Supporting Information

Gold-catalyzed [4+1]-Annulation Reactions between Anthranils and 4-Methoxy-1,2-dienyl-5-ynes Involving a 1,2-Allene Shift

Hsiang-Chu Hsieh,[+] Kuo-Chen Tan,[+] Antony Sekar Kulandai Raj and Rai-Shung Liu*

Frontier Research Centers on Fundamental and Applied Science of Matters and Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan, ROC----------email:rsliu@mx.nthu.edu.tw

+ H.-C. Hsien and K.-C. Tan contributed equally.

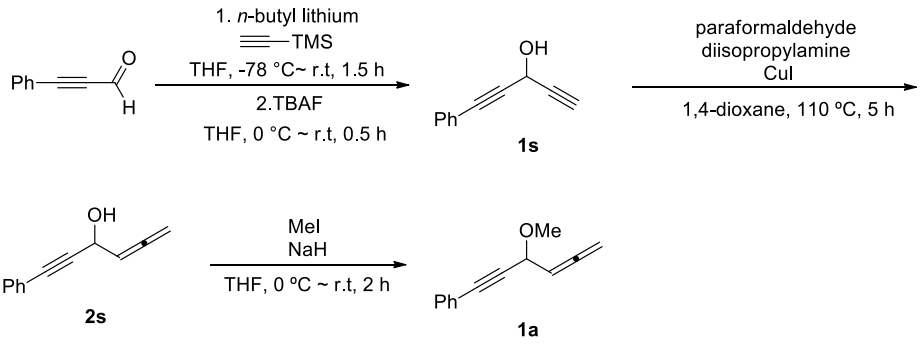
Contents:

(1) General procedure:

Unless otherwise noted, the reactions were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. Tetrahydrofuran (THF) and hexane were dried with sodium, benzophenone and distilled before use. Dichloromethane (DCM), ether and 1,2-dichloroethane (DCE) were dried over CaH_2 and distilled before use. Reagents from commercial sources were used without purifications. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz, 500 MHz, 600 MHz or Varian 500 MHz, spectrometers using chloroform-*d* ($CDCl_3$) as the internal standards. For HRMS, the data of the choro- and bromo-containing compounds are referred to Cl-35 and Br-79, which are the first peaks of their isotopes.

(2) Representative synthetic procedures:

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



Compound **1s** was prepared from 3-phenylpropiolaldehyde according to a literature procedure.[s1]

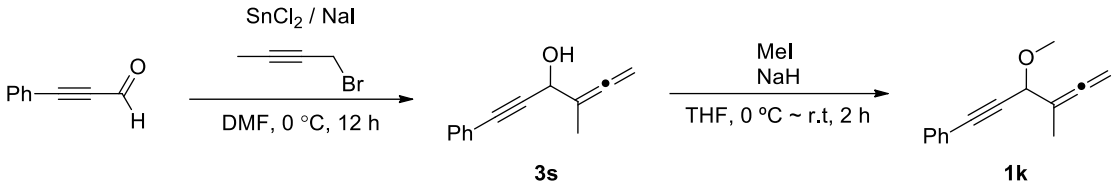
To a dried flask was added CuI (0.3 g, 1.6 mmol), paraformaldehyde (0.76 g, 25.6 mmol) and 1,4-dioxane (10 mL). The resulting mixture was stirred at room temperature before subsequent addition of iPr_2NH (2.3 g, 22.4 mmol), **1s** (2.5 g, 16 mmol) and 1,4-dioxane (5 mL). The mixture was stirred at 110 °C without protection of an inert atmosphere. After 5 h, the crude reaction mixture was cooled to room temperature, filtered through a celite bed (Et_2O), and concentrated in vacuo. The residue was purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford 1-phenylhexa-4,5-dien-1-yn-3-ol (**2s**) as brown oil (1.9 g, 11.2 mmol, 72%).

The compound **2s** (1.9 g, 11.2 mmol) was added to a stirred solution of NaH

(0.54 g, 13.4 mmol) in THF (30 mL) at 0 °C, and the resulting mixture was stirred at 0 °C for 30 min. MeI (3.1 g, 22.4 mmol) was added, and the resulting mixture was stirred at rt for 2 h. The reaction was quenched with water and extracted with Et_2O. The organic layer was washed with water and brine, dried over $MgSO_4$, and concentrated. The residue was purified by silica gel chromatography (SiO_2, eluent: EtOAc/hexane) to afford (3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (**1a**) as brown oil (1.3 g, 7.1mmol, 63%).

1b-1j were synthesized by similar procedure using the corresponding aldehydes..

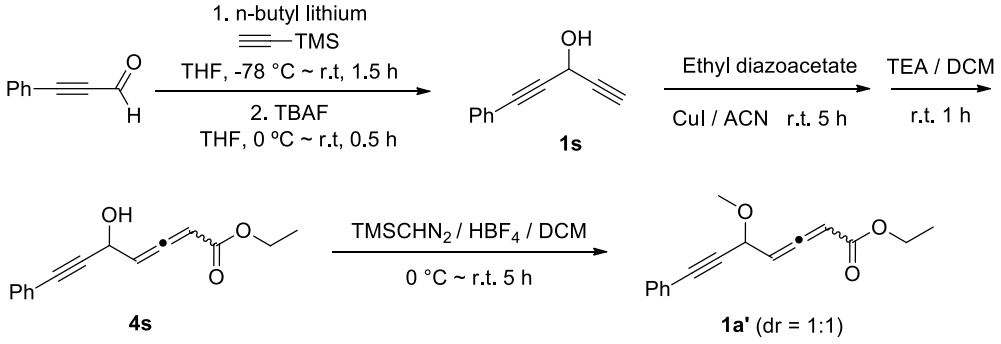
(B) Preparation of (3-methoxy-4-methylhexa-4,5-dien-1-yn-1-yl)benzene (1k)



Compound **3s** was prepared from 3-phenylpropiolaldehyde according to a literature procedure.[s2]

The compound **3s** (2 g, 10.8mmol) was added to a stirred solution of NaH (0.52 g, 13.0 mmol) in THF (30 mL) at 0 °C, and the resulting mixture was stirred at 0 °C for 30 min. MeI (3.0 g, 21.6 mmol) was added, and the resulting mixture was stirred at rt for 2 h. The reaction was quenched with water and extracted with Et_2O. The organic layer was washed with water and brine, dried over $MgSO_4$, and concentrated. The residue was purified by silica gel chromatography (SiO_2, eluent: EtOAc/hexane) to afford (3-methoxy-4-methylhexa-4,5-dien-1-yn-1-yl)benzene (**1k**) as yellow oil (1.6 g, 8.1 mmol, 75%).

(C)Preparation of ethyl 5-methoxy-7-phenylhepta-2,3-dien-6-ynoate (1a')



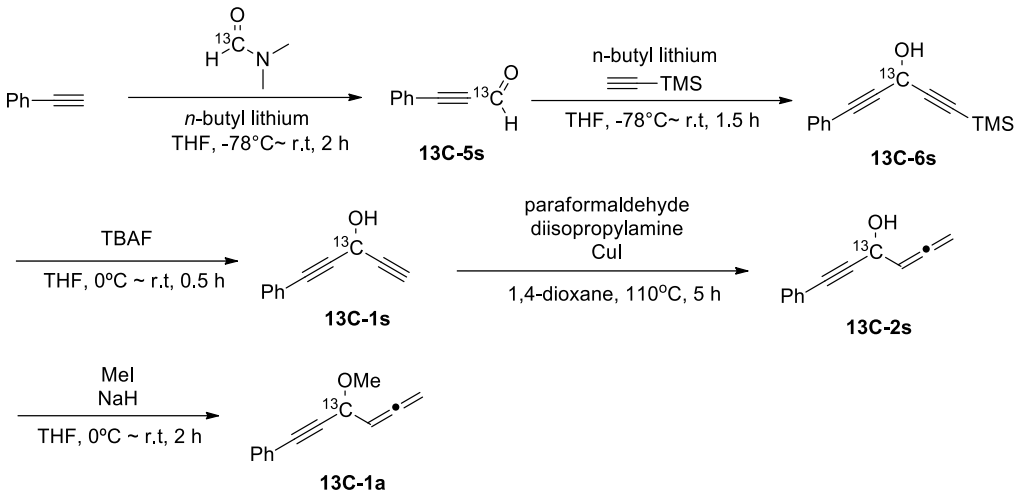
Compound **1s** was prepared from 3-phenylpropiolaldehyde according to a literature procedure.[s1]

To the mixture of the corresponding propargylic alcohol **1s** (30 mmol, 1.0 equiv.) and CuI (1.5 mmol, 0.05 equiv.) in acetonitrile (30 mL) was added ethyl diazoacetate (30 mmol, 1.0 equiv.). The reaction mixture was stirred at room temperature for 5 h. The mixture was filtered, washed with DCM and the solvent was evaporated under reduced pressure. For the mixture (10 mmol, 1.0 equiv.) was dissolved in DCM (30 mL). Et_3N (12 mmol, 1.2 equiv.) was added slowly. After the reaction mixture was stirred for 1 h at room temperature, the mixture was evaporated under reduced pressure. The residue was directly subjected to silica gel column chromatography (SiO_2, eluent: EtOAc/hexane) to give the product **4s** in 80% yield.[s3]

To a vigorously stirred mixture of **4s** (30 mg, 0.11 mmol) and fluoroboric acid (50% w/v in Et_2O, 0.22 mmol) in DCM (4 mL) was added dropwise of $TMSCHN_2$ (2.0 M in hexane, 0.11 mmol) at 0 ℃. The yellow color of $TMSCHN_2$ disappeared immediately accompany with the evolution of nitrogen. The stirring was continued at 0 ℃ and a further portions of $TMSCHN_2$ (0.22mmol) was added dropwise within 10 minutes. The mixture returned to room temperature and stirred for 5 h, the reaction mixture was then poured into saturated NaCl (5 mL), extracted with DCM (5 mL x3), washed with saturated brines, dried over anhydrous $MgSO_4$, and concentrated in vacuo to yield a yellow liquid. The brown liquid was purified by chromatography on silica gel column (SiO_2, eluent: EtOAc/hexane) to afford yellow liquid in 60% yield (**1a'**).[s4]

.**1b'-1k'** were synthesized by similar procedure using the corresponding aldehydes..

(D) Preparation of (3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (13C-1a)



Phenylacetylene (1 g, 9.8mmol) was dissolved into dry THF (10 mL) and the solution was cooled to -78 ℃. To this solution, *n*-butyllithium (4.7 mL, 11.8mmol, 2.5 M in hexane) was added. After being stirred for 30 minutes at -78 ℃, DMF (1.4g, 19.6 mmol) (90% dimethylformamide : 10% dimethylformamide-(carbonyl-13C)) was added. The reaction mixture was stirred at room temperature for 2h and then the reaction was quenched by saturated $KH_2PO_{4(aq)}$ and extracted three times with ether. The combined organic layer was dried over $MgSO_4$ and the solvent was removed under a reduced pressure. The residue was purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 3-phenylpropiolaldehyde (**13C-5s**) as yellow liquid (1.2 g, 9.3 mmol, 95%).

(3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene **(13C-1a)** was synthesized by similar procedure **(A)**.

(E) Preparation of benzisoxazoles (2a-2l, 2b'-2g')

Benzisoxazoles (**2a-2l, 2b'-2g'**) were prepared according to literature procedure.[s5][s6]

References

[s1] : R. D. Kardile, B. S. Kale, P. Sharma and R.-S. Liu, *Org.Lett.* 2018, **20**, 3806−3809.

[s2] : D. Xu, Z. Liand and S. Ma, *Tetrahedron Asymmetry* 2003, **14**, 3657-3666

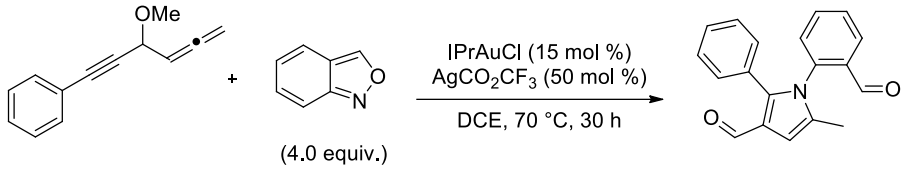
[s3] : W. Dong, P. Hu, J. Hu and X. Tong, *Tetrahedron Lett.* 2014, **55**, 1682–1685.

[s4] : X.-D. Zuo, S.-M. Guo, R. Yang, J.-H. Xie and Q.-L Zhou, *Chem. Sci*. 2017, **8**, 6202–6206.

[s5] : R. L. Sahani and R.-S. Liu, *Angew. Chem. Int. Ed*. 2017, **56***,* 1026.
[s6] : J. Chauhana and S. Fletcher, *Tetrahedron Lett.* 2012, **53**, 4951.

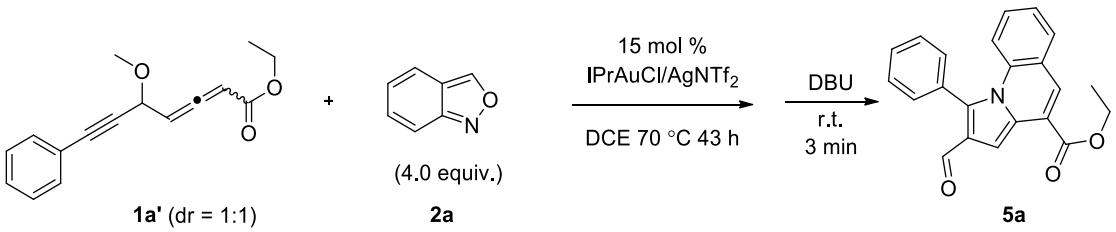
(3) Standard procedures for catalytic operations:

(A) Preparation of 1-(2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3a)



A suspension of chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (25.4 mg, 0.041mmol) and silver trifluoroacetate (30.2 mg, 0.137 mmol) in dry DCE (1 mL) was fitted with N_2 balloon, and the mixture was stirred for 10 min. To the solution was added a DCE (1 mL) solution of (3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (**1a**) (50 mg, 0.273 mmol) and benzisoxazole (**2a**) (129 mg, 1.09 mmol) at room temperature. The resulting solution was placed in an oil bath at 70 °C, and the mixture was stirred for 30 h. The solution was filtered over a short celite bed and evaporated under reduced pressure. The residues were purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 1-(2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (**3a**) as yellow solid (51 mg, 0.177 mmol, 65%).

(B) Preparation of ethyl 2-formyl-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate (5a)

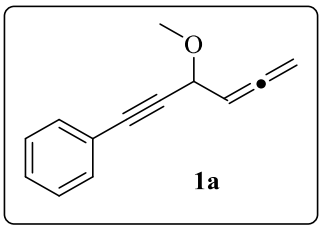


A suspension of (chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (18.2 mg, 0.029 mmol) and silver bis(trifluoromethanesulfonyl)imide (11.4 mg, 0.029

mmol) in dry DCE (1 mL) was fitted with N_2 balloon, and the mixture was stirred for 10 min. To the solution was added to a DCE (1 mL) solution of ethyl 5-methoxy-7-phenylhepta-2,3-dien-6-ynoate (50 mg, 0.195 mmol) and benzisoxazole (**2a**) (93.0 mg, 0.781 mmol) at room temperature. The resulting solution was placed in an oil bath at 70 ℃, and the mixture was stirred for 43 h. Then cool the mixture to room temperature. Add DBU(1,8-Diazabicyclo(5.4.0)undec-7-ene) (29.7 mg, 0.195 mmol) to the mixture. It was stirred for 3 min. The solution was filtered over a short celite bed, and evaporated under reduced pressure. The residues were purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired ethyl 2-formyl-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate (**5a**) as yellow solid (67 mg, 0.099 mmol, 51%).

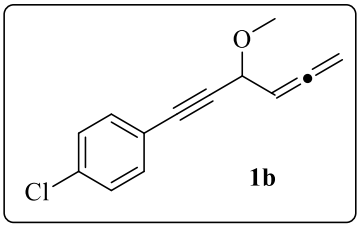
(4) Spectral data for compounds:

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



Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.43 (m, 2H), 7.31-7.28 (m, 3H), 5.36 (q, *J* = 6.6 Hz, 1H), 4.95 (dd, *J* = 6.6, 1.9 Hz, 2H), 4.79 (dt, *J* = 7.0, 2.0 Hz, 1H), 3.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 131.8, 128.5, 128.2, 122.4, 90.3, 86.7, 86.0, 77.7, 69.7, 55.5; EI-MS calcd. for $C_{13}H_{12}O[M^+]$: 184.0888; found: 184.0874.

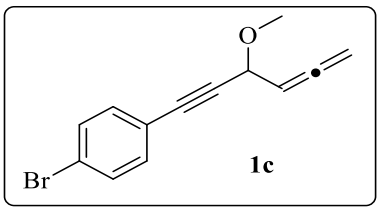
1-chloro-4-(3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (1b):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (dt, *J* = 8.9, 2.3 Hz, 2H), 7.26 (dt, *J* = 9.0, 2.3 Hz, 2H), 5.33 (q, *J* = 6.6 Hz, 1H), 4.94 (dd, *J* = 6.6, 2.1 Hz, 2H), 4.76 (dt, *J* =

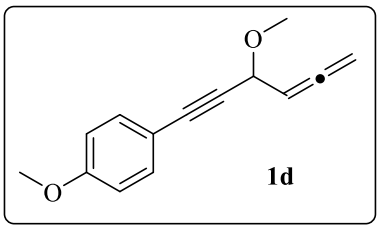
7.1, 2.0 Hz, 1H), 3.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 134.6, 133.0, 128.6, 120.9, 90.2, 87.0, 85.5, 77.8, 69.6, 55.6; EI-MS calcd. for $C_{13}H_{11}{}^{35}ClO[M^+]$: 218.0498; found: 218.0495.

1-bromo-4-(3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (1c):



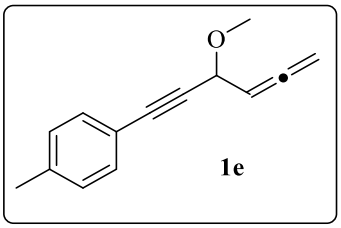
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (dt, *J* = 8.5, 1.9 Hz, 2H), 7.29 (dt, *J* = 8.8, 2.1 Hz, 2H), 5.33 (q, *J* = 6.7 Hz, 1H), 4.95-4.93 (m, 2H), 4.76 (dt, *J* = 7.0, 1.9 Hz, 1H), 3.43 (s, 3H); ^{13}CNMR (100 MHz, $CDCl_3$): δ 209.0, 133.2, 131.5, 122.8, 121.4, 90.2, 87.3, 85.6, 77.8, 69.7, 55.6; ESI-MS calcd. for $C_{13}H_{12}{}^{79}BrO[M+H]$: 263.0072; found: 263.0056.

1-methoxy-4-(3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (1d):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (dt, *J* = 9.6, 2.7 Hz, 2H), 6.81 (dt, *J* = 9.6, 2.7 Hz, 2H), 5.34 (q, *J* = 6.7 Hz, 1H), 4.95-4.92 (m, 2H), 4.76 (dt, *J* = 7.1, 1.9 Hz, 1H), 3.79 (s, 3H), 3.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 159.8, 133.3, 114.5, 113.9, 90.5, 86.6, 84.6, 77.6, 69.8, 55.5, 55.3; ESI-MS calcd. for $C_{14}H_{14}NaO_2[M+Na]$: 237.0891; found: 237.0882.

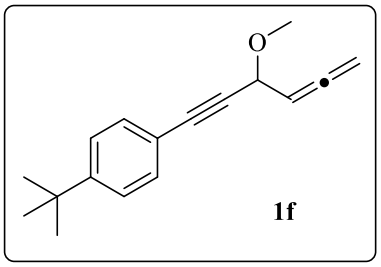
1-(3-methoxyhexa-4,5-dien-1-yn-1-yl)-4-methylbenzene (1e):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43-7.32 (m, 2H), 7.10-7.08 (m, 2H),

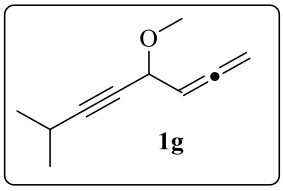
5.35 (q, *J* = 6.5 Hz, 1H), 4.95-4.93 (m, 2H), 4.77 (dt, *J* = 7.0, 1.9 Hz, 1H), 3.44 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 138.7, 131.7, 129.0, 119.3, 90.5, 86.8, 85.3, 77.6, 69.8, 55.5, 21.5; EI-MS calcd. for $C_{14}H_{14}O[M^+]$: 198.1045; found: 198.1040.

1-(tert-butyl)-4-(3-methoxyhexa-4,5-dien-1-yn-1-yl)benzene (1f):



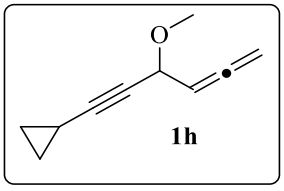
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.36 (m, 2H), 7.33-7.30 (m, 2H), 5.35 (q, *J* = 6.6 Hz, 1H), 4.94 (dd, *J* = 6.6, 2.0 Hz, 2H), 4.78 (dt, *J* = 7.0, 1.9 Hz, 1H), 3.44 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 151.8, 131.5, 125.2, 119.4, 90.5, 86.8, 85.3, 77.6, 69.7, 55.5, 34.8, 31.1; ESI-MS calcd. for $C_{17}H_{21}O[M+H]$: 241.1592; found: 241.1593.

4-methoxy-7-methylocta-1,2-dien-5-yne (1g):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.23 (q, *J* = 6.7Hz, 1H), 4.89-4.87 (m, 2H), 4.52 (dq, *J* = 7.0, 1.9 Hz, 1H), 3.35 (s, 3H), 2.62-2.55 (m, 1H), 1.15 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 208.9, 93.1, 90.8, 77.3, 76.2, 69.4, 55.2, 22.9, 20.5; FI-MS calcd. for $C_{10}H_{14}O[M^+]$: 150.1045; found: 150.1042.

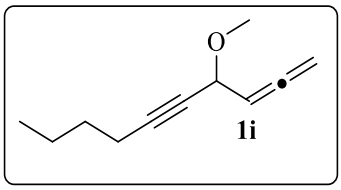
(3-methoxyhexa-4,5-dien-1-yn-1-yl)cyclopropane (1h):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.21 (q, *J* = 6.7 Hz, 1H), 4.88-4.86 (m, 2H), 4.49 (dq, *J* = 5.5, 1.9 Hz, 1H), 3.33 (s, 3H), 1.28-1.23 (m, 1H), 0.78-0.74 (m,

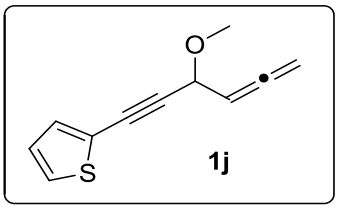
2H), 0.70-0.66 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 208.8, 90.7, 77.3, 72.2, 69.5, 55.3, 8.3, -0.6 (one quarternary carbon is merged with others); FI-MS calcd. for $C_{10}H_{12}O[M^+]$: 148.0888; found: 148.0886.

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



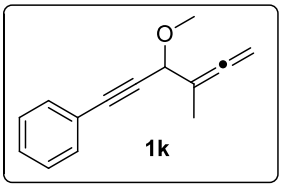
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.23 (q, *J* = 6.7 Hz, 1H), 4.88 (dd, *J* = 6.5, 1.8 Hz, 2H), 4.54-4.50 (m, 1H), 3.35 (s, 3H), 2.22 (td, *J* = 6.9, 1.9 Hz, 2H), 1.52-1.35 (m, 4H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 208.8, 90.8, 87.6, 69.5, 55.3, 30.6, 21.9, 21.6, 18.4, 13.5 (one quarternary carbon is merged with others); FI-MS calcd. for $C_{11}H_{16}O[M^+]$: 164.1201; found: 164.1198.

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



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.22-7.21 (m, 1H), 6.95 (dd, *J* = 5.1, 3.6 Hz, 1H), 5.34 (q, *J* = 6.8 Hz, 1H), 4.95 (dd, *J* = 6.5 , 2.0 Hz, 2H), 4.78 (dt, *J* = 7.0, 1.9 Hz, 1H), 3.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.0, 132.5, 127.4, 126.9, 122.2, 90.1, 89.9, 79.9, 77.8, 69.9, 55.6; FI-MS calcd. for $C_{11}H_{10}OS[M^+]$: 190.0452; found: 190.1350.

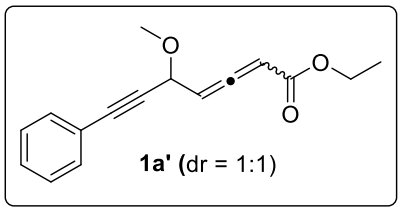
(3-methoxy-4-methylhexa-4,5-dien-1-yn-1-yl)benzene (1k):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45-7.43 (m, 2H), 7.31-7.28 (m, 3H), 4.83-4.81 (m, 2H), 4.71 (t, *J* = 1.2 Hz, 1H), 3.41 (d, *J* = 1.2 Hz, 3H), 1.82 (t, *J* = 3.2

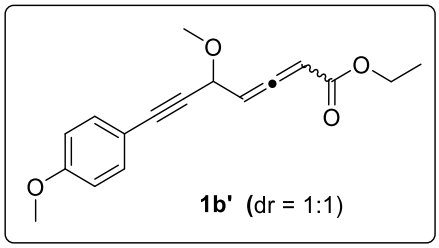
Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 207.2, 131.8, 128.4, 128.2, 122.5, 97.3, 86.6, 85.8, 76.0, 73.4, 55.6, 13.9; FI-MS calcd. for $C_{14}H_{14}O[M^+]$: 198.1039; found: 198.1034.

ethyl 5-methoxy-7-phenylhepta-2,3-dien-6-ynoate (1a'):



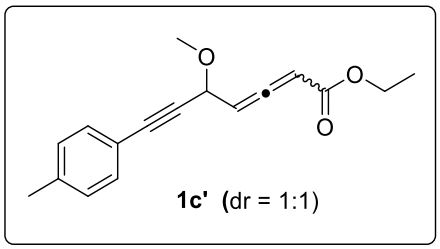
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43-7.41 (m, 2H), 7.32-7.28 (m, 3H), 5.83-5.77 (m, 2H), 4.94 (dd, *J* = 6.2, 2.5 Hz, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.6, 212.5, 165.0, 131.8, 128.7, 128.3, 122.1, 95.3, 95.1, 91.0, 90.7, 87.3, 87.1, 85.0, 84.7, 68.8, 68.1, 61.1, 55.7, 55.1, 14.2; ESI-MS calcd. for $C_{16}H_{16}NaO_3$[M+Na]: 279.0997; found: 279.0999.

ethyl 5-methoxy-7-(4-methoxyphenyl)hepta-2,3-dien-6-ynoate (1b'):



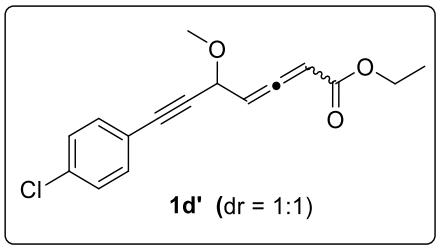
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (d, *J* = 8.9 Hz, 2H), 6.81 (d, *J* = 8.9 Hz, 2H), 5.83-5.76 (m, 2H), 4.92 (dd, *J* = 6.2, 2.5 Hz, 1H), 4.19 (q, *J* = 7.0 Hz, 2H), 3.79 (s, 3H), 3.45 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.6, 212.5,165.1, 165.0, 159.9, 133.3, 113.9, 95.5, 95.3, 91.0, 90.6, 87.3, 87.1, 85.0, 83.4, 68.9, 68.3, 61.1, 55.6, 55.3, 55.1, 14.2; ESI-MS calcd. for $C_{17}H_{19}O_4$[M+H]: 287.1283; found: 287.1281.

ethyl 5-methoxy-7-(p-tolyl)hepta-2,3-dien-6-ynoate (1c'):



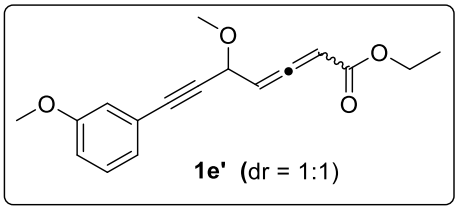
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (d, *J* = 7.9 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 5.83-5.75 (m, 2H), 4.93 (dd, *J* = 6.0, 2.4 Hz, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 3H), 2.33 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 212.6, 212.4, 165.0, 164.9, 138.8, 131.7, 129.0, 119.0, 95.3, 95.2, 90.9, 90.6, 87.4, 84.3, 84.0, 68.8, 68.1, 61.0, 55.5, 54.9, 21.4, 14.1; ESI-MS calcd. for $C_{17}H_{18}NaO_3$[M+Na]: 293.1154; found: 293.1151.

ethyl 7-(4-chlorophenyl)-5-methoxyhepta-2,3-dien-6-ynoate (1d'):



Yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 5.81-5.74 (m, 2H), 4.91 (dd, *J* = 6.2, 2.1 Hz, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.45 (s, 3H), 1.24 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.6, 212.5, 165.0, 164.9, 134.8, 133.0, 128.7, 120.5, 95.2, 95.0, 91.1, 90.8, 86.2, 86.0, 85.9, 85.8, 68.8, 68.2, 61.2, 55.8, 55.2, 14.2; ESI-MS calcd. for $C_{16}H_{16}{}^{35}ClO_3$[M+H]: 291.0788; found: 291.0783.

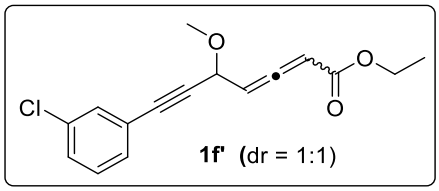
ethyl 5-methoxy-7-(3-methoxyphenyl)hepta-2,3-dien-6-ynoate (1e'):



Yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.19 (td, *J* = 8.0, 1.6 Hz, 1H), 7.01 (dq, *J* = 8.0, 1.1 Hz, 1H), 6.95-6.94 (m, 1H), 6.87-6.85 (m, 1H), 5.83-5.75 (m, 2H), 4.93 (dd, *J* = 6.3, 2.3 Hz, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.76 (s, 3H), 3.45 (s, 3H), 1.25 (t, *J*

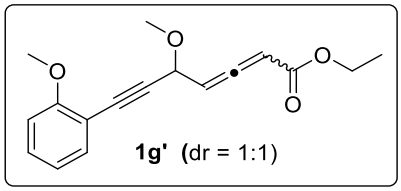
= 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 212.6, 212.5, 165.0, 164.9, 159.2, 129.3, 124.3, 124.2, 123.1, 123.0, 116.6, 116.5, 115,4, 115.3, 95.2, 95.1, 91.0, 90.7, 87.2, 87.0, 84.8, 84.5, 68.8, 68.1, 61.1, 61.0, 55.7, 55.2, 55.1, 14.1; ESI-MS calcd. for $C_{17}H_{19}O_4$[M+H]: 287.1283; found: 287.1279.

ethyl 7-(3-chlorophenyl)-5-methoxyhepta-2,3-dien-6-ynoate (1f'):



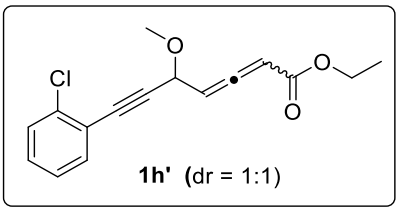
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.40 (m, 1H), 7.30-7.28 (m, 2H), 7.23-7.20 (m, 1H), 5.84-5.74 (m, 2H), 4.92 (dd, *J* = 6.0, 2.3 Hz, 1H), 4.19 (q, *J* = 7.0 Hz, 2H), 3.45 (s, 3H), 1.26 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.7, 212.5, 165.0, 164.9, 134.2, 131.7, 129.9, 129.5, 129.0, 123.8, 95.1, 94.9, 91.2, 90.8, 86.3, 86.0, 85.9, 68.7, 68.1, 61.2, 55.8, 55.2, 14.2; ESI-MS calcd. for $C_{16}H_{16}{}^{35}ClO_3$[M+H]: 291.0788; found: 291.0786.

ethyl 5-methoxy-7-(2-methoxyphenyl)hepta-2,3-dien-6-ynoate (1g'):



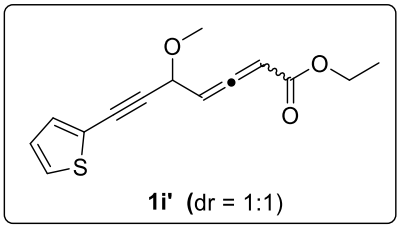
Yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 (d, *J* = 7.5 Hz, 1H), 7.28 (t, *J* = 7.9 Hz, 1H), 6.89-6.84 (m, 2H), 5.81-5.78 (m, 2H), 5.06-4.93 (m, 1H), 4.18 (q, *J* = 7.0 Hz, 2H), 3.84 (s, 3H), 3.47 (s, 3H), 1.24 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.7, 212.6, 165.2, 165.0, 160.2, 133.8, 130.2, 120.3, 111.3,110.6, 95.3, 95.2, 91.0, 90.6, 89.0, 88.6, 83.8, 83.5, 69.0, 68.3, 61.1, 55.7, 55.6, 54.9, 14.2; ESI-MS calcd. for $C_{17}H_{19}O_4$[M+H]: 287.1283; found: 287.1257.

ethyl 7-(2-chlorophenyl)-5-methoxyhepta-2,3-dien-6-ynoate (1h'):



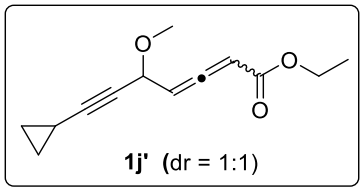
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.38-7.36 (m, 1H), 7.27-7.17 (m, 2H), 5.84-5.78 (m, 2H), 5.03 (dd, *J* = 5.9, 2.4 Hz, 1H), 4.18 (q, *J* = 7.0 Hz, 2H), 3.49 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.6, 165.1, 165.0, 136.1, 133.6, 129.7, 129.3, 126.4, 122.1, 95.0, 91.3, 91.0, 90.1, 89.8, 84.0, 83.9, 68.7, 68.1, 61.1, 55.6, 54.9, 14.2; ESI-MS calcd. for $C_{16}H_{16}{}^{35}ClO_3$[M+H]: 291.0788; found: 291.0792.

ethyl 5-methoxy-7-(thiophen-2-yl)hepta-2,3-dien-6-ynoate (1i'):



Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.20 (m, 2H), 6.96-6.94 (m, 1H), 5.83-5.74 (m, 2H), 4.93 (dd, *J* = 6.2, 2.3 Hz, 1H), 4.22-4.16 (m, 2H), 3.45 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.6, 212.4, 165.0, 132.7, 127.7, 126.9, 121.9, 95.0, 94.9, 91.1, 90.8, 88.9, 88.7, 80.6, 68.9, 68.3, 61.1, 55.7, 55.2, 14.2; ESI-MS calcd. for $C_{14}H_{14}NaO_3S$[M+Na]: 285.0561; found: 285.0549.

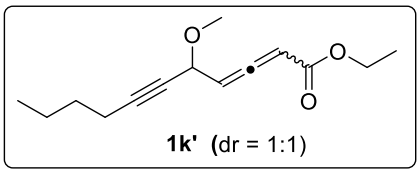
ethyl 7-cyclopropyl-5-methoxyhepta-2,3-dien-6-ynoate (1j'):



Yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$): 5.74-5.60 (m, 2H), 4.68-4.56 (m, 1H), 4.19-4.14 (m, 2H), 3.34 (s, 3H), 1.26-1.22 (m, 4H), 0.75-0.73 (m, 2H), 0.66-0.64 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 212.4, 212.2, 165.0, 164.9, 95.6, 95.3, 91.4, 91.2, 90.6, 90.2, 71.3, 71.0, 68.5, 67.8, 60.9, 60.8, 55.3, 54.7, 47.9, 33.8, 27.2, 22.6, 21.1,

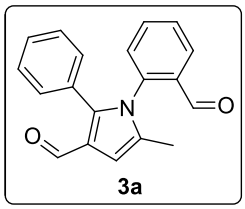
14.1, 10.7, 8.3, 8.2, -0.7; ESI-MS calcd. for $C_{13}H_{16}NaO_3$[M+Na]: 243.0992; found: 243.0999.

ethyl 5-methoxyundeca-2,3-dien-6-ynoate (1k'):



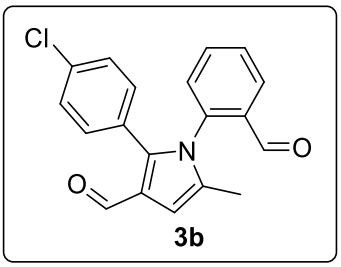
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): 5.74-5.61 (m, 2H), 4.73-4.60 (m, 1H), 4.19-4.12 (m, 2H), 3.34 (s, 3H), 2.19 (t, *J* = 6.8 Hz, 2H), 1.48-1.41 (m, 2H), 1.39-1.32 (m, 2H), 1.23 (t, *J* = 7.1 Hz, 3H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 212.4, 212.3, 165.1, 165.0, 95.6, 95.5, 90.8, 90.3, 88.3, 88.1, 76.1, 75.7, 68.5, 67.8, 60.9, 55.3, 54.7, 30.4, 21.8, 18.3, 14.1, 13.5; ESI-MS calcd. for $C_{14}H_{21}O_3$[M+H]: 237.1491; found: 237.1498.

1-(2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3a):



Yellow solid; mp: 184.1-185.9 ºC; 1H NMR (600 MHz, $CDCl_3$): δ 9.63 (s, 1H), 9.51 (s, 1H), 7.86 (dd, *J*= 7.8, 1.3 Hz, 1H), 7.65 (td, *J*= 7.7, 1.5 Hz, 1H), 7.50 (t, *J*=7.6 Hz, 1H), 7.31 (d, *J*=7.9 Hz, 1H), 7.23-7.18 (m, 3H), 7.09-7.08 (m, 2H), 6.65 (s, 1H), 2.05 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 188.5, 186.8, 144.5, 139.4, 134.7, 133.1, 132.9, 130.8, 130.0, 129.6, 128.9, 128.7, 128.3, 123.9, 106.1, 12.9 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{19}H_{15}NNaO_2$[M+Na]: 312.1000; found: 312.0992.

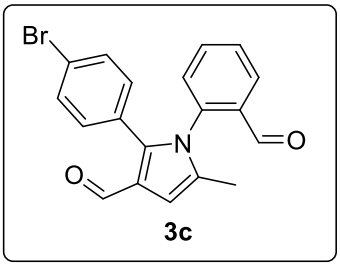
2-(4-chlorophenyl)-1-(2-formylphenyl)-5-methyl-1H-pyrrole-3-carbaldehyde (3b):



3b

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.60 (s, 1H), 9.49 (s, 1H), 7.87 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.66 (td, *J* = 7.7, 1.7 Hz, 1H), 7.55-7.50 (m, 1H), 7.30 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.18-7.15 (m, 2H), 7.03-7.00 (m, 2H), 6.63 (s, 1H), 2.02 (d, *J* = 1.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3, 186.2, 142.6, 138.9, 135.0, 134.8, 133.3, 132.8, 131.9, 130.0, 129.7, 129.3, 128.6, 127.4, 124.0, 106.3, 12.8; ESI-MS calcd. for $C_{19}H_{15}{}^{35}ClNO_2$[M+H]: 324.0791; found: 324.0781.

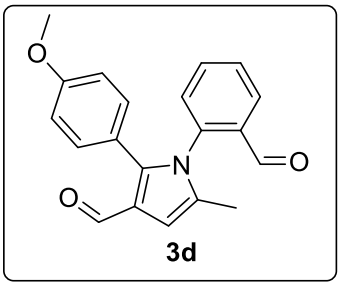
2-(4-bromophenyl)-1-(2-formylphenyl)-5-methyl-1H-pyrrole-3-carbaldehyde (3c):



3c

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.50 (s, 1H), 7.89 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.68-7.65 (m, 1H), 7.56-7.52 (m, 1H), 7.35-7.32 (m, 2H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.00-6.94 (m, 2H), 6.64 (s, 1H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3, 186.2, 142.7, 138.9, 134.8, 133.4, 132.9, 132.1, 131.6, 130.0, 129.8, 129.4, 127.9, 124.1, 123.3, 106.5, 12.8; ESI-MS calcd. for $C_{19}H_{15}{}^{79}BrNO_2$[M+H]: 368.0286; found: 368.0279.

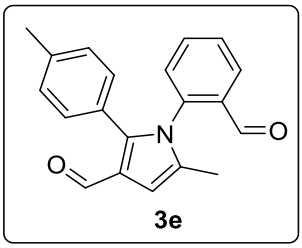
1-(2-formylphenyl)-2-(4-methoxyphenyl)-5-methyl-1H-pyrrole-3-carbaldehyde (3d):



3d

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.60 (s, 1H), 9.47 (s, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.65 (td, *J* = 7.6, 1.5 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.9Hz, 1H), 7.01-6.97 (m, 2H), 6.72-6.68 (m, 2H), 6.61 (s, 1H), 3.70 (d, *J* = 0.9 Hz, 3H), 2.03 (d, *J* = 0.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.5, 186.7, 159.8, 144.6, 139.5, 134.6, 132.9, 132.8, 132.0, 130.0, 129.5, 128.8, 123.6, 120.9, 113.8, 105.9, 55.1, 12.8; ESI-MS calcd. for $C_{20}H_{18}NO_3$[M+H]: 320.1287; found: 320.1280.

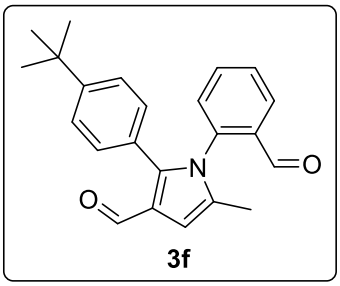
1-(2-formylphenyl)-5-methyl-2-(p-tolyl)-1H-pyrrole-3-carbaldehyde (3e):



3e

Yellow solid; mp: 180.8-183.3 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (s, 1H), 9.49 (d, *J* = 0.6 Hz, 1H), 7.86 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.65 (td, *J* = 7.7, 1.7 Hz, 1H), 7.52-7.48 (m, 1H), 7.31 (dd, *J* = 7.8 ,1.0 Hz, 1H), 7.00-6.95 (m, 4H), 6.63 (s, 1H), 2.24 (s, 3H), 2.04 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.5, 186.8, 144.8, 139.6, 138.8, 134.6, 132.9, 130.6, 130.0, 129.5, 129.1, 128.7, 125.8, 123.7, 106.0, 21.2, 12.8 (one C-H carbon is merged with others); ESI-MS calcd. for $C_{20}H_{18}NO_2$[M+H]: 304.1338; found: 304.1336.

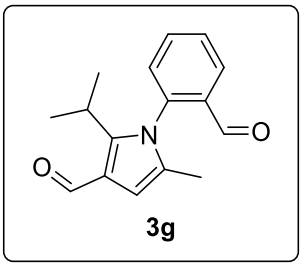
2-(4-(tert-butyl)phenyl)-1-(2-formylphenyl)-5-methyl-1H-pyrrole-3-carbaldehyde (3f):



3f

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.49 (d, *J* = 0.6 Hz, 1H), 7.87 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.65 (td, *J* = 7.6 , 1.6 Hz, 1H), 7.52-7.50 (m, 1H), 7.31 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.21-7.18 (m, 2H), 7.01-7.00 (m, 2H), 6.63 (d, *J* = 0.7 Hz, 1H), 2.02 (d, *J* = 1.0 Hz, 3H), 1.21 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.5, 186.9, 151.8, 144.8, 139.6, 134.6, 133.0, 132.9, 130.4, 130.0, 129.5, 128.7, 125.7, 125.2, 123.8, 106.0, 34.6, 31.0, 12.8; ESI-MS calcd. for $C_{23}H_{24}NO_2$[M+H]: 346.1807; found: 346.1803.

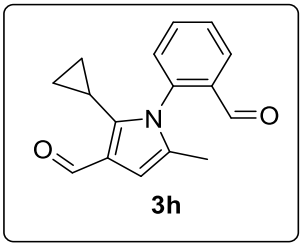
1-(2-formylphenyl)-2-isopropyl-5-methyl-1H-pyrrole-3-carbaldehyde (3g):



3g

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.08 (s, 1H), 9.44 (s, 1H), 8.07 (dd, *J* = 3.9, 1.6 Hz, 1H), 7.77 (td, *J* = 7.7, 1.6 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 6.48 (s, 1H), 2.81-2.74 (m, 1H), 1.86 (s, 3H), 1.25 (q, *J* = 3.7 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7, 185.3, 149.0, 140.0, 135.1, 133.5, 130.8, 130.1, 129.6, 128.8, 122.0, 107.6, 27.4, 23.4, 23.3, 12.6; ESI-MS calcd. for $C_{16}H_{18}NO_2$[M+H]: 256.1338; found: 256.1334.

2-cyclopropyl-1-(2-formylphenyl)-5-methyl-1H-pyrrole-3-carbaldehyde (3h):

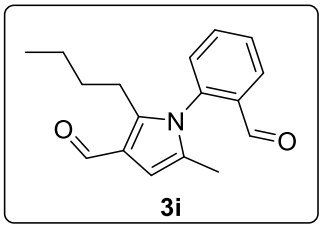


3h

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.09 (s, 1H), 9.52 (d, *J* = 0.7 Hz, 1H),

8.06 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.76 (td, *J* = 7.6, 1.6 Hz, 1H), 7.66-7.62 (m, 1H), 7.33 (dd, *J* = 7.8, 1.0 Hz, 1H), 6.43 (d, *J* = 1.0 Hz, 1H), 1.93 (d, *J* = 0.9 Hz, 3H), 1.58-1.51 (m, 1H), 0.75-0.70 (m, 1H), 0.68-0.62 (m, 1H), 0.58-0.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.0, 185.6, 144.2, 140.3, 135.0, 133.2, 131.6, 129.7, 129.5, 128.8, 123.7, 105.6, 12.6, 7.2, 6.8, 6.7; ESI-MS calcd. for $C_{16}H_{16}NO_2$[M+H]: 254.1181; found: 254.1186.

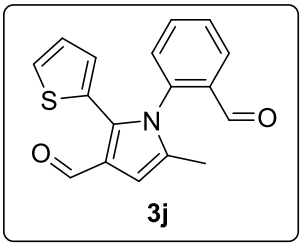
2-butyl-1-(2-formylphenyl)-5-methyl-1H-pyrrole-3-carbaldehyde (3i):



3i

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.88 (s, 1H), 9.43 (s, 1H), 8.08 (dd, *J* = 7.8 , 1.2 Hz, 1H), 7.78 (td, *J* = 7.7, 1.7 Hz, 1H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.33 (dd, *J* = 7.8, 0.6 Hz, 1H), 6.44 (s, 1H), 2.76-2.68 (m, 1H), 2.56-2.49 (m, 1H), 1.91 (s, 3H), 1.31-1.23 (m, 2H), 1.19-1.12 (m, 2H), 0.70 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8, 185.3, 144.1, 139.3, 135.1, 133.3, 131.6, 130.0, 129.6, 128.8, 122.3, 106.6, 32.7, 24.7, 22.2, 13.5, 12.6; ESI-MS calcd. for $C_{17}H_{20}NO_2$[M+H]: 270.1494; found: 270.1491.

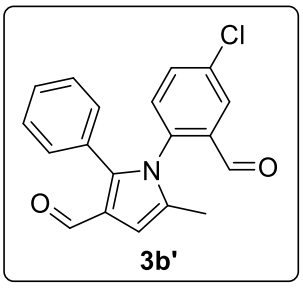
1-(2-formylphenyl)-5-methyl-2-(thiophen-2-yl)-1H-pyrrole-3-carbaldehyde (3j):



3j

Brown solid; mp: 141.8-144.8º C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.79 (s, 1H), 9.52 (s, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.71-7.67 (m, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 1H), 7.26-7.24 (m, 1H), 6.91-6.87 (m, 2H), 6.64 (s, 1H), 2.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3, 186.4, 139.2, 136.7, 134.8, 133.9, 133.4, 130.6, 130.1, 130.0, 129.2, 128.9, 128.7, 127.1, 124.9, 106.5, 12.9; ESI-MS calcd. for $C_{17}H_{13}NNaO_2S$ [M+Na]: 318.0565; found: 318.0560.

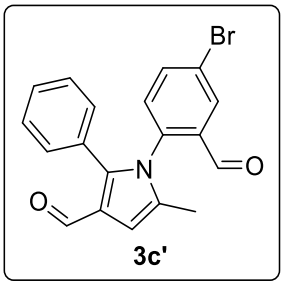
1-(4-chloro-2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3b'):



3b'

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.43 (s, 1H), 7.81 (d, *J* = 2.5 Hz, 1H), 7.60 (dd, *J* = 8.4, 2.5 Hz, 1H), 7.28-7.21 (m, 4H), 7.09-7.06 (m, 2H), 6.65 (d, *J* = 0.8 Hz, 1H), 2.05 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.1, 186.6, 144.5, 137.8, 136.0, 134.6, 133.9, 133.1, 131.3, 130.8, 129.0, 128.7, 128.6, 124.1, 106.4, 12.9 (one C-H carbon is merged with others); ESI-MS calcd. for $C_{19}H_{15}{}^{35}ClNO_2$[M+H]: 324.0791; found: 324.0780.

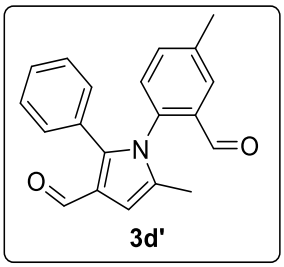
1-(4-bromo-2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3c'):



3c'

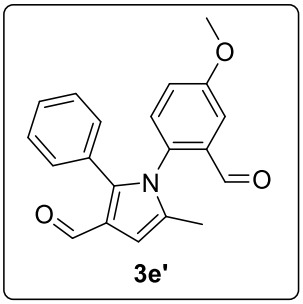
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.43 (s, 1H), 7.97 (d, *J* = 2.3 Hz, 1H), 7.75 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.28-7.22 (m, 3H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.09-7.06 (m, 2H), 6.65 (s, 1H), 2.05 (d, *J* = 1.1Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.0, 186.6, 144.4, 138.2, 137.5, 134.0, 133.0, 131.7, 131.5, 130.8, 129.0, 128.6, 128.5, 124.1, 123.8, 106.4, 12.9; ESI-MS calcd. for $C_{19}H_{14}{}^{79}BrNNaO_2$[M+Na]: 390.0106; found: 390.0094.

1-(2-formyl-4-methylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3d'):



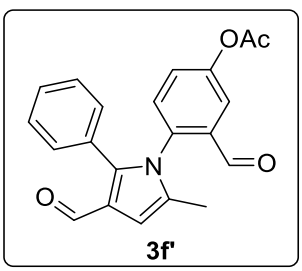
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.48 (d, *J* = 0.6 Hz, 1H), 7.65 (s, 1H), 7.45-7.42 (m, 1H), 7.24-7.18 (m, 4H), 7.10-7.08 (m, 2H), 6.64 (s, 1H), 2.40 (s, 3H), 2.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7, 186.7, 144.6, 139.9, 136.9, 135.4, 133.2, 132.5, 130.8, 129.8, 129.1, 129.0, 128.6, 128.3, 123.8, 105.9, 21.1, 12.8; ESI-MS calcd. for $C_{20}H_{18}NO_2$[M+H]: 304.1338; found: 304.1346.

1-(2-formyl-4-methoxyphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3e'):



Yellow solid; mp: 139.3-140.9ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.43 (s, 1H), 7.30 (d, *J* = 3.0 Hz, 1H), 7.24-7.19 (m, 4H), 7.16-7.13 (m, 1H), 7.10-7.08 (m, 2H), 6.63 (d, *J* = 0.7 Hz, 1H), 3.83 (s, 3H), 2.04 (d, *J* = 0.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.4, 186.7, 159.9, 144.8, 133.7, 133.5, 132.4, 131.1, 130.8, 129.0, 128.7, 128.4, 123.8, 121.7, 111.2, 105.9, 55.8, 12.8; ESI-MS calcd. for $C_{20}H_{18}NO_3$[M+H]: 320.1287; found: 320.1279.

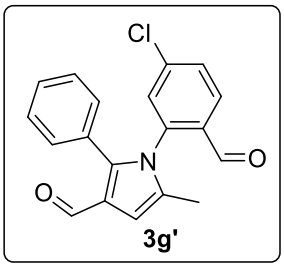
3-formyl-4-(3-formyl-5-methyl-2-phenyl-1H-pyrrol-1-yl)phenyl acetate (3f'):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.63 (s, 1H), 9.45 (s, 1H), 7.58 (d, *J* = 2.7

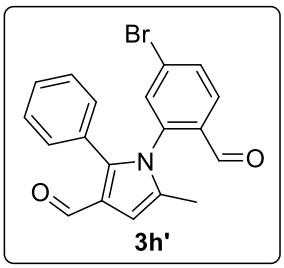
Hz, 1H), 7.41 (dd, *J* = 8.5, 2.7 Hz, 1H), 7.33 (d, *J* = 8.5 Hz, 1H), 7.25-7.20 (m, 3H), 7.09-7.07 (m, 2H), 6.65 (s, 1H), 2.30 (s, 3H), 2.07 (d, *J* = 1.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.4, 186.7, 168.5, 151.1, 144.6, 136.6, 133.9, 133.2, 131.1, 130.8, 128.9, 128.7, 128.5, 127.8, 124.0, 121.5, 106.3, 21.0, 12.9; ESI-MS calcd. for $C_{21}H_{17}NNaO_4$[M+Na]: 370.1055; found: 370.1047.

1-(5-chloro-2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3g'):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.42 (d, *J* = 0.7Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.49-7.46 (m, 1H), 7.35 (d, *J* = 2.0 Hz, 1H), 7.28-7.22 (m, 3H), 7.11-7.08 (m, 2H), 6.65 (d, *J* = 0.8 Hz, 1H), 2.08 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.2, 186.6, 144.4, 140.9, 140.4, 133.0, 131.4, 130.7, 130.1, 129.9, 129.0, 128.6, 128.5, 124.1, 106.5, 12.9 (one C-H carbon is merged with others); ESI-MS calcd. for $C_{19}H_{15}{}^{35}ClNO_2$[M+H]: 324.0791; found: 324.0761.

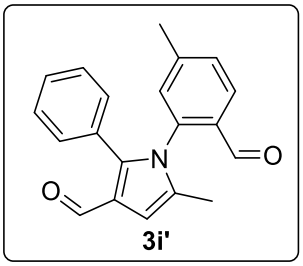
1-(5-bromo-2-formylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3h'):



Yellow solid;mp: 165.2-167.1ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.63 (s, 1H), 9.43 (s, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.65-7.63 (m, 1H), 7.52 (d, *J* = 1.8Hz, 1H), 7.28-7.23 (m, 3H), 7.09 (dd, *J* = 7.6, 1.5 Hz, 2H), 6.65 (s, 1H), 2.08 (d, *J* = 1.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.4, 186.6, 144.4, 140.3, 133.1, 133.0, 131.8, 130.8, 129.9, 129.2, 129.0, 128.6, 128.5, 124.1, 106.5, 12.9 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{19}H_{14}{}^{79}BrNNaO_2$[M+Na]: 390.0106; found:

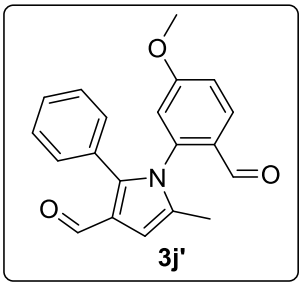
390.0099.

1-(2-formyl-5-methylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3i'):



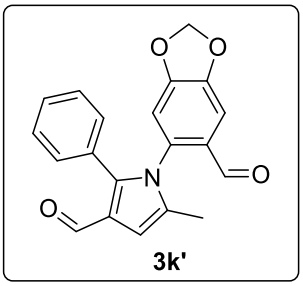
Yellow solid; mp: 161.3-163.7 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 9.45 (d, *J* = 0.6 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.30-7.28 (m, 1H), 7.24-7.18 (m, 3H), 7.10-7.08 (m, 3H), 6.63 (d, *J* = 1.1 Hz, 1H), 2.42 (s, 3H), 2.04 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.3, 186.8, 146.2, 144.5, 139.4, 133.1, 130.7, 130.6, 130.4, 130.3, 128.9, 128.8, 128.7, 128.3, 123.8, 106.0, 21.7, 12.9; ESI-MS calcd. for $C_{20}H_{18}NO_2$[M+H]: 304.1338; found: 304.1338.

1-(2-formyl-5-methoxyphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3j'):



Yellow solid; mp: 164.3-166.1 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (s, 1H), 9.38 (d, *J* = 0.6 Hz, 1H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.27-7.20 (m, 3H), 7.14-7.11 (m, 2H), 6.99-6.96 (m, 1H), 6.74 (d, *J* = 2.5 Hz, 1H), 6.63 (s, 1H), 3.83 (s, 3H), 2.06 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.3, 186.7, 164.4, 144.4, 141.3, 133.0, 130.8, 128.9, 128.7, 128.3, 126.4, 123.8, 115.4, 115.0, 106.0, 56.0, 12.8 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{20}H_{18}NO_3$[M+H]: 320.1287; found: 320.1274.

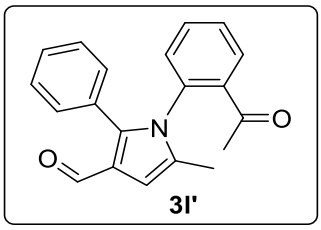
1-(6-formylbenzo[d][1,3]dioxol-5-yl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3k'):



3k'

Yellow solid; mp: 187.6-188.4 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (s, 1H), 9.25 (d, *J* = 0.5 Hz, 1H), 7.28-7.24 (m, 4H), 7.15-7.12 (m, 2H), 6.7 (d, *J* = 0.5 Hz, 1H), 6.62 (s, 1H), 6.11 (s, 2H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.9, 186.7, 152.9, 148.8, 144.7, 136.3, 133.4, 130.7, 128.9, 128.8, 128.5, 128.3, 123.9, 109.7, 106.4, 106.0, 103.0, 12.8; ESI-MS calcd. for $C_{20}H_{16}NO_4$[M+H]: 334.1079; found: 334.1076.

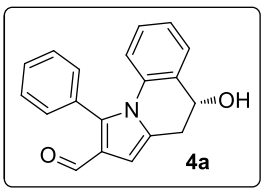
1-(2-acetylphenyl)-5-methyl-2-phenyl-1H-pyrrole-3-carbaldehyde (3l'):



3l'

Yellow solid; mp: 133.5-134.9 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (s, 1H), 7.60-7.53 (m, 2H), 7.43 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.29 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.23-7.17 (m, 3H), 7.06-7.03 (m, 2H), 6.64 (d, *J* = 0.9 Hz, 1H), 2.07 (d, *J* = 0.8 Hz, 3H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.2, 186.8, 143.3, 137.8, 135.3, 132.3, 130.8, 130.3, 129.6, 129.1, 128.9, 128.5, 128.2, 124.0, 106.1, 28.2, 12.9 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{20}H_{18}NO_2$: 304.1338[M+H]; found: 304.1331.

(R)-5-hydroxy-1-phenyl-4,5-dihydropyrrolo[1,2-a]quinoline-2-carbaldehyde (4a):

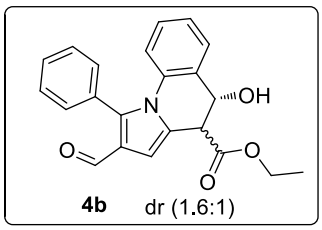


4a

White semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.55 (s, 1H), 7.53-7.51 (m, 1H), 7.47-7.41 (m, 3H), 7.39-7.37 (m, 2H), 7.14 (dt, *J* = 7.5, 0.9Hz, 1H), 6.98 (dt,*J* = 7.8 ,

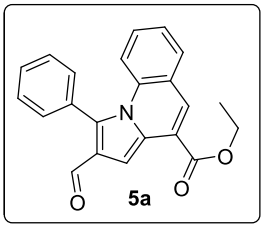
1.5 Hz, 1H), 6.65 (s, 1H), 6.57 (d, *J* = 8.2 Hz, 1H), 4.98 (s, 1H), 3.18-3.01 (m, 2H), 2.25 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 186.8, 134.1, 132.6, 130.6, 130.3, 129.3, 129.2, 128.8, 128.2, 126.9, 125.7, 120.7, 105.5, 66.6, 32.4 (two quarternary carbons are merged with others); ESI-MS calcd. for $C_{19}H_{15}NNaO_2$[M+Na].: 312.0995; found: 312.1000.

(5R)-ethyl 2-formyl-5-hydroxy-1-phenyl-4,5-dihydropyrrolo[1,2-a]quinoline-4-carboxylate (4b):



White semi-solid; ^{1}H NMR (600 MHz, $CDCl_3$)(*major isomer*): δ 9.59 (s, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.48-7.40 (m, 5H), 7.19-7.14 (m, 1H), 7.00-6.96 (m, 1H), 6.80 (s, 1H), 6.55-6.53 (m, 1H), 5.16-5.15(m, 1H), 4.19-4.15 (m, 2H), 4.09 (d, *J* = 3.3 Hz, 1H), 3.86 (d, *J* = 1.3Hz, 1H), 1.16 (t, *J* = 7.1Hz, 3H);^{1}H NMR (600 MHz, $CDCl_3$)(*minor isomer, major peaks*): δ 9.58 (s, 1H), 7.67 (d, *J* = 7.6Hz, 1H), 6.72 (d, *J* = 1.4 Hz, 1H), 5.26 (d, *J* = 7.7 Hz, 1H), 4.35-4.32 (m, 2H), 3.85-3.84 (m, 1H), 1.34 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) (*major isomer*): δ 186.7, 170.8, 140.3, 133.9, 130.7, 129.8, 129,3, 128.8, 127.2, 125.9, 125.1, 120.7, 106.9, 67.8, 62.0, 45.9, 14.0;^{13}C NMR (150 MHz, $CDCl_3$) (*minor isomer, major peaks*): δ 186.6, 170.2, 140.5, 133.3, 130.6, 129.4, 128.9, 126.1, 125.9, 105.7, 67.6, 62.1, 49.1, 14.2; ESI-MS calcd. for $C_{22}H_{20}NO_4$ [M+H]: 362.1392; found: 362.1367.

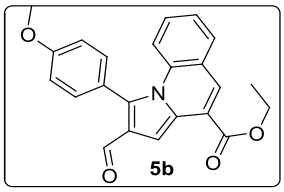
ethyl 2-formyl-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate (5a):



Yellow solid; mp: 139.7-141.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.67 (s, 1H), 7.93 (s, 1H), 7.74 (s, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.60-7.49 (m, 5H), 7.30-7.26 (m, 1H), 7.16-7.15 (m, 2H), 4.47 (q, *J* = 7.1 Hz, 2H), 1.47 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.9, 164.8, 137.1, 135.4, 131.6, 130.8, 130.6, 129.6, 129.1, 128.0, 127.4, 125.0, 124.4, 121.7, 117.9, 103.3, 61.5, 14.4 (one C-H carbon and one

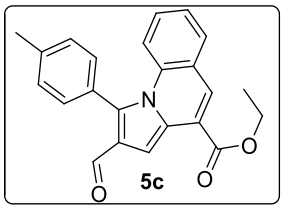
quarternary carbon are merged with others); ESI-MS calcd. for $C_{22}H_{17}NNaO_3$[M+Na]: 366.1106; found: 366.1083.

ethyl 2-formyl-1-(4-methoxyphenyl)pyrrolo[1,2-a]quinoline-4-carboxylate (5b):



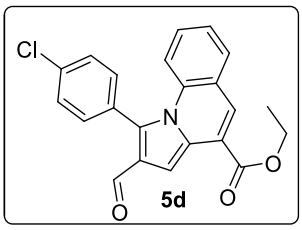
Yellow solid; mp: 175.7-176.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.67 (s, 1H), 7.90 (s, 1H), 7.72 (s, 1H), 7.68 (d, *J* = 7.7 Hz, 1H), 7.41-7.39 (m, 2H), 7.30-7.26 (m, 2H), 7.20-7.15 (m, 1H), 7.08-7.05 (m, 2H), 4.47 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.0, 164.8, 160.6, 137.3, 135.6, 132.1, 130.6, 129.6, 129.5, 127.9, 127.5, 124.9, 124.5, 123.5, 121.7, 117.9, 114.6 103.2, 61.5, 55.4, 14.4; ESI-MS calcd. for $C_{23}H_{20}NO_4$[M+H]: 374.1392; found: 374.1400.

ethyl 2-formyl-1-(p-tolyl)pyrrolo[1,2-a]quinoline-4-carboxylate (5c):



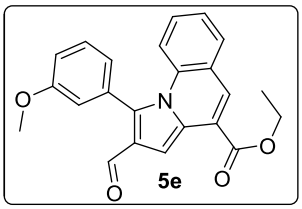
Yellow solid; mp: 113.4-115.6 ℃; ^{1}H NMR (400 MHz, CD_2Cl_2): δ 9.66 (s, 1H), 7.95 (s, 1H), 7.73 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.68 (s, 1H), 7.42-7.38 (m, 4H), 7.34-7.20 (m, 3H), 4.47 (q, *J* = 7.1 Hz, 2H), 2.51 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.0, 164.8, 139.7, 137.5, 135.5, 130.7, 130.5, 129.8, 129.6, 129.5, 128.5, 127.9, 127.4, 124.9, 124.4, 121.7, 118.0, 103.2, 61.5, 21.5, 14.4; ESI-MS calcd. for $C_{23}H_{20}NO_3$[M+H]: 358.1443; found: 358.1438.

ethyl 1-(4-chlorophenyl)-2-formylpyrrolo[1,2-a]quinoline-4-carboxylate (5d):



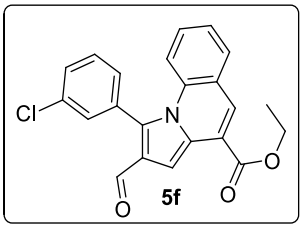
Yellow solid; mp: 145.3-147.1℃;^{1}H NMR (400 MHz, $(CD_3)_2CO$): δ 9.69 (s, 1H), 8.05 (s, 1H), 7.94 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.70-7.69 (m, 5H), 7.45-7.34 (m, 2H), 7.28-7.26 (m, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 1.45 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150 MHz, $(CD_3)_2CO$): δ 187.0, 164.8, 136.1, 135.9, 135.8, 133.4, 131.8, 131.3, 130.8, 130.4, 130.1, 128.6, 128.3, 126.1, 125.2, 121.9, 118.5, 103.8, 61.9, 14.5; ESI-MS calcd. for $C_{22}H_{17}{}^{35}ClNO_3$[M+H]: 378.0897; found: 378.0896.

ethyl 2-formyl-1-(3-methoxyphenyl)pyrrolo[1,2-a]quinoline-4-carboxylate (5e):



Yellow solid; mp: 148.7-149.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.70 (s, 1H), 7.93 (s, 1H), 7.74 (s, 1H), 7.70 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.31-7.27 (m, 1H), 7.23-7.19 (m, 2H), 7.12-7.07 (m, 2H), 7.02-7.01 (m, 1H), 4.48 (q, *J* = 7.0 Hz, 2H), 3.82 (s, 3H), 1.47 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.9, 164.8, 160.0, 136.9, 135.4, 132.8, 130.6, 130.2, 129.7, 129.5, 128.0, 127.3, 125.0, 124.4, 123.2, 121.7, 118.0, 116.1, 115.5, 103.2, 61.5, 55.4, 14.4; ESI-MS calcd. for $C_{23}H_{20}NO_4$[M+H]: 374.1392; found: 374.1392.

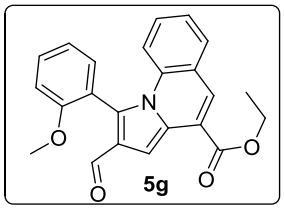
ethyl 1-(3-chlorophenyl)-2-formylpyrrolo[1,2-a]quinoline-4-carboxylate (5f):



Yellow solid; mp: 146.2-148.4 ℃; ^{1}H NMR (600 MHz,$CDCl_3$): δ 9.70 (s, 1H), 7.95 (s, 1H), 7.7 (s, 1H), 7.71 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.57-7.55 (m, 1H), 7.52-7.48 (m, 2H), 7.41-7.39 (m, 1H), 7.32 (td, *J* = 8.4, 1.2 Hz, 1H), 7.24-7.21 (m, 1H), 7.17 (d, *J* = 8.4

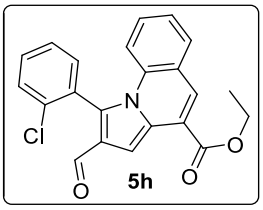
Hz, 1H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.4, 164.7, 135.2, 134.8, 133.5, 130.8, 130.7, 130.4, 129.9, 129.0, 128.2, 127.6, 125.2, 124.5, 121.7, 117.8, 103.8, 61.6, 14.4(two C-H carbons and one quarternary carbon are merged with others); ESI-MS calcd. for $C_{22}H_{17}{}^{35}ClNO_3$[M+H]: 378.0897; found: 378.0899.

ethyl 2-formyl-1-(2-methoxyphenyl)pyrrolo[1,2-a]quinoline-4-carboxylate (5g):



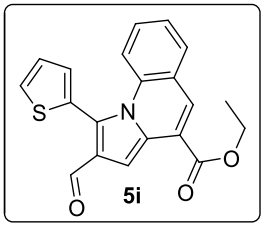
Yellow solid; mp: 185.1-187.4 ℃;^{1}H NMR (400 MHz, $CDCl_3$): δ 9.65 (s, 1H), 7.93 (s, 1H), 7.76 (s, 1H), 7.68 (dd, *J* = 7.8, 1.5Hz, 1H), 7.59-7.54 (m, 1H), 7.42 (dd, *J*= 7.4, 1.8 Hz, 1H), 7.32-7.26 (m, 2H), 7.20-7.12 (m, 2H), 7.03 (d, *J*= 8.4 Hz, 1H), 4.47 (q, *J* = 7.1 Hz, 2H), 3.57 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.1, 164.9, 158.3, 136.1, 134.1, 132.7, 131.6, 130.3, 129.7, 129.6, 127.9, 127.0, 124.8, 124.1, 121.7, 120.9, 120.5, 116.8, 111.2, 103.2, 61.5, 55.4, 14.4; ESI-MS calcd. for $C_{23}H_{20}NO_4$[M+H]: 374.1392; found: 374.1396.

ethyl 1-(2-chlorophenyl)-2-formylpyrrolo[1,2-a]quinoline-4-carboxylate (5h):



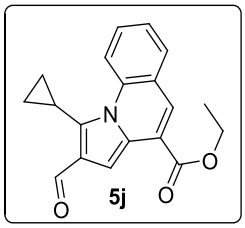
Yellow solid; mp: 150.2-152.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.64 (s, 1H), 7.97 (s, 1H), 7.80 (s, 1H), 7.73-7.72 (m, 1H), 7.61-7.46 (m, 4H), 7.34-7.19 (m, 2H), 7.11 (d, *J* = 8.6 Hz, 1H), 4.48 (q, *J* = 7.0 Hz, 2H), 1.48 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz,$CDCl_3$): δ 187.2, 164.8, 135.9, 135.6, 133.1, 131.4, 131.3, 130.7, 130.3, 129.9, 128.1, 127.4, 127.2, 125.2, 124.2, 121.6, 116.4, 103.7, 61.6, 14.4 (one C-H carbon and one quarternary carbon are merged with others); ESI-MS calcd. for $C_{22}H_{17}{}^{35}ClNO_3$[M+H]: 378.0897; found: 378.0897.

ethyl 2-formyl-1-(thiophen-2-yl)pyrrolo[1,2-a]quinoline-4-carboxylate (5i):



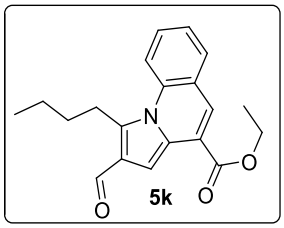
Yellow solid; mp: 143.2-145.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.79 (s, 1H), 7.97 (s, 1H), 7.76 (s, 1H), 7.72-7.71 (m, 1H), 7.66 (dt, *J* = 5.0, 0.9 Hz, 1H), 7.35-7.24 (m, 5H), 4.48 (q, *J* = 7.0 Hz, 2H), 1.47 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.6, 164.7, 135.5, 131.6, 130.7, 130.5, 130.1, 129.7, 129.3, 128.5, 128.2, 127.8, 125.2, 124.4, 121.5, 117.6, 103.5, 61.6, 14.4 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{20}H_{16}NO_3S$[M+H]: 350.0851; found: 350.0847.

ethyl 1-cyclopropyl-2-formylpyrrolo[1,2-a]quinoline-4-carboxylate (5j):



Yellow solid; mp: 142.2-144.8 ℃; ^{1}H NMR (600 MHz,$CDCl_3$): δ 10.49 (s, 1H), 8.86 (d, *J* = 8.6 Hz, 1H), 7.84 (s, 1H), 7.70 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.57-7.54 (m, 2H), 7.40 (td, *J* = 7.5, 0.8 Hz,1H), 4.43 (q, *J* = 7.1 Hz, 2H), 2.46-2.41 (m, 1H), 1.43 (t, *J* = 7.1 Hz, 3H), 1.38-1.35 (m, 2H), 0.85-0.83 (m, 2H); ^{13}C NMR (150 MHz,$CDCl_3$): δ 187.8, 164.8, 138.3, 135.9, 130.2, 129.3, 128.7, 127.4, 125.0, 124.7, 121.6, 118.6, 103.8, 61.4, 14.3, 10.8, 9.8 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{19}H_{18}NO_3$[M+H]: 308.1281; found: 308.1280.

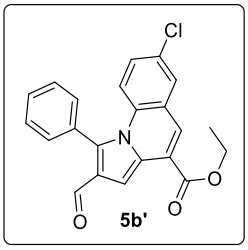
ethyl 1-butyl-2-formylpyrrolo[1,2-a]quinoline-4-carboxylate (5k):



Yellow solid; mp: 76.3-77.6 ℃; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.20 (s, 1H), 8.16 (d, *J* = 8.7Hz, 1H), 7.82 (s, 1H), 7.73 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.64 (s, 1H), 7.60-7.57 (m, 1H), 7.42-7.40 (m, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 3.67-3.64 (m, 2H), 1.83-1.78 (m,

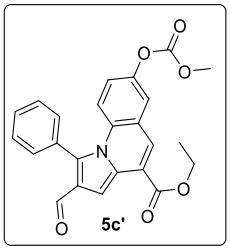
2H), 1.55-1.49 (m, 2H), 1.45 (t, *J* = 7.2 Hz, 3H), 0.99 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.7, 164.8, 137.3, 136.1, 130.8, 129.9, 129.1, 126.8, 125.4, 125.1, 124.9, 121.7, 117.2, 106.3, 61.4, 30.8, 27.2, 22.4, 14.4, 13.8; ESI-MS calcd. for $C_{20}H_{22}NO_3$[M+H]: 324.1600; found: 324.1598.

ethyl 7-chloro-2-formyl-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate(5b'):



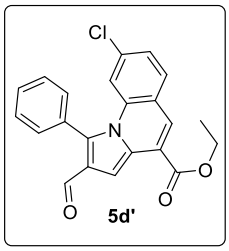
Yellow solid; mp: 169.2-170.1 ℃; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.67 (s, 1H), 7.82 (s, 1H), 7.76 (s, 1H), 7.66 (d, *J* = 2.2 Hz, 1H), 7.59-7.54 (m, 3H), 7.49-7.48 (m, 2H), 7.11-7.07 (m, 2H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.7, 164.4, 137.2, 133.8, 131.2, 130.7, 130.5, 129.9, 129.5, 129.4, 129.4, 129.3, 127.5, 126.5, 125.9, 123.0, 119.2, 104.0, 61.7, 14.4; ESI-MS calcd. for $C_{22}H_{17}{}^{35}ClNO_3$[M+H]: 378.0897; found: 378.0894

ethyl
2-formyl-7-((methoxycarbonyl)oxy)-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate(5c'):



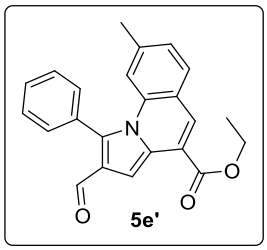
Yellow semi-solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.67 (s, 1H), 7.87 (s, 1H), 7.76 (s, 1H), 7.58-7.49 (m, 6H), 7.17 (d, *J* = 9.4 Hz, 1H), 6.98 (dd, *J* = 9.4, 2.7 Hz, 1H), 4.48 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.7, 164.5, 154.0, 147.5, 137.2, 133.2, 131.3, 130.8, 129.8, 129.4, 129.3, 127.4, 127.0, 125.6, 122.8, 122.5, 121.7, 119.1, 103.8, 61.7, 55.7, 14.4 (two C-H carbons are merged with others); ESI-MS calcd. for $C_{24}H_{20}NO_6$[M+H]: 418.1291; found: 418.1280

ethyl 8-chloro-2-formyl-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate(5d'):



Yellow solid; mp: 158.1-159.8 ℃; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.70 (s, 1H), 7.88 (s, 1H), 7.75 (s, 1H), 7.64-7.57 (m, 4H), 7.51-7.49 (m, 2H), 7.25 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.07 (d, *J* = 1.3Hz, 2H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.7, 164.6, 137.3, 135.9, 135.3, 131.4, 130.9, 130.7, 130.1, 129.6, 129.4, 127.6, 127.0, 125.4, 122.9, 121.9, 118.3, 103.7, 61.7, 14.4; ESI-MS calcd. for $C_{22}H_{17}{}^{35}ClNO_3$[M+H]: 378.0897; found: 378.0899

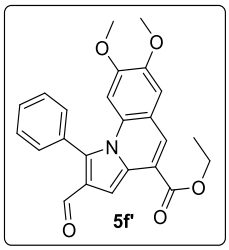
ethyl 2-formyl-8-methyl-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate(5e'):



Yellow semi-solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.70 (s, 1H), 7.90 (s, 1H), 7.72 (s, 1H), 7.57-7.53 (m, 4H), 7.50-7.48 (m, 2H), 7.10-7.09 (m, 1H), 6.88 (s, 1H), 4.47 (q, *J* = 7.1 Hz, 2H), 2.08 (s, 3H) 1.46 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.9, 164.9, 140.3, 137.0, 135.4, 131.8, 130.8, 130.3, 129.8, 129.3, 129.0, 128.1, 127.2, 126.1, 122.0, 120.7, 118.6, 103.0, 61.4, 22.0, 14.4; ESI-MS calcd. for $C_{23}H_{20}NO_3$[M+H]: 358.1443; found: 358.1443

ethyl

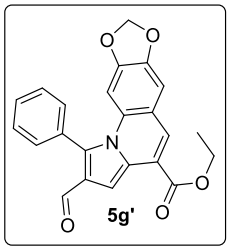
2-formyl-7,8-dimethoxy-1-phenylpyrrolo[1,2-a]quinoline-4-carboxylate(5f'):



Yellow solid; mp: 133.5-134.6 ℃; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.69 (s, 1H), 7.90 (s, 1H), 7.58-7.53 (m, 5H), 7.05 (s, 1H), 6.82 (s, 1H) 4.46 (q, *J* = 7.2 Hz, 2H), 3.90 (s, 3H), 3.26 (s, 3H), 1.46 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 187.8, 165.0, 150.6, 146.7, 135.2, 132.2, 131.7, 130.5, 129.6, 129.5, 129.0, 127.8, 127.2, 119.4, 117.7, 110.5, 102.4, 101.4, 61.3, 56.0, 55.1, 14.4; ESI-MS calcd. for $C_{24}H_{22}NO_5$[M+H]: 404.1498; found: 404.1498

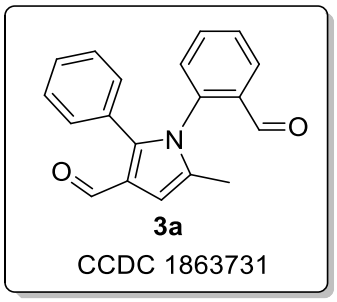
ethyl

2-formyl-1-phenyl-[1,3]dioxolo[4,5-g]pyrrolo[1,2-a]quinoline-4-carboxylate(5g'):



Yellow solid; mp: 235.1-236.2 ℃; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.66 (s, 1H), 7.82 (s, 1H), 7.69 (s, 1H), 7.57-7.53 (m, 3H), 7.48-7.46 (m, 2H), 7.03 (s, 1H), 6.59 (d, *J* = 0.4 Hz, 1H), 5.95 (s, 2H), 4.46 (q, *J* = 7.2 Hz, 2H), 1.46 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 188.0, 165.0, 149.4, 145.2, 135.8, 131.6, 131.5, 130.9, 129.7, 129.1, 127.9, 127.3, 119.5, 119.3, 107.8, 102.3, 102.1, 99.0, 61.4, 14.4 (one quarternary carbon is merged with others); ESI-MS calcd. for $C_{23}H_{18}NO_5$[M+H]: 388.1185; found: 388.1185

(5) X-ray crystallographic structure and data for compound 3a, 4a and **5a:**



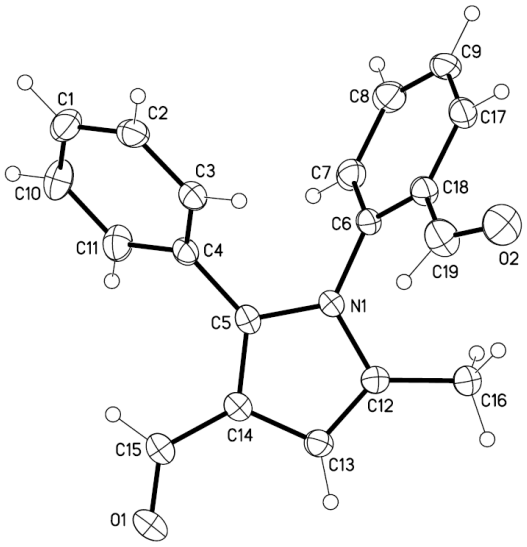


Table S1.Crystal data and structure refinement for 170932LT_0M.

Identification code	170932LT_0m	
Empirical formula	C19 H15 N O2	
Formula weight	289.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 8.3810(3) Å	α= 90°.
	b = 13.1650(5) Å	β= 97.823(2)°.
	c = 13.3041(5) Å	γ = 90°.
Volume	1454.26(9) Å ^{3}	
Z	4	
Density (calculated)	1.321 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	608	
Crystal size	0.15 x 0.12 x 0.02 mm^3	
Theta range for data collection	2.186 to 26.397°.	

Index ranges	-10<=h<=9, -13<=k<=16, -16<=l<=16
Reflections collected	13024
Independent reflections	2987 [R(int) = 0.0305]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8947
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2987 / 0 / 204
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.0957
R indices (all data)	R1 = 0.0507, wR2 = 0.1031
Extinction coefficient	n/a
Largest diff. peak and hole	0.251 and -0.249 e.Å $^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3)
for 170932LT_0M. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5624(1)	8226(1)	-64(1)	32(1)
N(1)	1212(1)	7546(1)	1513(1)	20(1)
C(1)	4077(2)	4133(1)	2328(1)	31(1)
C(2)	3920(2)	4892(1)	3025(1)	26(1)
C(3)	3423(2)	5855(1)	2695(1)	23(1)
C(4)	3095(2)	6067(1)	1661(1)	20(1)
C(5)	2603(2)	7095(1)	1302(1)	19(1)
C(6)	31(2)	7081(1)	2052(1)	20(1)
C(7)	-930(2)	6307(1)	1595(1)	25(1)
C(8)	-2107(2)	5885(1)	2101(1)	29(1)
C(9)	-2341(2)	6238(1)	3050(1)	28(1)
C(10)	3744(2)	4334(1)	1302(1)	35(1)
C(11)	3266(2)	5299(1)	966(1)	29(1)
C(12)	1061(2)	8515(1)	1076(1)	21(1)
C(13)	2370(2)	8670(1)	597(1)	22(1)
C(14)	3359(2)	7784(1)	730(1)	21(1)
C(15)	4922(2)	7628(1)	424(1)	24(1)
C(16)	-377(2)	9161(1)	1165(1)	26(1)

C(17)	-1388(2)	7006(1)	3505(1)	27(1)
C(18)	-174(2)	7436(1)	3016(1)	23(1)
C(19)	851(2)	8230(1)	3533(1)	34(1)
O(2)	530(2)	8722(1)	4250(1)	38(1)
O(2')	2215(6)	8447(4)	3433(4)	38(1)

Table S3. Bond lengths [Å] and angles [°] for 170932LT_0M.

O(1)-C(15)	1.2215(17)
N(1)-C(5)	1.3704(17)
N(1)-C(12)	1.4013(17)
N(1)-C(6)	1.4356(17)
C(1)-C(10)	1.380(2)
C(1)-C(2)	1.382(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.387(2)
C(2)-H(12)	0.9500
C(3)-C(4)	1.3933(19)
C(3)-H(13)	0.9500
C(4)-C(11)	1.391(2)
C(4)-C(5)	1.4752(19)
C(5)-C(14)	1.3907(19)
C(6)-C(7)	1.387(2)
C(6)-C(18)	1.3976(19)
C(7)-C(8)	1.385(2)
C(7)-H(11)	0.9500
C(8)-C(9)	1.384(2)
C(8)-H(10)	0.9500
C(9)-C(17)	1.376(2)
C(9)-H(2)	0.9500
C(10)-C(11)	1.389(2)
C(10)-H(15)	0.9500
C(11)-H(14)	0.9500
C(12)-C(13)	1.3563(19)
C(12)-C(16)	1.4930(19)
C(13)-C(14)	1.4271(19)
C(13)-H(4)	0.9500

C(14)-C(15)	1.4388(19)
C(15)-H(3)	0.9500
C(16)-H(5)	0.9800
C(16)-H(6)	0.9800
C(16)-H(7)	0.9800
C(17)-C(18)	1.399(2)
C(17)-H(9)	0.9500
C(18)-C(19)	1.465(2)
C(19)-O(2')	1.203(5)
C(19)-O(2)	1.212(2)
C(19)-H(8)	0.9569
C(19)-H(8')	0.9597

C(5)-N(1)-C(12)	109.90(11)
C(5)-N(1)-C(6)	125.56(11)
C(12)-N(1)-C(6)	124.45(11)
C(10)-C(1)-C(2)	120.04(14)
C(10)-C(1)-H(1)	120.0
C(2)-C(1)-H(1)	120.0
C(1)-C(2)-C(3)	119.99(14)
C(1)-C(2)-H(12)	120.0
C(3)-C(2)-H(12)	120.0
C(2)-C(3)-C(4)	120.42(13)
C(2)-C(3)-H(13)	119.8
C(4)-C(3)-H(13)	119.8
C(11)-C(4)-C(3)	119.13(13)
C(11)-C(4)-C(5)	120.03(13)
C(3)-C(4)-C(5)	120.83(12)
N(1)-C(5)-C(14)	107.04(12)
N(1)-C(5)-C(4)	122.62(12)
C(14)-C(5)-C(4)	130.34(12)
C(7)-C(6)-C(18)	120.74(13)
C(7)-C(6)-N(1)	119.53(12)
C(18)-C(6)-N(1)	119.70(12)
C(8)-C(7)-C(6)	119.41(14)
C(8)-C(7)-H(11)	120.3
C(6)-C(7)-H(11)	120.3
C(9)-C(8)-C(7)	120.54(14)

C(9)-C(8)-H(10)	119.7
C(7)-C(8)-H(10)	119.7
C(17)-C(9)-C(8)	120.10(13)
C(17)-C(9)-H(2)	119.9
C(8)-C(9)-H(2)	119.9
C(1)-C(10)-C(11)	120.30(15)
C(1)-C(10)-H(15)	119.9
C(11)-C(10)-H(15)	119.9
C(10)-C(11)-C(4)	120.12(14)
C(10)-C(11)-H(14)	119.9
C(4)-C(11)-H(14)	119.9
C(13)-C(12)-N(1)	107.35(12)
C(13)-C(12)-C(16)	131.70(13)
N(1)-C(12)-C(16)	120.93(12)
C(12)-C(13)-C(14)	108.20(12)
C(12)-C(13)-H(4)	125.9
C(14)-C(13)-H(4)	125.9
C(5)-C(14)-C(13)	107.49(12)
C(5)-C(14)-C(15)	124.17(13)
C(13)-C(14)-C(15)	128.14(13)
O(1)-C(15)-C(14)	125.56(14)
O(1)-C(15)-H(3)	117.2
C(14)-C(15)-H(3)	117.2
C(12)-C(16)-H(5)	109.5
C(12)-C(16)-H(6)	109.5
H(5)-C(16)-H(6)	109.5
C(12)-C(16)-H(7)	109.5
H(5)-C(16)-H(7)	109.5
H(6)-C(16)-H(7)	109.5
C(9)-C(17)-C(18)	120.55(14)
C(9)-C(17)-H(9)	119.7
C(18)-C(17)-H(9)	119.7
C(6)-C(18)-C(17)	118.64(13)
C(6)-C(18)-C(19)	122.15(13)
C(17)-C(18)-C(19)	119.21(13)
O(2')-C(19)-C(18)	128.5(3)
O(2)-C(19)-C(18)	124.89(15)
O(2)-C(19)-H(8)	117.1

C(18)-C(19)-H(8)	118.0
O(2')-C(19)-H(8')	113.0
C(18)-C(19)-H(8')	118.4

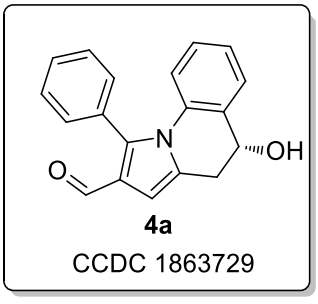
Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 170932LT_0M. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	28(1)	38(1)	33(1)	2(1)	14(1)	-3(1)
N(1)	18(1)	20(1)	22(1)	0(1)	6(1)	0(1)
C(1)	27(1)	22(1)	43(1)	5(1)	4(1)	4(1)
C(2)	21(1)	29(1)	29(1)	7(1)	4(1)	-1(1)
C(3)	20(1)	24(1)	25(1)	0(1)	6(1)	0(1)
C(4)	15(1)	21(1)	24(1)	-1(1)	5(1)	-1(1)
C(5)	16(1)	22(1)	19(1)	-3(1)	4(1)	0(1)
C(6)	16(1)	21(1)	24(1)	4(1)	5(1)	2(1)
C(7)	22(1)	24(1)	29(1)	0(1)	3(1)	1(1)
C(8)	20(1)	25(1)	42(1)	3(1)	2(1)	-4(1)
C(9)	19(1)	28(1)	40(1)	12(1)	9(1)	1(1)
C(10)	39(1)	26(1)	39(1)	-8(1)	5(1)	7(1)
C(11)	31(1)	30(1)	27(1)	-3(1)	5(1)	6(1)
C(12)	21(1)	20(1)	23(1)	1(1)	4(1)	-1(1)
C(13)	20(1)	22(1)	23(1)	2(1)	4(1)	-1(1)
C(14)	19(1)	23(1)	20(1)	-1(1)	3(1)	-1(1)
C(15)	22(1)	28(1)	22(1)	-2(1)	6(1)	0(1)
C(16)	22(1)	25(1)	32(1)	4(1)	8(1)	3(1)
C(17)	25(1)	30(1)	27(1)	6(1)	8(1)	7(1)
C(18)	21(1)	25(1)	24(1)	2(1)	5(1)	2(1)
C(19)	30(1)	38(1)	34(1)	-7(1)	7(1)	-3(1)
O(2)	45(1)	41(1)	26(1)	-8(1)	2(1)	-1(1)
O(2')	45(1)	41(1)	26(1)	-8(1)	2(1)	-1(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x 10^3$) for 170932LT_0M.

	x	y	z	U(eq)
H(1)	4414	3473	2554	37
H(12)	4153	4755	3731	32
H(13)	3305	6373	3176	27
H(11)	-782	6068	940	30
H(10)	-2760	5349	1795	35
H(2)	-3161	5950	3388	34
H(15)	3842	3809	825	42
H(14)	3055	5436	259	35
H(4)	2590	9264	236	26
H(3)	5452	7006	617	29
H(5)	-260	9816	832	39
H(6)	-468	9273	1883	39
H(7)	-1349	8818	837	39
H(9)	-1556	7245	4156	32
H(8)	1850	8377	3290	45
H(8')	441	8622	4050	45



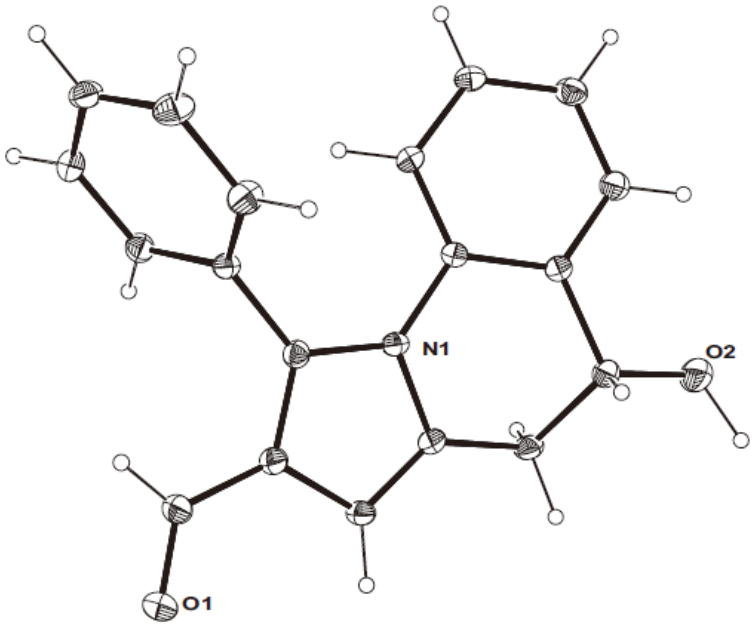


Table S6.Crystal data and structure refinement for d19507a.

Identification code	d19507a	
Empirical formula	C19 H15 N O2	
Formula weight	289.32	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.2847(12) Å	α= 90°.
	b = 16.3302(19) Å	β= 111.856(3)°.
	c = 9.0650(9) Å	γ = 90°.
Volume	1413.0(3) Å ^{3}	
Z	4	
Density (calculated)	1.360 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	608	
Crystal size	0.15 x 0.14 x 0.03 mm^3	
Theta range for data collection	2.47 to 25.15°.	
Index ranges	-12<=h<=12, -19<=k<=19, -10<=l<=10	
Reflections collected	14688	
Independent reflections	2503 [R(int) = 0.0704]	
Completeness to theta = 25.15°	98.7 %	
Absorption correction	multi-scan	

Max. and min. transmission	0.9974 and 0.9869
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2503 / 0 / 200
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0679, wR2 = 0.1451
R indices (all data)	R1 = 0.1011, wR2 = 0.1621
Extinction coefficient	0.026(3)
Largest diff. peak and hole	0.960 and -0.226 e.Å $^{-3}$

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for d19507a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8755(4)	4058(2)	1398(4)	37(1)
C(2)	7532(3)	3970(2)	1788(4)	32(1)
C(3)	7553(3)	3793(2)	3295(4)	30(1)
C(4)	8782(3)	3586(2)	4727(3)	29(1)
C(5)	9468(3)	2855(2)	4755(4)	36(1)
C(6)	10620(4)	2626(2)	6069(4)	41(1)
C(7)	11087(4)	3127(2)	7380(4)	41(1)
C(8)	10421(4)	3856(2)	7369(4)	49(1)
C(9)	9274(4)	4090(2)	6043(4)	43(1)
C(10)	5588(3)	3676(2)	4380(3)	29(1)
C(11)	6299(4)	3234(2)	5757(4)	35(1)
C(12)	5684(4)	3115(2)	6856(4)	38(1)
C(13)	4358(4)	3405(2)	6580(4)	41(1)
C(14)	3634(4)	3825(2)	5188(4)	42(1)
C(15)	4233(3)	3971(2)	4076(4)	32(1)
C(16)	3466(3)	4444(2)	2563(4)	40(1)
C(17)	3772(3)	4025(2)	1219(4)	35(1)
C(18)	5302(3)	4004(2)	1628(3)	31(1)
C(19)	6110(3)	4100(2)	761(4)	33(1)
N(1)	6176(3)	3825(2)	3196(3)	29(1)
O(1)	8745(3)	4281(2)	106(3)	49(1)
O(2)	2031(3)	4472(2)	2269(3)	56(1)

Table S8.Bond lengths [Å] and angles [°] for d19507a.

C(1)-O(1)	1.222(4)
C(1)-C(2)	1.435(5)
C(1)-H(1)	0.9500
C(2)-C(3)	1.388(4)
C(2)-C(19)	1.427(4)
C(3)-N(1)	1.386(4)
C(3)-C(4)	1.475(4)
C(4)-C(9)	1.380(4)
C(4)-C(5)	1.383(4)
C(5)-C(6)	1.383(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.374(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.372(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.388(5)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.391(4)
C(10)-C(15)	1.402(4)
C(10)-N(1)	1.436(4)
C(11)-C(12)	1.378(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.375(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.384(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.384(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.514(4)
C(16)-O(2)	1.399(4)
C(16)-C(17)	1.529(5)
C(16)-H(16)	1.0000
C(17)-C(18)	1.476(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(18)-C(19)	1.349(4)
C(18)-N(1)	1.401(4)
C(19)-H(19)	0.9500
O(2)-H(1A)	1.0707

O(1)-C(1)-C(2)	124.8(3)
O(1)-C(1)-H(1)	117.6
C(2)-C(1)-H(1)	117.6
C(3)-C(2)-C(19)	108.0(3)
C(3)-C(2)-C(1)	124.7(3)
C(19)-C(2)-C(1)	127.1(3)
N(1)-C(3)-C(2)	106.7(3)
N(1)-C(3)-C(4)	125.9(3)
C(2)-C(3)-C(4)	127.4(3)
C(9)-C(4)-C(5)	118.6(3)
C(9)-C(4)-C(3)	122.9(3)
C(5)-C(4)-C(3)	118.6(3)
C(6)-C(5)-C(4)	121.1(3)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(7)-C(6)-C(5)	119.7(3)
C(7)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(8)-C(7)-C(6)	119.8(3)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	120.4(3)
C(7)-C(8)-H(8)	119.8
C(9)-C(8)-H(8)	119.8
C(4)-C(9)-C(8)	120.3(3)
C(4)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(11)-C(10)-C(15)	120.5(3)
C(11)-C(10)-N(1)	122.1(3)
C(15)-C(10)-N(1)	117.4(3)
C(12)-C(11)-C(10)	119.5(3)
C(12)-C(11)-H(11)	120.3
C(10)-C(11)-H(11)	120.3

C(13)-C(12)-C(11)	120.7(3)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(12)-C(13)-C(14)	119.8(3)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(15)-C(14)-C(13)	121.0(3)
C(15)-C(14)-H(14)	119.5
C(13)-C(14)-H(14)	119.5
C(14)-C(15)-C(10)	118.5(3)
C(14)-C(15)-C(16)	121.7(3)
C(10)-C(15)-C(16)	119.9(3)
O(2)-C(16)-C(15)	110.3(3)
O(2)-C(16)-C(17)	112.2(3)
C(15)-C(16)-C(17)	107.5(3)
O(2)-C(16)-H(16)	108.9
C(15)-C(16)-H(16)	108.9
C(17)-C(16)-H(16)	108.9
C(18)-C(17)-C(16)	109.1(3)
C(18)-C(17)-H(17A)	109.9
C(16)-C(17)-H(17A)	109.9
C(18)-C(17)-H(17B)	109.9
C(16)-C(17)-H(17B)	109.9
H(17A)-C(17)-H(17B)	108.3
C(19)-C(18)-N(1)	108.2(3)
C(19)-C(18)-C(17)	132.9(3)
N(1)-C(18)-C(17)	118.8(3)
C(18)-C(19)-C(2)	107.9(3)
C(18)-C(19)-H(19)	126.1
C(2)-C(19)-H(19)	126.1
C(3)-N(1)-C(18)	109.2(2)
C(3)-N(1)-C(10)	130.5(2)
C(18)-N(1)-C(10)	120.3(3)
C(16)-O(2)-H(1A)	109.6

Symmetry transformations used to generate equivalent atoms:

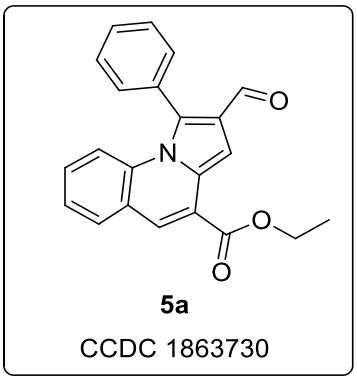
Table S9. Anisotropic displacement parameters ($Å^2 x 10^3$)for d19507a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	41(2)	37(2)	37(2)	4(1)	19(2)	4(2)
C(2)	33(2)	33(2)	29(2)	1(1)	10(1)	2(1)
C(3)	30(2)	29(2)	31(2)	-1(1)	11(1)	2(1)
C(4)	29(2)	32(2)	25(2)	2(1)	10(1)	0(1)
C(5)	35(2)	40(2)	31(2)	-6(1)	11(2)	3(2)
C(6)	35(2)	47(2)	42(2)	5(2)	14(2)	11(2)
C(7)	34(2)	57(2)	29(2)	9(2)	7(2)	-2(2)
C(8)	52(2)	51(2)	33(2)	-6(2)	3(2)	-6(2)
C(9)	48(2)	36(2)	38(2)	-5(2)	10(2)	3(2)
C(10)	30(2)	31(2)	25(2)	0(1)	11(1)	0(1)
C(11)	35(2)	38(2)	30(2)	8(1)	11(1)	8(2)
C(12)	44(2)	40(2)	32(2)	10(1)	15(2)	3(2)
C(13)	41(2)	51(2)	35(2)	3(2)	17(2)	-5(2)
C(14)	34(2)	55(2)	36(2)	2(2)	13(2)	2(2)
C(15)	30(2)	38(2)	27(2)	1(1)	9(1)	3(1)
C(16)	24(2)	62(2)	31(2)	6(2)	7(1)	6(2)
C(17)	32(2)	44(2)	24(2)	4(1)	5(1)	1(2)
C(18)	30(2)	35(2)	26(2)	2(1)	7(1)	2(1)
C(19)	38(2)	37(2)	24(2)	3(1)	12(1)	3(2)
N(1)	30(2)	32(1)	23(1)	3(1)	9(1)	1(1)
O(1)	54(2)	60(2)	42(2)	15(1)	27(1)	8(1)
O(2)	40(2)	73(2)	53(2)	13(1)	16(1)	9(1)

Table S10. Hydrogen coordinates ($x 10^4$) and isotropic displacement parameters ($Å^2 x 10^3$) for d19507a.

	x	y	z	U(eq)
H(1)	9637	3935	2202	44
H(5)	9142	2504	3855	43
H(6)	11087	2124	6066	50

H(7)	11869	2969	8293	49
H(8)	10747	4203	8274	58
H(9)	8826	4599	6041	51
H(11)	7201	3015	5938	42
H(12)	6182	2831	7815	46
H(13)	3941	3317	7342	50
H(14)	2712	4015	4994	50
H(16)	3839	5016	2689	48
H(17A)	3394	3460	1068	42
H(17B)	3314	4329	214	42
H(19)	5790	4230	-338	40
H(1A)	1550	4948	1431	59



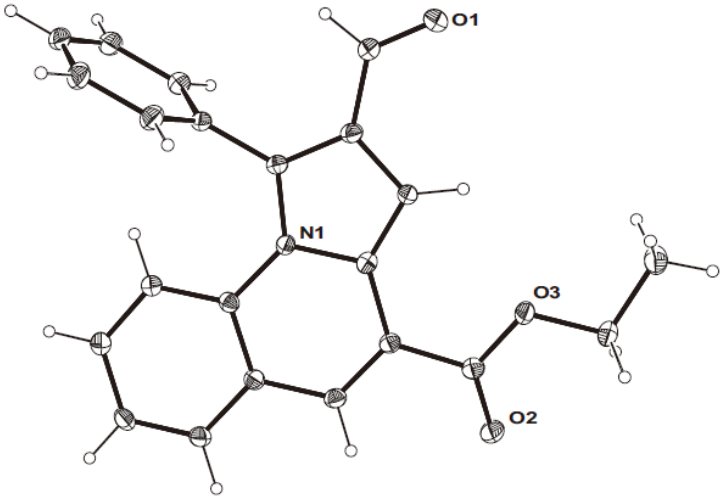


Table S11.Crystal data and structure refinement for d20154b.

Identification code	d20154b
Empirical formula	C22 H17 N O3
Formula weight	343.37

Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.161(2) Å	α= 90.00(3)°.
	b = 13.323(3) Å	β= 95.42(3)°.
	c = 35.586(7) Å	γ = 90.00(3)°.
Volume	3379.7(14) Å^3	
Z	8	
Density (calculated)	1.350 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	1440	
Crystal size	0.68 x 0.07 x 0.02 mm^3	
Theta range for data collection	2.30 to 25.01°.	
Index ranges	-8<=h<=8, -15<=k<=14, -42<=l<=41	
Reflections collected	31920	
Independent reflections	5915 [R(int) = 0.0802]	
Completeness to theta = 25.01°	99.2 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9982 and 0.9413	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5915 / 0 / 471	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.1086	
R indices (all data)	R1 = 0.1005, wR2 = 0.1362	
Largest diff. peak and hole	0.179 and -0.247 e.Å^{-3}	

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for d20154b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2025(4)	1545(2)	6838(1)	42(1)
C(2)	1955(3)	2490(2)	6635(1)	34(1)
C(3)	1878(3)	3428(2)	6800(1)	32(1)
C(4)	1871(4)	3648(2)	7210(1)	35(1)
C(5)	3526(4)	3644(2)	7445(1)	45(1)
C(6)	3482(5)	3839(2)	7827(1)	55(1)

C(7)	1811(5)	4037(2)	7974(1)	52(1)
C(8)	162(5)	4034(2)	7743(1)	52(1)
C(9)	191(4)	3834(2)	7362(1)	44(1)
C(10)	1678(3)	5198(2)	6530(1)	30(1)
C(11)	1884(3)	5739(2)	6868(1)	35(1)
C(12)	1773(4)	6773(2)	6866(1)	40(1)
C(13)	1470(4)	7298(2)	6529(1)	41(1)
C(14)	1296(4)	6777(2)	6195(1)	39(1)
C(15)	1413(3)	5726(2)	6186(1)	32(1)
C(16)	1335(3)	5196(2)	5833(1)	33(1)
C(17)	1552(3)	4193(2)	5817(1)	30(1)
C(18)	1567(3)	3728(2)	5436(1)	33(1)
C(19)	1513(4)	2230(2)	5078(1)	39(1)
C(20)	1552(4)	1120(2)	5154(1)	50(1)
C(21)	1737(3)	3611(2)	6162(1)	30(1)
C(22)	1880(3)	2608(2)	6238(1)	31(1)
C(23)	6854(4)	1634(2)	6892(1)	45(1)
C(24)	6756(3)	2195(2)	6540(1)	32(1)
C(25)	6794(3)	1762(2)	6187(1)	30(1)
C(26)	6956(3)	681(2)	6102(1)	30(1)
C(27)	5458(4)	34(2)	6133(1)	39(1)
C(28)	5629(4)	-982(2)	6062(1)	48(1)
C(29)	7289(4)	-1371(2)	5957(1)	45(1)
C(30)	8796(4)	-736(2)	5932(1)	42(1)
C(31)	8646(4)	280(2)	6006(1)	37(1)
C(32)	6588(3)	2507(2)	5524(1)	28(1)
C(33)	6457(3)	1610(2)	5317(1)	33(1)
C(34)	6338(4)	1644(2)	4927(1)	38(1)
C(35)	6330(3)	2543(2)	4736(1)	37(1)
C(36)	6451(3)	3427(2)	4936(1)	34(1)
C(37)	6570(3)	3430(2)	5331(1)	29(1)
C(38)	6588(3)	4361(2)	5535(1)	31(1)
C(39)	6576(3)	4385(2)	5914(1)	28(1)
C(40)	6498(3)	5398(2)	6093(1)	33(1)
C(41)	6620(4)	6310(2)	6669(1)	41(1)
C(42)	6853(4)	6078(2)	7083(1)	53(1)
C(43)	6630(3)	3464(2)	6125(1)	28(1)
C(44)	6652(3)	3245(2)	6500(1)	31(1)

N(1)	1752(3)	4135(1)	6512(1)	30(1)
N(2)	6705(3)	2537(1)	5926(1)	28(1)
O(1)	2135(3)	723(1)	6693(1)	51(1)
O(2)	1669(3)	4208(1)	5152(1)	50(1)
O(3)	1459(2)	2728(1)	5440(1)	38(1)
O(4)	6824(3)	2021(1)	7203(1)	55(1)
O(5)	6283(3)	6170(1)	5919(1)	52(1)
O(6)	6702(2)	5358(1)	6471(1)	38(1)

Table S13.Bond lengths [Å] and angles [°] for d20154b.

C(1)-O(1)	1.216(3)
C(1)-C(2)	1.450(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.384(3)
C(2)-C(22)	1.416(3)
C(3)-N(1)	1.388(3)
C(3)-C(4)	1.489(3)
C(4)-C(5)	1.384(4)
C(4)-C(9)	1.387(3)
C(5)-C(6)	1.387(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.376(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.375(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.383(3)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.397(3)
C(10)-C(15)	1.410(3)
C(10)-N(1)	1.419(3)
C(11)-C(12)	1.380(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.388(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.371(3)

C(13)-H(13)	0.9500
C(14)-C(15)	1.402(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.437(3)
C(16)-C(17)	1.347(3)
C(16)-H(16)	0.9500
C(17)-C(21)	1.446(3)
C(17)-C(18)	1.494(3)
C(18)-O(2)	1.203(3)
C(18)-O(3)	1.335(3)
C(19)-O(3)	1.453(3)
C(19)-C(20)	1.503(3)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.366(3)
C(21)-N(1)	1.428(3)
C(22)-H(22)	0.9500
C(23)-O(4)	1.222(3)
C(23)-C(24)	1.455(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.386(3)
C(24)-C(44)	1.406(3)
C(25)-N(2)	1.386(3)
C(25)-C(26)	1.478(3)
C(26)-C(27)	1.388(3)
C(26)-C(31)	1.394(3)
C(27)-C(28)	1.385(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.381(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.381(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.386(3)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500

C(32)-C(33)	1.401(3)
C(32)-C(37)	1.408(3)
C(32)-N(2)	1.425(3)
C(33)-C(34)	1.383(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.377(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.375(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.400(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.436(3)
C(38)-C(39)	1.351(3)
C(38)-H(38)	0.9500
C(39)-C(43)	1.438(3)
C(39)-C(40)	1.495(3)
C(40)-O(5)	1.203(3)
C(40)-O(6)	1.338(3)
C(41)-O(6)	1.456(3)
C(41)-C(42)	1.499(3)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(44)	1.365(3)
C(43)-N(2)	1.426(3)
C(44)-H(44)	0.9500

O(1)-C(1)-C(2)	124.9(2)
O(1)-C(1)-H(1)	117.6
C(2)-C(1)-H(1)	117.6
C(3)-C(2)-C(22)	108.9(2)
C(3)-C(2)-C(1)	125.0(2)
C(22)-C(2)-C(1)	126.1(2)
C(2)-C(3)-N(1)	107.58(19)
C(2)-C(3)-C(4)	126.7(2)
N(1)-C(3)-C(4)	125.7(2)

C(5)-C(4)-C(9)	119.4(2)
C(5)-C(4)-C(3)	120.6(2)
C(9)-C(4)-C(3)	120.0(2)
C(4)-C(5)-C(6)	119.6(3)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(7)-C(6)-C(5)	120.7(3)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(8)-C(7)-C(6)	120.0(3)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	119.8(3)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(8)-C(9)-C(4)	120.6(3)
C(8)-C(9)-H(9)	119.7
C(4)-C(9)-H(9)	119.7
C(11)-C(10)-C(15)	118.9(2)
C(11)-C(10)-N(1)	123.5(2)
C(15)-C(10)-N(1)	117.5(2)
C(12)-C(11)-C(10)	120.7(2)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(11)-C(12)-C(13)	120.7(2)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(14)-C(13)-C(12)	119.2(2)
C(14)-C(13)-H(13)	120.4
C(12)-C(13)-H(13)	120.4
C(13)-C(14)-C(15)	121.7(2)
C(13)-C(14)-H(14)	119.2
C(15)-C(14)-H(14)	119.2
C(14)-C(15)-C(10)	118.8(2)
C(14)-C(15)-C(16)	120.9(2)
C(10)-C(15)-C(16)	120.3(2)
C(17)-C(16)-C(15)	122.0(2)
C(17)-C(16)-H(16)	119.0

C(15)-C(16)-H(16)	119.0
C(16)-C(17)-C(21)	119.8(2)
C(16)-C(17)-C(18)	117.4(2)
C(21)-C(17)-C(18)	122.8(2)
O(2)-C(18)-O(3)	123.2(2)
O(2)-C(18)-C(17)	123.3(2)
O(3)-C(18)-C(17)	113.5(2)
O(3)-C(19)-C(20)	106.90(19)
O(3)-C(19)-H(19A)	110.3
C(20)-C(19)-H(19A)	110.3
O(3)-C(19)-H(19B)	110.3
C(20)-C(19)-H(19B)	110.3
H(19A)-C(19)-H(19B)	108.6
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-N(1)	108.10(19)
C(22)-C(21)-C(17)	133.8(2)
N(1)-C(21)-C(17)	118.1(2)
C(21)-C(22)-C(2)	107.5(2)
C(21)-C(22)-H(22)	126.2
C(2)-C(22)-H(22)	126.2
O(4)-C(23)-C(24)	124.0(2)
O(4)-C(23)-H(23)	118.0
C(24)-C(23)-H(23)	118.0
C(25)-C(24)-C(44)	109.2(2)
C(25)-C(24)-C(23)	124.3(2)
C(44)-C(24)-C(23)	126.5(2)
N(2)-C(25)-C(24)	107.01(19)
N(2)-C(25)-C(26)	126.12(19)
C(24)-C(25)-C(26)	126.8(2)
C(27)-C(26)-C(31)	118.5(2)
C(27)-C(26)-C(25)	120.8(2)
C(31)-C(26)-C(25)	120.6(2)
C(28)-C(27)-C(26)	120.6(3)

C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(29)-C(28)-C(27)	120.7(3)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(30)-C(29)-C(28)	119.0(2)
C(30)-C(29)-H(29)	120.5
C(28)-C(29)-H(29)	120.5
C(29)-C(30)-C(31)	120.8(3)
C(29)-C(30)-H(30)	119.6
C(31)-C(30)-H(30)	119.6
C(30)-C(31)-C(26)	120.3(2)
C(30)-C(31)-H(31)	119.8
C(26)-C(31)-H(31)	119.8
C(33)-C(32)-C(37)	119.40(19)
C(33)-C(32)-N(2)	123.1(2)
C(37)-C(32)-N(2)	117.49(19)
C(34)-C(33)-C(32)	119.6(2)
C(34)-C(33)-H(33)	120.2
C(32)-C(33)-H(33)	120.2
C(35)-C(34)-C(33)	121.5(2)
C(35)-C(34)-H(34)	119.3
C(33)-C(34)-H(34)	119.3
C(36)-C(35)-C(34)	119.4(2)
C(36)-C(35)-H(35)	120.3
C(34)-C(35)-H(35)	120.3
C(35)-C(36)-C(37)	121.2(2)
C(35)-C(36)-H(36)	119.4
C(37)-C(36)-H(36)	119.4
C(36)-C(37)-C(32)	119.0(2)
C(36)-C(37)-C(38)	120.4(2)
C(32)-C(37)-C(38)	120.61(19)
C(39)-C(38)-C(37)	121.6(2)
C(39)-C(38)-H(38)	119.2
C(37)-C(38)-H(38)	119.2
C(38)-C(39)-C(43)	120.0(2)
C(38)-C(39)-C(40)	116.9(2)
C(43)-C(39)-C(40)	123.17(19)

O(5)-C(40)-O(6)	123.2(2)
O(5)-C(40)-C(39)	124.0(2)
O(6)-C(40)-C(39)	112.8(2)
O(6)-C(41)-C(42)	106.9(2)
O(6)-C(41)-H(41A)	110.3
C(42)-C(41)-H(41A)	110.3
O(6)-C(41)-H(41B)	110.3
C(42)-C(41)-H(41B)	110.3
H(41A)-C(41)-H(41B)	108.6
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-N(2)	107.61(19)
C(44)-C(43)-C(39)	133.7(2)
N(2)-C(43)-C(39)	118.69(18)
C(43)-C(44)-C(24)	107.9(2)
C(43)-C(44)-H(44)	126.1
C(24)-C(44)-H(44)	126.1
C(3)-N(1)-C(10)	130.17(18)
C(3)-N(1)-C(21)	107.87(19)
C(10)-N(1)-C(21)	121.96(18)
C(25)-N(2)-C(32)	130.14(18)
C(25)-N(2)-C(43)	108.34(17)
C(32)-N(2)-C(43)	121.42(18)
C(18)-O(3)-C(19)	116.03(18)
C(40)-O(6)-C(41)	116.53(18)

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for d20154b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	60(2)	35(2)	31(1)	1(1)	7(1)	-1(1)

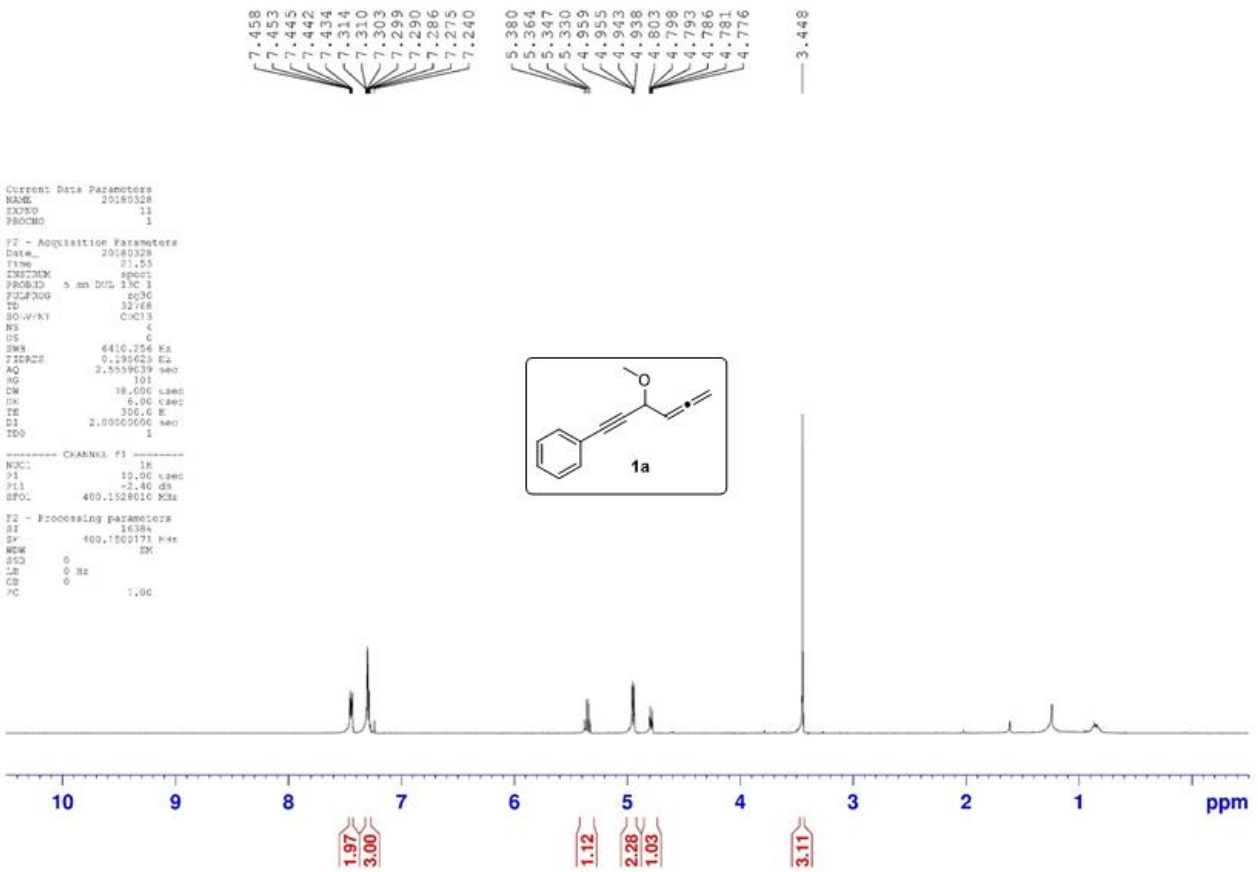
C(2)	40(2)	33(2)	30(1)	5(1)	4(1)	-3(1)
C(3)	38(2)	31(2)	28(1)	4(1)	2(1)	0(1)
C(4)	51(2)	26(2)	28(1)	2(1)	6(1)	-3(1)
C(5)	59(2)	38(2)	35(1)	-1(1)	-2(1)	5(1)
C(6)	82(3)	43(2)	35(2)	-2(1)	-13(2)	2(2)
C(7)	97(3)	31(2)	30(1)	-2(1)	10(2)	-11(2)
C(8)	76(2)	42(2)	40(2)	-4(1)	24(2)	-12(2)
C(9)	55(2)	44(2)	34(1)	-1(1)	8(1)	-7(1)
C(10)	28(1)	29(2)	34(1)	1(1)	7(1)	2(1)
C(11)	42(2)	32(2)	32(1)	1(1)	4(1)	1(1)
C(12)	49(2)	36(2)	36(1)	-3(1)	8(1)	2(1)
C(13)	52(2)	27(2)	45(2)	0(1)	12(1)	7(1)
C(14)	48(2)	34(2)	36(1)	6(1)	11(1)	8(1)
C(15)	33(2)	31(2)	32(1)	2(1)	9(1)	2(1)
C(16)	36(2)	35(2)	30(1)	6(1)	6(1)	2(1)
C(17)	29(2)	32(2)	28(1)	2(1)	5(1)	-1(1)
C(18)	31(2)	36(2)	33(1)	2(1)	6(1)	-1(1)
C(19)	45(2)	43(2)	30(1)	-8(1)	5(1)	-2(1)
C(20)	58(2)	46(2)	45(2)	-10(1)	10(1)	-9(1)
C(21)	28(2)	35(2)	28(1)	-1(1)	4(1)	-5(1)
C(22)	39(2)	26(2)	28(1)	0(1)	4(1)	-2(1)
C(23)	68(2)	31(2)	34(2)	2(1)	0(1)	2(1)
C(24)	42(2)	24(2)	29(1)	2(1)	0(1)	1(1)
C(25)	33(2)	27(2)	31(1)	2(1)	0(1)	1(1)
C(26)	42(2)	21(1)	25(1)	2(1)	-2(1)	-1(1)
C(27)	47(2)	33(2)	37(1)	-3(1)	5(1)	-5(1)
C(28)	68(2)	33(2)	42(2)	-6(1)	3(1)	-16(1)
C(29)	78(2)	21(2)	36(1)	-1(1)	-3(1)	-1(1)
C(30)	58(2)	28(2)	39(1)	-1(1)	3(1)	12(1)
C(31)	46(2)	27(2)	37(1)	0(1)	0(1)	0(1)
C(32)	27(1)	29(2)	26(1)	-1(1)	1(1)	1(1)
C(33)	41(2)	26(1)	31(1)	0(1)	0(1)	3(1)
C(34)	47(2)	33(2)	32(1)	-6(1)	2(1)	4(1)
C(35)	41(2)	42(2)	27(1)	-1(1)	4(1)	1(1)
C(36)	36(2)	35(2)	32(1)	5(1)	5(1)	-1(1)
C(37)	28(1)	30(2)	29(1)	2(1)	3(1)	-1(1)
C(38)	33(2)	25(1)	35(1)	5(1)	3(1)	-1(1)
C(39)	27(1)	23(1)	34(1)	3(1)	2(1)	0(1)

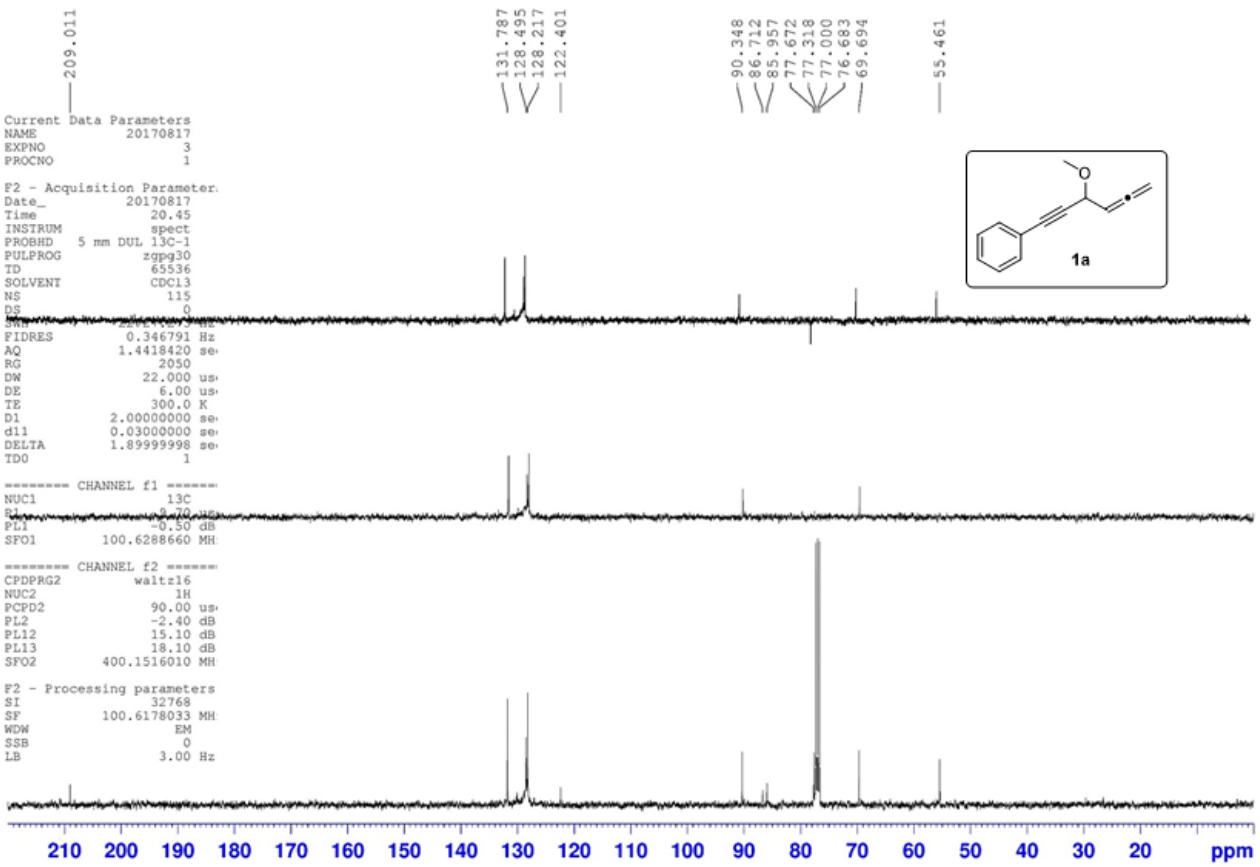
C(40)	34(2)	28(2)	36(1)	2(1)	2(1)	-2(1)
C(41)	52(2)	24(2)	45(2)	-7(1)	6(1)	4(1)
C(42)	72(2)	41(2)	44(2)	-9(1)	0(2)	7(2)
C(43)	29(1)	22(1)	32(1)	-1(1)	1(1)	0(1)
C(44)	38(2)	25(2)	29(1)	-3(1)	0(1)	2(1)
N(1)	36(1)	29(1)	25(1)	-2(1)	4(1)	-2(1)
N(2)	34(1)	20(1)	28(1)	0(1)	2(1)	1(1)
O(1)	80(2)	31(1)	44(1)	2(1)	11(1)	-1(1)
O(2)	78(2)	43(1)	31(1)	6(1)	13(1)	-2(1)
O(3)	53(1)	35(1)	27(1)	-4(1)	7(1)	-4(1)
O(4)	91(2)	45(1)	30(1)	-1(1)	2(1)	4(1)
O(5)	88(2)	22(1)	45(1)	3(1)	-4(1)	3(1)
O(6)	55(1)	24(1)	35(1)	-3(1)	5(1)	3(1)

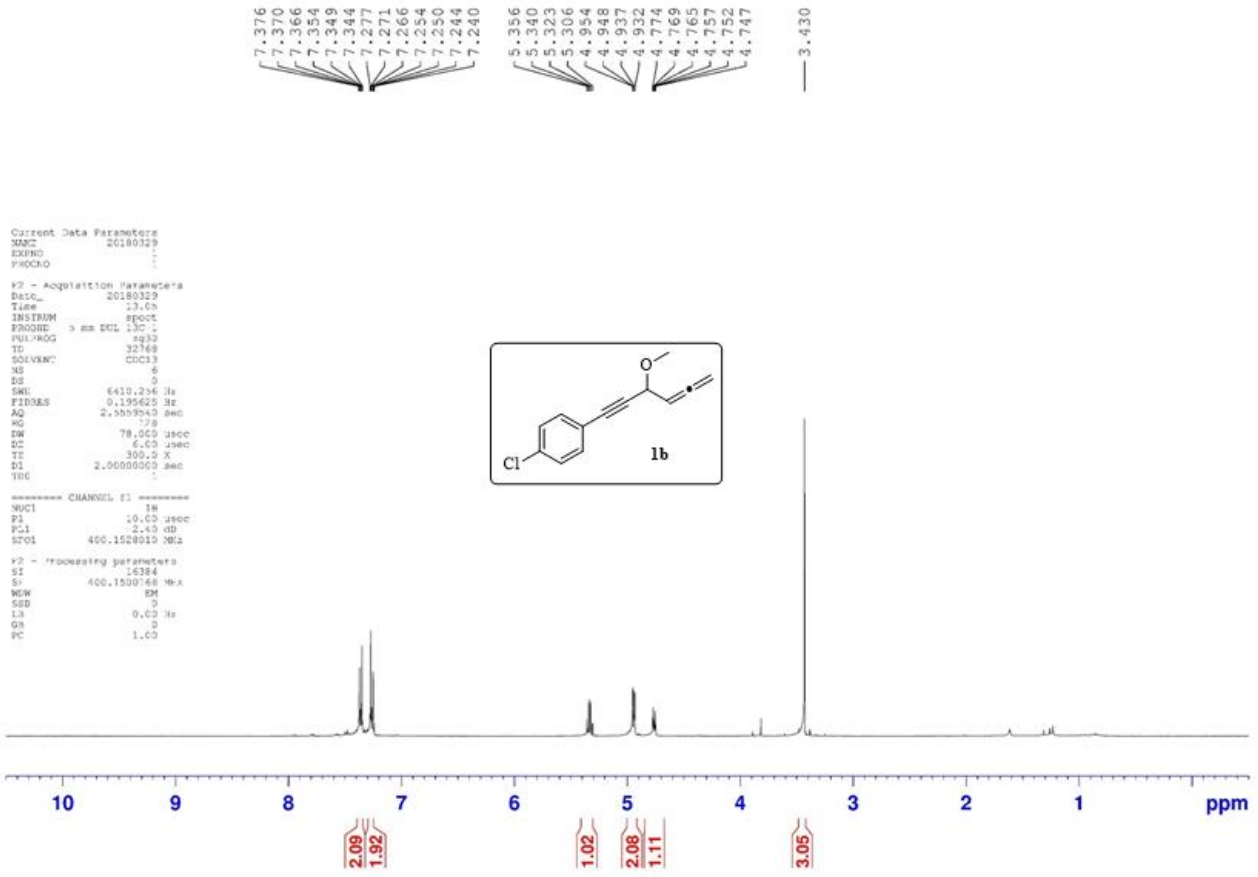
Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for d20154b.

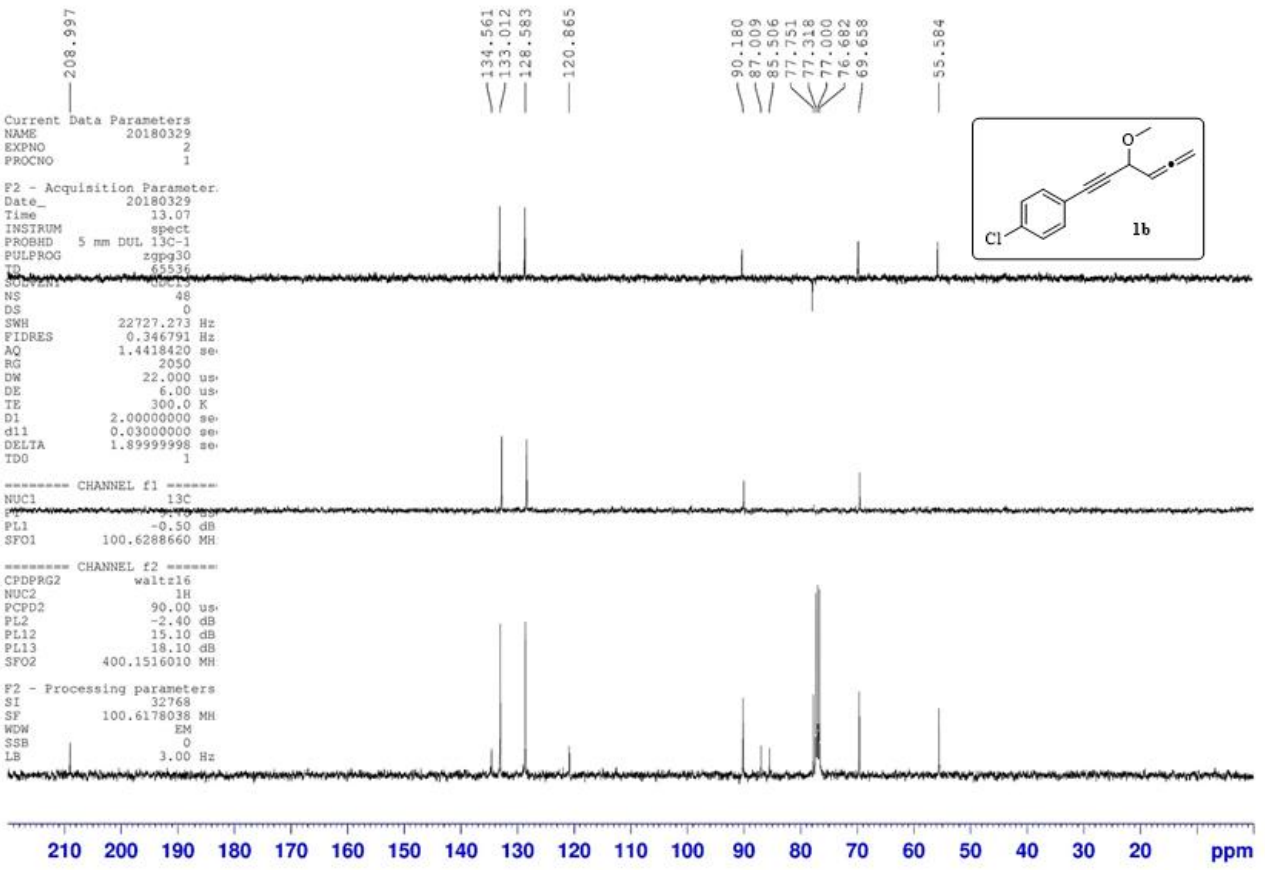
	x	y	z	U(eq)
H(1)	1981	1570	7104	50
H(5)	4685	3508	7345	54
H(6)	4616	3836	7988	65
H(7)	1798	4175	8236	63
H(8)	-993	4169	7844	62
H(9)	-952	3824	7203	53
H(11)	2103	5392	7101	42
H(12)	1906	7130	7098	48
H(13)	1384	8009	6529	49
H(14)	1091	7136	5964	46
H(16)	1124	5563	5604	40
H(19A)	2645	2436	4958	47
H(19B)	391	2409	4907	47
H(20A)	1646	756	4917	75
H(20B)	398	922	5262	75
H(20C)	2638	958	5332	75
H(22)	1921	2085	6058	37

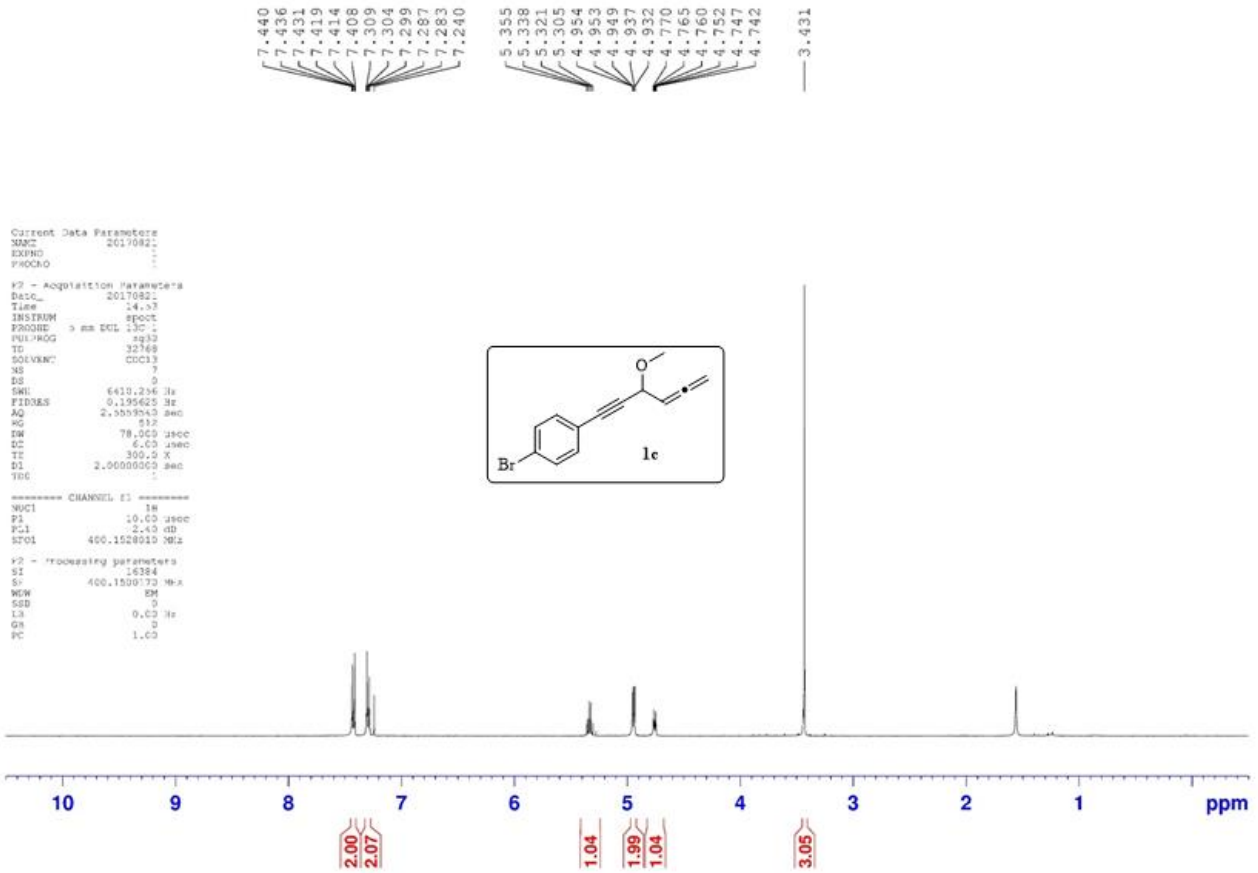
H(23)	6948	924	6880	54
H(27)	4304	292	6204	47
H(28)	4595	-1416	6087	57
H(29)	7391	-2066	5901	55
H(30)	9950	-999	5863	50
H(31)	9701	706	5992	44
H(33)	6449	983	5444	40
H(34)	6261	1034	4789	45
H(35)	6242	2552	4468	44
H(36)	6454	4046	4804	41
H(38)	6609	4975	5399	37
H(41A)	5399	6644	6601	49
H(41B)	7634	6762	6601	49
H(42A)	5859	5617	7144	79
H(42B)	6774	6700	7227	79
H(42C)	8079	5763	7147	79
H(44)	6607	3717	6699	37

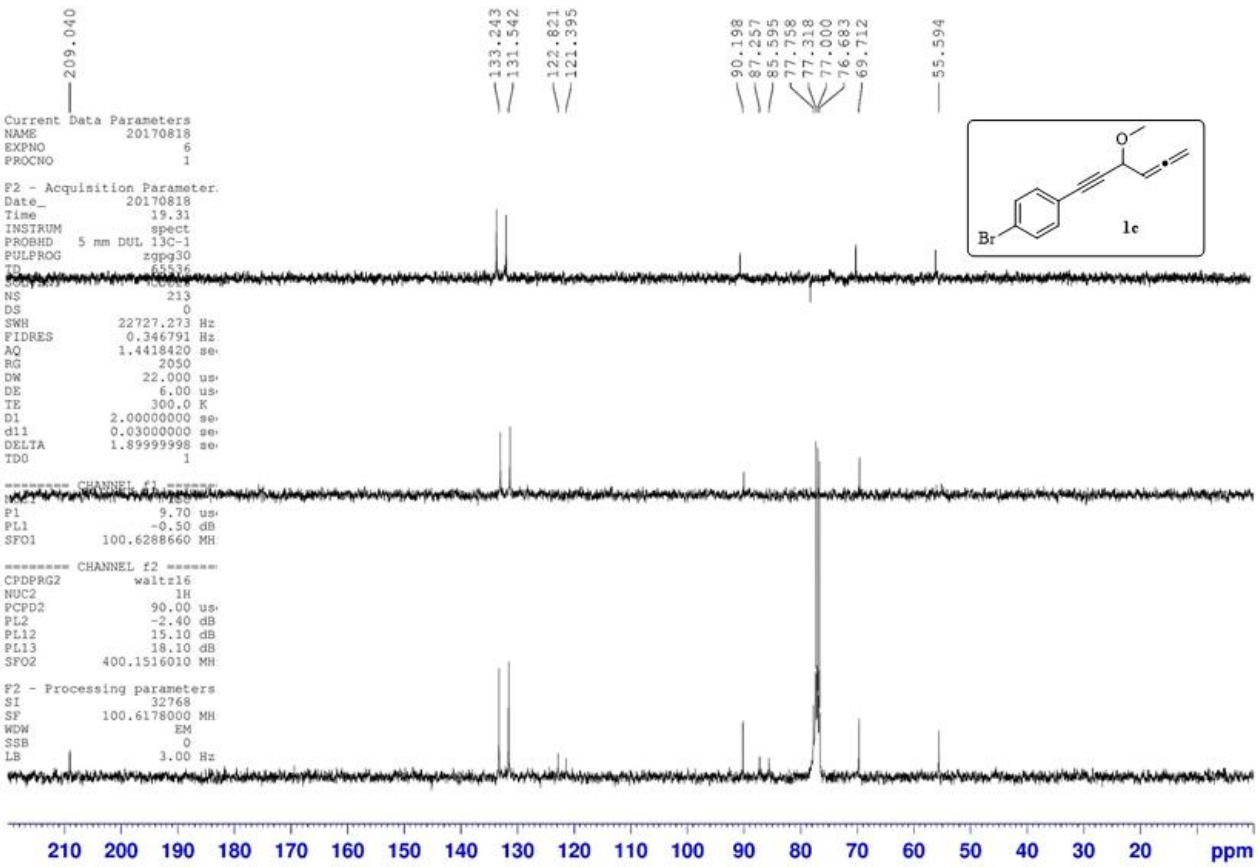

7.458
7.453
7.445
7.442
7.434
7.314
7.310
7.303
7.299
7.290
7.286
7.275
7.240
5.380
5.364
5.347
5.330
4.959
4.955
4.943
4.938
4.803
4.798
4.793
4.786
4.781
4.776
3.448
1a
10
9
8
7
6
5
4
3
2
1
ppm
1.97
3.00
1.12
2.28
1.03
3.11

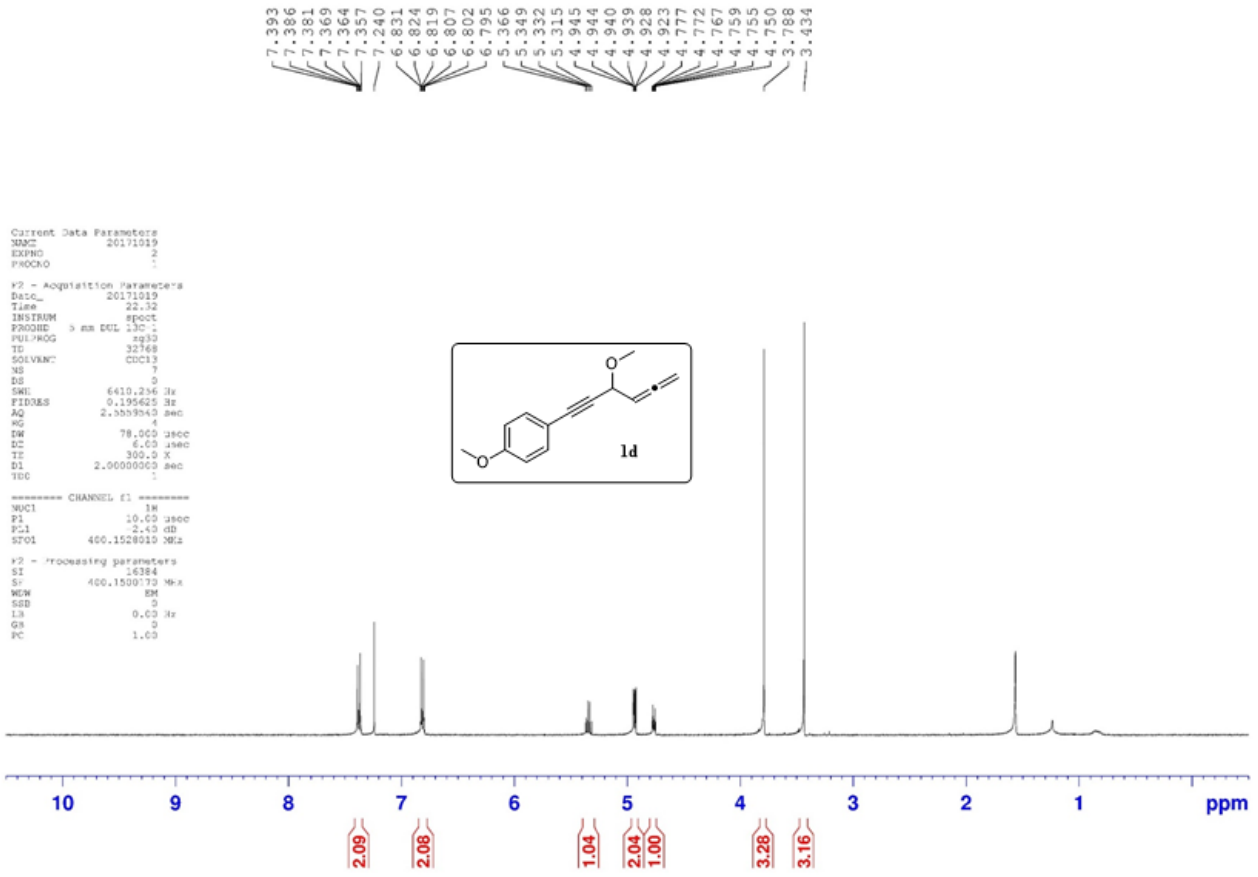

209.011
131.787
128.495
128.217
122.401
90.348
86.712
85.957
77.672
77.318
77.000
76.683
69.694
55.461
Current Data Parameters
NAME 20170817
EXPNO 3
PROCNO 1
F2 - Acquisition Parameter
Date_ 20170817
Time 20.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 115
DS 0
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
======== CHANNEL f1 ======
NUC1 13C
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178033 MH
WDW EM
SSB 0
LB 3.00 Hz
O
1a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

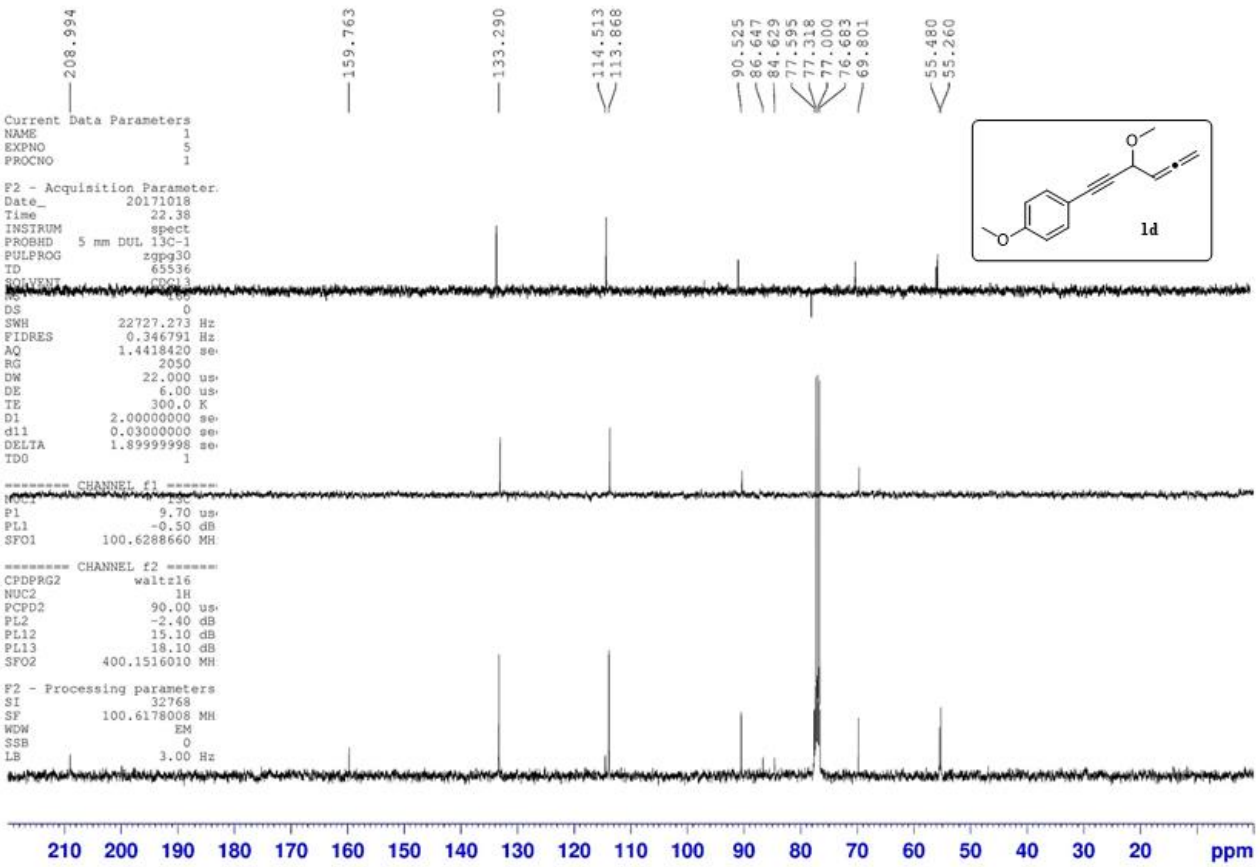

7.376
7.370
7.366
7.354
7.349
7.344
7.277
7.271
7.266
7.254
7.250
7.244
7.240
5.356
5.340
5.323
5.306
4.954
4.948
4.937
4.932
4.774
4.769
4.765
4.757
4.752
4.747
3.430
Cl
O
1b
10
9
8
7
6
5
4
3
2
1
ppm
2.09
1.92
1.02
2.08
1.11
3.05

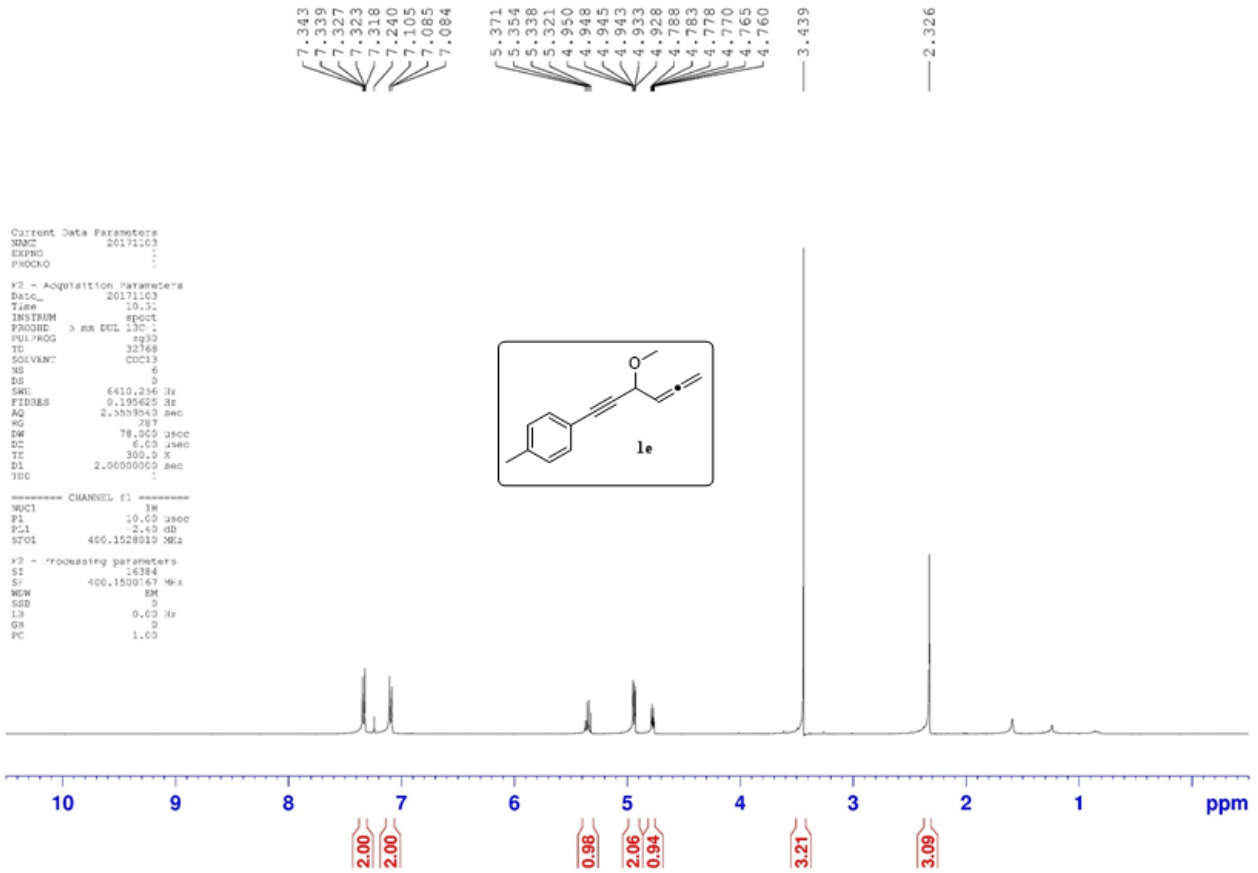

208.997
134.561
133.012
128.583
120.865
90.180
87.009
85.506
77.751
77.318
77.000
76.682
69.658
55.584
Current Data Parameters
NAME 20180329
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20180329
Time 13.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 48
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
======== CHANNEL f1 ======
NUC1 13C
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178038 MH
WDW EM
SSB 0
LB 3.00 Hz
O
Cl
1b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

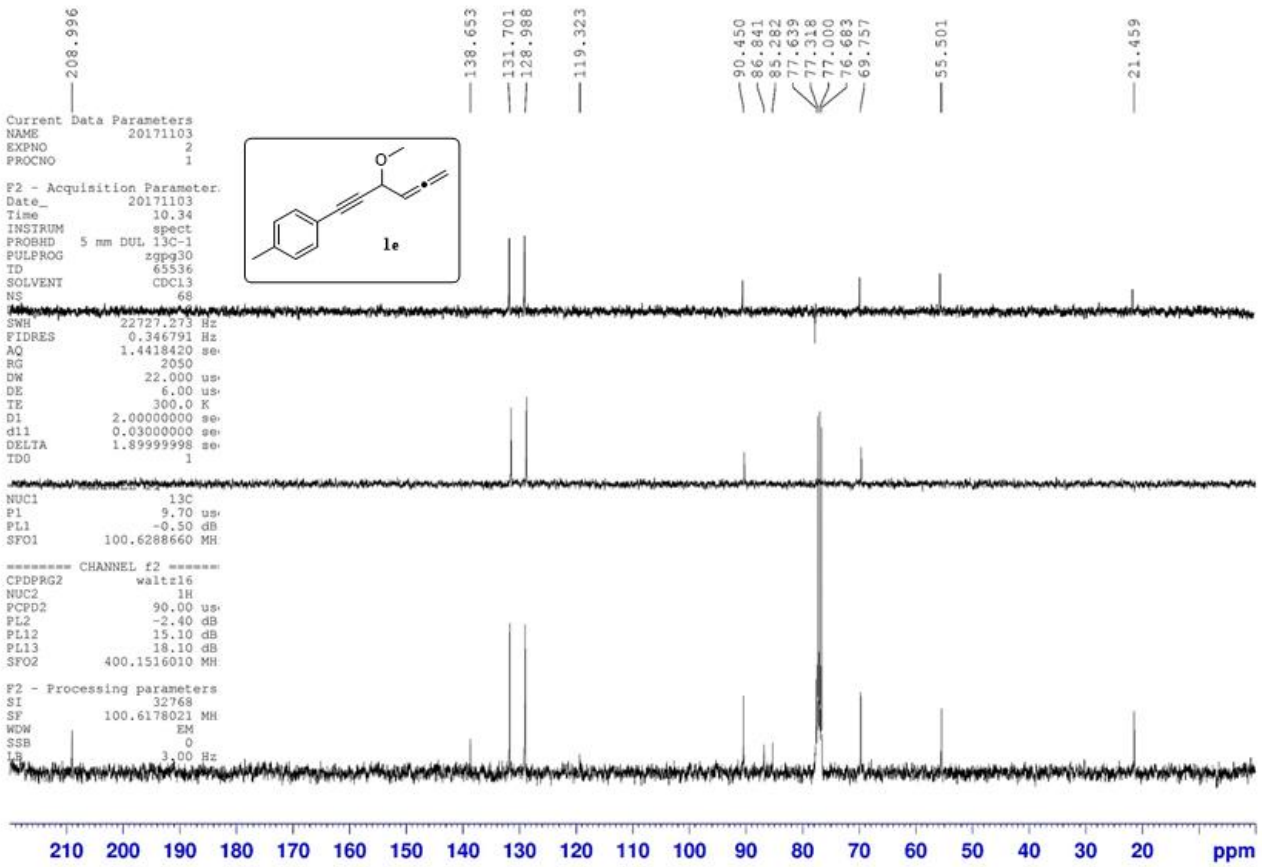

7.440
7.436
7.431
7.419
7.414
7.408
7.309
7.304
7.299
7.287
7.283
7.240
5.355
5.338
5.321
5.305
4.954
4.953
4.949
4.937
4.932
4.770
4.765
4.760
4.752
4.747
4.742
3.431
Br
1c
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.07
1.04
1.99
1.04
3.05

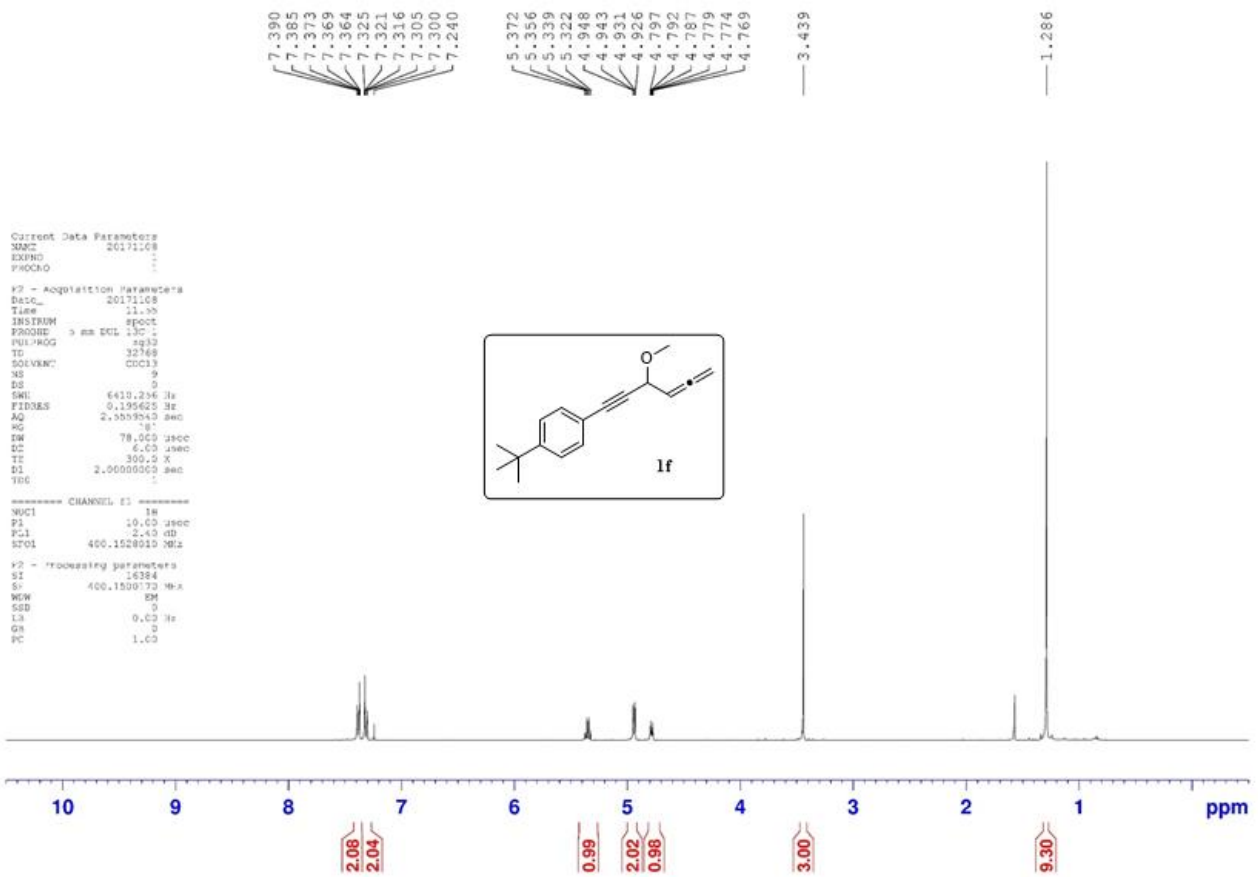

209.040
133.243
131.542
122.821
121.395
90.198
87.257
85.595
77.758
77.318
77.000
76.683
69.712
55.594
Current Data Parameters
NAME 20170818
EXPNO 6
PROCNO 1
F2 - Acquisition Parameter
Date_ 20170818
Time 19.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 213
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178000 MH
WDW EM
SSB 0
LB 3.00 Hz
O
Br
1c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

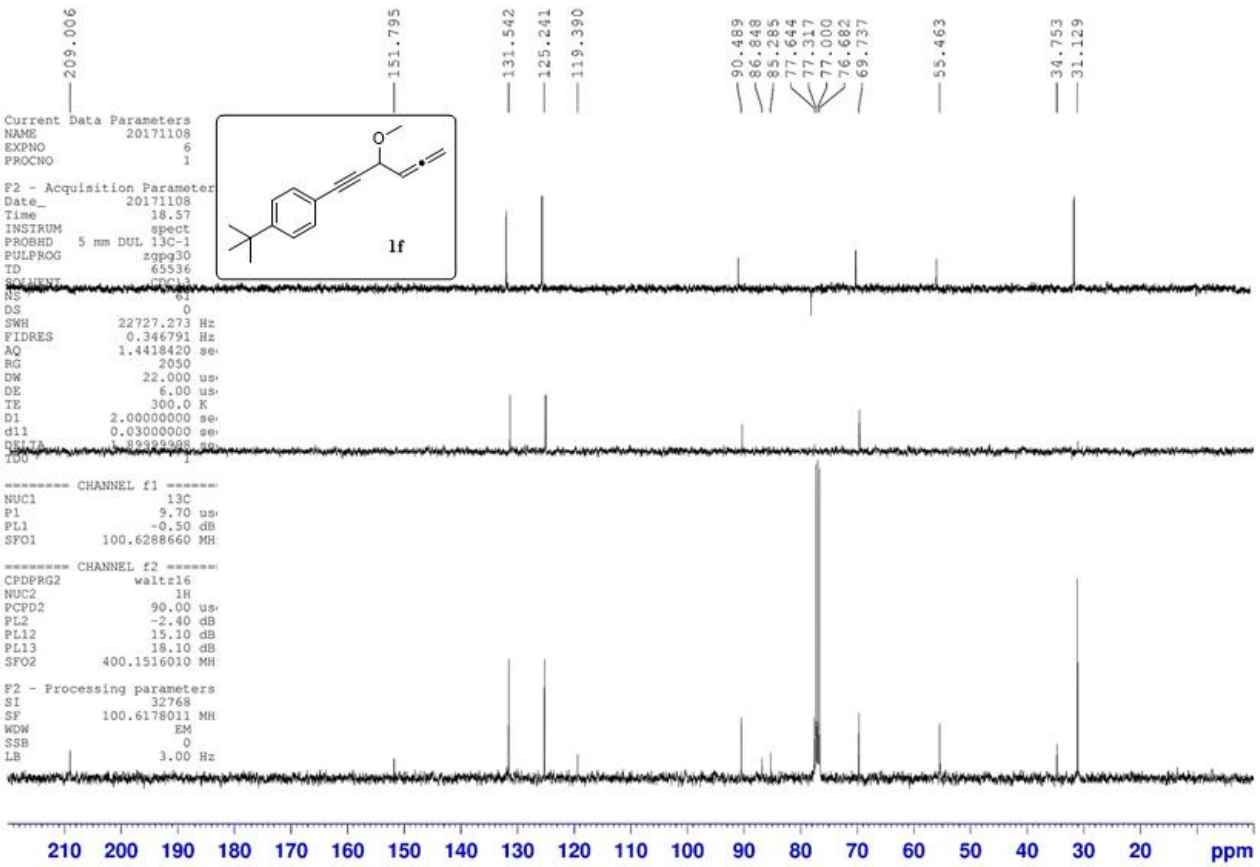

7.393
7.386
7.381
7.369
7.364
7.357
7.240
6.831
6.824
6.819
6.807
6.802
6.795
5.366
5.349
5.332
5.315
4.945
4.944
4.940
4.939
4.928
4.923
4.777
4.772
4.767
4.759
4.755
4.750
3.788
3.434
1d
10
9
8
7
6
5
4
3
2
1
ppm
2.09
2.08
1.04
2.04
1.00
3.28
3.16

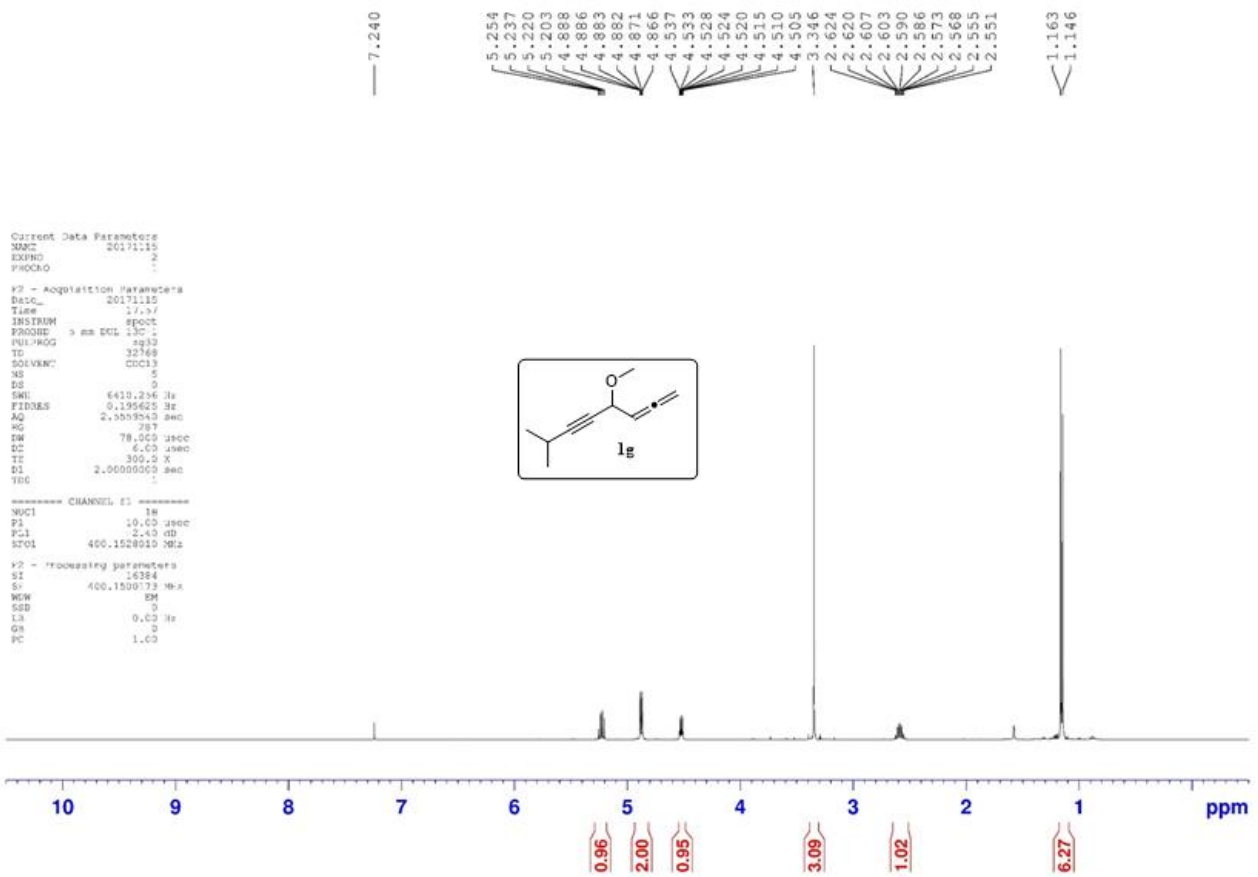

208.994
159.763
133.290
114.513
113.868
90.525
86.647
84.629
77.595
77.318
77.000
76.683
69.801
55.480
55.260
1d
Current Data Parameters
NAME 1
EXPNO 5
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171018
Time 22.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
======== CHANNEL f1 ======
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178008 MH
WDW EM
SSB 0
LB 3.00 Hz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

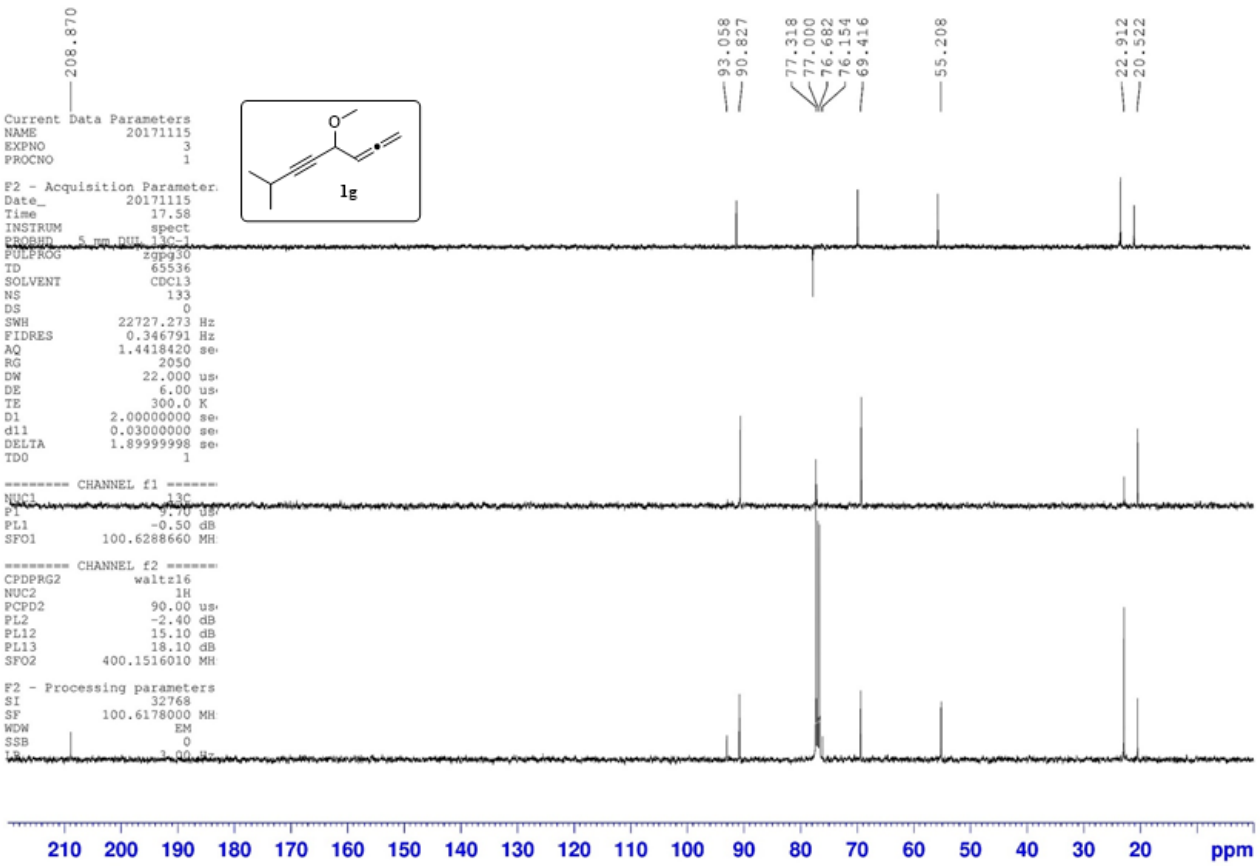

7.343
7.339
7.327
7.323
7.318
7.240
7.105
7.085
7.084
5.371
5.354
5.338
5.321
4.950
4.948
4.945
4.943
4.933
4.928
4.788
4.783
4.778
4.770
4.765
4.760
3.439
2.326
1e
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
0.98
2.06
0.94
3.21
3.09

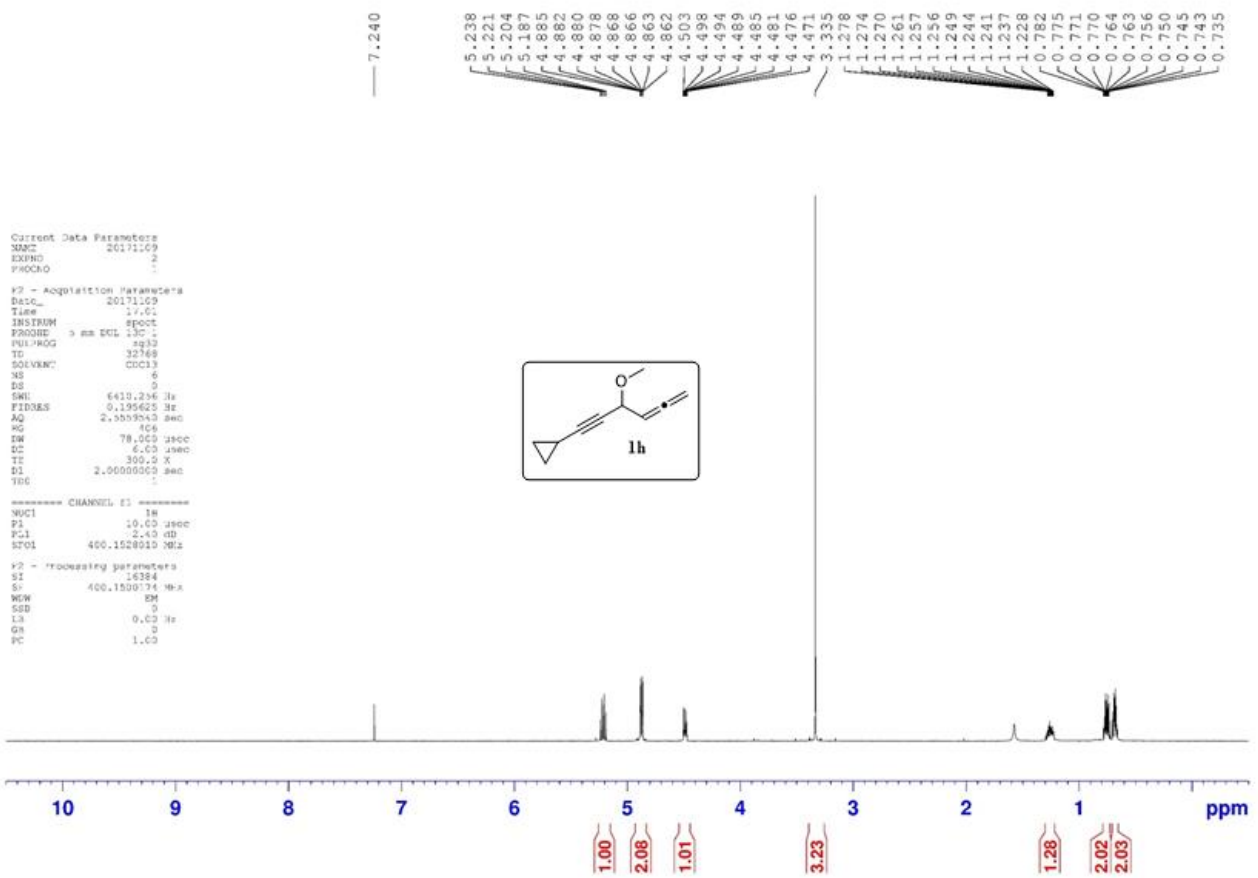

208.996
138.653
131.701
128.988
119.323
90.450
86.841
85.282
77.639
77.318
77.000
76.683
69.757
55.501
21.459
1e
Current Data Parameters
NAME 20171103
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171103
Time 10.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 68
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
NUC1 13C
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178021 MH
WDW EM
SSB 0
LB 3.00 Hz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

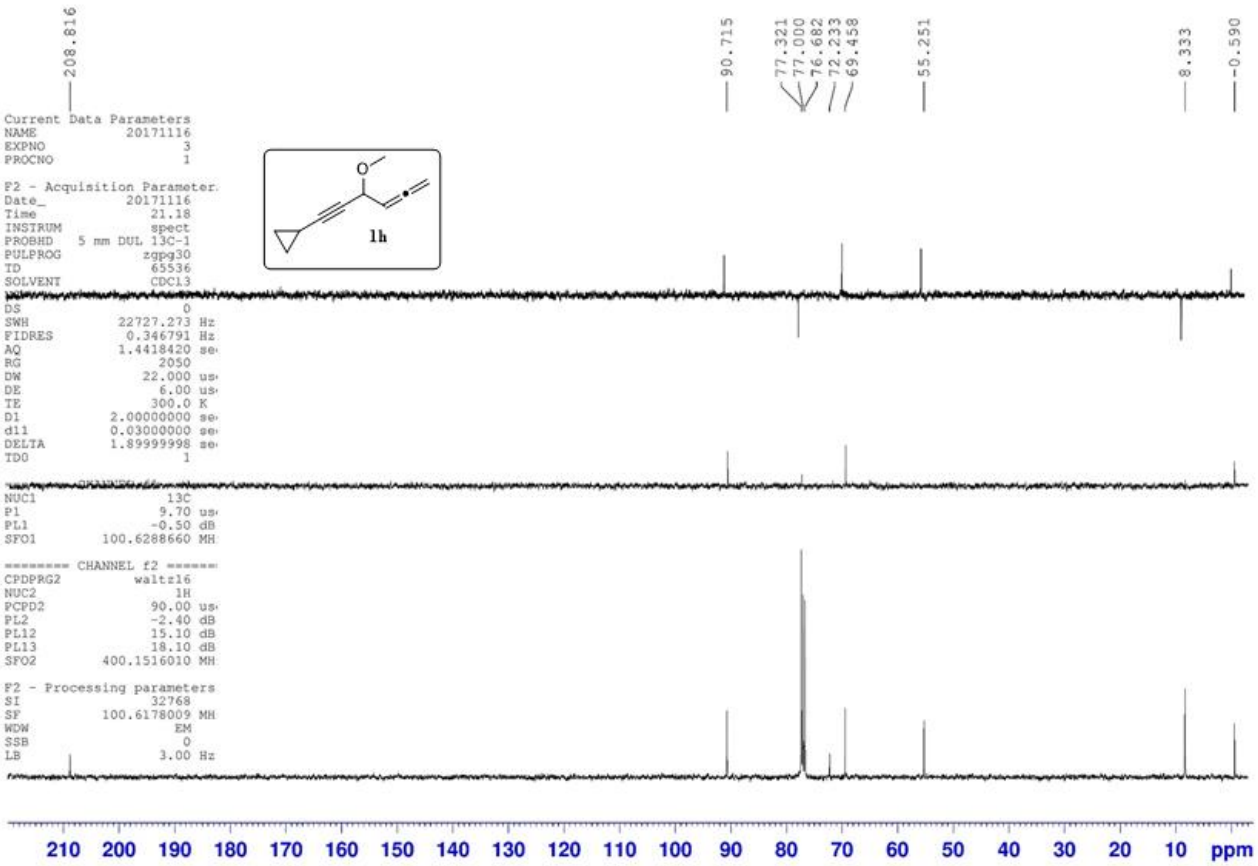

7.390
7.385
7.373
7.369
7.364
7.325
7.321
7.316
7.305
7.300
7.240
5.372
5.356
5.339
5.322
4.948
4.943
4.931
4.926
4.797
4.792
4.787
4.779
4.774
4.769
3.439
1.286
1f
10
9
8
7
6
5
4
3
2
1
ppm
2.08
2.04
0.99
2.02
0.98
3.00
9.30

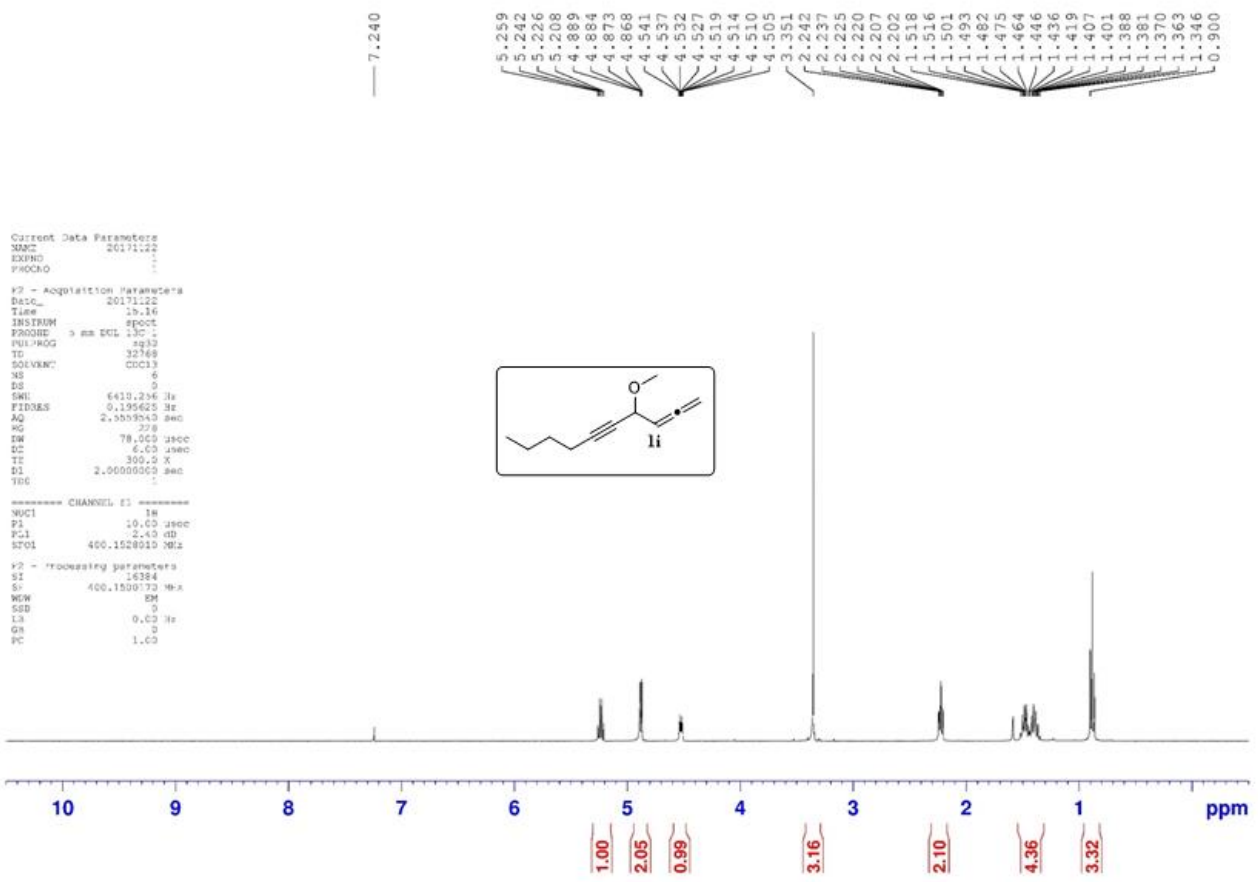

209.006
151.795
131.542
125.241
119.390
90.489
86.848
85.285
77.644
77.317
77.000
76.682
69.737
55.463
34.753
31.129
1f
Current Data Parameters
NAME 20171108
EXPNO 6
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171108
Time 18.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 61
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
ID0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178011 MH
WDW EM
SSB 0
LB 3.00 Hz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

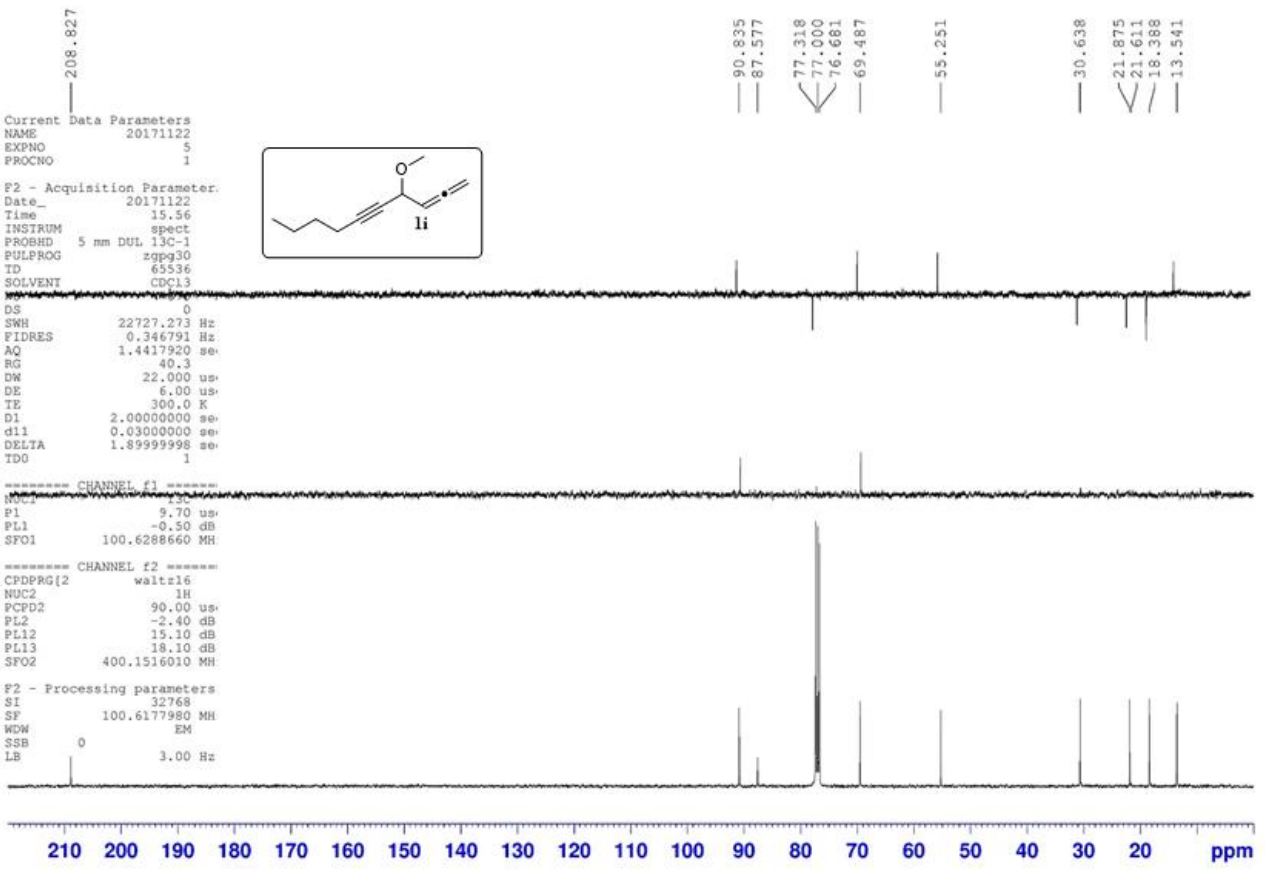

7.240
5.254
5.237
5.220
5.203
4.888
4.886
4.883
4.882
4.871
4.866
4.537
4.533
4.528
4.524
4.520
4.515
4.510
4.505
3.346
2.624
2.620
2.607
2.603
2.590
2.586
2.573
2.568
2.555
2.551
1.163
1.146
Current Data Parameters
NAME 20171115
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171115
Time 17.57
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559543 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
1g
10
9
8
7
6
5
4
3
2
1
ppm
0.96
2.00
0.95
3.09
1.02
6.27

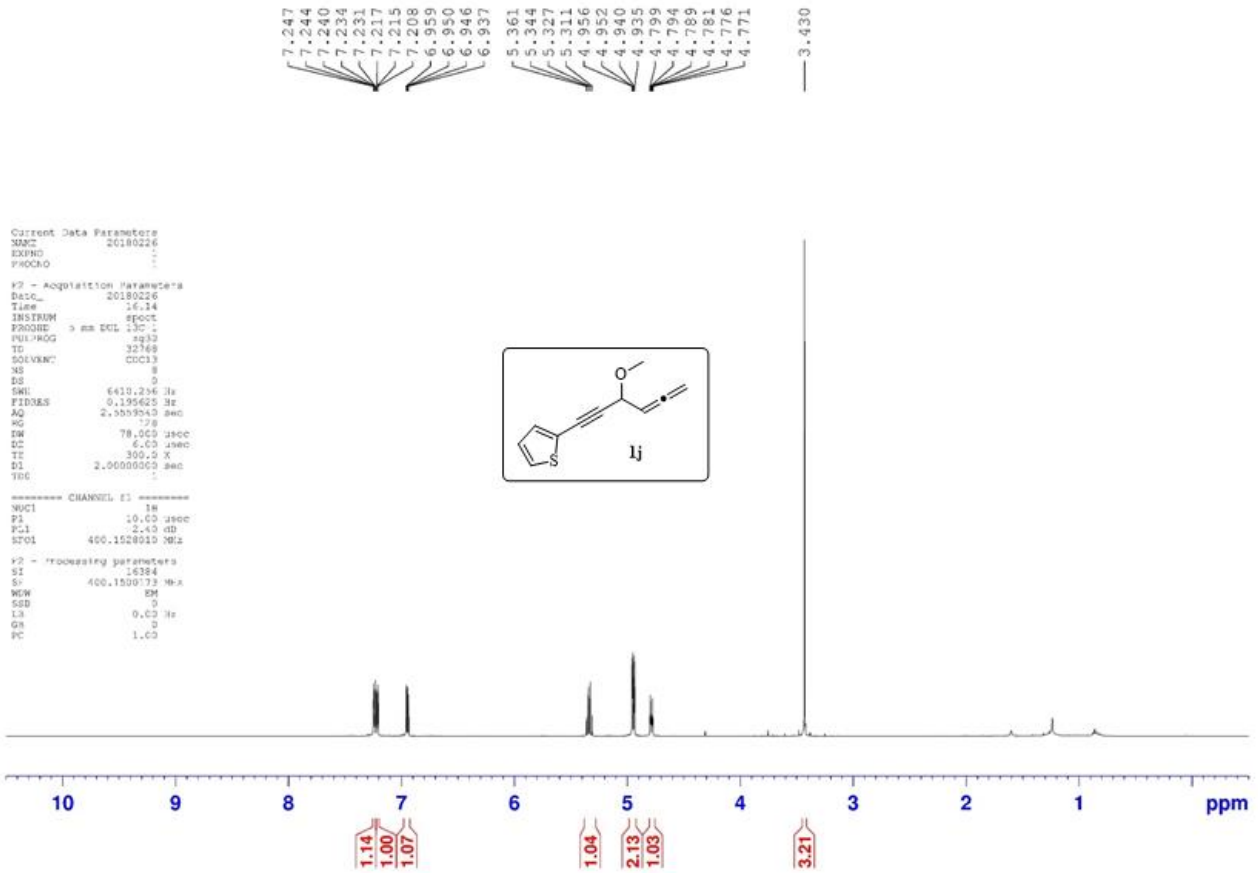

208.870
93.058
90.827
77.318
77.000
76.682
76.154
69.416
55.208
22.912
20.522
1g
Current Data Parameters
NAME 20171115
EXPNO 3
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171115
Time 17.58
INSTRUM spect
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 133
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
======== CHANNEL f1 ======
NUC1 13C
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178000 MH
WDW EM
SSB 0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

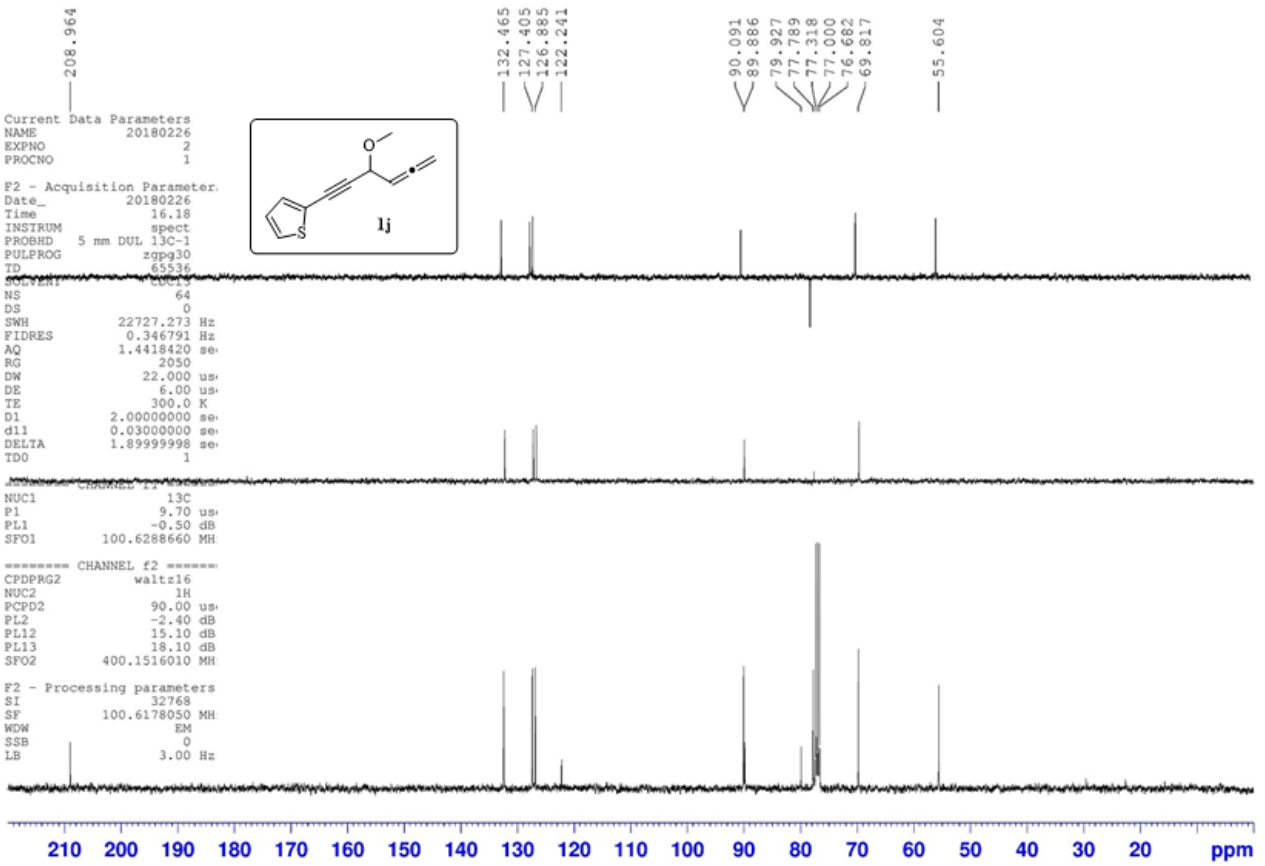

7.240
5.238
5.221
5.204
5.187
4.885
4.882
4.880
4.878
4.868
4.866
4.863
4.862
4.503
4.498
4.494
4.489
4.485
4.481
4.476
4.471
3.335
1.278
1.274
1.270
1.261
1.257
1.256
1.249
1.244
1.241
1.237
1.228
0.782
0.775
0.771
0.770
0.764
0.763
0.756
0.750
0.745
0.743
0.735
1h
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.08
1.01
3.23
1.28
2.02
2.03

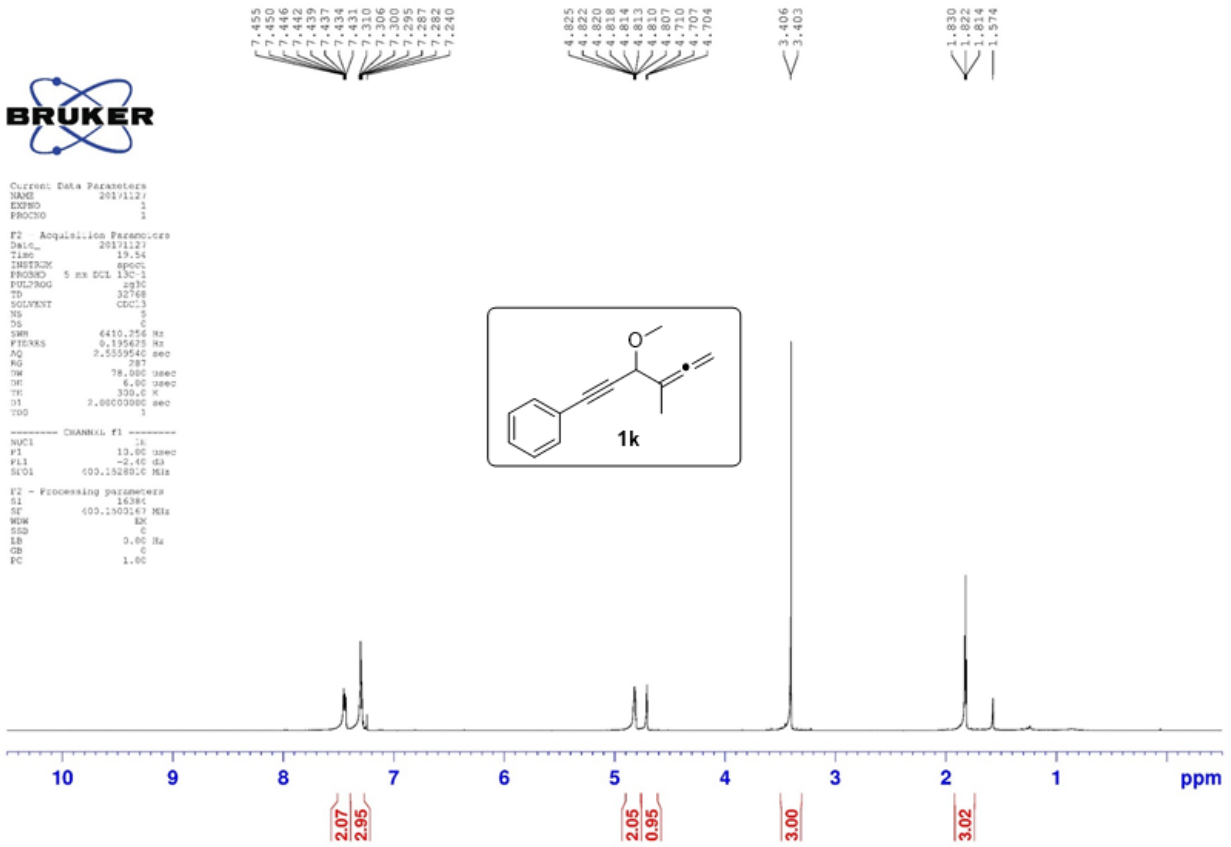

208.816
90.715
77.321
77.000
76.682
72.233
69.458
55.251
8.333
-0.590
Current Data Parameters
NAME 20171116
EXPNO 3
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171116
Time 21.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
NUC1 13C
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178009 MH
WDW EM
SSB 0
LB 3.00 Hz
1h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

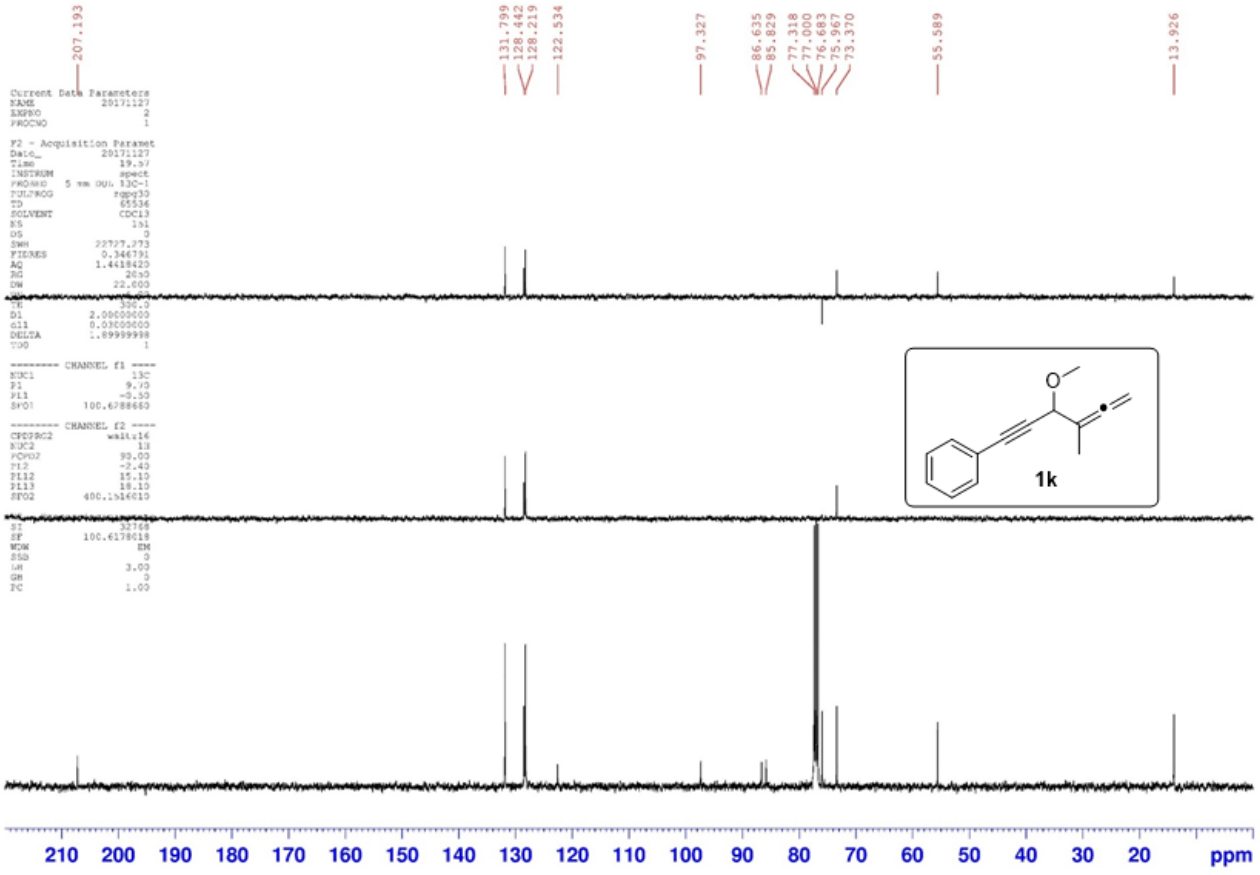

7.240
5.259
5.242
5.226
5.208
4.889
4.884
4.873
4.868
4.541
4.537
4.532
4.527
4.519
4.514
4.510
4.505
3.351
2.242
2.237
2.225
2.220
2.207
2.202
1.518
1.516
1.501
1.493
1.482
1.475
1.464
1.446
1.436
1.419
1.407
1.401
1.388
1.381
1.370
1.363
1.346
0.900
Current Data Parameters
NAME 20171122
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171122
Time 15.16
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559543 sec
RG 228
DW 78.000 usec
DE 6.00 usec
TE 300.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 2.40 dB
SFO1 400.1520010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
1i
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.05
0.99
3.16
2.10
4.36
3.32

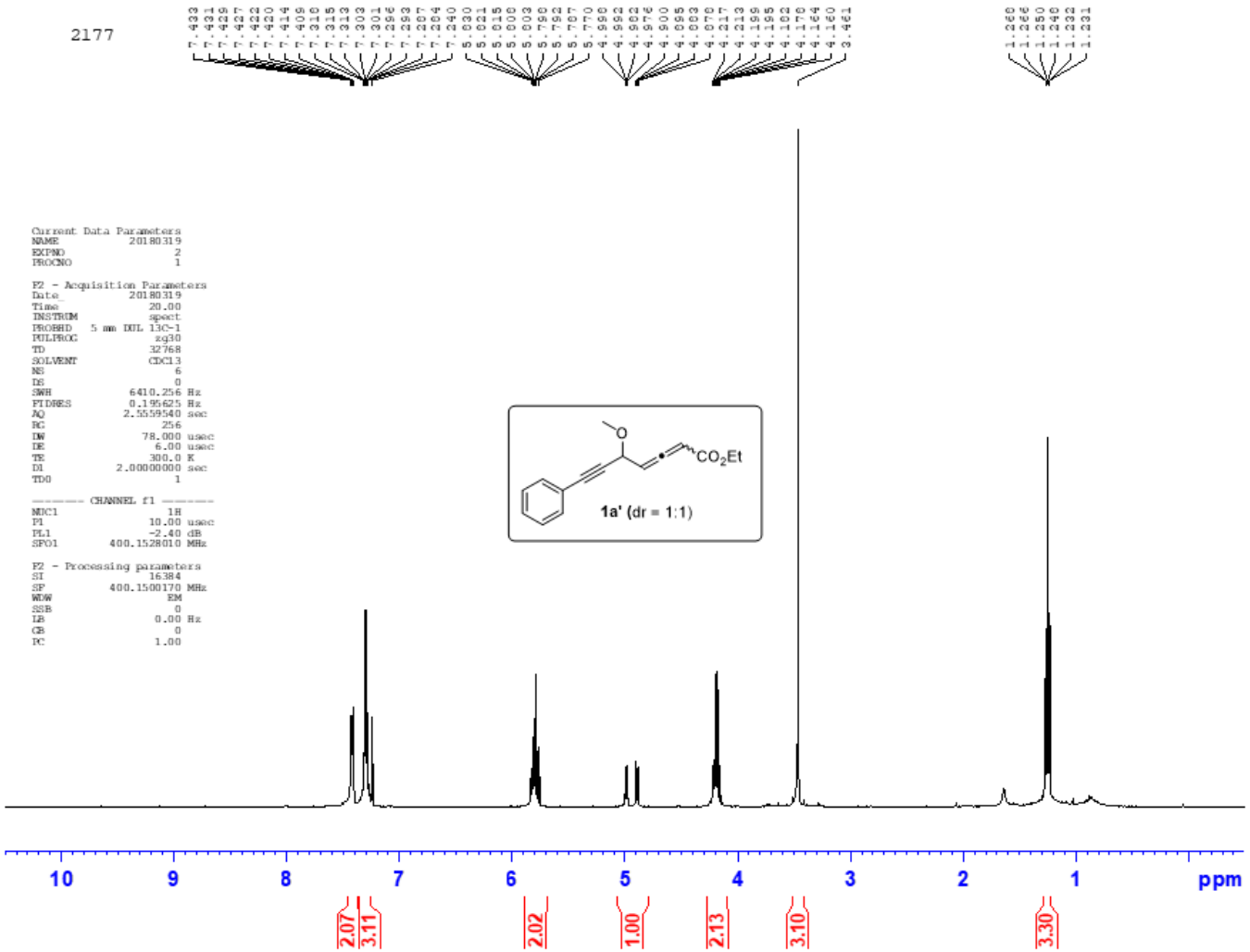

208.827
90.835
87.577
77.318
77.000
76.681
69.487
55.251
30.638
21.875
21.611
18.388
13.541
1i
Current Data Parameters
NAME 20171122
EXPNO 5
PROCNO 1
F2 - Acquisition Parameter
Date_ 20171122
Time 15.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4417920 se
RG 40.3
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
======== CHANNEL f1 ======
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6177980 MH
WDW EM
SSB 0
LB 3.00 Hz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

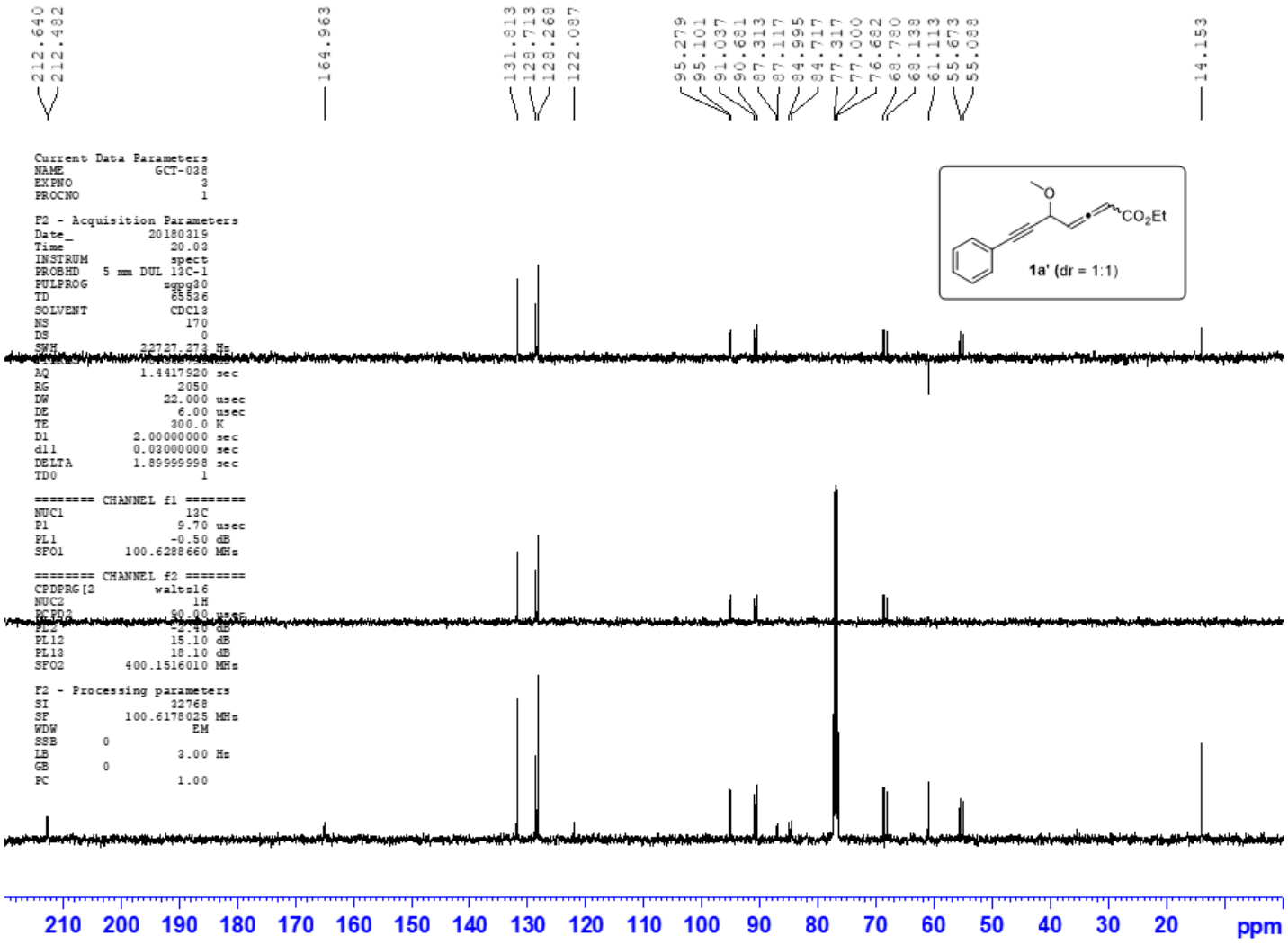

7.247
7.244
7.240
7.234
7.231
7.217
7.215
7.208
6.959
6.950
6.946
6.937
5.361
5.344
5.327
5.311
4.956
4.952
4.940
4.935
4.799
4.794
4.789
4.781
4.776
4.771
3.430
1j
10
9
8
7
6
5
4
3
2
1
ppm
1.14
1.00
1.07
1.04
2.13
1.03
3.21

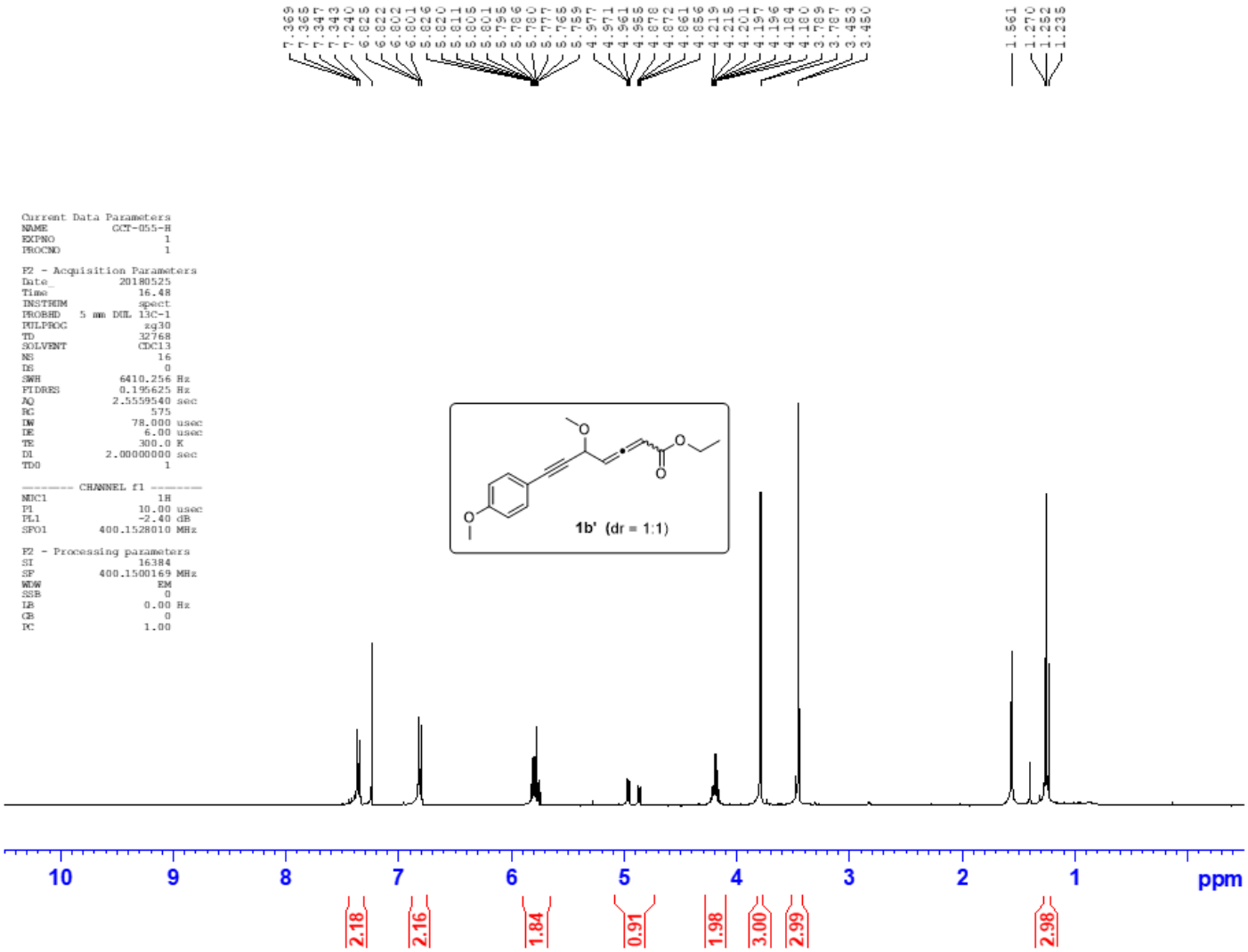

208.964
132.465
127.405
126.885
122.241
90.091
89.886
79.927
77.789
77.318
77.000
76.682
69.817
55.604
O
S
1j
Current Data Parameters
NAME 20180226
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20180226
Time 16.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 64
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 se
RG 2050
DW 22.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1
NUC1 13C
P1 9.70 us
PL1 -0.50 dB
SFO1 100.6288660 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 us
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MH
F2 - Processing parameters
SI 32768
SF 100.6178050 MH
WDW EM
SSB 0
LB 3.00 Hz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

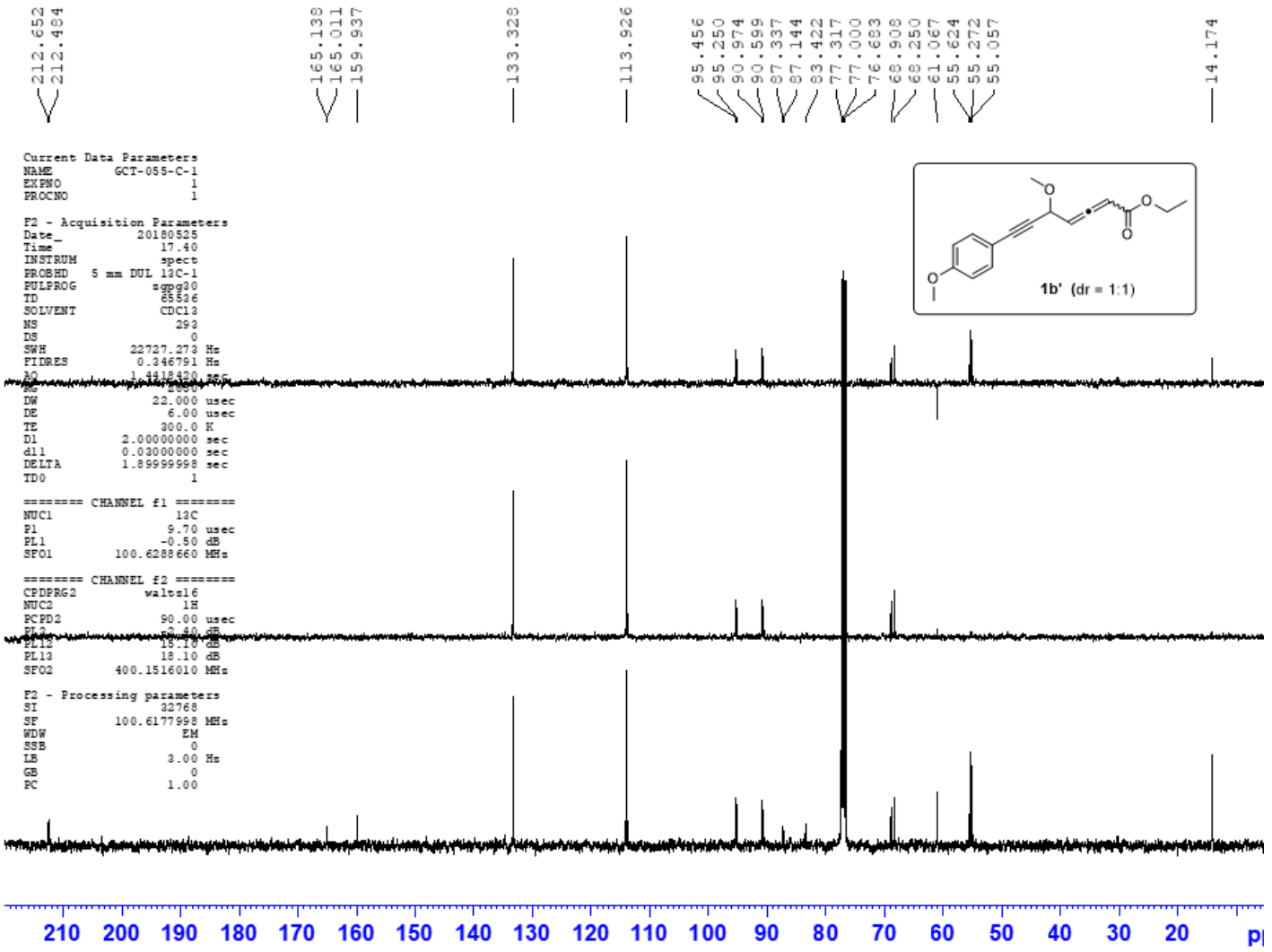

7.455
7.450
7.446
7.442
7.439
7.437
7.434
7.431
7.310
7.306
7.300
7.295
7.287
7.282
7.240
4.825
4.822
4.820
4.818
4.814
4.813
4.810
4.807
4.710
4.707
4.704
3.406
3.403
1.830
1.822
1.814
1.574
BRUKER
Current Data Parameters
NAME 20171127
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171127
Time 19.54
INSTRUM spect
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -2.40 dB
SFO1 600.1328800 MHz
F2 - Processing parameters
SI 16384
SF 600.1300167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
1k
10
9
8
7
6
5
4
3
2
1
ppm
2.07
2.95
2.05
0.95
3.00
3.02

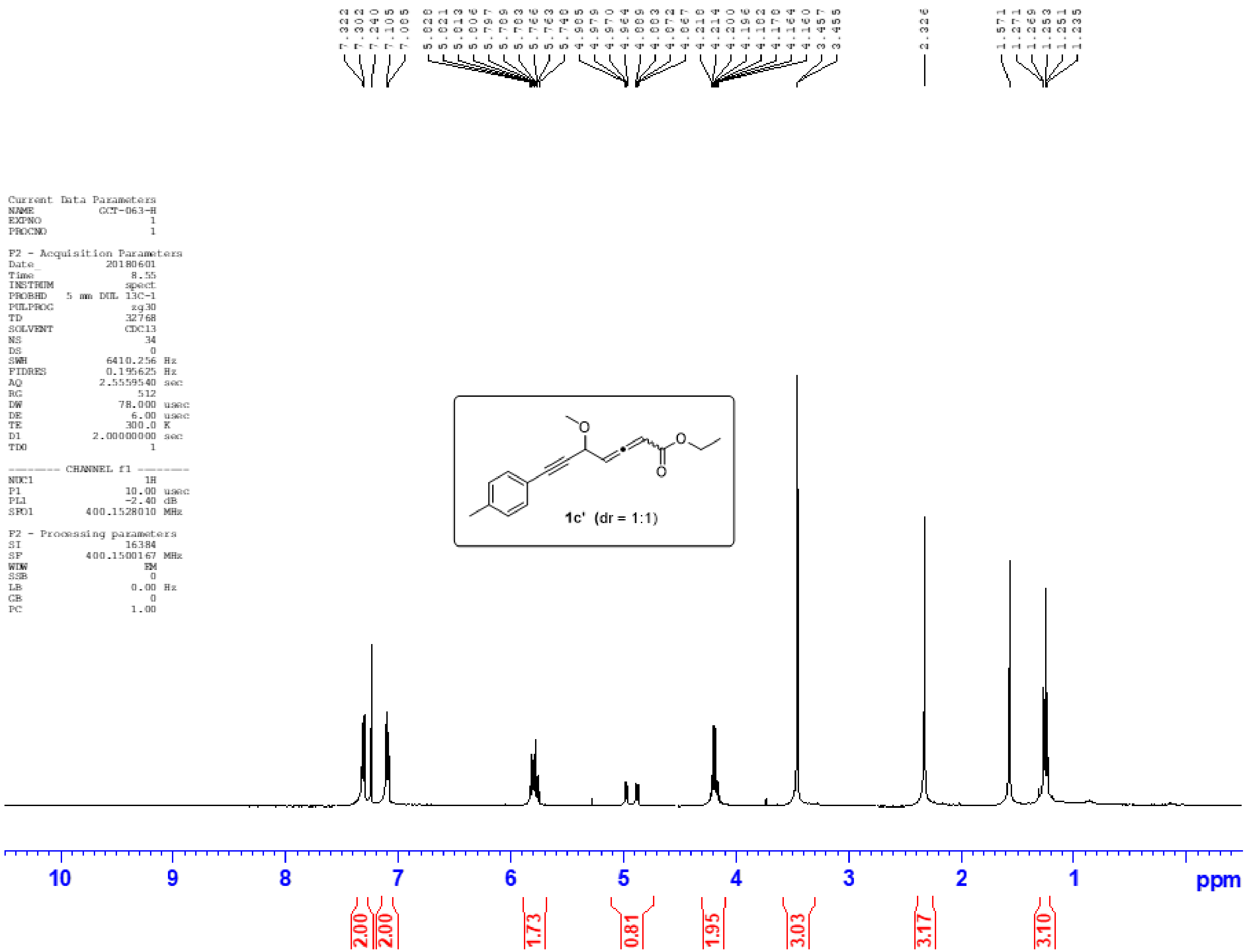

207.193
131.799
128.442
128.219
122.534
97.327
86.635
85.829
77.318
77.000
76.683
75.967
73.370
55.589
13.926
1k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

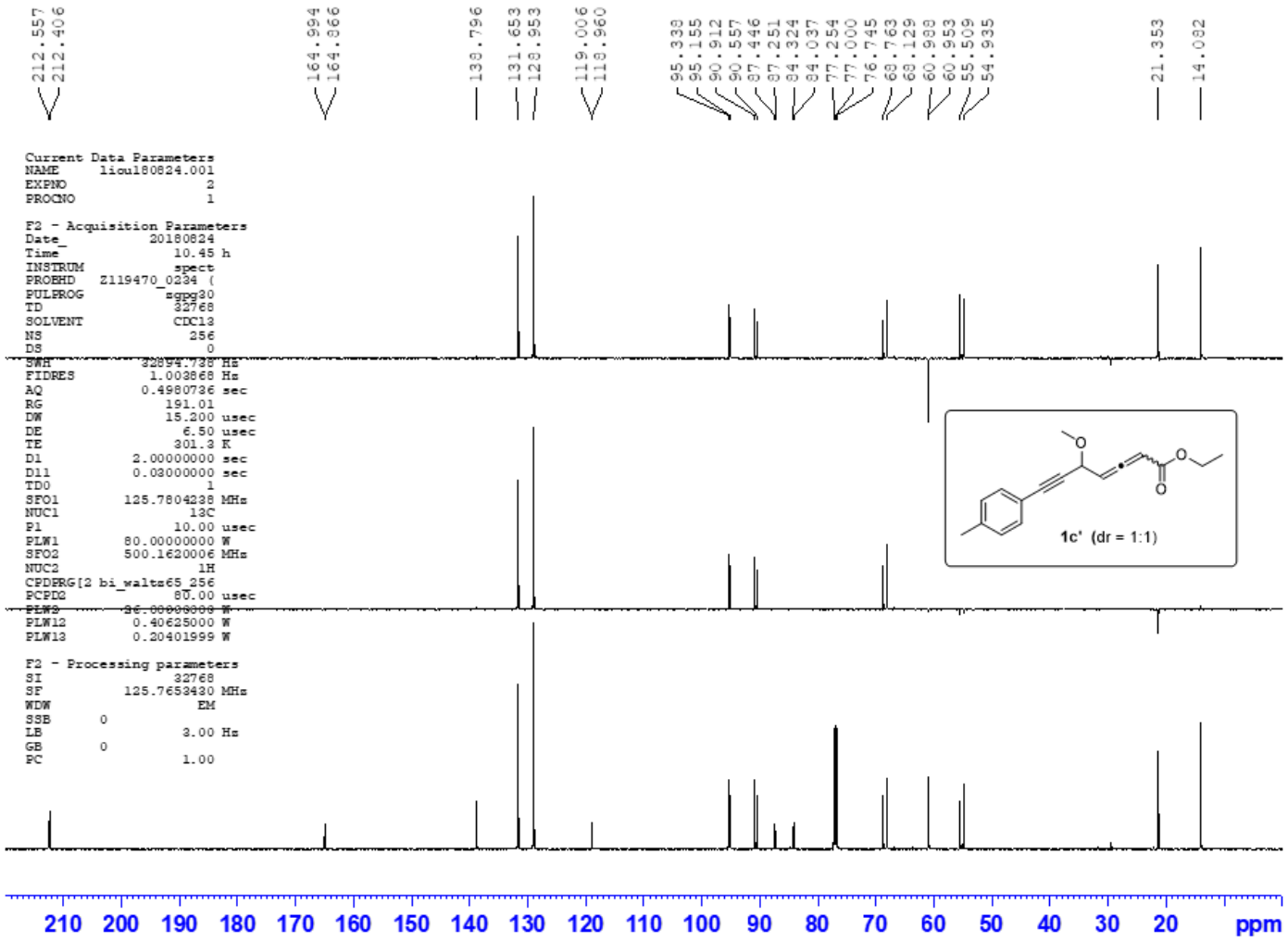

2177
Current Data Parameters
NAME 20180319
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180319
Time 20.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 256
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 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 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
CO2Et
1a' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
2.07
3.11
2.02
1.00
2.13
3.10
3.30

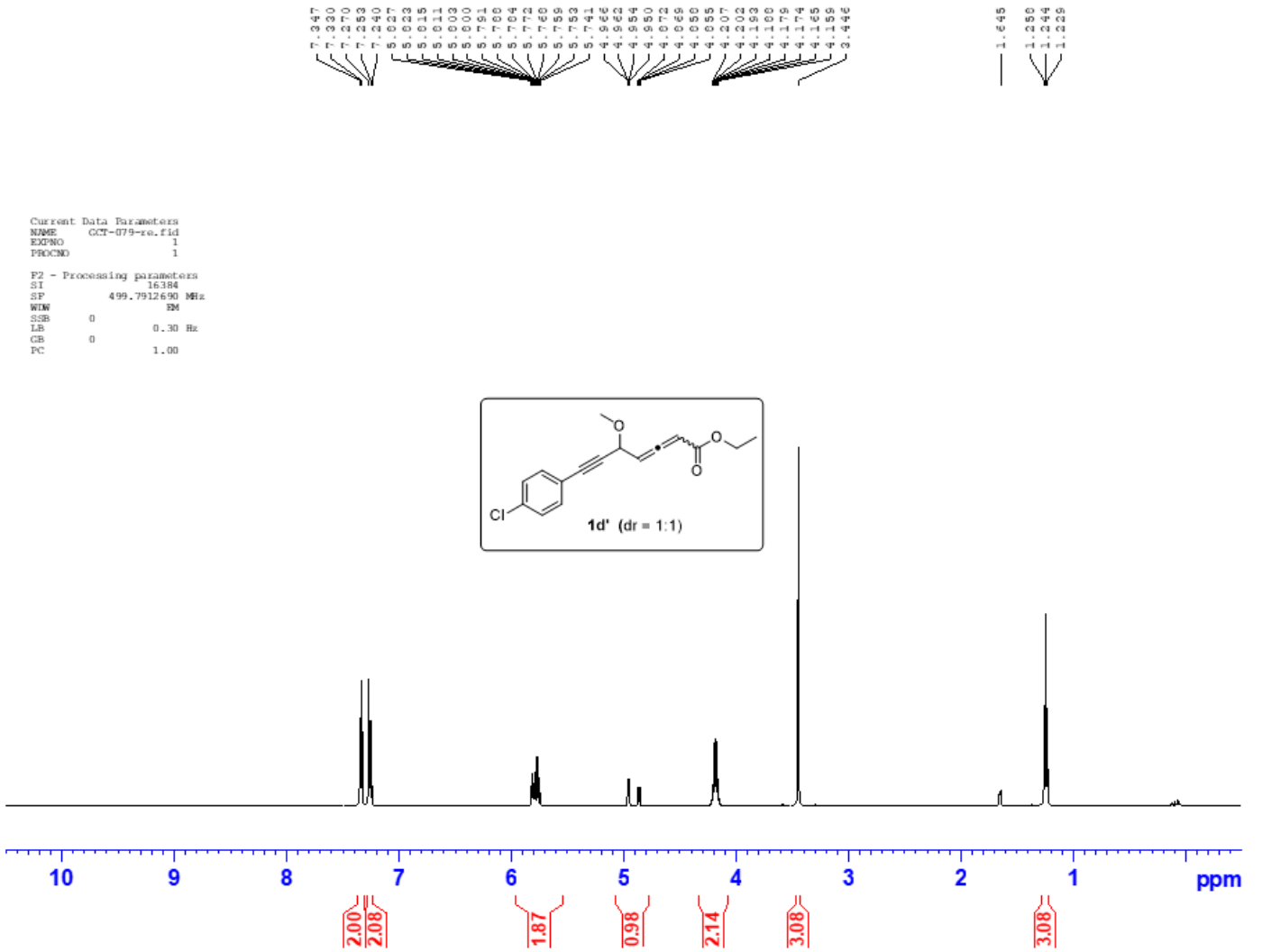

212.640
212.482
164.963
131.813
128.713
128.260
122.087
95.279
95.101
91.037
90.681
87.313
87.117
84.995
84.717
77.317
77.000
76.682
69.780
69.138
61.113
55.673
55.088
14.153
Current Data Parameters
NAME GCT-038
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180319
Time 20.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 170
DS 0
AQ 1.4417920 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178025 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
CO2Et
1a' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

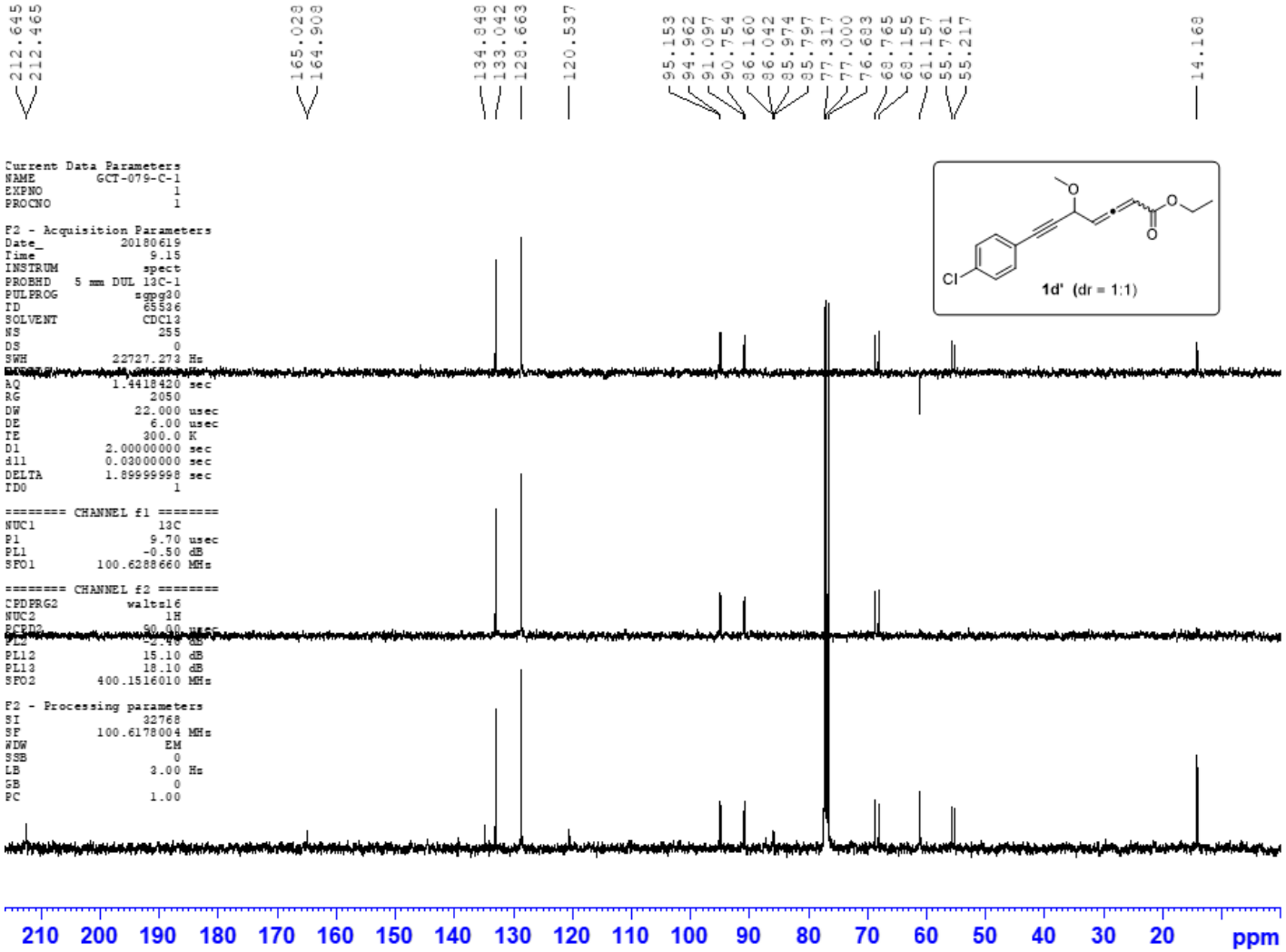

7.369
7.365
7.347
7.343
7.240
6.625
6.622
6.602
6.601
5.626
5.620
5.611
5.605
5.601
5.795
5.786
5.780
5.777
5.768
5.759
4.577
4.571
4.561
4.555
4.678
4.672
4.661
4.656
4.219
4.215
4.201
4.197
4.196
4.184
4.180
3.789
3.787
3.483
3.480
1.561
1.270
1.252
1.235
Current Data Parameters
NAME GCT-055-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180525
Time 16.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1b' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
2.18
2.16
1.84
0.91
1.98
3.00
2.99
2.98

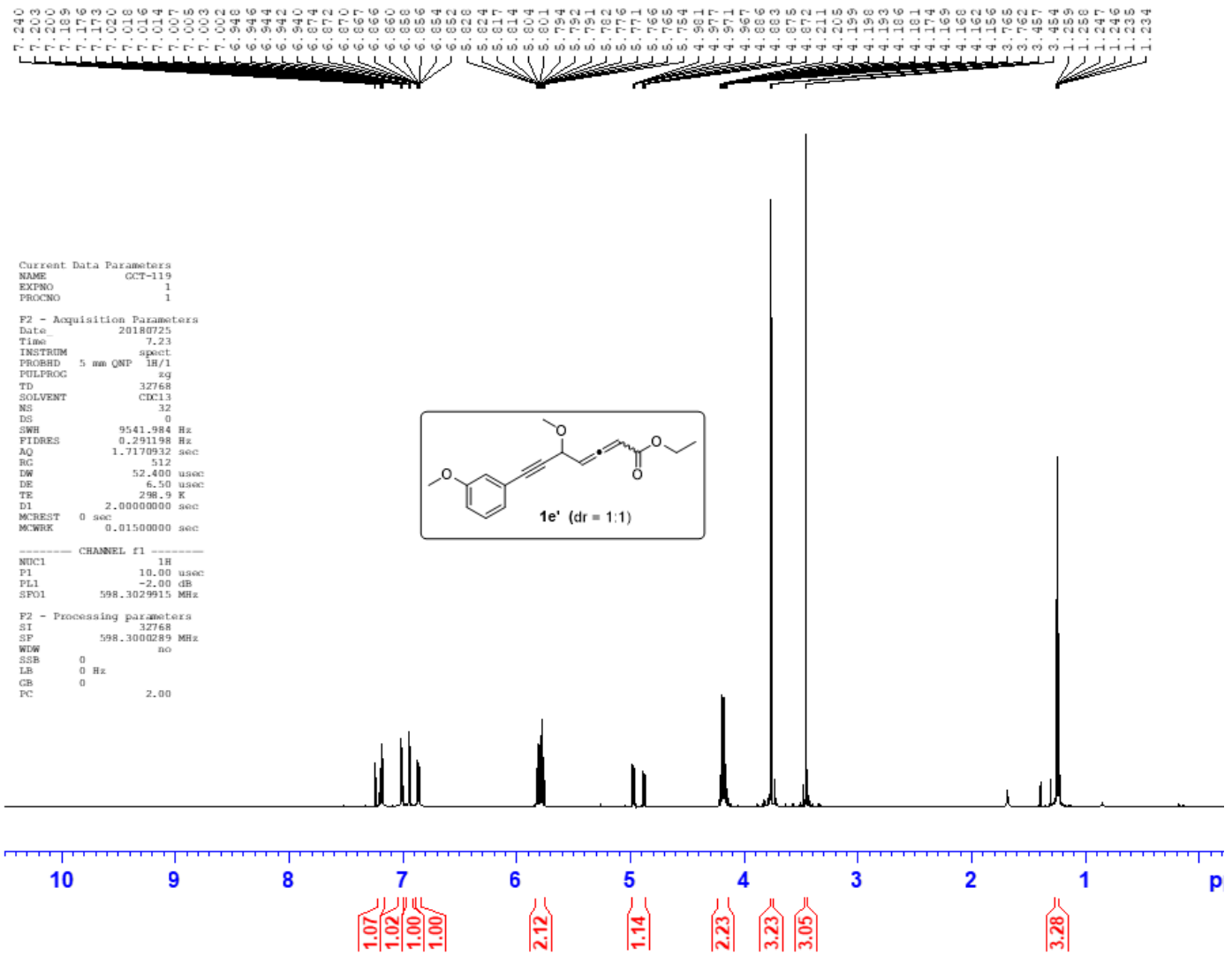

212.652
212.484
165.138
165.011
159.937
133.328
113.926
95.456
95.250
90.974
90.599
87.337
87.144
83.422
77.317
77.000
76.683
68.908
68.250
61.067
55.624
55.272
55.057
14.174
Current Data Parameters
NAME GCT-055-C-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180525
Time 17.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 293
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 18.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177998 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1b' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 p

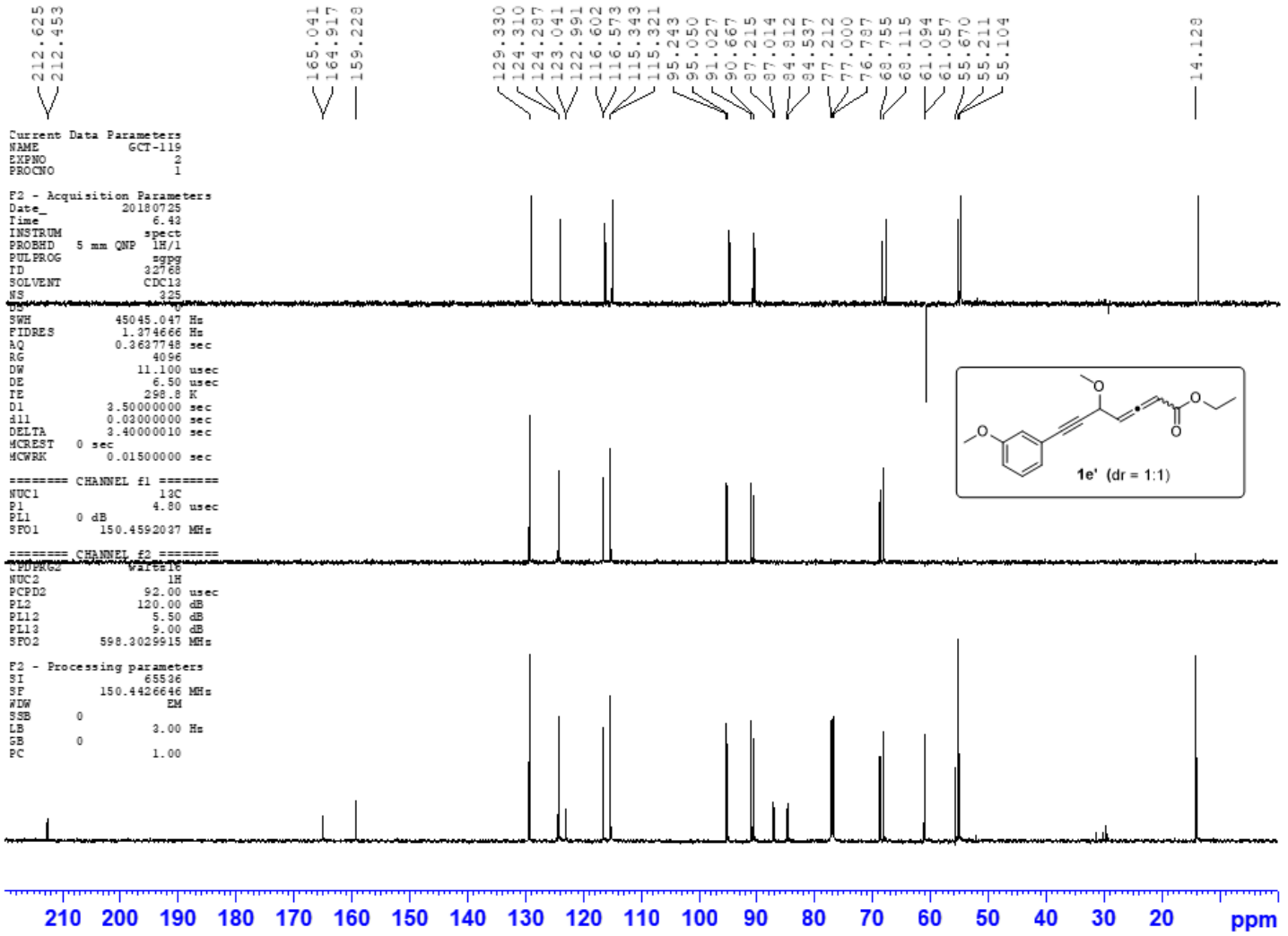

7.322
7.302
7.240
7.105
7.085
5.828
5.821
5.813
5.806
5.797
5.789
5.783
5.766
5.763
5.740
4.985
4.979
4.970
4.964
4.889
4.883
4.872
4.867
4.218
4.214
4.200
4.196
4.182
4.178
4.164
4.160
3.457
3.455
2.326
1.571
1.271
1.269
1.253
1.251
1.235
Current Data Parameters
NAME GCT-063-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180601
Time 8.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 34
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
O
O
1c' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
1.73
0.81
1.95
3.03
3.17
3.10

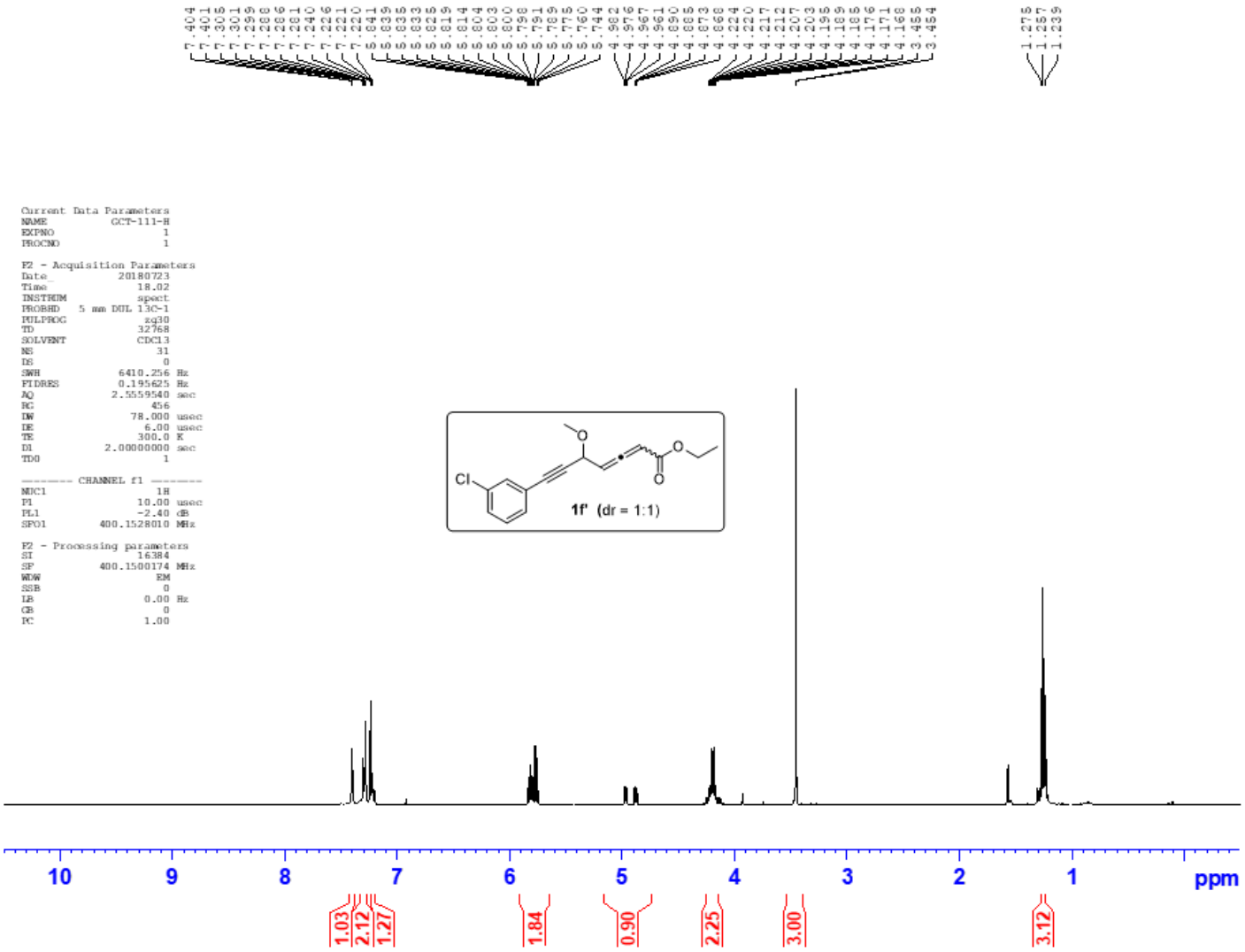

212.557
212.406
164.994
164.866
139.796
131.653
128.953
119.006
118.960
95.338
95.155
90.912
90.557
87.446
87.251
84.324
84.037
77.254
77.000
76.745
68.763
68.129
60.988
60.953
55.509
54.935
21.353
14.082
Current Data Parameters
NAME liou180824.001
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180824
Time 10.45 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 256
DS 0
SWH 32894.738 Hz
FIDRES 1.003868 Hz
AQ 0.4980736 sec
RG 191.01
DW 15.200 usec
DE 6.50 usec
TE 301.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804238 MHz
NUC1 13C
P1 10.00 usec
PLW1 80.00000000 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 bi_walts65_256
PCPD2 80.00 usec
PLW2 36.00000000 W
PLW12 0.40625000 W
PLW13 0.20401999 W
F2 - Processing parameters
SI 32768
SF 125.7653430 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1c' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

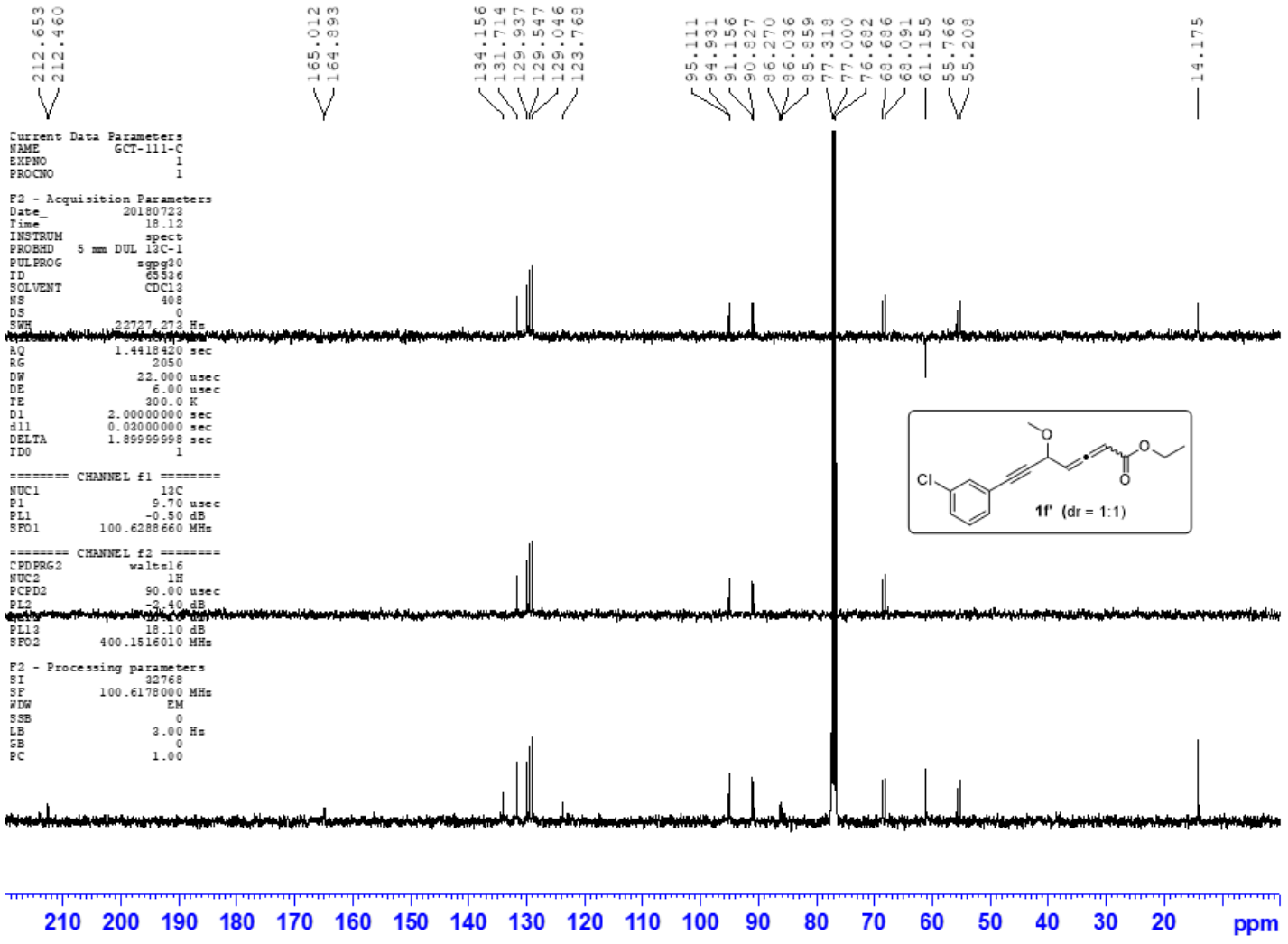

7.347
7.330
7.270
7.253
7.240
5.627
5.623
5.615
5.611
5.603
5.600
5.761
5.760
5.764
5.772
5.760
5.756
5.753
5.741
4.966
4.962
4.954
4.950
4.672
4.656
4.650
4.207
4.203
4.193
4.180
4.179
4.174
4.165
4.159
3.946
1.645
1.250
1.244
1.229
Current Data Parameters
NAME GCT-079-re.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 16384
SF 499.7912690 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
O
Cl
1d' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.08
1.87
0.98
2.14
3.08
3.08

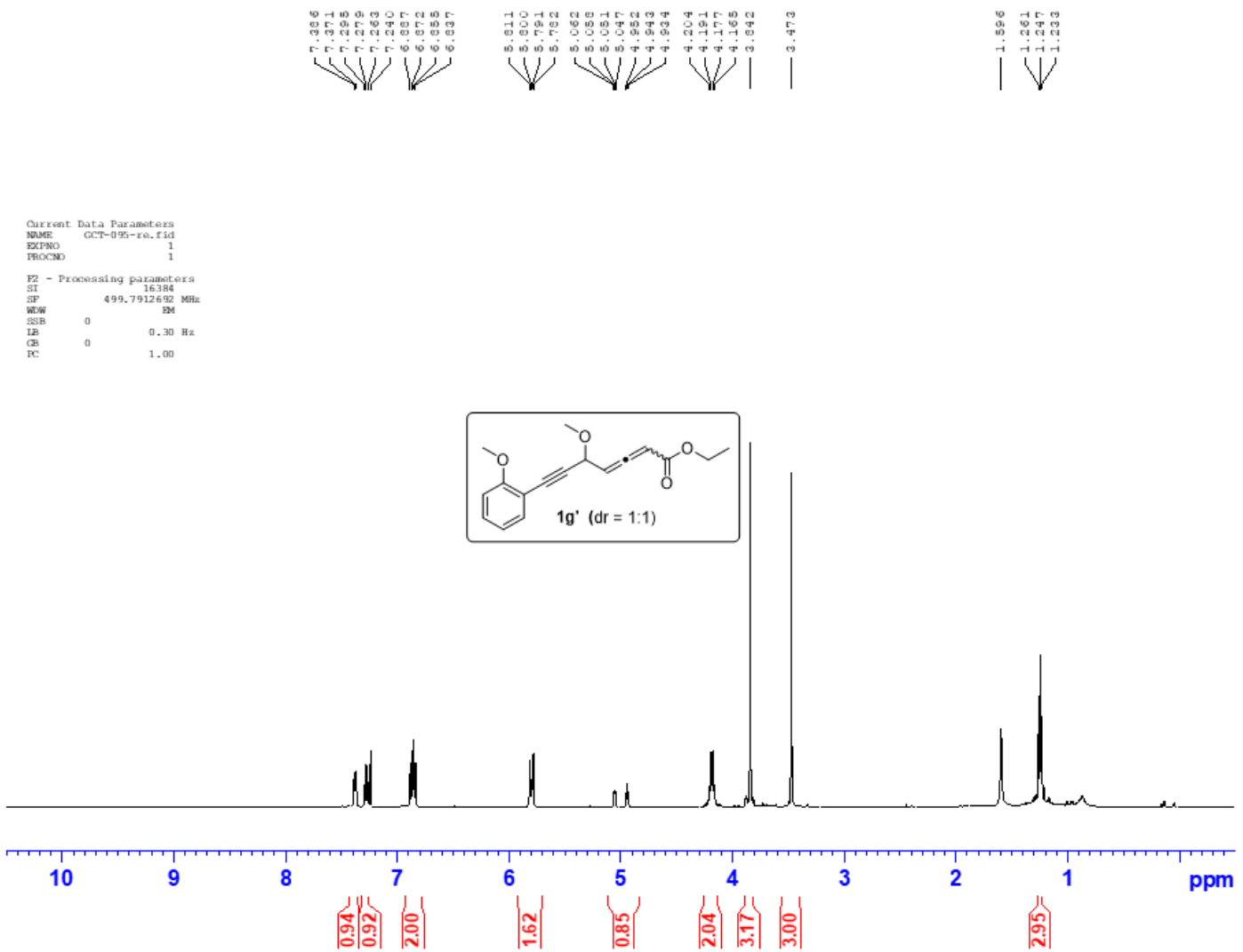

212.645
212.465
165.028
164.908
134.848
133.042
128.663
120.537
95.153
94.962
91.097
90.754
86.160
86.042
85.974
85.797
77.317
77.000
76.683
68.765
68.155
61.157
55.761
55.217
14.168
Current Data Parameters
NAME GCT-079-C-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180619
Time 9.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 255
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======= CHANNEL f1 =======
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======= CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178004 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
O
Cl
1d' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

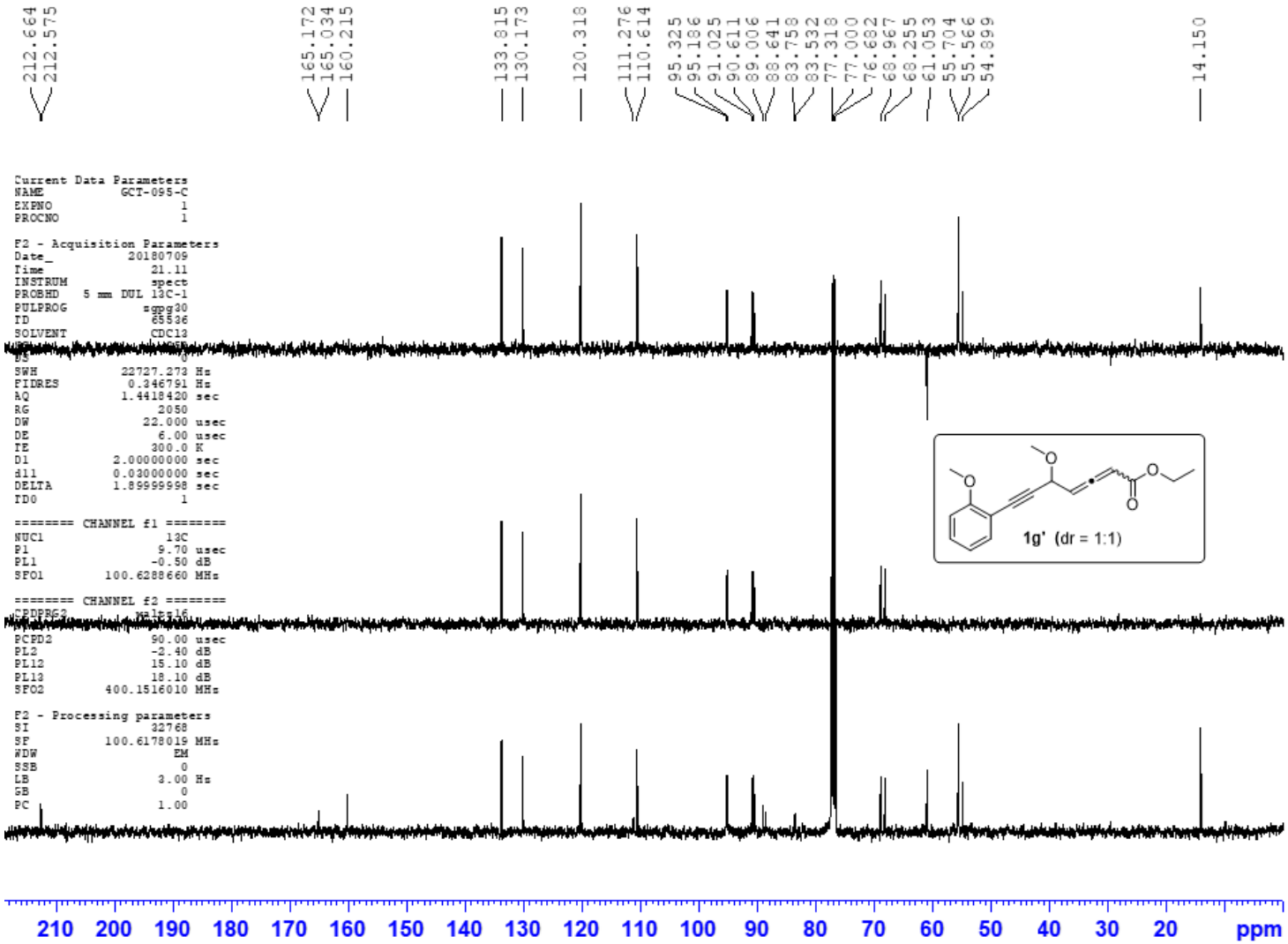

Current Data Parameters
NAME GCT-119
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180725
Time 7.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.3029915 MHz
F2 - Processing parameters
SI 32768
SF 598.3000289 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
1e' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
p
1.07
1.02
1.00
1.00
2.12
1.14
2.23
3.23
3.05
3.28

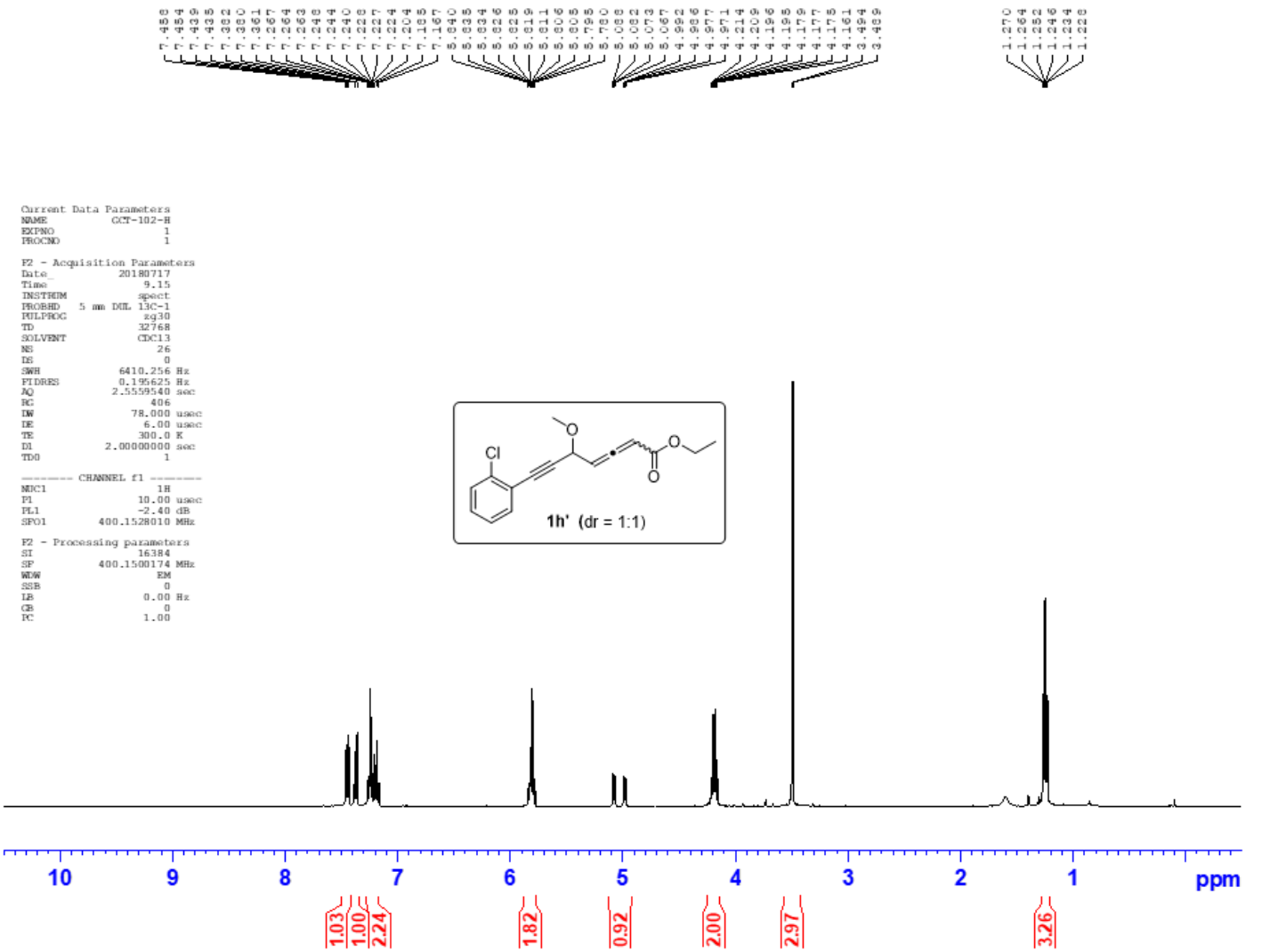

212.625
212.453
165.041
164.917
159.228
129.330
124.310
124.287
123.041
122.991
116.602
116.573
115.343
115.321
95.243
95.050
91.027
90.667
87.215
87.014
84.812
84.537
77.212
77.000
76.787
68.755
68.115
61.094
61.057
55.670
55.211
55.104
14.128
Current Data Parameters
NAME GCT-119
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180725
Time 6.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 325
DS 4
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 298.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426646 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1e' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

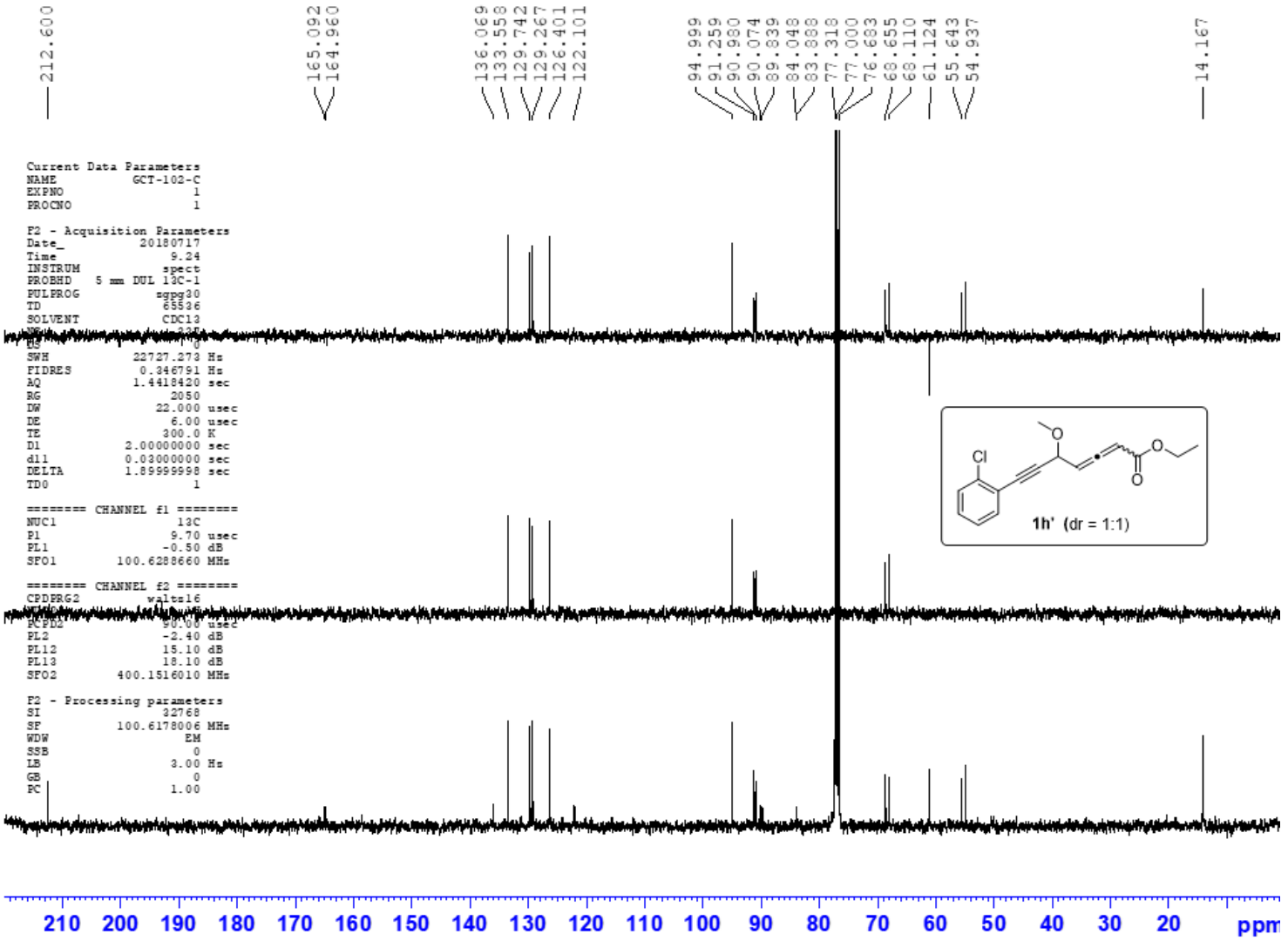

7.404
7.401
7.305
7.301
7.299
7.288
7.281
7.240
7.226
7.221
7.220
5.641
5.639
5.633
5.625
5.615
5.614
5.604
5.603
5.600
5.598
5.591
5.589
5.775
5.760
5.744
4.962
4.957
4.956
4.961
4.950
4.935
4.873
4.868
4.224
4.220
4.217
4.212
4.207
4.203
4.195
4.189
4.185
4.176
4.171
4.168
3.454
1.275
1.267
1.239
Current Data Parameters
NAME GCT-111-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180723
Time 18.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 31
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 456
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 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
O
O
O
1f' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
1.03
2.12
1.27
1.84
0.90
2.25
3.00
3.12

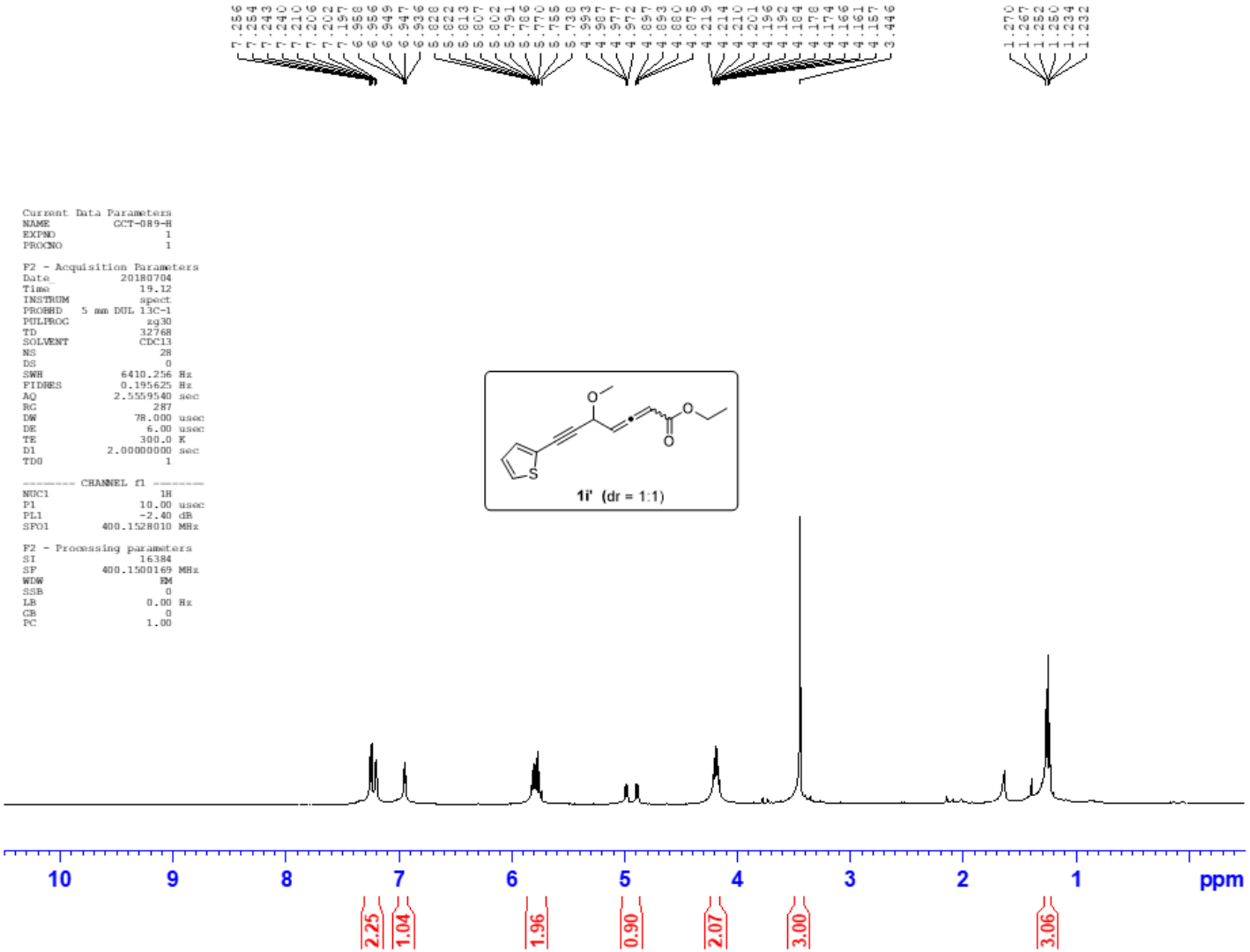

212.653
212.460
165.012
164.893
134.156
131.714
129.937
129.547
129.046
123.768
95.111
94.931
91.156
90.827
86.270
86.036
85.859
77.318
77.000
76.682
68.686
68.091
61.155
55.766
55.208
14.175
Current Data Parameters
NAME GCT-111-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180723
Time 18.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 408
DS 0
SWH 23727.273 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178000 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
O
O
O
1f' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

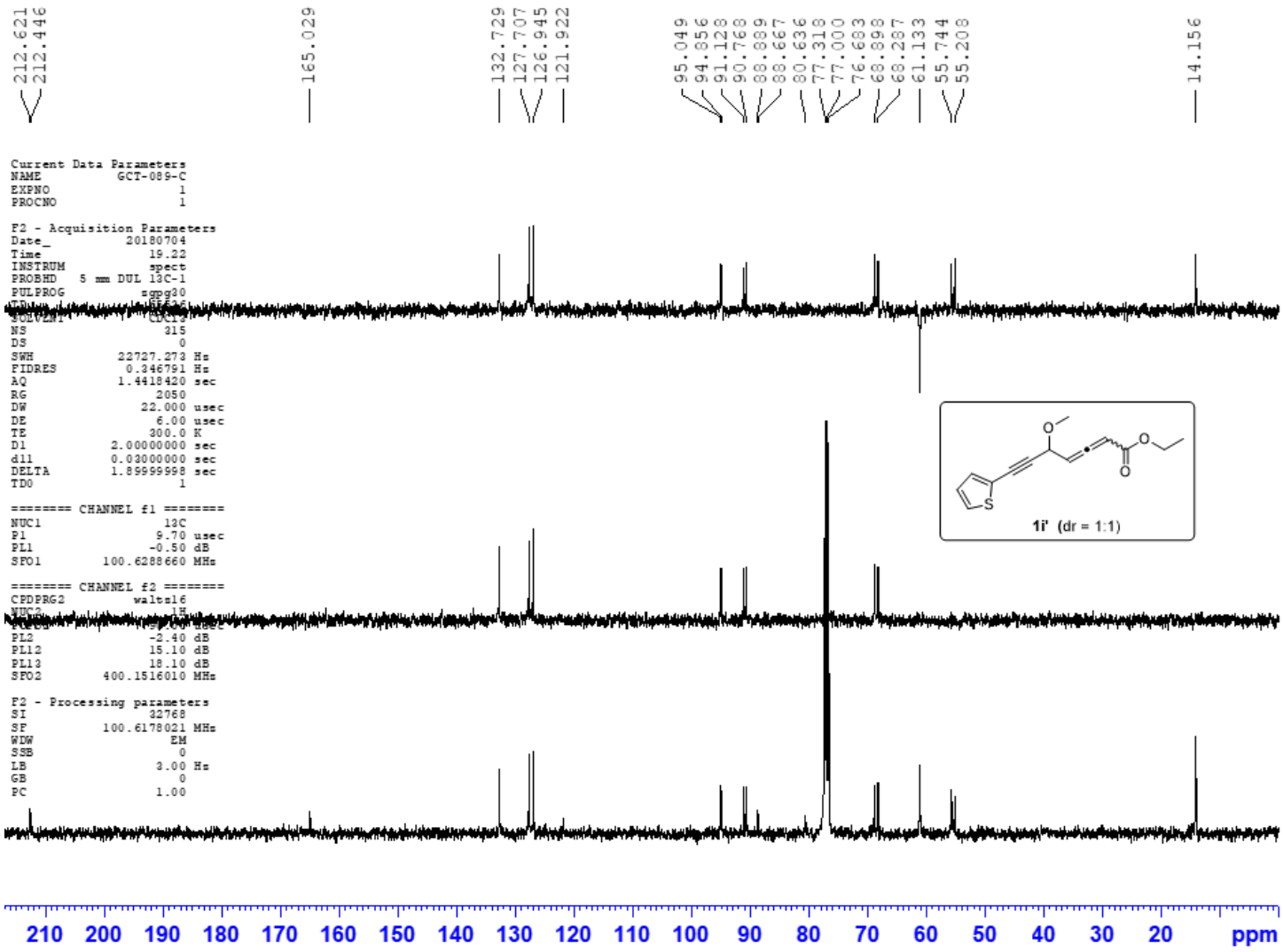

7.386
7.371
7.269
7.263
7.240
6.687
6.672
6.636
6.637
5.811
5.800
5.791
5.782
5.062
5.058
5.051
5.047
4.952
4.943
4.934
4.204
4.191
4.177
4.168
3.642
3.473
1.596
1.261
1.247
1.233
Current Data Parameters
NAME GCT-095-re.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 16384
SF 499.7912692 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1g' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
0.94
0.92
2.00
1.62
0.85
2.04
3.17
3.00
2.95

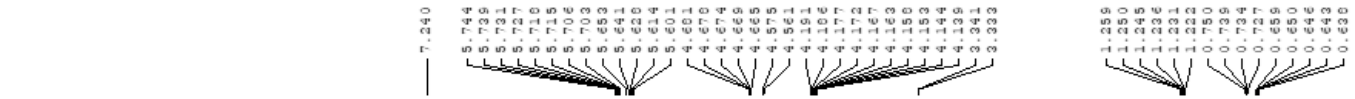

212.664
212.575
165.172
165.034
160.215
133.815
130.173
120.318
111.276
110.614
95.325
95.186
91.025
90.611
89.006
88.641
83.758
83.532
77.318
77.000
76.682
68.967
68.255
61.053
55.704
55.566
54.899
14.150
Current Data Parameters
NAME GCT-095-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180709
Time 21.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
SWH 22727.272 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
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 100.6178019 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1g' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.458
7.454
7.439
7.435
7.382
7.380
7.361
7.267
7.264
7.263
7.248
7.244
7.240
7.228
7.227
7.224
7.204
7.185
7.167
6.640
6.638
6.634
6.626
6.625
6.619
6.611
6.606
6.605
6.598
6.580
5.082
5.073
5.067
4.992
4.988
4.977
4.971
4.214
4.209
4.196
4.195
4.179
4.177
4.175
4.161
3.484
3.469
1.270
1.264
1.252
1.246
1.234
1.228
Current Data Parameters
NAME GCT-102-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180717
Time 9.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 26
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
O
O
O
1h' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
1.03
1.00
2.24
1.82
0.92
2.00
2.97
3.26

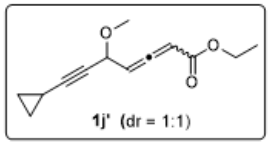

212.600
165.092
164.960
136.069
133.558
129.742
129.267
126.401
122.101
94.999
91.259
90.980
90.074
89.839
84.048
83.888
77.318
77.000
76.683
68.655
68.110
61.124
55.643
54.937
14.167
Current Data Parameters
NAME GCT-102-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180717
Time 9.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG sgpg30
TD 65536
SOLVENT CDC13
NS 8
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
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 100.6178006 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
O
O
O
1h' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

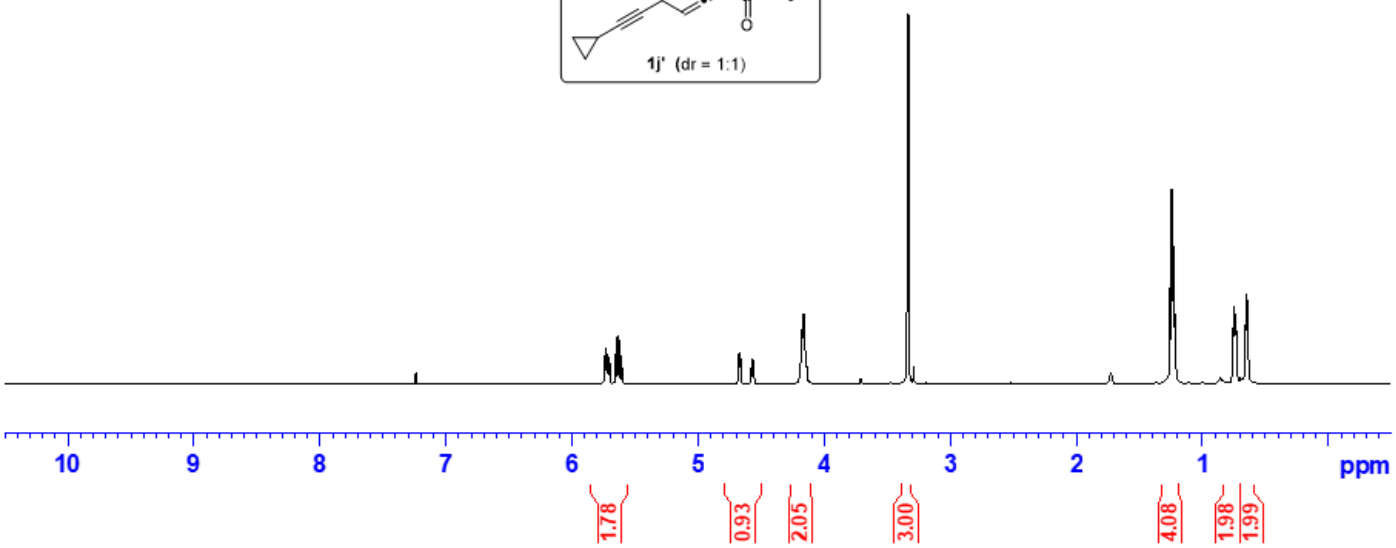

7.256
7.254
7.243
7.240
7.210
7.206
7.202
7.197
6.956
6.956
6.945
6.936
5.822
5.813
5.807
5.802
5.791
5.786
5.770
5.755
5.738
4.993
4.987
4.977
4.972
4.957
4.893
4.880
4.875
4.215
4.214
4.210
4.201
4.196
4.192
4.184
4.178
4.174
4.166
4.161
4.157
3.446
1.270
1.267
1.262
1.250
1.234
1.232
Current Data Parameters
NAME GCT-089-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20180704
Time 19.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 28
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1i' (dr = 1:1)
10
9
8
7
6
5
4
3
2
1
ppm
2.25
1.04
1.96
0.90
2.07
3.00
3.06

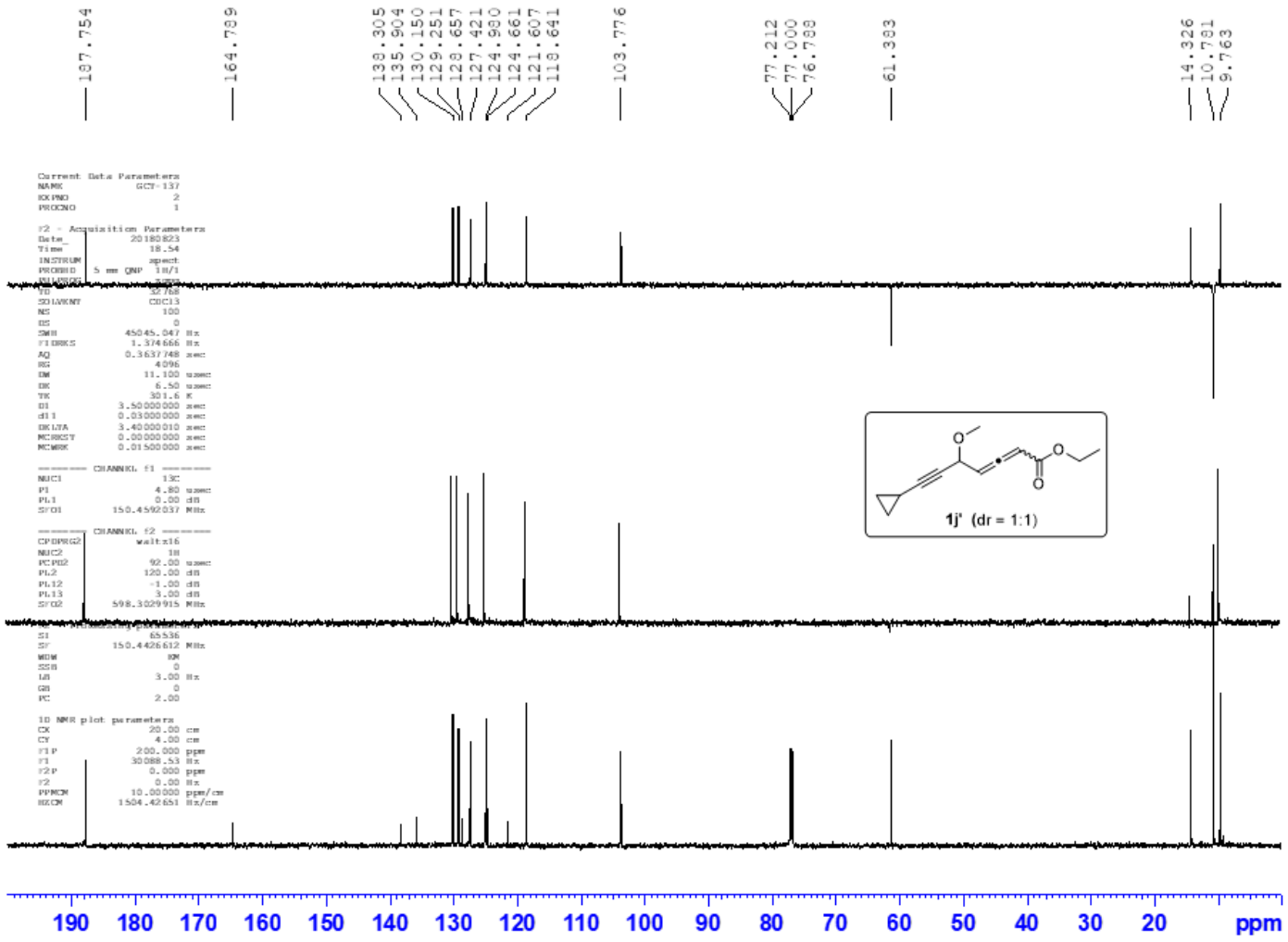

212.621
212.446
165.029
132.729
127.707
126.945
121.922
95.049
94.856
91.128
90.768
88.889
88.667
80.636
77.318
77.000
76.683
68.898
68.287
61.133
55.744
55.208
14.156
Current Data Parameters
NAME GCT-089-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180704
Time 19.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
NS 315
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178021 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1i' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

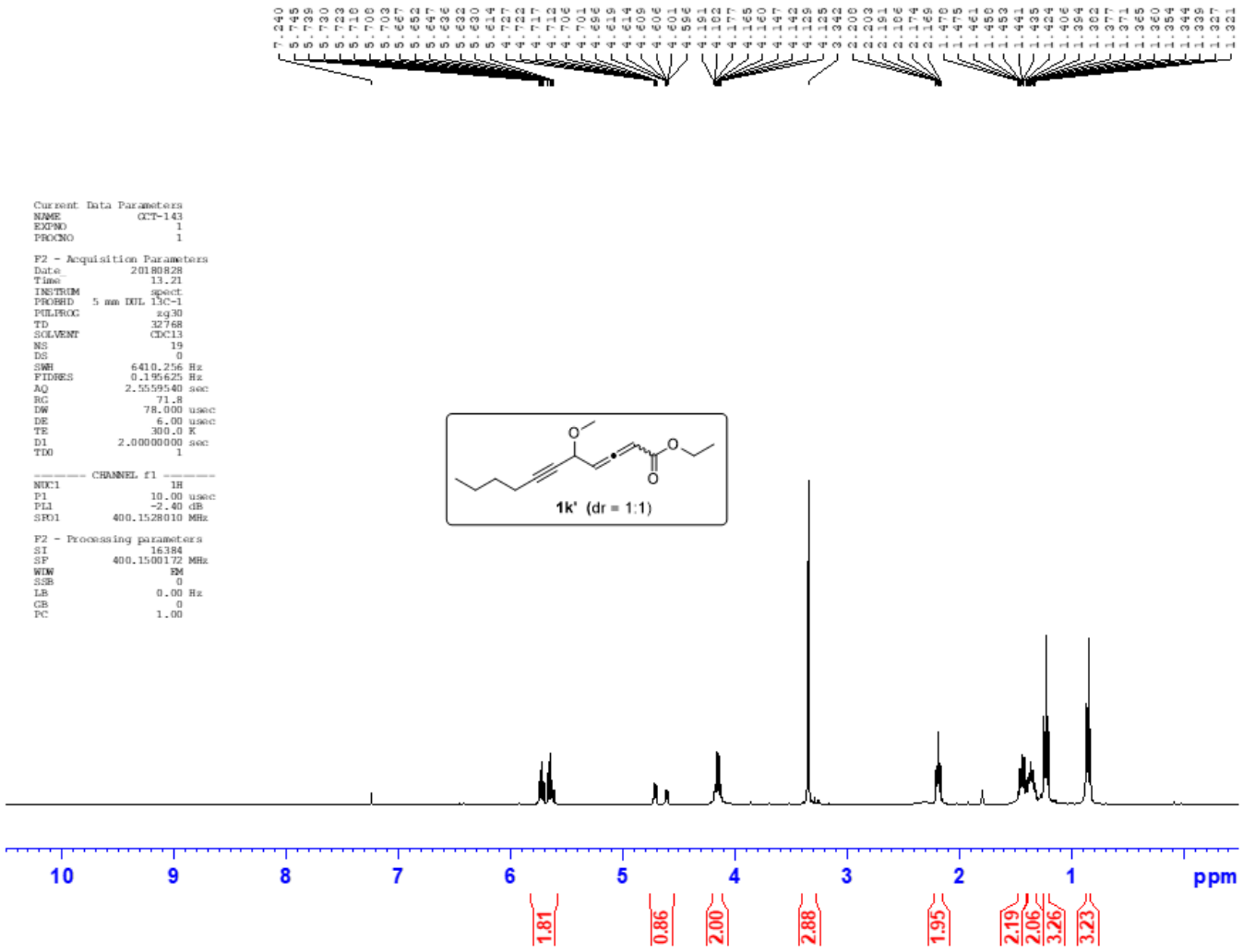


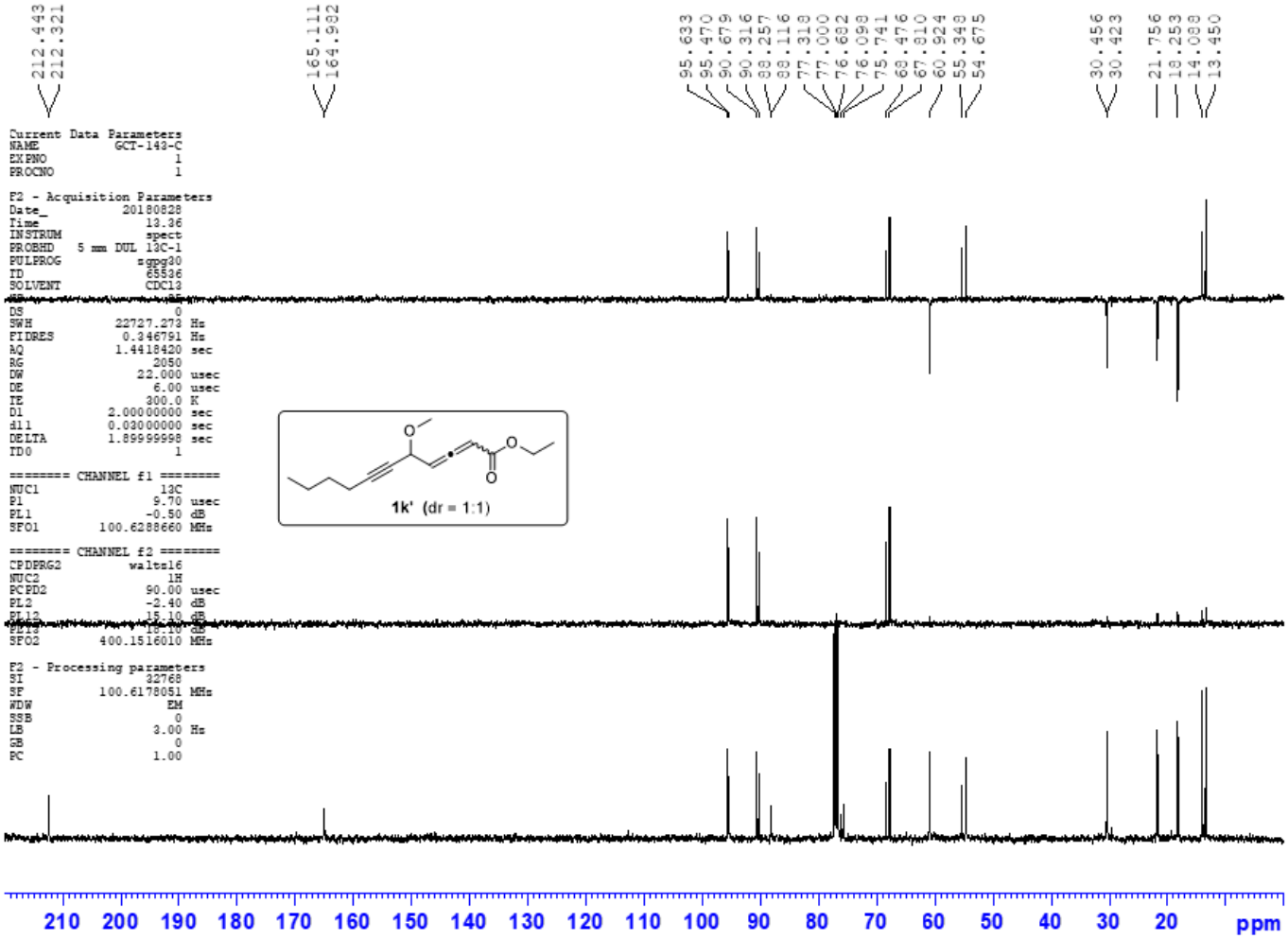

```
Current Data Parameters
NAME      QCT-136-re.fid
EXPNO                1
PROCNO               1

F2 - Processing parameters
SI               16384
SF          499.7912689 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

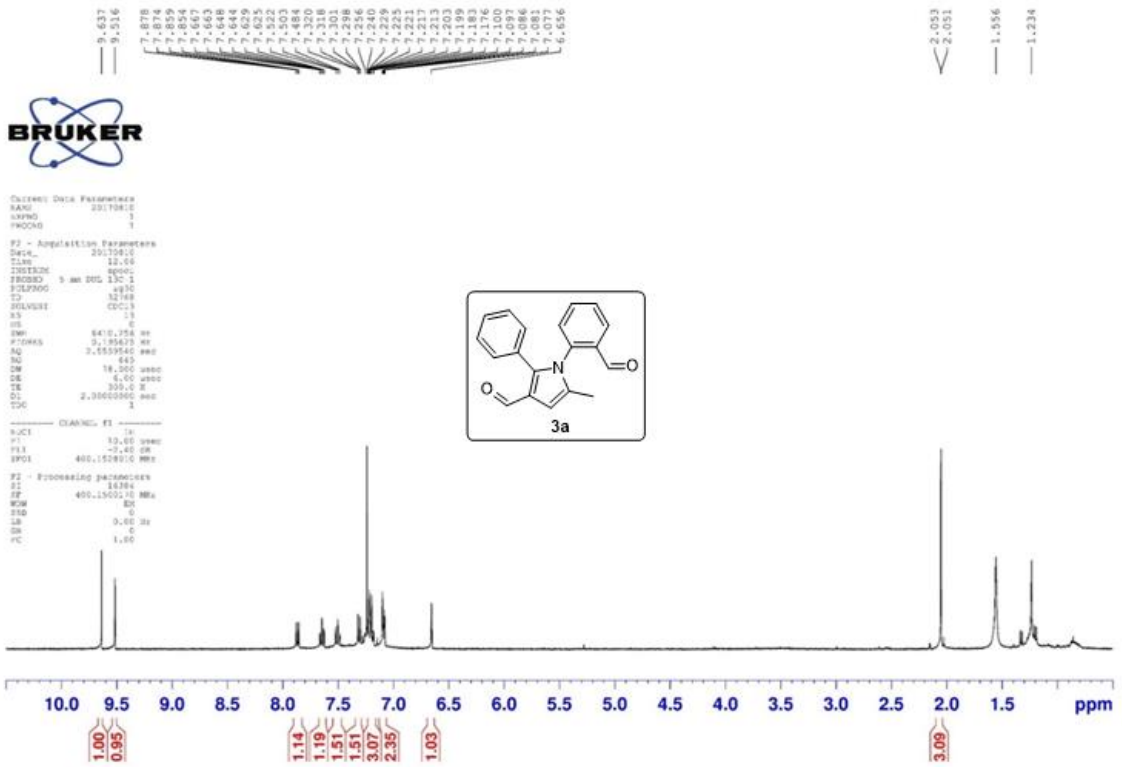


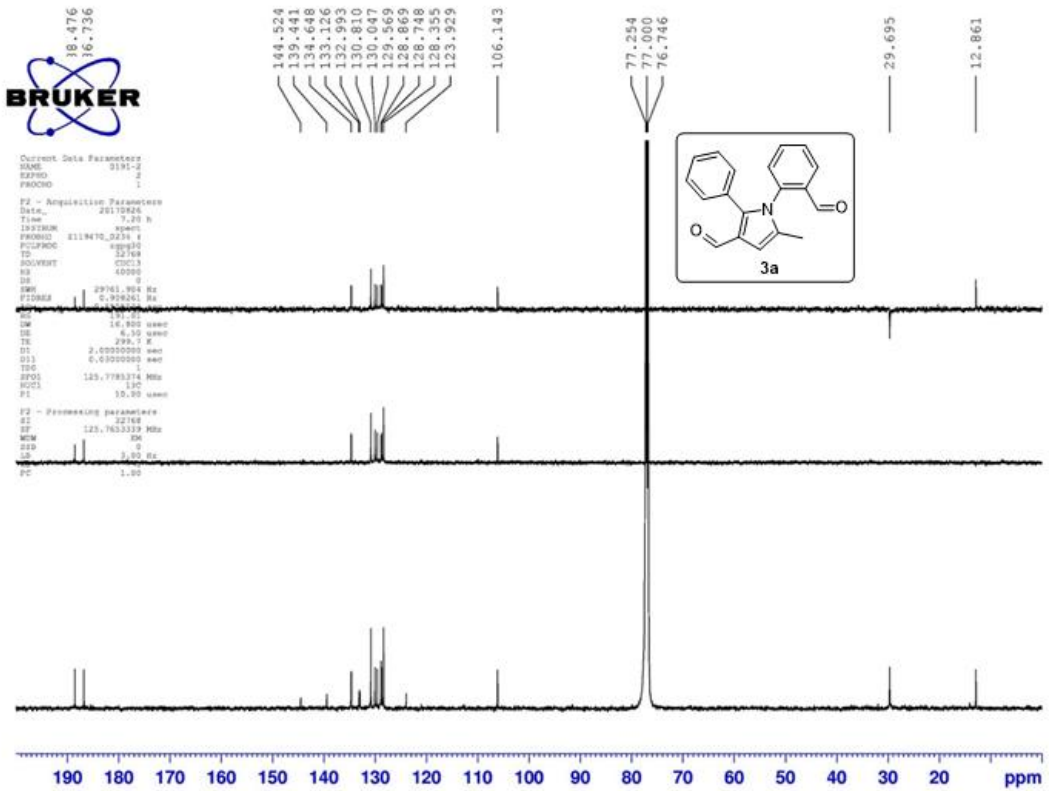


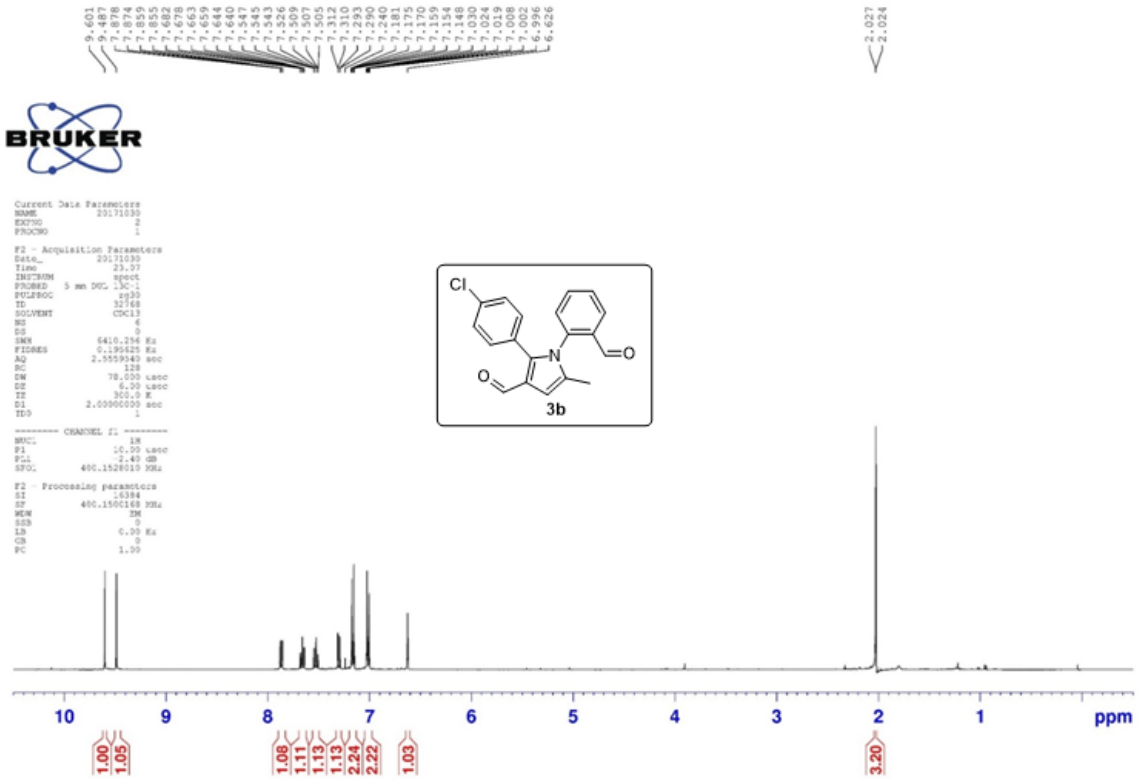

187.754
164.789
130.305
135.904
130.150
129.251
128.657
127.421
124.980
124.661
121.607
118.641
103.776
77.212
77.000
76.788
61.383
14.326
10.781
9.763
1j' (dr = 1:1)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

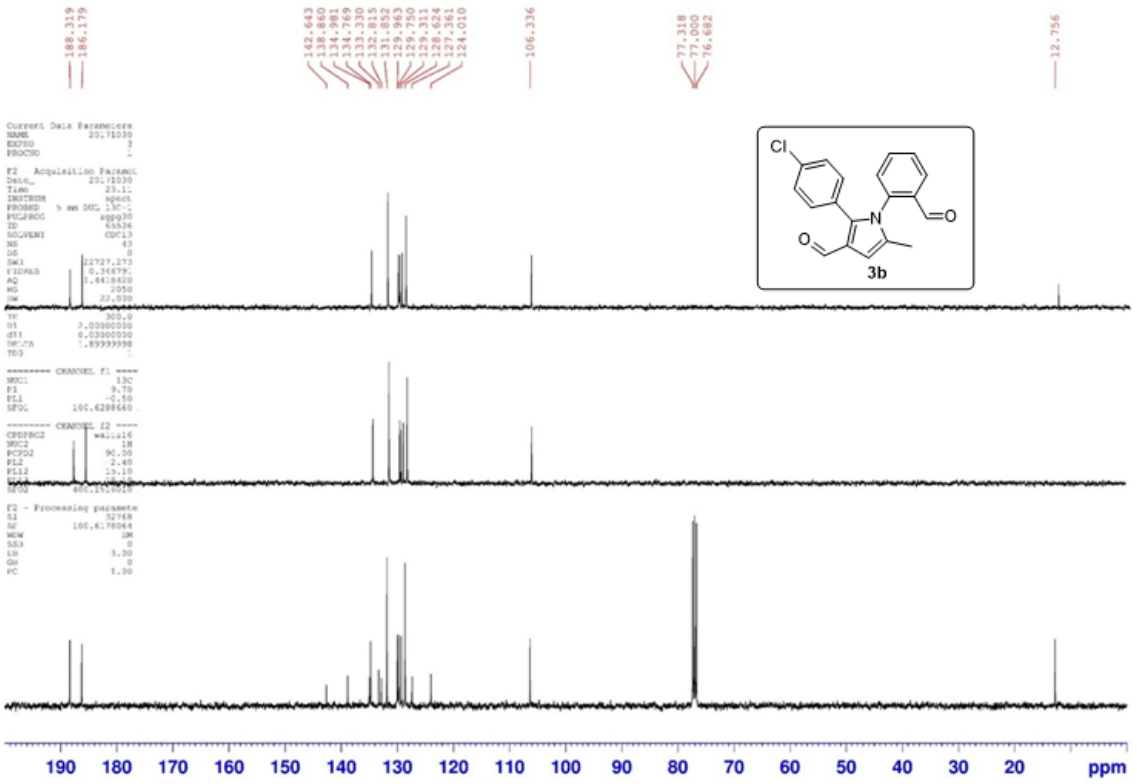

7.240 7.745 7.739 7.730 7.723 7.716 7.706 7.703 7.652 7.647 7.636 7.632 7.630 7.614 7.727 7.722 7.717 7.712 7.705 7.701 7.696 7.619 7.614 7.609 7.605 7.601 7.596 4.191 4.182 4.177 4.165 4.160 4.147 4.142 4.125 3.942 2.200 2.203 2.191 2.186 2.174 2.168 1.470 1.475 1.461 1.456 1.453 1.441 1.435 1.424 1.406 1.394 1.377 1.371 1.365 1.360 1.354 1.344 1.338 1.327 1.321
Current Data Parameters
NAME OCT-143
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20180828
Time 13.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 19
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 71.8
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1k' (dr = 1:1)
10 9 8 7 6 5 4 3 2 1 ppm
1.81 0.86 2.00 2.88 1.95 2.19 2.06 3.26 3.23

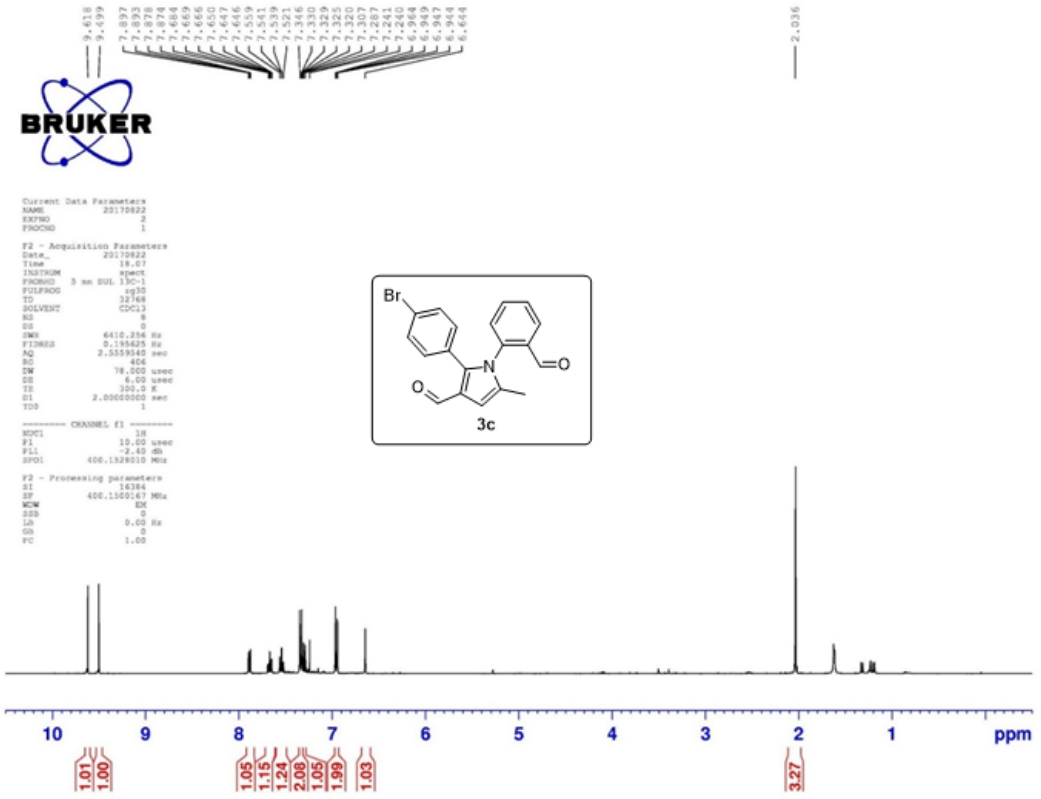

212.443
212.321
165.111
164.982
95.633
95.470
90.679
90.316
88.257
88.116
77.313
77.000
76.682
76.093
75.741
68.476
67.810
60.924
55.348
54.675
30.456
30.423
21.756
18.253
14.083
13.450
Current Data Parameters
NAME GCT-143-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180828
Time 13.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178051 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
O
1k' (dr = 1:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

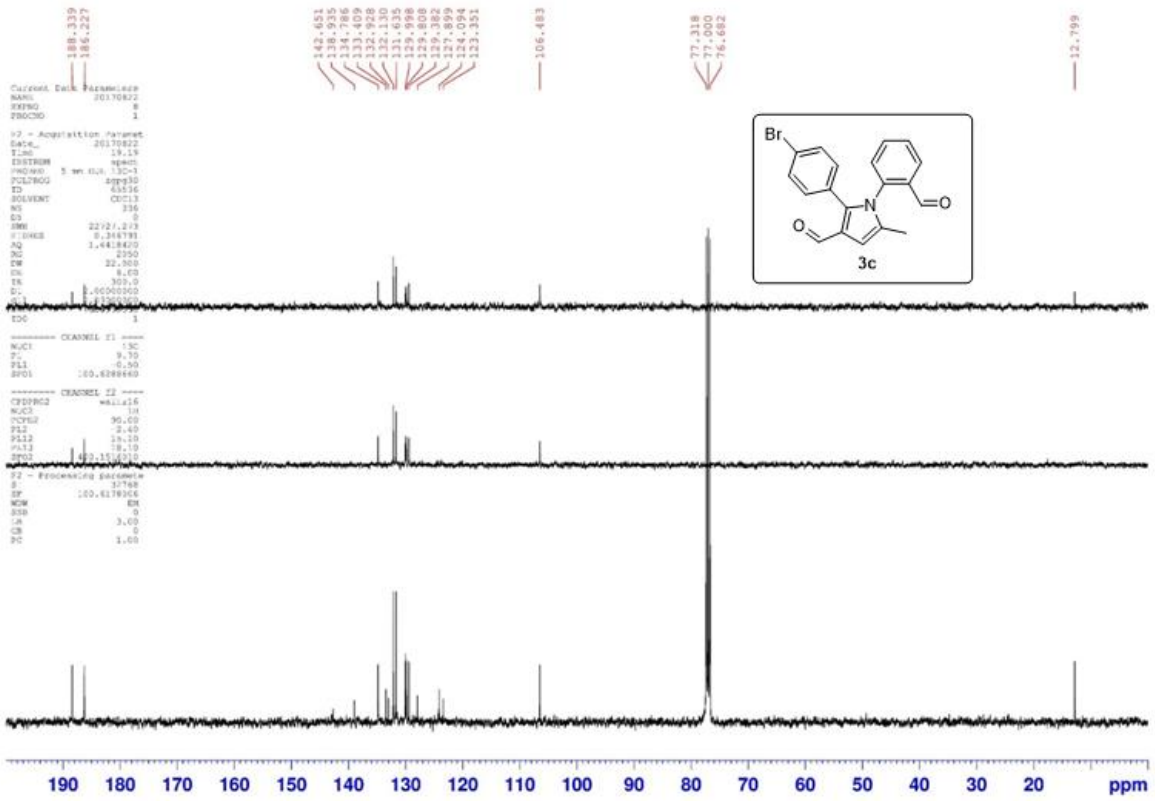

9.637
9.516
7.878
7.874
7.859
7.854
7.667
7.663
7.648
7.644
7.629
7.625
7.522
7.503
7.484
7.320
7.318
7.301
7.298
7.246
7.240
7.229
7.225
7.221
7.217
7.213
7.203
7.199
7.183
7.176
7.100
7.097
7.086
7.081
7.077
6.656
2.053
2.051
1.556
1.234
BRUKER
3a
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
0.95
1.14
1.19
1.51
1.51
3.07
2.35
1.03
3.09

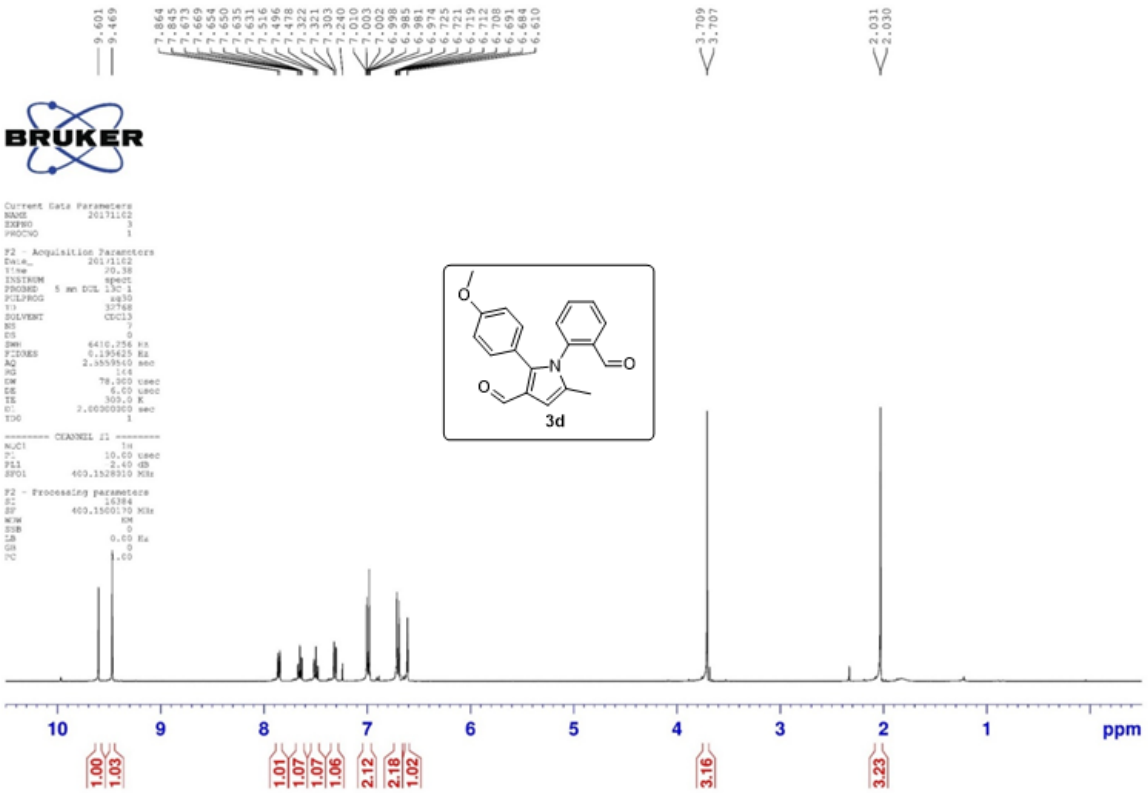

38.476
36.736
144.524
139.441
134.648
133.126
132.993
130.810
130.047
129.569
128.869
128.748
128.355
123.929
106.143
77.254
77.000
76.746
29.695
12.861
3a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

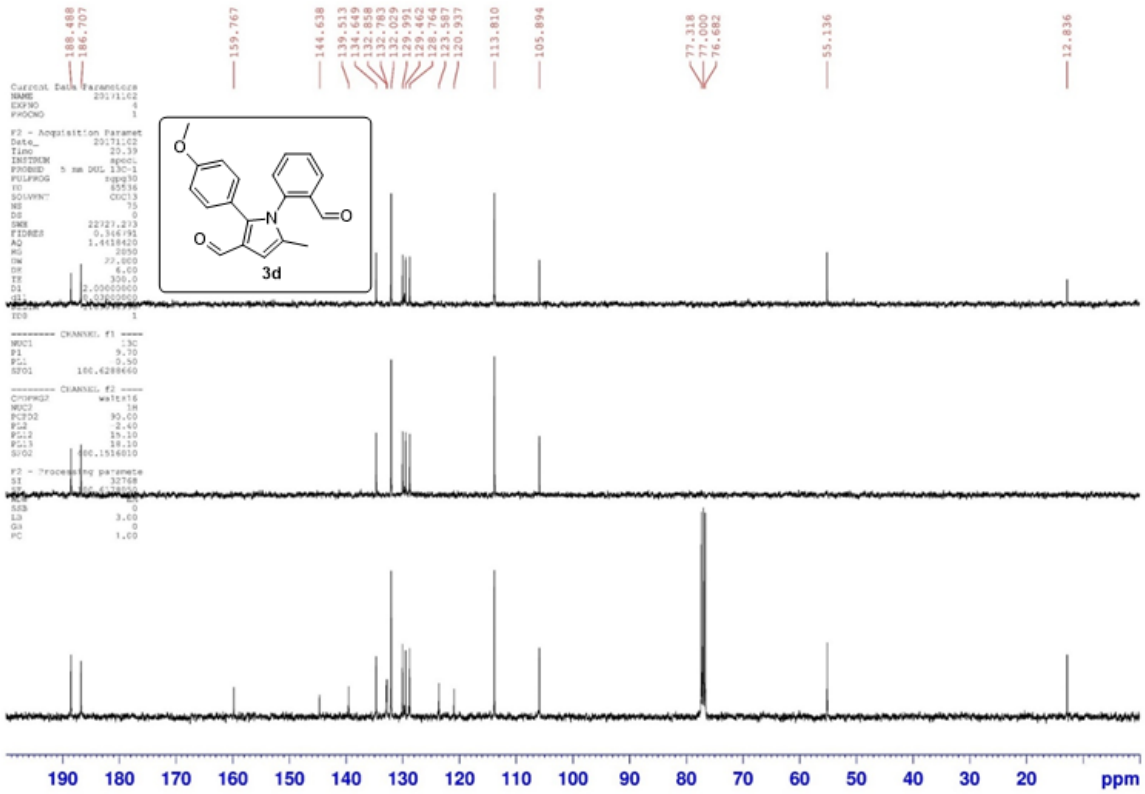

9.601
9.487
7.878
7.874
7.859
7.855
7.682
7.678
7.663
7.659
7.644
7.640
7.547
7.543
7.526
7.509
7.507
7.505
7.312
7.310
7.293
7.290
7.240
7.181
7.175
7.170
7.159
7.154
7.148
7.030
7.024
7.019
7.008
7.002
6.996
6.626
2.027
2.024
BRUKER
Current Data Parameters
NAME 20171030
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171030
Time 23.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
N
O
O
3b
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.05
1.08
1.11
1.13
1.13
2.24
2.22
1.03
3.20

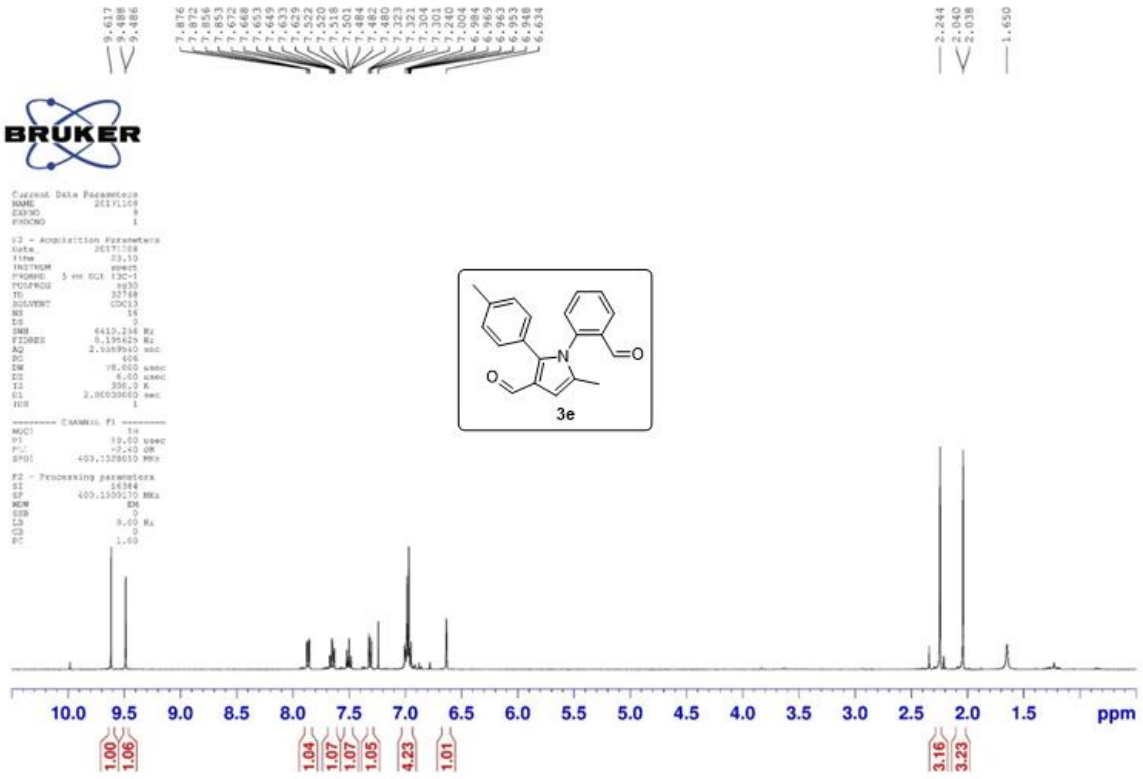

188.319
186.179
142.643
138.860
134.981
134.769
133.330
132.815
131.852
129.963
129.750
129.311
128.584
127.361
124.010
106.336
77.318
77.000
76.682
12.756
Cl
N
O
O
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

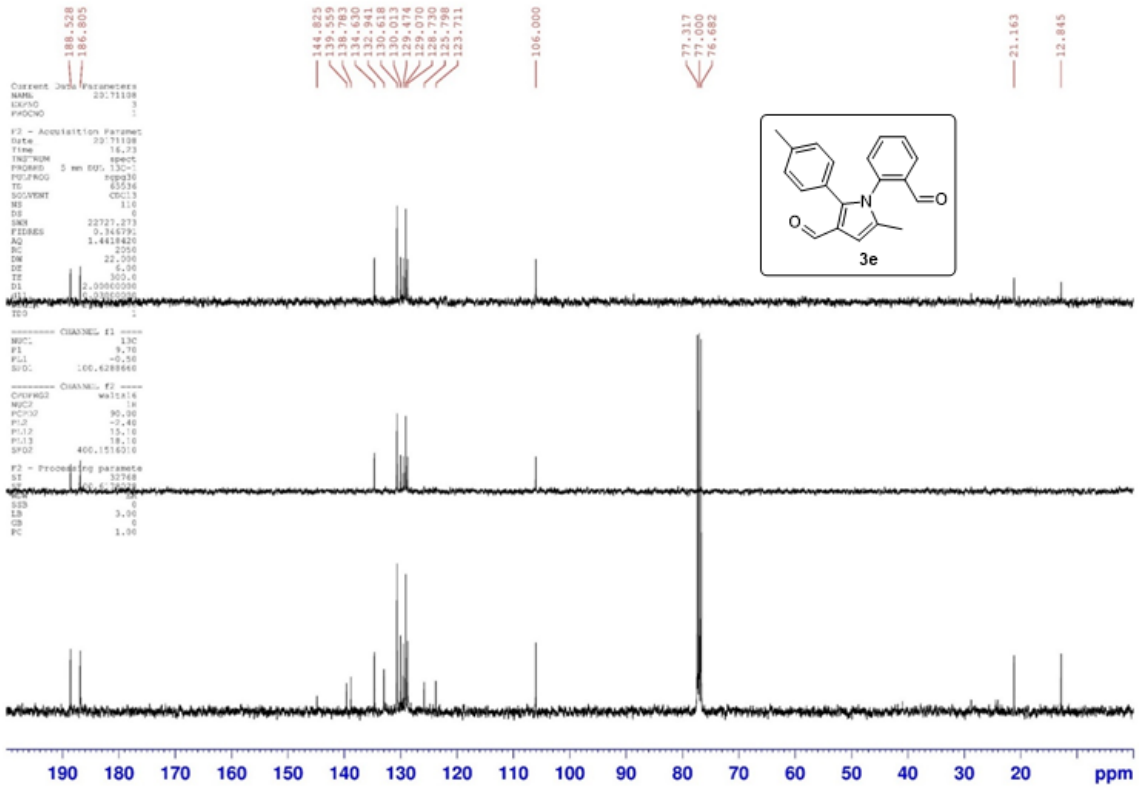

9.618
9.499
7.897
7.893
7.878
7.874
7.684
7.669
7.666
7.650
7.647
7.646
7.549
7.541
7.539
7.521
7.346
7.330
7.329
7.325
7.320
7.307
7.297
7.241
7.240
6.964
6.949
6.947
6.944
6.644
2.036
BRUKER
Br
N
O
O
3c
10
9
8
7
6
5
4
3
2
1
ppm
1.01
1.00
1.05
1.15
1.24
2.06
1.05
1.99
1.03
3.27

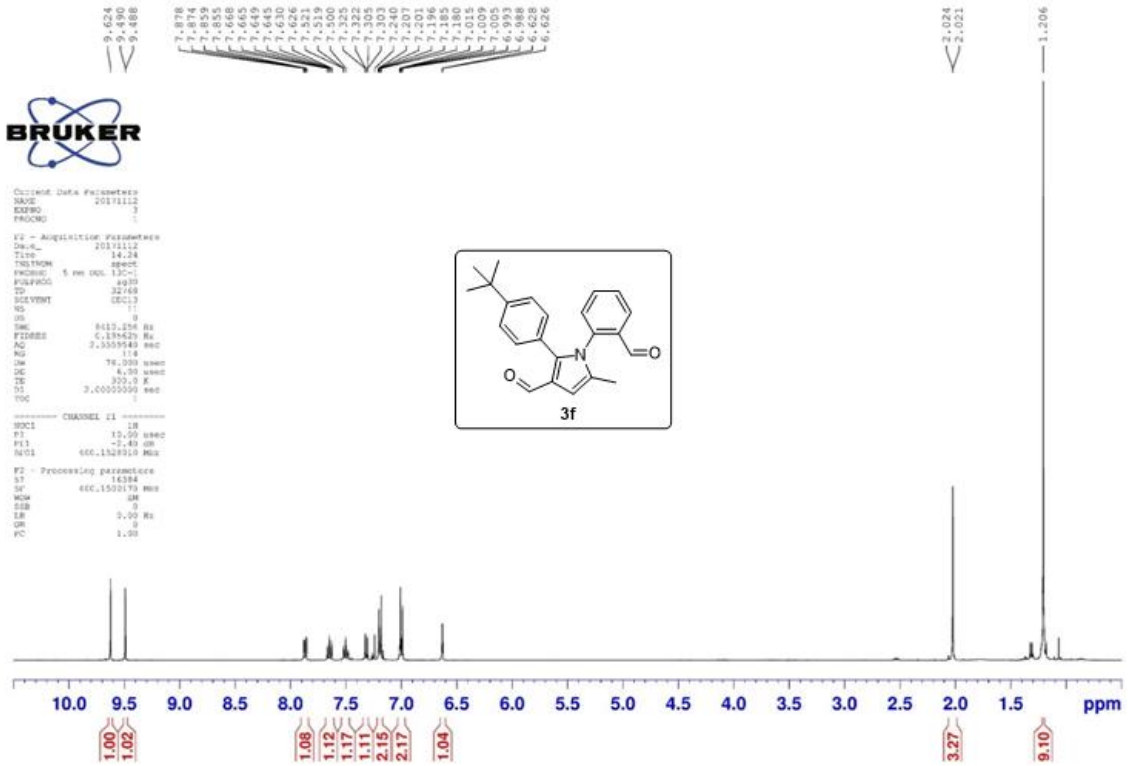

188.339
186.227
142.651
138.935
134.786
133.409
132.928
132.130
131.635
129.998
129.808
129.382
127.899
124.084
123.351
106.483
77.318
77.000
76.682
12.799
Br
O
N
O
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

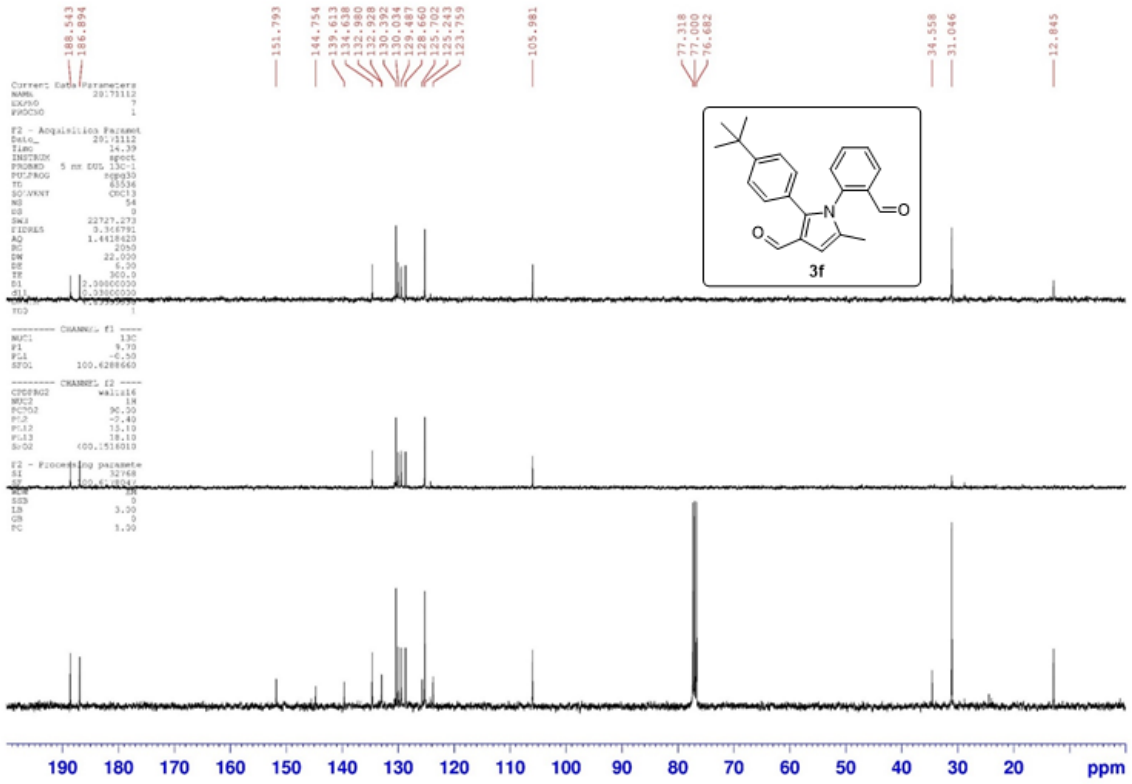

9.601
9.469
7.864
7.845
7.673
7.669
7.654
7.650
7.635
7.631
7.516
7.496
7.478
7.322
7.321
7.303
7.240
7.010
7.003
7.002
6.998
6.985
6.981
6.974
6.725
6.721
6.719
6.712
6.708
6.691
6.684
6.610
3.709
3.707
2.031
2.030
BRUKER
3d
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.01
1.07
1.07
1.06
2.12
2.18
1.02
3.16
3.23

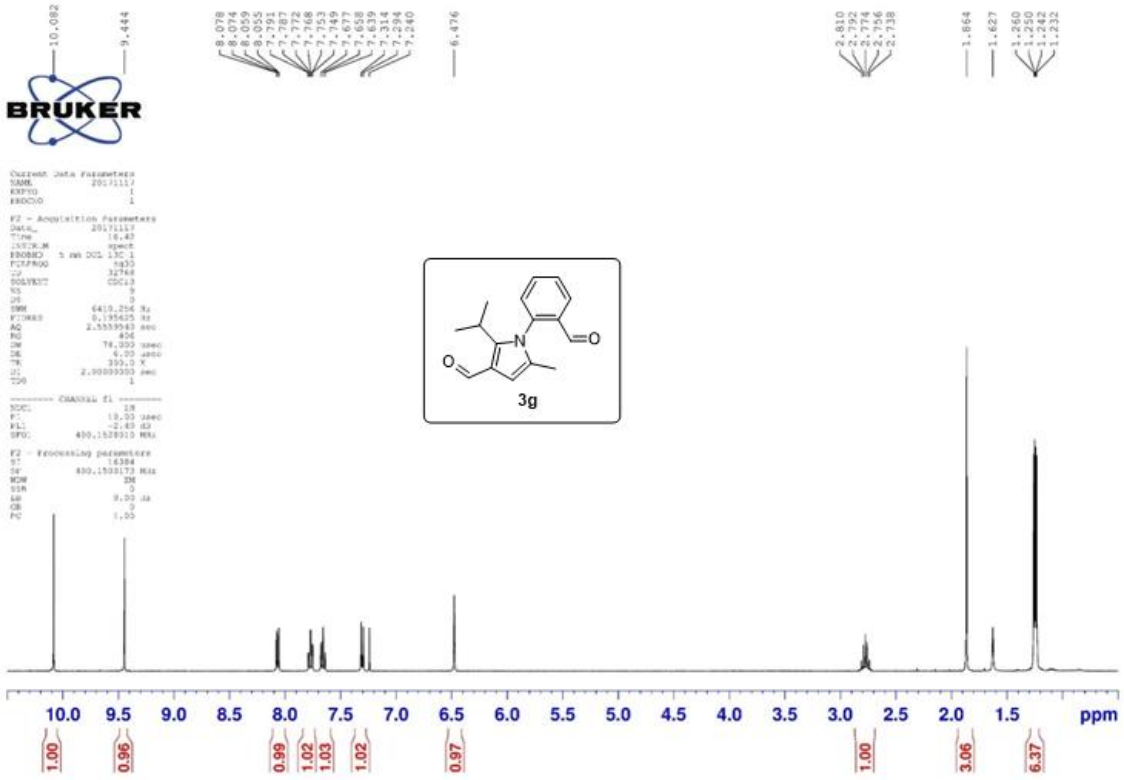

188.488
186.707
159.767
144.638
139.513
134.649
132.858
132.783
132.029
129.991
129.462
128.764
123.587
120.937
113.810
105.894
77.318
77.000
76.682
55.136
12.836
3d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

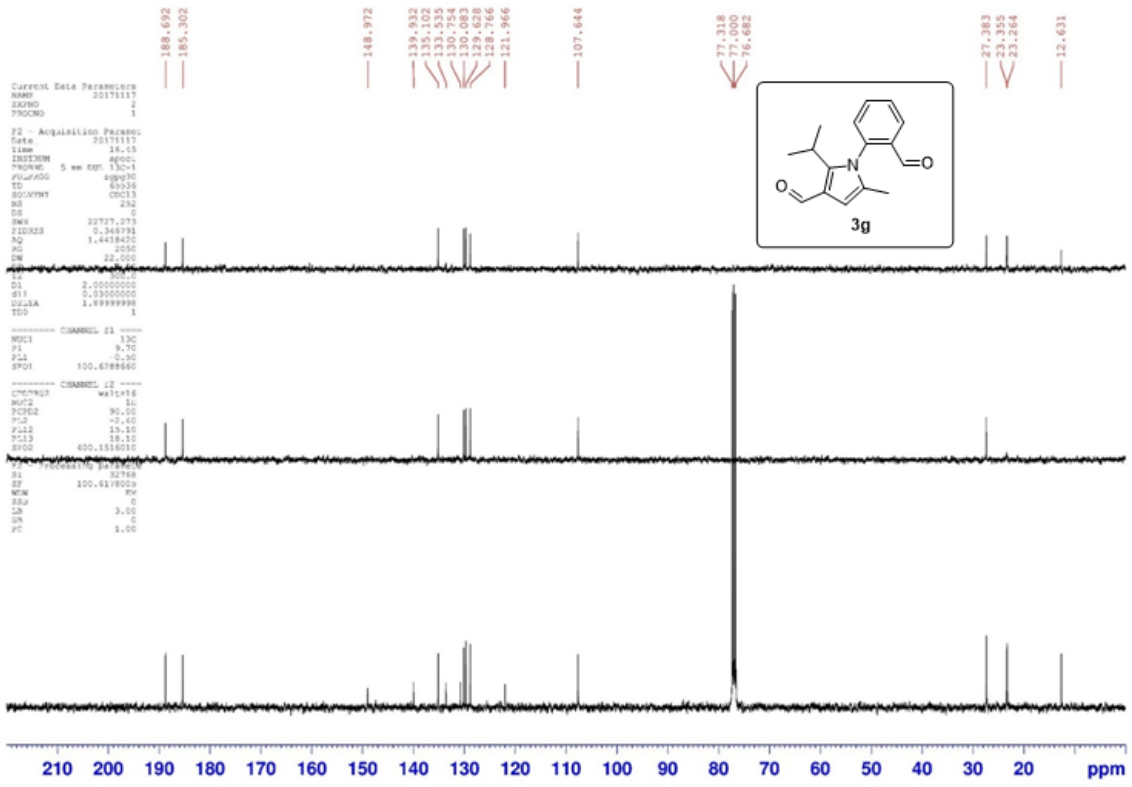

9.617
9.488
9.486
7.876
7.872
7.856
7.853
7.672
7.668
7.653
7.649
7.633
7.629
7.522
7.520
7.518
7.501
7.484
7.482
7.480
7.323
7.321
7.304
7.301
7.240
7.004
6.984
6.969
6.963
6.953
6.948
6.634
2.244
2.040
2.038
1.650
BRUKER
3e
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
1.06
1.04
1.07
1.07
1.05
4.23
1.01
3.16
3.23

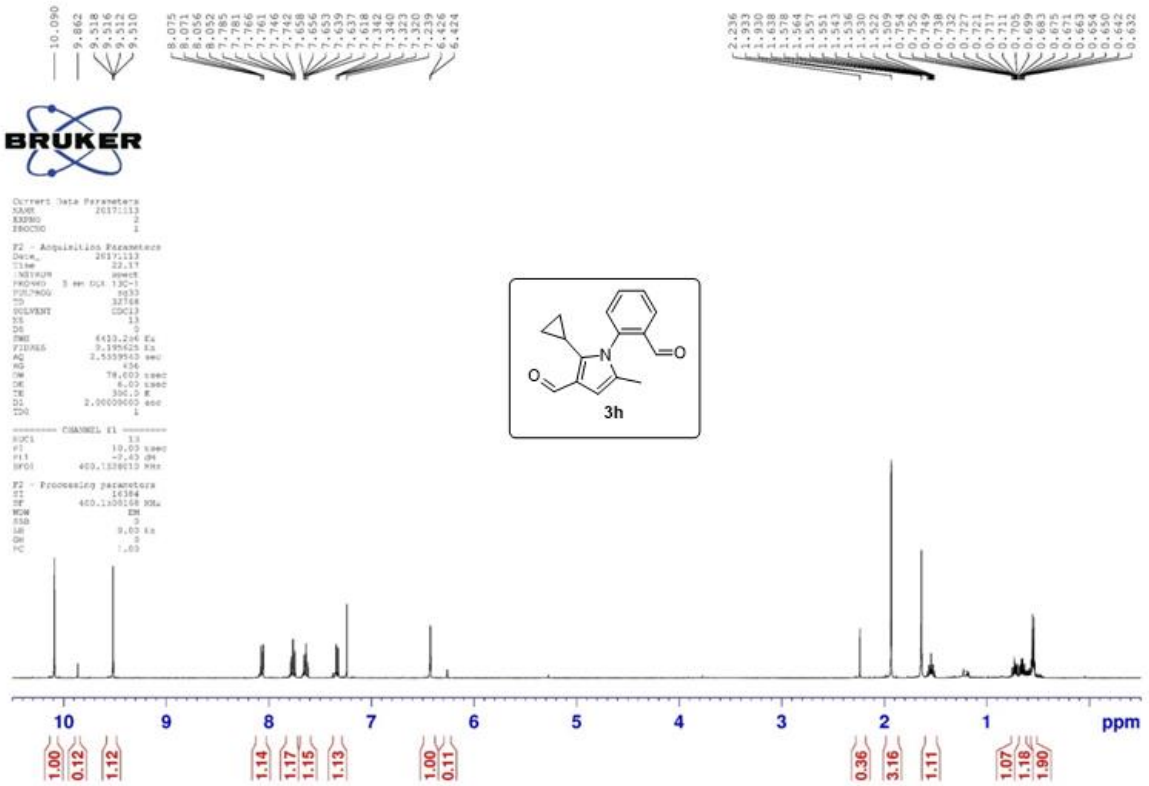

188.528
186.805
144.825
139.559
138.783
134.630
132.941
130.618
130.013
129.474
129.070
128.730
125.798
123.711
106.000
77.317
77.000
76.682
21.163
12.845
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

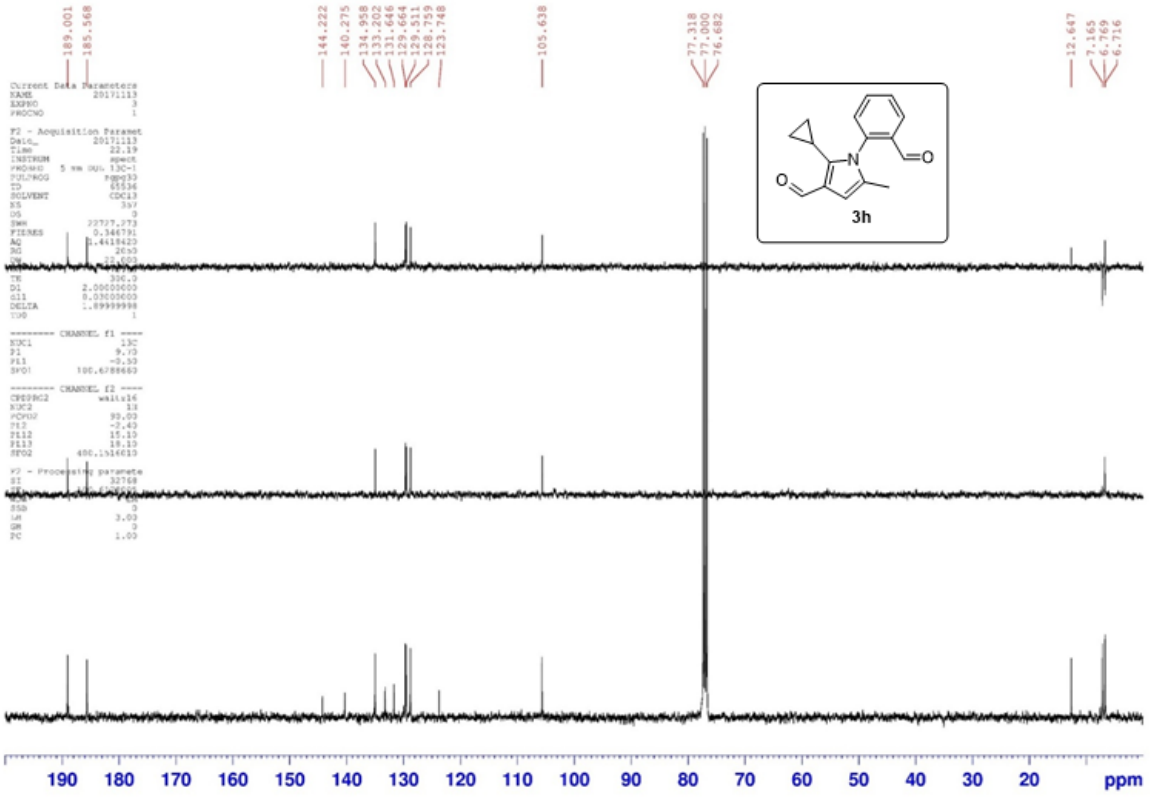

9.624
9.490
9.488
7.878
7.874
7.859
7.855
7.668
7.665
7.649
7.645
7.630
7.626
7.521
7.519
7.500
7.325
7.322
7.305
7.303
7.240
7.207
7.201
7.196
7.185
7.180
7.015
7.009
7.005
6.993
6.988
6.628
6.626
2.024
2.021
1.206
BRUKER
3f
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
1.02
1.08
1.12
1.17
1.11
2.15
2.17
1.04
3.27
9.10

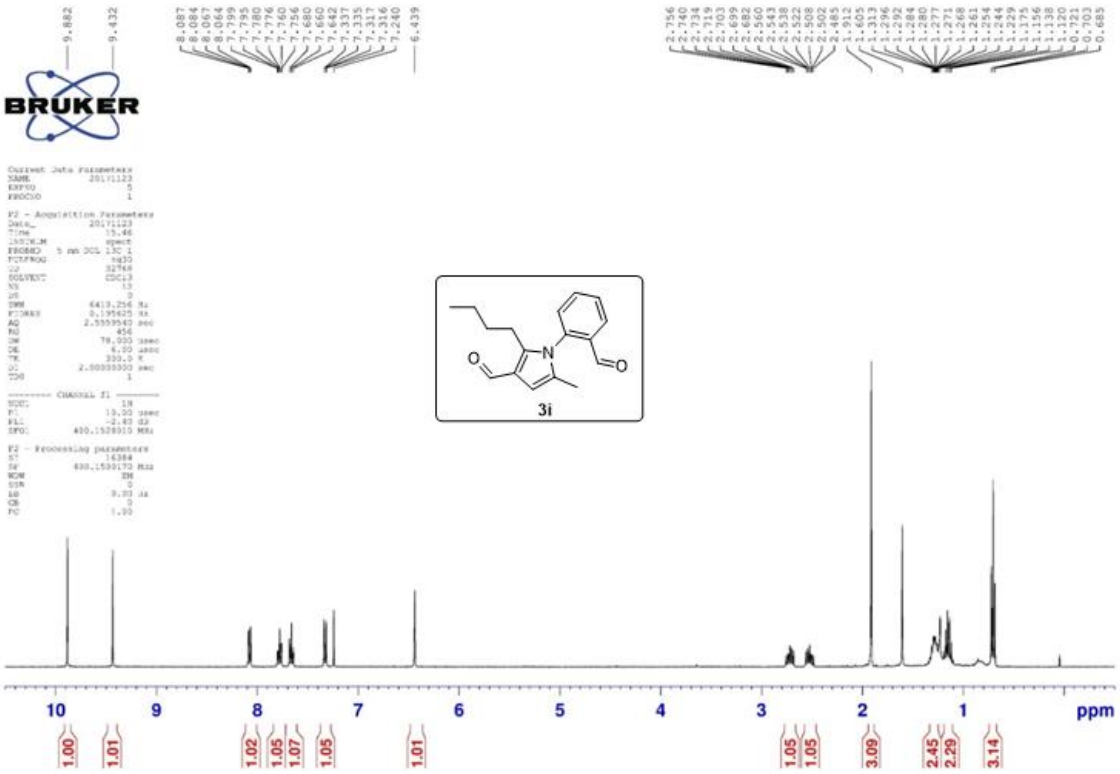

188.543
186.894
151.793
144.754
139.613
134.638
132.980
132.928
130.392
130.034
129.487
128.660
125.702
125.243
123.759
105.981
77.318
77.000
76.682
34.558
31.046
12.845
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

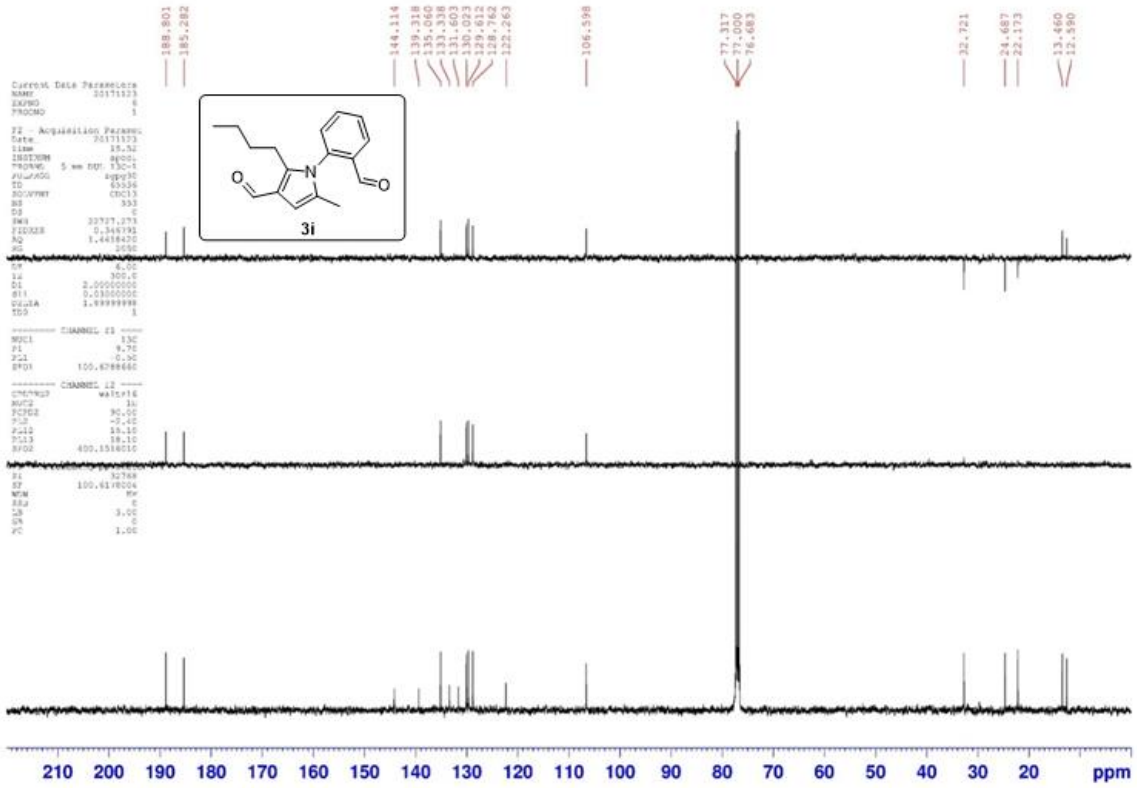

10.082
9.444
8.078
8.074
8.069
8.055
7.791
7.787
7.772
7.768
7.753
7.749
7.677
7.658
7.639
7.314
7.294
7.240
6.476
2.810
2.792
2.774
2.756
2.738
1.864
1.627
1.260
1.240
1.242
1.232
BRUKER
3g
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
0.96
0.99
1.02
1.03
1.02
0.97
1.00
3.06
6.37

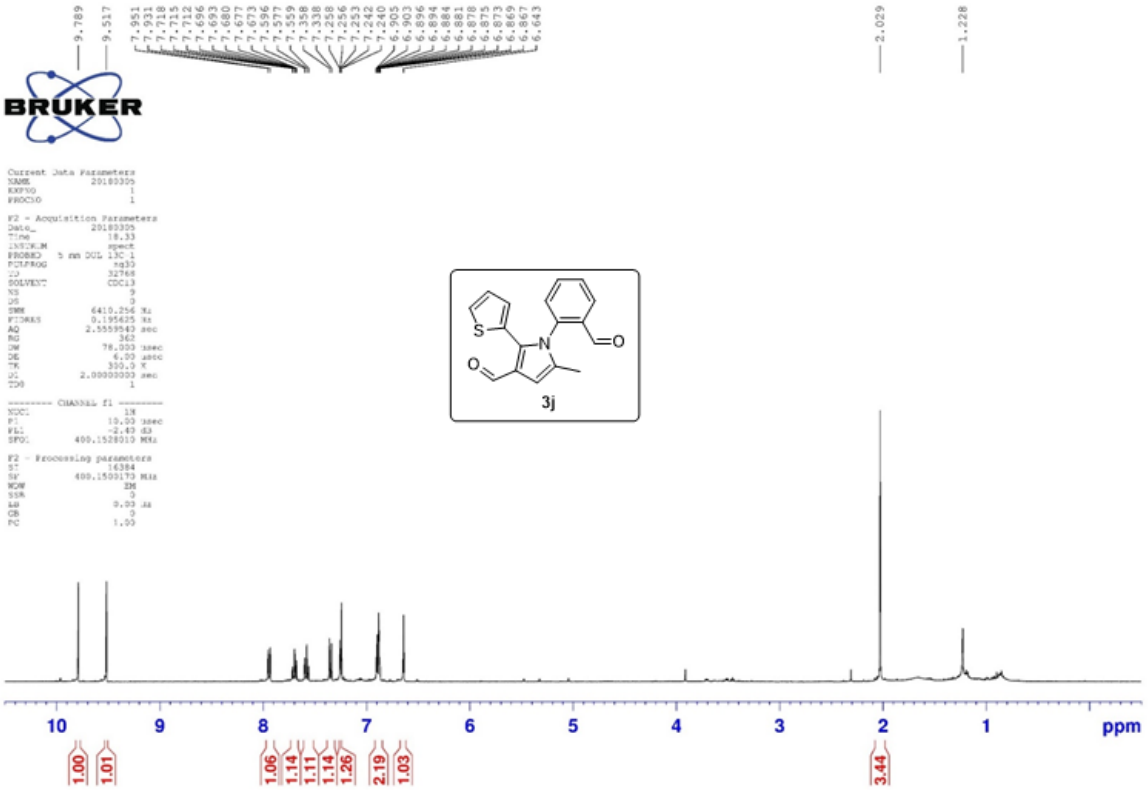

188.692
185.302
148.972
139.932
135.102
133.535
130.754
130.083
129.628
128.766
121.966
107.644
77.318
77.000
76.682
27.383
23.355
23.264
12.631
3g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

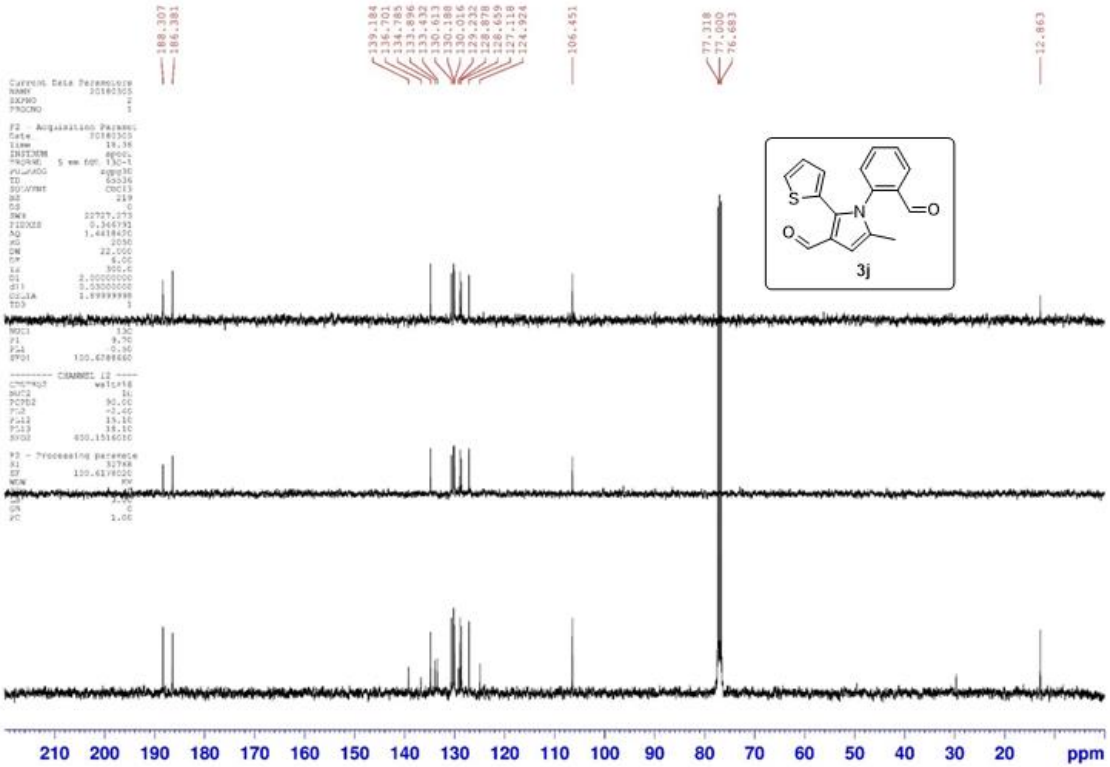

10.090
9.862
9.518
9.516
9.512
9.510
8.075
8.071
8.056
8.052
7.785
7.781
7.766
7.761
7.746
7.742
7.658
7.656
7.639
7.633
7.618
7.342
7.340
7.323
7.320
7.239
6.426
6.424
2.236
1.933
1.930
1.638
1.578
1.564
1.557
1.551
1.543
1.536
1.530
1.522
1.509
1.504
0.752
0.749
0.738
0.732
0.727
0.721
0.717
0.711
0.705
0.699
0.683
0.675
0.671
0.663
0.654
0.650
0.642
0.632
BRUKER
3h
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.12
1.12
1.14
1.17
1.15
1.13
1.00
0.11
0.36
3.16
1.11
1.07
1.18
1.90

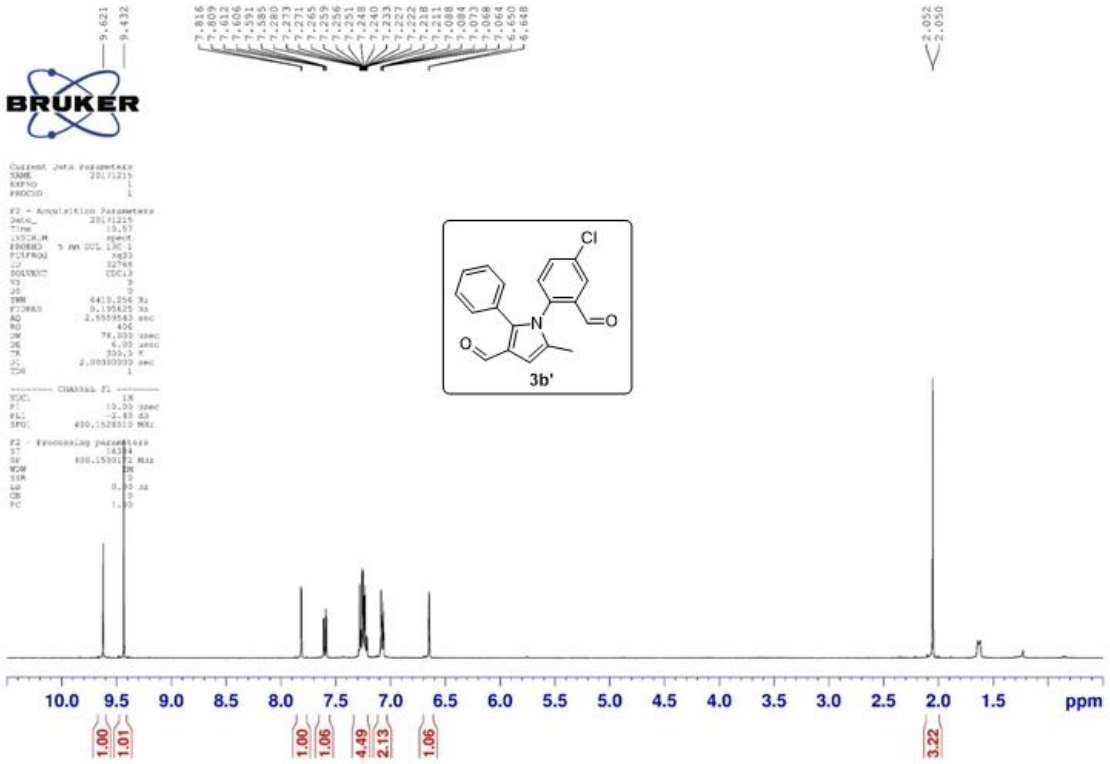

189.001
185.568
144.222
140.275
134.958
133.202
131.646
129.664
129.511
128.759
123.748
105.638
77.318
77.000
76.682
12.647
7.165
6.769
6.716
3h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

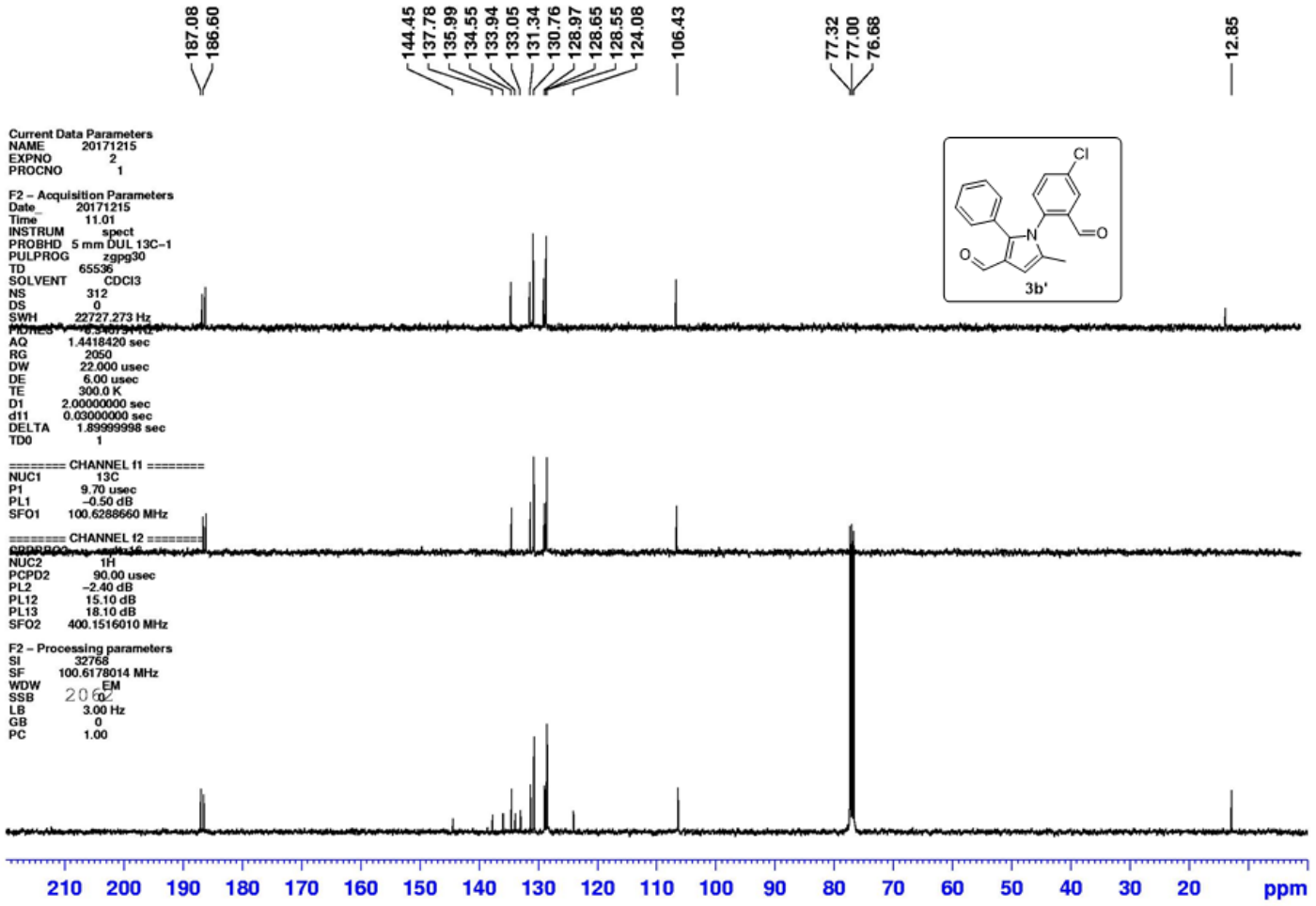

9.882
9.432
8.087
8.084
8.067
8.064
7.799
7.795
7.780
7.776
7.760
7.756
7.680
7.660
7.652
7.337
7.335
7.317
7.316
7.240
6.439
2.756
2.750
2.734
2.719
2.703
2.699
2.682
2.560
2.543
2.538
2.522
2.508
2.502
2.485
1.912
1.605
1.313
1.296
1.292
1.284
1.280
1.277
1.271
1.268
1.261
1.254
1.244
1.229
1.175
1.156
1.138
1.120
0.701
0.685
BRUKER
3i
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.02
1.05
1.07
1.05
1.01
1.05
1.05
3.09
2.45
2.29
3.14

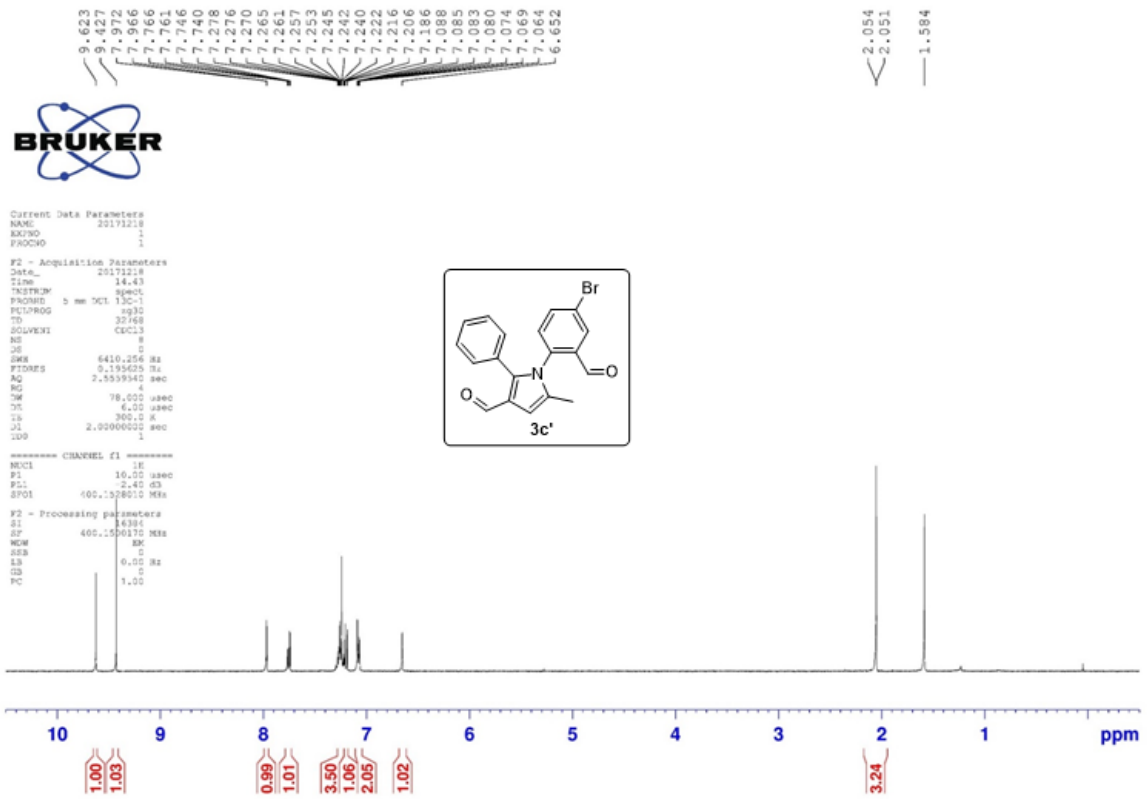

188.801
185.282
144.114
139.318
135.060
133.338
131.603
130.023
129.622
128.742
122.263
106.598
77.317
77.000
76.683
32.721
24.687
22.173
13.460
12.590
O
N
O
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

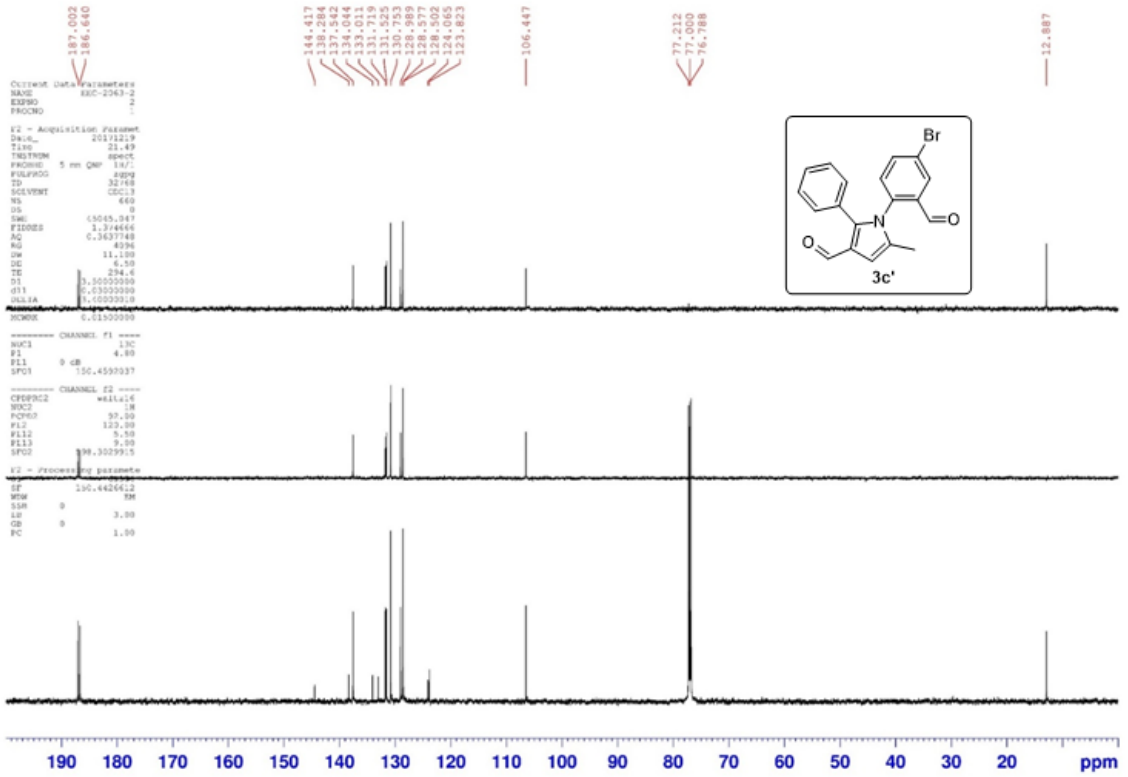

9.789
9.517
7.951
7.931
7.718
7.715
7.712
7.696
7.693
7.680
7.677
7.673
7.596
7.577
7.559
7.358
7.338
7.258
7.256
7.253
7.242
7.240
6.905
6.903
6.896
6.894
6.884
6.881
6.878
6.875
6.873
6.869
6.867
6.643
2.029
1.228
BRUKER
3j
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.06
1.14
1.11
1.14
1.26
2.19
1.03
3.44

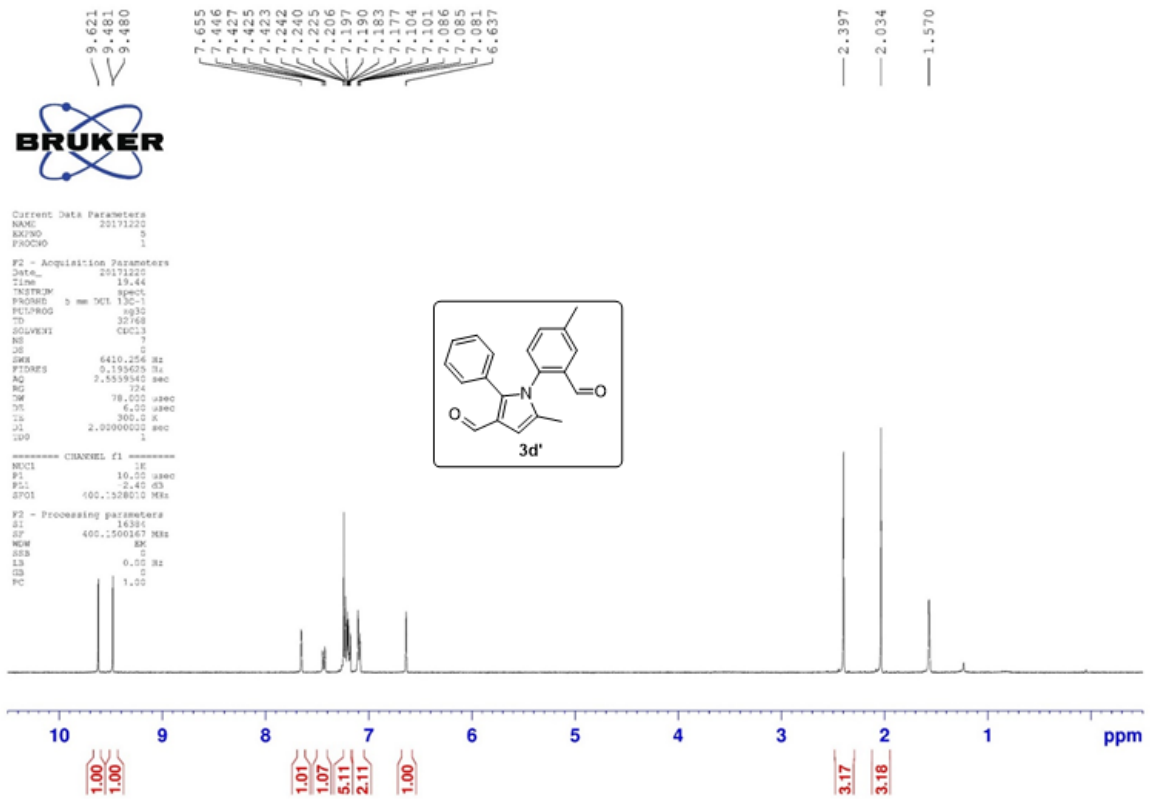

188.307
186.381
139.184
136.701
134.788
133.896
133.432
130.613
130.188
130.016
129.232
128.878
128.659
126.118
124.324
106.451
77.318
77.000
76.683
12.863
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

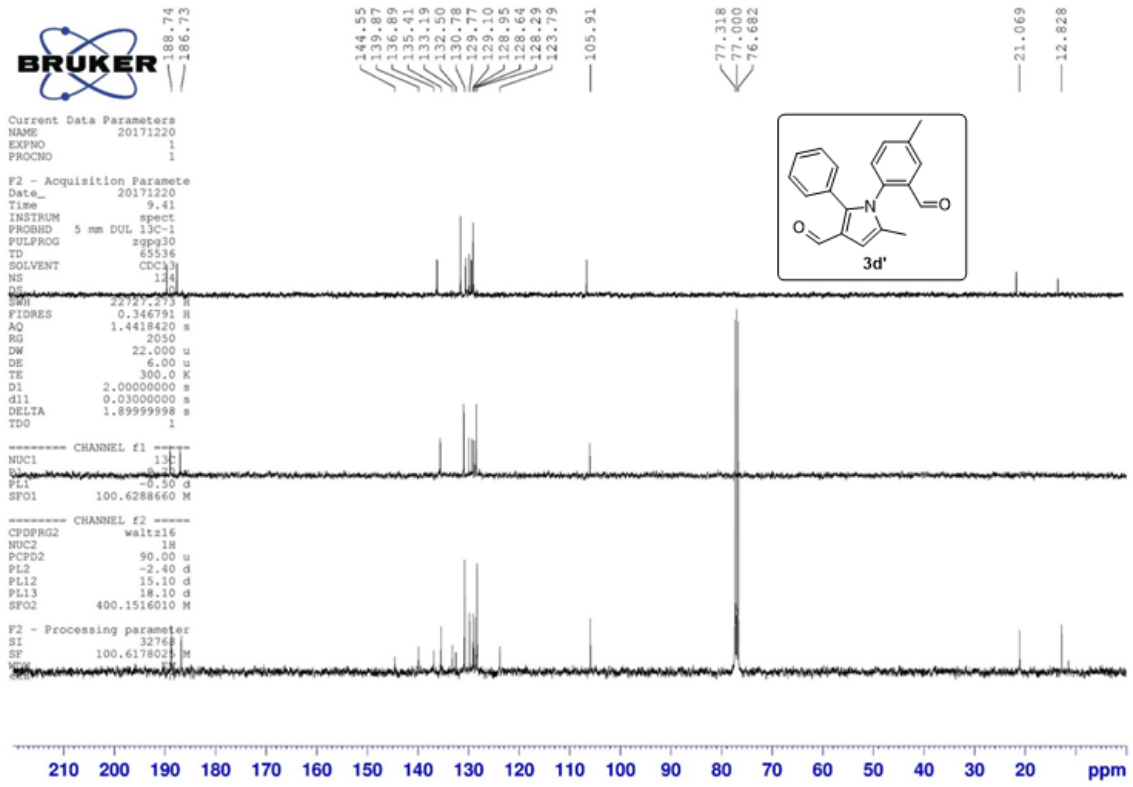

9.621
9.432
7.816
7.809
7.612
7.606
7.591
7.585
7.280
7.273
7.271
7.265
7.259
7.256
7.251
7.248
7.240
7.233
7.227
7.218
7.211
7.088
7.084
7.073
7.068
7.064
6.650
6.648
2.052
2.050
BRUKER
Cl
O
N
O
3b'
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
1.01
1.00
1.06
4.49
2.13
1.06
3.22

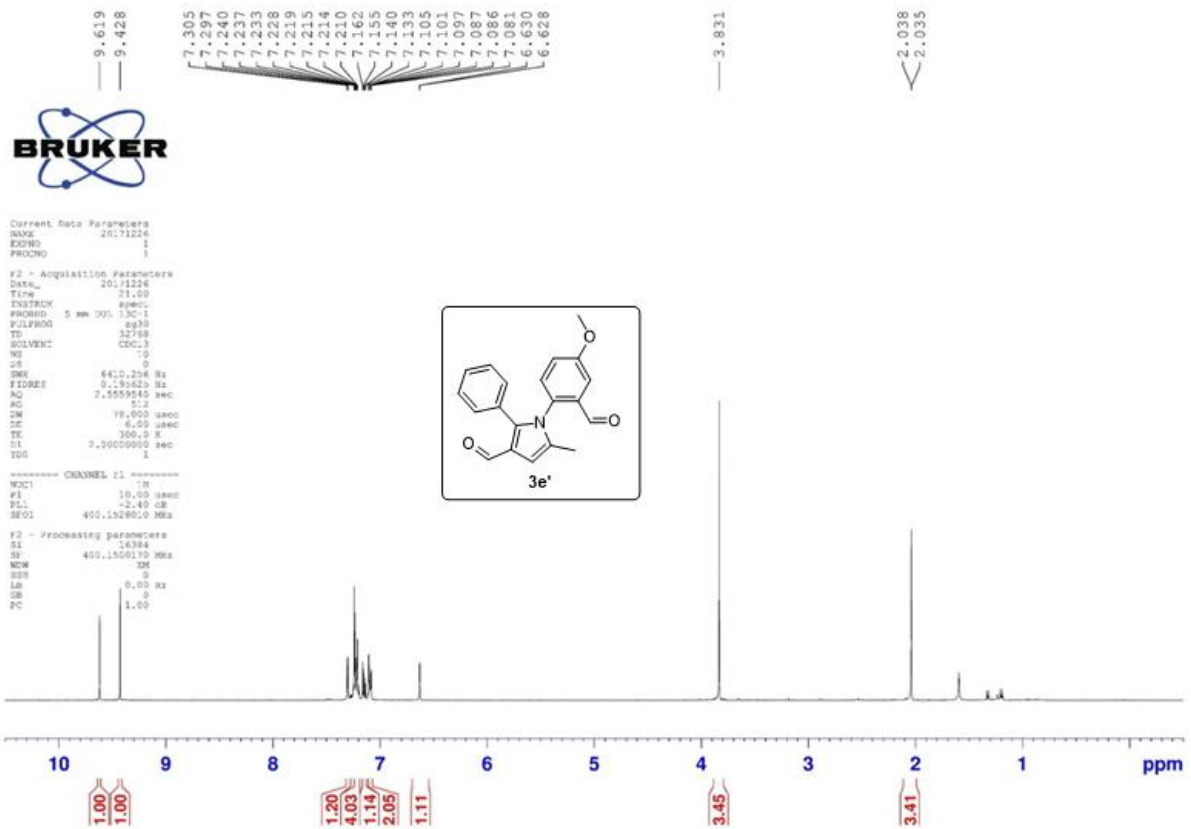

187.08
186.60
144.45
137.78
135.99
134.55
133.94
133.05
131.34
130.76
128.97
128.65
128.55
124.08
106.43
77.32
77.00
76.68
12.85
Current Data Parameters
NAME 20171215
EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
Date_ 20171215
Time 11.01
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 312
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 –0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 –2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 – Processing parameters
SI 32768
SF 100.6178014 MHz
WDW EM
SSB 2062
LB 3.00 Hz
GB 0
PC 1.00
Cl
N
O
O
3b'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

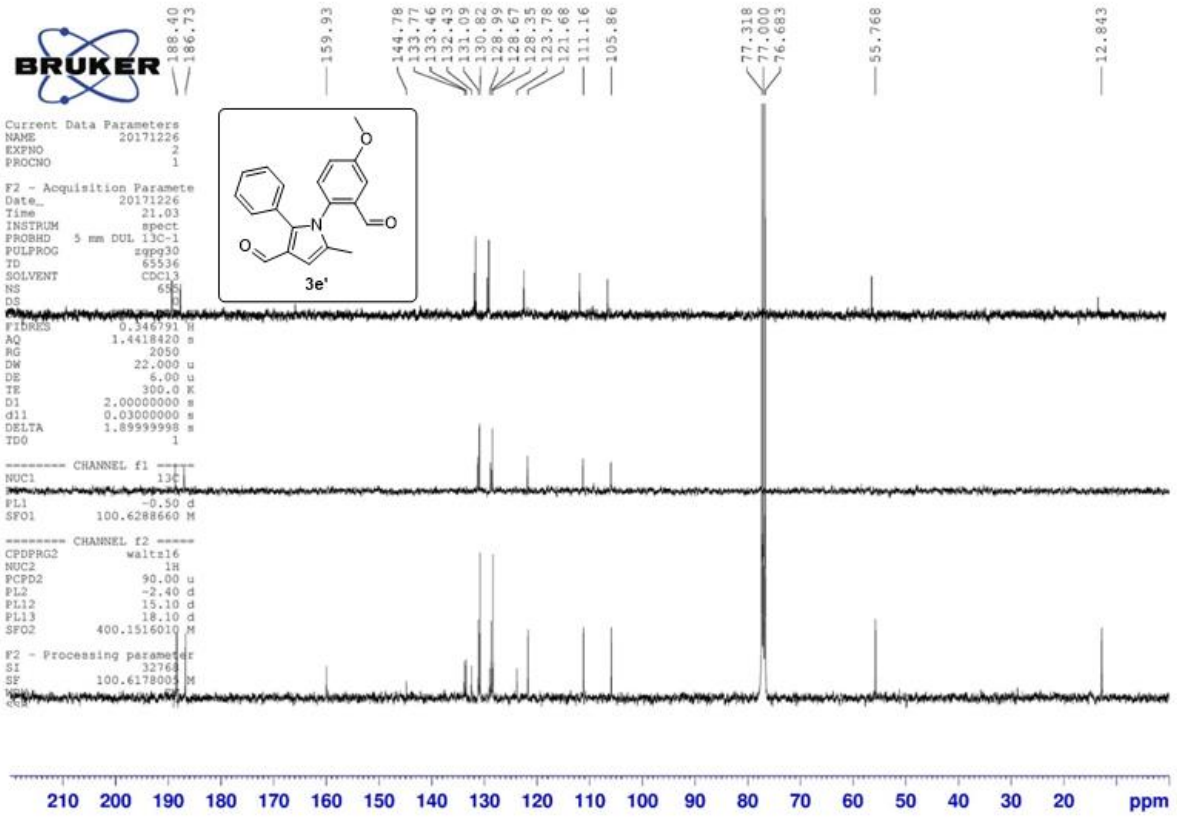

9.623
9.427
7.972
7.967
7.966
7.766
7.761
7.746
7.740
7.278
7.276
7.270
7.265
7.261
7.257
7.253
7.245
7.242
7.240
7.222
7.216
7.206
7.186
7.088
7.085
7.083
7.080
7.074
7.069
7.064
7.030
6.652
2.054
2.051
1.584
BRUKER
Br
N
O
O
3c'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
0.99
1.01
3.50
1.06
2.05
1.02
3.24

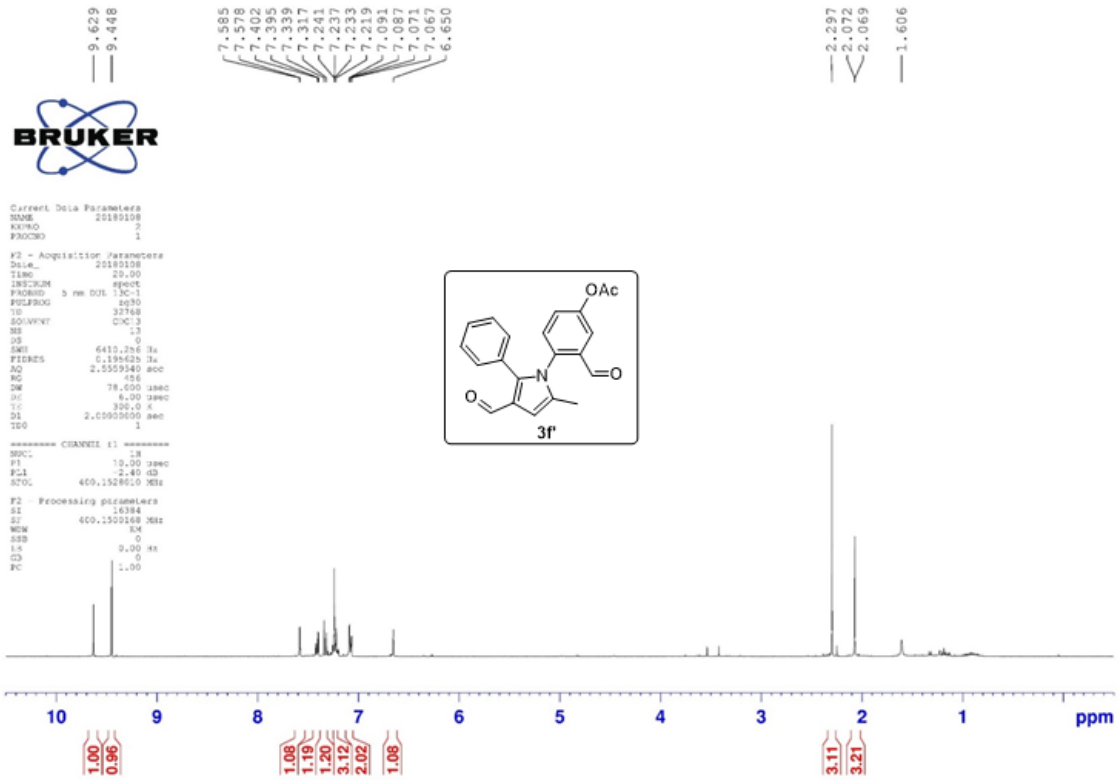

187.002
186.640
144.417
138.284
137.642
134.044
133.011
131.719
131.525
130.753
128.989
128.577
128.502
124.065
123.823
106.447
77.212
77.000
76.788
12.887
Br
O
N
O
3c'
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

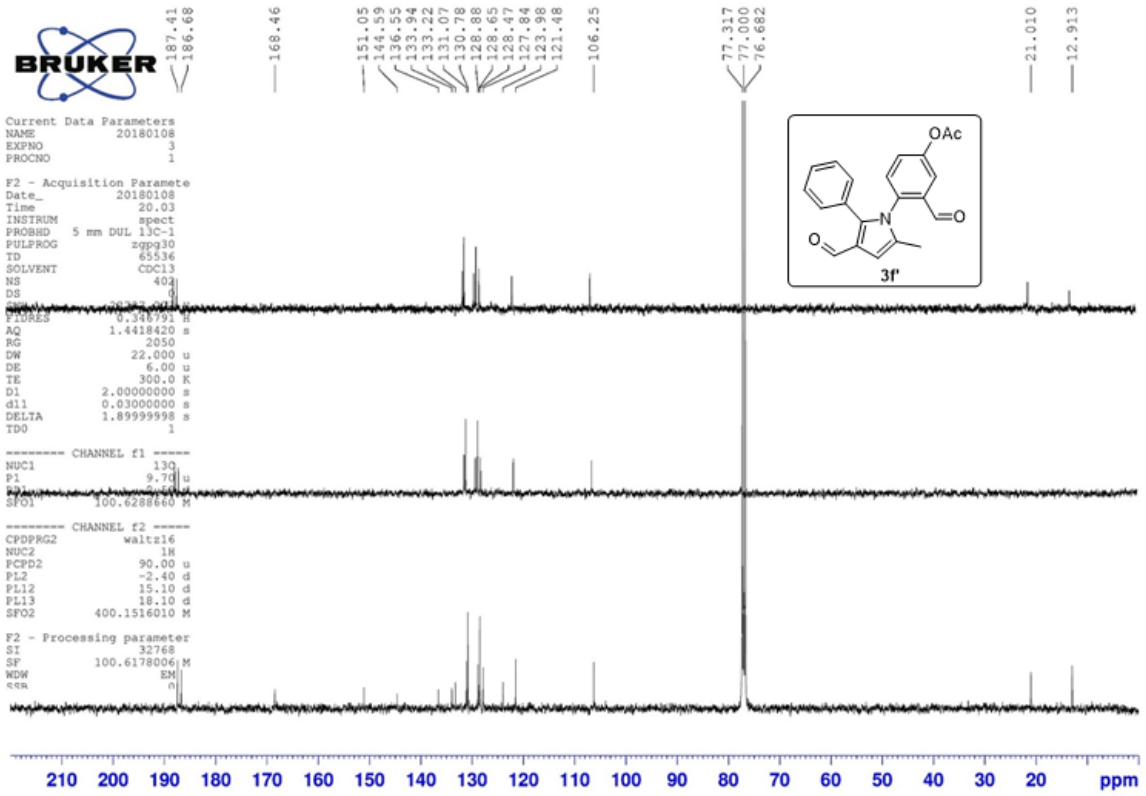

9.621
9.481
9.480
7.655
7.446
7.427
7.425
7.423
7.242
7.240
7.225
7.206
7.197
7.190
7.183
7.177
7.104
7.101
7.086
7.085
7.081
6.637
2.397
2.034
1.570
BRUKER
Current Data Parameters
NAME 20171220
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171220
Time 19.44
INSTRM spect
PROBHD 5 mm TCI 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5539542 sec
RG 724
DW 78.000 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
D9 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.2500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
3d'
O
N
O
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.01
1.07
5.11
2.11
1.00
3.17
3.18

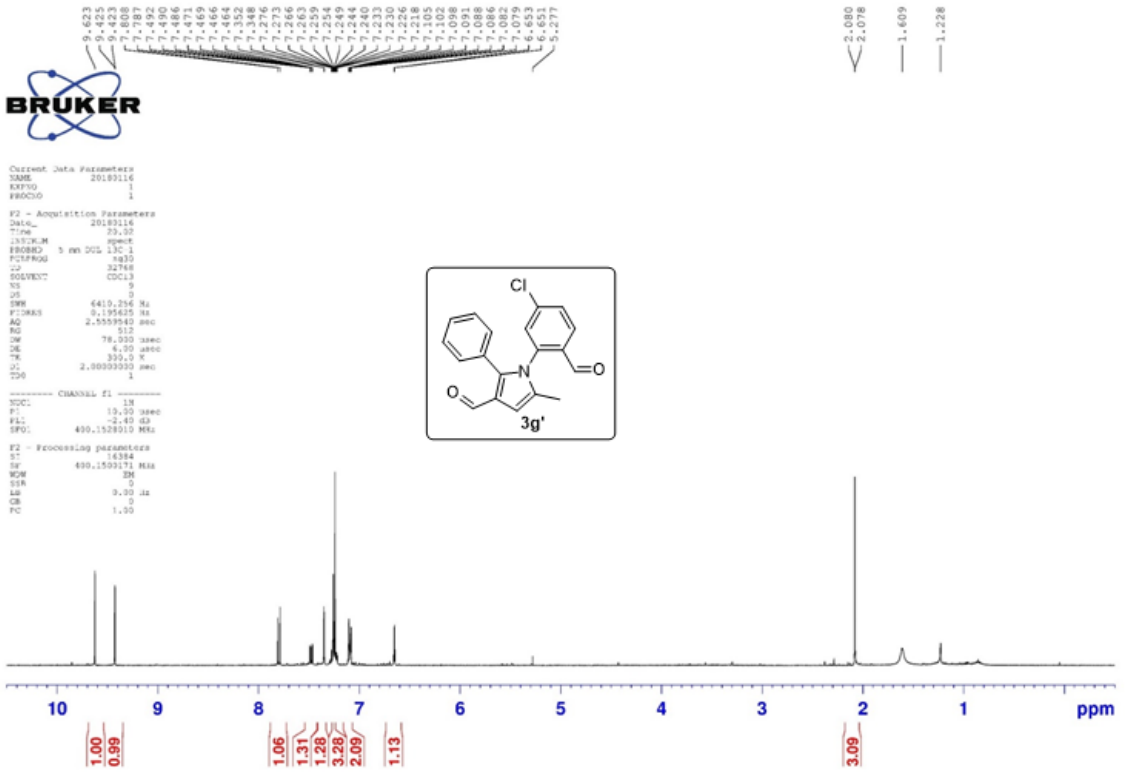

188.74
186.73
144.55
139.87
136.89
135.41
133.19
132.50
130.78
129.77
129.10
128.95
128.64
128.29
123.79
105.91
77.318
77.000
76.682
21.069
12.828
3d'
Current Data Parameters
NAME 20171220
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171220
Time 9.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 124
DS 4
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.75 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 100.6178025 MHz
WDW EM
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

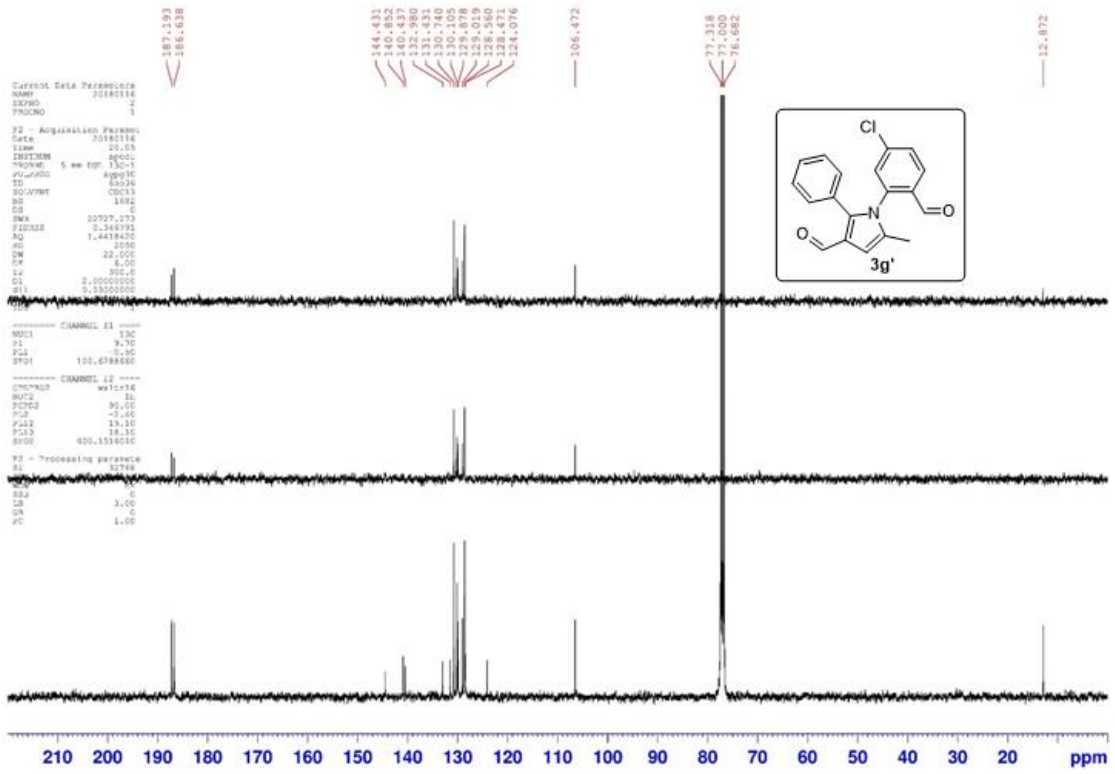

9.619
9.428
7.305
7.297
7.240
7.237
7.233
7.228
7.219
7.215
7.214
7.210
7.162
7.155
7.140
7.133
7.105
7.101
7.097
7.087
7.086
7.081
6.630
6.628
3.831
2.038
2.035
BRUKER
3e'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.20
4.03
1.14
2.05
1.11
3.45
3.41

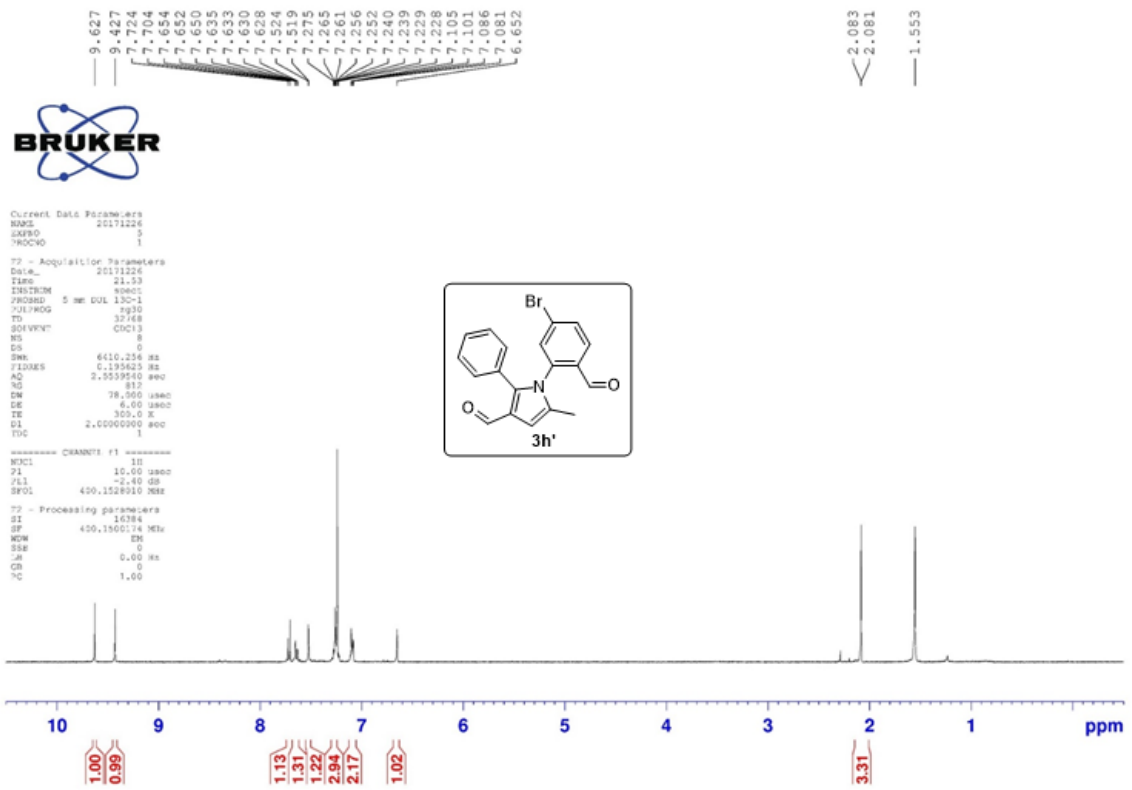

188.40
186.73
159.93
144.78
133.77
133.46
132.43
131.09
130.82
128.99
128.67
128.35
123.78
121.68
111.16
105.86
77.318
77.000
76.683
55.768
12.843
3e'
Current Data Parameters
NAME 20171226
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171226
Time 21.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 68
DS 0
SWH 31446.541 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
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 100.6178005 MHz
WDW EM
SSB 0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

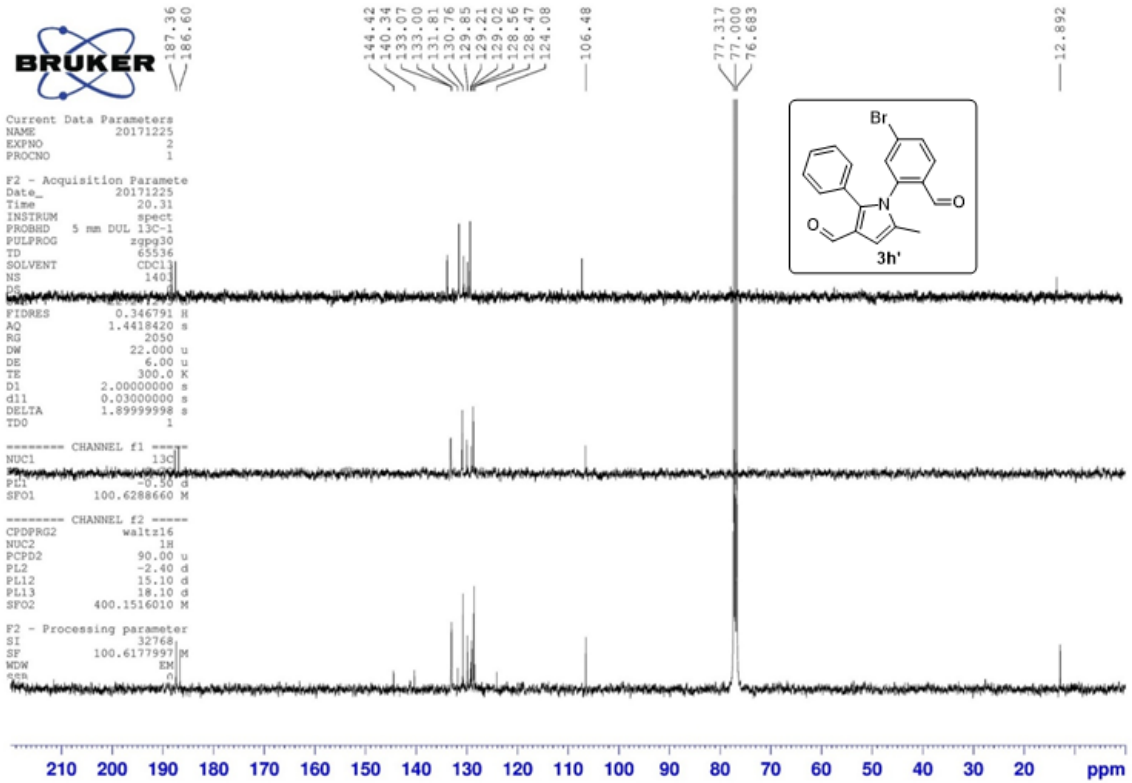

9.629
9.448
7.585
7.578
7.402
7.395
7.339
7.317
7.241
7.237
7.233
7.219
7.091
7.087
7.071
7.067
6.650
2.297
2.072
2.069
1.606
BRUKER
OAc
O
N
O
3f'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.96
1.08
1.19
1.20
3.12
2.02
1.06
3.11
3.21

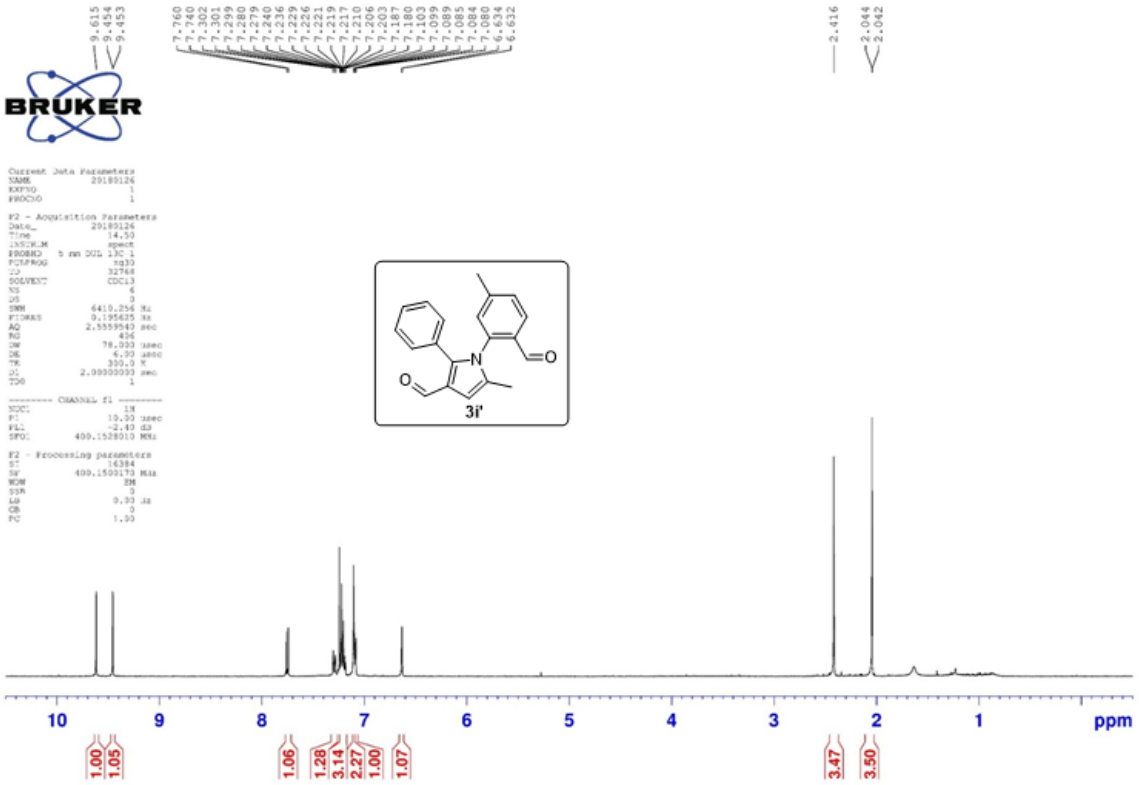

187.41
186.68
168.46
151.05
144.59
136.55
133.94
133.22
131.07
130.78
128.88
128.65
128.47
127.84
123.98
121.48
106.25
77.317
77.000
76.682
21.010
12.913
OAc
O
O
N
3f'
Current Data Parameters
NAME 20180108
EXPNO 3
PROCNO 1
F2 - Acquisition Paramete
Date_ 20180108
Time 20.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 402
DS 0
FIDRES 0.346791 H
AQ 1.4418420 s
RG 2050
DW 22.000 u
DE 6.00 u
TE 300.0 K
D1 2.00000000 s
d11 0.03000000 s
DELTA 1.89999998 s
TD0 1
======== CHANNEL f1 =====
NUC1 13C
P1 9.70 u
SFO1 100.6288660 M
======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 -2.40 d
PL12 15.10 d
PL13 18.10 d
SFO2 400.1516010 M
F2 - Processing parameter
SI 32768
SF 100.6178006 M
WDW EM
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

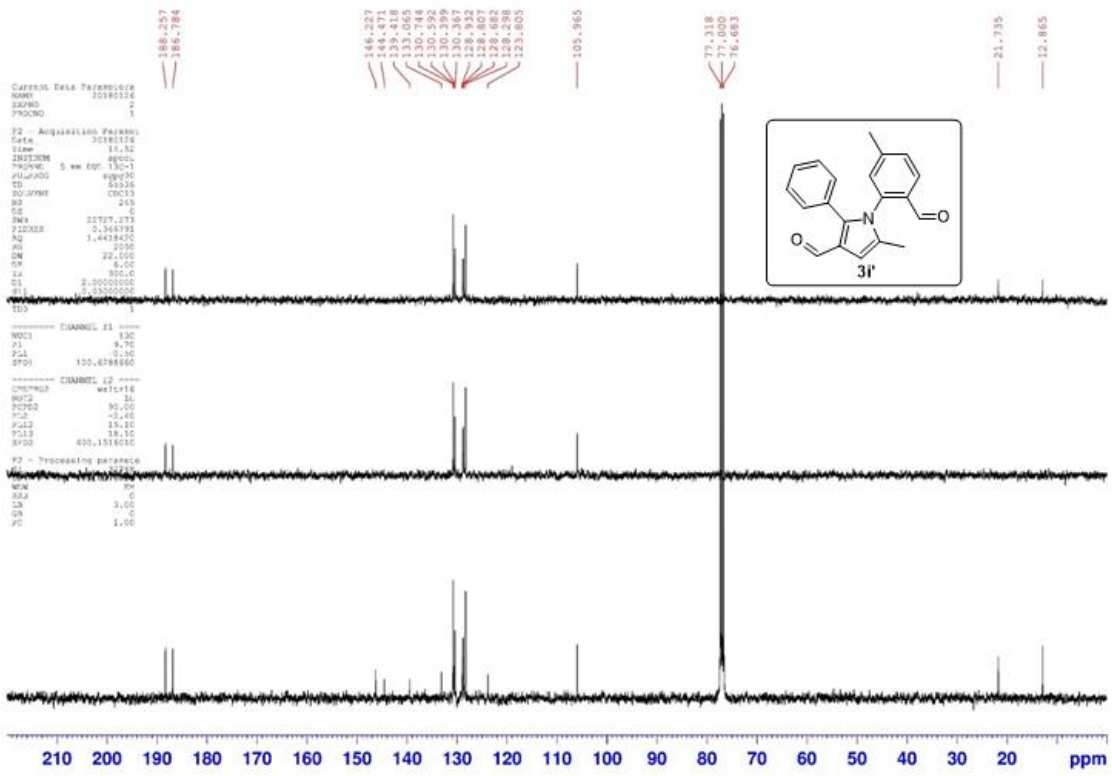

BRUKER
3g'
Cl
N
O
O
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.99
1.06
1.31
1.28
3.28
2.09
1.13
3.09

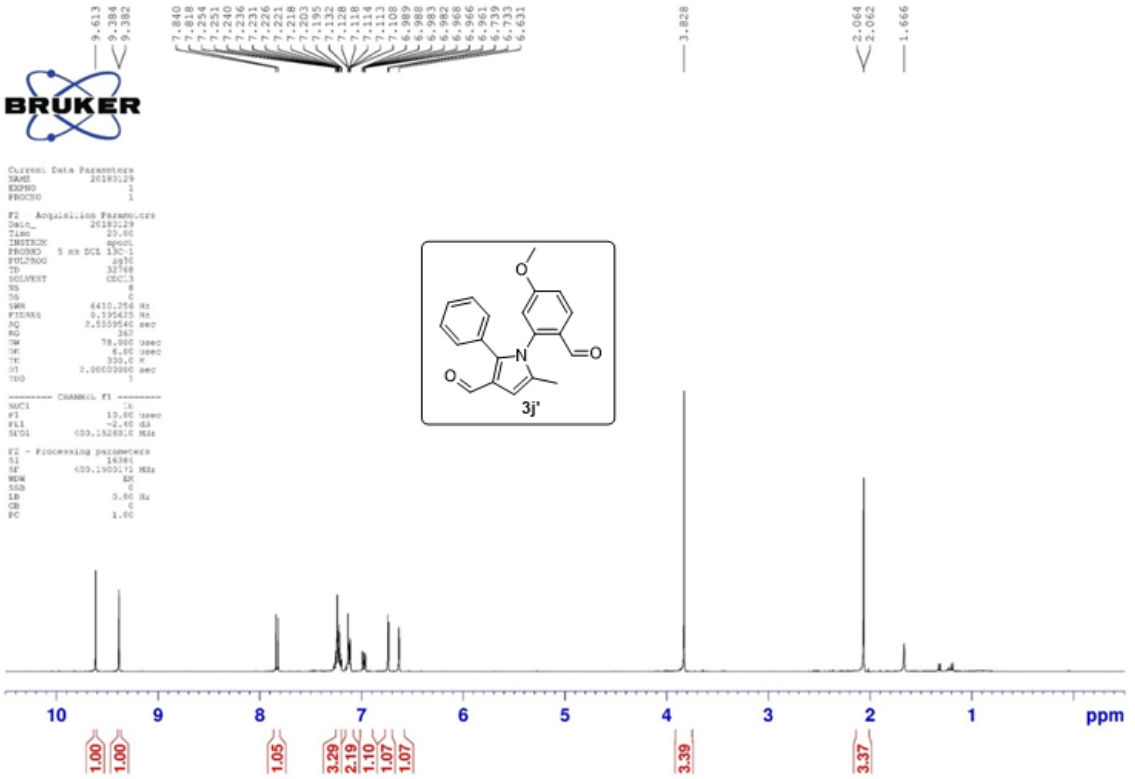

187.193
186.638
144.431
140.852
140.437
132.980
131.431
130.740
130.105
129.878
129.019
128.560
128.471
124.076
106.472
77.318
77.000
76.682
12.872
Cl
N
O
O
3g'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

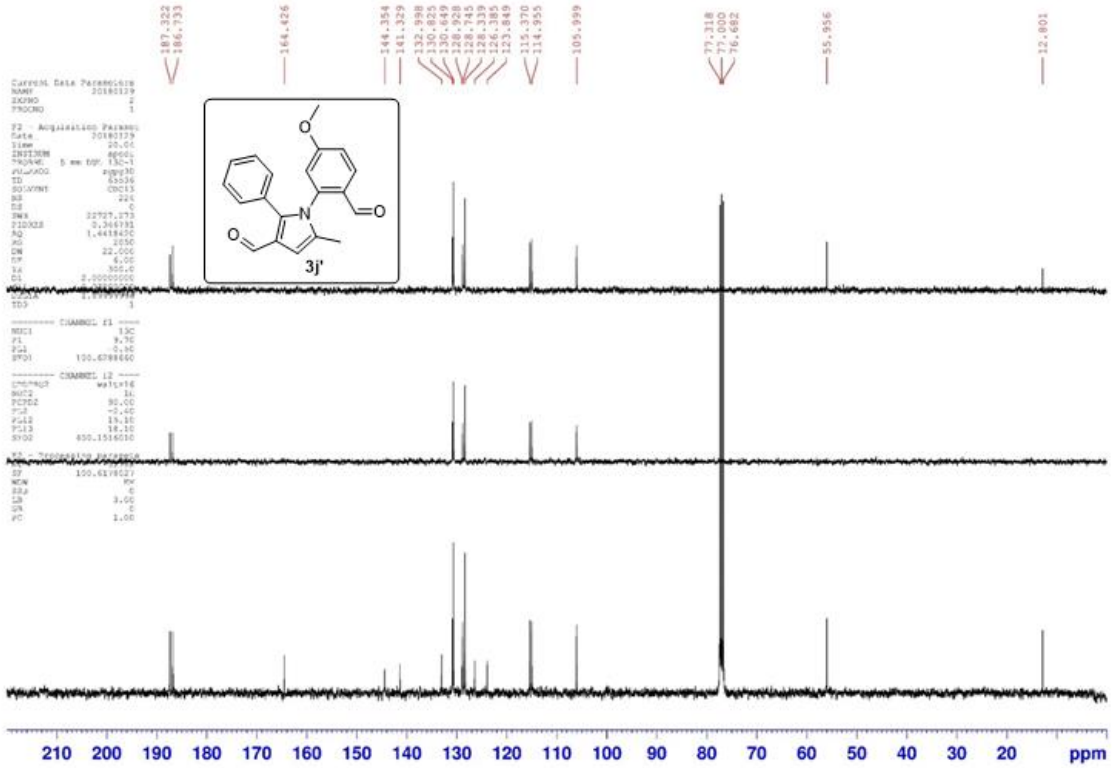

9.627
9.427
7.724
7.704
7.654
7.652
7.650
7.635
7.633
7.630
7.628
7.524
7.519
7.275
7.265
7.261
7.256
7.252
7.240
7.239
7.229
7.228
7.105
7.101
7.086
7.081
6.652
2.083
2.081
1.553
BRUKER
Br
N
O
O
3h'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.99
1.13
1.31
1.22
2.94
2.17
1.02
3.31

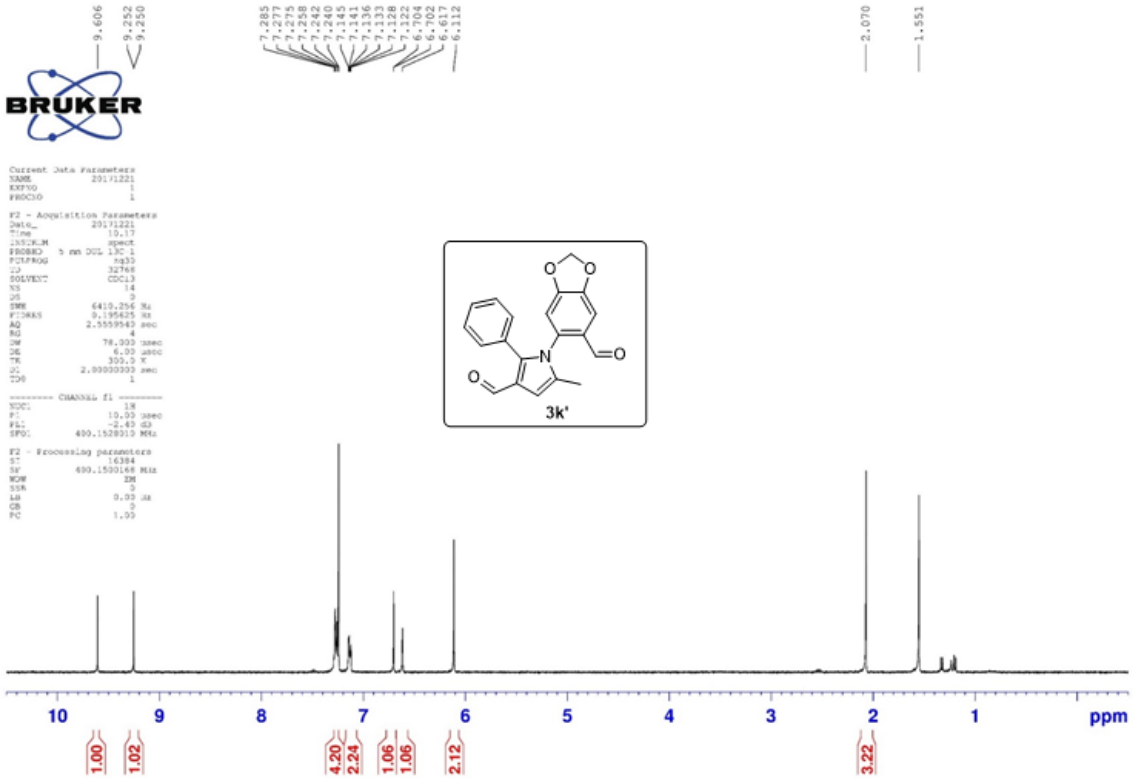

187.36
186.60
144.42
140.34
133.07
133.00
131.81
130.76
129.85
129.21
129.02
128.56
128.47
124.08
106.48
77.317
77.000
76.683
12.892
Br
N
O
O
3h'
Current Data Parameters
NAME 20171225
EXPNO 2
PROCNO 1
F2 - Acquisition Paramete
Date_ 20171225
Time 20.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1401
FIDRES 0.346791 H
AQ 1.4418420 s
RG 2050
DW 22.000 u
DE 6.00 u
TE 300.0 K
D1 2.00000000 s
d11 0.03000000 s
DELTA 1.89999998 s
TD0 1
======== CHANNEL f1 ======
NUC1 13C
PL1 -0.50 d
SFO1 100.6288660 M
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 -2.40 d
PL12 15.10 d
PL13 18.10 d
SFO2 400.1516010 M
F2 - Processing parameter
SI 32768
SF 100.6177997 M
WDW EM
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

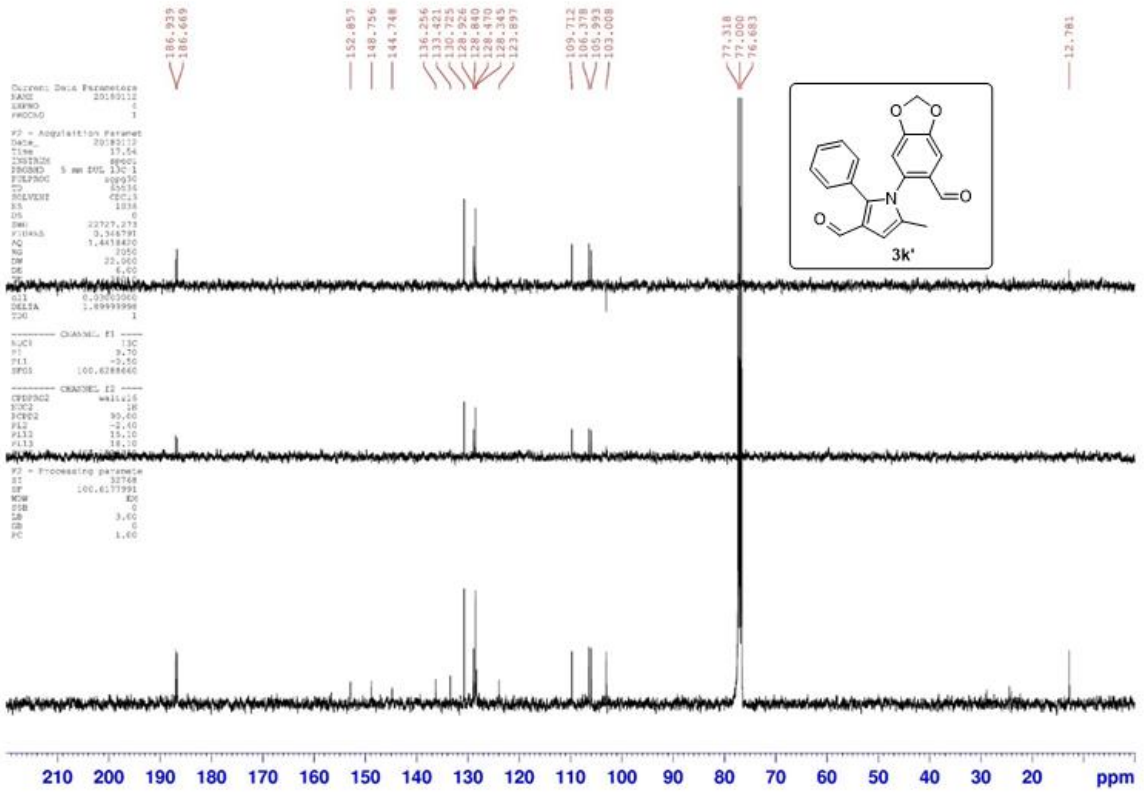

9.615
9.454
9.453
7.760
7.740
7.302
7.301
7.299
7.280
7.279
7.240
7.236
7.229
7.226
7.221
7.219
7.217
7.210
7.206
7.203
7.187
7.180
7.103
7.099
7.089
7.085
7.064
7.080
6.634
6.632
2.416
2.044
2.042
BRUKER
3i'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.05
1.06
1.28
3.14
2.27
1.00
1.07
3.47
3.50

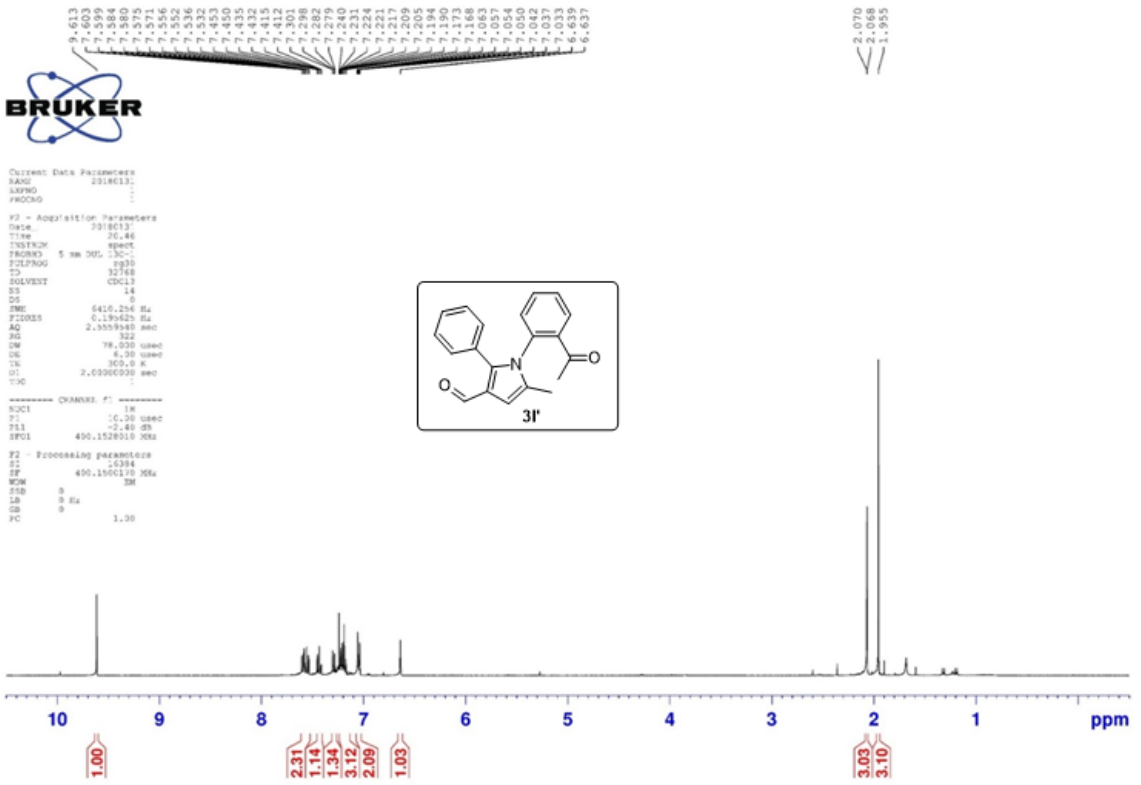

188.257
186.784
146.227
144.471
139.418
133.065
130.744
130.592
130.399
130.367
128.932
128.857
128.682
128.298
123.805
105.965
77.318
77.000
76.683
21.735
12.865
O
N
O
3i'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

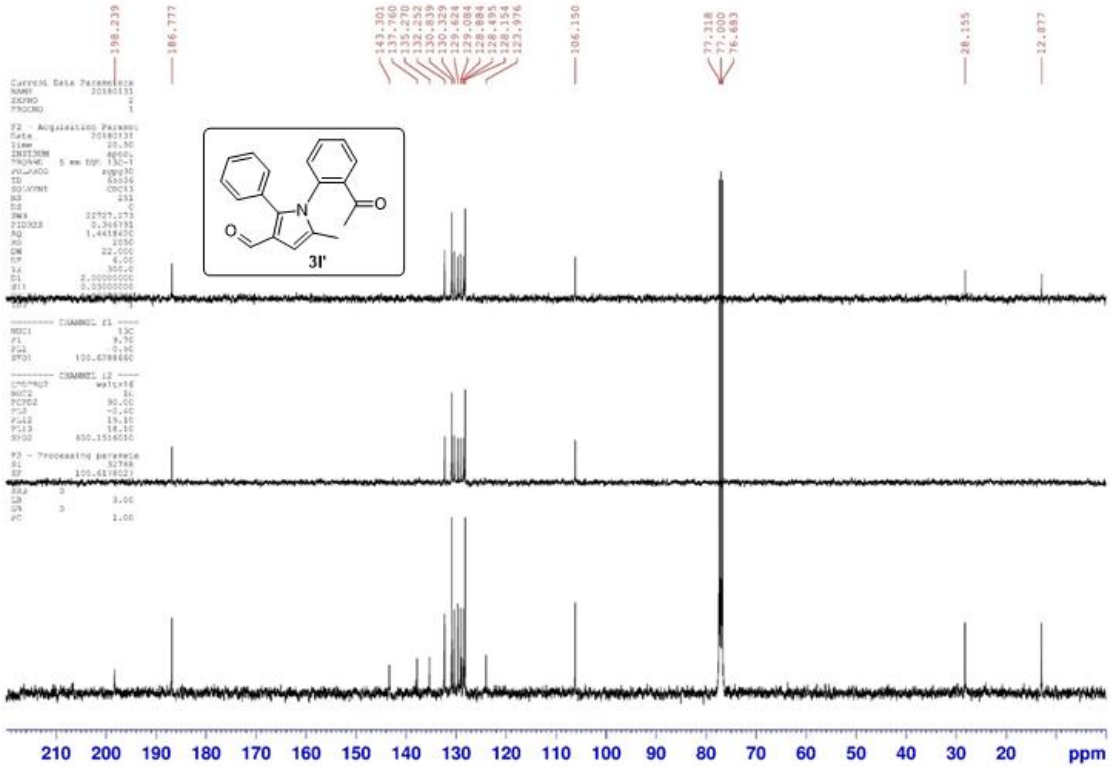

9.613
9.384
9.382
7.840
7.818
7.254
7.251
7.240
7.236
7.231
7.226
7.221
7.218
7.203
7.195
7.132
7.128
7.118
7.114
7.113
7.108
6.989
6.988
6.983
6.982
6.968
6.966
6.961
6.739
6.733
6.631
3.828
2.064
2.062
1.666
BRUKER
3j'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.05
3.29
2.19
1.10
1.07
1.07
3.39
3.37

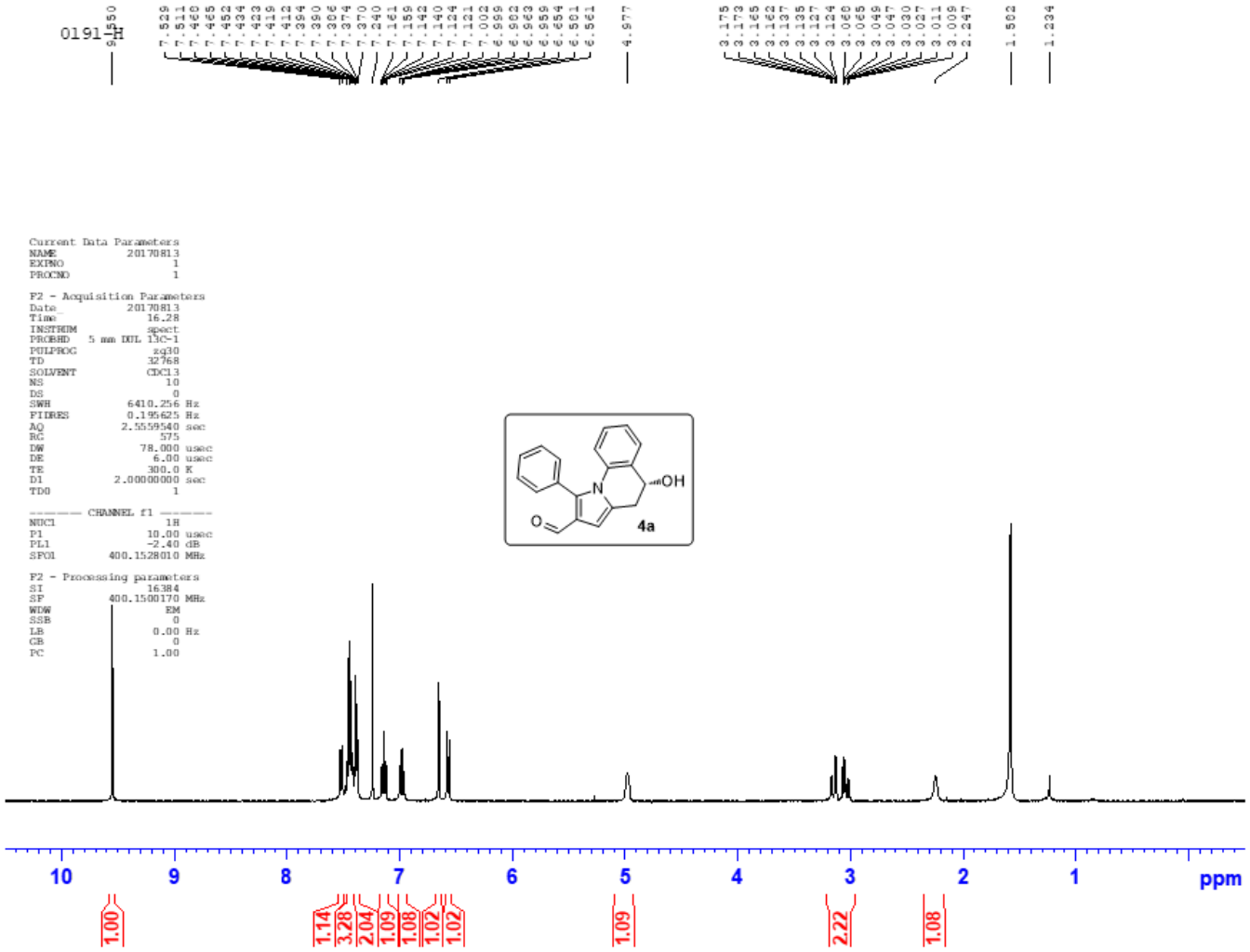

187.322
186.733
164.426
144.354
141.329
132.998
130.825
130.649
130.028
128.748
128.339
126.385
123.849
115.370
114.955
105.999
77.318
77.000
76.682
55.956
12.801
3j'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

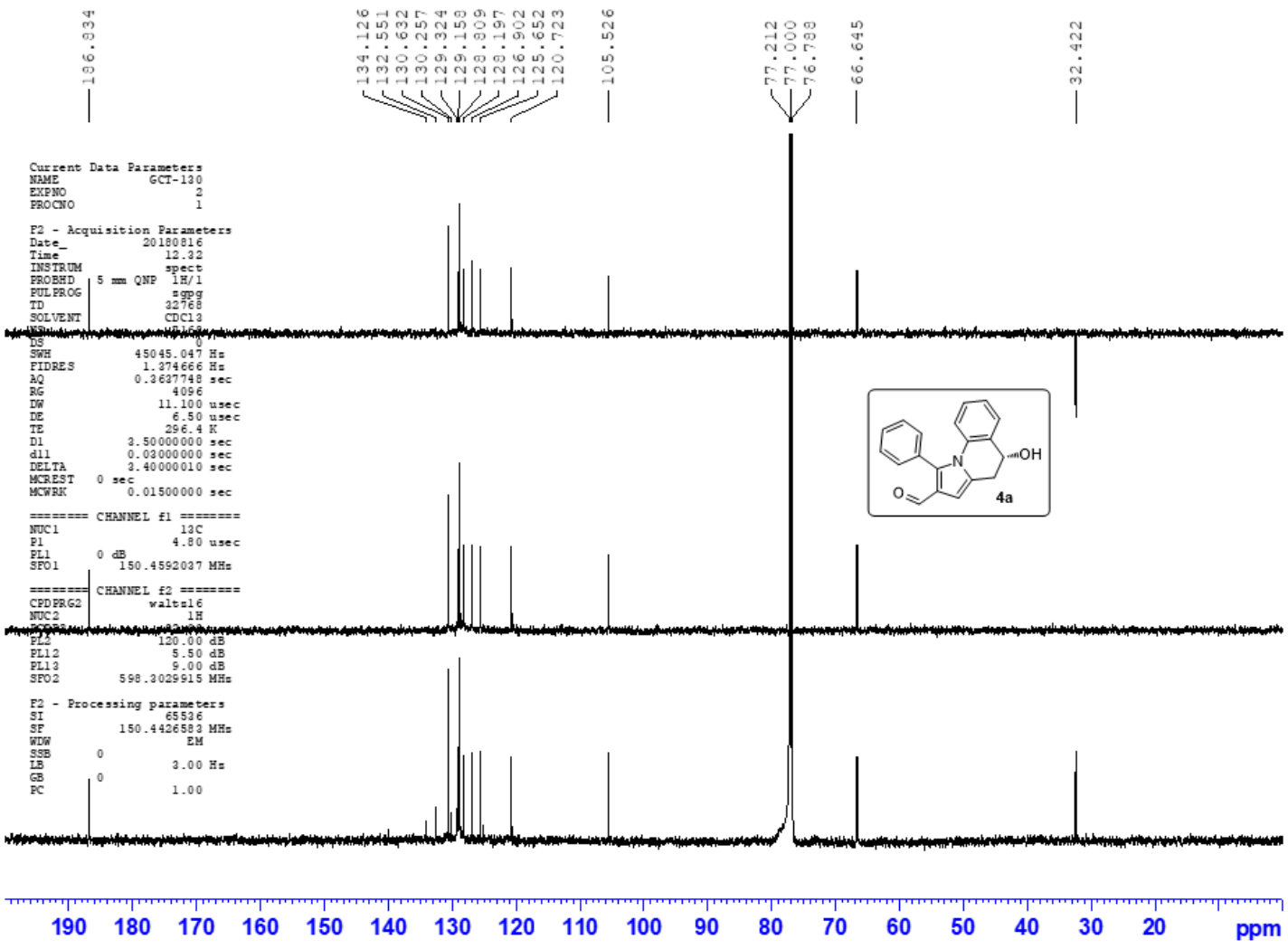

9.606
9.252
9.250
7.285
7.277
7.275
7.258
7.242
7.240
7.145
7.141
7.136
7.133
7.128
7.122
7.104
6.702
6.617
6.112
2.070
1.551
BRUKER
3k'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
4.20
2.24
1.06
1.06
2.12
3.22

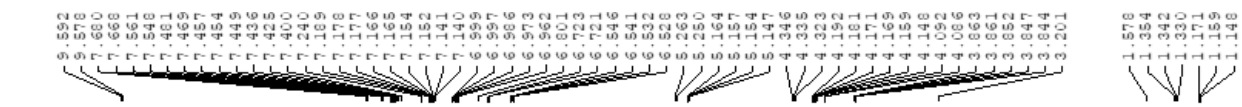

186.939
186.669
152.857
148.756
144.748
136.256
133.421
130.725
128.926
128.840
128.470
128.345
123.897
109.712
106.378
105.993
103.008
77.318
77.000
76.683
12.781
3k'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

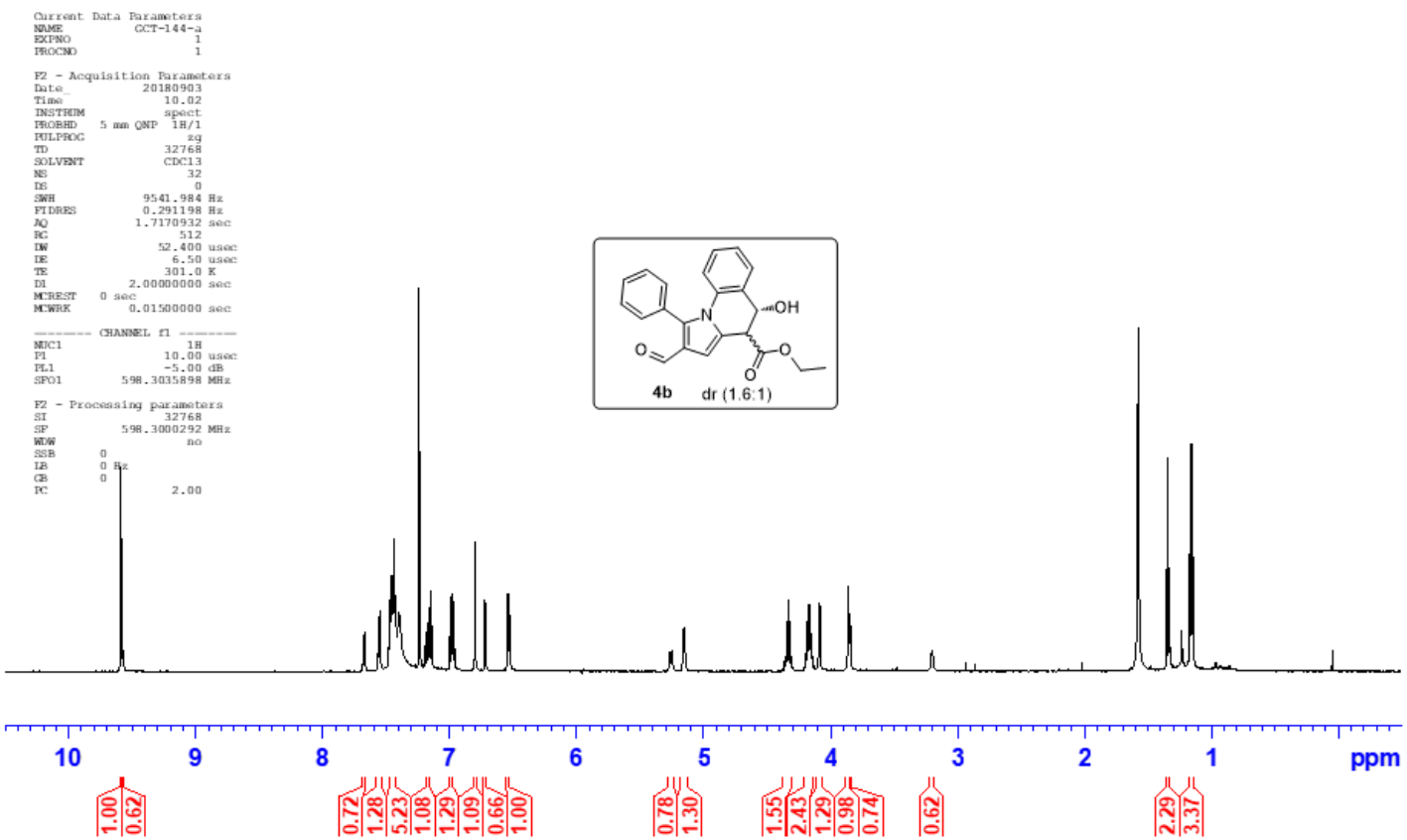

9.613
8.003
7.999
7.584
7.580
7.575
7.571
7.556
7.552
7.536
7.532
7.453
7.450
7.435
7.432
7.415
7.412
7.301
7.298
7.282
7.279
7.240
7.231
7.224
7.211
7.209
7.205
7.194
7.190
7.173
7.168
7.063
7.057
7.054
7.050
7.042
7.037
7.033
6.639
6.637
2.070
2.068
1.955
BRUKER
3l'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.31
1.14
1.34
3.12
2.09
1.03
3.03
3.10

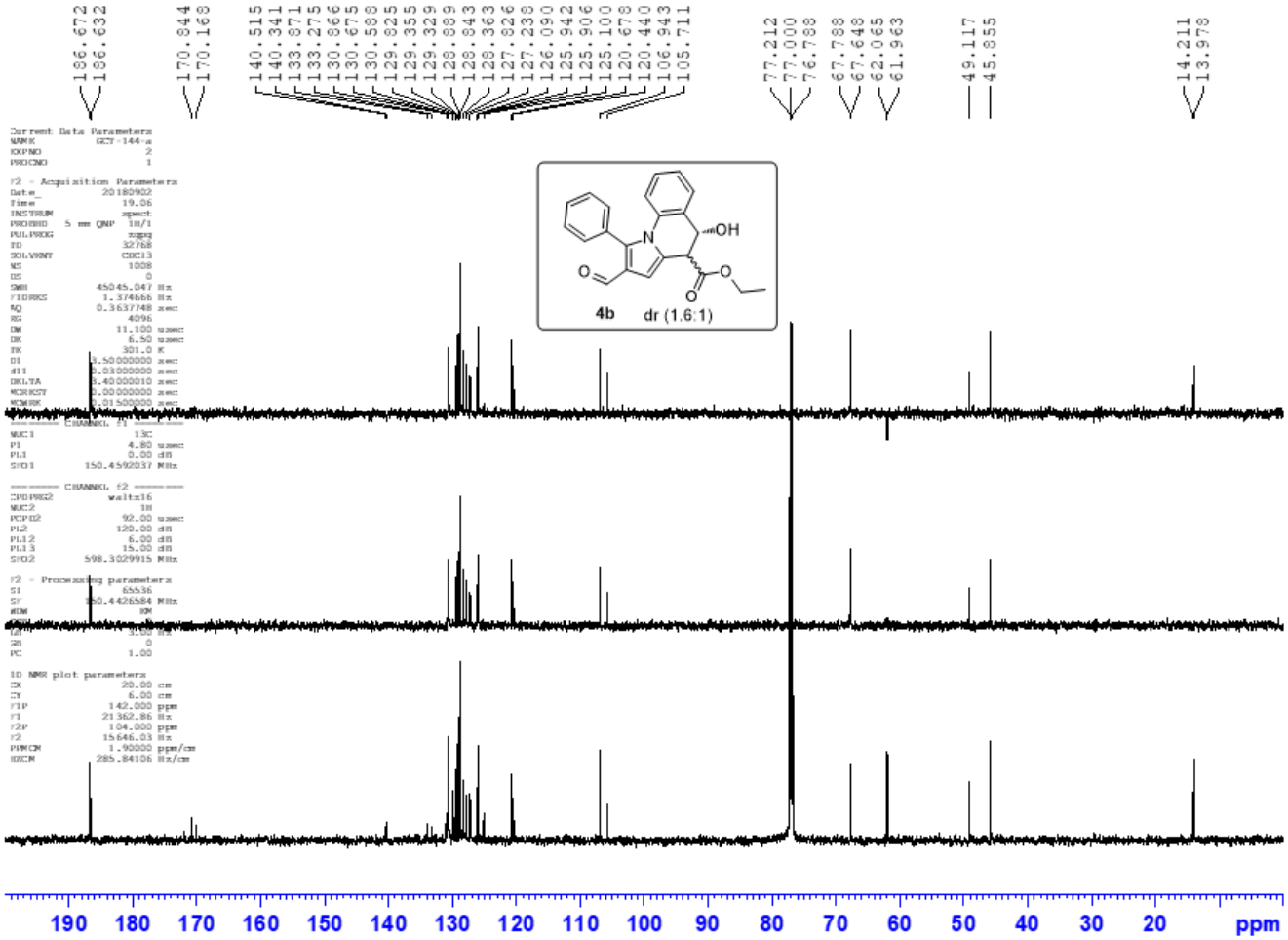

198.239
186.777
143.301
137.760
135.270
132.252
130.329
130.039
129.624
129.084
128.884
128.495
128.154
123.976
106.150
77.318
77.000
76.683
28.155
12.877
O
N
O
3l'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

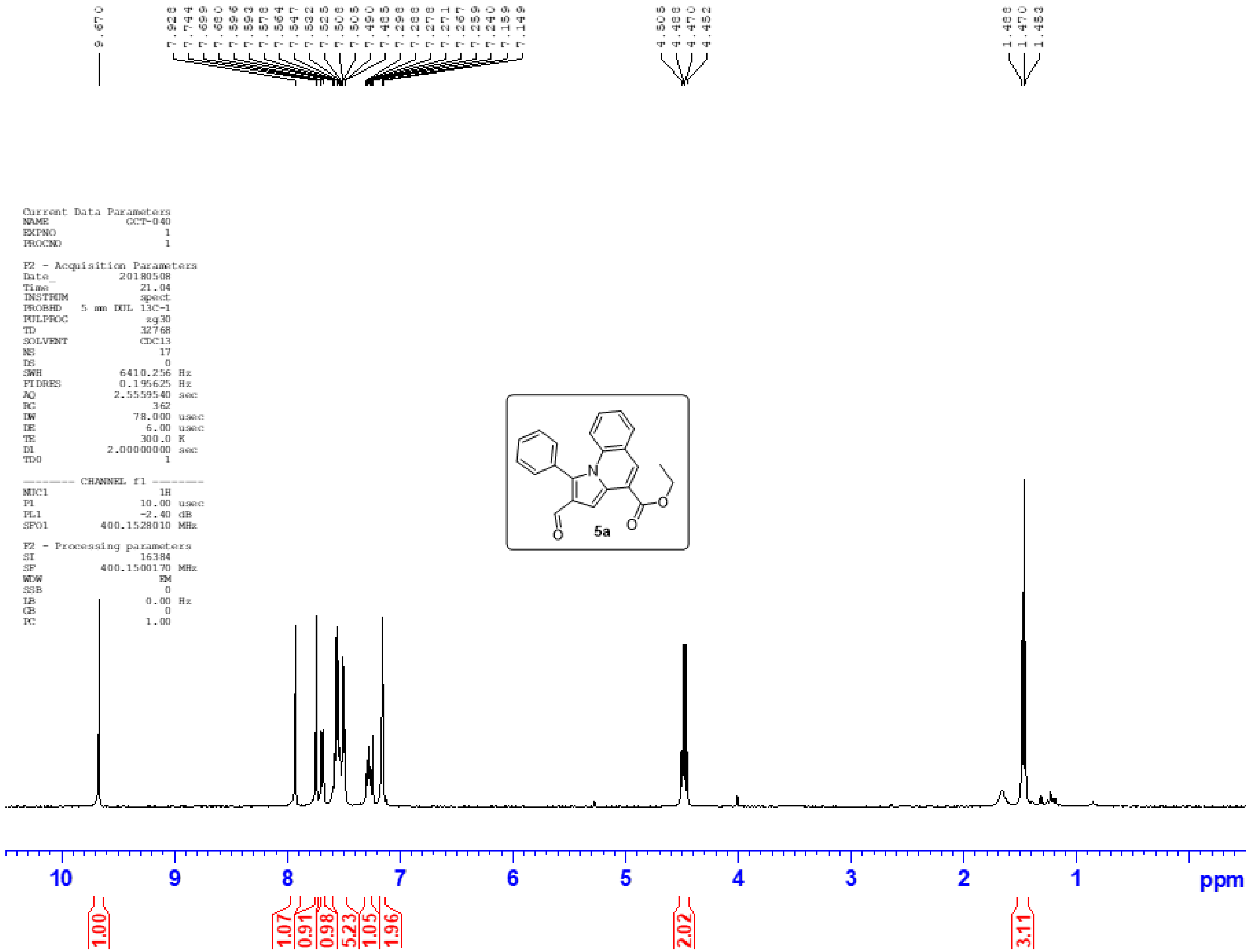

0191_1H
9.550
7.529
7.516
7.460
7.455
7.452
7.434
7.433
7.419
7.412
7.394
7.390
7.386
7.374
7.370
7.240
7.161
7.158
7.142
7.140
7.124
7.121
7.002
6.999
6.963
6.959
6.959
6.654
6.651
6.561
4.977
3.175
3.173
3.165
3.162
3.137
3.135
3.127
3.124
3.060
3.055
3.049
3.047
3.030
3.027
3.011
3.009
2.247
1.562
1.234
Current Data Parameters
NAME 20170813
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20170813
Time 16.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
O
N
4a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.14
3.28
2.04
1.09
1.08
1.02
1.02
1.09
2.22
1.08

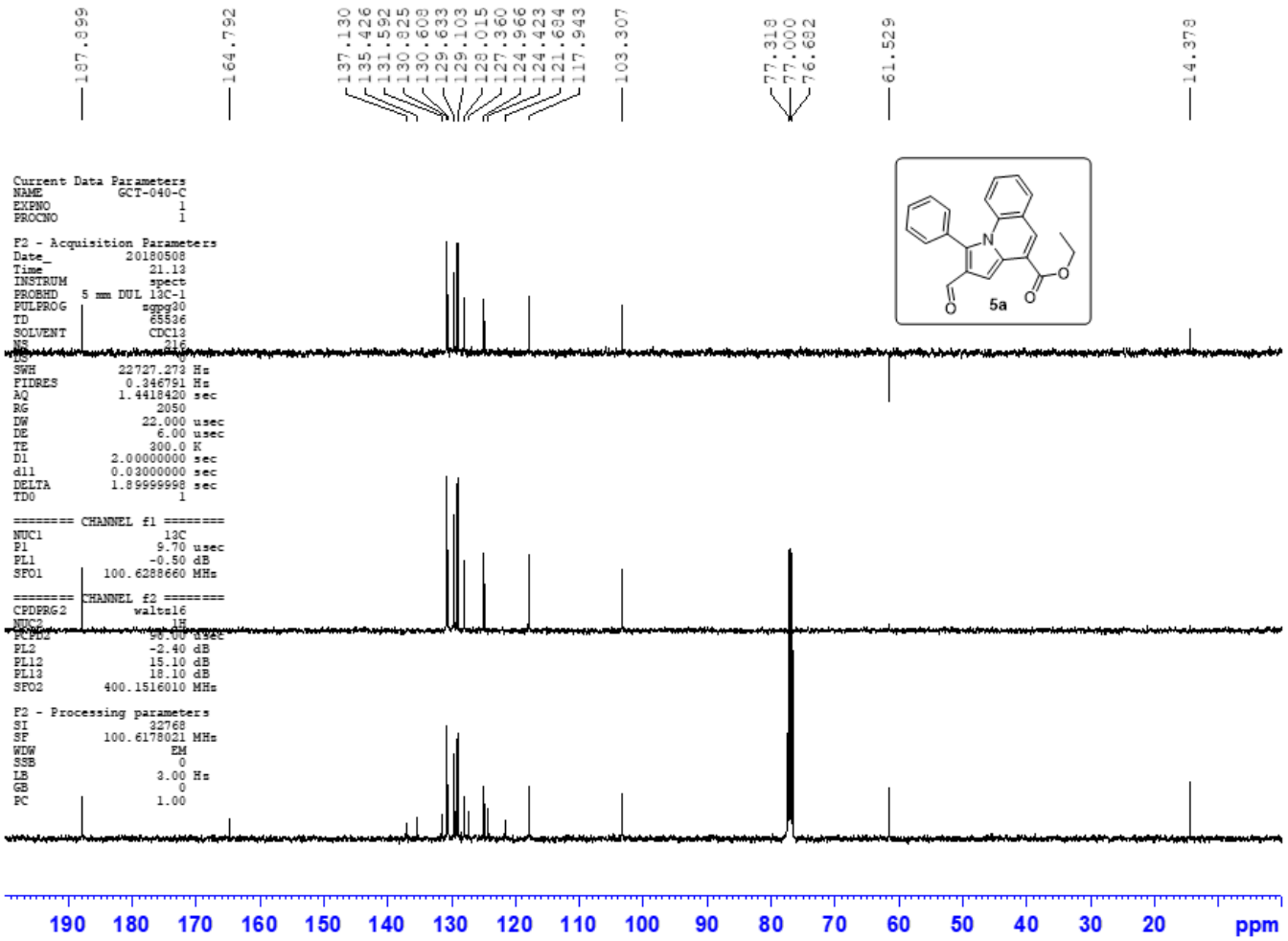

186.034
134.126
132.551
130.632
130.257
129.324
129.158
128.809
128.197
126.902
125.652
120.723
105.526
77.212
77.000
76.788
66.645
32.422
Current Data Parameters
NAME GCT-130
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180816
Time 12.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426583 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
N
O
4a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

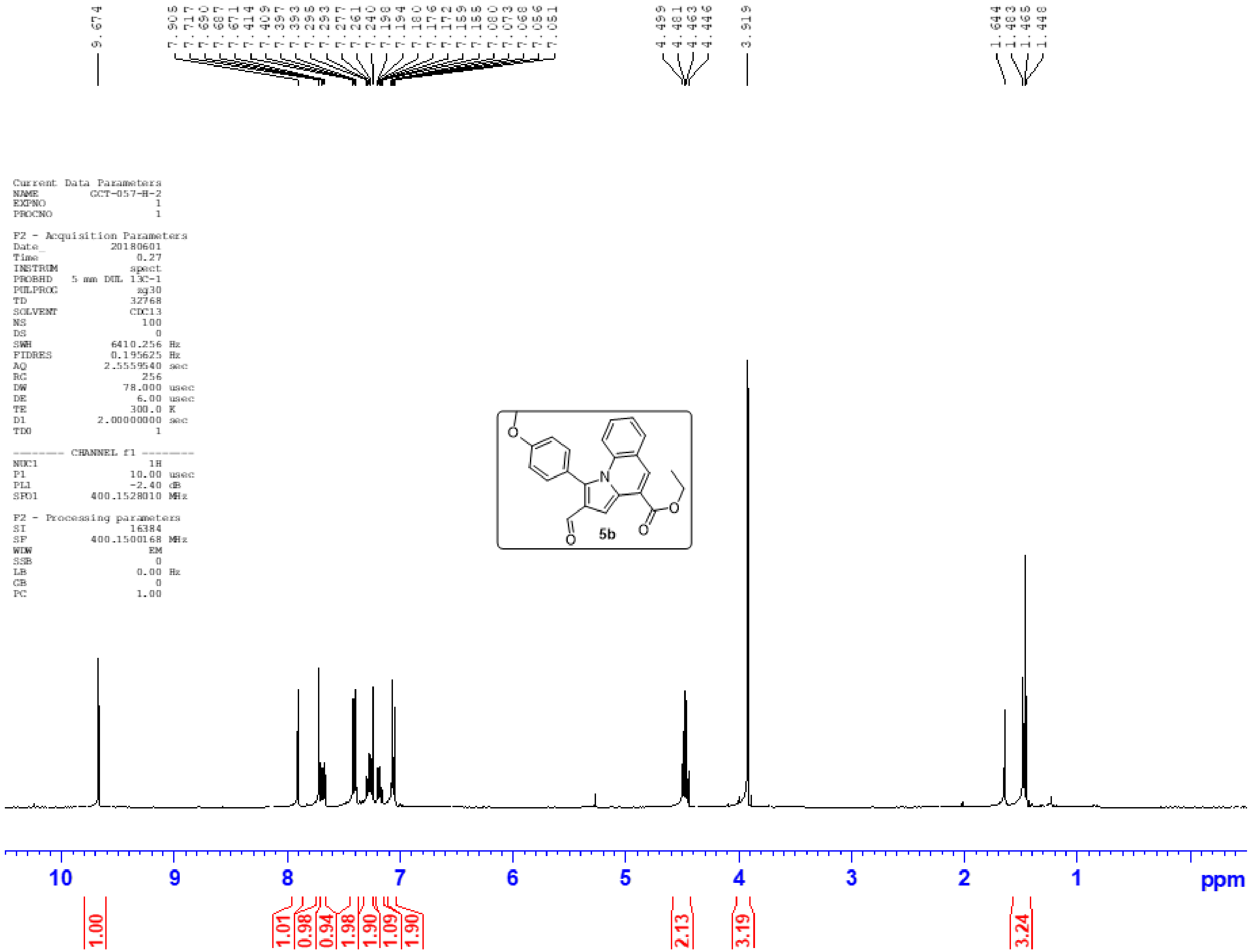


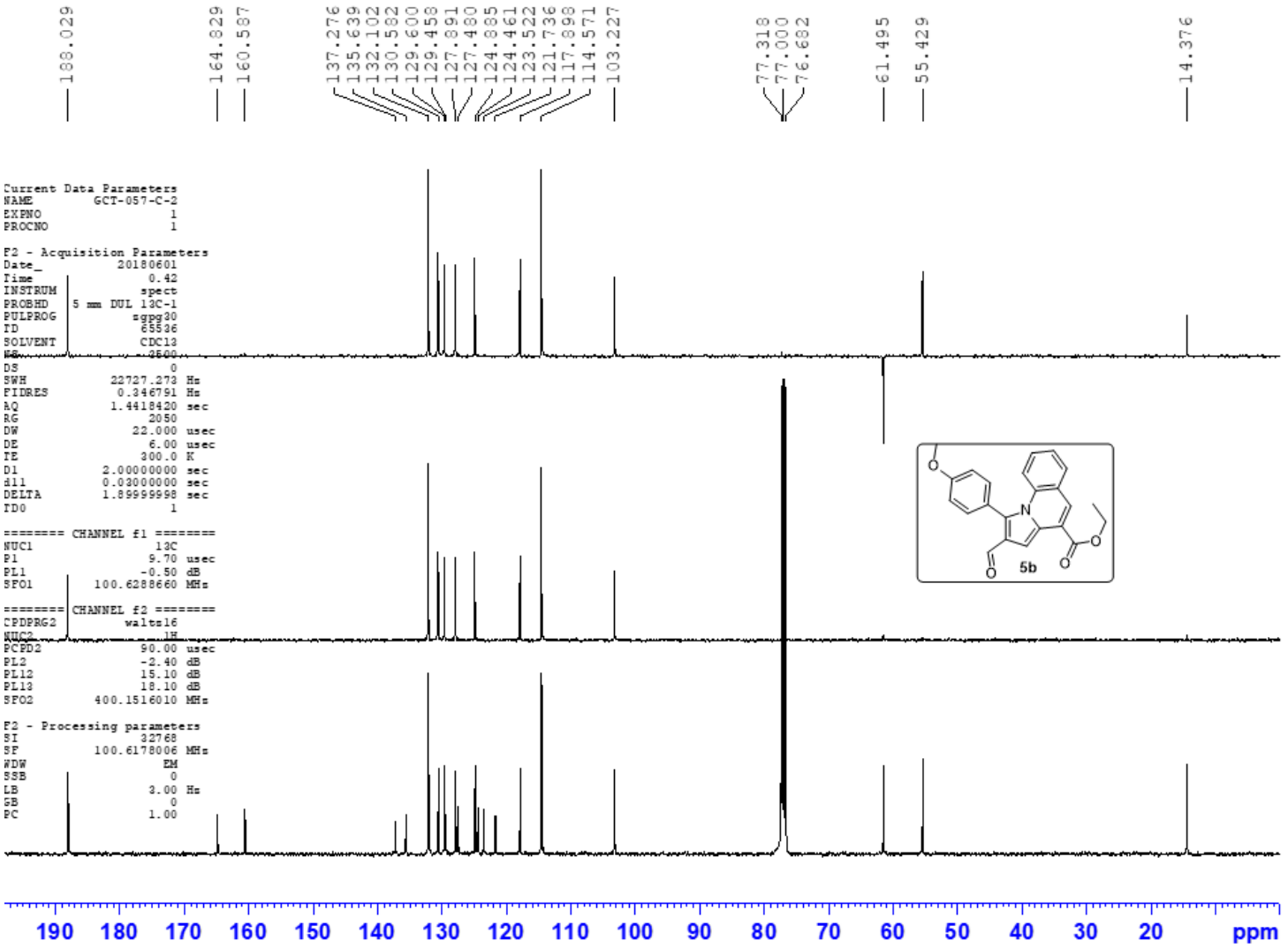

Current Data Parameters
NAME GCT-144-a
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180903
Time 10.02
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 301.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000292 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
OH
O
N
O
O
4b dr (1.6:1)
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.62
0.72
1.28
5.23
1.08
1.29
1.09
0.66
1.00
0.78
1.30
1.55
2.43
1.29
0.98
0.74
0.62
2.29
3.37

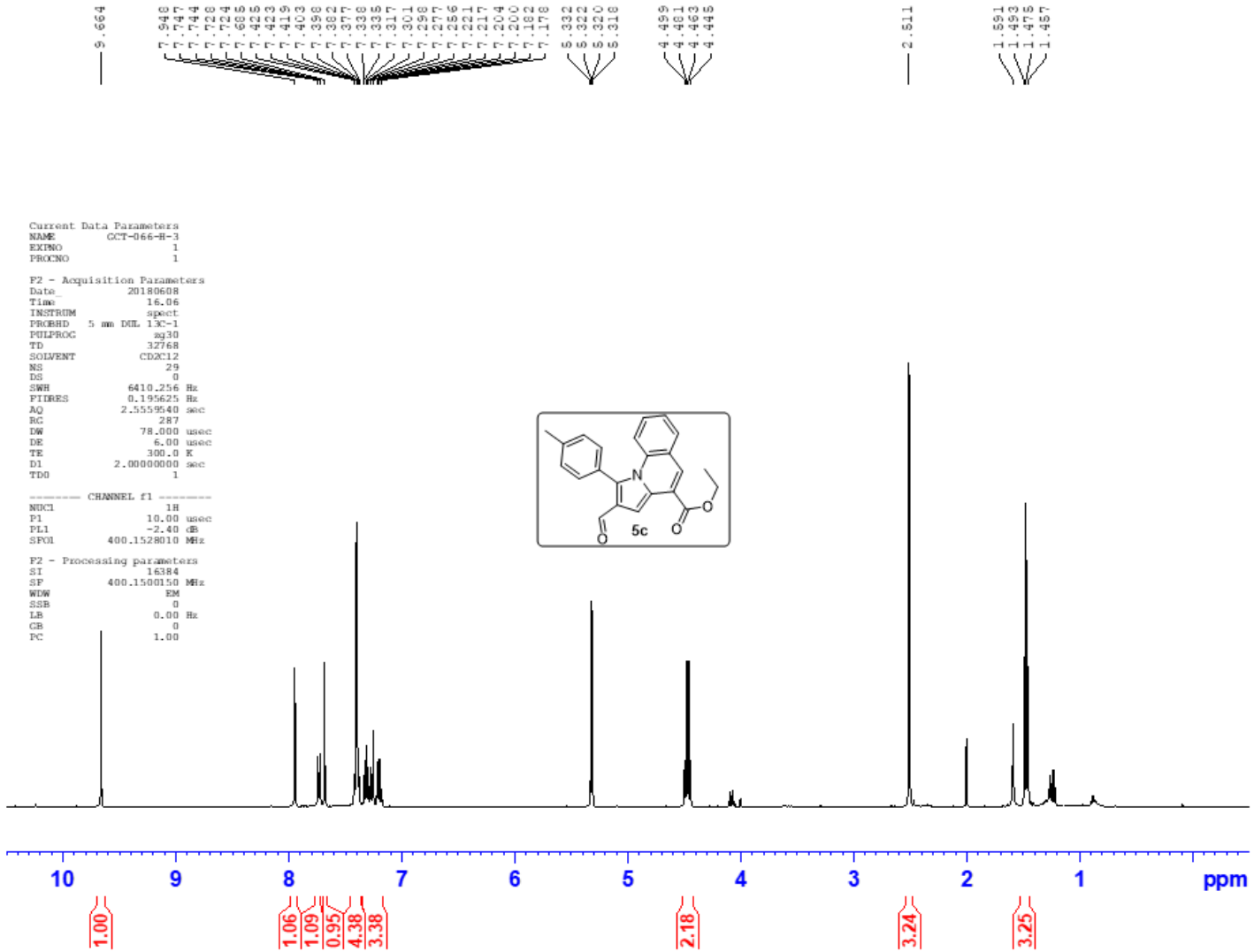

186.672
186.632
170.844
170.168
140.515
140.341
133.871
133.275
130.666
130.675
130.583
129.825
129.355
129.329
128.889
128.843
128.363
127.826
127.238
126.090
125.942
125.906
125.100
120.678
120.440
106.943
105.711
77.212
77.000
76.788
67.788
67.648
62.065
61.963
49.117
45.855
14.211
13.978
OH
N
O
O
O
4b dr (1.6:1)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

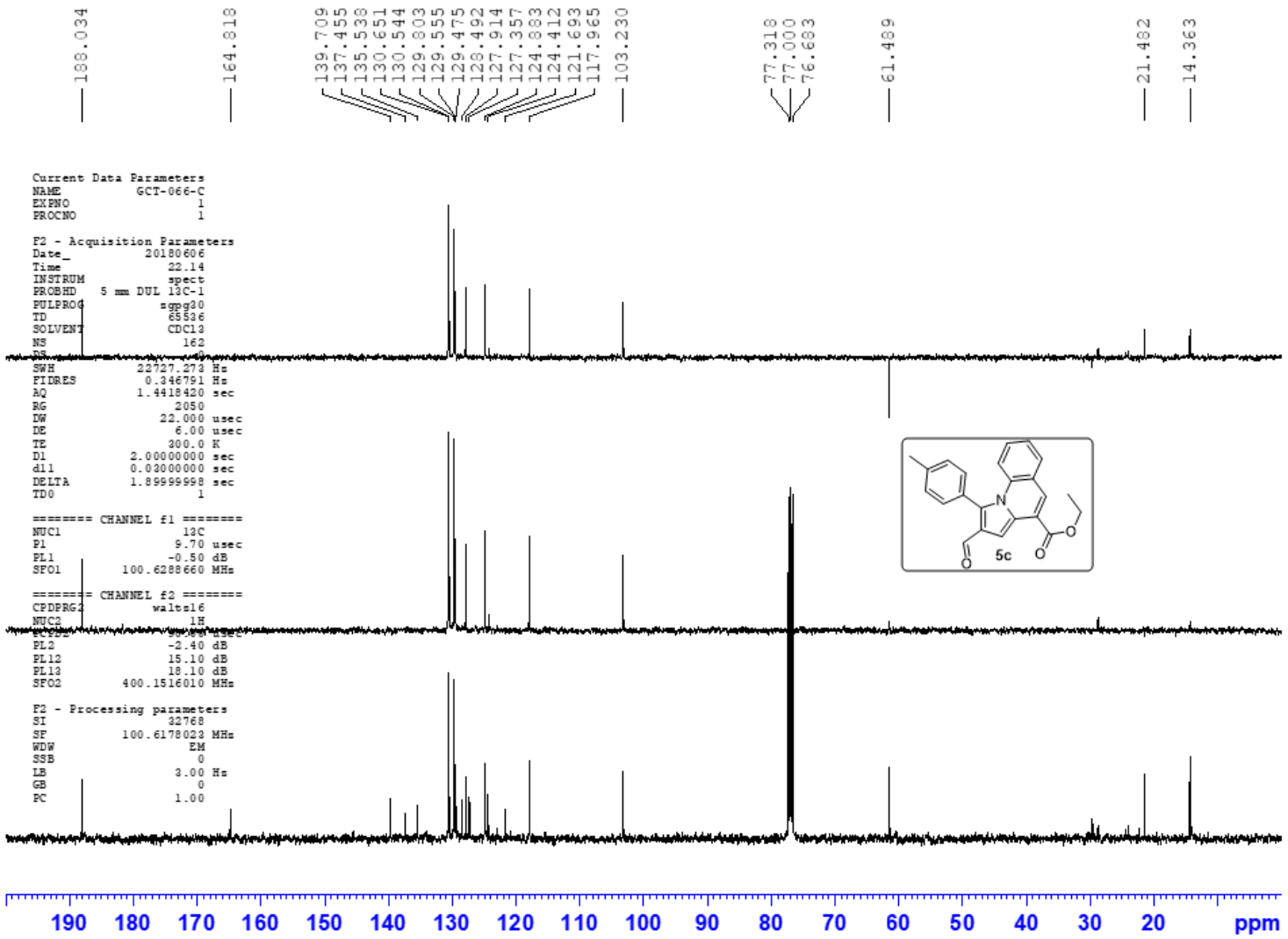

9.670
7.928 7.744 7.699 7.680 7.596 7.593 7.578 7.564 7.547 7.532 7.525 7.508 7.505 7.490 7.485 7.298 7.288 7.278 7.271 7.267 7.259 7.240 7.159 7.149
4.505 4.488 4.470 4.452
1.488 1.470 1.453
Current Data Parameters
NAME GCT-040
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180508
Time 21.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 17
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 362
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
O
O
O
5a
10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.07 0.91 0.98 5.23 1.05 1.96 2.02 3.11

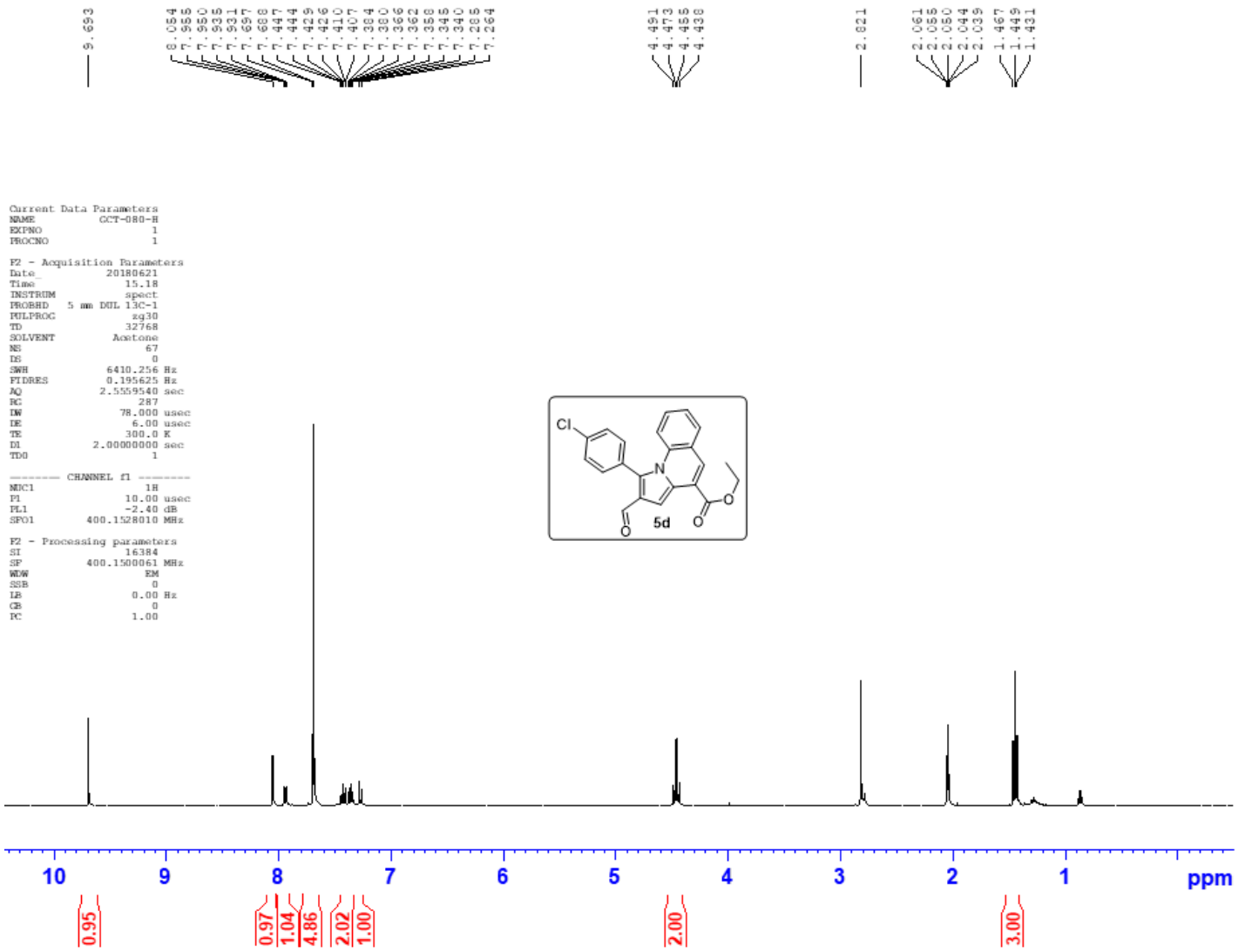

187.899
164.792
137.130
135.426
131.592
130.825
130.608
129.633
129.103
128.015
127.360
124.966
124.423
121.684
117.943
103.307
77.318
77.000
76.682
61.529
14.378
Current Data Parameters
NAME GCT-040-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180508
Time 21.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 216
DS 4
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178021 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5a
O
O
O
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

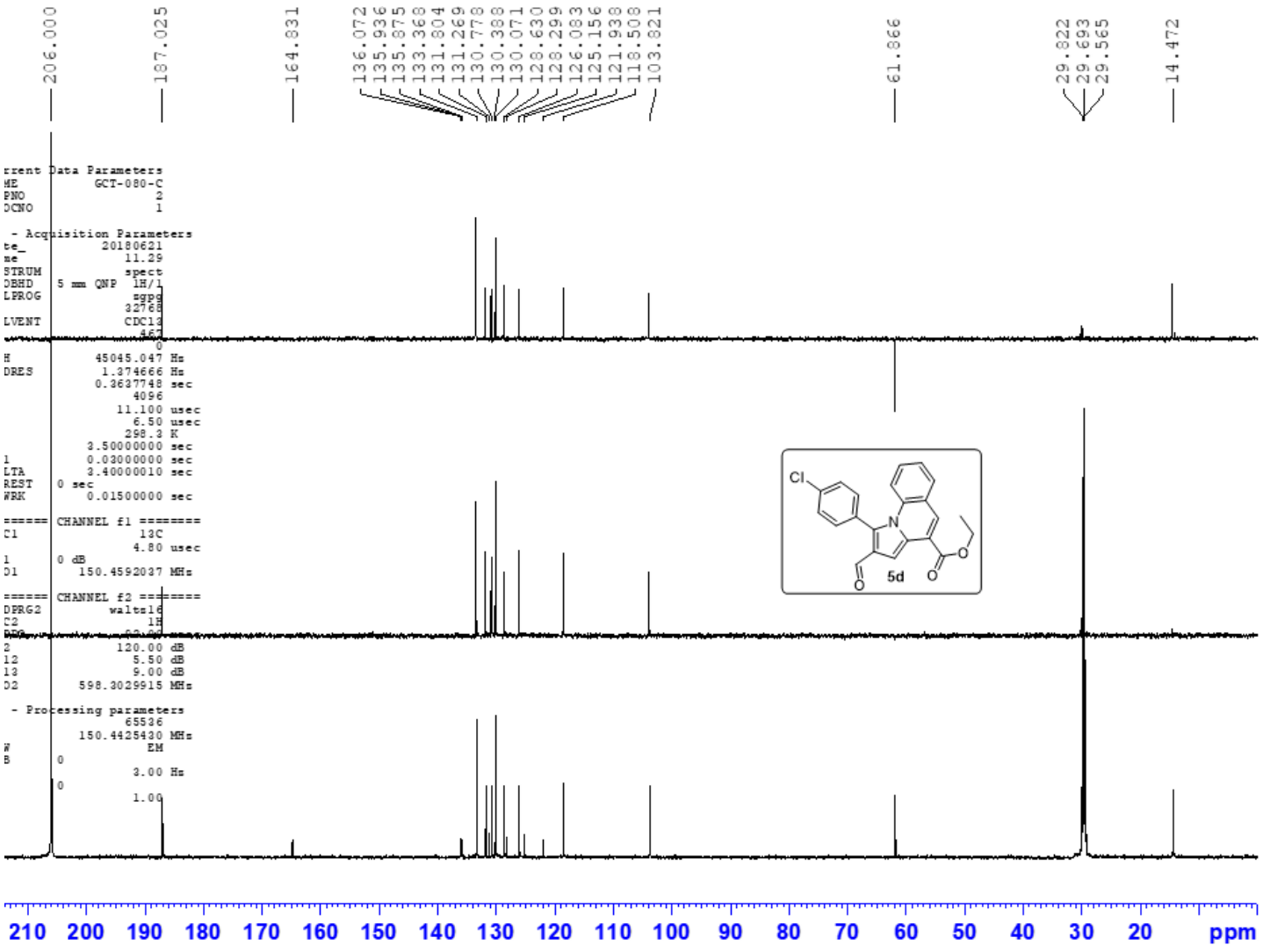

9.674
7.905
7.717
7.690
7.687
7.671
7.414
7.409
7.397
7.393
7.296
7.293
7.277
7.261
7.240
7.198
7.194
7.180
7.176
7.172
7.159
7.155
7.080
7.073
7.068
7.056
7.051
4.499
4.481
4.463
4.446
3.919
1.644
1.483
1.465
1.448
Current Data Parameters
NAME GCT-057-H-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180601
Time 0.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 100
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 0.00 Hz
GB 0
PC 1.00
O
N
O
O
O
5b
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
0.98
0.94
1.98
1.90
1.09
1.90
2.13
3.19
3.24

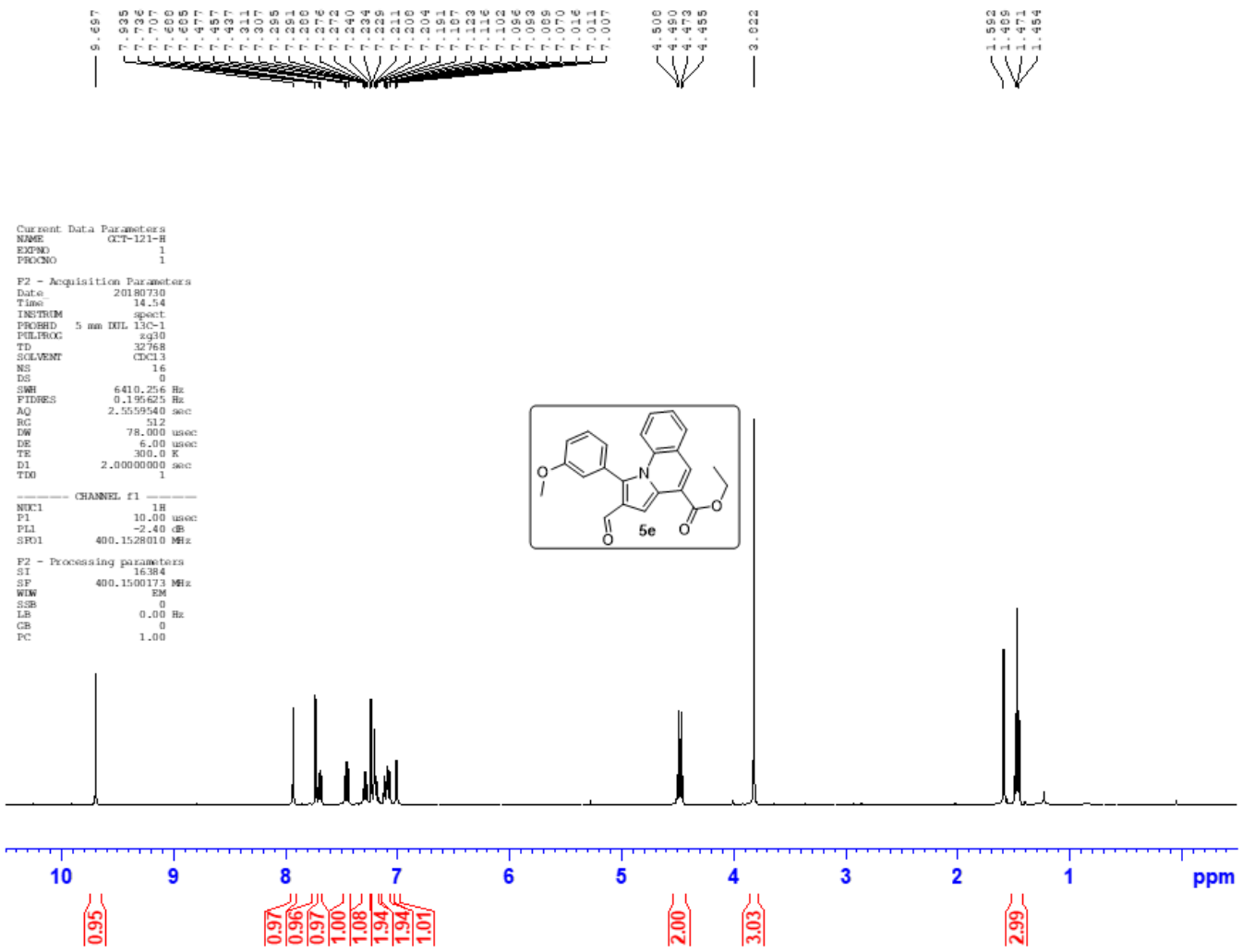

188.029
164.829
160.587
137.276
135.639
132.102
130.582
129.600
129.458
127.891
127.480
124.885
124.461
123.522
121.736
117.898
114.571
103.227
77.318
77.000
76.682
61.495
55.429
14.376
Current Data Parameters
NAME GCT-057-C-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180601
Time 0.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2500
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178006 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

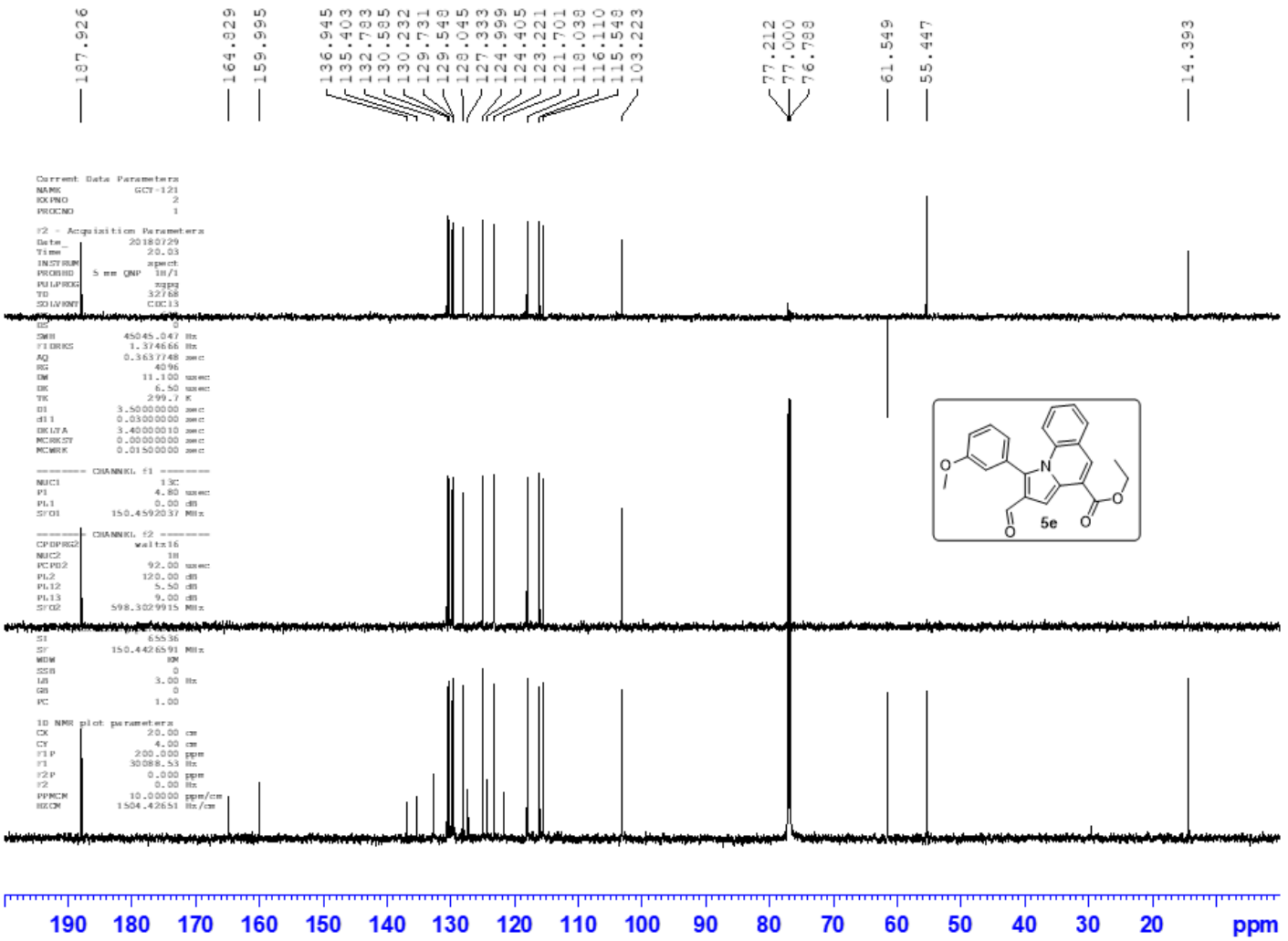

9.664
7.948
7.747
7.744
7.728
7.724
7.685
7.425
7.423
7.419
7.403
7.398
7.382
7.377
7.338
7.335
7.317
7.301
7.298
7.277
7.256
7.221
7.217
7.204
7.200
7.182
7.178
6.332
6.322
6.320
6.316
4.499
4.481
4.463
4.445
2.511
1.591
1.493
1.475
1.457
Current Data Parameters
NAME GCT-066-H-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20180608
Time 16.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CD2C12
NS 29
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500150 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5c
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
1.09
0.95
4.38
3.38
2.18
3.24
3.25

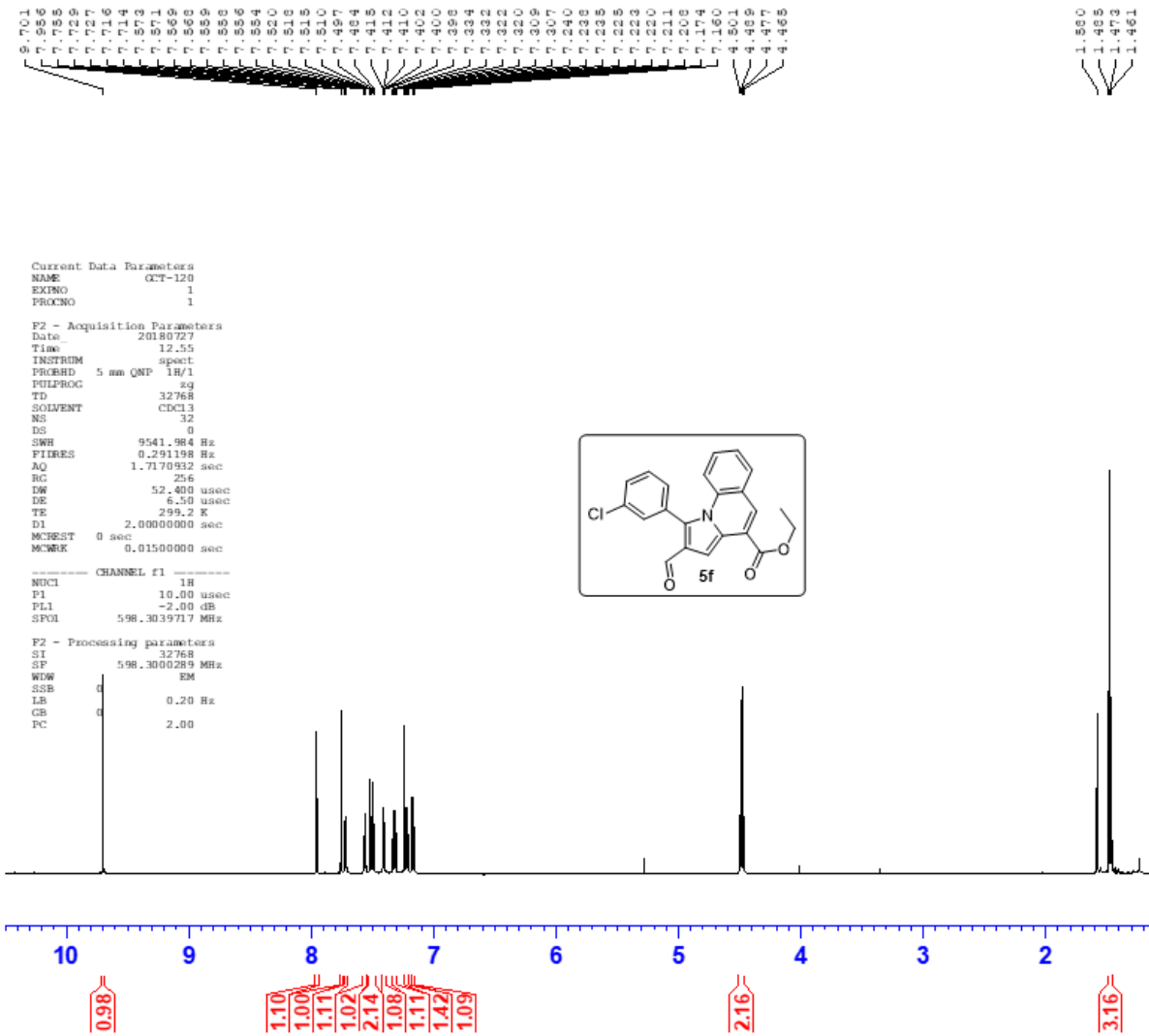

188.034
164.818
139.709
137.455
135.538
130.651
130.544
129.803
129.555
129.475
128.492
127.914
127.357
124.883
124.412
121.693
117.965
103.230
77.318
77.000
76.683
61.489
21.482
14.363
Current Data Parameters
NAME GCT-066-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180606
Time 22.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 162
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178023 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

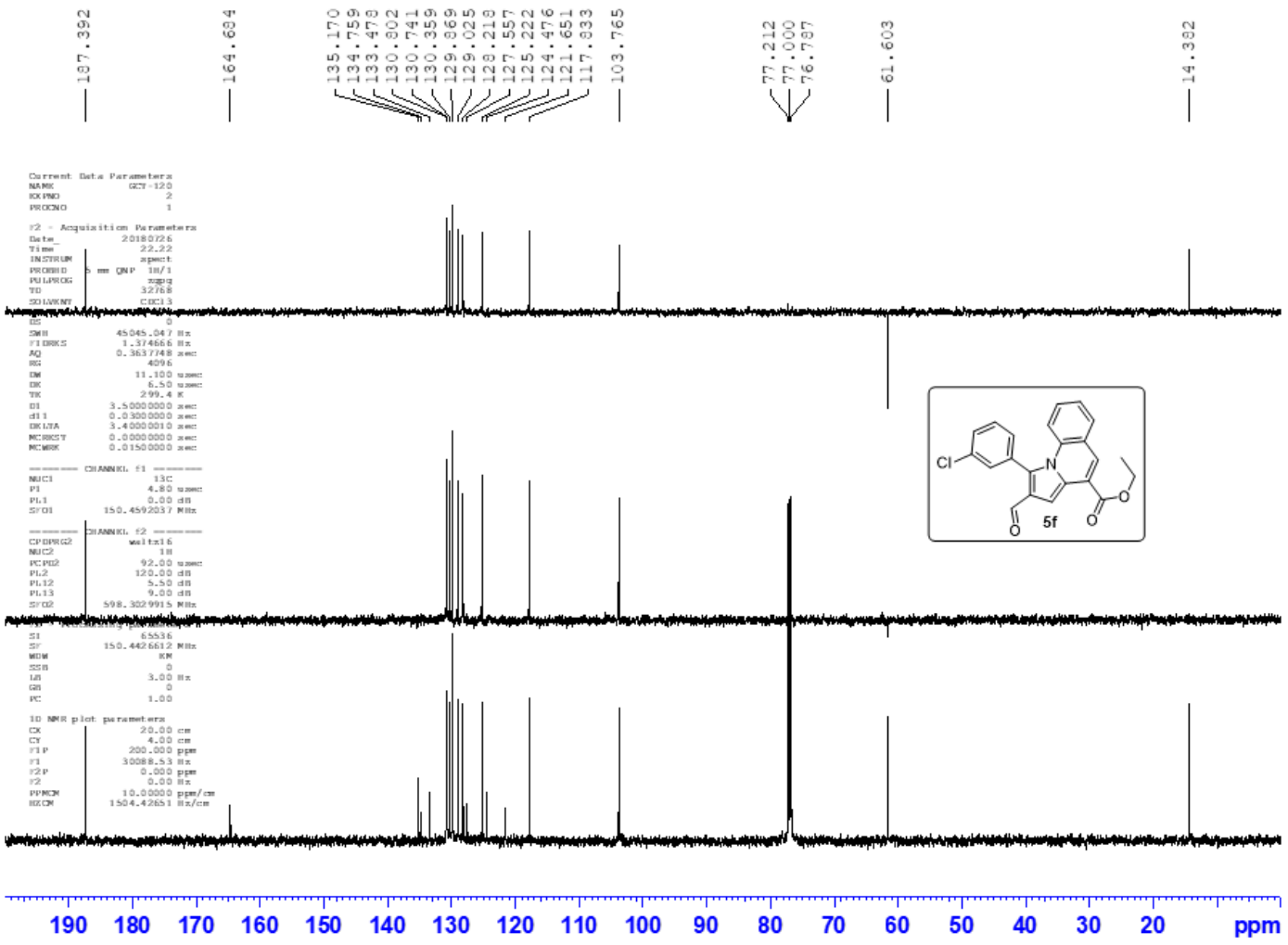

9.693
8.054
7.956
7.950
7.935
7.931
7.697
7.688
7.447
7.444
7.425
7.426
7.410
7.407
7.384
7.380
7.366
7.362
7.358
7.345
7.340
7.265
7.264
4.491
4.473
4.456
4.438
2.821
2.061
2.055
2.050
2.044
2.039
1.467
1.449
1.431
Current Data Parameters
NAME GCT-080-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180621
Time 15.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 67
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500061 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
N
O
O
O
5d
10
9
8
7
6
5
4
3
2
1
ppm
0.95
0.97
1.04
4.86
2.02
1.00
2.00
3.00

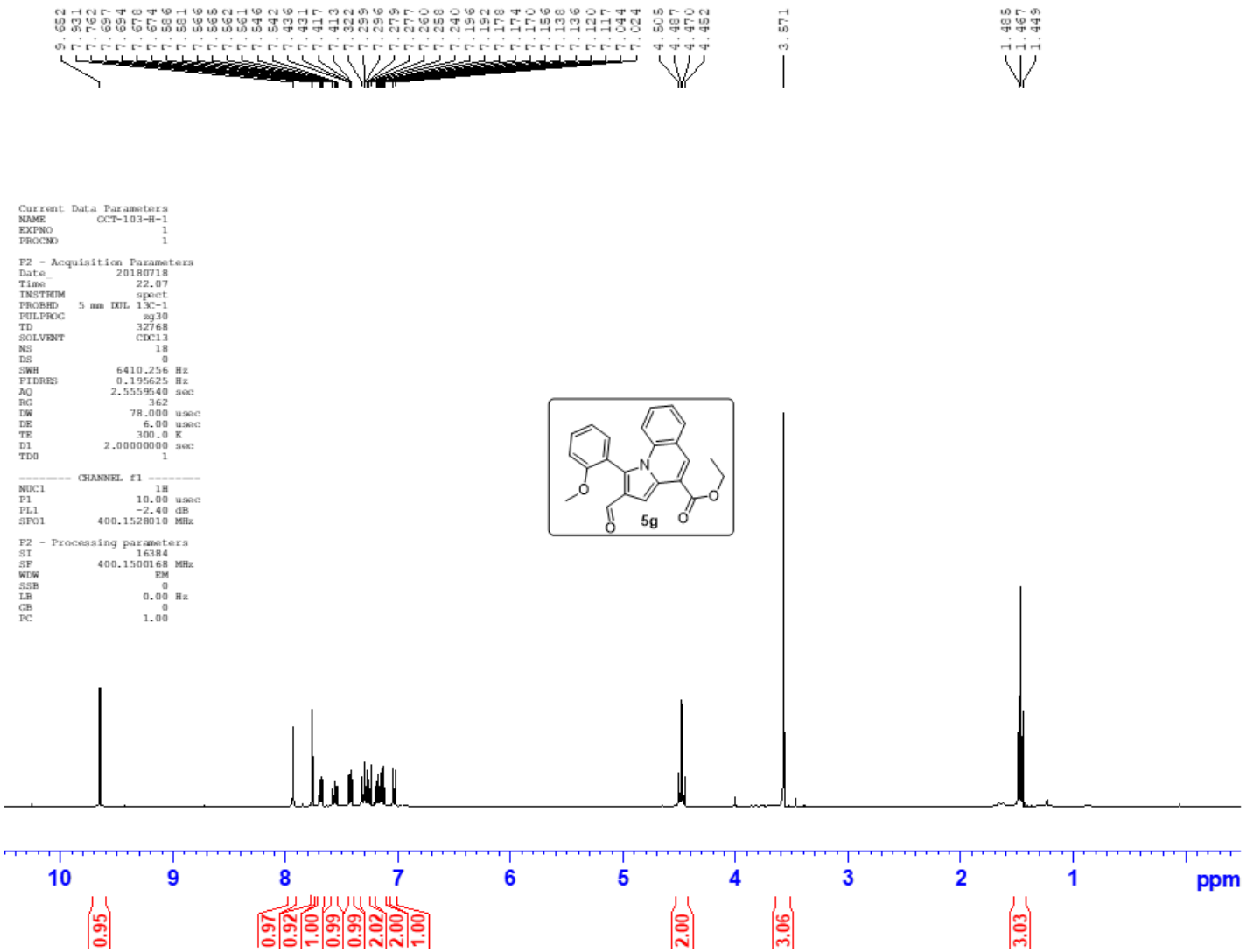

206.000
187.025
164.831
136.072
135.936
135.875
133.368
131.804
131.269
130.778
130.388
130.071
128.630
128.299
126.083
125.156
121.938
118.508
103.821
61.866
29.822
29.693
29.565
14.472
rrent Data Parameters
ME GCT-080-C
PNO 2
DCNO 1
- Acquisition Parameters
te_ 20180621
me 11.29
STRUM spect
OBHD 5 mm QNP 1H/1
LPROG zgpg
32768
LVENT CDCl3
467
0
H 45045.047 Hz
DRES 1.374666 Hz
0.3637748 sec
4096
11.100 usec
6.50 usec
298.3 K
3.50000000 sec
1 0.03000000 sec
LTA 3.40000010 sec
REST 0 sec
WRK 0.01500000 sec
====== CHANNEL f1 ========
C1 13C
4.80 usec
1 0 dB
O1 150.4592037 MHz
====== CHANNEL f2 ========
DPRG2 waltz16
C2 1H
2 120.00 dB
12 5.50 dB
13 9.00 dB
O2 598.3029915 MHz
- Processing parameters
65536
150.4425430 MHz
W EM
B 0
3.00 Hz
0
1.00
Cl
N
O
O
O
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


9.657
7.935
7.926
7.907
7.600
7.605
7.477
7.457
7.437
7.311
7.307
7.295
7.261
7.250
7.237
7.232
7.240
7.234
7.229
7.211
7.206
7.204
7.191
7.187
7.123
7.116
7.102
7.095
7.093
7.089
7.070
7.016
7.011
7.007
4.500
4.490
4.473
4.455
3.622
1.582
1.569
1.471
1.454
Current Data Parameters
NAME GCT-121-H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20180730
Time 14.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5e
10
9
8
7
6
5
4
3
2
1
ppm
0.95
0.97
0.96
0.97
1.00
1.08
1.94
1.94
1.01
2.00
3.03
2.99

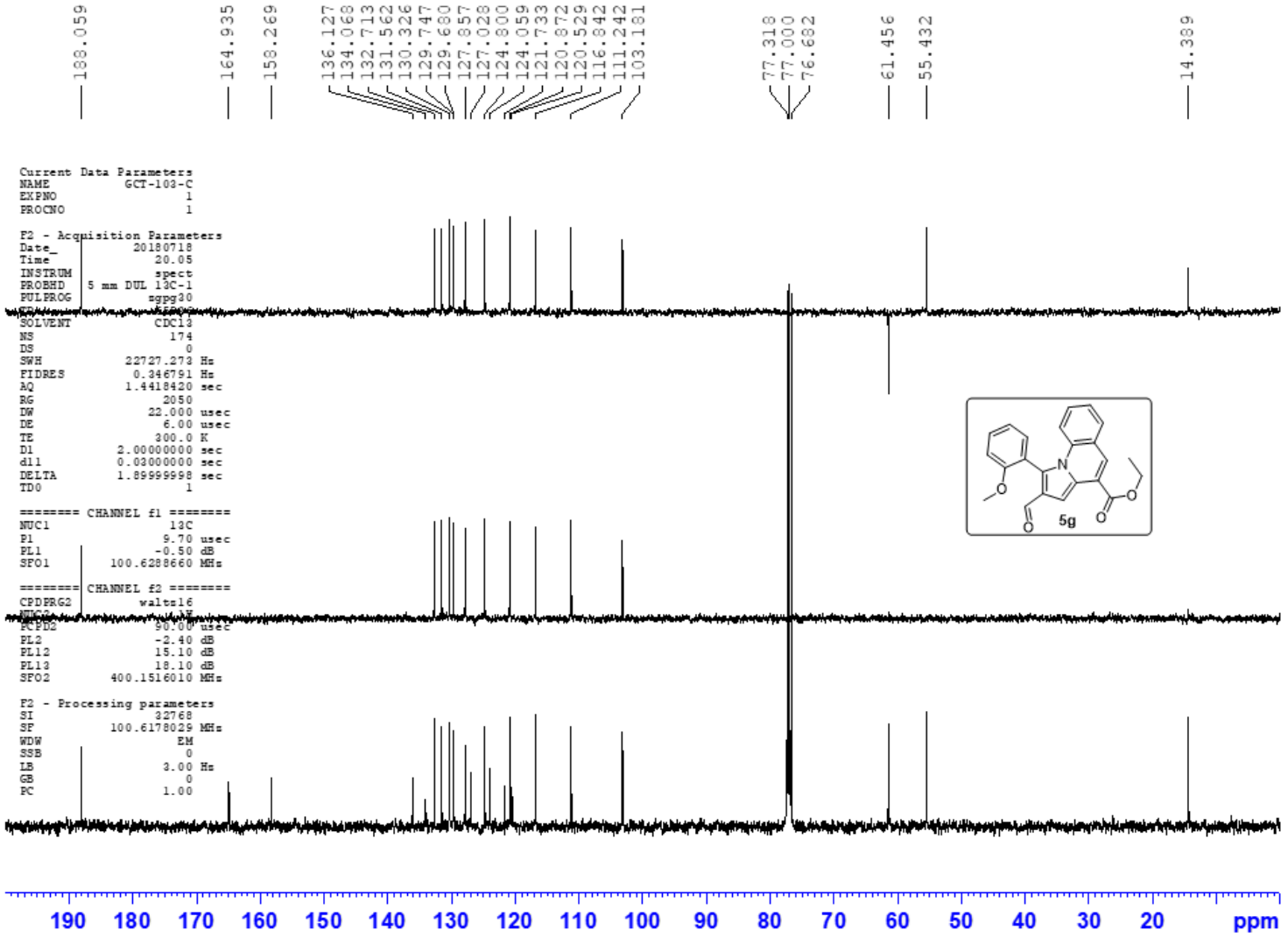

187.926
164.029
159.995
136.945
135.403
132.783
130.585
130.232
129.731
129.548
128.045
127.333
124.999
124.405
123.221
121.701
118.038
116.110
115.548
103.223
77.212
77.000
76.788
61.549
55.447
14.393
5e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

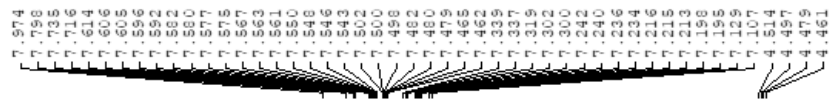

Current Data Parameters
NAME CCT-120
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20180727
Time 12.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.3039717 MHz
F2 - Processing parameters
SI 32768
SF 598.3000289 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00
Cl
N
O
O
O
5f
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.10
1.00
1.11
1.02
2.14
1.08
1.11
1.42
1.09
2.16
3.16


187.392
164.604
135.170
134.759
133.476
130.802
130.741
130.359
129.869
129.025
128.218
127.557
125.222
124.476
121.651
117.833
103.765
77.212
77.000
76.787
61.603
14.382
Cl
N
O
O
O
5f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

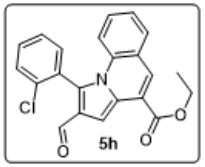


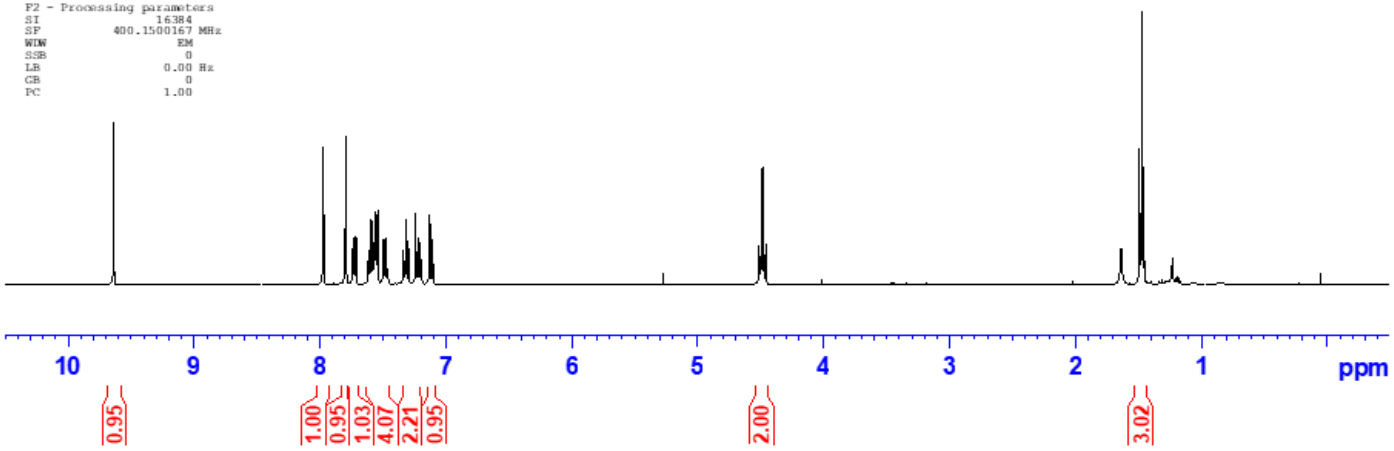

```
Current Data Parameters
NAME         GCT-103-H-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180718
Time              22.07
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                 32768
SOLVENT            CDCl3
NS                    18
DS                     0
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              2.5559540 sec
RG                   362
DW                78.000 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
TD0                    1

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

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

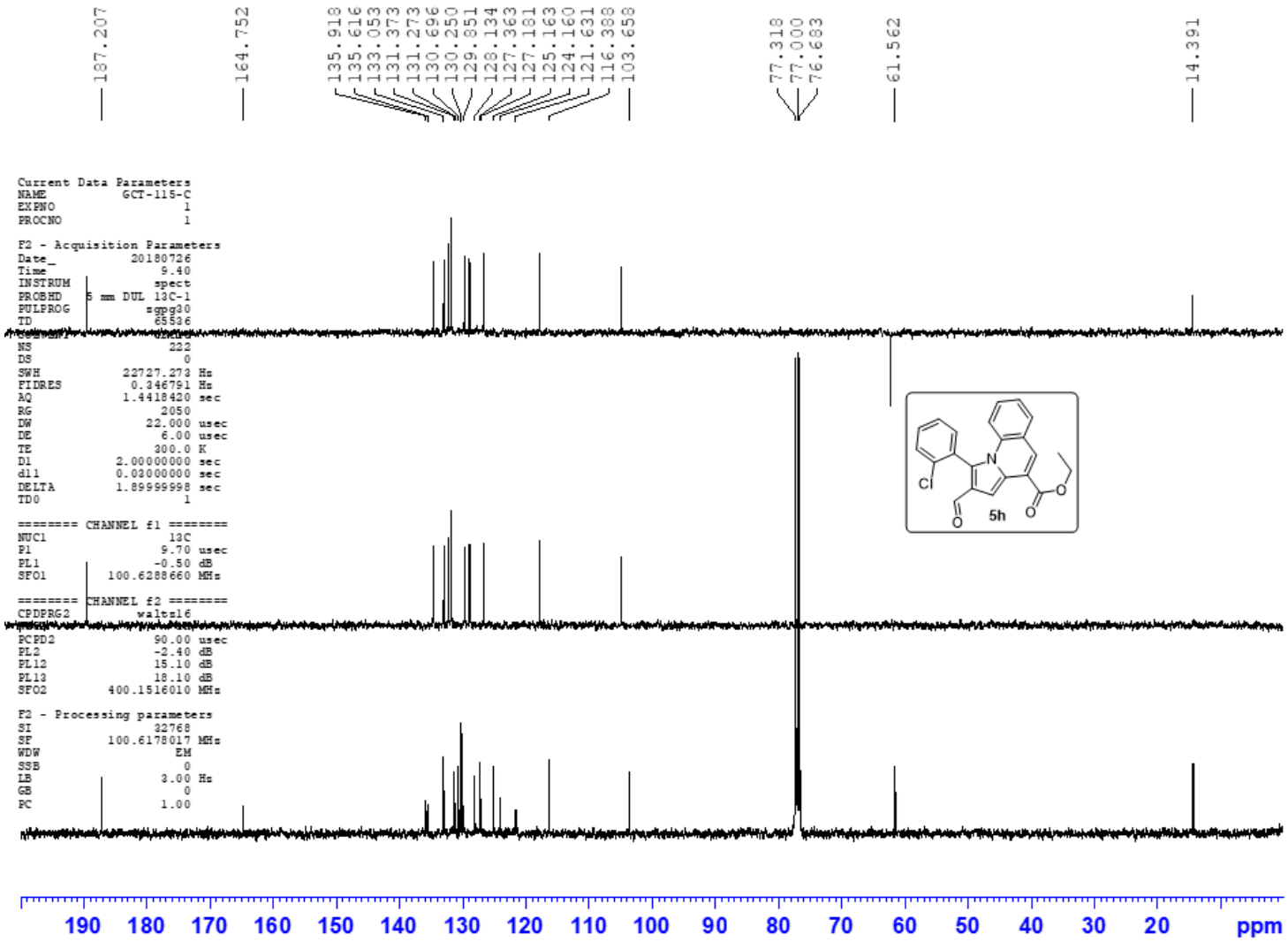

188.059
164.935
158.269
136.127
134.068
132.713
131.562
130.326
129.747
129.680
127.857
127.028
124.800
124.059
121.733
120.872
120.529
116.842
111.242
103.181
77.318
77.000
76.682
61.456
55.432
14.389
Current Data Parameters
NAME GCT-103-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180718
Time 20.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
SOLVENT CDCl3
NS 174
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
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 100.6178029 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

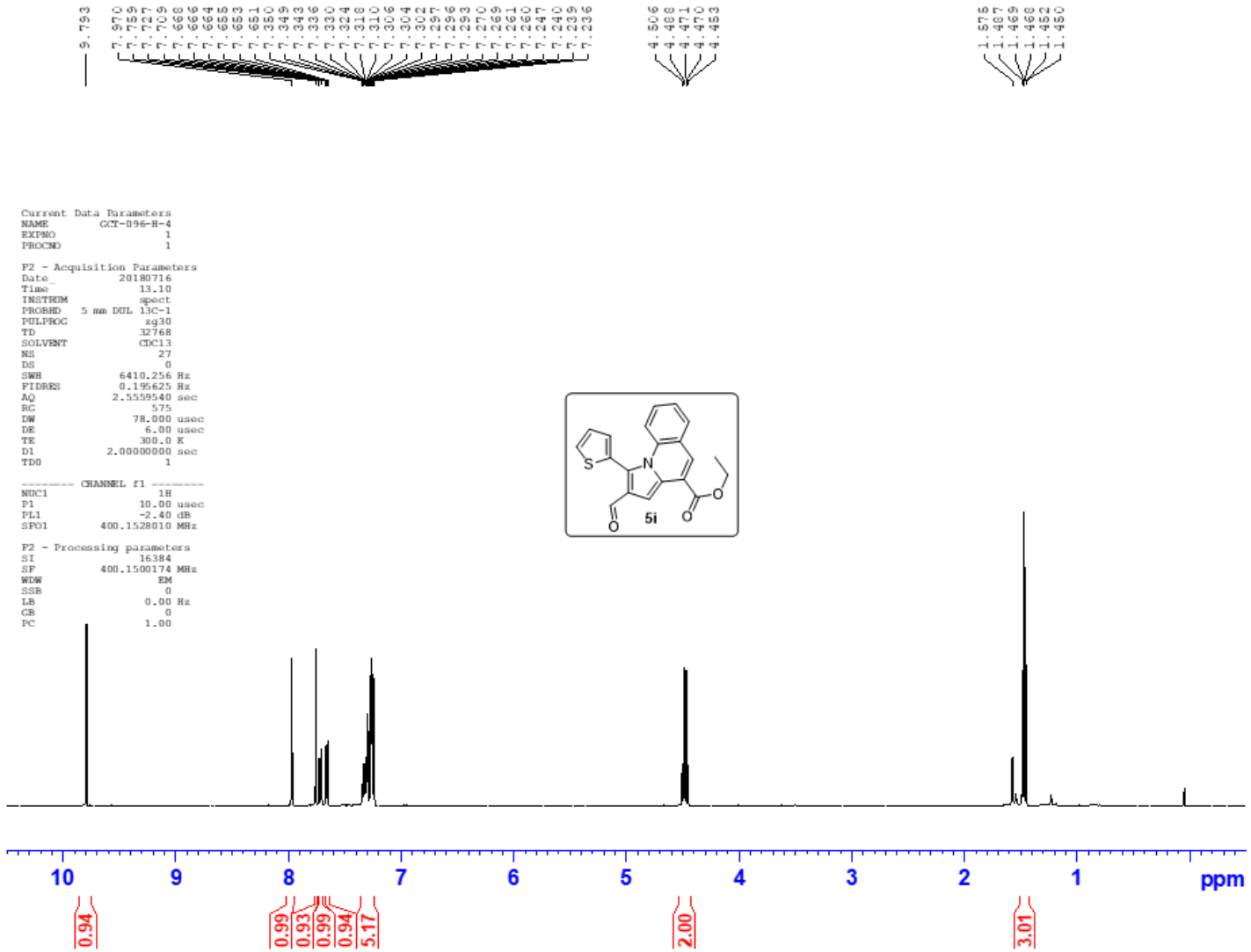


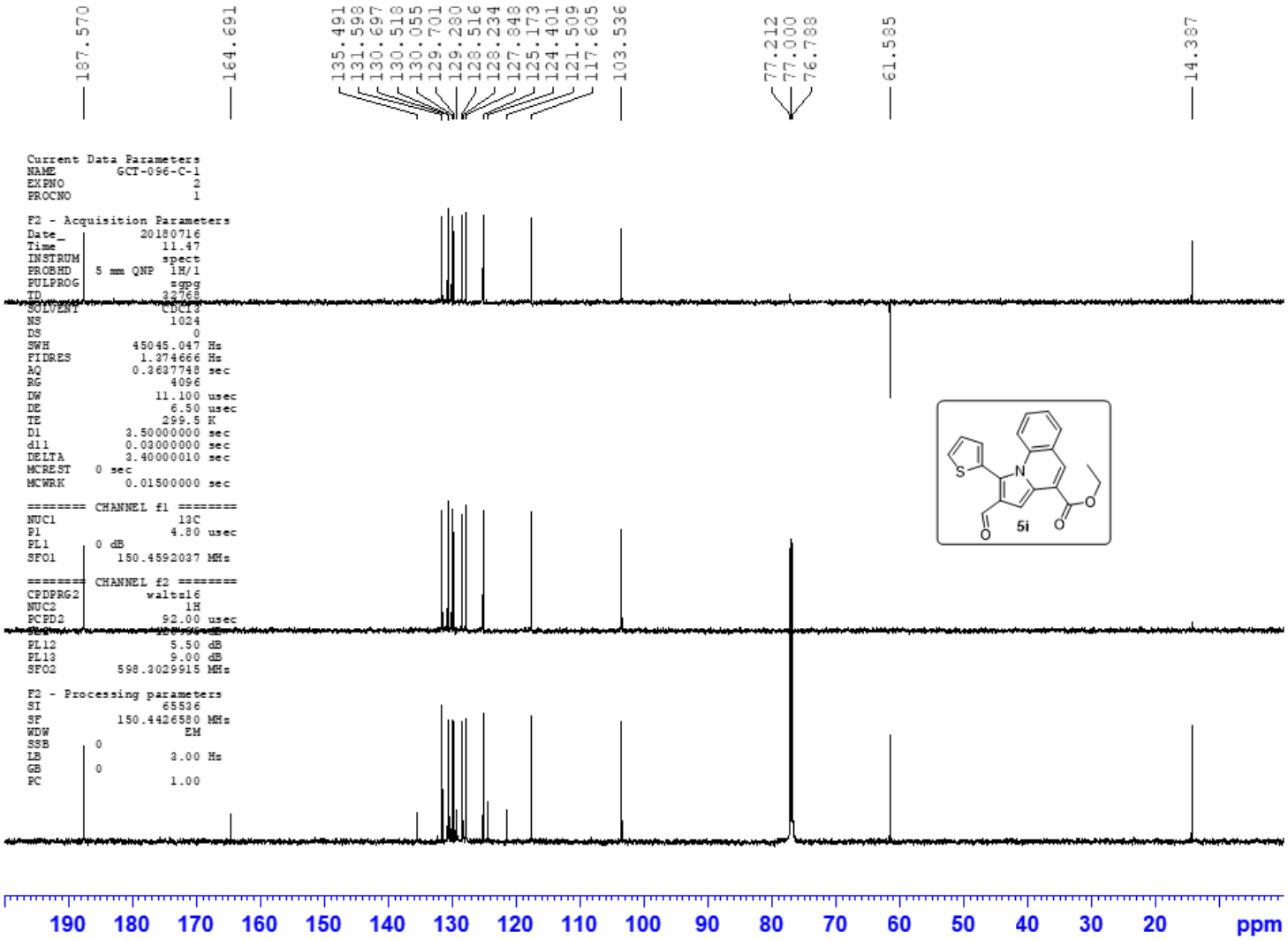
```
Current Data Parameters
NAME          GCT-115-H-1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20180726
Time               9.30
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  31
DS                   0
SWH           6410.256 Hz
FIDRES        0.195625 Hz
AQ            2.5559540 sec
RG                 362
DW               78.000 usec
DE                6.00 usec
TE               300.0 K
D1           2.00000000 sec
TD0                  1

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

F2 - Processing parameters
SI                16384
SF          400.1500167 MHz
WDW                  EM
SSB                  0
LB                0.00 Hz
GB                   0
PC                1.00
```

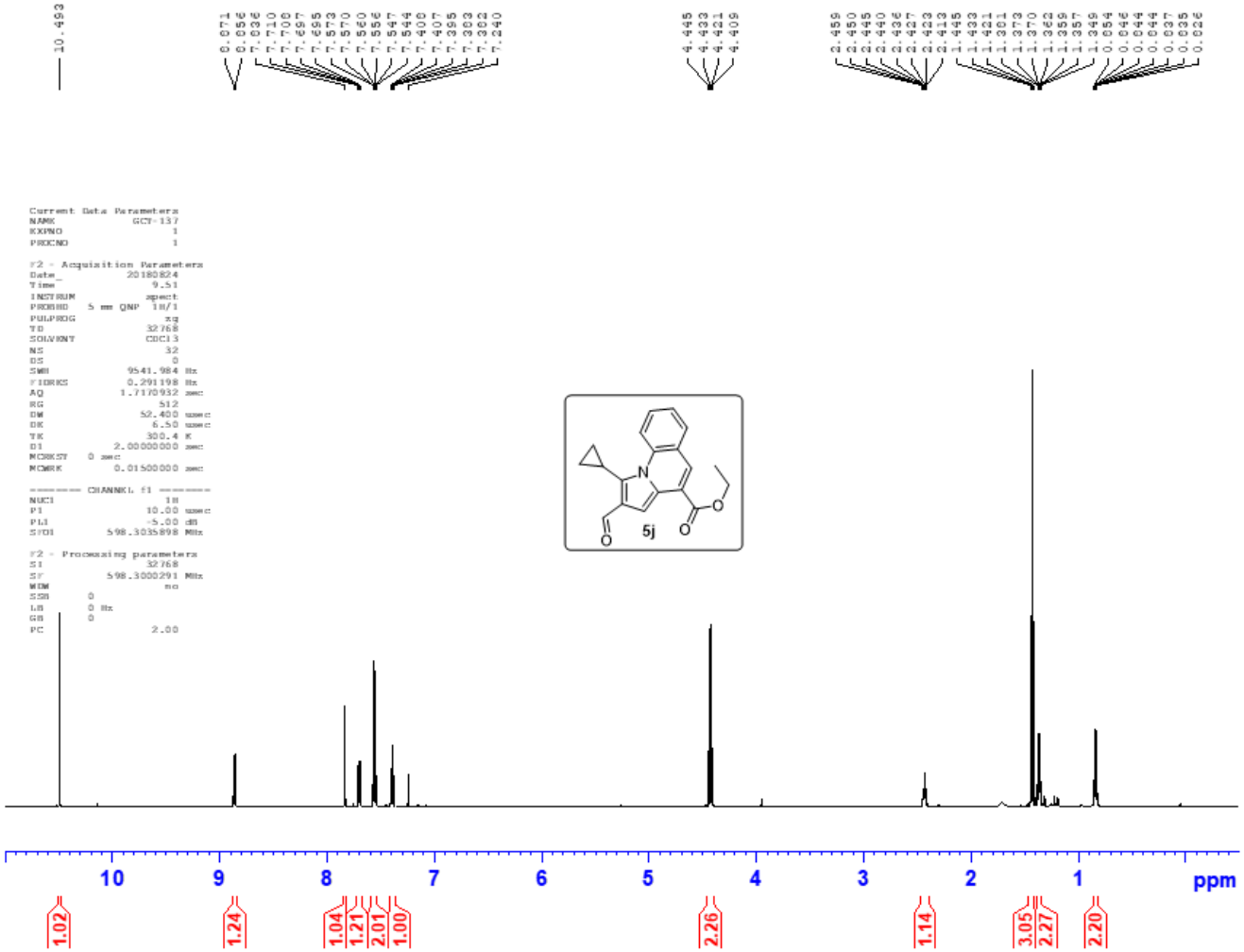


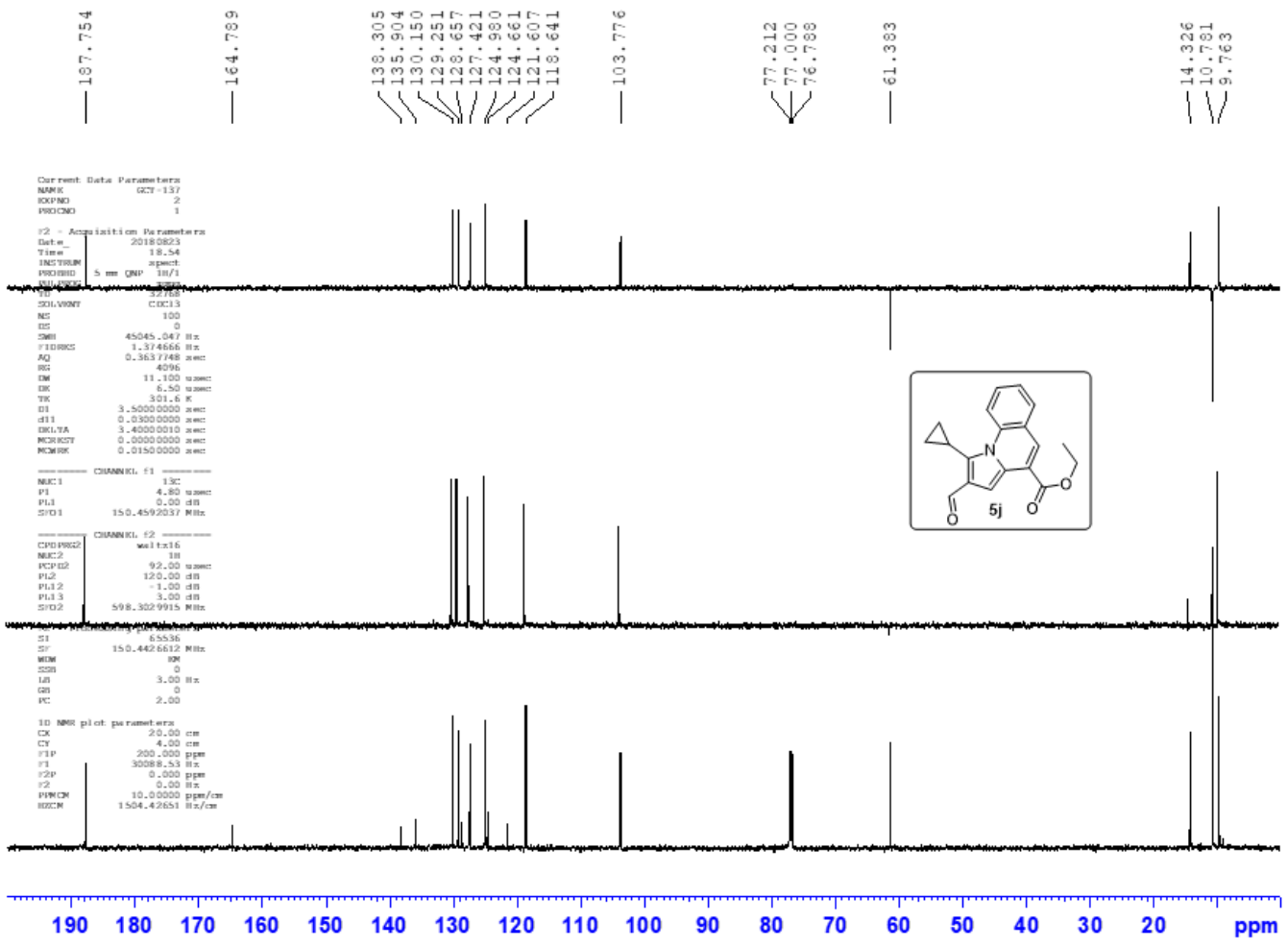


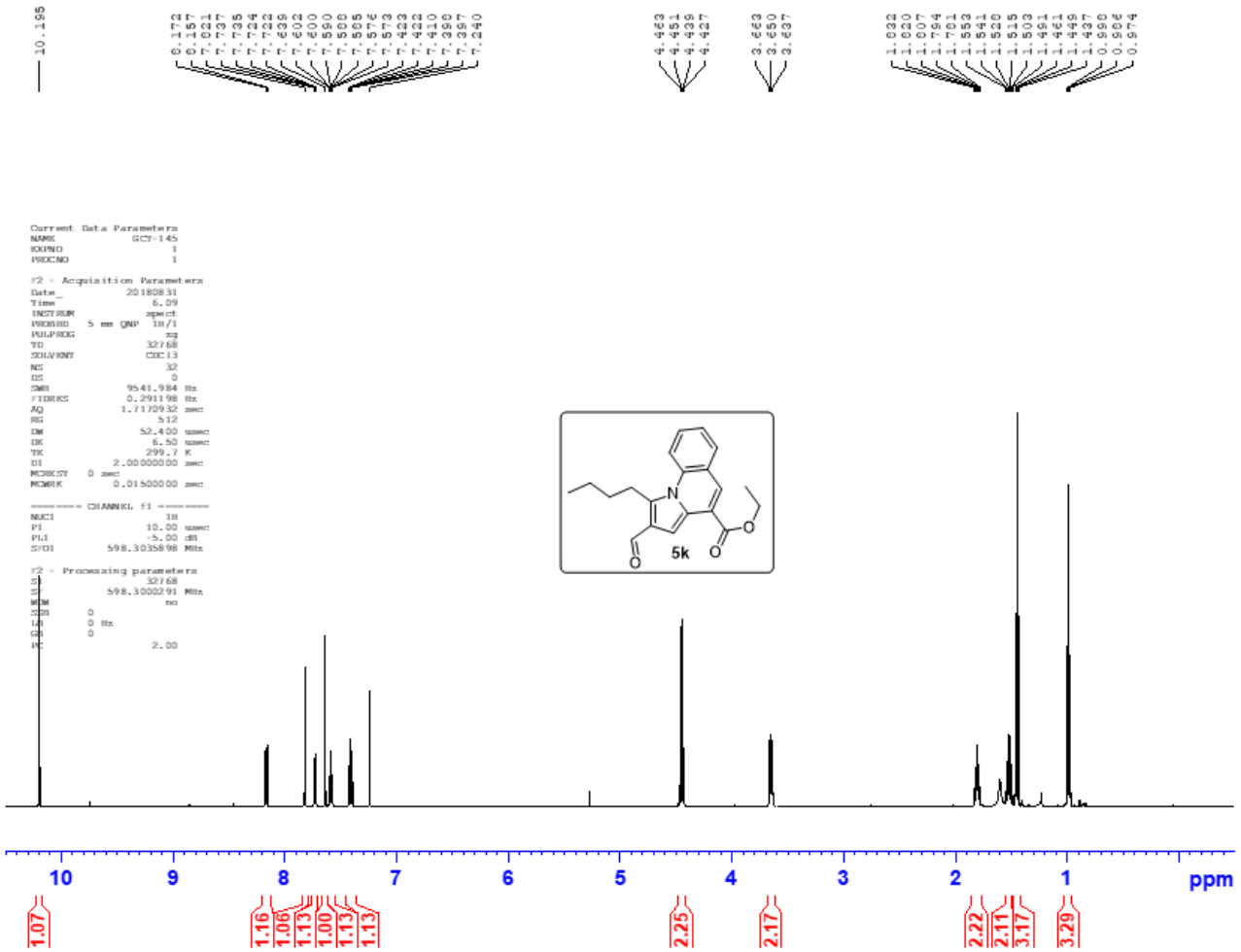

187.207
164.752
135.918
135.616
133.053
131.373
131.273
130.696
130.250
129.851
128.134
127.363
127.181
125.163
124.160
121.631
116.388
103.658
77.318
77.000
76.683
61.562
14.391
Current Data Parameters
NAME GCT-115-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180726
Time 9.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 222
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
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 100.6178017 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
N
O
O
O
5h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

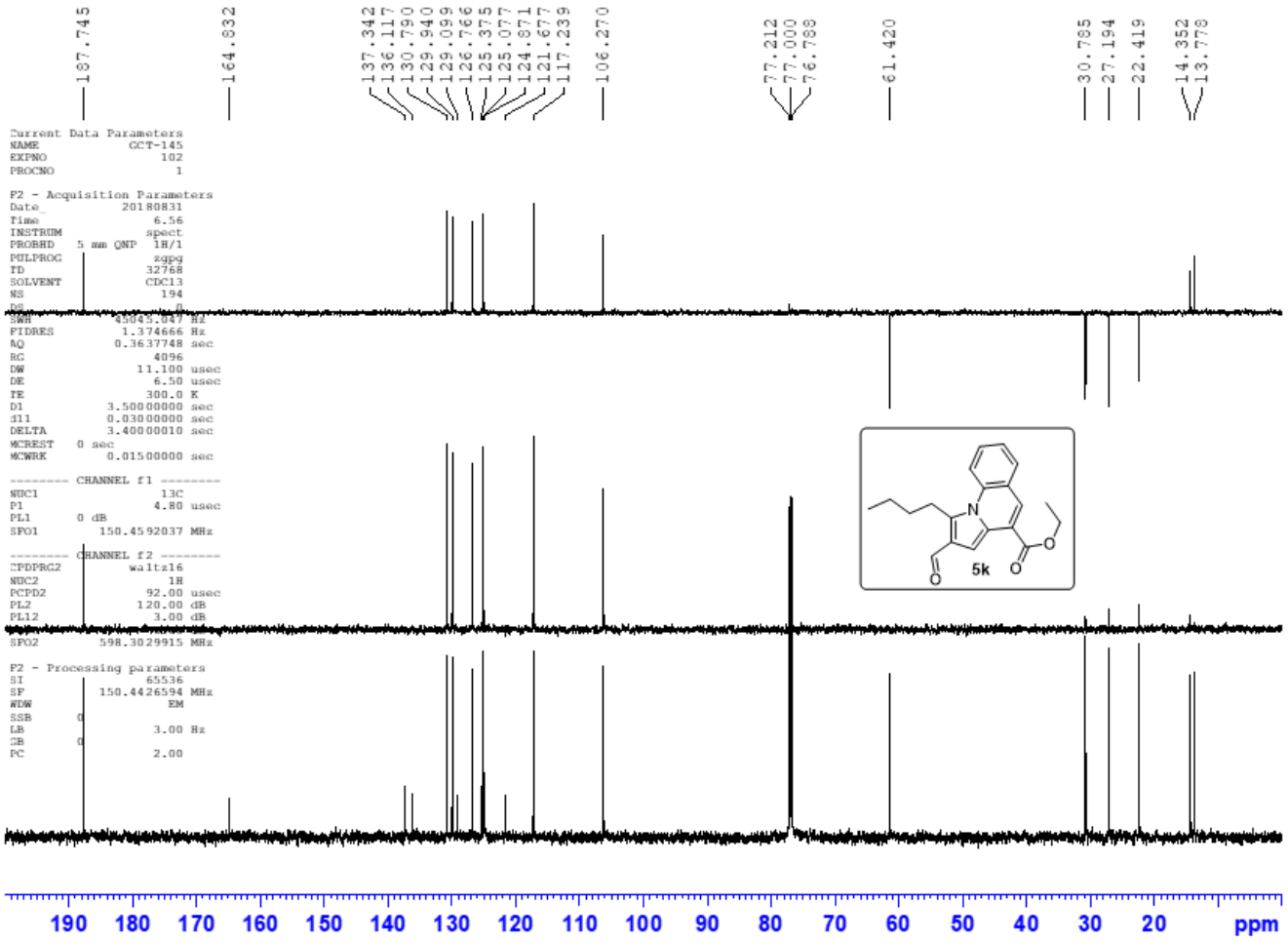

9.793
7.670
7.659
7.727
7.709
7.668
7.666
7.664
7.685
7.683
7.651
7.350
7.349
7.343
7.336
7.330
7.324
7.318
7.310
7.306
7.304
7.302
7.297
7.296
7.293
7.270
7.269
7.261
7.260
7.247
7.240
7.239
7.236
4.506
4.488
4.471
4.470
4.453
1.575
1.487
1.469
1.468
1.452
1.450
Current Data Parameters
NAME GCT-096-H-4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180716
Time 13.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 27
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
S
N
O
O
O
5i
10
9
8
7
6
5
4
3
2
1
ppm
0.94
0.99
0.93
0.99
0.94
5.17
2.00
3.01

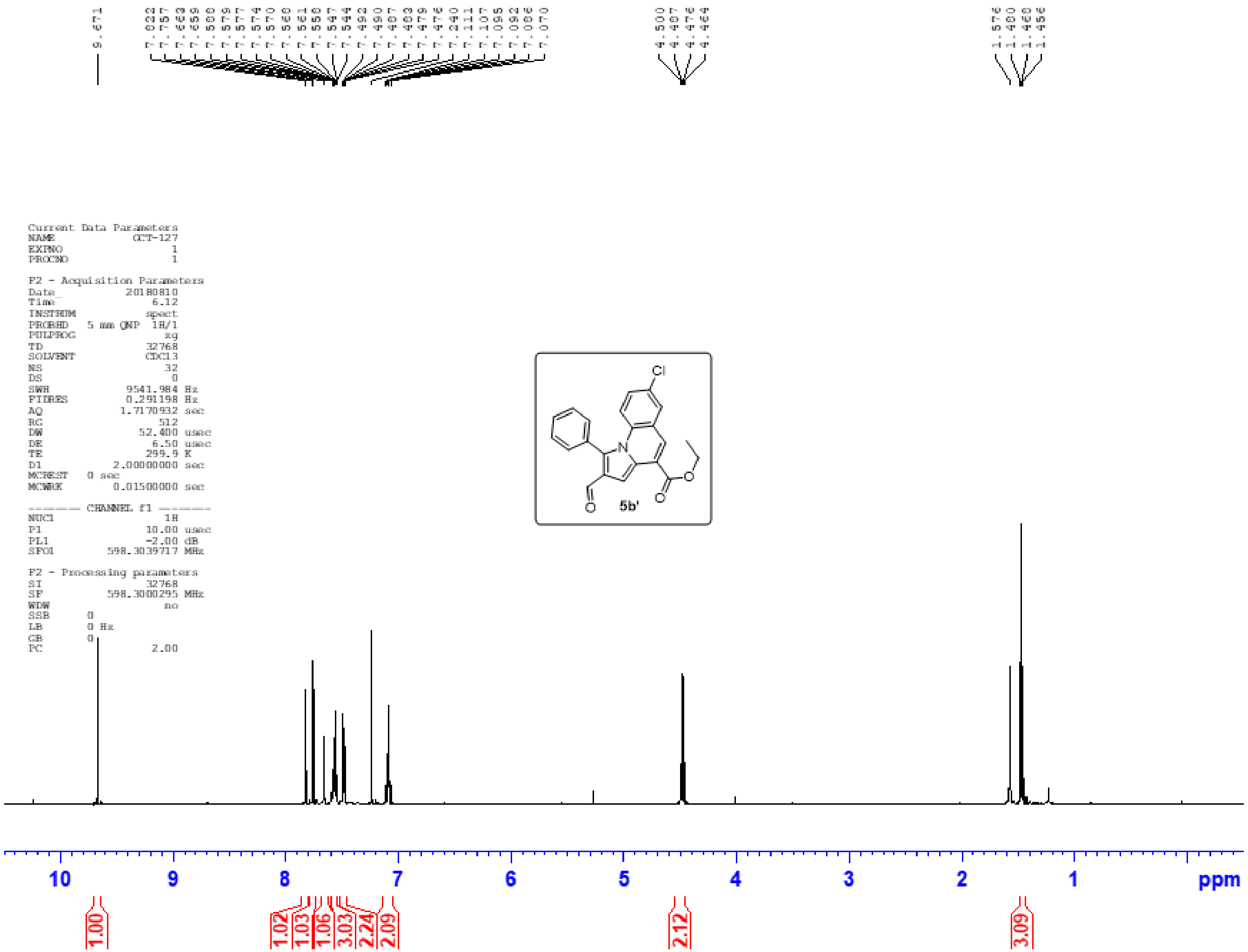

187.570
164.691
135.491
131.598
130.697
130.518
130.055
129.701
129.280
128.516
128.234
127.848
125.173
124.401
121.509
117.605
103.536
77.212
77.000
76.788
61.585
14.387
Current Data Parameters
NAME GCT-096-C-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180716
Time 11.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1024
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426580 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
S
N
O
O
O
5i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

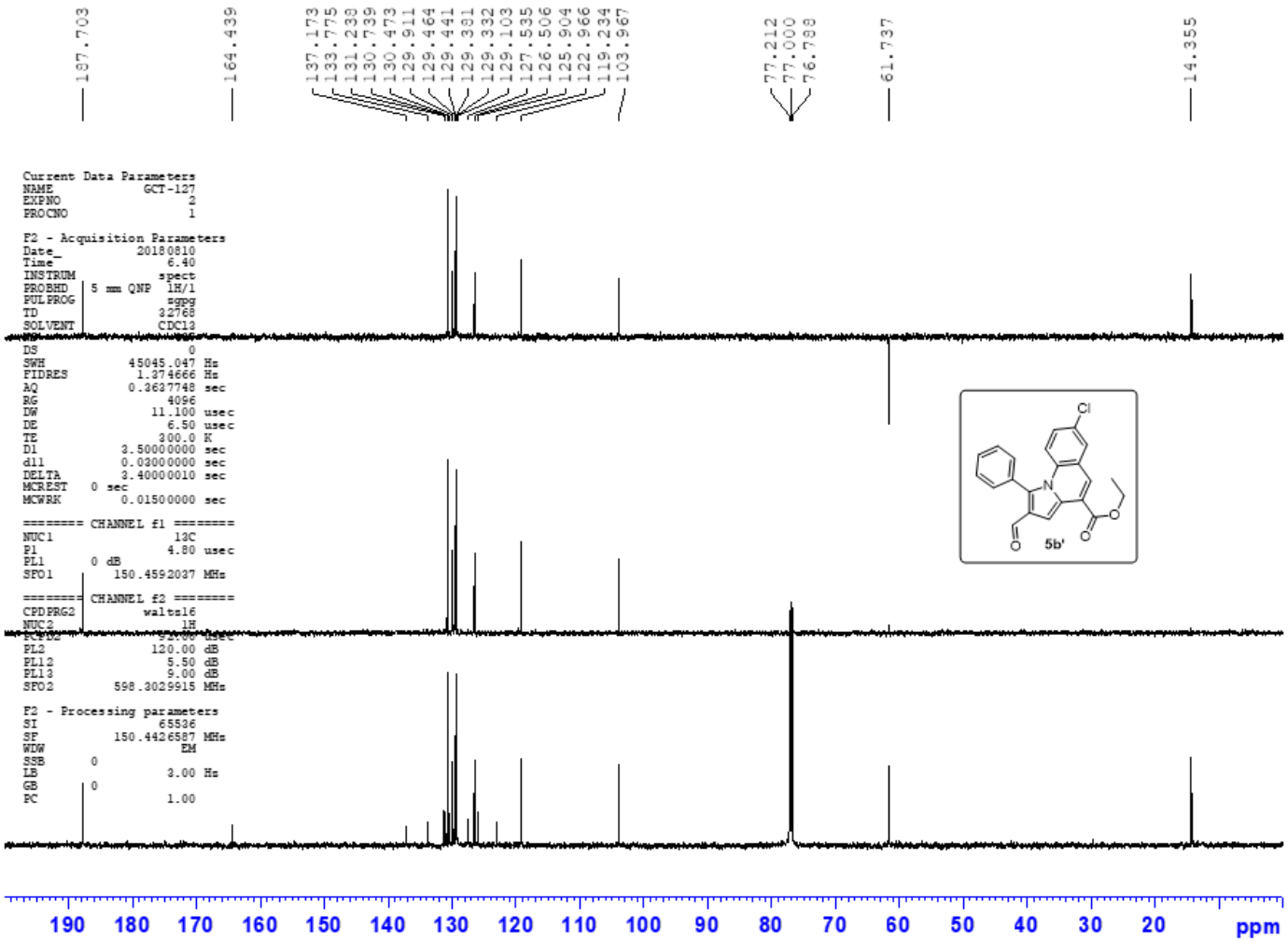

10.463
9.071
9.056
7.736
7.710
7.706
7.697
7.695
7.573
7.570
7.560
7.555
7.547
7.544
7.406
7.407
7.395
7.393
7.392
7.240
4.445
4.433
4.421
4.409
2.459
2.450
2.445
2.440
2.436
2.427
2.423
2.413
1.445
1.433
1.421
1.361
1.373
1.370
1.362
1.356
1.357
1.349
0.654
0.646
0.644
0.644
0.637
0.635
0.626
Current Data Parameters
NAME GCT-137
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180824
Time 9.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000291 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
5j
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.24
1.04
1.21
2.01
1.00
2.26
1.14
3.05
2.27
2.20

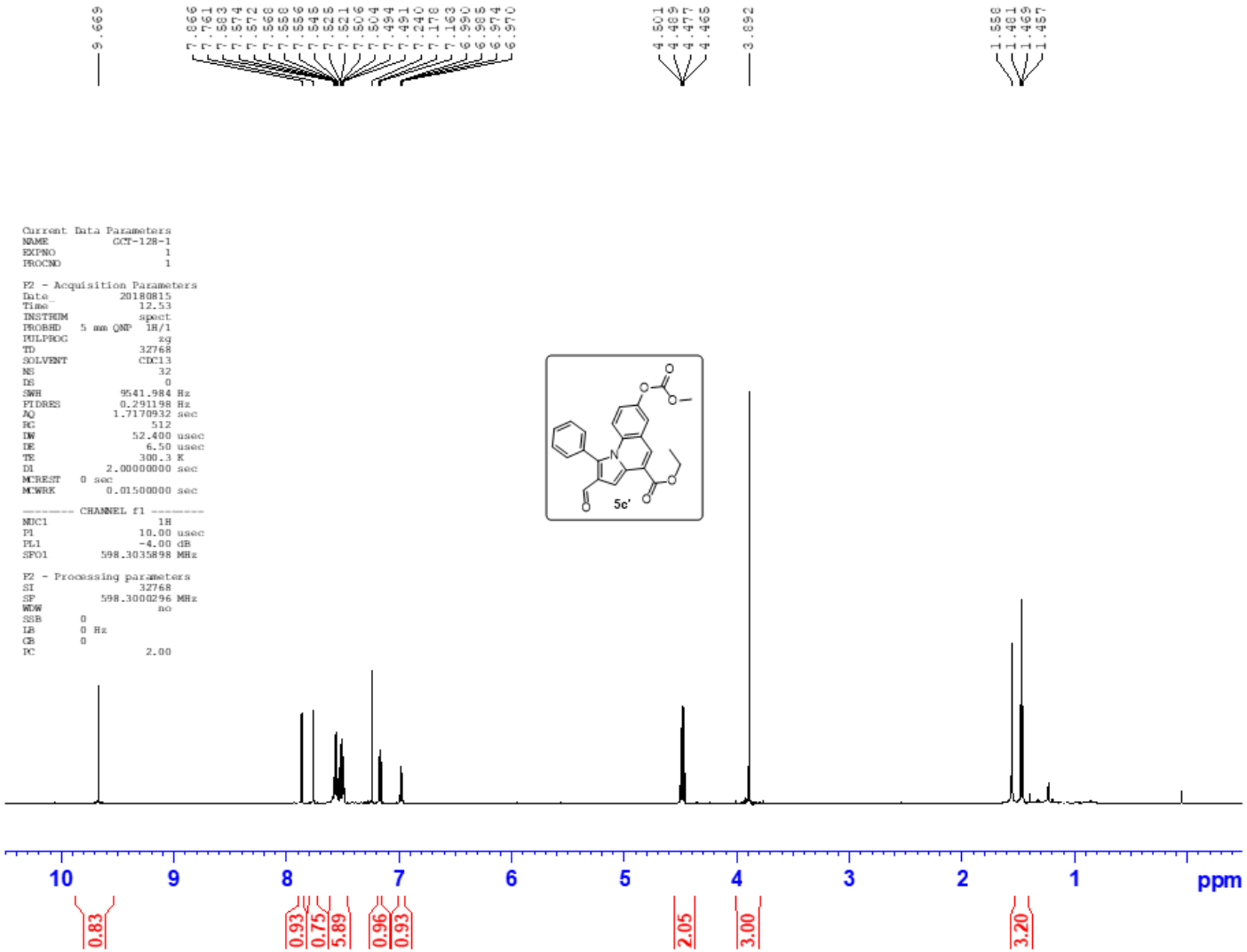

187.754
164.799
138.305
135.904
130.150
129.251
128.657
127.421
124.980
124.661
121.607
118.641
103.776
77.212
77.000
76.788
61.383
14.326
10.781
9.763
5j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

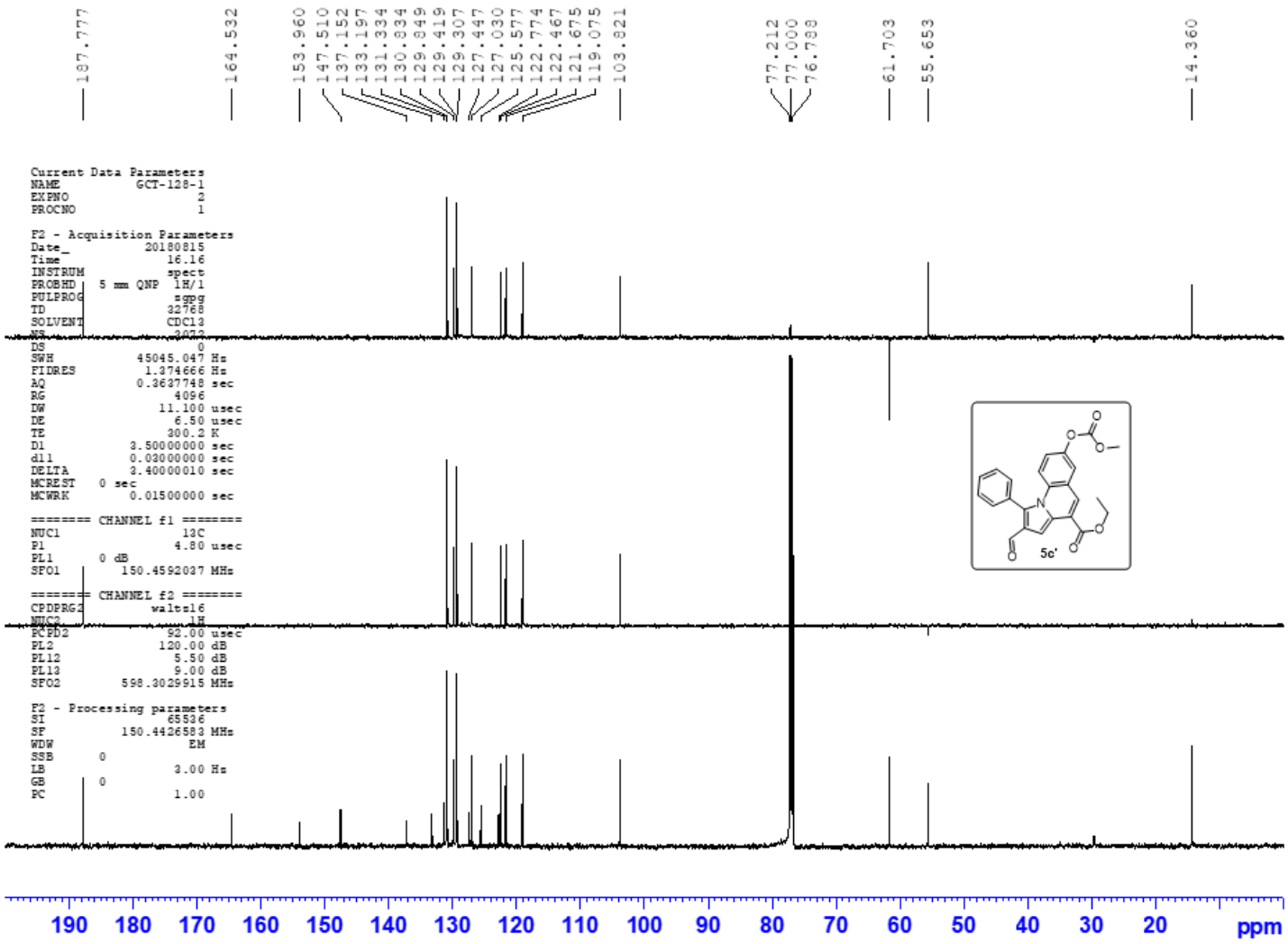

10.195
8.172
8.157
8.041
7.737
7.735
7.724
7.722
7.716
7.602
7.600
7.560
7.558
7.555
7.553
7.543
7.423
7.410
7.396
7.387
7.240
4.463
4.451
4.439
4.427
3.663
3.650
3.637
1.632
1.630
1.607
1.594
1.591
1.583
1.541
1.536
1.515
1.503
1.491
1.481
1.446
1.437
0.960
0.956
0.974
Current Data Parameters
NAME GCT-145
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180831
Time 6.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 299.7 K
D1 2.0000000 sec
MCREST 0 sec
MCWRK 0.0150000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -5.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000291 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
5k
10
9
8
7
6
5
4
3
2
1
ppm
1.07
1.16
1.06
1.13
1.00
1.13
1.13
2.25
2.17
2.22
2.11
3.17
3.29

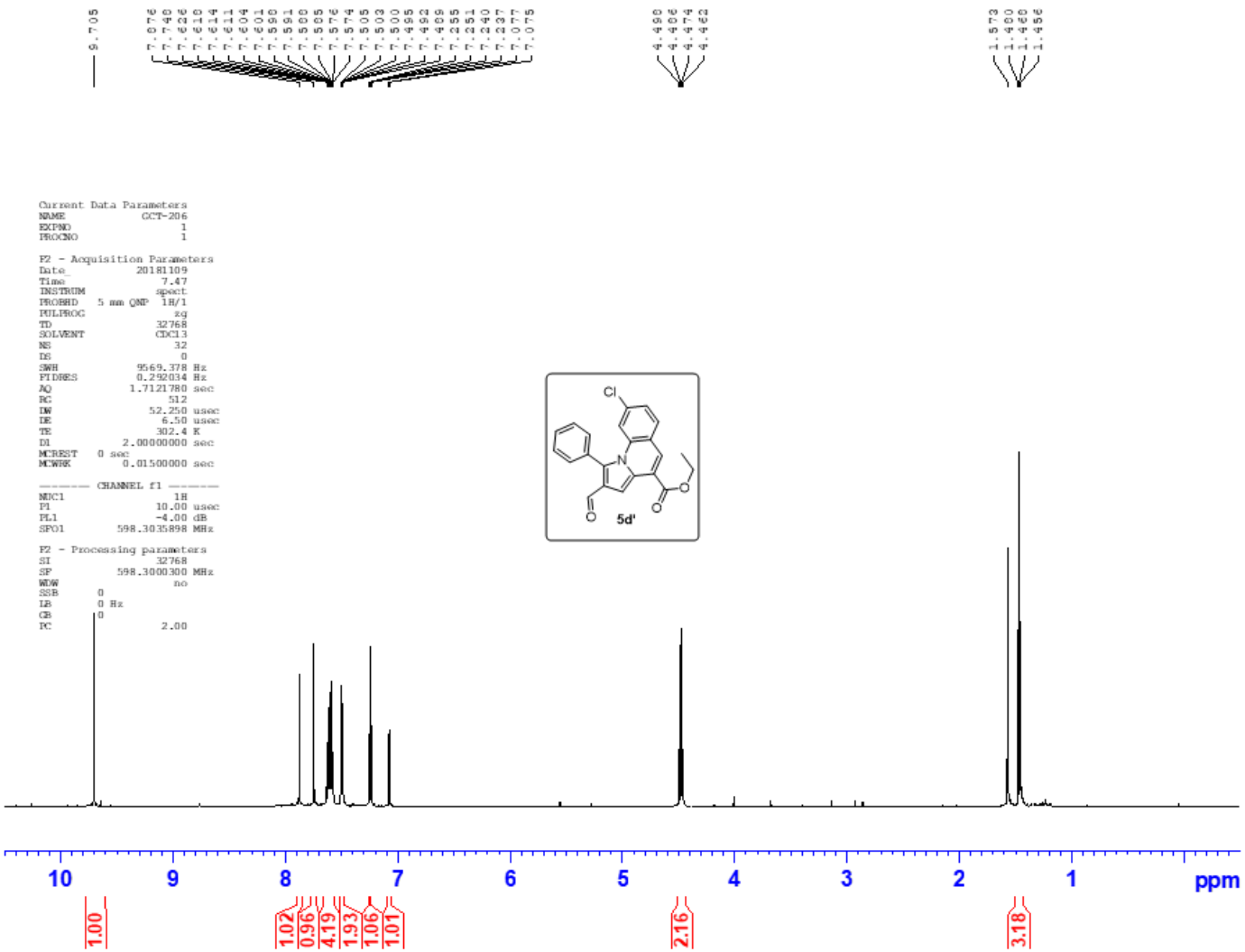

187.745
164.832
137.342
136.117
130.790
129.940
129.099
126.766
125.375
125.077
124.871
121.677
117.239
106.270
77.212
77.000
76.788
61.420
30.785
27.194
22.419
14.352
13.778
Current Data Parameters
NAME CCT-145
EXPNO 102
PROCNO 1
P2 - Acquisition Parameters
Date_ 20180831
Time 6.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 194
DS 0
SWH 43843.847 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 3.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426594 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00
N
O
O
O
5k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

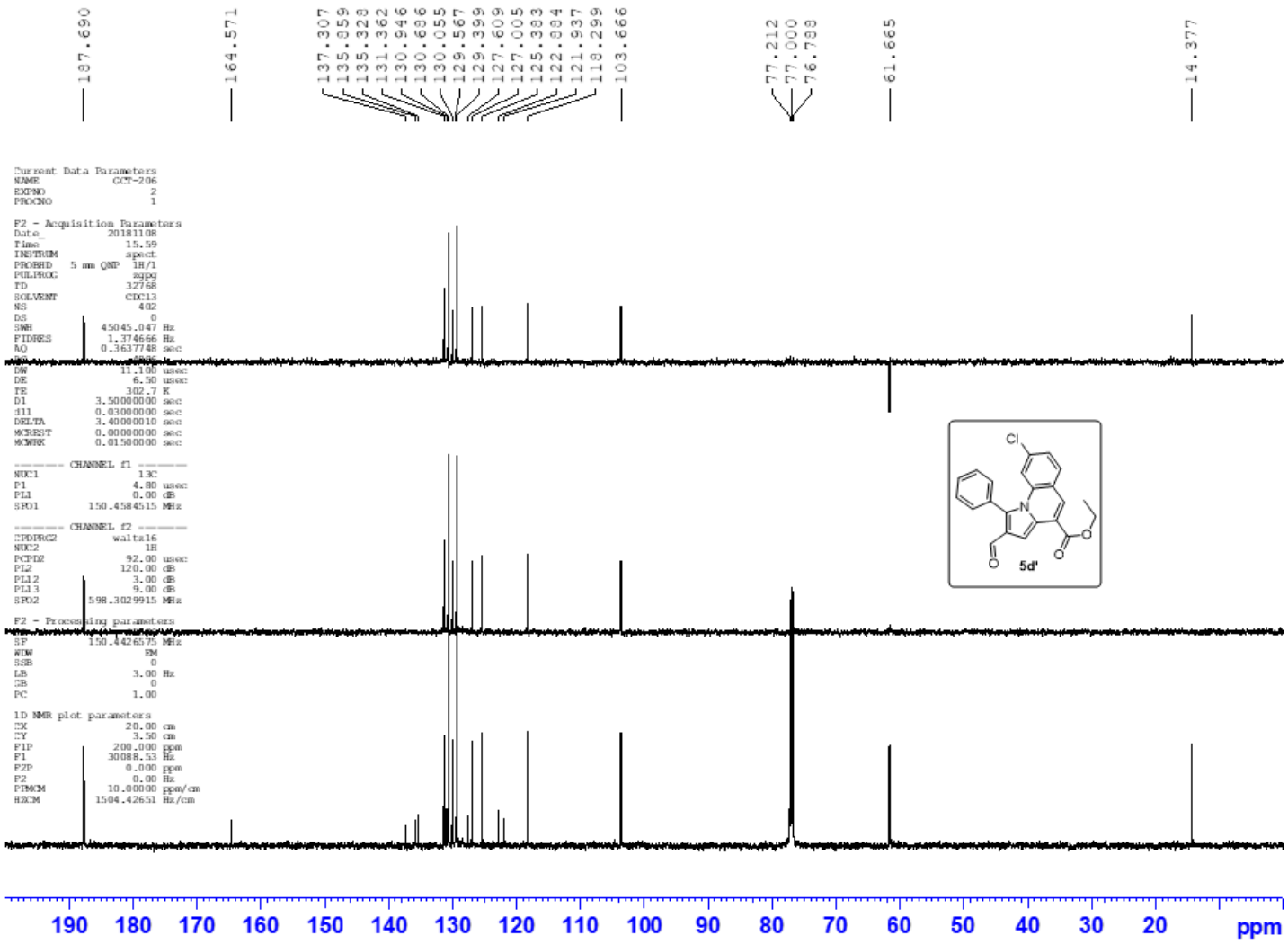

Current Data Parameters
NAME CCT-127
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180810
Time 6.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.3039717 MHz
F2 - Processing parameters
SI 32768
SF 598.3000295 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Cl
O
O
O
N
5b'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
1.03
1.06
3.03
2.24
2.09
2.12
3.09

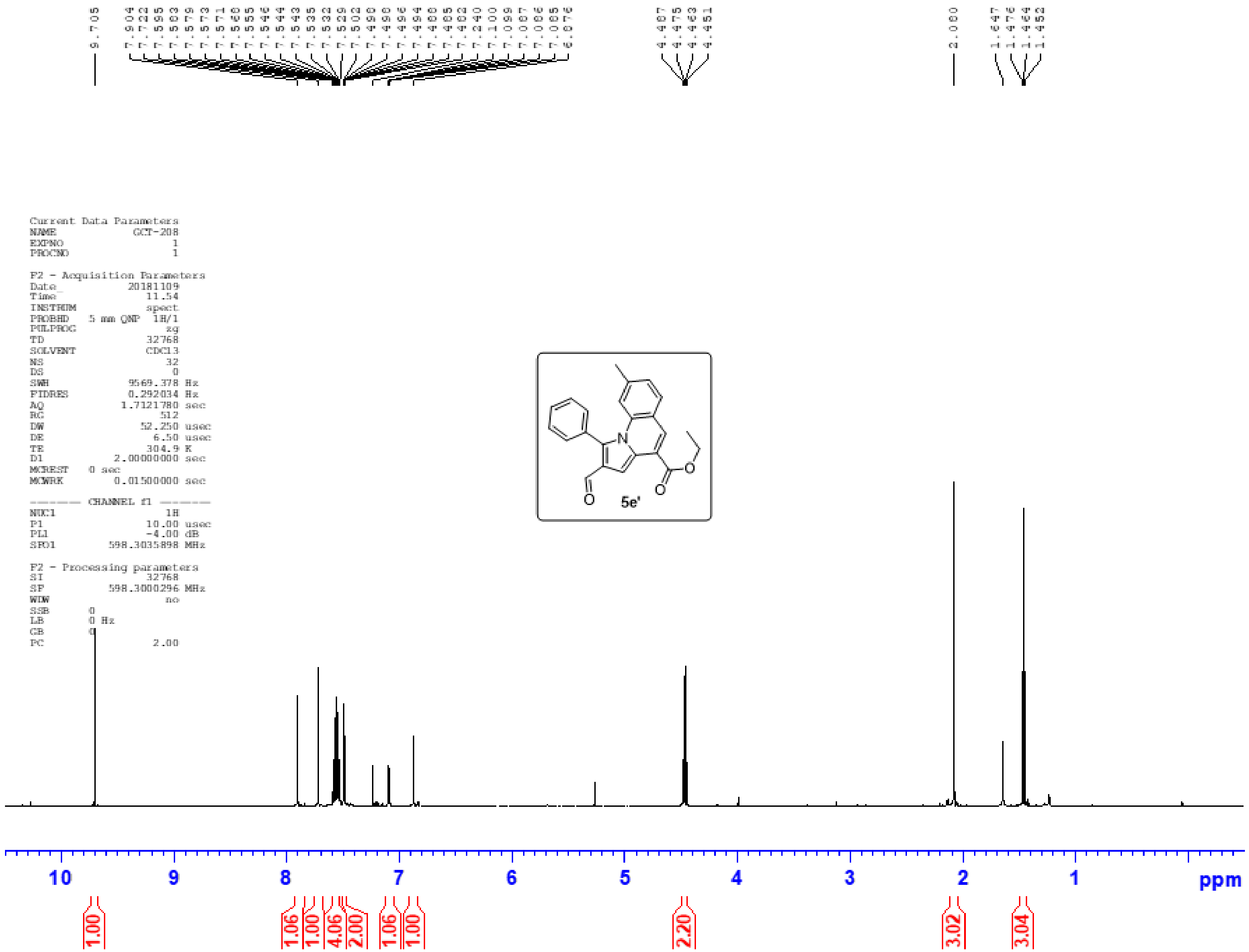

187.703
164.439
137.173
133.775
131.239
130.739
130.473
129.911
129.464
129.441
129.381
129.332
129.103
127.535
126.506
125.904
122.966
119.234
103.967
77.212
77.000
76.788
61.737
14.355
Current Data Parameters
NAME GCT-127
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180810
Time_ 6.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426587 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
O
N
O
O
5b'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

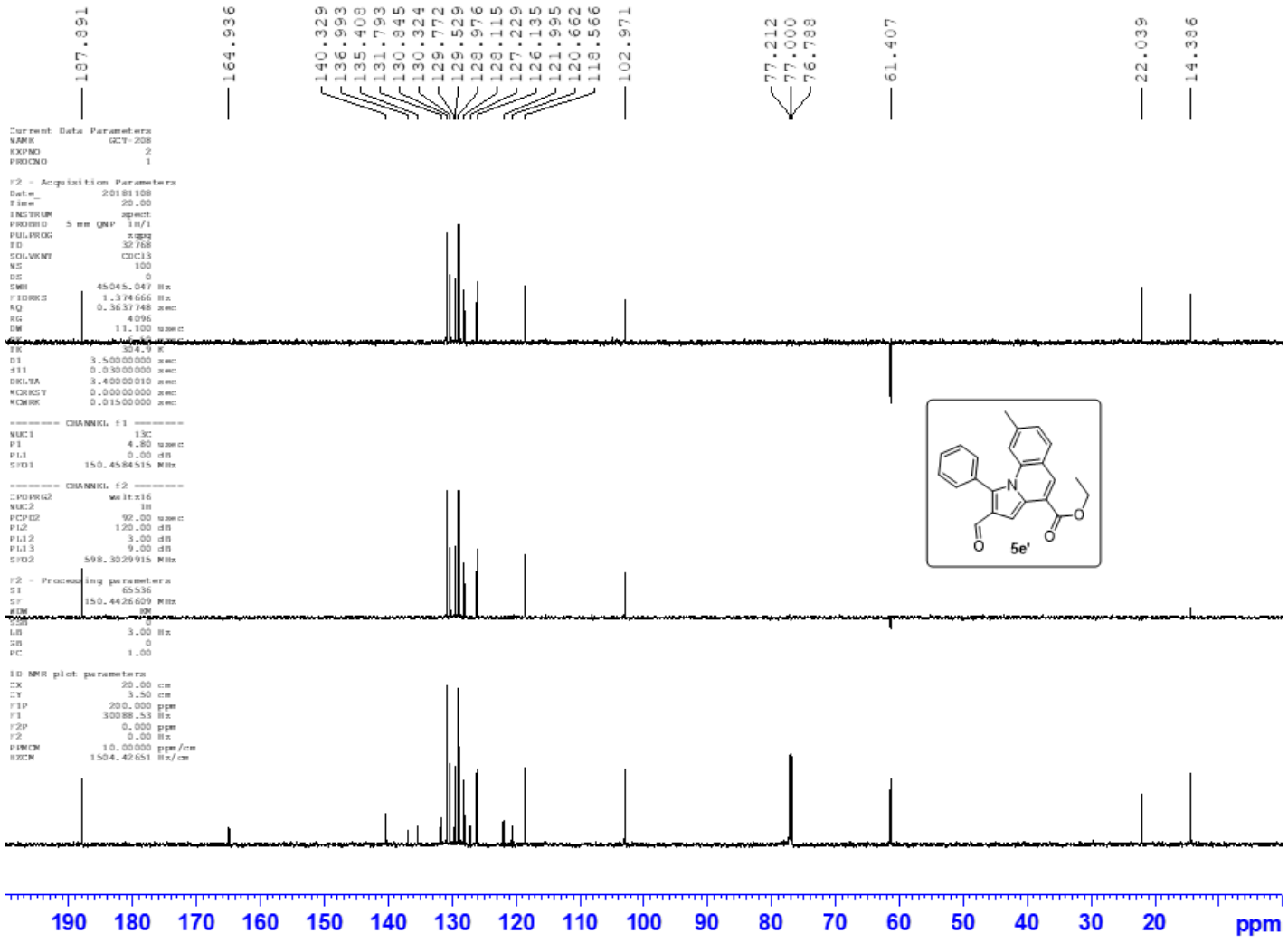

9.669
7.966
7.761
7.683
7.674
7.672
7.566
7.558
7.556
7.545
7.526
7.521
7.506
7.504
7.494
7.491
7.240
7.178
7.163
6.990
6.985
6.974
6.970
4.501
4.489
4.477
4.466
3.892
1.558
1.481
1.469
1.457
Current Data Parameters
NAME GCT-128-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180815
Time 12.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000296 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
5c'
10
9
8
7
6
5
4
3
2
1
ppm
0.83
0.93
0.75
5.89
0.96
0.93
2.05
3.00
3.20

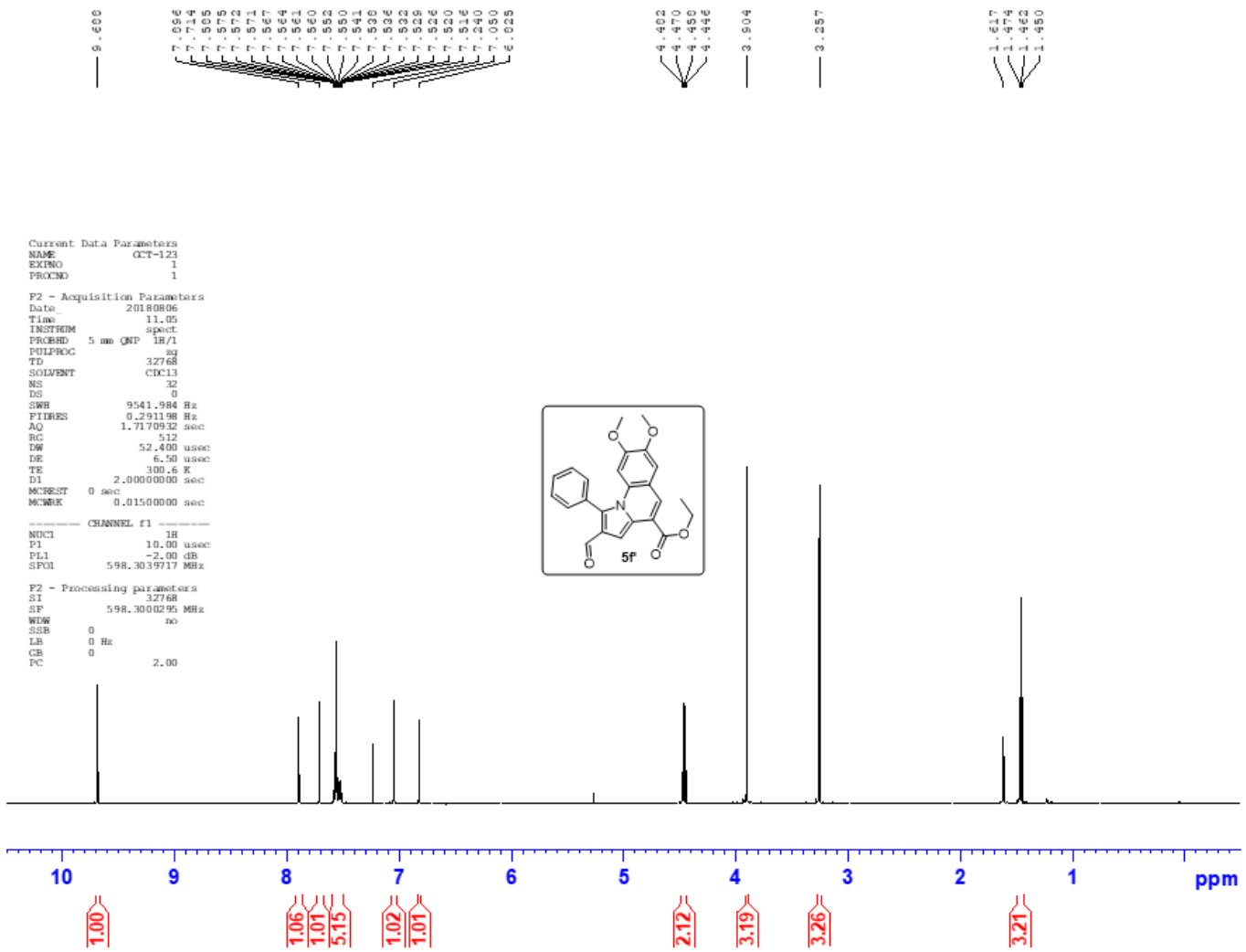

187.777
164.532
153.960
147.510
137.152
133.197
131.334
130.834
129.849
129.419
129.307
127.447
127.030
125.577
122.774
122.467
121.675
119.075
103.821
77.212
77.000
76.788
61.703
55.653
14.360
Current Data Parameters
NAME GCT-128-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180815
Time_ 16.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3072
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426583 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5c'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

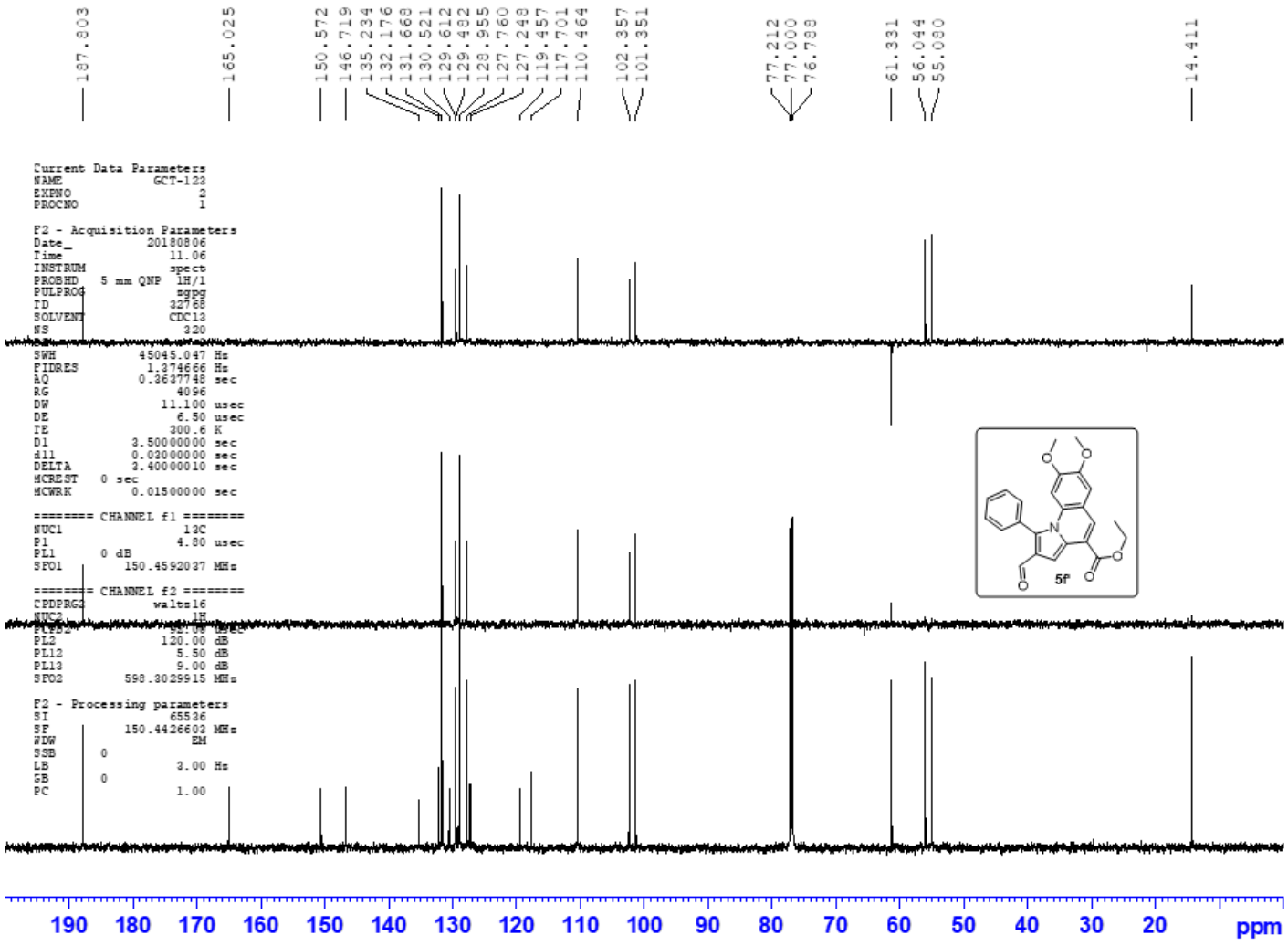

9.705
7.675
7.640
7.626
7.619
7.614
7.611
7.604
7.596
7.591
7.560
7.557
7.574
7.505
7.503
7.500
7.495
7.492
7.459
7.255
7.251
7.240
7.237
7.077
7.075
4.490
4.486
4.474
4.462
1.573
1.460
1.456
1.452
Current Data Parameters
NAME CCT-206
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181109
Time 7.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9569.378 Hz
FIDRES 0.292034 Hz
AQ 1.7121780 sec
RG 512
DW 52.250 usec
DE 6.50 usec
TE 302.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000300 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Cl
N
O
O
O
5d'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
0.96
4.19
1.93
1.06
1.01
2.16
3.18

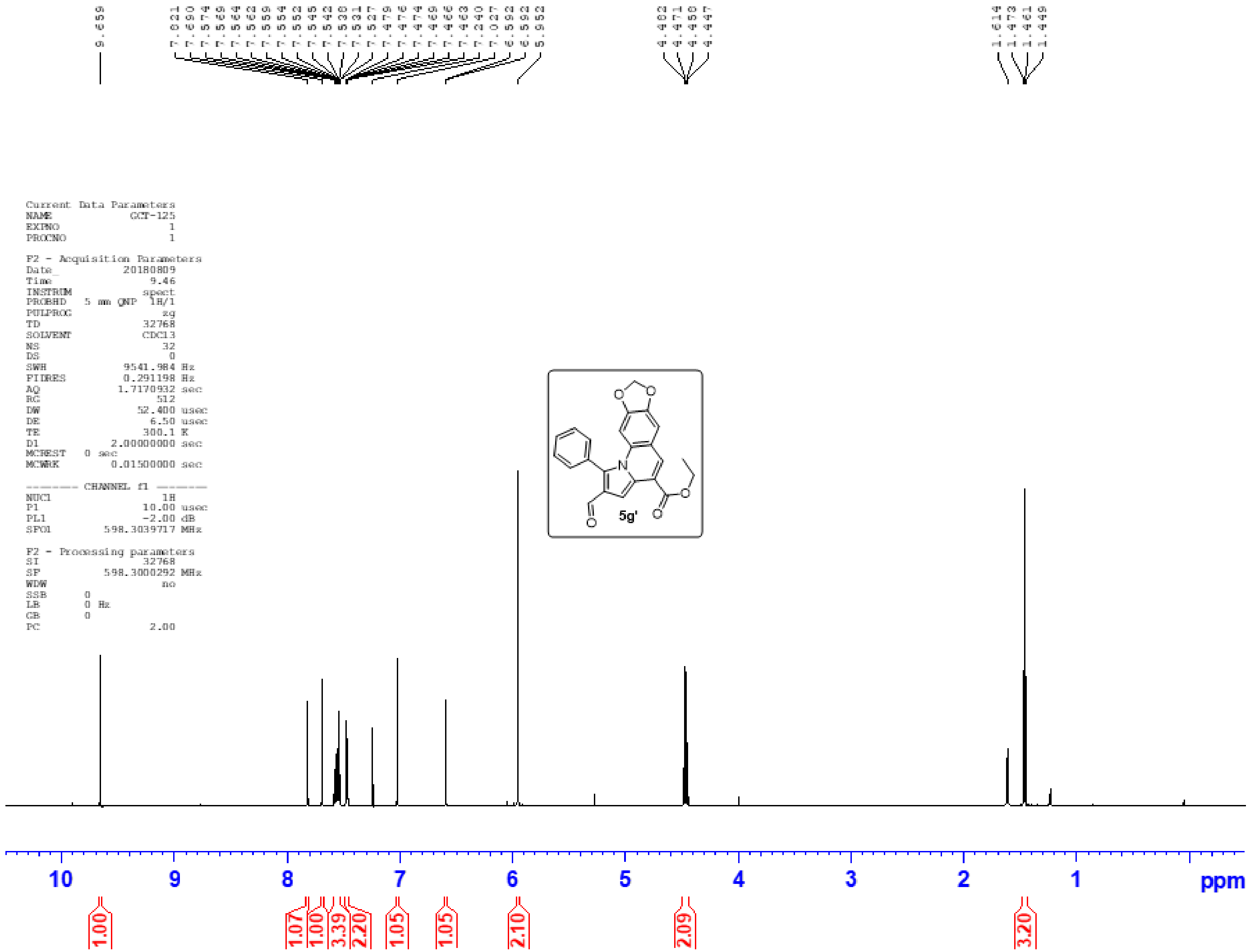

187.690
164.571
137.307
135.859
135.328
131.362
130.946
130.636
130.055
129.567
129.399
127.609
127.005
125.383
122.884
121.937
118.299
103.666
77.212
77.000
76.788
61.665
14.377
Current Data Parameters
NAME GCT-206
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181108
Time 15.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDC13
NS 402
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2050
DW 11.100 usec
DE 6.50 usec
TE 302.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.4584515 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 3.00 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SF 150.1426575 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 3.50 cm
F1P 200.000 ppm
F1 30088.53 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.42651 Hz/cm
Cl
N
O
O
O
5d'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

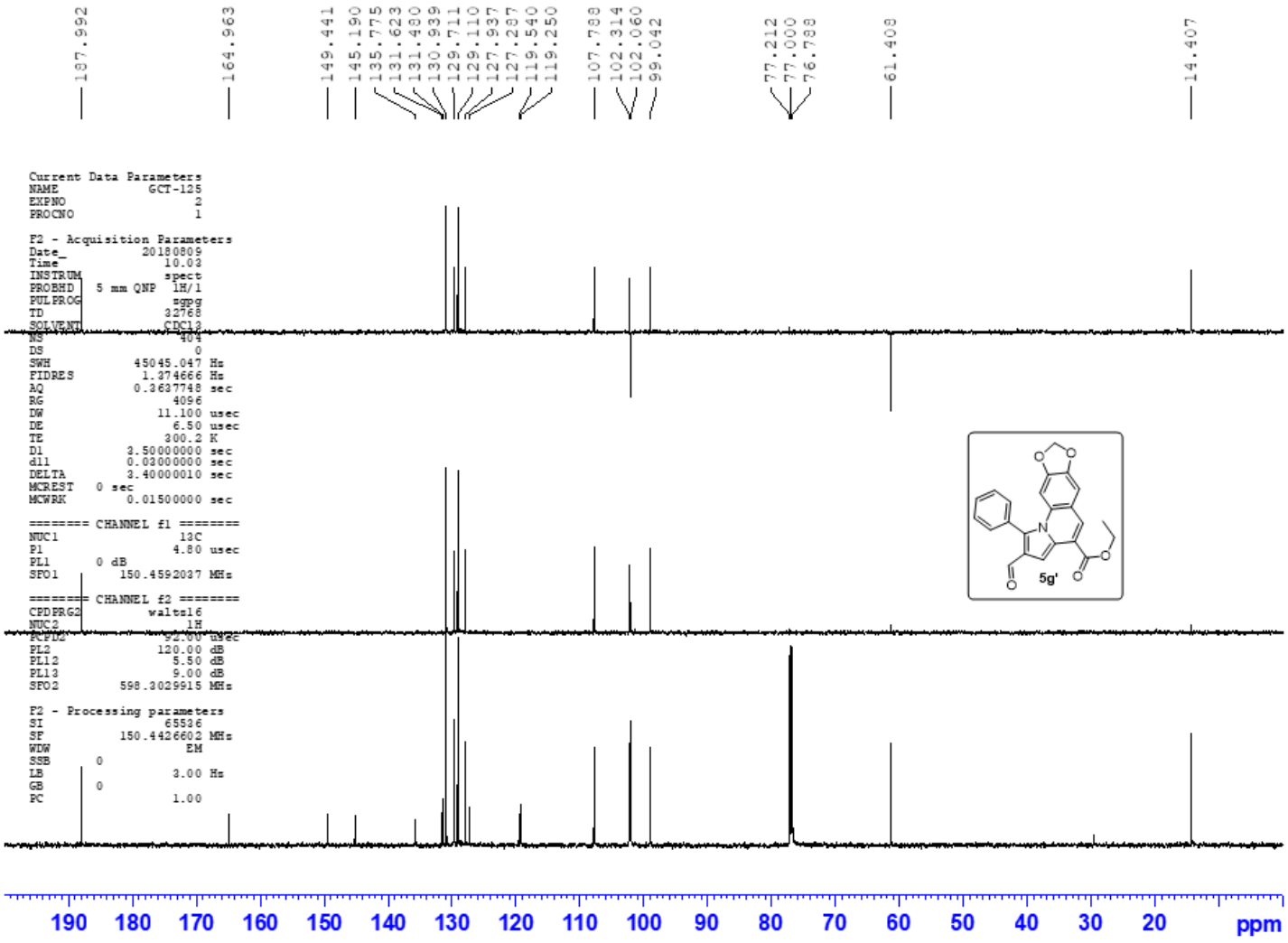

9.705
7.904
7.722
7.595
7.583
7.579
7.573
7.571
7.560
7.555
7.546
7.544
7.543
7.535
7.532
7.529
7.502
7.490
7.490
7.496
7.494
7.480
7.485
7.482
7.240
7.100
7.099
7.087
7.086
7.085
6.876
4.487
4.475
4.463
4.451
2.080
1.647
1.476
1.464
1.452
Current Data Parameters
NAME GCT-208
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181109
Time 11.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9569.378 Hz
FIDRES 0.292034 Hz
AQ 1.7121780 sec
RG 512
DW 52.250 usec
DE 6.50 usec
TE 304.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 10.00 usec
PL1 -4.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000296 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
5e'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
1.00
4.06
2.00
1.06
1.00
2.20
3.02
3.04

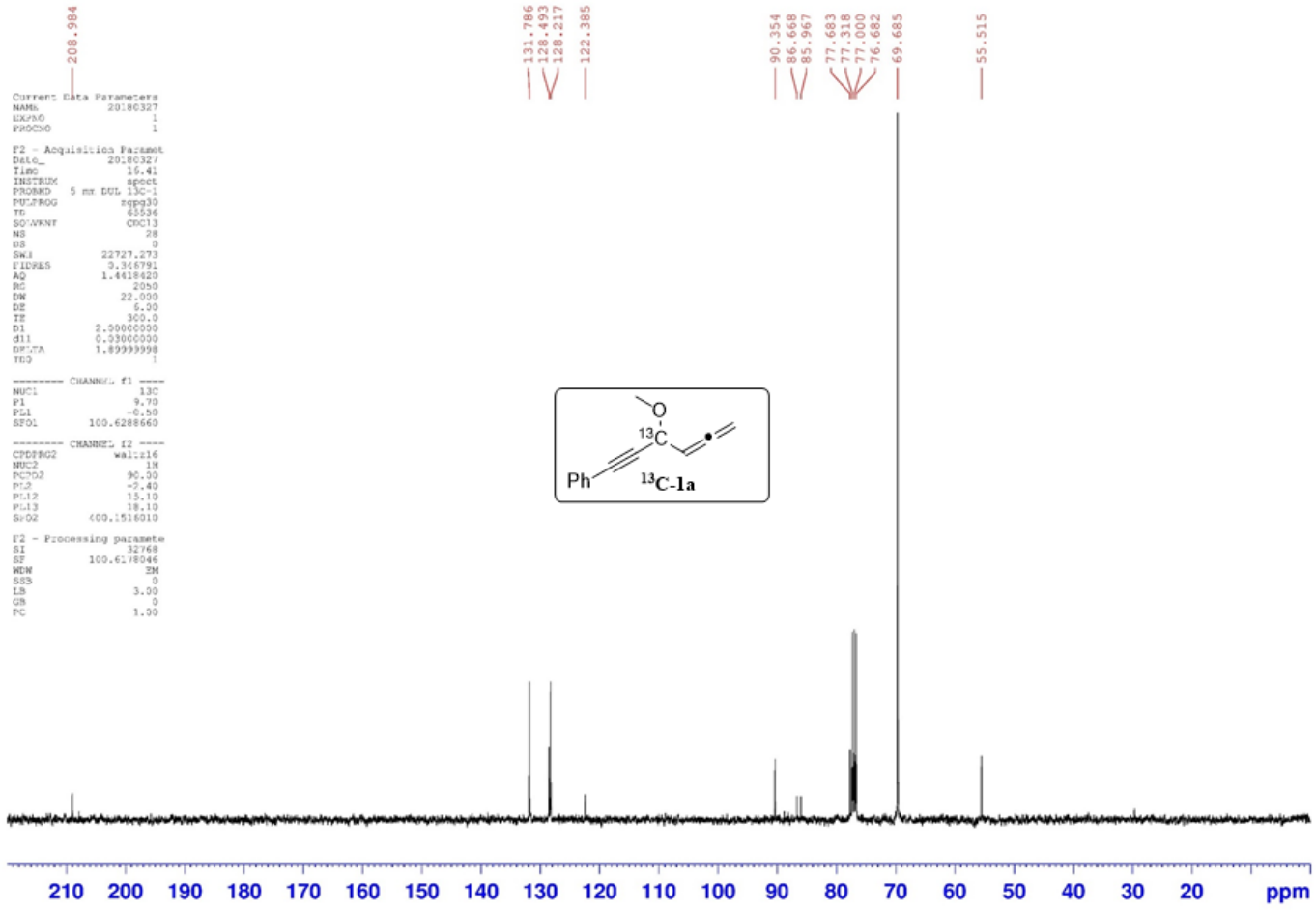

187.691
164.936
140.329
136.993
135.408
131.793
130.845
130.324
129.772
129.529
128.976
128.115
127.229
126.135
121.995
120.662
118.566
102.971
77.212
77.000
76.788
61.407
22.039
14.386
5e'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

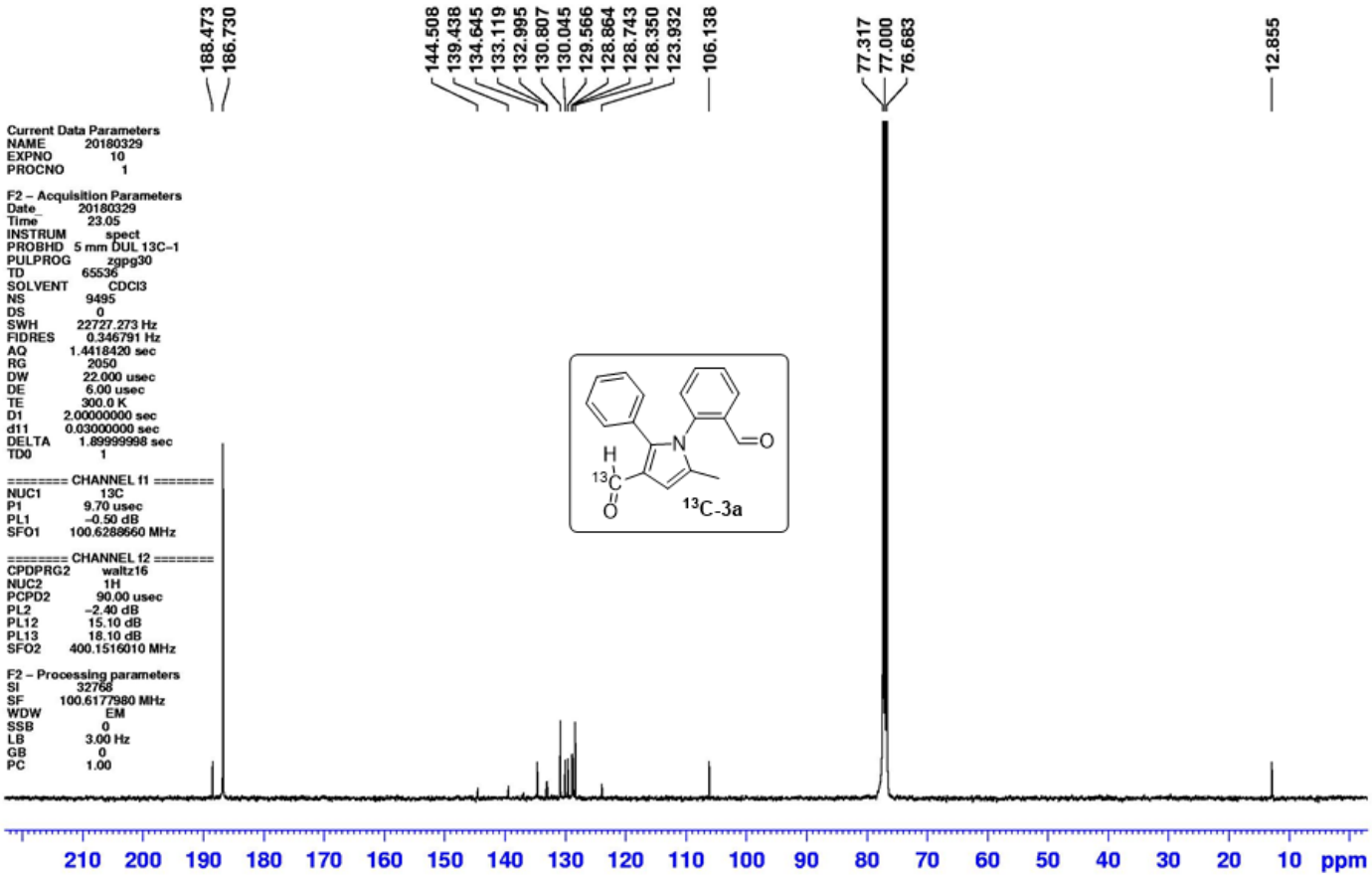

9.600
7.996
7.714
7.695
7.575
7.572
7.571
7.567
7.564
7.561
7.560
7.552
7.550
7.541
7.536
7.532
7.526
7.525
7.520
7.516
7.240
7.050
6.825
4.482
4.470
4.458
4.446
3.504
3.257
1.617
1.474
1.462
1.450
Current Data Parameters
NAME CCT-123
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180806
Time 11.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.3039717 MHz
F2 - Processing parameters
SI 32768
SF 598.3000295 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
5f'
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
1.01
5.15
1.02
1.01
2.12
3.19
3.26
3.21


187.803
165.025
150.572
146.719
135.234
132.176
131.668
130.521
129.612
129.482
128.955
127.760
127.248
119.457
117.701
110.464
102.357
101.351
77.212
77.000
76.788
61.331
56.044
55.080
14.411
Current Data Parameters
NAME GCT-123
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180806
Time 11.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 320
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 2.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426603 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


9.659
7.821 7.690 7.574 7.569 7.564 7.562 7.559 7.554 7.552 7.545 7.542 7.530 7.531 7.527 7.479 7.476 7.474 7.469 7.466 7.463 7.240 7.027 6.592 6.592 5.952
4.482 4.471 4.450 4.447
1.614 1.473 1.461 1.449
Current Data Parameters
NAME GCT-125
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180809
Time 9.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 598.3039717 MHz
F2 - Processing parameters
SI 32768
SF 598.3000292 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
N
O
5g'
10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.07 1.00 3.39 2.20 1.05 1.05 2.10 2.09 3.20


187.992
164.963
149.441
145.190
135.775
131.623
131.480
130.939
129.711
129.110
127.937
127.287
119.540
119.250
107.788
102.314
102.060
99.042
77.212
77.000
76.788
61.408
14.407
Current Data Parameters
NAME GCT-125
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180809
Time 10.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 404
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 300.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426602 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
5g'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


208.984
131.786
128.493
128.217
122.385
90.354
86.668
85.967
77.683
77.318
77.000
76.682
69.685
55.515
Current Data Parameters
NAME 20180327
EXPNO 1
PROCNO 1
F2 - Acquisition Paramet
Date_ 20180327
Time 16.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 28
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418429
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
-------- CHANNEL f1 ----
NUC1 13C
P1 9.70
PL1 -0.50
SFO1 100.6288660
-------- CHANNEL f2 ----
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6278046
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
O
13C
Ph
13C-1a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


188.473
186.730
144.508
139.438
134.645
133.119
132.995
130.807
130.045
129.566
128.864
128.743
128.350
123.932
106.138
77.317
77.000
76.683
12.855
Current Data Parameters
NAME 20180329
EXPNO 10
PROCNO 1
F2 – Acquisition Parameters
Date_ 20180329
Time 23.05
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9495
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 –0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 –2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 – Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
H
13C
O
N
O
13C-3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm