

Supporting Information

Gold-catalyzed (4+1)-Annulation Reactions between 1,4-Diyn-3-ols and Isoxazoles to Construct a Pyrrole Core

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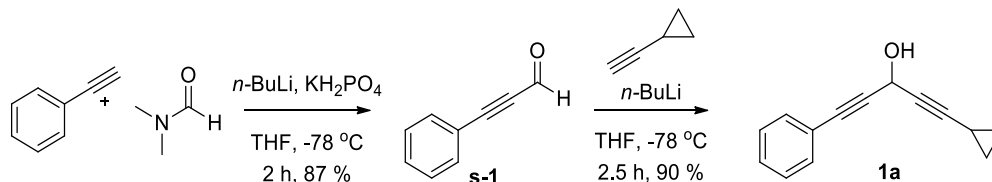
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(1) Representative Synthetic Procedures:

(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. Dichloromethane, DCE, Ether and Toluene 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. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60_f - 254) using UV light as a visualizing agents. ^1H NMR and ^{13}C NMR spectra were recorded on a Varian 400 and 600 MHz, Bruker 400 MHz Spectrometers using *d*-chloroform, *d*-benzene and *d*-acetone as the internal standards. The isoxazoles **2a** and **2b** were purchased commercially. Other isoxazole derivatives **2c-2d**,⁶ **2e-2f**,³ and **2g-2i**.⁴ were prepared according to the literature reports. Benzoisoxazole **5a-5c** were prepared according to reported literature procedures.⁵

(b) Preparation of 1-cyclopropyl-5-phenylpenta-1,4-diyn-3-ol (**1a**).²



n-BuLi (9.4 mL, 23.0 mmol) was added slowly to a solution of phenyl acetylene (2.0 g, 19.5 mmol) in THF (25 mL) at -78°C ; the mixture was stirred for 30 minutes at same temperature. Then DMF (3 mL, 39.2 mmol) was added to this reaction mixture and stirred for additional 2.0 h. The whole mixture then poured cautiously to the pre-cooled (0°C) biphasic mixture of KH_2PO_4 (10.6 g, 78.0 mmol) in water (100 mL) and diethyl ether (100 mL). The mixture was stirred for additional 1 h and extracted with Et_2O (50 mL x 2). The organic extracts were washed with brine (20 mL), dried over MgSO_4 and concentrated under reduced pressure. Crude product was directly used for the next step.

n-BuLi (3.7 mL, 9.1 mmol) was added slowly to a THF solution (25 mL) of cyclopropyl acetylene (1.0 g, 7.6 mmol) at -78 °C; the mixture was stirred for 30 minutes at same temperature before treatment with compound **s-1** in THF (0.60 g, 9.1 mmol); and the mixture was stirred for additional 2.0 h, quenched with sat. solution of NH₄Cl in water and extracted with Et₂O (50 mL x 2). The organic extracts were washed with brine (20 mL), dried over MgSO₄ and concentrated under reduced pressure to get 1-cyclopropyl-5-phenylpenta-1,4-diyn-3-ol (**1a**) (1.35 g, 6.8 mmol, 90 %) as yellow oil.

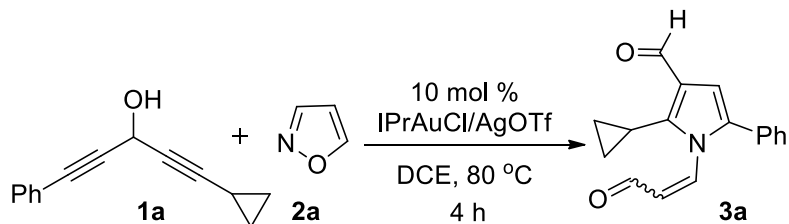
Other substrate **1b-1w** were prepared with the above procedure.

(2) References.

- (1) Zeng, M.; Wu, F.; Chen, K.; Zhu, S. *Org. Lett.* **2016**, *18*, 3554
- (2) Wang, T.; Shi, S.; Hansmann, M. M.; Rettenmeier, E.; Rudolph, M.; Hashmi, A. S. K. *Angew. Chem. Int. Ed.* **2014**, *53*, 3715.
- (3) Tang, S.; He, J.; Sun, Y.; He, L.; she, X., *Org. Lett.* **2009**, *11*, 3982
- (4) Sahani, R. L.; Liu, R.-S. *Angew. Chem. Int. Ed.* **2017**, *56*, 1026.
- (5) Sahani, R. L.; Liu, R.-S. *Angew. Chem. Int. Ed.* **2017**, *56*, 12736.
- (6) Pravin, C.; Kalyanasundaram, A.; Perumal, P.T.; *synlett.*, **2010**, *5*, 777

(3) Standard procedures for catalytic operations.

(a) Typical procedure for the synthesis of (Z)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (**3a**)

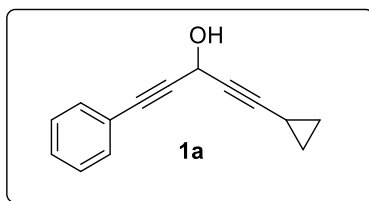


A suspension of IPrAuCl (0.063 g, 0.1 mmol) and AgOTf (0.026 g, 0.1 mmol) in dry DCE (2 mL) was fitted with N₂ balloon, and to this solution was added a DCE (4 mL) solution of 1-cyclopropyl-5-phenylpenta-1,4-diyn-3-ol **1a** (0.2 g, 1.0 mmol) and isoxazole **2a** (0.14 g, 2.0

mmol) at room temperature. The resulting mixture was stirred for 4 h at 80 °C. After completion of the reaction, the solution was filtered over a short celite bed. The solvent was evaporated to dryness under reduced pressure, and the residue was purified on a silica gel column using ethyl acetate/hexane (15:85) as the eluent to give compound **3a** (0.224 g, 0.84 mmol, 83 %) as brown oil.

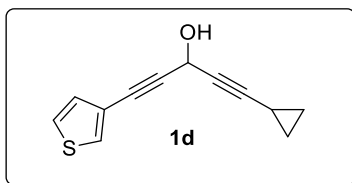
(4) Spectral data for key compounds:

Spectra data for 1-cyclopropyl-5-phenylpenta-1,4-diyn-3-ol (**1a**)



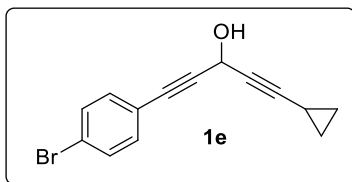
Yellow oil (1.35 g, 6.8 mmol, 90 %); ^1H NMR (400 MHz, CDCl_3): δ 7.45 ~ 7.42 (m, 2H), 7.32 ~ 7.25 (m, 3H), 5.2 (s, 1H), 2.4 (bs, 1H), 1.31 ~ 1.23 (m, 1H), 0.81 ~ 0.79 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 131.7, 128.6, 128.2, 122.0, 88.7, 86.5, 83.8, 72.5, 52.8, 8.2, 0.5; ESI-MS calcd for $\text{C}_{14}\text{H}_{12}\text{O}$ [$\text{M}+\text{Na}$]: 219.0786, found: 219.0775.

Spectra data for 1-cyclopropyl-5-(thiophen-3-yl)penta-1,4-diyn-3-ol (**1d**)



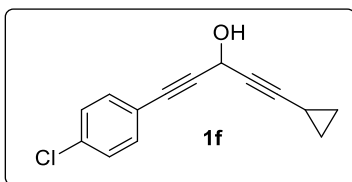
Brown oil (1.26 g, 6.2 mmol, 85 %); ^1H NMR (400 MHz, CDCl_3): δ 7.44 ~ 7.43 (m, 1H), 7.21 ~ 7.19 (m, 1H), 7.08 ~ 7.06 (m, 1H), 5.27 (s, 1H), 2.88 (bs, 1H), 1.28 ~ 1.21 (m, 1H), 0.77 ~ 0.73 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ 129.4, 129.2, 125.0, 120.8, 88.1, 86.2, 78.6, 72.5, 52.1, 7.8; ESI-MS calcd for $\text{C}_{12}\text{H}_{10}\text{OS}$ [$\text{M}+\text{Na}$]: 225.0350, found: 225.0328.

Spectra data for 1-(4-bromophenyl)-5-cyclopropylpenta-1,4-diyn-3-ol (**1e**)



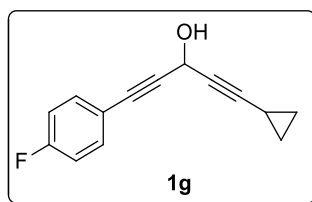
Brown oil (0.92 g, 3.3 mmol, 70 %); ^1H NMR (400 MHz, CDCl_3): δ 7.42 (d, J = 8 Hz, 2H), 7.29 (d, J = 6.6 Hz, 2H), 5.27 (s, 1H), 2.35 (d, J = 5.8 Hz, 1H), 1.29 ~ 1.24 (m, 1H), 0.79 ~ 0.72 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ 133.2, 131.5, 123.0, 121.0, 89.0, 87.6, 82.8, 72.2, 52.8, 8.2, 0.5; ESI-MS calcd for $\text{C}_{14}\text{H}_{11}\text{BrO}[\text{M}+\text{Na}]$: 296.9891, found: 296.9849.

Spectra data for 1-(4-chlorophenyl)-5-cyclopropylpenta-1,4-diyne-3-ol (1f)



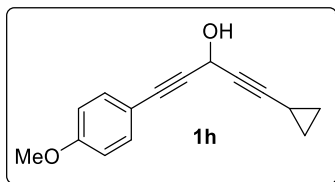
Colourless oil (1.03 g, 4.5 mmol, 74 %); ^1H NMR (400 MHz, CDCl_3): δ 7.37 ~ 7.33 (m, 2H), 7.28 ~ 7.25 (m, 2H), 5.26 (d, J = 5.6 Hz, 1H), 2.28 (d, J = 6.8 Hz, 1H), 1.32 ~ 1.23 (m, 1H), 0.81 ~ 0.71 (m, 4H); ^{13}C NMR (100 MHz, $d\text{-CDCl}_3$): δ 134.6, 132.9, 128.5, 120.4, 89.01, 87.4, 82.7, 72.34, 52.8, 8.4, -0.3; ESI-MS calcd for $\text{C}_{14}\text{H}_{11}\text{ClO}[\text{M}-\text{H}]$: 229.0420, found: 229.0405.

Spectral data for 1-cyclopropyl-5-(4-fluorophenyl)penta-1,4-diyne-3-ol (1g):



Yellow oil (1.12 g, 5.2 mmol, 78 %); ^1H NMR (500 MHz, CDCl_3): δ 7.42 ~ 7.39 (m, 2H), 6.97 (t, J = 8.6 Hz, 2H), 5.27 (d, J = 6.0 Hz, 1H), 2.42 (d, J = 6.9 Hz, 1H), 1.30 ~ 1.25 (m, 1H), 0.78 ~ 0.76 (m, 2H), 0.74 ~ 0.72 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3): δ 163.6, (d, J = 248.7 Hz), 133.7 (d, J = 8.3 Hz), 118.0 (d, J = 3.4 Hz), 115.5 (d, J = 22 Hz), 88.8, 86.2, 82.8, 72.4, 52.7, 8.2, -0.6; ESI-MS calcd for $\text{C}_{14}\text{H}_{11}\text{FO}[\text{M}+\text{H}]$: 215.0872, found: 215.0884.

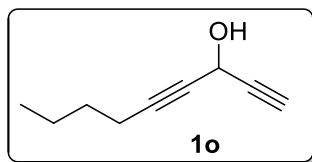
Spectra data for 1-cyclopropyl-5-(4-methoxyphenyl)penta-1,4-diyne-3-ol (1h)



Brown oil (1.21 g, 5.3 mmol, 86 %); ^1H NMR (500 MHz, CDCl_3): δ 7.79 (d, J = 9.0 Hz, 2H), 7.23 (d, J = 8.5 Hz, 2H), 5.71 (d, J = 6.0 Hz, 1H), 4.20 (s, 3H), 2.98 (d, J = 7.0 Hz, 1H), 1.72 ~

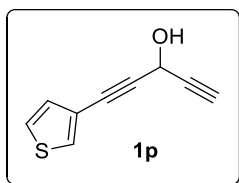
1.66 (m, 1H), 1.20 ~ 1.14 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3): δ 159.7, 133.2, 113.8, 88.4, 85.2, 83.8, 72.7, 55.2, 52.7, 8.1, -0.6; ESI-MS calcd for $\text{C}_{15}\text{H}_{14}\text{O}_2$ [M-H]: 225.0916, found: 225.0925.

Spectral data for nona-1,4-diyn-3-ol (1o):



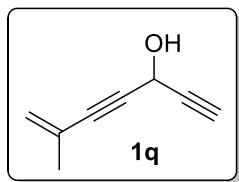
Yellow oil (0.45 g, 3.4 mmol, 70 %); ^1H NMR (500 MHz, CDCl_3): δ 5.07 (d, J = 4 Hz, 1H), 2.52 (s, 1H), 2.22 ~ 2.20 (m, 3H), 1.51 ~ 1.45 (m, 2H), 1.42 ~ 1.34 (m, 2H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 86.0, 81.4, 76.9, 72.1, 52.1, 30.2, 21.8, 18.3, 13.5; ESI-MS calcd for $\text{C}_9\text{H}_{12}\text{O}$ [M+H] : 137.0966, found : 137.0935.

Spectral data for 1-(thiophen-3-yl)penta-1,4-diyn-3-ol (1p):



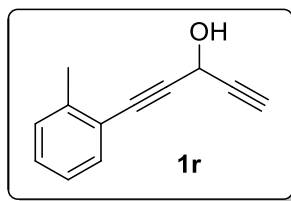
Yellow oil (0.449 g, 2.7 mmol, 65 %); ^1H NMR (500 MHz, CDCl_3): δ 7.49 (s, 1H), 7.26 ~ 7.24 (m, 1H), 7.12 (d, J = 4.9 Hz, 1H), 5.30 (d, J = 7.5 Hz, 1H), 2.59 (s, 1H), 2.31 (d, J = 7.6 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 129.9, 129.7, 125.4, 120.6, 85.0, 80.6, 80.0, 72.9, 52.5.

Spectral data for 6-methylhepta-6-en-1,4-diyn-3-ol (1q):



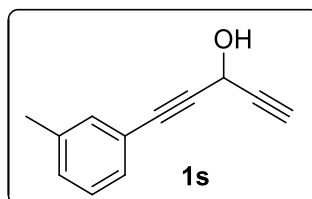
Pale yellow oil (0.37 g, 3.1 mmol, 60 %); ^1H NMR (400 MHz, CDCl_3): δ 5.35 (s, 1H), 5.28 ~ 5.27 (m, 1H), 5.21 (d, J = 1.9 Hz, 1H), 2.55 (d, J = 2.3 Hz, 1H), 2.36 (bs, 1H), 1.87 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 125.3, 122.9, 85.0, 84.4, 80.5, 72.4, 51.5, 22.6.

Spectral data for 1-(o-tolyl)penta-1,4-diyn-3-ol (1r):



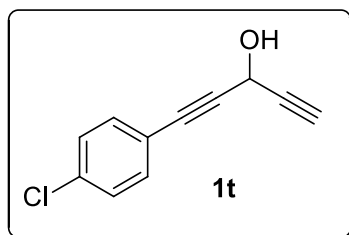
Yellow oil (0.49 g, 2.8 mmol, 71 %); ^1H NMR (400 MHz, CDCl_3): δ 7.41 (dd, J = 7.6, 0.7 Hz, 1H), 7.24 ~ 7.18 (m, 2H), 7.13 ~ 7.09 (m, 1H), 5.37 (d, J = 4.5 Hz, 1H), 2.60 (d, J = 2.2 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 140.4, 132.0, 129.3, 128.7, 125.3, 121.3, 89.2, 83.6, 80.9, 72.7, 52.5, 20.6; ESI-MS calcd for $\text{C}_{12}\text{H}_{10}\text{O}$ [$\text{M}+\text{Na}$] : 193.0629, found : 193.0615.

Spectral data for 1-(m-tolyl)penta-1,4-diyn-3-ol (1s):



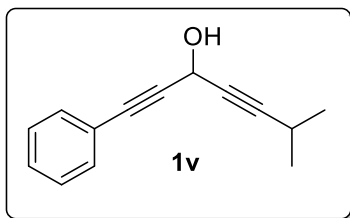
Yellow oil (0.519 g, 3.0 mmol, 74 %); ^1H NMR (500 MHz, CDCl_3): δ 7.26 (s, 1H), 7.24 (d, J = 7.6 Hz, 1H), 7.18 (t, J = 7.5 Hz, 1H), 7.13 (d, J = 7.6 Hz, 1H), 5.32 (d, J = 1.7 Hz, 1H), 2.61 (bs, 1H), 2.59 (d, J = 2.2 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 137.9, 132.3, 129.7, 128.8, 128.1, 121.4, 85.1, 84.8, 80.8, 72.8, 52.4, 21.0; ESI-MS calcd for $\text{C}_{12}\text{H}_{10}\text{O}$ [$\text{M}+\text{Na}$] : 193.0629, found : 193.0619.

Spectral data for 1-(4-chlorophenyl)penta-1,4-diyn-3-ol (1t)



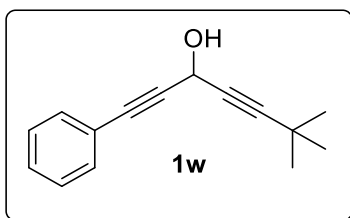
Yellow oil (0.50 g, 2.6 mmol, 69 %); ^1H NMR (400 MHz, CDCl_3): δ 7.38 ~ 7.36 (m, 2H), 7.29 ~ 7.27 (m, 2H), 5.31 (dd, J = 7.5, 2.2 Hz, 1H), 2.60 (d, J = 2.3 Hz, 1H), 2.37 (d, J = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 135.1, 133.0, 128.7, 120.1, 86.2, 83.5, 80.5, 73.1, 52.4; ESI-MS calcd for $\text{C}_{11}\text{H}_7\text{ClO}$ [$\text{M}+\text{Na}$] : 213.0083, found : 213.0074.

Spectra data for 6-methyl-1-phenylhepta-1,4-diyn-3-ol (1v)



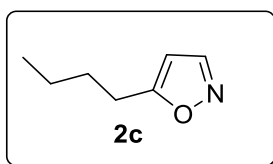
Brown oil (1.75 g, 8.8 mmol, 60 %); ^1H NMR (400 MHz, CDCl_3): δ 7.45 ~ 7.42 (m, 2H), 7.29 ~ 7.24 (m, 3H), 5.36 (d, J = 4.9 Hz, 1H), 2.94 (d, J = 5.8 Hz, 1H), 2.63 ~ 2.56 (m, 1H), 1.18 (s, 3H), 1.16 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 131.6, 128.1, 122.0, 90.7, 86.7, 83.6, 76.6, 52.5, 22.4, 20.3; ESI-MS calcd for $\text{C}_{14}\text{H}_{14}\text{O}$ [$\text{M}+\text{Na}$] : 221.0942, found: 221.1586.

Spectra data for 6,6-dimethyl-1-phenylhepta-1,4-dien-3-ol (1w)



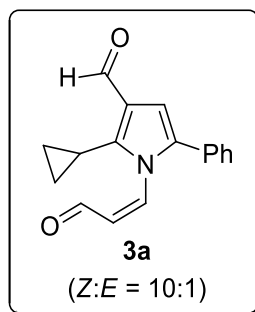
Colourless oil (1.54 g, 7.3 mmol, 60 %); ^1H NMR (400 MHz, $d\text{-CDCl}_3$): δ 7.45 ~ 7.40 (m, 2H), 7.33 ~ 7.26 (m, 3H), 5.33 (d, J = 7.0 Hz, 1H), 2.47 (d, J = 7.1 Hz, 1H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ 131.6, 128.4, 128.0, 122.0, 93.5, 86.7, 83.6, 75.9, 52.8, 30.7, 27.4; ESI-MS calcd for $\text{C}_{15}\text{H}_{16}\text{O}$ [M] : 212.1201, found: 212.1220.

Spectra data for 5-butylisoxazole (2c)



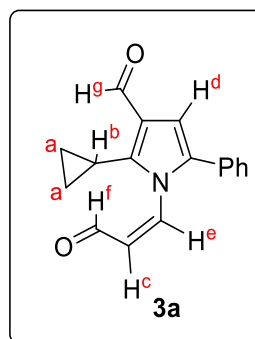
Colourless oil (1.21 g, 5.3 mmol, 86 %); ^1H NMR (400 MHz, CDCl_3): δ 8.11 (d, J = 1.7 Hz, 1H), 5.94 (t, J = 0.7 Hz, 1H), 2.74 (t, J = 7.6 Hz, 2H), 1.69 ~ 1.62 (m, 2H), 1.41 ~ 1.31 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 172.7, 149.9, 99.6, 29.6, 26.2, 22.2, 13.7; CI-MS calcd for $\text{C}_7\text{H}_{11}\text{NO}$ [$\text{M}+\text{H}$] : 126.0919, found: 126.0915.

Spectral data for (Z)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (3a):



Brown oil (0.114 g, 0.43 mmol, 85 %); ^1H NMR for major isomer (500 MHz, CDCl_3) : δ 10.19 (s, 1H), 9.48 (d, $J = 7.7$ Hz, 1H), 7.49 (d, $J = 8.5$ Hz, 1H), 7.36 ~ 7.33 (m, 2H), 7.31 ~ 7.27 (m, 3H), 6.70 (s, 1H), 5.98 (t, $J = 8.1$ Hz, 1H), 1.86 ~ 1.18 (m, 1H), 1.17 ~ 1.13 (m, 2H), 0.84 ~ 0.91 (m, 2H); ^1H NMR for minor isomer: δ 10.27 (s, 1H), 9.42 (d, $J = 7.5$ Hz, 1H), 7.83 (d, $J = 14.7$ Hz, 1H), 7.41 (d, $J = 6.5$ Hz, 3H), 6.33 (s, 1H), 6.15 (dd, $J = 14.7, 7.5$ Hz, 1H), 1.29 ~ 1.25 (m, 2H), 0.91 ~ 0.83 (m, 2H) rest of peaks merged with others; ^{13}C NMR for major isomer (125 MHz, CDCl_3): δ 188.7, 185.8, 145.0, 138.8, 136.3, 130.4, 128.9, 128.8, 128.1, 125.5, 125.4, 108.6, 7.8, 6.0; ^{13}C NMR for minor isomer δ 191.6, 129.3, 110.3, 8.0, 6.5, rest of peaks merged with others; ESI-MS calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_2$ [M+H] $^+$: 266.1181, found : 266.1173.

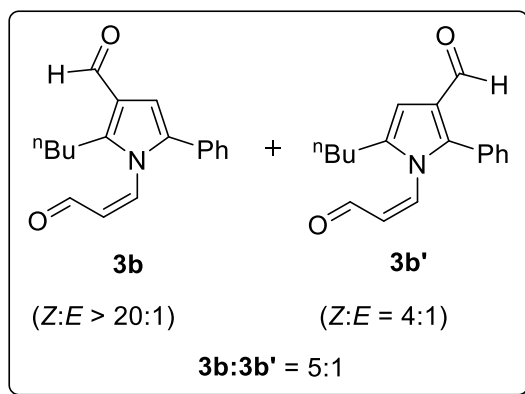
^1H NOE map of compound **3a**:



Irradiation	Enhancement (%)
H^a (δ 0.84 ~ -0.91)	H^a (δ 1.17 ~ 1.13, 19.79 %), H^e (δ 7.49, 1.32 %), H^g (δ 10.19, 4.09 %)
H^a (δ 1.17 ~ 1.13)	H^a (δ 0.84 ~ -0.91, 22.38 %), H^b (δ 1.86 ~ 1.18, 3.99 %)

H^b (δ 1.86 ~ 1.18)	H^a (δ 1.17 ~ 1.13, 7.17 %), H^e (δ 7.49, 1.94 %), H^f (δ 9.48, 4.45 %), H^g (δ 10.19, 1.54 %)
H^c (δ 5.98)	H^e (δ 7.49, 9.80 %), H^f (δ 9.48, 2.48 %)
H^d (δ 6.70)	H^{Ph} (δ 7.36 ~ 7.27, 5.04 %), H^g (δ 10.19, 1.61 %)
H^e (δ 7.49)	H^b (δ 1.86 ~ 1.18, 1.70 %), H^c (δ 5.98, 9.43 %)
H^f (δ 9.48)	H^b (δ 1.86 ~ 1.18, 3.64 %), H^c (δ 5.98, 2.24 %), H^{Ph} (δ 7.36 ~ 7.27, 2.55 %)
H^g (δ 10.19)	H^a (δ 0.84 ~ -0.91, 3.87 %), H^b (δ 1.86 ~ 1.18, 1.74 %), H^d (δ 6.70, 1.54 %)

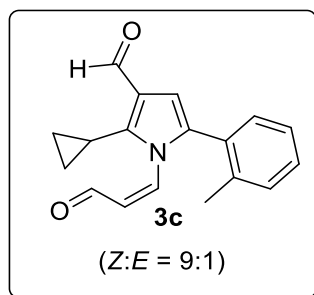
Spectral data for (Z)-2-butyl-1-(3-oxoprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (3b) and (Z)-5-butyl-1-(3-oxoprop-1-en-1-yl)-2-phenyl-1H-pyrrole-3-carbaldehyde (3b'):



Brown oil (0.132 g, 0.47 mmol, 83 %); 1H NMR for **3b** major isomer (500 MHz, $CDCl_3$): δ 9.94 (s, 1H), 9.30 (d, J = 7.7 Hz, 1H), 7.43 (d, J = 8.4 Hz, 1H), 7.34 ~ 7.31 (m, 2H), 7.28 ~ 7.26 (m, 3H), 6.72 (s, 1H), 5.98 (t, J = 8.0 Hz, 1H), 2.97 (t, J = 7.9 Hz, 2H), 1.60 ~ 1.54 (m, 2H), 1.39 ~ 1.32 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H); 1H NMR for **3b'** major isomer: δ 9.61 (s, 1H), 9.37 (d, J = 7.7 Hz, 1H), 7.41 ~ 7.38 (m, 3H), 6.59 (s, 1H), 5.92 (t, J = 9.0 Hz, 1H), 2.55 (t, J = 7.7 Hz, 2H), 1.64 ~ 1.60 (m, 2H), 1.46 ~ 1.45 (m, 2H), 0.97 ~ 0.96 (m, 3H); rest of peaks merged with others;); 1H NMR for **3b'** minor isomer: δ 9.50 (s, 1H), 9.42 (d, J = 7.4 Hz, 1H), 7.58 (d, J = 14.7 Hz, 1H), 6.6 (s, 1H), 5.83 (dd, J = 14.7 Hz, 1H), rest of peaks merged with others; ^{13}C NMR for **3b** major isomer (125 MHz, $CDCl_3$): δ 185.8, 185.3, 144.5, 137.8, 131.1, 130.2, 129.0, 128.7, 127.9, 127.3, 123.4, 109.9, 32.2, 24.8, 22.3, 13.6; ^{13}C NMR for **3b'** major isomer: δ 191.2, 186.6, 143.4, 136.5, 130.9, 129.2, 128.7, 126.9, 124.5, 106.1, 30.2, 26.5, 22.2, 13.7, rest of peaks

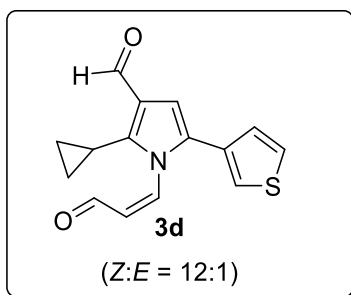
merged with others; ^{13}C NMR for **3b'** minor isomer: δ 191.6, 186.5, 144.3, 138.4, 130.3, 129.2, 128.8, 121.3, 11.8, rest of peaks merged with others; ESI-MS calcd for $\text{C}_{18}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{H}]$: 282.1494, found : 282.1489.

Spectra data for (Z)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-5-(o-tolyl)-1H-pyrrole-3-carbaldehyde (3c)



Brown oil (0.100 g, 0.36 mmol, 76 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 10.21 (s, 1H), 9.44 (d, $J = 7.6$ Hz, 1H), 7.35 (d, $J = 8.6$ Hz, 1H), 7.28 ~ 7.13 (m, 4H), 6.60 (s, 1H), 5.85 ~ 5.78 (m, 1H), 2.15 (s, 3H), 1.88 ~ 1.81 (m, 1H), 1.18 ~ 1.13 (m, 2H), 0.85 ~ 0.81 (m, 2H); ^1H NMR for minor isomer δ 10.28 (s, 1H), 9.33 (d, $J = 7.4$ Hz, 1H), 7.76 (d, $J = 14.7$ Hz, 1H), 6.54 (s, 1H), 2.08 (s, 3H), 1.99 ~ 1.91 (m, 1H), 1.31 ~ 1.26 (m, 2H), rest of the peaks merged with others; ^{13}C NMR for major isomer (100 MHz, CDCl_3): δ 188.5, 185.7, 144.1, 138.2, 137.3, 135.2, 131.4, 130.6, 129.9, 129.1, 125.9, 125.1, 124.8, 109.2, 20.1, 7.8, 6.1; ^{13}C NMR for minor isomer δ 191.7, 185.9, 144.9, 137.8, 130.8, 130.5, 129.7, 126.3, 118.7, 110.5, 19.7, 7.8, 6.2, rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{H}]$: 280.1338, found: 280.1329.

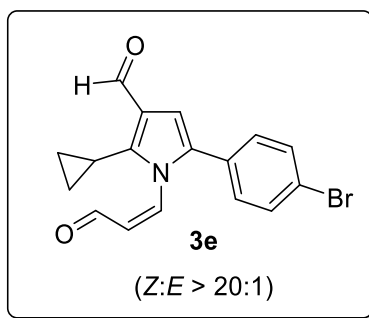
Spectra data for (Z)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-5-(thiophen-3-yl)-1H-pyrrole-3-carbaldehyde (3d)



Brown oil (0.108 g, 0.39 mmol, 81 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 10.18 (s, 1H), 9.51 (d, $J = 7.6$ Hz, 1H), 7.51 (d, $J = 8.4$ Hz, 1H), 7.34 ~ 7.32 (m, 1H), 7.25 ~ 7.23

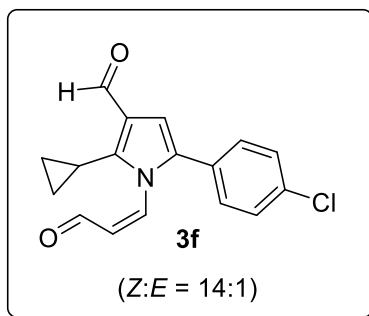
(m, 1H), 7.06 ~ 7.05 (m, 1H), 6.71 (s, 1H), 6.05 (t, $J = 8.2$ Hz, 1H), 1.84 ~ 1.77 (m, 1H), 1.17 ~ 1.13 (m, 2H), 0.83 ~ 0.79 (m, 2H); ^1H NMR for minor isomer δ 10.25 (s, 1H), 9.46 (d, $J = 7.4$ Hz, 1H), 7.85 (d, $J = 14.4$ Hz, 1H), 7.42 ~ 7.40 (m, 1H), 7.30 ~ 7.29 (m, 1H), 7.40 ~ 7.02 (m, 1H), 6.69 (s, 1H), 6.20 (dd, $J = 14.6, 7.4$ Hz, 1H), 1.97 ~ 1.90 (m, 1H), 1.29 ~ 1.12 (m, 2H), 0.92 ~ 0.87 (m, 2H); ^{13}C NMR for major isomer (100 MHz, CDCl_3): 188.3, 185.4, 144.61, 138.6, 131.3, 130.9, 127.3, 126.5, 125.9, 125.1, 123.5, 108.1, 8.1, 6.2; ^{13}C NMR for minor isomer δ 191.3, 185.6, 144.8, 127.8, 127.4, 126.8, 125.1, 120.7, 110.3, 8.2, 6.7 rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{15}\text{H}_{13}\text{NO}_2\text{S}$ [$\text{M}+\text{Na}$] : 294.0565, found: 294.0563.

Spectra data for (Z)-5-(4-bromophenyl)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-1H-pyrrole-3-carbaldehyde (3e)



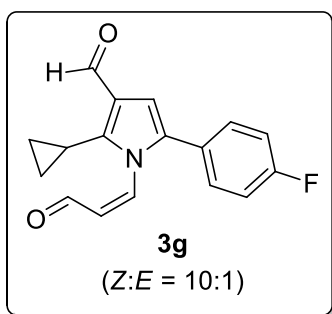
Brown oil (0.114 g, 0.33 mmol, 91 %); ^1H NMR (400 MHz, CDCl_3): δ 10.19 (s, 1H), 9.49 (d, $J = 7.6$ Hz, 1H), 7.49 ~ 7.46 (m, 3H), 7.18 (d, $J = 8.4$ Hz, 2H), 6.71 (s, 1H), 6.01 (t, $J = 8.4$ Hz, 1H), 1.86 ~ 1.79 (m, 1H), 1.19 ~ 1.11 (m, 2H), 0.89 ~ 0.71 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): 188.3, 185.3, 145.1, 138.5, 135.0, 131.9, 130.1, 129.2, 125.8, 125.4, 122.4, 109.0, 8.1, 6.2; ESI-MS calcd for $\text{C}_{17}\text{H}_{14}\text{BrNO}_2$ [$\text{M}+\text{H}$] : 344.0286, found: 344.0272.

Spectra data for (Z)-5-(4-chlorophenyl)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-1H-pyrrole-3-carbaldehyde (3f)



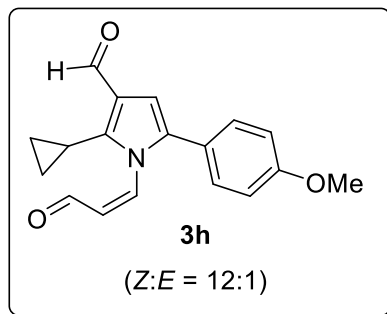
Brown oil (0.129 g, 0.39 mmol, 90 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 10.18 (s, 1H), 9.47 (d, J = 7.6 Hz, 1H), 7.48 (d, J = 8.5 Hz, 1H), 7.33 ~ 7.31 (m, 2H), 7.25 ~ 7.22 (m, 2H), 6.70 (s, 1H), 6.01 (t, J = 8.4 Hz, 1H), 1.86 ~ 1.17 (m, 1H), 1.19 ~ 1.14 (m, 2H), 0.84 ~ 0.80 (m, 2H); ^1H NMR for minor isomer δ 10.25 (s, 1H), 9.44 (d, J = 7.4 Hz, 1H), 7.80 (d, J = 14.6 Hz, 1H), 7.39 (d, J = 8.3 Hz, 2H), 6.63 (s, 1H), 6.13 (dd, J = 14.6, 7.4 Hz, 1H), 1.98 ~ 1.91 (m, 1H), 1.32 ~ 1.25 (m, 2H), 0.95 ~ 0.88 (m, 2H), rest of the peaks merged with others; ^{13}C NMR for major isomer (125 MHz, CDCl_3): δ 188.6, 185.6, 145.2, 138.6, 135.1, 134.3, 130.0, 128.9, 125.9, 125.4, 109.0, 7.8, 6.0; ^{13}C NMR for minor isomer δ 191.3, 185.8, 130.5, 129.2, 121.3, 110.9, 7.9, 6.4, rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{17}\text{H}_{14}\text{ClNO}_2$ [$\text{M}+\text{H}$] : 300.0791, found: 300.0800.

Spectral data for (Z)-2-cyclopropyl-5-(4-fluorophenyl)-1-(3-oxoprop-1-en-1-yl)-1H-pyrrole-3-carbaldehyde (3g):



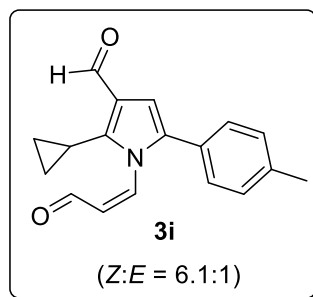
Brown oil (0.117 g, 0.41 mmol, 89 %); ^1H NMR for major isomer (500 MHz, CDCl_3): δ 10.19 (s, 1H), 9.47 (d, J = 7.7 Hz, 1H), 7.47 (d, J = 8.6 Hz, 1H), 7.29 ~ 7.26 (m, 2H), 7.05 (t, J = 8.6 Hz, 2H), 6.67 (s, 1H), 5.99 (t, J = 8.2 Hz, 1H), 1.85 ~ 1.80 (m, 1H), 1.18 ~ 1.14 (m, 2H), 0.84 ~ 0.80 (m, 2H); ^1H NMR for minor isomer δ 10.26 (s, 1H), 9.43 (d, J = 7.5 Hz, 1H), 7.80 (d, J = 14.7 Hz, 1H), 7.11 (t, J = 8.6 Hz, 2H), 6.61 (s, 1H), 6.10 (dd, J = 14.7, 7.4 Hz, 1H), 1.97 ~ 1.92 (m, 1H), 1.29 ~ 1.26 (m, 2H), 0.91 ~ 0.87 (m, 2H); ^{13}C NMR for major isomer (125 MHz, CDCl_3): δ 188.6, 185.7, 162.4 (d, J = 248.7), 145.0, 138.6, 135.2, 130.8, 130.7, 125.7, 116.1, 115.9, 108.7, 7.8, 6.0; ^{13}C NMR for minor isomer δ 191.4, 126.5, 125.3, 121.0 rest of peaks merged with others; ESI-MS calcd for $\text{C}_{17}\text{H}_{14}\text{FNO}_2$ [$\text{M}+\text{Na}$] : 306.0906, found : 306.0936.

Spectra data for (Z)-2-cyclopropyl-5-(4-methoxyphenyl)-1-(3-oxoprop-1-en-1-yl)-1H-pyrrole-3-carbaldehyde (3h)



Brown oil (0.100 g, 0.33 mmol, 77 %); ^1H NMR for major isomer (500 MHz, CDCl_3): δ 10.18 (s, 1H), 9.47 (d, $J = 7.7$ Hz, 1H), 7.46 (d, $J = 8.6$ Hz, 1H), 7.21 (d, $J = 8.7$ Hz, 2H), 6.86 (d, $J = 8.6$ Hz, 2H), 6.61 (s, 1H), 5.96 (t, $J = 8.1$ Hz, 1H), 3.78 (s, 3H), 1.84 ~ 1.79 (m, 1H), 1.15 ~ 1.12 (m, 2H), 0.82 ~ 0.79 (m, 2H); ^1H NMR for minor isomer δ 10.26 (s, 1H), 9.40 (d, $J = 7.4$ Hz, 1H), 7.81 (d, $J = 14.4$ Hz, 1H), 6.96 ~ 6.91 (m, 2H), 6.56 (s, 1H), 6.17 (dd, $J = 14.7, 7.5$ Hz, 1H), 3.82 (s, 3H), 1.98 ~ 1.91 (m, 1H), 1.31 ~ 1.26 (m, 2H), 0.93 ~ 0.84 (m, 2H), rest of the peaks merged with others; ^{13}C NMR for major isomer (125 MHz, CDCl_3): δ 188.7, 185.7, 159.5, 144.6, 138.9, 136.2, 130.3, 125.4, 125.3, 122.7, 114.2, 107.8, 55.2, 7.8, 6.0; ^{13}C NMR for minor isomer δ 191.7, 185.9, 145.3, 132.3, 131.3, 130.7, 129.4, 114.3, 8.0, 6.5, rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_3$ [M+H]: 296.1287, found: 296.1285.

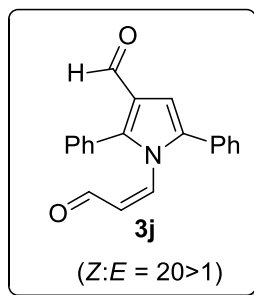
Spectra data for (Z)-2-cyclopropyl-1-(3-oxoprop-1-en-1-yl)-5-(p-tolyl)-1H-pyrrole-3-carbaldehyde (3i)



Brown oil (0.083 g, 0.29 mmol, 63 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 10.19 (s, 1H), 9.47 (d, $J = 7.7$ Hz, 1H), 7.47 (d, $J = 8.5$ Hz, 1H), 7.20 ~ 7.14 (m, 4H), 6.66 (s, 1H), 5.96 (t, $J = 8.4$ Hz, 1H), 2.32 (s, 3H), 1.85 ~ 1.78 (m, 1H), 1.17 ~ 1.12 (m, 2H), 0.83 ~ 0.79 (m, 2H); ^1H NMR for minor isomer δ 10.26 (s, 1H), 9.41 (d, $J = 7.4$ Hz, 1H), 7.82 (d, $J = 14.6$ Hz, 1H), 7.29 (d, $J = 8.0$ Hz, 2H), 7.08 (d, $J = 7.8$ Hz, 2H), 6.59 (s, 1H), 6.16 (dd, $J = 14.8, 7.6$ Hz, 1H), 2.38 (s, 3H), 1.97 ~ 1.91 (m, 1H), 1.28 ~ 1.23 (m, 2H), 0.91 ~ 0.85 (m, 2H); ^{13}C NMR for major isomer (100 MHz, CDCl_3): δ 188.8, 185.7, 144.8, 138.9, 138.2, 131.5, 129.5, 128.8, 127.5,

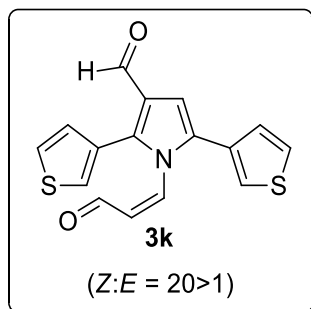
125.5, 120.8, 108.2, 21.2, 7.8, 6.1; ^{13}C NMR for minor isomer: δ 191.6, 185.9, 145.3, 139.0, 138.5, 136.5, 129.6, 129.2, 129.0, 125.4, 119.4, 110.1, 21.4, 8.0, 6.5; ESI-MS calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_2$ [M+H]: 280.1338, found: 280.1327.

Spectra data for (Z)-1-(3-oxoprop-1-en-1-yl)-2,5-diphenyl-1H-pyrrole-3-carbaldehyde (3j)



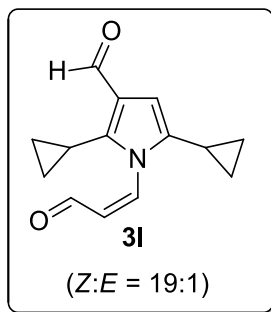
Brown oil (0.121 g, 0.40 mmol, 94 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 9.68 (s, 1H), 9.32 (d, $J = 7.6$ Hz, 1H), 7.47 ~ 7.46 (m, 3H), 7.46 ~ 7.38 (m, 7H), 7.22 (d, $J = 8.8$ Hz, 1H), 6.91 (s, 1H), 5.77 (t, $J = 8.4$ Hz, 1H); ^{13}C NMR for major isomer (100 MHz, CDCl_3): δ 187.7, 186.5, 144.4, 137.9, 137.5, 131.2, 130.9, 130.2, 129.6, 129.2, 128.8, 128.4, 127.9, 125.4, 125.0, 108.9; ESI-MS calcd for $\text{C}_{20}\text{H}_{16}\text{NO}_2$ [M+H]: 302.1181, found: 302.1164.

Spectra data for (Z)-1-(3-oxoprop-1-en-1-yl)-2,5-di(thiophen-3-yl)-1H-pyrrole-3-carbaldehyde (3k)



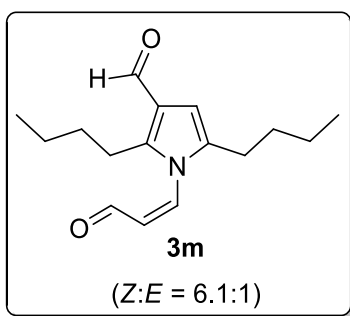
Brown oil (0.119 g, 0.38 mmol, 93 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 9.75 (s, 1H), 9.35 (d, $J = 7.6$ Hz, 1H), 7.47 ~ 7.45 (m, 2H), 7.38 ~ 7.36 (m, 1H), 7.31 ~ 7.30 (m, 1H), 7.28 (d, $J = 8.6$ Hz, 1H), 7.11 ~ 7.09 (m, 2H), 6.90 (s, 1H), 5.88 (t, $J = 8.2$ Hz, 1H); ^{13}C NMR for major isomer (100 MHz, CDCl_3): δ 187.44, 186.23, 139.05, 137.63, 132.76, 130.76, 128.91, 128.45, 127.97, 127.76, 127.19, 126.80, 125.75, 125.34, 124.34, 108.74. ; ESI-MS calcd for $\text{C}_{16}\text{H}_{11}\text{NO}_2\text{S}_2$ [M+H]: 314.0309, found: 314.0301.

Spectra data for (Z)-2,5-dicyclopropyl-1-(3-oxoprop-1-en-1-yl)-1H-pyrrole-3-carbaldehyde (3l)



Brown oil (0.124 g, 0.54 mmol, 87 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 10.05 (d, $J = 1.2$ Hz, 1H), 9.64 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.56 (dd, $J = 8.4, 1.6$ Hz, 1H), 6.02 ~ 6.16 (m, 2H), 1.80 ~ 1.73 (m, 1H), 1.72 ~ 1.71 (m, 1H), 1.69 ~ 1.54 (m, 2H), 1.54 ~ 1.14 (m, 2H), 1.09 ~ 1.05 (m, 2H), 1.05 ~ 0.886 (m, 2H); ^1H NMR for minor isomer δ 10.14 (d, $J = 1.2$ Hz, 1H), 9.57 (dd, $J = 7.6, 1.6$ Hz, 1H), 8.12 (dd, $J = 14.8, 1.2$ Hz, 1H), 6.83 ~ 6.77 (m, 1H), 6.29 (s, 1H), rest of the peaks merged with others; ^{13}C NMR for major isomer (100 MHz, CDCl_3): δ 189.6, 185.7, 143.8, 139.3, 138.0, 125.9, 124.5, 104.0, 7.8, 7.5, 7.3, 5.9; ^{13}C NMR for minor isomer δ 192.1, 185.5, 126.7, 107.81, 7.5, rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{14}\text{H}_{15}\text{NO}_2$ [M+H] : 230.1181, found: 230.1175.

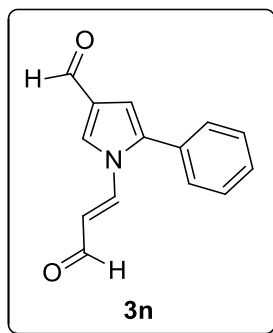
Spectra data for (Z)-2,5-dibutyl-1-(3-oxoprop-1-en-1-yl)-1H-pyrrole-3-carbaldehyde (3m)



Brown oil (0.120 g, 0.46 mmol, 88 %); ^1H NMR for major isomer (400 MHz, CDCl_3): δ 9.80 (s, 1H), 9.41 (d, $J = 8.0$ Hz, 1H), 7.36 (d, $J = 8.0$ Hz, 1H), 6.35 (s, 1H), 6.22 (t, $J = 8.0$ Hz, 1H), 1.83 ~ 1.80 (m, 2H), 2.42 ~ 2.38 (m, 2H), 1.59 ~ 1.52 (m, 4H), 1.50 ~ 1.43 (m, 4H), 1.31 ~ 1.29 (m, 6H); ^1H NMR for minor isomer δ 9.85 (s, 1H), 9.55 (d, $J = 7.2$ Hz, 1H), 7.60 (d, $J = 14.8$ Hz, 1H), 6.39 (s, 1H), 6.28 (dd, $J = 14.8, 7.6$ Hz, 1H), 3.01 ~ 2.98 (m, 2H), rest of the peaks merged with others; ^{13}C NMR for major isomer (100 MHz, CDCl_3): δ 189.4, 185.0, 143.2, 139.2, 136.0,

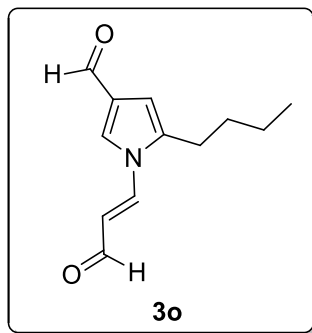
129.5, 122.8, 106.5, 32.2, 30.2, 26.3, 24.4, 22.1, 22.0, 13.6, 13.5; ^{13}C NMR for minor isomer δ 191.7, 185.1, 144.3, 136.3, 124.1, 119.5, 108.6, 31.9, 29.8, 27.6, 24.2, 22.2, 13.7, rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{16}\text{H}_{23}\text{NO}_2$ $[\text{M}+\text{H}]$: 262.1807, found: 262.1806.

Spectral data for (*E*)-1-(3-oxoprop-1-en-1-yl)-5-phenyl-1*H*-pyrrole-3-carbaldehyde (3n):



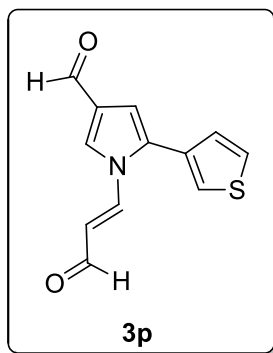
Brown solid (0.092 g, 0.40 mmol, 64 %); ^1H NMR (600 MHz, CDCl_3): δ 9.90 (s, 1H), 9.49 (d, 7.4 Hz, 1H), 7.75 (d, J = 1.5 Hz, 1H), 7.61 (d, J = 14.3 Hz, 1H), 7.49 ~ 7.46 (m, 3H), 7.36 (dd, J = 8.1, 1.9 Hz, 2H), 6.77 (d, J = 1.6 Hz, 1H), 6.35 (dd, J = 14.4, 7.5 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 190.5, 185.2, 144.9, 138.2, 129.7, 129.4, 129.2, 129.1, 125.7, 117.1, 110.0, one carbon merged with other; ESI-MS calcd for $\text{C}_{14}\text{H}_{11}\text{NO}_2$ $[\text{M}+\text{Na}]$: 248.0687, found : 248.06957.

Spectral data for (*E*)-5-butyl-1-(3-oxoprop-1-en-1-yl)-1*H*-pyrrole-3-carbaldehyde (3o):



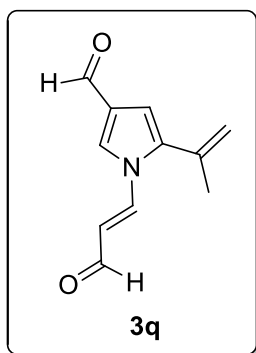
Brown oil (0.103 g, 0.50 mmol, 64 %); ^1H NMR (500 MHz, CDCl_3): δ 9.80 (s, 1H), 9.61 (d, J = 7.3 Hz, 1H), 7.61 (d, J = 14.3 Hz, 1H), 7.58 (s, 1H), 6.48 (s, 1H), 6.31 (dd, J = 14.2, 7.2 Hz, 1H), 2.66 (t, J = 7.6 Hz, 2H), 1.67 ~ 1.61 (m, 2H), 1.46 ~ 1.39 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 190.5, 185.1, 143.4, 137.8, 129.0, 125.3, 116.4, 107.8, 30.2, 25.5, 22.2, 13.7; ESI-MS calcd for $\text{C}_{12}\text{H}_{15}\text{NO}_2$ $[\text{M}+\text{H}]$: 206.1181, found : 206.1183.

Spectral data for (*E*)-1-(3-oxoprop-1-en-1-yl)-5-(thiophen-3-yl)-1*H*-pyrrole-3-carbaldehyde (3p):



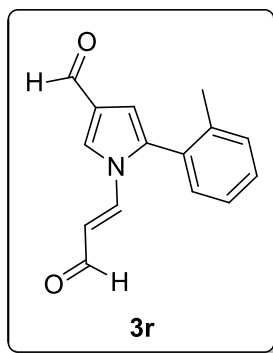
Brown oil (0.096 g, 0.41 mmol, 68 %); ^1H NMR (500 MHz, CDCl_3): δ 9.88 (s, 1H), 9.53 (d, J = 7.5 Hz, 1H), 7.72 (s, 1H), 7.68 (d, J = 14.4 Hz, 1H), 7.49 ~ 7.48 (m, 1H), 7.36 (d, J = 1.5 Hz, 1H), 7.12 (d, J = 5.0 Hz, 1H), 6.77 (s, 1H), 6.35 (dd, J = 14.4, 7.3 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 190.5, 185.1, 144.6, 133.2, 129.7, 129.1, 128.2, 127.3, 125.8, 125.4, 117.1, 110.1; ESI-MS calcd for $\text{C}_{12}\text{H}_9\text{NO}_2\text{S}$ $[\text{M}+\text{H}]$: 232.0432, found : 232.0433.

Spectral data for (*E*)-1-(3-oxoprop-1-en-1-yl)-5-(prop-1-en-2-yl)-1*H*-pyrrole-3-carbaldehyde (3q):



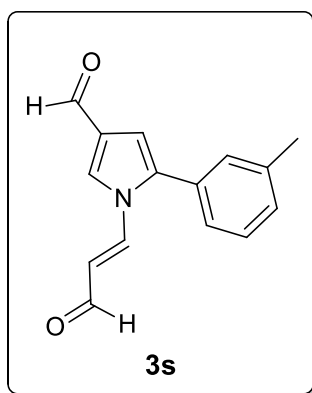
Brown oil (0.096 g, 0.50 mmol, 61 %); ^1H NMR (600 MHz, CDCl_3): δ 9.84 (s, 1H), 9.60 (d, J = 7.4 Hz, 1H), 7.82 (d, J = 14.3 Hz, 1H), 7.63 (s, 1H), 6.67 (s, 1H), 6.35 (dd, J = 14.4, 7.4 Hz, 1H), 5.45 (s, 1H), 5.00 (d, J = 0.5 Hz, 1H), 2.10 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 190.5, 185.1, 145.2, 139.8, 133.8, 128.8, 126.2, 119.2, 117.1, 108.8, 23.6; ESI-MS calcd for $\text{C}_{11}\text{H}_{11}\text{NO}_2$ $[\text{M}+\text{Na}]$: 212.0687, found : 212.0689.

Spectral data for (*E*)-1-(3-oxoprop-1-en-1-yl)-5-(*o*-tolyl)-1*H*-pyrrole-3-carbaldehyde (3r):



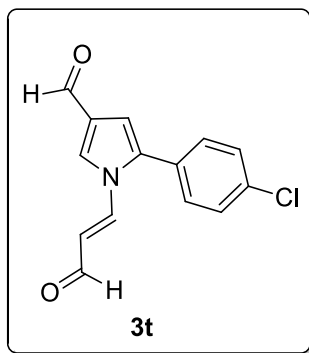
Brown oil (0.098 g, 0.41 mmol, 70 %); ^1H NMR (400 MHz, CDCl_3): δ 9.91 (s, 1H), 9.39 (d, J = 7.4 Hz, 1H), 7.76 (s, 1H), 7.42 ~ 7.38 (m, 1H), 7.34 ~ 7.27 (m, 2H), 7.23 ~ 7.20 (m, 2H), 7.68 (d, J = 1.0 Hz, 1H), 6.28 (dd, J = 14.4, 7.4 Hz, 1H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 190.6, 188.3, 144.4, 138.4, 137.0, 131.5, 130.6, 130.0, 129.1, 128.7, 126.2, 125.0, 116.6, 110.3, 19.9; ESI-MS calcd for $\text{C}_{15}\text{H}_{13}\text{NO}_2$ [$\text{M}+\text{H}$] : 240.1025, found : 240.1026.

Spectral data for (*E*)-1-(3-oxoprop-1-en-1-yl)-5-(*m*-tolyl)-1*H*-pyrrole-3-carbaldehyde (3s):



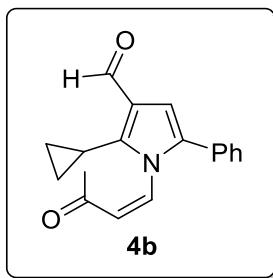
Brown oil (0.101 g, 0.42 mmol, 72 %); ^1H NMR (500 MHz, CDCl_3): δ 9.89 (s, 1H), 9.48 (d, J = 7.4 Hz, 1H), 7.76 (s, 1H), 7.62 (d, J = 14.4 Hz, 1H), 7.37 (t, J = 7.5 Hz, 1H), 7.27 (d, J = 7.5 Hz, 1H), 7.17 (s, 1H), 7.14 (d, J = 7.4 Hz, 1H), 6.75 (s, 1H), 6.35 (dd, J = 14.4, 7.5 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 190.6, 185.2, 145.0, 139.0, 138.4, 130.4, 130.0, 129.3, 129.1, 128.9, 126.8, 125.5, 116.9, 109.9, 21.4; ESI-MS calcd for $\text{C}_{15}\text{H}_{13}\text{NO}_2$ [$\text{M}+\text{H}$] : 240.1025, found : 240.1023.

Spectral data for (*E*)-5-(4-chlorophenyl)-1-(3-oxoprop-1-en-1-yl)-1*H*-pyrrole-3-carbaldehyde (3t):



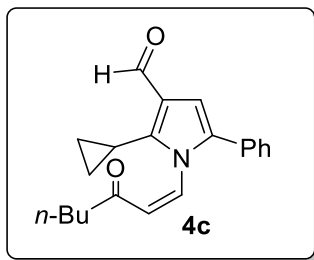
Brown oil (0.099 g, 0.38 mmol, 73 %); ^1H NMR (400 MHz, CDCl_3): δ 9.88 (s, 1H), 9.49(d, J = 7.4 Hz, 1H), 7.77 (s, 1H), 7.55 (d, J = 14.3 Hz, 1H), 7.46 (d, J = 8.0, Hz, 2H), 7.29 (d, J = 8 Hz, 2H), 6.76 (s, 1H), 6.36 (dd, J = 14.4, 7.4 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 190.3, 185.1, 144.3, 136.8, 135.5, 130.9, 129.3, 129.0, 127.8, 125.9, 117.3, 110.4; ESI-MS calcd for $\text{C}_{14}\text{H}_{10}\text{ClNO}_2$ [$\text{M}+\text{H}$] : 260.0478, found : 260.0476.

Spectra data for (Z)-2-cyclopropyl-1-(3-oxobut-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4b)



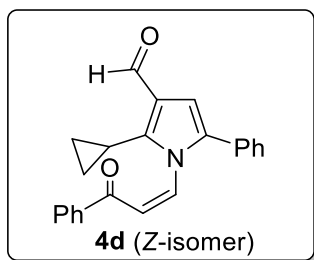
Brown oil (0.138 g, 0.49 mmol, 97 %); ^1H NMR (400 MHz, CDCl_3): δ 10.14 (s, 1H), 7.34 ~ 7.23 (m, 5H), 6.95 (d, J = 8.9 Hz, 1H), 6.64 (s, 1H), 6.09 (d, J = 8.9 Hz, 1H), 1.79 ~ 1.72 (m, 4H), 1.09 ~ 1.04 (m, 2H), 0.81 ~ 0.77 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 196.8, 185.7, 144.3, 135.0, 132.1, 131.1, 128.7, 128.4, 127.9, 127.6, 124.8, 107.8, 29.2, 7.3, 6.1; ESI-MS calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_2$ [$\text{M}+\text{H}$] : 280.1338, found: 280.1332.

Spectra data for (Z)-2-cyclopropyl-1-(3-oxohept-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4c)



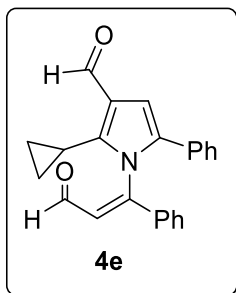
Brown oil (0.140 g, 0.43 mmol, 86 %); ^1H NMR (400 MHz, CDCl_3): δ 10.14 (s, 1H), 7.33 ~ 7.23 (m, 5H), 6.90 (d, J = 8.9 Hz, 1H), 6.63 (s, 1H), 6.10 (d, J = 8.9 Hz, 1H), 1.96 (t, J = 7.1 Hz, 2H), 1.80 ~ 1.73 (m, 1H), 1.31 ~ 1.23 (m, 2H), 1.15 ~ 1.04 (m, 4H), 0.80 ~ 0.75 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3): δ 198.83, 185.54, 144.26, 134.84, 131.54, 131.24, 128.63, 128.24, 127.44, 126.96, 124.61, 107.70, 42.37, 25.41, 22.18, 13.86, 7.41, 6.38; ESI-MS calcd for $\text{C}_{21}\text{H}_{23}\text{NO}_2$ [M+H] : 322.1807, found: 322.1805.

Spectra data for (Z)-2-cyclopropyl-1-(3-oxo-3-phenylprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4d)



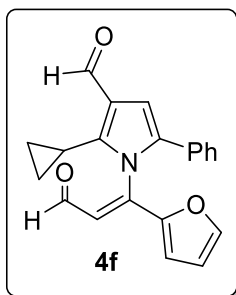
Brown oil (0.170 g, 0.49 mmol, 98 %); ^1H NMR (400 MHz, CDCl_3): δ 10.11 (s, 1H), 7.61 ~ 7.59 (m, 2H), 7.49 ~ 7.44 (m, 1H), 7.31 (t, J = 7.8 Hz, 2H), 7.26 ~ 7.17 (m, 4H), 7.13 ~ 7.09 (m, 2H), 6.72 (d, J = 9.0 Hz, 1H), 6.55 (s, 1H), 1.79 ~ 1.72 (m, 1H), 1.04 ~ 0.99 (m, 2H), 0.83 ~ 0.79 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 189.5, 185.9, 144.5, 136.3, 135.0, 133.3, 133.3, 131.3, 128.9, 128.3, 128.2, 128.2, 127.5, 124.9, 123.9, 107.8, 7.4, 6.3; ESI-MS calcd for $\text{C}_{23}\text{H}_{19}\text{NO}_2$ [M+H] : 342.1494, found: 342.2394.

Spectra data for (Z)-2-cyclopropyl-1-(3-oxo-1-phenylprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4e)



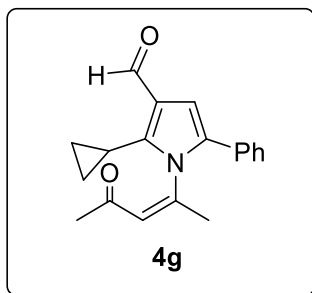
Brown oil (0.168 g, 0.49 mmol, 97 %); ^1H NMR (400 MHz, CDCl_3): δ 10.21 (s, 1H), 9.35 (d, J = 7.4 Hz, 1H), 7.46 (t, J = 7.2 Hz, 1H), 7.39 (t, J = 7.9 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.18 (bs, 5H), 6.81 (s, 1H), 6.58 (d, J = 7.4 Hz, 1H), 1.47 ~ 1.40 (m, 1H), 0.93 ~ 0.66 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ 190.1, 185.8, 152.8, 145.2, 137.8, 135.2, 132.0, 130.7, 129.3, 128.5, 128.0, 124.9, 124.5, 107.8, 7.3, 7.0, 7.0; ESI-MS calcd for $\text{C}_{23}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 342.1494, found: 342.1479.

Spectra data for (Z)-2-cyclopropyl-1-(1-(furan-2-yl)-3-oxoprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4f)



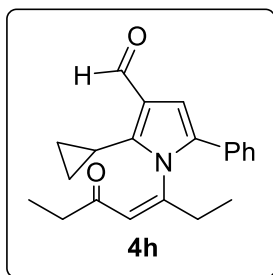
Brown oil (0.199 g, 0.48 mmol, 95 %); ^1H NMR (400 MHz, CDCl_3): δ 10.21 (s, 1H), 9.35 (d, J = 7.4 Hz, 1H), 7.56 (t, J = 7.2 Hz, 1H), 7.18 (bs, 5H), 6.81 (s, 1H), 6.77 (s, 1H), 6.48 ~ 6.44 (m, 2H), 6.58 (d, J = 7.6 Hz, 1H), 1.71 ~ 1.67 (m, 1H), 0.93 ~ 0.93 (m, 4H), 0.92 ~ 0.89 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 189.5, 186.6, 149.6, 146.7, 145.3, 142.1, 137.3, 130.7, 128.5, 128.1, 127.7, 124.7, 121.9, 116.0, 113.1, 107.7, 7.1, 6.7, 6.3 ; ESI-MS calcd for $\text{C}_{23}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 342.1494, found: 342.1479.

Spectra data for (Z)-2-cyclopropyl-1-(4-oxopent-2-en-2-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4g)



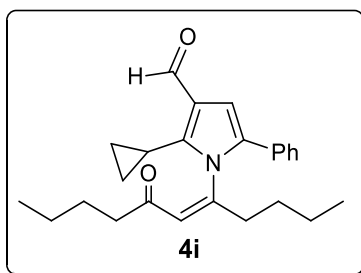
Brown oil (0.149 g, 0.34 mmol, 67 %); ^1H NMR (400 MHz, CDCl_3): δ 10.12 (s, 1H), 7.33 ~ 7.26 (m, 5H), 6.68 (s, 1H), 6.26 (d, J = 1.0 Hz, 1H), 2.20 (s, 3H), 1.86 (s, 3H), 1.75 ~ 1.68 (m, 1H), 1.06 ~ 0.90 (m, 3H), 0.70 ~ 0.64 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 196.3, 185.7, 144.7, 143.2, 133.7, 131.6, 128.7, 128.6, 127.8, 127.7, 124.7, 108.1, 29.2, 24.6, 6.7, 6.4, 6.3; ESI-MS calcd for $\text{C}_{19}\text{H}_{19}\text{NO}_2$ [$\text{M}+\text{H}$] : 294.1494, found: 294.1492.

Spectra data for (Z)-2-cyclopropyl-1-(5-oxohept-3-en-3-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4h)



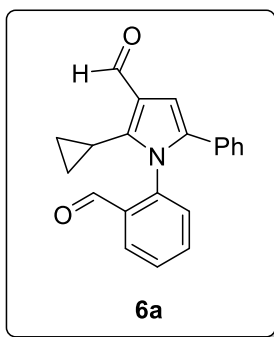
Brown oil (0.116 g, 0.36 mmol, 71 %); ^1H NMR (400 MHz, CDCl_3): δ 10.12 (s, 1H), 7.32 ~ 7.25 (m, 5H), 6.68 (s, 1H), 6.24 (s, 1H), 2.36 ~ 2.21 (m, 3H), 2.08 ~ 1.98 (m, 1H), 1.74 ~ 1.64 (m, 1H), 1.04 (t, J = 7.2 Hz, 3H), 0.98 ~ 0.89 (m, 7H); ^{13}C NMR (100 MHz, CDCl_3): δ 198.9, 185.5, 149.1, 143.0, 133.5, 131.8, 128.3, 127.7, 127.5, 125.1, 124.3, 108.1, 36.0, 30.8, 10.7, 7.6, 6.9, 6.8, 6.7; ESI-MS calcd for $\text{C}_{21}\text{H}_{23}\text{NO}_2$ [$\text{M}+\text{H}$]: 322.1807, found: 322.1808.

Spectra data for (Z)-2-cyclopropyl-1-(7-oxoundec-5-en-5-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4i)



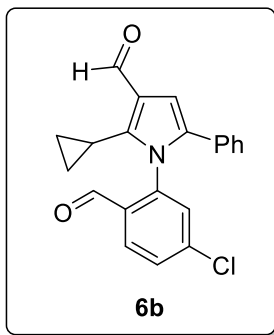
Brown oil (0.103 g, 0.29 mmol, 58 %); ^1H NMR (400 MHz, CDCl_3): δ 10.09 (s, 1H), 7.31 ~ 7.26 (m, 5H), 6.67 (s, 1H), 6.23 (s, 1H), 2.30 ~ 2.17 (m, 3H), 2.08 ~ 2.00 (m, 1H), 1.74 ~ 1.67 (m, 1H), 1.44 ~ 1.33 (m, 4H), 1.28 ~ 1.13 (m, 5H), 0.99 ~ 0.91 (m, 3H), 0.81 ~ 0.78 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) : δ 198.5, 185.4, 148.1, 143.1, 133.5, 131.9, 128.3, 127.8, 127.5, 125.6, 124.2, 108.1, 42.6, 37.3, 28.2, 25.5, 22.3, 22.1, 13.9, 13.8, 7.1, 6.9, 6.9; ESI-MS calcd for $\text{C}_{25}\text{H}_{31}\text{NO}_2$ $[\text{M}+\text{H}]$: 378.2433, found: 378.2429.

Spectra data for 2-cyclopropyl-1-(2-formylphenyl)-5-phenyl-1H-pyrrole-3-carbaldehyde (6a)



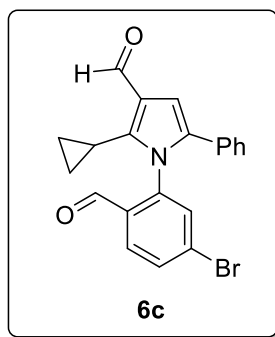
Brown solid (0.157 g, 0.50 mmol, 98 %); ^1H NMR (400 MHz, CDCl_3): δ 10.16 (s, 1H), 9.54 (s, 1H), 7.88 (d, J = 7.7 Hz, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.36 (d, J = 7.8 Hz, 1H), 7.09 ~ 7.07 (m, 3H), 6.96 ~ 6.94 (m, 2H), 6.77 (s, 1H), 1.70 ~ 1.63 (m, 1H), 0.77 ~ 0.58 (m, 3H), 0.49 ~ 0.43 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 188.4, 185.6, 145.1, 140.3, 136.8, 134.4, 132.6, 130.8, 129.8, 129.2, 128.6, 128.2, 128.2, 127.3, 124.2, 107.2, 6.9, 6.9, 6.7; ESI-MS calcd for $\text{C}_{21}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{H}]$: 316.1338, found: 316.1332.

Spectra data for 1-(5-chloro-2-formylphenyl)-2-cyclopropyl-5-phenyl-1H-pyrrole-3-carbaldehyde (6b)



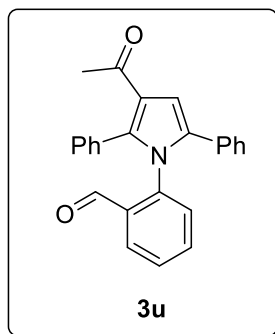
Brown sticky oil (0.172 g, 0.49 mmol, 96 %); ^1H NMR (400 MHz, CDCl_3): δ 10.19 (s, 1H), 9.50 (s, 1H), 7.86 (d, J = 2.4 Hz, 1H), 7.61 (dd, J = 8.4, 2.4 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.16 (t, J = 2.8 Hz, 3H), 6.98 ~ 6.96 (m, 2H), 6.79 (s, 1H), 1.70 ~ 1.63 (m, 1H), 0.87 ~ 0.74 (m, 2H), 0.66 ~ 0.61 (m, 1H), 0.52 ~ 0.47 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 187.1, 185.7, 145.13, 138.9, 137.0, 135.7, 134.4, 133.8, 131.2, 130.6, 128.5, 128.5, 127.7, 124.6, 107.7, 7.3, 7.2, 6.8; ESI-MS calcd for $\text{C}_{21}\text{H}_{16}\text{ClNO}_2$ [M+H] : 350.0948, found: 350.0940.

Spectra data for 1-(5-bromo-2-formylphenyl)-2-cyclopropyl-5-phenyl-1H-pyrrole-3-carbaldehyde (6c)



Brown sticky oil (0.190 g, 0.48 mmol, 94 %); ^1H NMR (400 MHz, CDCl_3): δ 10.19 (s, 1H), 9.49 (s, 1H), 8.01 (d, J = 2.2 Hz, 1H), 7.78 (dd, J = 2.2, 8.3 Hz, 1H), 7.25 (d, J = 8.4 Hz, 1H), 7.16 (t, J = 2.9 Hz, 3H), 6.99 ~ 6.96 (m, 2H), 6.79 (s, 1H), 1.70 ~ 1.63 (m, 1H), 0.87 ~ 0.75 (m, 2H), 0.66 ~ 0.61 (m, 1H), 0.52 ~ 0.47 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 187.0, 185.7, 145.0, 139.4, 137.3, 137.0, 134.0, 131.5, 131.4, 130.6, 128.5, 128.5, 127.8, 124.6, 123.5, 107.7, 7.3, 7.2, 6.8; ESI-MS calcd for $\text{C}_{21}\text{H}_{16}\text{BrNO}_2$ [M+H] : 394.0443, found: 394.0436.

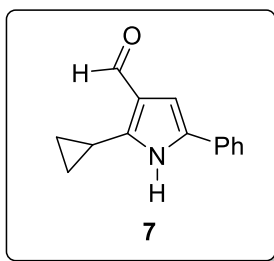
Spectra data for 2-(3-acetyl-2,5-diphenyl-1H-pyrrol-1-yl)benzaldehyde (3u)



Brown sticky solid (0.120 g, 0.32 mmol, 81 %); ^1H NMR (400 MHz, CDCl_3): δ 9.56 (s, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.41 (t, J = 7.2 Hz, 1H), 7.33 (t, J = 7.2 Hz, 1H), 7.24 ~ 7.18 (m, 2H),

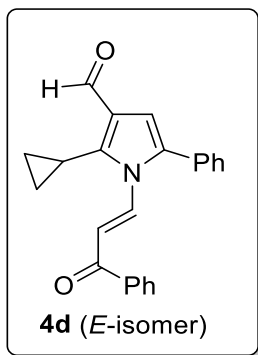
7.17 ~ 7.13 (m, 1H), 7.13 ~ 7.11 (m, 6H), 7.05 ~ 7.02 (m, 2H), 6.98 (s, 1H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 194.3, 188.4, 140.3, 140.0, 136.6, 134.0, 132.9, 131.3, 131.2, 131.1, 130.6, 129.0, 128.7, 128.6, 128.3, 128.3, 128.0, 127.5, 124.5, 124.5, 110.2, 29.2; ESI-MS calcd for $\text{C}_{25}\text{H}_{19}\text{NO}_2$ [M+H] : 366.1494, found: 366.1475.

Spectra data for 2-cyclopropyl-5-phenyl-1H-pyrrole-3-carbaldehyde (7)



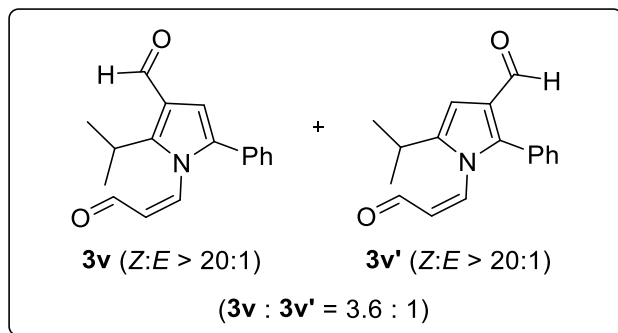
Yellow oil (0.040 g, 0.19 mmol, 65 %); ^1H NMR (400 MHz, CDCl_3): δ 10.04 (s, 1H), 8.45 (bs, 1H), 7.43 (d, $J = 8.0$ Hz, 2H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.24 (t, $J = 6.4$ Hz, 1H), 6.80 (d, $J = 2.4$ Hz, 1H), 2.37 ~ 2.30 (m, 1H), 1.13 ~ 1.08 (m, 2H), 0.89 ~ 0.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3): δ 185.5, 144.1, 131.5, 131.2, 129.0, 127.1, 124.4, 124.0, 105.1, 7.3, 7.2 ; ESI-MS calcd for $\text{C}_{14}\text{H}_{13}\text{NO}$ [M+H] : 212.1075, found: 212.1079.

Spectra data for (E)-2-cyclopropyl-1-(3-oxo-3-phenylprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (4d)



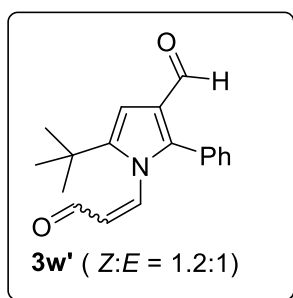
Brown oil (0.170 g, 0.49 mmol, 98 %); ^1H NMR (400 MHz, CDCl_3): δ 10.27 (s, 1H), 8.33 (d, $J = 14.0$ Hz, 1H), 7.60 (d, $J = 8$ Hz, 2H), 7.51 (t, $J = 7.6$ Hz, 1H), 7.46 ~ 7.35 (m, 7H), 6.70 (d, $J = 14.4$ Hz, 1H), 6.65 (s, 1H), 2.02 ~ 1.98 (m, 1H), 1.31 ~ 1.26 (m, 2H), 0.95 ~ 0.91 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 188.8, 185.9, 145.0, 137.5, 135.5, 133.0, 131.9, 129.4, 128.8, 128.5, 128.4, 128.0, 125.7, 114.9, 110.4, 7.57, 6.18; ESI-MS calcd for $\text{C}_{23}\text{H}_{19}\text{NO}_2$ [M+H] : 342.1494, found: 342.2394.

Spectra data for (Z)-2-isopropyl-1-(3-oxoprop-1-en-1-yl)-5-phenyl-1H-pyrrole-3-carbaldehyde (3v+3v')



Brown oil (0.095 g, 0.35 mmol, 70 %); ^1H NMR for major isomer (**3u**) (400 MHz, CDCl_3): δ 10.11 (s, 1H), 9.24 (d, $J = 7.6$ Hz, 1H), 7.57 (d, $J = 7.2$ Hz, 1H), 7.39 ~ 7.23 (m, 5H), 6.74 (s, 1H), 5.98 (t, $J = 8.1$ Hz, 1H), 3.47 ~ 3.40 (m, 1H), 1.45 (s, 3H), 1.43 (s, 3H); ^1H NMR for minor isomer (**3u'**) δ 9.59 (s, 1H), 9.30 (d, $J = 7.6$ Hz, 1H), 6.60 (s, 1H), 5.90 (t, $J = 8.2$ Hz, 1H), 2.90 ~ 2.84 (m, 1H), 1.26 (s, 3H), 1.24 (s, 3H), rest of the peaks merged with others; ^{13}C NMR for major isomer (**3u**) (100 MHz, CDCl_3): δ 188.18, 185.08, 148.85, 138.75, 136.12, 131.06, 129.12, 128.52, 128.45, 127.78, 123.13, 110.26, 27.14, 22.80; ^{13}C NMR for minor isomer (**3u'**): δ 188.0, 186.4, 143.7, 138.0, 130.2, 29.0, 128.6, 127.1, 124.2, 103.8, 26.22, 22.4, rest of the peaks merged with others; ESI-MS calcd for $\text{C}_{17}\text{H}_{17}\text{NO}_2$ [$\text{M}+\text{H}$] : 268.1332, found: 268.1334.

Spectra data for (Z)-5-(tert-butyl)-1-(3-oxoprop-1-en-1-yl)-2-phenyl-1H-pyrrole-3-carbaldehyde (3w')



Brown oil (0.098 g, 0.35 mmol, 71 %); ^1H NMR for major isomer (400 MHz, $d\text{-CDCl}_3$): δ 9.57 (s, 1H), 9.20 (d, $J = 7.6$ Hz, 1H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.45 ~ 7.24 (m, 5H), 6.65 (s, 1H), 5.88 (t, $J = 7.8$ Hz, 1H), 1.38 (s, 9H); ^1H NMR for minor isomer δ 9.48 (s, 1H), 9.39 (d, $J = 7.2$ Hz, 1H), 7.87 (d, $J = 14.4$ Hz, 1H), 7.45 ~ 7.24 (m, 5H), 6.65 (s, 1H), 5.29 (dd, $J = 14.4, 7.2$ Hz, 1H), 1.45 (s, 9H); ^{13}C NMR for major isomer (100 MHz, $d\text{-CDCl}_3$): δ 187.99, 186.74, 145.71, 145.35,

143.38, 140.2, 130.39, 129.03, 128.59, 128.15, 123.11, 105.20, 32.64, 30.26; ^{13}C NMR for minor isomer: δ 190.5, 186.6, 145.9, 145.2, 144.3, 131.3, 129.6, 128.9, 128.0, 125.8, 123.5, 106.0, 32.4, 30.7; ESI-MS calcd for $\text{C}_{18}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{H}]$: 282.1494, found: 282.1486.

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

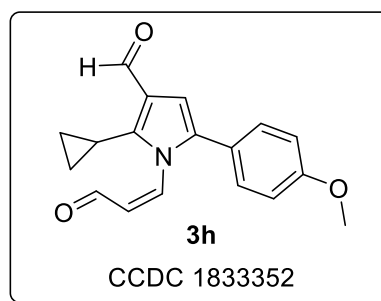
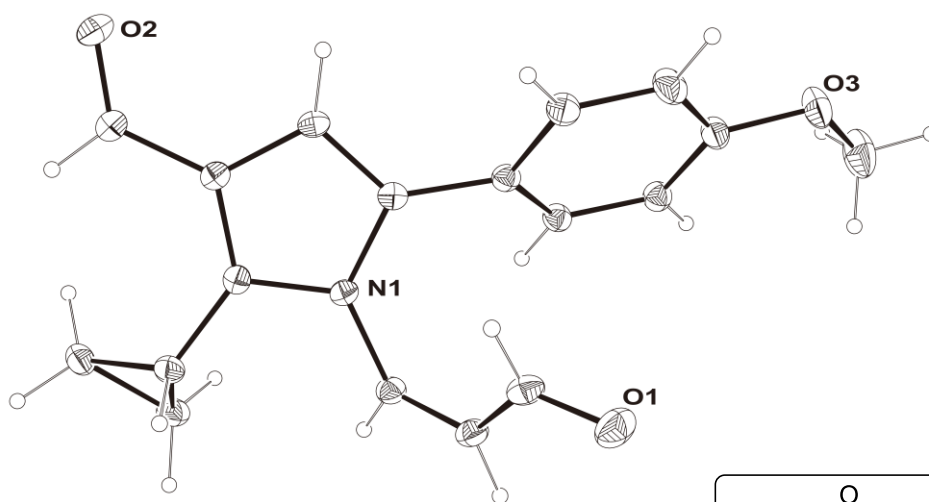


Table S1. Crystal data and structure refinement for d19782.

Identification code	d19782	
Empirical formula	$\text{C}_{18}\text{H}_{17}\text{N O}_3$	
Formula weight	295.33	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	$a = 9.6853(4)$ Å	$\alpha = 90^\circ$.
	$b = 6.6511(2)$ Å	$\beta = 100.113(2)^\circ$.
	$c = 24.7893(12)$ Å	$\gamma = 90^\circ$.
Volume	$1572.06(11)$ Å ³	
Z	4	

Density (calculated)	1.248 Mg/m ³
Absorption coefficient	0.085 mm ⁻¹
F(000)	624
Crystal size	0.41 x 0.14 x 0.06 mm ³
Theta range for data collection	2.47 to 25.04°.
Index ranges	-11<=h<=11, -7<=k<=7, -29<=l<=29
Reflections collected	16974
Independent reflections	2754 [R(int) = 0.0435]
Completeness to theta = 25.04°	99.4 %
Absorption correction	multi-scan
Max. and min. transmission	0.9949 and 0.9659
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2754 / 0 / 201
Goodness-of-fit on F ²	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.0911
R indices (all data)	R1 = 0.0538, wR2 = 0.1022
Extinction coefficient	0.023(3)
Largest diff. peak and hole	0.171 and -0.164 e.Å ⁻³

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for d19782. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1297(2)	7142(2)	5182(1)	35(1)
C(2)	538(2)	8001(2)	5515(1)	38(1)
C(3)	1066(2)	9288(2)	5979(1)	42(1)
C(4)	3459(2)	7485(2)	4810(1)	30(1)
C(5)	2648(2)	7855(2)	4258(1)	36(1)
C(6)	1857(2)	6156(3)	3938(1)	44(1)
C(7)	3102(2)	7052(3)	3752(1)	44(1)
C(8)	4874(2)	7569(2)	5020(1)	30(1)
C(9)	5991(2)	7898(2)	4713(1)	35(1)
C(10)	5041(2)	7233(2)	5594(1)	32(1)
C(11)	3760(2)	6935(2)	5731(1)	31(1)
C(12)	3415(2)	6240(2)	6254(1)	32(1)
C(13)	4083(2)	7087(3)	6746(1)	42(1)

C(14)	3835(2)	6382(3)	7242(1)	49(1)
C(15)	2902(2)	4806(3)	7260(1)	43(1)
C(16)	1725(3)	2662(4)	7805(1)	80(1)
C(17)	2241(2)	3923(2)	6779(1)	38(1)
C(18)	2504(2)	4640(2)	6281(1)	35(1)
N(1)	2772(1)	7129(2)	5244(1)	30(1)
O(1)	346(1)	9838(2)	6306(1)	59(1)
O(2)	7234(1)	7889(2)	4913(1)	45(1)
O(3)	2707(2)	4232(2)	7772(1)	60(1)

Table S3. Bond lengths [Å] and angles [°] for d19782.

C(1)-C(2)	1.328(2)
C(1)-N(1)	1.4093(19)
C(1)-H(1)	0.9500
C(2)-C(3)	1.451(2)
C(2)-H(2)	0.9500
C(3)-O(1)	1.216(2)
C(3)-H(3)	0.9500
C(4)-C(8)	1.379(2)
C(4)-N(1)	1.3824(19)
C(4)-C(5)	1.473(2)
C(5)-C(7)	1.500(2)
C(5)-C(6)	1.510(2)
C(5)-H(5)	1.0000
C(6)-C(7)	1.490(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(10)	1.420(2)
C(8)-C(9)	1.446(2)
C(9)-O(2)	1.2190(19)
C(9)-H(9)	0.9500
C(10)-C(11)	1.357(2)
C(10)-H(10)	0.9500

C(11)-N(1)	1.4076(19)
C(11)-C(12)	1.470(2)
C(12)-C(18)	1.391(2)
C(12)-C(13)	1.395(2)
C(13)-C(14)	1.376(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(3)
C(14)-H(14)	0.9500
C(15)-O(3)	1.370(2)
C(15)-C(17)	1.383(2)
C(16)-O(3)	1.424(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.387(2)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(2)-C(1)-N(1)	126.57(15)
C(2)-C(1)-H(1)	116.7
N(1)-C(1)-H(1)	116.7
C(1)-C(2)-C(3)	126.09(15)
C(1)-C(2)-H(2)	117.0
C(3)-C(2)-H(2)	117.0
O(1)-C(3)-C(2)	122.79(16)
O(1)-C(3)-H(3)	118.6
C(2)-C(3)-H(3)	118.6
C(8)-C(4)-N(1)	107.13(13)
C(8)-C(4)-C(5)	132.63(14)
N(1)-C(4)-C(5)	120.01(13)
C(4)-C(5)-C(7)	122.02(14)
C(4)-C(5)-C(6)	120.09(13)
C(7)-C(5)-C(6)	59.33(11)
C(4)-C(5)-H(5)	114.7
C(7)-C(5)-H(5)	114.7
C(6)-C(5)-H(5)	114.7
C(7)-C(6)-C(5)	60.02(11)

C(7)-C(6)-H(6A)	117.8
C(5)-C(6)-H(6A)	117.8
C(7)-C(6)-H(6B)	117.8
C(5)-C(6)-H(6B)	117.8
H(6A)-C(6)-H(6B)	114.9
C(6)-C(7)-C(5)	60.65(11)
C(6)-C(7)-H(7A)	117.7
C(5)-C(7)-H(7A)	117.7
C(6)-C(7)-H(7B)	117.7
C(5)-C(7)-H(7B)	117.7
H(7A)-C(7)-H(7B)	114.8
C(4)-C(8)-C(10)	107.67(13)
C(4)-C(8)-C(9)	126.35(15)
C(10)-C(8)-C(9)	125.97(14)
O(2)-C(9)-C(8)	124.16(16)
O(2)-C(9)-H(9)	117.9
C(8)-C(9)-H(9)	117.9
C(11)-C(10)-C(8)	108.96(13)
C(11)-C(10)-H(10)	125.5
C(8)-C(10)-H(10)	125.5
C(10)-C(11)-N(1)	106.64(13)
C(10)-C(11)-C(12)	128.78(14)
N(1)-C(11)-C(12)	123.99(13)
C(18)-C(12)-C(13)	117.86(15)
C(18)-C(12)-C(11)	121.83(14)
C(13)-C(12)-C(11)	120.14(14)
C(14)-C(13)-C(12)	121.11(16)
C(14)-C(13)-H(13)	119.4
C(12)-C(13)-H(13)	119.4
C(13)-C(14)-C(15)	120.15(16)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
O(3)-C(15)-C(17)	124.22(16)
O(3)-C(15)-C(14)	115.89(16)
C(17)-C(15)-C(14)	119.88(15)
O(3)-C(16)-H(16A)	109.5

O(3)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(3)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-C(18)	119.42(16)
C(15)-C(17)-H(17)	120.3
C(18)-C(17)-H(17)	120.3
C(17)-C(18)-C(12)	121.56(15)
C(17)-C(18)-H(18)	119.2
C(12)-C(18)-H(18)	119.2
C(4)-N(1)-C(11)	109.57(12)
C(4)-N(1)-C(1)	122.09(13)
C(11)-N(1)-C(1)	128.16(13)
C(15)-O(3)-C(16)	117.46(15)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d19782. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	28(1)	38(1)	39(1)	3(1)	3(1)	-4(1)
C(2)	27(1)	38(1)	48(1)	5(1)	6(1)	0(1)
C(3)	33(1)	36(1)	55(1)	1(1)	7(1)	7(1)
C(4)	34(1)	22(1)	34(1)	0(1)	9(1)	1(1)
C(5)	36(1)	33(1)	38(1)	4(1)	5(1)	6(1)
C(6)	40(1)	51(1)	38(1)	-4(1)	-1(1)	2(1)
C(7)	49(1)	51(1)	33(1)	6(1)	7(1)	6(1)
C(8)	30(1)	22(1)	38(1)	-1(1)	7(1)	2(1)
C(9)	34(1)	27(1)	43(1)	-3(1)	10(1)	-1(1)
C(10)	27(1)	28(1)	38(1)	-4(1)	2(1)	0(1)
C(11)	31(1)	27(1)	33(1)	-3(1)	3(1)	0(1)
C(12)	31(1)	33(1)	33(1)	-2(1)	5(1)	4(1)
C(13)	41(1)	46(1)	39(1)	-6(1)	4(1)	-7(1)
C(14)	55(1)	56(1)	34(1)	-10(1)	1(1)	-8(1)

C(15)	48(1)	50(1)	31(1)	2(1)	8(1)	5(1)
C(16)	106(2)	87(2)	53(1)	16(1)	29(1)	-18(2)
C(17)	39(1)	37(1)	38(1)	2(1)	9(1)	0(1)
C(18)	36(1)	35(1)	33(1)	-3(1)	4(1)	0(1)
N(1)	26(1)	29(1)	34(1)	-1(1)	5(1)	-1(1)
O(1)	50(1)	64(1)	66(1)	-14(1)	19(1)	11(1)
O(2)	30(1)	52(1)	56(1)	-10(1)	10(1)	-4(1)
O(3)	77(1)	71(1)	33(1)	6(1)	13(1)	-5(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d19782.

	x	y	z	U(eq)
H(1)	796	6467	4870	42
H(2)	-443	7750	5444	45
H(3)	2015	9719	6028	50
H(5)	2164	9188	4212	43
H(6A)	1957	4794	4101	53
H(6B)	920	6457	3722	53
H(7A)	2935	7903	3419	53
H(7B)	3972	6241	3798	53
H(9)	5741	8138	4330	41
H(10)	5909	7219	5841	38
H(13)	4720	8168	6738	51
H(14)	4303	6974	7573	59
H(16A)	811	3032	7592	120
H(16B)	1635	2457	8189	120
H(16C)	2055	1418	7659	120
H(17)	1610	2834	6788	46
H(18)	2053	4025	5951	42

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

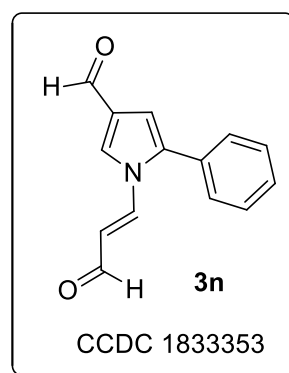
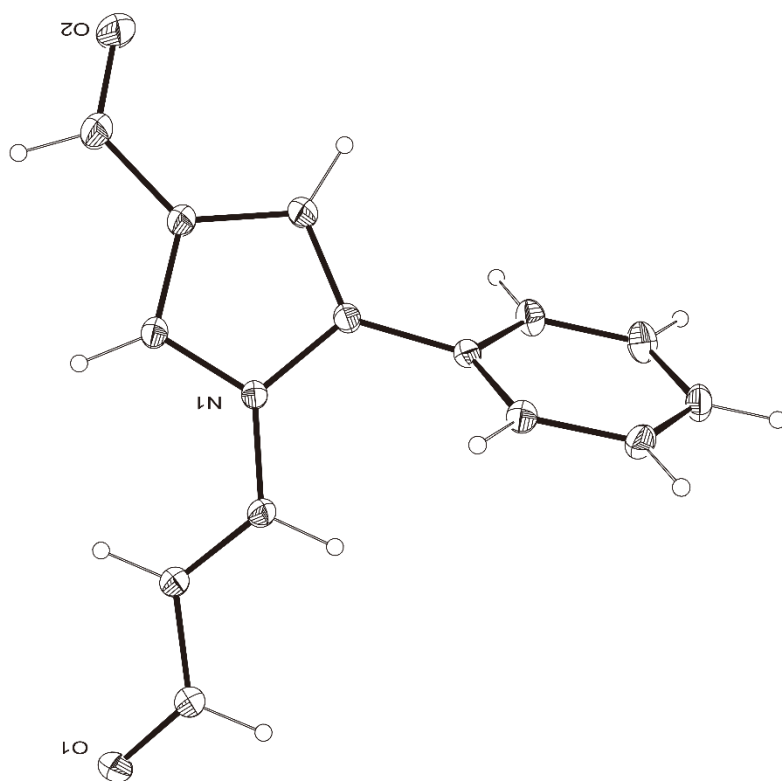


Table S6. Crystal data and structure refinement for d19435.

Identification code	d19435	
Empirical formula	C ₁₄ H ₁₁ N O ₂	
Formula weight	225.24	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 14.4905(6) Å b = 16.4449(7) Å c = 15.5684(8) Å	α = 90°. β = 111.546(2)°. γ = 90°.
Volume	3450.6(3) Å ³	

Z	12
Density (calculated)	1.301 Mg/m ³
Absorption coefficient	0.088 mm ⁻¹
F(000)	1416
Crystal size	0.35 x 0.34 x 0.05 mm ³
Theta range for data collection	2.41 to 25.04°.
Index ranges	-17<=h<=17, -19<=k<=19, -18<=l<=18
Reflections collected	41471
Independent reflections	6070 [R(int) = 0.0907]
Completeness to theta = 25.04°	99.6 %
Absorption correction	multi-scan
Max. and min. transmission	0.9956 and 0.9699
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6070 / 0 / 460
Goodness-of-fit on F ²	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.1046
R indices (all data)	R1 = 0.0891, wR2 = 0.1301
Largest diff. peak and hole	0.170 and -0.230 e.Å ⁻³

Table S7. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for d19435. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8426(2)	-1394(1)	6200(2)	38(1)
C(2)	8098(2)	-670(1)	5661(2)	35(1)
C(3)	7217(1)	-634(1)	4976(1)	31(1)
C(4)	5832(1)	171(1)	3863(1)	29(1)
C(5)	5057(1)	-456(1)	3672(1)	29(1)
C(6)	5128(2)	-1202(1)	3286(2)	35(1)
C(7)	4352(2)	-1753(1)	3051(2)	40(1)
C(8)	3499(2)	-1565(2)	3206(2)	43(1)
C(9)	3423(2)	-827(2)	3590(2)	45(1)
C(10)	4191(2)	-273(1)	3818(2)	38(1)
C(11)	5753(2)	945(1)	3557(2)	39(1)
C(12)	6712(2)	1311(1)	3909(2)	38(1)
C(13)	7355(2)	748(1)	4443(2)	34(1)

C(14)	7014(2)	2120(2)	3757(2)	54(1)
C(15)	4577(2)	3888(1)	2537(2)	41(1)
C(16)	4910(2)	4634(1)	3041(2)	37(1)
C(17)	5537(2)	4609(1)	3909(2)	38(1)
C(18)	6625(2)	5259(1)	5380(2)	36(1)
C(19)	7214(2)	4532(1)	5781(2)	38(1)
C(20)	7692(2)	4084(2)	5311(2)	47(1)
C(21)	8288(2)	3432(2)	5735(2)	57(1)
C(22)	8412(2)	3219(2)	6625(2)	56(1)
C(23)	7950(2)	3663(2)	7095(2)	56(1)
C(24)	7356(2)	4315(2)	6681(2)	48(1)
C(25)	6670(2)	6011(2)	5749(2)	40(1)
C(26)	5931(2)	6505(1)	5107(2)	38(1)
C(27)	5452(2)	6037(1)	4351(2)	40(1)
C(28)	5689(2)	7346(2)	5224(2)	50(1)
C(29)	5537(2)	3726(1)	570(2)	40(1)
C(30)	5844(2)	4436(1)	1149(2)	36(1)
C(31)	6727(1)	4473(1)	1825(1)	31(1)
C(32)	8026(1)	5196(1)	3140(1)	30(1)
C(33)	8799(1)	4560(1)	3409(1)	29(1)
C(34)	8603(2)	3743(1)	3504(1)	34(1)
C(35)	9377(2)	3188(1)	3841(2)	40(1)
C(36)	10347(2)	3446(2)	4093(2)	44(1)
C(37)	10544(2)	4251(2)	4003(2)	45(1)
C(38)	9781(2)	4806(1)	3661(2)	37(1)
C(39)	8068(2)	5939(1)	3524(2)	35(1)
C(40)	7144(1)	6340(1)	3076(2)	32(1)
C(41)	6559(1)	5825(1)	2410(1)	31(1)
C(42)	6821(2)	7130(1)	3268(2)	40(1)
N(1)	6841(1)	42(1)	4424(1)	29(1)
N(2)	5867(1)	5275(1)	4497(1)	36(1)
N(3)	7078(1)	5121(1)	2435(1)	29(1)
O(1)	9205(1)	-1452(1)	6860(1)	51(1)
O(2)	6472(1)	2650(1)	3305(2)	82(1)
O(3)	3987(1)	3847(1)	1744(1)	49(1)
O(4)	6159(1)	7766(1)	5880(1)	68(1)

O(5)	4754(1)	3670(1)	-80(1)	54(1)
O(6)	7325(1)	7608(1)	3845(1)	55(1)

Table S8. Bond lengths [Å] and angles [°] for d19435.

C(1)-O(1)	1.219(2)
C(1)-C(2)	1.433(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.331(3)
C(2)-H(2)	0.9500
C(3)-N(1)	1.387(3)
C(3)-H(3)	0.9500
C(4)-C(11)	1.349(3)
C(4)-N(1)	1.417(2)
C(4)-C(5)	1.473(3)
C(5)-C(6)	1.387(3)
C(5)-C(10)	1.388(3)
C(6)-C(7)	1.385(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.378(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.375(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.380(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.426(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.359(3)
C(12)-C(14)	1.446(3)
C(13)-N(1)	1.375(3)
C(13)-H(13)	0.9500
C(14)-O(2)	1.211(3)
C(14)-H(14)	0.9500
C(15)-O(3)	1.218(2)
C(15)-C(16)	1.442(3)
C(15)-H(15)	0.9500

C(16)-C(17)	1.322(3)
C(16)-H(16)	0.9500
C(17)-N(2)	1.395(3)
C(17)-H(17)	0.9500
C(18)-C(25)	1.355(3)
C(18)-N(2)	1.410(3)
C(18)-C(19)	1.469(3)
C(19)-C(24)	1.386(3)
C(19)-C(20)	1.390(3)
C(20)-C(21)	1.383(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.376(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.370(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.377(3)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.421(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.363(3)
C(26)-C(28)	1.454(3)
C(27)-N(2)	1.371(3)
C(27)-H(27)	0.9500
C(28)-O(4)	1.215(3)
C(28)-H(28)	0.9500
C(29)-O(5)	1.216(2)
C(29)-C(30)	1.441(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.326(3)
C(30)-H(30)	0.9500
C(31)-N(3)	1.394(3)
C(31)-H(31)	0.9500
C(32)-C(39)	1.352(3)
C(32)-N(3)	1.414(2)
C(32)-C(33)	1.477(3)

C(33)-C(38)	1.390(3)
C(33)-C(34)	1.393(3)
C(34)-C(35)	1.391(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.380(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.372(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.382(3)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(39)-C(40)	1.425(3)
C(39)-H(39)	0.9500
C(40)-C(41)	1.365(3)
C(40)-C(42)	1.448(3)
C(41)-N(3)	1.373(3)
C(41)-H(41)	0.9500
C(42)-O(6)	1.216(3)
C(42)-H(42)	0.9500
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(1)	121.4(2)
C(3)-C(2)-H(2)	119.3
C(1)-C(2)-H(2)	119.3
C(2)-C(3)-N(1)	125.12(19)
C(2)-C(3)-H(3)	117.4
N(1)-C(3)-H(3)	117.4
C(11)-C(4)-N(1)	107.10(17)
C(11)-C(4)-C(5)	129.05(18)
N(1)-C(4)-C(5)	123.85(18)
C(6)-C(5)-C(10)	118.61(19)
C(6)-C(5)-C(4)	122.29(19)
C(10)-C(5)-C(4)	118.92(19)
C(7)-C(6)-C(5)	120.7(2)
C(7)-C(6)-H(6)	119.7

C(5)-C(6)-H(6)	119.7
C(8)-C(7)-C(6)	120.1(2)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(9)-C(8)-C(7)	119.6(2)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(8)-C(9)-C(10)	120.5(2)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(9)-C(10)-C(5)	120.5(2)
C(9)-C(10)-H(10)	119.8
C(5)-C(10)-H(10)	119.8
C(4)-C(11)-C(12)	108.57(19)
C(4)-C(11)-H(11)	125.7
C(12)-C(11)-H(11)	125.7
C(13)-C(12)-C(11)	107.45(19)
C(13)-C(12)-C(14)	123.0(2)
C(11)-C(12)-C(14)	129.5(2)
C(12)-C(13)-N(1)	108.55(17)
C(12)-C(13)-H(13)	125.7
N(1)-C(13)-H(13)	125.7
O(2)-C(14)-C(12)	125.9(2)
O(2)-C(14)-H(14)	117.1
C(12)-C(14)-H(14)	117.1
O(3)-C(15)-C(16)	124.7(2)
O(3)-C(15)-H(15)	117.7
C(16)-C(15)-H(15)	117.7
C(17)-C(16)-C(15)	119.8(2)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(16)-C(17)-N(2)	125.9(2)
C(16)-C(17)-H(17)	117.0
N(2)-C(17)-H(17)	117.0
C(25)-C(18)-N(2)	107.19(19)
C(25)-C(18)-C(19)	129.3(2)

N(2)-C(18)-C(19)	123.5(2)
C(24)-C(19)-C(20)	118.5(2)
C(24)-C(19)-C(18)	119.1(2)
C(20)-C(19)-C(18)	122.2(2)
C(21)-C(20)-C(19)	120.3(2)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	120.4(3)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(23)-C(22)-C(21)	119.6(2)
C(23)-C(22)-H(22)	120.2
C(21)-C(22)-H(22)	120.2
C(22)-C(23)-C(24)	120.6(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(23)-C(24)-C(19)	120.6(3)
C(23)-C(24)-H(24)	119.7
C(19)-C(24)-H(24)	119.7
C(18)-C(25)-C(26)	108.4(2)
C(18)-C(25)-H(25)	125.8
C(26)-C(25)-H(25)	125.8
C(27)-C(26)-C(25)	107.3(2)
C(27)-C(26)-C(28)	125.1(2)
C(25)-C(26)-C(28)	127.5(2)
C(26)-C(27)-N(2)	108.66(19)
C(26)-C(27)-H(27)	125.7
N(2)-C(27)-H(27)	125.7
O(4)-C(28)-C(26)	124.1(2)
O(4)-C(28)-H(28)	118.0
C(26)-C(28)-H(28)	118.0
O(5)-C(29)-C(30)	124.1(2)
O(5)-C(29)-H(29)	117.9
C(30)-C(29)-H(29)	117.9
C(31)-C(30)-C(29)	121.3(2)
C(31)-C(30)-H(30)	119.3

C(29)-C(30)-H(30)	119.4
C(30)-C(31)-N(3)	125.47(19)
C(30)-C(31)-H(31)	117.3
N(3)-C(31)-H(31)	117.3
C(39)-C(32)-N(3)	107.22(17)
C(39)-C(32)-C(33)	127.52(18)
N(3)-C(32)-C(33)	125.23(18)
C(38)-C(33)-C(34)	118.64(19)
C(38)-C(33)-C(32)	117.68(19)
C(34)-C(33)-C(32)	123.39(18)
C(35)-C(34)-C(33)	120.3(2)
C(35)-C(34)-H(34)	119.8
C(33)-C(34)-H(34)	119.8
C(36)-C(35)-C(34)	120.1(2)
C(36)-C(35)-H(35)	119.9
C(34)-C(35)-H(35)	119.9
C(37)-C(36)-C(35)	119.7(2)
C(37)-C(36)-H(36)	120.1
C(35)-C(36)-H(36)	120.1
C(36)-C(37)-C(38)	120.7(2)
C(36)-C(37)-H(37)	119.6
C(38)-C(37)-H(37)	119.6
C(37)-C(38)-C(33)	120.5(2)
C(37)-C(38)-H(38)	119.8
C(33)-C(38)-H(38)	119.8
C(32)-C(39)-C(40)	108.65(18)
C(32)-C(39)-H(39)	125.7
C(40)-C(39)-H(39)	125.7
C(41)-C(40)-C(39)	107.12(19)
C(41)-C(40)-C(42)	123.75(19)
C(39)-C(40)-C(42)	129.11(19)
C(40)-C(41)-N(3)	108.74(17)
C(40)-C(41)-H(41)	125.6
N(3)-C(41)-H(41)	125.6
O(6)-C(42)-C(40)	125.5(2)
O(6)-C(42)-H(42)	117.3

C(40)-C(42)-H(42)	117.3
C(13)-N(1)-C(3)	125.25(16)
C(13)-N(1)-C(4)	108.31(16)
C(3)-N(1)-C(4)	125.72(17)
C(27)-N(2)-C(17)	125.81(18)
C(27)-N(2)-C(18)	108.36(18)
C(17)-N(2)-C(18)	125.59(19)
C(41)-N(3)-C(31)	124.50(16)
C(41)-N(3)-C(32)	108.25(16)
C(31)-N(3)-C(32)	127.16(17)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d19435. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	33(1)	31(1)	45(1)	1(1)	9(1)	0(1)
C(2)	32(1)	27(1)	42(1)	0(1)	10(1)	-1(1)
C(3)	29(1)	24(1)	39(1)	-1(1)	12(1)	0(1)
C(4)	25(1)	30(1)	31(1)	-2(1)	7(1)	-1(1)
C(5)	28(1)	28(1)	28(1)	0(1)	6(1)	-1(1)
C(6)	33(1)	33(1)	38(1)	-1(1)	11(1)	-2(1)
C(7)	45(1)	30(1)	38(1)	-3(1)	9(1)	-8(1)
C(8)	34(1)	47(2)	40(1)	1(1)	6(1)	-16(1)
C(9)	32(1)	57(2)	49(2)	-9(1)	17(1)	-8(1)
C(10)	32(1)	43(1)	40(1)	-10(1)	12(1)	-3(1)
C(11)	28(1)	33(1)	50(2)	4(1)	8(1)	3(1)
C(12)	32(1)	27(1)	49(1)	0(1)	10(1)	-3(1)
C(13)	28(1)	28(1)	43(1)	-1(1)	10(1)	-4(1)
C(14)	41(1)	33(2)	81(2)	5(1)	14(1)	-5(1)
C(15)	33(1)	37(1)	46(2)	2(1)	7(1)	1(1)
C(16)	31(1)	36(1)	38(1)	1(1)	8(1)	-2(1)
C(17)	33(1)	35(1)	41(1)	2(1)	8(1)	-6(1)
C(18)	31(1)	44(2)	30(1)	3(1)	8(1)	-4(1)
C(19)	32(1)	43(2)	34(1)	4(1)	6(1)	-4(1)

C(20)	51(1)	50(2)	36(1)	-1(1)	10(1)	3(1)
C(21)	55(2)	50(2)	56(2)	-7(1)	8(1)	6(1)
C(22)	47(1)	41(2)	64(2)	10(1)	-1(1)	-1(1)
C(23)	50(2)	63(2)	45(2)	19(1)	6(1)	-3(1)
C(24)	41(1)	63(2)	37(1)	9(1)	10(1)	2(1)
C(25)	38(1)	50(2)	31(1)	-1(1)	9(1)	-2(1)
C(26)	39(1)	40(1)	36(1)	1(1)	13(1)	-4(1)
C(27)	40(1)	40(2)	35(1)	6(1)	8(1)	-5(1)
C(28)	53(2)	48(2)	43(2)	0(1)	10(1)	-3(1)
C(29)	34(1)	36(1)	43(1)	-5(1)	7(1)	2(1)
C(30)	30(1)	32(1)	40(1)	-6(1)	7(1)	2(1)
C(31)	30(1)	26(1)	35(1)	-4(1)	11(1)	0(1)
C(32)	28(1)	29(1)	29(1)	0(1)	7(1)	-1(1)
C(33)	30(1)	29(1)	25(1)	-2(1)	7(1)	1(1)
C(34)	35(1)	31(1)	35(1)	1(1)	12(1)	-1(1)
C(35)	50(1)	31(1)	36(1)	4(1)	13(1)	7(1)
C(36)	39(1)	46(2)	37(1)	0(1)	3(1)	15(1)
C(37)	29(1)	49(2)	49(2)	-5(1)	4(1)	3(1)
C(38)	32(1)	36(1)	40(1)	-2(1)	7(1)	-3(1)
C(39)	35(1)	29(1)	34(1)	-3(1)	6(1)	-2(1)
C(40)	32(1)	25(1)	37(1)	-1(1)	11(1)	-1(1)
C(41)	26(1)	29(1)	36(1)	1(1)	8(1)	3(1)
C(42)	39(1)	32(1)	50(2)	-2(1)	16(1)	1(1)
N(1)	23(1)	25(1)	35(1)	-1(1)	7(1)	-1(1)
N(2)	35(1)	37(1)	31(1)	2(1)	7(1)	-4(1)
N(3)	25(1)	25(1)	32(1)	-3(1)	7(1)	-2(1)
O(1)	40(1)	41(1)	55(1)	11(1)	-3(1)	3(1)
O(2)	55(1)	37(1)	135(2)	30(1)	11(1)	2(1)
O(3)	41(1)	47(1)	46(1)	-4(1)	1(1)	-2(1)
O(4)	73(1)	59(1)	57(1)	-21(1)	8(1)	-2(1)
O(5)	41(1)	50(1)	51(1)	-16(1)	-5(1)	-2(1)
O(6)	51(1)	37(1)	70(1)	-21(1)	13(1)	-5(1)

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for d19435.

	x	y	z	U(eq)
H(1)	8009	-1859	6032	46
H(2)	8518	-206	5796	42
H(3)	6814	-1107	4856	37
H(6)	5715	-1337	3180	42
H(7)	4407	-2261	2783	48
H(8)	2967	-1943	3049	51
H(9)	2836	-697	3700	55
H(10)	4127	237	4077	46
H(11)	5158	1203	3173	47
H(13)	8044	829	4773	40
H(14)	7700	2246	4036	65
H(15)	4836	3392	2845	49
H(16)	4681	5142	2752	44
H(17)	5785	4090	4153	45
H(20)	7609	4226	4696	57
H(21)	8614	3129	5409	68
H(22)	8815	2766	6912	68
H(23)	8041	3521	7712	67
H(24)	7041	4618	7015	58
H(25)	7119	6180	6338	48
H(27)	4919	6209	3814	48
H(28)	5129	7580	4757	60
H(29)	5975	3274	705	48
H(30)	5405	4885	1045	43
H(31)	7155	4019	1900	37
H(34)	7936	3564	3339	41
H(35)	9238	2630	3897	48
H(36)	10876	3068	4327	52
H(37)	11212	4428	4177	54
H(38)	9928	5361	3598	45

H(39)	8623	6158	4011	41
H(41)	5902	5935	1998	37
H(42)	6159	7287	2912	48

(C) X-ray crystallographic data of compound (6a).

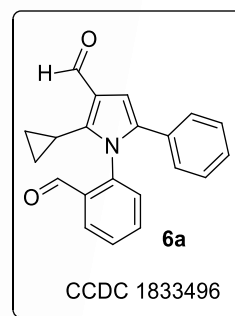
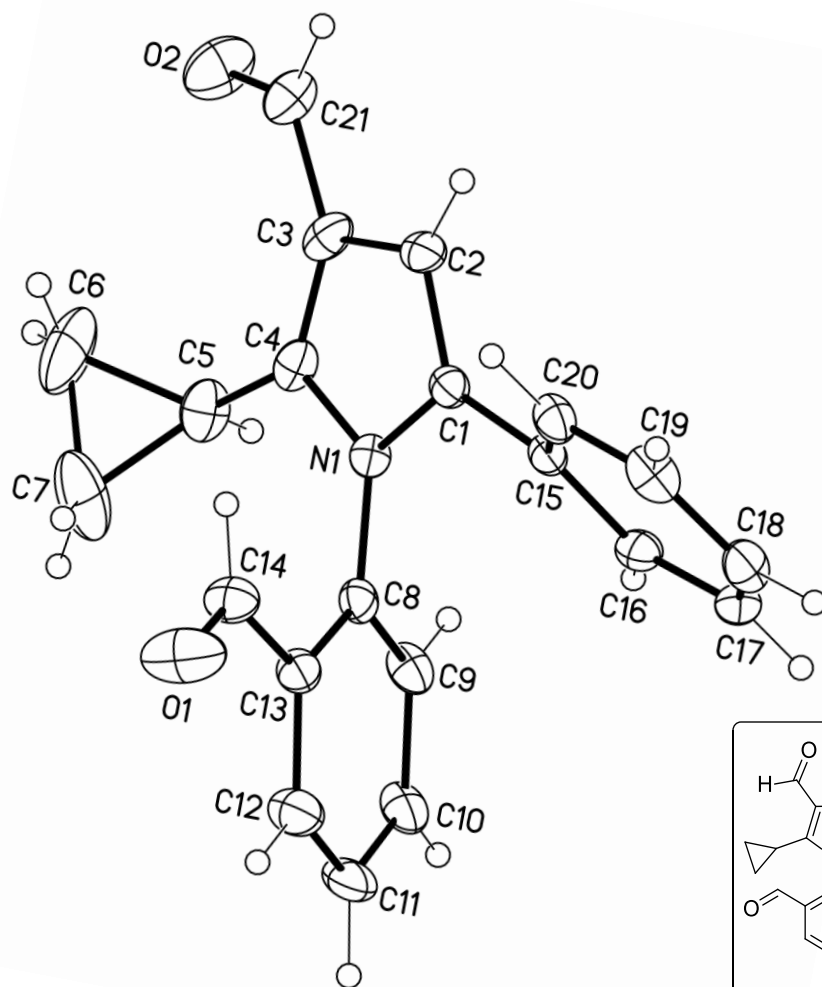


Table S11. Crystal data and structure refinement for 171016LT_0M_A.

Identification code	171016lt_0m_a
Empirical formula	C ₂₁ H ₁₇ N O ₂

Formula weight	315.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.9072(2) Å	$\alpha = 90^\circ$.
	b = 16.7423(5) Å	$\beta = 90.1880(10)^\circ$.
	c = 12.1333(4) Å	$\gamma = 90^\circ$.
Volume	1606.26(8) Å ³	
Z	4	
Density (calculated)	1.304 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	664	
Crystal size	0.20 x 0.15 x 0.14 mm ³	
Theta range for data collection	2.073 to 26.372°.	
Index ranges	-9<=h<=8, -20<=k<=20, -15<=l<=15	
Reflections collected	13209	
Independent reflections	3282 [R(int) = 0.0288]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8870	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3282 / 39 / 237	
Goodness-of-fit on F ²	1.270	
Final R indices [I>2sigma(I)]	R1 = 0.0903, wR2 = 0.1958	
R indices (all data)	R1 = 0.0945, wR2 = 0.1975	
Extinction coefficient	0.0088(14)	
Largest diff. peak and hole	0.285 and -0.335 e.Å ⁻³	

Table S12. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for 171016LT_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)	4935(4)	3812(2)	6123(3)	18(1)
C(2)	4009(5)	4412(2)	6584(3)	21(1)
C(3)	4861(5)	4669(2)	7554(3)	24(1)

C(4)	6333(5)	4219(2)	7656(3)	21(1)
C(5)	7679(5)	4217(2)	8498(3)	29(1)
C(6)	8389(7)	4983(3)	8906(5)	55(2)
C(7)	9463(6)	4441(4)	8224(4)	50(1)
C(8)	7744(4)	3170(2)	6519(3)	19(1)
C(9)	8030(5)	2498(2)	7161(3)	23(1)
C(10)	9304(5)	1975(2)	6871(3)	27(1)
C(11)	10270(5)	2114(2)	5941(4)	32(1)
C(12)	10007(5)	2793(2)	5311(3)	29(1)
C(13)	8744(4)	3337(2)	5604(3)	20(1)
C(14)	8563(5)	4089(2)	4973(3)	25(1)
C(15)	4539(4)	3308(2)	5157(3)	18(1)
C(16)	4631(4)	2475(2)	5215(3)	21(1)
C(17)	4113(5)	2013(2)	4326(3)	24(1)
C(18)	3527(5)	2373(2)	3362(3)	26(1)
C(19)	3479(5)	3200(3)	3296(3)	27(1)
C(20)	3978(4)	3666(2)	4181(3)	23(1)
N(1)	6366(4)	3697(2)	6782(2)	17(1)
O(1)	9342(5)	4249(2)	4142(3)	46(1)
C(21)	4030(20)	5300(11)	8196(11)	28(3)
O(2)	4530(8)	5528(4)	9095(5)	43(2)
C(21')	4460(20)	5251(12)	8436(14)	25(3)
O(2')	3199(10)	5664(4)	8357(6)	42(2)

Table S13. Bond lengths [Å] and angles [°] for 171016LT_0M_A.

C(1)-C(2)	1.364(5)
C(1)-N(1)	1.396(4)
C(1)-C(15)	1.476(5)
C(2)-C(3)	1.421(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.392(5)
C(3)-C(21)	1.470(15)
C(3)-C(21')	1.482(16)
C(4)-N(1)	1.374(4)
C(4)-C(5)	1.473(5)

C(5)-C(6)	1.483(6)
C(5)-C(7)	1.498(6)
C(5)-H(5)	1.0000
C(6)-C(7)	1.495(8)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.387(5)
C(8)-C(13)	1.393(5)
C(8)-N(1)	1.440(4)
C(9)-C(10)	1.381(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.384(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.384(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.398(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.481(5)
C(14)-O(1)	1.213(5)
C(14)-H(14)	0.9500
C(15)-C(20)	1.398(5)
C(15)-C(16)	1.398(5)
C(16)-C(17)	1.388(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.394(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.384(5)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-O(2)	1.221(11)
C(21)-H(21)	0.9500
C(21')-O(2')	1.219(13)

C(21')-H(21')	0.9500
C(2)-C(1)-N(1)	107.5(3)
C(2)-C(1)-C(15)	129.3(3)
N(1)-C(1)-C(15)	123.0(3)
C(1)-C(2)-C(3)	108.0(3)
C(1)-C(2)-H(2)	126.0
C(3)-C(2)-H(2)	126.0
C(4)-C(3)-C(2)	107.7(3)
C(4)-C(3)-C(21)	135.9(6)
C(2)-C(3)-C(21)	116.4(6)
C(4)-C(3)-C(21')	118.1(6)
C(2)-C(3)-C(21')	134.1(6)
N(1)-C(4)-C(3)	107.0(3)
N(1)-C(4)-C(5)	121.3(3)
C(3)-C(4)-C(5)	131.7(3)
C(4)-C(5)-C(6)	120.1(4)
C(4)-C(5)-C(7)	121.6(4)
C(6)-C(5)-C(7)	60.2(3)
C(4)-C(5)-H(5)	114.7
C(6)-C(5)-H(5)	114.7
C(7)-C(5)-H(5)	114.7
C(5)-C(6)-C(7)	60.4(3)
C(5)-C(6)-H(6A)	117.7
C(7)-C(6)-H(6A)	117.7
C(5)-C(6)-H(6B)	117.7
C(7)-C(6)-H(6B)	117.7
H(6A)-C(6)-H(6B)	114.9
C(6)-C(7)-C(5)	59.4(3)
C(6)-C(7)-H(7A)	117.8
C(5)-C(7)-H(7A)	117.8
C(6)-C(7)-H(7B)	117.8
C(5)-C(7)-H(7B)	117.8
H(7A)-C(7)-H(7B)	115.0
C(9)-C(8)-C(13)	121.3(3)
C(9)-C(8)-N(1)	119.7(3)
C(13)-C(8)-N(1)	119.0(3)

C(10)-C(9)-C(8)	119.2(3)
C(10)-C(9)-H(9)	120.4
C(8)-C(9)-H(9)	120.4
C(9)-C(10)-C(11)	120.5(3)
C(9)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(10)-C(11)-C(12)	120.3(4)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	120.0(4)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(8)-C(13)-C(12)	118.6(3)
C(8)-C(13)-C(14)	121.9(3)
C(12)-C(13)-C(14)	119.4(3)
O(1)-C(14)-C(13)	124.7(4)
O(1)-C(14)-H(14)	117.7
C(13)-C(14)-H(14)	117.7
C(20)-C(15)-C(16)	119.1(3)
C(20)-C(15)-C(1)	119.6(3)
C(16)-C(15)-C(1)	121.2(3)
C(17)-C(16)-C(15)	120.1(3)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.5(4)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	119.3(3)
C(19)-C(18)-H(18)	120.4
C(17)-C(18)-H(18)	120.4
C(20)-C(19)-C(18)	120.7(4)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(15)	120.3(3)
C(19)-C(20)-H(20)	119.8
C(15)-C(20)-H(20)	119.8

C(4)-N(1)-C(1)	109.7(3)
C(4)-N(1)-C(8)	125.3(3)
C(1)-N(1)-C(8)	124.7(3)
O(2)-C(21)-C(3)	123.6(12)
O(2)-C(21)-H(21)	118.2
C(3)-C(21)-H(21)	118.2
O(2')-C(21')-C(3)	119.4(12)
O(2')-C(21')-H(21')	120.3
C(3)-C(21')-H(21')	120.3

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 171016LT_0M_A. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(2)	16(2)	22(2)	4(1)	0(1)	0(1)
C(2)	21(2)	15(2)	27(2)	6(1)	4(1)	2(1)
C(3)	35(2)	16(2)	20(2)	0(1)	8(2)	-2(2)
C(4)	29(2)	20(2)	14(2)	-1(1)	3(1)	-5(2)
C(5)	36(2)	31(2)	19(2)	-1(2)	-4(2)	-7(2)
C(6)	74(4)	36(3)	55(3)	-10(2)	-29(3)	-14(3)
C(7)	38(3)	82(4)	29(2)	1(2)	-8(2)	-26(3)
C(8)	16(2)	19(2)	21(2)	0(1)	-3(1)	-2(1)
C(9)	18(2)	27(2)	24(2)	8(2)	-2(1)	-1(2)
C(10)	17(2)	22(2)	43(2)	14(2)	-5(2)	2(2)
C(11)	18(2)	25(2)	53(3)	8(2)	6(2)	6(2)
C(12)	25(2)	28(2)	34(2)	5(2)	6(2)	4(2)
C(13)	20(2)	19(2)	22(2)	2(1)	-1(1)	0(1)
C(14)	27(2)	24(2)	25(2)	5(2)	2(2)	5(2)
C(15)	14(2)	20(2)	19(2)	-2(1)	1(1)	-1(1)
C(16)	19(2)	21(2)	23(2)	1(2)	-1(1)	4(1)
C(17)	21(2)	22(2)	30(2)	-6(2)	6(2)	0(2)
C(18)	22(2)	38(2)	19(2)	-11(2)	0(1)	-5(2)
C(19)	23(2)	40(2)	17(2)	5(2)	-1(1)	-2(2)
C(20)	18(2)	23(2)	26(2)	5(2)	0(1)	-3(1)

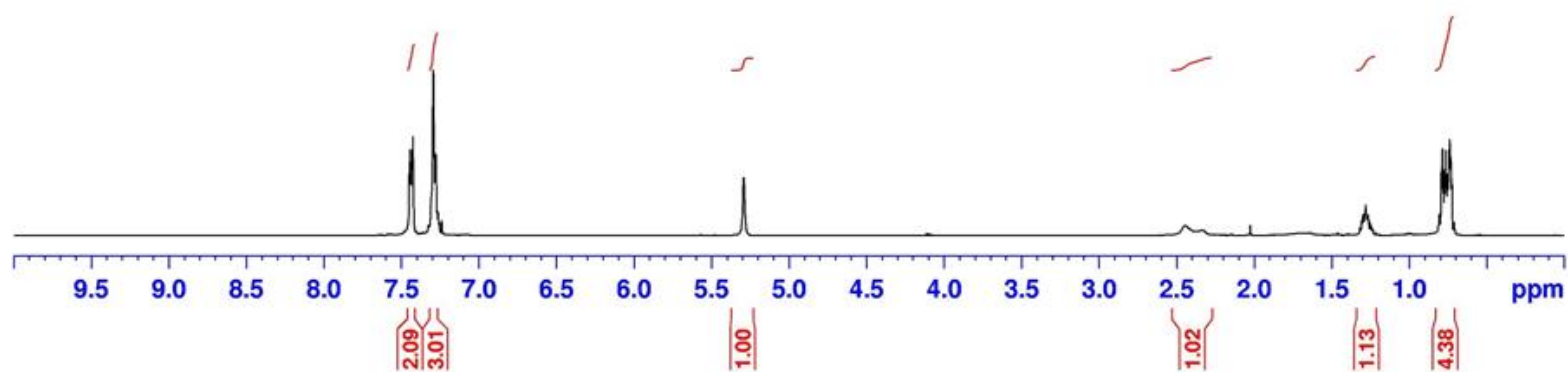
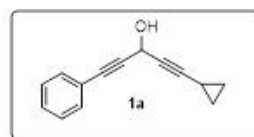
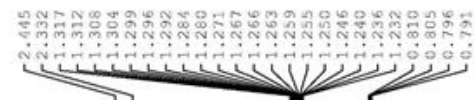
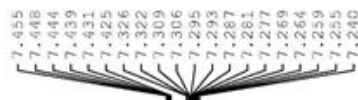
N(1)	18(1)	17(1)	16(1)	2(1)	-2(1)	0(1)
O(1)	61(2)	40(2)	38(2)	16(2)	24(2)	17(2)
C(21)	37(7)	21(4)	27(6)	0(5)	-3(4)	1(5)
O(2)	59(4)	41(4)	27(3)	-12(3)	-4(3)	5(3)
C(21')	36(7)	20(4)	19(7)	-2(5)	-1(5)	11(5)
O(2')	51(5)	38(4)	39(4)	-8(3)	-1(3)	27(4)

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 171016LT_0M_A.

	x	y	z	U(eq)
H(2)	2976	4621	6305	25
H(5)	7566	3792	9072	34
H(6A)	8652	5025	9702	66
H(6B)	7978	5482	8561	66
H(7A)	10386	4147	8600	59
H(7B)	9711	4604	7457	59
H(9)	7357	2398	7794	28
H(10)	9519	1517	7312	33
H(11)	11119	1742	5734	38
H(12)	10685	2889	4680	35
H(14)	7781	4474	5238	30
H(16)	5048	2225	5863	25
H(17)	4159	1447	4375	29
H(18)	3164	2056	2757	31
H(19)	3100	3449	2636	32
H(20)	3938	4232	4125	27
H(21)	3045	5544	7895	34
H(21')	5189	5302	9058	30

Current Data Parameters
NAME BK-C-131-A-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 399.7611794 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Fmoc-hyp (TBDMS)
 Current Data Parameters
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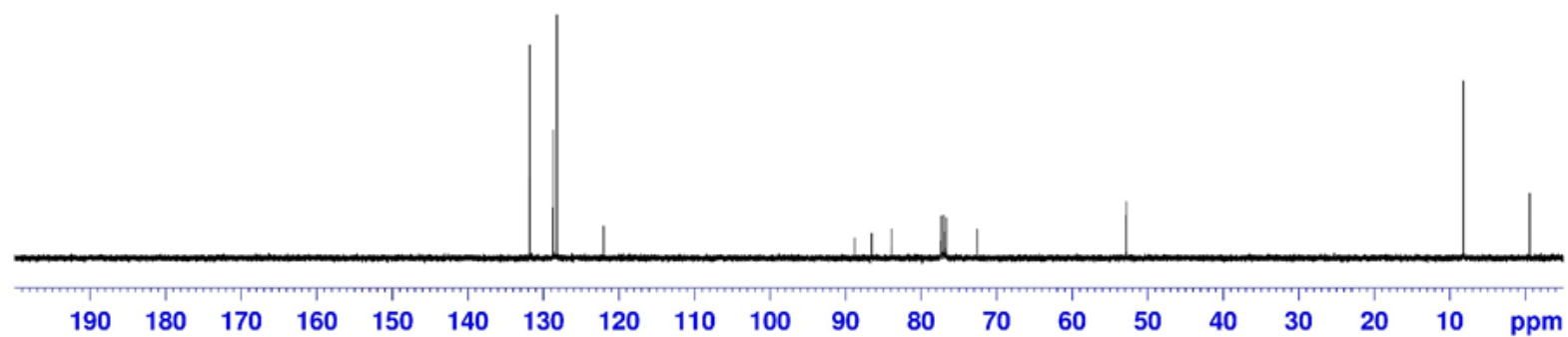
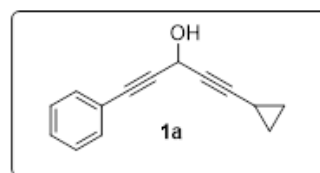
131.78
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 128.20
 122.04

88.765
 86.544
 83.869
 77.319
 77.000
 76.682
 72.587

52.822

8.205

-0.590



52-B-H1

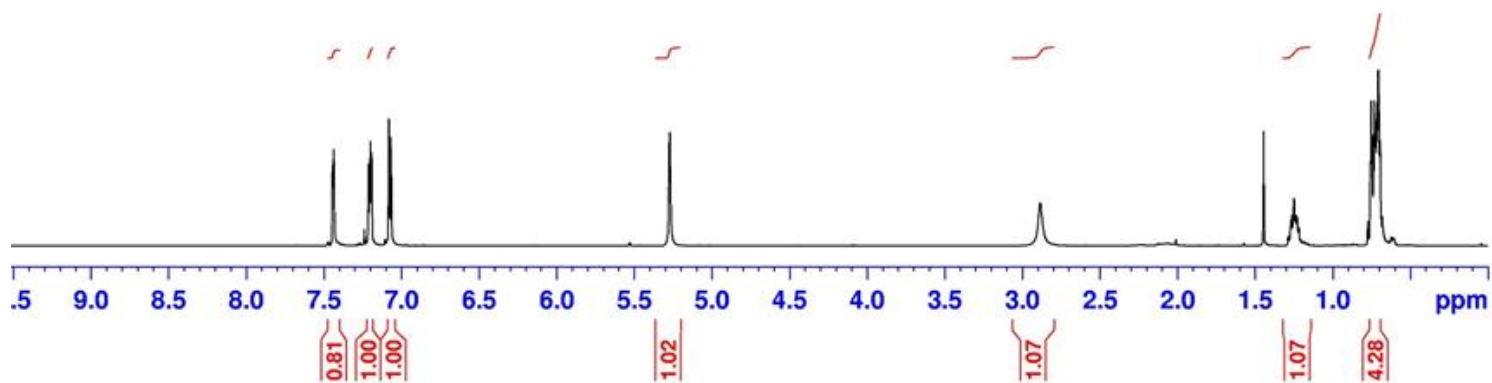
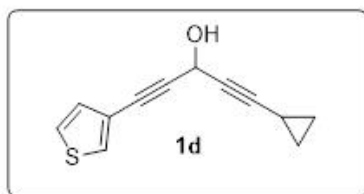
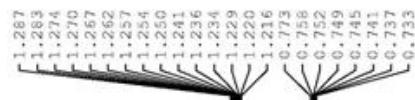
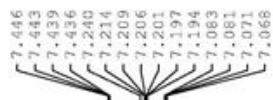
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Bk-C-152-b-h1.fid

Processing parameters

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EM

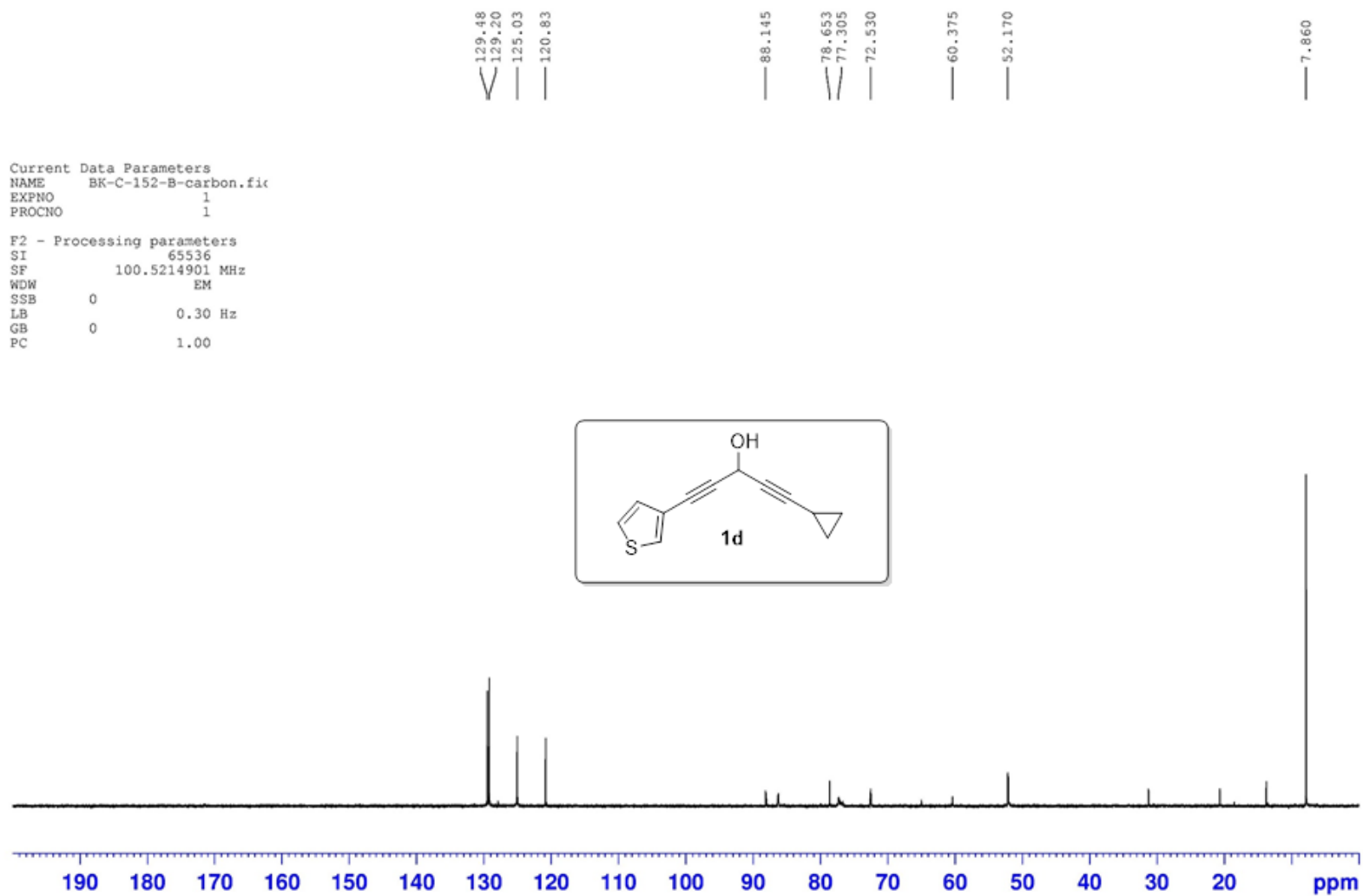
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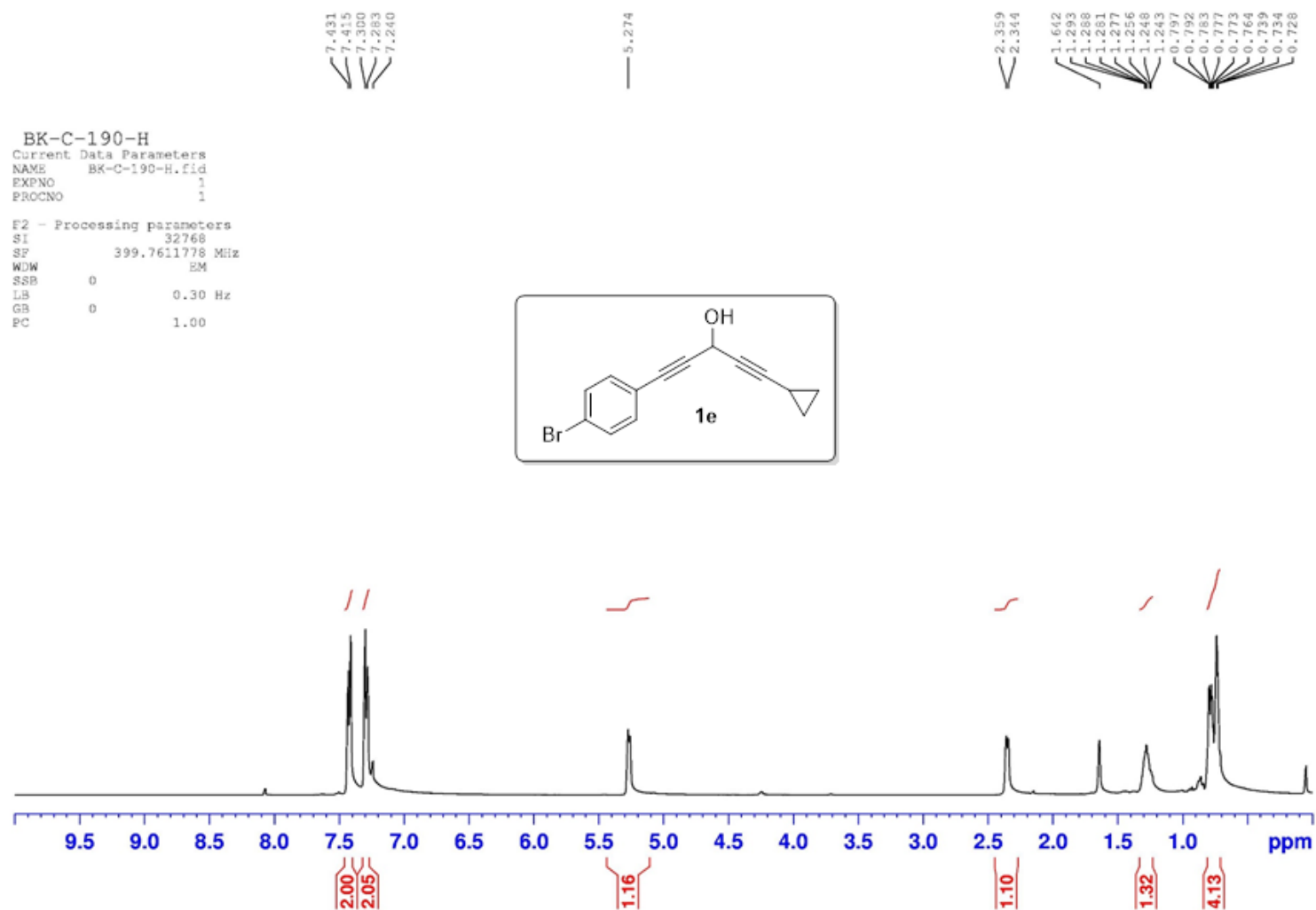
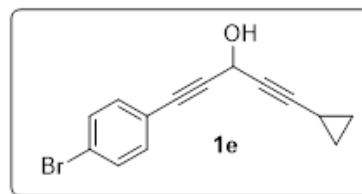


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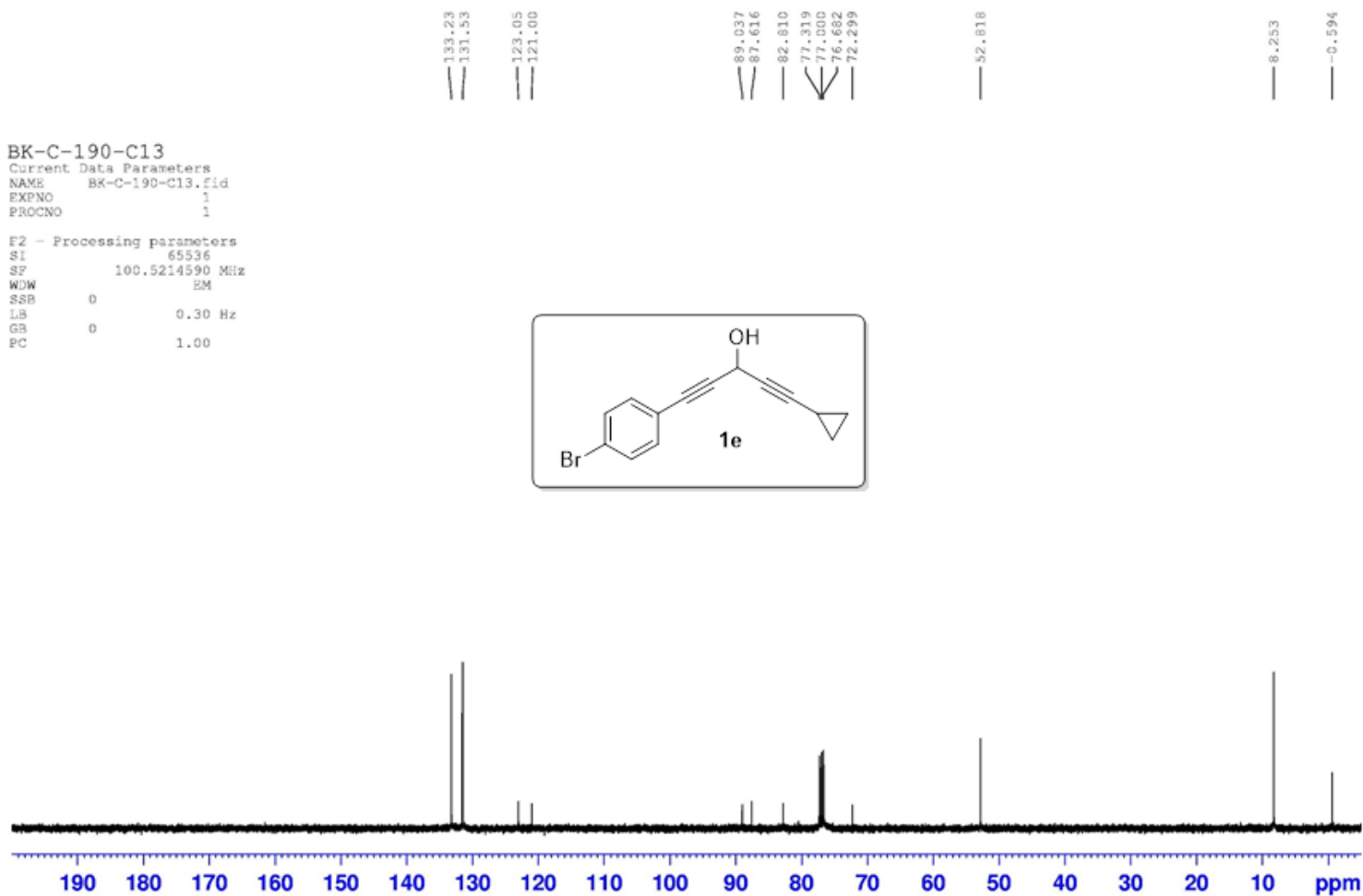
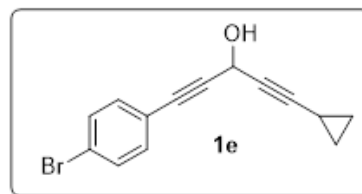


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 PROCNO 1
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 PC 1.00



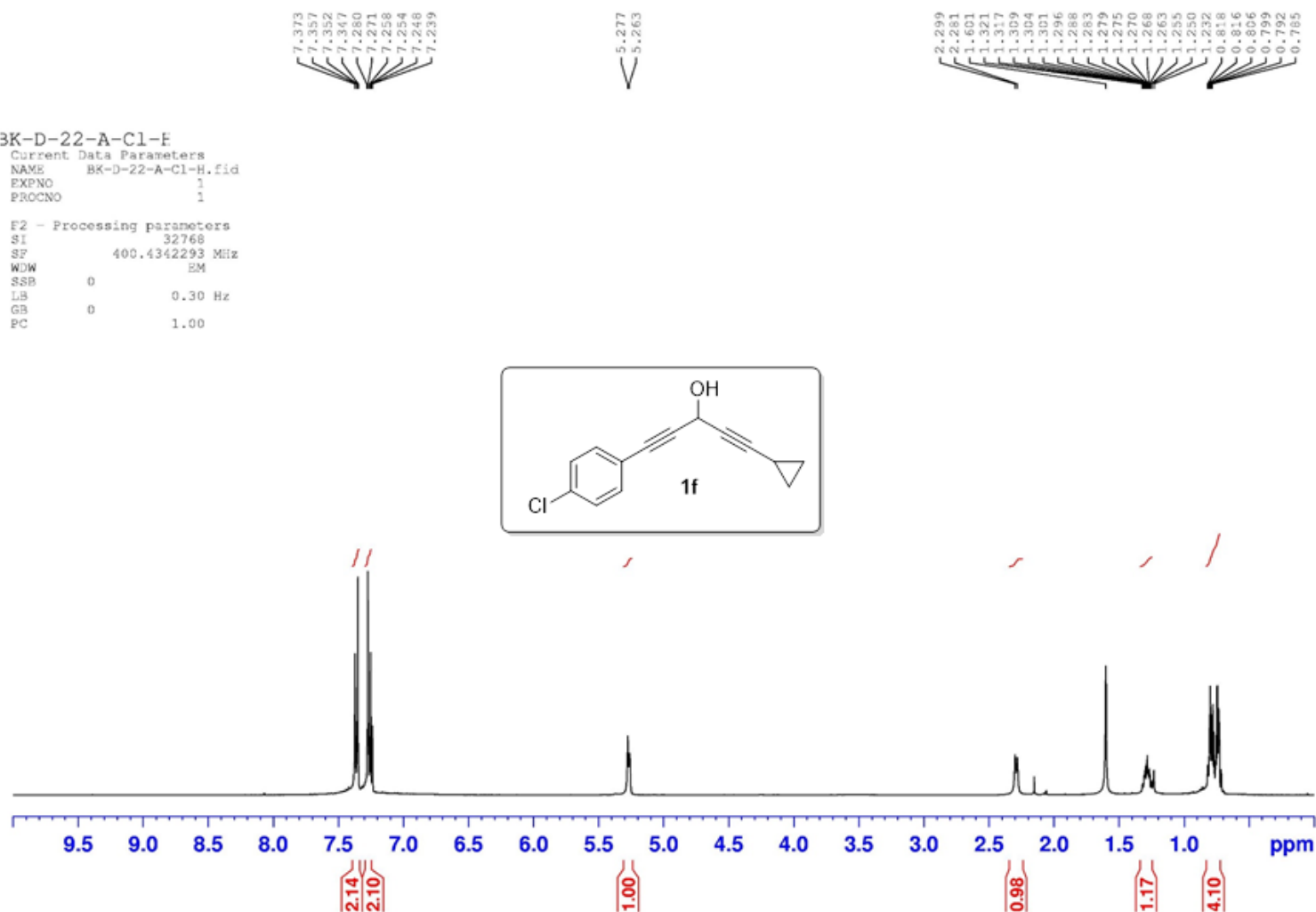
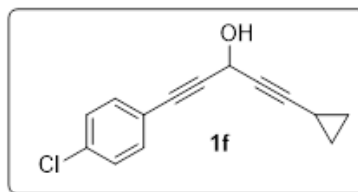
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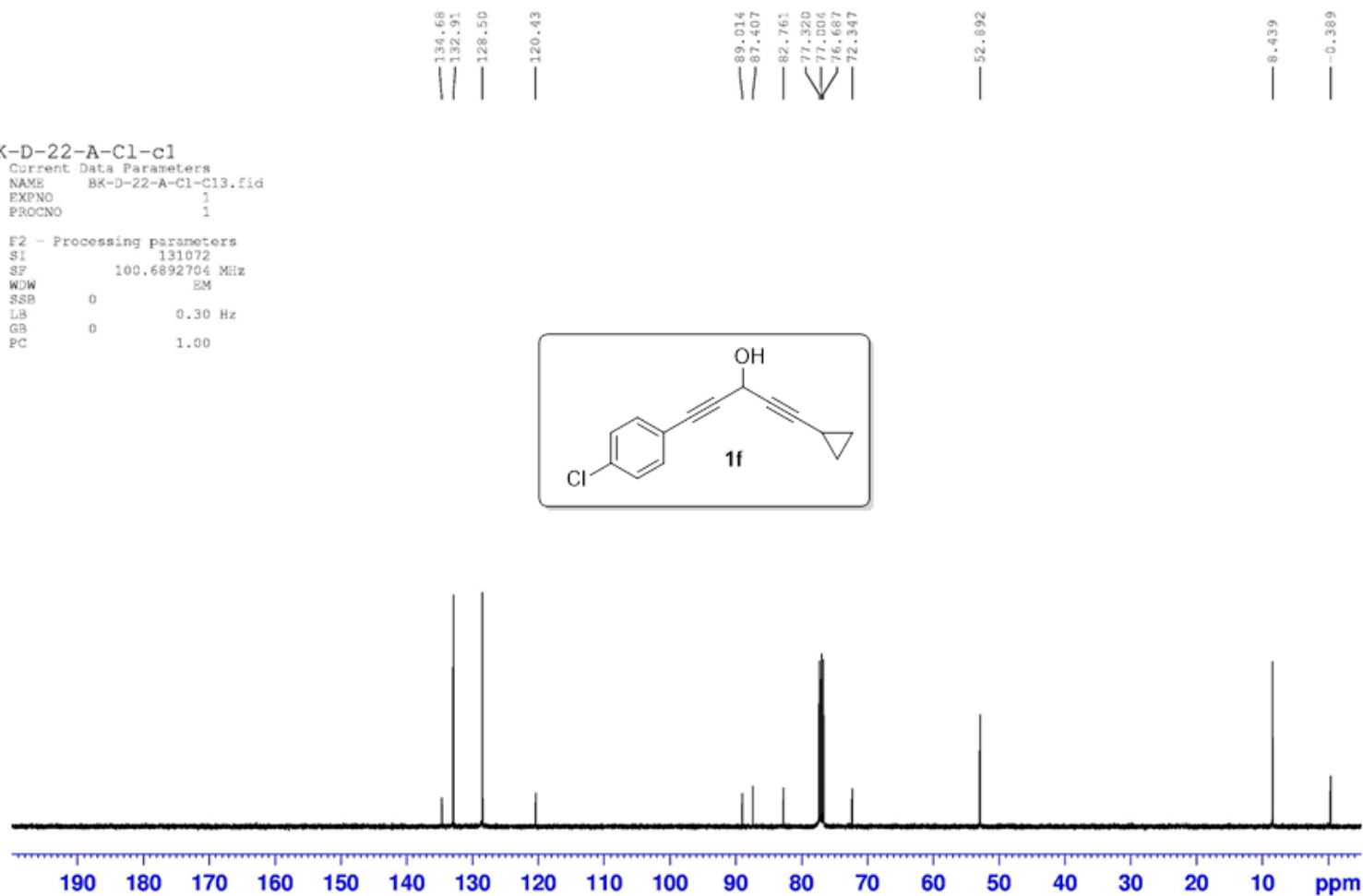
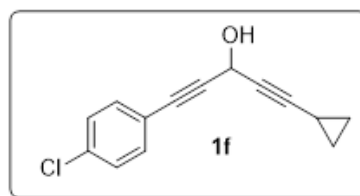
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 PC 1.00



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 PC 1.00



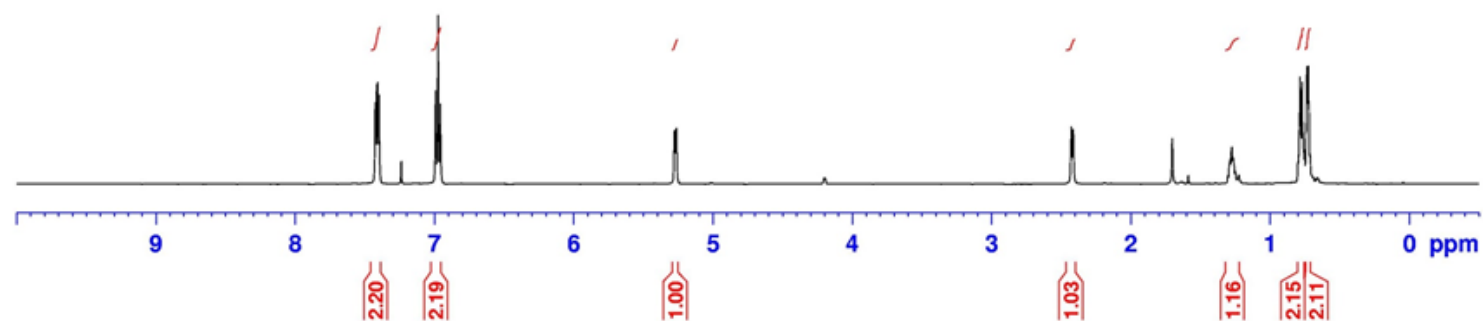
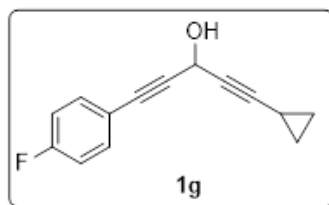
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7.410
7.399
7.240
6.994
6.976
6.959

5.277
5.265

2.428
2.414
1.702
1.304
1.301
1.294
1.288
1.285
1.277
1.274
1.268
1.263
1.258
1.251
0.789
0.785
0.779
0.773
0.769
0.763
0.741
0.735
0.731
0.725
0.721

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Processing parameters
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SF 499.7938788 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



163.68
161.69

133.79
133.72

118.10
118.07
115.64
115.46

88.876
86.203
82.827
77.254
77.000
76.746
72.431

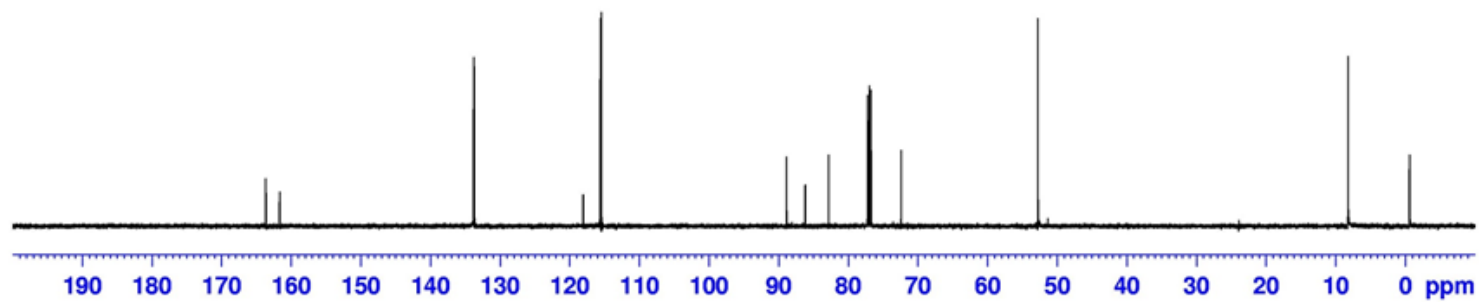
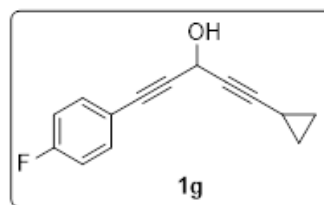
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8.231

-0.604

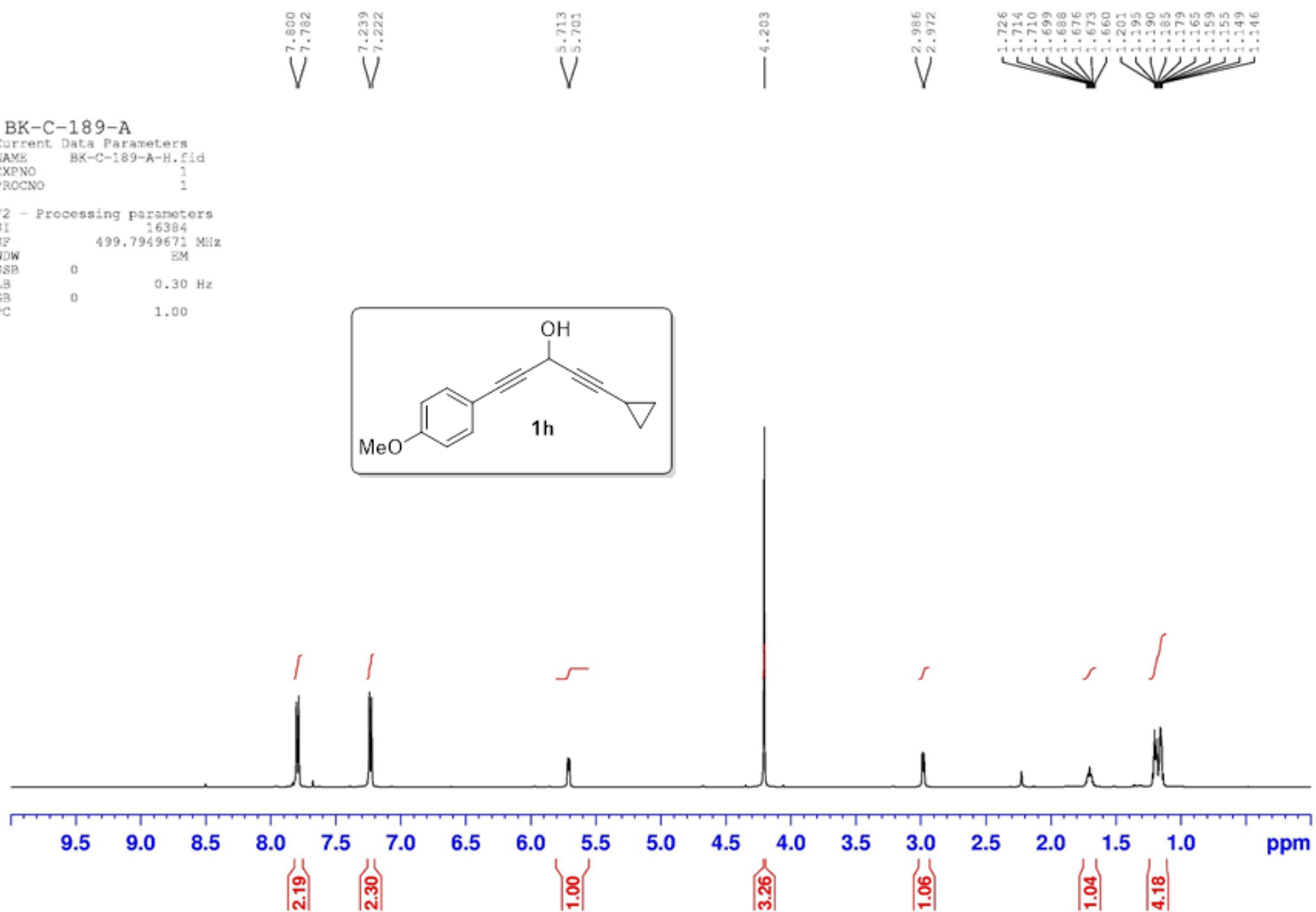
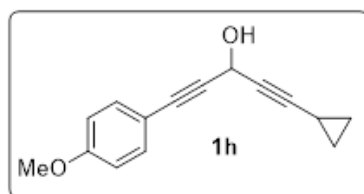
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EXPNO 1
PROCNO 1

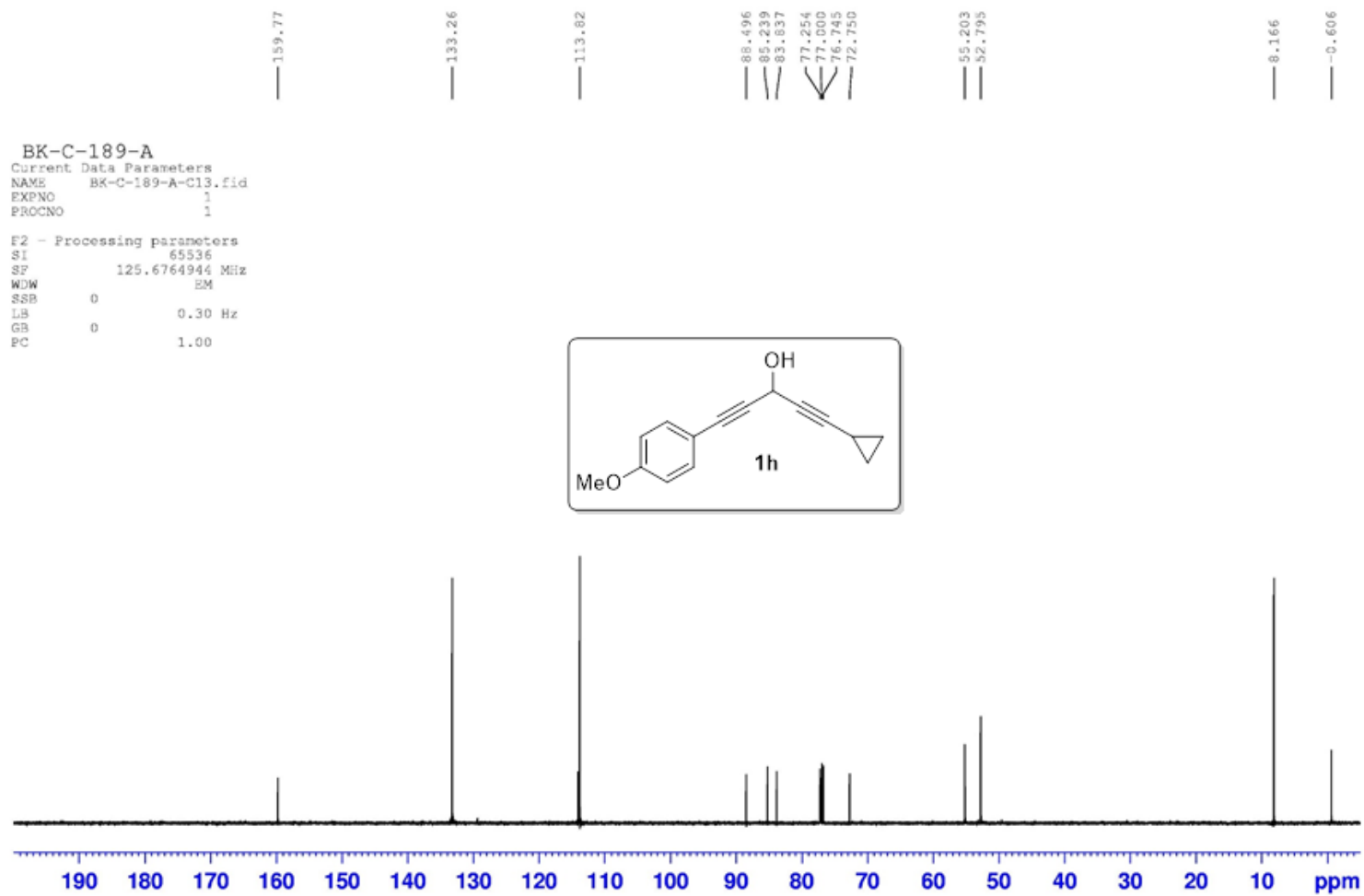
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PC 1.00



BK-C-189-A
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 PROCNO 1

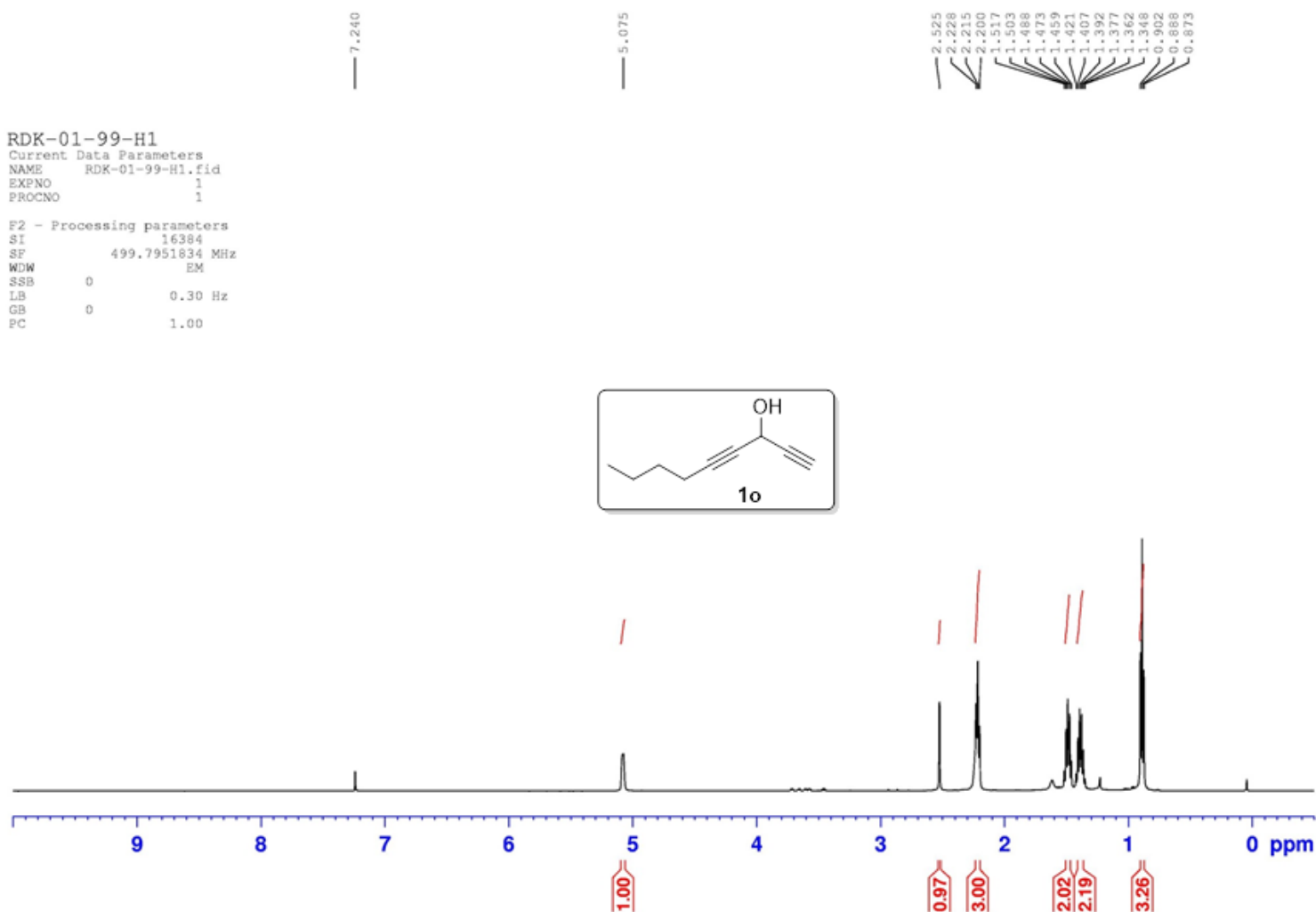
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 PC 1.00





RDk-01-99-H1
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 PROCNO 1

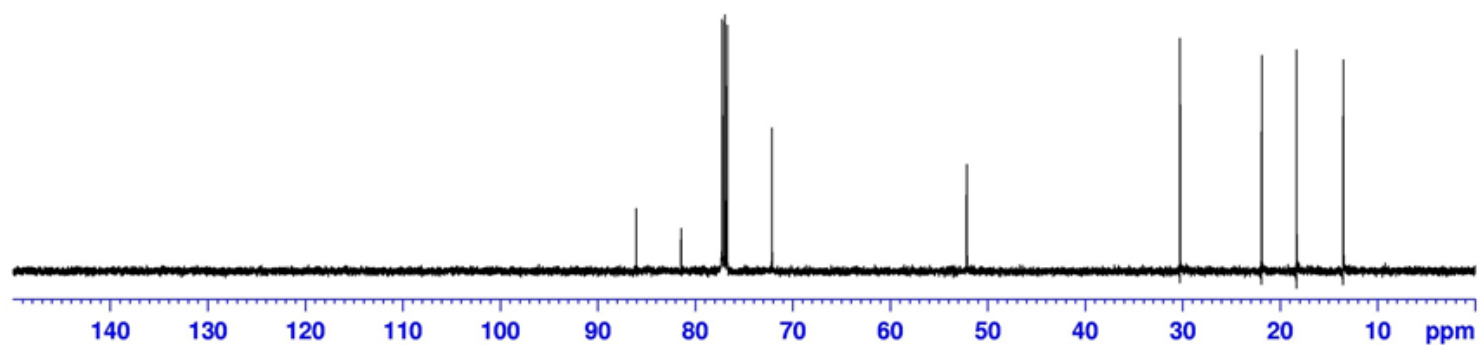
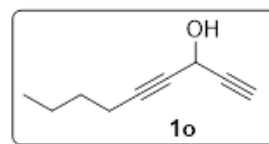
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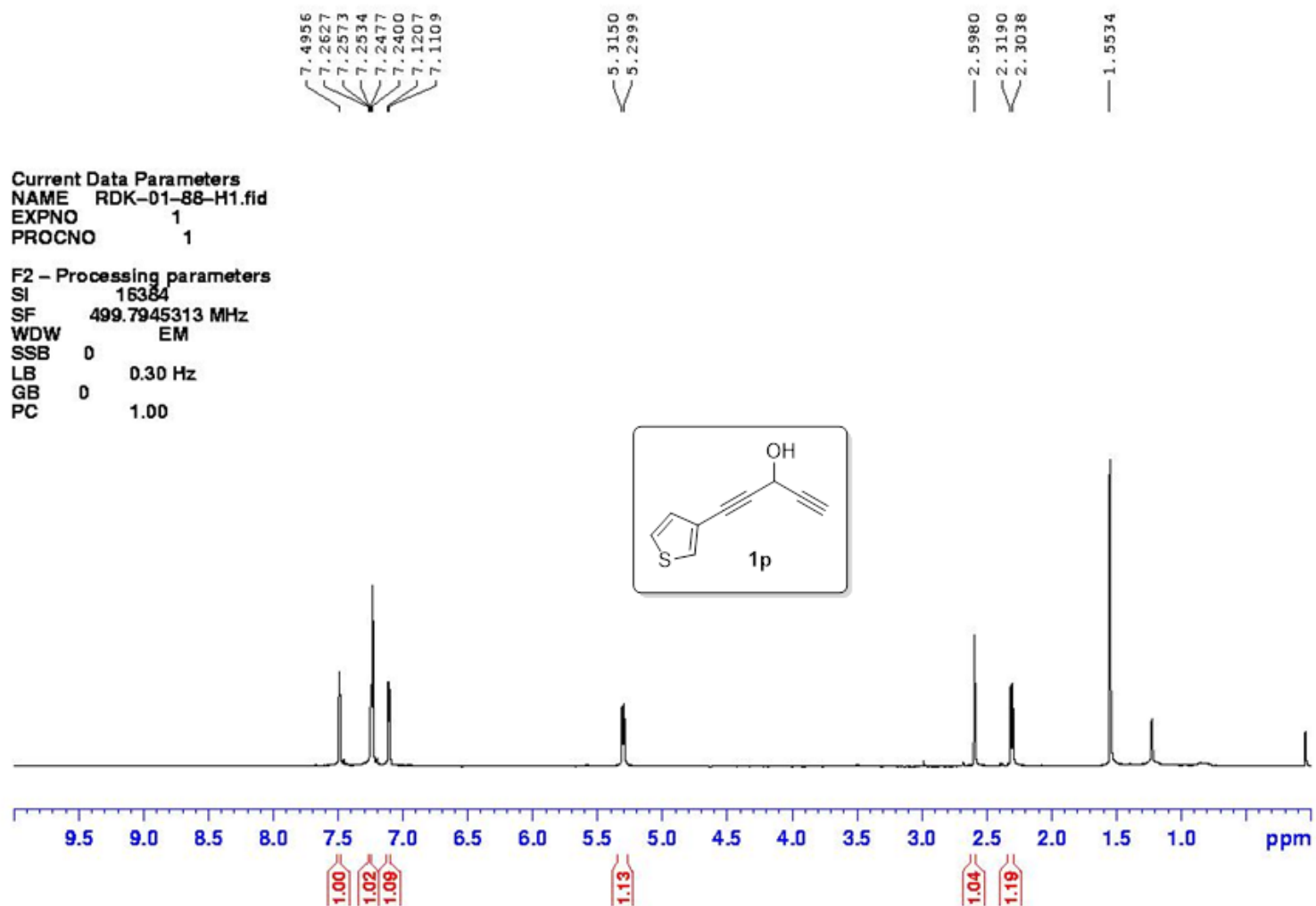


RDK-01-99-C13

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PROCNO 1

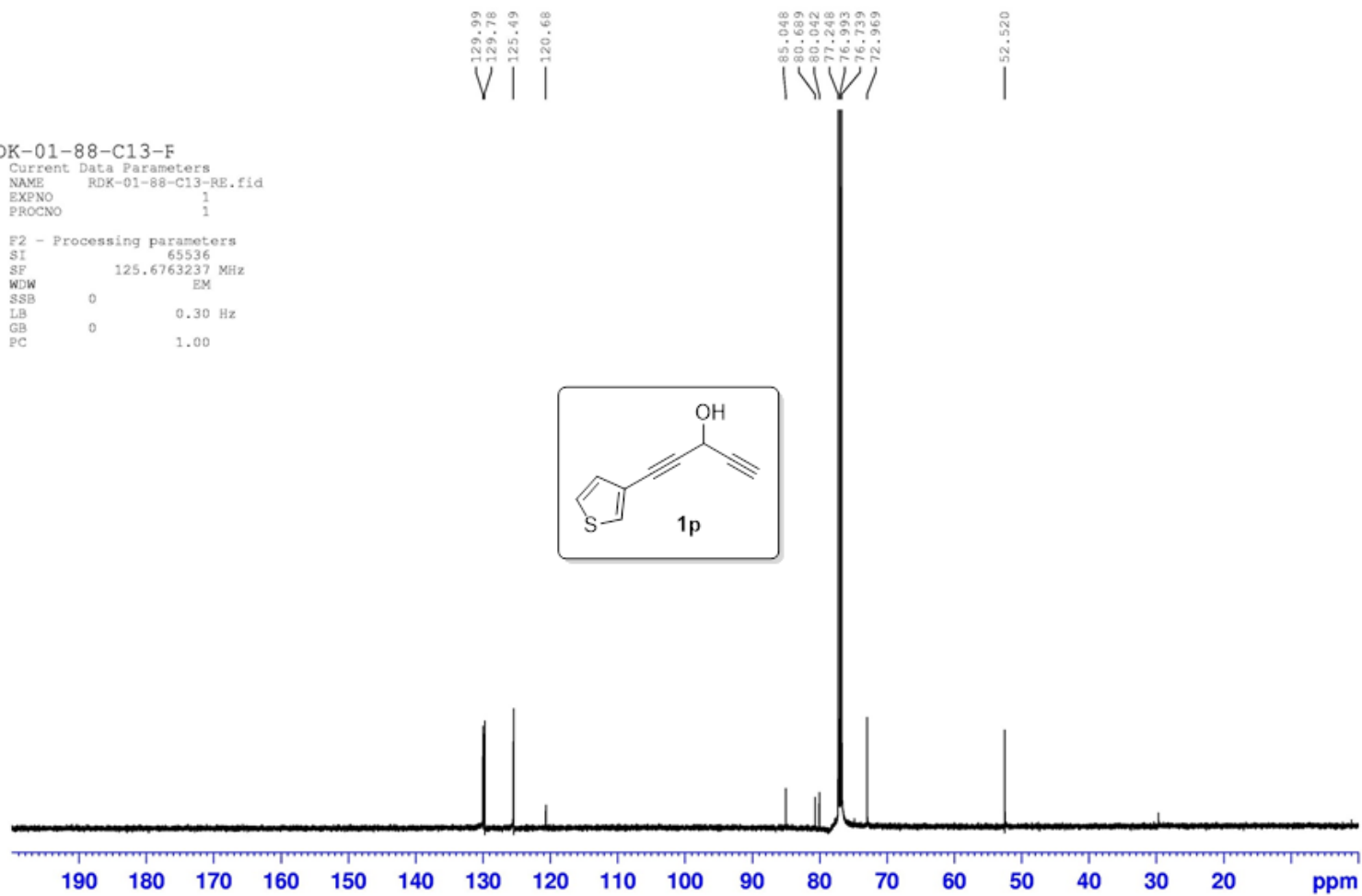
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GB 0
PC 1.00

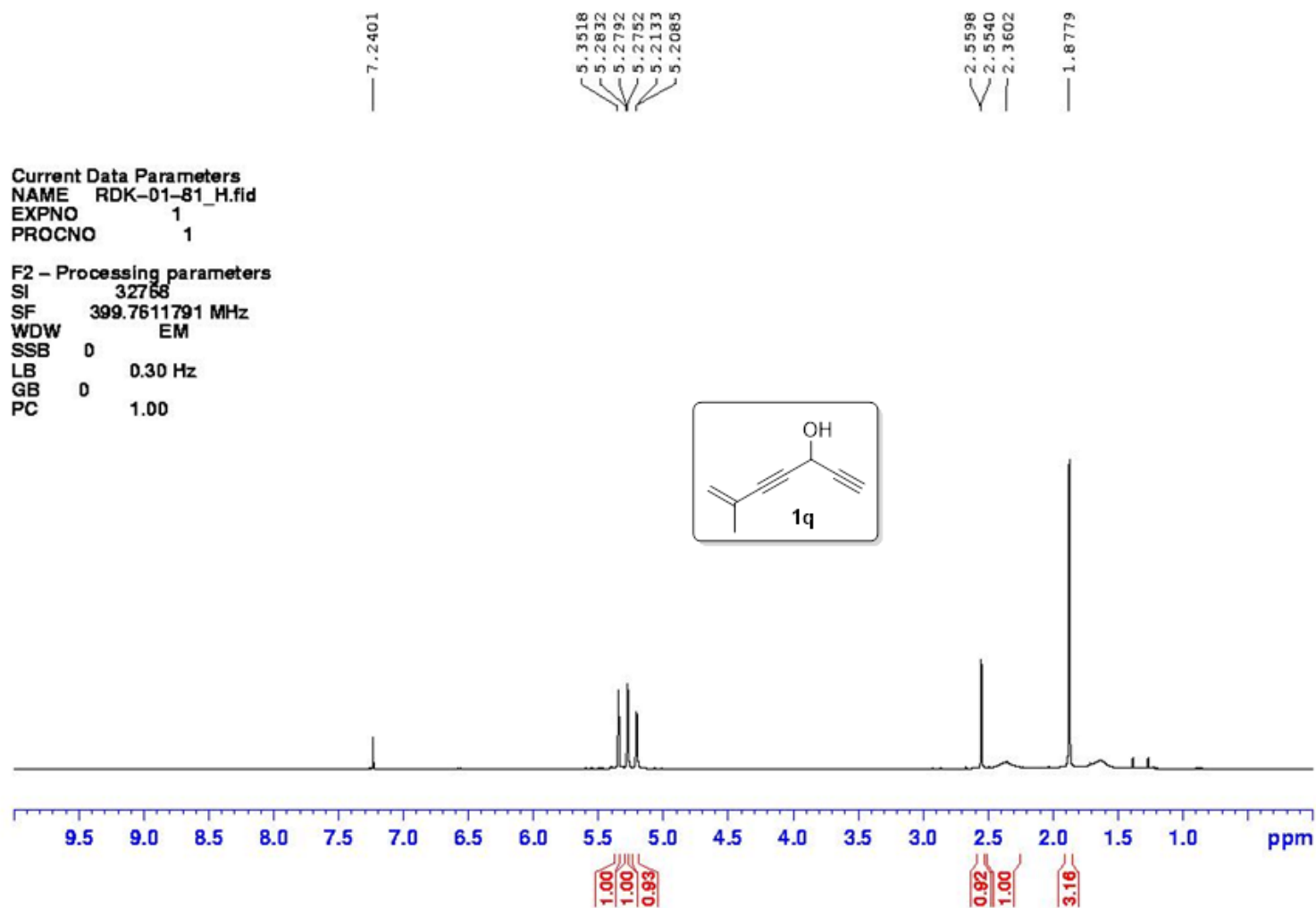




JK-01-88-C13-F
 Current Data Parameters
 NAME RDK-01-88-C13-RE.fid
 EXPNO 1
 PROCNO 1

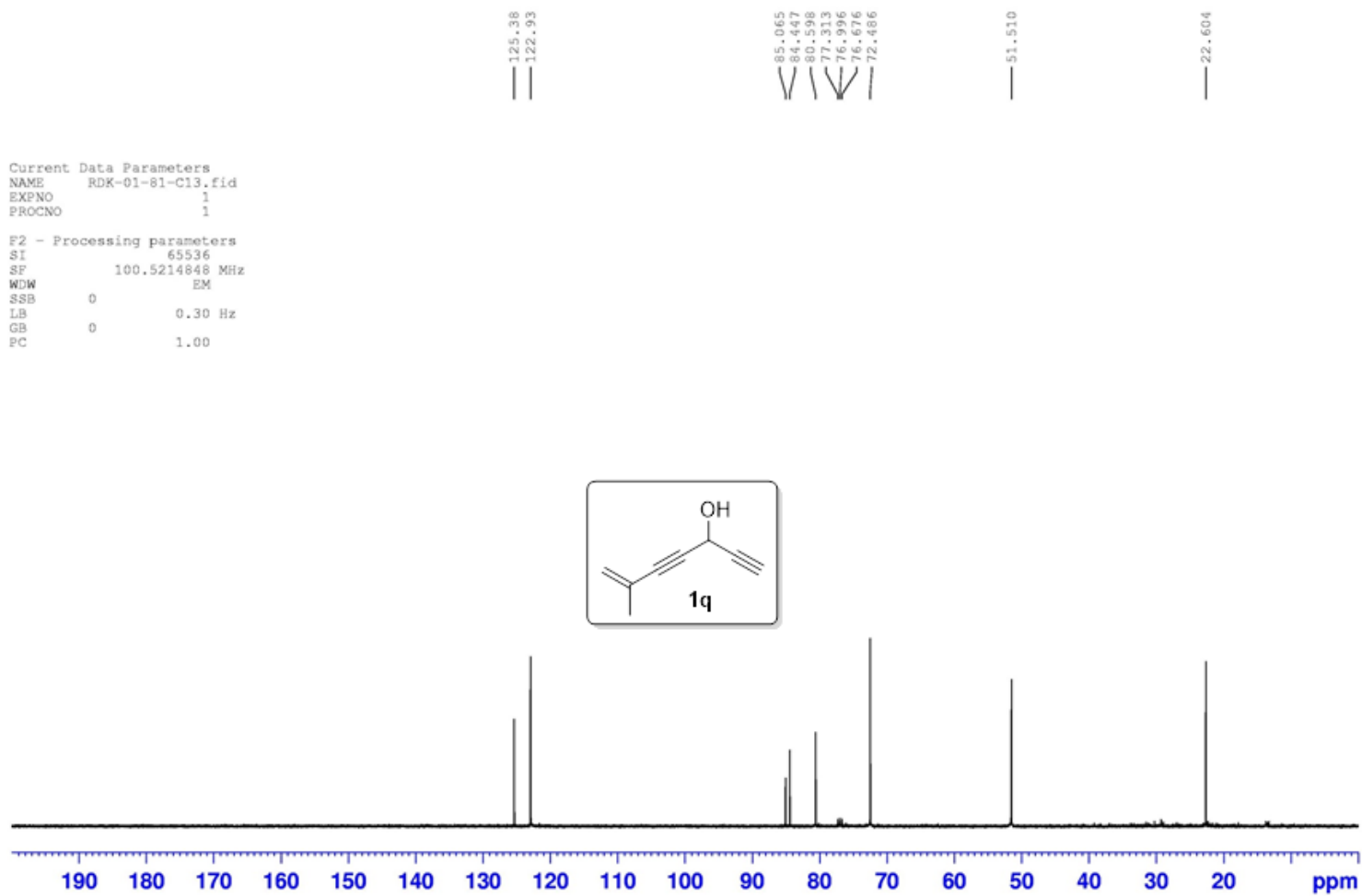
F2 - Processing parameters
 SI 65536
 SF 125.6763237 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME RDK-01-81-C13.fid
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 100.5214848 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



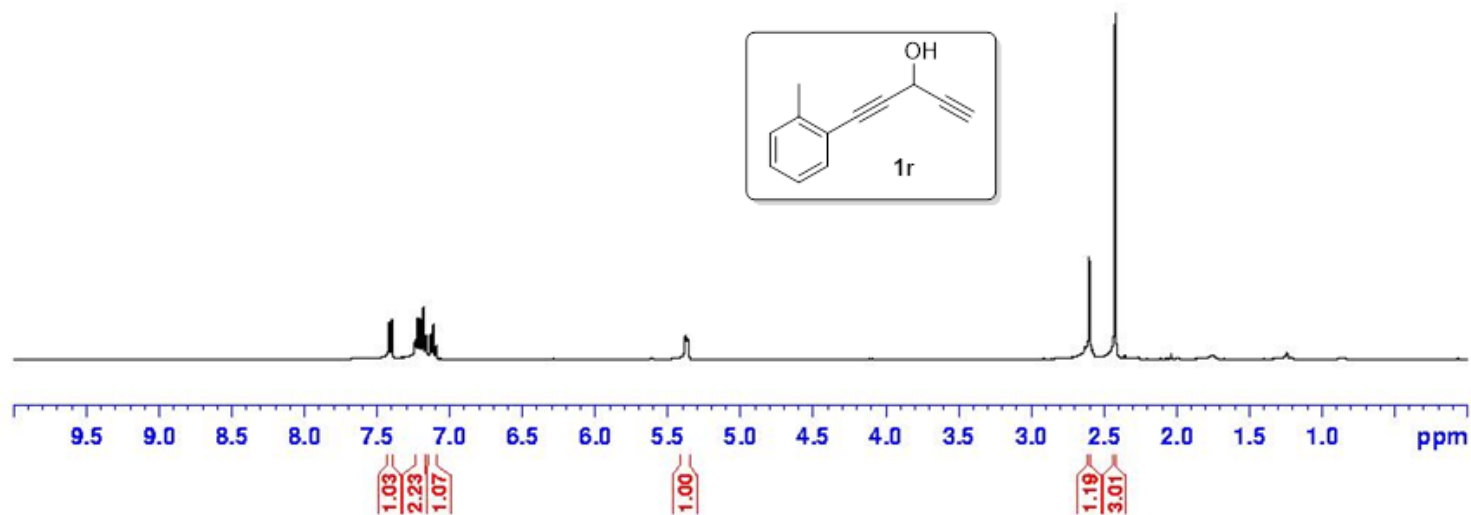
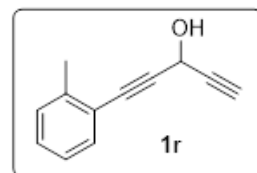
7.4235
7.4216
7.4045
7.4028
7.2477
7.2444
7.2400
7.2288
7.2260
7.2107
7.2075
7.1881
7.1869
7.1370
7.1346
7.1181
7.1000
7.0978

5.3811
5.3697

2.6057
2.6000
2.4266

Current Data Parameters
NAME RDK-01-83-H1.fid
EXPNO 1
PROCNO 1

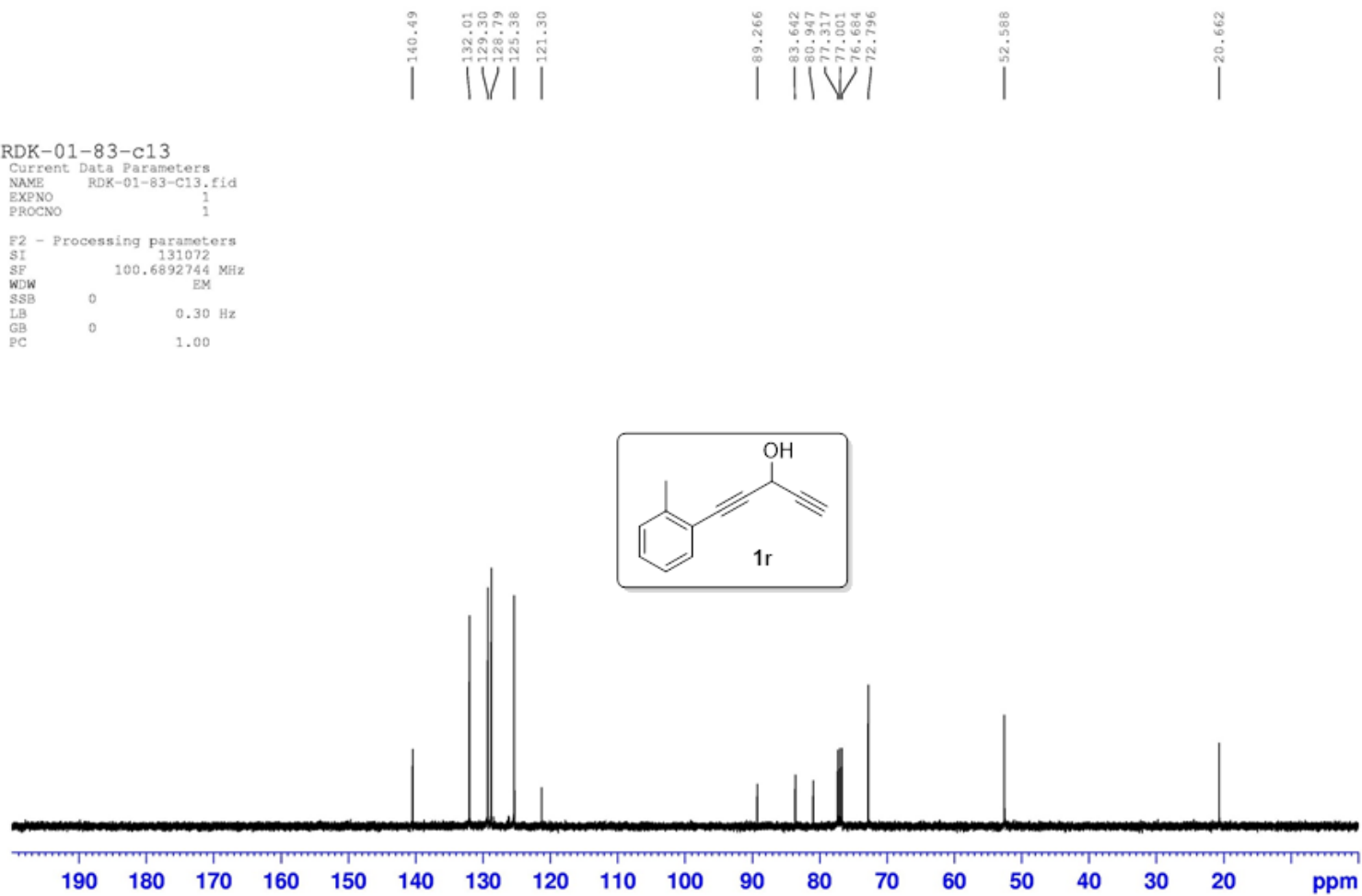
F2 - Processing parameters
SI 32768
SF 400.4342288 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



RDk-01-83-c13

Current Data Parameters
NAME RDk-01-83-c13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 131072
SF 100.6892744 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



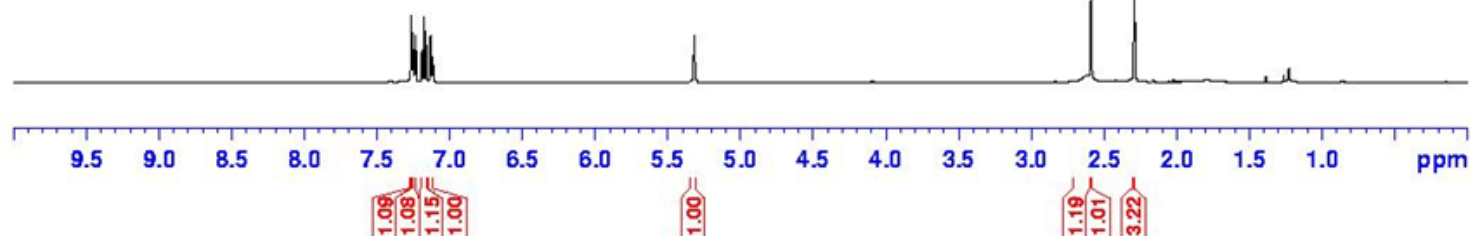
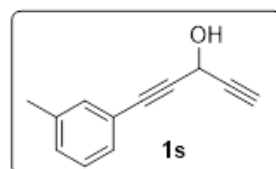
7.2699
7.2558
7.2405
7.1953
7.1801
7.1650
7.1378
7.1226

5.3252
5.3217

2.6156
2.5932
2.5888
2.2959

Current Data Parameters
NAME RDK-01-62-H1.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 16384
SF 499.7945336 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



RDk-01-62-C13

Current Data Parameters
NAME RDk-01-62-C13.fid
EXPNO 1
PROCNO 1

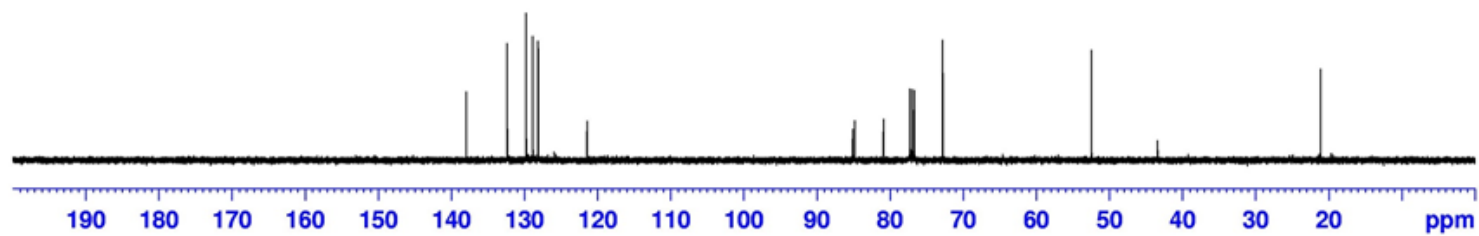
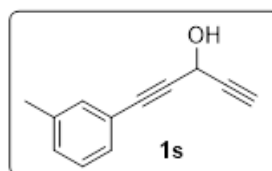
F2 - Processing parameters
SI 65536
SF 100.5214615 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

137.98
132.38
129.79
128.89
128.16
121.47

85.104
84.842
80.882
77.313
76.995
76.677
72.810

52.444

21.098



7.3871
7.3826
7.3706
7.3606
7.2918
7.2870
7.2749
7.2705
7.2400

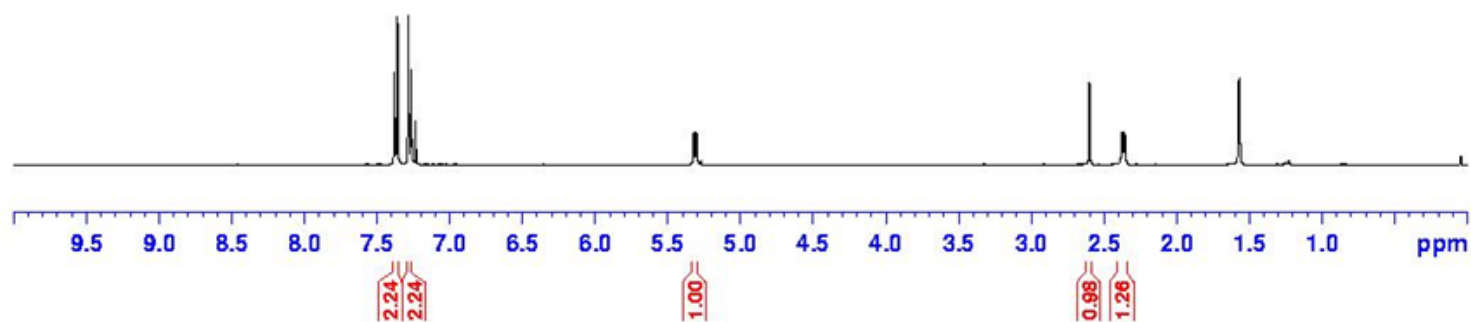
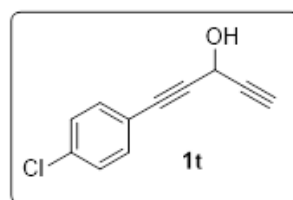
5.3289
5.3233
5.3101
5.3045

2.6076
2.6018
2.3804
2.3615

— 1.5736

Current Data Parameters
NAME RDK-01-85_H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 399.7611793 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

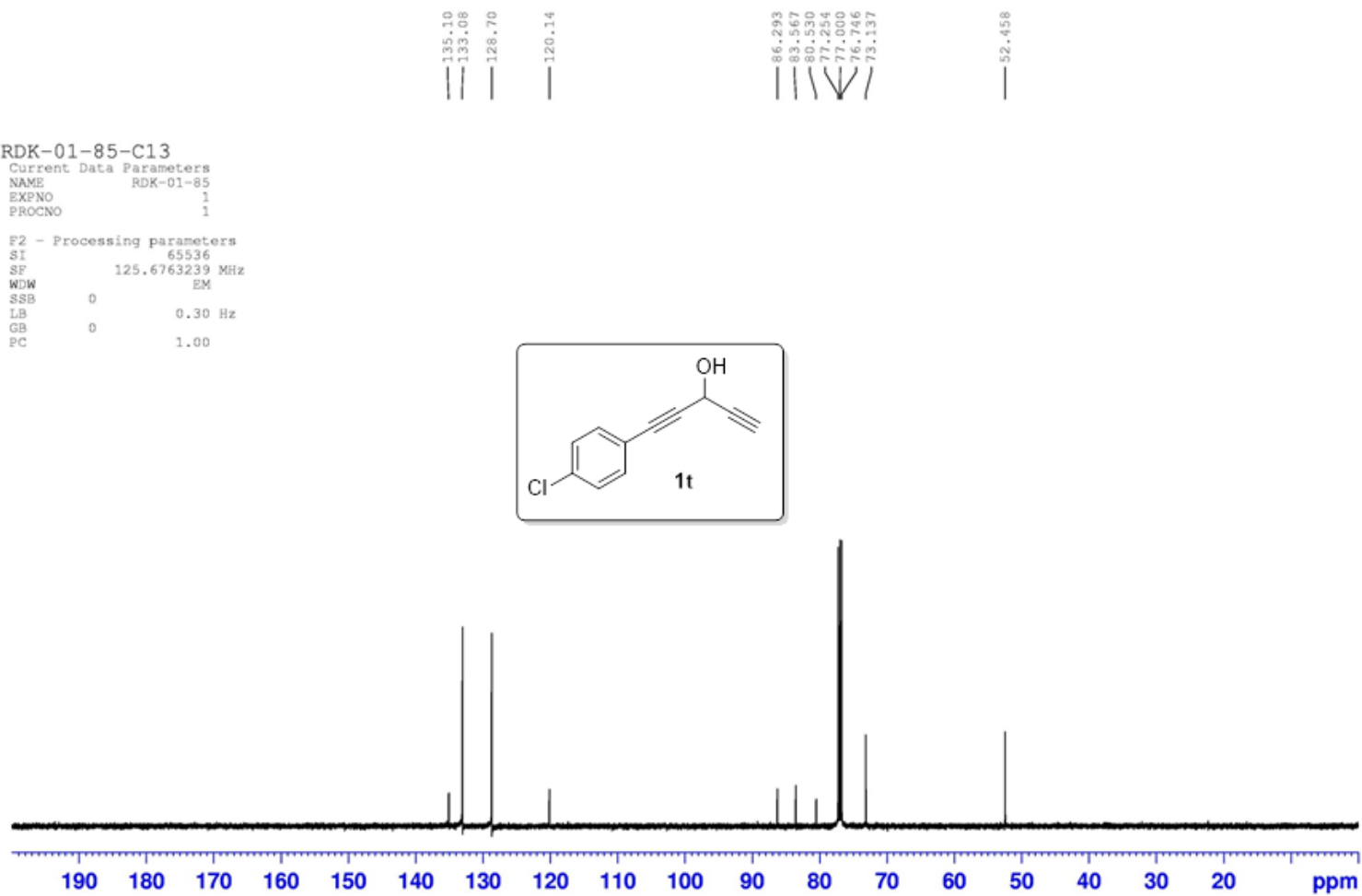
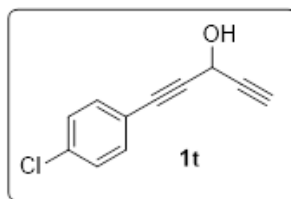


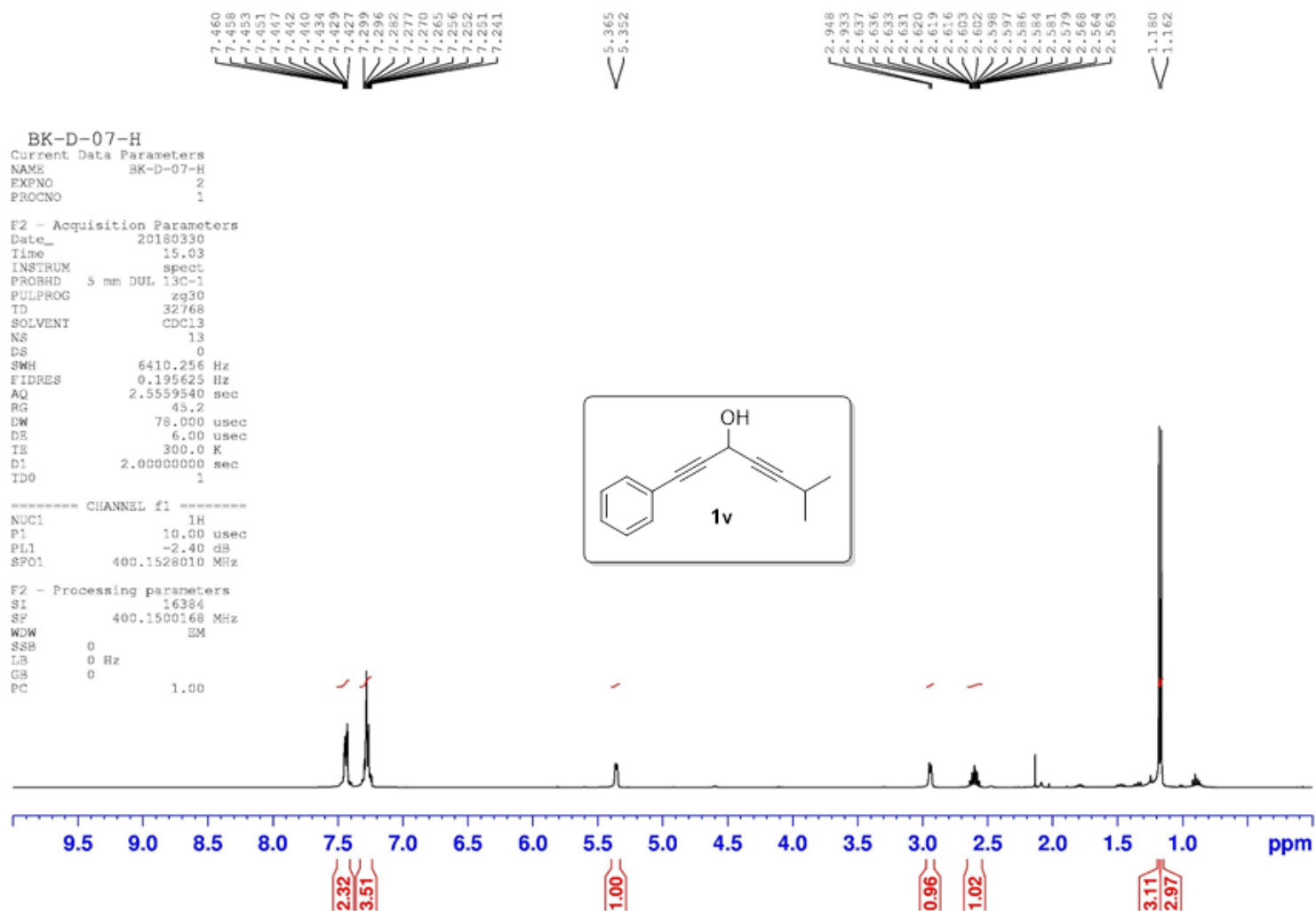
```
Current Data Parameters
NAME          RDK-01-85
EXPNO          1
PROCNO         1
```

```

F2 - Processing parameters
SI                65536
SF                125.6763239 MHz
WDW              EM
SSB              0
LB                0.30 Hz
GB              0
PC                1.00

```





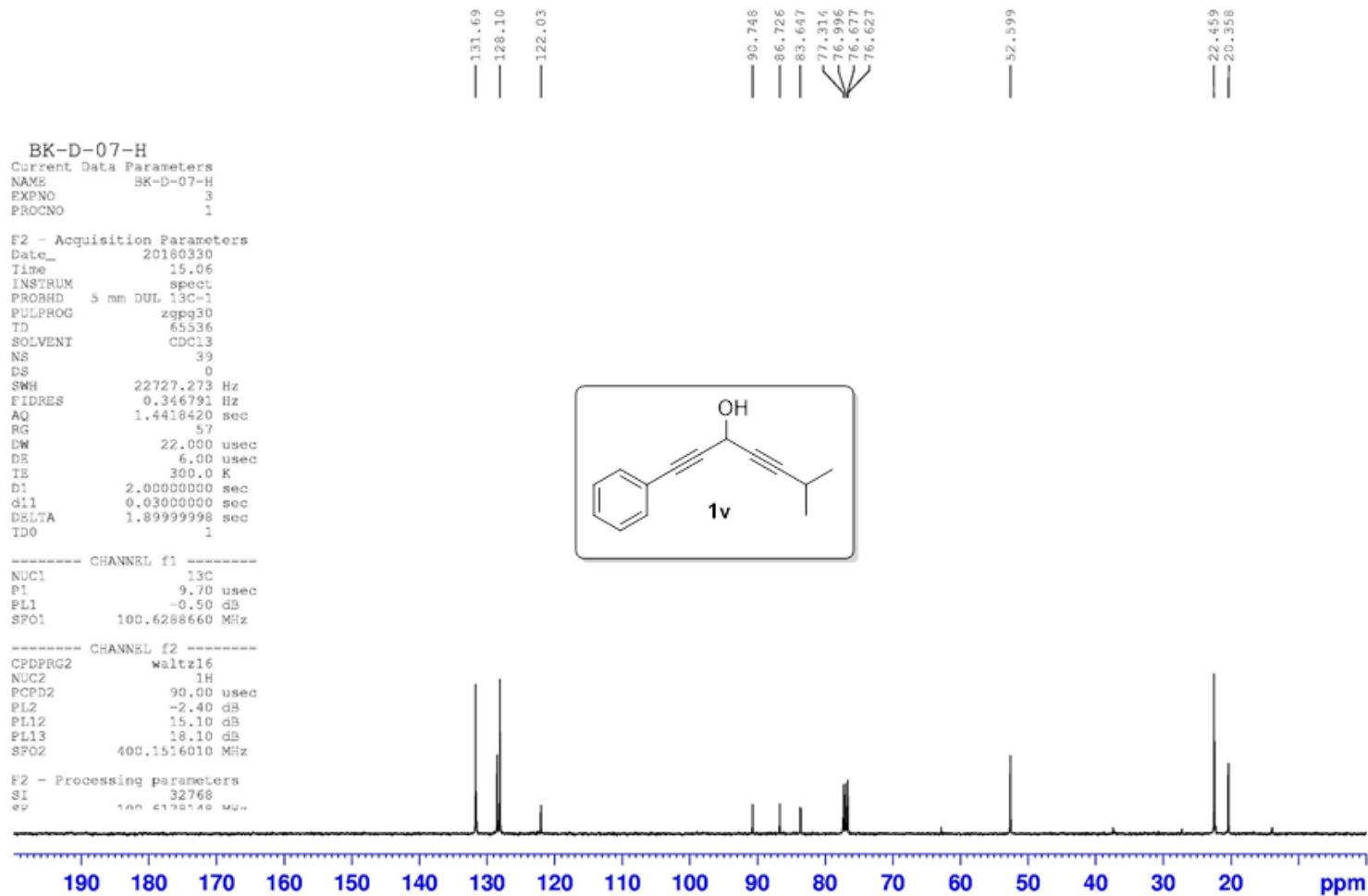
BK-D-07-H
 Current Data Parameters
 NAME BK-D-07-H
 EXPNO 3
 PROCNO 1

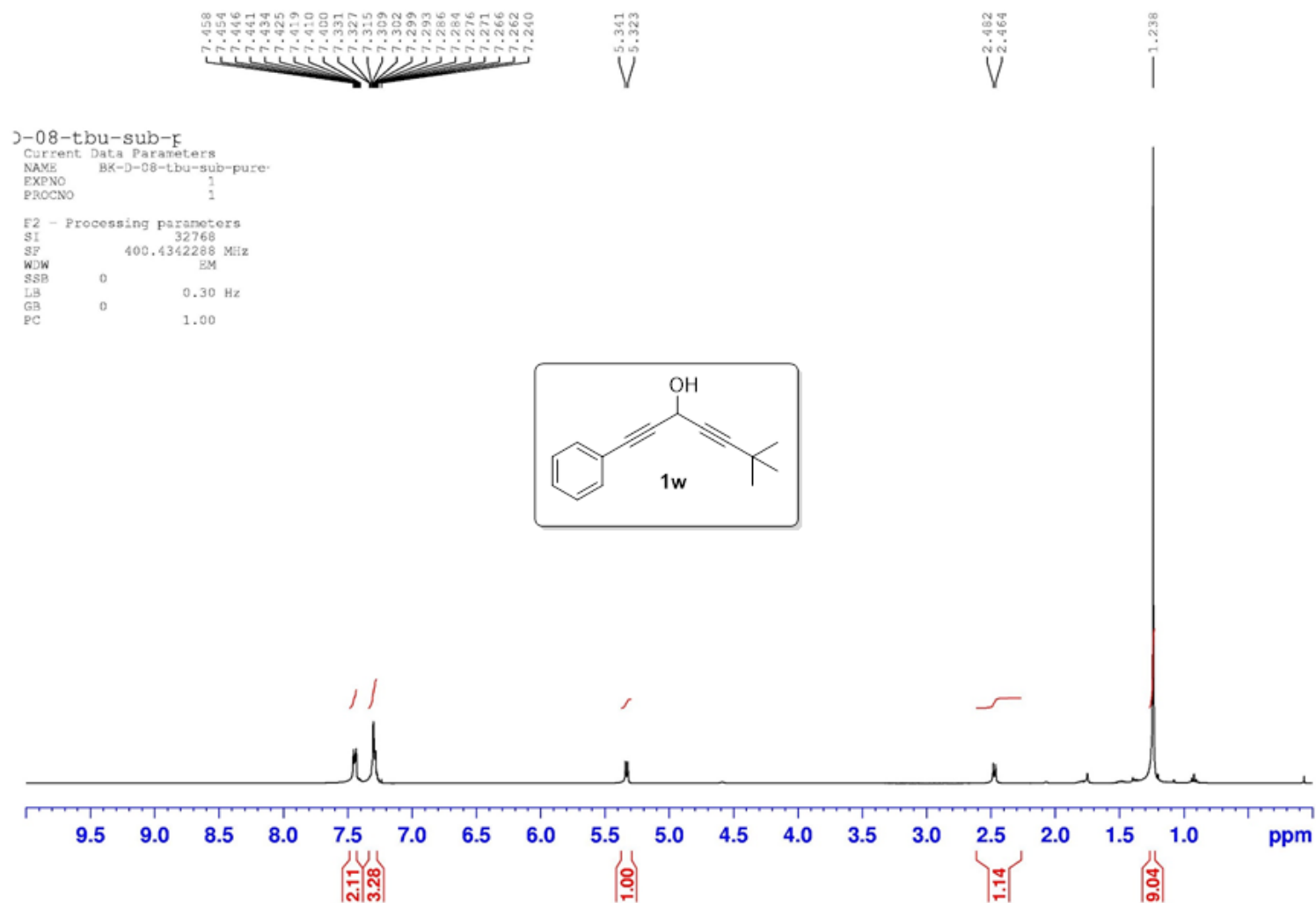
F2 - Acquisition Parameters
 Date_ 20180330
 Time 15.06
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 39
 DS 0
 SWH 22727.273 Hz
 FIDRES 0.346791 Hz
 AQ 1.4418420 sec
 RG 57
 DW 22.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 ID0 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

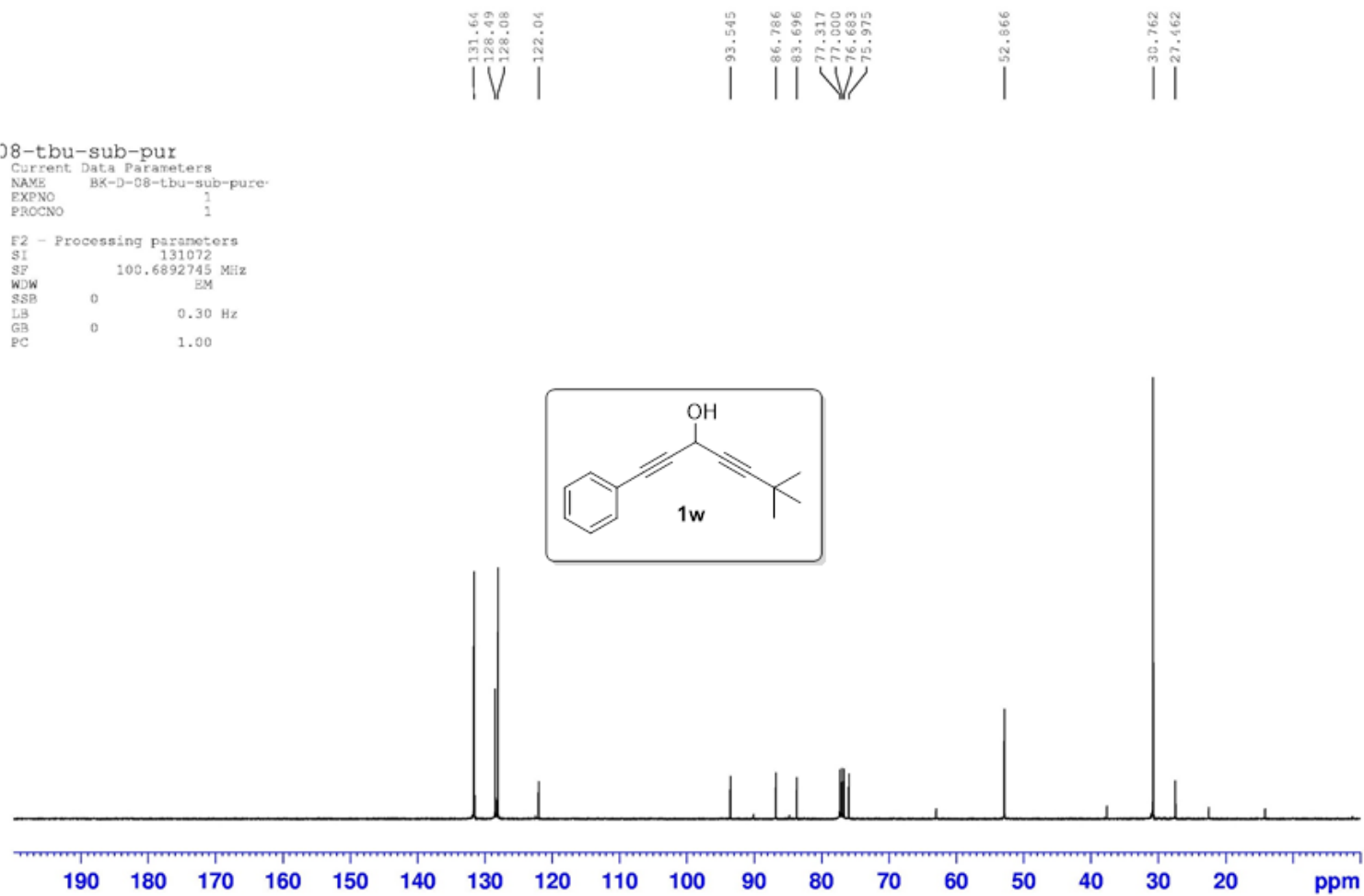
F2 - Processing parameters
 SI 32768
 SF 100.6176140 MHz





08-tbu-sub-pur
 Current Data Parameters
 NAME BK-D-08-tbu-sub-pure
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 SI 131072
 SF 100.6892745 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

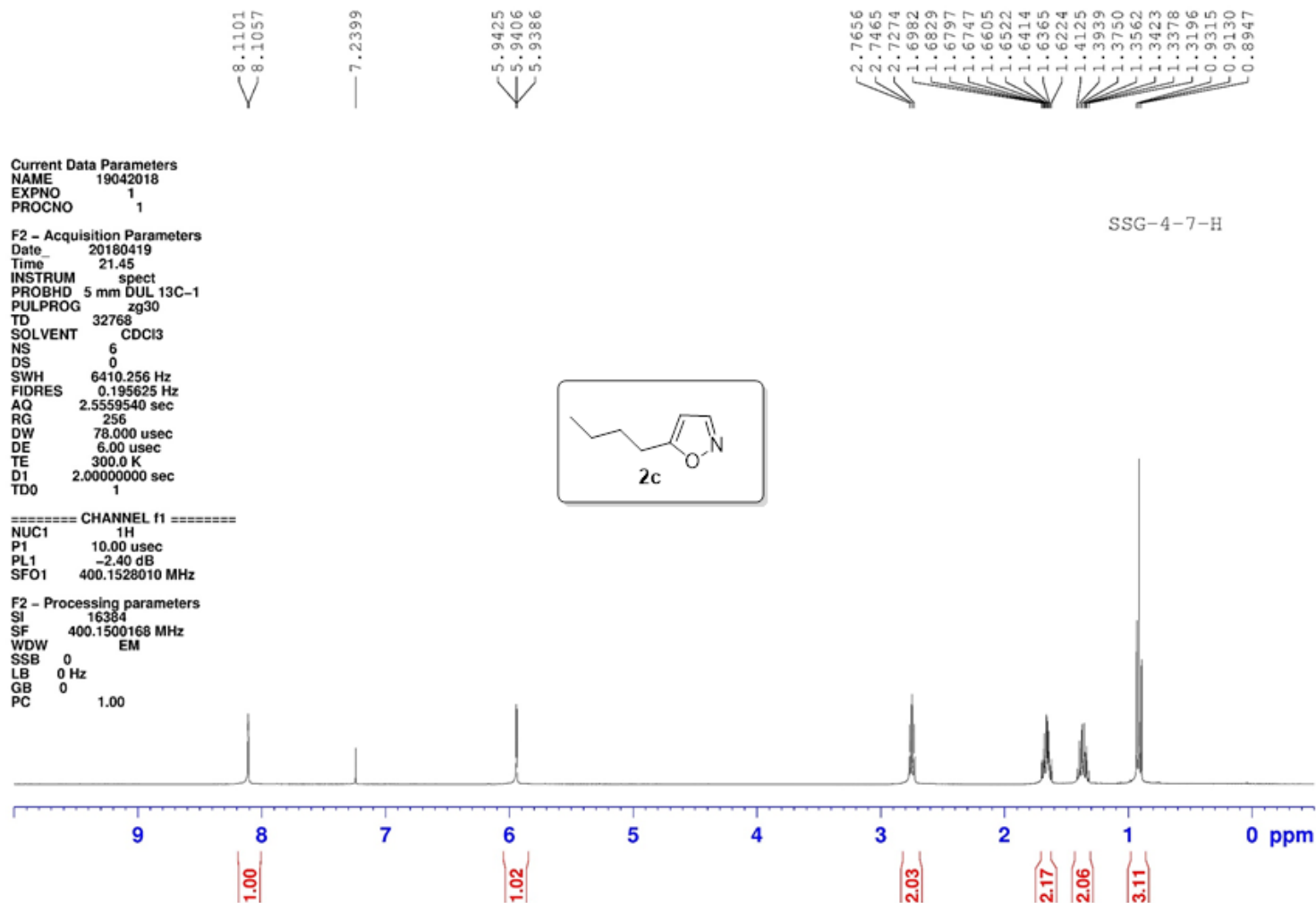
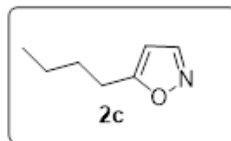


Current Data Parameters
 NAME 19042018
 EXPNO 1
 PROCNO 1

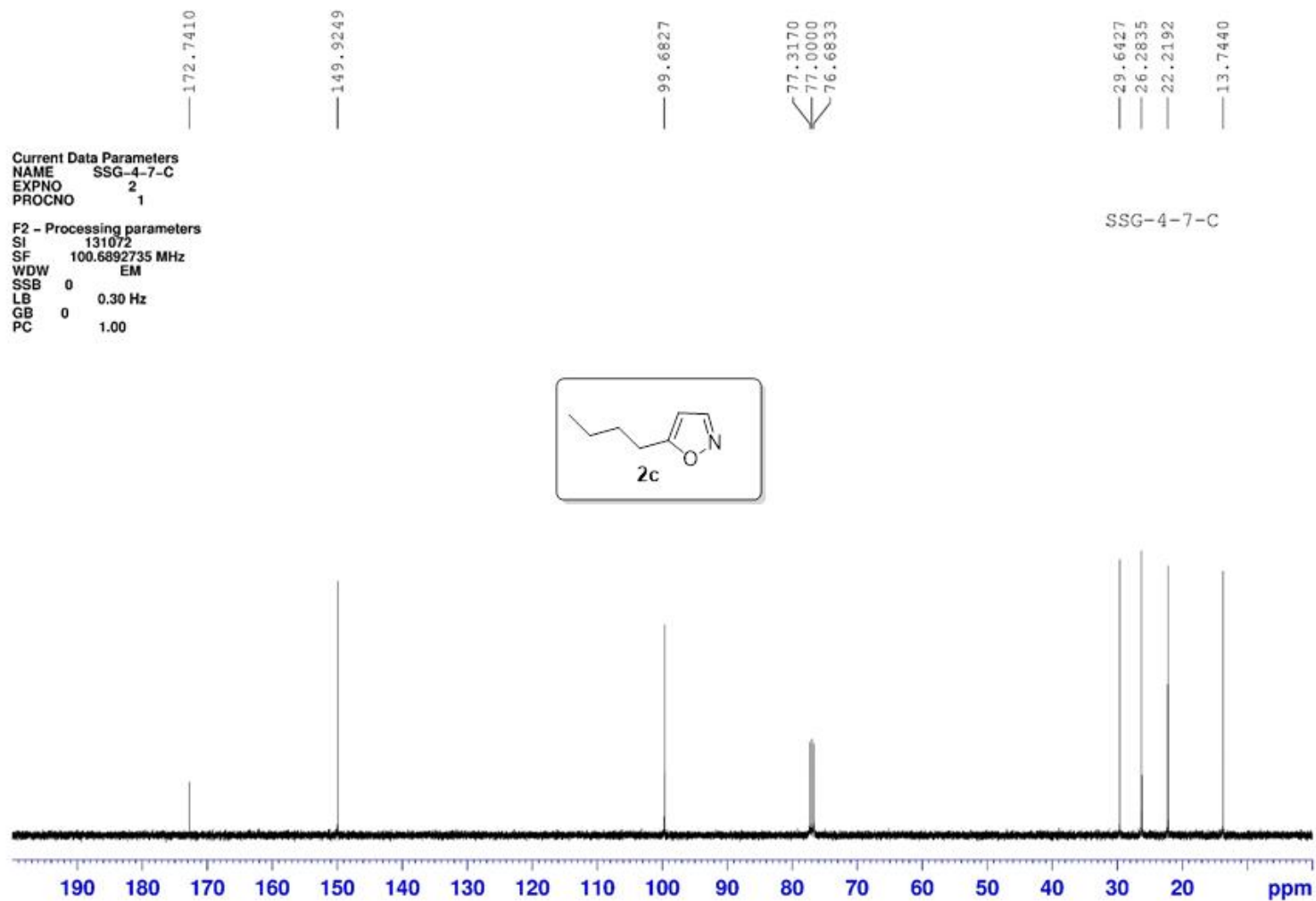
F2 - Acquisition Parameters
 Date_ 20180419
 Time 21.45
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 6
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 256
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== 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



SSG-4-7-H



10.2727
10.1997

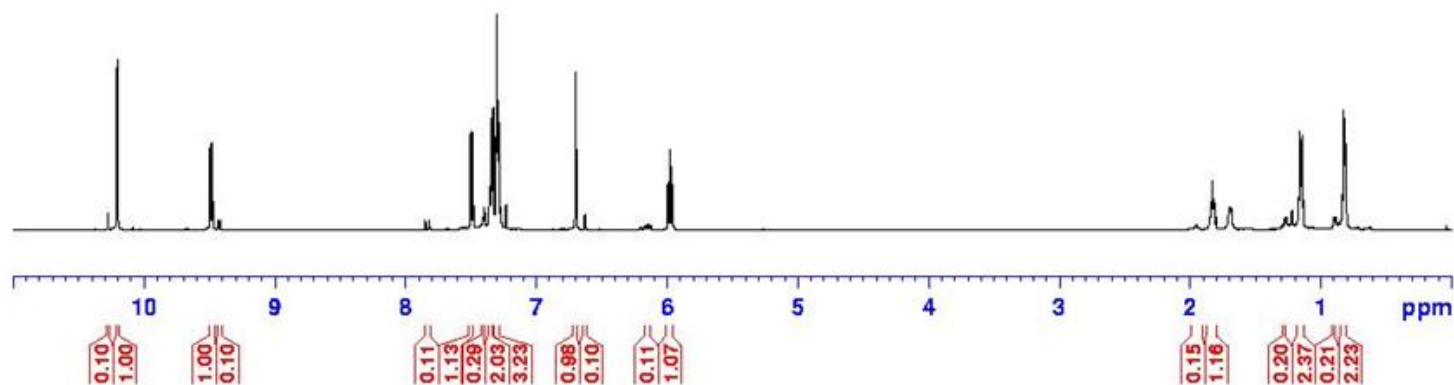
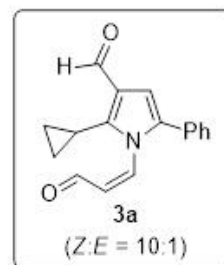
9.4891
9.4737
9.4287
9.4138

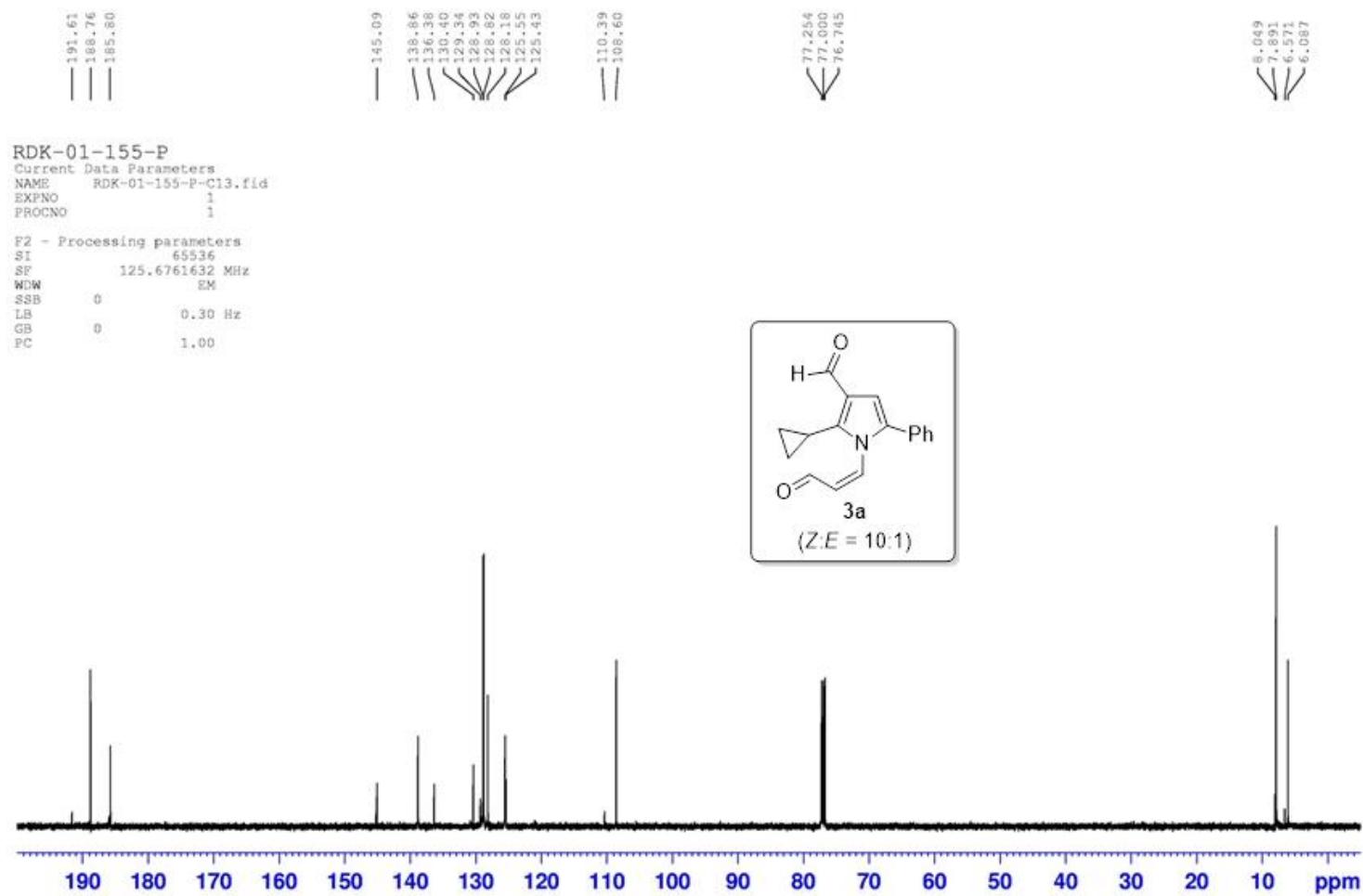
7.8446
7.8153
7.5081
7.4911
7.4170
7.4040
7.3660
7.3509
7.3363
7.3114
7.2966
7.2779
7.2400
6.7037
6.6319
6.1746
6.1596
6.1452
6.1303
5.9969
5.9807
5.9645

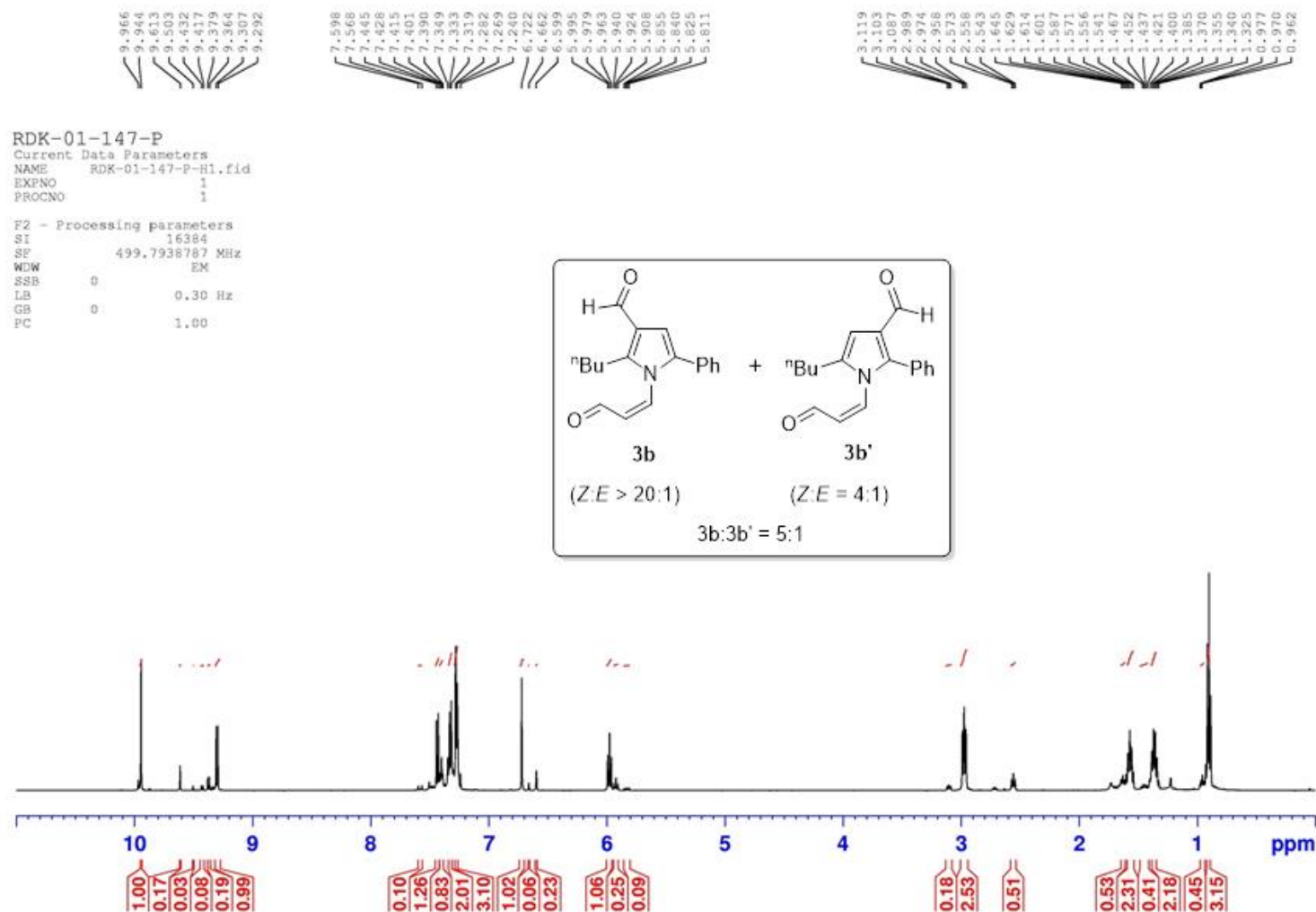
1.9685
1.9576
1.9466
1.9415
1.8605
1.8494
1.8440
1.8331
1.8221
1.8167
1.8056
1.7085
1.6931
1.2941
1.2810
1.2666
1.2551
1.1777
1.1657
1.1513
1.1396
0.9156

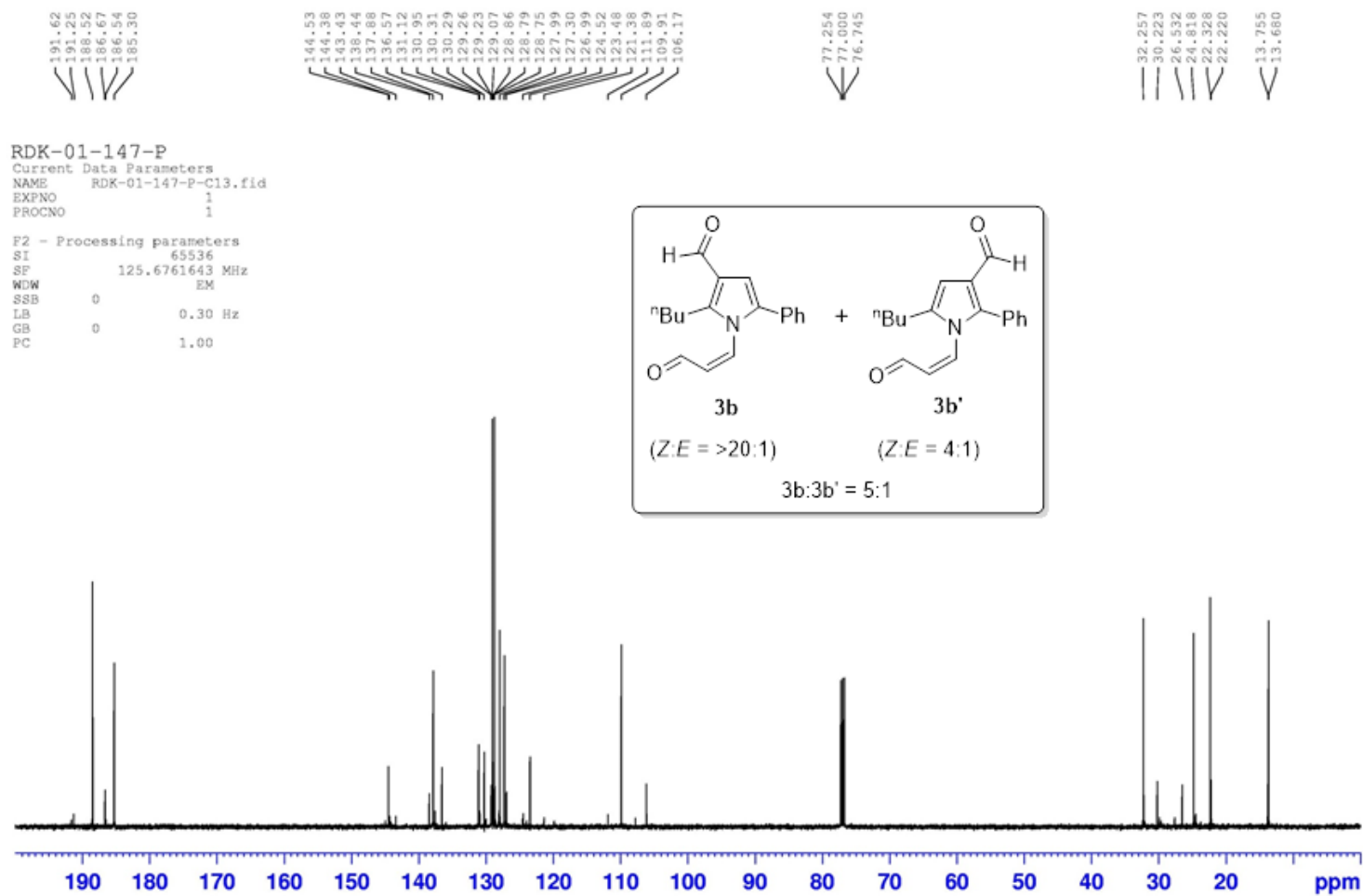
Current Data Parameters
NAME RDK-01-155-P-H1.fid
EXPNO 1
PROCNO 1

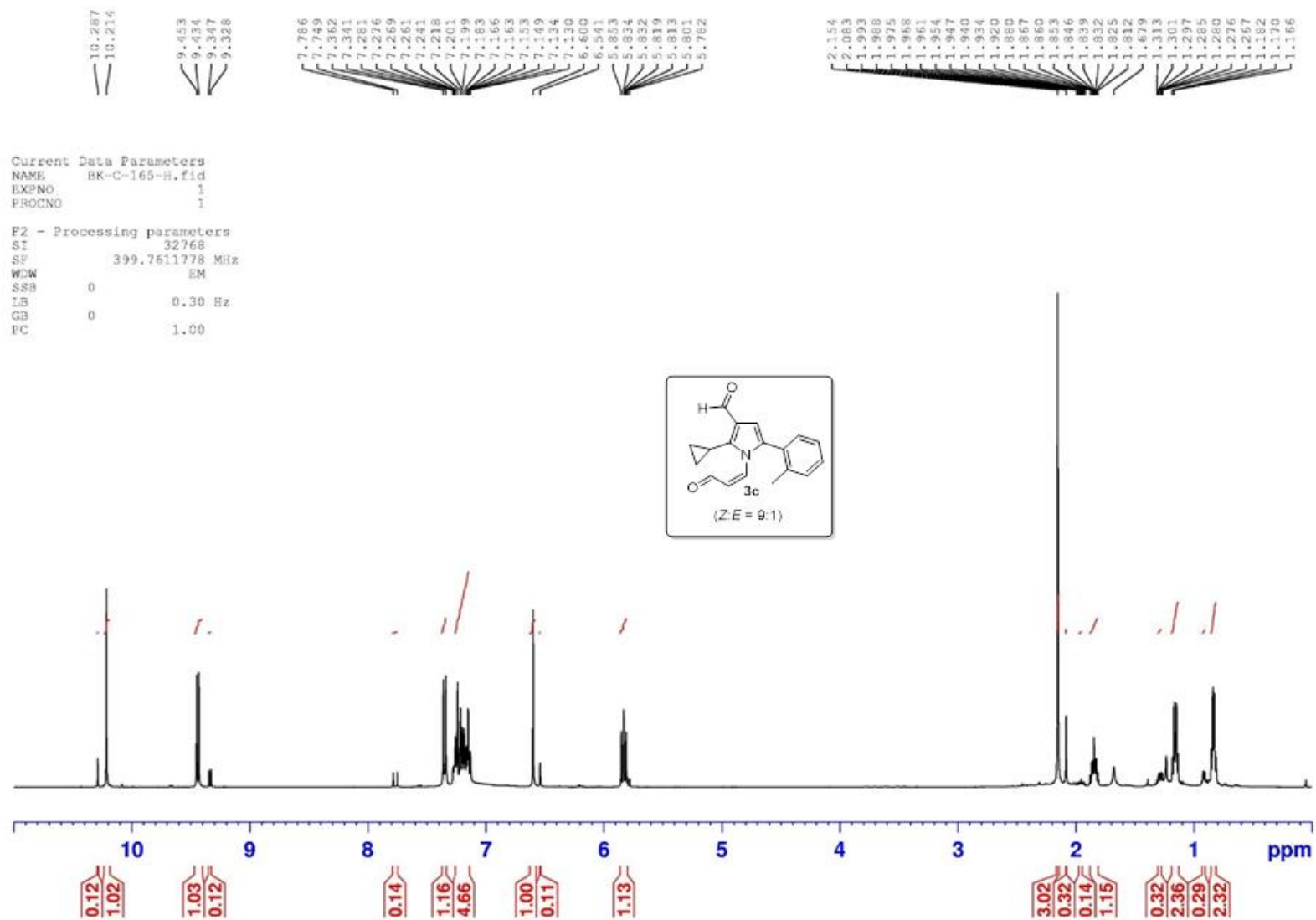
F2 - Processing parameters
SI 16384
SF 499.7938788 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00











191.76
188.50
185.92
183.76

144.91
144.14
138.22
137.80
137.31
135.25
131.42
130.83
130.67
130.57
129.98
129.78
129.11
126.34
125.99
125.15
124.82
118.75
110.51
109.28

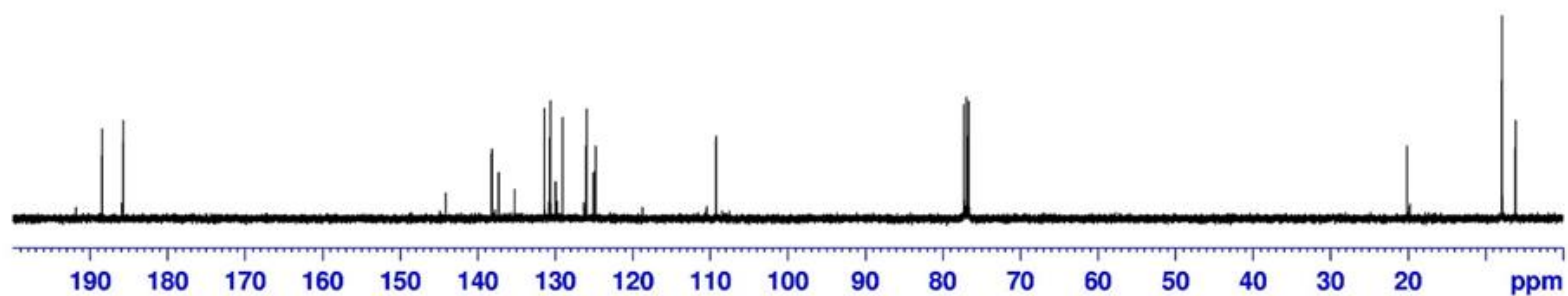
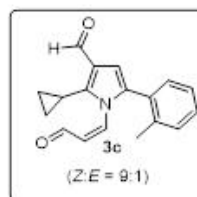
77.318
77.000
76.662

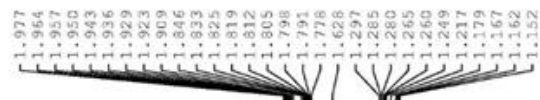
20.131
19.792

7.894
7.824
6.203
6.122

Current Data Parameters
NAME BK-C-165-13C-1.fid
EXPNO 1
PROCNO 1

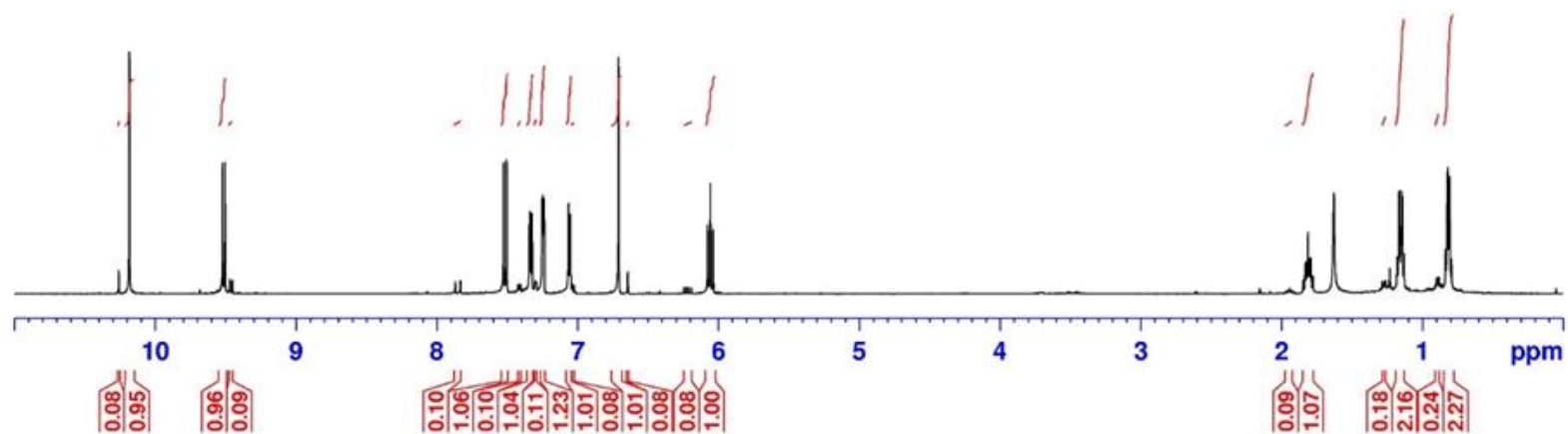
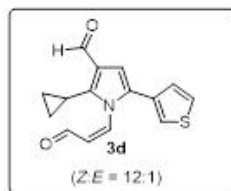
F2 - Processing parameters
SI 65536
SF 100.5214601 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





BK-D-17-A-H
Current Data Parameters
NAME BK-D-17-A-H.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



191.35
188.35
185.64
185.46

144.89
144.61
138.60
131.38
130.90
127.69
127.40
126.85
126.53
125.98
125.17
125.15
123.54
120.73
110.37
108.15

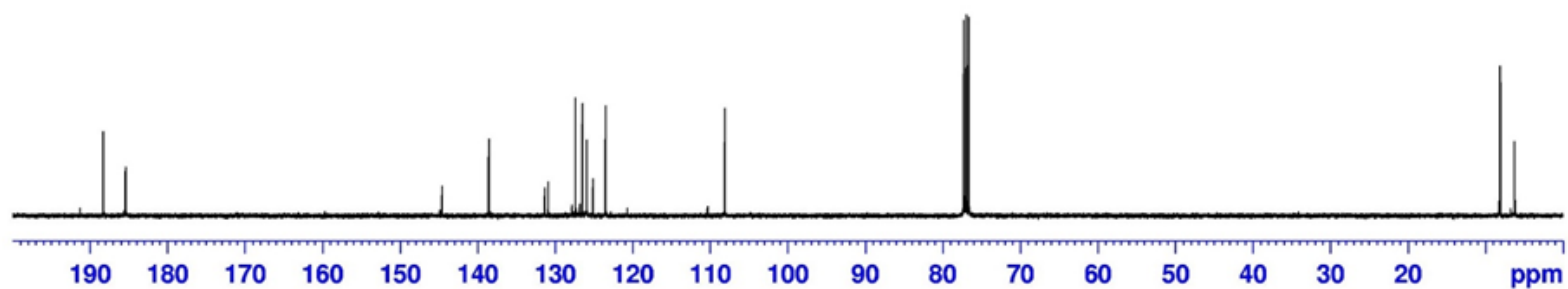
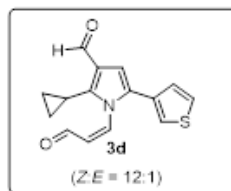
77.317
77.000
76.884

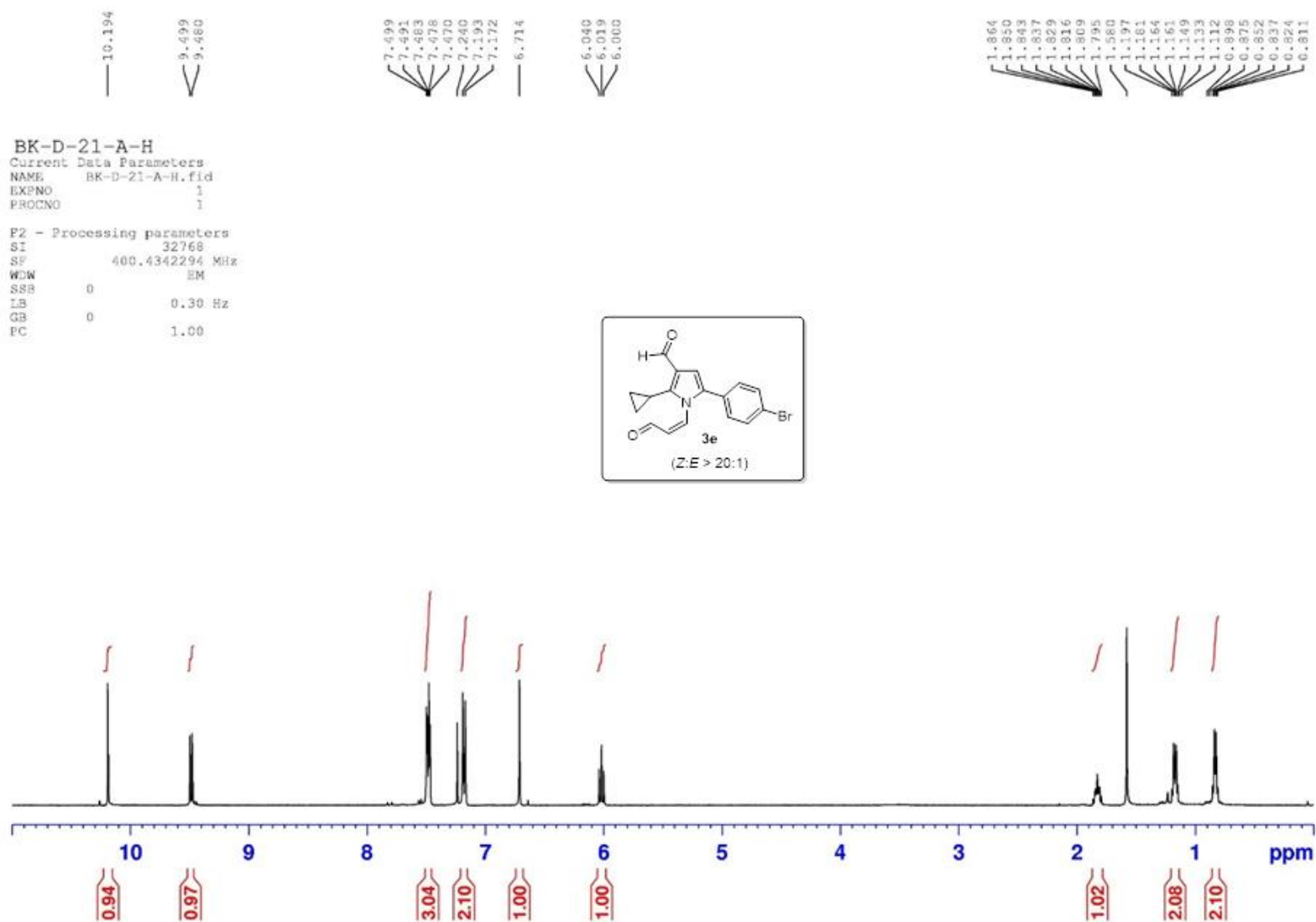
8.258
8.112
8.053
6.237

BK-D-17-A-C13

Current Data Parameters
NAME BK-D-17-A-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 131072
SF 100.6892717 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





188.33
185.37

145.15
138.52
135.04
131.97
130.14
129.26
125.90
125.41
122.40

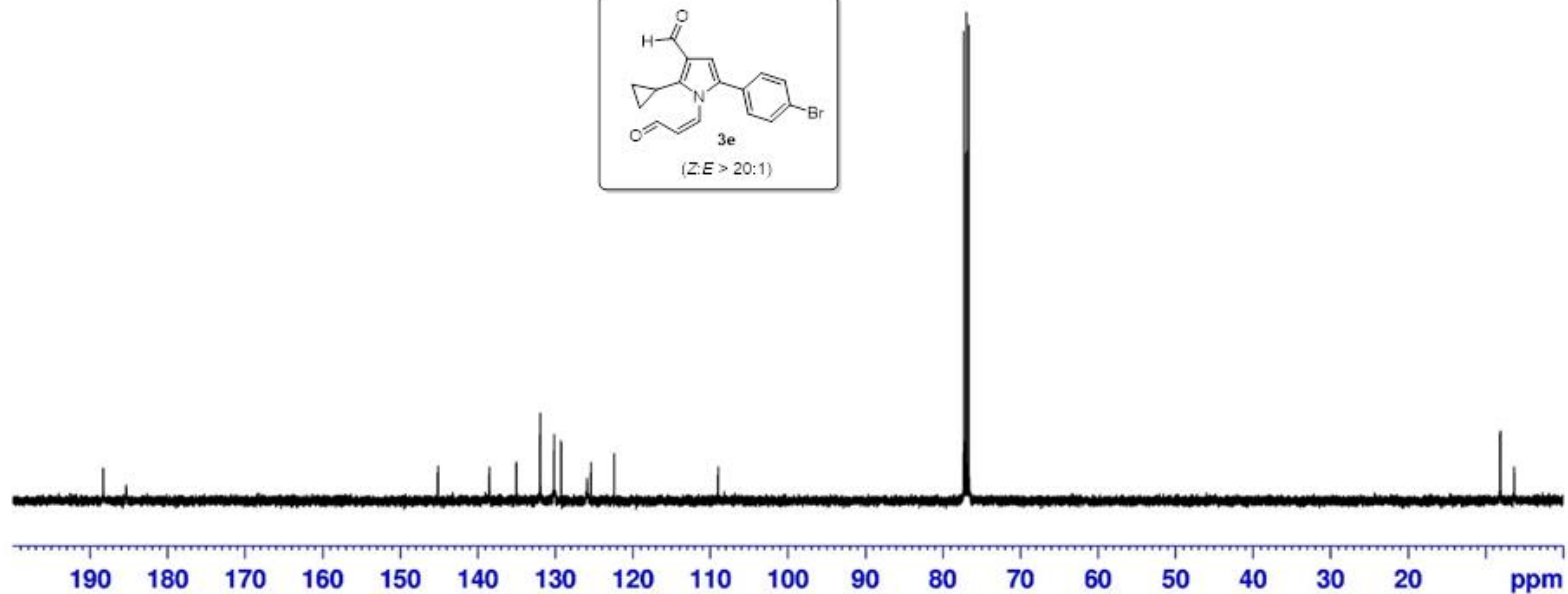
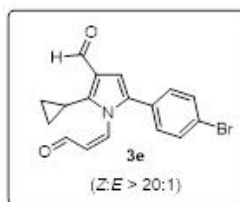
109.00

77.317
77.001
76.684

8.106
6.295

Current Data Parameters
NAME BK-D-21-A-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 131072
SF 100.6892706 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10.258
10.187

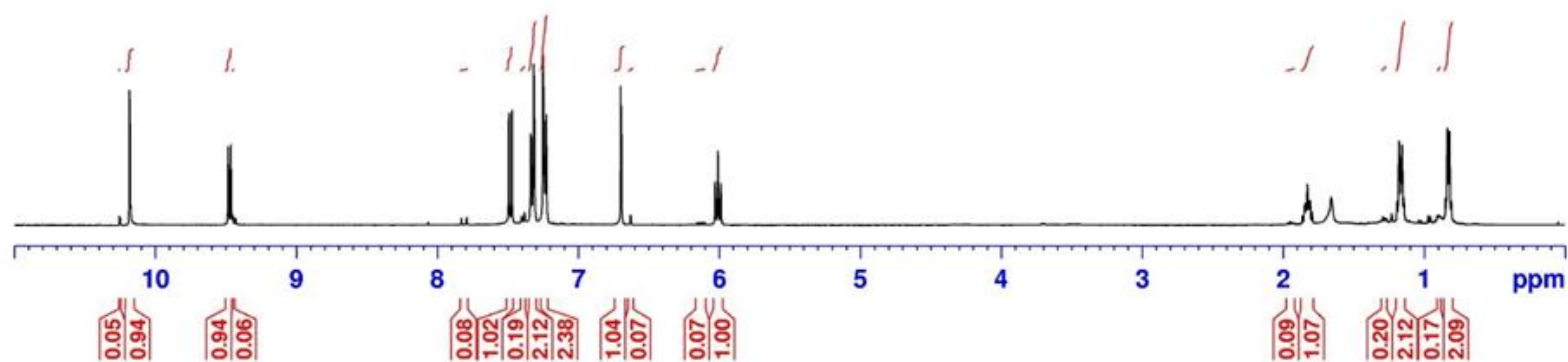
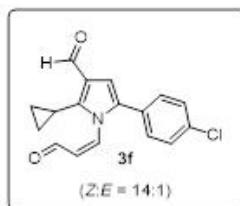
9.488
9.469
9.455
9.436

7.830
7.794
7.495
7.473
7.404
7.383
7.338
7.335
7.322
7.317
7.251
7.241
7.230
6.700
6.631
6.162
6.143
6.125
6.106
6.032
6.011
5.992

1.984
1.970
1.965
1.951
1.937
1.931
1.917
1.883
1.850
1.843
1.827
1.829
1.823
1.815
1.809
1.795
1.659
1.626
1.308
1.292
1.271
1.259
1.192
1.177
1.165
1.160
1.156
1.145

BK-D-22-A-H
Current Data Parameters
NAME BK-D-22-AA-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 400.4342266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



191.34
188.62
185.83
183.65

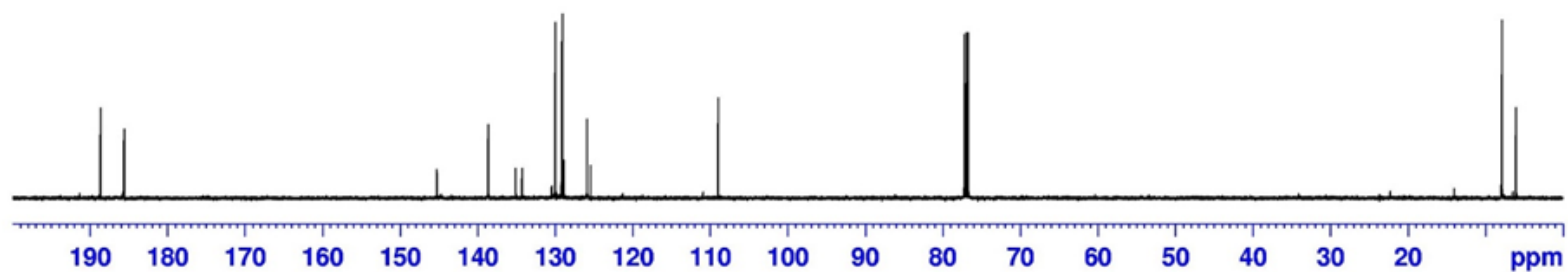
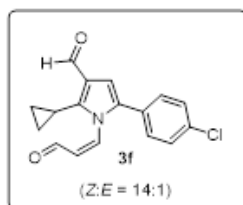
145.29
138.67
133.14
134.30
130.50
130.03
129.24
129.13
128.90
125.91
125.47
121.33

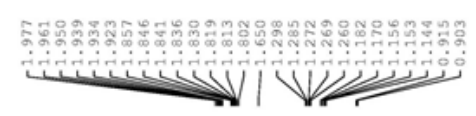
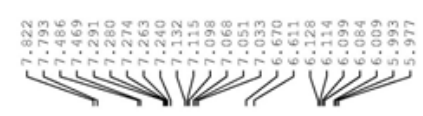
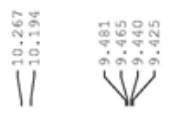
110.95
109.01

77.254
77.000
76.746

7.994
7.894
6.482
6.081

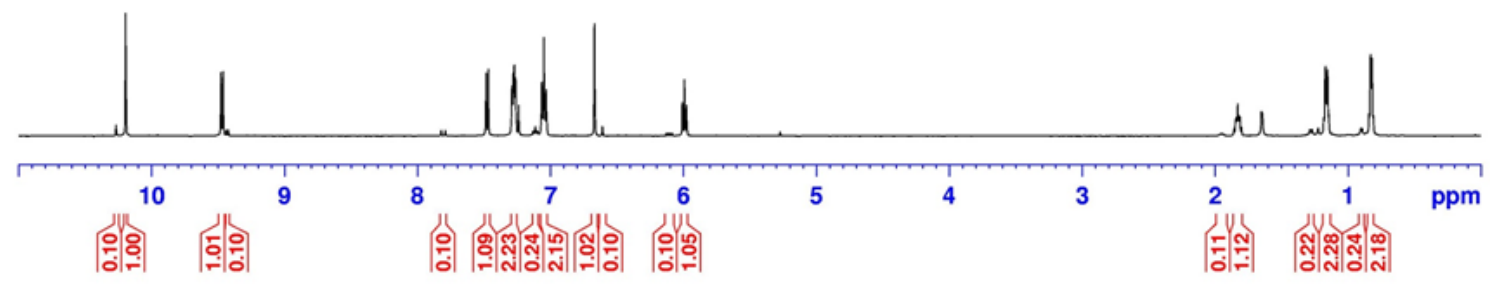
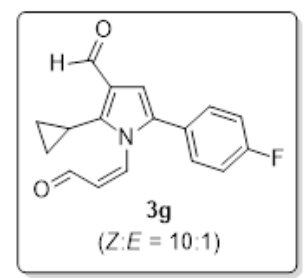
BK-D-22-A
Current Data Parameters
NAME BK-D-22-A-C13.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 125.6761614 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





RDK-01-161-P
Current Data Parameters
NAME RDK-01-161-P.-H1.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 16384
SF 499.7938790 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



191.43
188.61
185.70

163.44
161.45

145.04

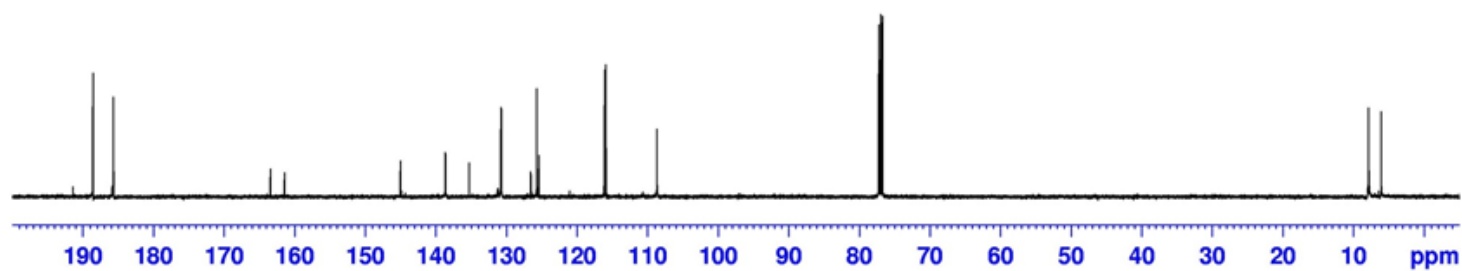
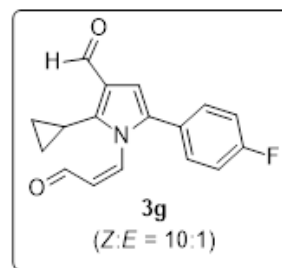
138.67
135.29
130.91
130.74
126.58
126.55
125.72
125.39
121.07
116.10
115.93
108.70

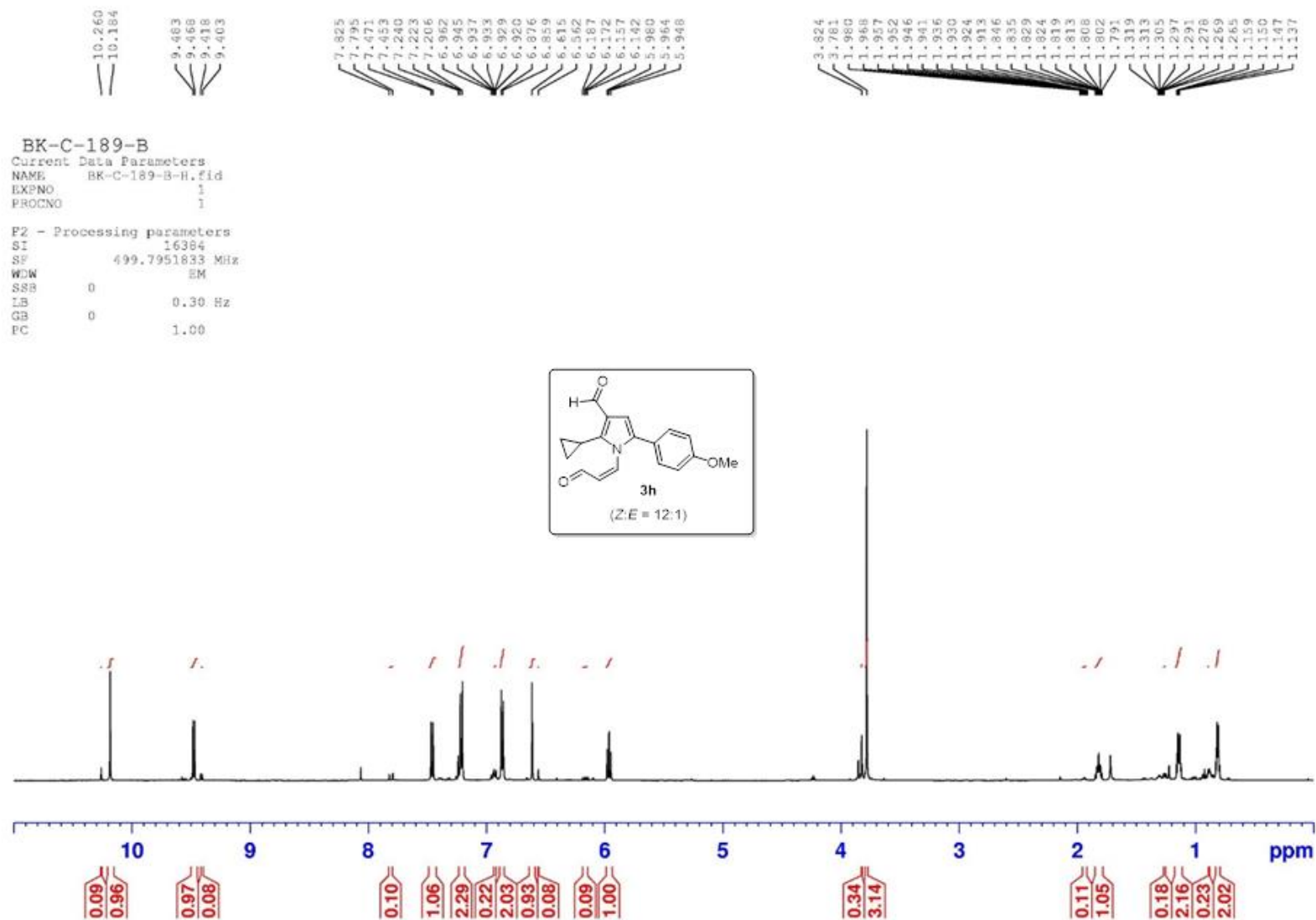
77.254
77.000
76.745

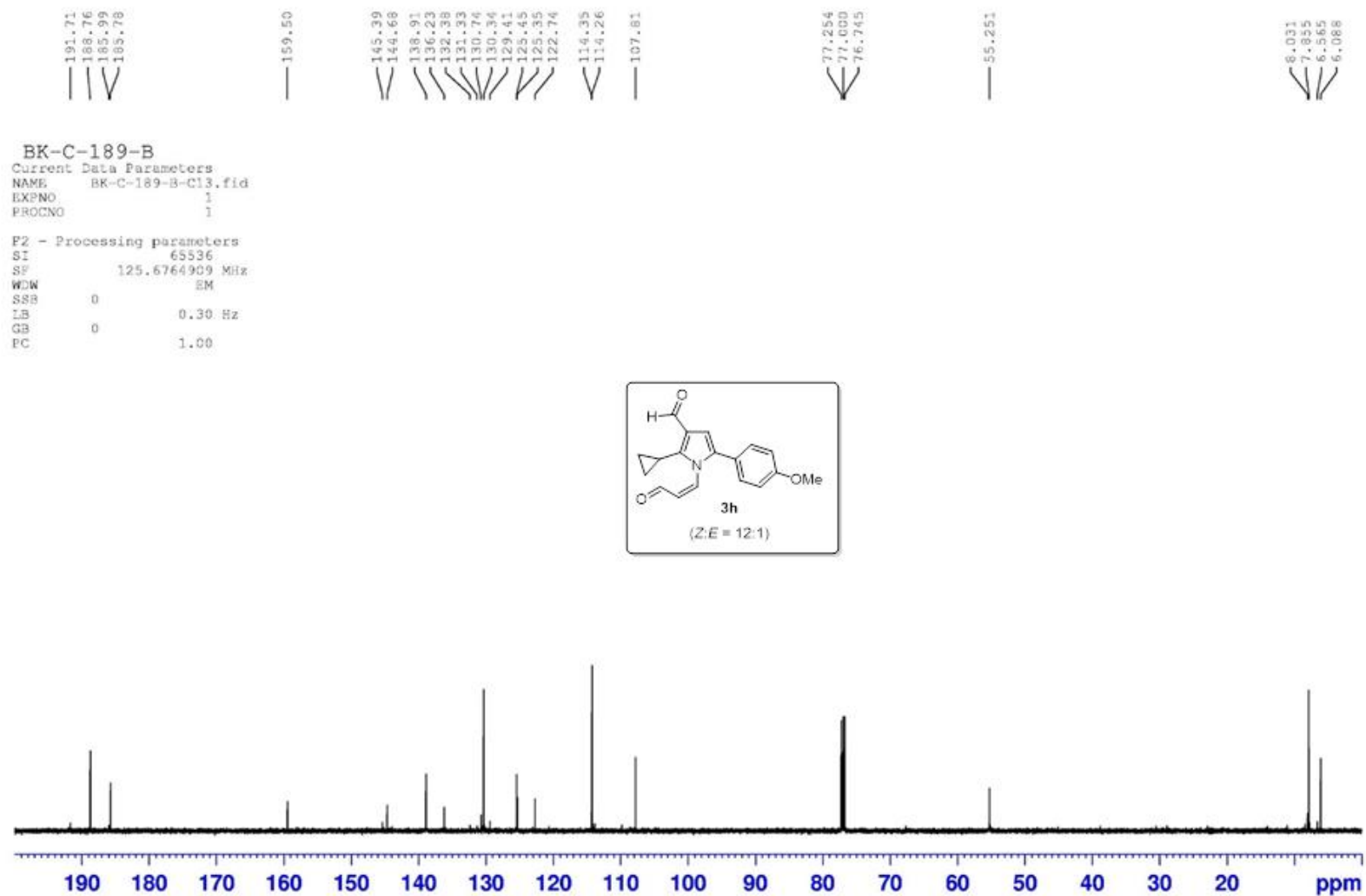
7.867
6.078

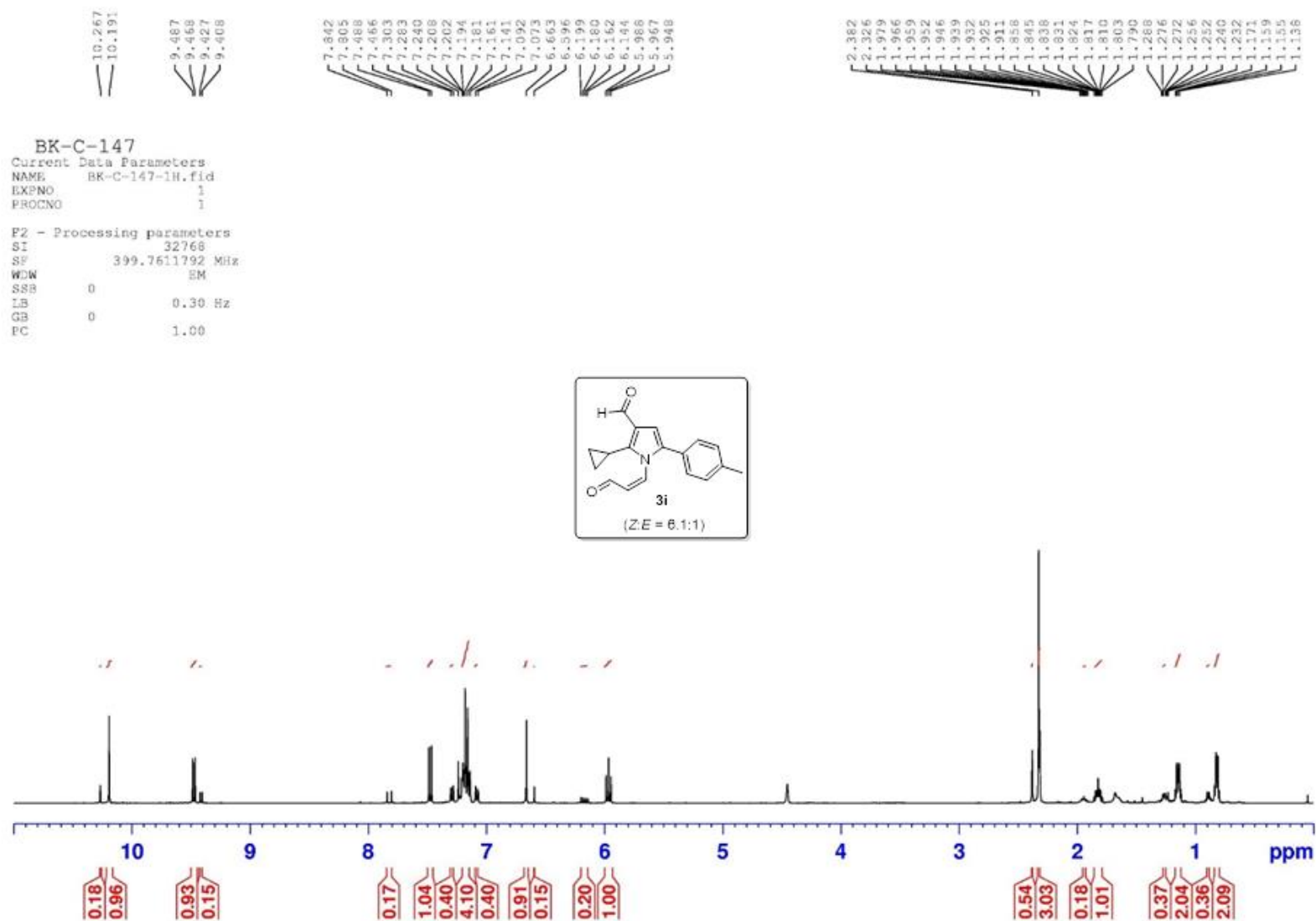
RDK-01-161-P
Current Data Parameters
NAME RDK-01-161-P-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 125.6761614 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00









191.68
188.84
185.99
185.79

145.37
144.86
139.01
138.94
138.56
138.22
136.51
131.53
129.62
129.52
129.28
129.01
128.87
127.53
125.56
125.42
120.85
119.46
110.11
108.24

77.319
77.001
76.683

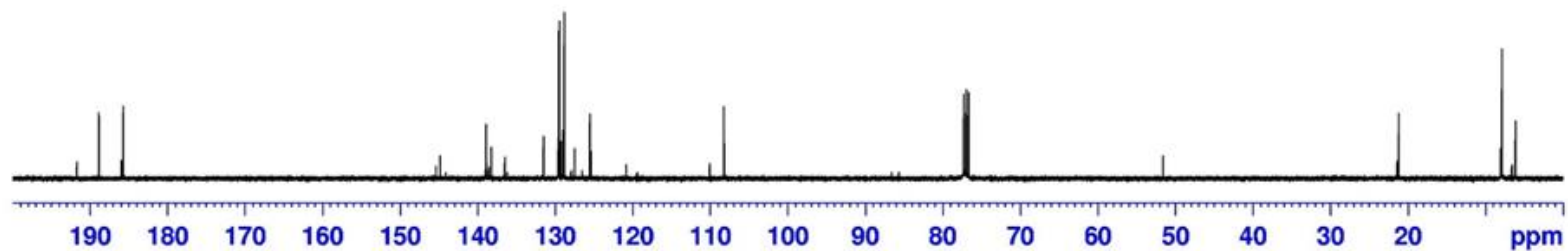
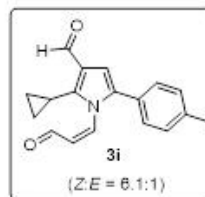
21.409
21.264

8.054
7.887
6.595
6.129

BK-C-147

Current Data Parameters
NAME BK-C-147-13C.fid
EXPNO 1
PROCNO 1

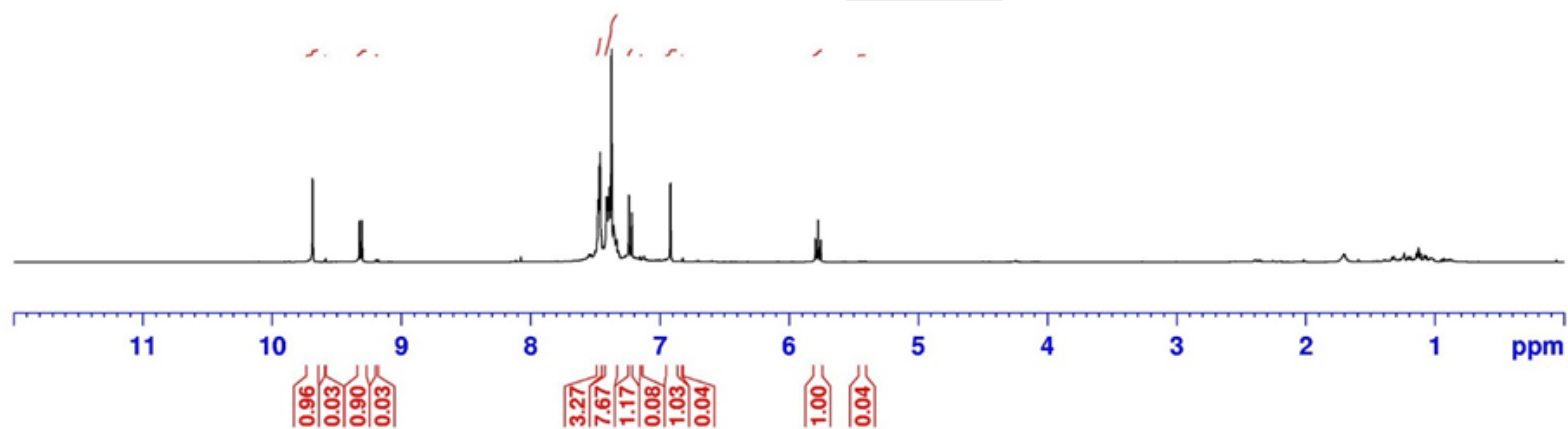
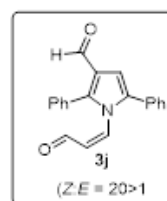
F2 - Processing parameters
SI 65536
SF 100.5214589 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BK-C-156-H

Current Data Parameters
 NAME BK-C-156-H.fid
 EXPNO 1
 PROCNO 1
 F2 - Processing parameters
 SI 32768
 SF 399.7611794 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.688
9.588
9.325
9.306
9.197
9.178
7.476
7.467
7.462
7.414
7.410
7.406
7.395
7.389
7.356
7.359
7.343
7.340
7.333
7.239
7.217
7.151
7.122
6.918
6.823
5.795
5.774
5.754
5.459
5.440
5.422
5.404



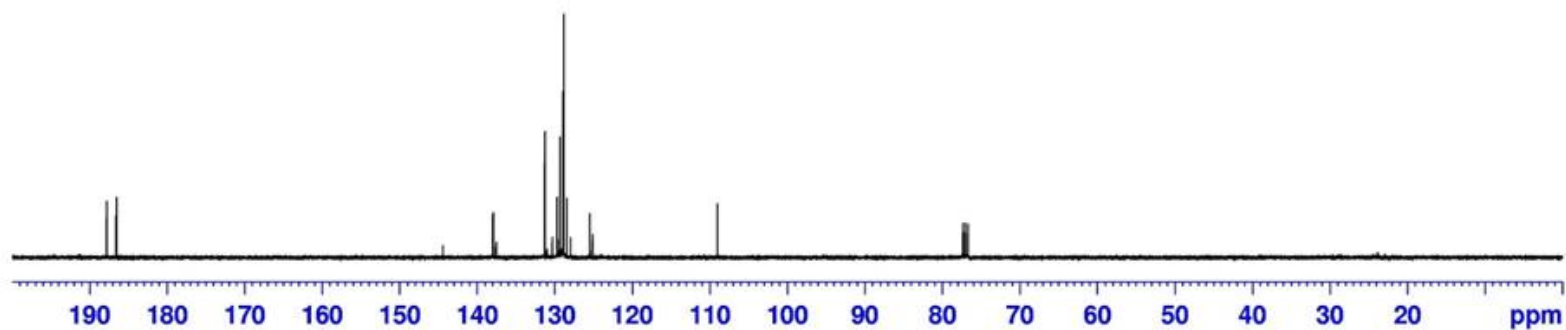
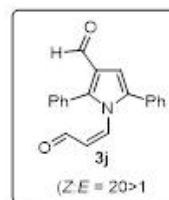
187.77
186.54
3K-C-156-C13

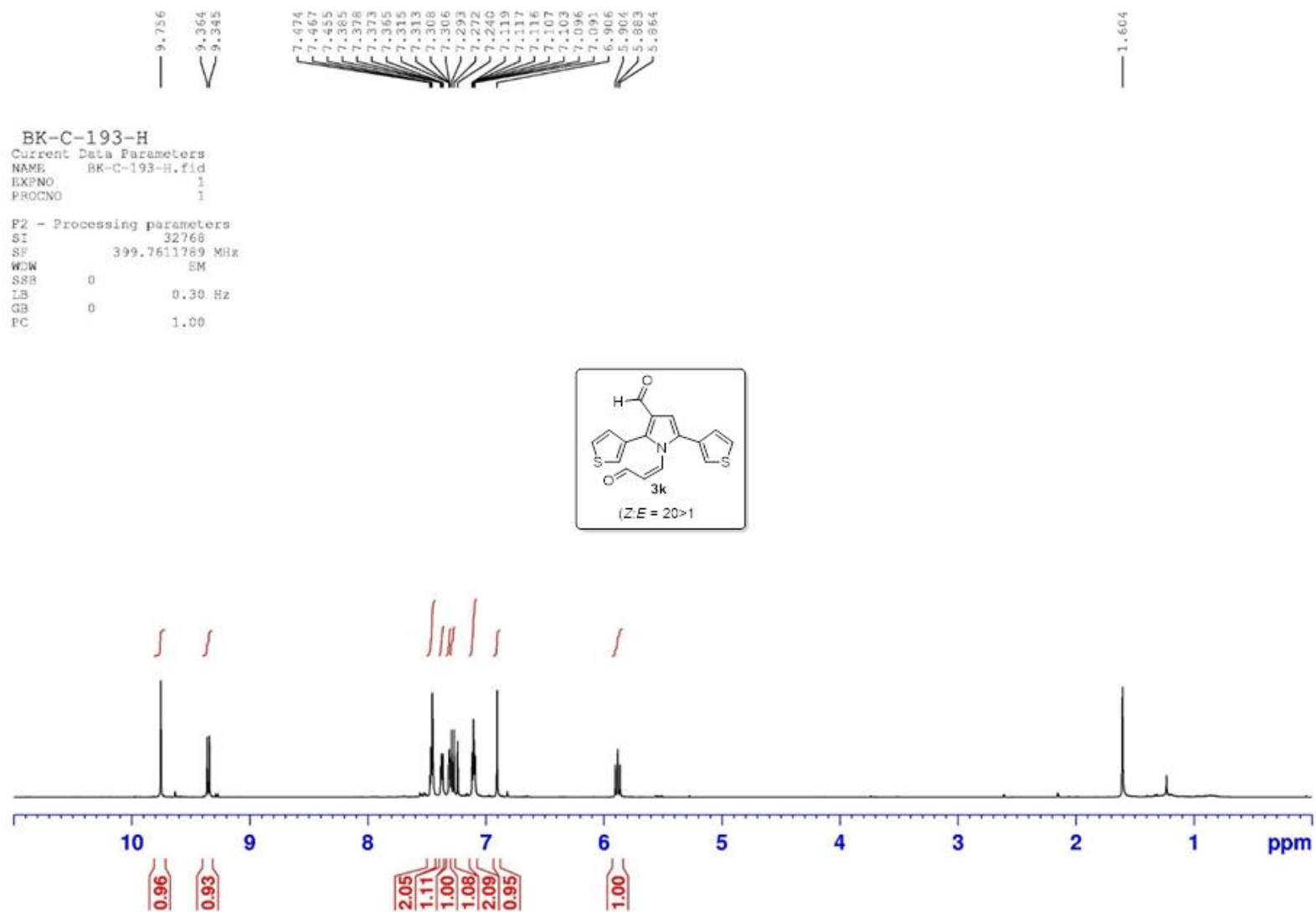
144.40
137.96
137.55
131.27
130.99
130.26
129.56
129.29
128.63
128.44
127.92
125.45
125.08
108.97

77.318
77.000
76.682

Current Data Parameters
NAME BK-C-156-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214616 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



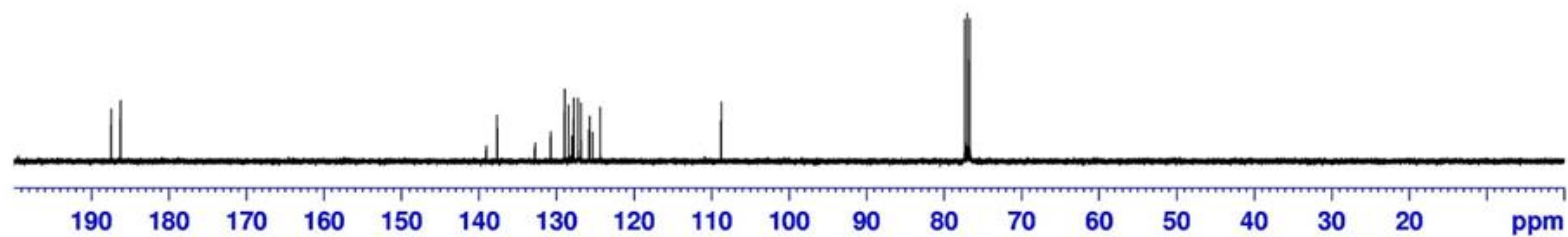
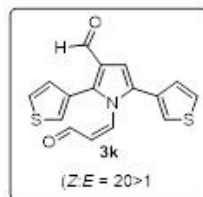


187.44
186.23
3K-C-193-C13

139.05
137.63
132.76
130.76
128.91
128.45
127.97
127.76
127.19
126.80
125.75
125.34
124.34
108.74

77.318
77.000
76.682

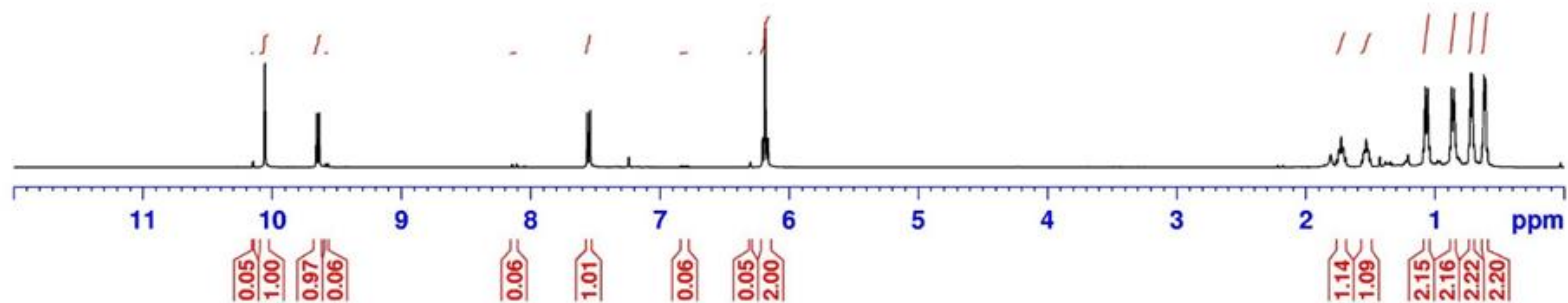
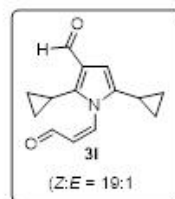
Current Data Parameters
NAME BK-C-193-c13.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214581 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BK-C-162-H

Current Data Parameters
 NAME BK-C-162-A-1H.fid
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 399.7611766 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



192.14
189.60
185.75
185.54
3K-C-162-c13

143.60
139.35
138.02

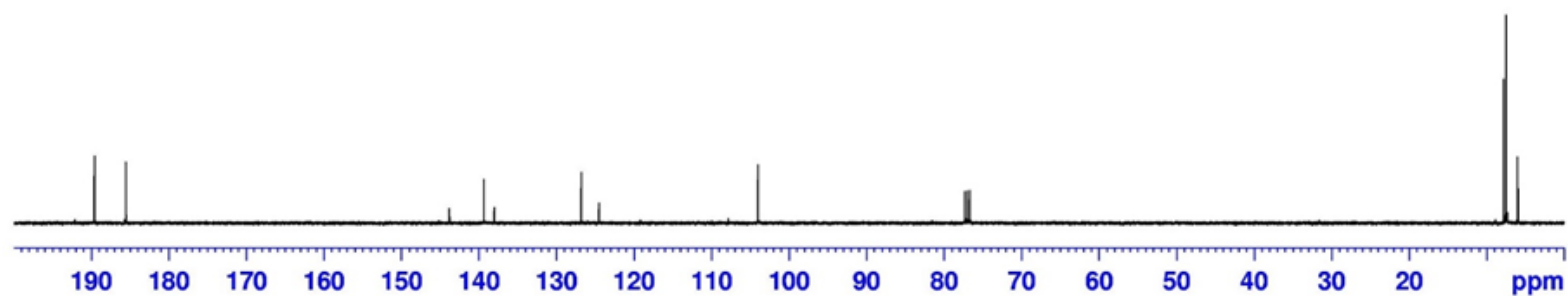
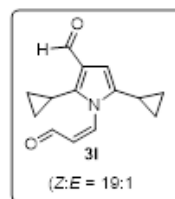
126.78
125.97
124.51

107.61
104.01

77.318
77.000
76.682

7.813
7.572
7.501
7.316
5.970

Current Data Parameters
NAME BK-C-162-c13.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214618 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BK-C-157-H1

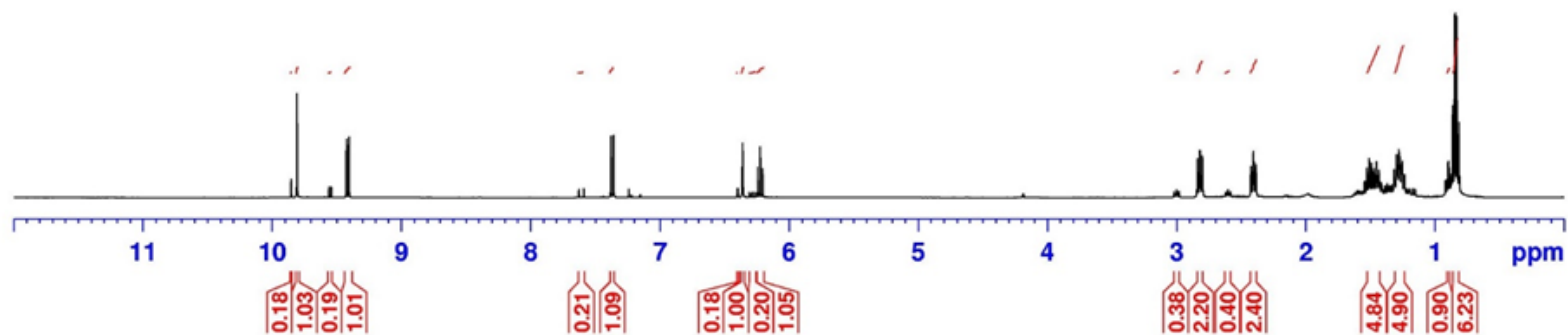
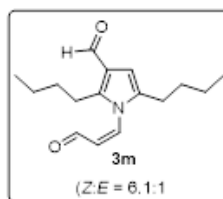
Current Data Parameters
 NAME BK-C-157-H.fid
 EXPNO 1
 PROCNO 1
 F2 - Processing parameters
 SI 32768
 SF 399.7611769 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.854
9.809
9.561
9.543
9.426
9.406

7.626
7.589
7.379
7.359
7.240

6.337
6.339
6.309
6.290
6.272
6.254
6.242
6.222
6.203

3.019
3.000
2.980
2.838
2.819
2.800
2.620
2.618
2.600
2.582
2.560
2.424
2.422
2.416
2.404
2.386
2.384
1.599
1.583
1.580
1.567
1.561
1.545
1.527
1.522
1.507
1.501
1.497
1.488
1.472
1.469
1.452
1.445
1.433
1.416
1.296



191.73
189.46
185.12
185.02

144.30
143.21
139.21
136.36
136.01
129.50
124.14
122.80
119.51

108.60
106.51

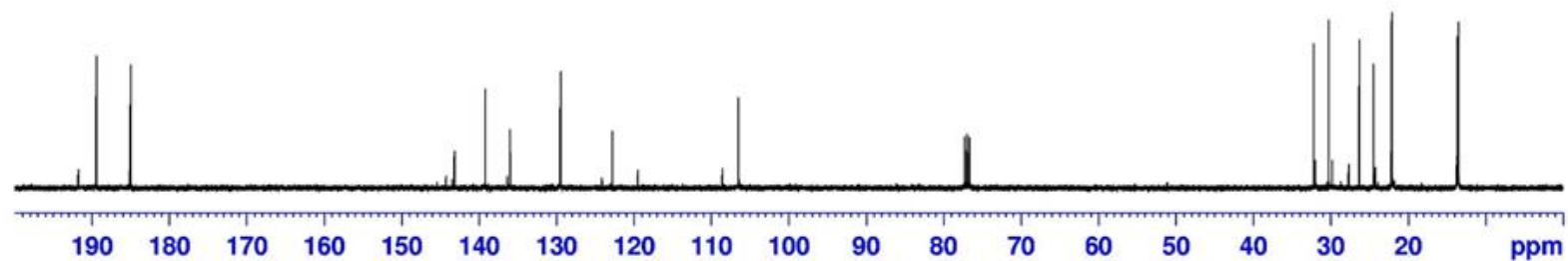
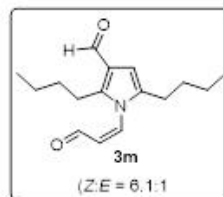
77.318
77.000
76.662

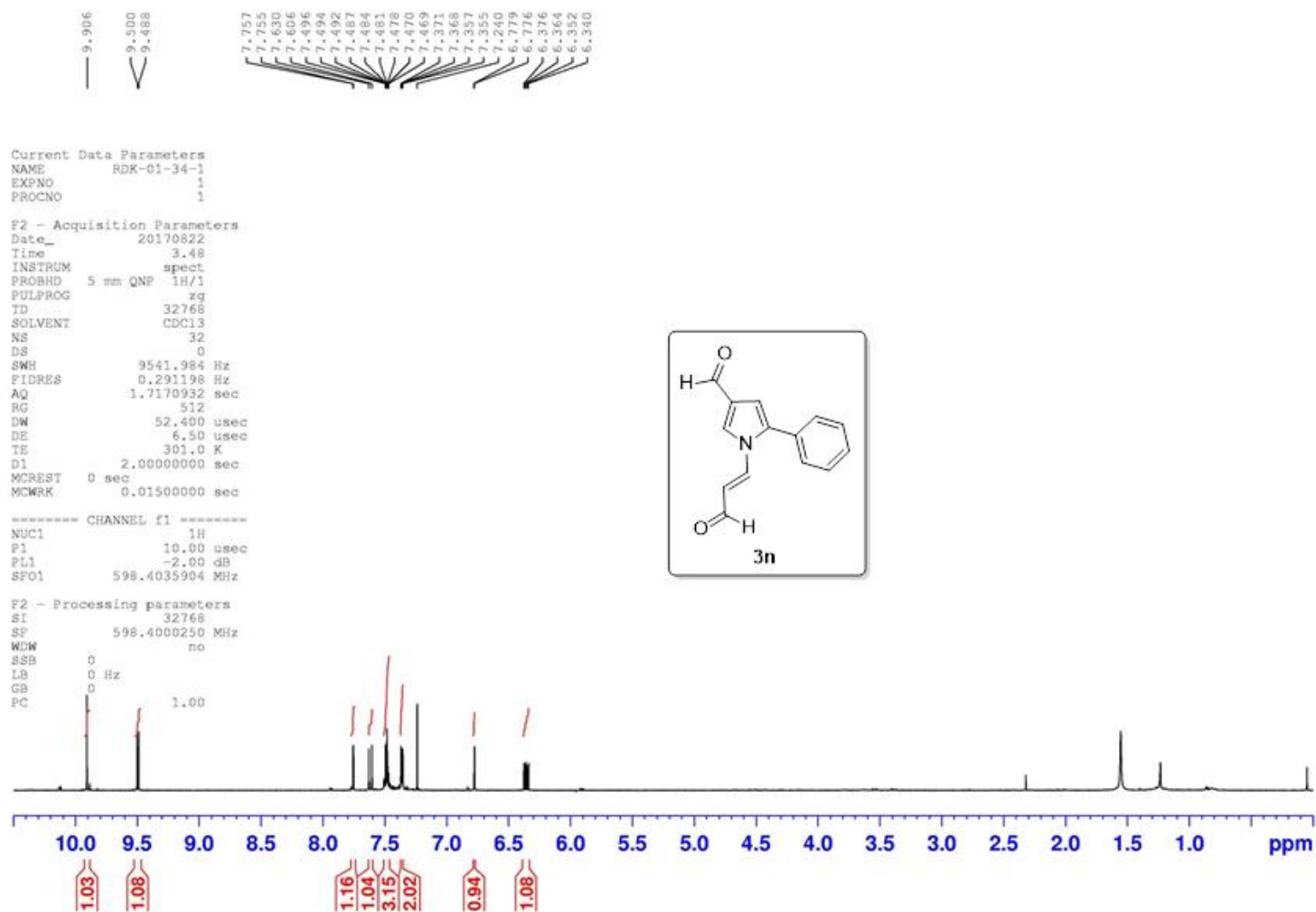
32.224
31.999
30.269
29.814
27.694
26.333
24.496
24.256
22.212
22.142
22.079
13.735
13.645
13.561

BK-C-157-C13

Current Data Parameters
NAME BK-C-157-Carbon.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214643 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





190.59
185.28

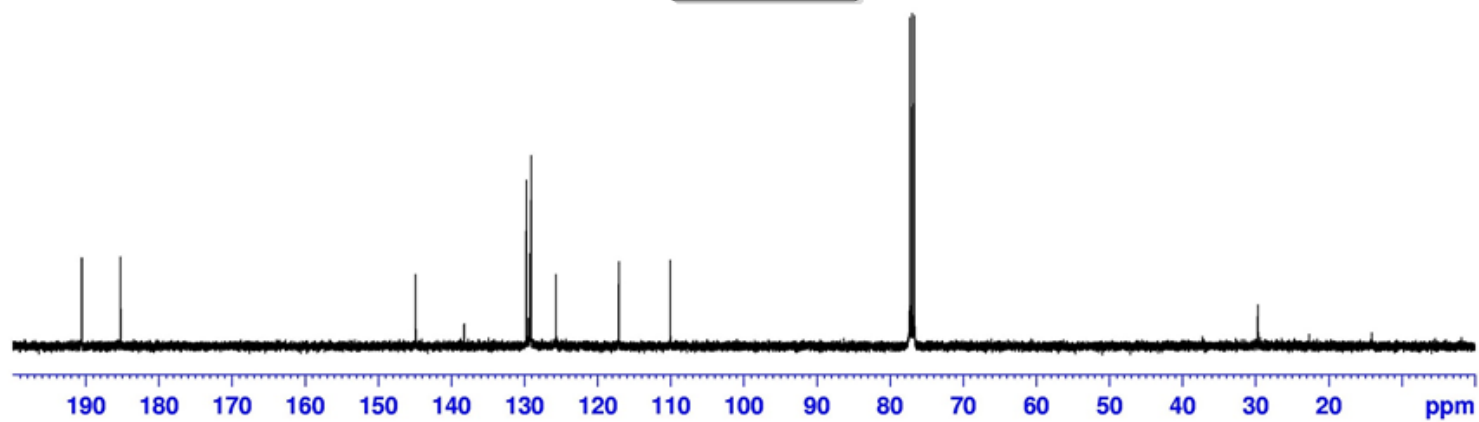
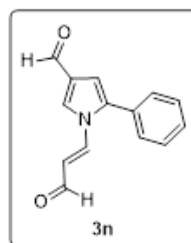
144.93
138.28
129.76
129.46
129.28
129.12
125.72
117.11
110.08

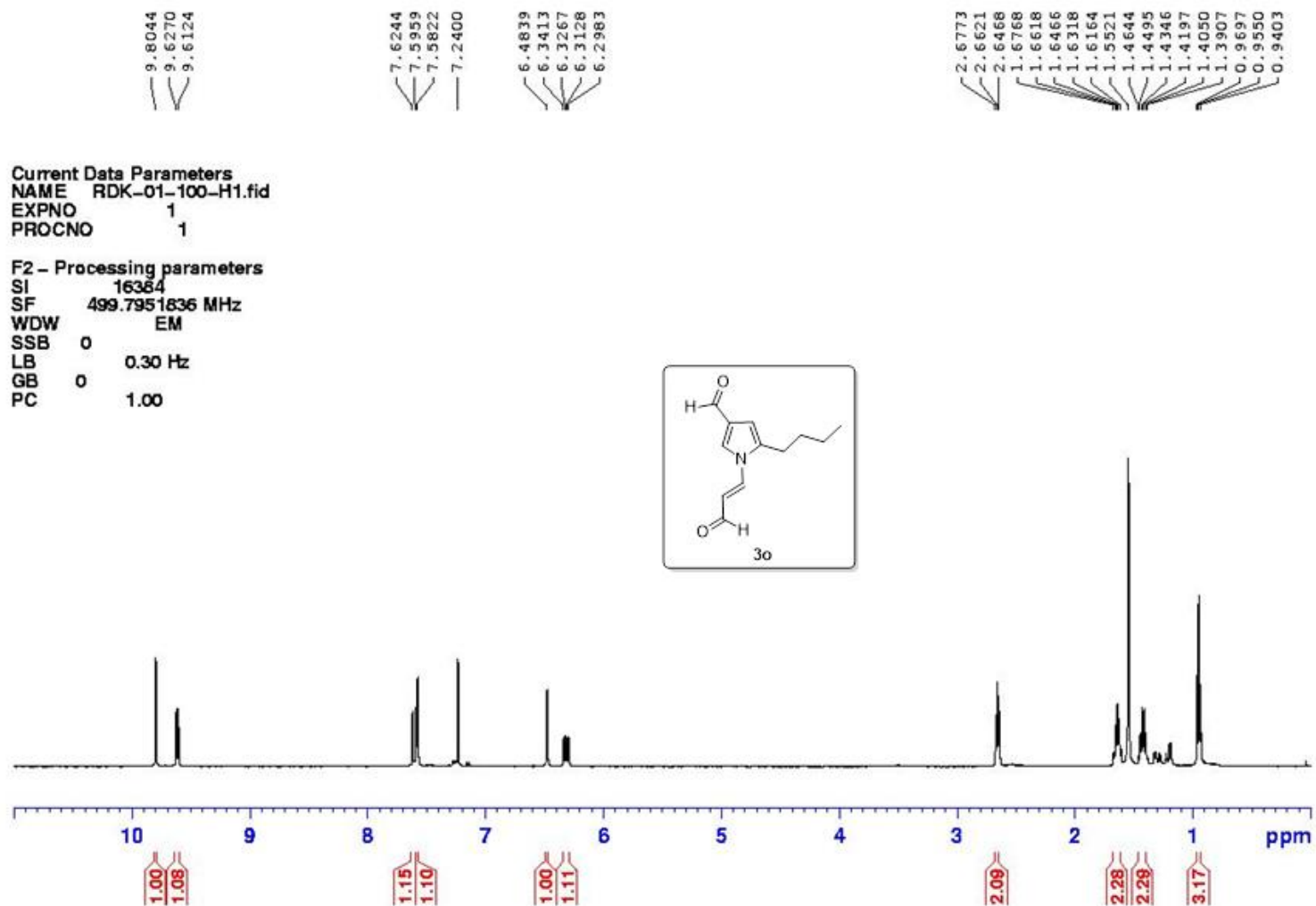
77.318
77.000
76.682

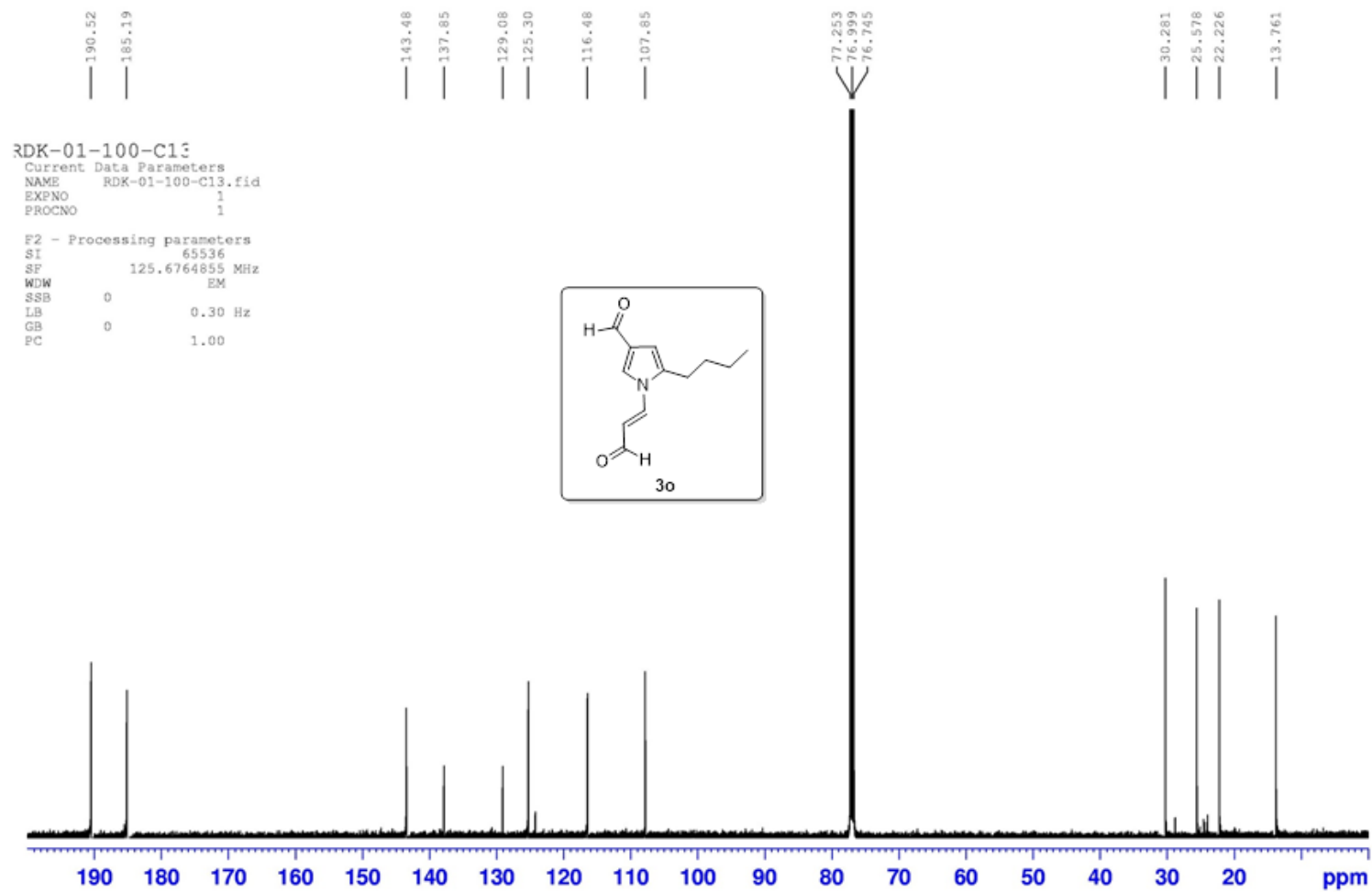
RDK-01-34-C13

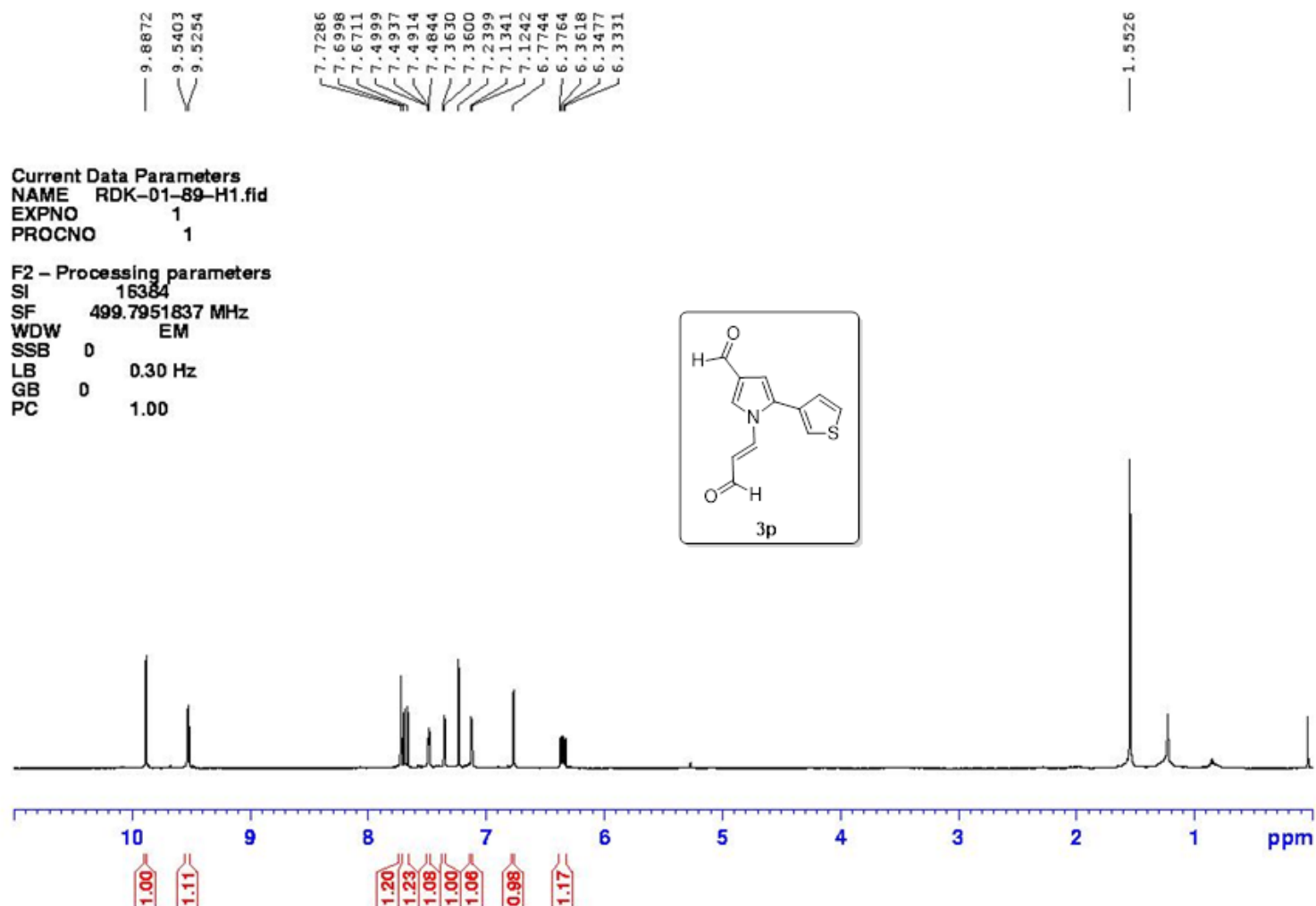
Current Data Parameters
NAME RDK-01-34-C13.fid
EXPNO 1
PROCNO 1

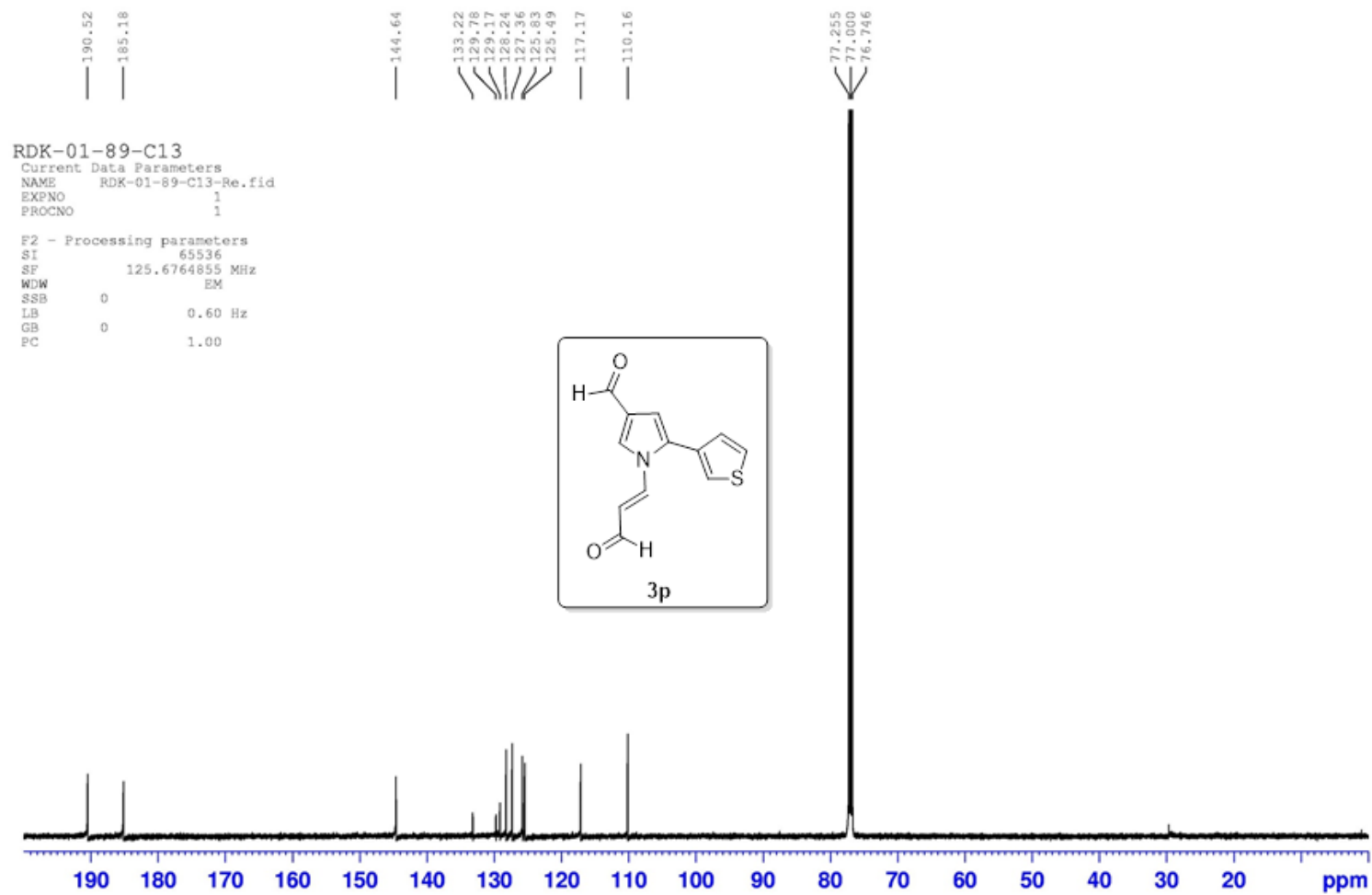
F2 - Processing parameters
SI 65536
SF 100.5214578 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00











Current Data Parameters
 NAME 826-01-88
 EXPNO 1
 PROCNO 1

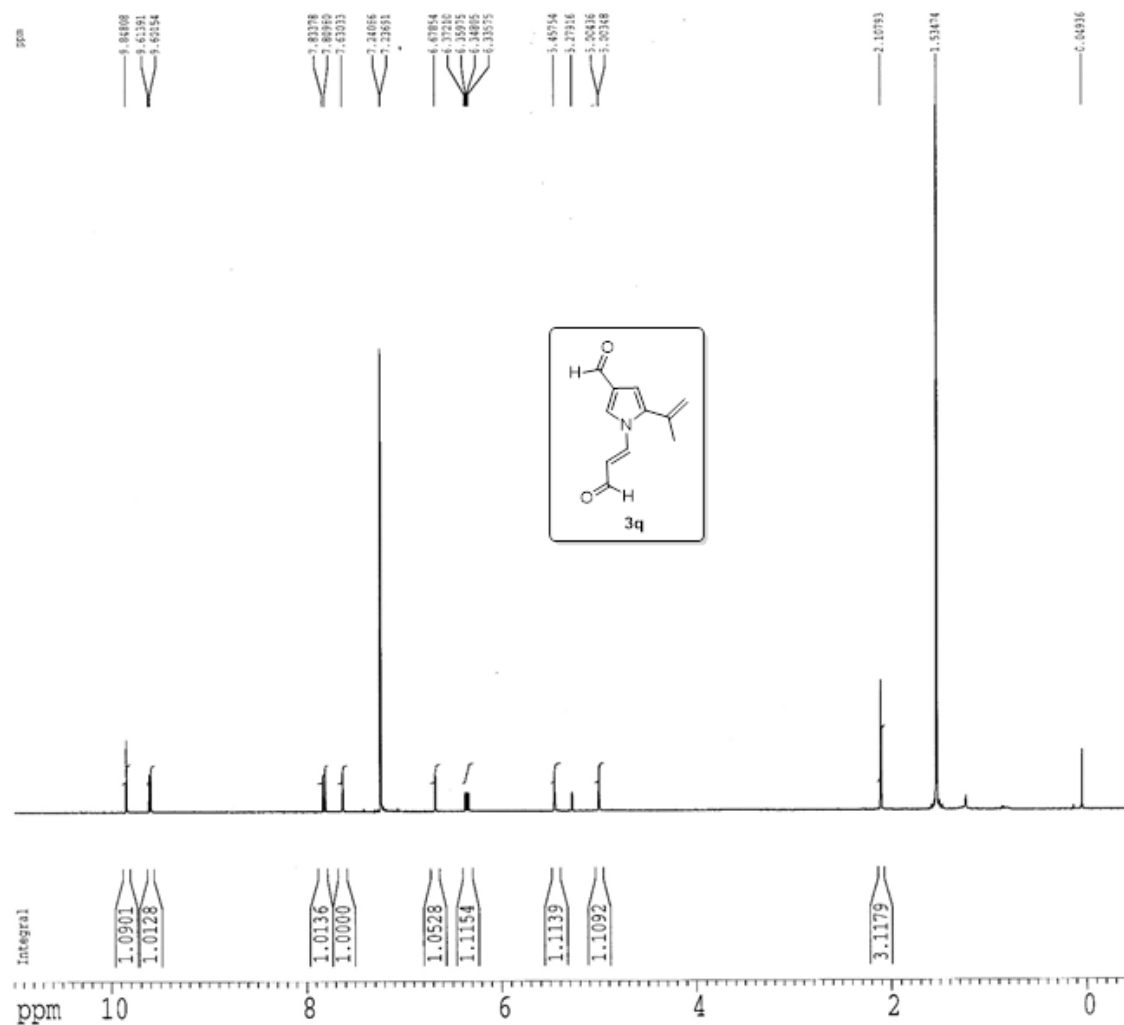
Acquisition Parameters
 Date_ 2017-01-11
 Time 14:28
 INSTRUM spect
 PULPROG zgpg30
 PRGPGM 1 me zgpg30
 F2 500.136
 F1 500.136
 SOLVENT CDCl3
 NS 64
 DS 4
 SC 0
 EX 1273.867 Hz
 FIDRES 0.138857 Hz
 AQ 1.5204912 sec
 LG 322
 FWHM 41.401 Hz
 SFO 500.136 MHz
 TE 303.2 K
 DE 2.00000000 sec
 ACQRES 1.5204912 sec
 FREQ 500.136000 MHz

===== CHANNEL f1 =====
 NUC1 13C
 P1 1.60 sec
 PL1 0.00 dB
 PL2 1.00 dB
 PL3 199.100000 dB

===== CHANNEL f2 =====
 NUC2 1H
 P2 0.00 sec
 PL2 0.00 dB
 PL3 0.00 dB

===== CHANNEL f3 =====
 NUC3 13C
 P3 0.00 sec
 PL3 0.00 dB
 PL4 199.100000 dB

===== CHANNEL f4 =====
 NUC4 1H
 P4 0.00 sec
 PL4 0.00 dB
 PL5 199.100000 dB



Current Data Parameters
NAME RDC-01-84
EXPNO 7
PROCNO 1

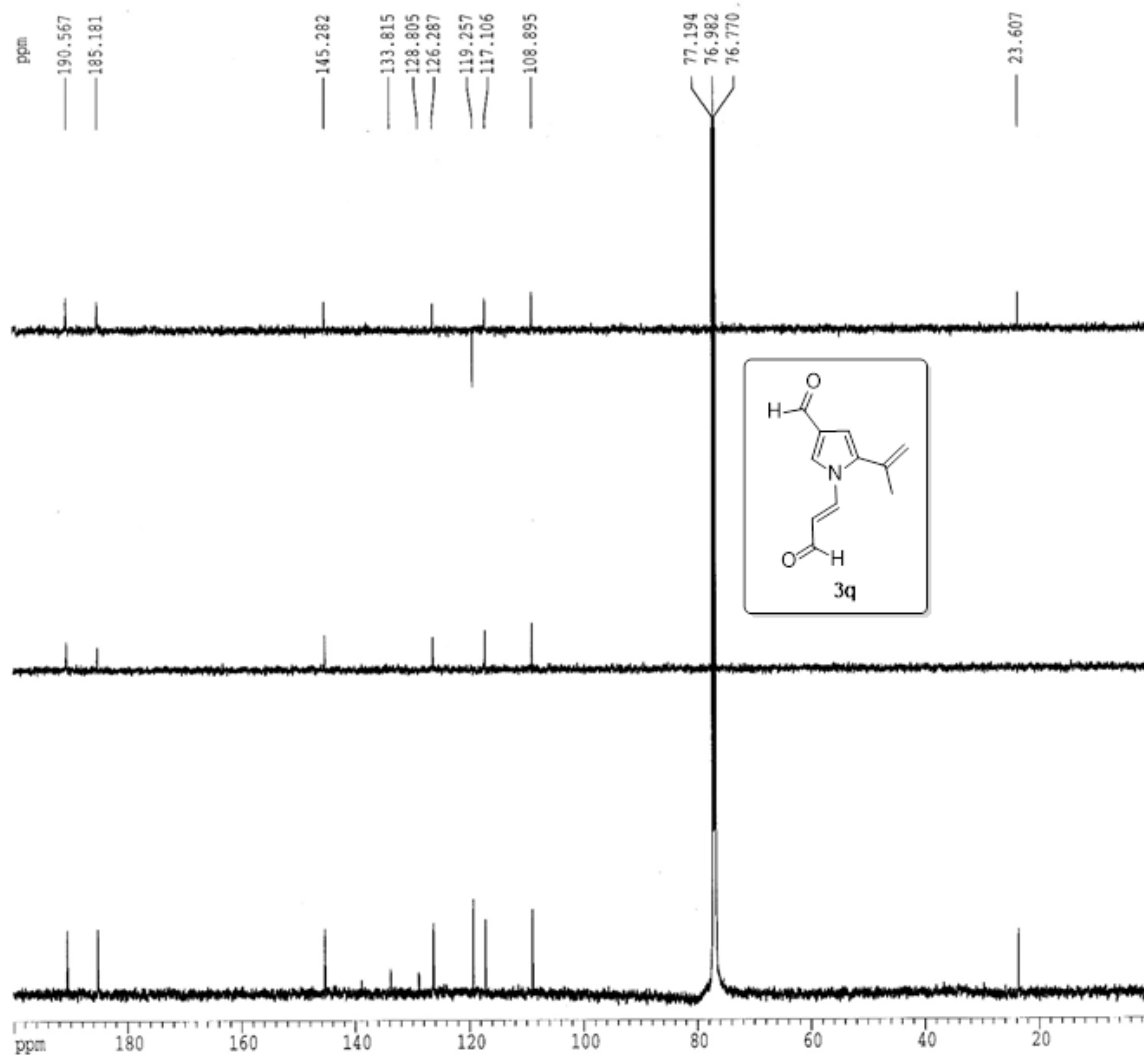
F2 - Acquisition Parameters
Date_ 20171101
Time 23.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6192
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.1617748 sec
RG 4096
RT 11.100 usec
GB 0.50 usec
LB 301.9 K
PC 3.5000000 sec
GC 0.0300000 sec
DELTA 3.4000000 sec
MTELT 0.0000000 sec
MTRF 0.7150000 sec

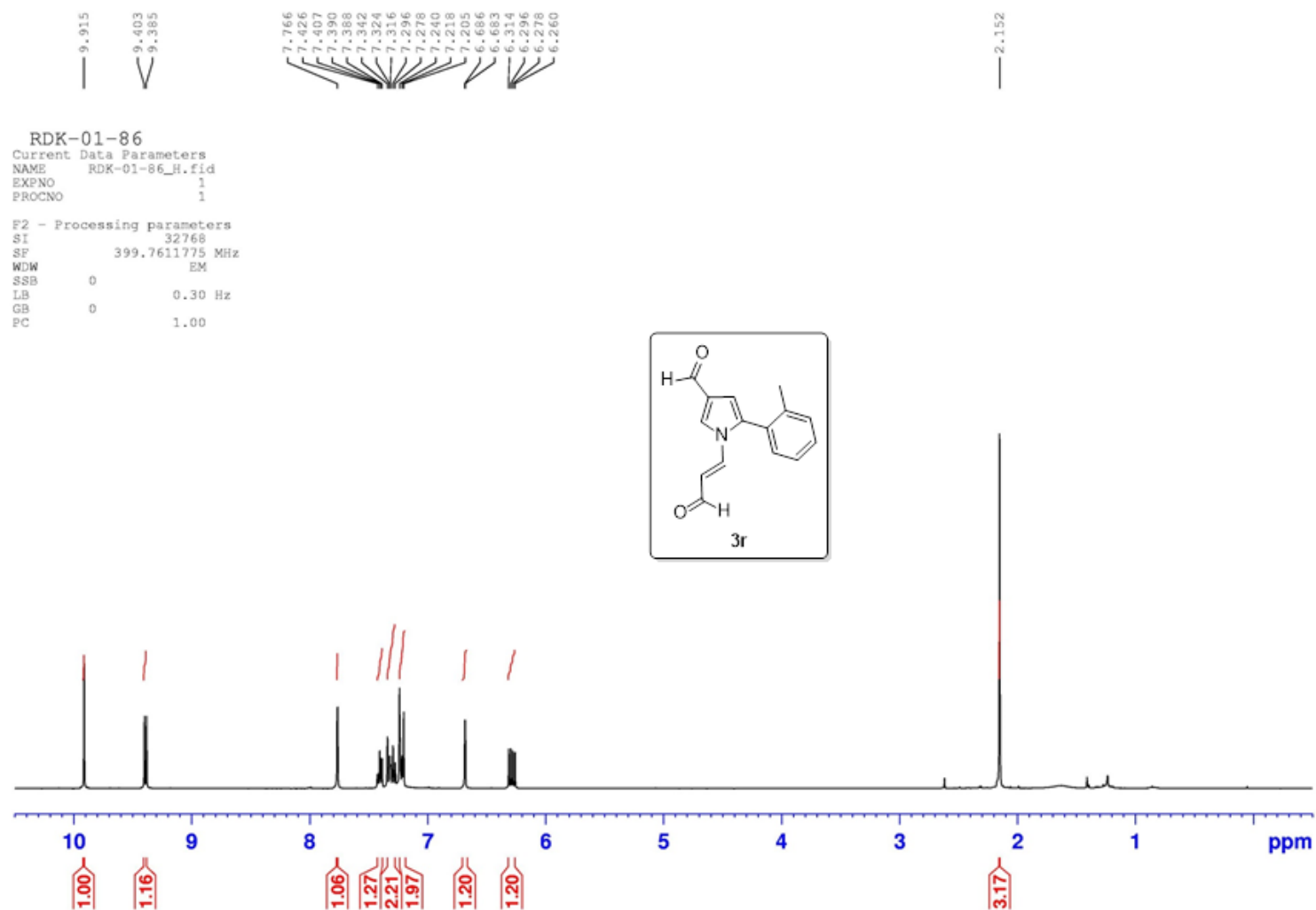
***** CHANNEL f1 *****
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4628468 MHz

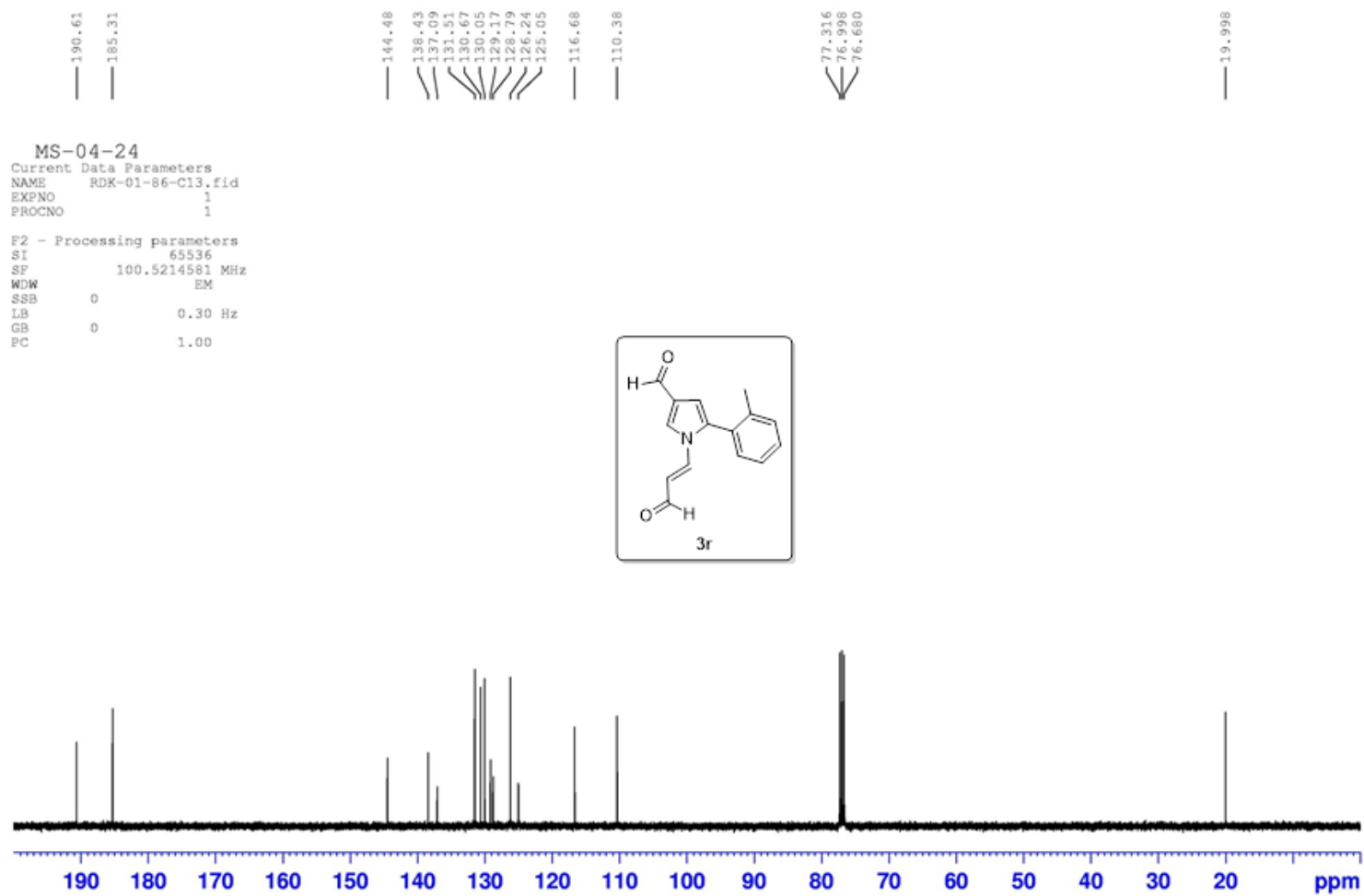
***** CHANNEL f2 *****
NUC2 1H
P2 12.00 usec
PL2 100.00 dB
PL12 5.50 dB
PL13 5.00 dB
SFO2 500.4079920 MHz

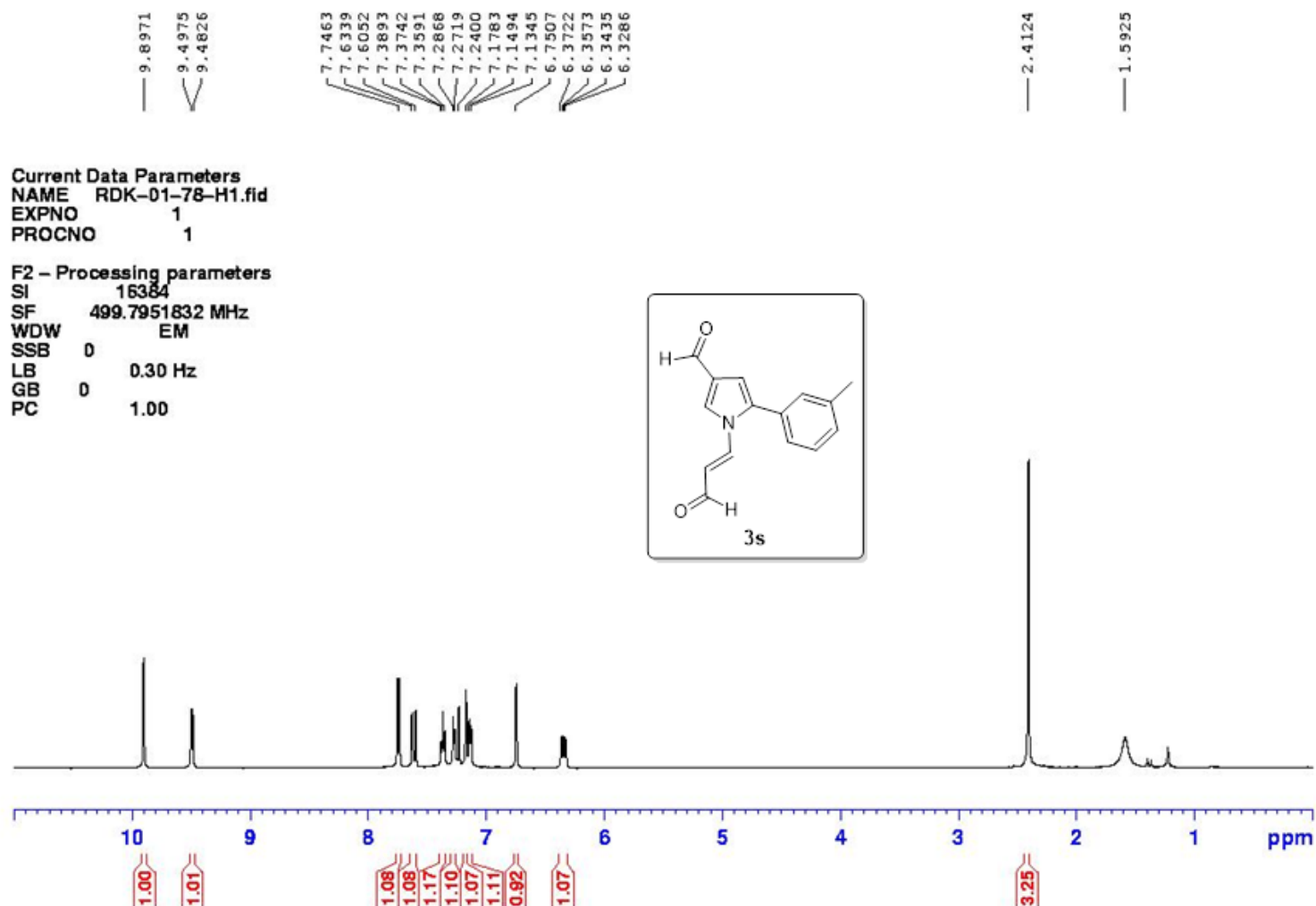
F1 - Processing parameters
SI 65536
SF 150.4678943 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

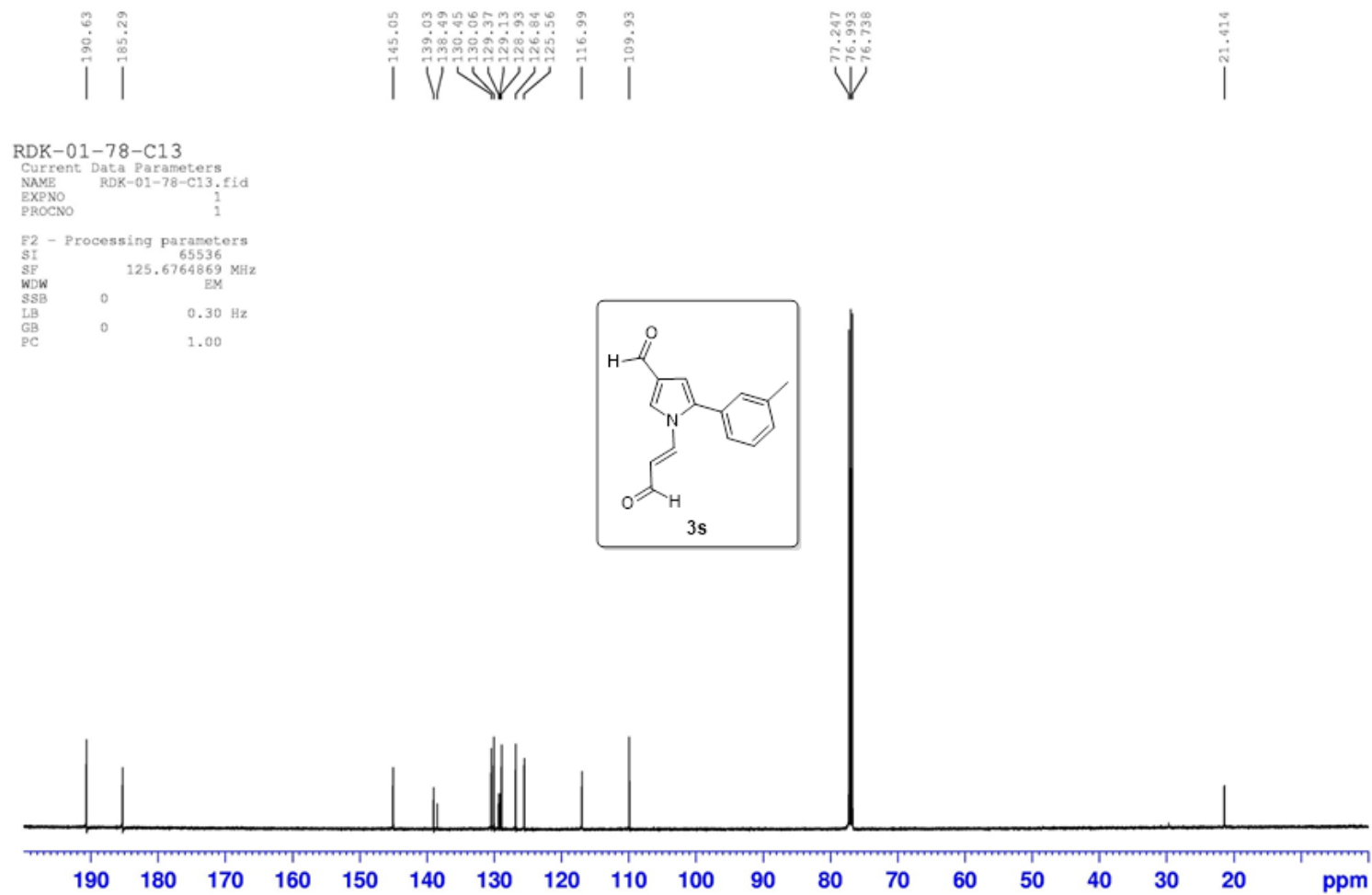
1D 13C plot parameters
SI 65536
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
F2 10.0000000 ppm/cm
F2CM 1504.67796 Hz/cm







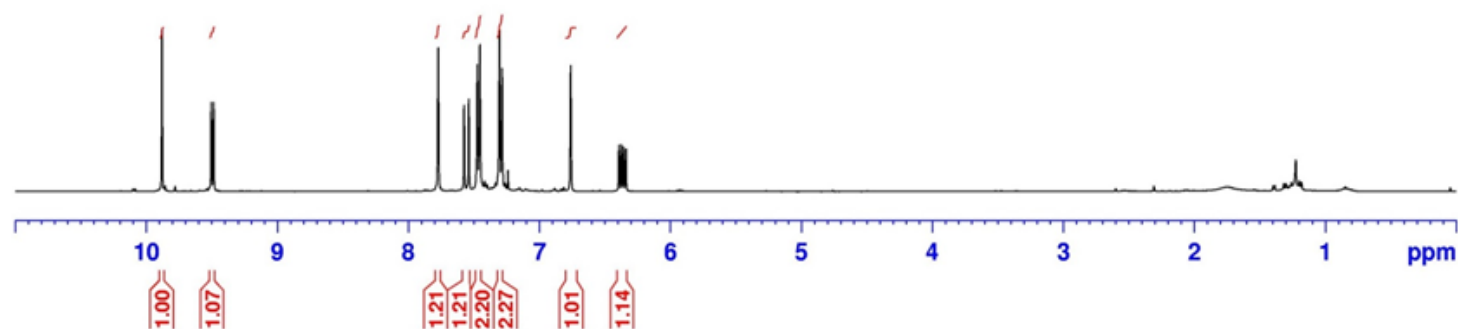
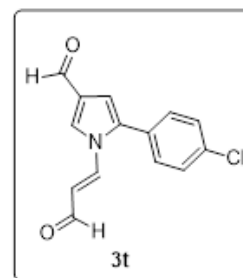


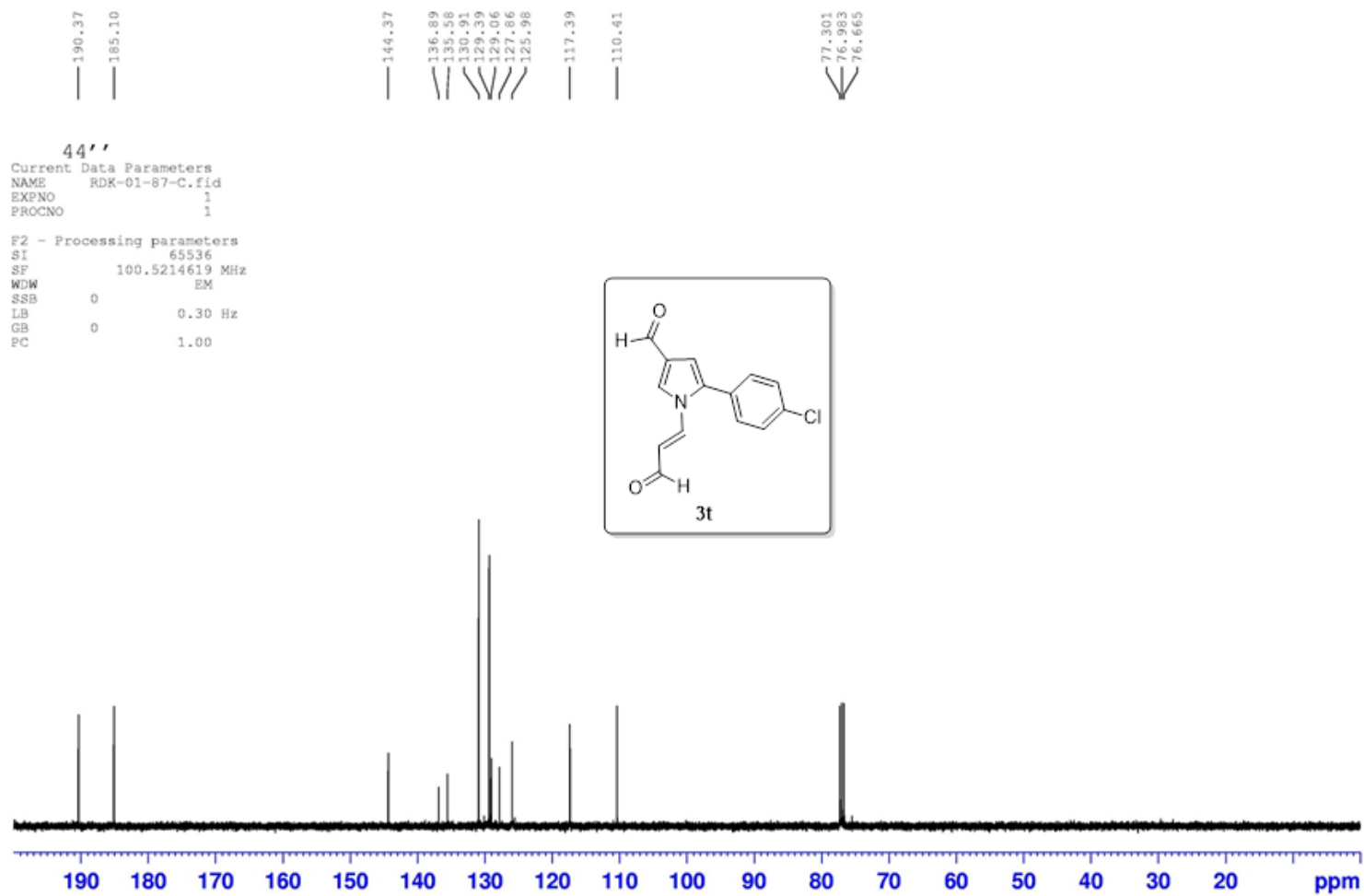


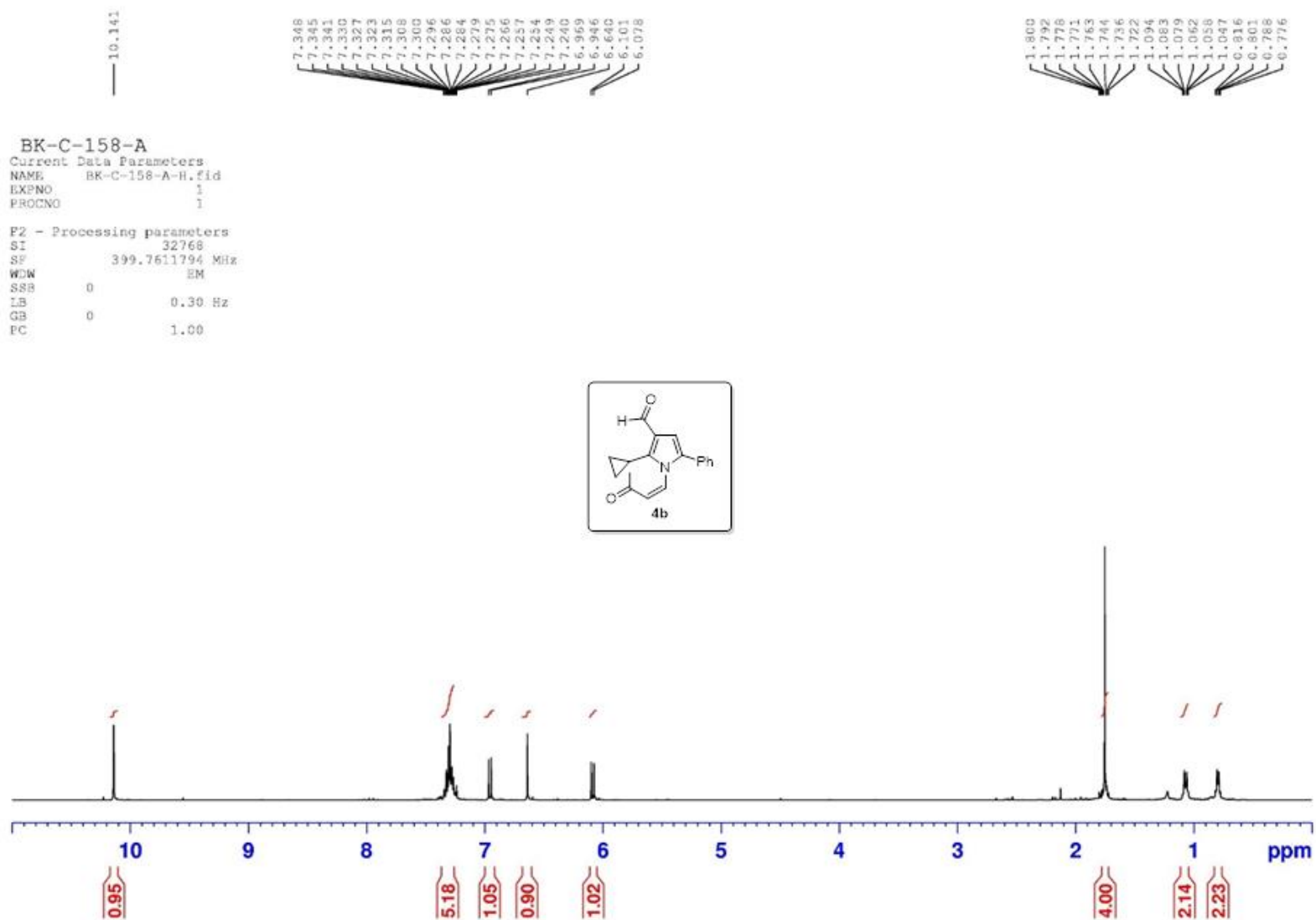
9.882
9.505
9.487

7.774
7.575
7.539
7.475
7.455
7.306
7.286
7.240
6.762
6.393
6.375
6.357
6.339

RDK-01-87
Current Data Parameters
NAME RDK-01-870_H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611786 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







— 196.84
 — 195.72
 — 144.30
 135.08
 132.11
 131.15
 128.73
 128.46
 127.98
 127.69
 124.87

— 107.85

77.319
 77.000
 76.682

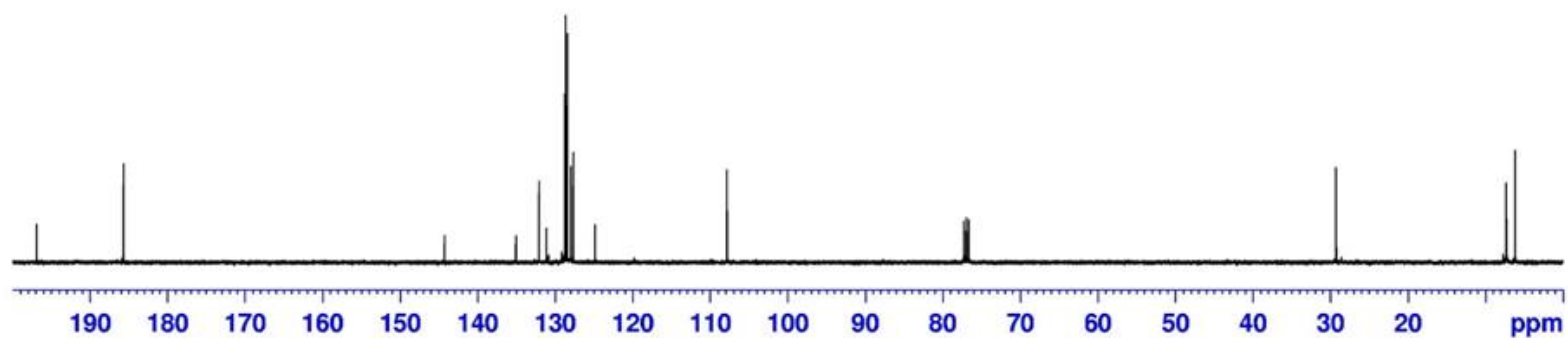
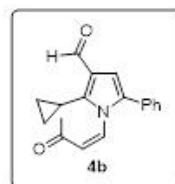
— 29.273

7.344
 6.194

3K-C-158-A-c13

Current Data Parameters
 NAME BK-C-158-A-C13.fid
 EXPNO 1
 PROCNO 1

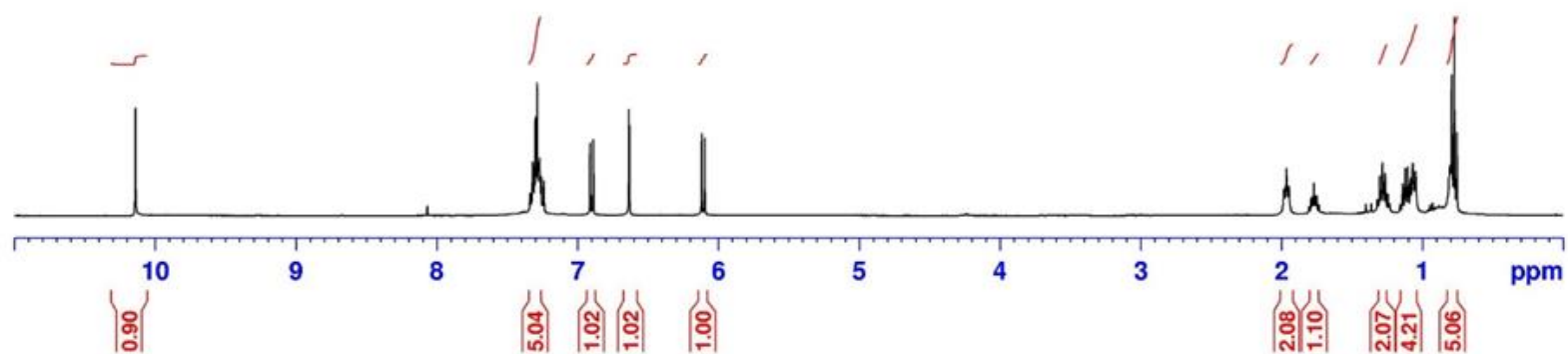
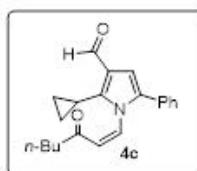
F2 - Processing parameters
 SI 65536
 SF 100.5214632 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BK-C-173-AA-H
 Current Data Parameters
 NAME BK-C-173-AA-H.fid
 EXPNO 1
 PROCNO 1
 F2 - Processing parameters
 SI 32768
 SF 400.4342266 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.338
 7.334
 7.330
 7.326
 7.309
 7.301
 7.288
 7.280
 7.279
 7.276
 7.272
 7.267
 7.260
 7.252
 7.248
 7.240
 6.912
 6.890
 6.636
 6.120
 6.098

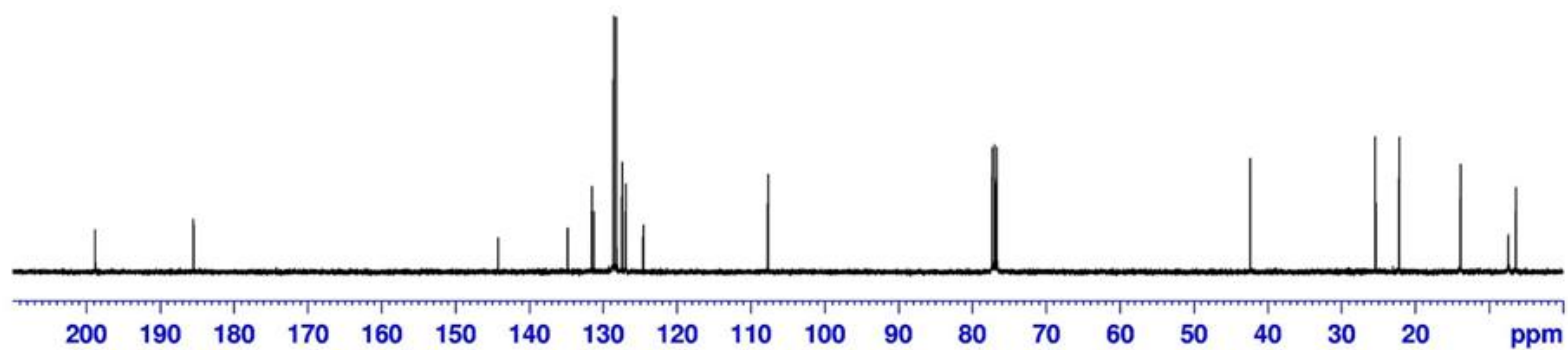
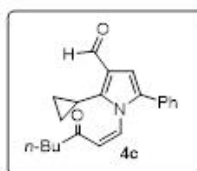
1.983
 1.945
 1.947
 1.864
 1.790
 1.777
 1.763
 1.770
 1.762
 1.756
 1.749
 1.735
 1.319
 1.302
 1.283
 1.264
 1.245
 1.221
 1.188
 1.139
 1.121
 1.101
 1.083
 1.067
 1.050

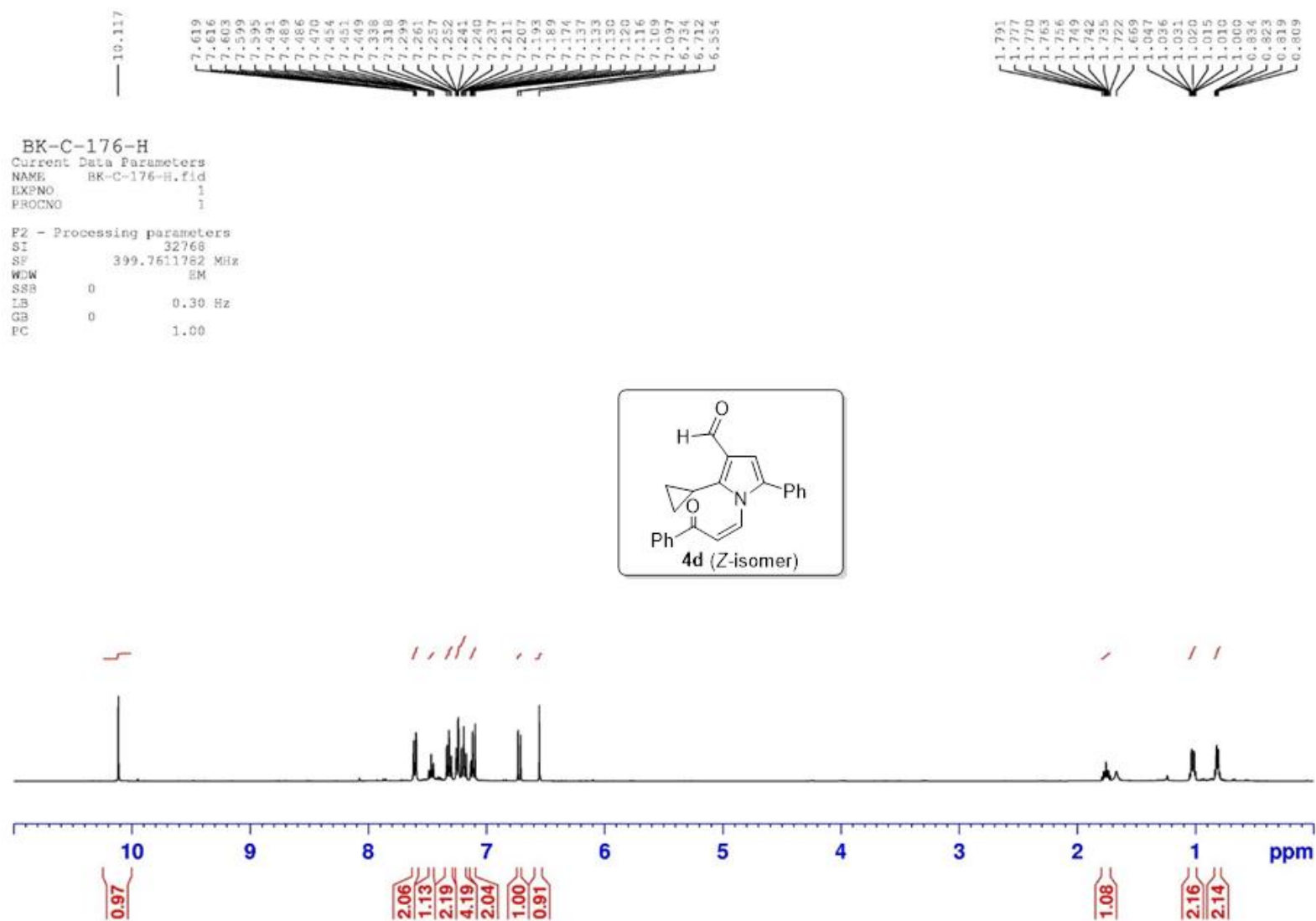




Current Data Parameters
 NAME BK-C-173-AA-C13.fid
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 SI 131072
 SF 100.6892742 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





189.54
185.90

144.52
136.35
135.01
133.33
133.30
131.32
128.96
128.35
128.27
128.24
127.50
124.94
123.91

107.84

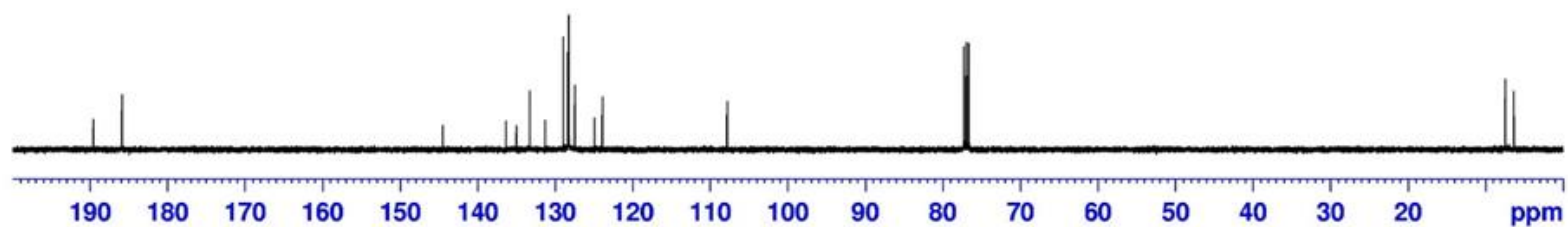
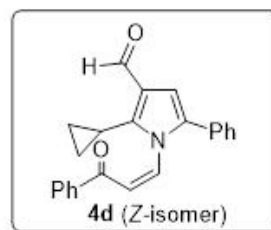
77.318
77.000
76.682

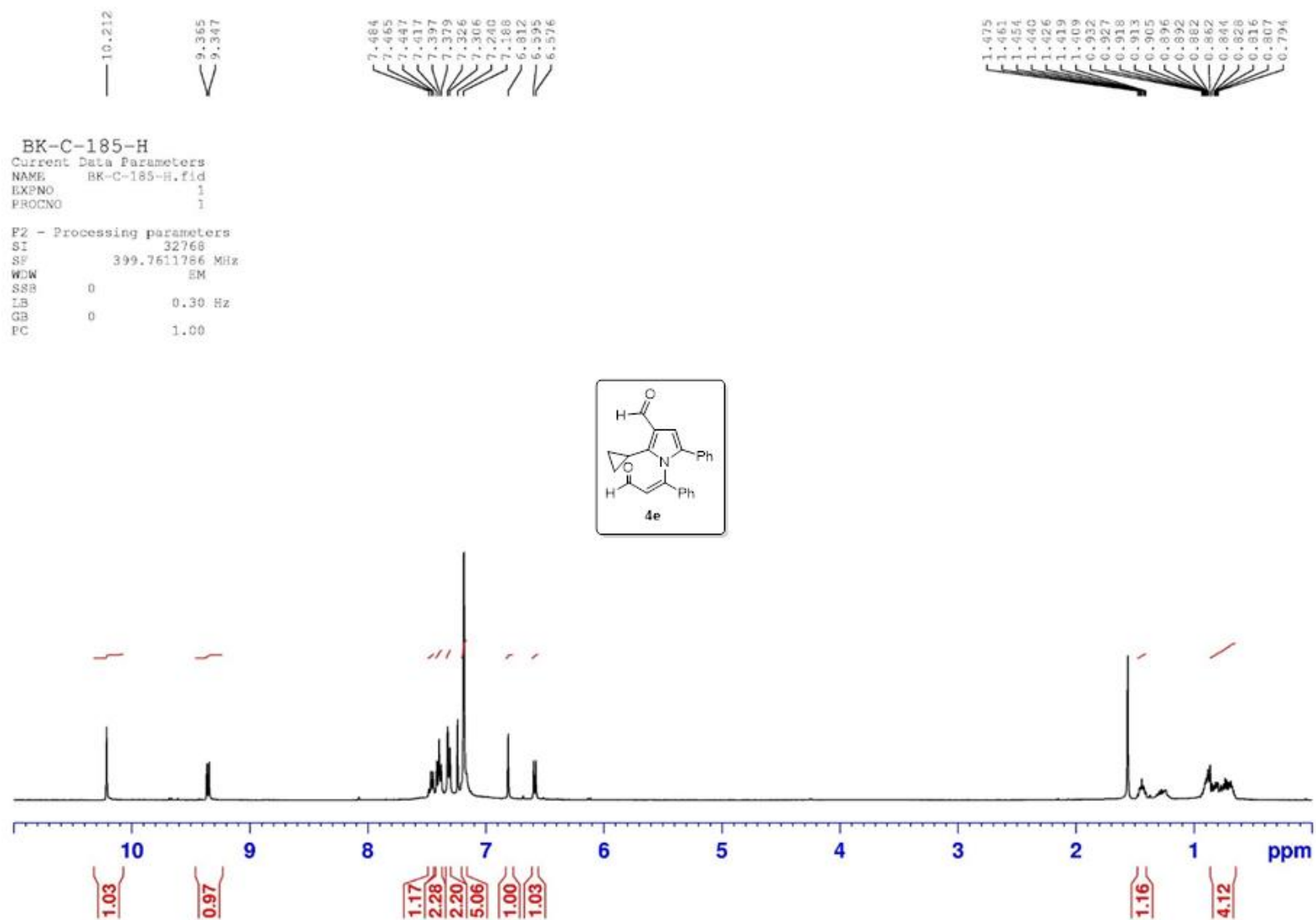
7.451
6.362

BK-C-176-C13

Current Data Parameters
NAME BK-C-176-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214589 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





190.10
185.86

152.82
145.27
137.83
135.23
132.01
130.77
129.37
128.56
128.05
124.98
124.53

107.85

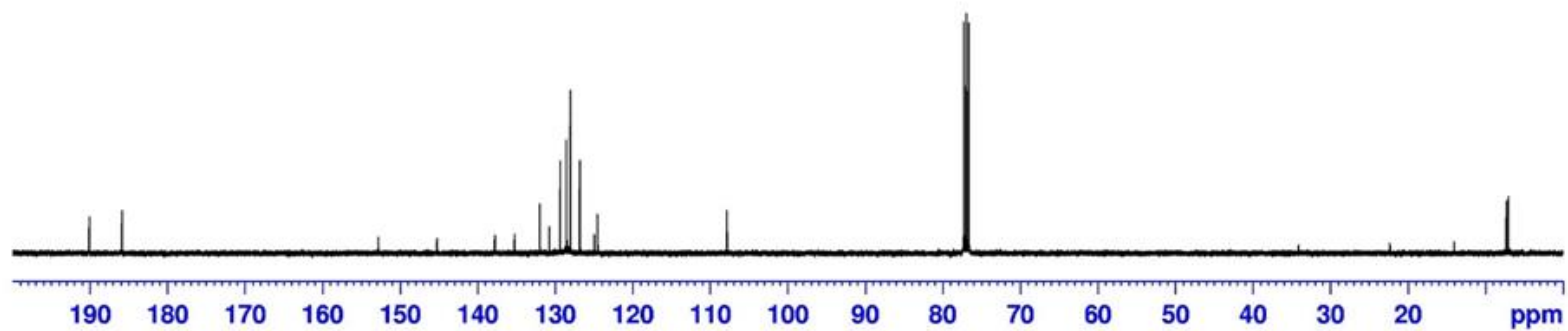
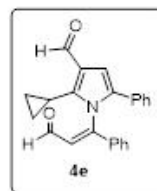
77.318
77.000
76.682

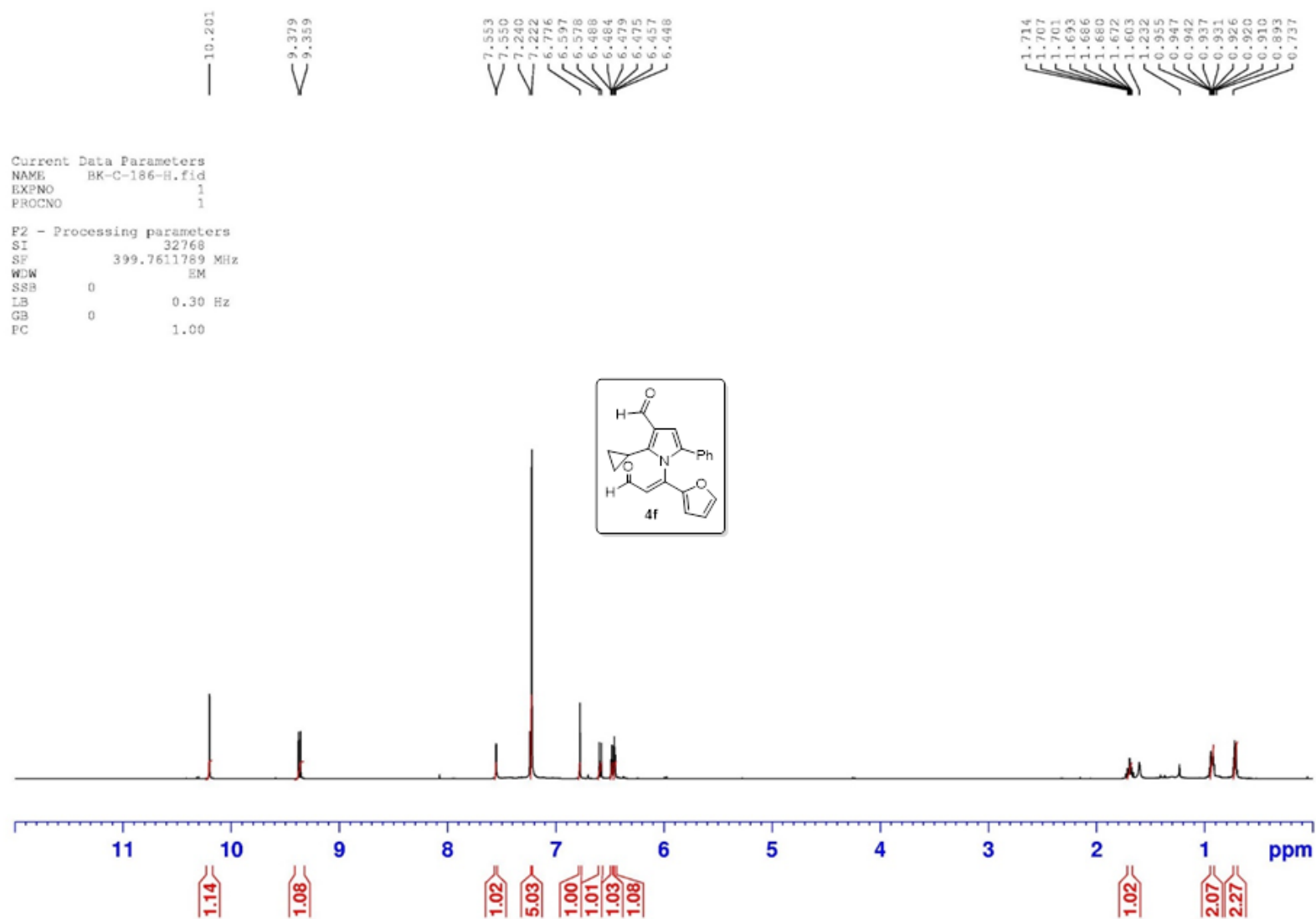
7.310
7.056
7.025

BK-C-185-C13

Current Data Parameters
NAME BK-C-185-C13-2.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214567 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





189.55
185.69

149.60
146.74
145.37
142.11
137.31
130.77
128.55
128.10
127.79
124.73
121.91
116.04
113.19
107.70

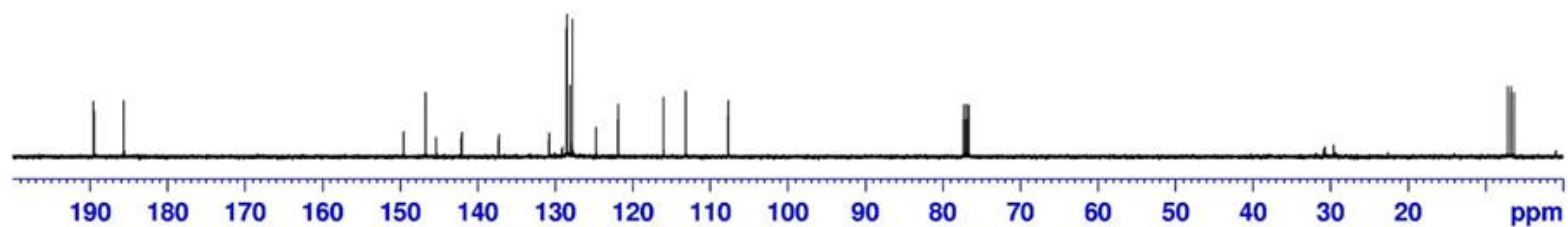
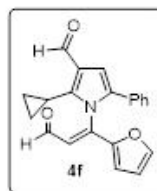
77.317
77.000
76.681

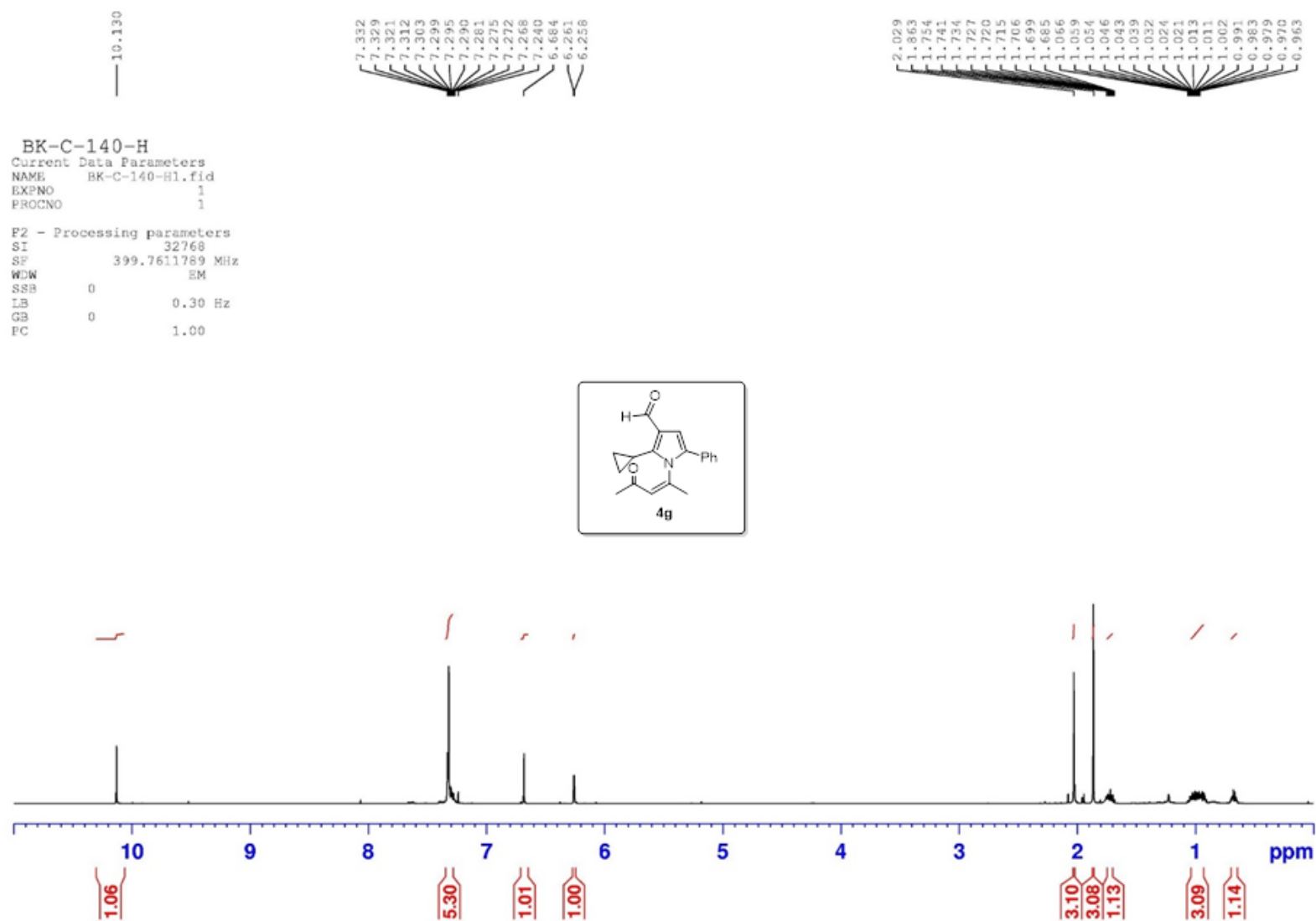
7.155
6.744
6.320

BK-C-186-C13

Current Data Parameters
NAME BK-C-186-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214629 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



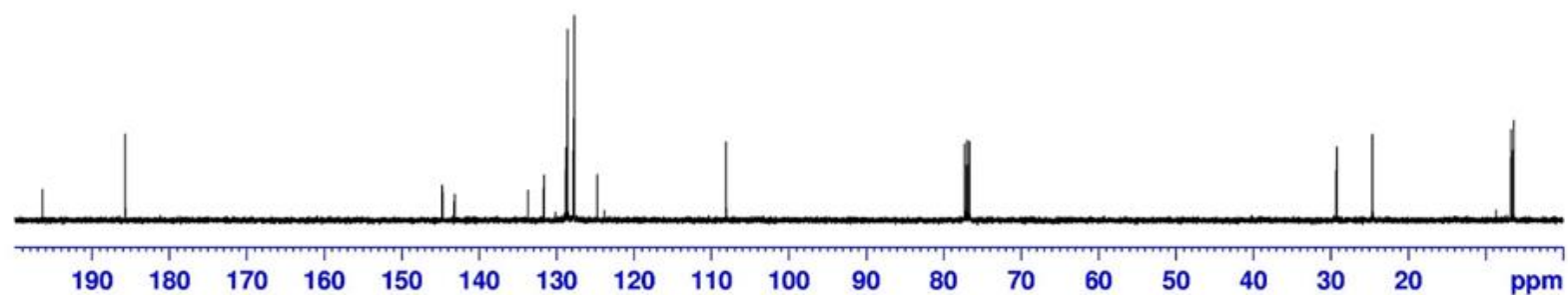
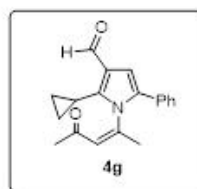


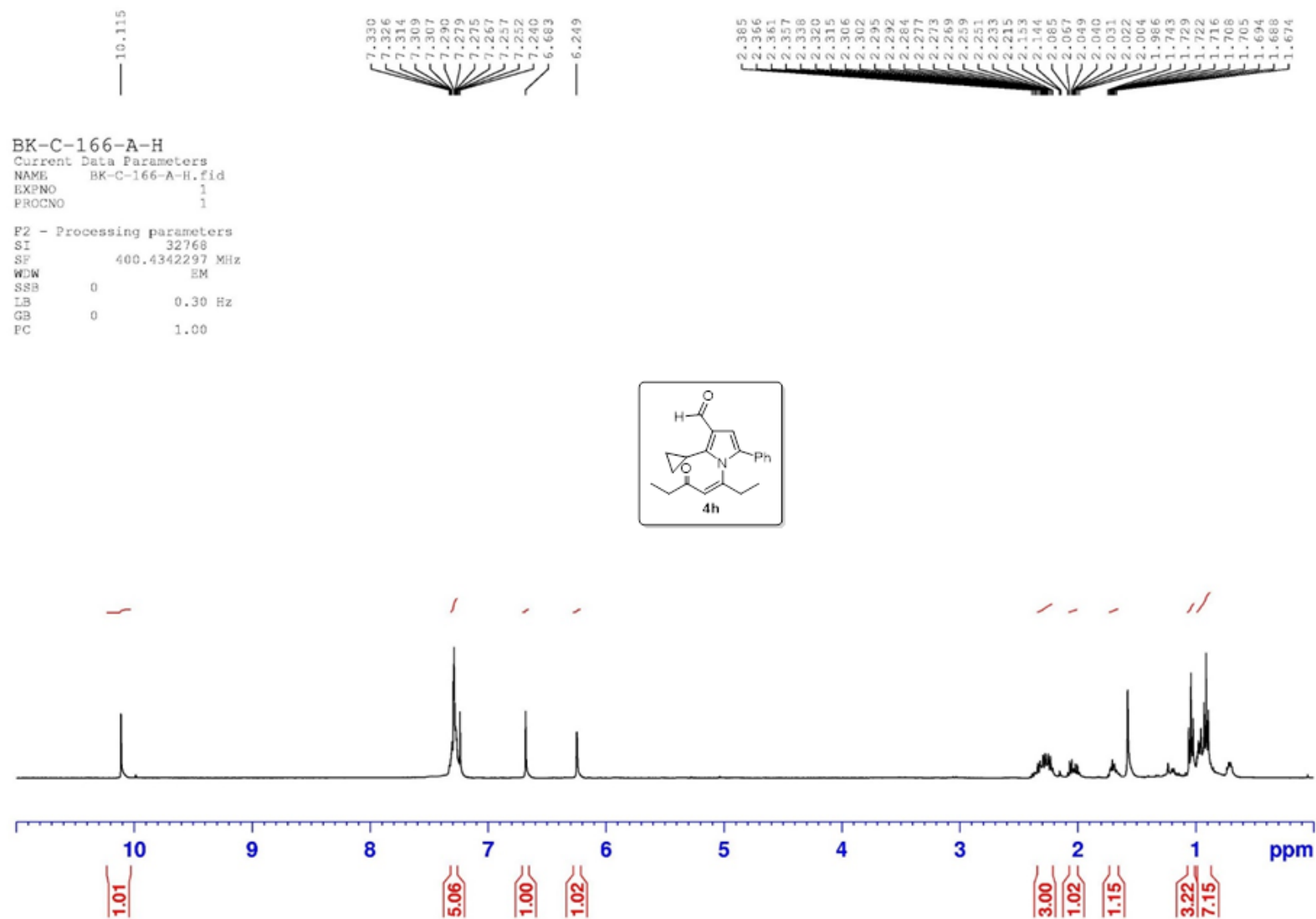


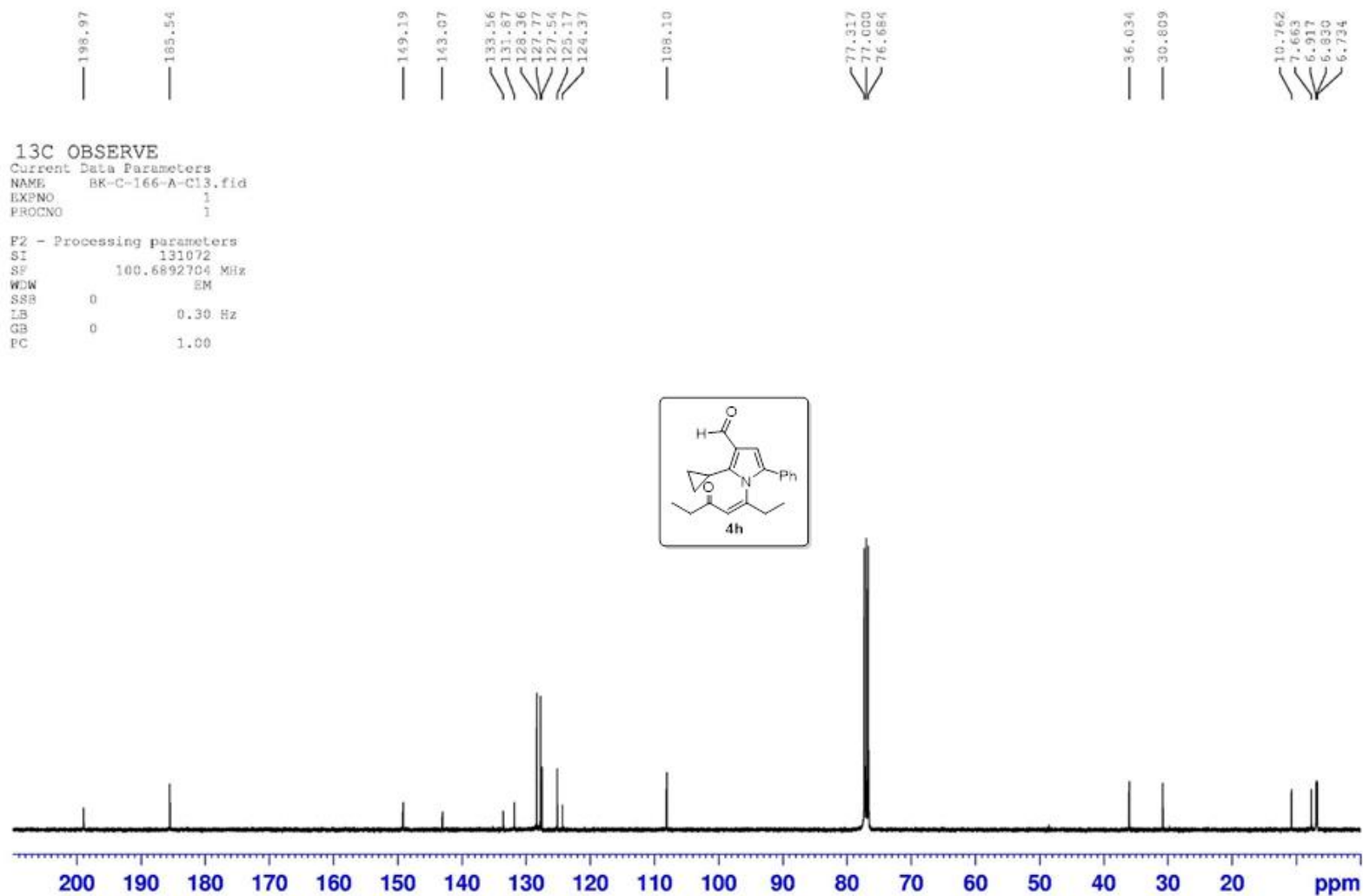
BK-C-140-c13

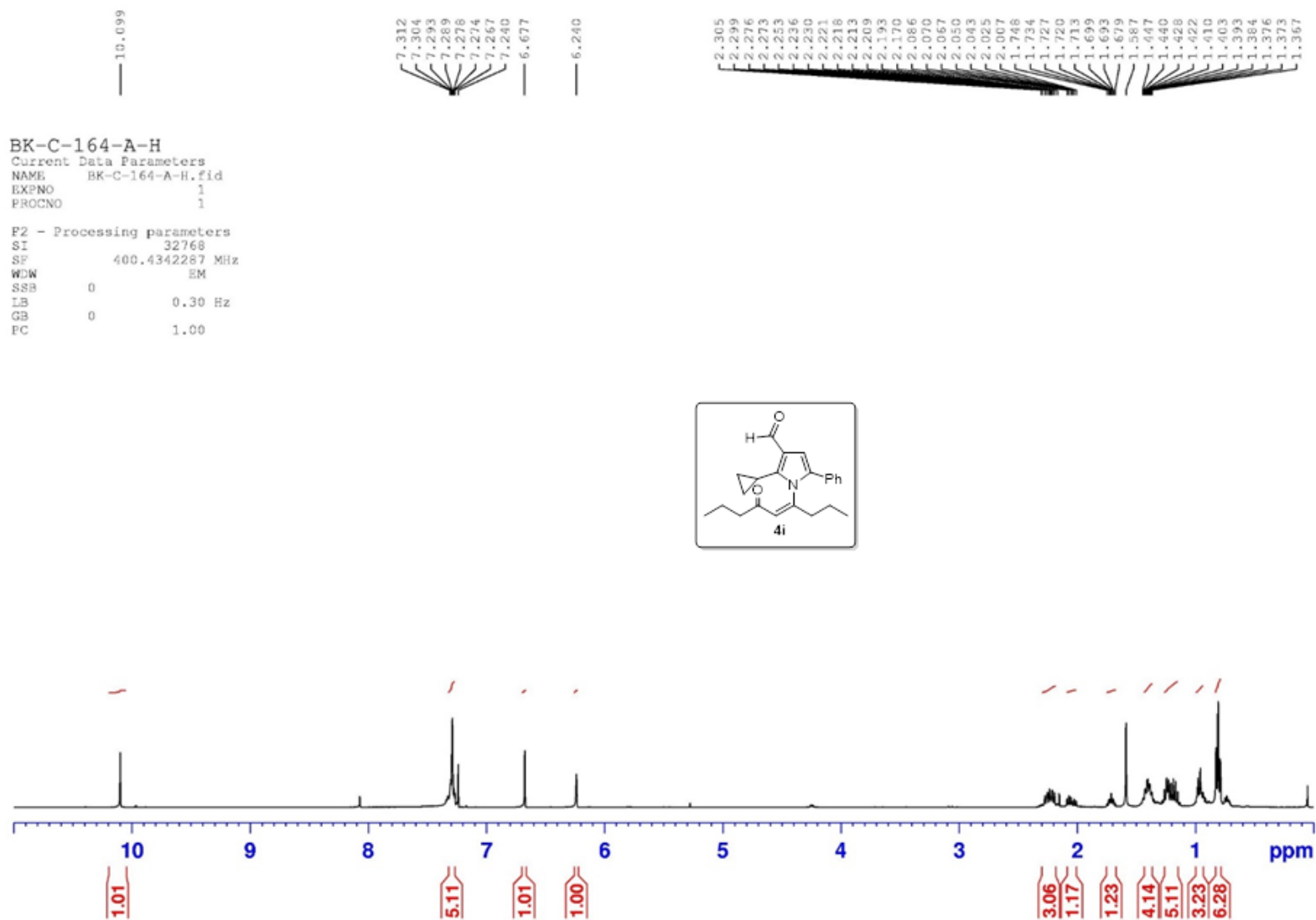
Current Data Parameters
NAME BK-C-140-c13.fid
EXPNO 1
PROCNO 1

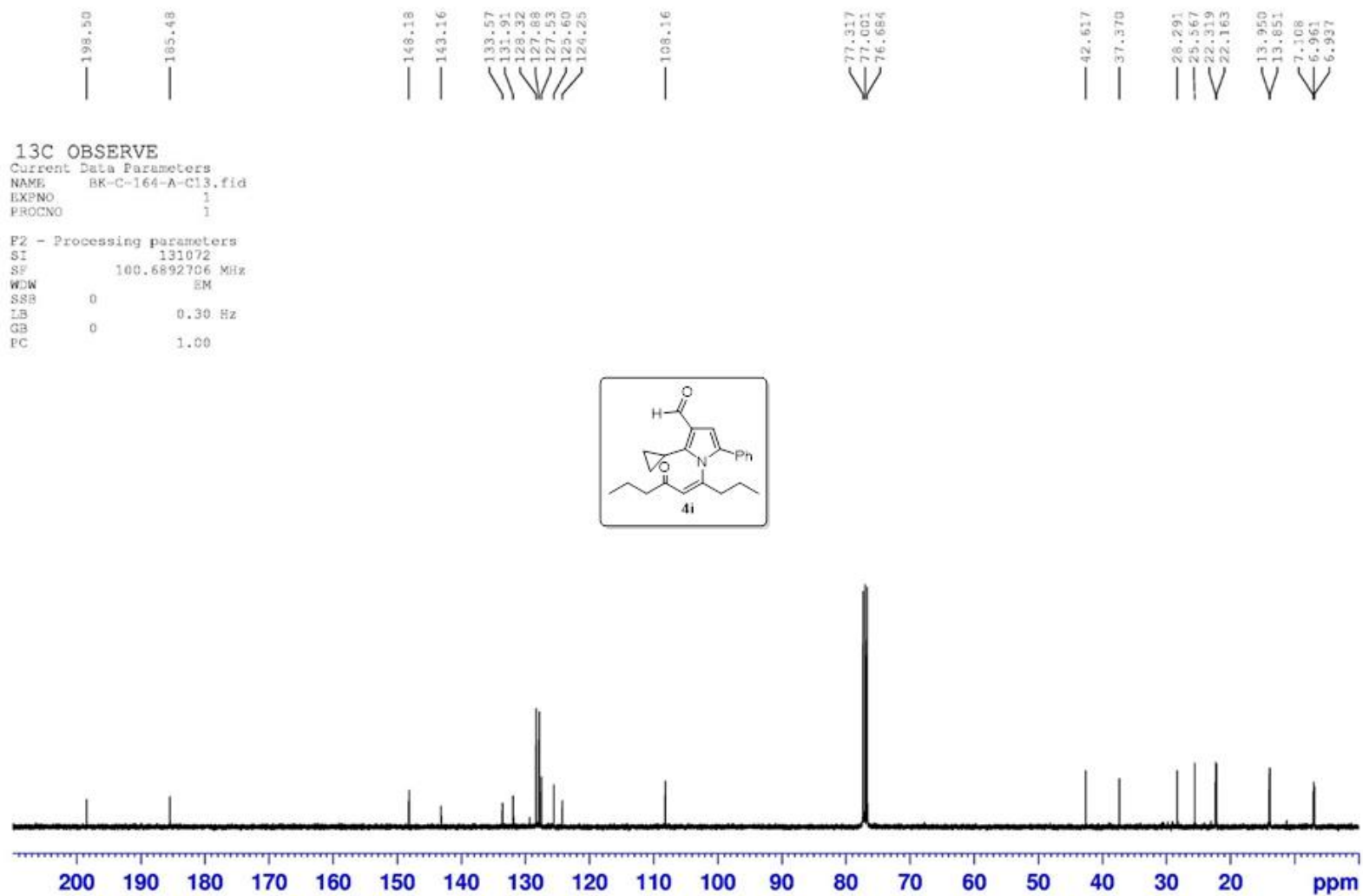
F2 - Processing parameters
SI 65536
SF 100.5214609 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

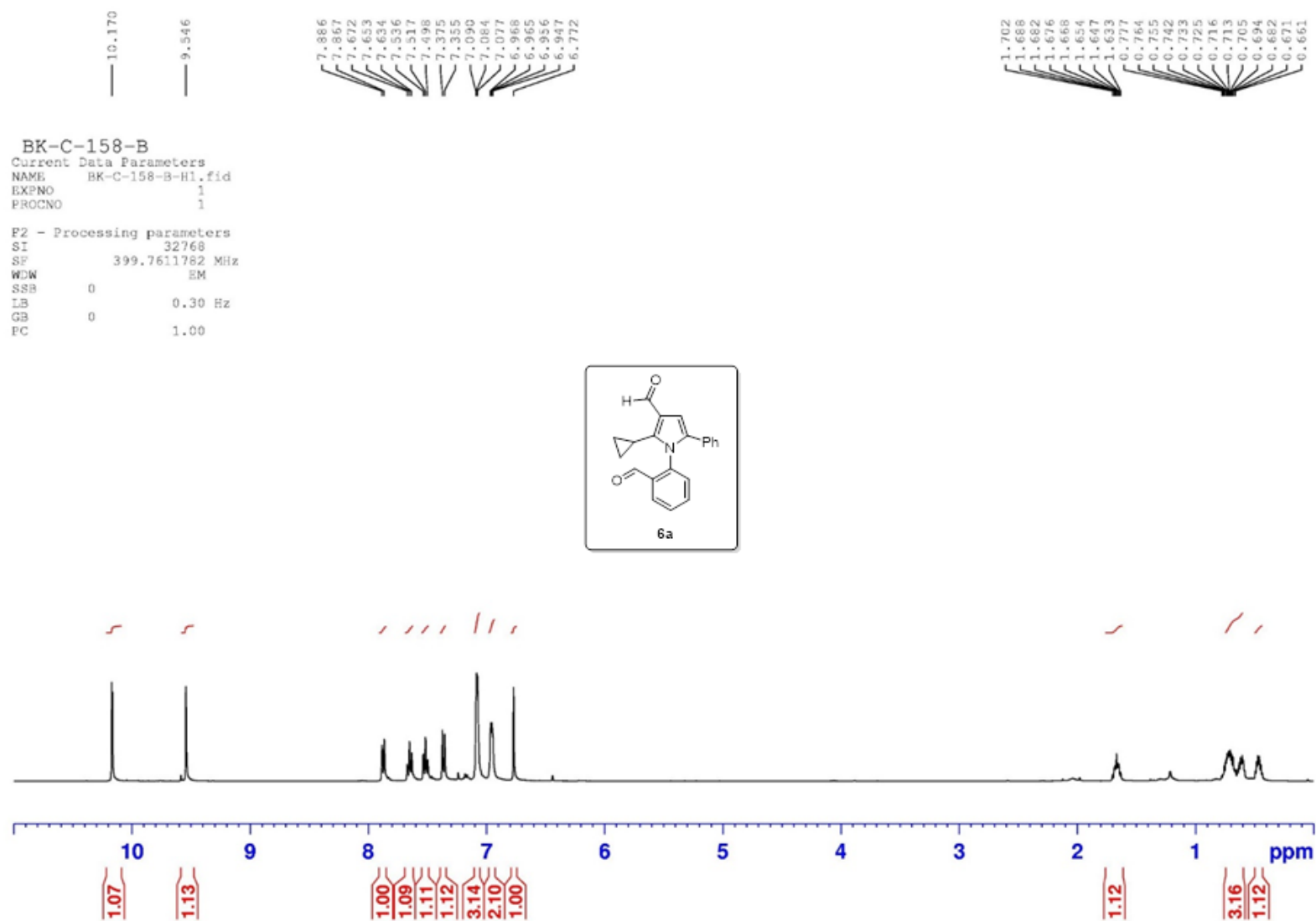












188.43
185.61
C-158-B-C1

145.18
140.36
136.65
134.47
132.66
130.83
129.87
129.25
128.65
128.26
128.22
127.58
124.25

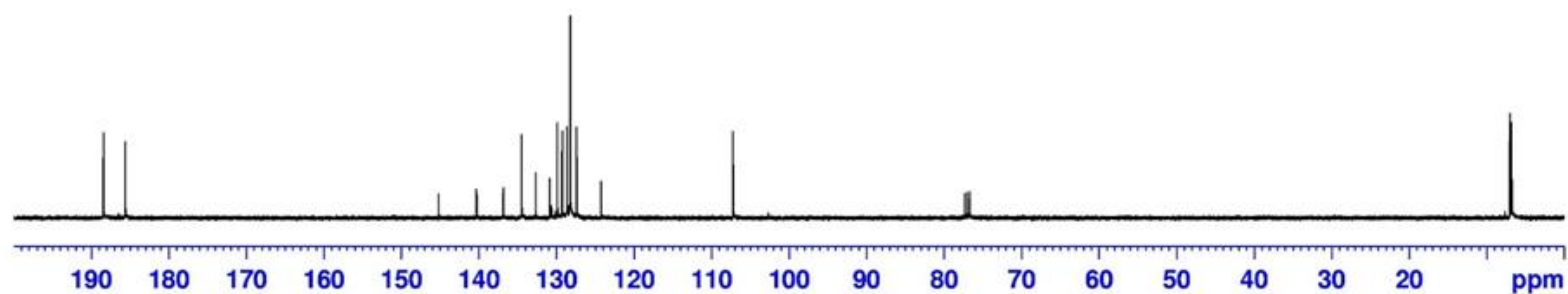
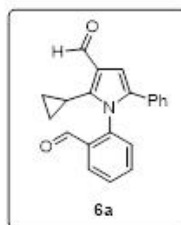
107.20

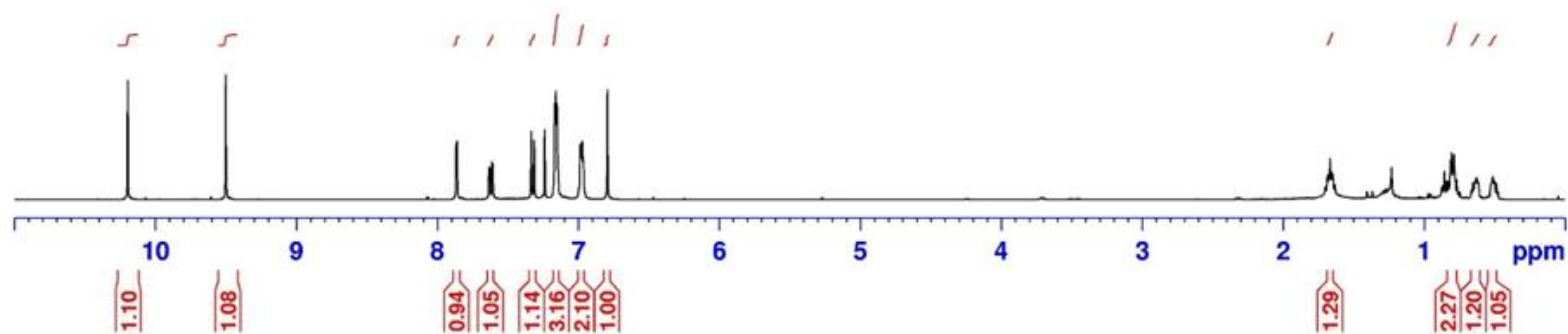
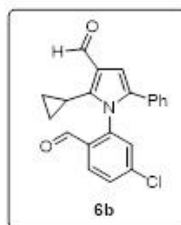
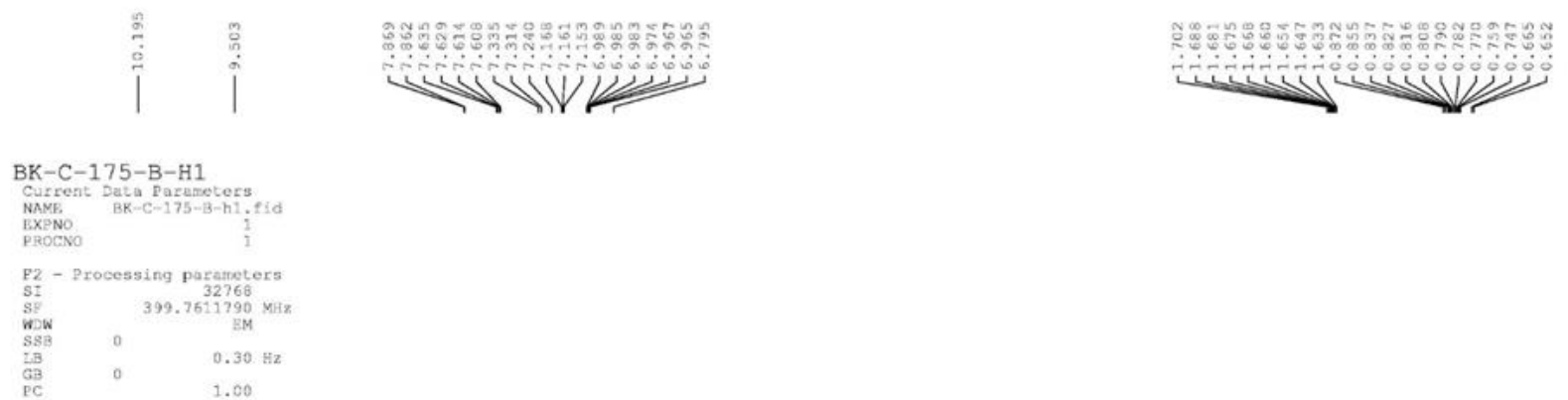
77.319
77.001
76.682

6.995
6.970
6.752

Current Data Parameters
NAME BK-C-158-B-C13.fid
EXPNO 1
PROCNO 1

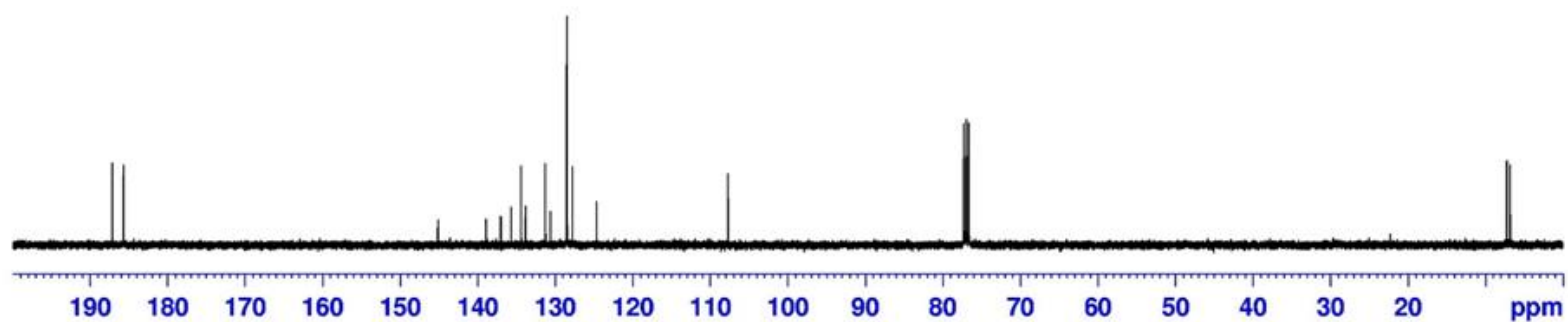
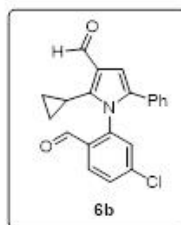
F2 - Processing parameters
SI 65536
SF 100.5214724 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





$$\begin{array}{r} 7.309 \\ 7.256 \\ \hline 6.819 \end{array}$$

F2 - Processing parameters	
SI	65536
SF	100.5214563 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



10.197
9.499

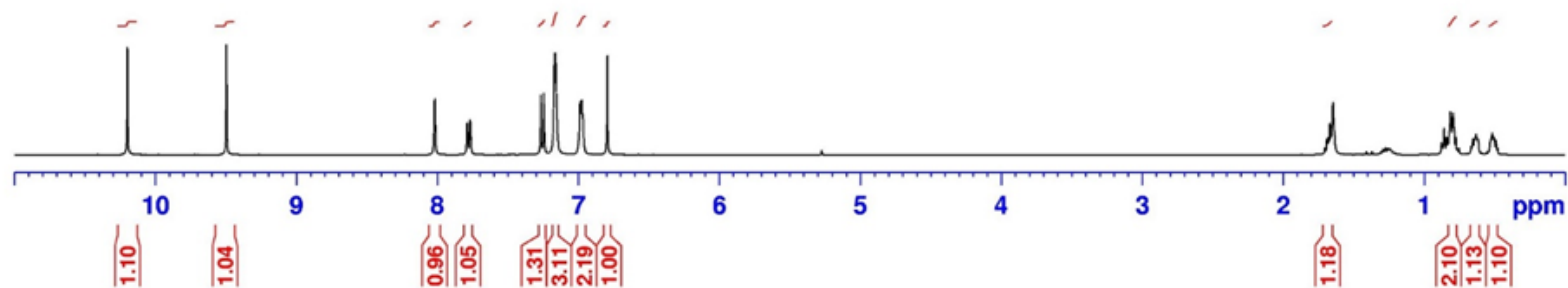
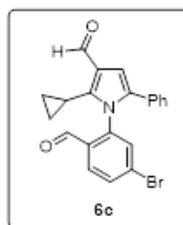
8.024
8.018
7.791
7.786
7.771
7.765
7.268
7.247
7.174
7.167
7.158
6.992
6.986
6.981
6.977
6.968
6.796

1.704
1.690
1.683
1.677
1.670
1.662
1.655
1.647
0.876
0.859
0.841
0.832
0.814
0.796
0.793
0.775
0.763
0.753
0.687
0.653
0.644

BK-C-175-A-H1

Current Data Parameters
NAME BK-C-175-A-H1.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 399.7611778 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



187.06
185.70
C-175-A-C1

145.07
139.44
137.38
137.00
134.00
131.56
131.48
130.64
128.58
128.50
127.60
124.68
123.52

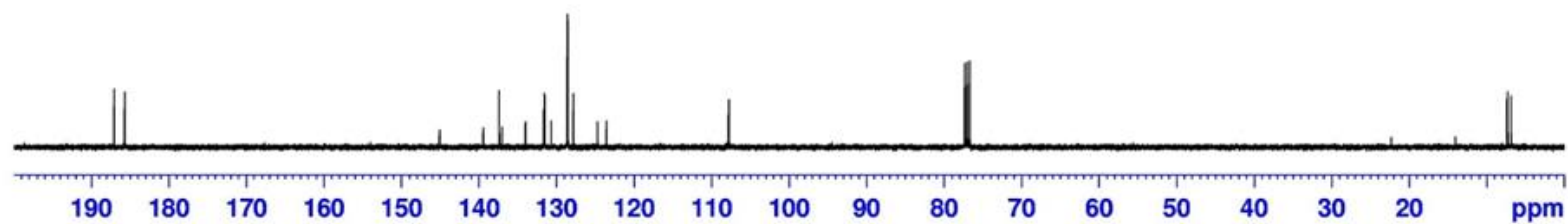
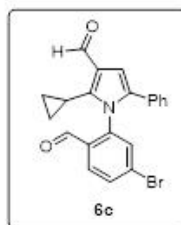
107.74

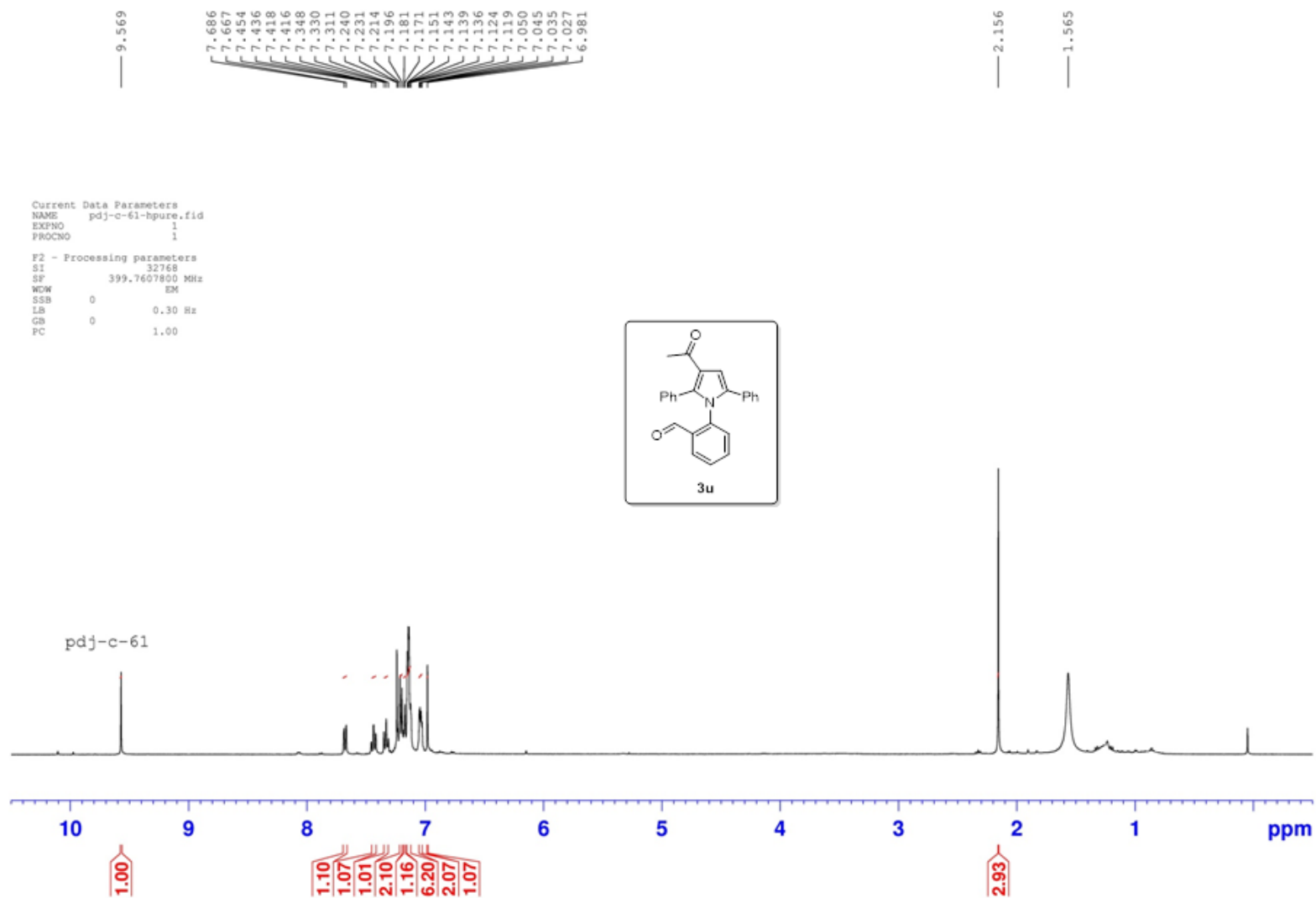
77.318
77.000
76.682

7.326
7.273
6.820

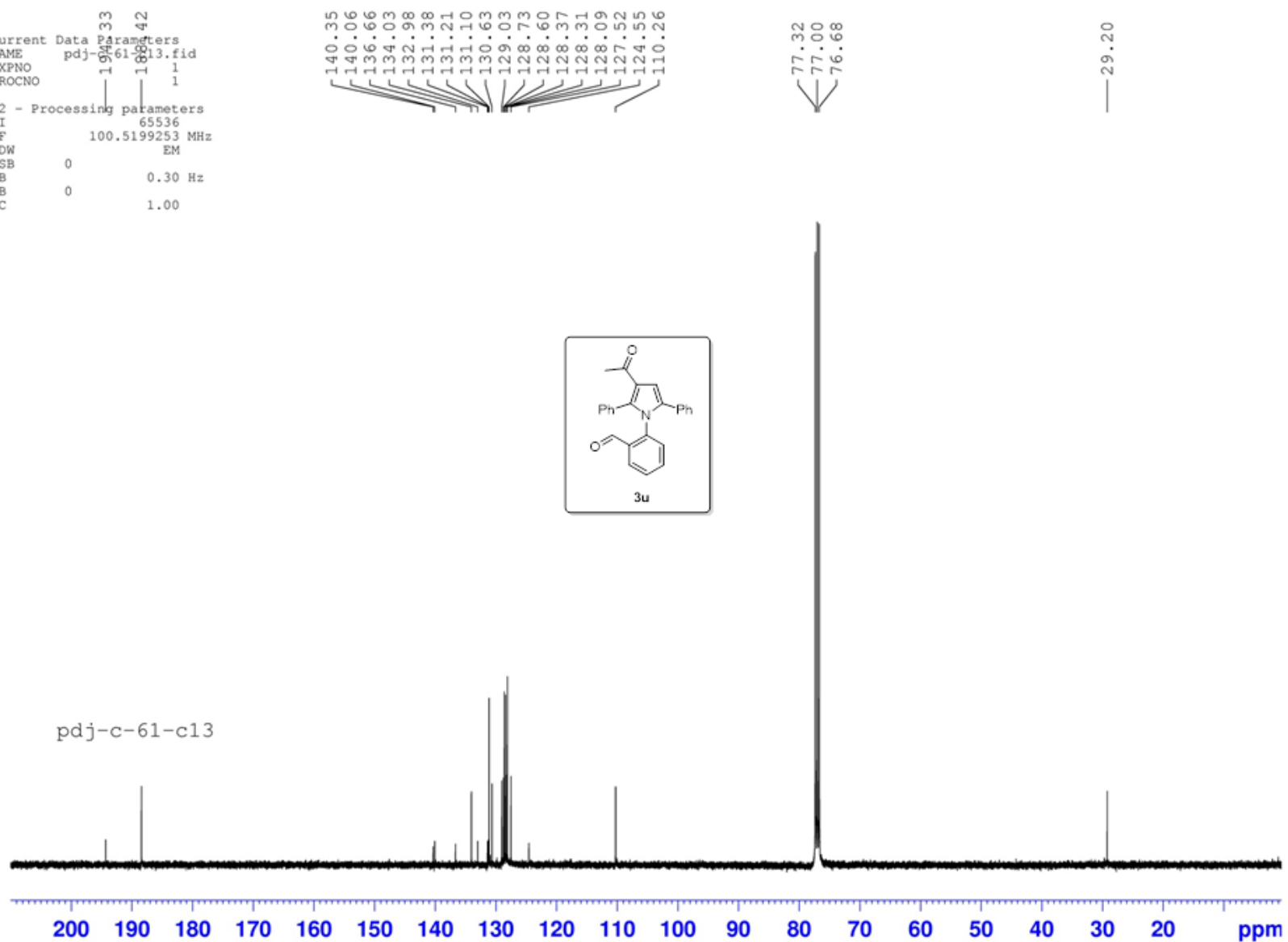
Current Data Parameters
NAME BK-C-175-A-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214584 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



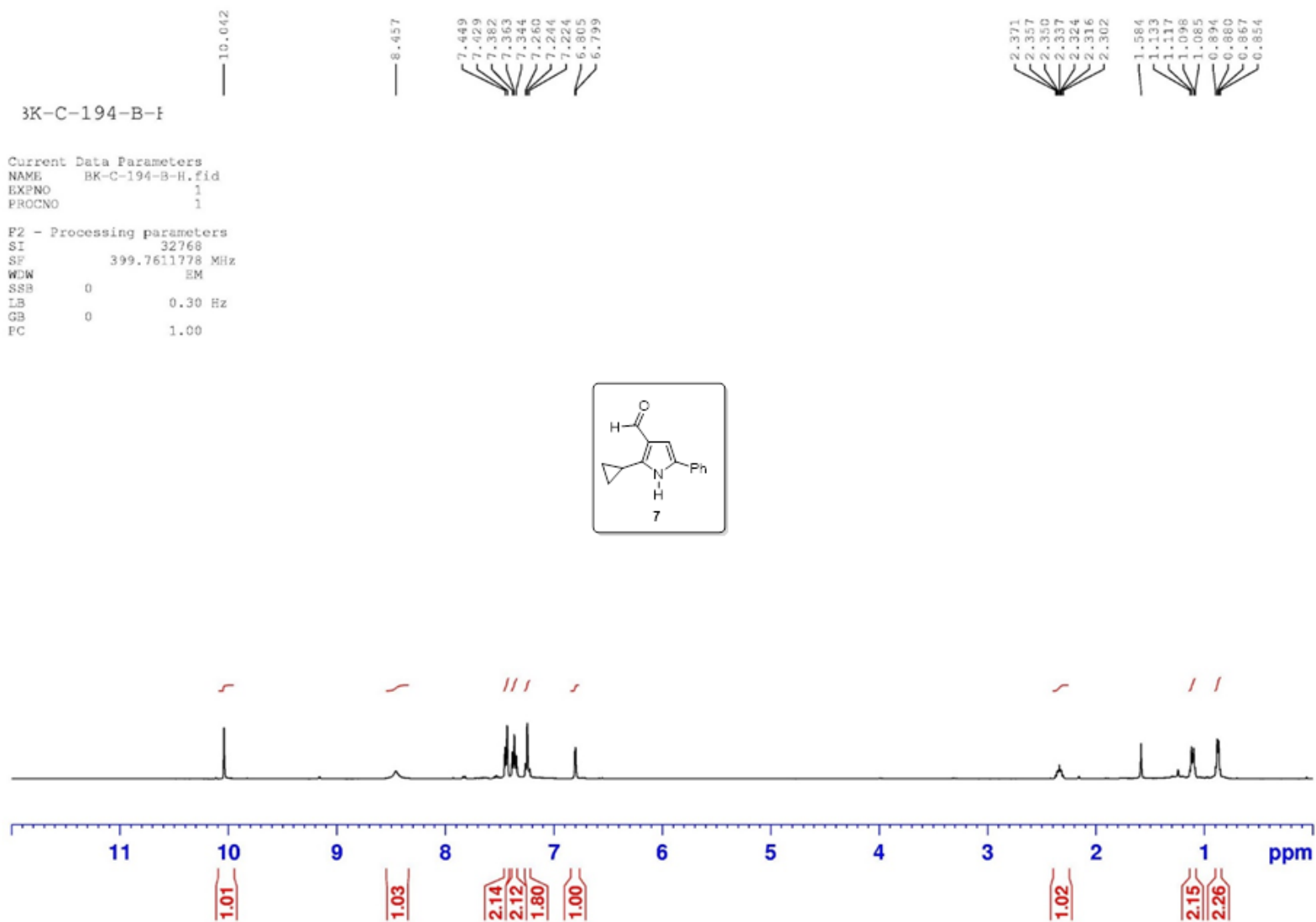
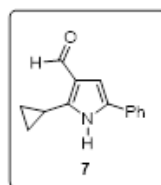


Current Data Parameters
NAME pdj-c-61-c13.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5199253 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3K-C-194-B-I

Current Data Parameters
 NAME BK-C-194-B-H.fid
 EXPNO 1
 PROCNO 1
 F2 - Processing parameters
 SI 32768
 SF 399.7611778 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



185.50
—C-194-B-C1

144.12

131.59
131.28
129.00
127.17
124.44
124.07

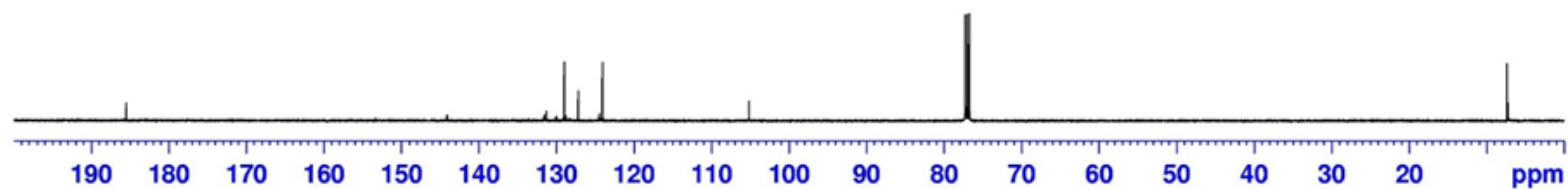
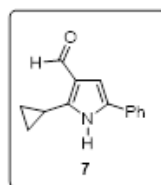
105.15

77.254
77.000
76.746

7.321
7.216

Current Data Parameters
NAME BK-C-194-B-C13.fid
EXPNO 1
PROCNO 1

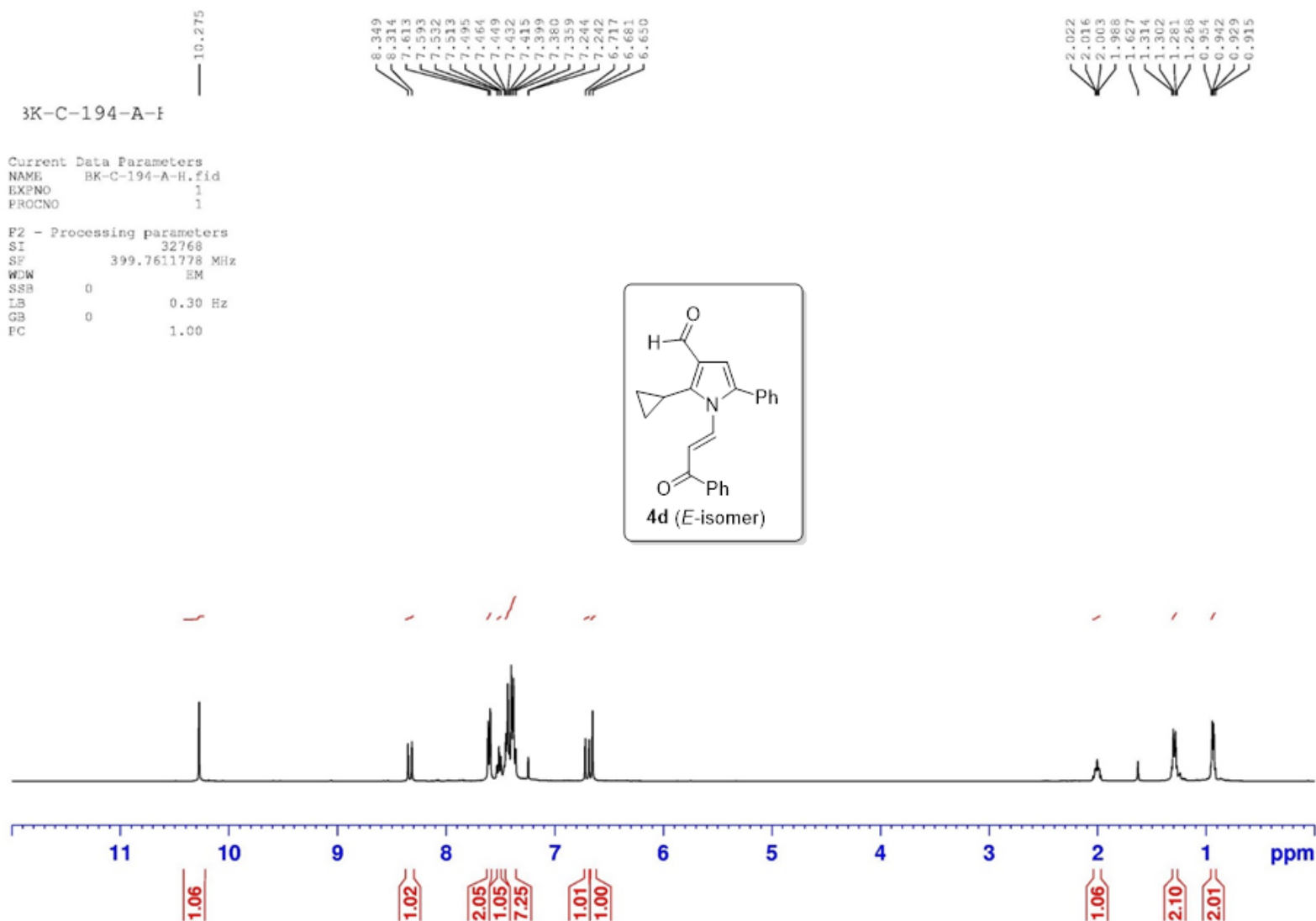
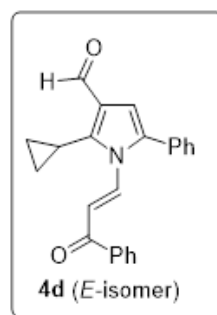
F2 - Processing parameters
SI 65536
SF 125.6764859 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3K-C-194-A-f

Current Data Parameters
NAME BK-C-194-A-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 399.7611778 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



188.83
185.91
(-C-194-A-C)

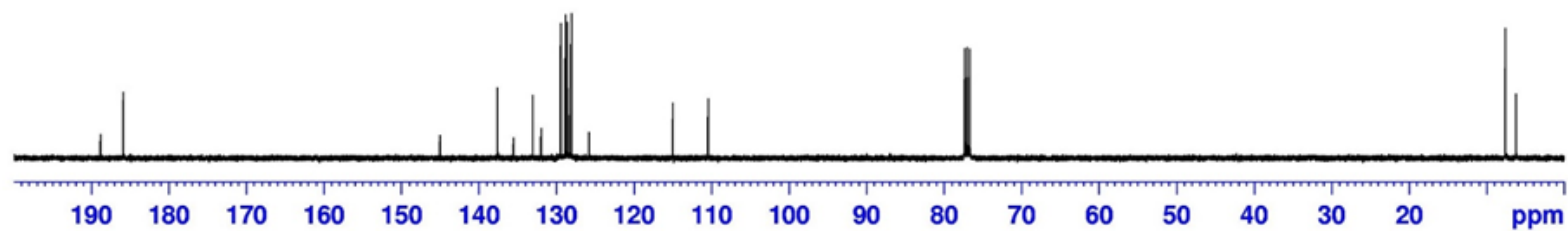
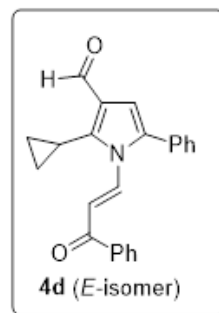
145.01
137.59
135.51
133.06
131.97
129.45
128.86
128.58
128.49
128.09
125.78
114.97
110.42

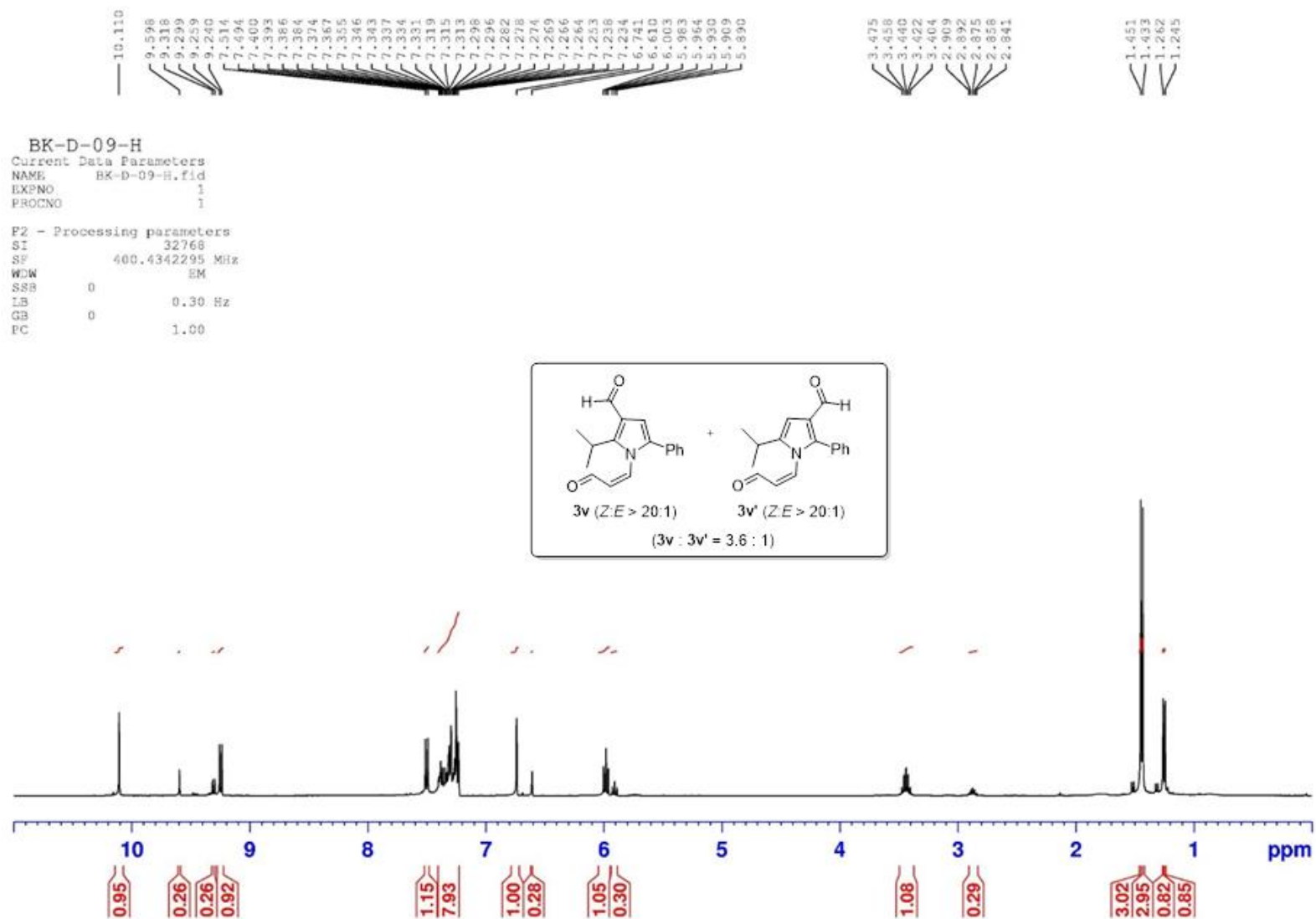
77.318
77.000
76.682

7.571
6.188

Current Data Parameters
NAME BK-C-194-A-C13.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 100.5214587 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





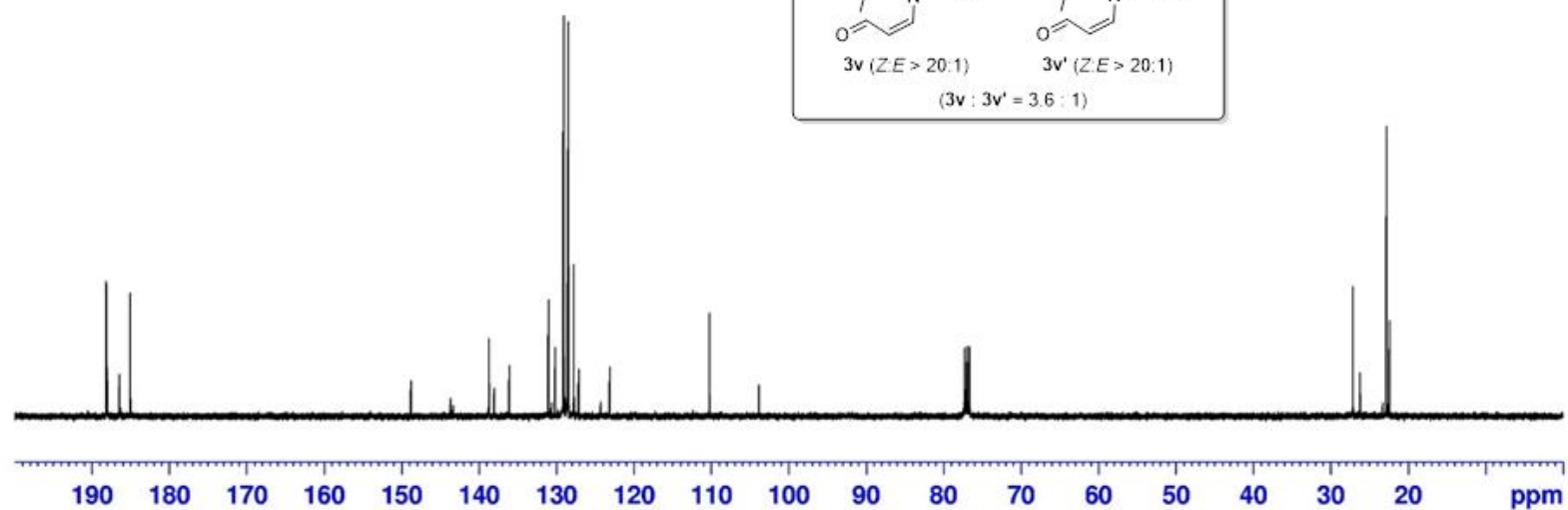
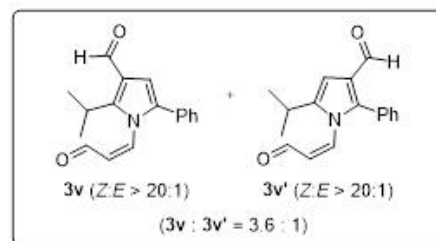
188.19
188.06
186.47
185.08

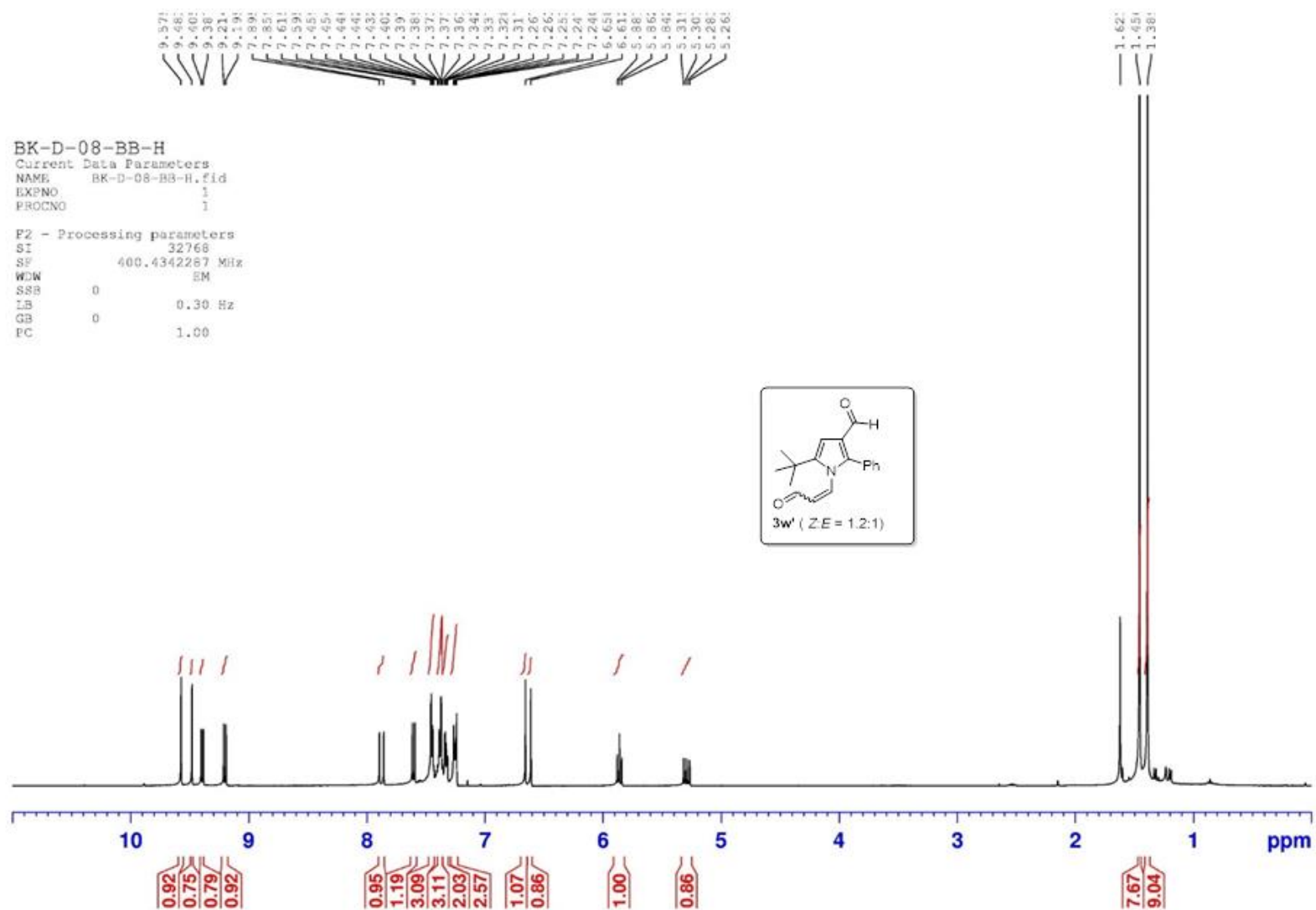
148.85
143.71
138.76
138.08
136.12
131.06
130.21
129.12
129.06
128.61
128.52
128.45
127.78
127.16
124.28
123.13
110.26
103.88

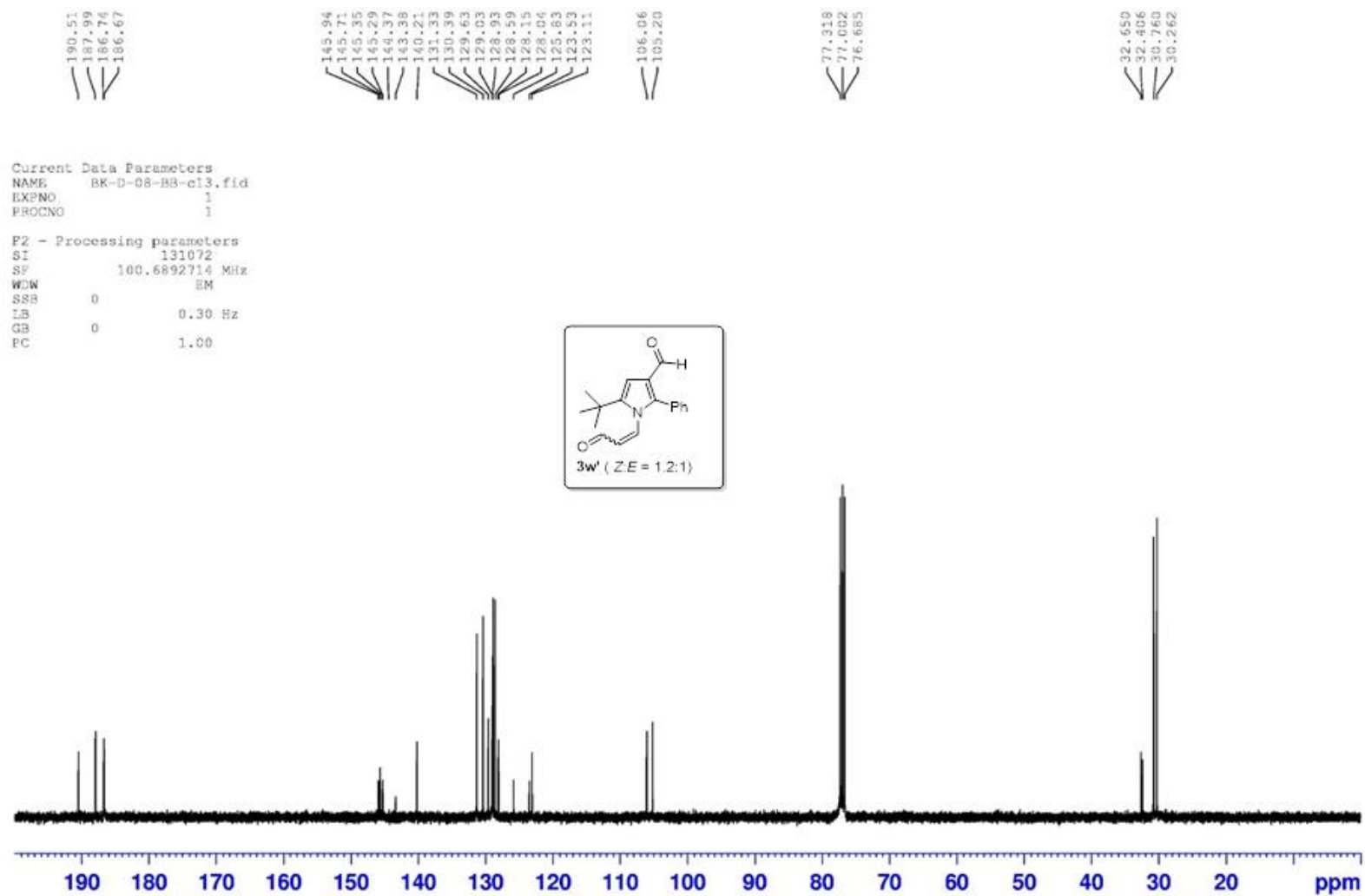
77.318
77.000
76.684

27.145
26.221
22.601
22.429

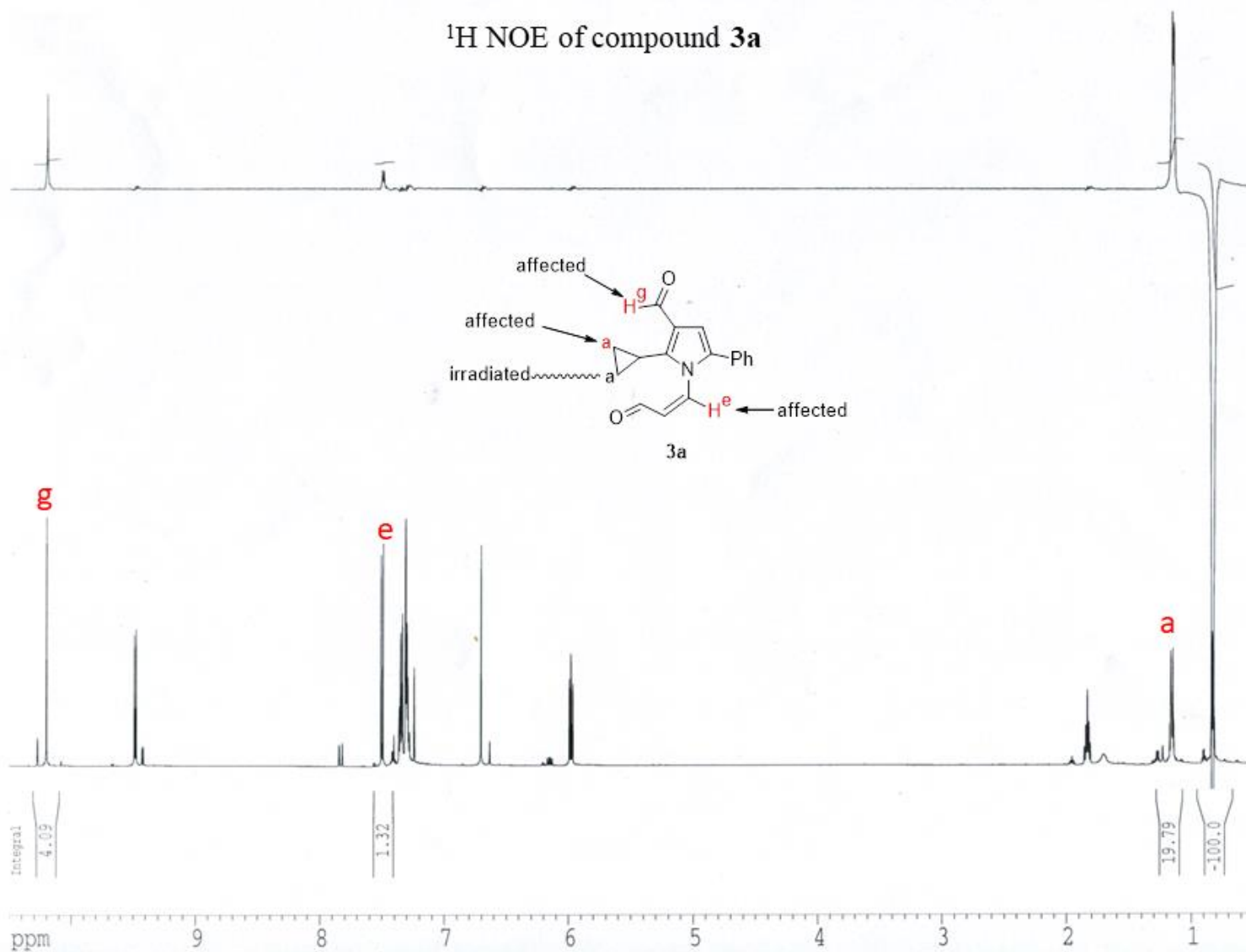
BK-D-09-C13
Current Data Parameters
NAME BK-D-09-C13.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 131072
SF 100.6892779 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



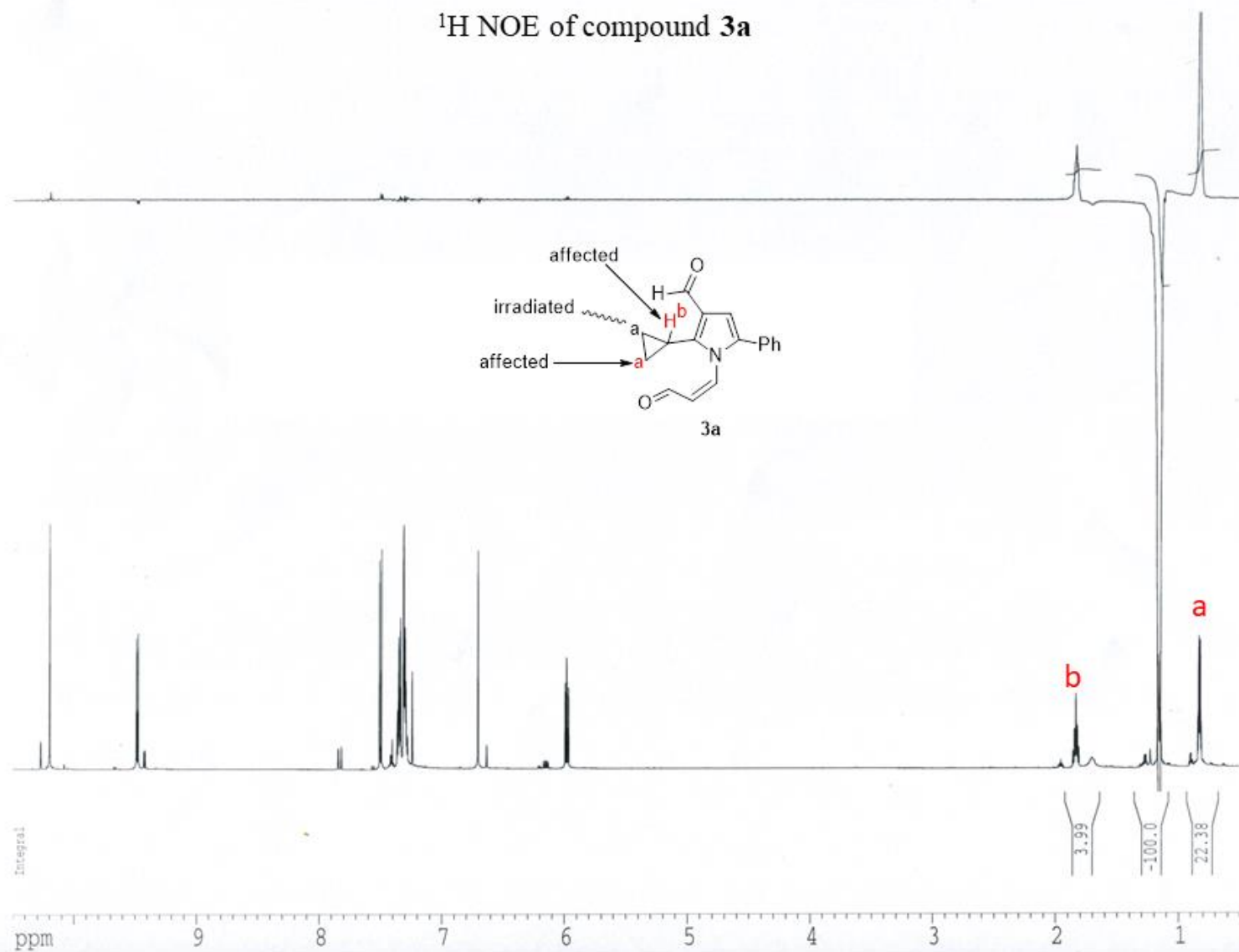




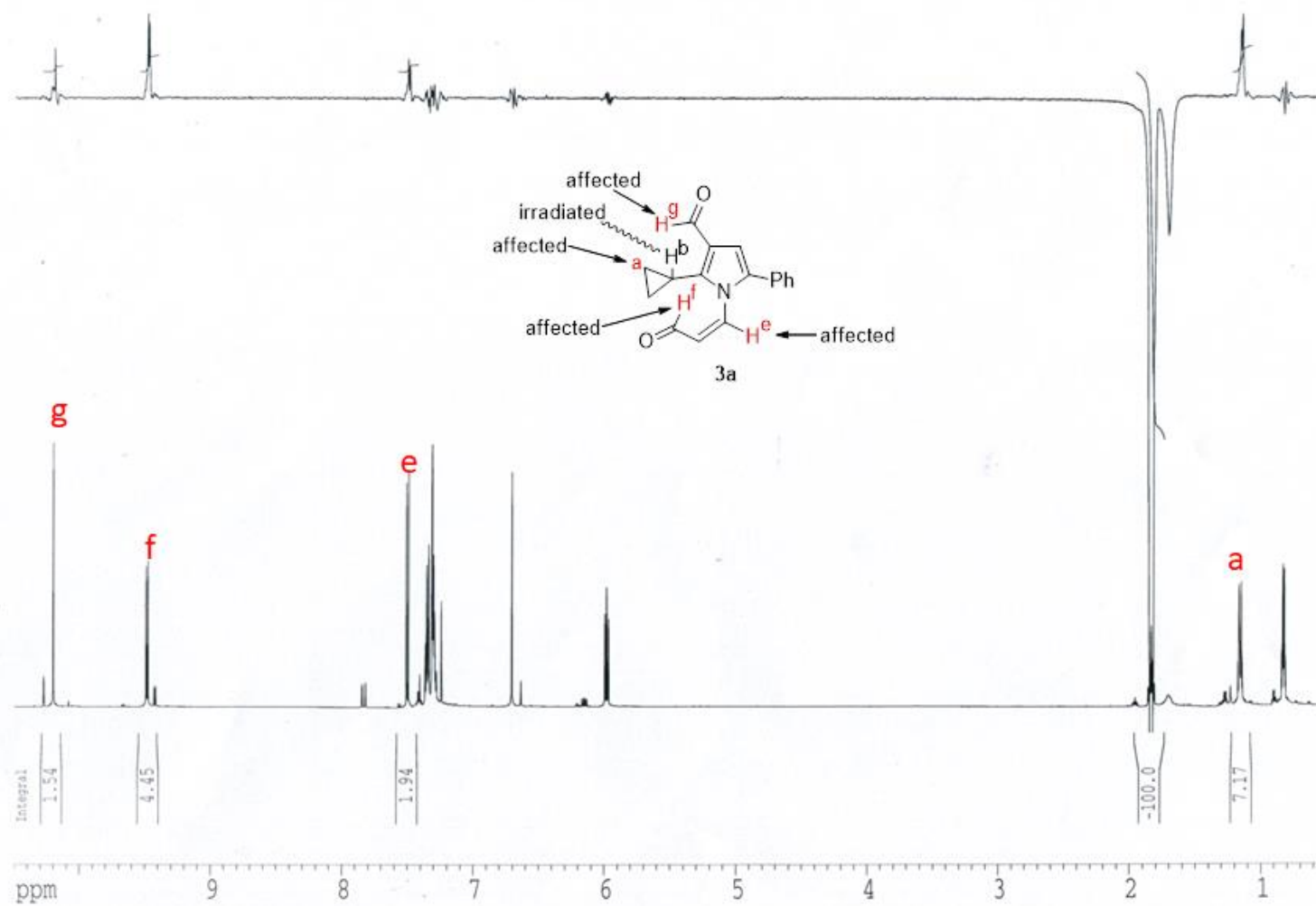
^1H NOE of compound **3a**



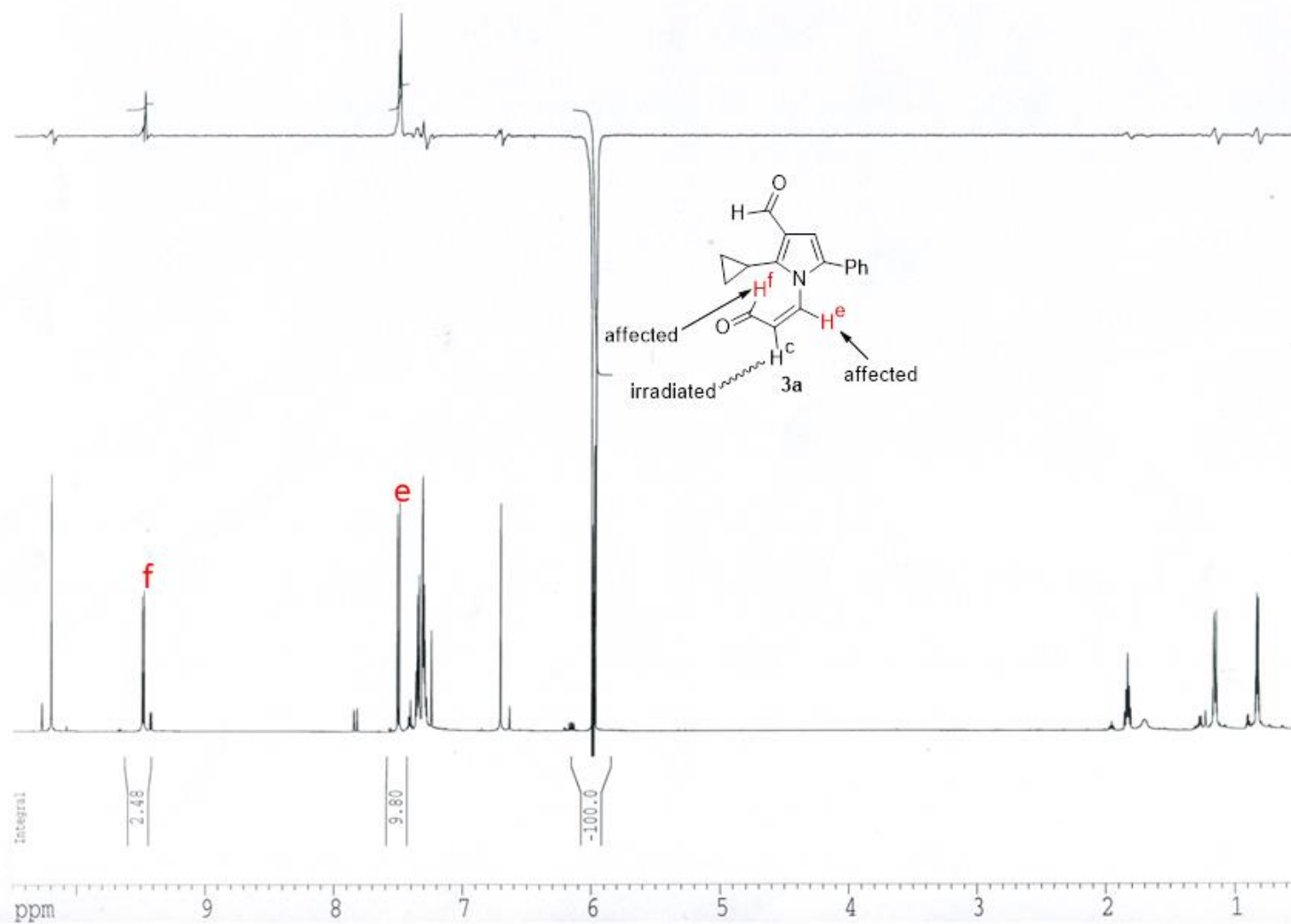
^1H NOE of compound **3a**



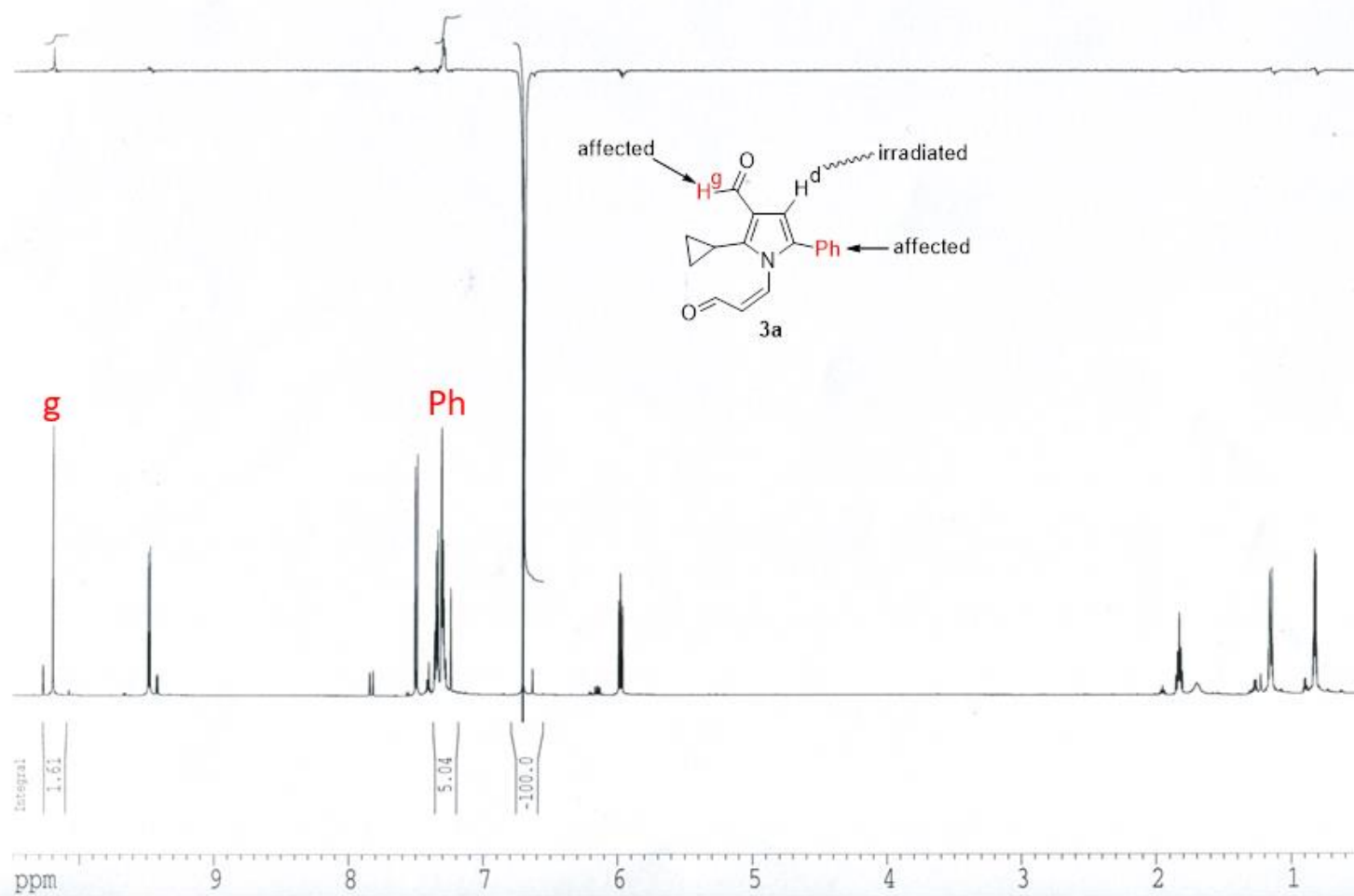
^1H NOE of compound **3a**



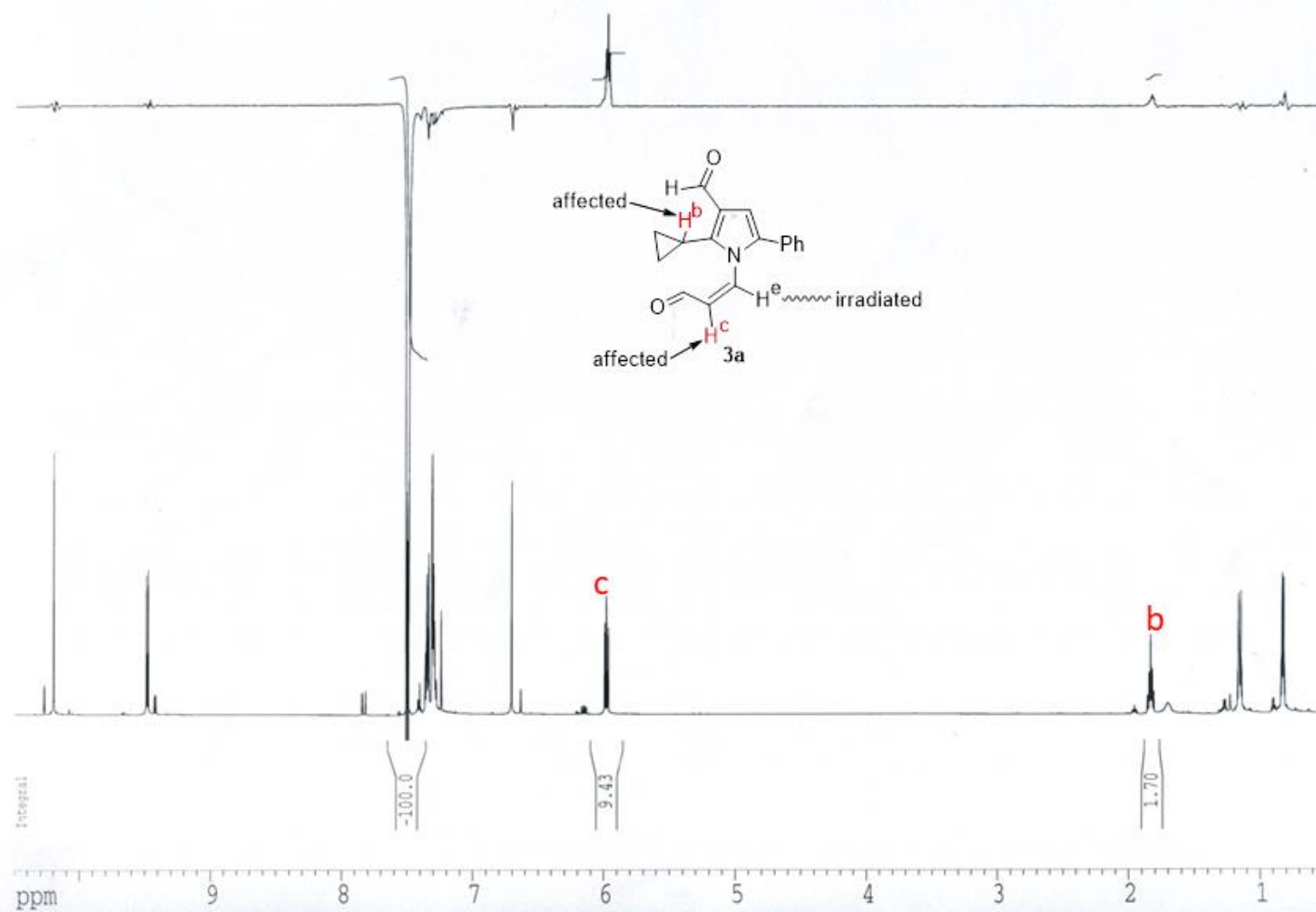
^1H NOE of compound **3a**



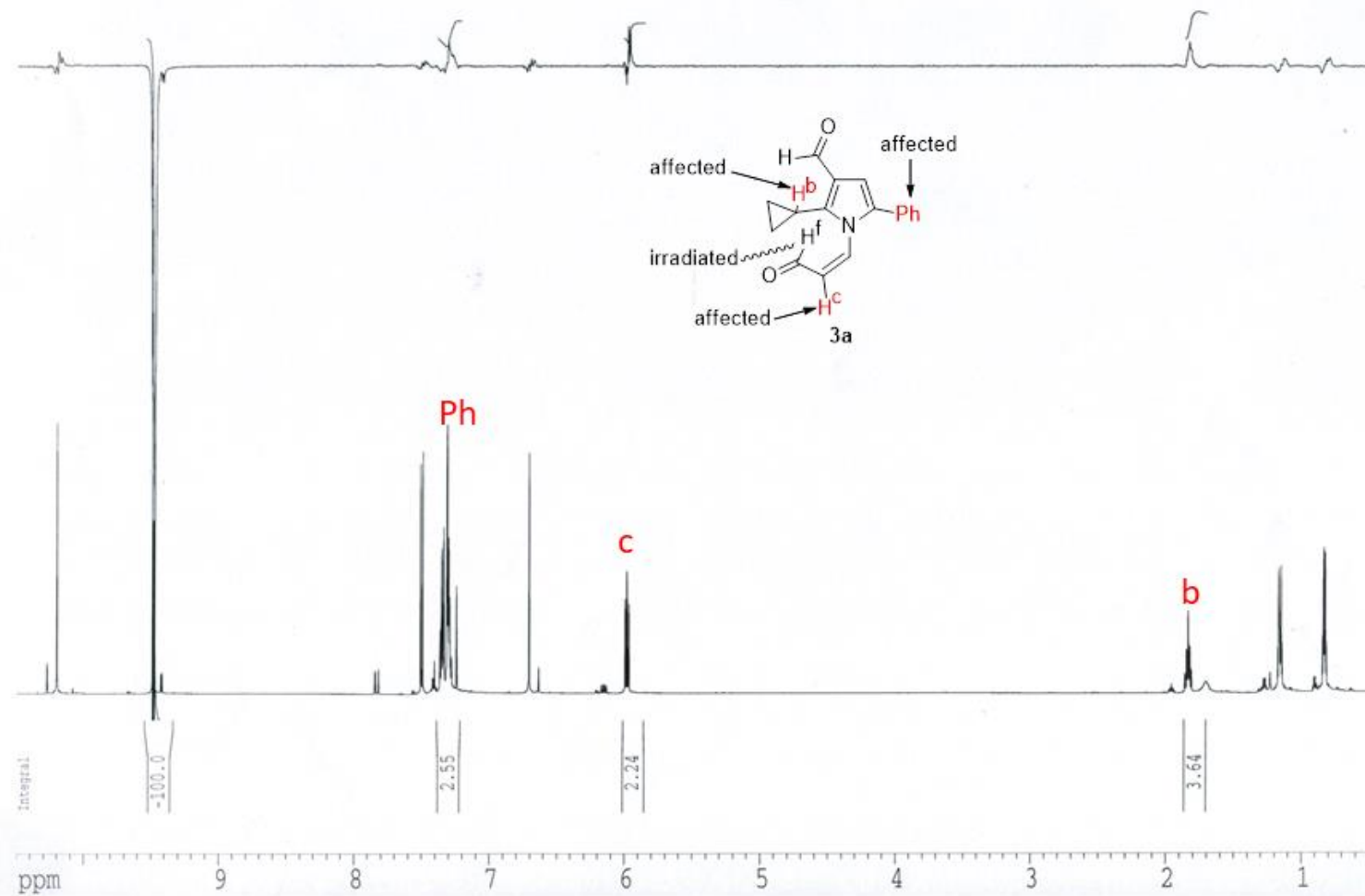
^1H NOE of compound **3a**



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



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



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

