075776359	1.1159961294	1.9035967926
C14	-4.3277056974	0.0305120587	-0.1750667476
H15	-2.4494590845	-0.6152438430	-1.0108739798
C16	-4.1942509133	1.2357657559	1.9163354278
H17	-2.2126832515	1.5311907719	2.7106089302
C18	-4.9575087232	0.6948888226	0.8795790888
H19	-4.9183954324	-0.3950367935	-0.9812381312
H20	-4.6817928361	1.7498637438	2.7394145233
H21	-6.0395327727	0.7880289861	0.8947817721

O22	2.3500580085	2.7805652633	3.9418411393
C23	3.1652917648	3.9447543225	3.8725883109
H24	3.1121176748	4.4115353832	4.8568787375
H25	4.2066122204	3.6857369133	3.6421053269
H26	2.7919181880	4.6450257151	3.1145523498
Au27	4.8012948840	0.5741346202	0.0843101929
C28	8.5369411452	-1.4392699391	-0.5107907330
C29	8.9782079366	-0.3138018570	0.1051244518
H30	9.0626122588	-2.3097607226	-0.8692902476
H31	9.9680954819	0.0010205551	0.3941439174
C32	6.7303681000	-0.1348086720	-0.1068473530
N33	7.1593824349	-1.3140226918	-0.6339013965
N34	7.8603857808	0.4734018729	0.3438618373
N35	2.2710517789	1.9998030716	-0.6763333309
C36	2.5268363317	1.9776354524	-1.9734976636
C37	1.5947617644	2.7827132940	-2.6564352233
H38	3.3654200582	1.4029330929	-2.3384432805
C39	0.7895856432	3.2783089775	-1.6701936256
H40	1.5481900636	2.9776671657	-3.7163754885
H41	-0.0500926962	3.9594621287	-1.6633876136
O42	1.1615466975	2.8194893596	-0.4704338309
C43	7.9105720549	1.7604786238	1.0019118292
C44	8.1257586898	2.9074872085	0.2128436128
C45	7.7711652327	1.8030999226	2.4028921945
C46	8.1914195081	4.1372532181	0.8772588819
C47	7.8490740580	3.0610726499	3.0124312371
C48	8.0560612316	4.2141084676	2.2605304021
H49	8.3575777832	5.0452341734	0.3048502894
H50	7.7540182858	3.1365763851	4.0917421227

H51	8.1191299942	5.1786458580	2.7568170961
C52	6.3172250263	-2.3355044853	-1.2174313479
C53	5.7836780869	-3.3273302330	-0.3710541427
C54	6.1051231544	-2.3182271340	-2.6099363794
C55	4.9892133765	-4.3145762055	-0.9658864812
C56	5.3055339664	-3.3325848884	-3.1485586630
C57	4.7495434156	-4.3168335908	-2.3366780939
H58	4.5594063584	-5.0968866917	-0.3472347295
H59	5.1222621988	-3.3565873240	-4.2189062565
H60	4.1345515746	-5.0967996461	-2.7768338629
C61	8.2836183683	2.8512144634	-1.3050764462
H62	8.2377735194	1.8030697897	-1.6157475390
C63	7.1272563409	3.5838721759	-2.0130997649
H64	7.2260667562	3.4933996767	-3.1003905627
H65	6.1592588167	3.1638112177	-1.7186566399
H66	7.1197575981	4.6514710856	-1.7687771516
C67	9.6503305124	3.4010897338	-1.7568031729
H68	10.4754983992	2.8653761583	-1.2769694334
H69	9.7638808328	3.2953896448	-2.8408307850
H70	9.7593097632	4.4635968075	-1.5155854449
C71	6.7194822561	-1.2665046487	-3.5302808957
H72	7.2730435585	-0.5534539283	-2.9127616164
C73	5.6360099004	-0.4684108269	-4.2797978170
H74	5.0516368232	-1.1067310205	-4.9507474174
H75	4.9416453618	0.0002211958	-3.5732336732
H76	6.0920154066	0.3210779799	-4.8867923195
C77	7.7232593775	-1.8982738724	-4.5157790224
H78	8.1891838793	-1.1251451191	-5.1361033178
H79	8.5195661736	-2.4331196390	-3.9881444265

H80	7.2328794602	-2.6118567704	-5.1864200648
C81	6.0552224903	-3.3750235929	1.1308178910
H82	6.6842580107	-2.5192473619	1.3930346927
C83	6.8340074650	-4.6486565358	1.5163733359
H84	7.0705748337	-4.6416206722	2.5855978973
H85	6.2521818816	-5.5535907282	1.3119835706
H86	7.7751005794	-4.7261944830	0.9622589646
C87	4.7549909431	-3.2487023526	1.9478902626
H88	4.2276354899	-2.3197138047	1.7072822674
H89	4.0729809799	-4.0835540113	1.7551455898
H90	4.9784536428	-3.2453031210	3.0201383130
C91	7.5572887970	0.5554406621	3.2569183572
H92	7.5034414020	-0.3102006855	2.5900098848
C93	6.2233226957	0.6180959167	4.0269111908
H94	6.2134635380	1.4419325462	4.7487775562
H95	5.3761904483	0.7554174573	3.3471140908
H96	6.0645297835	-0.3096720306	4.5873934061
C97	8.7428042803	0.3217062180	4.2143948028
H98	8.5985131145	-0.6045274516	4.7806578945
H99	9.6893431331	0.2412726444	3.6700409672
H100	8.8429653670	1.1386139858	4.9368349317

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C1	2.4490594681	-0.9444942378	0.1695682375
C2	3.4081926840	-1.9912651120	0.8044054272
C3	3.2727057224	-3.3963895477	0.2968425051
C4	2.4917561746	-3.7821983525	-0.7283553037

H5	2.7499853409	0.0633291795	0.4748091601
H6	2.5949154681	-0.9873680971	-0.9123355997
H7	3.9316885436	-4.1161912343	0.7730148945
H8	1.8217158763	-3.1042808218	-1.2487796493
C9	1.0124110241	-1.0905322225	0.5128761534
C10	0.0123836252	-1.3315460221	1.2050004434
C11	-1.0472453823	-1.6695062088	2.1065516967
C12	-1.5746378020	-0.6935029449	2.9759376593
C13	-1.5392921838	-2.9899176356	2.1551754196
C14	-2.5749524180	-1.0385927692	3.8785855621
H15	-1.1992470151	0.3238184124	2.9316250885
C16	-2.5397075099	-3.3219889815	3.0636988964
H17	-1.1331424502	-3.7379336769	1.4823240027
C18	-3.0588532982	-2.3489861516	3.9220627208
H19	-2.9819994289	-0.2850214587	4.5459206425
H20	-2.9192998250	-4.3385921782	3.0995756903
H21	-3.8434605879	-2.6120348057	4.6254150306
O22	2.4170747522	-5.0052099982	-1.2905350927
C23	3.2449253464	-6.0371372857	-0.7578027208
H24	3.0417751634	-6.9271341789	-1.3539679817
H25	4.3058858264	-5.7707094963	-0.8410380625
H26	3.0009537955	-6.2362304792	0.2931579763
Au27	5.4041079288	-1.2745931756	0.4202548748
C28	9.1265816838	0.7581997504	0.2407114781
C29	9.3177741874	-0.0823365823	-0.8088769993
H30	9.7583433605	1.5208188529	0.6677600485
H31	10.1521381130	-0.2032515374	-1.4815401424
C32	7.2713444093	-0.5200280300	0.0405757675
N33	7.8662934929	0.4741217667	0.7514148088

N34	8.1708878040	-0.8574858494	-0.9187929227
N35	3.1884049413	-2.0006119267	2.2734091331
C36	3.7461619447	-1.3671249217	3.2935549971
C37	3.0809599138	-1.7097374401	4.4869430514
H38	4.5936746695	-0.7162305607	3.1290762175
C39	2.1166380720	-2.5948695241	4.0986845776
H40	3.3096491666	-1.3670080755	5.4842303372
H41	1.3711059479	-3.1695173506	4.6310069711
O42	2.1432348952	-2.7856758799	2.7728530819
Au43	-0.5739551678	-0.3372276942	-0.9030986724
C44	-1.6130997701	0.3799848520	-2.4889555917
N45	-2.1464691142	1.6147512449	-2.6691331575
N46	-1.9142429559	-0.3155603314	-3.6173109525
C47	-2.7792662657	1.6916609933	-3.8994459834
C48	-2.6341627357	0.4785653940	-4.4949561193
H49	-3.2671382922	2.5947146552	-4.2303017857
H50	-2.9718848904	0.1089653905	-5.4502342133
C51	-1.5590917643	-1.6988567793	-3.8697789507
C52	-0.3560320806	-1.9728061416	-4.5519802867
C53	-2.4472741737	-2.7010678242	-3.4314658847
C54	-0.0379656453	-3.3194037333	-4.7643364066
C55	-2.0761793940	-4.0304085112	-3.6736000658
C56	-0.8848717609	-4.3350532477	-4.3275017014
H57	0.8792104662	-3.5755782899	-5.2865715815
H58	-2.7324434440	-4.8343907597	-3.3542055233
H59	-0.6181124084	-5.3727312000	-4.5070762787
C60	-2.0735350735	2.7191166586	-1.7322246209
C61	-3.1146328949	2.8723017419	-0.7969027503
C62	-0.9898233177	3.6130283458	-1.8361059560

C63	-3.0359915489	3.9664437513	0.0743263916
C64	-0.9645911891	4.6866862133	-0.9382743672
C65	-1.9731222045	4.8622800879	0.0053513184
H66	-3.8237417026	4.1250840648	0.8044935257
H67	-0.1507053860	5.4031853596	-0.9857852940
H68	-1.9356516591	5.7101473971	0.6837029165
C69	7.9702720575	-1.8767502272	-1.9301458207
C70	8.2523846087	-3.2177246780	-1.6037573298
C71	7.5201487654	-1.4696090602	-3.2002007363
C72	8.0315885898	-4.1779832387	-2.5983361950
C73	7.3234458691	-2.4730756041	-4.1560906315
C74	7.5681121862	-3.8114668298	-3.8584443908
H75	8.2397492912	-5.2222983757	-2.3883754473
H76	6.9794809304	-2.2026185919	-5.1502099433
H77	7.4106020237	-4.5721667259	-4.6182367937
C78	7.2563700925	1.1528570662	1.8741010027
C79	7.5274592748	0.6719488634	3.1732501465
C80	6.4373005447	2.2723789405	1.6224737033
C81	6.9263014371	1.3478224213	4.2447542834
C82	5.8635903064	2.9083621977	2.7319141739
C83	6.1073797598	2.4541885156	4.0262369543
H84	7.1225592803	1.0192191325	5.2612869241
H85	5.2342395409	3.7807187212	2.5812964071
H86	5.6670783212	2.9754675441	4.8721523366
C87	-4.3139927105	1.9323455591	-0.7332434706
H88	-4.1582158825	1.1285271171	-1.4589168870
C89	-5.6115231752	2.6659898838	-1.1283626915
H90	-6.4587642420	1.9727051967	-1.1268977833
H91	-5.8420296670	3.4753869094	-0.4279177142

H92	-5.5366295631	3.1056797156	-2.1283142517
C93	-4.4425005140	1.2671075646	0.6490246105
H94	-3.5324846065	0.7168263558	0.9104167687
H95	-4.6298623751	2.0030929809	1.4381500625
H96	-5.2800663528	0.5616008849	0.6539995997
C97	0.1194516534	3.4555618678	-2.8745951854
H98	-0.1001008125	2.5713910363	-3.4801476097
C99	1.4866385565	3.2146858914	-2.2054856016
H100	1.4603387824	2.3295437124	-1.5601765208
H101	2.2609683889	3.0607546798	-2.9650543190
H102	1.7901704814	4.0696092578	-1.5916230077
C103	0.1749306939	4.6597757588	-3.8333987607
H104	0.4198259741	5.5846311169	-3.3021570498
H105	0.9421372986	4.5035592668	-4.5989849858
H106	-0.7824591534	4.8120433765	-4.3411694806
C107	-3.7667424459	-2.3878919790	-2.7281143791
H108	-3.8704425316	-1.3004294569	-2.6595164267
C109	-4.9725400481	-2.9088818523	-3.5348476759
H110	-4.9656043312	-4.0009500312	-3.6127687472
H111	-5.9094525658	-2.6181940291	-3.0484996876
H112	-4.9798336933	-2.5031206704	-4.5514010669
C113	-3.7813368138	-2.9338510235	-1.2872265850
H114	-2.9521519193	-2.5273924294	-0.6978703055
H115	-4.7174776879	-2.6629301468	-0.7873638278
H116	-3.7021619303	-4.0261668601	-1.2718928290
C117	0.5806821704	-0.8809344250	-5.0647691709
H118	0.1295975903	0.0905429813	-4.8423733146
C119	0.7601878743	-0.9579002658	-6.5938308843
H120	-0.2017692274	-0.9014137209	-7.1127906185

H121	1.3825749700	-0.1286001612	-6.9465303556
H122	1.2479573106	-1.8893838297	-6.8994073259
C123	1.9421852089	-0.9249240885	-4.3456011430
H124	1.8163552172	-0.8089109737	-3.2629705106
H125	2.4631654946	-1.8713350143	-4.5265567714
H126	2.5885643547	-0.1150433414	-4.6995149244
C127	6.1756155458	2.8073924451	0.2159233551
H128	6.6985302483	2.1626184153	-0.4958484755
C129	4.6770714227	2.7521936987	-0.1415658351
H130	4.2945604744	1.7279607038	-0.0686440312
H131	4.0788259012	3.3872633671	0.5211566695
H132	4.5173639463	3.1008464541	-1.1676131189
C133	6.7393919652	4.2316872542	0.0423060355
H134	7.8110059973	4.2655392908	0.2605114157
H135	6.5947869014	4.5764505542	-0.9869444038
H136	6.2422999046	4.9478626623	0.7049029091
C137	7.2557974842	-0.0080614013	-3.5565593346
H138	7.4769737424	0.6050540279	-2.6776515908
C139	5.7743561420	0.2245970649	-3.9112129049
H140	5.4819322630	-0.3399570312	-4.8030443117
H141	5.1192441960	-0.0822963924	-3.0885644433
H142	5.5940903095	1.2857153545	-4.1176913173
C143	8.1812477275	0.4732983242	-4.6916765415
H144	8.0186500516	1.5377581063	-4.8918057116
H145	9.2365816174	0.3358613031	-4.4352830662
H146	7.9941485224	-0.0706029546	-5.6235147999
C147	8.8086621107	-3.6397403050	-0.2464186289
H148	8.9276737042	-2.7420136360	0.3669797727
C149	7.8370525301	-4.5729615644	0.5014498014

H150	6.8610125900	-4.0941871197	0.6418654752
H151	7.6796864422	-5.5094489833	-0.0446392940
H152	8.2380912165	-4.8305114253	1.4875748726
C153	10.2026340758	-4.2840323740	-0.3878604152
H154	10.9043500844	-3.6127524223	-0.8929367737
H155	10.6143421775	-4.5234309387	0.5982735606
H156	10.1608980912	-5.2146752401	-0.9632440290
C157	8.4469819731	-0.5187858053	3.4416970315
H158	8.7457631052	-0.9432128492	2.4800296842
C159	7.7297616834	-1.6382091900	4.2190768477
H160	7.4009855327	-1.3023453768	5.2087781980
H161	6.8536864984	-2.0018173884	3.6693886602
H162	8.4028250945	-2.4881391373	4.3702937435
C163	9.7334728138	-0.0741418892	4.1653968113
H164	10.4045337882	-0.9267575660	4.3099142561
H165	10.2731231093	0.6861961229	3.5919275893
H166	9.5129692944	0.3487692278	5.1505170921

C’’D’-TS

C1	2.3867064813	0.0185145369	0.0600442226
C2	3.4577200898	-0.1720728144	1.1678788528
C3	3.8639378662	-1.5693600655	1.4935137572
C4	3.5965413967	-2.6430392175	0.7217332880
H5	2.3114053919	1.0802483203	-0.1992882696
H6	2.7225129627	-0.4881395975	-0.8465401688
H7	4.4193782702	-1.6808560215	2.4185624630
H8	3.0457228550	-2.5729984619	-0.2113738190

C9	1.0335110822	-0.4527538414	0.4605227227
C10	0.0966971792	-0.5915706947	1.2623921630
C11	-0.9242540536	-0.6984905438	2.2543271687
C12	-1.8170113604	0.3727439378	2.4620297980
C13	-1.0093230859	-1.8515788897	3.0605929585
C14	-2.7721469138	0.2895633265	3.4690995145
H15	-1.7495391069	1.2565820579	1.8350633067
C16	-1.9727634174	-1.9232610658	4.0605377777
H17	-0.3184084520	-2.6725391217	2.8964244508
C18	-2.8518371143	-0.8558365519	4.2662261383
H19	-3.4564673366	1.1163059802	3.6335069919
H20	-2.0400460570	-2.8110715454	4.6820018893
H21	-3.6011249811	-0.9167174249	5.0503160878
O22	3.9447189008	-3.9221189205	0.9455294490
C23	4.6731501864	-4.2273640980	2.1365499167
H24	4.8464307045	-5.3033495378	2.1157345767
H25	5.6333968981	-3.6986068039	2.1548555939
H26	4.0917776948	-3.9637271513	3.0282743032
Au27	5.3563313902	0.6525312228	0.3457422921
C28	9.2056872186	1.8880680158	-0.9400969396
C29	8.4627079710	2.3662675708	-1.9711691400
H30	10.2661131883	1.9252368910	-0.7470086673
H31	8.7421273513	2.9035889658	-2.8634522997
C32	7.0534903711	1.3568781240	-0.5273750216
N33	8.3250719623	1.2701904142	-0.0634176336
N34	7.1432001302	2.0305813052	-1.7021654417
N35	3.2460146693	0.5906559626	2.2971194543
C36	3.3109144822	1.8485194357	2.7082170536
C37	2.5433400861	2.1358143818	3.8381078029

H38	3.9806336861	2.5326126048	2.2028713424
C39	1.9287753600	0.9542498093	4.2136464508
H40	2.5225510389	3.0780096280	4.3638043163
H41	1.3544202672	0.7614681820	5.1193034280
O42	2.1326855206	-0.0463054203	3.4191770685
Au43	-0.4195498148	-1.5285473089	-0.9108714869
C44	-1.5152565025	-2.4668481629	-2.3492012059
N45	-1.1819085443	-2.7021410037	-3.6435797377
N46	-2.7630996318	-2.9816108546	-2.2031222574
C47	-2.2138646866	-3.3558510766	-4.3027934551
C48	-3.2069914227	-3.5319700888	-3.3963891531
H49	-2.1366933103	-3.6300607934	-5.3428262556
H50	-4.1791491537	-3.9908318199	-3.4807574245
C51	6.0281155814	2.3195052386	-2.5766066851
C52	5.3630603496	3.5523877170	-2.4343638331
C53	5.6703573230	1.3524867596	-3.5376914587
C54	4.2835317789	3.7957878375	-3.2913142277
C55	4.5763167638	1.6480966093	-4.3587199396
C56	3.8911101604	2.8540259859	-4.2378771229
H57	3.7480820148	4.7380855641	-3.2214775820
H58	4.2622101975	0.9269750457	-5.1073042448
H59	3.0527205912	3.0683692980	-4.8952991462
C60	8.7244713344	0.6040668860	1.1582198459
C61	8.8058233636	1.3651240465	2.3403633458
C62	9.0355830461	-0.7690580697	1.0968518785
C63	9.2019516399	0.6939240442	3.5026572034
C64	9.4266601057	-1.3843971269	2.2916063970
C65	9.5068216965	-0.6639918509	3.4800532428
H66	9.2821945026	1.2436492361	4.4357481400

H67	9.6832683511	-2.4397898034	2.2888537389
H68	9.8200995270	-1.1623658926	4.3931449207
C69	-3.5590649040	-2.9825410974	-0.9941969232
C70	-3.4241671380	-4.0685172303	-0.1067055479
C71	-4.4830608570	-1.9362034669	-0.8065364415
C72	-4.2606064234	-4.0773862282	1.0152179228
C73	-5.2906496865	-2.0000649137	0.3346395726
C74	-5.1833523461	-3.0579808196	1.2327629434
H75	-4.1993427084	-4.9018233609	1.7196147991
H76	-6.0216875100	-1.2175808019	0.5153107595
H77	-5.8314343486	-3.0938975742	2.1040927940
C78	0.0688853315	-2.3696662971	-4.2887265448
C79	0.1764124663	-1.1256547308	-4.9398122953
C80	1.0842118052	-3.3471600953	-4.3060366057
C81	1.3665295006	-0.8736465389	-5.6318986916
C82	2.2524762340	-3.0363729790	-5.0109641486
C83	2.3882258989	-1.8185358785	-5.6728669025
H84	1.4848293120	0.0663362170	-6.1631107151
H85	3.0569795697	-3.7644466735	-5.0589810398
H86	3.2922007255	-1.6127152034	-6.2400687829
C87	8.4950240752	2.8596267866	2.3906972807
H88	8.2197643140	3.1881437485	1.3834747828
C89	8.9830830056	-1.5814330022	-0.1958377128
H90	8.6349076901	-0.9261953985	-1.0005085761
C91	7.2910318939	3.1519622476	3.3077394398
H92	7.0491273653	4.2203786144	3.2921451183
H93	6.4065946131	2.5915162147	2.9823529486
H94	7.4971144659	2.8738442289	4.3467216373
C95	9.7286484971	3.6801544819	2.8171269077

H96	10.5802396564	3.4954523056	2.1548350610
H97	9.5036441837	4.7513829184	2.7873269801
H98	10.0426421479	3.4364576064	3.8372887957
C99	7.9779017387	-2.7457346473	-0.0941131842
H100	8.2730929952	-3.4656258734	0.6772178107
H101	6.9722002172	-2.3833520940	0.1462635547
H102	7.9255287614	-3.2880228217	-1.0445922618
C103	10.3836928989	-2.0890774667	-0.5943076844
H104	10.3390101957	-2.6233240775	-1.5492323881
H105	11.0936891098	-1.2629265484	-0.7024652367
H106	10.7891403346	-2.7796080981	0.1525565807
C107	6.4231503700	0.0342524938	-3.7131873172
H108	7.2974854230	0.0476988836	-3.0553932966
C109	5.5564454609	-1.1695049458	-3.2931896092
H110	5.2510508005	-1.0914722415	-2.2433011448
H111	4.6499073480	-1.2442762744	-3.9033208296
H112	6.1175766773	-2.1032800467	-3.4114899669
C113	6.9462726309	-0.1343651473	-5.1534123147
H114	7.5727547943	0.7107303885	-5.4548250332
H115	7.5477117714	-1.0458102769	-5.2337756996
H116	6.1283533624	-0.2152676310	-5.8772258960
C117	5.7772262139	4.6079911663	-1.4114888992
H118	6.6261177493	4.2189054939	-0.8409940513
C119	4.6451360757	4.8893862430	-0.4035993321
H120	3.7606863734	5.3109686157	-0.8932519522
H121	4.3380528526	3.9678940046	0.1059176971
H122	4.9772815577	5.6078161773	0.3536045093
C123	6.2428283579	5.9066012164	-2.1009373197
H124	6.5855275079	6.6330884543	-1.3567864563

H125	7.0691634773	5.7174253585	-2.7934674074
H126	5.4327679058	6.3734622949	-2.6710734631
C127	0.9460481159	-4.7015414044	-3.6129100446
H128	-0.0626314884	-4.7725500949	-3.1945137321
C129	1.9337384593	-4.8303176465	-2.4367345087
H130	1.7670299471	-4.0421546167	-1.6939962110
H131	1.8092609428	-5.7958568828	-1.9355543269
H132	2.9735550220	-4.7642635812	-2.7747658741
C133	1.1076975375	-5.8691925746	-4.6058508890
H134	2.1150263585	-5.9028291326	-5.0333751859
H135	0.9335800020	-6.8239006417	-4.0990728252
H136	0.3967698934	-5.7925303498	-5.4344946191
C137	-0.9376689121	-0.0813121603	-4.9269652839
H138	-1.7890849779	-0.4945612087	-4.3775518636
C139	-0.4948946524	1.1941453892	-4.1830494445
H140	-1.3128923066	1.9217026272	-4.1510509364
H141	-0.1995121340	0.9687863770	-3.1520900500
H142	0.3561835667	1.6729944302	-4.6795968517
C143	-1.4294529213	0.2443330806	-6.3508478193
H144	-2.2721195323	0.9421166508	-6.3109493798
H145	-0.6443082402	0.7101120333	-6.9554821100
H146	-1.7622483441	-0.6566569981	-6.8757316528
C147	-4.6344605212	-0.7743201867	-1.7863836518
H148	-3.9255605564	-0.9213956547	-2.6072270704
C149	-4.2803780492	0.5692446459	-1.1196481182
H150	-3.2636086797	0.5527007601	-0.7115369029
H151	-4.3432077107	1.3850444665	-1.8475256383
H152	-4.9681829923	0.8043415363	-0.3005234435
C153	-6.0462362290	-0.7354865189	-2.4048238283

H154	-6.1171978549	0.0699384033	-3.1432511412
H155	-6.2901458833	-1.6767224317	-2.9078816581
H156	-6.8150029666	-0.5562475376	-1.6460181636
C157	-2.4506680606	-5.2212413274	-0.3431279005
H158	-1.8452742162	-4.9852951786	-1.2239450164
C159	-3.2062639287	-6.5317480478	-0.6422888304
H160	-3.8635538604	-6.4263522873	-1.5115288057
H161	-2.4998645157	-7.3422227691	-0.8497081871
H162	-3.8261471331	-6.8387485995	0.2064045640
C163	-1.4744457985	-5.3983363435	0.8360336899
H164	-0.9151573174	-4.4759369380	1.0284723021
H165	-1.9961371743	-5.6752976169	1.7582987480
H166	-0.7535516979	-6.1929868893	0.6158548981

D’

C1	2.7618532106	0.3560442954	0.6976532664
C2	3.0129367722	-0.9133096232	1.5225517978
C3	3.7295950816	-2.0765597905	0.9099456718
C4	3.3944172736	-2.5632010481	-0.3515114503
H5	3.3727863692	1.1504870144	1.1466543349
H6	3.1512253084	0.2243147614	-0.3159929772
H7	4.1002670173	-2.7781100023	1.6523168479
H8	2.8134143443	-1.9736933228	-1.0570881107
C9	1.3789138503	0.8716998351	0.5895215880
C10	0.5863949796	1.8235994013	0.6681110422
C11	-0.2471682332	2.9662715278	0.8395544349
C12	-0.3148134965	3.9497167845	-0.1694414756
C13	-0.9550927015	3.1472325383	2.0454448344

C14	-1.0769409619	5.0947185692	0.0328102584
H15	0.2309423902	3.8033015679	-1.0965003205
C16	-1.7170775603	4.2950274560	2.2321496501
H17	-0.8892510313	2.3923413365	2.8225640418
C18	-1.7796977957	5.2665029189	1.2291612142
H19	-1.1279631147	5.8540120711	-0.7415843131
H20	-2.2613428028	4.4368498610	3.1607800707
H21	-2.3759874100	6.1614999496	1.3810831611
O22	3.6439391896	-3.7607128038	-0.8358717751
C23	4.3704953557	-4.7204272245	-0.0337507768
H24	4.4471875360	-5.6131618210	-0.6513516103
H25	5.3672146785	-4.3308137455	0.1971996092
H26	3.8182393503	-4.9405669125	0.8837999877
Au27	5.5273940649	-1.1049988208	-0.0977301759
C28	8.3717507798	1.7546848390	-1.3859740536
C29	9.1022716605	0.6208844777	-1.5558445237
H30	8.6133056240	2.7908182438	-1.5633212319
H31	10.1095311856	0.4693385834	-1.9104607119
C32	7.0877365206	0.0151051083	-0.7583902426
N33	7.1333140588	1.3664052383	-0.8939570863
N34	8.2976725339	-0.4373720070	-1.1637770147
N35	2.7550510773	-1.0400357020	2.7570978102
C36	2.1686897770	-0.2524091973	3.7062593294
C37	0.8543683987	-0.2251867518	4.0559933243
H38	2.8923694312	0.2567571630	4.3463548846
C39	-0.1966580024	-0.9115989596	3.3192810818
H40	0.5821328121	0.3004748363	4.9659703026
H41	-1.1902729100	-0.9294946432	3.8094144843
O42	-0.0518687091	-1.4483909985	2.2213248826

Au43	-0.3206269672	-0.1835163939	-0.4178071739
C44	-1.6323470768	-1.3783784236	-1.4303451377
N45	-1.8091924019	-1.4112896528	-2.7806678094
N46	-2.5111867086	-2.2934574543	-0.9394741259
C47	-2.7885239823	-2.3282927905	-3.1253272821
C48	-3.2287491688	-2.8823639397	-1.9680026787
H49	-3.0825998813	-2.4875368758	-4.1502092909
H50	-3.9834781155	-3.6274548570	-1.7736457827
C51	6.0602866297	2.2850325308	-0.5632047268
C52	5.9539995743	2.7443311595	0.7666747818
C53	5.1887032637	2.6966749349	-1.5927883829
C54	4.9093259311	3.6347892524	1.0532457941
C55	4.1642857799	3.5890908331	-1.2470294819
C56	4.0284232048	4.0546190225	0.0588730488
H57	4.8024414961	4.0244863429	2.0612832368
H58	3.4799606459	3.9365943032	-2.0154317352
H59	3.2365336947	4.7579082742	0.3023163809
C60	8.7080411429	-1.8283060331	-1.1239532506
C61	9.3256969924	-2.2985505321	0.0527237190
C62	8.4701884755	-2.6358539769	-2.2532463670
C63	9.7001595007	-3.6469646757	0.0749415456
C64	8.8664477524	-3.9770533656	-2.1704272955
C65	9.4725301486	-4.4763600499	-1.0204740195
H66	10.1830117027	-4.0512318379	0.9597017224
H67	8.7079179648	-4.6342566943	-3.0201004489
H68	9.7801733187	-5.5174960193	-0.9804352947
C69	-2.7723534410	-2.6299529006	0.4469503217
C70	-3.7246346762	-1.8669873813	1.1492276645
C71	-2.1429577773	-3.7672419467	0.9863755169

C72	-4.0365846247	-2.2816234583	2.4495612798
C73	-2.5061253433	-4.1416310101	2.2841723537
C74	-3.4420846840	-3.4092991439	3.0080252782
H75	-4.7700286518	-1.7245072006	3.0251063990
H76	-2.0516518423	-5.0189609923	2.7346312749
H77	-3.7147203232	-3.7228333694	4.0119460588
C78	-1.1541909051	-0.5707811087	-3.7602160168
C79	-1.7769575681	0.6398552371	-4.1194701106
C80	0.0337000831	-1.0378262400	-4.3583702494
C81	-1.1580065393	1.4009916131	-5.1184798848
C82	0.6030171786	-0.2369254143	-5.3537538851
C83	0.0145385074	0.9687594509	-5.7288260457
H84	-1.6099618340	2.3374860164	-5.4315769418
H85	1.5104434186	-0.5636479876	-5.8518008262
H86	0.4682115393	1.5694544662	-6.5122610805
C87	5.3254296988	2.2214641760	-3.0376292359
H88	6.1909366271	1.5558701206	-3.0994603724
C89	5.5825489462	3.3997917869	-3.9982345427
H90	5.7428443173	3.0317882660	-5.0168629264
H91	4.7339191440	4.0913940987	-4.0265142636
H92	6.4673384365	3.9726512957	-3.7036537702
C93	4.0975425038	1.4021430900	-3.4786138934
H94	3.9505582353	0.5318627612	-2.8286225375
H95	3.1796323758	1.9993843955	-3.4578383259
H96	4.2305503613	1.0371365154	-4.5022857825
C97	6.9321893408	2.3451138677	1.8698706194
H98	7.6534395623	1.6373438921	1.4504804840
C99	7.7271805076	3.5667471603	2.3753432207
H100	7.0717245197	4.3077592521	2.8448243143

H101	8.4654292413	3.2576704715	3.1222805660
H102	8.2603106001	4.0642314950	1.5591596590
C103	6.2196965106	1.6288714783	3.0341601908
H104	5.6875152500	0.7345100779	2.6892856909
H105	6.9470352582	1.3155725174	3.7898520325
H106	5.4967358961	2.2865547823	3.5296480279
C107	9.5937199165	-1.4115777557	1.2680592991
H108	9.2545509074	-0.3965302299	1.0371932247
C109	11.1002474062	-1.3227418727	1.5832610469
H110	11.2737780108	-0.6327488067	2.4154825948
H111	11.5112898473	-2.2956162500	1.8706006854
H112	11.6698990498	-0.9620935362	0.7210418632
C113	8.7956837522	-1.8870942421	2.4986808053
H114	7.7184481727	-1.9013856467	2.2949870003
H115	9.0926080317	-2.8950464961	2.8062852682
H116	8.9710443560	-1.2185493587	3.3484330742
C117	7.8191065611	-2.1097571813	-3.5298305453
H118	7.6021920474	-1.0462070696	-3.3900640214
C119	6.4769745509	-2.8152395015	-3.8072726310
H120	6.6168055161	-3.8863131425	-3.9880171995
H121	5.7855741699	-2.7050230146	-2.9638772342
H122	5.9993379024	-2.3913215465	-4.6970349046
C123	8.7695704983	-2.2282534509	-4.7376272221
H124	8.3080254160	-1.7938551293	-5.6305120162
H125	9.7139828225	-1.7054850388	-4.5567966809
H126	9.0062535663	-3.2730944346	-4.9630730851
C127	-3.0863987380	1.1219081603	-3.4991455881
H128	-3.3787489590	0.4138057147	-2.7179813702
C129	-2.9243640794	2.4958285496	-2.8208273347

H130	-3.8646855817	2.7965581396	-2.3463219334
H131	-2.1493531645	2.4679423294	-2.0478371798
H132	-2.6564458225	3.2763620675	-3.5411760529
C133	-4.2210729063	1.1443980937	-4.5434838354
H134	-4.3714909603	0.1585147311	-4.9955951927
H135	-5.1634429673	1.4478802537	-4.0760193159
H136	-4.0084665577	1.8510816117	-5.3524703175
C137	0.6577569133	-2.3798925387	-3.9851058999
H138	0.2823667682	-2.6589146496	-2.9950541084
C139	2.1912816301	-2.3067242970	-3.8834050563
H140	2.5098179365	-1.4559613436	-3.2708083346
H141	2.5858758954	-3.2280644608	-3.4414220436
H142	2.6646669546	-2.1945977900	-4.8646746582
C143	0.2372737101	-3.4886562212	-4.9725283135
H144	0.6765384670	-4.4492952976	-4.6822333967
H145	-0.8491327245	-3.6141928285	-5.0033515557
H146	0.5750301068	-3.2556077578	-5.9877226462
C147	-4.4235976667	-0.6458340402	0.5555051261
H148	-4.0807063840	-0.5178873481	-0.4759830594
C149	-5.9522499697	-0.8350128943	0.5076568611
H150	-6.4277211756	0.0219070120	0.0191473563
H151	-6.2256406450	-1.7365359102	-0.0488949773
H152	-6.3810473254	-0.9215831822	1.5112213444
C153	-4.0468649172	0.6378538695	1.3203314953
H154	-4.3703285056	0.5867965950	2.3651268326
H155	-2.9642855551	0.8040614192	1.3104486167
H156	-4.5289203014	1.5105616226	0.8663132445
C157	-1.1078153060	-4.5845785435	0.2185974460
H158	-0.8907503431	-4.0647557081	-0.7205240710

C159	-1.6484278734	-5.9834342075	-0.1371679870
H160	-0.9063625930	-6.5499944080	-0.7097612053
H161	-1.8834856878	-6.5585576145	0.7644952009
H162	-2.5621259681	-5.9233992525	-0.7374018107
C163	0.2191114513	-4.6849181811	0.9976706343
H164	0.5748980305	-3.6935312673	1.2925007972
H165	0.1072133351	-5.2838758000	1.9078066242
H166	0.9795562826	-5.1753916913	0.3775261744

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C1	3.2185388761	-0.4156359141	0.8992633816
C2	2.3736433449	0.8336123929	0.6392373339
C3	1.1432102653	0.9858628238	1.3978097728
C4	0.7537433960	0.1389940341	2.3829726861
H5	3.5387864889	-0.4171330587	1.9504020114
H6	2.6057468643	-1.3134017950	0.7633316302
H7	0.5067072944	1.8211400415	1.1337348690
H8	1.3433296692	-0.7227866245	2.6832582303
C9	4.4363807425	-0.5017491372	0.0697836821
C10	5.6326454893	-0.4108459599	-0.2298707071
O11	-0.3540021843	0.2017493844	3.1206545493
C12	-1.2678841987	1.2833136360	2.8998708997
H13	-2.0779185389	1.1378199787	3.6135454962
H14	-0.7780910216	2.2458388370	3.0827971983
H15	-1.6616487727	1.2550379190	1.8780570744
Au16	4.3805915908	-1.3846853192	-2.0356322793
C17	3.9284915487	-2.3472057850	-3.7691799804

N18	4.5852655495	-3.4217106715	-4.2813519901
N19	2.8827932535	-2.1305195128	-4.6092682757
C20	3.9529916033	-3.8752888702	-5.4291385720
C21	2.8809198197	-3.0680362224	-5.6315138389
H22	4.3269912849	-4.7185385456	-5.9872197481
H23	2.1275697105	-3.0618067859	-6.4029336927
N24	2.8179345856	1.6578210137	-0.2557340627
C25	2.2479855425	2.9012474719	-0.4594274717
C26	3.0474888575	3.0781227104	-2.8057239533
C27	2.3538034307	3.5864638928	-1.6235639059
H28	1.7344540215	3.3812947759	0.3780380920
H29	3.5428373559	2.0952148642	-2.6874150480
H30	1.9067945440	4.5724521888	-1.7096209633
O31	3.0960986591	3.6879477445	-3.8660696788
C32	7.0341813792	-0.2381554775	-0.4685162387
C33	7.9385914401	-1.2791210896	-0.1824382428
C34	7.5107995708	0.9951259934	-0.9548496816
C35	9.3017188042	-1.0792848422	-0.3743284726
H36	7.5647725867	-2.2279807732	0.1890252041
C37	8.8766868991	1.1808884780	-1.1425394285
H38	6.8067012068	1.7920410689	-1.1722195428
C39	9.7712043742	0.1468657137	-0.8533995257
H40	10.0001999722	-1.8794559497	-0.1493086772
H41	9.2445389145	2.1323689731	-1.5141258162
H42	10.8367342805	0.2974727462	-1.0010874328
C43	5.7828415537	-4.0288305684	-3.7365304936
C44	7.0351105151	-3.5185811288	-4.1340657329
C45	5.6389311624	-5.1357851811	-2.8766847110
C46	8.1736779757	-4.1526465342	-3.6209496637

C47	6.8125932577	-5.7286243738	-2.3948779053
C48	8.0646492882	-5.2426661839	-2.7619476931
H49	9.1571502801	-3.7948805771	-3.9097061307
H50	6.7439361710	-6.5870665986	-1.7335609771
H51	8.9623700034	-5.7243718868	-2.3844451162
C52	1.9180873445	-1.0518398642	-4.5068704118
C53	0.7865710096	-1.2333077719	-3.6875021017
C54	2.1468616399	0.1133360197	-5.2690803053
C55	-0.1203192927	-0.1688463767	-3.6115189966
C56	1.2162108418	1.1512137653	-5.1349256127
C57	0.0992039975	1.0116444969	-4.3157802756
H58	-1.0121751956	-0.2693654008	-3.0004438968
H59	1.3697874248	2.0788506637	-5.6747255420
H60	-0.6124148756	1.8286247490	-4.2354332930
C61	4.2794892854	-5.7090207368	-2.4846475588
H62	3.5021189384	-5.0846093251	-2.9346924784
C63	4.0618792815	-5.6681137705	-0.9601949680
H64	4.7866682542	-6.2944303510	-0.4298487020
H65	4.1553576474	-4.6465792445	-0.5760468584
H66	3.0618747481	-6.0377685012	-0.7095771049
C67	4.0966120672	-7.1364205801	-3.0380615958
H68	3.0999524337	-7.5171860802	-2.7920262780
H69	4.2085863529	-7.1623671798	-4.1270298597
H70	4.8314394745	-7.8282709383	-2.6135900375
C71	0.4983275112	-2.5382574673	-2.9488753345
H72	1.3821916884	-3.1788804756	-3.0270270270
C73	0.2390800468	-2.3135341489	-1.4484905995
H74	1.0722452794	-1.7758862088	-0.9846009546
H75	-0.6720279893	-1.7324164255	-1.2726288266

H76	0.1193042254	-3.2738609603	-0.9355618541
C77	-0.6759334361	-3.2921541733	-3.6054995681
H78	-0.4786595792	-3.4995076891	-4.6622471072
H79	-0.8499117635	-4.2479849050	-3.0999640353
H80	-1.6012017139	-2.7091924177	-3.5493416000
C81	7.1865925132	-2.3588146764	-5.1149143336
H82	6.1936948177	-1.9452090055	-5.3134494530
C83	7.7570517984	-2.8499417866	-6.4612701930
H84	7.8202191415	-2.0209452051	-7.1738245064
H85	8.7634690083	-3.2643770985	-6.3404556303
H86	7.1285487674	-3.6293332447	-6.9048272726
C87	8.0382890016	-1.2159214223	-4.5329761256
H88	7.6190094455	-0.8447661080	-3.5929364158
H89	9.0688027736	-1.5318324556	-4.3400617743
H90	8.0787256554	-0.3806887161	-5.2402254329
C91	3.3434288666	0.2659262154	-6.2087920659
H92	3.7631064995	-0.7296648471	-6.3849302641
C93	4.4549750500	1.1291889198	-5.5781294570
H94	4.0930168279	2.1329987291	-5.3351063301
H95	4.8317869382	0.6733067006	-4.6552273481
H96	5.2966479650	1.2244265801	-6.2736024464
C97	2.9289155310	0.8206765116	-7.5856894408
H98	3.7843249854	0.7987984804	-8.2687329128
H99	2.1230031854	0.2301141939	-8.0339159155
H100	2.5914207942	1.8598806114	-7.5240884563

EF-TS

C1	3.2073480523	-1.0565684049	0.6343991154
C2	3.1459864536	0.0124908096	1.7274120320
C3	2.5390037521	-0.2867716192	3.0097919199
C4	2.1095754380	-1.5280566273	3.3529519006
H5	3.7328229286	-1.9444283446	1.0077922734
H6	2.1934265838	-1.3910857493	0.3846870957
H7	2.4291985722	0.5374036627	3.7053396574
H8	2.1907117778	-2.3770617142	2.6800160435
C9	3.9113713737	-0.5376965081	-0.5769889820
C10	4.4799002502	0.5966089003	-0.7027472830
O11	1.5525286331	-1.9122338960	4.4965007079
C12	1.3586769916	-0.9444228622	5.5382012313
H13	0.9035538368	-1.4882338352	6.3651401752
H14	2.3183455440	-0.5214878363	5.8534020700
H15	0.6891207702	-0.1457329542	5.2030237827
Au16	4.0187086867	-1.5328904579	-2.4462962928
C17	4.0176116697	-2.5762853908	-4.2098686096
N18	4.5428463840	-3.8111262837	-4.4283081996
N19	3.4311191606	-2.2308259301	-5.3869972948
C20	4.2835753925	-4.2351656874	-5.7239103498
C21	3.5835588367	-3.2409265171	-6.3269839907
H22	4.6216384209	-5.1924708850	-6.0869544867
H23	3.1853390907	-3.1520910583	-7.3249955501
N24	3.6310144317	1.1645400718	1.4015570357
C25	3.7725678278	2.2398816359	2.2712284513
C26	2.7978008083	3.9027241783	0.7019495044
C27	3.4400290037	3.5134188513	1.9639359881
H28	4.2317519579	2.0264397451	3.2393961558
H29	2.5706131572	3.0644040724	0.0120659601

H30	3.6314453262	4.3067575057	2.6806268833
O31	2.5207967889	5.0526291674	0.4099646731
C32	5.2674198835	1.6649787992	-1.2086469544
C33	6.6593677603	1.6912315930	-0.9634661180
C34	4.6754095559	2.6969438704	-1.9694590761
C35	7.4328648458	2.7314793529	-1.4623561983
H36	7.1132919448	0.8900623193	-0.3893604556
C37	5.4590667765	3.7332527860	-2.4621941448
H38	3.6103990753	2.6631035941	-2.1727170646
C39	6.8329949784	3.7532948530	-2.2052434808
H40	8.5022877782	2.7503679596	-1.2758249877
H41	5.0007892755	4.5277851731	-3.0420989658
H42	7.4402272621	4.5686239481	-2.5878286016
C43	5.3074364184	-4.5728579537	-3.4646640342
C44	6.7077255214	-4.4141690169	-3.4487899259
C45	4.6230763733	-5.4470427267	-2.5986345185
C46	7.4235407110	-5.1535168231	-2.5002410171
C47	5.3921989252	-6.1605169526	-1.6719401403
C48	6.7749663195	-6.0131821422	-1.6187179662
H49	8.5042013028	-5.0562232836	-2.4534303757
H50	4.9013102290	-6.8443293031	-0.9857685502
H51	7.3518863532	-6.5774326485	-0.8912907962
C52	2.7739778449	-0.9708009843	-5.6646074045
C53	1.4076130849	-0.8390530114	-5.3531086143
C54	3.5296092795	0.0547136495	-6.2683764564
C55	0.8001194207	0.3849810895	-5.6568567100
C56	2.8679858052	1.2562509945	-6.5506465579
C57	1.5194412047	1.4201697241	-6.2471347989
H58	-0.2533524178	0.5267661110	-5.4346887472

H59	3.4156063973	2.0700330931	-7.0166246305
H60	1.0236802394	2.3589506517	-6.4780013093
C61	3.1096938995	-5.6423858041	-2.6406927562
H62	2.7056223471	-5.0186335098	-3.4438776946
C63	2.4477024110	-5.1787531490	-1.3283545787
H64	2.7944682636	-5.7702265177	-0.4741363892
H65	2.6746611817	-4.1262059763	-1.1262704743
H66	1.3594775336	-5.2886777296	-1.3893828696
C67	2.7377292286	-7.1025468689	-2.9658781089
H68	1.6511005219	-7.2092224815	-3.0498829983
H69	3.1835162471	-7.4283945757	-3.9110457355
H70	3.0777616701	-7.7896349876	-2.1839859729
C71	0.5867000174	-1.9633822615	-4.7270992810
H72	1.2500450212	-2.8163469046	-4.5552865906
C73	0.0171088732	-1.5498788227	-3.3564827048
H74	0.8192387928	-1.2543275081	-2.6716123478
H75	-0.6775914012	-0.7080935897	-3.4451709563
H76	-0.5303278495	-2.3842412111	-2.9046061284
C77	-0.5316343291	-2.4362335858	-5.6769862166
H78	-0.1273419263	-2.7601642111	-6.6414603106
H79	-1.0748383706	-3.2795127548	-5.2373617746
H80	-1.2574108796	-1.6395931654	-5.8714898763
C81	7.4527567075	-3.4865179721	-4.4064272504
H82	6.7251364897	-3.0451118204	-5.0942644042
C83	8.4761148287	-4.2589988263	-5.2622429240
H84	8.9502279550	-3.5878474393	-5.9860650130
H85	9.2711319212	-4.6939644290	-4.6475822905
H86	8.0019947123	-5.0747100085	-5.8174418795
C87	8.1256887673	-2.3247908265	-3.6493672416

H88	7.3909698165	-1.7459643959	-3.0799658465
H89	8.8838943600	-2.6905935122	-2.9487140372
H90	8.6227853935	-1.6486665559	-4.3535406664
C91	5.0081233949	-0.0971092653	-6.6187373233
H92	5.3331738182	-1.0964630185	-6.3139401858
C93	5.8743918468	0.9141301142	-5.8426865127
H94	5.6314188758	1.9458893728	-6.1184985456
H95	5.7332620136	0.8127587600	-4.7619700803
H96	6.9352801580	0.7555246953	-6.0655796989
C97	5.2423981906	0.0147017551	-8.1385231981
H98	6.2992222406	-0.1483869325	-8.3751170934
H99	4.6543216627	-0.7259171848	-8.6905550306
H100	4.9672122988	1.0048321423	-8.5171655372

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C1	2.6120704421	1.1549659761	-0.9524778397
C2	2.7515372310	1.7303139451	0.4296778499
C3	2.1302988285	2.8778385477	0.9961511829
C4	1.1931956139	3.5883667905	0.3037769823
H5	1.5770866531	0.8475758642	-1.1534934844
H6	2.8570206889	1.9096585555	-1.7108103625
H7	2.4323286753	3.1878366016	1.9895377328
H8	0.8793223771	3.2983782576	-0.6956347522
C9	3.5559251004	-0.0266826405	-0.9960424493
C10	4.1394896365	-0.1119990213	0.2211609366
O11	0.5499100765	4.6708731667	0.6991993713
C12	0.8300693197	5.2240116925	1.9983741040

H13	0.1901983232	6.1001530728	2.0877807752
H14	0.5854835750	4.4992836960	2.7811187292
H15	1.8818171496	5.5180832693	2.0677050863
Au16	3.8252211834	-1.2369787571	-2.6276809876
C17	4.0596404513	-2.4360764564	-4.2919909825
N18	5.1479604178	-3.1245275246	-4.7305415586
N19	3.0977040909	-2.6883996748	-5.2212354391
C20	4.8682930118	-3.7955125507	-5.9147555458
C21	3.5762031974	-3.5207419650	-6.2243500500
H22	5.6095200001	-4.3984508307	-6.4142693919
H23	2.9577768262	-3.8339636370	-7.0502165969
N24	3.6439726760	0.9841448901	1.0748361374
C25	4.0525025189	1.2398884296	2.4233638467
C26	6.4184065845	1.8380602767	1.8280623957
C27	5.2964806332	1.5927653015	2.7696601741
H28	3.2670800126	1.1106647965	3.1636755207
H29	6.1929878238	1.7320086132	0.7493601745
H30	5.5280766622	1.7345393735	3.8217862209
O31	7.5215652525	2.1587156100	2.2181159228
C32	5.1074335811	-1.0768470310	0.7789098245
C33	4.8284405652	-1.7938255238	1.9544218962
C34	6.3239980386	-1.3063555580	0.1185562705
C35	5.7479324908	-2.7085836929	2.4612892034
H36	3.8812227013	-1.6473757868	2.4674510445
C37	7.2424195190	-2.2244542110	0.6269462473
H38	6.5453822688	-0.7620654894	-0.7942279763
C39	6.9600731246	-2.9221144303	1.8011532631
H40	5.5175464837	-3.2581181664	3.3694514185
H41	8.1786658297	-2.3898062841	0.1032724163

H42	7.6796423712	-3.6301051314	2.2022528945
C43	6.4324830763	-3.1987621100	-4.0691165034
C44	6.6659494677	-4.2701617815	-3.1842643882
C45	7.4092152864	-2.2316190725	-4.3782665886
C46	7.9364748627	-4.3540441839	-2.6026067734
C47	8.6599522166	-2.3647565971	-3.7634377084
C48	8.9236951550	-3.4156577429	-2.8898487117
H49	8.1560235499	-5.1676444826	-1.9176792181
H50	9.4401111469	-1.6406437285	-3.9796395484
H51	9.9064852880	-3.5071292048	-2.4349477210
C52	1.7490312226	-2.1709624966	-5.1700020861
C53	1.4736798179	-0.9507200697	-5.8163051935
C54	0.7712685480	-2.9157213209	-4.4822158586
C55	0.1583438311	-0.4764210811	-5.7522693290
C56	-0.5263418407	-2.3925947790	-4.4520004356
C57	-0.8308603542	-1.1872456763	-5.0782954935
H58	-0.0949040910	0.4605294158	-6.2398905976
H59	-1.3088198561	-2.9386623710	-3.9330942174
H60	-1.8467218684	-0.8028648903	-5.0462951827
C61	7.1606952374	-1.0741438945	-5.3416837833
H62	6.1432367304	-1.1669615371	-5.7314606336
C63	7.2461506050	0.2841288271	-4.6165420984
H64	6.5201251440	0.3383076279	-3.7984613217
H65	8.2433957676	0.4530859611	-4.1957698062
H66	7.0377794833	1.1035817278	-5.3132497820
C67	8.1187017611	-1.1263399074	-6.5477697000
H68	8.0404600087	-2.0801415618	-7.0794643007
H69	7.8841015080	-0.3241336082	-7.2555810993
H70	9.1623937662	-1.0014439278	-6.2406070499

C71	5.6000960803	-5.3058826841	-2.8338316002
H72	4.7214704248	-5.1165511405	-3.4570448450
C73	5.1555491340	-5.1626064972	-1.3642703513
H74	5.9896476159	-5.3394581313	-0.6775872938
H75	4.7661770624	-4.1597539524	-1.1630309445
H76	4.3698133379	-5.8899295872	-1.1312543023
C77	6.0706799202	-6.7409105217	-3.1403648099
H78	5.2645430063	-7.4549875806	-2.9413222771
H79	6.3680698794	-6.8502821887	-4.1883922867
H80	6.9251648396	-7.0309196898	-2.5201774994
C81	2.5407480154	-0.1453212873	-6.5551328880
H82	3.4802027937	-0.7045044574	-6.5152581237
C83	2.7905226372	1.2120797164	-5.8677187996
H84	1.8907335583	1.8370764212	-5.8779276752
H85	3.0971474816	1.0720393193	-4.8255265819
H86	3.5834199317	1.7629657799	-6.3854154424
C87	2.1852925588	0.0391907624	-8.0427452913
H88	2.9925146266	0.5638810729	-8.5644600639
H89	2.0315116435	-0.9241186219	-8.5393775839
H90	1.2716902555	0.6289664732	-8.1708681668
C91	1.0770359151	-4.2376723593	-3.7807602195
H92	2.1334966017	-4.4723734051	-3.9392682393
C93	0.8617840017	-4.1280639081	-2.2576850273
H94	1.4806809348	-3.3333361676	-1.8280359236
H95	-0.1844453873	-3.9128194795	-2.0146654038
H96	1.1286376040	-5.0703741988	-1.7669049539
C97	0.2591936173	-5.3992546977	-4.3789768692
H98	0.4339460936	-5.5012288760	-5.4549286858
H99	0.5366561714	-6.3444889155	-3.9005967885

H100	-0.8161174619	-5.2562445368	-4.2287982318

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C1	-4.1573163975	-1.7210856139	-0.0860761656
C2	-3.0857510087	-1.1002932462	-0.0227225518
C3	-1.6035722717	-0.9505400566	0.0598396778
H4	-1.1831825954	-1.7151802647	-0.6167717832
O5	-1.2651789316	0.3391132795	-0.3988027113
C6	0.0889693370	0.4510210786	-0.8342554097
H7	0.2094336943	1.4737331431	-1.1923651533
H8	0.7947645415	0.2643022681	-0.0177572608
H9	0.2946111508	-0.2471036739	-1.6576543253
C10	-1.1261892534	-1.2640838316	1.4768012247
C11	-0.7296933694	-0.3618229316	2.3385065379
C12	-0.3025052024	0.5136163418	3.2071501394
H13	-0.9815089083	0.9912965679	3.9093853734
H14	0.7476127791	0.7909443793	3.2661080570
Au15	-4.4096271785	0.7021125731	0.0946969907
C16	-5.7749569287	4.7057518009	-0.0924226970
C17	-6.6360317798	4.2332610006	0.8445208634
H18	-5.6640156361	5.6838886710	-0.5322026887
H19	-7.4326153618	4.7140731476	1.3891370208
C20	-5.2935849686	2.5255831249	0.2331279782
N21	-6.3270791778	2.8946219532	1.0347302379
N22	-4.9586372032	3.6459364997	-0.4571920991
C23	-5.3511156057	-2.4984678595	-0.1900573435
C24	-6.1013913968	-2.8123250401	0.9611853215
C25	-5.7598203564	-2.9824933769	-1.4494593510

C26	-7.2405369340	-3.6012501393	0.8470382526
H27	-5.7832439981	-2.4335131693	1.9271256663
C28	-6.8996593970	-3.7726161082	-1.5488571740
H29	-5.1766150709	-2.7380491615	-2.3317019710
C30	-7.6399850117	-4.0806755042	-0.4040283261
H31	-7.8185588356	-3.8450665973	1.7330276838
H32	-7.2124729848	-4.1490631524	-2.5179207823
H33	-8.5303007383	-4.6973656389	-0.4871588040
C34	-7.0436997654	2.0335657510	1.9516346831
C35	-8.2140766060	1.3978101249	1.4916956576
C36	-6.5661030685	1.9118394732	3.2703059347
C37	-8.9082197389	0.6005811753	2.4089188875
C38	-7.3000176814	1.0977391700	4.1405076275
C39	-8.4561294592	0.4494667899	3.7165378633
H40	-9.8185770224	0.0979209782	2.0956021959
H41	-6.9672012419	0.9788385900	5.1672462065
H42	-9.0145205495	-0.1696987052	4.4131242170
C43	-3.9065960969	3.7493062410	-1.4468443982
C44	-2.6316577959	4.1735789568	-1.0244224120
C45	-4.2221830668	3.4662329438	-2.7901233543
C46	-1.6457106003	4.3023050144	-2.0094591932
C47	-3.1931065650	3.6065468211	-3.7282826677
C48	-1.9206786446	4.0193063717	-3.3443282362
H49	-0.6520771897	4.6375302398	-1.7273220352
H50	-3.3942528405	3.3988504171	-4.7749861647
H51	-1.1403936375	4.1297099887	-4.0921501144
C52	-5.3218141779	2.6376145383	3.7750400034
H53	-4.8962023253	3.2086013162	2.9443634132
C54	-5.6762201073	3.6438298393	4.8884169144

H55	-6.0810983567	3.1397554253	5.7722450926
H56	-4.7839051730	4.1959404447	5.2017199372
H57	-6.4218205185	4.3704334099	4.5497525699
C58	-4.2398568790	1.6460702101	4.2447388115
H59	-3.9479305781	0.9657375849	3.4378958533
H60	-3.3479813788	2.1908176561	4.5735964458
H61	-4.5860485157	1.0401985508	5.0886453900
C62	-8.7489154564	1.5636243516	0.0714908884
H63	-8.0389582869	2.1754289675	-0.4927491037
C64	-8.8565499546	0.2116544282	-0.6592136438
H65	-9.5818017947	-0.4527195645	-0.1778440711
H66	-9.1873463135	0.3659285669	-1.6919730878
H67	-7.8918448297	-0.3052288187	-0.6830973411
C68	-10.0990163749	2.3090809737	0.0696378182
H69	-10.8693939487	1.7440138000	0.6049833539
H70	-10.0172291796	3.2911487913	0.5471283102
H71	-10.4502853802	2.4606909605	-0.9564384736
C72	-2.3112973230	4.5238342626	0.4262520732
H73	-3.1803560185	4.2657412131	1.0389311057
C74	-1.1224550631	3.7088236198	0.9684540635
H75	-0.1925329373	3.9546959487	0.4437248593
H76	-0.9650867569	3.9357010612	2.0285943802
H77	-1.2958904036	2.6340650433	0.8686335746
C78	-2.0687176824	6.0381476122	0.5860593306
H79	-1.1981789113	6.3641166044	0.0072274790
H80	-2.9297002269	6.6241150386	0.2472656005
H81	-1.8829154254	6.2864678656	1.6361856262
C82	-5.6166958727	3.0454072084	-3.2483218163
H83	-6.2613163057	2.9737003654	-2.3666991657

C84	-5.5997348837	1.6539284108	-3.9095747177
H85	-5.1888742160	0.8991401989	-3.2305901741
H86	-6.6161811382	1.3514791141	-4.1836650909
H87	-4.9960291866	1.6481376379	-4.8230552642
C88	-6.2388041268	4.1001762578	-4.1856835706
H89	-5.6595609366	4.2082637510	-5.1087226646
H90	-7.2569871783	3.8094442236	-4.4653972804
H91	-6.2871978550	5.0838113158	-3.7071968783
H92	-1.1343220949	-2.3184847506	1.7544619839

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C1	-3.7825245621	-2.0473162221	-0.1696722702
C2	-3.1693094292	-0.9844877634	0.2420182368
N3	-2.6533038679	-3.6315201993	-0.0604307382
C4	-2.1601894836	-4.4519290826	-0.9623186993
C5	-2.1611288899	-5.5362133112	0.9358406583
C6	-1.8160538560	-5.6928896543	-0.3728881322
H7	-2.0741791666	-4.1286962790	-1.9912887858
H8	-2.1059035297	-6.1726795906	1.8071553399
H9	-1.3826700393	-6.5574864333	-0.8510669180
O10	-2.6719440930	-4.3082737114	1.1455541230
C11	-1.7473123924	-0.8648085813	0.7477923121
H12	-1.1442020623	-1.6430226512	0.2483350351
O13	-1.2575265626	0.4103934644	0.3848360153
C14	0.1609279401	0.4861615039	0.3120273463
H15	0.3989247976	1.5055695297	0.0038886212
H16	0.6364433608	0.2821563007	1.2785901310

H17	0.5567894299	-0.2156584175	-0.4369867834
C18	-1.6949375190	-1.1380963146	2.2490948057
C19	-1.3606909234	-0.2639979138	3.1641689095
C20	-1.0050567870	0.5795785292	4.0961065481
H21	-1.7341910773	1.2128596053	4.5960253253
H22	0.0324119757	0.6797577846	4.4082585702
Au23	-4.3881387972	0.7381009176	0.1976404365
C24	-6.0786374514	4.6479973476	0.0336771893
C25	-7.0652008011	4.0174589896	0.7185759753
H26	-5.9699275877	5.6737520491	-0.2799644803
H27	-7.9956788639	4.3791199462	1.1257551891
C28	-5.4729082230	2.4770965461	0.2486911787
N29	-6.6790625904	2.6896854840	0.8418788783
N30	-5.1114954965	3.6921283473	-0.2455761248
C31	-4.9795722612	-2.6295194648	-0.7512830751
C32	-5.9121438648	-3.3156806889	0.0458915921
C33	-5.1873717884	-2.5406740776	-2.1401526489
C34	-7.0338676797	-3.8968277955	-0.5385691576
H35	-5.7512501589	-3.3832663096	1.1174379225
C36	-6.3121063238	-3.1240800530	-2.7179189382
H37	-4.4691677785	-2.0023396599	-2.7519659300
C38	-7.2331372839	-3.8053553787	-1.9185811746
H39	-7.7555226171	-4.4208483420	0.0809389263
H40	-6.4718200995	-3.0464294314	-3.7894193011
H41	-8.1082475643	-4.2626705592	-2.3715305179
C42	-3.8953343361	3.9845273126	-0.9730199645
C43	-2.7700553173	4.4274987856	-0.2511959649
C44	-3.9081506950	3.8625391778	-2.3761064689
C45	-1.6241590571	4.7493577570	-0.9876567925

C46	-2.7318222786	4.1931900680	-3.0584717015
C47	-1.6027410950	4.6325035866	-2.3740049765
H48	-0.7384179719	5.1011229047	-0.4669960201
H49	-2.7025205544	4.1119422473	-4.1411069232
H50	-0.7027657226	4.8912008102	-2.9251219305
C51	-7.4832089848	1.6798427474	1.4934022230
C52	-8.4813015288	1.0350850081	0.7367904533
C53	-7.2569438872	1.4104474534	2.8567734437
C54	-9.2614297225	0.0762112412	1.3923794577
C55	-8.0661259397	0.4393426685	3.4581088682
C56	-9.0555510821	-0.2210738063	2.7362817545
H57	-10.0427456766	-0.4410416773	0.8431377901
H58	-7.9244471983	0.2041417818	4.5088603357
H59	-9.6758815615	-0.9665145330	3.2264078626
C60	-8.7371053137	1.3453034246	-0.7362971160
H61	-8.0291034718	2.1170575725	-1.0522405218
C62	-8.4830120184	0.1110752816	-1.6223539606
H63	-7.4619098141	-0.2620523927	-1.4980071615
H64	-9.1714409173	-0.7060029513	-1.3814911345
H65	-8.6288960962	0.3657741725	-2.6781411196
C66	-10.1547269398	1.9090899852	-0.9568296283
H67	-10.3283192700	2.8064964034	-0.3540526430
H68	-10.2997001686	2.1758162393	-2.0092235070
H69	-10.9255371744	1.1775083199	-0.6920097820
C70	-6.2051123616	2.1420619409	3.6864218255
H71	-5.6667175818	2.8295688308	3.0273339364
C72	-5.1644252493	1.1682938913	4.2719351061
H73	-5.6250971527	0.4456878523	4.9542103991
H74	-4.6541533590	0.6099665730	3.4805158422

H75	-4.4101105634	1.7224402687	4.8419222976
C76	-6.8632188572	2.9888919752	4.7946561126
H77	-6.1032659028	3.5511385116	5.3478646767
H78	-7.5790551100	3.7061651823	4.3798549571
H79	-7.4006249993	2.3615628804	5.5139088746
C80	-2.7671219179	4.5876916372	1.2661392165
H81	-3.7146966728	4.1992700003	1.6518671221
C82	-2.6814224518	6.0747189992	1.6643993701
H83	-1.7467595080	6.5267174594	1.3155845911
H84	-3.5081630621	6.6546891450	1.2405241241
H85	-2.7170876363	6.1821080565	2.7537059559
C86	-1.6424487007	3.7661271448	1.9234361980
H87	-0.6522295829	4.1362963940	1.6346913952
H88	-1.7103069164	3.8414937649	3.0144505026
H89	-1.7045270504	2.7100419235	1.6468887476
C90	-5.1350002036	3.4013085076	-3.1584373959
H91	-5.9401614426	3.1988330412	-2.4459152220
C92	-5.6370287735	4.4989495727	-4.1174426147
H93	-4.8924090809	4.7349296650	-4.8850926293
H94	-6.5480366812	4.1718587052	-4.6300744902
H95	-5.8652968714	5.4256398996	-3.5808864466
C96	-4.8572026039	2.0860003761	-3.9116977510
H97	-4.0710507097	2.2120433017	-4.6638226335
H98	-4.5404161929	1.2981473822	-3.2203339170
H99	-5.7606888312	1.7463594120	-4.4301509562
H100	-1.9571684451	-2.1528493452	2.5474015632

β

C1	-3.9640419022	-2.2043075183	0.7696878580
C2	-3.6420150570	-1.1444505513	-0.0153435646
N3	-3.5131638983	-3.5310706251	0.3901485201
C4	-3.8554657443	-4.3671270796	-0.5732076598
C5	-2.3442454039	-5.3690195409	0.6602924642
C6	-3.1209999272	-5.5629457261	-0.4476528053
H7	-4.6059418397	-4.0721727534	-1.2936967259
H8	-1.6256489204	-5.9857378470	1.1821300896
H9	-3.1745894358	-6.4369728704	-1.0778559058
O10	-2.5474720299	-4.1547025444	1.1881225261
C11	-2.6654461765	-1.2978297069	-1.1727540255
H12	-2.4828760093	-2.3566756238	-1.4287717150
O13	-3.2239048898	-0.6572529963	-2.3061666985
C14	-2.6278718303	-1.0397881658	-3.5382206535
H15	-3.1640223789	-0.5034328718	-4.3235526052
H16	-1.5663515561	-0.7730692501	-3.5837478377
H17	-2.7291942870	-2.1224058029	-3.7134243531
C18	-1.3162926324	-0.7278074265	-0.7363530708
C19	-0.7773352067	0.3615044551	-1.2200795213
C20	-0.2285680712	1.4389051202	-1.7150270384
H21	-0.4340427854	2.4206719174	-1.2931749909
H22	0.4399065459	1.3923340284	-2.5729664211
Au23	-4.4974724489	0.7299688283	0.2347282792
C24	-5.9901564474	4.7529642723	0.0201950645
C25	-7.1563348755	4.0640423225	0.0191214208
H26	-5.7826741384	5.8084629781	-0.0500354002
H27	-8.1804181868	4.3943681944	-0.0492512444

C28	-5.4768226761	2.5531390114	0.2141171599
N29	-6.8277159790	2.7204498110	0.1423130769
N30	-4.9714606523	3.8135015606	0.1335103406
C31	-4.7015405192	-2.2525689150	2.0624496937
C32	-5.7633139671	-3.1509648194	2.2465026046
C33	-4.2917228234	-1.4567014718	3.1423385646
C34	-6.4115500722	-3.2432156326	3.4755119852
H35	-6.0927965786	-3.7792250387	1.4221910568
C36	-4.9354220253	-1.5572241055	4.3774811164
H37	-3.4551836690	-0.7764042419	3.0113001864
C38	-5.9939733488	-2.4516241260	4.5471157126
H39	-7.2375002250	-3.9375422953	3.6005089321
H40	-4.5984923879	-0.9464794835	5.2112231404
H41	-6.4903394128	-2.5333499211	5.5100806162
C42	-3.5724693127	4.1805484064	0.1384014765
C43	-2.9025041080	4.2811489907	1.3729037560
C44	-2.9673185048	4.5115672328	-1.0925567963
C45	-1.5770792006	4.7317209279	1.3492798180
C46	-1.6497245358	4.9806291675	-1.0496268353
C47	-0.9595357373	5.0930717451	0.1553449872
H48	-1.0264484600	4.8121759367	2.2811285842
H49	-1.1538037441	5.2580107896	-1.9754418116
H50	0.0627755212	5.4616111373	0.1644453429
C51	-7.7895803092	1.6459494163	0.2366516165
C52	-8.1252510516	0.9383424072	-0.9336136146
C53	-8.3476192720	1.3449050104	1.4973303199
C54	-9.0253407844	-0.1251432788	-0.8046537108
C55	-9.2366984955	0.2678814292	1.5635876973
C56	-9.5675253845	-0.4674508858	0.4289017194

H57	-9.3079772775	-0.6902476095	-1.6880442430
H58	-9.6793809474	0.0013297984	2.5186918753
H59	-10.2659049977	-1.2966297705	0.5029391709
C60	-7.5737122000	1.2943560316	-2.3120483646
H61	-6.8105833068	2.0676854477	-2.1850569874
C62	-8.6858086401	1.8835040005	-3.2047930335
H63	-8.2789384948	2.1815021573	-4.1770759953
H64	-9.4804253535	1.1513082595	-3.3848030796
H65	-9.1452714882	2.7653834482	-2.7459170244
C66	-6.8898372880	0.0958185165	-2.9980840827
H67	-6.0580991927	-0.2807999802	-2.3952563677
H68	-7.5933001567	-0.7262362502	-3.1738596638
H69	-6.4903517090	0.3987125084	-3.9718703646
C70	-7.9890231380	2.1046501748	2.7748351529
H71	-7.3327503587	2.9373740501	2.5097294920
C72	-7.2091776057	1.2084707712	3.7550443854
H73	-7.8067421916	0.3463458667	4.0701466480
H74	-6.2954037225	0.8233249563	3.2932237296
H75	-6.9340626846	1.7720273874	4.6537844480
C76	-9.2351991371	2.7136754282	3.4467853761
H77	-8.9423598723	3.3107081769	4.3169754556
H78	-9.7845923560	3.3656320592	2.7599269447
H79	-9.9280462471	1.9412327816	3.7969133194
C80	-3.5519677300	3.9141312354	2.7043194772
H81	-4.5920883513	3.6341958429	2.5126345476
C82	-2.8634850321	2.6847740284	3.3284885992
H83	-1.8109162758	2.8853706933	3.5538922464
H84	-3.3581722587	2.4019362653	4.2647092681
H85	-2.9069867520	1.8314157949	2.6435307038

C86	-3.5693791747	5.1047474552	3.6824877490
H87	-2.5575540888	5.4131040177	3.9660990786
H88	-4.0718616690	5.9749771841	3.2474243599
H89	-4.0993793554	4.8320085182	4.6016006577
C90	-3.6684771817	4.3586874992	-2.4425436495
H91	-4.6944247740	4.0271100219	-2.2630492511
C92	-2.9837192133	3.2668206926	-3.2928272441
H93	-2.9484194702	2.3107612531	-2.7618318860
H94	-3.5312015049	3.1231814665	-4.2315691211
H95	-1.9558927270	3.5466342017	-3.5487638040
C96	-3.7483033378	5.6946990395	-3.2069297082
H97	-4.3123634130	5.5671852451	-4.1370467186
H98	-4.2451185898	6.4695611200	-2.6136312961
H99	-2.7548578468	6.0694741022	-3.4756274355
H100	-0.8004526896	-1.2888438455	0.0438108436

βγ-TS

C1	-3.7419663688	-2.2188357733	-0.1117820865
C2	-3.2777090361	-0.9472189103	0.2524571876
N3	-2.8318053984	-3.1218889761	-0.5565383588
C4	-2.4327527836	-3.6872475231	-1.6742903543
C5	-1.5903681016	-5.1254841852	-0.1846698661
C6	-1.6738749512	-4.8513365979	-1.5420749037
H7	-2.6979675646	-3.1995606782	-2.6078839280
H8	-1.0426614193	-5.9472848596	0.2791922962
H9	-1.2289292316	-5.4133810515	-2.3479982907
O10	-2.2035000074	-4.3079245194	0.5967229556
C11	-1.8085317778	-0.7583741616	0.5177255489

H12	-1.1903328360	-1.4184486049	-0.1136357057
O13	-1.4598683563	0.5864806184	0.2909314134
C14	-0.0571189905	0.8245194335	0.2543103954
H15	0.0665614129	1.8852320910	0.0317895335
H16	0.4241539326	0.5945841374	1.2125260278
H17	0.4259171294	0.2327539090	-0.5373715346
C18	-1.6249947927	-1.2172221237	1.9751283107
C19	-1.5663387788	-0.4070154350	3.0038024864
C20	-1.4618053229	0.3750908593	4.0440373211
H21	-2.3352785052	0.6692555910	4.6216339157
H22	-0.4979269853	0.7574032893	4.3736875607
Au23	-4.4557335338	0.7351028559	0.3219807280
C24	-6.0093897554	4.6938192846	-0.1149104849
C25	-7.1026160798	4.1170300126	0.4433324866
H26	-5.8245228134	5.7029956125	-0.4462495739
H27	-8.0691433907	4.5183718895	0.7024268435
C28	-5.5091528199	2.5155133333	0.2633660919
N29	-6.7799471733	2.7858284555	0.6668134188
N30	-5.0441109063	3.7029164399	-0.2157375312
C31	-5.1540062649	-2.6830704473	-0.0096349371
C32	-5.7056972507	-3.5614948129	-0.9555595857
C33	-5.9452349375	-2.2760976424	1.0761000593
C34	-7.0208878967	-4.0020856958	-0.8324977013
H35	-5.1137747789	-3.9039382932	-1.8000467541
C36	-7.2591552075	-2.7229997379	1.2010410403
H37	-5.5230402334	-1.6188509268	1.8291713677
C38	-7.8012672713	-3.5848835475	0.2476648712
H39	-7.4361449530	-4.6736370291	-1.5783639791
H40	-7.8566543709	-2.3957940980	2.0461182396

H41	-8.8240187586	-3.9369941530	0.3477911747
C42	-3.7259557644	3.9472475167	-0.7585429296
C43	-2.7421261487	4.4823054519	0.0954581712
C44	-3.5037580791	3.7000065418	-2.1270291392
C45	-1.4936682051	4.7703853590	-0.4684283570
C46	-2.2327688943	3.9964832734	-2.6320575346
C47	-1.2396636814	4.5291997088	-1.8155345161
H48	-0.7124666434	5.1936481957	0.1563282011
H49	-2.0223391058	3.8198651872	-3.6827853409
H50	-0.2645987969	4.7650073306	-2.2330880808
C51	-7.7148145700	1.8475852526	1.2443472648
C52	-8.6463633547	1.2267216136	0.3895199799
C53	-7.7055568098	1.6591192128	2.6398243173
C54	-9.6033854412	0.3957342697	0.9825639045
C55	-8.6819151760	0.8109001887	3.1760451675
C56	-9.6254402128	0.1933287155	2.3597482053
H57	-10.3436139692	-0.0947617714	0.3573095173
H58	-8.7129029420	0.6450024195	4.2489597099
H59	-10.3860064617	-0.4454325584	2.8006506452
C60	-8.6445390306	1.4291290107	-1.1237944651
H61	-7.8181479545	2.0992741580	-1.3782716094
C62	-9.9443882422	2.1014896700	-1.6082274383
H63	-9.9028126966	2.2783163762	-2.6883281538
H64	-10.8207924911	1.4754304880	-1.4092065231
H65	-10.1065611773	3.0654572767	-1.1146158966
C66	-8.3915943543	0.1011191538	-1.8633454772
H67	-7.4533722304	-0.3593312637	-1.5386841424
H68	-9.1973257853	-0.6188658622	-1.6854514981
H69	-8.3355296044	0.2741243271	-2.9437064302

C70	-6.7041738466	2.3467093484	3.5644287183
H71	-6.0432727309	2.9675302591	2.9524959755
C72	-5.8138226637	1.3192039213	4.2906452139
H73	-6.4039389085	0.6544343999	4.9306894858
H74	-5.2628878879	0.7003727447	3.5742816589
H75	-5.0863316034	1.8329524655	4.9291827378
C76	-7.4111235099	3.2801374515	4.5669757582
H77	-6.6740876849	3.8078247471	5.1816738493
H78	-8.0215862040	4.0299330150	4.0534410309
H79	-8.0676879800	2.7232236366	5.2436638225
C80	-2.9859222290	4.7567637354	1.5769210168
H81	-3.9972246854	4.4205836502	1.8249144854
C82	-2.0137857328	3.9514436421	2.4612604652
H83	-0.9778728587	4.2782786241	2.3180430730
H84	-2.2577077359	4.0952051687	3.5198107617
H85	-2.0646265477	2.8818442084	2.2369595179
C86	-2.9114944162	6.2640483963	1.8920714450
H87	-1.9149875128	6.6683704718	1.6840760601
H88	-3.6316645229	6.8368709890	1.2982298118
H89	-3.1277129778	6.4441715825	2.9505786923
C90	-4.5808022391	3.1501177777	-3.0586515749
H91	-5.4930819308	2.9960649913	-2.4748836777
C92	-4.1779590401	1.7797962234	-3.6374225861
H93	-3.9848330611	1.0588918100	-2.8360223066
H94	-4.9796332936	1.3838727991	-4.2706227072
H95	-3.2747012461	1.8537523643	-4.2526771286
C96	-4.9182954640	4.1518941268	-4.1807418517
H97	-5.7316790270	3.7665169590	-4.8048052109
H98	-5.2331669415	5.1181115005	-3.7734608118

H99	-4.0573654723	4.3312338734	-4.8334516787
H100	-1.5593101026	-2.2939408291	2.1242588605

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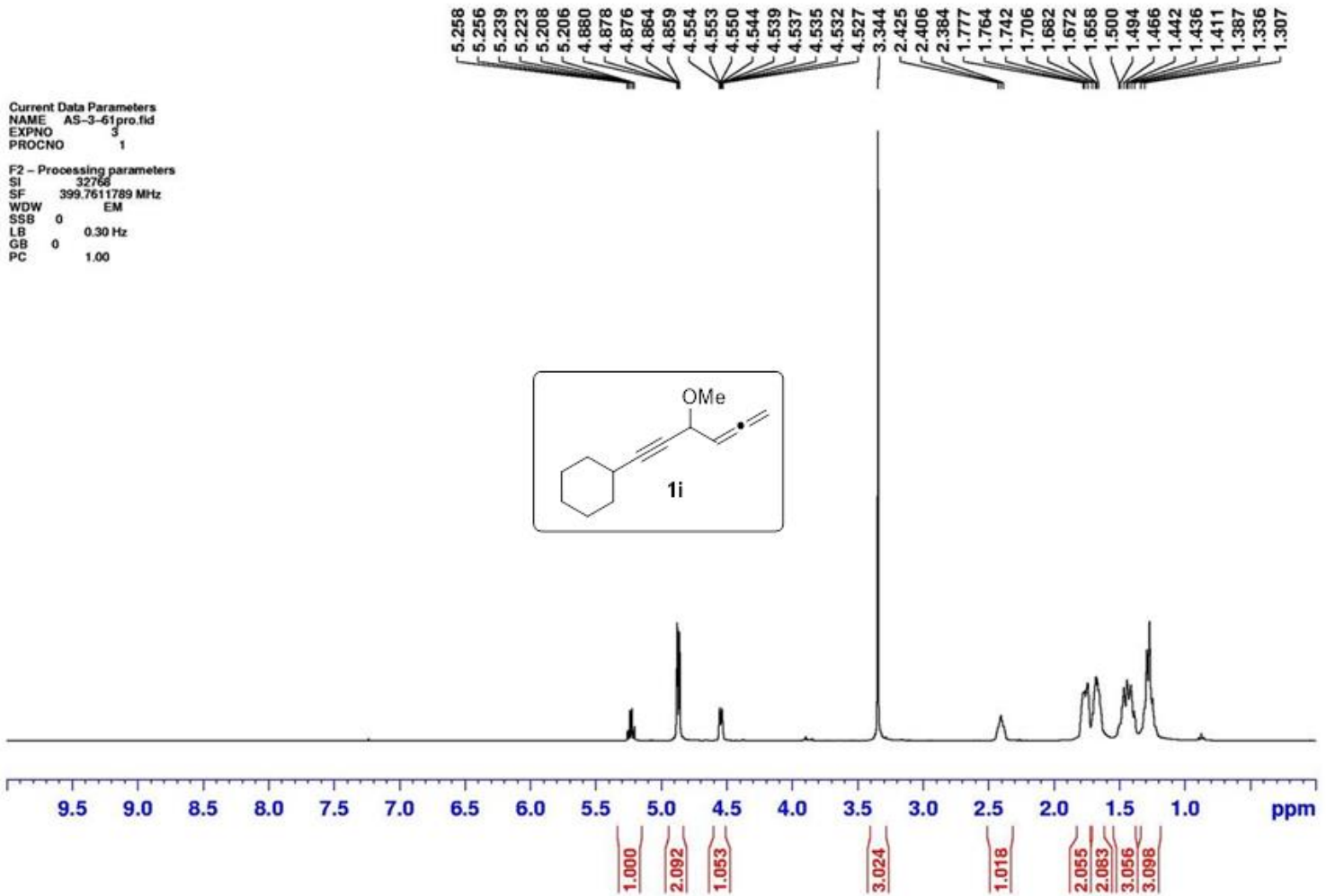
C1	-3.5512564120	-2.1248779274	-0.3721970149
C2	-3.0869608214	-0.7906637614	0.1566118542
N3	-2.7103972966	-2.7351685401	-1.1272793968
C4	-2.7700666796	-3.9587132257	-1.7384293635
C5	-2.0964143709	-5.3424309281	0.2262645062
C6	-2.4546374629	-5.1548404603	-1.1749445593
H7	-2.9503459114	-3.9122844793	-2.8140326595
H8	-1.8614869268	-6.3893896290	0.5060328027
H9	-2.4321413234	-6.0282934586	-1.8191101358
O10	-2.0270827892	-4.4588944201	1.0761179844
C11	-1.6537934319	-0.6463138721	0.2608350257
H12	-1.0452646826	-1.3485728133	-0.3192412502
O13	-1.1656505843	0.6397107939	0.3035306755
C14	0.2426170610	0.7173043590	0.5357393125
H15	0.5044257555	1.7735767093	0.4734946101
H16	0.5054353348	0.3324893108	1.5292763568
H17	0.7996995925	0.1576623969	-0.2262215222
C18	-1.9489476115	-1.3503821092	1.6533346924
C19	-2.1350625152	-0.6568175806	2.7663137317
C20	-2.2556155849	0.0012914641	3.8797018154
H21	-3.2305852157	0.2079748763	4.3148270345
H22	-1.3788544878	0.3646649440	4.4123520934
Au23	-4.3436292012	0.8337514790	0.3308913750

C24	-6.1096621895	4.6906970400	-0.0472357250
C25	-7.1749936637	4.0563290224	0.5039437064
H26	-5.9735731912	5.7108793566	-0.3684179216
H27	-8.1597580826	4.4094343730	0.7645794390
C28	-5.5108827628	2.5350142351	0.3028897455
N29	-6.7937433449	2.7374983659	0.7109515862
N30	-5.1011967870	3.7467673197	-0.1638990921
C31	-4.9115947457	-2.6239875644	-0.0358276522
C32	-5.6519038068	-3.3650848938	-0.9716237273
C33	-5.4696721654	-2.3824127311	1.2299751487
C34	-6.9133194632	-3.8571138504	-0.6476756621
H35	-5.2546940074	-3.5404412137	-1.9658786731
C36	-6.7240413186	-2.8907564331	1.5580452006
H37	-4.9126547844	-1.8127444996	1.9652812750
C38	-7.4488622663	-3.6277791391	0.6209007943
H39	-7.4785005463	-4.4178254990	-1.3863469843
H40	-7.1384999939	-2.7047268540	2.5439915071
H41	-8.4297490446	-4.0188505585	0.8754971161
C42	-3.8142913551	4.0293741806	-0.7653529718
C43	-2.7741737457	4.5012907258	0.0569963595
C44	-3.6784304816	3.8594341969	-2.1578923362
C45	-1.5556557869	4.8006493272	-0.5630928301
C46	-2.4353082824	4.1693862925	-2.7204577642
C47	-1.3858803620	4.6350359095	-1.9342338375
H48	-0.7304562225	5.1738767220	0.0363859024
H49	-2.2899669577	4.0511112171	-3.7901881309
H50	-0.4319243087	4.8766684524	-2.3947711592
C51	-7.7018770792	1.7415300297	1.2412317421
C52	-8.5348831872	1.0514416975	0.3373244143

C53	-7.7772797051	1.5694314164	2.6370732205
C54	-9.4635019217	0.1537528044	0.8786235310
C55	-8.7241264677	0.6584098457	3.1221500439
C56	-9.5593809051	-0.0390943199	2.2538702589
H57	-10.1268590659	-0.3912074475	0.2138537035
H58	-8.8179522830	0.5052637177	4.1931216910
H59	-10.2962956520	-0.7309297379	2.6524674658
C60	-8.4803129278	1.2689033250	-1.1728462405
H61	-7.6518137695	1.9490859208	-1.3911323045
C62	-9.7715445919	1.9392554210	-1.6842930702
H63	-9.7051948481	2.1248023138	-2.7615380011
H64	-10.6479064985	1.3063661015	-1.5086734661
H65	-9.9507689486	2.8985806145	-1.1873637637
C66	-8.1943511684	-0.0427469979	-1.9276679094
H67	-7.2679953736	-0.5086161994	-1.5780700559
H68	-9.0040316549	-0.7689071407	-1.7998247206
H69	-8.0969705758	0.1538746980	-3.0009329516
C70	-6.8968644087	2.3438573072	3.6135149700
H71	-6.1978937874	2.9526251213	3.0329099556
C72	-6.0526219615	1.3927503403	4.4827147190
H73	-6.6772716788	0.7768985094	5.1381474454
H74	-5.4614548072	0.7193185526	3.8523369273
H75	-5.3691434321	1.9644145269	5.1204461801
C76	-7.7315062305	3.3033799151	4.4846409369
H77	-7.0817477963	3.8774463920	5.1536763860
H78	-8.2946472408	4.0134236053	3.8702316268
H79	-8.4507789569	2.7584339218	5.1050138428
C80	-2.9294935582	4.7012130360	1.5618935339
H81	-3.9342143991	4.3753899531	1.8483269972

C82	-1.9296077748	3.8315880396	2.3485183204
H83	-0.8956275553	4.1391516620	2.1568989533
H84	-2.1057786786	3.9312298272	3.4254229280
H85	-2.0237385248	2.7760492975	2.0756811031
C86	-2.7994874204	6.1886835145	1.9463328319
H87	-1.8055589573	6.5796770319	1.7037529250
H88	-3.5353229552	6.8057064293	1.4203017616
H89	-2.9542139836	6.3214902367	3.0224066557
C90	-4.8148585227	3.3724751905	-3.0544804510
H91	-5.6930731428	3.1889353994	-2.4282427750
C92	-4.4605752664	2.0386116437	-3.7406822554
H93	-4.2133631012	1.2681190174	-3.0029532967
H94	-5.3067015503	1.6822012981	-4.3384172646
H95	-3.6037038140	2.1478147199	-4.4137902795
C96	-5.2112462849	4.4421759011	-4.0917527228
H97	-6.0648648084	4.0991354144	-4.6860170571
H98	-5.4915243438	5.3845654451	-3.6101207608
H99	-4.3903253799	4.6545467611	-4.7847017106
H100	-1.8675917968	-2.4378167344	1.6527148283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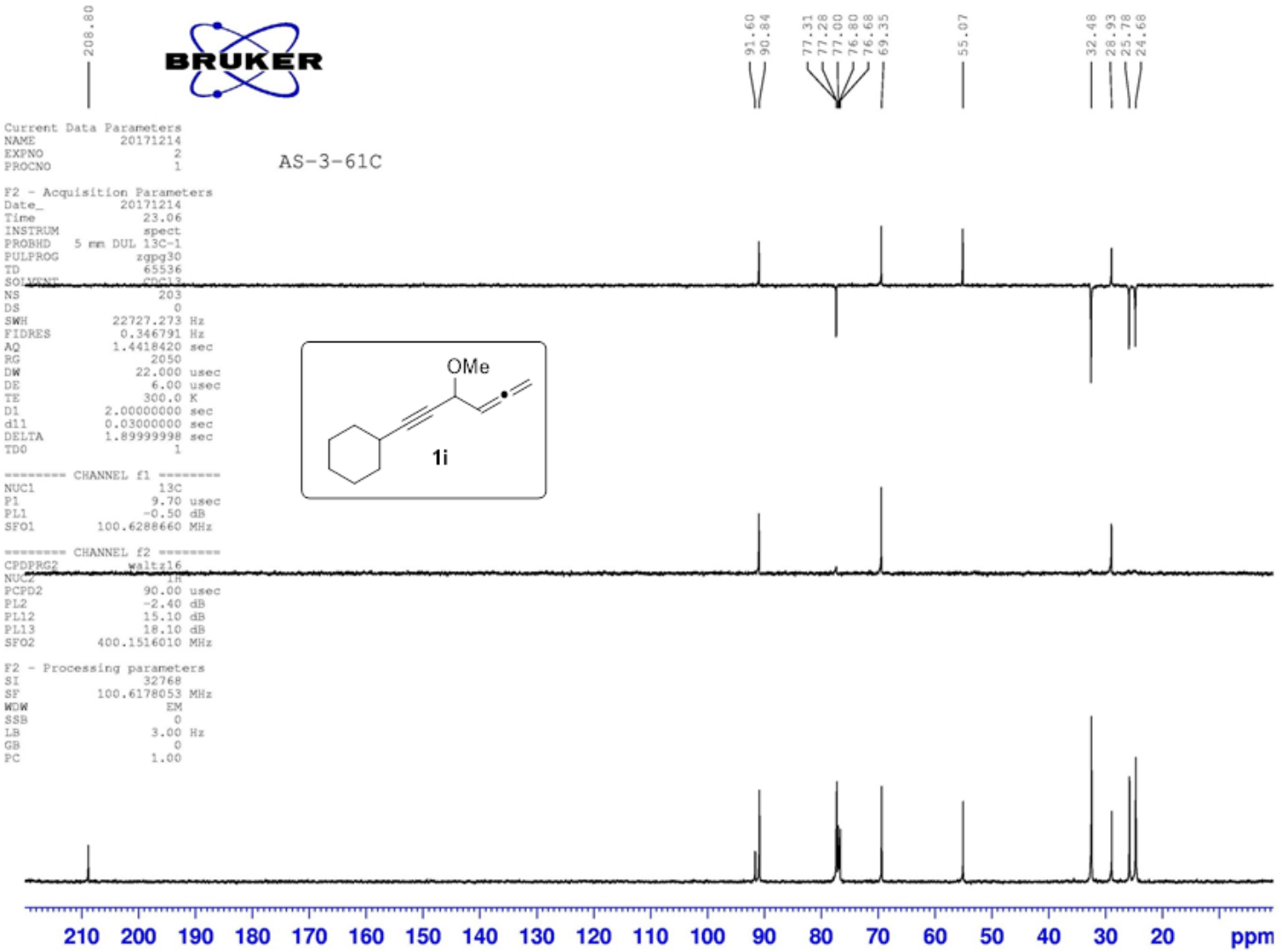
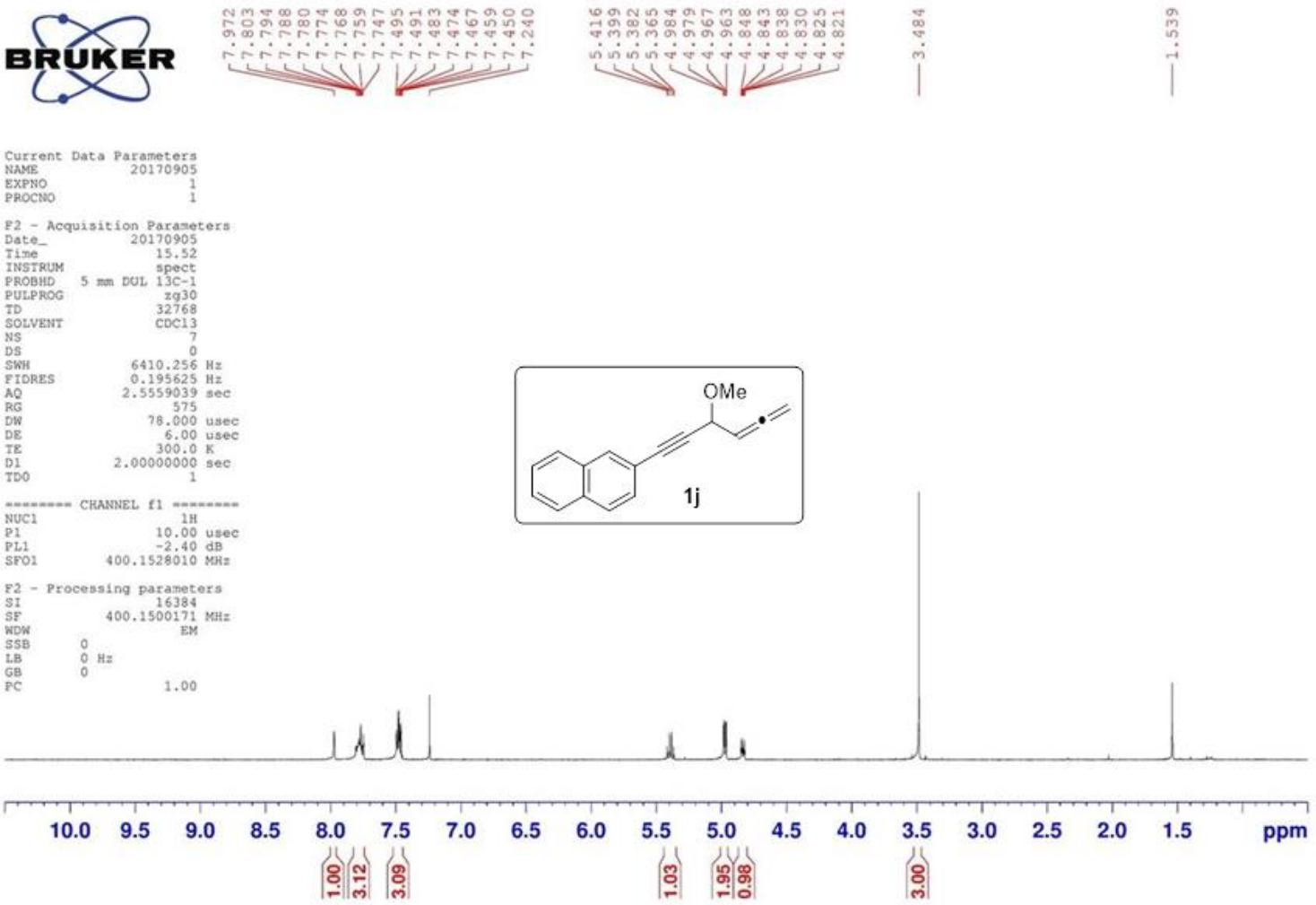
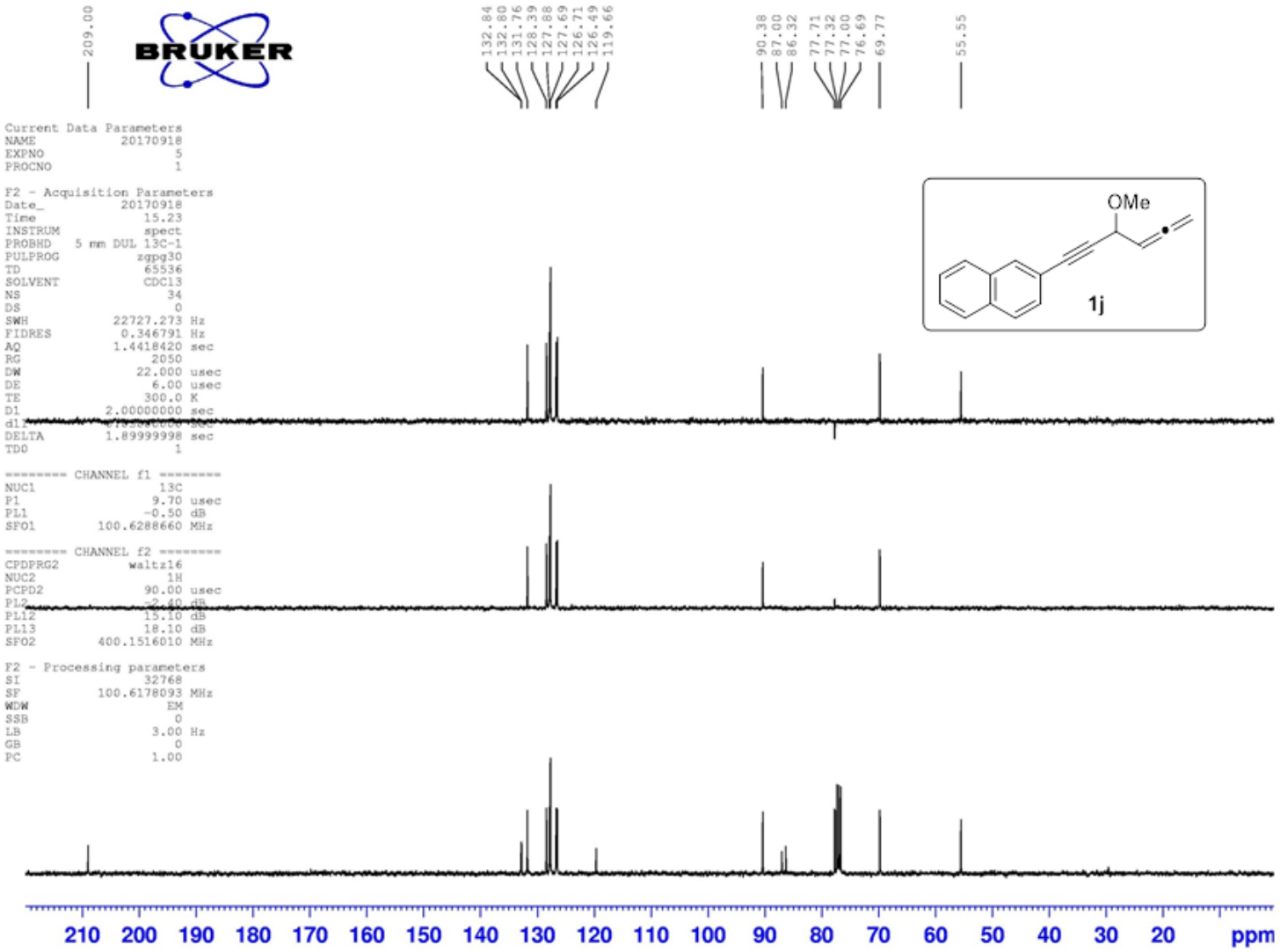
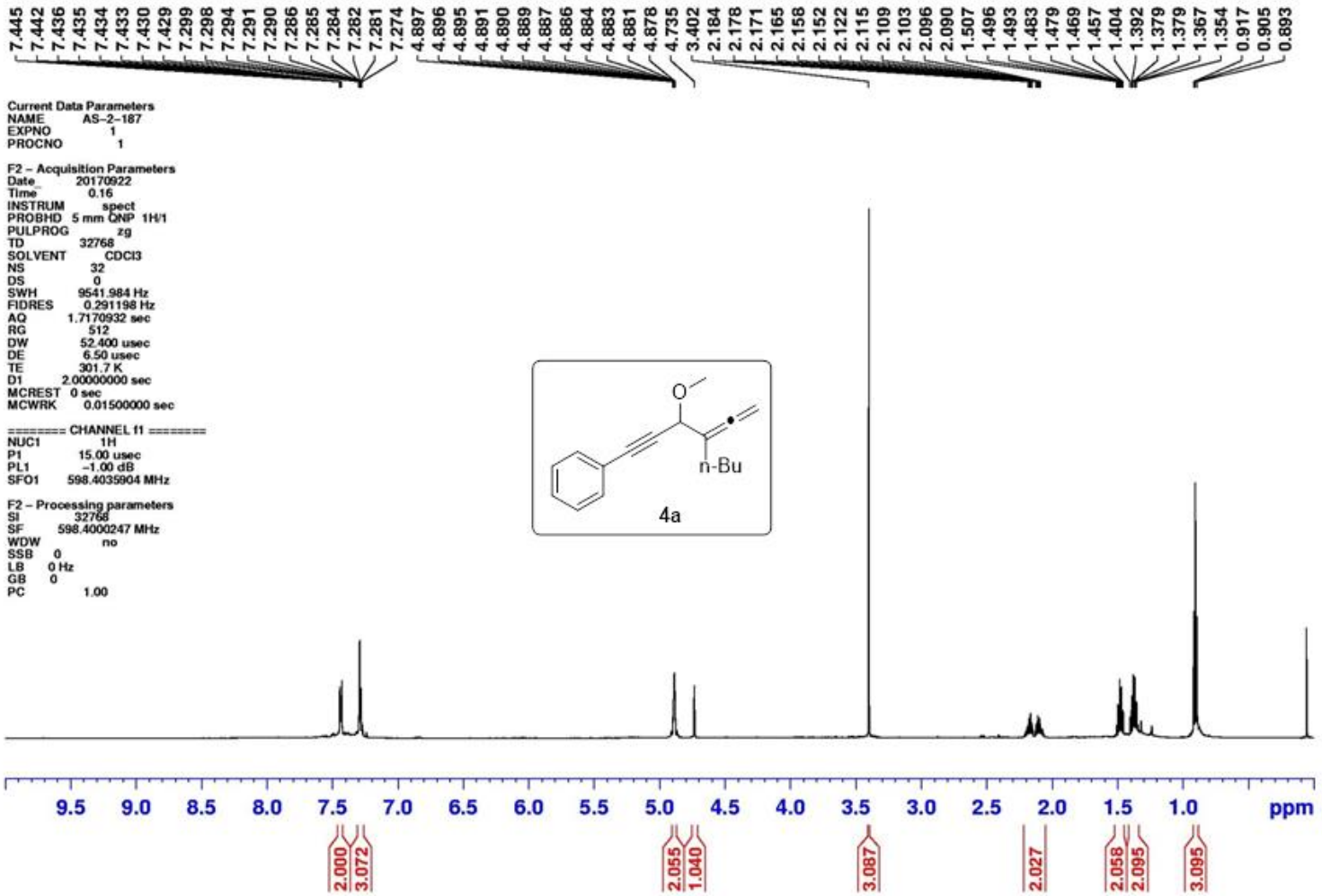
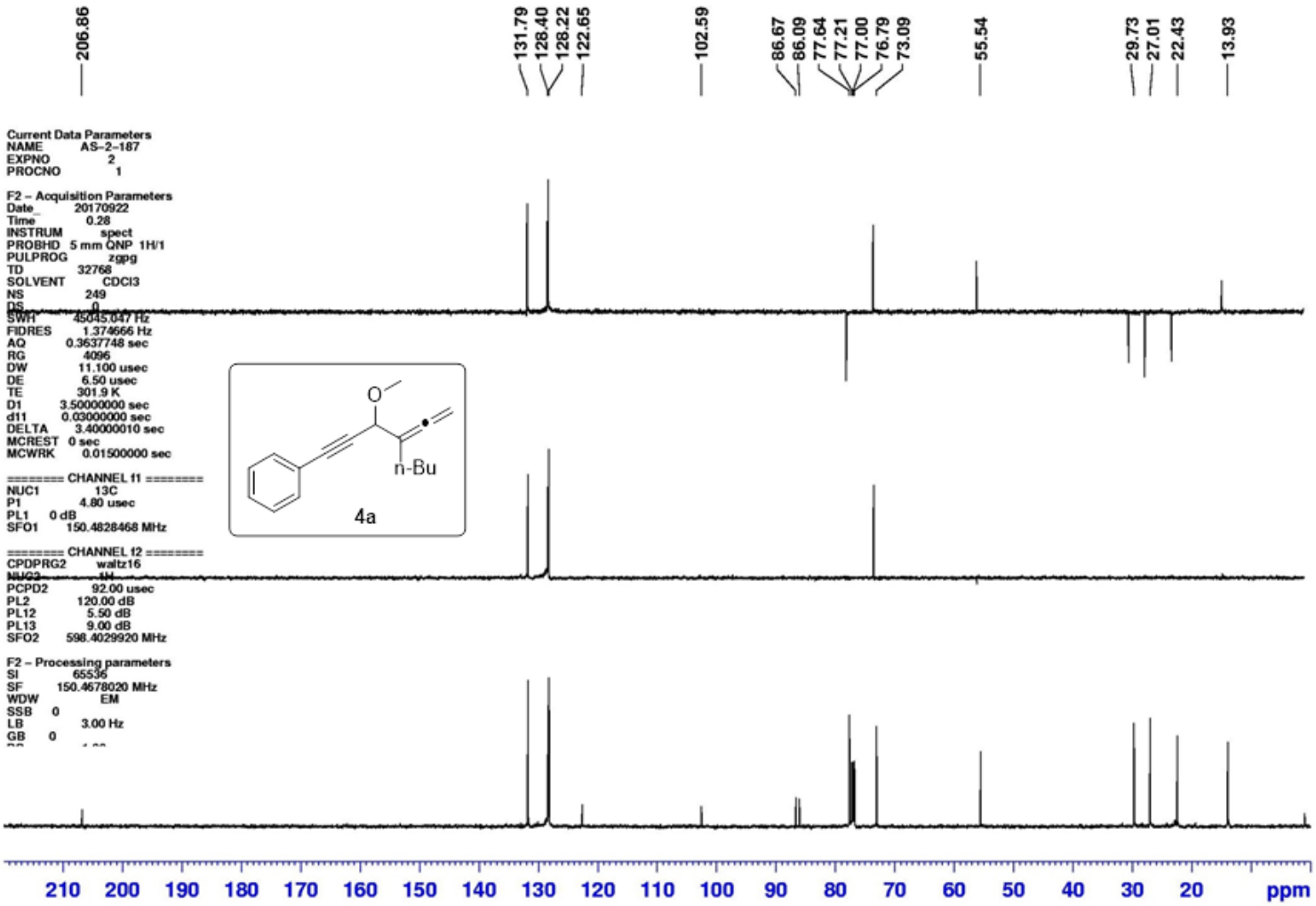
5.256
5.239
5.223
5.208
5.206
4.880
4.878
4.876
4.864
4.859
4.554
4.553
4.550
4.544
4.539
4.537
4.535
4.532
4.527
3.344
2.425
2.406
2.384
1.777
1.764
1.742
1.706
1.682
1.672
1.658
1.500
1.494
1.466
1.442
1.436
1.411
1.387
1.336
1.307
Current Data Parameters
NAME AS-3-61pro.fid
EXPNO 3
PROCNO 1
F2 – Processing parameters
SI 32768
SF 399.7611789 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
1i
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.000
2.092
1.053
3.024
1.018
2.055
2.083
3.056
3.098

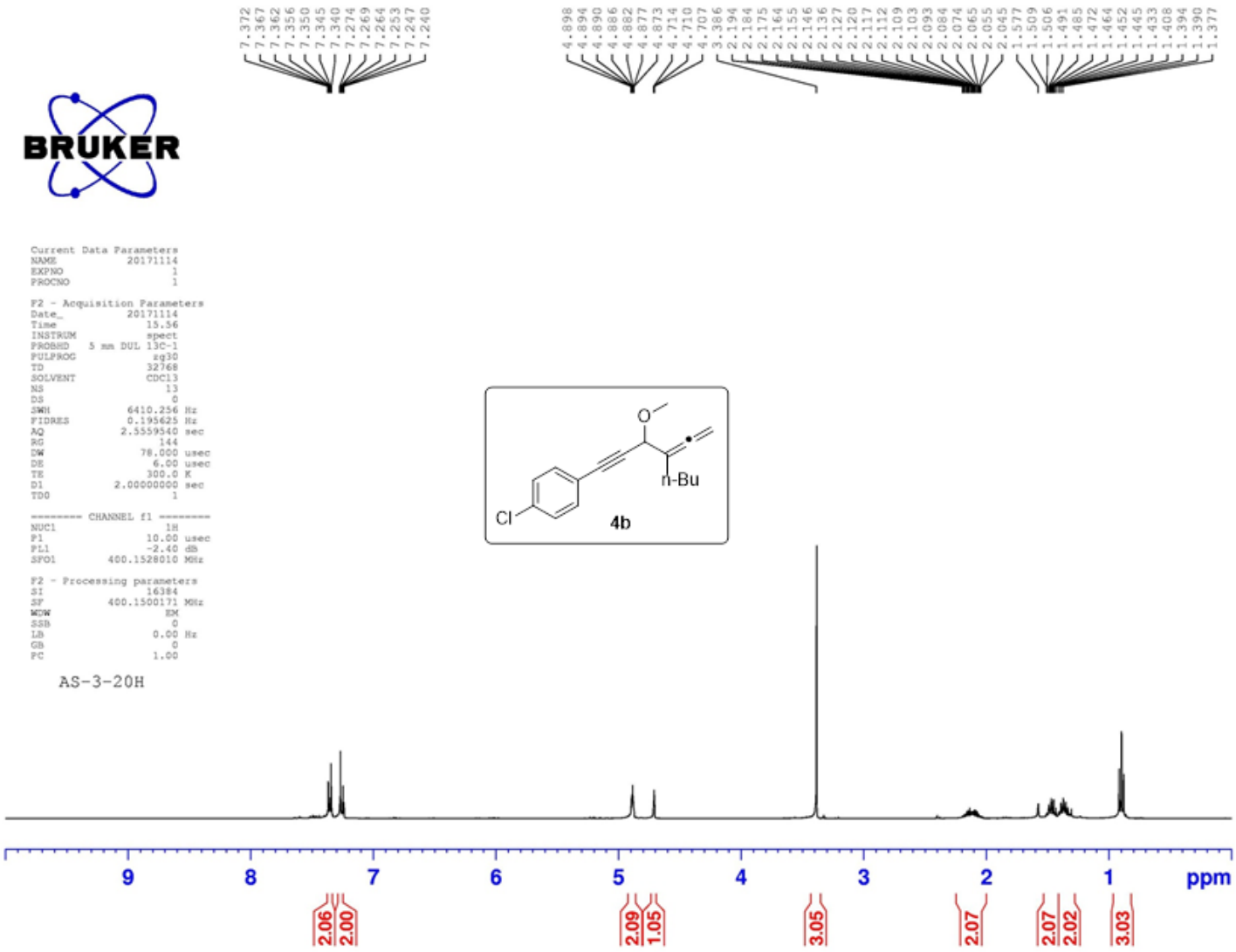

208.80
91.60
90.84
77.31
77.28
77.00
76.80
76.68
69.35
55.07
32.48
28.93
25.78
24.68
BRUKER
Current Data Parameters
NAME 20171214
EXPNO 2
PROCNO 1
AS-3-61C
F2 - Acquisition Parameters
Date_ 20171214
Time 23.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 100.6178053 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
1i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

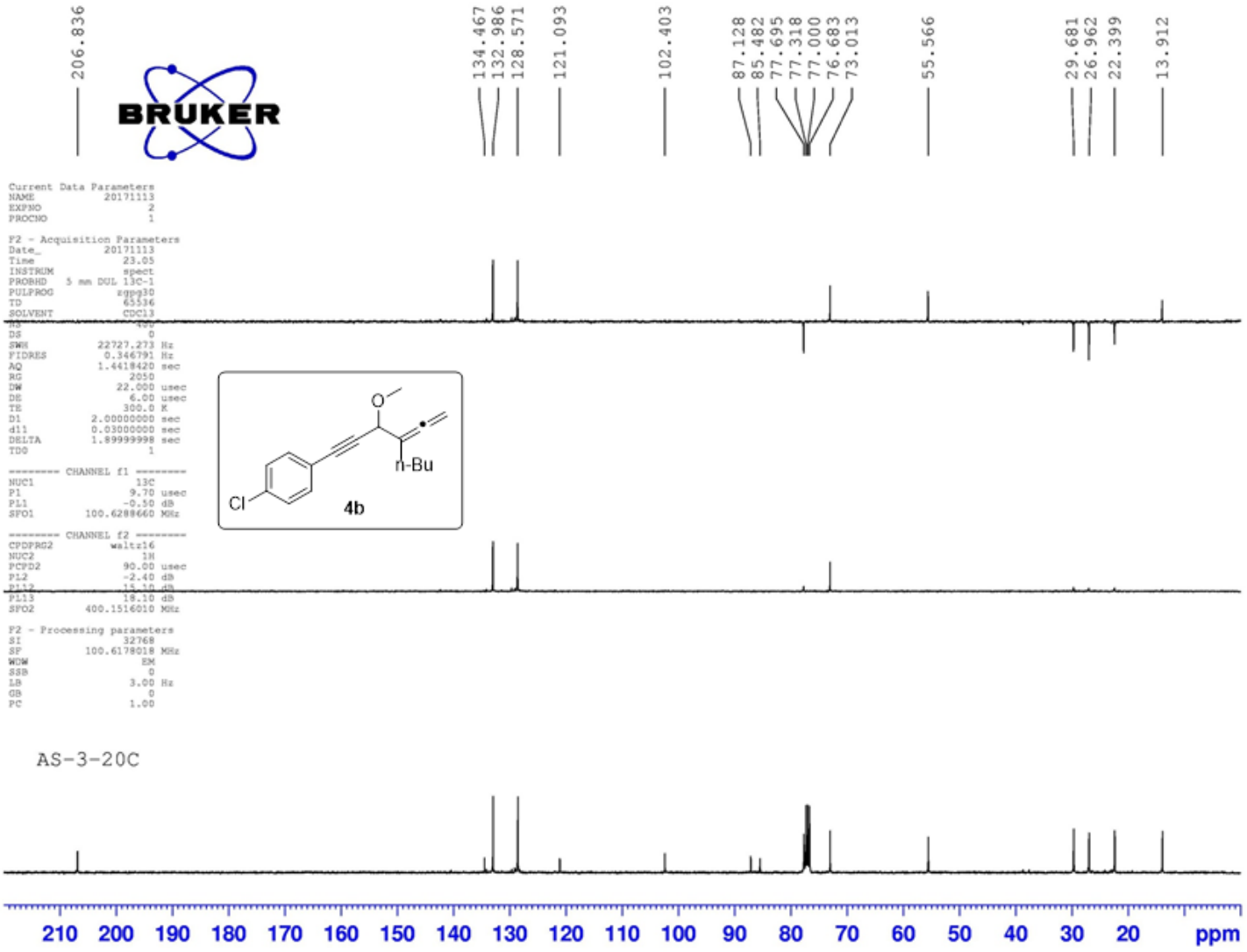

7.972
7.803
7.794
7.788
7.780
7.774
7.768
7.759
7.747
7.495
7.491
7.483
7.474
7.467
7.459
7.450
7.240
5.416
5.399
5.382
5.365
4.984
4.979
4.967
4.963
4.848
4.843
4.838
4.830
4.825
4.821
3.484
1.539
Current Data Parameters
NAME 20170905
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170905
Time 15.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 575
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 400.1500171 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
OMe
1j
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
3.12
3.09
1.03
1.95
0.98
3.00

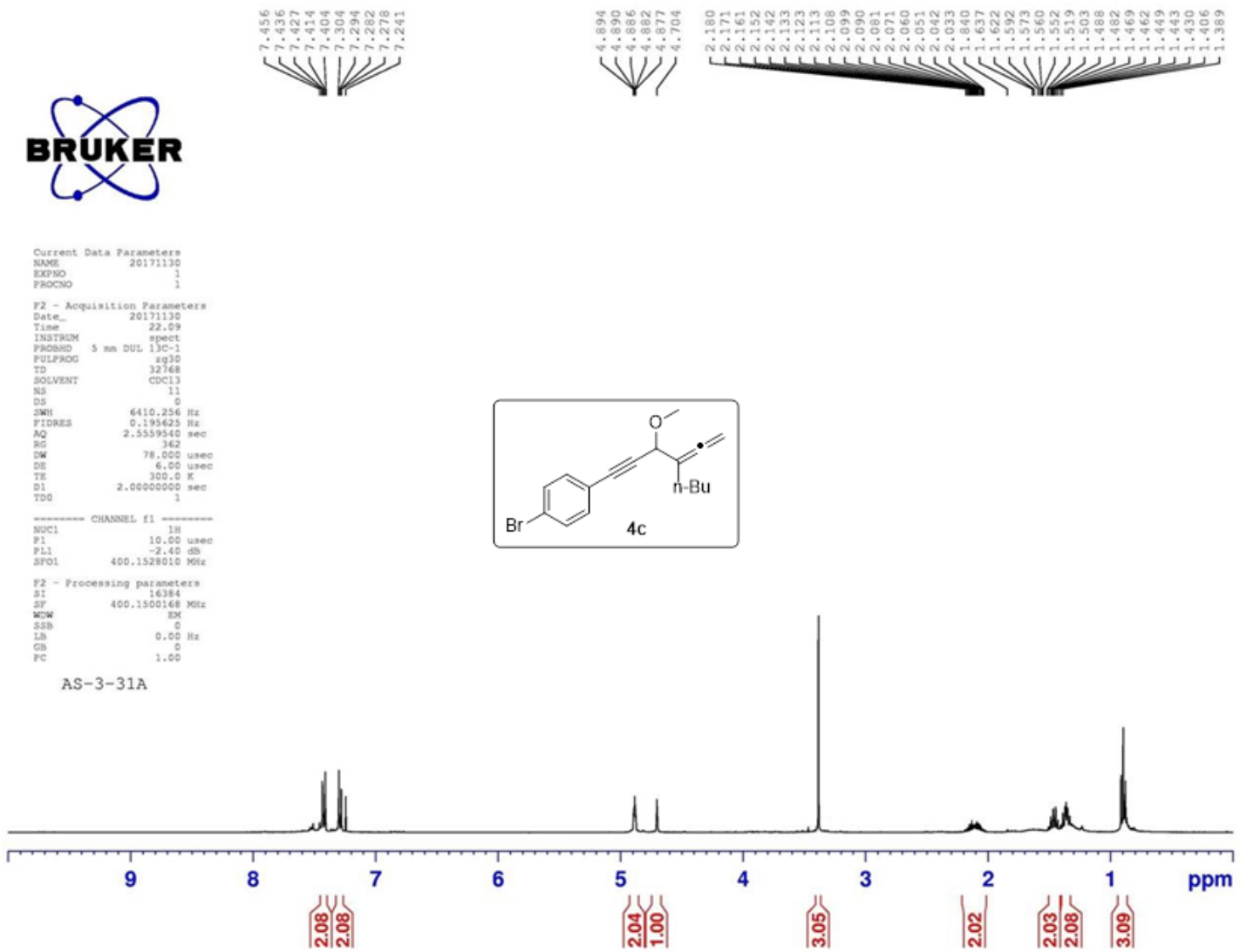

209.00
132.84
132.80
131.76
128.39
127.88
127.69
126.71
126.49
119.66
90.38
87.00
86.32
77.71
77.32
77.00
76.69
69.77
55.55
OMe
1j
Current Data Parameters
NAME 20170918
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170918
Time 15.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 34
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178093 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

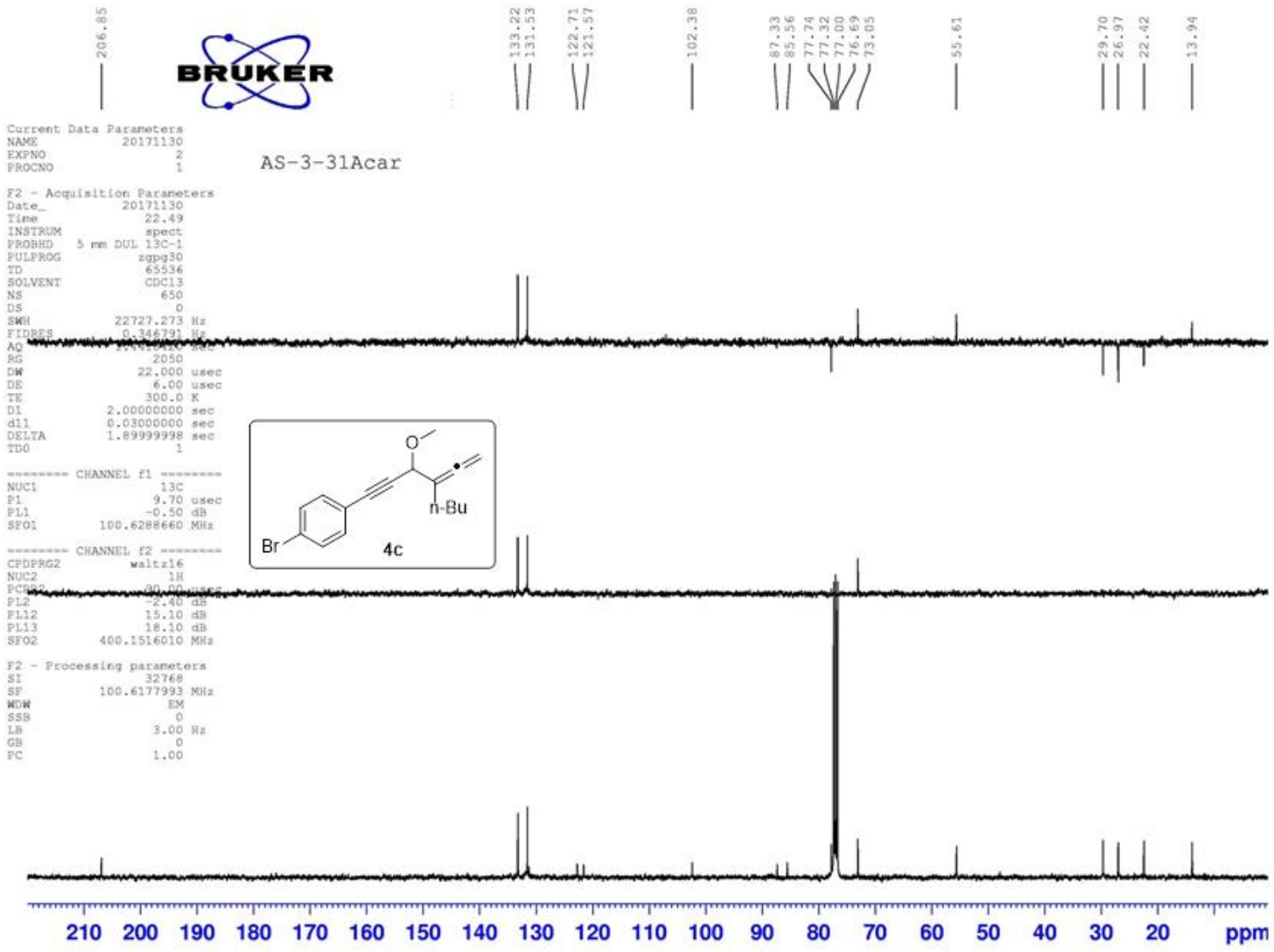

7.445 7.442 7.436 7.435 7.434 7.433 7.430 7.429 7.299 7.298 7.294 7.291 7.290 7.286 7.285 7.284 7.282 7.281 7.274
4.897 4.896 4.895 4.891 4.890 4.889 4.887 4.886 4.884 4.883 4.881 4.878 4.735
3.402
2.184 2.178 2.171 2.165 2.158 2.152 2.122 2.115 2.109 2.103 2.096 2.090 2.507 1.496 1.493 1.483 1.479 1.469 1.457 1.404 1.392 1.379 1.379 1.367 1.354 0.917 0.905 0.893
Current Data Parameters
NAME AS-2-187
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170922
Time 0.16
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 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000247 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
n-Bu
4a
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.000 3.072 2.055 1.040 3.087 2.027 2.058 2.095 3.095

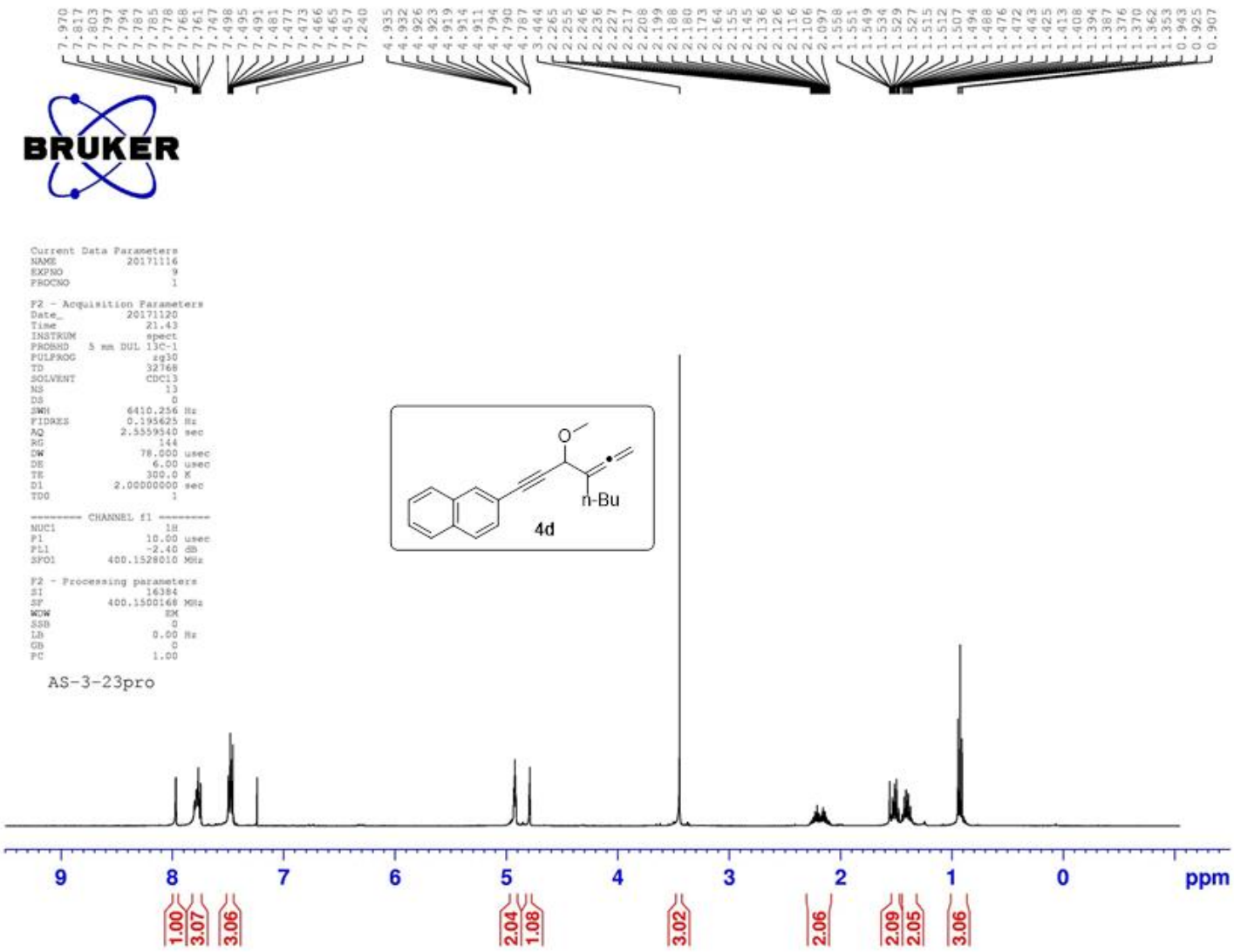

206.86
131.79
128.40
128.22
122.65
102.59
86.67
86.09
77.64
77.21
77.00
76.79
73.09
55.54
29.73
27.01
22.43
13.93
Current Data Parameters
NAME AS-2-187
EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
Date_ 20170922
Time 0.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 249
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 – Processing parameters
SI 65536
SF 150.4678020 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
O
n-Bu
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.372
7.367
7.362
7.356
7.350
7.345
7.340
7.274
7.269
7.264
7.253
7.247
7.240
4.898
4.894
4.890
4.886
4.882
4.877
4.873
4.714
4.710
4.707
3.386
2.194
2.184
2.175
2.164
2.155
2.146
2.136
2.127
2.120
2.117
2.112
2.109
2.103
2.093
2.084
2.074
2.065
2.055
2.045
1.577
1.509
1.506
1.491
1.485
1.472
1.464
1.452
1.445
1.433
1.408
1.394
1.390
1.377
BRUKER
Current Data Parameters
NAME 20171114
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171114
Time 15.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 13
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 144
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 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-20H
O
n-Bu
Cl
4b
9
8
7
6
5
4
3
2
1
ppm
2.06
2.00
2.09
1.05
3.05
2.07
2.07
2.02
3.03


206.836
134.467
132.986
128.571
121.093
102.403
87.128
85.482
77.695
77.318
77.000
76.683
73.013
55.566
29.681
26.962
22.399
13.912
BRUKER
Current Data Parameters
NAME 20171113
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171113
Time 23.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 100.6178018 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
n-Bu
Cl
4b
AS-3-20C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.456
7.436
7.427
7.414
7.404
7.304
7.294
7.282
7.278
7.241
4.894
4.890
4.886
4.882
4.877
4.704
2.180
2.171
2.161
2.152
2.142
2.133
2.123
2.113
2.108
2.099
2.090
2.081
2.071
2.060
2.051
2.042
2.033
1.840
1.637
1.622
1.592
1.573
1.560
1.552
1.519
1.503
1.488
1.482
1.469
1.462
1.449
1.443
1.430
1.406
1.389
BRUKER
Current Data Parameters
NAME 20171130
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171130
Time 22.09
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 362
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
AS-3-31A
O
n-Bu
Br
4c
9
8
7
6
5
4
3
2
1
ppm
2.08
2.08
2.04
1.00
3.05
2.02
2.03
2.08
3.09


206.85
133.22
131.53
122.71
121.57
102.38
87.33
85.56
77.74
77.32
77.00
76.69
73.05
55.61
29.70
26.97
22.42
13.94
BRUKER
AS-3-31Acar
Current Data Parameters
NAME 20171130
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171130
Time 22.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4417920 sec
RG 2050
DW 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 80.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177993 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
n-Bu
Br
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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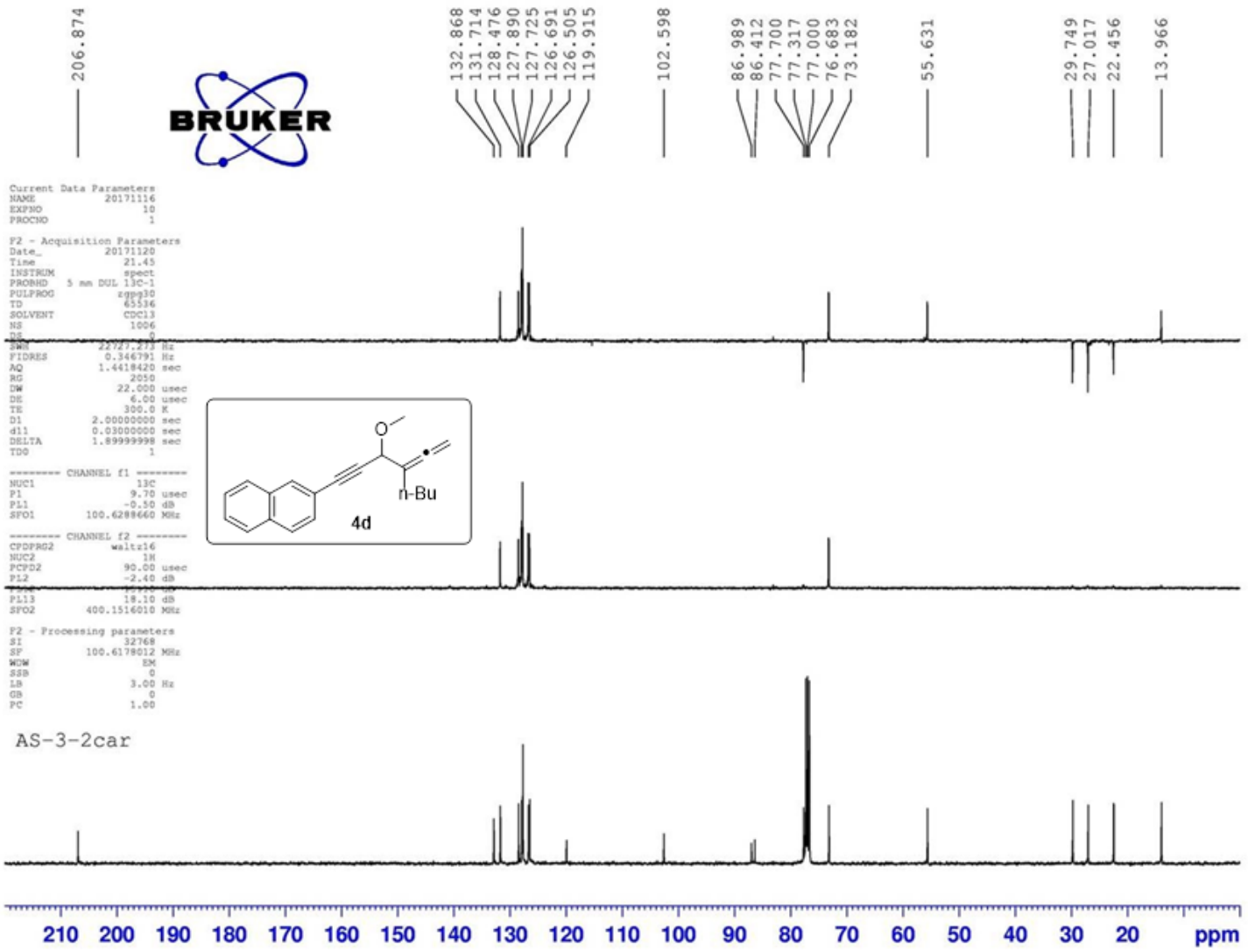
4.935 4.932 4.926 4.923 4.919 4.914 4.911 4.794 4.790 4.787 3.444 2.265 2.255 2.246 2.236 2.227 2.217 2.208 2.199 2.188 2.180 2.173 2.164 2.155 2.145 2.136 2.126 2.116 2.106 2.097 1.558 1.551 1.549 1.534 1.529 1.527 1.515 1.512 1.507 1.494 1.488 1.476 1.472 1.443 1.425 1.413 1.408 1.394 1.387 1.376 1.370 1.362 1.353 0.943 0.925 0.907
BRUKER
Current Data Parameters
NAME 20171116
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171120
Time 21.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 13
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 144
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
AS-3-23pro
O
n-Bu
4d
9 8 7 6 5 4 3 2 1 0 ppm
1.00 3.07 3.06 2.04 1.08 3.02 2.06 2.09 2.05 3.06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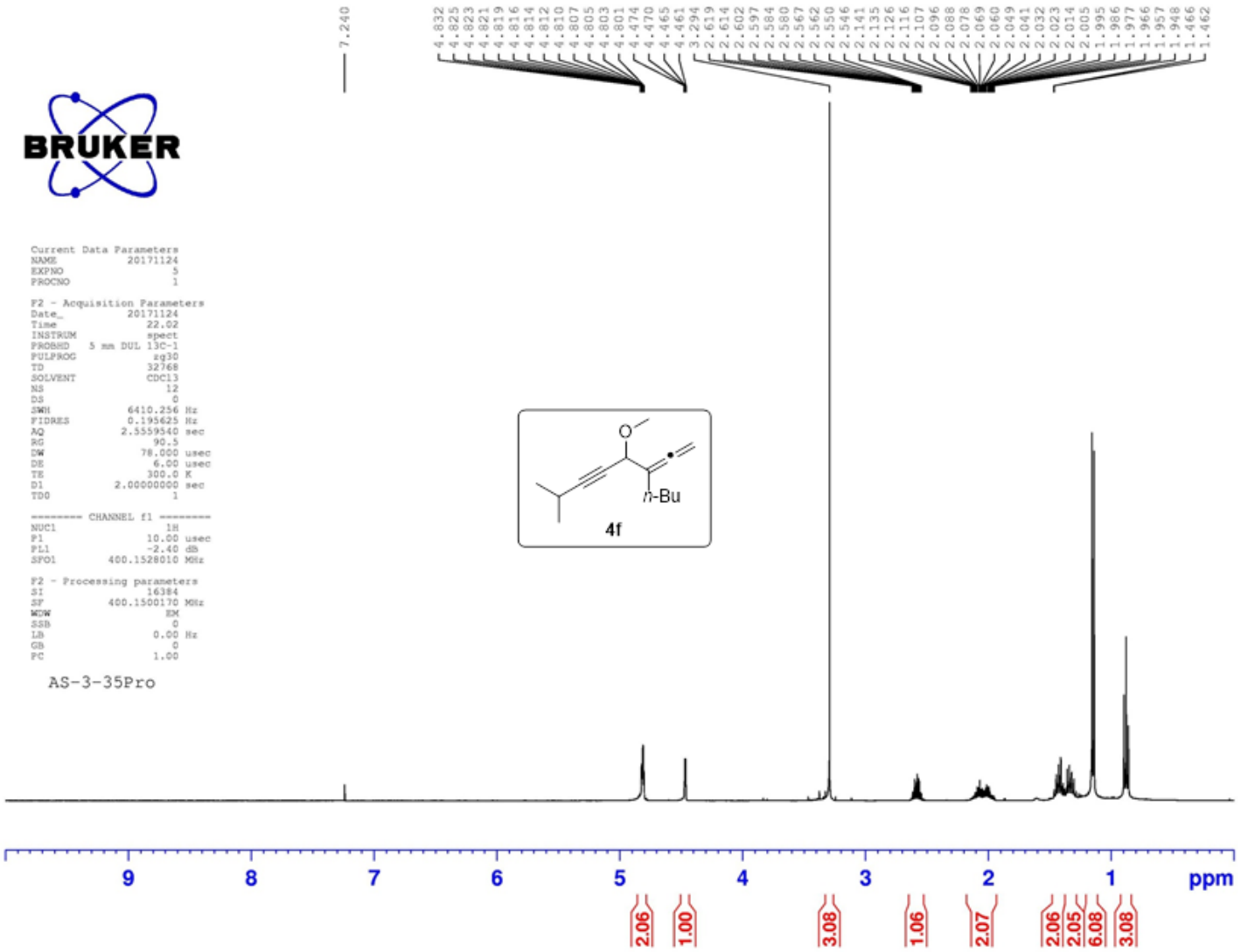
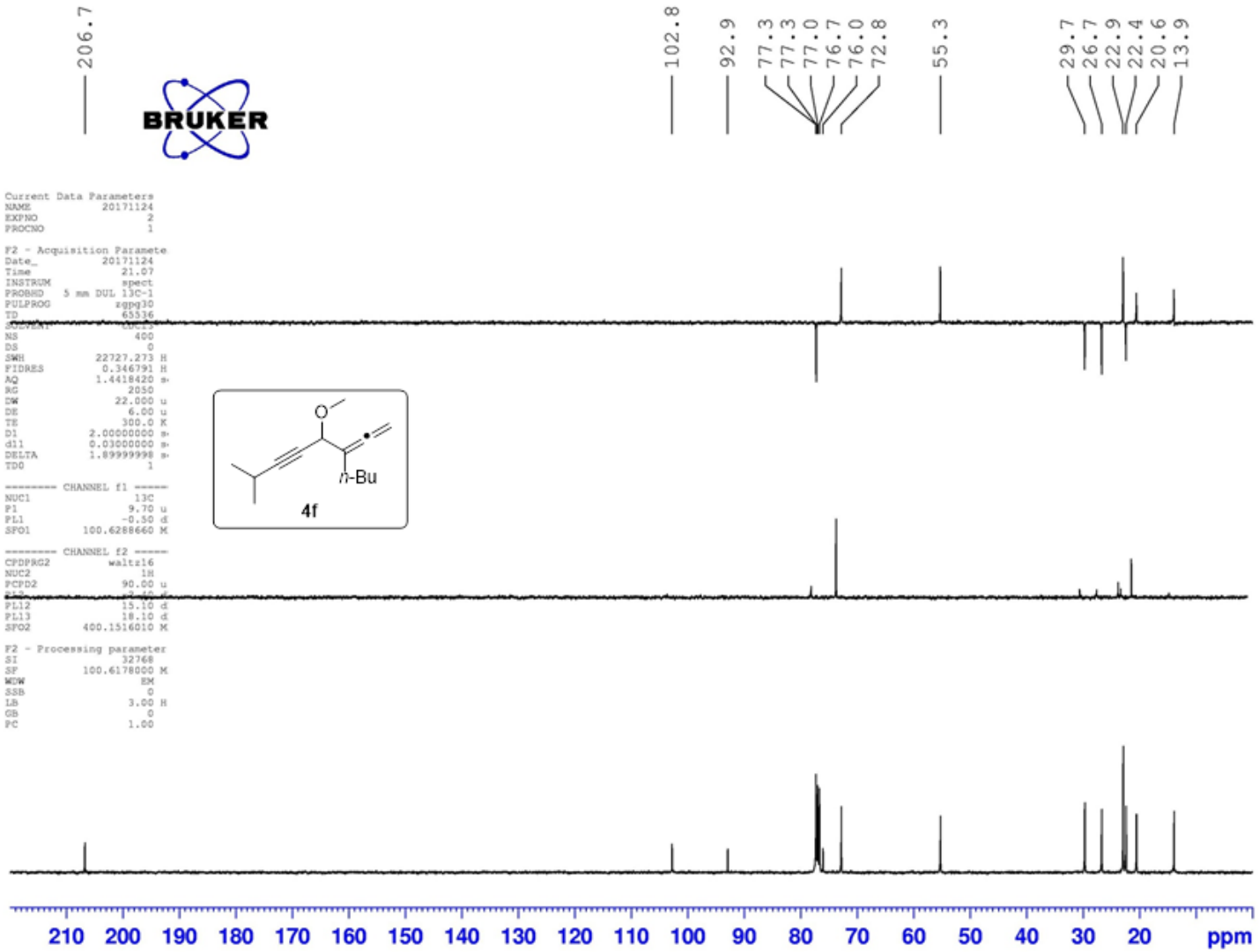
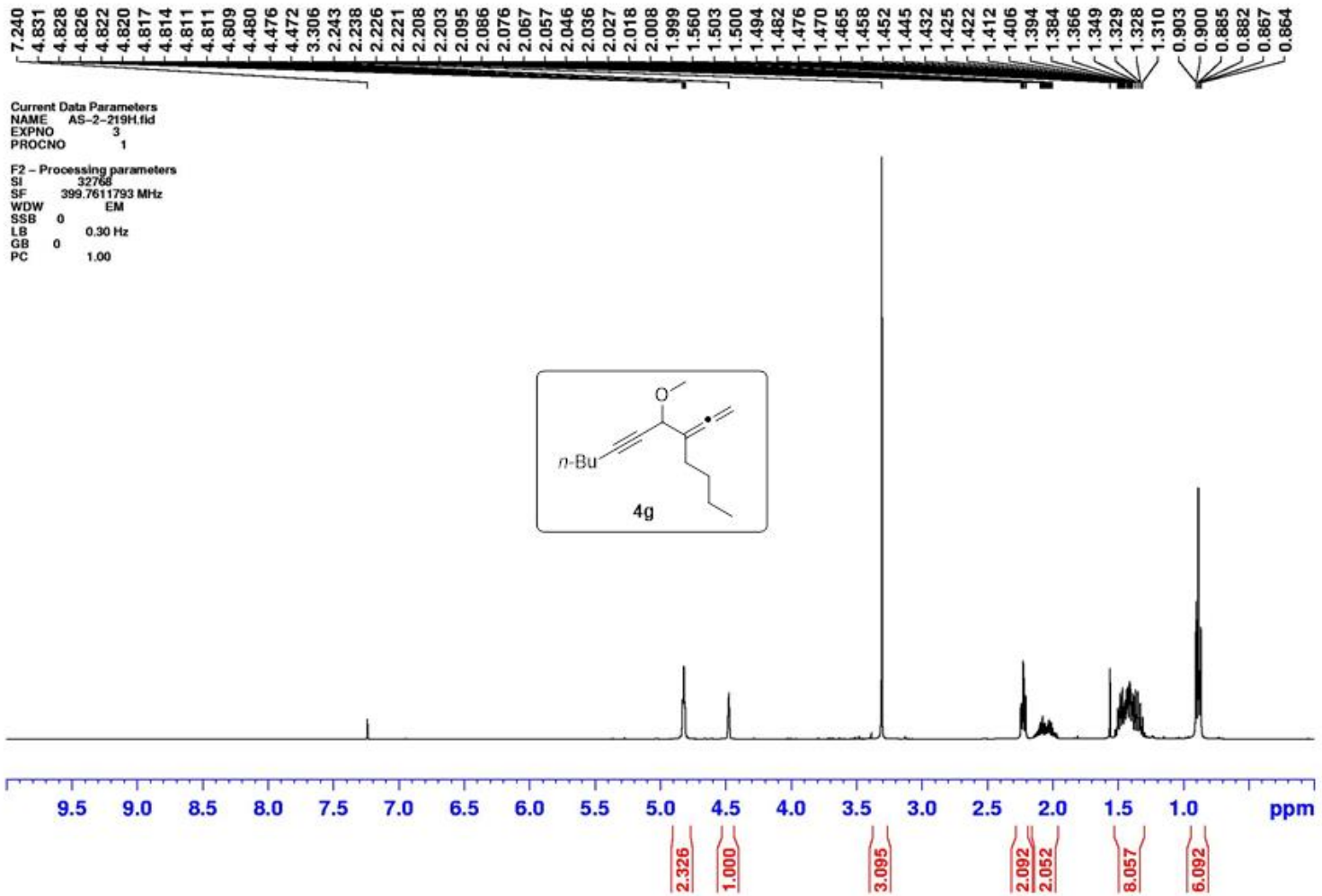
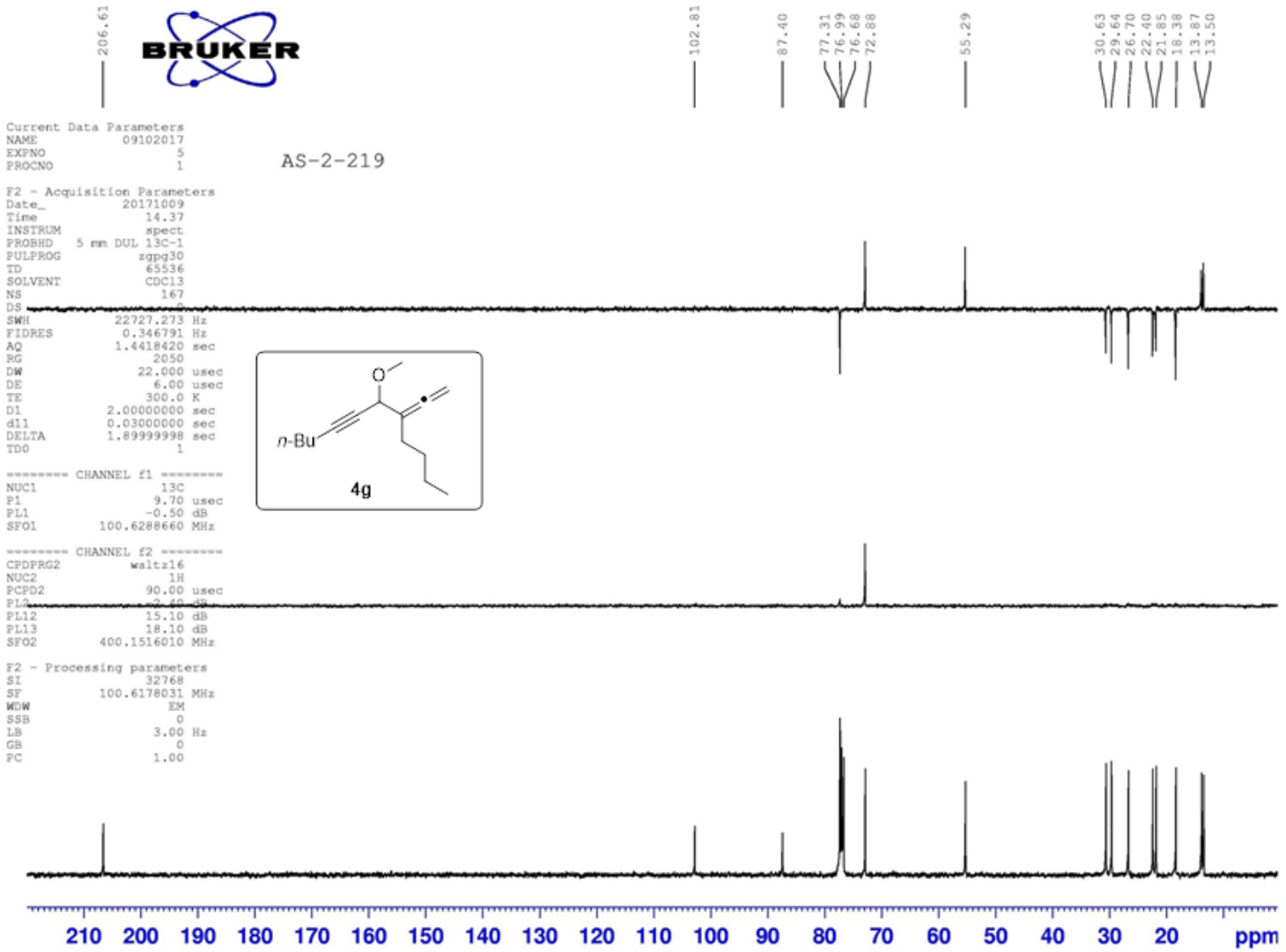
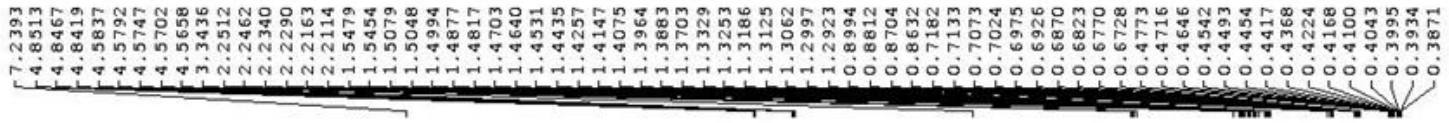
132.868
131.714
128.476
127.890
127.725
126.691
126.505
119.915
102.598
86.989
86.412
77.700
77.317
77.000
76.683
73.182
55.631
29.749
27.017
22.456
13.966
BRUKER
Current Data Parameters
NAME 20171116
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171120
Time 21.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1006
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 18.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178012 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
n-Bu
4d
AS-3-2car
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


BRUKER
Current Data Parameters
NAME 20171124
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171124
Time 22.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 90.5
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 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-35Pro
7.240
4.832
4.825
4.823
4.821
4.819
4.816
4.814
4.812
4.810
4.807
4.805
4.803
4.801
4.474
4.470
4.465
4.461
3.294
2.619
2.614
2.602
2.597
2.584
2.580
2.567
2.562
2.550
2.546
2.141
2.135
2.126
2.116
2.107
2.096
2.088
2.078
2.069
2.060
2.049
2.041
2.032
2.023
2.014
2.005
1.995
1.966
1.977
1.966
1.957
1.948
1.466
1.462
O
n-Bu
4f
9
8
7
6
5
4
3
2
1
ppm
2.06
1.00
3.08
1.06
2.07
2.06
2.05
6.08
3.08


206.7
102.8
92.9
77.3
77.3
77.0
76.7
76.0
72.8
55.3
29.7
26.7
22.9
22.4
20.6
13.9
BRUKER
Current Data Parameters
NAME 20171124
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171124
Time 21.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 400
DS 0
SWH 22727.273 H
FIDRES 0.346791 H
AQ 1.4418420 s
RG 2050
DW 22.000 u
DE 6.00 u
TE 300.0 K
D1 2.00000000 s
d11 0.03000000 s
DELTA 1.89999998 s
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.70 u
PL1 -0.50 d
SFO1 100.6288660 M
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL12 15.10 d
PL13 18.10 d
SFO2 400.1516010 M
F2 - Processing parameter
SI 32768
SF 100.6178000 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.00
O
n-Bu
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

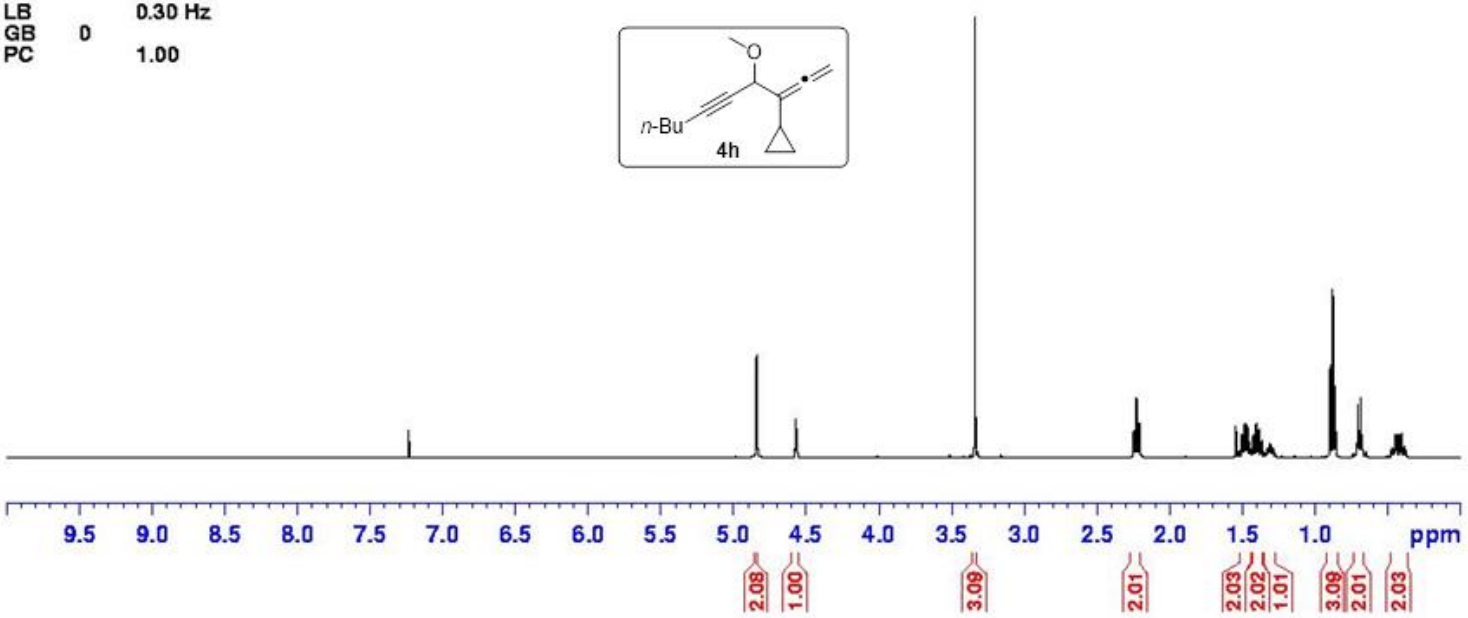

7.240
4.831
4.828
4.826
4.822
4.820
4.817
4.814
4.811
4.811
4.809
4.480
4.476
4.472
3.306
2.243
2.238
2.226
2.221
2.208
2.203
2.095
2.086
2.076
2.067
2.057
2.046
2.036
2.027
2.018
2.008
1.999
1.560
1.503
1.500
1.494
1.482
1.476
1.470
1.465
1.458
1.452
1.445
1.432
1.425
1.422
1.412
1.406
1.394
1.384
1.366
1.349
1.329
1.328
1.310
0.903
0.900
0.885
0.882
0.867
0.864
Current Data Parameters
NAME AS-2-219H.fid
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611793 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
n-Bu
O
4g
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.326
1.000
3.095
2.092
2.052
8.057
6.092

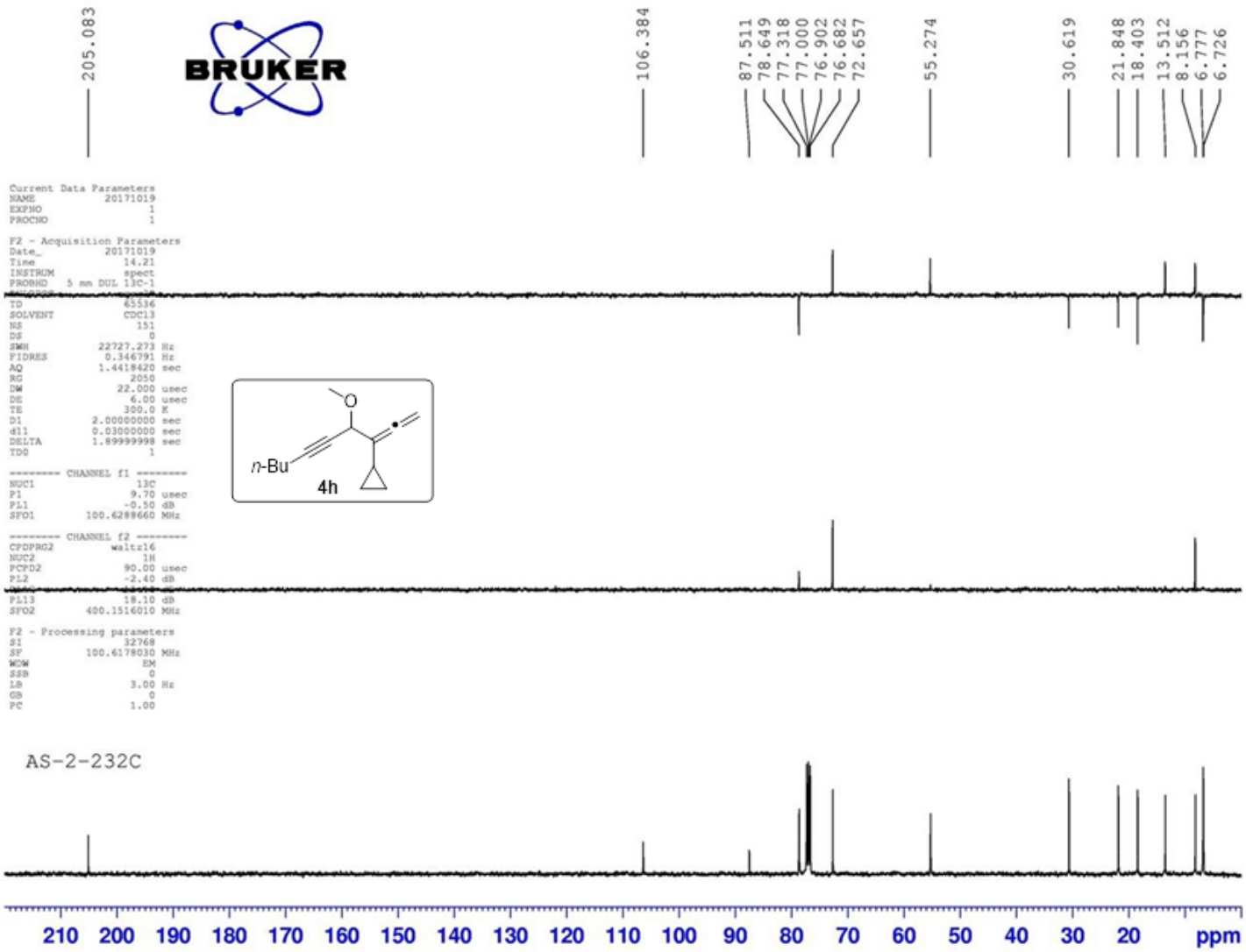

206.61
102.81
87.40
77.31
76.99
76.68
72.88
55.29
30.63
29.64
26.70
22.40
21.85
18.38
13.87
13.50
Current Data Parameters
NAME 09102017
EXPNO 5
PROCNO 1
AS-2-219
F2 - Acquisition Parameters
Date_ 20171009
Time 14.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 167
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 100.6178031 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
n-Bu
4g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

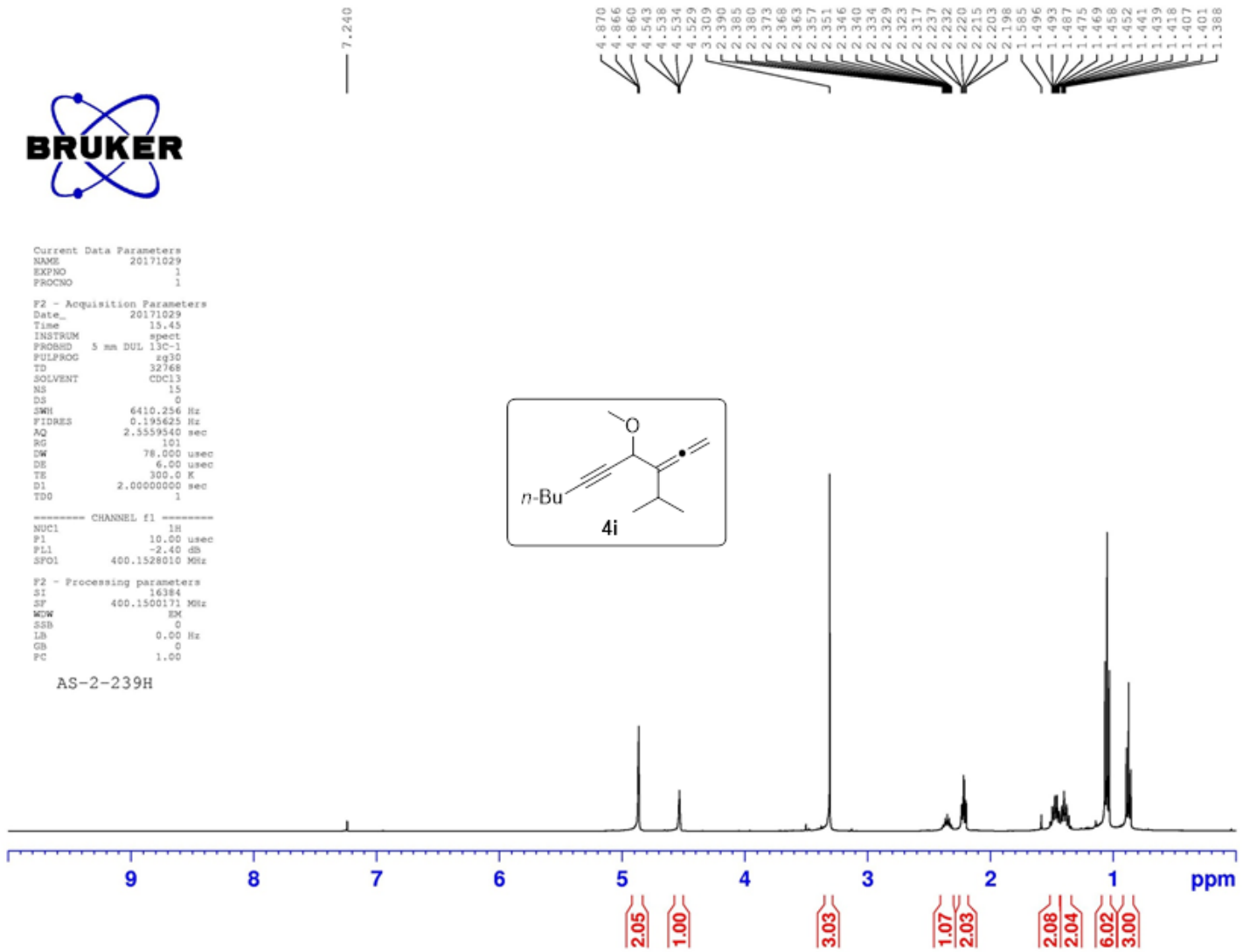


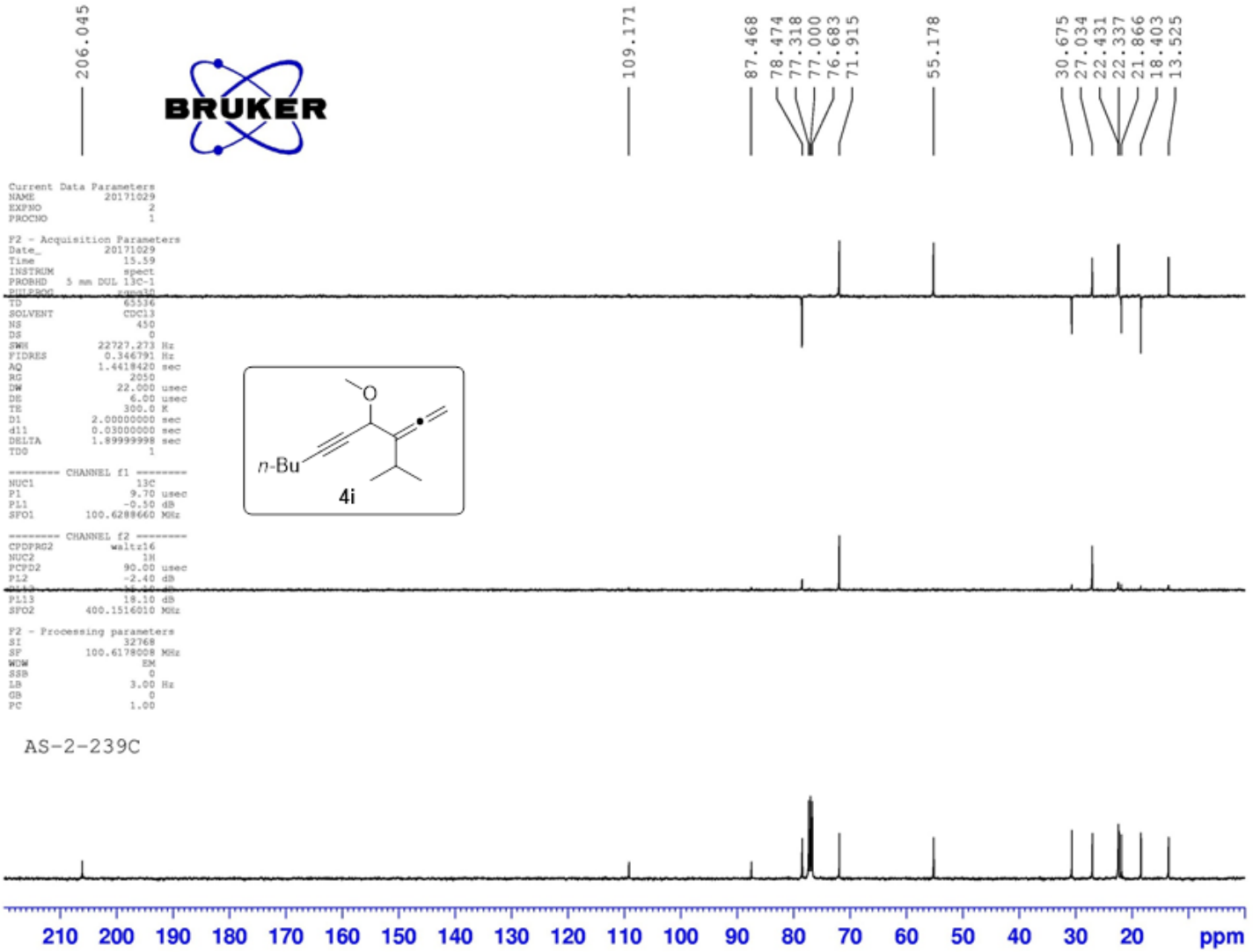
Current Data Parameters
NAME AS–2–232H.fid
EXPNO 2
PROCNO 1

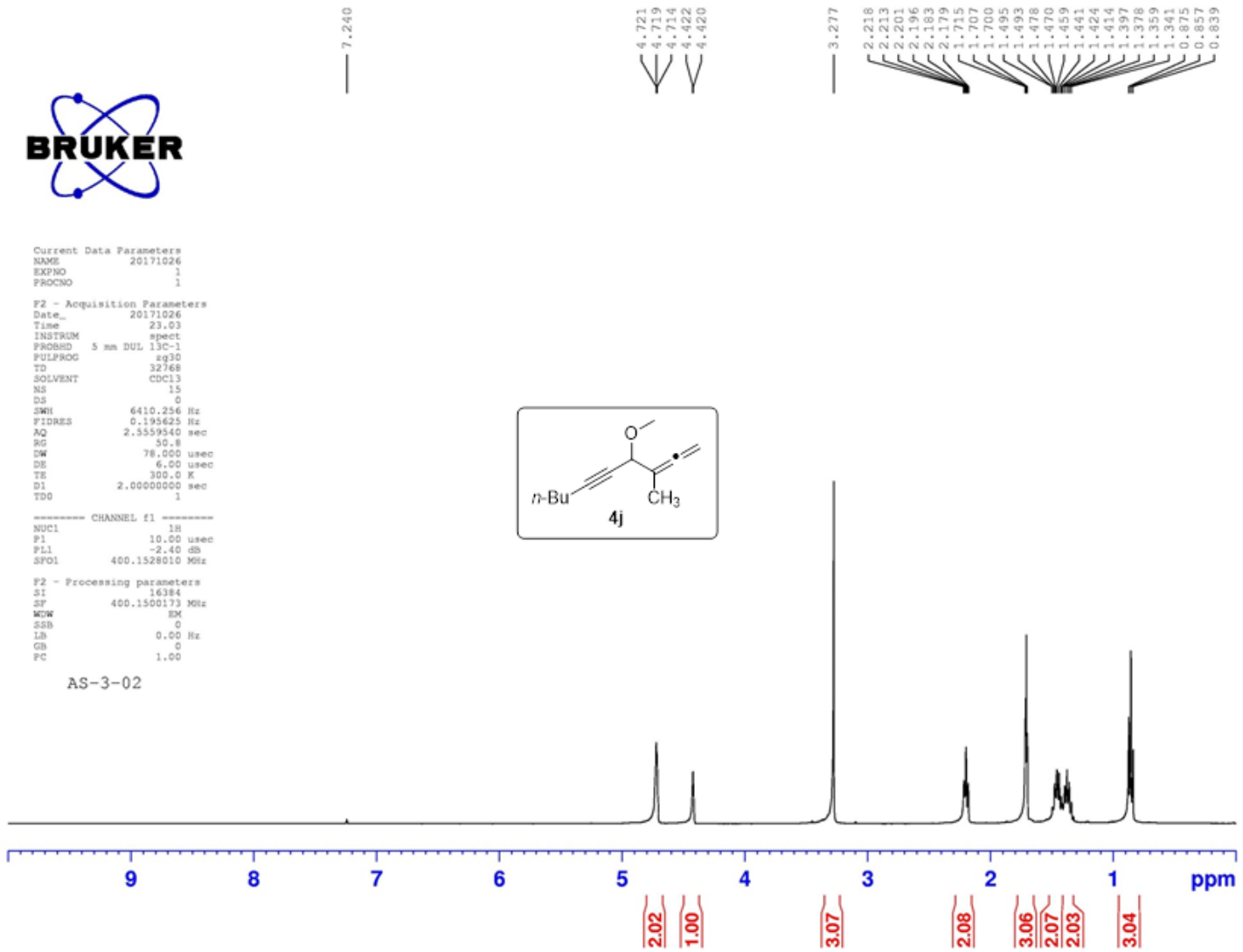
F2 – Processing parameters
SI 32768
SF 399.7611797 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

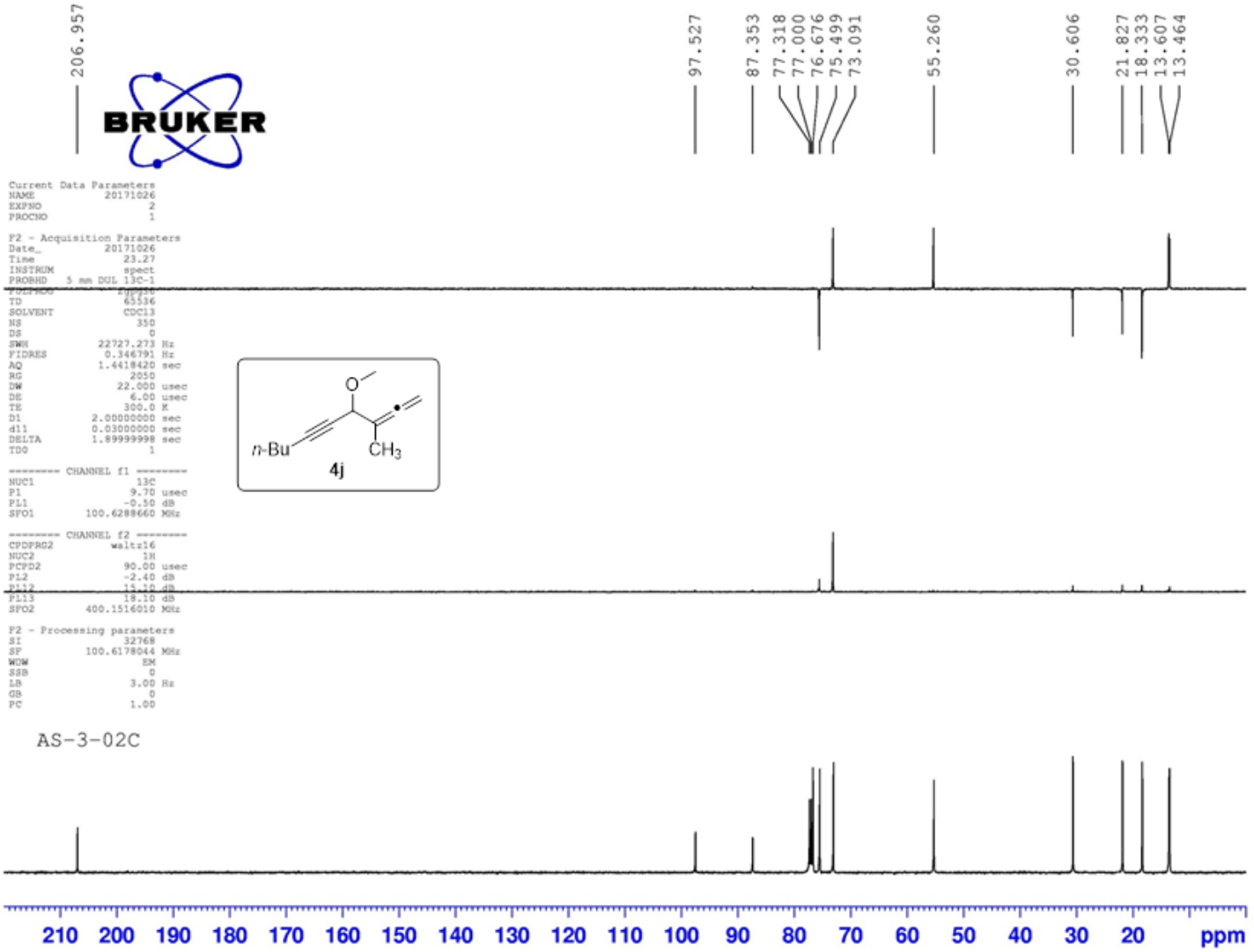


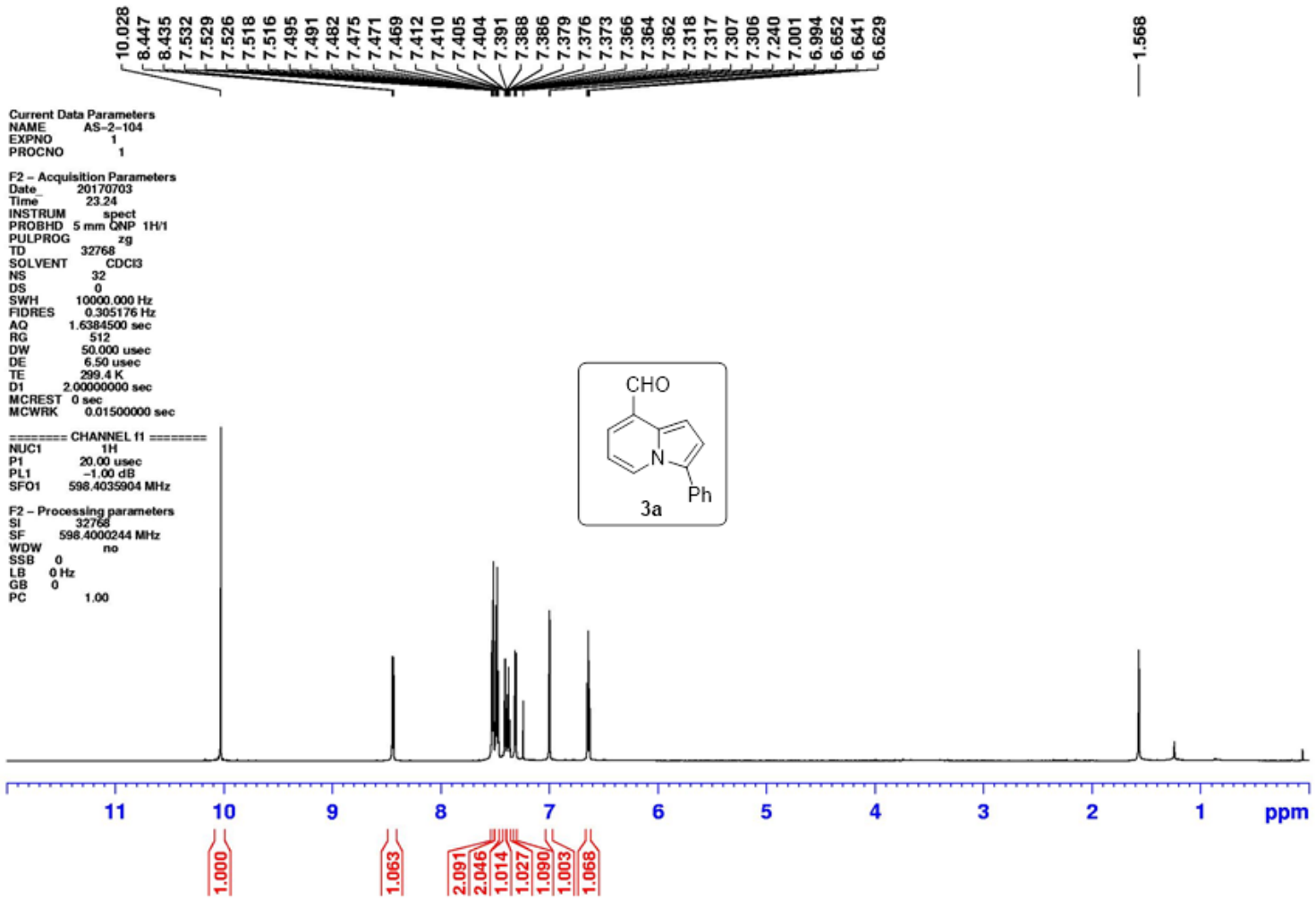

205.083
106.384
87.511
78.649
77.318
77.000
76.902
76.682
72.657
55.274
30.619
21.848
18.403
13.512
8.156
6.777
6.726
Current Data Parameters
NAME 20171019
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171019
Time 14.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
TD 65536
SOLVENT CDCl3
NS 151
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178030 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
n-Bu
O
4h
AS-2-232C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

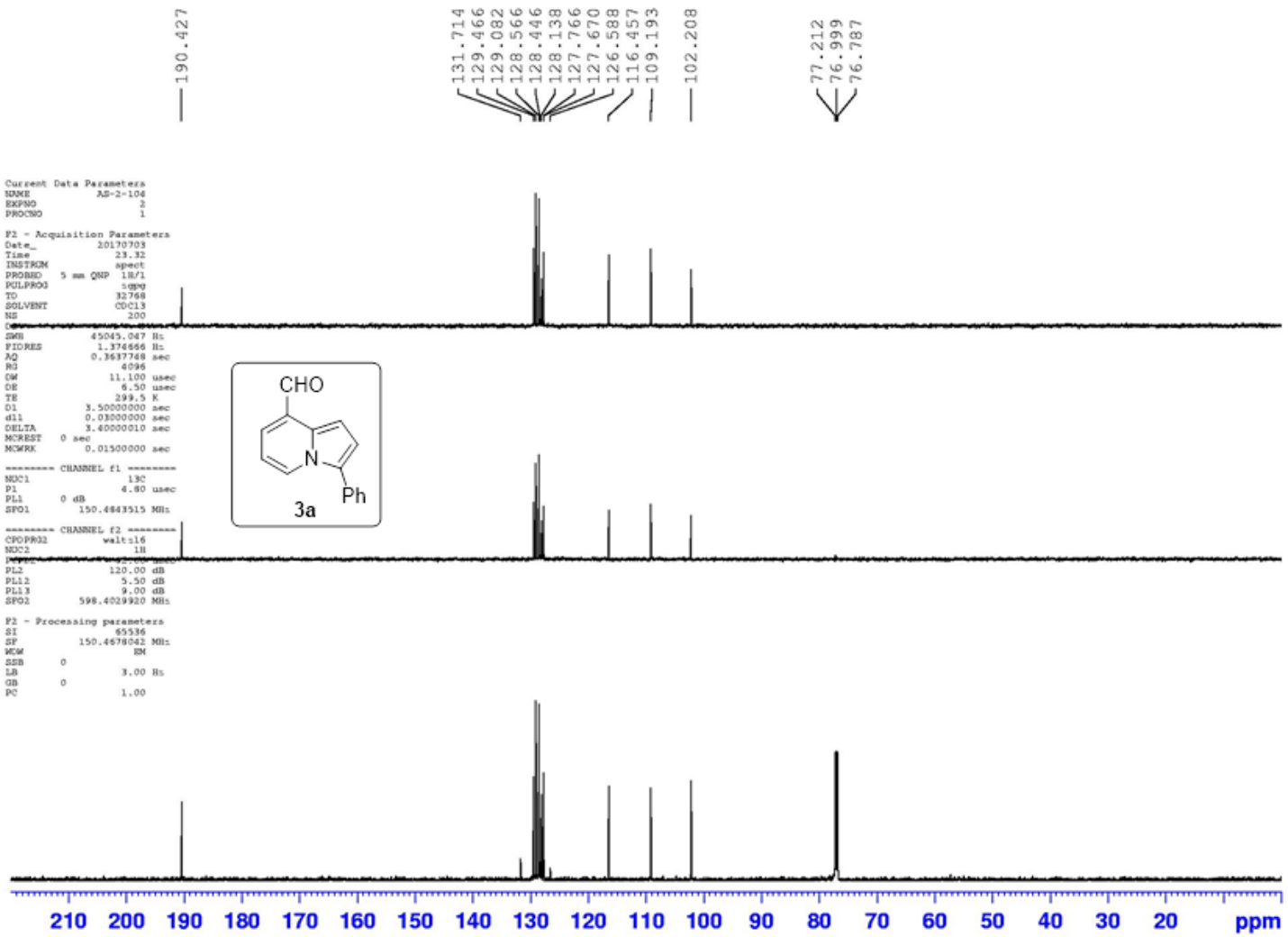

7.240
4.870
4.866
4.860
4.543
4.538
4.534
4.529
3.309
2.390
2.385
2.380
2.373
2.368
2.363
2.357
2.351
2.346
2.340
2.334
2.329
2.323
2.317
2.237
2.232
2.220
2.215
2.203
2.198
1.585
1.496
1.493
1.487
1.475
1.469
1.458
1.452
1.441
1.439
1.418
1.407
1.401
1.388
BRUKER
Current Data Parameters
NAME 20171029
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171029
Time 15.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 101
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 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-2-239H
O
n-Bu
4i
9
8
7
6
5
4
3
2
1
ppm
2.05
1.00
3.03
1.07
2.03
2.08
2.04
6.02
3.00


206.045
109.171
87.468
78.474
77.318
77.000
76.683
71.915
55.178
30.675
27.034
22.431
22.337
21.866
18.403
13.525
BRUKER
Current Data Parameters
NAME 20171029
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171029
Time 15.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 450
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 18.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178008 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
n-Bu
4i
AS-2-239C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

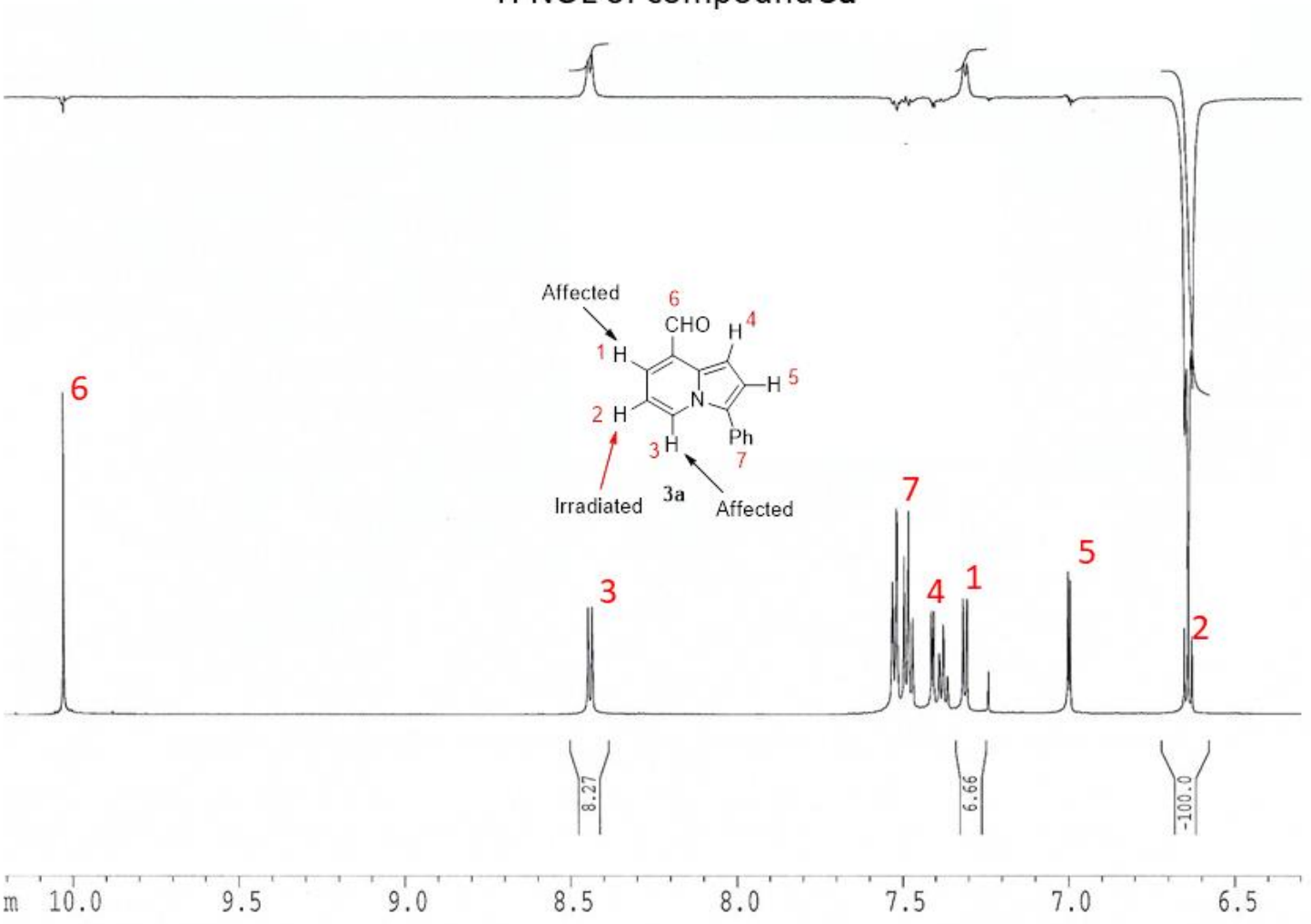

7.240
4.721
4.719
4.714
4.422
4.420
3.277
2.218
2.213
2.201
2.196
2.183
2.179
2.175
1.715
1.707
1.700
1.495
1.493
1.478
1.470
1.459
1.441
1.424
1.414
1.397
1.378
1.359
1.341
0.875
0.857
0.839
BRUKER
Current Data Parameters
NAME 20171026
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171026
Time 23.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 50.8
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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-02
O
n-Bu
CH3
4j
9
8
7
6
5
4
3
2
1
ppm
2.02
1.00
3.07
2.08
3.06
2.07
2.03
3.04


206.957
97.527
87.353
77.318
77.000
76.676
75.499
73.091
55.260
30.606
21.827
18.333
13.607
13.464
BRUKER
Current Data Parameters
NAME 20171026
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171026
Time 23.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
TD 65536
SOLVENT CDCl3
NS 350
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 100.6178044 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
n-Bu
O
CH3
4j
AS-3-02C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

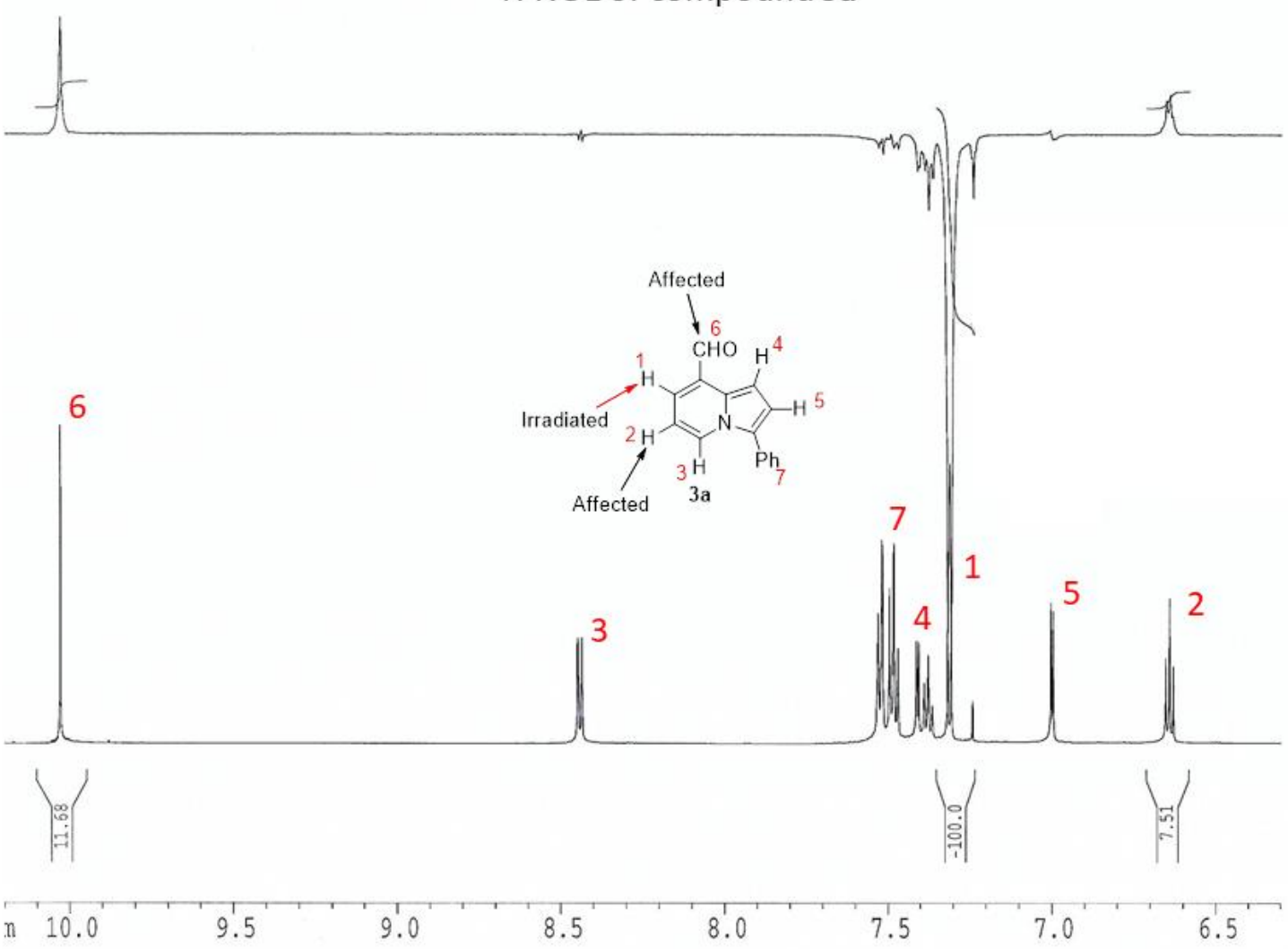

10.028
8.447
8.435
7.532
7.529
7.526
7.518
7.516
7.495
7.491
7.482
7.475
7.471
7.469
7.412
7.410
7.405
7.404
7.391
7.388
7.386
7.379
7.376
7.373
7.366
7.364
7.362
7.318
7.317
7.307
7.306
7.240
7.001
6.994
6.652
6.641
6.629
1.568
Current Data Parameters
NAME AS-2-104
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20170703
Time 23.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 512
DW 50.000 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000244 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
CHO
N
Ph
3a
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.063
2.091
2.046
1.014
1.027
1.090
1.003
1.068


190.427
131.714
129.466
129.082
128.566
128.446
128.138
127.766
127.670
126.588
116.457
109.193
102.208
77.212
76.999
76.787
Current Data Parameters
NAME AS-2-104
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170703
Time 23.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678042 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CHO
N
Ph
3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

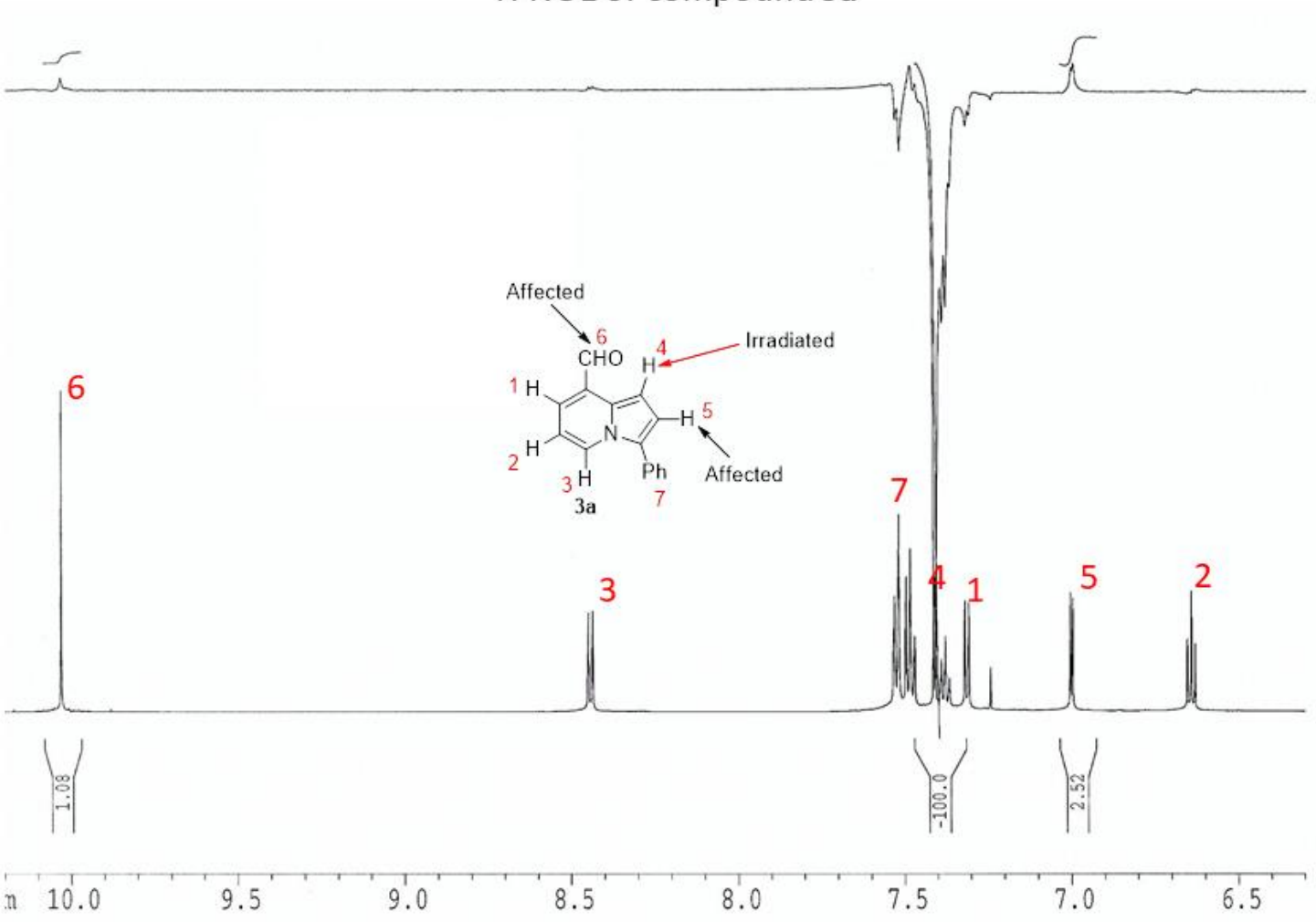
^{1}H NOE of compound **3a**



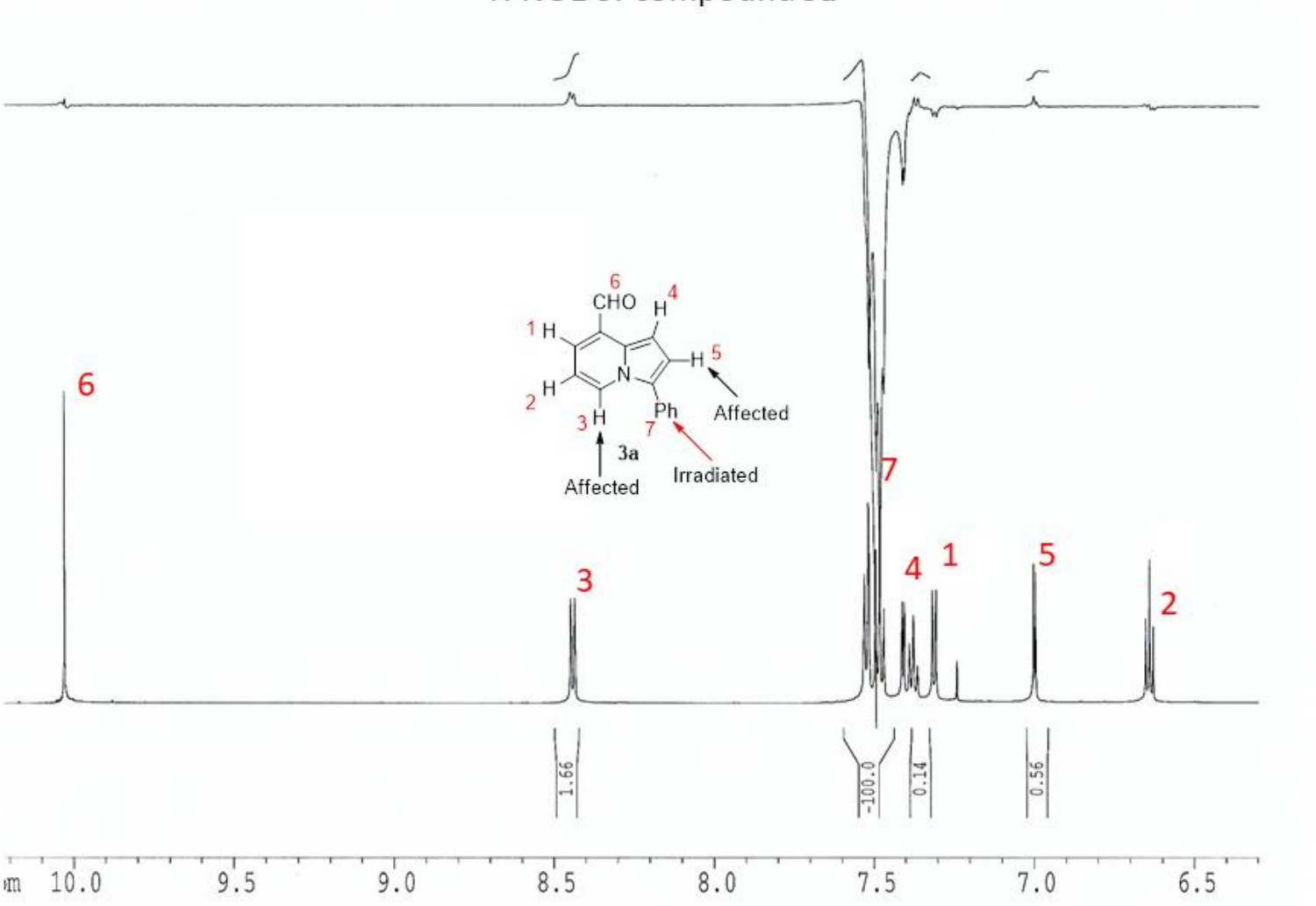
^{1}H NOE of compound **3a**



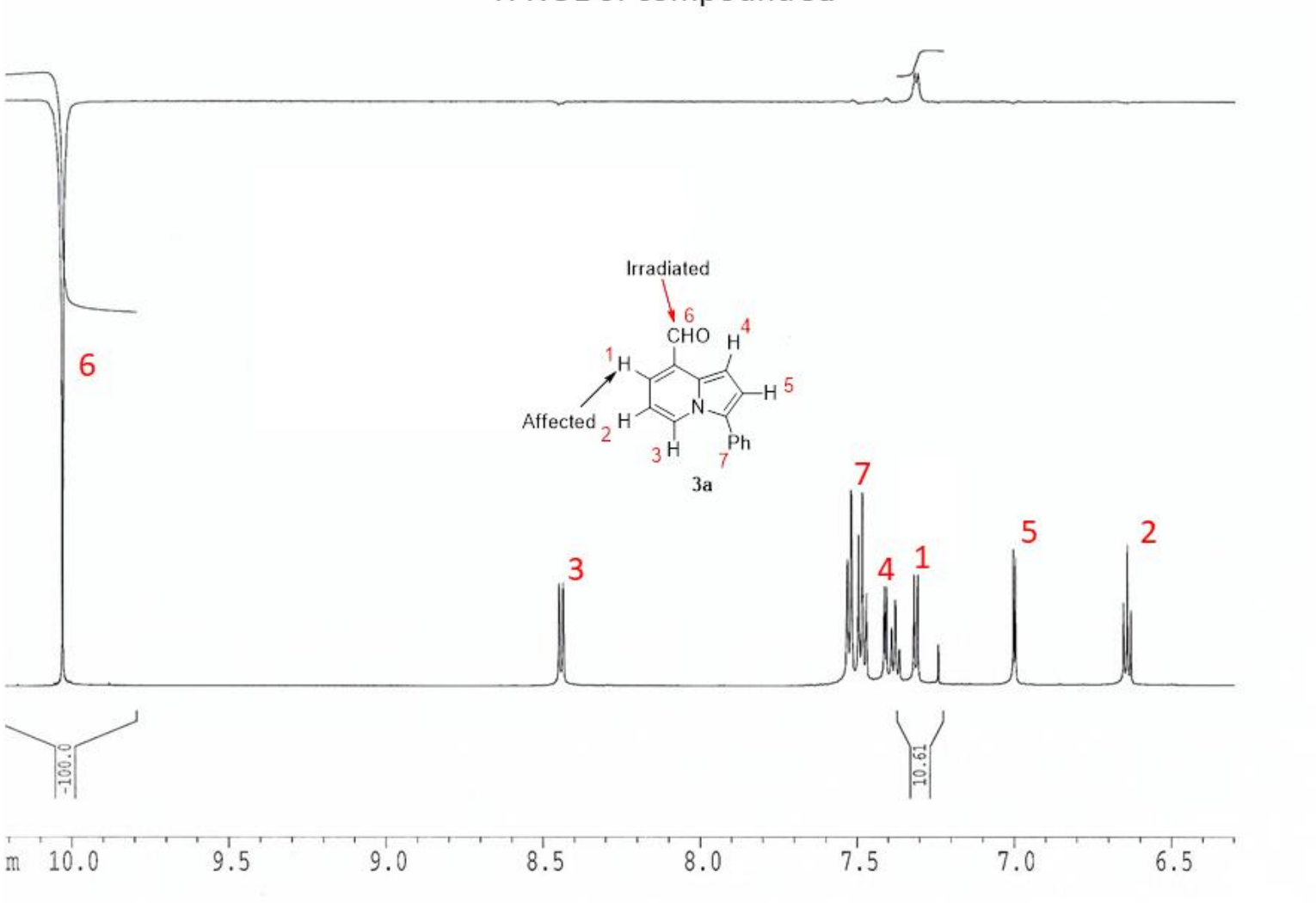
^{1}H NOE of compound **3a**

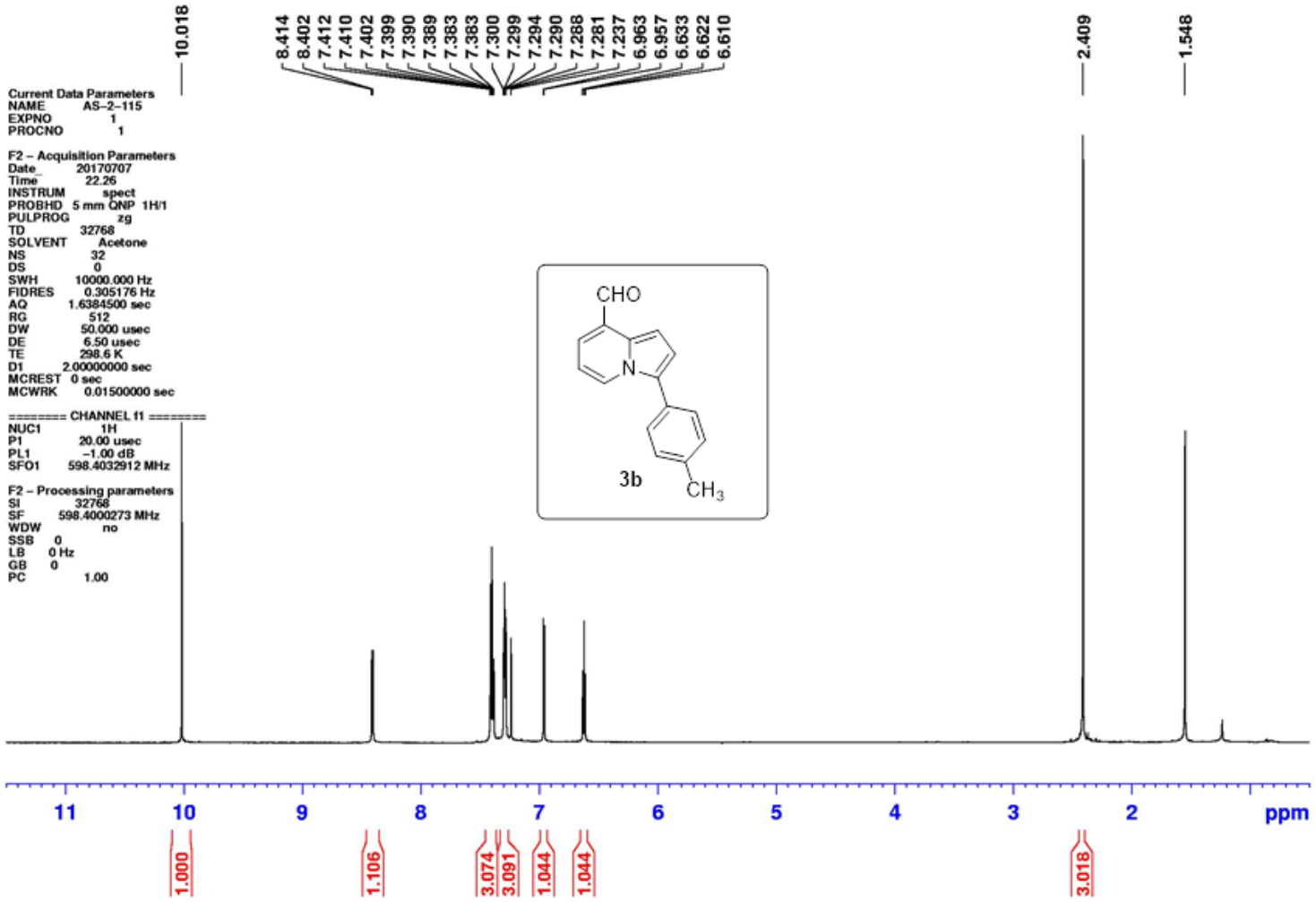


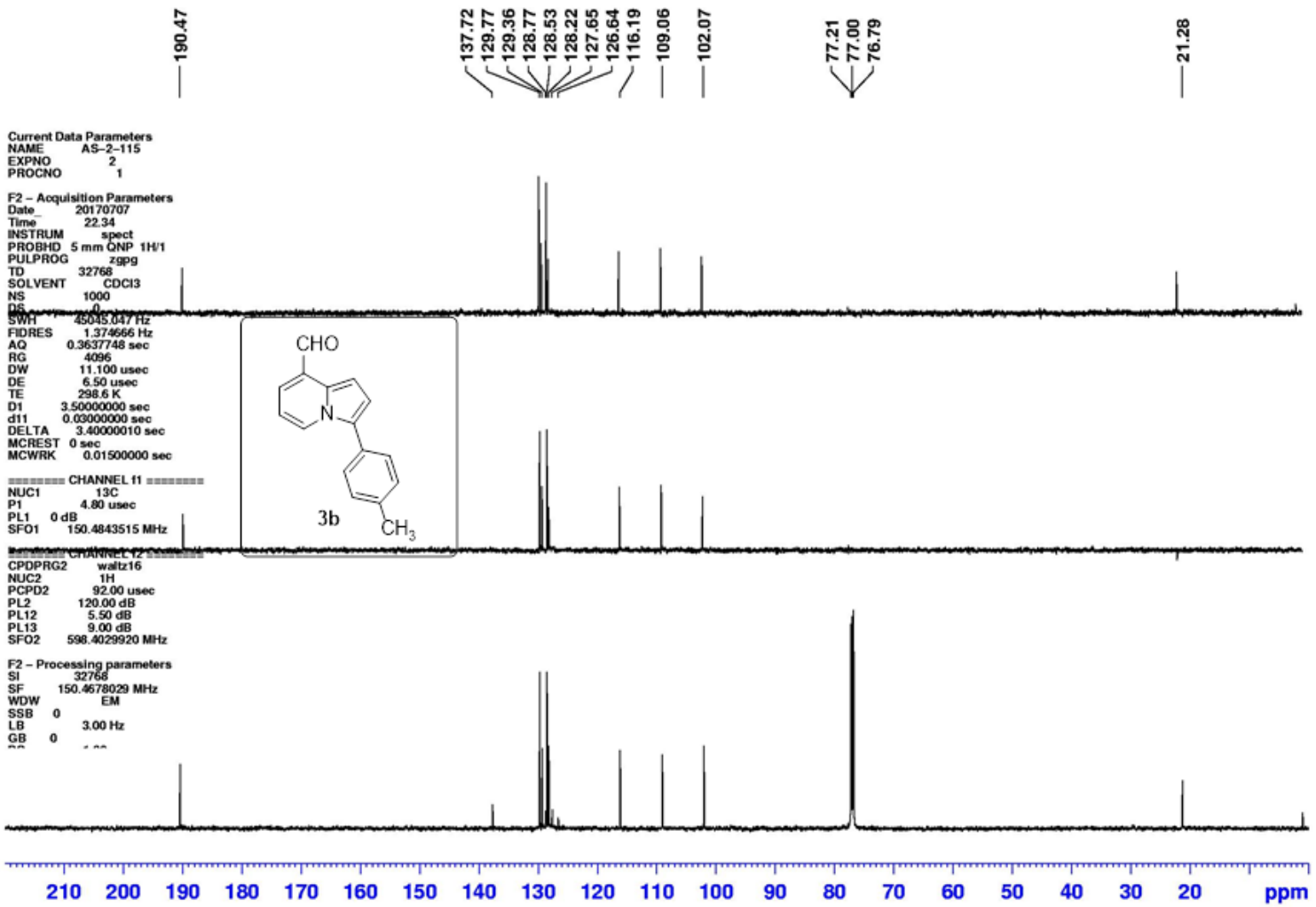
^{1}H NOE of compound **3a**

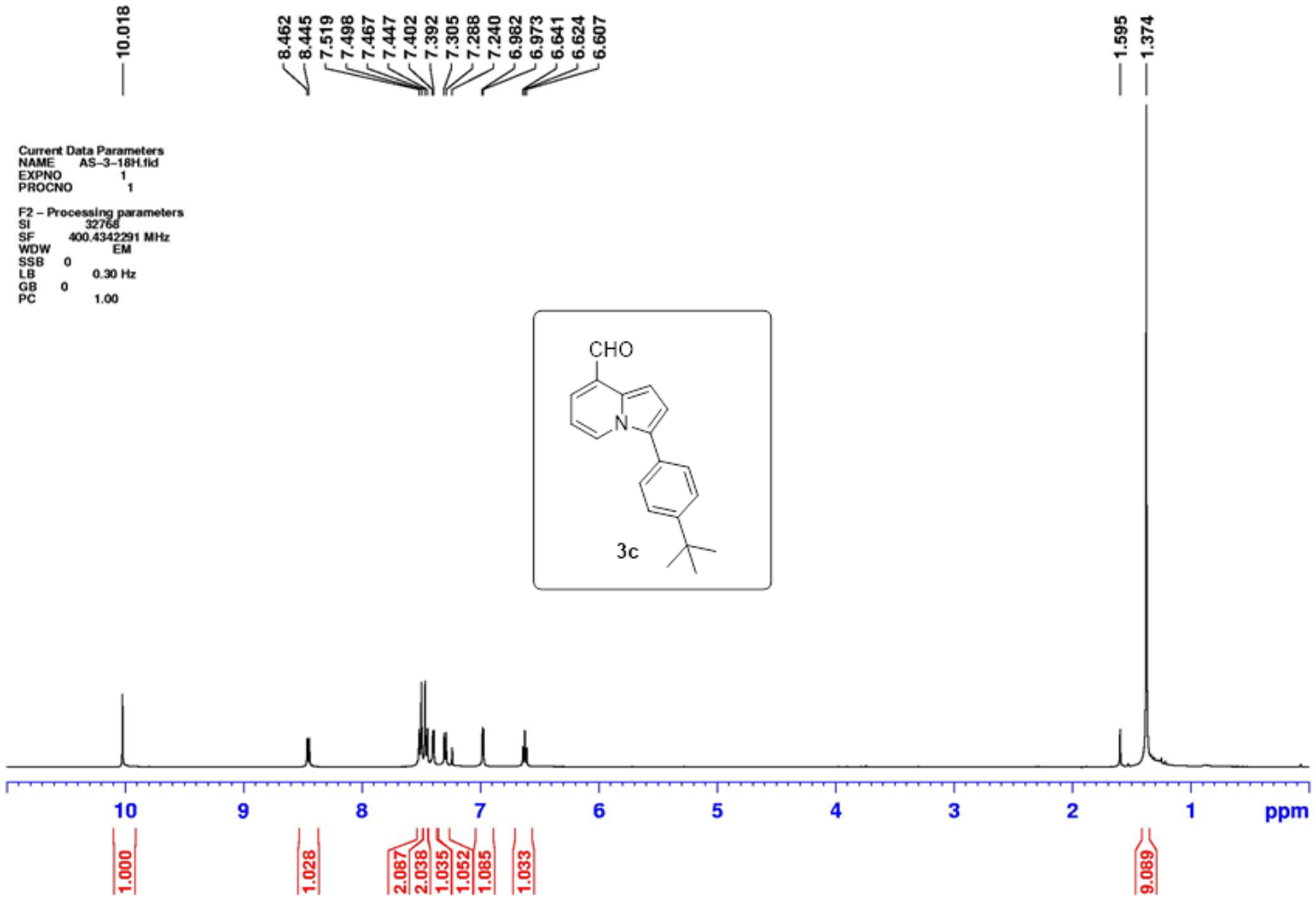


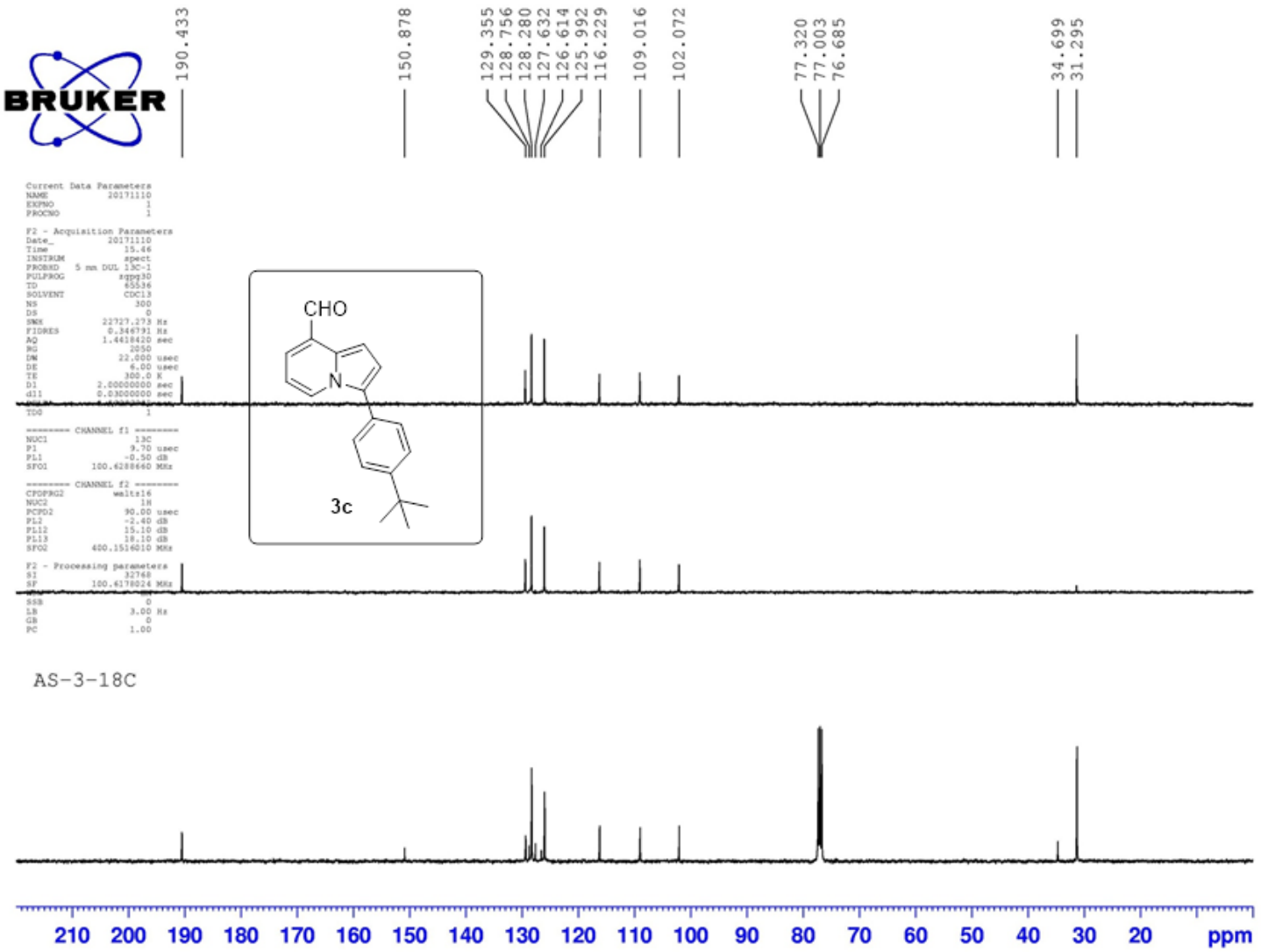
^{1}H NOE of compound **3a**

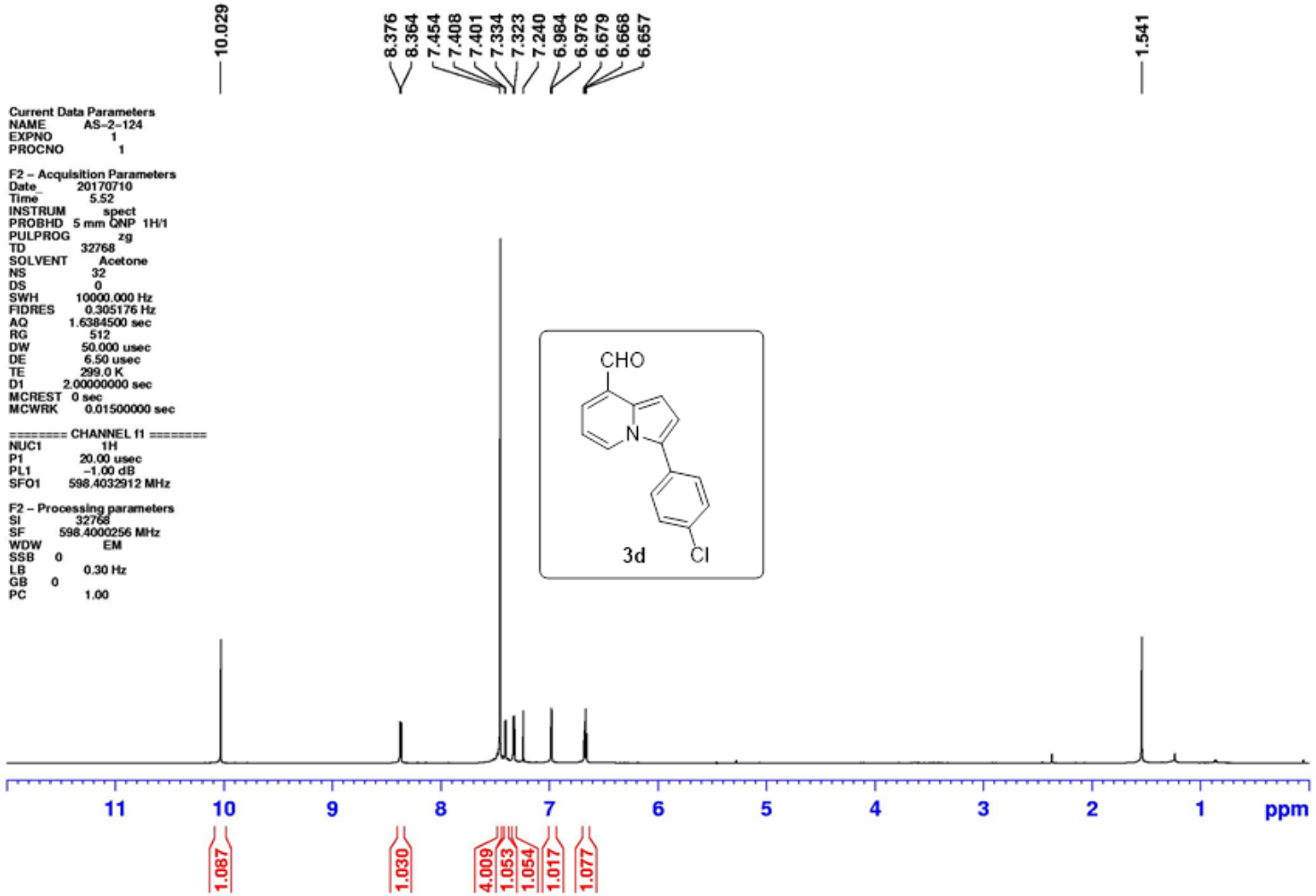


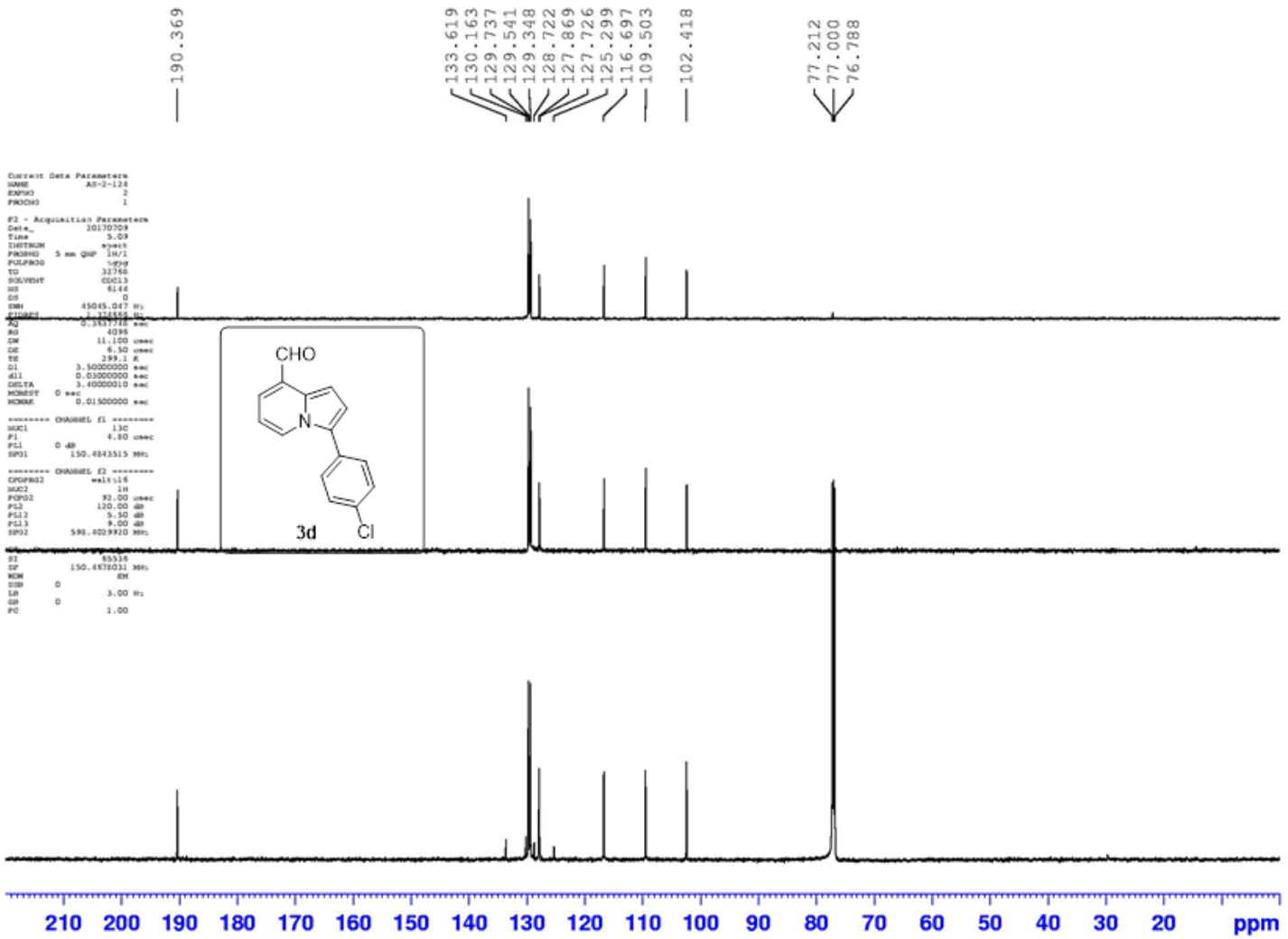

10.018
8.414
8.402
7.412
7.410
7.402
7.399
7.390
7.389
7.383
7.383
7.300
7.299
7.294
7.290
7.288
7.281
7.237
6.963
6.957
6.633
6.622
6.610
2.409
1.548
Current Data Parameters
NAME AS–2–115
EXPNO 1
PROCNO 1
F2 – Acquisition Parameters
Date_ 20170707
Time 22.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 512
DW 50.000 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 –1.00 dB
SFO1 598.4032912 MHz
F2 – Processing parameters
SI 32768
SF 598.4000273 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
CHO
N
3b
CH3
11
10
9
8
7
6
5
4
3
2
ppm
1.000
1.106
3.074
3.091
1.044
1.044
3.018

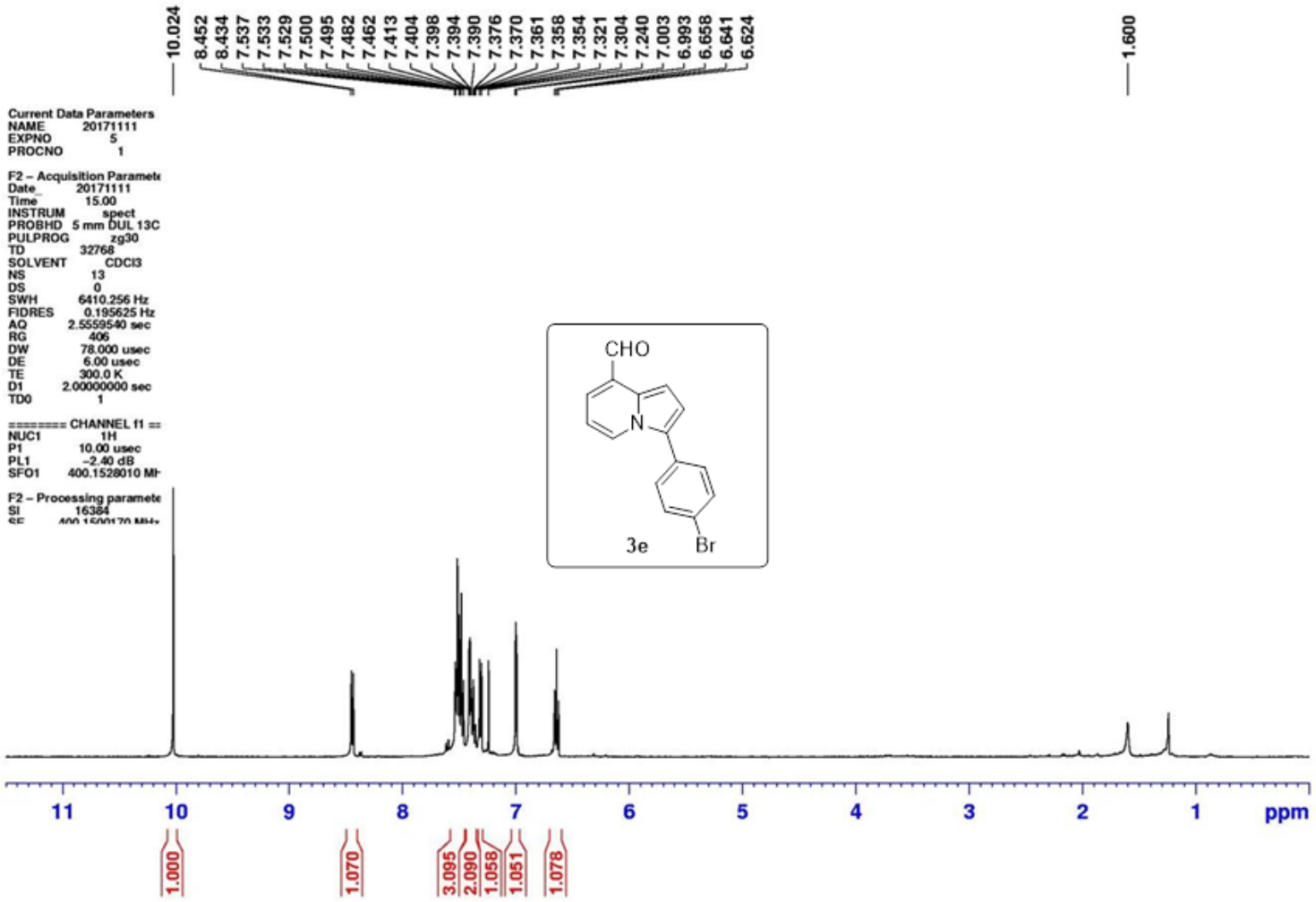

190.47
137.72
129.77
129.36
128.77
128.53
128.22
127.65
126.64
116.19
109.06
102.07
77.21
77.00
76.79
21.28
Current Data Parameters
NAME AS-2-115
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170707
Time 22.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 45045.047 Hz
FIDRES 1.374566 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 298.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 150.4678029 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
CHO
N
3b
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

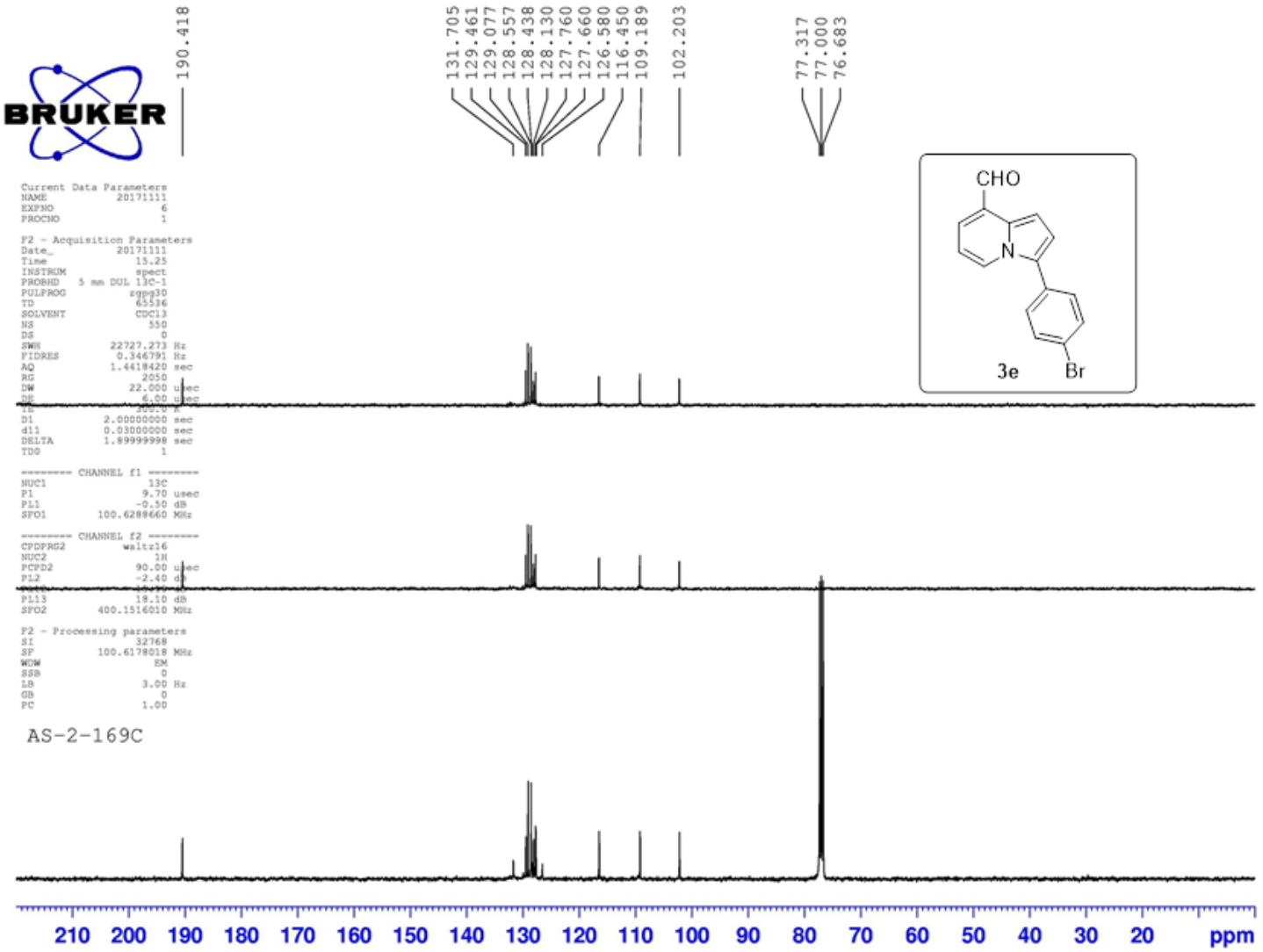

10.018
8.462
8.445
7.519
7.498
7.467
7.447
7.402
7.392
7.305
7.288
7.240
6.982
6.973
6.641
6.624
6.607
1.595
1.374
Current Data Parameters
NAME AS-3-18H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 400.4342291 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3c
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.028
2.087
2.038
1.035
1.052
1.085
1.033
9.089

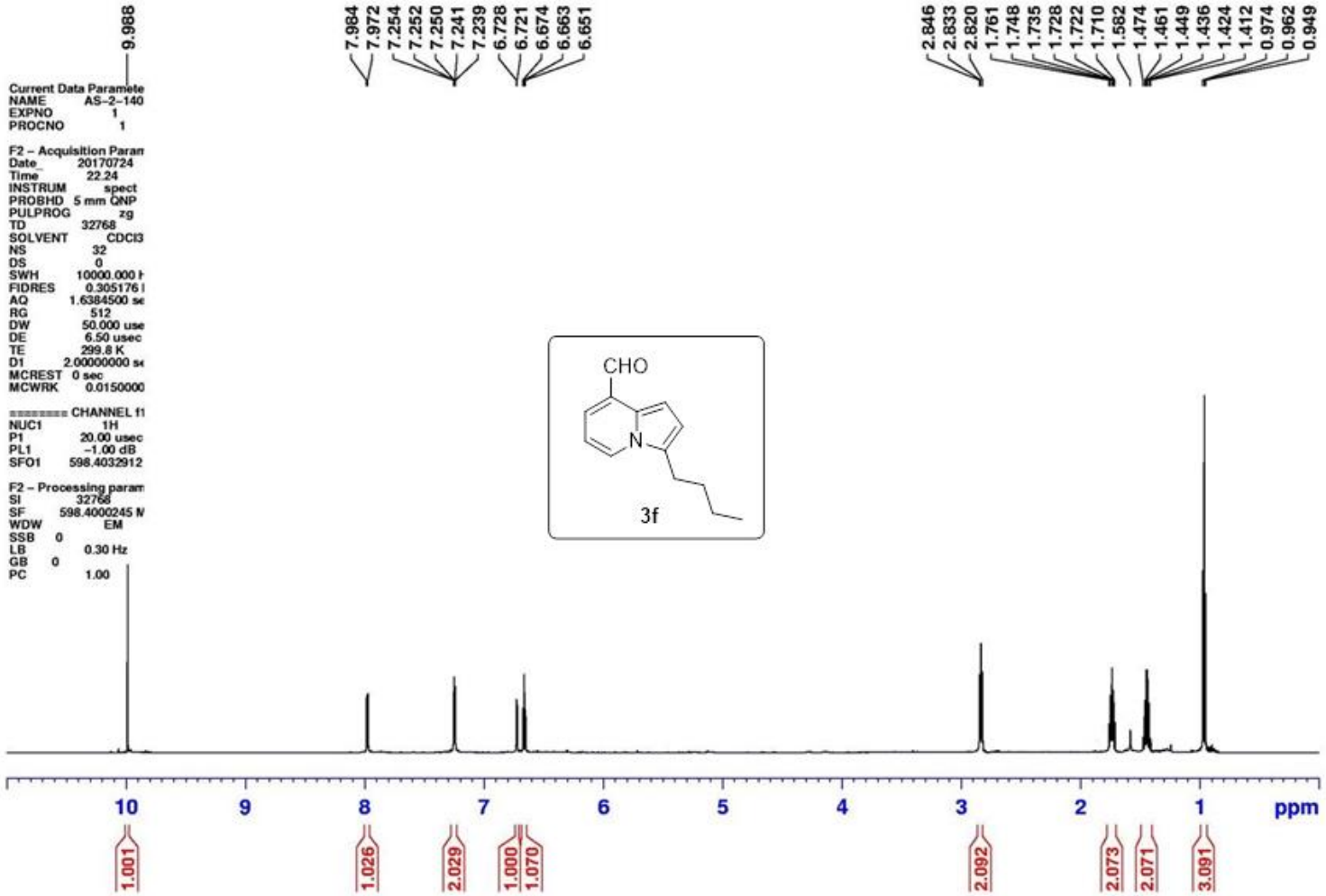

190.433
150.878
129.355
128.756
128.280
127.632
126.614
125.992
116.229
109.016
102.072
77.320
77.003
76.685
34.699
31.295
CHO
N
3c
AS-3-18C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

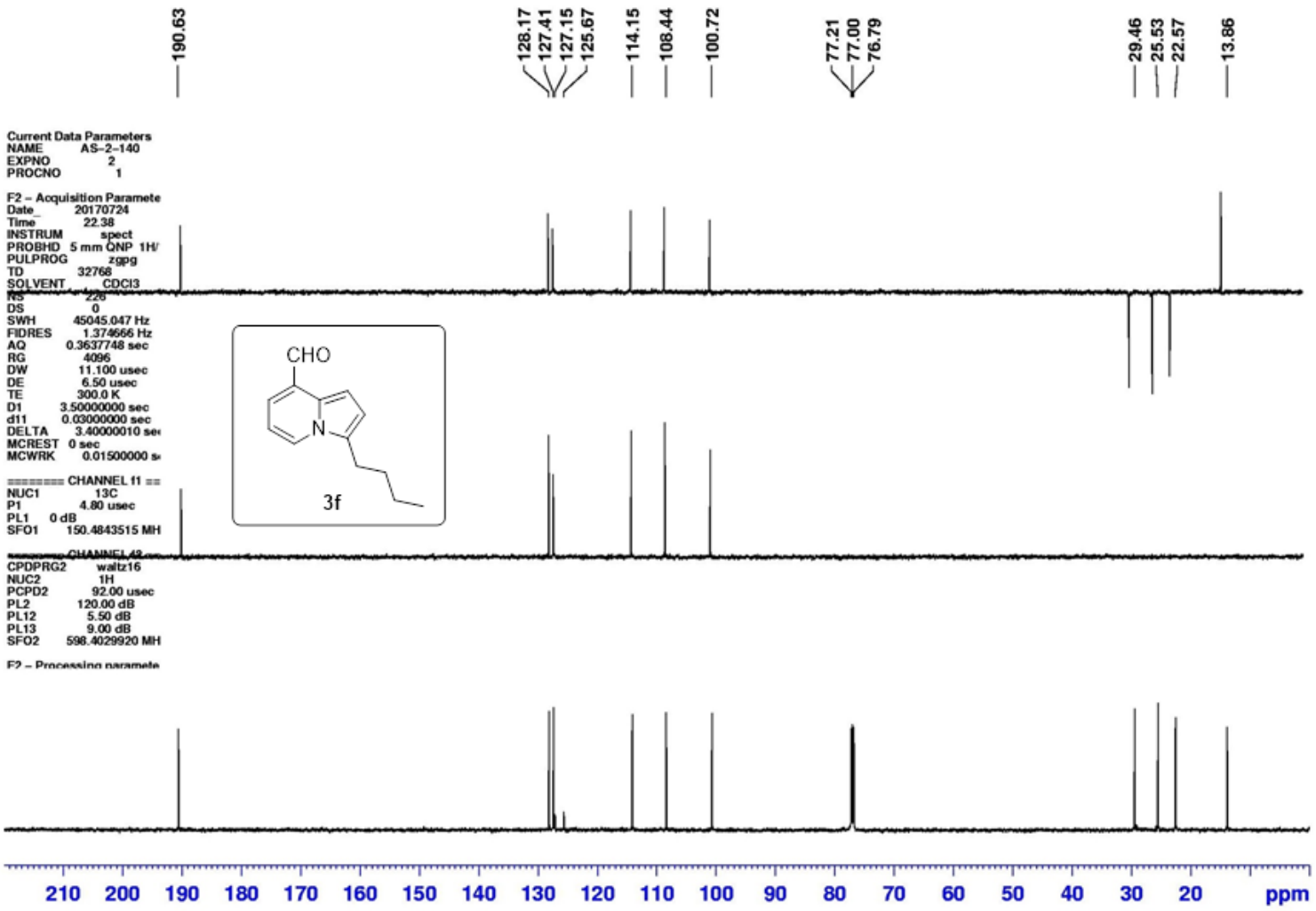

10.029
8.376
8.364
7.454
7.408
7.401
7.334
7.323
7.240
6.984
6.978
6.679
6.668
6.657
1.541
Current Data Parameters
NAME AS-2-124
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170710
Time 5.52
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 512
DW 50.000 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 -1.00 dB
SFO1 598.4032912 MHz
F2 - Processing parameters
SI 32768
SF 598.4000256 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3d
Cl
11
10
9
8
7
6
5
4
3
2
1
ppm
1.087
1.030
4.009
1.053
1.054
1.017
1.077

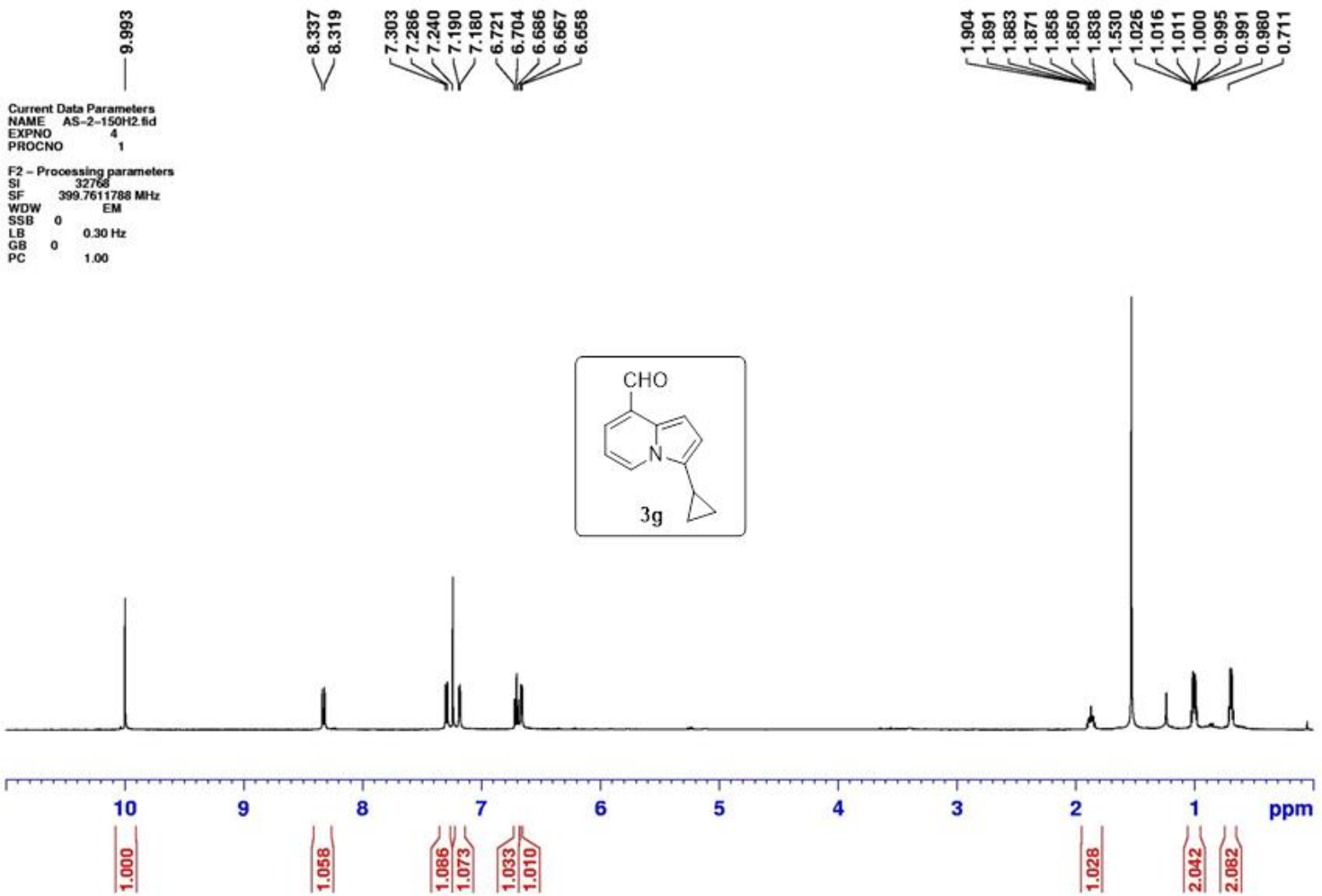

190.369
133.619
130.163
129.737
129.541
129.348
128.722
127.869
127.726
125.299
116.697
109.503
102.418
77.212
77.000
76.788
CHO
N
Cl
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

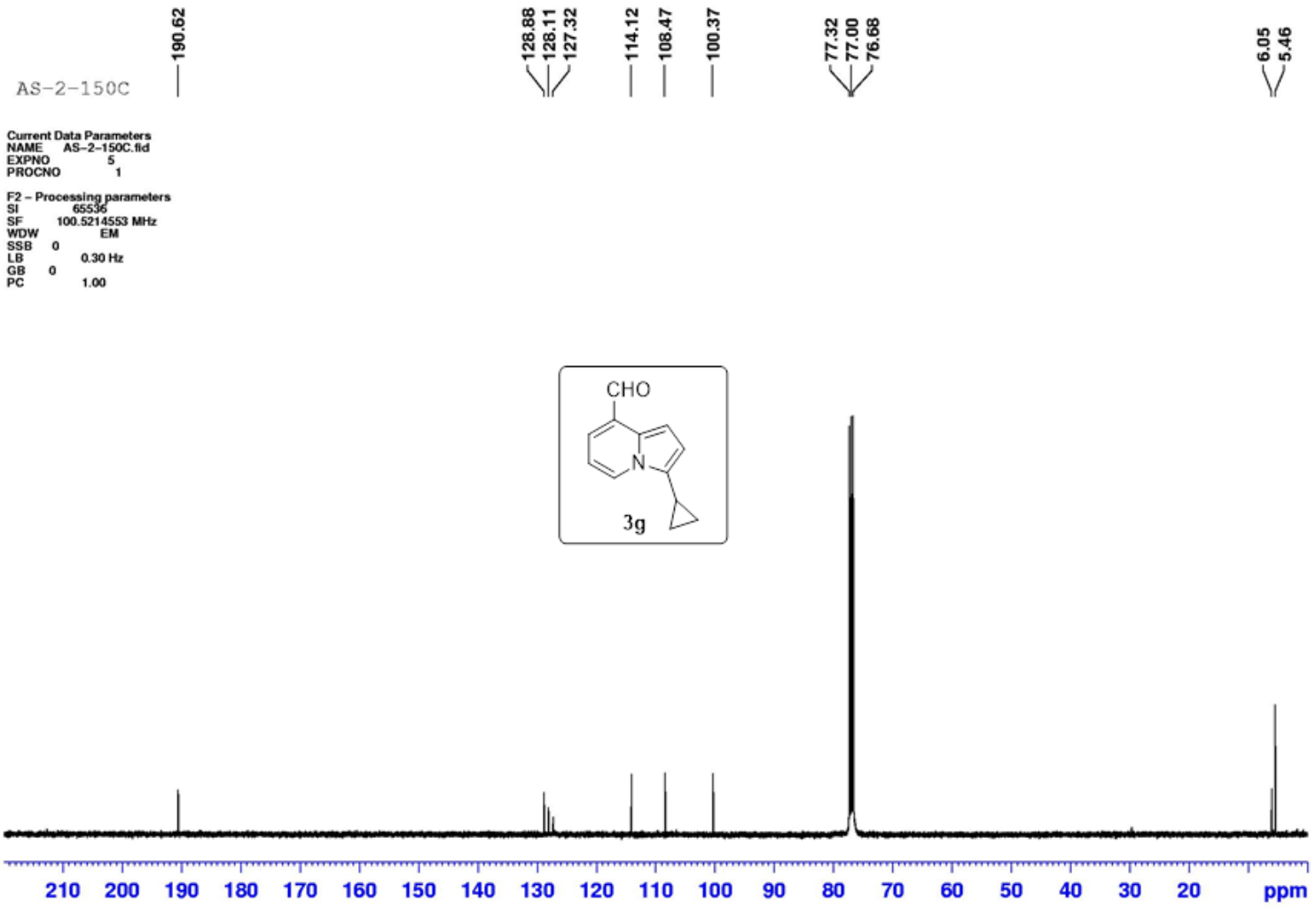

10.024
8.452
8.434
7.537
7.533
7.529
7.500
7.495
7.482
7.462
7.413
7.404
7.398
7.394
7.390
7.376
7.370
7.361
7.358
7.354
7.321
7.304
7.240
7.003
6.993
6.658
6.641
6.624
1.600
Current Data Parameters
NAME 20171111
EXPNO 5
PROCNO 1
F2 – Acquisition Parameter
Date_ 20171111
Time 15.00
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 13
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
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 MH
F2 – Processing parameter
SI 16384
CHO
N
Br
3e
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.070
3.095
2.090
1.058
1.051
1.078

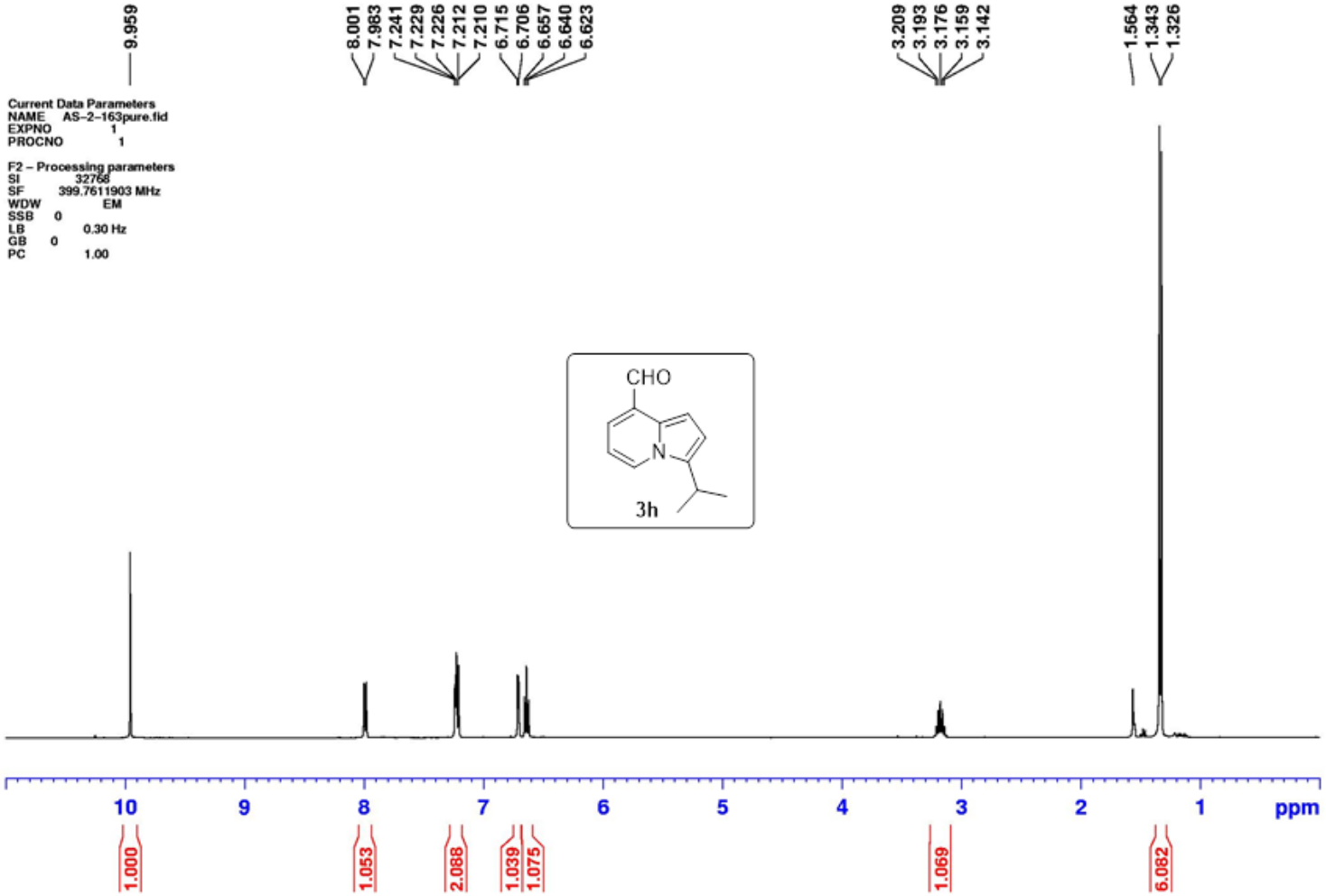

190.418
131.705
129.461
129.077
128.557
128.438
128.130
127.760
127.660
126.580
116.450
109.189
102.203
77.317
77.000
76.683
CHO
N
3e
Br
AS-2-169C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

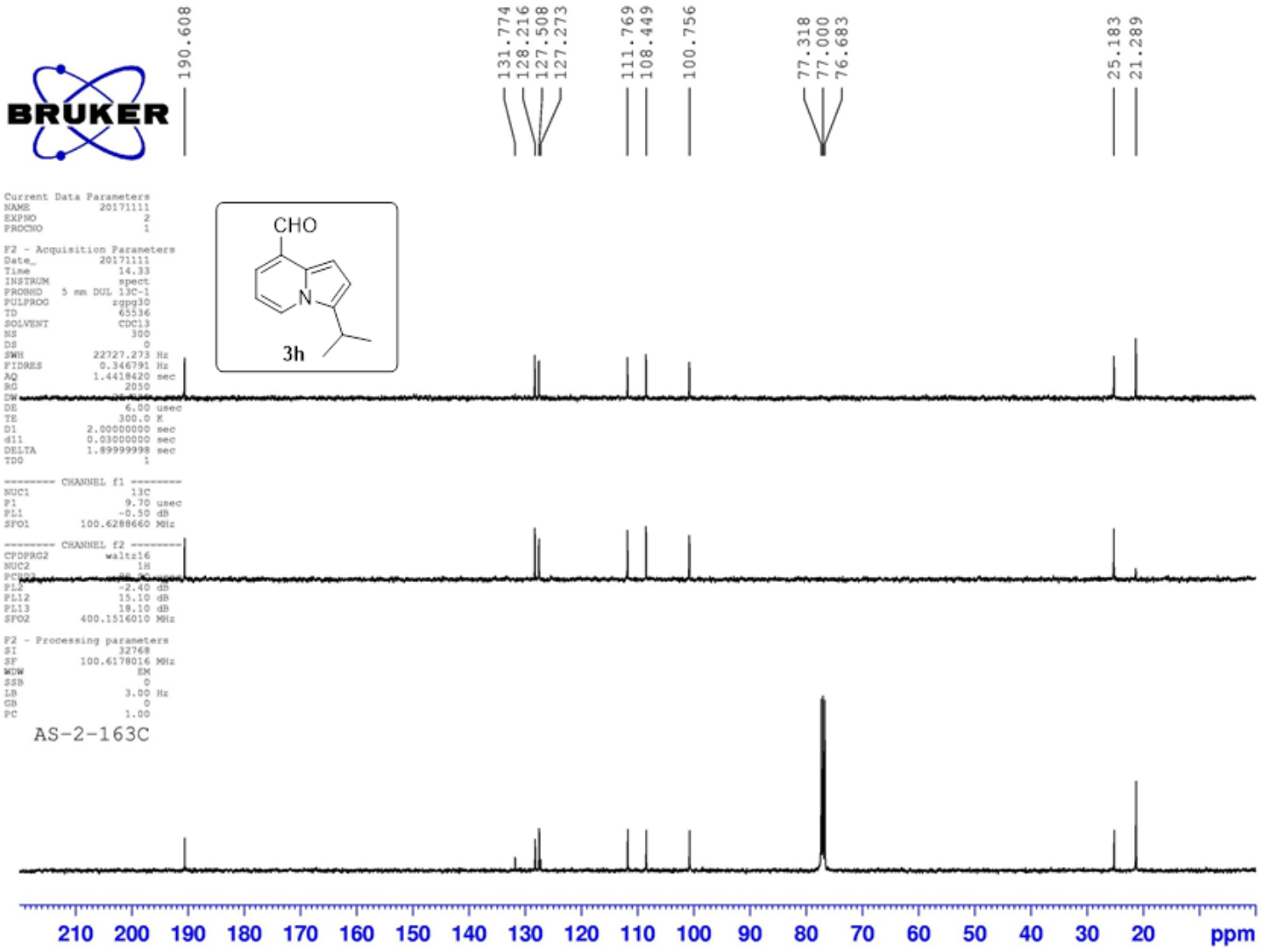

9.988
7.984
7.972
7.254
7.252
7.250
7.241
7.239
6.728
6.721
6.674
6.663
6.651
2.846
2.833
2.820
1.761
1.748
1.735
1.728
1.722
1.710
1.582
1.474
1.461
1.449
1.436
1.424
1.412
0.974
0.962
0.949
Current Data Paramete
NAME AS-2-140
EXPNO 1
PROCNO 1
F2 - Acquisition Param
Date_ 20170724
Time 22.24
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 H
FIDRES 0.305176 H
AQ 1.6384500 se
RG 512
DW 50.000 use
DE 6.50 usec
TE 299.8 K
D1 2.00000000 se
MCREST 0 sec
MCWRK 0.0150000
======== CHANNEL f1
NUC1 1H
P1 20.00 usec
PL1 -1.00 dB
SFO1 598.4032912
F2 - Processing param
SI 32768
SF 598.4000245 M
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3f
10
9
8
7
6
5
4
3
2
1
ppm
1.001
1.026
2.029
1.000
1.070
2.092
2.073
2.071
3.091

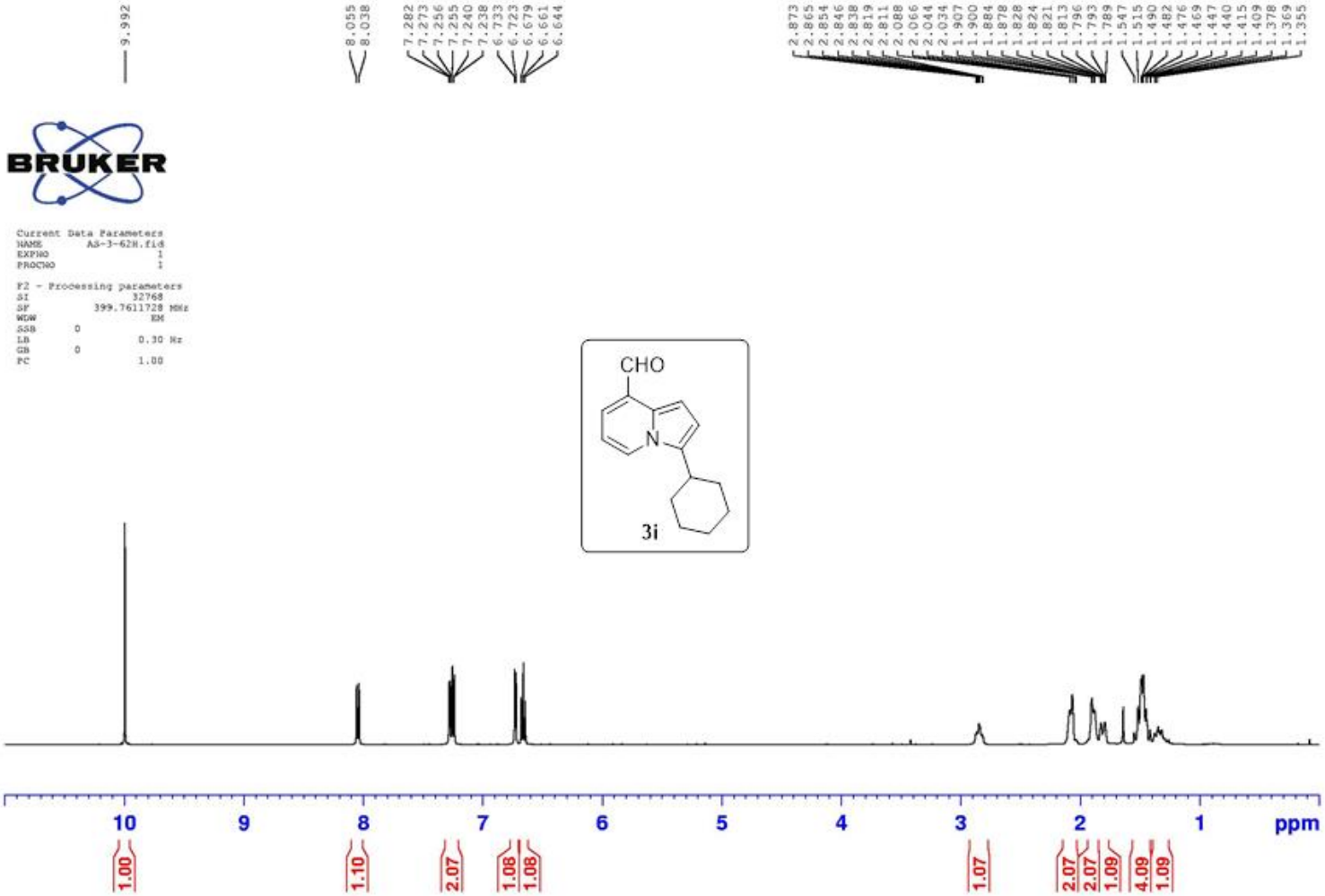

190.63
128.17
127.41
127.15
125.67
114.15
108.44
100.72
77.21
77.00
76.79
29.46
25.53
22.57
13.86
Current Data Parameters
NAME AS-2-140
EXPNO 2
PROCNO 1
F2 - Acquisition Paramete
Date_ 20170724
Time 22.38
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 226
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 se
MCREST 0 sec
MCWRK 0.01500000 s
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MH
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MH
F2 - Processing paramete
CHO
N
3f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

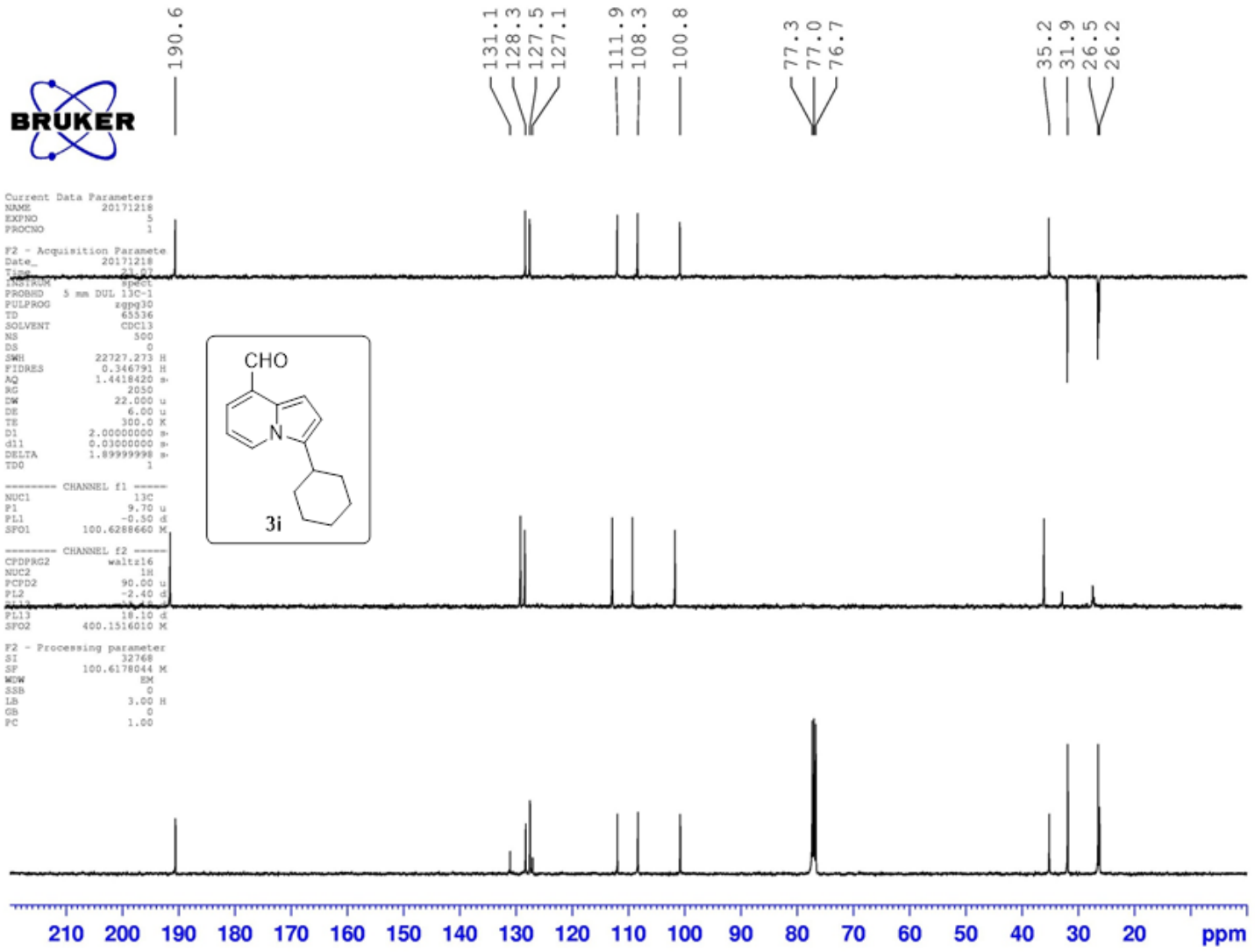

9.993
8.337
8.319
7.303
7.286
7.240
7.190
7.180
6.721
6.704
6.686
6.667
6.658
1.904
1.891
1.883
1.871
1.858
1.850
1.838
1.530
1.026
1.016
1.011
1.000
0.995
0.991
0.980
0.711
Current Data Parameters
NAME AS-2-150H2.fid
EXPNO 4
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611788 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3g
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.058
1.086
1.073
1.033
1.010
1.028
2.042
2.082

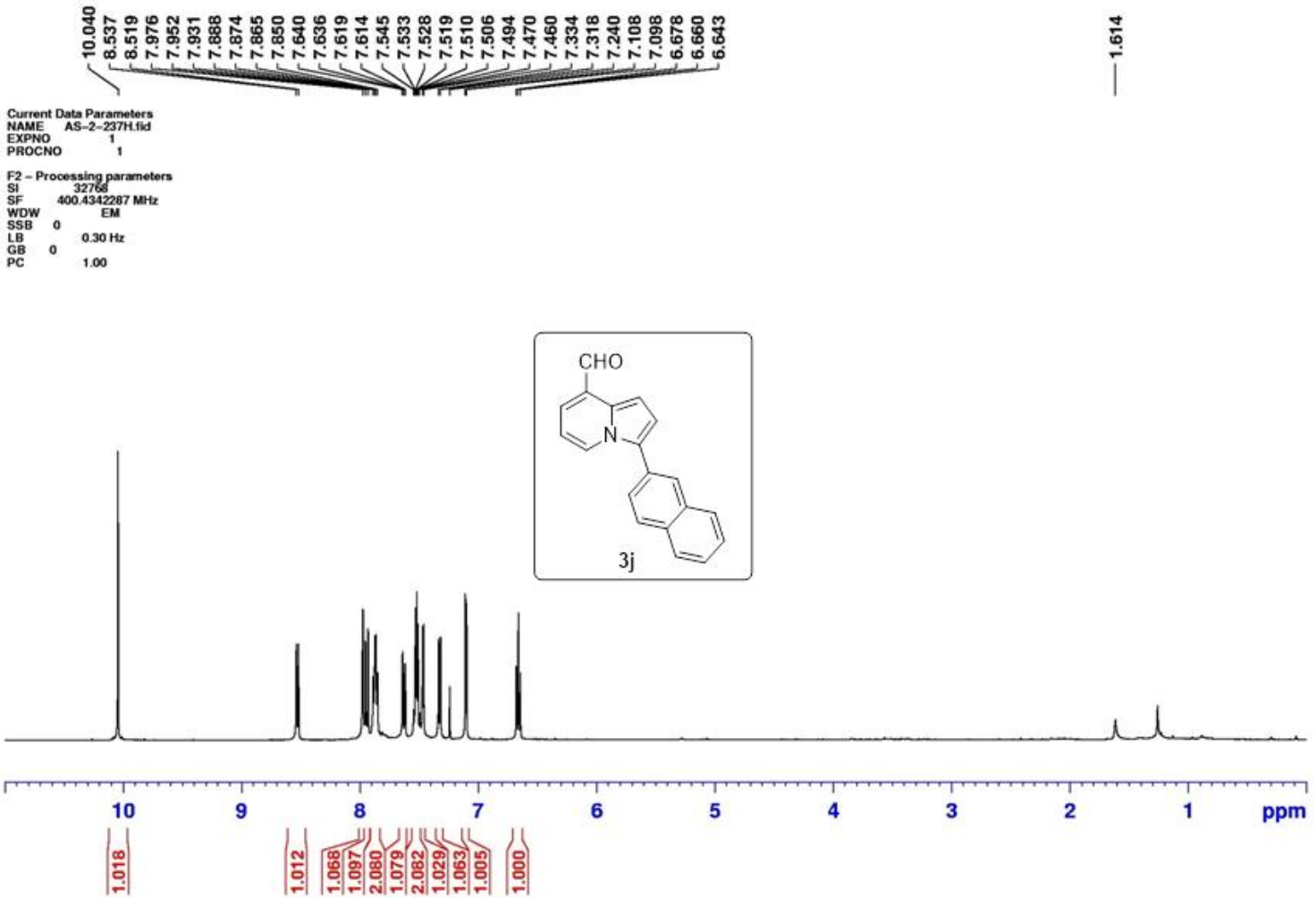

190.62
128.88
128.11
127.32
114.12
108.47
100.37
77.32
77.00
76.68
6.05
5.46
AS-2-150C
Current Data Parameters
NAME AS-2-150C.fid
EXPNO 5
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214553 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

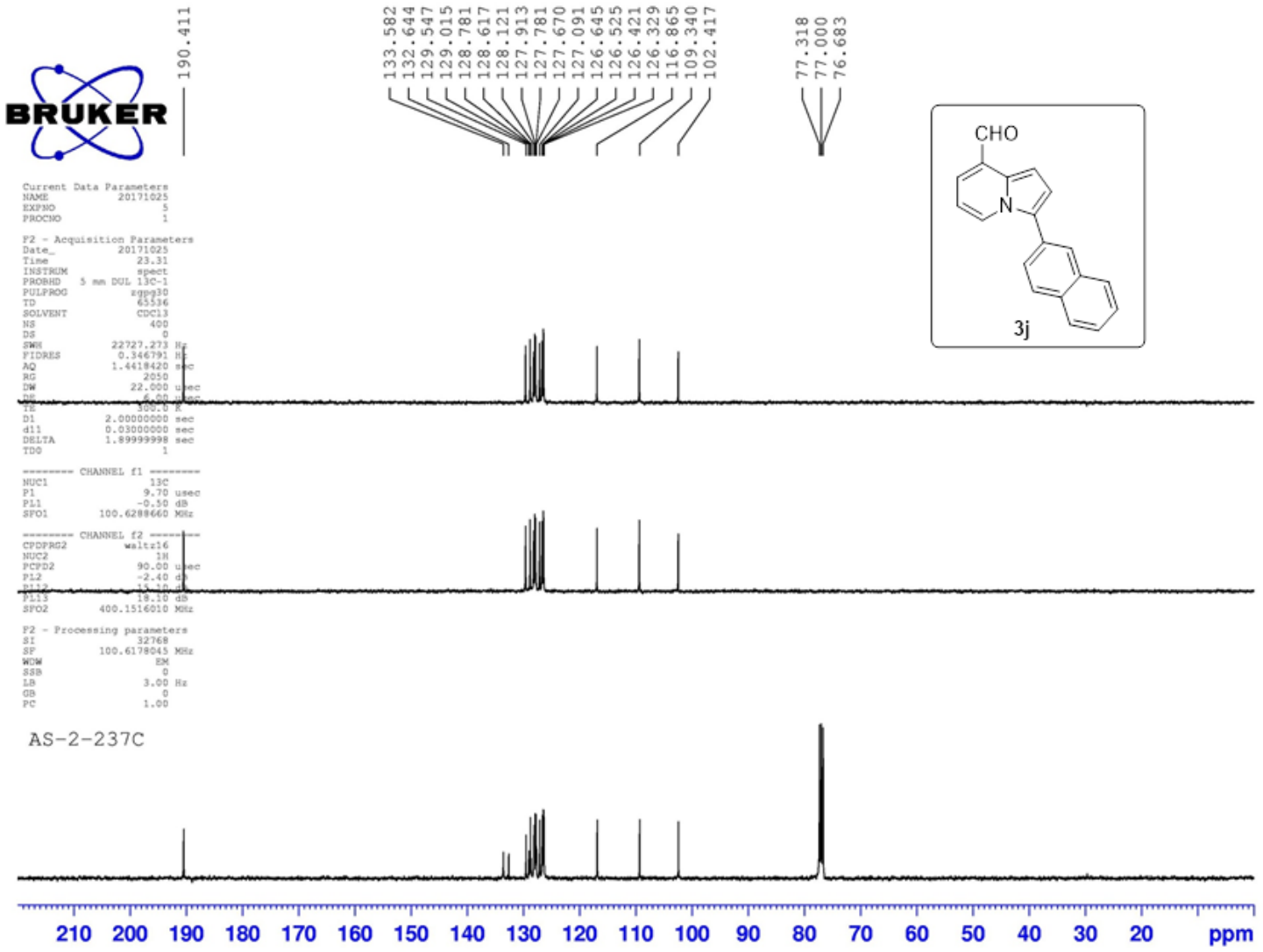

9.959
8.001
7.983
7.241
7.229
7.226
7.212
7.210
6.715
6.706
6.657
6.640
6.623
3.209
3.193
3.176
3.159
3.142
1.564
1.343
1.326
Current Data Parameters
NAME AS-2-163pure.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611903 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3h
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.053
2.088
1.039
1.075
1.069
6.082

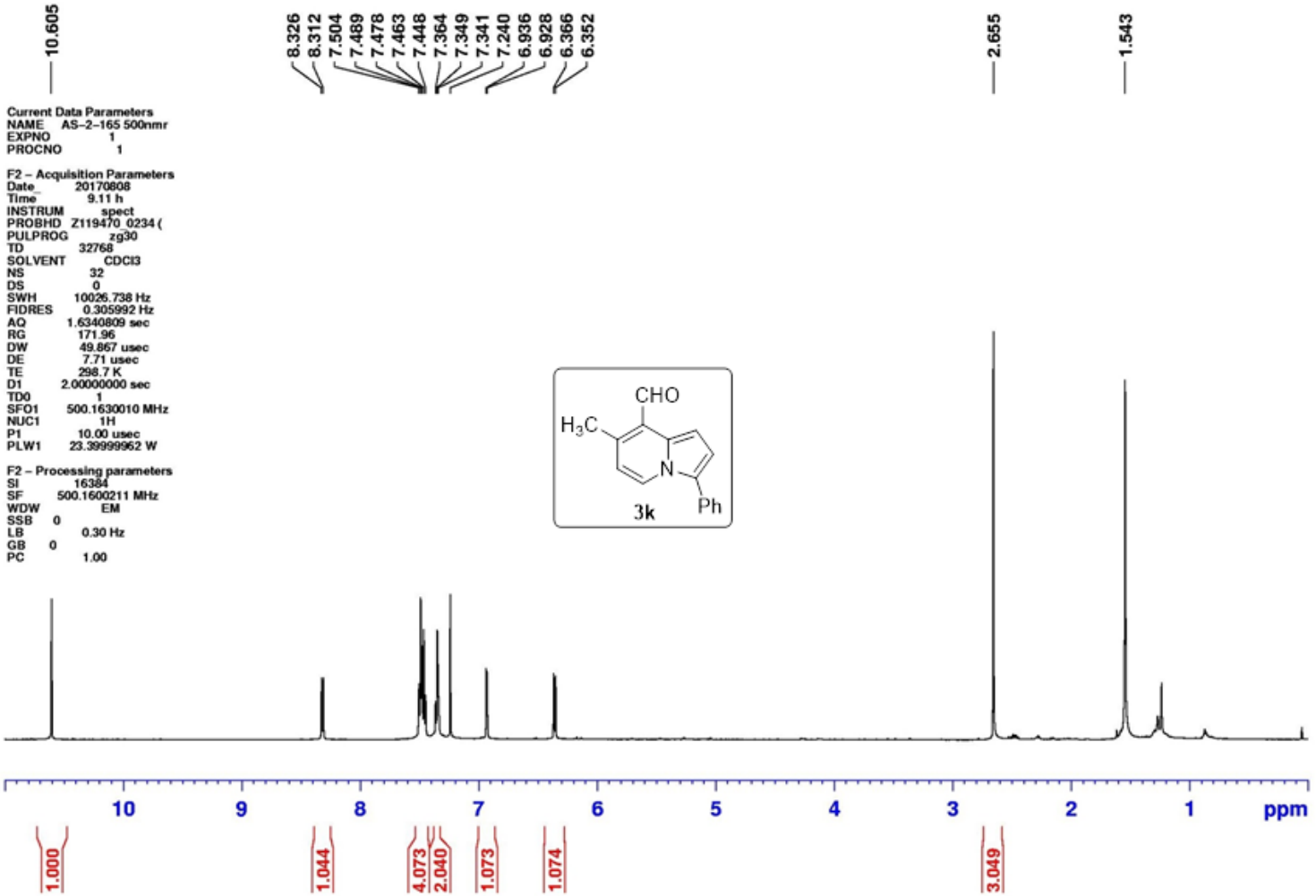

190.608
131.774
128.216
127.508
127.273
111.769
108.449
100.756
77.318
77.000
76.683
25.183
21.289
CHO
N
3h
AS-2-163C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

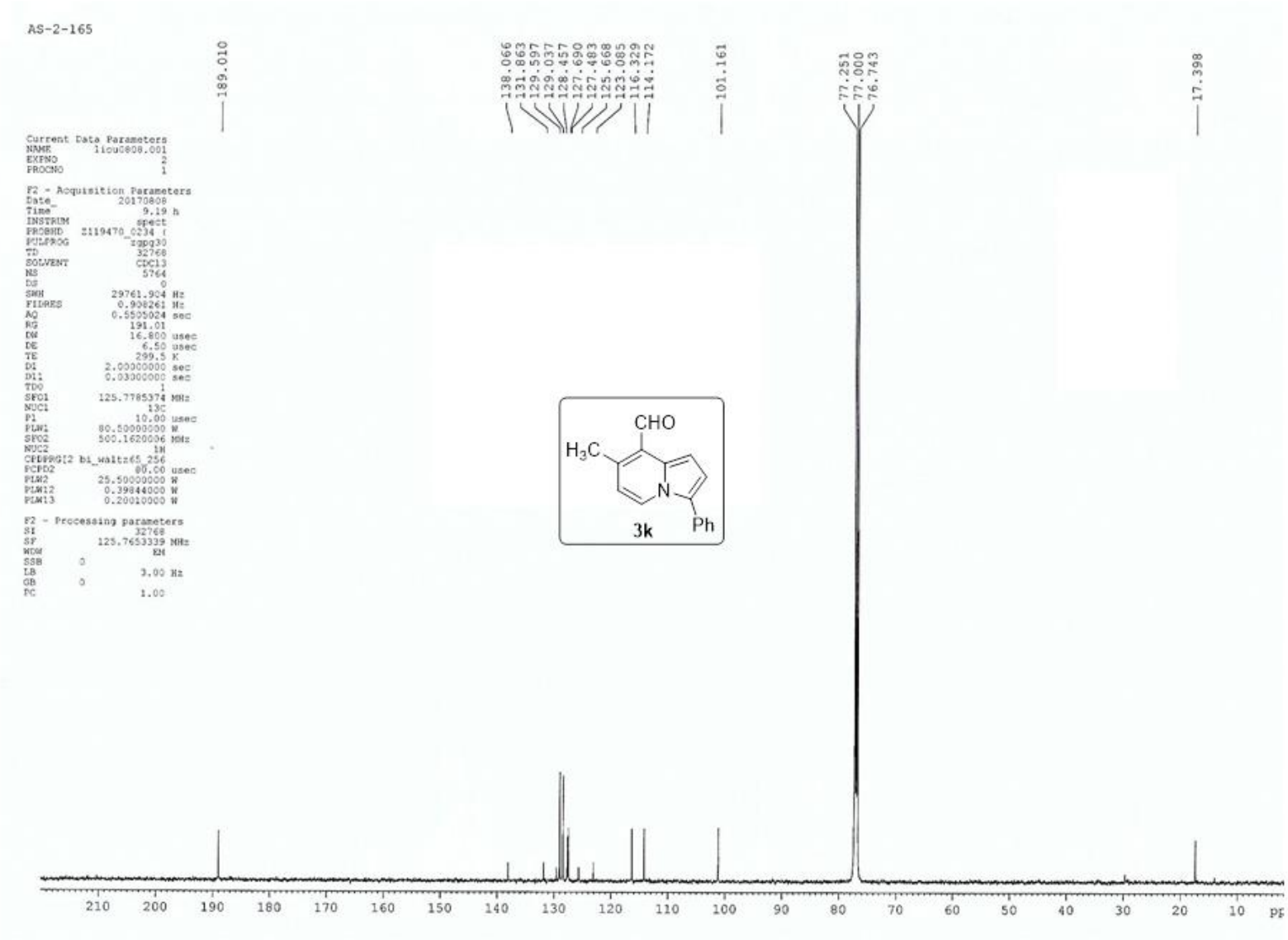

9.992
8.055
8.038
7.282
7.273
7.256
7.255
7.240
7.238
6.733
6.723
6.679
6.661
6.644
2.873
2.865
2.854
2.846
2.838
2.819
2.811
2.088
2.066
2.044
2.034
1.907
1.900
1.884
1.878
1.828
1.824
1.821
1.813
1.796
1.793
1.789
1.547
1.515
1.490
1.482
1.476
1.469
1.447
1.440
1.415
1.409
1.378
1.369
1.355
BRUKER
Current Data Parameters
NAME A3-3-62H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611728 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3i
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.10
2.07
1.08
1.08
1.07
2.07
2.07
1.09
4.09
1.09

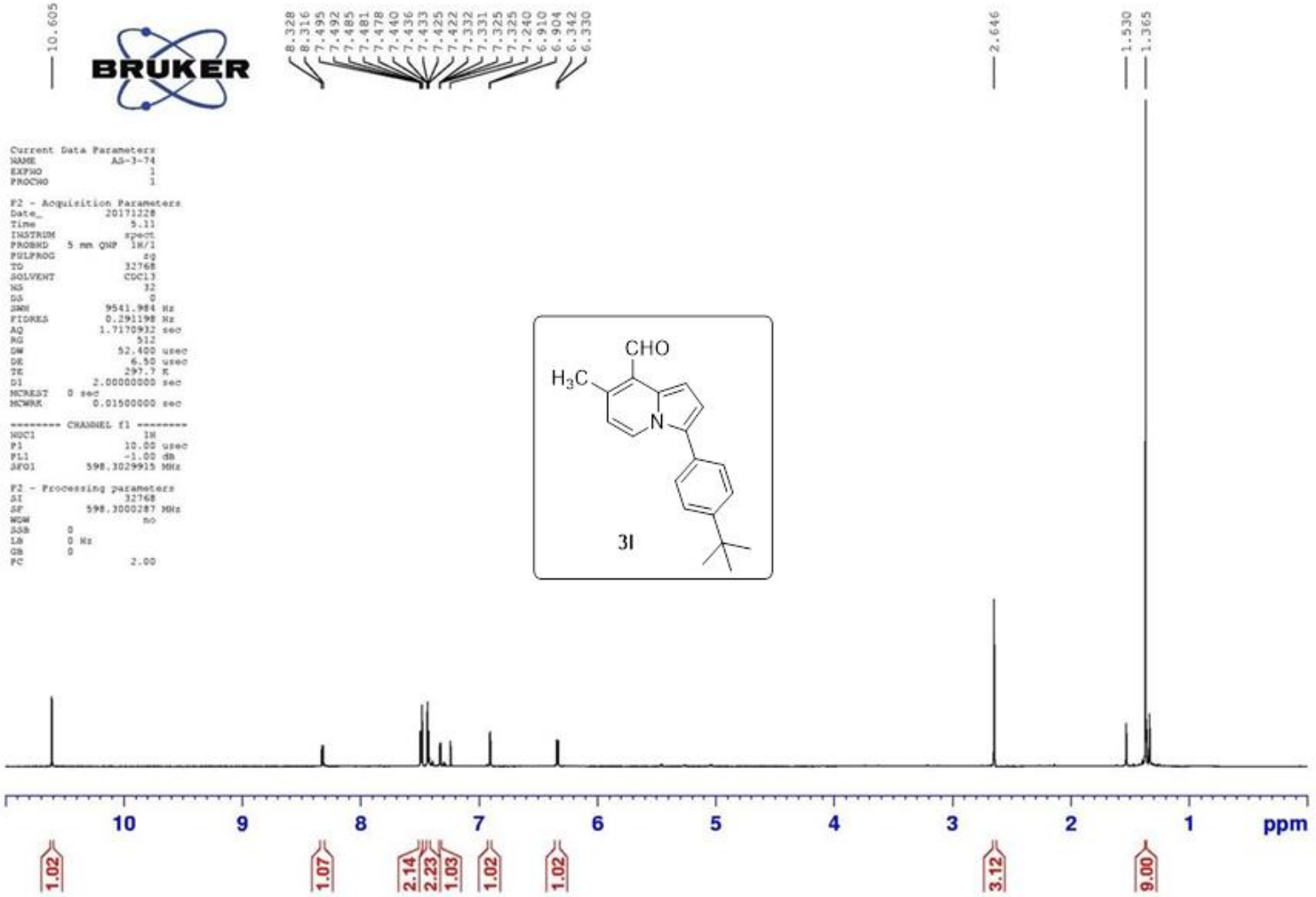

190.6
131.1
128.3
127.5
127.1
111.9
108.3
100.8
77.3
77.0
76.7
35.2
31.9
26.5
26.2
BRUKER
CHO
N
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

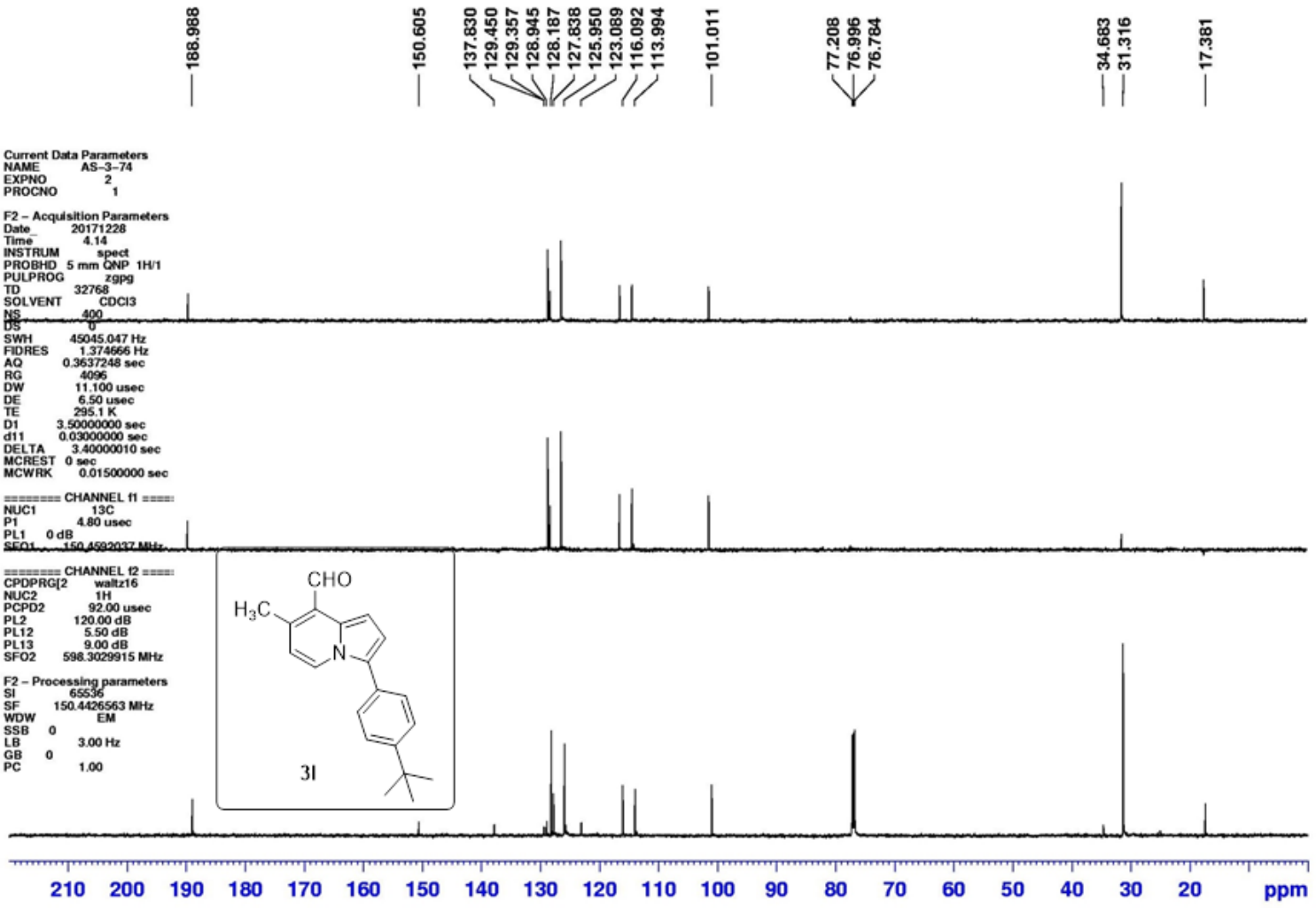

10.040
8.537
8.519
7.976
7.952
7.931
7.888
7.874
7.865
7.850
7.640
7.636
7.619
7.614
7.545
7.533
7.528
7.519
7.510
7.506
7.494
7.470
7.460
7.334
7.318
7.240
7.108
7.098
6.678
6.660
6.643
1.614
Current Data Parameters
NAME AS-2-237H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 400.4342287 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
N
3j
10
9
8
7
6
5
4
3
2
1
ppm
1.018
1.012
1.068
1.097
2.080
1.079
2.082
1.029
1.063
1.005
1.000

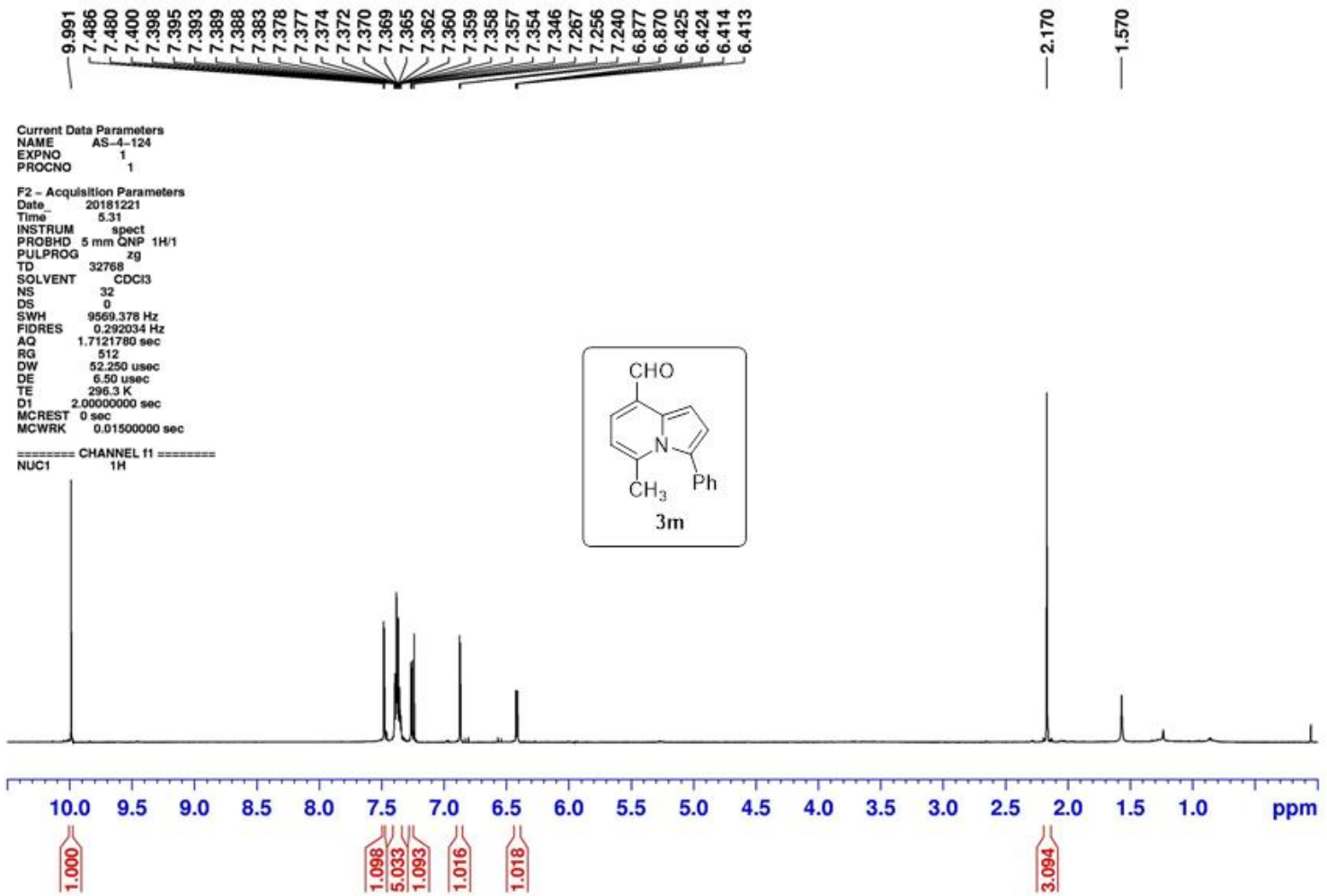

BRUKER
190.411
133.582
132.644
129.547
129.015
128.781
128.617
128.121
127.913
127.781
127.670
127.091
126.645
126.525
126.421
126.329
116.865
109.340
102.417
77.318
77.000
76.683
CHO
N
3j
Current Data Parameters
NAME 20171025
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171025
Time 23.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.1 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 13.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178045 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
AS-2-237C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

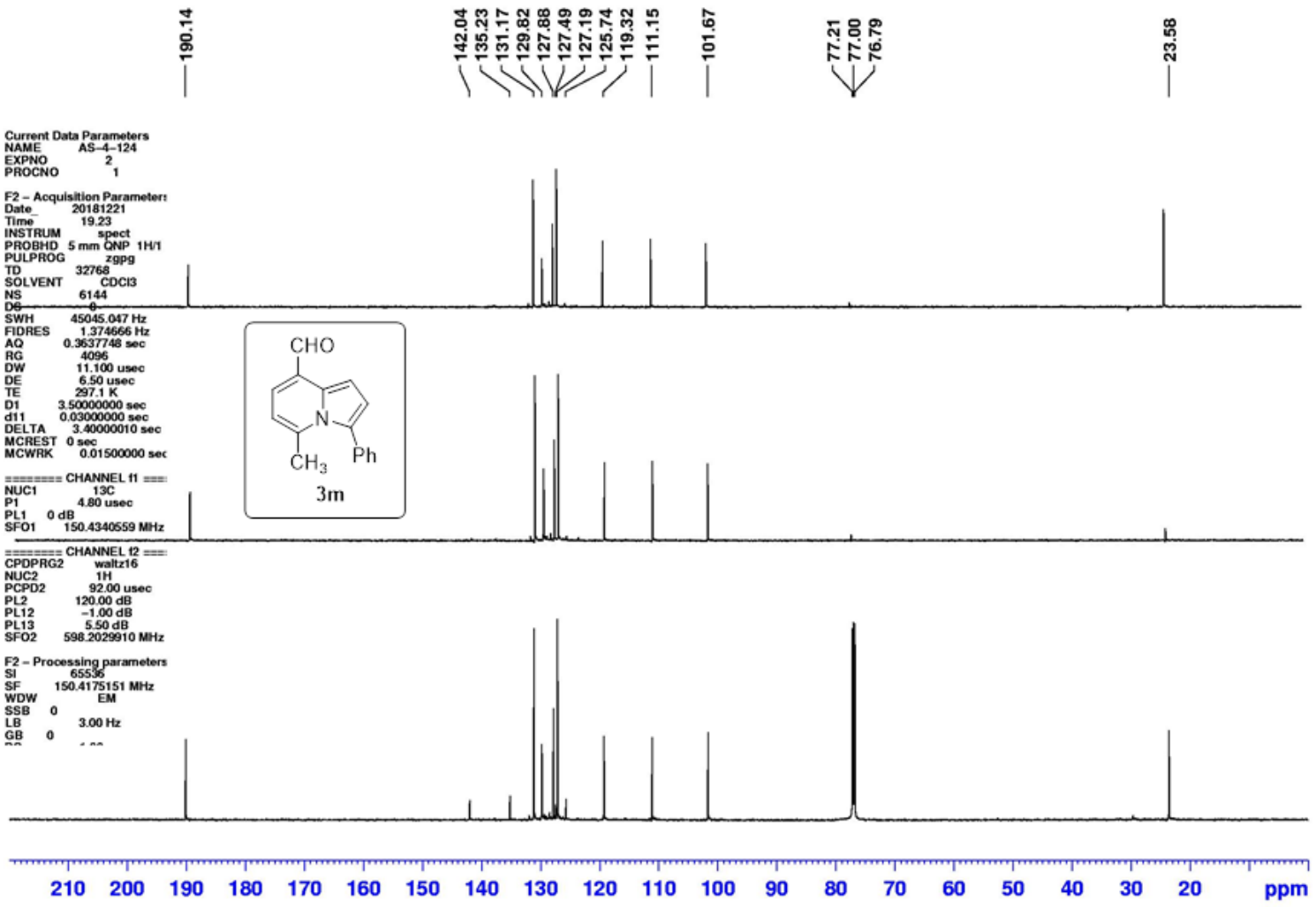

10.605
8.326
8.312
7.504
7.489
7.478
7.463
7.448
7.364
7.349
7.341
7.240
6.936
6.928
6.366
6.352
2.655
1.543
Current Data Parameters
NAME AS-2-165 500nmr
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170808
Time 9.11 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340809 sec
RG 171.96
DW 49.867 usec
DE 7.71 usec
TE 298.7 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.39999962 W
F2 - Processing parameters
SI 16384
SF 500.1600211 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CHO
H3C
N
Ph
3k
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.044
4.073
2.040
1.073
1.074
3.049


AS-2-165
189.010
138.066
131.863
129.597
129.037
128.457
127.690
127.483
125.668
123.085
116.329
114.172
101.161
77.251
77.000
76.743
17.398
Current Data Parameters
NAME 11cu0808.001
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170808
Time 9.19 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 5764
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
PLW1 80.50000000 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 80.00 usec
PLW2 25.50000000 W
PLW12 0.39844000 W
PLW13 0.20010000 W
F2 - Processing parameters
SI 32768
SF 125.7653339 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CHO
H3C
N
Ph
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

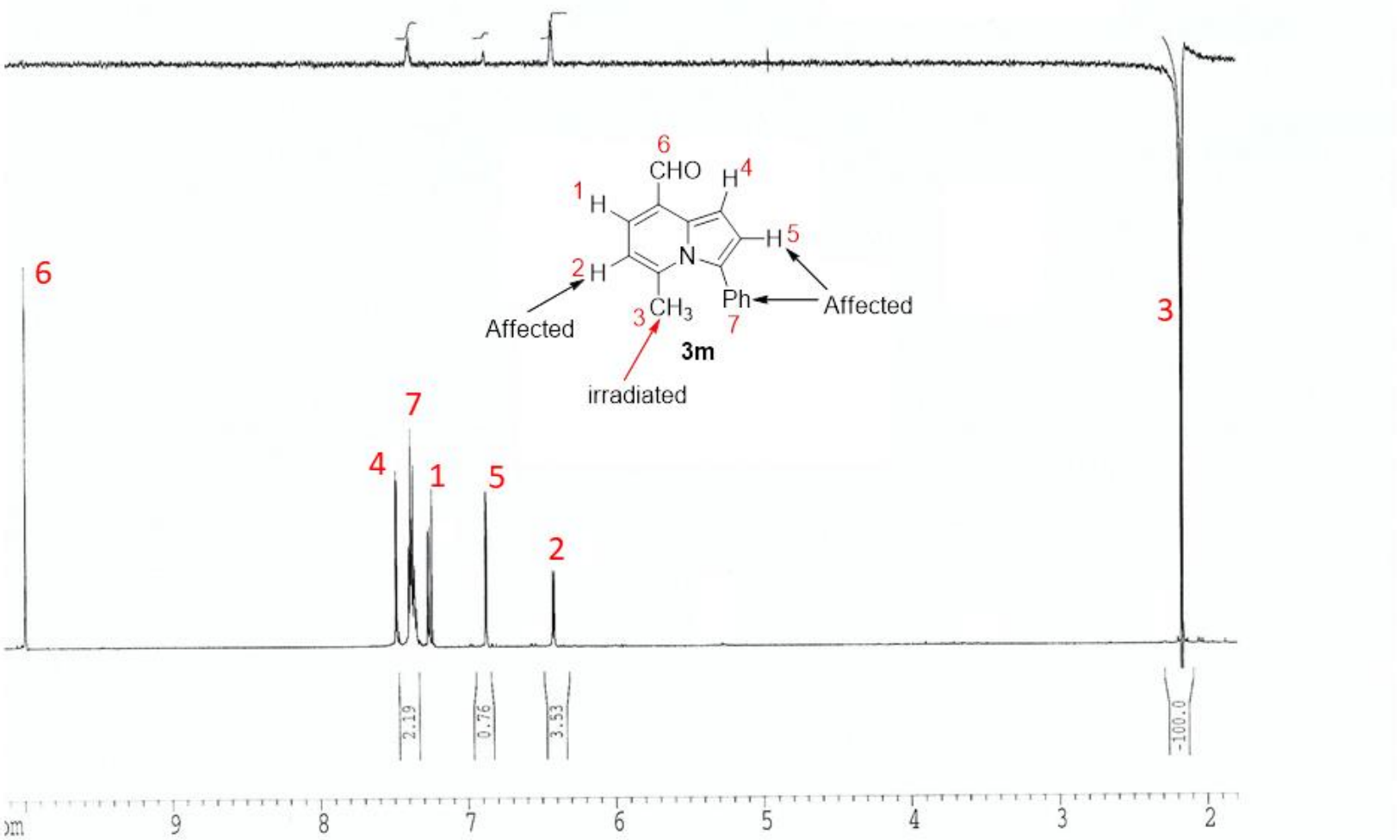

10.605
8.328
8.316
7.495
7.492
7.485
7.481
7.478
7.440
7.436
7.433
7.425
7.422
7.332
7.331
7.325
7.325
7.240
6.910
6.904
6.342
6.330
2.646
1.530
1.365
Current Data Parameters
NAME AS-3-74
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171228
Time 5.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.3029915 MHz
F2 - Processing parameters
SI 32768
SF 598.3000287 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
CHO
H3C
N
3l
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.07
2.14
2.23
1.03
1.02
1.02
3.12
9.00


188.988
150.605
137.630
129.450
129.357
128.945
128.187
127.838
125.950
123.089
116.092
113.994
101.011
77.208
76.996
76.784
34.663
31.316
17.381
Current Data Parameters
NAME AS-3-74
EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
Date 20171228
Time 4.14
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 400
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 – Processing parameters
SI 65536
SF 150.4426563 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
CHO
H3C
N
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

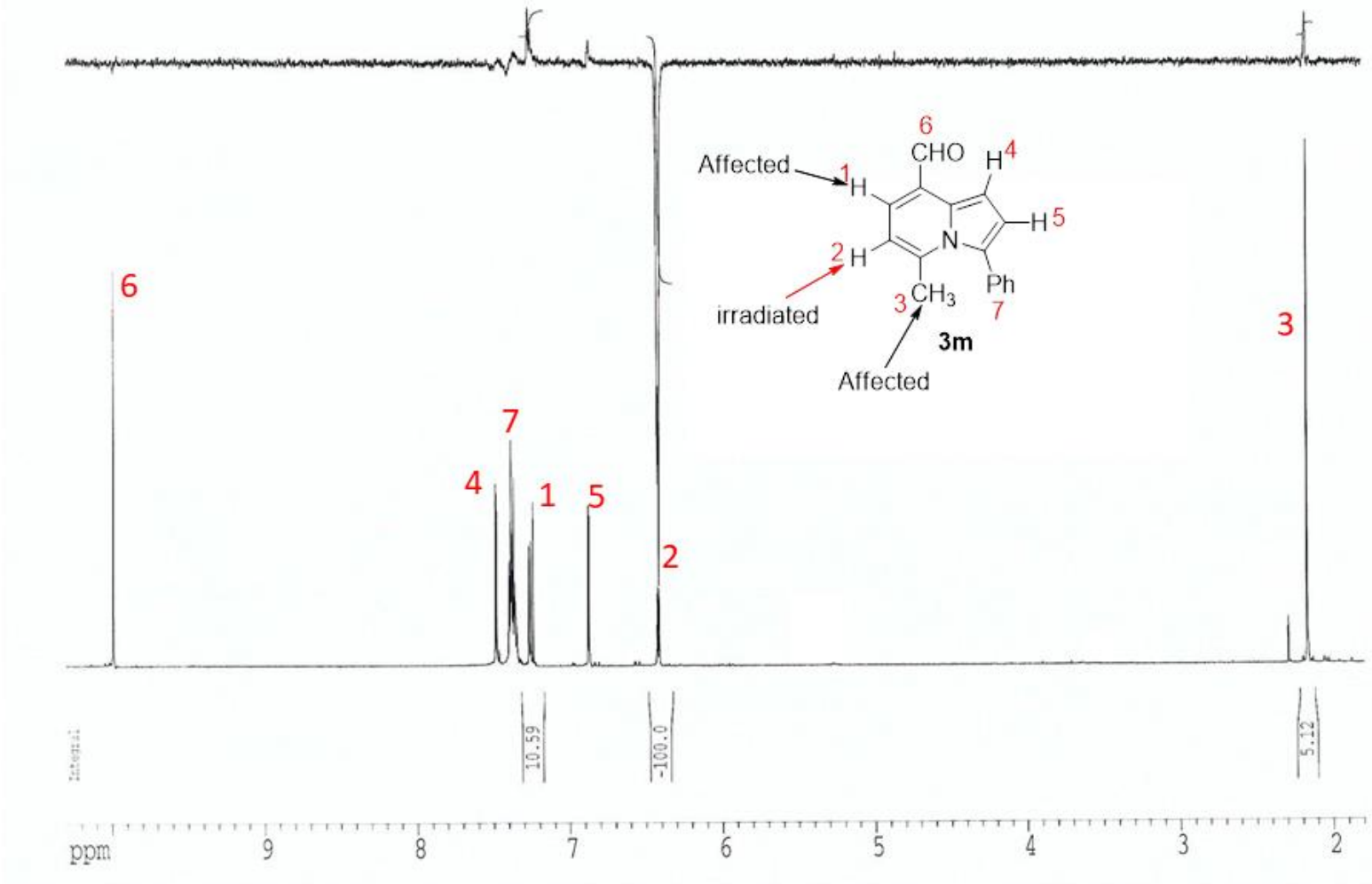

9.991
7.486
7.480
7.400
7.398
7.395
7.393
7.389
7.388
7.383
7.378
7.377
7.374
7.372
7.370
7.369
7.365
7.362
7.360
7.359
7.358
7.357
7.354
7.346
7.267
7.256
7.240
6.877
6.870
6.425
6.424
6.414
6.413
2.170
1.570
Current Data Parameters
NAME AS-4-124
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181221
Time 5.31
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
DW 52.250 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
CHO
N
CH3
Ph
3m
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.000
1.098
5.033
1.093
1.016
1.018
3.094


190.14
142.04
135.23
131.17
129.82
127.88
127.49
127.19
125.74
119.32
111.15
101.67
77.21
77.00
76.79
23.58
Current Data Parameters
NAME AS-4-124
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181221
Time 19.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4340559 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 -1.00 dB
PL13 5.50 dB
SFO2 598.2029910 MHz
F2 - Processing parameters
SI 65536
SF 150.4175151 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
CHO
N
CH3
Ph
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

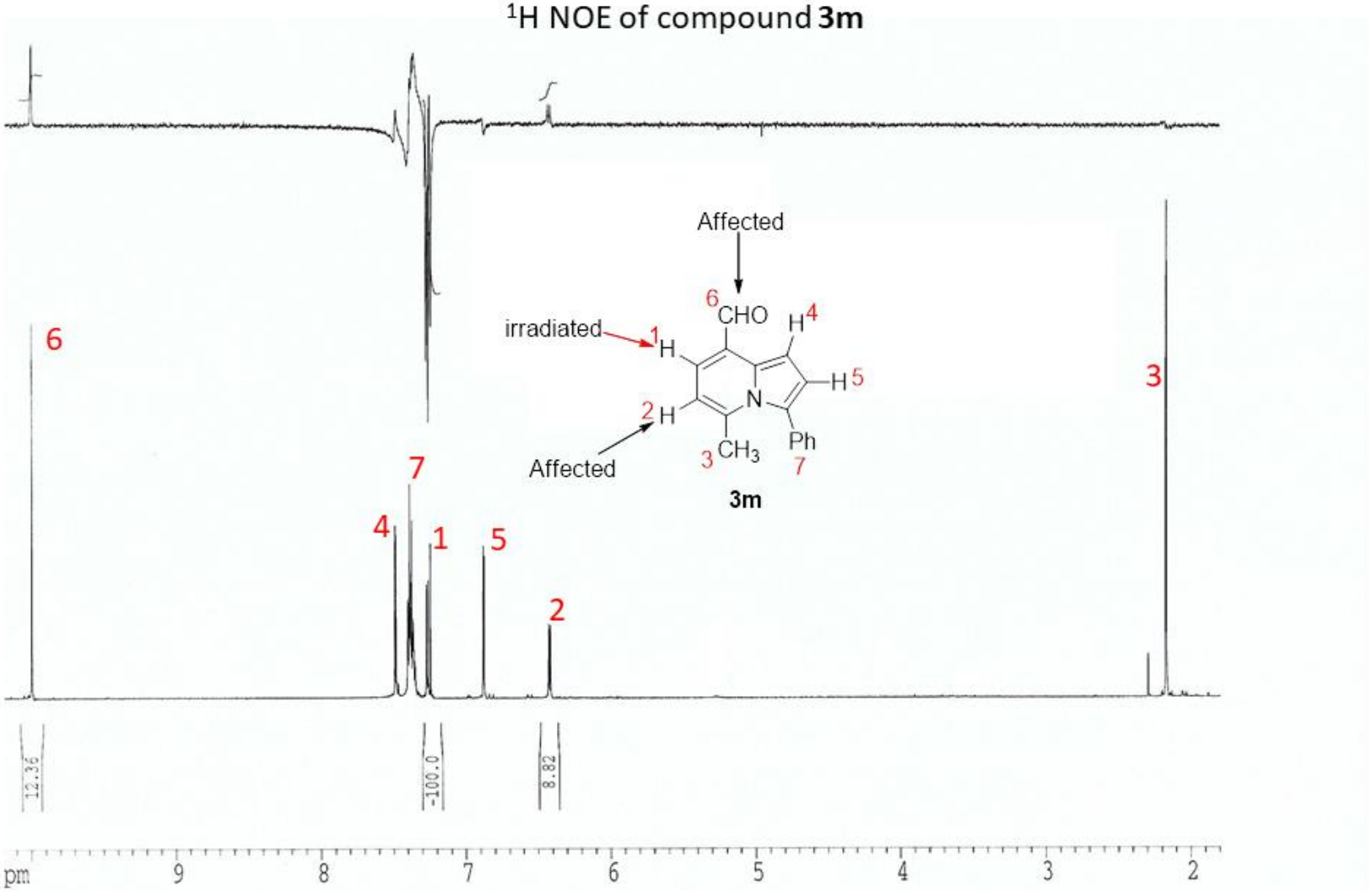
^{1}H NOE of compound **3m**



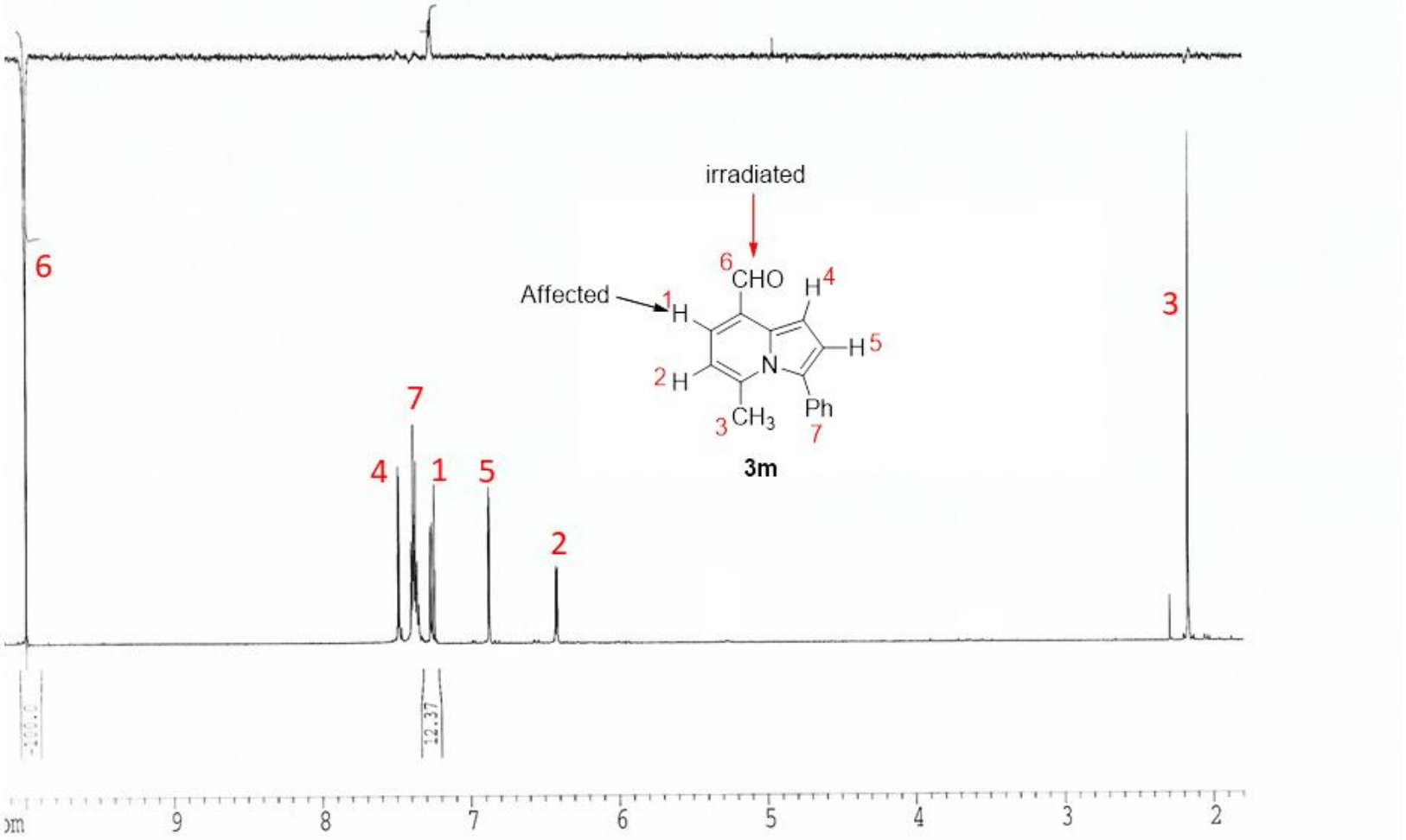
^{1}H NOE of compound **3m**

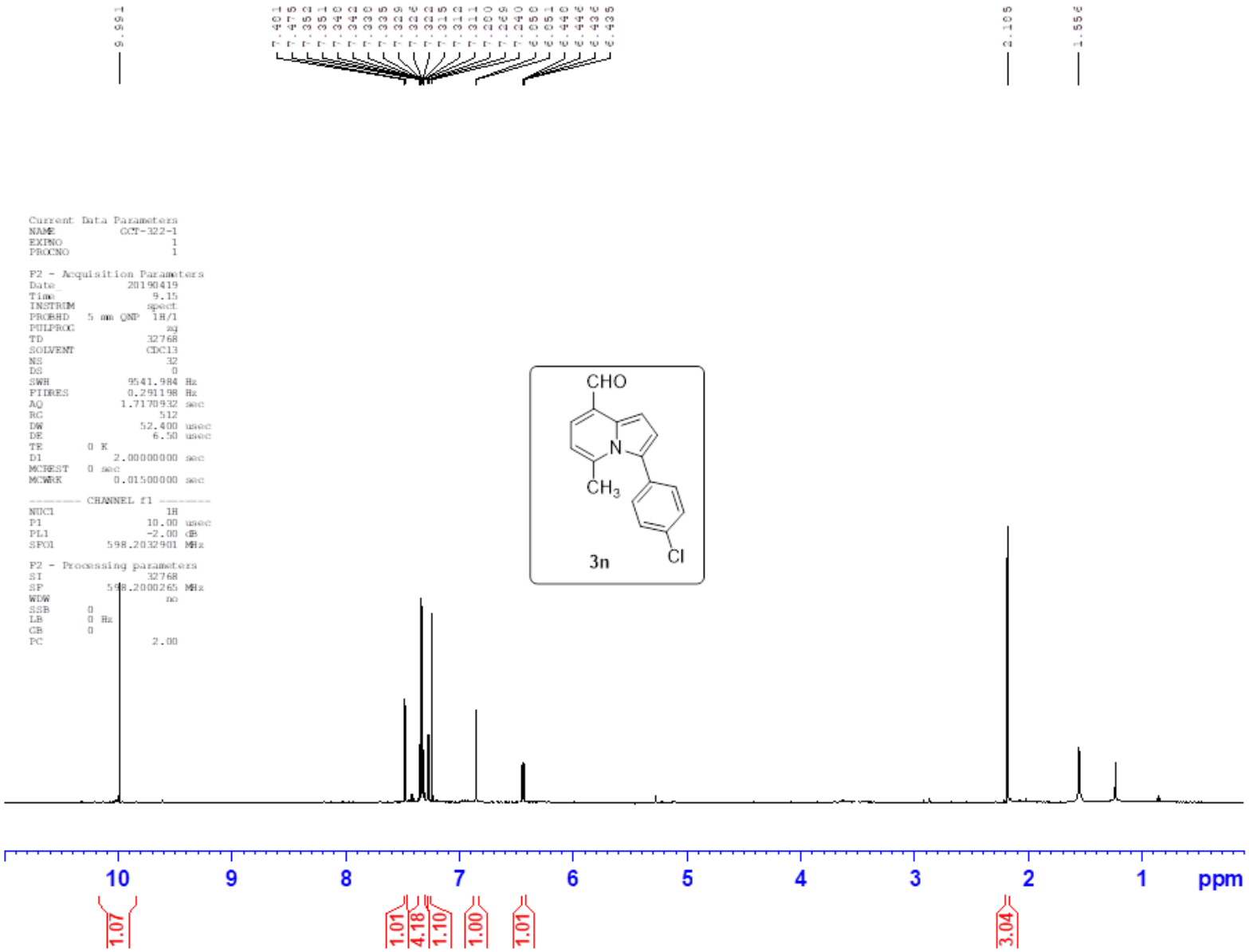


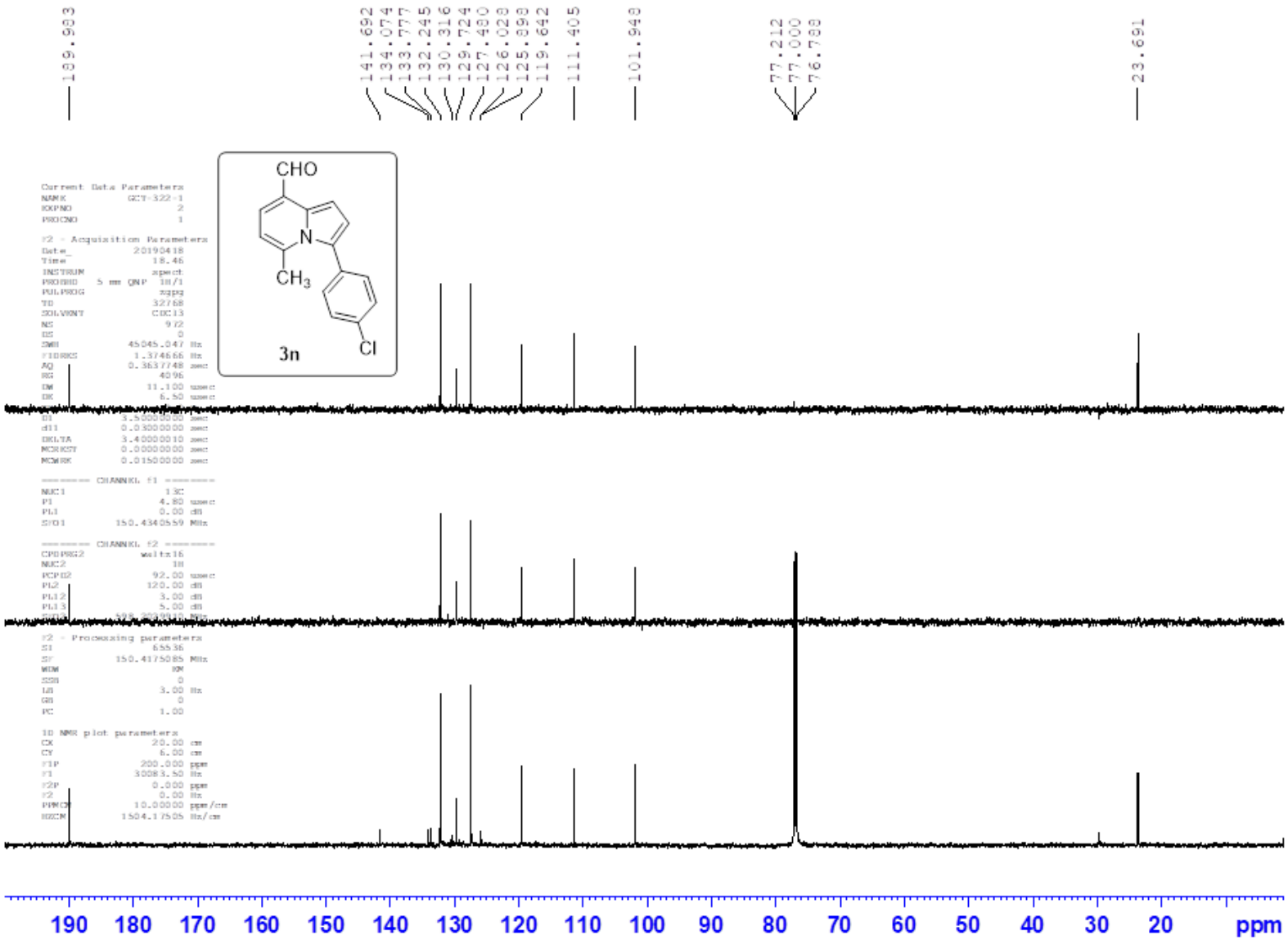
^{1}H NOE of compound **3m**

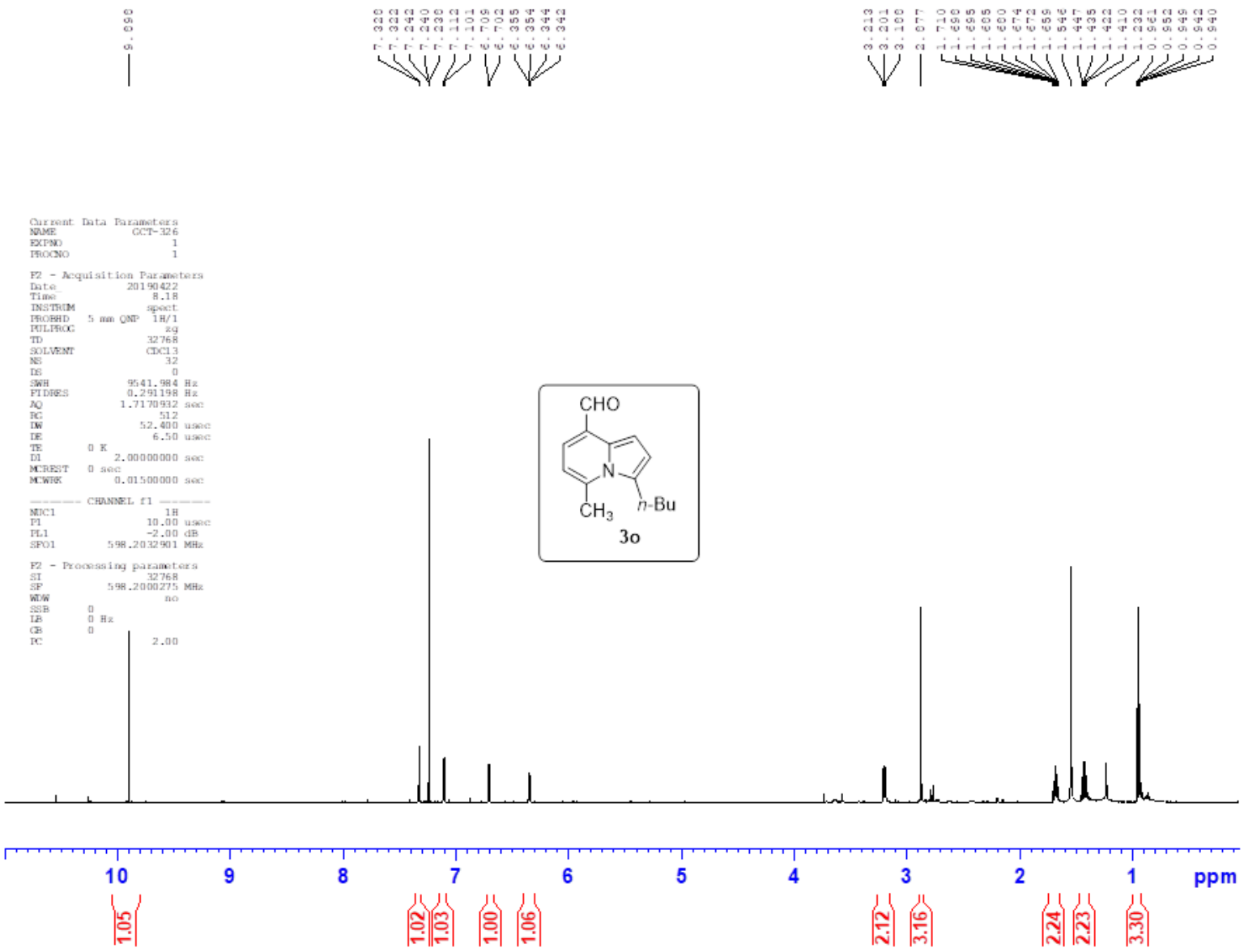


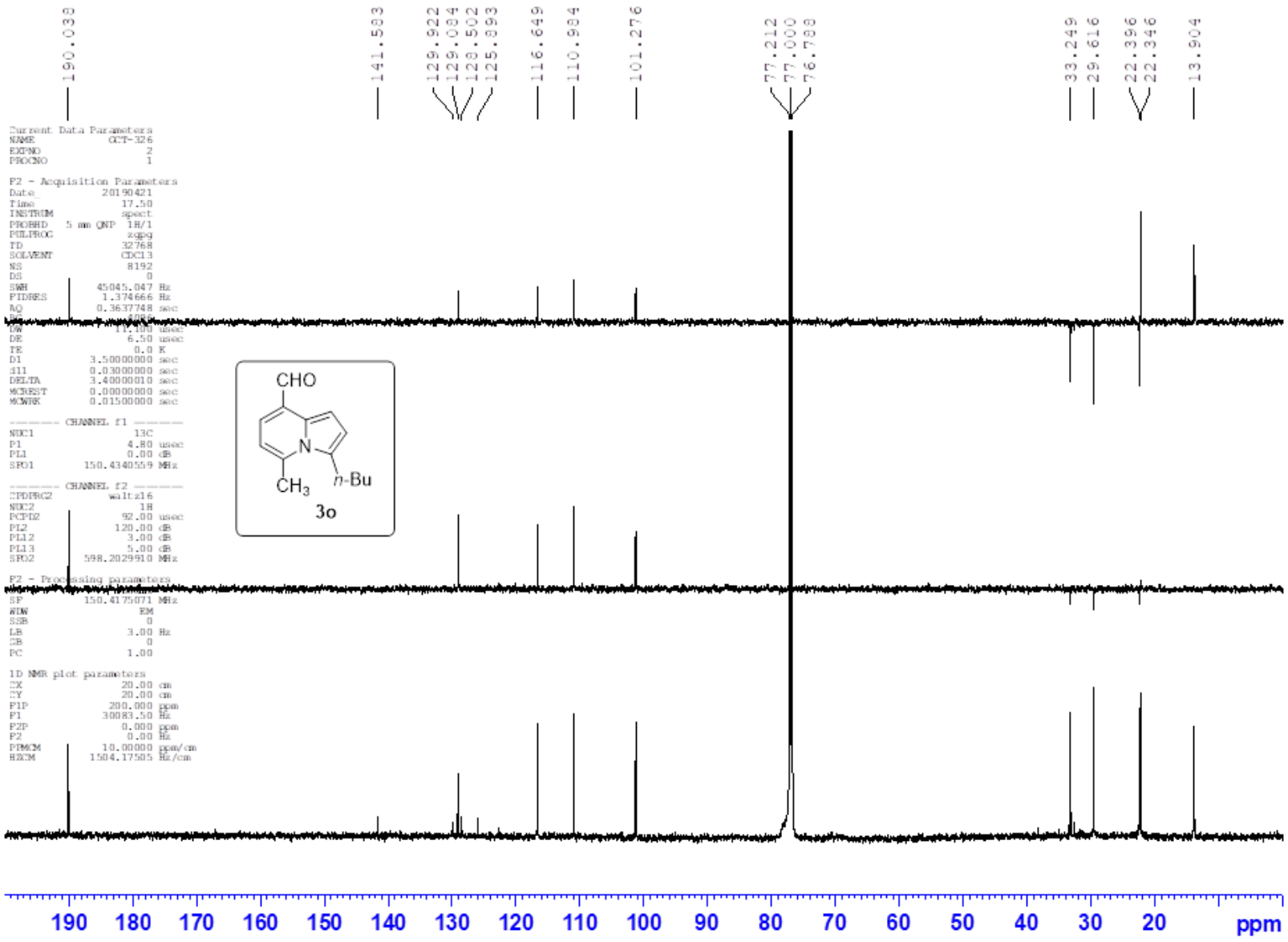
^{1}H NOE of compound **3m**

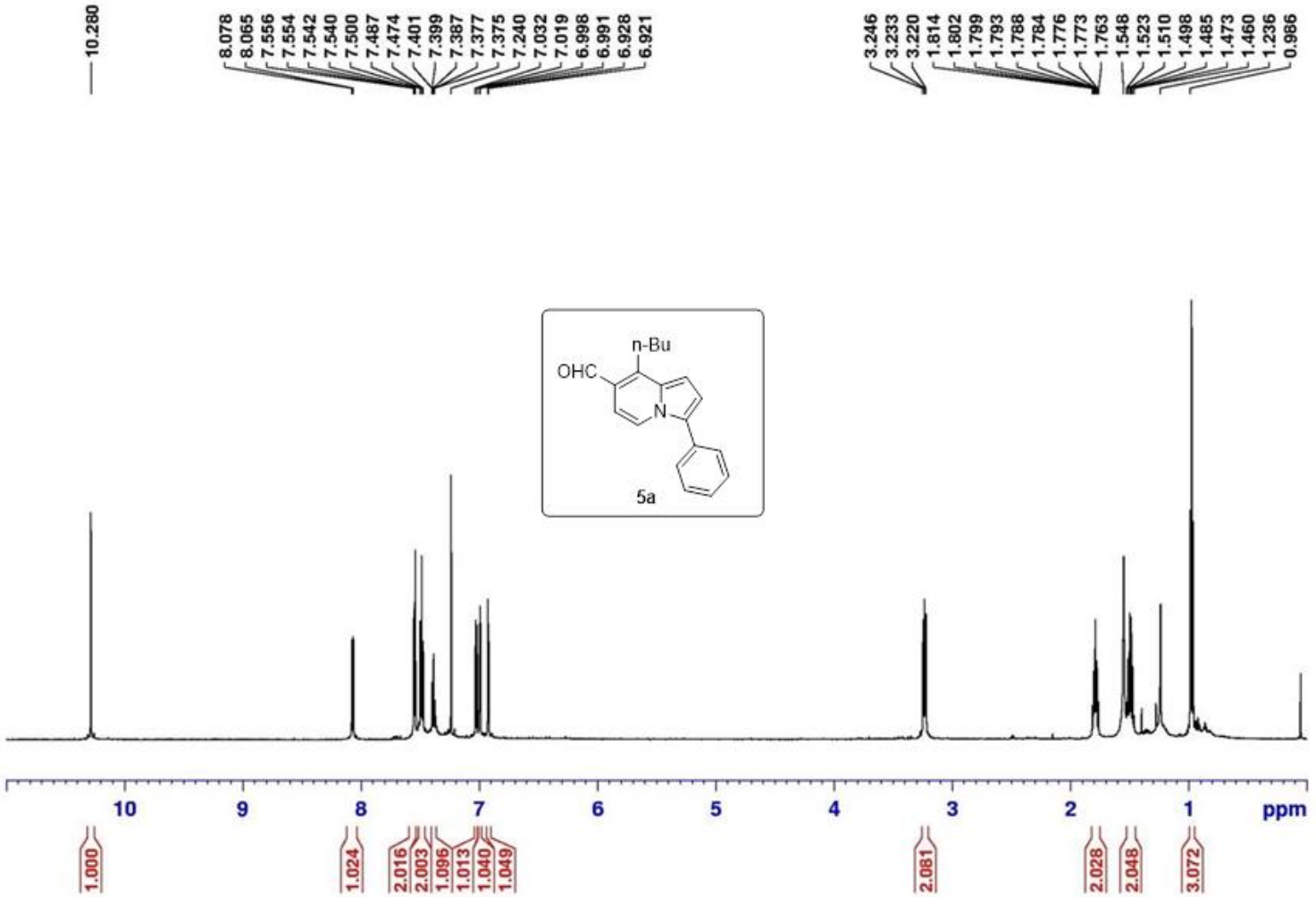


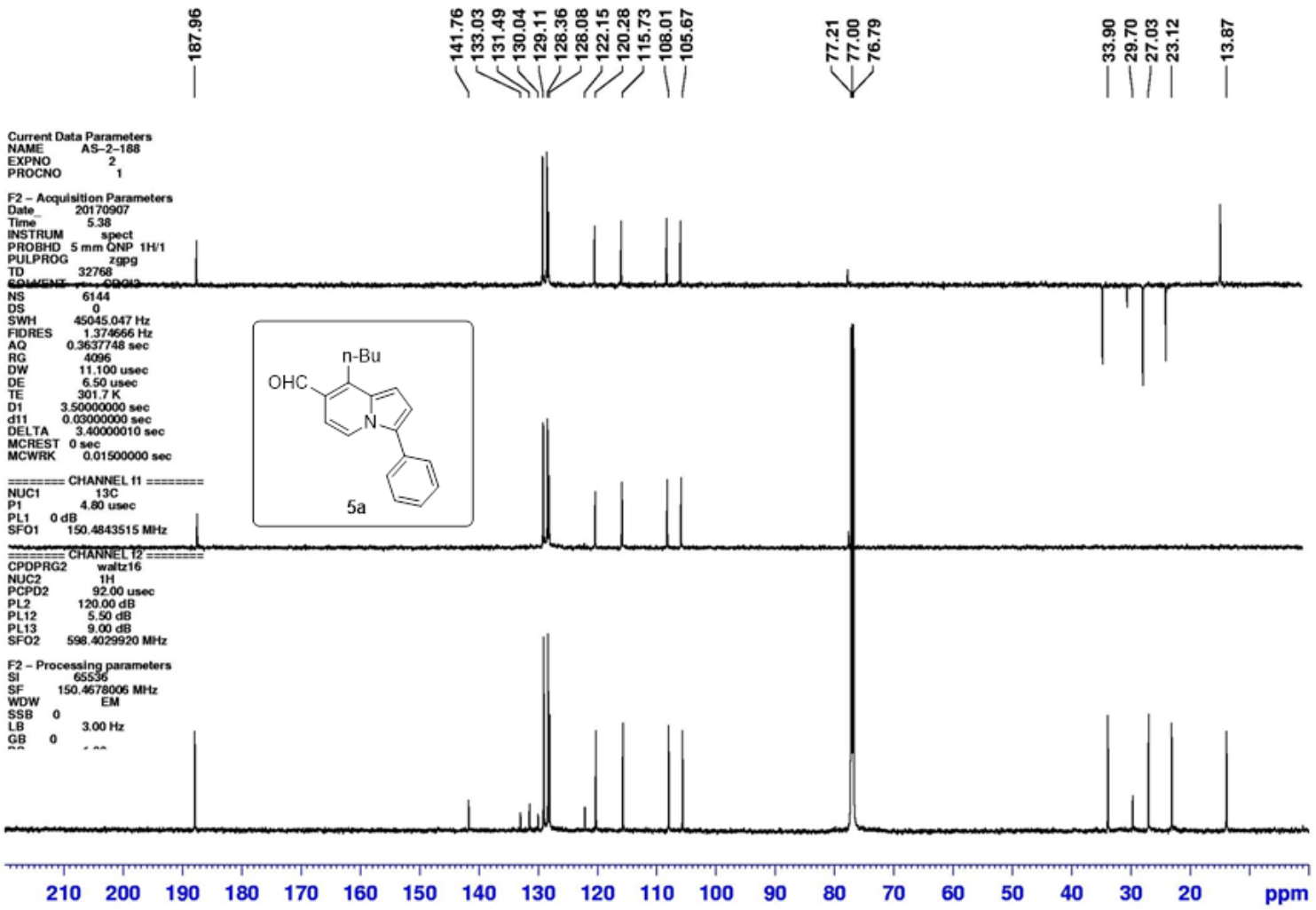

9.991
9.401
9.475
9.352
9.351
9.340
9.342
9.336
9.335
9.329
9.325
9.322
9.315
9.313
9.311
9.260
9.259
9.240
9.650
9.651
9.640
9.645
9.632
9.635
2.105
1.556
Current Data Parameters
NAME GCT-322-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190419
Time 9.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.2032901 MHz
F2 - Processing parameters
SI 32768
SF 598.2000265 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
CHO
N
CH3
Cl
3n
10
9
8
7
6
5
4
3
2
1
ppm
1.07
1.01
4.18
1.10
1.00
1.01
3.04

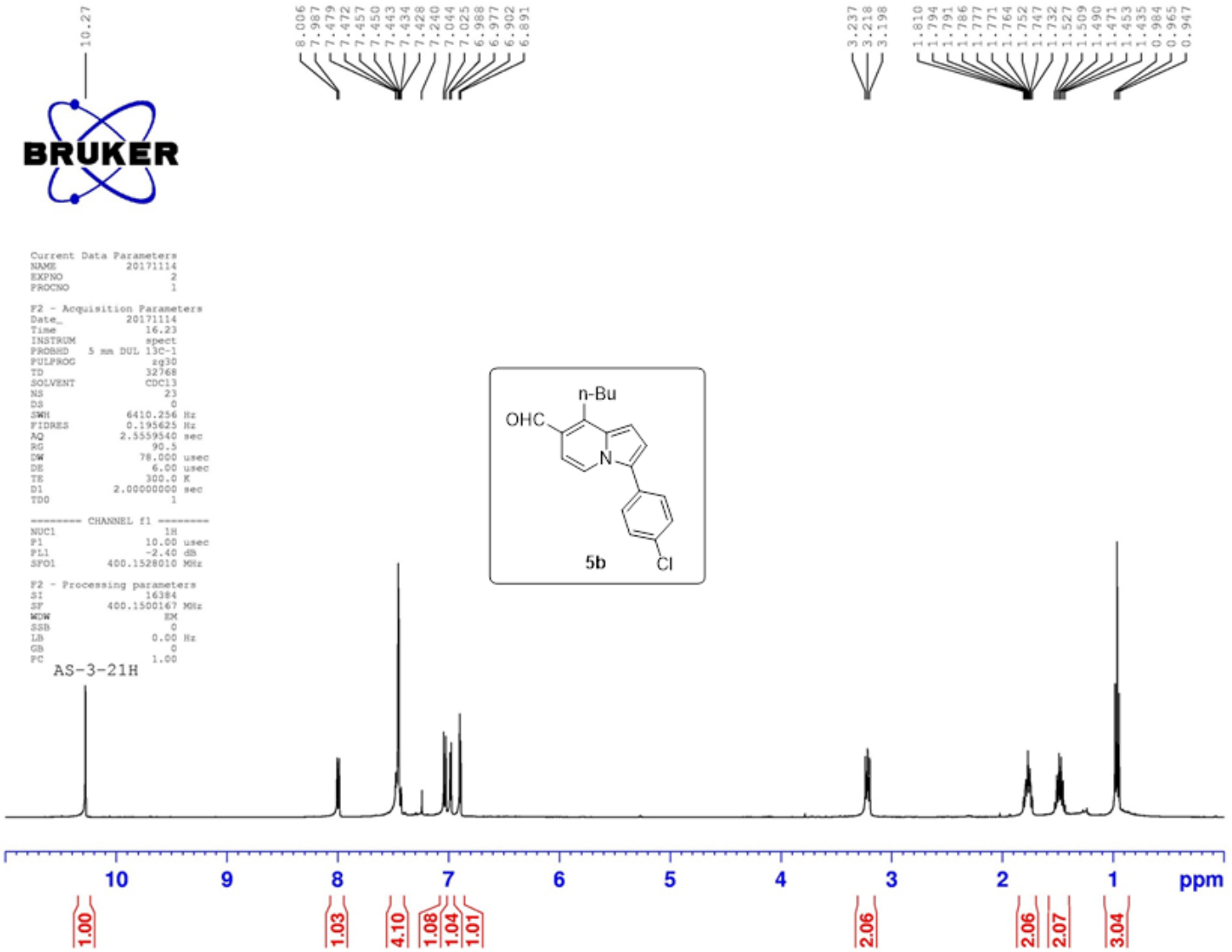

189.903
141.692
134.074
133.777
132.245
130.316
129.724
127.480
126.028
125.898
119.642
111.405
101.948
77.212
77.000
76.788
23.691
CHO
N
CH3
Cl
3n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

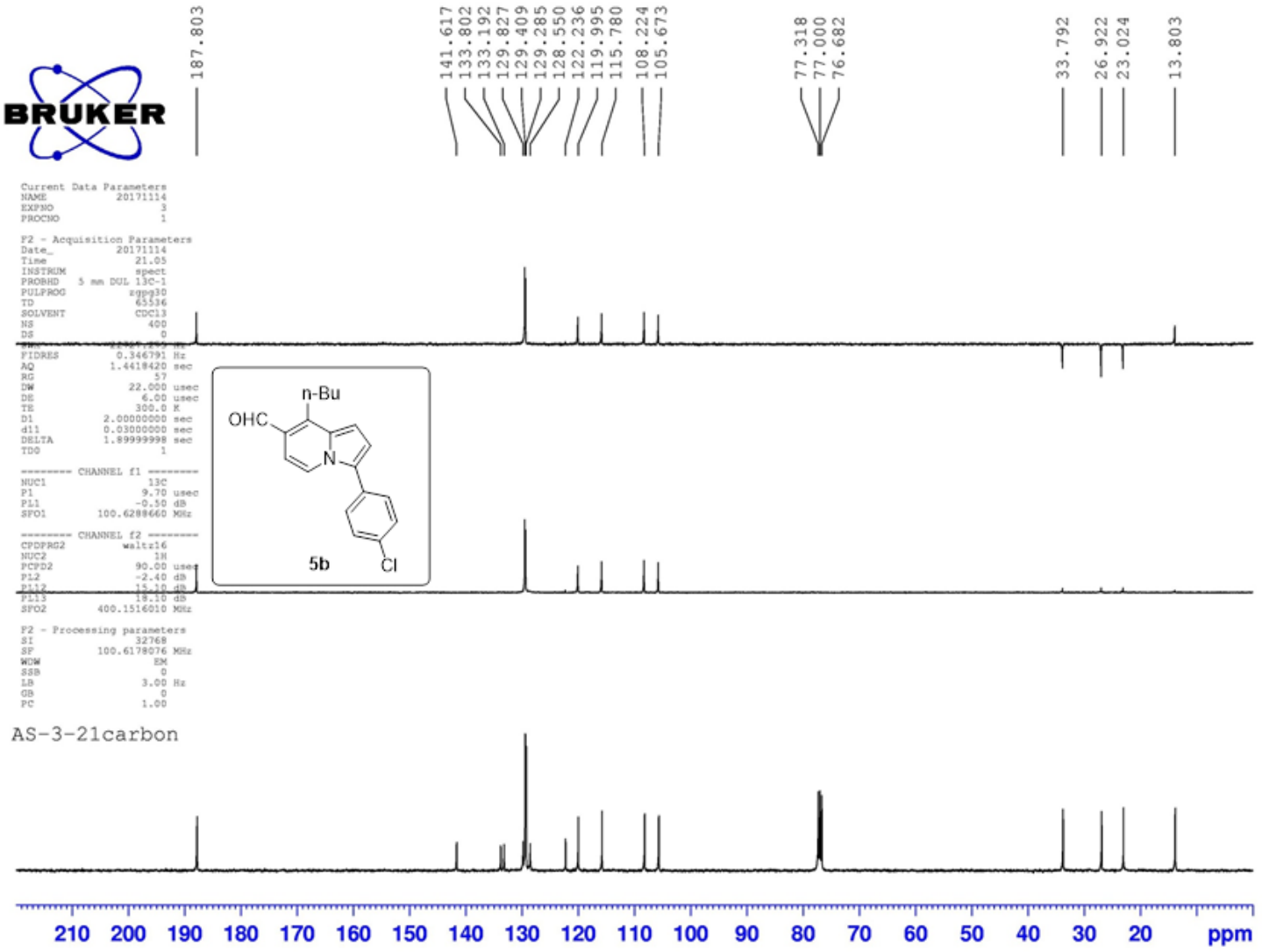

9.696
7.328
7.322
7.243
7.240
7.230
7.113
7.101
6.709
6.702
6.355
6.354
6.344
6.342
3.213
3.201
3.186
2.077
1.710
1.696
1.695
1.685
1.680
1.674
1.672
1.659
1.546
1.447
1.435
1.422
1.410
1.232
0.961
0.952
0.949
0.942
0.940
Current Data Parameters
NAME GCT-326
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20190422
Time 8.18
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 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.2032901 MHz
F2 - Processing parameters
SI 32768
SF 598.2000275 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
CHO
N
CH3
n-Bu
3o
10
9
8
7
6
5
4
3
2
1
ppm
1.05
1.02
1.03
1.00
1.06
2.12
3.16
2.24
2.23
3.30

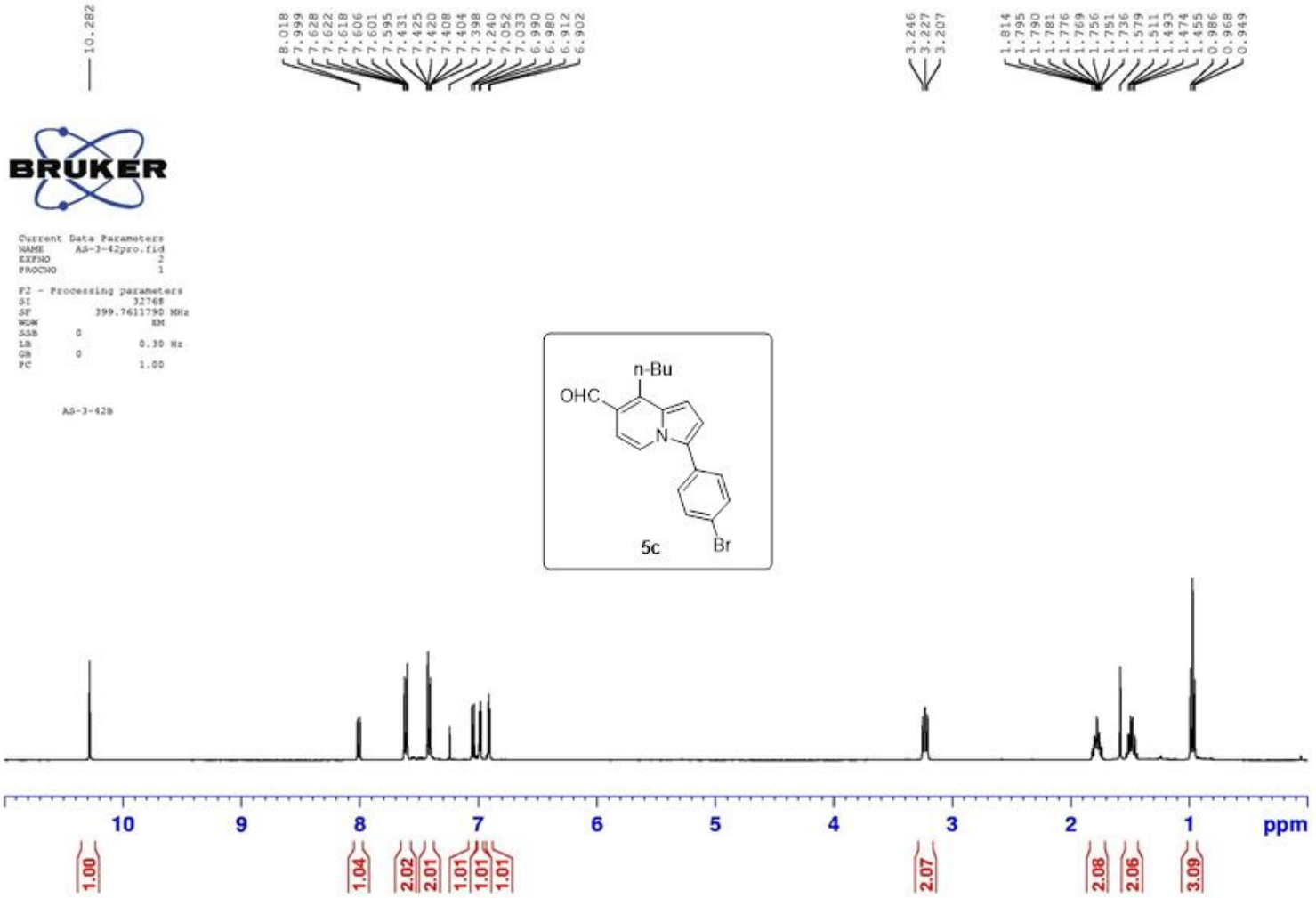

190.039
141.503
129.922
129.084
128.502
125.693
116.649
110.984
101.276
77.212
77.000
76.788
33.249
29.616
22.396
22.346
13.904
CHO
N
CH3
n-Bu
3o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

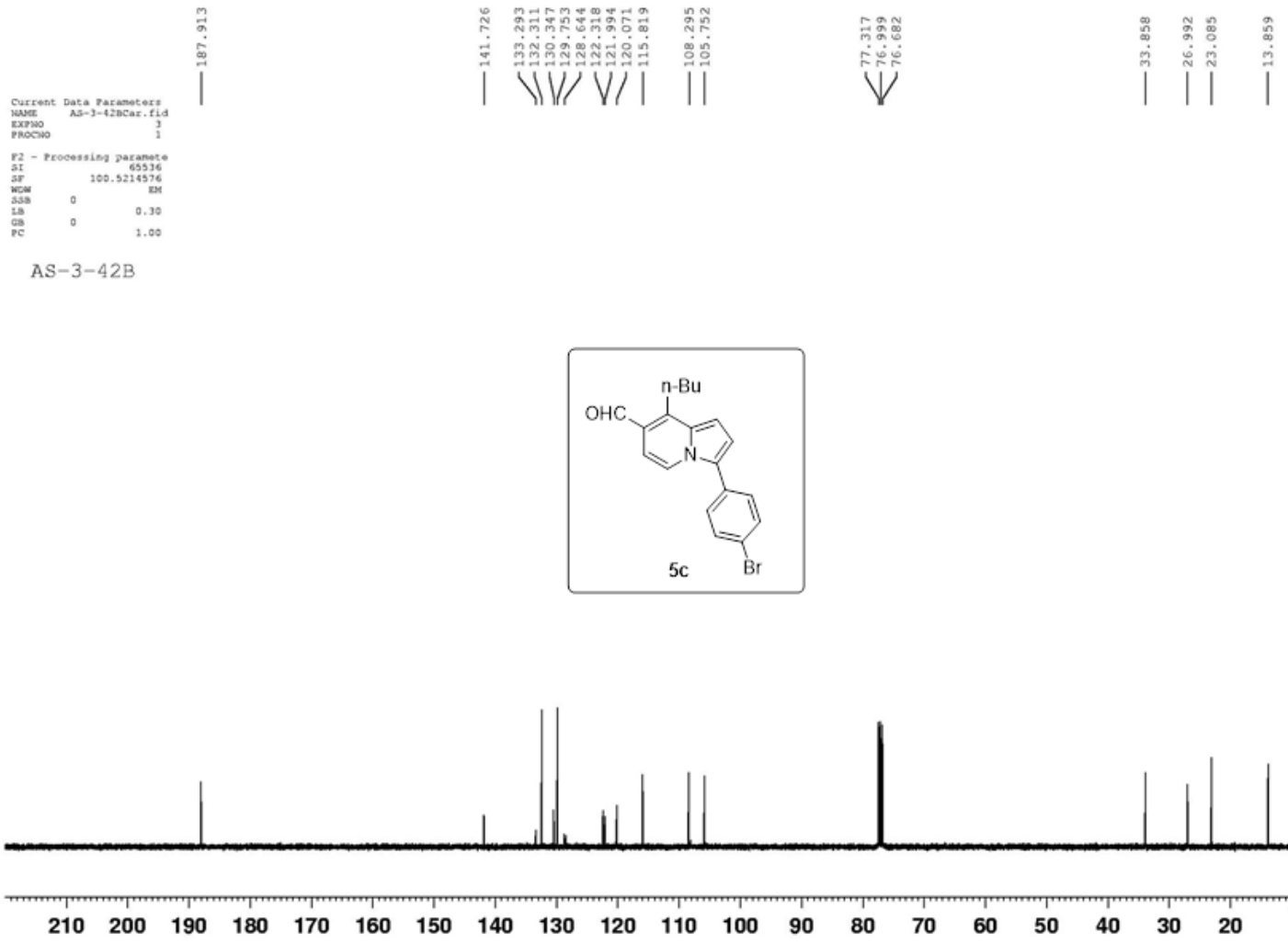

10.280
8.078
8.065
7.556
7.554
7.542
7.540
7.500
7.487
7.474
7.401
7.399
7.387
7.377
7.375
7.240
7.032
7.019
6.998
6.991
6.928
6.921
3.246
3.233
3.220
1.814
1.802
1.799
1.793
1.788
1.784
1.776
1.773
1.763
1.548
1.523
1.510
1.498
1.485
1.473
1.460
1.236
0.986
n-Bu
OHC
N
5a
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.024
2.016
2.003
1.096
1.013
1.040
1.049
2.081
2.028
2.048
3.072

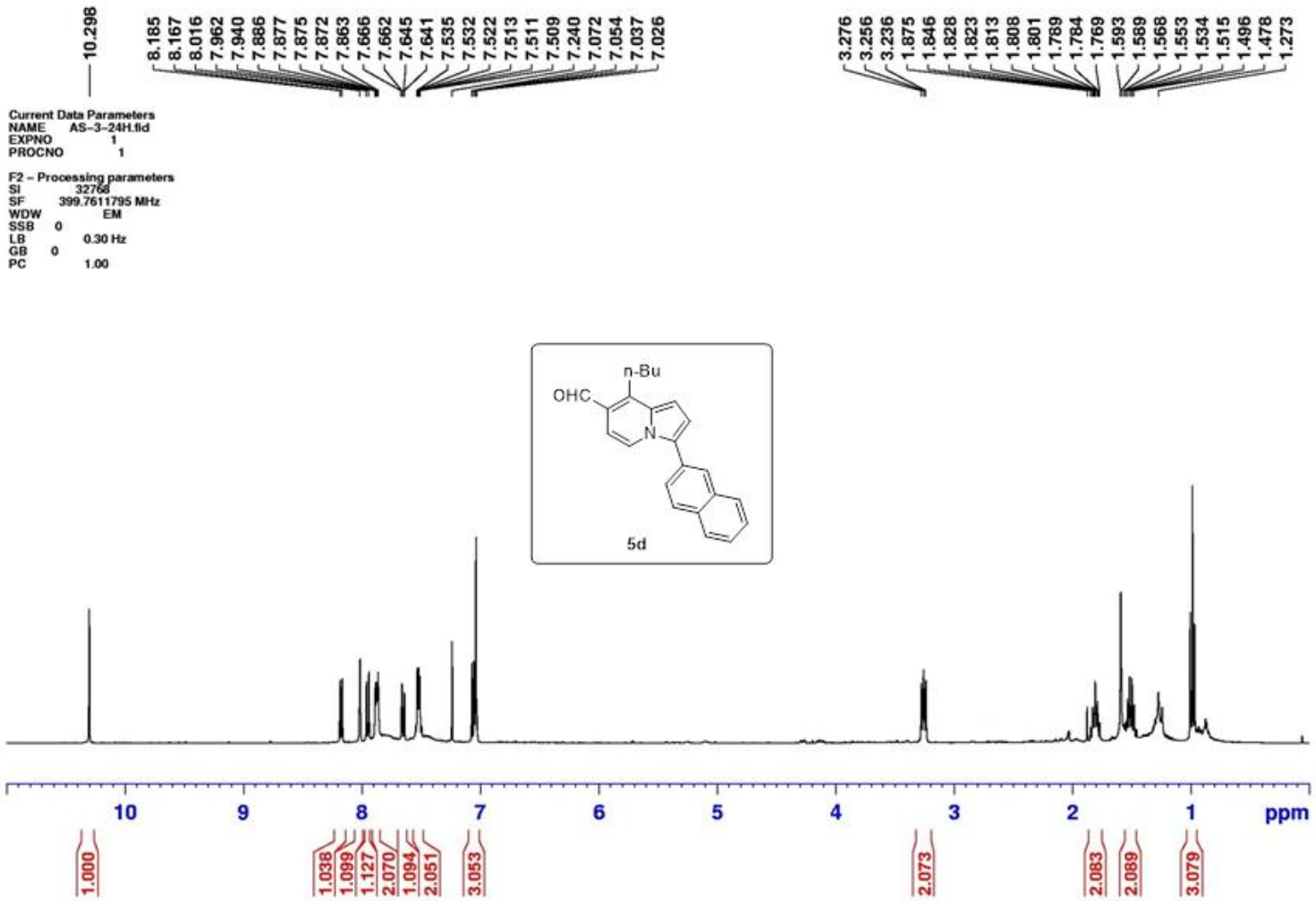

187.96
141.76
133.03
131.49
130.04
129.11
128.36
128.08
122.15
120.28
115.73
108.01
105.67
77.21
77.00
76.79
33.90
29.70
27.03
23.12
13.87
Current Data Parameters
NAME AS–2–188
EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
Date_ 20170907
Time 5.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 – Processing parameters
SI 65536
SF 150.4678006 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
n-Bu
OHC
N
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

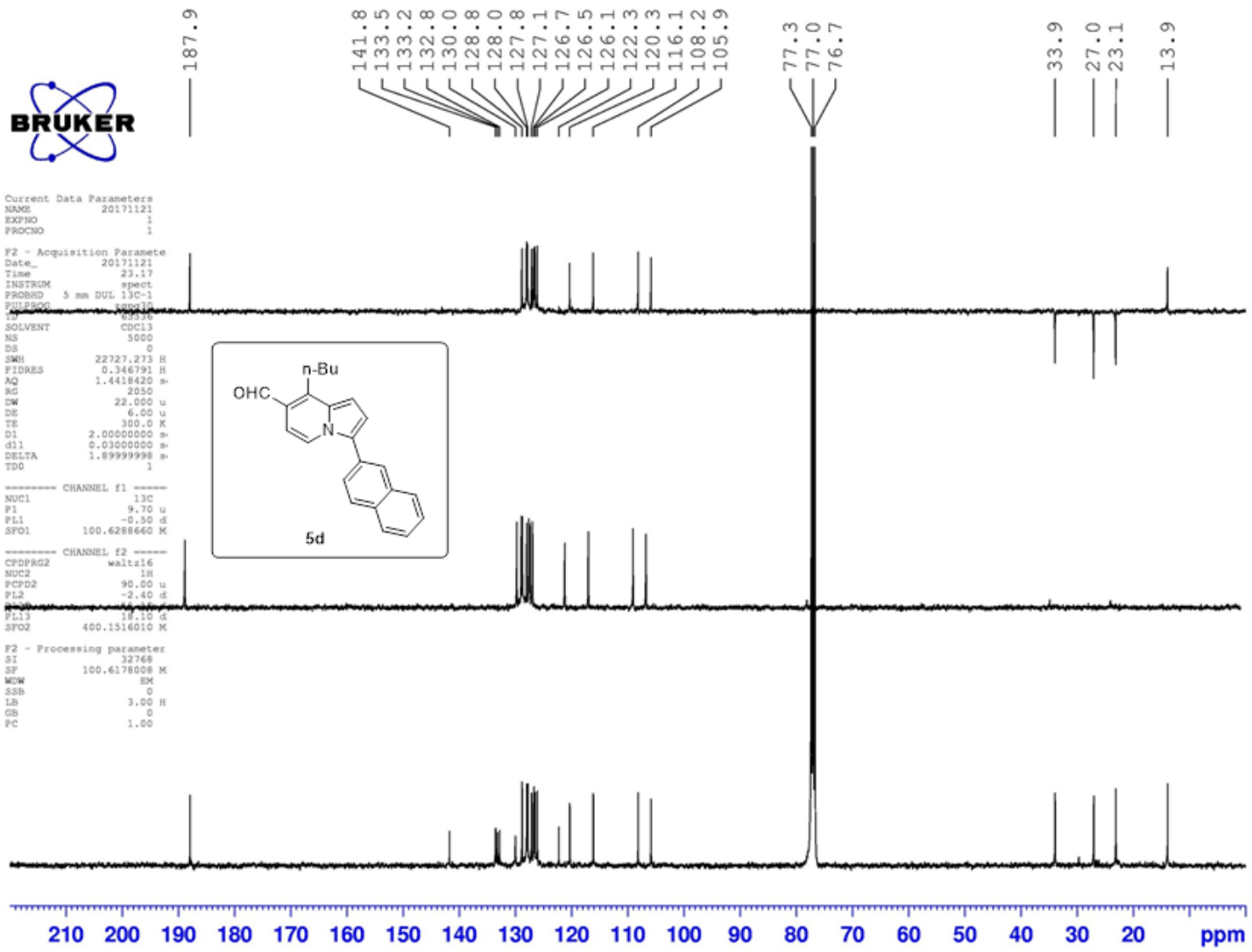

10.27
8.006
7.987
7.479
7.472
7.457
7.450
7.443
7.434
7.428
7.240
7.044
7.025
6.988
6.977
6.902
6.891
3.237
3.218
3.198
1.810
1.794
1.791
1.786
1.777
1.771
1.764
1.752
1.747
1.732
1.527
1.509
1.490
1.471
1.453
1.435
0.984
0.965
0.947
BRUKER
Current Data Parameters
NAME 20171114
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171114
Time 16.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 23
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 90.5
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 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-21H
n-Bu
OHC
N
5b
Cl
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
4.10
1.08
1.04
1.01
2.06
2.06
2.07
3.04

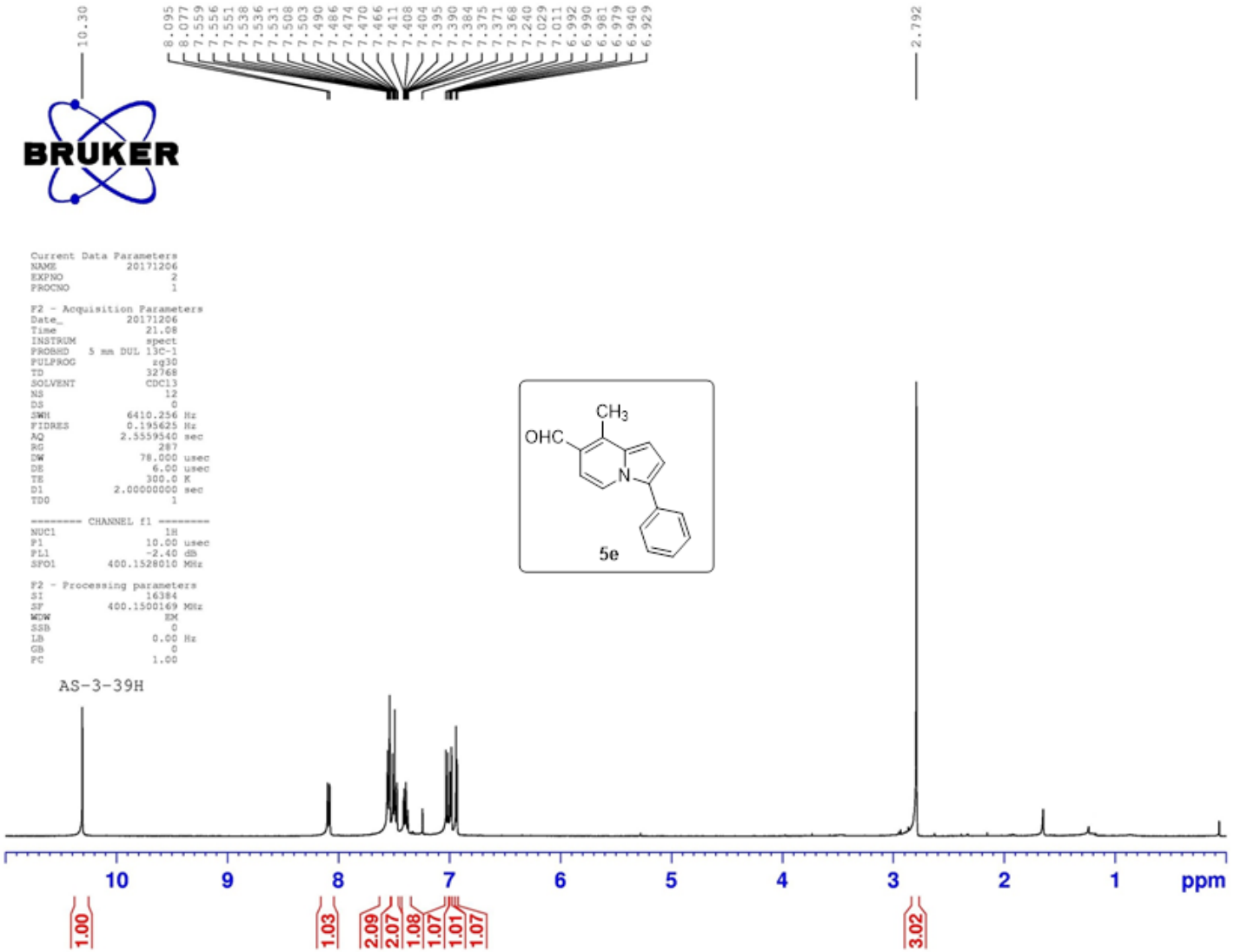

187.803
141.617
133.802
133.192
129.827
129.409
129.285
128.550
122.236
119.995
115.780
108.224
105.673
77.318
77.000
76.682
33.792
26.922
23.024
13.803
n-Bu
OHC
N
Cl
5b
AS-3-21carbon
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

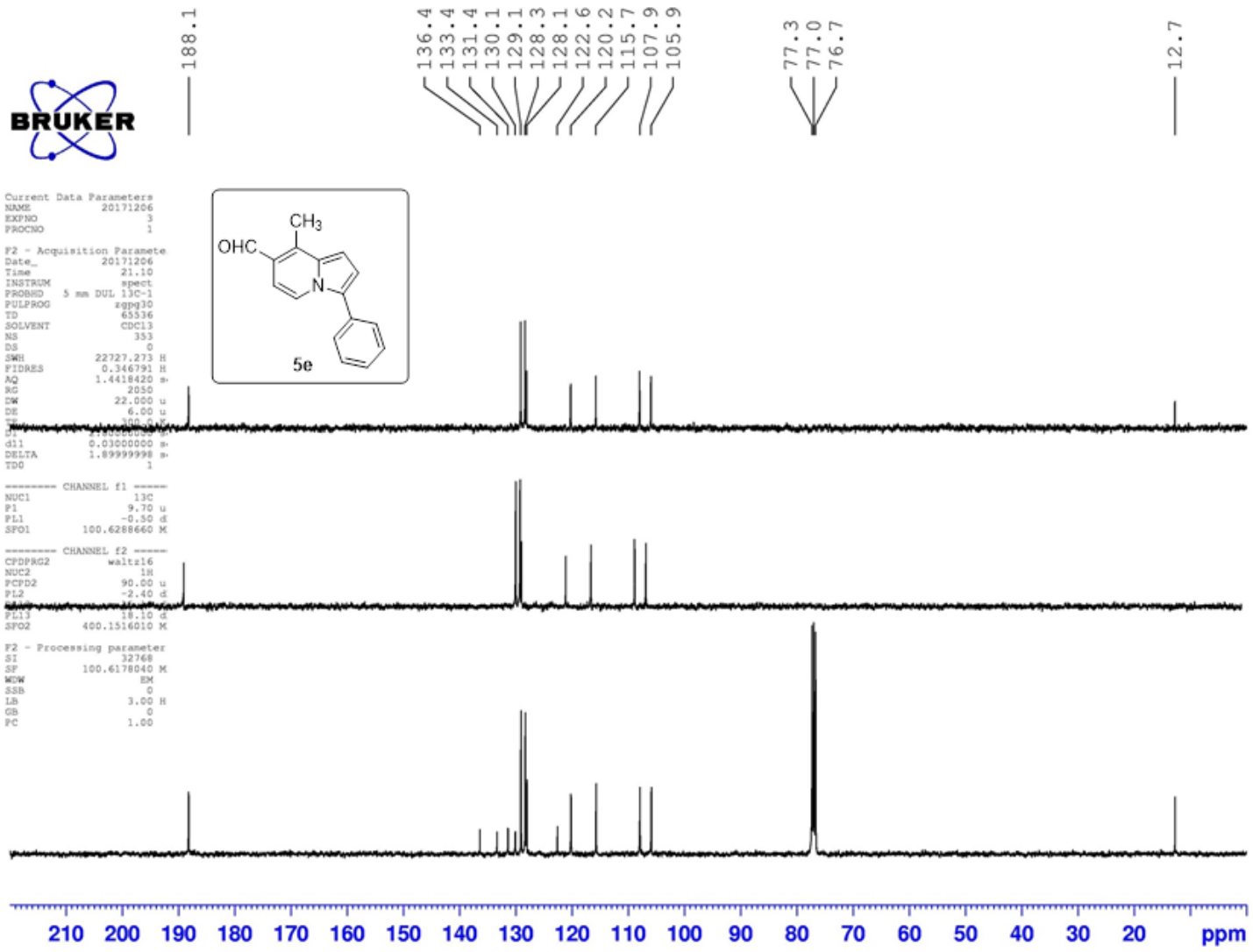

10.282
8.018
7.999
7.628
7.622
7.618
7.606
7.601
7.595
7.431
7.425
7.420
7.408
7.404
7.398
7.240
7.052
7.033
6.990
6.980
6.312
6.902
3.246
3.227
3.207
1.814
1.795
1.790
1.781
1.776
1.769
1.756
1.751
1.736
1.579
1.511
1.493
1.474
1.455
0.986
0.968
0.949
BRUKER
Current Data Parameters
NAME AS-3-42pro.fid
EXPNO 2
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611790 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
AS-3-42b
n-Bu
OHC
N
Br
5c
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
2.02
2.01
1.01
1.01
1.01
2.07
2.08
2.06
3.09

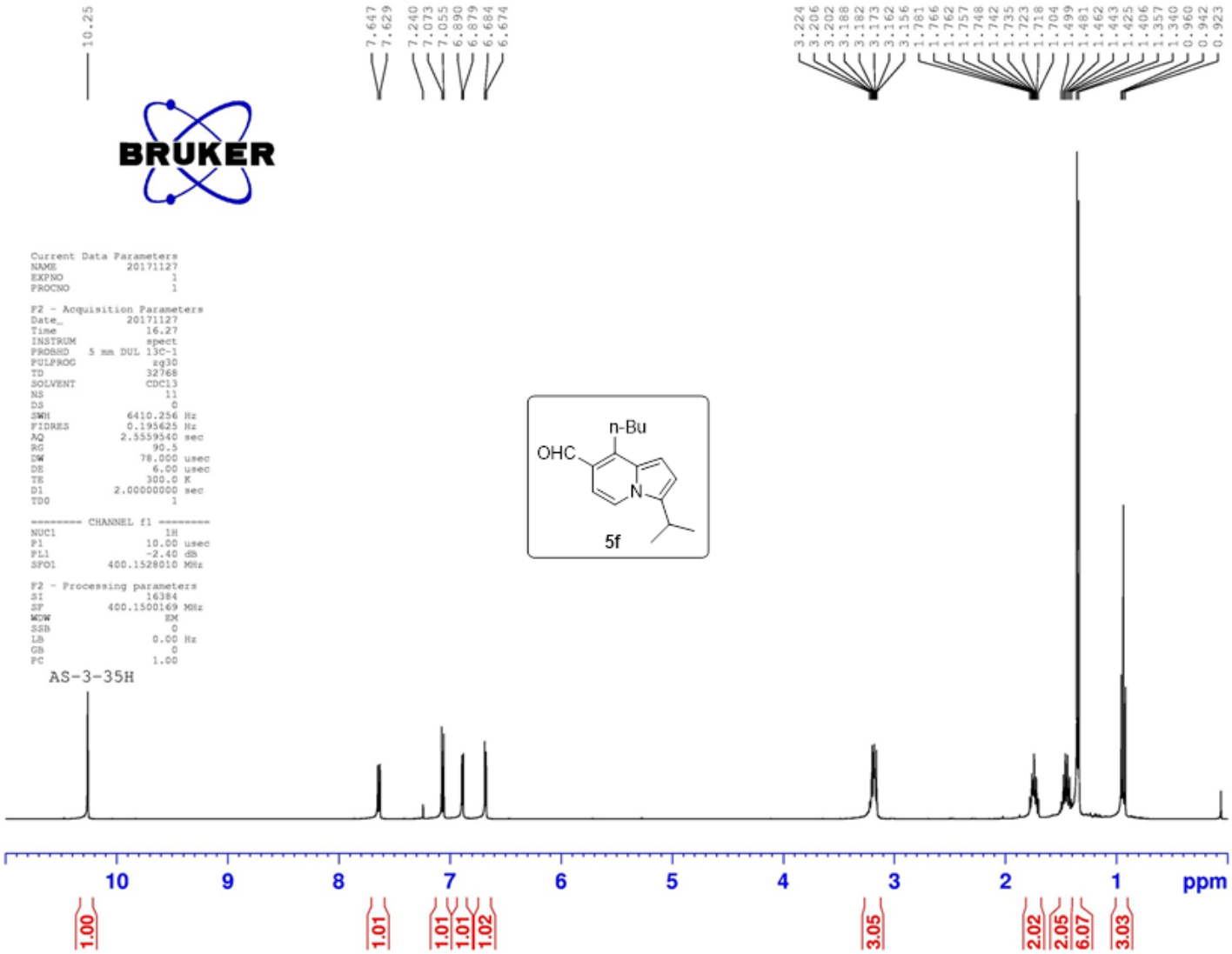

187.913
141.726
133.293
132.311
130.347
129.753
128.644
122.318
121.994
120.071
115.819
108.295
105.752
77.317
76.999
76.682
33.858
26.992
23.085
13.859
Current Data Parameters
NAME AS-3-42BCar.fid
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214576
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
AS-3-42B
n-Bu
OHC
N
Br
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

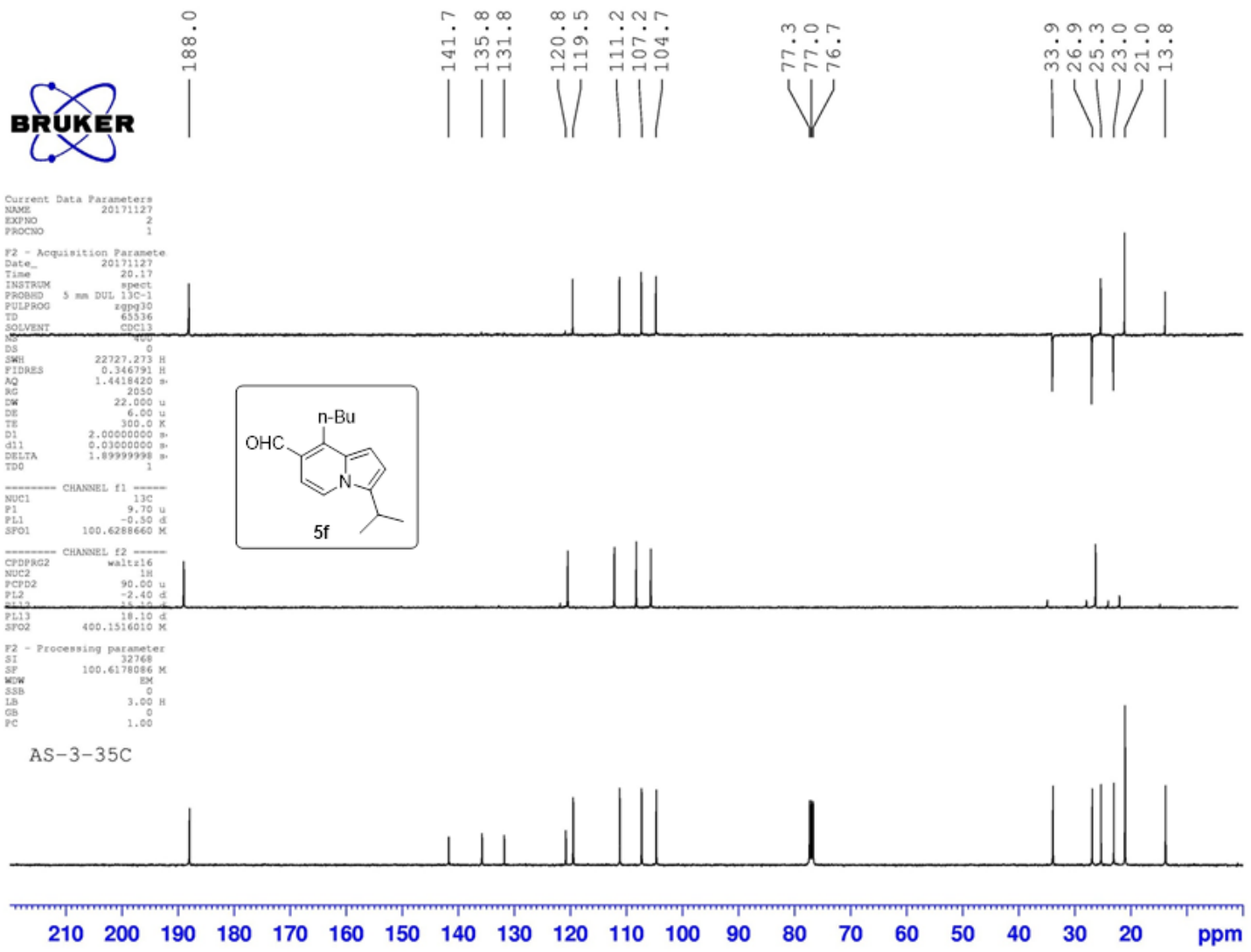

10.298
8.185
8.167
8.016
7.962
7.940
7.886
7.877
7.875
7.872
7.863
7.666
7.662
7.645
7.641
7.535
7.532
7.522
7.513
7.511
7.509
7.240
7.072
7.054
7.037
7.026
3.276
3.256
3.236
1.875
1.846
1.828
1.823
1.813
1.808
1.801
1.789
1.784
1.769
1.593
1.589
1.568
1.553
1.534
1.515
1.496
1.478
1.273
Current Data Parameters
NAME AS-3-24H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611795 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
n-Bu
OHC
N
5d
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.038
1.099
1.127
2.070
1.094
2.051
3.053
2.073
2.083
2.089
3.079

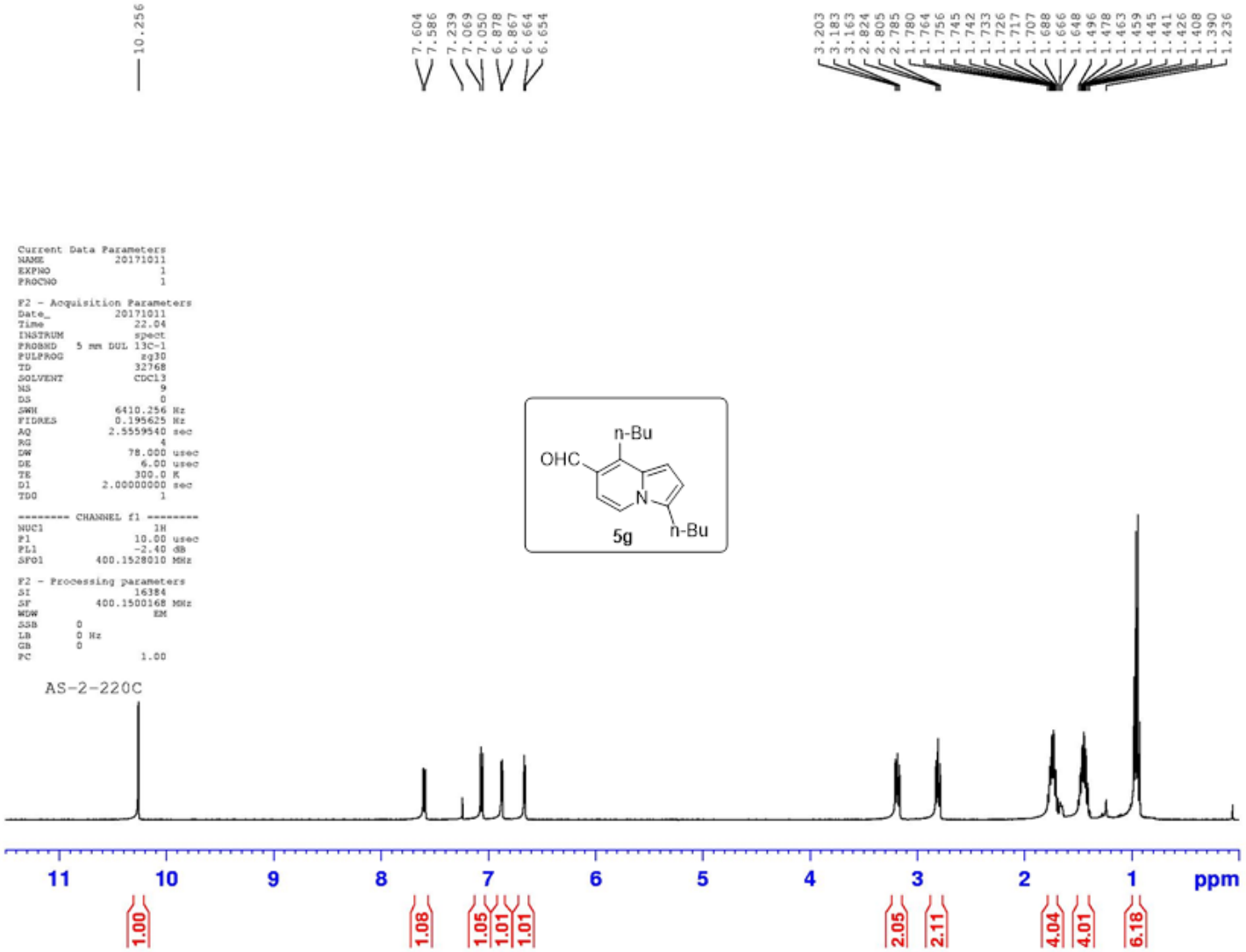

187.9
141.8
133.5
133.2
132.8
130.0
128.8
128.0
127.8
127.1
126.7
126.5
126.1
122.3
120.3
116.1
108.2
105.9
77.3
77.0
76.7
33.9
27.0
23.1
13.9
BRUKER
n-Bu
OHC
N
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

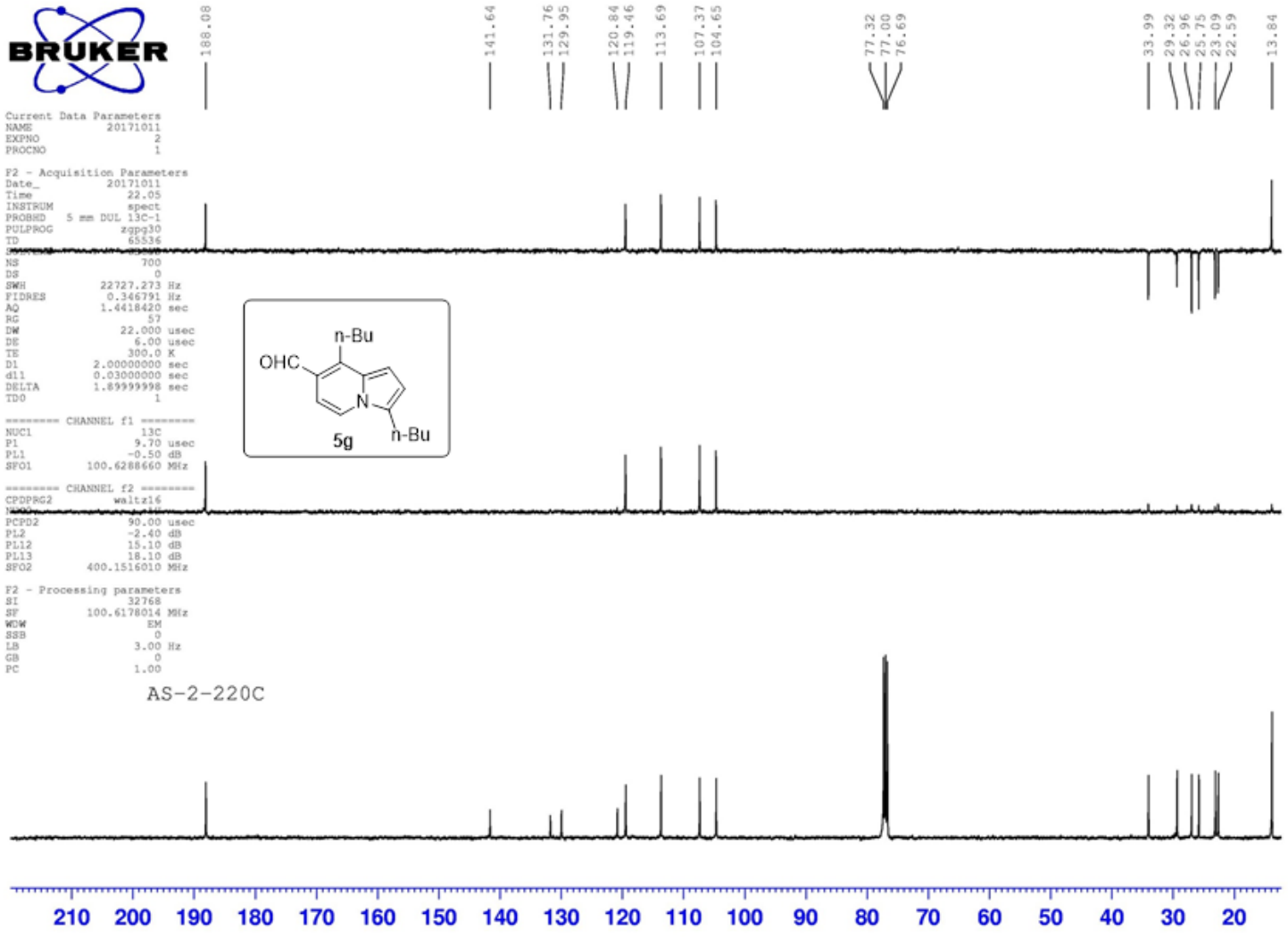

10.30
8.095
8.077
7.559
7.556
7.551
7.538
7.536
7.531
7.508
7.503
7.490
7.486
7.474
7.470
7.466
7.411
7.408
7.404
7.395
7.390
7.384
7.375
7.371
7.368
7.240
7.029
7.011
6.992
6.990
6.981
6.979
6.940
6.929
2.792
BRUKER
Current Data Parameters
NAME 20171206
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171206
Time 21.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
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 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-39H
CH3
OHC
N
5e
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
2.09
2.07
1.08
1.07
1.01
1.07
3.02

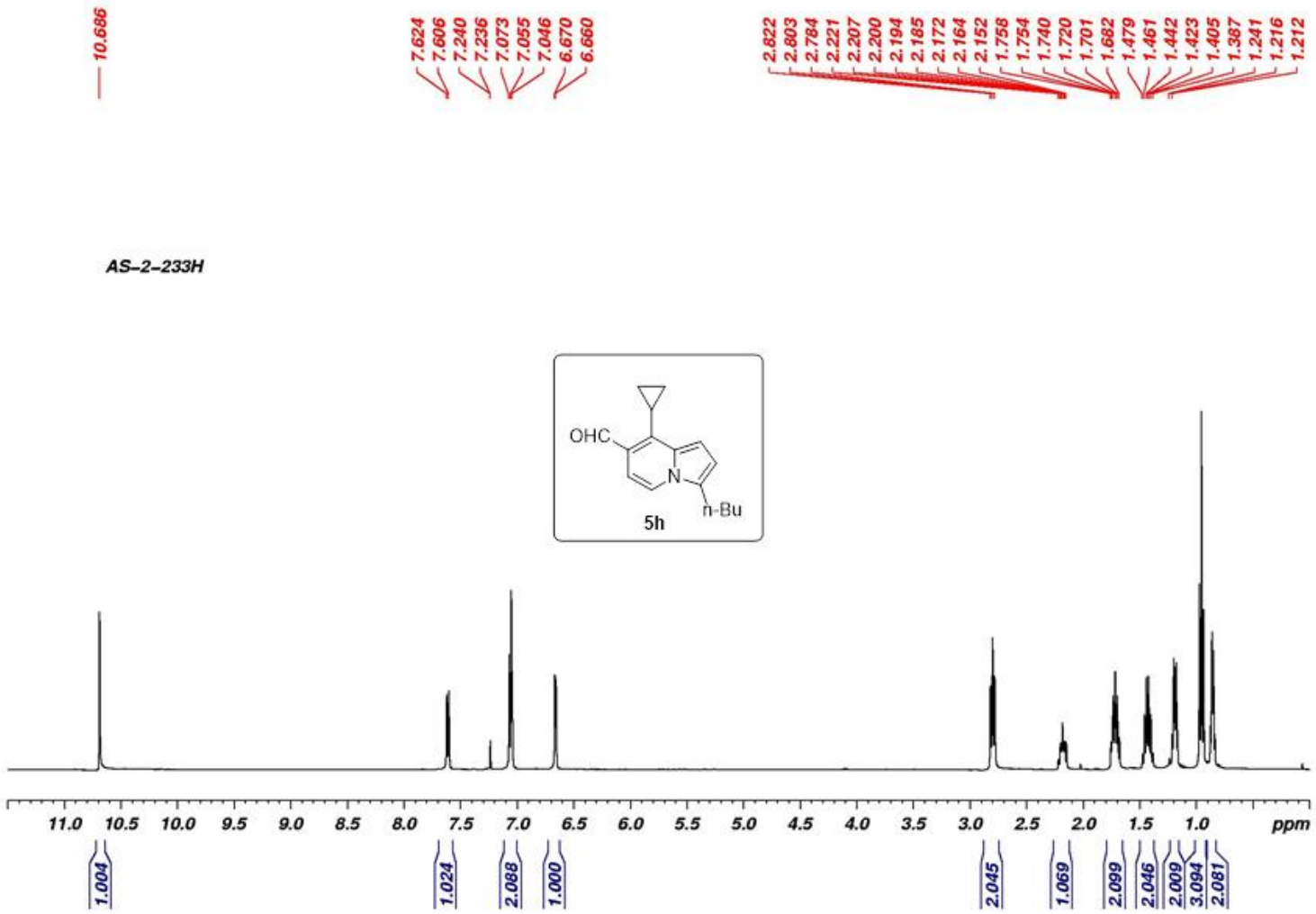

188.1
136.4
133.4
131.4
130.1
129.1
128.3
128.1
122.6
120.2
115.7
107.9
105.9
77.3
77.0
76.7
12.7
CH3
OHC
N
5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

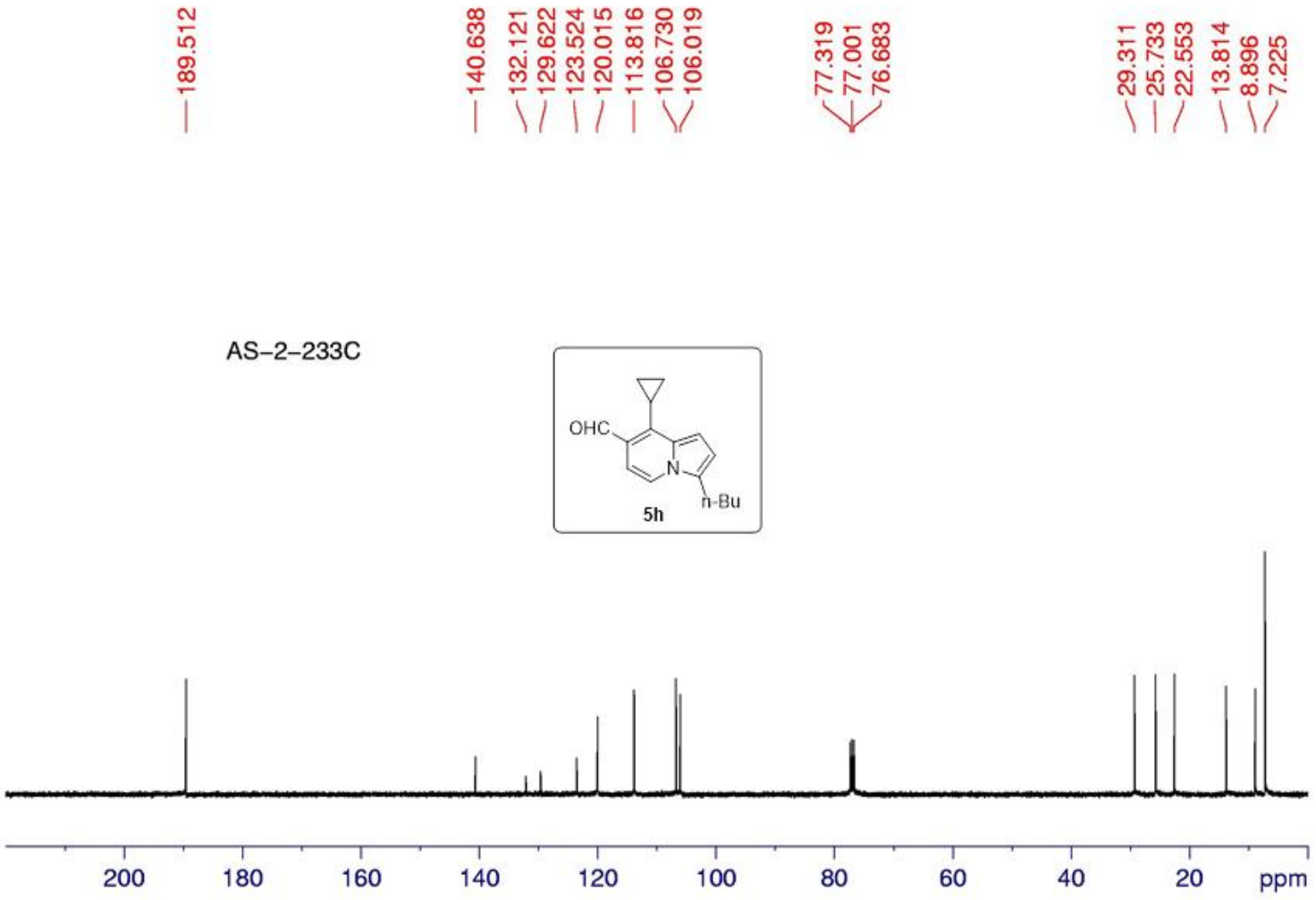

10.25
7.647
7.629
7.240
7.073
7.055
6.890
6.879
6.684
6.674
3.224
3.206
3.202
3.188
3.182
3.173
3.162
3.156
1.781
1.766
1.762
1.757
1.748
1.742
1.735
1.723
1.718
1.704
1.499
1.481
1.462
1.443
1.425
1.406
1.357
1.340
0.960
0.942
0.923
BRUKER
Current Data Parameters
NAME 20171127
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171127
Time 16.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 90.5
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 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-35H
n-Bu
OHC
N
5f
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.01
1.01
1.02
3.05
2.02
2.05
6.07
3.03

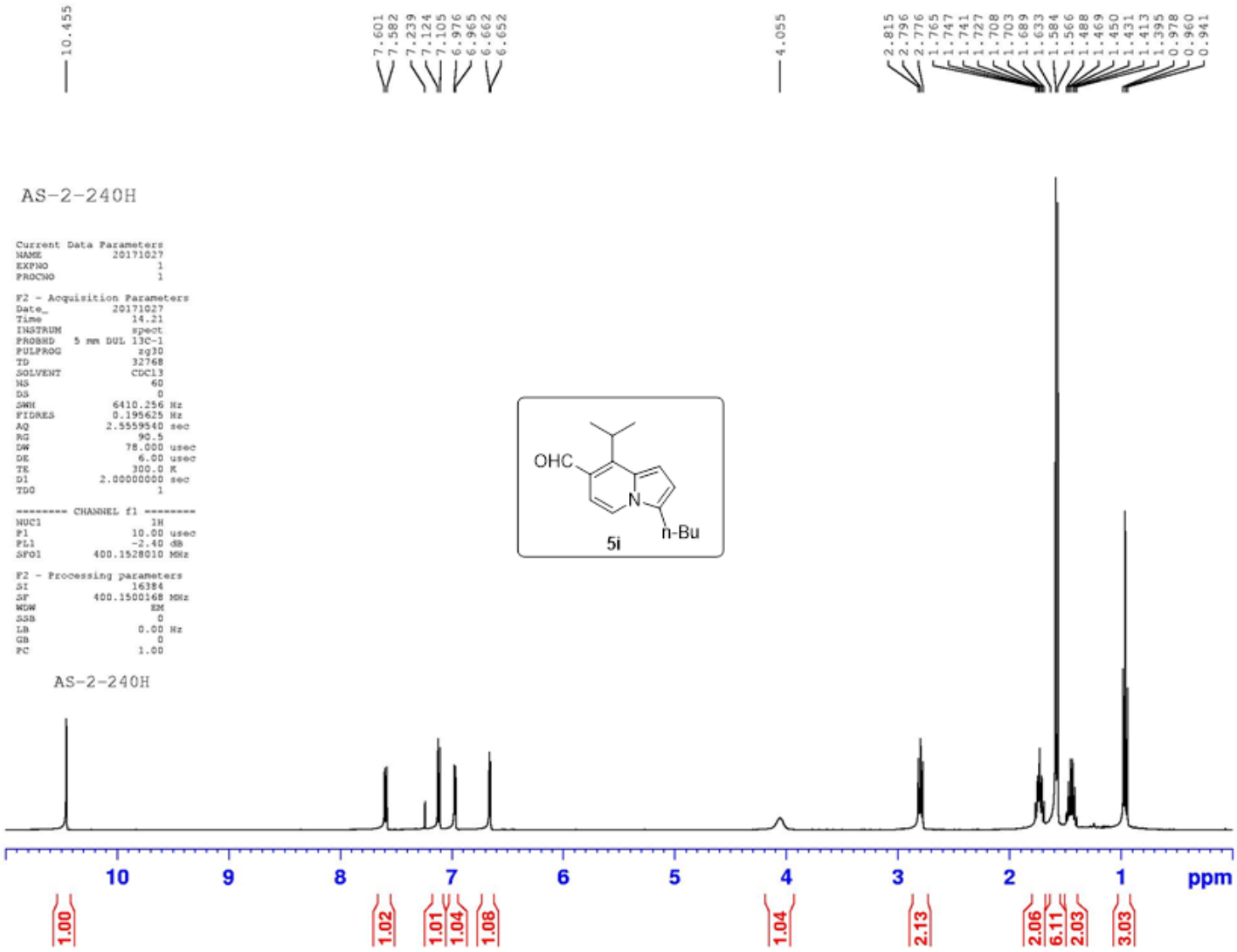

188.0
141.7
135.8
131.8
120.8
119.5
111.2
107.2
104.7
77.3
77.0
76.7
33.9
26.9
25.3
23.0
21.0
13.8
BRUKER
Current Data Parameters
NAME 20171127
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171127
Time 20.17
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 22727.273 H
FIDRES 0.346791 H
AQ 1.4418420 s
RG 2050
DW 22.000 u
DE 6.00 u
TE 300.0 K
D1 2.00000000 s
d11 0.03000000 s
DELTA 1.89999998 s
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.70 u
PL1 -0.50 d
SFO1 100.6288660 M
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 -2.40 d
PL13 18.10 d
SFO2 400.1516010 M
F2 - Processing parameter
SI 32768
SF 100.6178086 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.00
n-Bu
OHC
N
5f
AS-3-35C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

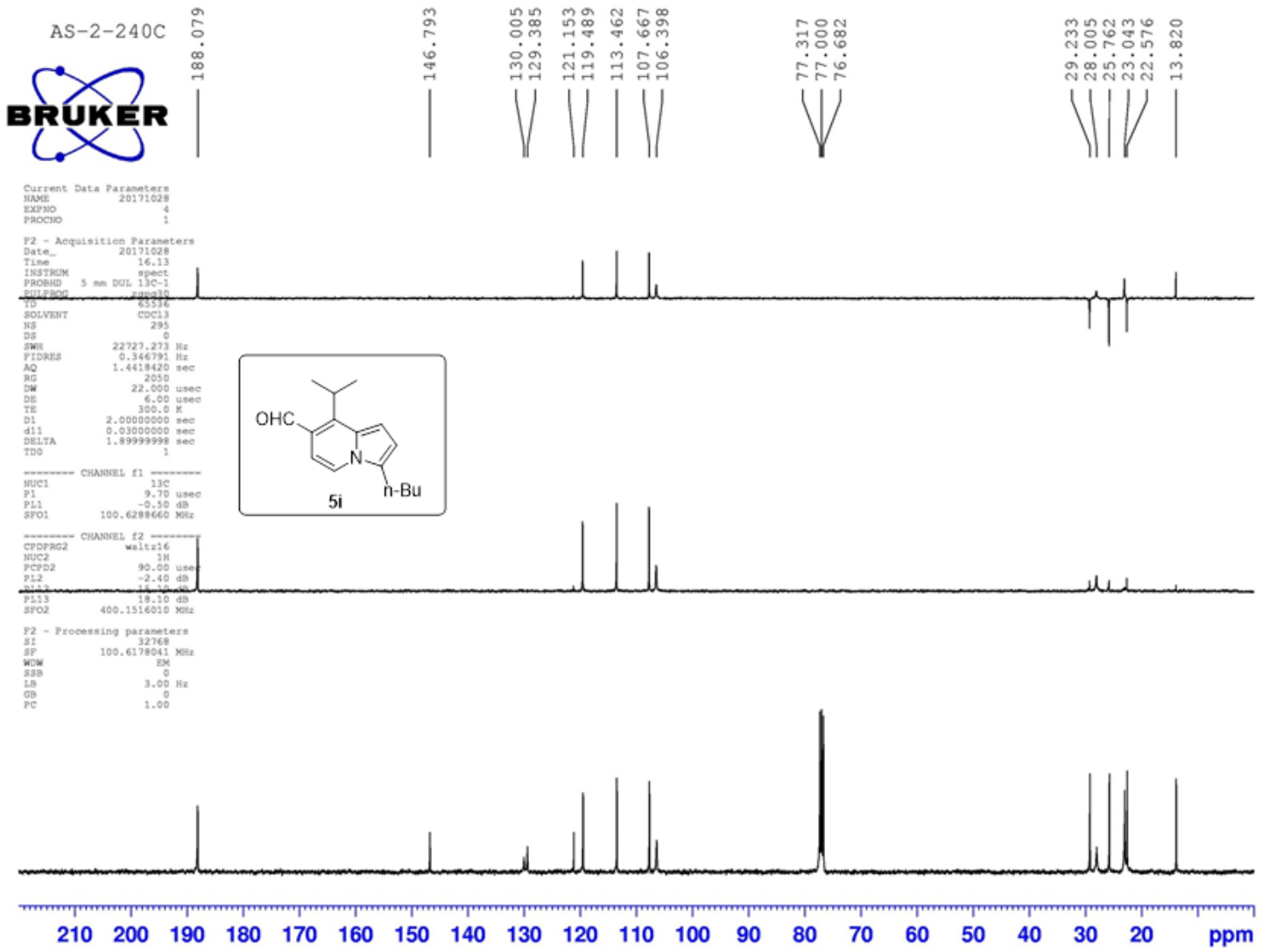

10.256
7.604
7.586
7.239
7.069
7.050
6.878
6.867
6.664
6.654
3.203
3.183
3.163
2.824
2.805
2.785
1.780
1.764
1.756
1.745
1.742
1.733
1.726
1.717
1.707
1.688
1.666
1.648
1.496
1.478
1.463
1.459
1.445
1.441
1.426
1.408
1.390
1.236
Current Data Parameters
NAME 20171011
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171011
Time 22.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 9
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
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 Hz
GB 0
PC 1.00
AS-2-220C
n-Bu
OHC
N
n-Bu
5g
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.08
1.05
1.01
1.01
2.05
2.11
4.04
4.01
6.18

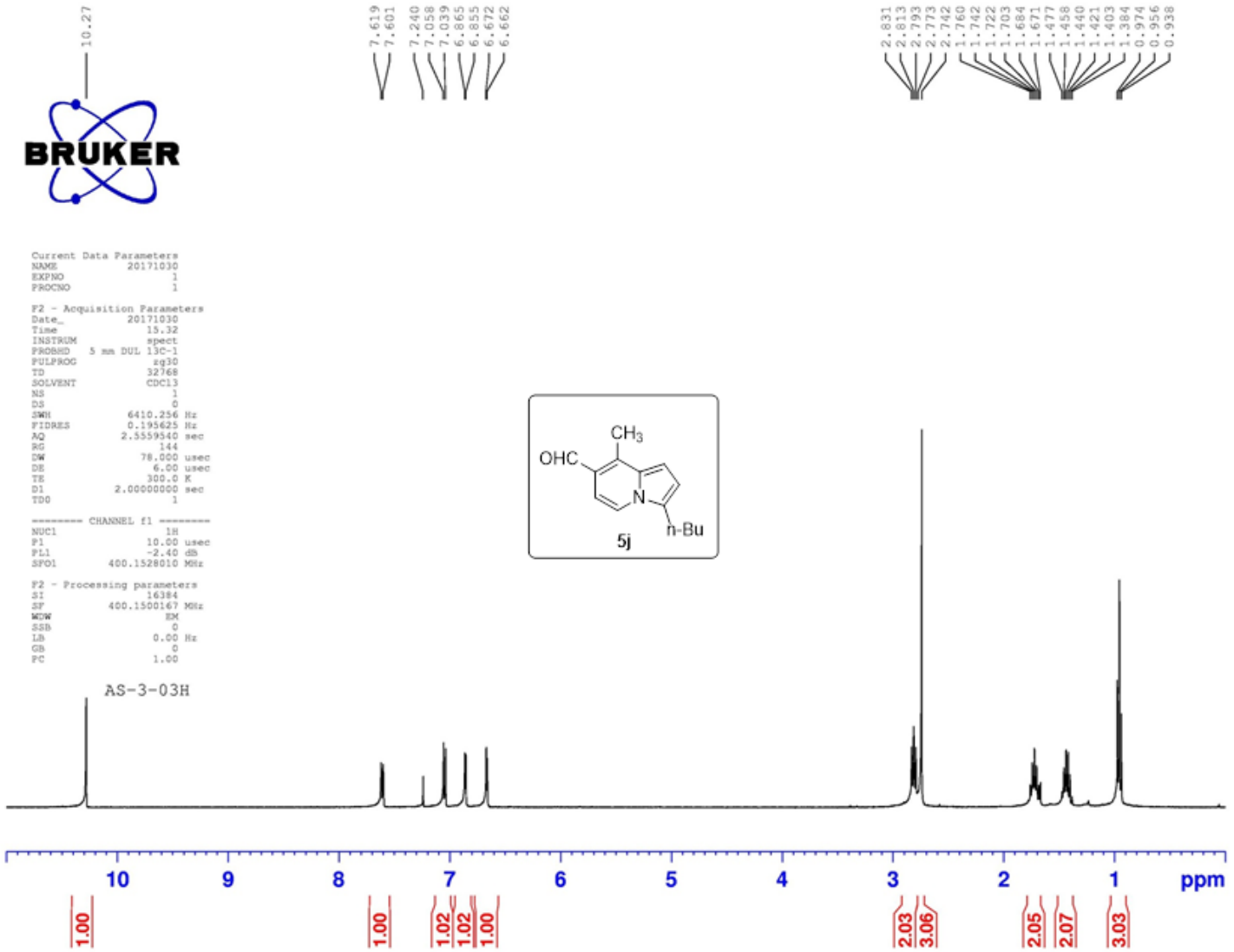

188.08
141.64
131.76
129.95
120.84
119.46
113.69
107.37
104.65
77.32
77.00
76.69
33.99
29.32
26.96
25.75
23.09
22.59
13.84
Current Data Parameters
NAME 20171011
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171011
Time 22.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 700
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 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
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 100.6178014 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
n-Bu
OHC
N
n-Bu
5g
AS-2-220C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20

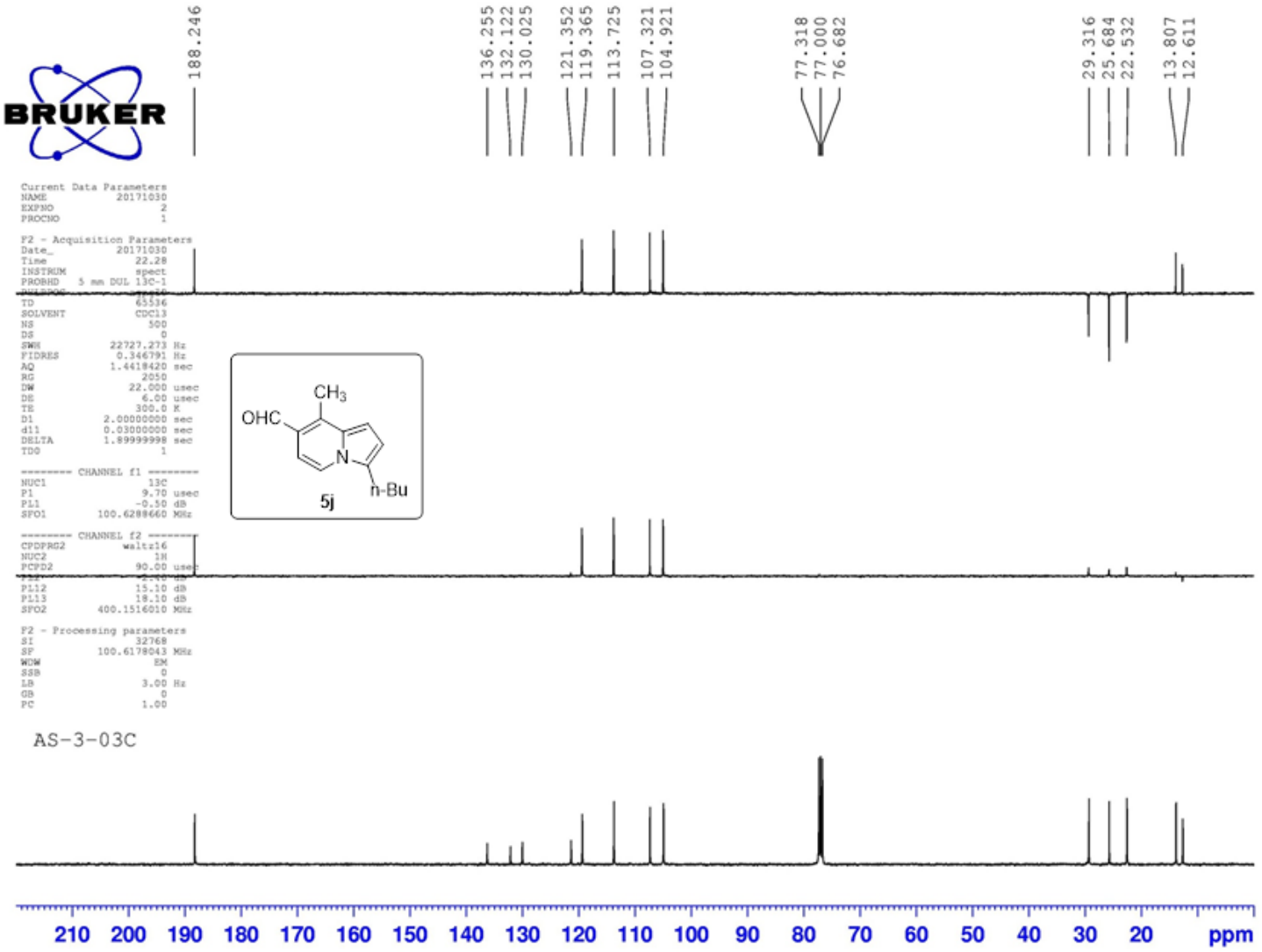

10.686
7.624
7.606
7.240
7.236
7.073
7.055
7.046
6.670
6.660
2.822
2.803
2.784
2.221
2.207
2.200
2.194
2.185
2.172
2.164
2.152
1.758
1.754
1.740
1.720
1.701
1.682
1.479
1.461
1.442
1.423
1.405
1.387
1.241
1.216
1.212
AS-2-233H
OHC
N
n-Bu
5h
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.004
1.024
2.088
1.000
2.045
1.069
2.099
2.046
2.009
3.094
2.081

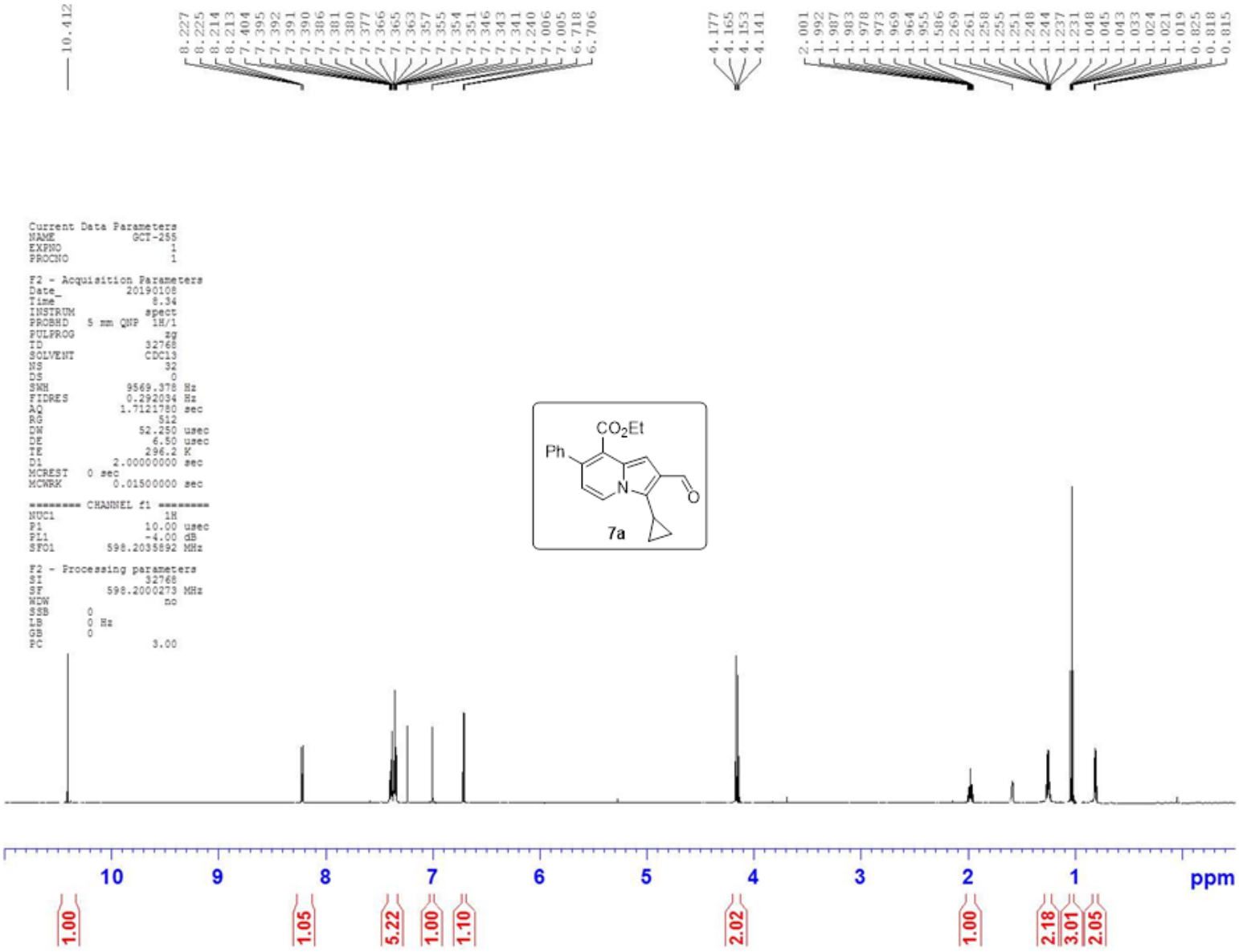

189.512
140.638
132.121
129.622
123.524
120.015
113.816
106.730
106.019
77.319
77.001
76.683
29.311
25.733
22.553
13.814
8.896
7.225
AS–2–233C
OHC
N
n-Bu
5h
200
180
160
140
120
100
80
60
40
20
ppm

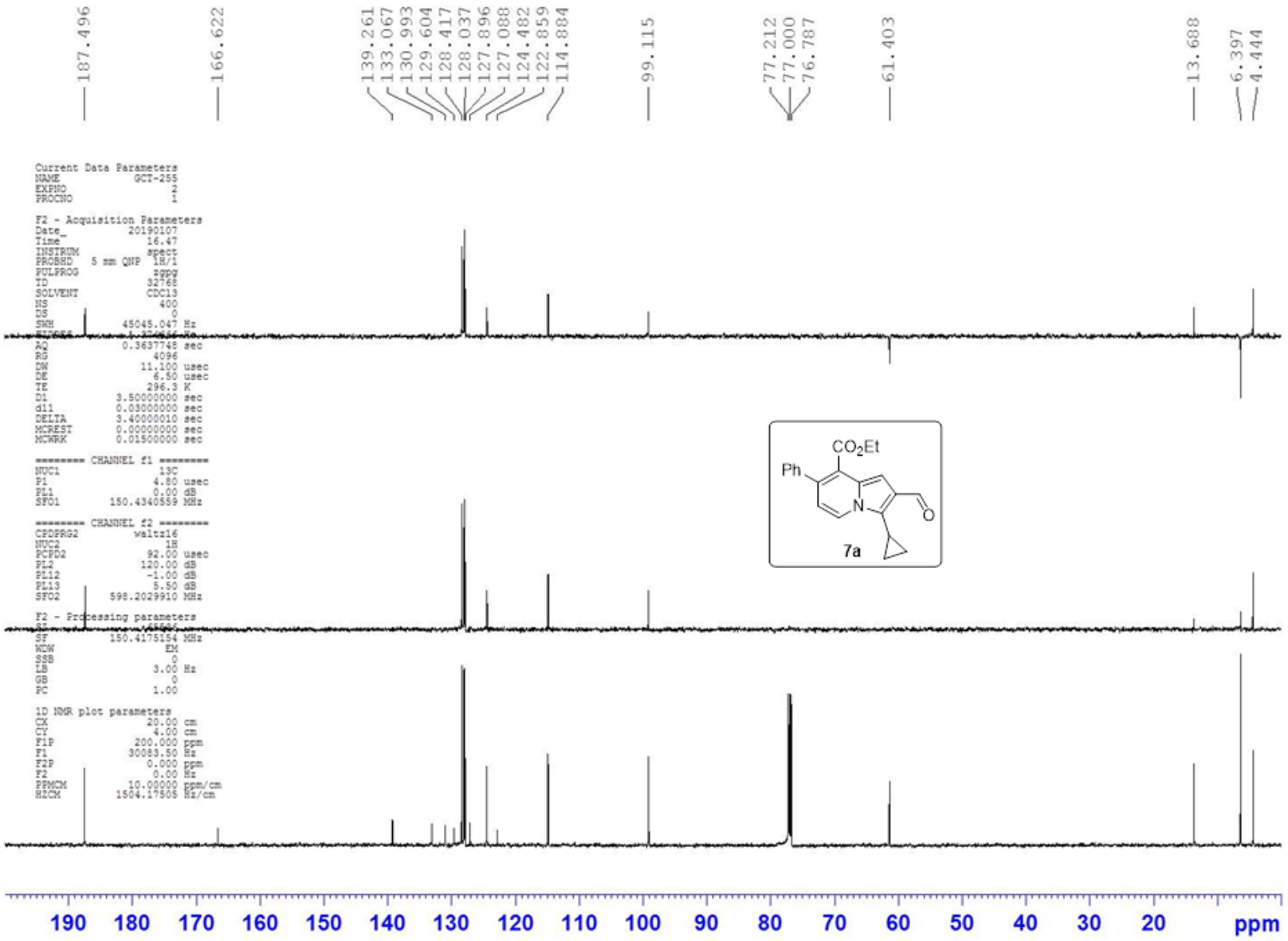

10.455
7.601
7.582
7.239
7.124
7.105
6.976
6.965
6.662
6.652
4.055
2.815
2.796
2.776
1.765
1.747
1.741
1.727
1.708
1.703
1.689
1.633
1.584
1.566
1.488
1.469
1.450
1.431
1.413
1.395
0.978
0.960
0.941
AS-2-240H
Current Data Parameters
NAME 20171027
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171027
Time 14.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 60
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 90.5
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
OHC
N
n-Bu
5i
AS-2-240H
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
1.01
1.04
1.08
1.04
2.13
2.06
6.11
2.03
3.03

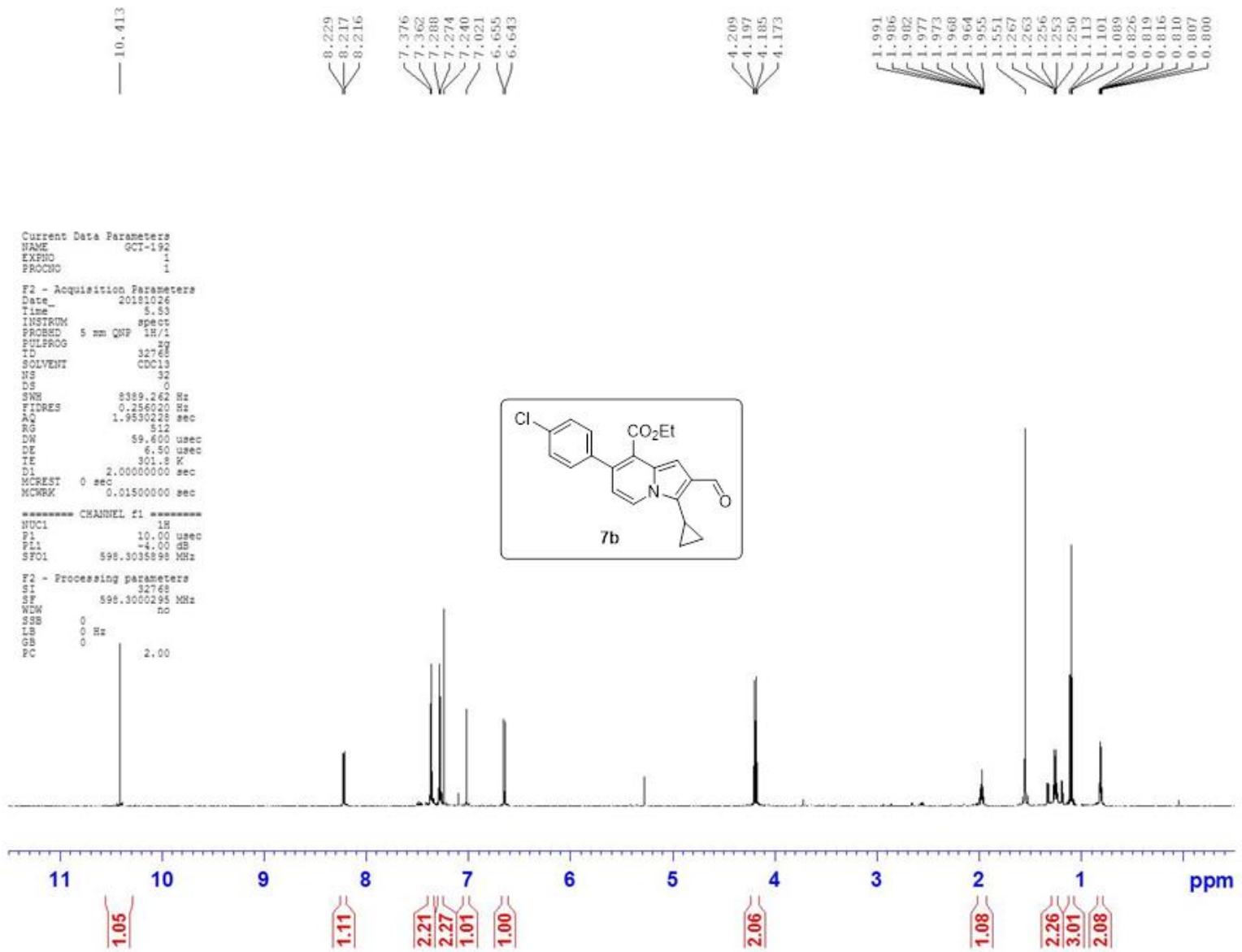

AS-2-240C
188.079
146.793
130.005
129.385
121.153
119.489
113.462
107.667
106.398
77.317
77.000
76.682
29.233
28.005
25.762
23.043
22.576
13.820
OHC
N
n-Bu
5i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

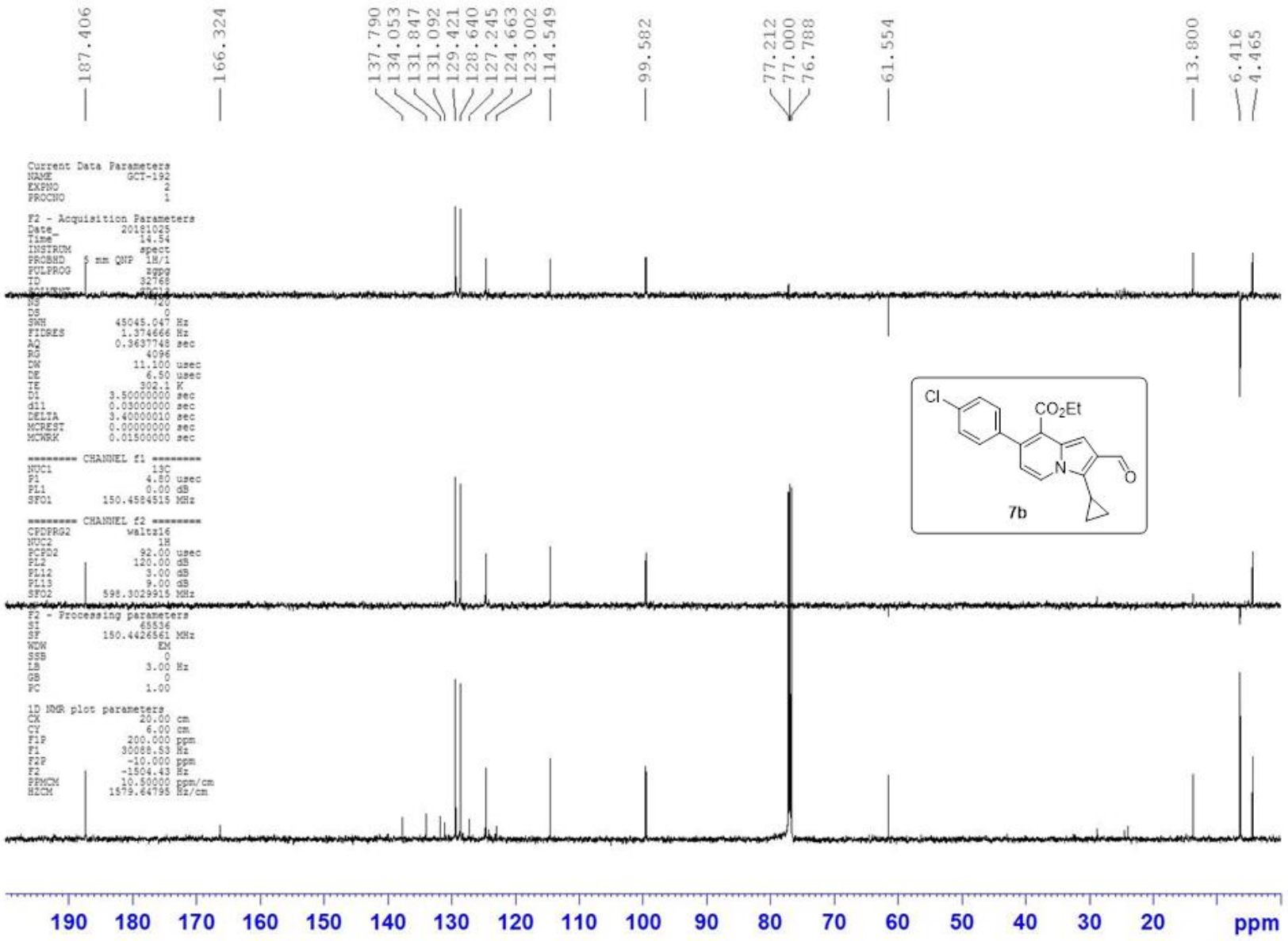

10.27
7.619
7.601
7.240
7.058
7.039
6.865
6.855
6.672
6.662
2.831
2.813
2.793
2.773
2.742
1.760
1.742
1.722
1.703
1.684
1.671
1.477
1.458
1.440
1.421
1.403
1.384
0.974
0.956
0.938
BRUKER
Current Data Parameters
NAME 20171030
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171030
Time 15.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 144
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 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
AS-3-03H
CH3
OHC
N
n-Bu
5j
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.02
1.02
1.00
2.03
3.06
2.05
2.07
3.03

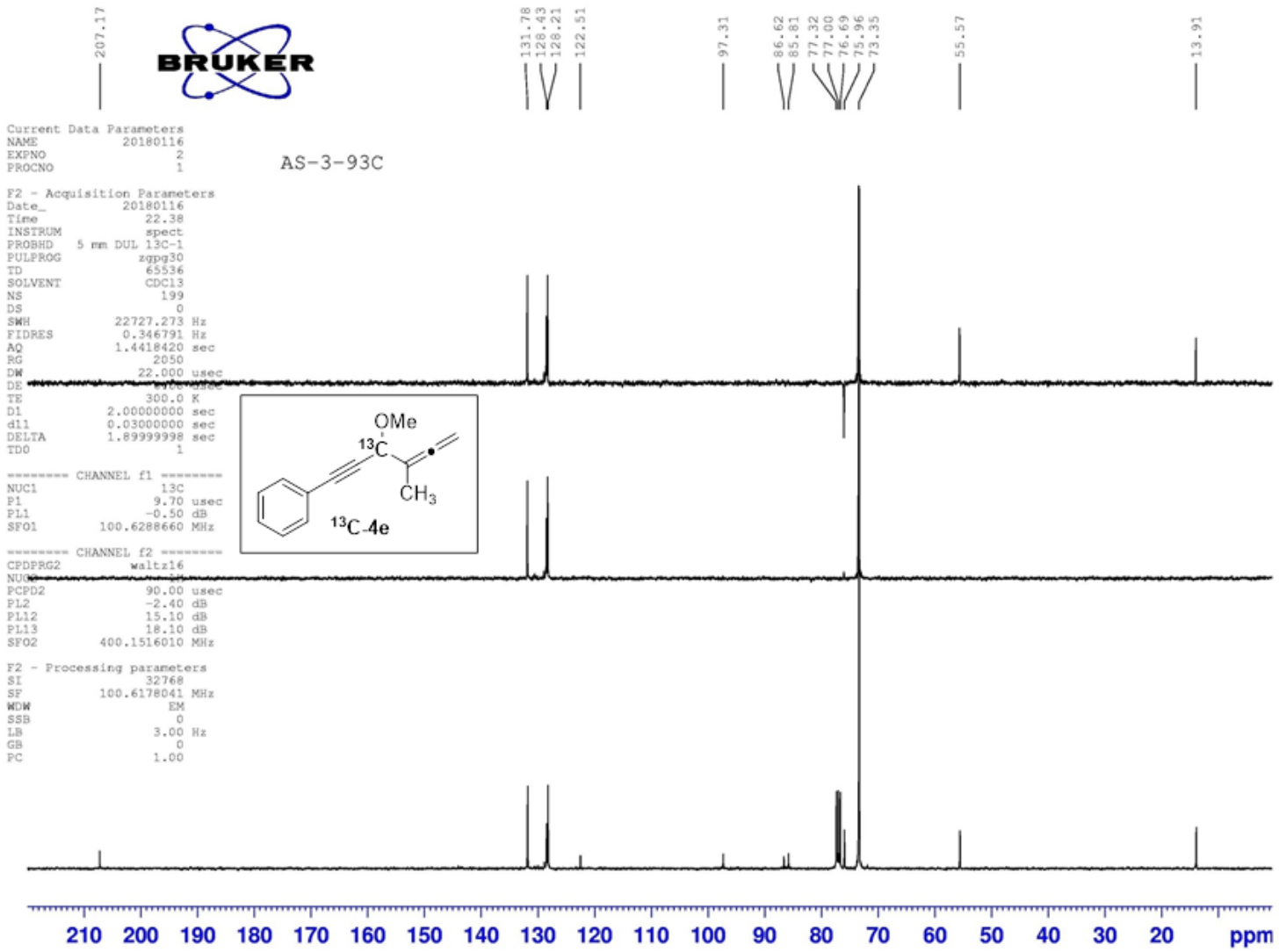

188.246
136.255
132.122
130.025
121.352
119.365
113.725
107.321
104.921
77.318
77.000
76.682
29.316
25.684
22.532
13.807
12.611
BRUKER
Current Data Parameters
NAME 20171030
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171030
Time 22.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
TD 65536
SOLVENT CDCl3
NS 500
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178043 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OHC
CH3
N
n-Bu
5j
AS-3-03C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

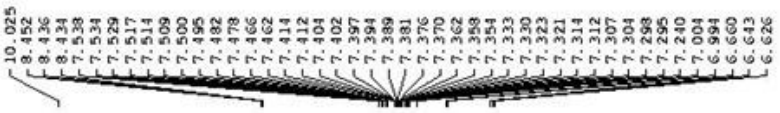

10.412
8.227
8.225
8.214
8.213
7.404
7.395
7.392
7.391
7.390
7.386
7.381
7.380
7.377
7.366
7.365
7.363
7.357
7.355
7.354
7.351
7.346
7.343
7.341
7.240
7.006
7.005
6.718
6.706
4.177
4.165
4.153
4.141
2.001
1.992
1.987
1.983
1.978
1.973
1.969
1.964
1.955
1.586
1.269
1.261
1.258
1.255
1.251
1.248
1.244
1.237
1.231
1.048
1.045
1.043
1.033
1.024
1.021
1.019
0.825
0.818
0.815
Current Data Parameters
NAME GCT-255
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190108
Time 8.34
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
DW 52.250 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
SFO1 598.2035892 MHz
F2 - Processing parameters
SI 32768
SF 598.2000273 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 3.00
CO2Et
Ph
N
O
7a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.05
5.22
1.00
1.10
2.02
1.00
2.18
3.01
2.05


187.496
166.622
139.261
133.067
130.993
129.604
128.417
128.037
127.896
127.088
124.482
122.859
114.884
99.115
77.212
77.000
76.787
61.403
13.688
6.397
4.444
Current Data Parameters
NAME GCT-255
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190107
Time 16.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 400
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4340559 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 -1.00 dB
PL13 5.50 dB
SFO2 598.2029910 MHz
F2 - Processing parameters
SF 150.4175154 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30083.50 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.17505 Hz/cm
CO2Et
Ph
N
O
7a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


10.413
8.229
8.217
8.216
7.376
7.362
7.288
7.274
7.240
7.021
6.655
6.643
4.209
4.197
4.185
4.173
1.991
1.986
1.982
1.977
1.973
1.968
1.964
1.955
1.551
1.267
1.263
1.256
1.253
1.250
1.113
1.101
1.089
0.826
0.819
0.816
0.810
0.807
0.800
Current Data Parameters
NAME GCT-192
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191026
Time 5.53
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 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 301.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000295 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Cl
CO2Et
N
O
7b
11
10
9
8
7
6
5
4
3
2
1
ppm
1.05
1.11
2.21
2.27
1.01
1.00
2.06
1.08
2.26
3.01
2.08

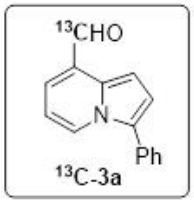

187.406
166.324
137.790
134.053
131.847
131.092
129.421
128.640
127.245
124.663
123.002
114.549
99.582
77.212
77.000
76.788
61.554
13.800
6.416
4.465
Cl
CO2Et
N
O
7b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

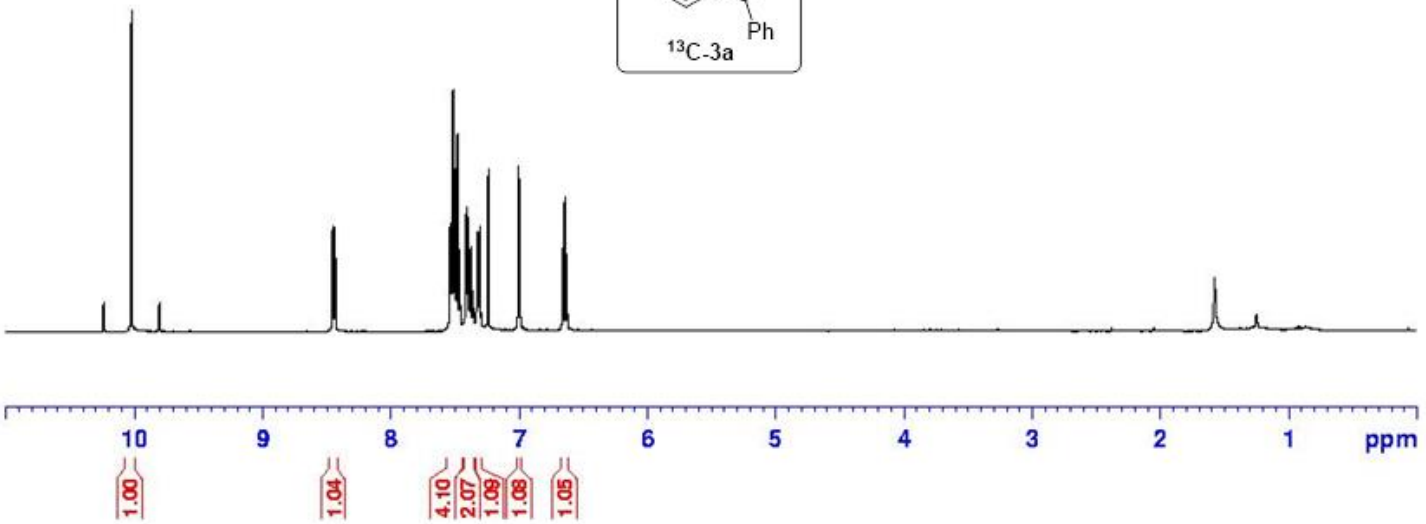

207.17
131.78
128.43
128.21
122.51
97.31
86.62
85.81
77.32
77.00
76.69
75.96
73.35
55.57
13.91
AS-3-93C
Current Data Parameters
NAME 20180116
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180116
Time 22.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 199
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 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
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 100.6178041 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
13C
CH3
13C-4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

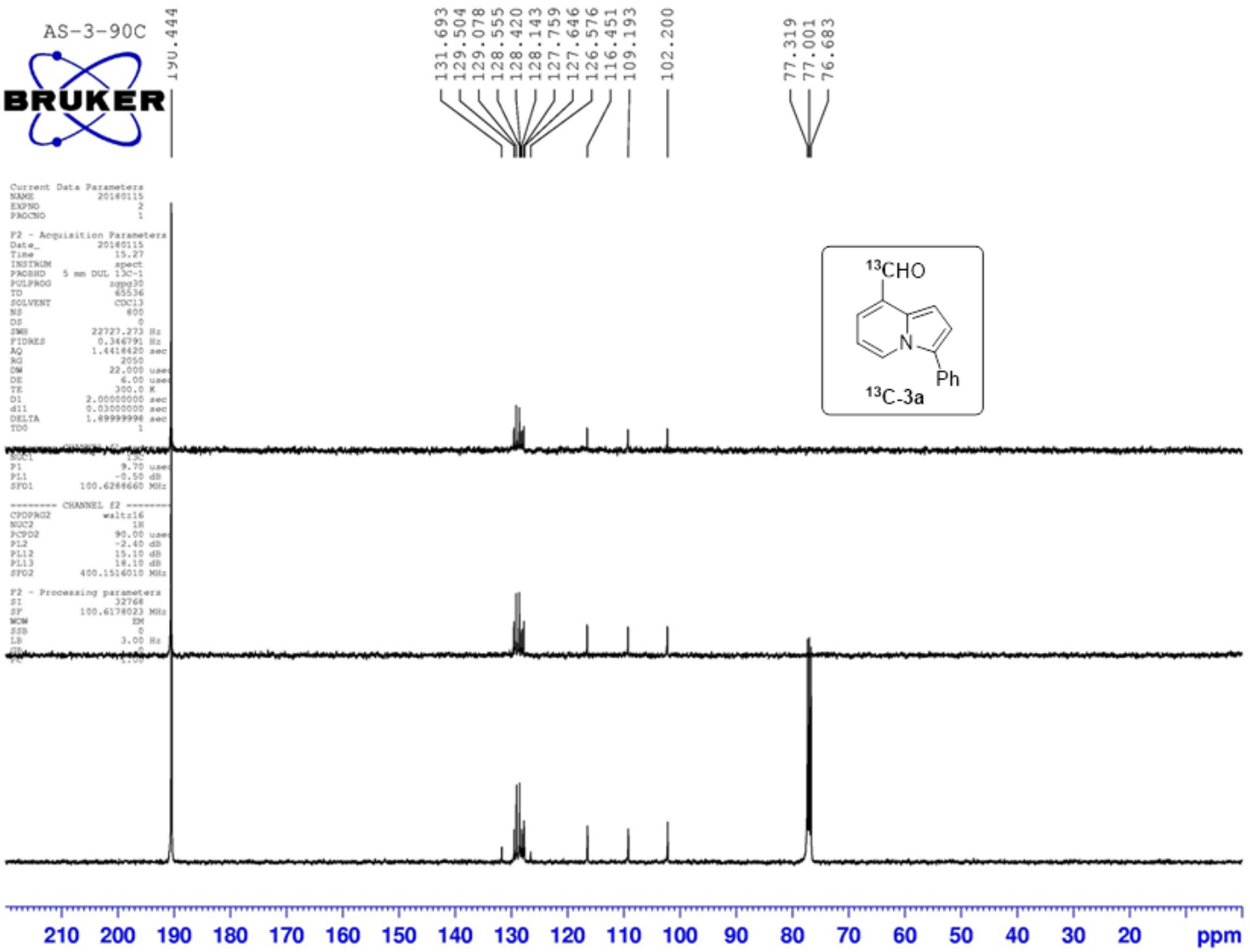


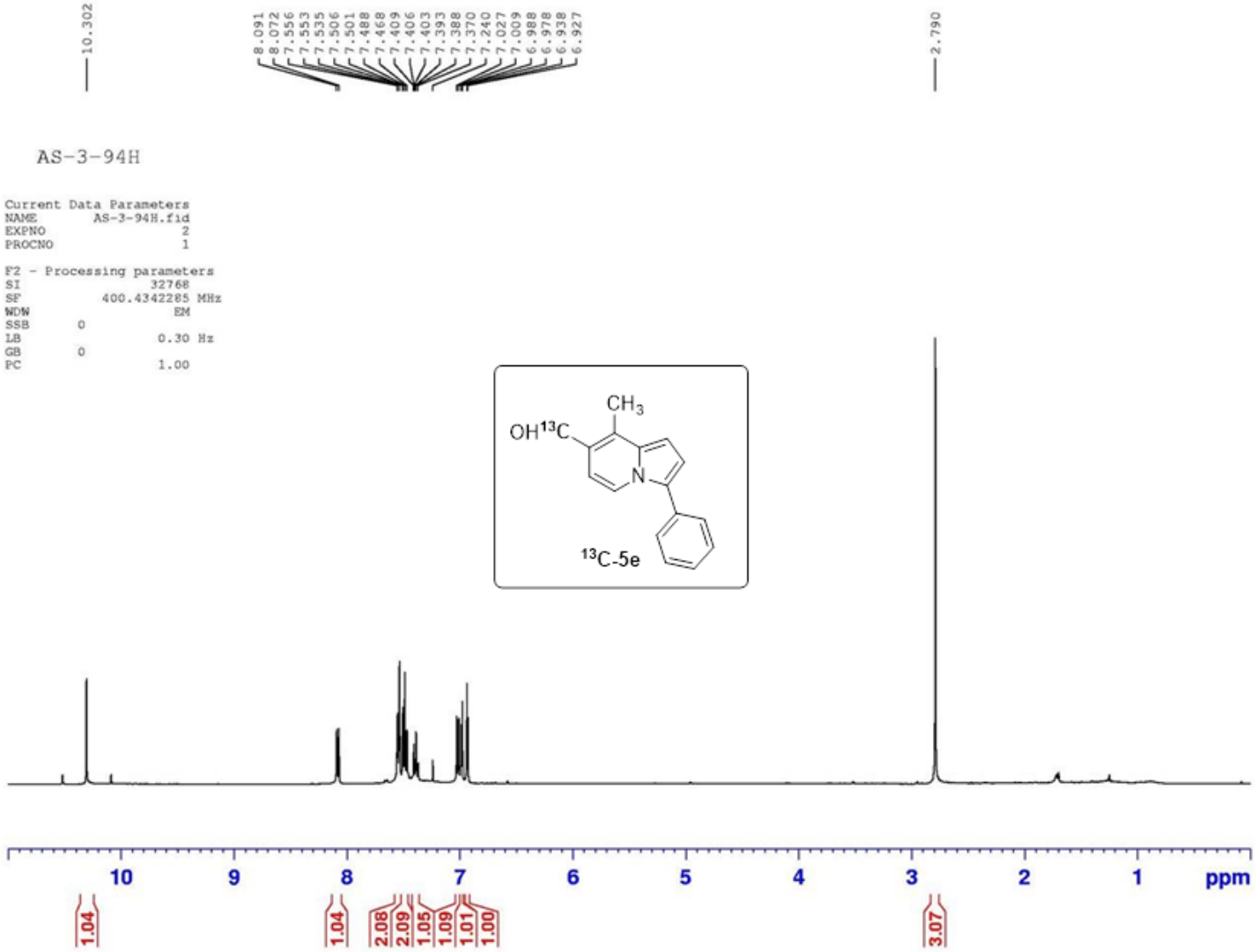
AS-3-90H

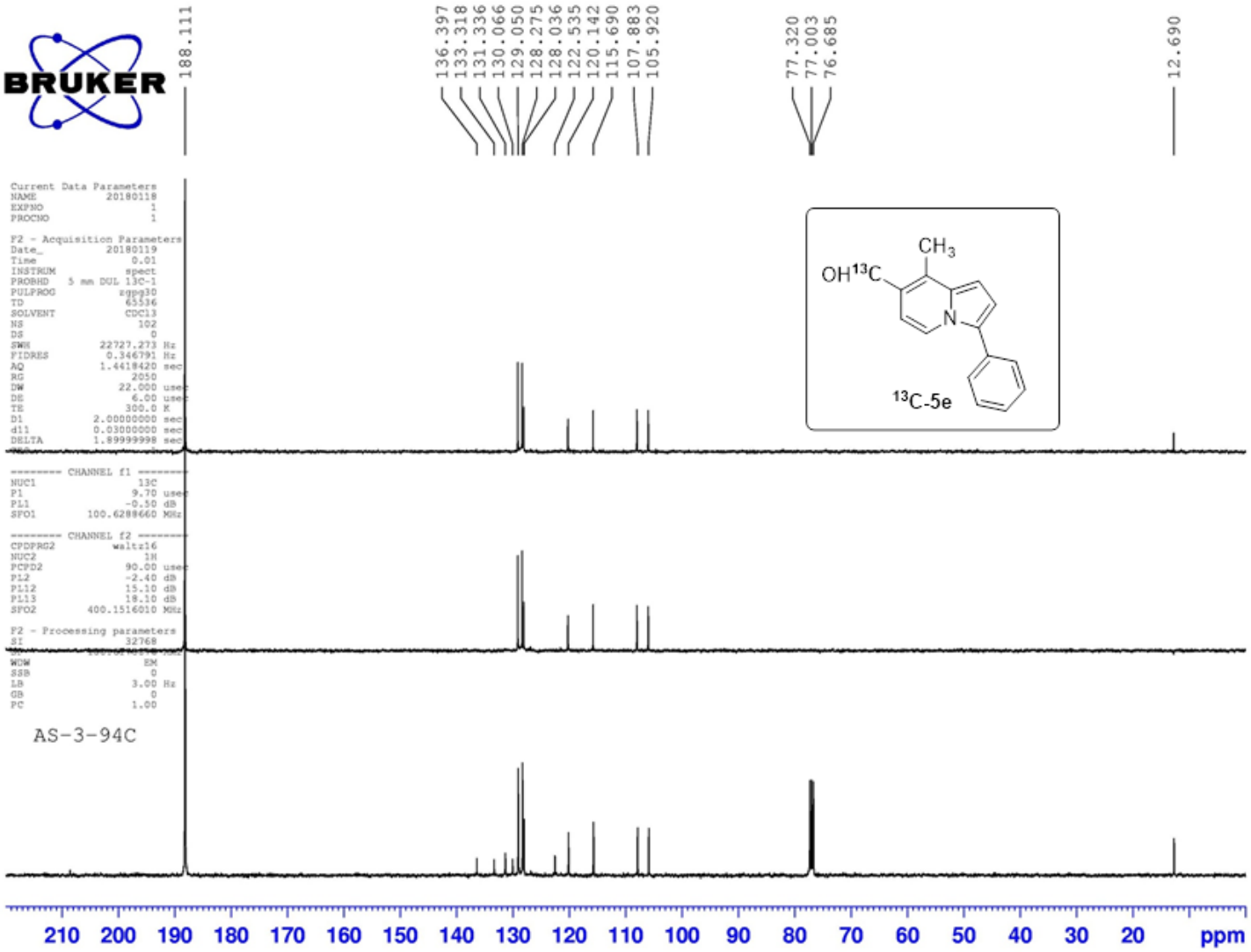
```
Current Data Parameters
NAME          AS-3-90H.fid
EXPNO                   1
PROCNO                  1

F2 - Processing parameters
SI                  32768
SF             400.4342287 MHz
WDW                    EM
SSB         0
LB                  0.30 Hz
GB          0
PC                  1.00
```

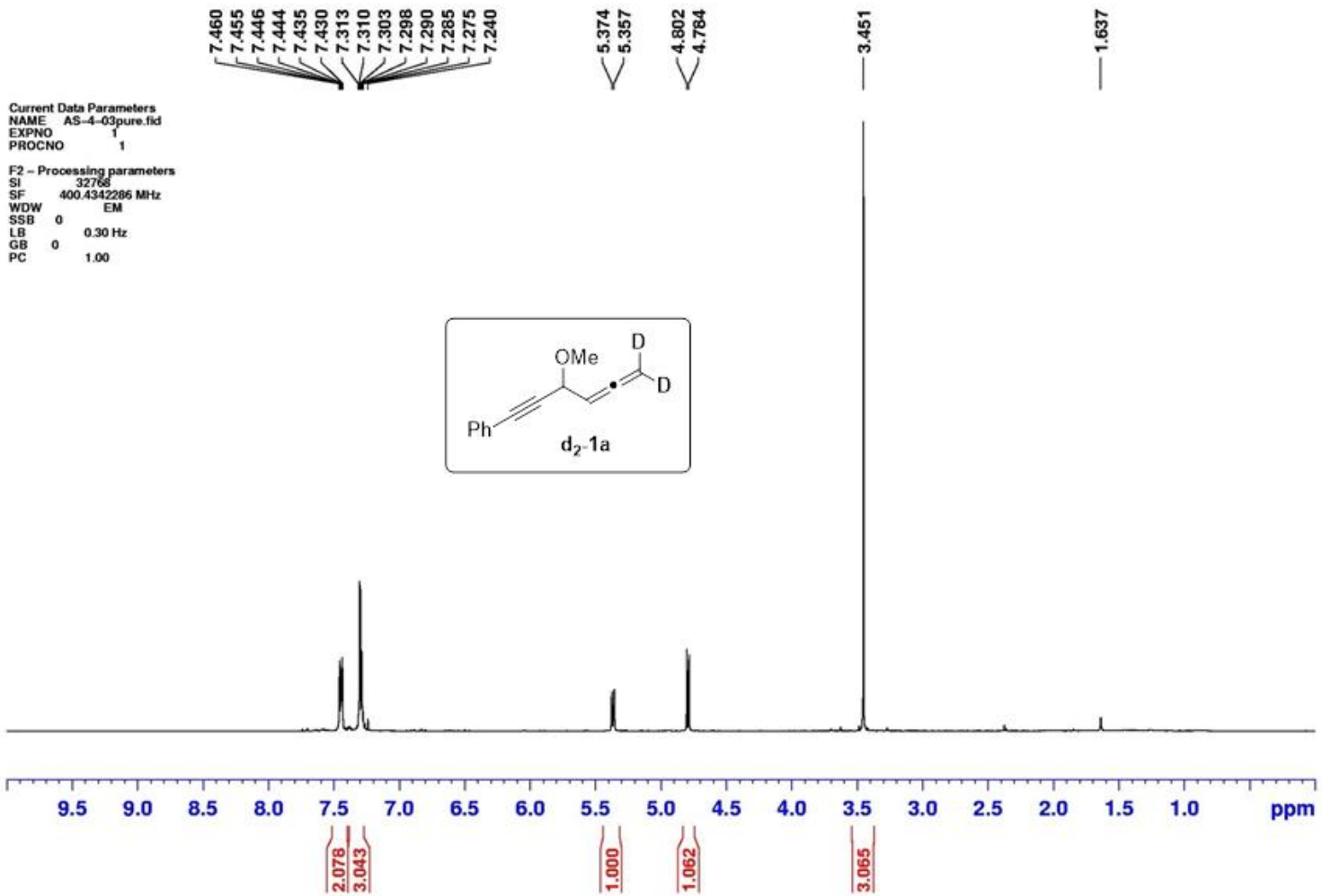


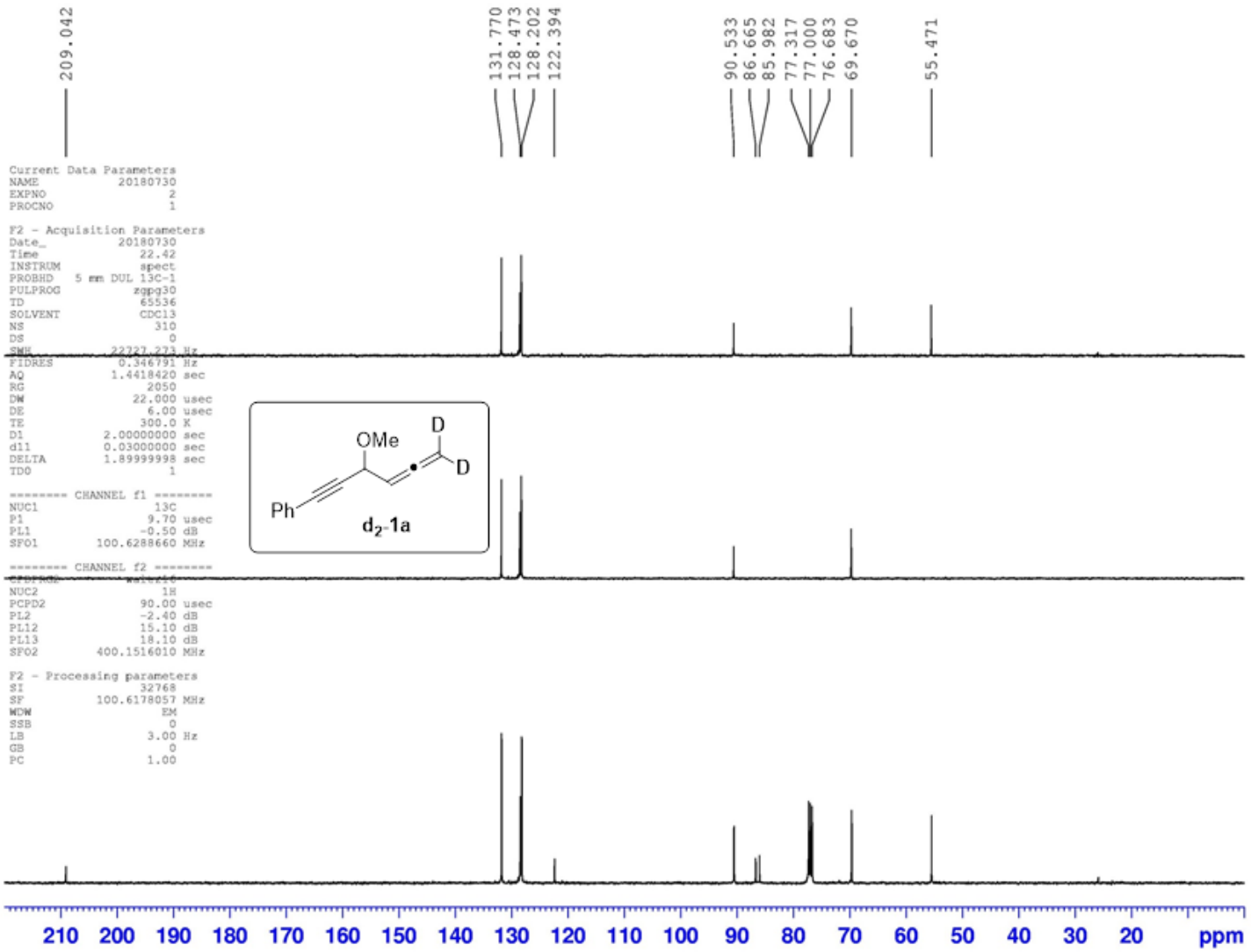


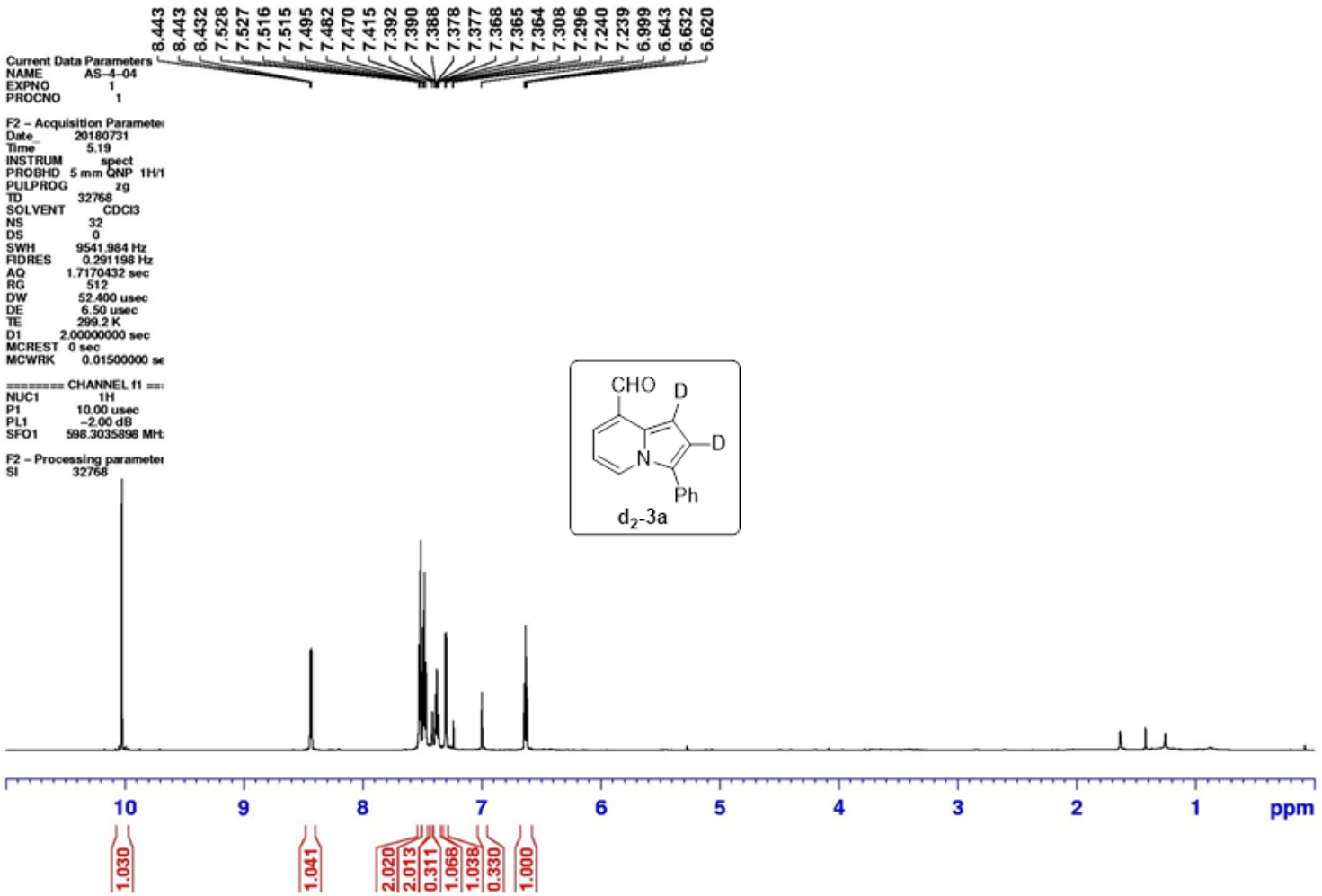

AS-3-90C
BRUKER
190.444
131.693
129.504
129.078
128.555
128.420
128.143
127.759
127.646
126.576
116.451
109.193
102.200
77.319
77.001
76.683
^{13}CHO
N
Ph
^{13}C-3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

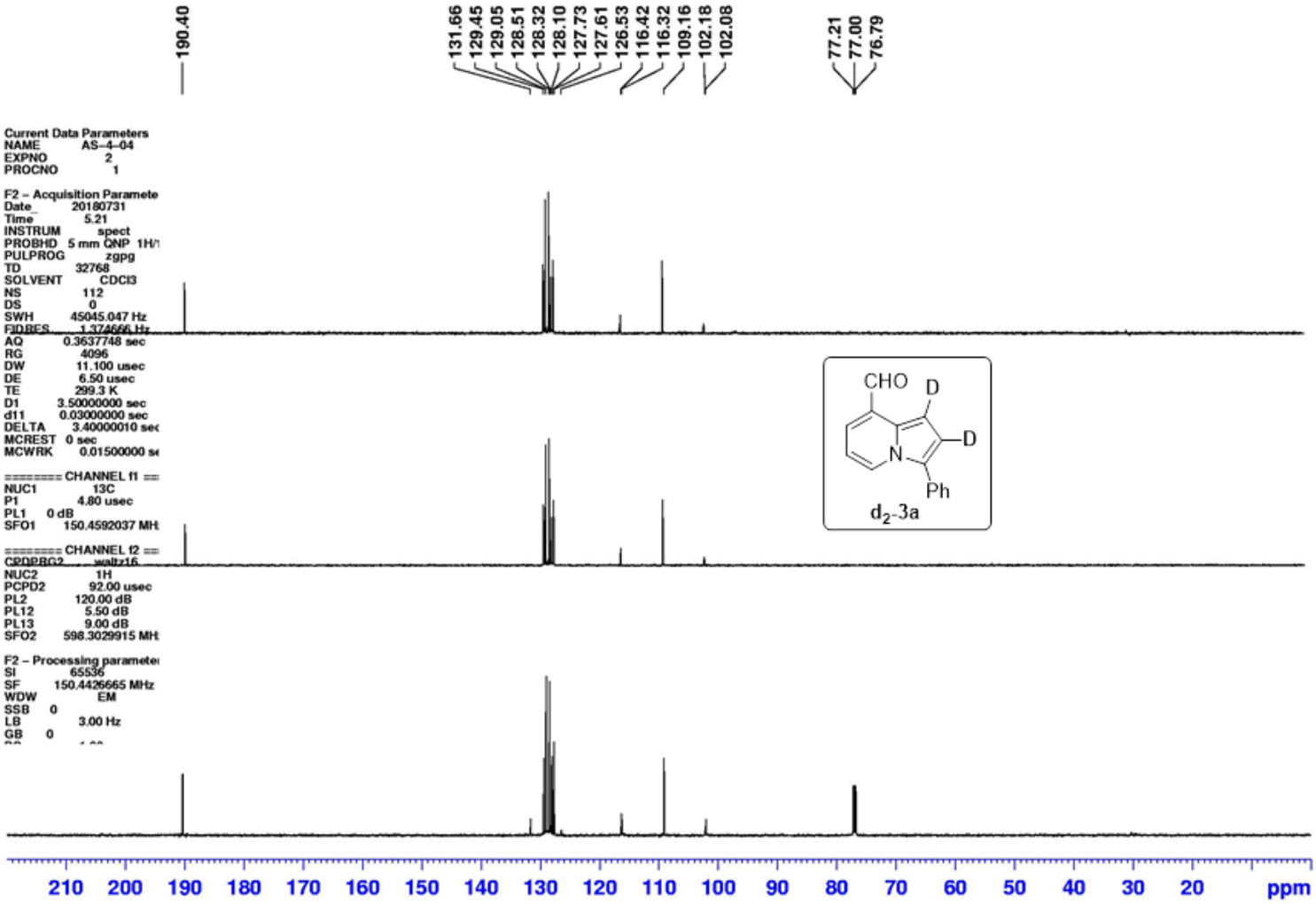

10.302
8.091
8.072
7.556
7.553
7.535
7.506
7.501
7.488
7.468
7.409
7.406
7.403
7.393
7.388
7.370
7.240
7.027
7.009
6.988
6.978
6.938
6.927
2.790
AS-3-94H
Current Data Parameters
NAME AS-3-94H.fid
EXPNO 2
PROCNO 1
F2 - Processing parameters
SI 32768
SF 400.4342285 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CH3
OH13C
N
13C-5e
10
9
8
7
6
5
4
3
2
1
ppm
1.04
1.04
2.08
2.09
1.05
1.09
1.01
1.00
3.07


188.111
136.397
133.318
131.336
130.066
129.050
128.275
128.036
122.535
120.142
115.690
107.883
105.920
77.320
77.003
76.685
12.690
Current Data Parameters
NAME 20180118
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180119
Time 0.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
======== 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
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
AS-3-94C
CH3
OH13C
N
13C-5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.460
7.455
7.446
7.444
7.435
7.430
7.313
7.310
7.303
7.298
7.290
7.285
7.275
7.240
5.374
5.357
4.802
4.784
3.451
1.637
Current Data Parameters
NAME AS-4-03pure.fid
EXPNO 1
PROCNO 1
F2 – Processing parameters
SI 32768
SF 400.4342286 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
D
D
Ph
d2-1a
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.078
3.043
1.000
1.062
3.065


209.042
131.770
128.473
128.202
122.394
90.533
86.665
85.982
77.317
77.000
76.683
69.670
55.471
Current Data Parameters
NAME 20180730
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180730
Time 22.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 310
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 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 ========
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 100.6178057 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
D
D
Ph
d2-1a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.443
8.443
8.432
7.528
7.527
7.516
7.515
7.495
7.482
7.470
7.415
7.392
7.390
7.388
7.378
7.377
7.368
7.365
7.364
7.308
7.296
7.240
7.239
6.999
6.643
6.632
6.620
Current Data Parameters
NAME AS-4-04
EXPNO 1
PROCNO 1
F2 - Acquisition Parameter
Date_ 20180731
Time 5.19
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 1.7170432 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 se
======== CHANNEL f1 ===
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.3035898 MH
F2 - Processing parameter
SI 32768
CHO
D
D
N
Ph
d2-3a
10
9
8
7
6
5
4
3
2
1
ppm
1.030
1.041
2.020
2.013
0.311
1.068
1.038
0.330
1.000


190.40
131.66
129.45
129.05
128.51
128.32
128.10
127.73
127.61
126.53
116.42
116.32
109.16
102.18
102.08
77.21
77.00
76.79
Current Data Parameters
NAME AS--4--04
EXPNO 2
PROCNO 1
F2 – Acquisition Parameter
Date_ 20180731
Time 5.21
INSTRUM spect
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 112
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
CHANNEL f2
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 – Processing parameter
SI 65536
SF 150.4426665 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
CHO
D
D
N
Ph
d2-3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm