Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Gold-catalyzed *N,O*-functionalizations of 1,4-diyn-3-ols with *N*-hydroxyanilines to form highly functionalized pyrrole derivatives

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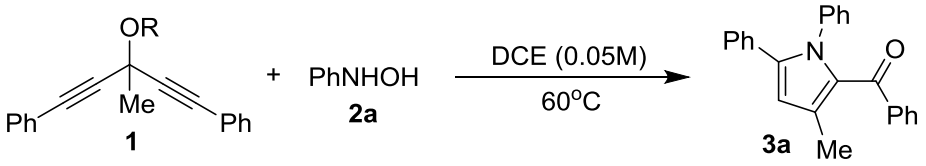
Contents:

(1) Table S1-Catalytic reaction over various Lewis acid:



Entry	R	Catalyst (mol%)	Lewis acid (mol%)	Time (h)	Yield (%)
1	Bn	JohnPhosAuCl(10)/$AgNTf_2$ (10)	PTSA (20)	6.5	14.8
2	Bn	JohnPhosAuCl(10)/$AgNTf_2$ (10)	$Zn(OTf)_2$ (20)	5	38.5
3	Bn	JohnPhosAuCl(10)/$AgNTf_2$ (10)	$Cu(OTf)_2$ (20)	13	0
4	Bn	JohnPhosAuCl(10)/$AgNTf_2$ (10)	$Sc(OTf)_3$ (20)	11	4.2
5[a]	H	JohnPhosAuCl(20)/$AgNTf_2$ (50)	-	2	78

1 (1.0 equiv). **2a** (3.0 equiv). [a]Room temperature.

(2) Representative synthetic procedures:

(A) General procedure:

Unless otherwise noted, all the reaction for the preparation of the substrates 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. All other commercial reagents were used without further purification, unless otherwise indicated. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60_f-254) using UV light as visualizing agents. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz, 600MHz, Varian 400 MHz, 500MHz and 700 MHz. Spectrometers using chloroform-*d* ($CDCl_3$) and acetone-*d* as the internal standards. The preparations of *N*-phenyl hydroxyl-amines were prepared according to literature procedure.[S1-3]

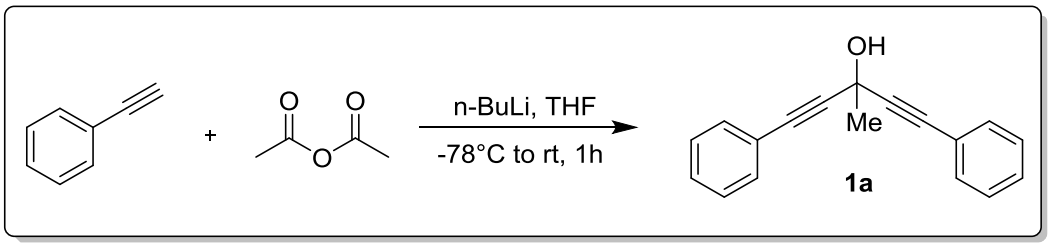
[S1] F. G. Bordwell, W.Z. Liu, *J. Am. Chem. Soc.* **1996**, *118*, 8777-8781.

[S2] S. Ung, A. Falguieres, A. Guy, C. Ferroud, *Tetrahedron Letters.*, **2005**, *46*, 5913–5917

[S3] Y. Wang, L. Liu, L. Zhang, *Chem. Sci.* **2013**, *4*, 739-746.

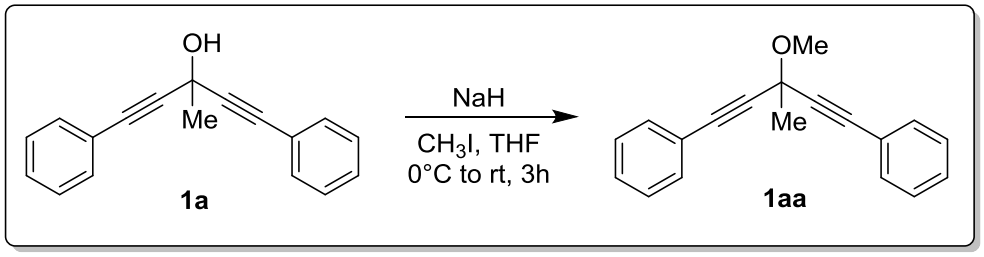
(B) Preparation of starting materials:

1.Preparation of 3-methyl-1,5-diphenylpenta-1,4-diyn-3-ol (1a)



Phenylacetylene (2.37 mL, 21.6 mmol) was dissolved into dry THF (10 mL), and the solution was cooled to -78℃. To this solution, *n*-Butyllithium (9.4 mL, 23.5 mmol, 2.5M in hexane) was added. After being stirred for 20 minutes at -78℃, acetic anhydride (0.93 mL, 9.8 mmol) was added. The reaction mixture was stirred at room temperature for 1h, and then the reaction was quenched by saturated $NH_4Cl_{(aq)}$, 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 collum chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 3-methyl-1,5-diphenylpenta-1,4-diyn-3-ol **1a** (2.1 g, 8.53mmol, 87%). The other symmetric 3-alkyl-1,4-diyne-3-ols **1b-1l** were synthesized by similar procedure using the corresponding alkynes and acetic anhydride or ester.

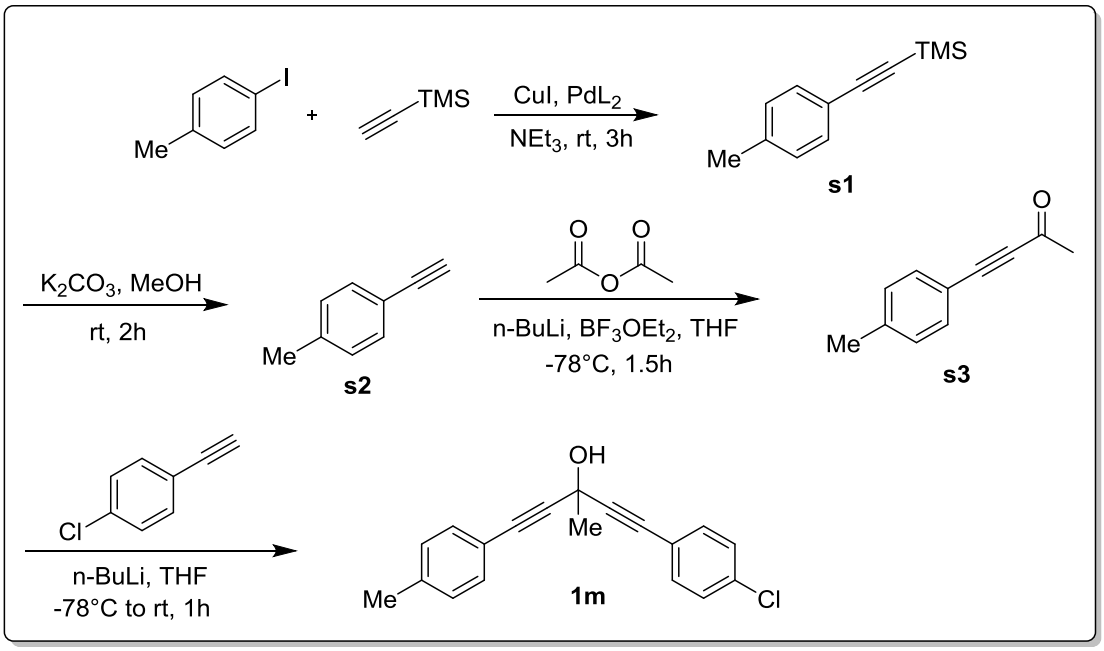
2.Preparation of (3-methoxy-3-methylpenta-1,4-diyne-1,5-diyl)dibenzene (1aa)



Compound **1a** (0.30 g, 1.2 mmol) was added to a stirred solution of NaH (0.073 g, 3.0 mmol) in THF (5 mL) at 0 ℃, and the resulting mixture was stirred at 0 ℃ for 5 min. MeI (0.86 g, 6.1 mmol) was added, and the resulting mixture was stirred at rt for 3 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 (hexane:EtOAc = 20:1), which furnished (3-methoxy-3-methylpenta-1,4-diyne-1,5-diyl)dibenzene **1aa** (0.21 g, 0.81 mmol, 66%) as a white solid.[S4] The other substrate **1ab** and **1ac** were synthesized by same procedure.

[S4] K. Tanaka, T. Osaka, K. Noguchi, M. Hirano, *Org. Lett.*, **2007**, *9*, 1307-1310.

3. Preparation of 1-(4-chlorophenyl)-3-methyl-5-(*p*-tolyl)penta-1,4- diyn-3-ol (1k)



Compound **s2** was prepared from 1-iodo-4-methylbenzene according to a literature procedure.[S5]

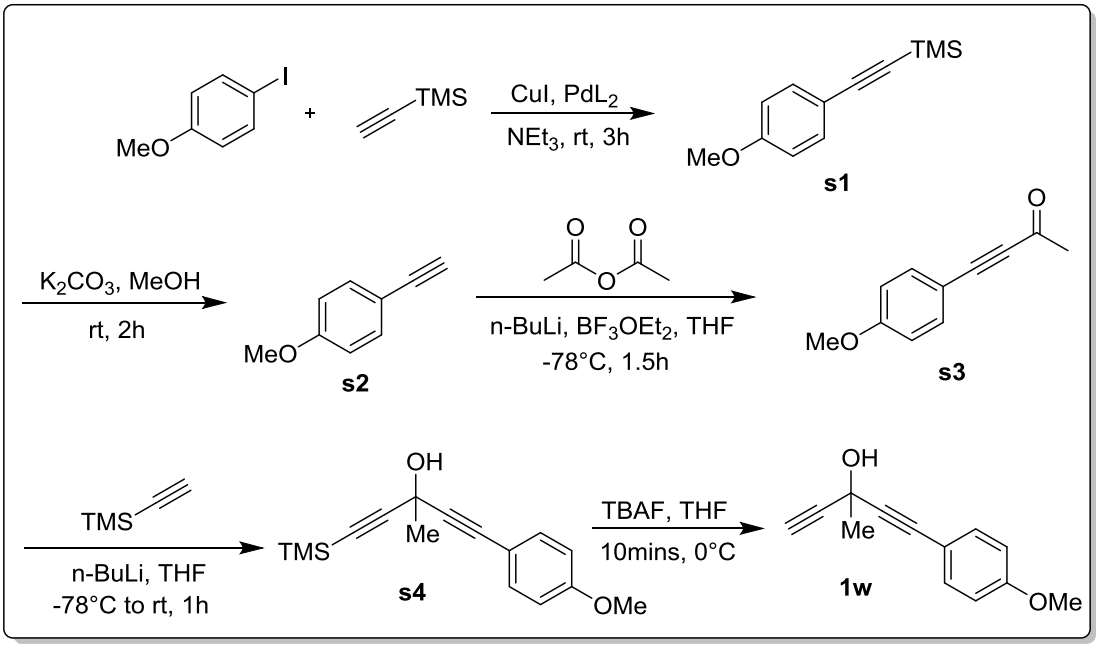
s2 (2 g, 17.2 mmol) was dissolved into dry THF (20 mL), and the solution was cooled to -78℃. To this solution, *n*-Butyllithium (8.2 mL, 20.6 mmol, 2.5M in hexane) was added. After being stirred for 20 minutes at -78℃, acetic anhydride (2.4 mL, 25.8 mmol) and BF_3OEt_2 (3.2 mL, 25.5 mmol) were added successively. The reaction was quenched by saturated $NH_4Cl_{(aq)}$, 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 collum chromatography (SiO_2, eluent: dichloromethane/hexane) to afford the desired **s3** (2 g, 12.6mmol, 74%).

1-chloro-4-ethynylbenzene (0.5 g, 3.67 mmol) was dissolved into THF (5 mL), and the solution was cooled to -78℃. To this solution, *n*-Butyllithium (5.1 mL, 12.8 mmol, 2.5M in hexane) was added. After being stirred for 20 minutes at -78℃, **s3** (0.48 g, 3.06 mmol) was added. The reaction mixture was stirred at room temperature for 1h, and then the reaction was quenched by saturated $NH_4Cl_{(aq)}$, 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 collum chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 1-(4-chlorophenyl)-3-methyl-5-(*p*-tolyl)penta-1,4-diyn-3-ol **1m** (0.51 g, 1.73mmol, 57%).

The other asymmetric 3-alkyl-1,4-diyne-3-ols **1n-1v, 1x and 1y** were synthesized by similar procedure using the corresponding alkynes and acetic anhydride.

[S5] D. Nishikawa, K. Hirano, M. Miura, *J. Am. Chem. Soc.* **2015**, *137*, 15620−15623

4. Preparation of 3-methyl-1-(p-tolyl)penta-1,4-diyn-3-ol (1w)



Compound **s2** was prepared from 1-iodo-4-methoxybenzene according to a literature procedure.[S5]

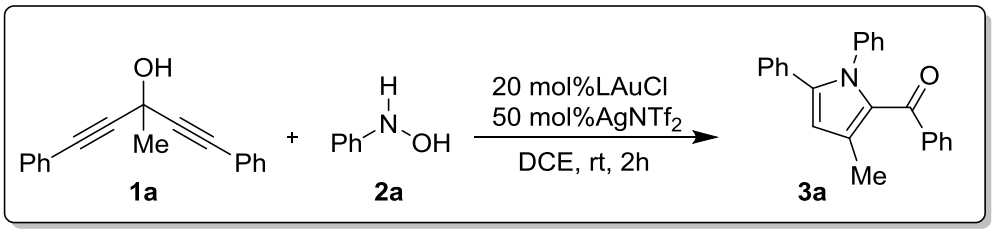
s2 (2 g, 17.2 mmol) was dissolved into dry THF (20 mL), and the solution was cooled to -78℃. To this solution, *n*-Butyllithium (8.2 mL, 20.6 mmol, 2.5M in hexane) was added. After being stirred for 20 minutes at -78℃, acetic anhydride (2.4 mL, 25.8 mmol) and BF_3OEt_2 (3.2 mL, 25.5 mmol) were added successively. The reaction was quenched by saturated $NH_4Cl_{(aq)}$, 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 collum chromatography (SiO_2, eluent: dichloromethane/hexane) to afford the desired **s3** (2 g, 12.6mmol, 74%).

Trimethylsilylacetylene (0.93mL, 6.51 mmol) was dissolved into THF (5 mL), and the solution was cooled to -78℃. To this solution, *n*-Butyllithium (2.87 mL, 7.16 mmol, 2.5M in hexane) was added. After being stirred for 20 minutes at -78℃, **s3** (567mg, 3.26mmol) was added. The reaction mixture was stirred at room temperature for 1h, and then the reaction was quenched by saturated $NH_4Cl_{(aq)}$, 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 collum chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 3-methyl-1,4-diyne-3-ols **s4** (596 mg, 2.19 mmol, 67%).

This silyl compound was then dissolved in THF (5 mL), added with Bu_4NF (1.0 M THF, 2.6 mL, 2.63 mmol); the mixture was stirred at 0℃ for 10 minutes before the treatment of water (5 mL). The solution was concentrated, extracted with diethyl ether,

and the residue was purified by collum chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 1-(4-methoxyphenyl)-3-methylpenta-1,4-diyn-3-ol **1w** (393 mg, 1.96 mmol, 90%).

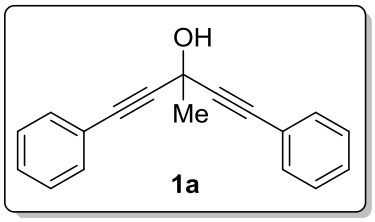
(3) Standard procedures for catalytic operations:



A suspension of chloro[(1,1'-biphenyl-2-yl)di-*tert*- butylphosphine] gold(I) (21.6 mg, 0.04 mmol) and silver bis(trifluoromethane-sulfonyl) imide (39.42 mg, 0.10 mmol) in dry DCE (1.5 mL) was fitted with N_2 balloon and to this solution was added DCE (1.5 mL) solution of 3-methyl-1,5-diphenylpenta-1,4-diyn-3-ol **1a** (50 mg, 0.20 mmol) and *N*-phenylhydroxylamine **2a** (33.3 mg, 0.30 mmol) at room temperature. The resulting mixture was stirred for 30 minutes at room temperature. In the TLC, we found *N*-phenylhydroxylamine was finished, and **3a** was remained. So we put the other *N*-phenylhydroxylamine (33.3 mg, 0.30 mmol) in the solution. The resulting mixture was stirred for another 1.5 h at room temperature. After completion of the reaction it was filtered over a short celite bed. The solvent was evaporated under reduced pressure, and The residue was purified by collum chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired (3-methyl-1,5-diphenyl-1*H*-pyrrol-2-yl) (phenyl)methanone **3a** (53 mg, 0.16 mmol, 78%) as yellow solid.

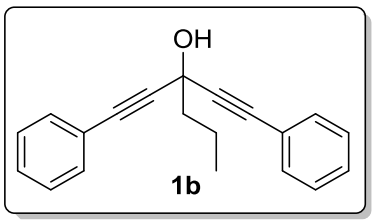
(4) Spectral data for compounds:

Spectral data for 3-methyl-1,5-diphenylpenta-1,4-diyn-3-ol (1a)



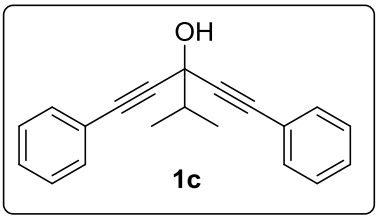
Yellow solid; mp: 108.5~110.5℃;(20% ethylacetate/hexane, R_f = 0.23, 2.1 g, 8.53 mmol, 87%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49~7.46 (m, 4H), 7.34~7.28 (m, 6H), 2.91 (s, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.8, 128.6, 128.2, 122.1, 90.0, 82.6, 60.8, 32.0; FI-MS (M) calcd. for $C_{18}H_{14}O$:246.1045; Found: 246.1039.

Spectral data for 1-phenyl-3-(phenylethynyl)hex-1-yn-3-ol (1b)



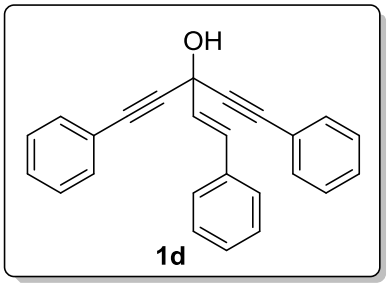
White solid; mp: 74.2~76.3℃ ;(20% ethylacetate/hexane, R_f = 0.33, 2.4 g, 8.75 mmol, 83%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.48~7.45 (m, 4H), 7.33~7.30 (m, 6H), 2.63 (s, 1H), 2.08~2.04 (m, 2H), 1.79~1.71 (m, 2H), 1.03 (t, *J* = 1.2Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ131.8, 128.6, 128.2, 122.2, 89.4, 83.5, 64.5, 46.1, 18.2, 13.9; ESI-MS (M+Na) calcd. for $C_{20}H_{18}ONa$:297.1255; Found: 297.1252.

Spectral data for 3-isopropyl-1,5-diphenylpenta-1,4-diyn-3-ol (1c)



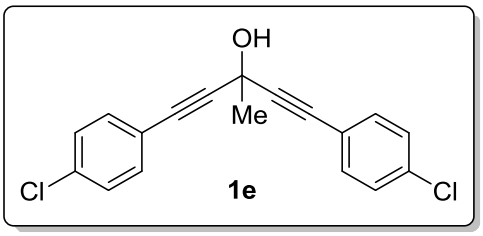
Yellow oil;(20% ethylacetate/hexane, R_f = 0.32, 3.23 g, 12 mmol, 85%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.49~7.46 (m, 4H), 7.34~7.29 (m, 6H), 2.66 (s, 1H), 2.26~2.20 (m, 1H), 1.24 (s, 3H), 1.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ131.8, 128.6, 128.2, 122.3, 88.5, 84.1, 68.8, 40.1, 17.6; ESI-MS (M+Na) calcd. for $C_{20}H_{18}ONa$: 297.1255; Found: 297.1243.

Spectral data for (*E*)-1,5-diphenyl-3-(phenylethynyl)pent-1-en-4-yn-3-ol (1d)



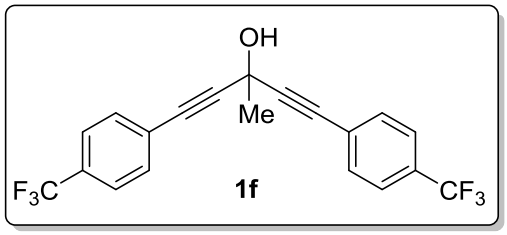
Yellow solid, mp: 136.1~137.5℃; (20% ethylacetate/hexane, R_f = 0.29, 5.4 g, 16.1 mmol, 95%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.55~7.53 (m, 4H), 7.49 (d, *J* = 7.4Hz, 2H), 7.37~7.27 (m, 9H), 7.17 (d, *J* = 15.6Hz, 1H), 6.54 (d, *J* = 15.6Hz, 1H), 3.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ135.7, 131.9, 130.9, 129.4, 128.9, 128.6, 128.3, 127.1, 121.9, 87.7, 85.1, 64.1; ESI-MS (M+Na) calcd. for $C_{25}H_{18}ONa$: 357.1255; Found: 357.1250.

Spectral data for 1,5-bis(4-chlorophenyl)-3-methylpenta-1,4-diyn-3-ol (1e)



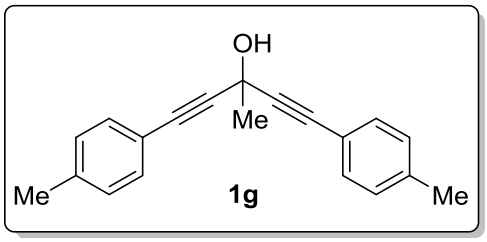
White solid; mp: 171.6~172.4℃;(20% ethylacetate/hexane, R_f = 0.24, 2.5 g, 7.93 mmol, 80%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.40~7.36 (m, 4H), 7.29~7.26 (m, 4H), 2.75 (s, 1H), 1.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ134.9, 133.0, 128.7, 120.5, 90.7, 81.7, 60.8, 31.9; FI-MS (M) calcd. for $C_{18}H_{12}Cl_2O$: 314.0265; Found: 314.0260.

Spectral data for 3-methyl-1,5-bis(4-(trifluoromethyl)phenyl)penta-1,4-diyn-3-ol (1f)



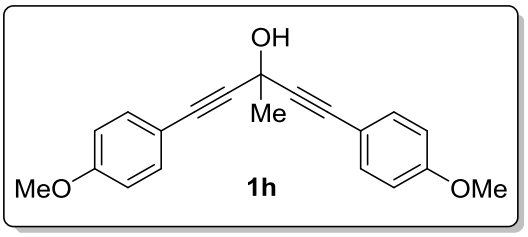
White solid; mp: 153.4~156.4℃;(20% ethylacetate/hexane, R_f = 0.23, 3.7 g, 9.68 mmol, 74%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.57 (s, 8H), 2.79 (s, 1H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ132.1, 125.3, 125.3, 125.2, 125.2, 91.9, 81.6, 60.8, 31.7; FI-MS (M) calcd. for $C_{20}H_{12}F_6O$: 382.0792; Found: 382.0787.

Spectral data for 3-methyl-1,5-di-p-tolylpenta-1,4-diyn-3-ol (1g)



Yellow oil;(20% ethylacetate/hexane, R_f = 0.26, 2.7 g, 9.84 mmol, 78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.36 (d, *J* = 7.6Hz, 4H), 7.10 (d, *J* = 7.6Hz, 4H), 2.71 (s, 1H), 2.33 (s, 6H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ138.8, 131.7, 129.0, 119.1, 89.5, 82.7, 60.9, 32.1, 21.5; ESI-MS (M+Na) calcd. for $C_{20}H_{18}ONa$: 297.1255; Found: 297.1252.

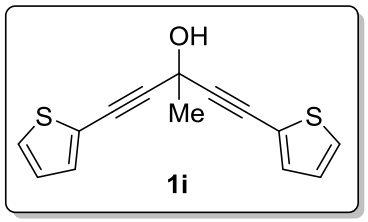
Spectral data for 1,5-bis(4-methoxyphenyl)-3-methylpenta-1,4-diyn-3-ol (1h)



1h

Orange solid; mp: 151.6~152.7℃;(20% ethylacetate/hexane, R_f = 0.21, 974 mg, 3.18 mmol, 64%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.41~7.38 (m, 4H), 6.84~6.81 (m, 4H), 3.80 (s, 6H), 2.62 (s, 1H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ159.8, 133.3, 114.2, 113.9, 89.0, 82.4, 60.9, 55.2, 32.1; ESI-MS (M+Na) calcd. for $C_{20}H_{18}O_3$: 329.1154; Found: 329.1147.

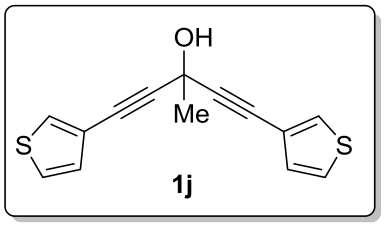
Spectral data for 3-methyl-1,5-di(thiophen-2-yl)penta-1,4-diyn-3-ol (1i)



1i

Red oil; (20% ethylacetate/hexane, R_f = 0.27, 674 mg, 2.61 mmol, 53%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.28~7.24 (m, 4H), 6.98~6.96 (m, 2H), 2.72 (s, 1H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ132.8, 127.8, 127.0, 121.9, 93.3, 76.4, 61.1, 31.6; FI-MS (M) calcd. for $C_{14}H_{10}OS_2$: 258.0173; Found: 258.0168.

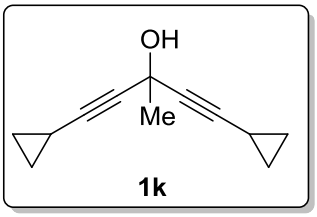
Spectral data for 3-methyl-1,5-di(thiophen-3-yl)penta-1,4-diyn-3-ol (1j)



1j

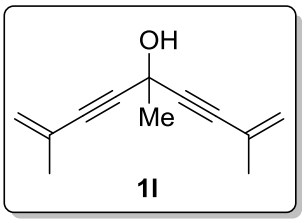
Red sticky solid; (20% ethylacetate/hexane, R_f = 0.18, 620 mg, 2.40 mmol, 49%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.49~7.48 (m, 2H), 7.26~7.25 (m, 2H), 7.13~7.12 (m, 2H), 2.67 (s, 1H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ129.9, 129.5, 125.4, 121.1, 89.6, 78.0, 60.9, 31.9; FI-MS (M) calcd. for $C_{14}H_{10}OS_2$: 258.0173; Found: 258.0168.

Spectral data for 1,5-dicyclopropyl-3-methylpenta-1,4-diyn-3-ol (1k)



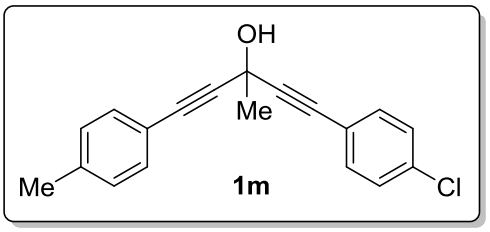
Yellow oil; (20% ethylacetate/hexane, R_f = 0.29, 1.2 g, 6.89 mmol, 71%); ^{1}H NMR (400 MHz, $CDCl_3$): δ2.31 (s, 1H), 1.65 (s, 3H), 1.26~1.20 (m, 2H), 0.77~0.71 (m, 4H), 0.70~0.69 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ85.9, 77.3, 60.1, 32.5, 8.2, -0.7; ESI-MS (M+H) calcd. for $C_{12}H_{15}O$: 175.1123; Found: 175.1117.

Spectral data for 2,5,8-trimethylnona-1,8-dien-3,6-diyn-5-ol (1l)



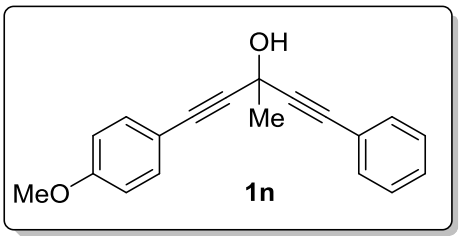
Red oil; (20% ethylacetate/hexane, R_f = 0.33, 671 mg, 3.85 mmol, 40%); ^{1}H NMR (400 MHz, $CDCl_3$): δ5.32 (s, 2H), 5.25 (s, 2H), 1.88 (s, 6H), 1.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ125.9, 122.9, 89.0, 83.6, 60.6, 31.9, 23.2; FI-MS (M) calcd. for $C_{12}H_{14}O$: 174.1045; Found: 174.1039.

Spectral data for 1-(4-chlorophenyl)-3-methyl-5-(p-tolyl)penta-1,4-diyn-3-ol (1m)



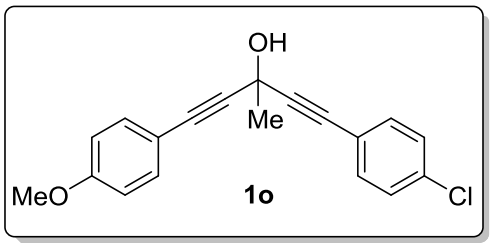
White solid; mp: 172.9~173.8℃;(20% ethylacetate/hexane, R_f = 0.33, 0.99 g, 3.36 mmol, 53%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.38 (d, *J* = 8.4Hz, 2H), 7.35 (d, *J* = 8.4Hz, 2H), 7.27 (d, *J* = 8.4Hz, 2H), 7.10 (d, *J* = 7.8Hz, 2H), 2.80 (s, 1H), 2.33 (s, 3H), 1.93 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ138.9, 134.7, 133.0, 131.7, 129.0, 128.6, 120.7, 118.9, 91.1, 89.2, 83.0, 81.4, 60.8, 32.0, 21.5; FI-MS (M) calcd. for $C_{19}H_{15}ClO$: 294.0811; Found: 294.0806.

Spectral data for 1-(4-methoxyphenyl)-3-methyl-5-phenylpenta-1,4-diyn-3-ol (1n)



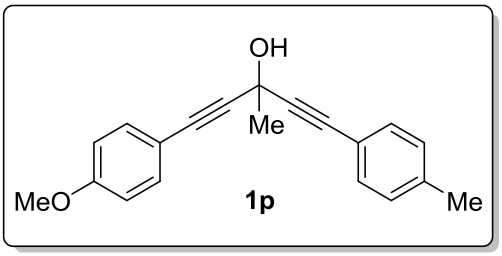
Yellow solid, mp: 106.0~108.0℃; (20% ethylacetate/hexane, R_f = 0.24, 2.11 g, 7.64 mmol, 78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.48~7.44 (m, 2H), 7.41~7.38 (m, 2H), 7.32~7.28 (m, 3H), 6.84~6.80 (m, 2H), 3.79 (s, 3H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ159.8, 133.3, 131.8, 128.6, 128.2, 122.2, 114.2, 113.9, 90.3, 88.8, 82.6, 82.4, 60.8, 55.2, 32.1; ESI-MS (M+Na) calcd. for $C_{19}H_{16}O_2Na$: 299.1048; Found: 299.1042.

Spectral data for 1-(4-chlorophenyl)-5-4-methoxyphenyl)-3-methylpenta-1,4-iyn-3-ol (1o)



White solid, mp: 164.6~165.4℃; (20% ethylacetate/hexane, R_f = 0.20, 1.30 g, 4.18 mmol, 73%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.40~7.37 (m, 4H), 7.29~7.26 (m, 2H), 6.84~6.81 (m, 2H), 3.80 (s, 3H), 2.70 (s, 1H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, CDCl3): δ160.0, 134.7, 133.3, 133.1, 128.6, 120.7, 113.9, 91.2, 88.5, 82.9, 81.4, 60.9, 55.3, 32.0; ESI-MS (M+Na) calcd. for $C_{19}H_{15}ClO_2Na$: 333.0658; Found: 333.0651.

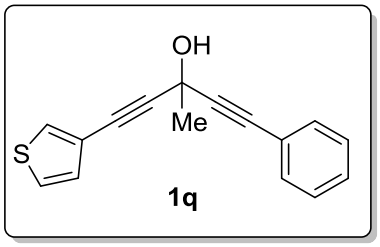
Spectral data for 1-(4-methoxyphenyl)-3-methyl-5-(p-tolyl)penta-1,4-diyn-3-ol (1p)



White solid, mp: 130.3~130.9℃; (20% ethylacetate/hexane, R_f = 0.29, 1.48 g, 5.10 mmol, 89%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.41~7.38 (m, 2H), 7.35 (d, *J* = 6.8Hz,

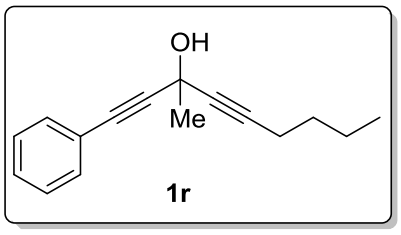
2H), 7.10 (d, *J* = 8Hz, 2H), 6.84~6.81 (m, 2H), 3.80 (s, 3H), 2.71 (s, 1H), 2.33 (s, 3H), 1.93 (s, 3H), ; ^{13}C NMR (100 MHz, $CDCl_3$): δ159.8, 138.8, 133.3, 131.7, 129.0, 119.1, 114.2, 113.9, 89.6, 88.9, 82.7, 82.6, 60.9, 55.3, 32.1, 21.5; FI-MS (M) calcd. for $C_{20}H_{18}O_2$: 290.1307; Found: 290.1301.

Spectral data for 3-methyl-1-phenyl-5-(thiophen-3-yl)penta-1,4-diyn-3-ol (1q)



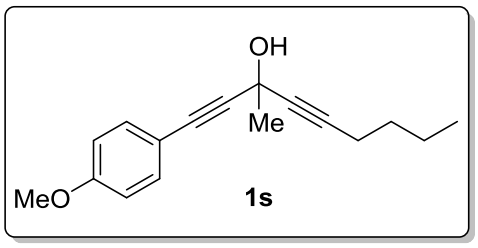
Orange oil; (20% ethylacetate/hexane, R_f = 0.40, 0.58 g, 2.30 mmol, 62%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.49~7.45 (m, 3H), 7.32~7.30 (m, 3H), 7.26~7.25 (m, 1H), 7.13 (t, *J* = 1.2Hz, 1H), 2.79 (s, 1H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ131.8, 129.9, 129.5, 128.7, 128.3, 125.3, 122.1, 121.1, 90.0, 89.6, 77.9, 60.8, 31.9; ESI-MS (M+Na) calcd. for $C_{16}H_{12}OSNa$: 275.0507; Found: 275.0501.

Spectral data for 3-methyl-1-phenylnona-1,4-diyn-3-ol (1r)



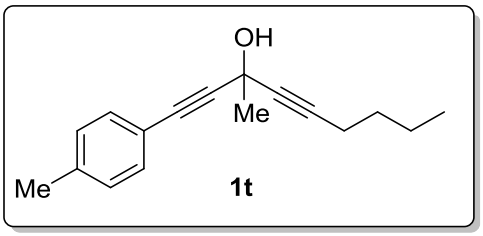
Orange oil; (20% ethylacetate/hexane, R_f = 0.36, 1.11 g, 4.90 mmol, 71%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.44~7.42 (m, 2H), 7.30~7.28 (m, 3H), 2.56 (s, 1H), 2.25~2.21 (m, 2H), 1.82 (s, 3H), 1.54~1.47 (m, 2H), 1.45~1.38 (m, 2H), 0.93~0.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ131.8, 128.5, 128.2, 122.2, 90.7, 83.8, 81.9, 81.5, 60.5, 32.2, 30.4, 21.9, 18.3, 13.6; ESI-MS (M+H) calcd. for $C_{16}H_{19}O$: 227.1436; Found: 227.1430.

Spectral data for 1-(4-methoxyphenyl)-3-methylnona-1,4-diyn-3-ol (1s)



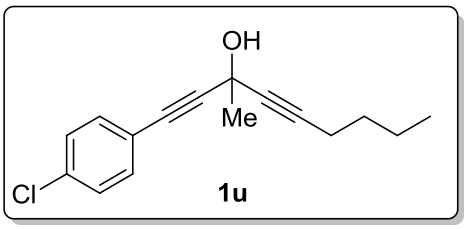
Yellow oil; (20% ethylacetate/hexane, R_f = 0.20, 0.90 g, 3.51 mmol, 61%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.37~7.31 (m, 2H), 6.81~6.79 (m, 2H), 3.77 (s, 3H), 2.68 (s, 1H), 2.23~2.19 (m, 2H), 1.80 (s, 3H), 1.49~1.48 (m, 2H), 1.46~1.35 (m, 2H), 0.91~0.87 (m, 3H); 13C NMR (100 MHz, CDCl3): δ159.7, 133.2, 133.0, 114.3, 113.8, 89.4, 83.5, 81.8, 60.5, 55.2, 32.3, 30.4, 21.9, 18.3, 13.6; ESI-MS (M+Na) calcd. for $C_{17}H_{20}O_2Na$: 279.1361; Found: 279.1356.

Spectral data for 3-methyl-1-(*p*-tolyl)nona-1,4-diyn-3-ol (1t)



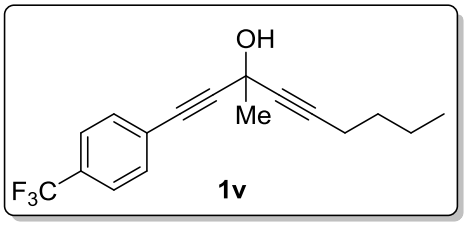
Red oil; (20% ethylacetate/hexane, R_f = 0.32, 517 mg, 2.15 mmol, 68%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.35~7.31 (m, 2H), 7.12~7.08 (m, 2H), 2.54 (s, 1H), 2.32 (s, 3H), 2.22 (t, *J* = 7.2Hz, 2H), 1.81 (s, 3H), 1.54~1.47 (m, 2H), 1.45~1.36 (m, 2H), 0.90 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ138.6, 131.7, 129.0, 119.2, 90.0, 83.6, 82.1, 81.7, 60.5, 32.3, 30.4, 21.9, 21.5, 18.4, 13.6; FI-MS (M) calcd. for $C_{17}H_{20}O$: 240.1514; Found: 240.1509.

Spectral data for 1-(4-chlorophenyl)-3-methylnona-1,4-diyn-3-ol (1u)



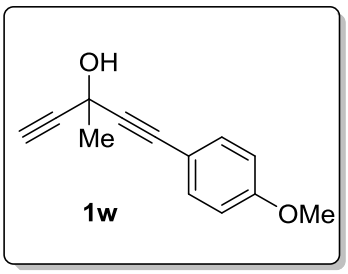
Orange oil; (20% ethylacetate/hexane, R_f = 0.34, 1.12 g, 4.30 mmol, 77%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.45~7.34 (m, 2H), 7.33~7.24 (m, 2H), 2.52 (s, 1H), 2.22 (t, *J* = 7.2Hz, 2H), 1.81 (s, 3H), 1.55~1.46 (m, 2H), 1.44~1.35 (m, 2H), 0.90 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ133.2, 133.0, 131.5, 128.6, 91.6, 84.0, 81.4, 80.8, 60.5, 32.2, 30.4, 21.9, 18.3, 13.6; ESI-MS (M+Na) calcd. for $C_{16}H_{17}ClONa$: 283.0866; Found: 283.0856.

Spectral data for 3-methyl-1-(4-(trifluoromethyl)phenyl)nona-1,4-diyn-3-ol (1v)



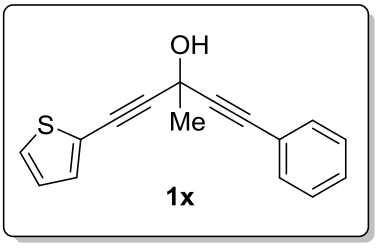
Yellow solid, mp: 154.2~155.7℃; (20% ethylacetate/hexane, R_f = 0.31, 0.96 g, 3.26 mmol, 69%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.57~7.52 (m, 4H), 2.56 (s, 1H), 2.23 (t, *J* = 7.2Hz, 2H), 1.82 (s, 3H), 1.54~1.47 (m, 2H), 1.45~1.36 (m, 2H), 0.90 (t, *J* = 7.1Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ132.0, 126.1, 125.2, 93.0, 84.3, 81.2, 80.5, 60.5, 32.1, 30.4, 21.9, 18.3, 13.6; ESI-MS (M+H) calcd. for $C_{17}H_{18}F_3O$: 295.1310; Found: 295.1304.

Spectral data for 3-methyl-1-(p-tolyl)penta-1,4-diyn-3-ol (1w)



Orange oil; (20% ethylacetate/hexane, R_f = 0.20, 393 mg, 1.96 mmol, 90%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.37 (d, *J* = 7.2Hz, 2H), 6.82 (d, *J* = 6.8Hz, 2H), 3.79 (s, 3H), 2.58 (s, 1H), 1.85 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ159.9, 133.3, 113.9, 88.2, 85.1, 82.8, 70.7, 60.2, 55.3, 31.8; ESI-MS (M+H) calcd. for $C_{13}H_{13}O_2$: 201.0916; Found: 201.0910.

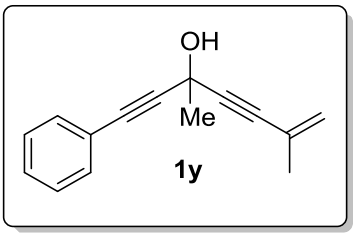
Spectral data for 3-methyl-1-phenyl-5-(thiophen-2-yl)penta-1,4-diyn-3-ol (1x)



Orange oil; (20% ethylacetate/hexane, R_f = 0.37, 878 mg, 3.48 mmol, 50%); ^{1}H NMR (700 MHz, $CDCl_3$): δ7.46 (d, *J* = 7.1Hz, 2H), 7.32~7.29 (m, 3H), 7.27 (d, *J* = 5.1Hz, 1H), 7.24 (d, *J* = 3.7Hz, 1H), 6.96 (t, *J* = 4Hz, 1H), 2.68 (s, 1H), 1.93 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ132.7, 131.8, 128.7, 128.3, 127.7, 127.0, 122.0, 122.0, 93.6, 89.7, 82.9, 76.2, 61.0, 31.8; ESI-MS (M+Na) calcd. for $C_{16}H_{12}OSNa$: 275.0507;

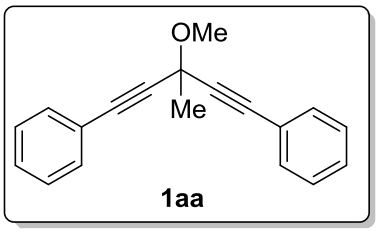
Found: 275.0501.

Spectral data for 3,6-dimethyl-1-phenylhepta-6-en-1,4-diyn-3-ol (1y)



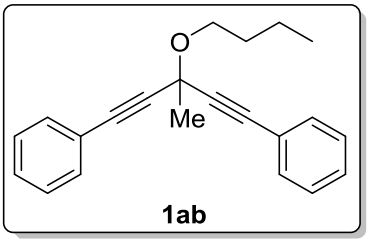
Orange oil; (20% ethylacetate/hexane, R_f = 0.37, 933 mg, 4.44 mmol, 64%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.46~7.43 (m, 2H), 7.32~7.28 (m, 3H), 5.35 (q, *J* = 1Hz, 1H), 5.27 (d, *J* = 1.5Hz, 1H), 2.61 (s, 1H), 1.90 (t, *J* = 1.4Hz, 3H), 1.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ131.8, 128.6, 128.2, 125.9, 123.0, 122.1, 90.1, 89.0, 83.8, 82.5, 60.7, 31.9, 23.2; ESI-MS (M+Na) calcd. for $C_{17}H_{20}O_2Na$: 279.1361; Found: 279.1356.

Spectral data for (3-methoxy-3-methylpenta-1,4-diyne-1,5-diyl)dibenzene (1aa)



White solid, mp: 88.8~90.8℃; (10% ethylacetate/hexane, R_f = 0.53, 210 mg, 0.81 mmol, 66%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.48~7.47 (m, 4H), 7.32~7.30 (m, 6H), 3.60 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ131.9, 128.6, 128.3, 122.2, 87.7, 84.1, 67.4, 53.4, 30.8; ESI-MS (M+H) calcd. for $C_{19}H_{17}O$: 260.1279; Found: 261.1283.

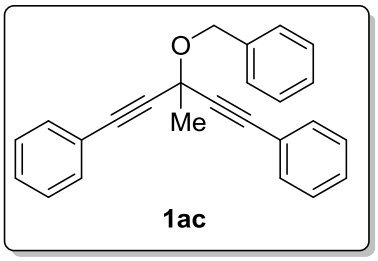
Spectral data for (3-butoxy-3-methylpenta-1,4-diyne-1,5-diyl)dibenzene (1ab)



White sticky solid; (10% ethylacetate/hexane, R_f = 0.60, 356 mg, 1.18 mmol, 58%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.48~7.46 (m, 4H), 7.32~7.29 (m, 6H), 3.85 (t, *J* =

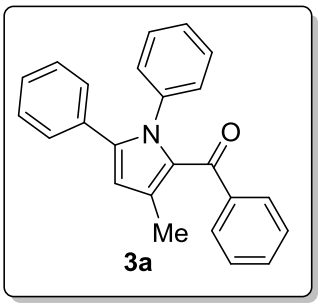
6.6Hz, 2H), 1.91 (s, 3H), 1.67~1.62 (m, 2H), 1.48~1.42 (m, 2H), 0.94 (t, *J* = 7.44Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ131.8, 128.5, 128.2, 122.4, 88.6, 83.6, 66.5, 65.8, 31.9, 31.1, 19.4, 13.9; ESI-MS (M+Na) calcd. for $C_{22}H_{22}ONa$: 325.1568; Found: 325.1563.

Spectral data for (3-(benzyloxy)-3-methylpenta-1,4-diyne-1,5-diyl)dibenzene (1ac)



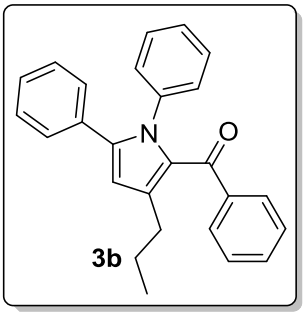
White solid, mp: 105.9~107.4℃; (10% ethylacetate/hexane, R_f = 0.53, 417 mg, 1.24 mmol, 61%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.51~7.49 (m, 4H), 7.46~7.45 (m, 2H), 7.37~7.27 (m, 9H), 4.94 (s, 2H), 2.00 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ138.3, 131.9, 128.6, 128.3, 128.1, 127.6, 122.2, 88.2, 84.2, 68.4, 66.9, 31.1; EI-MS (M) calcd. for $C_{25}H_{20}O$: 336.1514; Found: 336.1510.

Spectral data for (3-methyl-1,5-diphenyl-1*H*-pyrrol-2-yl)(phenyl)methanone (3a)



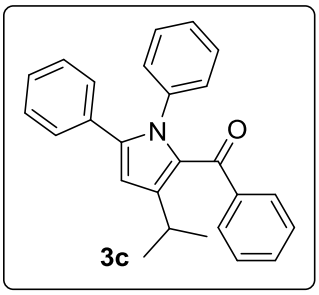
Yellow solid, mp: 142.6~143.1℃; (20% ethylacetate/hexane, R_f = 0.41, 53 mg, 0.157 mmol, 78%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.73 (d, *J* = 7.8Hz, 2H), 7.46 (t, *J* = 7.8Hz, 1H), 7.37 (t, *J* = 7.8Hz, 2H), 7.20~7.17 (m, 6H), 7.11~7.07 (m, 4H), 6.29 (s, 1H), 1.98 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.8, 140.2, 139.8, 139.2, 131.9, 131.9, 131.7, 129.3, 128.8, 128.8, 128.5, 128.2, 128.1, 128.0, 127.3, 113.0, 13.7; ESI-MS (M+H) calcd. for $C_{24}H_{20}NO$: 338.1545; Found: 338.1539.

Spectral data for (1,5-diphenyl-3-propyl-1*H*-pyrrol-2-yl)(phenyl)methanone (3b)



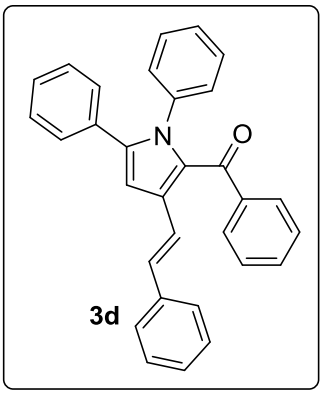
Red oil; (20% ethylacetate/hexane, R_f = 0.43, 36.6 mg, 0.100 mmol, 55%); ^{1}H NMR (600 MHz, $CDCl_3$): δ6.69 (d, *J* = 7.8Hz, 2H), 7.45~7.42 (m, 1H), 7.33 (t, *J* = 7.8Hz, 2H), 7.18~7.15 (m, 6H), 7.08~7.07 (m, 4H), 6.33 (s, 1H), 2.30 (t, *J* = 7.8Hz, 2H), 1.57~1.51 (m, 2H), 0.79 (t, *J* = 7.8Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ188.4, 140.3, 139.4, 139.1, 133.7, 132.1, 132.0, 131.5, 129.3, 128.8, 128.5, 128.1, 128.1, 128.0, 127.2, 111.5, 29.3, 24.2, 14.0; ESI-MS (M+Na) calcd. for $C_{26}H_{23}NONa$: 388.1677; Found: 388.1672.

Spectral data for (3-isopropyl-1,5-diphenyl-1*H*-pyrrol-2-yl)(phenyl)methanone (3c)



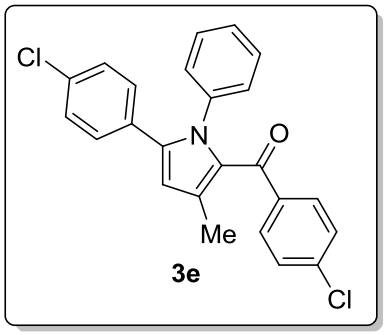
Red oil; (20% ethylacetate/hexane, R_f = 0.44, 32.0 mg, 0.087 mmol, 48%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.71 (dd, J = 8.0Hz & 1.0Hz, 2H), 7.44 (td, J = 6.7Hz & 1.2Hz, 1H), 7.33 (t, J = 7.8Hz, 2H), 7.19~7.13 (m, 6H), 7.10~7.06 (m, 4H), 6.39 (s, 1H), 2.81~2.71 (m, 1H), 1.17 (s, 3H), 1.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ188.7, 140.3, 140.0, 139.2, 139.0, 132.2, 132.1, 130.5, 129.3, 128.7, 128.5, 128.1, 128.0, 128.0, 127.2, 127.1, 108.6, 25.6, 24.4; ESI-MS (M+H) calcd. for $C_{26}H_{23}NONa$: 366.1858; Found: 366.1872.

Spectral data for (*E*)-(1,5-diphenyl-3-styryl-1*H*-pyrrol-2-yl)(phenyl)methanone (3d)



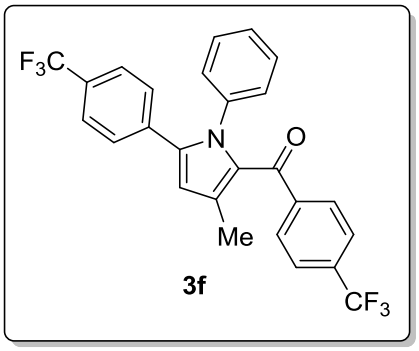
Orange oil; (20% ethylacetate/hexane, R_f = 0.41, 46.4 mg, 0.109 mmol, 73%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.78 (dd, J = 7.6Hz & 0.6Hz, 2H), 7.50 (t, J = 7.4Hz, 1H), 7.39 (t, J = 7.7Hz, 2H), 7.25~7.19 (m, 8H), 7.18~7.11 (m, 7H), 6.95 (d, J = 16.2Hz, 1H), 6.78 (s, 1H), 6.76 (d, J = 16.5Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ187.5, 140.5, 140.0, 138.7, 137.4, 132.3, 131.7, 131.6, 129.9, 129.8, 128.9, 128.6, 128.5, 128.2, 128.0, 127.6, 127.5, 127.2, 126.1, 121.1, 118.5, 115.0, 107.5; ESI-MS (M+H) calcd. for $C_{26}H_{23}NONa$: 426.1858; Found: 426.1859.

Spectral data for (4-chlorophenyl)(5-(4-chlorophenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl)methanone (3e)



Orange sticky solid; (20% ethylacetate/hexane, R_f = 0.47, 26.4 mg, 0.065 mmol, 41%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.65 (dd, *J* = 6.6Hz & 1.8Hz, 2H), 7.35~7.33 (m, 2H), 7.23~7.21 (m, 3H), 7.14 (d, *J* = 6.6Hz, 2H), 7.07~7.06 (m, 2H), 6.98 (d, *J* = 6.6Hz, 2H), 6.27 (s, 1H), 1.99 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ186.4, 138.8, 138.7, 138.4, 133.5, 131.6, 130.7, 130.2, 129.9, 128.8, 128.8, 128.6, 128.3, 128.1, 127.7, 113.3, 13.7; ESI-MS (M+H) calcd. for $C_{24}H_{18}C_{l2}NO$: 406.0765; Found: 406.0760.

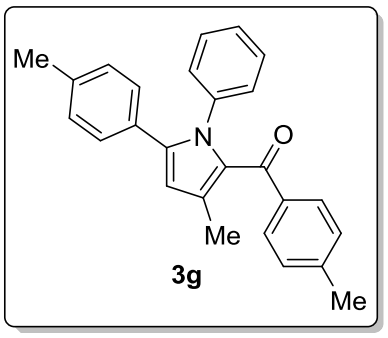
Spectral data for (3-methyl-1-phenyl-5-(4-(trifluoromethyl)phenyl)-1*H*-pyrrol-2-yl)(4-(trifluoromethyl)phenyl)methanone (3f)



3f

Yellow oil; (20% ethylacetate/hexane, R_f = 0.40, 13.6 mg, 0.029 mmol, 22%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.78 (d, *J* = 8Hz, 2H), 7.61 (d, *J* = 8.4Hz, 2H), 7.43 (d, *J* = 8.4Hz, 2H), 7.23~7.22 (m, 3H), 7.17 (d, *J* = 8Hz, 2H), 7.09~7.07 (m, 2H), 6.37 (s, 1H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ186.5, 143.0, 138.6, 138.5, 135.2, 131.9, 129.6, 129.4, 128.9, 128.8, 128.1, 128.0, 125.3, 125.3, 125.1, 125.1, 114.1, 13.8; ESI-MS (M+H) calcd. for $C_{26}H_{18}F_6NO$: 474.1293; Found: 474.1287.

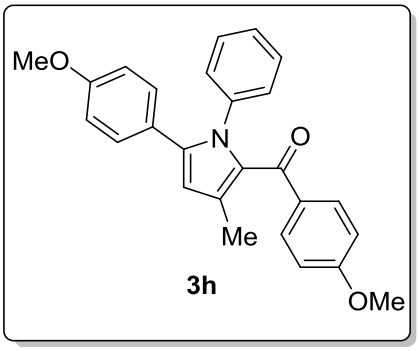
Spectral data for (3-methyl-1-phenyl-5-(*p*-tolyl)-1*H*-pyrrol-2-yl)(*p*-tolyl) methanone (3g)



3g

Yellow oil; (20% ethylacetate/hexane, R_f = 0.38, 38.6 mg, 0.106 mmol, 58%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.65 (d, *J* = 8Hz, 2H), 7.20~7.16 (m, 5H), 7.11~7.09 (m, 2H), 6.99~6.94 (m, 4H), 6.23 (s, 1H), 2.37 (s, 3H), 2.26 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ187.5, 142.6, 139.7, 139.4, 137.6, 137.1, 131.7, 129.6, 129.1, 128.9, 128.7, 128.6, 128.5, 128.2, 128.2, 127.2, 112.6, 21.6, 21.1, 13.7; ESI-MS (M+H) calcd. for $C_{26}H_{24}NO$: 366.1858; Found: 366.1852.

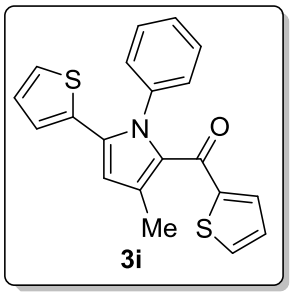
Spectral data for (4-methoxyphenyl)(5-(4-methoxyphenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl)methanone (3h)



3h

Orange sticky solid; (40% ethylacetate/hexane, R_f = 0.28, 59 mg, 0.148 mmol, 91%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.76~7.73 (m, 2H), 7.23~7.18 (m, 3H), 7.11~7.09 (m, 2H), 7.01~6.98 (m, 2H), 6.88~6.85 (m, 2H), 6.72~6.70 (m, 2H), 6.20 (s, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ186.6, 162.9, 158.8, 139.4, 139.3, 133.0, 131.7, 131.5, 130.0, 128.5, 128.1, 127.7, 127.2, 124.6, 113.5, 113.4, 112.2, 55.4, 55.1, 13.6; ESI-MS (M+H) calcd. for $C_{26}H_{24}NO_3$: 398.1756; Found: 398.1751.

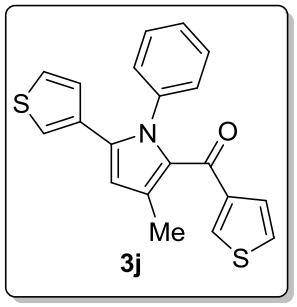
Spectral data for (3-methyl-1-phenyl-5-(thiophen-2-yl)-1*H*-pyrrol-2-yl) (thiophen-2-yl)methanone (3i)



3i

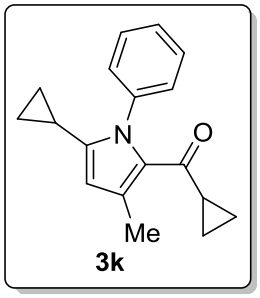
Yellow oil; (20% ethylacetate/hexane, R_f = 0.38, 33.1 mg, 0.095 mmol, 49%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.57 (d, *J* = 4.2Hz, 2H), 7.32~7.29 (m, 3H), 7.26~7.24 (m, 2H), 7.11 (dd, *J* = 5.4Hz & 1.2Hz, 1H), 7.05 (t, *J* = 4.2Hz, 1H), 6.82 (dd, *J* = 5.4Hz & 3.6Hz, 1H), 6.58 (dd, *J* = 3.6Hz & 1.2Hz, 1H), 6.39 (s, 1H), 2.13 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ179.1, 145.6, 138.7, 133.5, 133.3, 133.1, 132.2, 128.9, 128.7, 128.3, 127.5, 127.2, 127.0, 125.8, 125.5, 112.6, 29.7, 13.6; ESI-MS (M+H) calcd. for $C_{20}H_{16}NOS_2$: 350.0673; Found: 350.0668.

Spectral data for (3-methyl-1-phenyl-5-(thiophen-3-yl)-1*H*-pyrrol-2-yl) (thiophen-3-yl)methanone (3j)



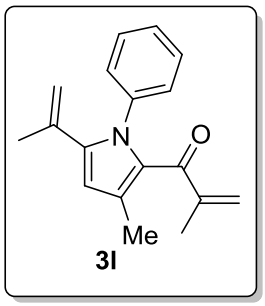
Red sticky solid; (20% ethylacetate/hexane, R_f = 0.27, 46.7 mg, 0.134 mmol, 69%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.82 (d, *J* = 3Hz, 1H), 7.36 (d, *J* = 5.4Hz, 1H), 7.30~7.29 (m, 3H), 7.24~7.23 (m, 1H), 7.21~7.19 (m, 2H), 7.14~7.13 (m, 1H), 6.82 (d, *J* = 4.8Hz, 1H), 6.64 (t, *J* = 1.8Hz, 1H), 6.32 (s, 1H), 2.07 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ181.0, 143.9, 139.4, 135.1, 132.2, 128.7, 128.3, 127.9, 127.8, 127.6, 125.8, 124.9, 122.2, 112.3, 13.6; ESI-MS (M+H) calcd. for $C_{20}H_{16}NOS_2$: 350.0673; Found: 350.0668.

Spectral data for cyclopropyl(5-cyclopropyl-3-methyl-1-phenyl-1*H*-pyrrol-2-yl)methanone (3k)



Yellow oil; (20% ethylacetate/hexane, R_f = 0.33, 23.6 mg, 0.089 mmol, 31%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.43~7.38 (m, 2H), 7.36~7.32 (m, 1H), 7.28~7.25 (m, 2H), 5.70 (s, 1H), 2.39 (s, 3H), 1.91~1.85 (m, 1H), 1.41~1.35 (m, 1H), 0.97~0.94 (m, 2H), 0.75~0.70 (m, 2H), 0.63~0.58 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ190.5, 143.0, 140.3, 131.8, 129.1, 128.7, 127.9, 127.5, 107.8, 20.3, 14.5, 10.1, 8.0, 7.9; ESI-MS (M+H) calcd. for $C_{18}H_{20}NO$: 266.1545; Found: 266.1539.

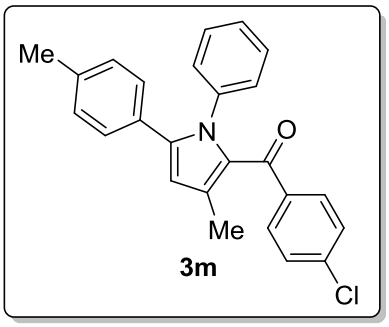
Spectral data for 2-methyl-1-(3-methyl-1-phenyl-5-(prop-1-en-2-yl)-1*H*-pyrrol-2-yl)prop-2-en-1-one (3l)



3l

Orange oil; (20% ethylacetate/hexane, R_f = 0.46, 25.1 mg, 0.095 mmol, 33%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.34~7.29 (m, 3H), 7.16~7.14 (m, 2H), 6.09 (s, 1H), 5.58~5.57 (m, 2H), 4.90 (t, *J* = 1.8Hz, 1H), 4.67 (d, *J* = 0.6Hz, 1H), 2.17 (s, 3H), 1.81 (t, *J* = 1.2Hz, 3H), 1.72 (d, *J* = 0.6Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ190.0, 146.2, 140.1, 139.8, 135.2, 131.5, 128.6, 127.7, 127.5, 127.0, 124.7, 116.4, 112.0, 22.8, 17.6, 13.4; ESI-MS (M+H) calcd. for $C_{18}H_{20}NO$: 266.1545; Found: 266.1539.

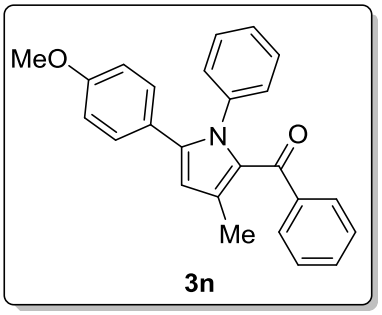
Spectral data for (4-chlorophenyl)(3-methyl-1-phenyl-5-(*p*-tolyl)-1*H*-pyrrol-2-yl)methanone (3m)



3m

Yellow oil; (20% ethylacetate/hexane, R_f = 0.39, 43.9 mg, 0.114 mmol, 67%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.65 (d, *J* = 8.4Hz, 2H), 7.33 (d, *J* = 8.4Hz, 2H), 7.21~7.20 (m, 3H), 7.09~7.07 (m, 2H), 6.97 (d, *J* = 8Hz, 2H), 6.95 (d, *J* = 8Hz, 2H), 6.25 (s, 1H), 2.26 (s, 3H), 1.98 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ186.2, 140.4, 139.2, 138.7, 138.1, 137.3, 130.7, 129.9, 128.8, 128.6, 128.5, 128.5, 128.3, 128.2, 128.1, 127.4, 113.0, 21.1, 13.8; FI-MS (M) calcd. for $C_{25}H_{20}ClNO$: 385.1223; Found: 385.1228.

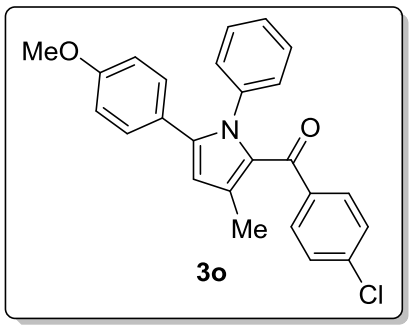
Spectral data for (5-(4-methoxyphenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl) (phenyl)methanone (3n)



3n

Yellow oil; (20% ethylacetate/hexane, R_f = 0.34, 47.2 mg, 0.128 mmol, 71%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.73~7.71 (m, 2H), 7.47~7.43 (m, 1H), 7.38~7.34 (m, 2H), 7.21~7.18 (m, 3H), 7.13~7.10 (m, 2H), 7.02~6.98 (m, 2H), 6.73~6.70 (m, 2H), 6.22 (s, 1H), 3.74 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ187.6, 158.9, 140.4, 139.9, 139.3, 131.8, 131.4, 130.0, 129.3, 129.0, 128.5, 128.2, 128.1, 127.2, 124.3, 113.5, 112.5, 55.1, 13.7; ESI-MS (M+Na) calcd. for $C_{25}H_{21}NO_2Na$: 390.1470; Found: 390.1464.

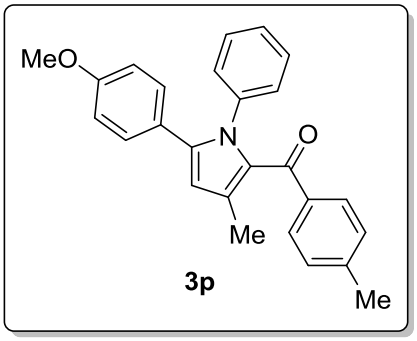
Spectral data for (4-chlorophenyl)(5-(4-methoxyphenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl)methanone (3o)



3o

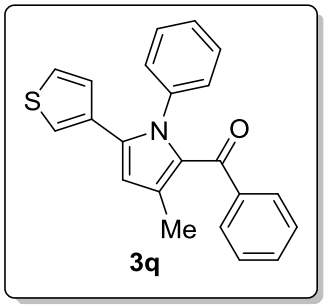
Yellow oil; (20% ethylacetate/hexane, R_f = 0.33, 40.1 mg, 0.100 mmol, 62%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.65~7.63 (m, 2H), 7.34~7.32 (m, 2H), 7.22~7.20 (m, 3H), 7.09~7.07 (m, 2H), 7.00~6.97 (m, 2H), 6.72~6.69 (m, 2H), 6.22 (s, 1H), 3.74 (s, 3H), 1.98 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ186.1, 159.0, 140.3, 139.2, 138.7, 138.1, 131.1, 130.7, 130.0, 129.3, 128.6, 128.5, 128.2, 127.4, 124.2, 113.6, 112.7, 55.2, 13.9; ESI-MS (M+H) calcd. for $C_{25}H_{21}ClNO_2$: 402.1261; Found: 402.1255.

Spectral data for (5-(4-methoxyphenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl)(*p*-tolyl)methanone (3p)



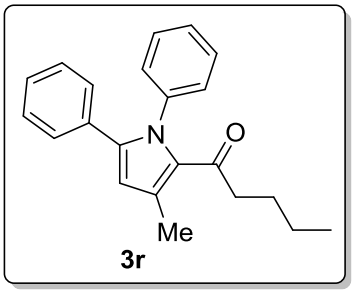
Yellow oil; (20% ethylacetate/hexane, R_f = 0.26, 43.4 mg, 0.114 mmol, 66%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.65 (d, *J* = 8Hz, 2H), 7.23~7.16 (m, 5H), 7.11~7.09 (m, 2H), 7.01~6.98 (m, 2H), 6.72~6.69 (m, 2H), 6.20 (s, 1H), 3.74 (s, 3H), 2.37 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ187.4, 158.9, 142.6, 139.6, 139.4, 137.7, 131.6, 130.0, 129.6, 128.9, 128.5, 128.3, 128.2, 127.2, 124.5, 113.5, 112.4, 55.1, 21.6, 13.7; ESI-MS (M+H) calcd. for $C_{26}H_{24}NO_2$: 382.1807; Found: 382.1802.

Spectral data for (3-methyl-1-phenyl-5-(thiophen-3-yl)-1*H*-pyrrol-2-yl)(phenyl) methanone (3q)



Orange oil; (20% ethylacetate/hexane, R_f = 0.46, 42.9 mg, 0.125 mmol, 63%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.70~7.69 (m, 2H), 7.47~7.44 (m, 1H), 7.38~7.30 (m, 2H), 7.30~7.28 (m, 3H), 7.21~7.20 (m, 2H), 7.14~7.13 (m, 1H), 6.83 (dd, *J* = 5.4Hz & 1.2Hz, 1H), 6.65 (dd, *J* = 3.0Hz & 1.2Hz, 1H), 6.32 (s, 1H), 1.94 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.4, 140.4, 139.5, 135.5, 132.2, 131.9, 129.2, 128.8, 128.7, 128.4, 128.2, 128.0, 127.9, 127.6, 124.9, 122.2, 112.4, 13.7; ESI-MS (M+H) calcd. for $C_{22}H_{18}NOS$: 344.1109; Found: 344.1104.

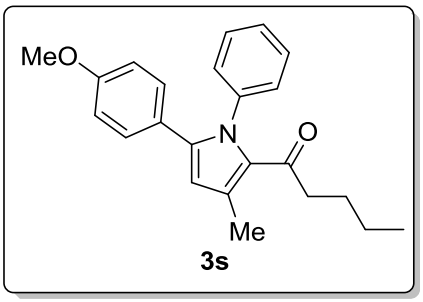
Spectral data for 1-(3-methyl-1,5-diphenyl-1*H*-pyrrol-2-yl)pentan-1-one (3r)



3r

White solid, mp: 106.5~107.0℃; (20% ethylacetate/hexane, R_f = 0.46, 35.8 mg, 0.113 mmol, 51%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.29~7.28 (m, 3H), 7.15~7.10 (m, 5H), 7.02~7.00 (m, 2H), 6.24 (s, 1H), 2.44 (s, 3H), 2.42 (t, *J* = 7.2Hz, 2H), 1.53~1.48 (m, 2H), 1.26~1.17 (m, 2H), 0.81 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ192.2, 140.1, 139.6, 132.2, 131.9, 128.9, 128.7, 128.6, 128.4, 127.9, 127.7, 127.3, 113.6, 41.7, 26.6, 22.4, 14.9, 13.9; ESI-MS (M+H) calcd. for $C_{22}H_{24}NO$: 318.1858; Found: 318.1852.

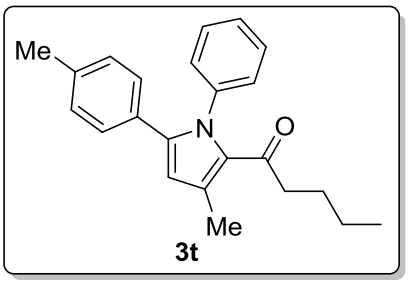
Spectral data for 1-(5-(4-methoxyphenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl) pentan-1-one (3s)



3s

Yellow oil; (20% ethylacetate/hexane, R_f = 0.36, 31.9 mg, 0.092 mmol, 47%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.30~7.28 (m, 3H), 7.11~7.10 (m, 2H), 6.94 (dt, *J* = 9.6Hz & 3Hz, 2H), 6.68~6.66 (m, 2H), 6.18 (s, 1H), 3.72 (s, 3H), 2.44 (s, 3H), 2.42 (t, *J* = 7.2Hz, 2H), 1.54~1.49 (m, 2H), 1.25~1.20 (m, 2H), 0.82 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ191.9, 158.9, 140.3, 139.7, 131.9, 130.2, 128.8, 128.6, 128.5, 127.6, 124.4, 113.4, 113.1, 55.1, 41.6, 26.6, 22.4, 15.0, 13.9; ESI-MS (M+H) calcd. for $C_{23}H_{26}NO_2$: 348.1964; Found: 348.1958.

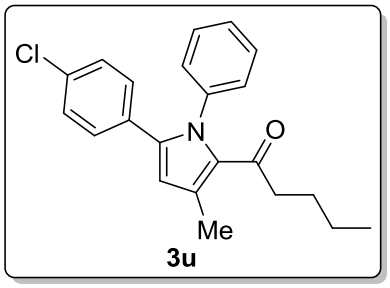
Spectral data for 1-(3-methyl-1-phenyl-5-(*p*-tolyl)-1*H*-pyrrol-2-yl)pentan-1-one (3t)



3t

Orange sticky solid; (20% ethylacetate/hexane, R_f = 0.36, 43.4 mg, 0.131 mmol, 63%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.30~7.29 (m, 3H), 7.12~7.11 (m, 2H), 6.95~6.94 (m, 2H), 6.90 (dd, *J* = 6.6Hz & 2.4Hz, 2H), 6.21 (s, 1H), 2.44 (s, 3H), 2.42 (t, *J* = 7.2Hz, 2H), 2.24 (s, 3H), 1.54~1.49 (m, 2H), 1.25~1.20 (m, 2H), 0.82 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ192.1, 140.3, 139.8, 137.2, 132.0, 129.0, 128.8, 128.7, 128.5, 128.4, 127.6, 113.3, 41.6, 26.6, 22.4, 21.1, 14.9, 13.9; ESI-MS (M+H) calcd. for $C_{23}H_{26}NO$: 332.2014; Found: 332.2009.

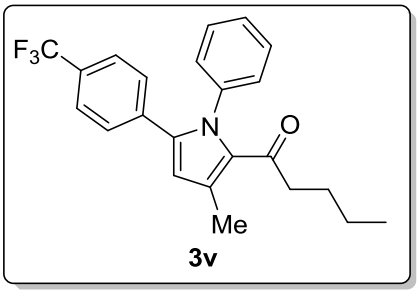
Spectral data for 1-(5-(4-chlorophenyl)-3-methyl-1-phenyl-1*H*-pyrrol-2-yl) pentan-1-one (3u)



3u

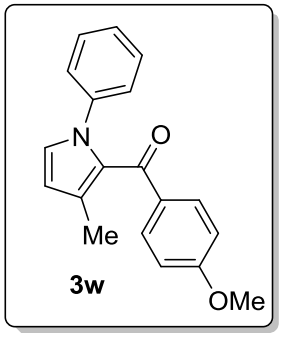
Yellow solid, mp: 142.4~145.0℃; (10% ethylacetate/hexane, R_f = 0.44, 21.6 mg, 0.061 mmol, 32%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.31 (s, 3H), 7.26 (d, *J* = 7.5Hz, 1H), 7.11~7.10 (m, 3H), 6.93 (d, *J* = 7.4Hz, 1H), 6.86 (d, *J* = 7.4Hz, 1H), 6.23 (s, 1H), 2.43~2.41 (m, 5H), 1.54~1.48 (m, 2H), 1.24~1.19 (m, 2H), 0.81 (t, *J* = 7.3Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ192.2, 139.9, 138.2, 131.1, 130.4, 130.3, 130.0, 128.7, 128.6, 128.3, 128.2, 127.9, 113.7, 41.7, 26.5, 22.4, 14.9, 13.8; ESI-MS (M+H) calcd. for $C_{22}H_{23}ClNO$: 352.1468; Found: 352.1464.

Spectral data for 1-(3-methyl-1-phenyl-5-(4-(trifluoromethyl)phenyl)-1*H*-pyrrol -2-yl)pentan-1-one (3v)



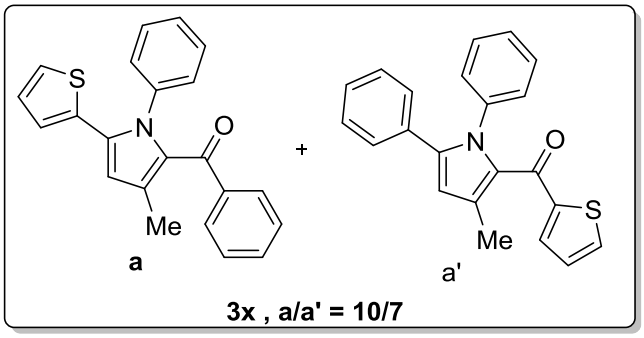
Yellow oil; (10% ethylacetate/hexane, R_f = 0.44, 7.9 mg, 0.020 mmol, 12%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.38 (d, *J* = 8.4Hz, 2H), 7.33~7.32 (m, 3H), 7.12~7.10 (m, 4H), 6.30 (s, 1H), 2.44~2.41 (m, 5H), 1.55~1.49 (m, 2H), 1.25~1.19 (m, 2H), 0.82 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ192.5, 139.8, 137.6, 135.5, 132.9, 128.9, 128.3, 128.1, 124.9, 124.9, 114.3, 41.8, 26.5, 22.4, 14.8, 13.8; ESI-MS (M+H) calcd. for $C_{23}H_{23}F_3NO$: 386.1732; Found: 386.1726.

Spectral data for (4-methoxyphenyl)(3-methyl-1-phenyl-1*H*-pyrrol-2-yl) methanone (3w)



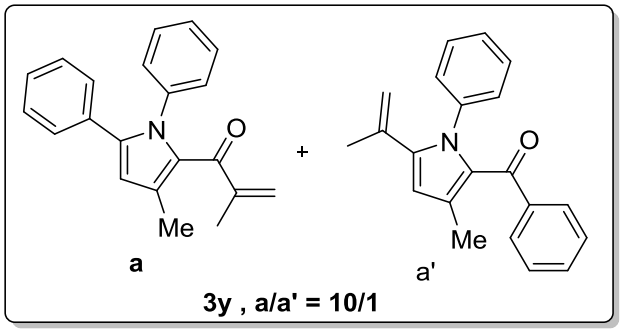
Orange sticky solid; (20% ethylacetate/hexane, R_f = 0.29, 67.7 mg, 0.232 mmol, 93%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.74~7.70 (m, 2H), 7.29~7.25 (m, 2H), 7.19~7.15 (m, 3H), 6.95 (d, *J* = 2.8Hz, 1H), 6.86~6.82 (m, 2H), 6.17 (d, *J* = 2.4Hz, 1H), 3.82 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ186.8, 162.9, 140.7, 132.4, 131.8, 129.7, 128.9, 127.4, 126.6, 124.6, 113.5, 112.0, 55.4, 13.5; ESI-MS (M+H) calcd. for $C_{19}H_{18}NO_2$: 292.1338; Found: 292.1332.

Spectral data for (3-methyl-1-phenyl-5-(thiophen-2-yl)-1*H*-pyrrol-2-yl)(phenyl) methanone and (3-methyl-1,5-diphenyl-1*H*-pyrrol-2-yl)(thiophen-2-yl) methanone (3x)



Orange oil; (20% ethylacetate/hexane, R_f = 0.45, 34.7 mg, 0.101 mmol, 51%); ^{1}H NMR (600 MHz, $CDCl_3$) major isomer: δ7.70 (dd, J = 7.9Hz & 0.9Hz, 2H), 7.48~7.45 (m, 1H), 7.37 (t, J = 7.9Hz, 2H), 7.33~7.30 (m, 3H), 7.27~7.24 (m, 2H), 7.04 (t, J = 4.5Hz, 1H), 6.83 (dd, J = 5.1Hz & 3.7Hz, 1H), 6.60 (dd, J = 3.7Hz & 1.1Hz, 1H), 6.39 (s, 1H), 1.93 (s, 3H); ^{1}H NMR (600 MHz, $CDCl_3$) minor isomer: δ7.57~7.56 (m, 2H), 7.21~7.19 (m, 3H), 7.18~7.16 (m, 2H), 7.12~7.10 (m, 4H), 7.08~7.07 (m, 2H), 6.30 (s, 1H), 2.17 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) major isomer: δ187.3, 140.3, 139.0, 133.9, 133.6, 133.1, 132.0, 131.9, 129.2, 128.9, 128.7, 128.7, 128.2, 127.2, 127.0, 125.6, 112.7, 13.7; ^{13}C NMR (150 MHz, $CDCl_3$) minor isomer: δ 179.7, 145.7, 139.2, 139.0, 133.5, 132.2, 131.8, 128.6, 128.3, 128.0, 128.0, 127.5, 127.4, 125.9, 112.9, 13.5, (remaining peaks merging with major isomer); ESI-MS (M+H) calcd. for $C_{22}H_{18}NOS$: 344.1109; Found: 344.1104.

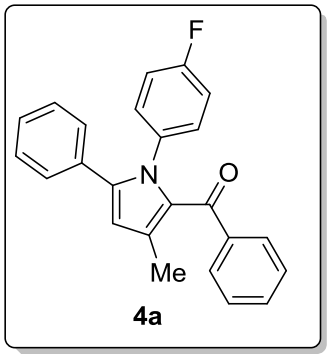
Spectral data for 2-methyl-1-(3-methyl-1,5-diphenyl-1*H*-pyrrol-2-yl)prop-2-en-1-one and (3-methyl-1-phenyl-5-(prop-1-en-2-yl)-1*H*-pyrrol-2-yl)(phenyl) methanone (3y)



Orange oil; (10% ethylacetate/hexane, R_f = 0.24, 52.3 mg, 0.174 mmol, 73%); ^{1}H NMR (600 MHz, $CDCl_3$) major isomer: δ7.25~7.24 (m, 3H), 7.17~7.15 (m, 3H), 7.06~7.03 (m, 4H), 6.25 (s, 1H), 5.63~5.61 (m, 2H), 2.25 (s, 3H), 1.85 (s, 3H); ^{1}H NMR (600 MHz, $CDCl_3$) minor isomer: δ7.69 (d, *J* = 8.2Hz, 2H), 7.46~7.44 (m, 1H), 7.35 (t, *J* = 7.8Hz, 2H), 6.14 (s, 1H), 4.95~4.73 (m, 2H), 1.90 (s, 3H), 1.76 (s, 3H), (remaining peaks merging with major isomer); ^{13}C NMR (150 MHz, $CDCl_3$) major

isomer: δ190.1, 146.1, 139.5, 138.7, 132.0, 128.7, 128.6, 128.5, 127.9, 127.8, 127.7, 127.2, 127.1, 124.8, 112.8, 17.6, 13.5; ^{13}C NMR (150 MHz, $CDCl_3$) minor isomer: δ131.9, 131.4, 129.2, 128.1, 116.7, 112.2, (remaining peaks merging with major isomer); ESI-MS (M+H) calcd. for $C_{21}H_{20}NO$: 302.1545; Found: 302.1539.

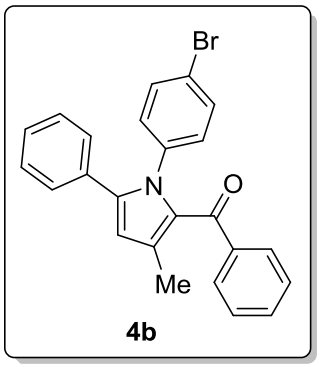
Spectral data for (1-(4-fluorophenyl)-3-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl) methanone (4a)



4a

White solid, mp: 164.0~165.9℃; (20% ethylacetate/hexane, R_f = 0.48, 42.6 mg, 0.120 mmol, 59%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.73~7.71 (m, 2H), 7.50~7.46 (m, 1H), 7.4~7.36 (m, 2H), 7.20~7.18 (m, 3H), 7.10~7.06 (m, 4H), 6.91~6.87 (m, 2H), 6.27 (s, 1H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ187.7, 140.2, 140.2, 132.1, 131.8, 131.6, 129.8, 129.7, 129.3, 129.0, 128.8, 128.3, 128.1, 127.5, 115.5, 115.4, 113.1, 13.8; ESI-MS (M+H) calcd. for $C_{24}H_{19}FNO$: 356.1451; Found: 356.1445.

Spectral data for (1-(4-bromophenyl)-3-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl) methanone (4b)

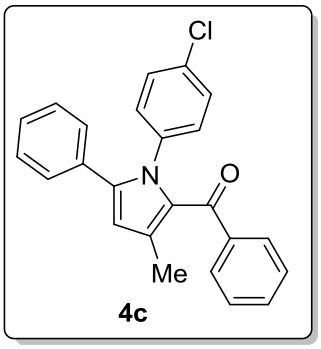


4b

Orange oil; (20% ethylacetate/hexane, R_f = 0.50, 75.2 mg, 0.181 mmol, 89%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.75~7.73 (m, 2H), 7.51~7.48 (m, 1H), 7.41~7.39 (m, 2H), 7.33 (dt, *J* = 9.6Hz & 3Hz, 2H), 7.22~7.20 (m, 3H), 7.10~7.08 (m, 2H), 6.99 (dt, *J* = 9.6Hz & 3Hz, 2), 6.28 (s, 1H), 1.95 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.6, 140.1, 138.3, 132.1, 131.7, 131.6, 131.5, 129.7, 129.3, 129.2, 128.8, 128.3, 128.2,

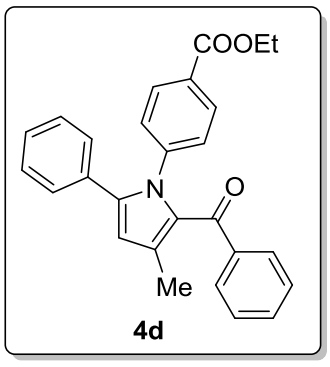
127.6, 121.2, 13.8; ESI-MS (M+H) calcd. for $C_{24}H_{19}BrNO$: 416.0650; Found: 416.0645.

Spectral data for (1-(4-chlorophenyl)-3-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl) methanone (4c)



White solid, mp: 146.2~147.3℃; (20% ethylacetate/hexane, R_f = 0.38, 55.9 mg, 0.150 mmol, 74%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.75~7.73 (m, 2H), 7.51~7.48 (m, 1H), 7.41~7.39 (m, 2H), 7.22~7.19 (m, 3H), 7.18 (dt, *J* = 8.3Hz & 2.9Hz, 2H), 7.09~7.07 (m, 2H), 7.05 (dt, *J* = 8.3Hz & 2.9Hz, 2H), 6.27 (s, 1H), 1.95 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.6, 140.1, 140.1, 137.8, 133.1, 132.2, 131.6, 131.5, 129.3, 129.3, 128.8, 128.7, 128.3, 128.2, 127.6, 113.3, 13.8; ESI-MS (M+H) calcd. for $C_{24}H_{19}ClNO$: 372.1155; Found: 372.1150.

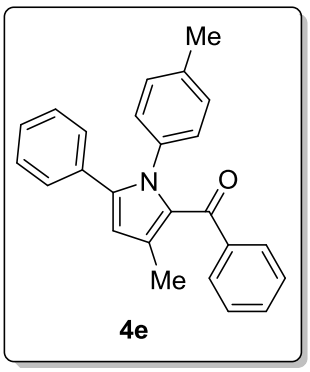
Spectral data for ethyl 4-(2-benzoyl-3-methyl-5-phenyl-1*H*-pyrrol-1-yl)benzoate (4d)



Yellow oil; (20% ethylacetate/hexane, R_f = 0.42, 75.6 mg, 0.185 mmol, 91%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.89 (dt, *J* = 9Hz & 2.4Hz, 2H), 7.75~7.74 (m, 2H), 7.50~7.47 (m, 1H), 7.40~7.38 (m, 2H), 7.20~7.17 (m, 3H), 7.15 (dt, *J* = 9Hz & 2.4Hz, 2H), 7.06~7.05 (m, 2H), 6.28 (s, 1H), 4.31 (q, *J* = 7.2Hz, 2H), 1.96 (s, 3H), 1.33 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.6, 165.9, 143.2, 140.0, 139.9, 132.2,

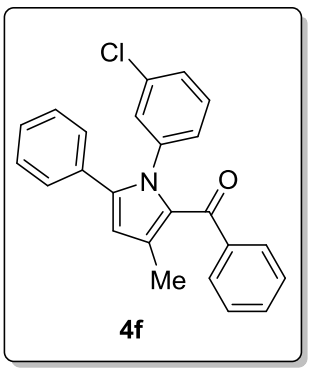
131.5, 130.0, 129.3, 129.2, 128.8, 128.3, 128.2, 127.9, 127.6, 113.6, 61.0, 14.3, 13.7; ESI-MS (M+H) calcd. for $C_{27}H_{24}NO_3$: 410.1756; Found: 410.1751.

Spectral data for (3-methyl-5-phenyl-1-(*p*-tolyl)-1*H*-pyrrol-2-yl)(phenyl) methanone (4e)



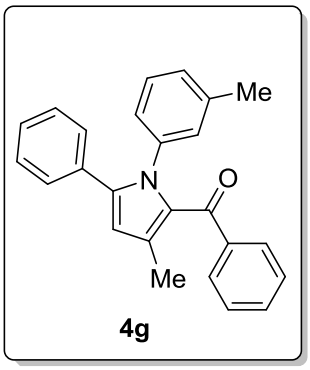
Orange oil; (20% ethylacetate/hexane, R_f = 0.46, 35.0 mg, 0.100 mmol, 49%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.74~7.73 (m, 2H), 7.48~7.45 (m, 1H), 7.39~7.36 (m, 2H), 7.19~7.17 (m, 3H), 7.11~7.10 (m, 2H), 7.00 (s, 4H), 6.27 (s, 1H), 2.27 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.8, 140.3, 139.8, 137.1, 136.6, 132.0, 131.9, 131.8, 129.4, 129.2, 128.8, 128.6, 128.2, 128.0, 127.8, 127.2, 112.9, 21.1, 13.7; ESI-MS (M+H) calcd. for $C_{25}H_{22}NO$: 352.1701; Found: 352.1696.

Spectral data for (1-(3-chlorophenyl)-3-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl) methanone (4f)



Yellow oil; (20% ethylacetate/hexane, R_f = 0.35, 43 mg, 0.116 mmol, 57%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.74 (d, *J* = 7.7Hz, 2H), 7.49 (t, *J* = 7.5Hz, 1H), 7.40 (t, *J* = 6.9Hz, 2H), 7.21 (s, 3H), 7.18 (d, *J* = 8.1Hz, 1H), 7.14~7.10 (m, 4H), 7.02 (d, *J* = 7.2Hz, 1H), 6.29 (s, 1H), 1.98 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ187.5, 140.3, 140.0, 140.0, 133.9, 132.0, 131.6, 131.4, 129.3, 129.2, 128.7, 128.3, 128.2, 128.1, 127.6, 127.6, 126.5, 113.4, 13.7; ESI-MS (M+H) calcd. for $C_{24}H_{18}ClNO$: 372.1155; Found: 372.1154.

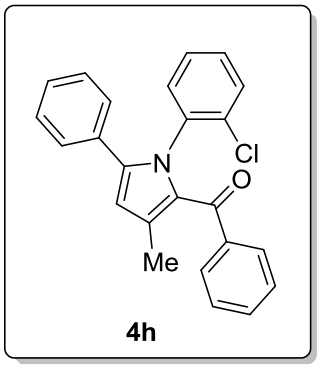
Spectral data for (3-methyl-5-phenyl-1-(*m*-tolyl)-1*H*-pyrrol-2-yl)(phenyl) methanone (4g)



4g

Orange oil; (20% ethylacetate/hexane, R_f = 0.37, 32.1 mg, 0.091 mmol, 45%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.72 (d, *J* = 7.5Hz, 2H), 7.45 (t, *J* = 7.5Hz, 1H), 7.36 (t, *J* = 7.5Hz, 2H), 7.18 (s, 3H), 7.09~7.05 (m, 3H), 6.98 (d, *J* = 7.5Hz, 1H), 6.90~6.89 (m, 2H), 6.28 (s, 1H), 2.20 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ187.9, 140.3, 139.6, 139.0, 138.3, 132.0, 131.8, 131.7, 129.2, 128.8, 128.7, 128.7, 128.2, 128.1, 128.1, 127.9, 127.2, 125.2, 113.0, 21.2, 13.7; ESI-MS (M+H) calcd. for $C_{25}H_{22}NO$: 352.1701; Found: 352.1696.

Spectral data for (1-(2-chlorophenyl)-3-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl) methanone (4h)

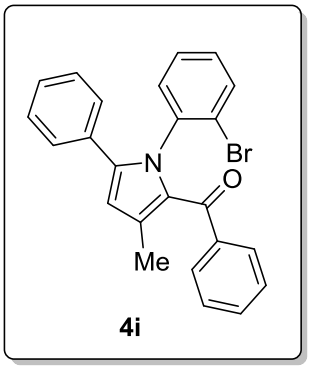


4h

Yellow solid, mp: 191.7~194.3℃; (20% ethylacetate/hexane, R_f = 0.31, 42.3 mg, 0.114 mmol, 56%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.75 (d, *J* = 7.3Hz, 2H), 7.48 (t, *J* = 7.6Hz, 1H), 7.40 (t, *J* = 6.7Hz, 2H), 7.34~7.29 (m, 2H), 7.21~7.18 (m, 5H), 7.14 (s, 2H), 6.32 (s, 1H), 1.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ187.4, 140.4, 140.0, 137.4, 132.9, 131.8, 131.5, 131.2, 129.7, 129.3, 129.1, 129.1, 128.5, 128.2, 128.1, 127.6, 126.9, 113.1, 14.0; ESI-MS (M+H) calcd. for $C_{24}H_{19}ClNO$: 372.1155; Found: 372.1150.

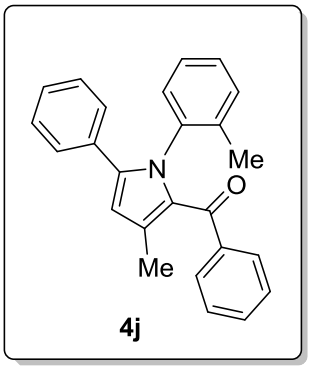
Spectral data for (1-(2-bromophenyl)-3-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl)

methanone (4i)



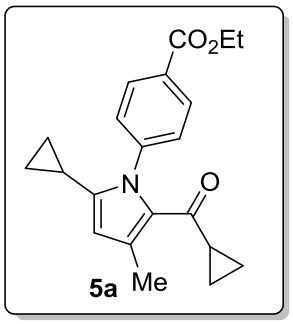
White solid, mp: 192.5~193.8℃; (20% ethylacetate/hexane, R_f = 0.34, 52.4 mg, 0.126 mmol, 62%); ^{1}H NMR (500 MHz, $CDCl_3$): δ7.84 (d, *J* = 7.5Hz, 2H), 7.56~7.52 (m, 2H), 7.46 (t, *J* = 7.9Hz, 3H), 7.31 (t, *J* = 7.5Hz, 1H), 7.25~7.18 (m, 6H), 6.38 (s, 1H), 1.98 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ187.3, 140.3, 140.0, 138.9, 132.8, 131.8, 131.6, 131.5, 131.4, 129.4, 129.4, 129.1, 128.6, 128.2, 128.1, 127.6, 127.4, 123.3, 113.1, 14.1; ESI-MS (M+H) calcd. for $C_{24}H_{19}BrNO$: 416.0650; Found: 416.0645.

Spectral data for (3-methyl-5-phenyl-1-(*o*-tolyl)-1*H*-pyrrol-2-yl)(phenyl) methanone (4j)



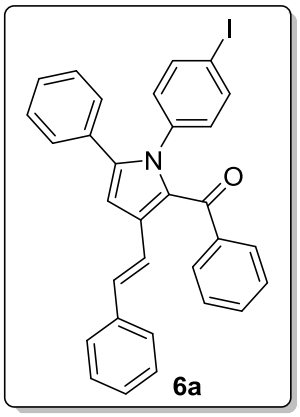
Orange oil; (20% ethylacetate/hexane, R_f = 0.37, 15.0 mg, 0.043 mmol, 21%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.72~7.70 (m, 2H), 7.47 (td, *J* = 7.9Hz & 1.1Hz, 1H), 7.38 (t, *J* = 7.4Hz, 2H), 7.23 (s, 1H), 7.17~7.14 (m, 4H), 7.12~7.09 (m, 3H), 7.07 (d, *J* = 7.5Hz, 1H), 6.32 (s, 1H), 1.94 (s, 3H), 1.93 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.3, 140.3, 138.6, 136.0, 131.9, 131.8, 130.4, 129.4, 129.3, 128.6, 128.2, 128.1, 128.1, 127.4, 126.0, 112.6, 17.7, 14.0; ESI-MS (M+H) calcd. for $C_{25}H_{22}NO$: 352.1701; Found: 352.1696.

Spectral data for ethyl 4-(2-(cyclopropanecarbonyl)-5-cyclopropyl-3-methyl-*1H*-pyrrol-1-yl)benzoate (5a)



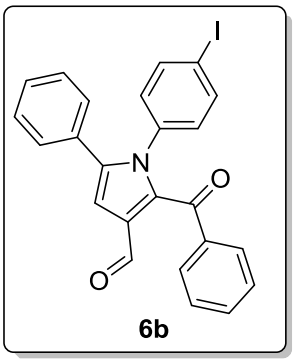
Yellow oil; (20% ethylacetate/hexane, R_f = 0.29, 62.0 mg, 0.184 mmol, 64%); ^{1}H NMR (600 MHz, $CDCl_3$): δ8.09 (dd, *J* = 8.5Hz & 0.5Hz, 2H), 7.31 (dd, *J* = =8.5Hz & 0.5Hz, 2H), 5.72 (s, 1H), 4.37 (qd, *J* = 7.1Hz & 0.7Hz, 2H), 2.41 (s, 3H), 2.02~1.98 (m, 1H), 1.38 (td, *J* = 7.1Hz & 0.7Hz, 3H), 0.99~0.96 (m, 2H), 0.74~0.67 (m, 4H), 0.62~0.59 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ190.3, 166.0, 144.5, 142.9, 131.6, 130.2, 129.4, 127.7, 108.6, 61.1, 20.2, 14.6, 14.3, 10.2, 8.0, 7.8; ESI-MS (M+H) calcd. for $C_{21}H_{24}NO_3$: 338.1756; Found: 338.1746.

Spectral data for (*E*)-(1-(4-iodophenyl)-5-phenyl-3-styryl-*1H*-pyrrol-2-yl) (phenyl)methanone (6a)



Orange oil; (20% ethylacetate/hexane, R_f = 0.33, 20.61 mg, 0.037 mmol, 25%); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.79 (d, *J* = 7.1Hz, 2H), 7.54 (d, *J* = 8.5Hz, 3H), 7.42 (t, *J* = 7.8Hz, 2H), 7.26~7.23 (m, 3H), 7.21 (d, *J* = 7.6Hz, 2H), 7.17~7.13 (m, 3H), 7.11~7.09 (m, 2H), 6.92 (d, *J* = 16.2Hz, 1H), 6.87 (dt, *J* = 8.5Hz & 1.9Hz, 2H), 6.75 (s, 1H), 6.67 (d, *J* = 16.2Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ187.2, 140.7, 139.9, 138.6, 137.8, 137.3, 132.6, 131.5, 131.2, 130.4, 129.9, 129.0, 128.9, 128.5, 128.4, 128.3, 127.9, 127.8, 127.4, 126.2, 120.9, 107.8, 93.0; ESI-MS (M+H) calcd. for $C_{31}H_{23}INO$: 552.0824; Found: 552.1790.

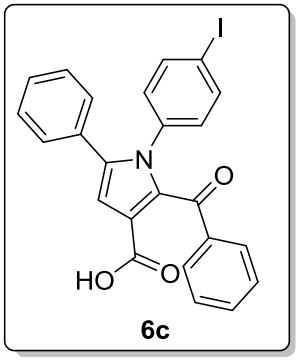
Spectral data for 2-benzoyl-1-(4-iodophenyl)-5-phenyl-*1H*-pyrrole-3-carbaldehyde (6b)



6b

Red oil; (20% ethylacetate/hexane, R_f = 0.23, 36.79 mg, 0.077 mmol, 85%); ^{1}H NMR (400 MHz, $CDCl_3$): δ9.55 (s, 1H), 7.79 (d, *J* = 7.1Hz, 2H), 7.57~7.54 (m, 3H), 7.42 (t, *J* = 7.7Hz, 2H), 7.27~7.23 (m, 3H), 7.12~7.08 (m, 2H), 6.94 (s, 1H), 6.85 (dt, *J* = 8.6Hz & 1.8Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ187.0, 185.7, 139.5, 139.0, 138.1, 138.0, 137.4, 137.2, 133.9, 130.3, 129.8, 129.6, 128.9, 128.7, 128.5, 128.3, 108.9, 94.1; ESI-MS (M+H) calcd. for $C_{24}H_{17}INO_2$: 478.0304; Found: 478.0293.

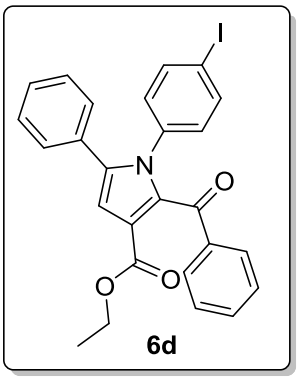
Spectral data for 2-benzoyl-1-(4-iodophenyl)-5-phenyl-*1H*-pyrrole-3-carboxylic acid (6c)



6c

Yellow oil; (50% ethylacetate/hexane, R_f = 0.25, 21.19 mg, 0.043 mmol, 41%); ^{1}H NMR (600 MHz, Acentone): δ10.76 (s, 1H), 7.82 (d, *J* = 7.3Hz, 2H), 7.67 (dt, *J* = 8.5Hz & 1.7Hz, 2H), 7.59 (t, *J* = 7.4Hz, 1H), 7.46 (t, *J* = 7.9Hz, 2H), 7.30~7.23 (m, 5H), 7.03 (dt, *J* = 8.5Hz & 1.7Hz, 2H), 6.87 (s, 1H); ^{13}C NMR (150 MHz, Acentone): δ190.9, 165.4, 140.2, 139.8, 139.4, 138.5, 138.2, 135.1, 132.9, 132.2, 131.0, 130.6, 130.3, 130.1, 129.5, 115.6, 112.1, 95.4; ESI-MS (M+H) calcd. for $C_{24}H_{17}INO_3$: 494.0253; Found: 494.0250.

Spectral data for ethyl 2-benzoyl-1-(4-iodophenyl)-5-phenyl-*1H*-pyrrole-3-carboxylate (6d)

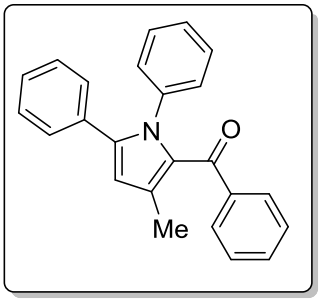


6d

Yellow solid, mp: 178.8~180.7℃; (50% ethylacetate/hexane, R_f = 0.59, 48.09 mg, 0.092 mmol, 91%); ^{1}H NMR (600 MHz, $CDCl_3$): δ7.82 (dd, *J* = 8.1Hz & 1.0Hz, 2H), 7.55~7.52 (m, 3H), 7.41 (t, *J* = 8.2Hz, 2H), 7.23~7.21 (m, 3H), 7.12~7.08 (m, 2H), 6.88 (s, 1H), 6.85 (dt, *J* = 8.7Hz & 1.9Hz, 2H), 3.92 (q, *J* = 7.1Hz, 2H), 0.85 (t, *J* = 7.1Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ189.1, 163.7, 138.6, 138.1, 137.3, 135.2, 133.4, 130.8, 129.8, 129.3, 128.7, 128.5, 128.4, 127.7, 118.9, 114.0, 110.8, 94.1, 60.3, 13.6; ESI-MS (M+H) calcd. for $C_{26}H_{21}INO_3$: 522.0566; Found: 522.0551.

(5)X-ray crystallographic structure and data for compound 3a and 4c

a) X-ray crystallographic structure and data for compound '3a'



3a(CCDC 1580644)

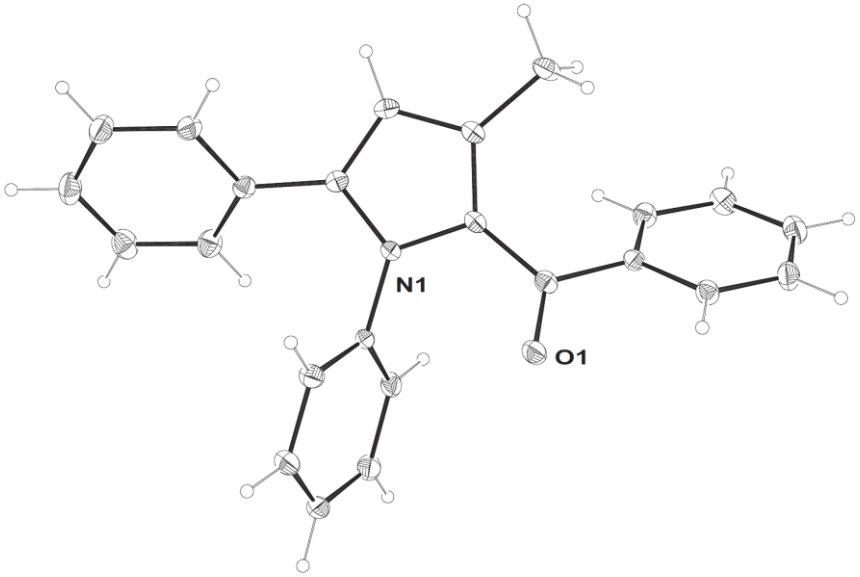


Table 1. Crystal data and structure refinement for d18758.

Identification code	d18758	
Empirical formula	C24 H19 N O	
Formula weight	337.40	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.6383(14) Å	α= 80.286(4)°.
	b = 9.7333(11) Å	β= 71.715(4)°.
	c = 10.4533(14) Å	γ = 74.791(4)°.
Volume	894.5(2) Å ^{3}	
Z	2	
Density (calculated)	1.253 Mg/m^3	

Absorption coefficient	0.076 mm^{-1}
F(000)	356
Crystal size	0.11 x 0.09 x 0.03 mm^3
Theta range for data collection	2.28 to 25.08°.
Index ranges	-11<=h<=11, -11<=k<=11, -12<=l<=12
Reflections collected	18760
Independent reflections	3156 [R(int) = 0.1026]
Completeness to theta = 25.08°	99.1 %
Absorption correction	multi-scan
Max. and min. transmission	0.9977 and 0.9917
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3156 / 0 / 236
Goodness-of-fit on F^2	1.129
Final R indices [I>2sigma(I)]	R1 = 0.0692, wR2 = 0.1179
R indices (all data)	R1 = 0.1081, wR2 = 0.1303
Largest diff. peak and hole	0.204 and -0.199 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d18758. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4669(3)	3566(3)	4255(2)	30(1)
C(2)	3311(3)	3148(2)	5239(2)	28(1)
C(3)	2014(3)	4201(3)	5621(3)	34(1)
C(4)	726(3)	3844(3)	6483(3)	43(1)
C(5)	693(3)	2442(3)	6965(3)	44(1)
C(6)	1967(3)	1379(3)	6566(3)	42(1)
C(7)	3270(3)	1738(3)	5712(3)	36(1)
C(8)	6158(3)	2742(2)	4309(2)	28(1)
C(9)	6700(3)	2120(2)	5409(2)	30(1)
C(10)	5850(3)	1993(3)	6886(3)	42(1)
C(11)	8261(3)	1730(3)	4914(3)	32(1)
C(12)	8679(3)	2084(2)	3536(3)	28(1)
C(13)	10197(3)	1823(2)	2588(3)	30(1)
C(14)	11362(3)	2026(3)	3005(3)	38(1)
C(15)	12811(3)	1777(3)	2175(3)	48(1)
C(16)	13131(3)	1322(3)	920(3)	51(1)

C(17)	11993(4)	1096(3)	499(3)	49(1)
C(18)	10531(3)	1340(3)	1328(3)	42(1)
C(19)	7321(3)	3265(3)	1816(2)	27(1)
C(20)	7967(3)	4394(3)	1161(3)	36(1)
C(21)	7890(3)	4907(3)	-133(3)	45(1)
C(22)	7147(3)	4325(3)	-755(3)	48(1)
C(23)	6516(3)	3196(3)	-101(3)	47(1)
C(24)	6621(3)	2648(3)	1185(3)	36(1)
N(1)	7392(2)	2718(2)	3166(2)	27(1)
O(1)	4509(2)	4586(2)	3413(2)	42(1)

Table 3. Bond lengths [Å] and angles [°] for d18758.

C(1)-O(1)	1.223(3)
C(1)-C(8)	1.461(3)
C(1)-C(2)	1.494(3)
C(2)-C(7)	1.384(3)
C(2)-C(3)	1.388(3)
C(3)-C(4)	1.376(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.377(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.382(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.385(4)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.393(3)
C(8)-N(1)	1.395(3)
C(9)-C(11)	1.397(3)
C(9)-C(10)	1.505(3)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.377(3)
C(11)-H(11)	0.9500
C(12)-N(1)	1.374(3)
C(12)-C(13)	1.473(4)

C(13)-C(18)	1.386(4)
C(13)-C(14)	1.394(4)
C(14)-C(15)	1.377(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.373(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.381(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.386(4)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.370(3)
C(19)-C(20)	1.379(3)
C(19)-N(1)	1.437(3)
C(20)-C(21)	1.379(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.373(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.371(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.385(4)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500

O(1)-C(1)-C(8)	121.4(2)
O(1)-C(1)-C(2)	119.1(2)
C(8)-C(1)-C(2)	119.5(2)
C(7)-C(2)-C(3)	118.9(2)
C(7)-C(2)-C(1)	122.3(2)
C(3)-C(2)-C(1)	118.7(2)
C(4)-C(3)-C(2)	120.1(2)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	120.9(3)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	119.5(3)
C(4)-C(5)-H(5)	120.2

C(6)-C(5)-H(5)	120.2
C(5)-C(6)-C(7)	119.7(3)
C(5)-C(6)-H(6)	120.2
C(7)-C(6)-H(6)	120.2
C(2)-C(7)-C(6)	120.9(2)
C(2)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(9)-C(8)-N(1)	107.3(2)
C(9)-C(8)-C(1)	130.7(2)
N(1)-C(8)-C(1)	120.8(2)
C(8)-C(9)-C(11)	106.9(2)
C(8)-C(9)-C(10)	128.7(2)
C(11)-C(9)-C(10)	124.1(2)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(9)	109.3(2)
C(12)-C(11)-H(11)	125.4
C(9)-C(11)-H(11)	125.4
N(1)-C(12)-C(11)	107.3(2)
N(1)-C(12)-C(13)	124.5(2)
C(11)-C(12)-C(13)	128.2(2)
C(18)-C(13)-C(14)	118.6(3)
C(18)-C(13)-C(12)	123.5(2)
C(14)-C(13)-C(12)	117.9(2)
C(15)-C(14)-C(13)	120.7(3)
C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6
C(16)-C(15)-C(14)	120.3(3)
C(16)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
C(15)-C(16)-C(17)	119.6(3)
C(15)-C(16)-H(16)	120.2
C(17)-C(16)-H(16)	120.2
C(16)-C(17)-C(18)	120.5(3)

C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(13)-C(18)-C(17)	120.2(3)
C(13)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(24)-C(19)-C(20)	120.5(2)
C(24)-C(19)-N(1)	119.5(2)
C(20)-C(19)-N(1)	120.0(2)
C(21)-C(20)-C(19)	119.3(3)
C(21)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
C(22)-C(21)-C(20)	120.5(3)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(23)-C(22)-C(21)	119.8(3)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.2(3)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(19)-C(24)-C(23)	119.6(3)
C(19)-C(24)-H(24)	120.2
C(23)-C(24)-H(24)	120.2
C(12)-N(1)-C(8)	109.2(2)
C(12)-N(1)-C(19)	125.7(2)
C(8)-N(1)-C(19)	125.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for d18758. 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)	36(2)	29(1)	25(1)	-8(1)	-6(1)	-6(1)
C(2)	30(2)	31(1)	23(1)	-6(1)	-7(1)	-6(1)
C(3)	35(2)	33(1)	31(2)	-7(1)	-6(1)	-5(1)
C(4)	33(2)	51(2)	39(2)	-11(1)	-2(1)	-5(1)

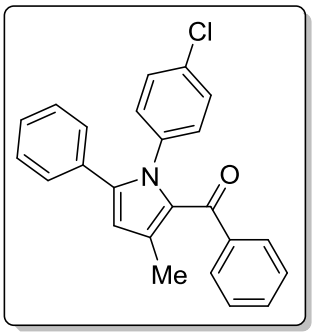
C(5)	40(2)	57(2)	36(2)	-8(1)	-3(1)	-20(2)
C(6)	51(2)	36(2)	42(2)	-3(1)	-9(2)	-19(1)
C(7)	37(2)	33(2)	37(2)	-10(1)	-8(1)	-4(1)
C(8)	33(2)	29(1)	23(1)	-2(1)	-5(1)	-12(1)
C(9)	36(2)	30(1)	24(1)	-1(1)	-7(1)	-10(1)
C(10)	52(2)	48(2)	25(2)	1(1)	-11(1)	-11(1)
C(11)	36(2)	33(1)	31(2)	0(1)	-17(1)	-7(1)
C(12)	30(2)	26(1)	31(2)	-3(1)	-11(1)	-6(1)
C(13)	31(2)	26(1)	33(2)	-2(1)	-10(1)	-5(1)
C(14)	35(2)	40(2)	40(2)	3(1)	-14(1)	-8(1)
C(15)	32(2)	51(2)	57(2)	2(2)	-13(2)	-7(1)
C(16)	31(2)	45(2)	63(2)	-2(2)	0(2)	-3(1)
C(17)	48(2)	45(2)	44(2)	-11(1)	-1(2)	-3(1)
C(18)	37(2)	40(2)	46(2)	-12(1)	-9(1)	-4(1)
C(19)	23(1)	35(1)	19(1)	-4(1)	-4(1)	-2(1)
C(20)	39(2)	37(2)	32(2)	-1(1)	-11(1)	-10(1)
C(21)	42(2)	49(2)	34(2)	8(1)	-5(1)	-6(1)
C(22)	34(2)	76(2)	23(2)	-1(2)	-5(1)	3(2)
C(23)	36(2)	80(2)	29(2)	-13(2)	-10(1)	-13(2)
C(24)	30(2)	52(2)	30(2)	-9(1)	-6(1)	-15(1)
N(1)	26(1)	33(1)	20(1)	-1(1)	-5(1)	-7(1)
O(1)	40(1)	41(1)	32(1)	5(1)	-3(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for d18758.

	x	y	z	U(eq)
H(3)	2015	5171	5286	40
H(4)	-153	4573	6750	52
H(5)	-199	2208	7568	53
H(6)	1949	407	6875	51
H(7)	4148	1007	5448	44
H(10A)	5113	2889	7112	64
H(10B)	6551	1799	7434	64
H(10C)	5332	1207	7074	64
H(11)	8928	1290	5443	38

H(14)	11154	2339	3873	46
H(15)	13594	1921	2473	57
H(16)	14130	1163	344	61
H(17)	12214	770	-366	59
H(18)	9756	1177	1033	50
H(20)	8459	4815	1598	43
H(21)	8355	5668	-599	54
H(22)	7069	4704	-1635	58
H(23)	6006	2790	-532	57
H(24)	6210	1848	1627	43

b) X-ray crystallographic structure and data for compound ‘4c’



4c (CCDC 1580618)

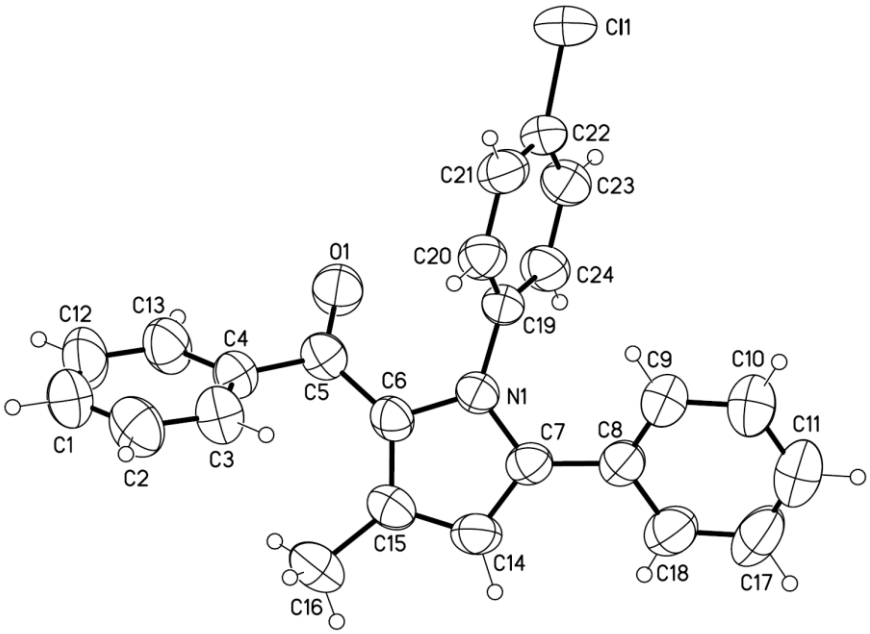


Table 1. Crystal data and structure refinement for 170328LT.

Identification code	170328LT	
Empirical formula	C24 H18 Cl N O	
Formula weight	371.84	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.0623(5) Å	α= 90°.
	b = 18.5108(9) Å	β= 98.868(2)°.
	c = 9.7609(4) Å	γ = 90°.
Volume	1974.87(15) Å ^{3}	
Z	4	

Density (calculated)	1.251 Mg/m^3
Absorption coefficient	0.206 mm^{-1}
F(000)	776
Crystal size	0.15 x 0.02 x 0.01 mm^3
Theta range for data collection	2.164 to 26.391°.
Index ranges	-13<=h<=13, -23<=k<=23, -6<=l<=12
Reflections collected	14743
Independent reflections	4036 [R(int) = 0.0319]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.9026
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4036 / 0 / 245
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.1095
R indices (all data)	R1 = 0.0820, wR2 = 0.1281
Extinction coefficient	n/a
Largest diff. peak and hole	0.309 and -0.362 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 170328LT. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	-3279(1)	8520(1)	357(1)	102(1)
O(1)	1422(1)	7380(1)	921(2)	71(1)
N(1)	1993(1)	8687(1)	2496(2)	47(1)
C(1)	3612(3)	5365(2)	3488(4)	94(1)
C(2)	3543(2)	5921(2)	4410(3)	80(1)
C(3)	3122(2)	6587(1)	3914(2)	64(1)
C(4)	2762(2)	6692(1)	2506(2)	52(1)
C(5)	2237(2)	7389(1)	1926(2)	53(1)
C(6)	2722(2)	8069(1)	2562(2)	50(1)
C(7)	2700(2)	9267(1)	3007(2)	50(1)
C(8)	2250(2)	9998(1)	3225(2)	53(1)
C(9)	1091(2)	10146(1)	3542(2)	64(1)
C(10)	739(3)	10844(1)	3801(3)	79(1)
C(11)	1532(3)	11406(1)	3770(3)	89(1)

C(12)	3253(3)	5465(2)	2096(3)	99(1)
C(13)	2823(2)	6122(1)	1610(2)	74(1)
C(14)	3879(2)	9013(1)	3351(2)	59(1)
C(15)	3908(2)	8274(1)	3090(2)	59(1)
C(16)	5053(2)	7824(2)	3302(3)	91(1)
C(17)	2681(3)	11273(1)	3468(3)	89(1)
C(18)	3038(2)	10579(1)	3186(2)	71(1)
C(19)	704(2)	8682(1)	2012(2)	48(1)
C(20)	-63(2)	8336(1)	2784(2)	56(1)
C(21)	-1298(2)	8300(1)	2289(2)	64(1)
C(22)	-1735(2)	8606(1)	1019(3)	64(1)
C(23)	-974(2)	8962(1)	260(2)	68(1)
C(24)	256(2)	8999(1)	756(2)	60(1)

Table 3. Bond lengths [Å] and angles [°] for 170328LT.

Cl(1)-C(22)	1.738(2)
O(1)-C(5)	1.226(2)
N(1)-C(7)	1.376(2)
N(1)-C(6)	1.395(2)
N(1)-C(19)	1.431(2)
C(1)-C(12)	1.368(4)
C(1)-C(2)	1.378(4)
C(1)-H(1)	0.9500
C(2)-C(3)	1.378(3)
C(2)-H(15)	0.9500
C(3)-C(4)	1.384(3)
C(3)-H(16)	0.9500
C(4)-C(13)	1.380(3)
C(4)-C(5)	1.490(3)
C(5)-C(6)	1.468(3)
C(6)-C(15)	1.387(3)
C(7)-C(14)	1.378(3)
C(7)-C(8)	1.468(3)
C(8)-C(18)	1.389(3)
C(8)-C(9)	1.391(3)
C(9)-C(10)	1.384(3)

C(9)-H(7)	0.9500
C(10)-C(11)	1.364(4)
C(10)-H(8)	0.9500
C(11)-C(17)	1.371(4)
C(11)-H(2)	0.9500
C(12)-C(13)	1.363(3)
C(12)-H(18)	0.9500
C(13)-H(17)	0.9500
C(14)-C(15)	1.392(3)
C(14)-H(3)	0.9500
C(15)-C(16)	1.504(3)
C(16)-H(4)	0.9800
C(16)-H(6)	0.9800
C(16)-H(5)	0.9800
C(17)-C(18)	1.384(4)
C(17)-H(10)	0.9500
C(18)-H(9)	0.9500
C(19)-C(20)	1.377(3)
C(19)-C(24)	1.381(3)
C(20)-C(21)	1.379(3)
C(20)-H(14)	0.9500
C(21)-C(22)	1.381(3)
C(21)-H(13)	0.9500
C(22)-C(23)	1.373(3)
C(23)-C(24)	1.375(3)
C(23)-H(12)	0.9500
C(24)-H(11)	0.9500

C(7)-N(1)-C(6)	109.37(16)
C(7)-N(1)-C(19)	127.32(16)
C(6)-N(1)-C(19)	123.28(16)
C(12)-C(1)-C(2)	120.7(2)
C(12)-C(1)-H(1)	119.6
C(2)-C(1)-H(1)	119.6
C(1)-C(2)-C(3)	119.2(2)
C(1)-C(2)-H(15)	120.4
C(3)-C(2)-H(15)	120.4
C(2)-C(3)-C(4)	120.3(2)

C(2)-C(3)-H(16)	119.8
C(4)-C(3)-H(16)	119.8
C(13)-C(4)-C(3)	119.1(2)
C(13)-C(4)-C(5)	118.42(18)
C(3)-C(4)-C(5)	122.32(18)
O(1)-C(5)-C(6)	121.74(18)
O(1)-C(5)-C(4)	119.21(18)
C(6)-C(5)-C(4)	119.05(17)
C(15)-C(6)-N(1)	107.39(18)
C(15)-C(6)-C(5)	130.96(19)
N(1)-C(6)-C(5)	120.85(17)
N(1)-C(7)-C(14)	106.55(18)
N(1)-C(7)-C(8)	125.81(17)
C(14)-C(7)-C(8)	127.50(19)
C(18)-C(8)-C(9)	117.2(2)
C(18)-C(8)-C(7)	118.8(2)
C(9)-C(8)-C(7)	123.93(19)
C(10)-C(9)-C(8)	121.3(2)
C(10)-C(9)-H(7)	119.4
C(8)-C(9)-H(7)	119.4
C(11)-C(10)-C(9)	120.5(3)
C(11)-C(10)-H(8)	119.7
C(9)-C(10)-H(8)	119.7
C(10)-C(11)-C(17)	119.2(3)
C(10)-C(11)-H(2)	120.4
C(17)-C(11)-H(2)	120.4
C(13)-C(12)-C(1)	119.9(3)
C(13)-C(12)-H(18)	120.0
C(1)-C(12)-H(18)	120.0
C(12)-C(13)-C(4)	120.7(2)
C(12)-C(13)-H(17)	119.7
C(4)-C(13)-H(17)	119.7
C(7)-C(14)-C(15)	109.79(18)
C(7)-C(14)-H(3)	125.1
C(15)-C(14)-H(3)	125.1
C(6)-C(15)-C(14)	106.87(18)
C(6)-C(15)-C(16)	128.9(2)
C(14)-C(15)-C(16)	124.2(2)

C(15)-C(16)-H(4)	109.5
C(15)-C(16)-H(6)	109.5
H(4)-C(16)-H(6)	109.5
C(15)-C(16)-H(5)	109.5
H(4)-C(16)-H(5)	109.5
H(6)-C(16)-H(5)	109.5
C(11)-C(17)-C(18)	120.8(3)
C(11)-C(17)-H(10)	119.6
C(18)-C(17)-H(10)	119.6
C(17)-C(18)-C(8)	120.9(2)
C(17)-C(18)-H(9)	119.5
C(8)-C(18)-H(9)	119.5
C(20)-C(19)-C(24)	121.12(19)
C(20)-C(19)-N(1)	119.28(17)
C(24)-C(19)-N(1)	119.56(17)
C(19)-C(20)-C(21)	119.47(19)
C(19)-C(20)-H(14)	120.3
C(21)-C(20)-H(14)	120.3
C(20)-C(21)-C(22)	119.1(2)
C(20)-C(21)-H(13)	120.5
C(22)-C(21)-H(13)	120.5
C(23)-C(22)-C(21)	121.5(2)
C(23)-C(22)-Cl(1)	119.49(18)
C(21)-C(22)-Cl(1)	119.01(19)
C(22)-C(23)-C(24)	119.4(2)
C(22)-C(23)-H(12)	120.3
C(24)-C(23)-H(12)	120.3
C(23)-C(24)-C(19)	119.5(2)
C(23)-C(24)-H(11)	120.3
C(19)-C(24)-H(11)	120.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 170328LT. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Cl(1)	55(1)	99(1)	138(1)	-19(1)	-26(1)	-11(1)
O(1)	80(1)	66(1)	57(1)	-3(1)	-16(1)	6(1)
N(1)	47(1)	49(1)	43(1)	2(1)	-2(1)	2(1)
C(1)	88(2)	58(2)	129(3)	16(2)	-4(2)	14(1)
C(2)	85(2)	84(2)	71(2)	28(1)	11(1)	13(1)
C(3)	80(2)	66(2)	50(1)	5(1)	15(1)	14(1)
C(4)	54(1)	55(1)	47(1)	0(1)	11(1)	6(1)
C(5)	56(1)	59(1)	43(1)	2(1)	6(1)	6(1)
C(6)	52(1)	52(1)	44(1)	5(1)	0(1)	7(1)
C(7)	52(1)	52(1)	43(1)	3(1)	0(1)	-6(1)
C(8)	62(1)	50(1)	44(1)	4(1)	-1(1)	-4(1)
C(9)	73(2)	53(1)	67(1)	-3(1)	14(1)	-3(1)
C(10)	95(2)	60(2)	85(2)	-5(1)	23(1)	7(1)
C(11)	123(3)	55(2)	90(2)	-5(1)	21(2)	2(2)
C(12)	105(2)	69(2)	113(2)	-26(2)	-18(2)	32(2)
C(13)	80(2)	73(2)	64(1)	-15(1)	-1(1)	21(1)
C(14)	48(1)	64(2)	60(1)	3(1)	-4(1)	-6(1)
C(15)	50(1)	65(2)	58(1)	6(1)	-2(1)	7(1)
C(16)	54(1)	88(2)	126(2)	9(2)	-2(1)	15(1)
C(17)	118(2)	52(2)	94(2)	-1(1)	6(2)	-23(2)
C(18)	74(2)	64(2)	73(2)	2(1)	3(1)	-14(1)
C(19)	45(1)	46(1)	48(1)	-1(1)	-3(1)	1(1)
C(20)	56(1)	58(1)	52(1)	0(1)	3(1)	-3(1)
C(21)	55(1)	63(1)	74(2)	-8(1)	9(1)	-11(1)
C(22)	47(1)	56(1)	82(2)	-15(1)	-9(1)	-2(1)
C(23)	64(1)	66(2)	66(1)	6(1)	-18(1)	3(1)
C(24)	57(1)	62(1)	58(1)	11(1)	-4(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^{-3}) for 170328LT.

	x	y	z	U(eq)
H(1)	3911	4907	3822	112
H(15)	3783	5847	5377	96
H(16)	3079	6975	4541	77
H(7)	531	9760	3582	77
H(8)	-61	10932	4001	95
H(2)	1291	11884	3955	107
H(18)	3304	5078	1469	119
H(17)	2562	6187	644	89
H(3)	4568	9299	3711	71
H(4)	5129	7580	4203	137
H(6)	5765	8136	3279	137
H(5)	5010	7462	2563	137
H(10)	3239	11662	3452	107
H(9)	3834	10499	2963	86
H(14)	256	8125	3652	68
H(13)	-1840	8066	2813	77
H(12)	-1295	9180	-600	82
H(11)	794	9242	239	72

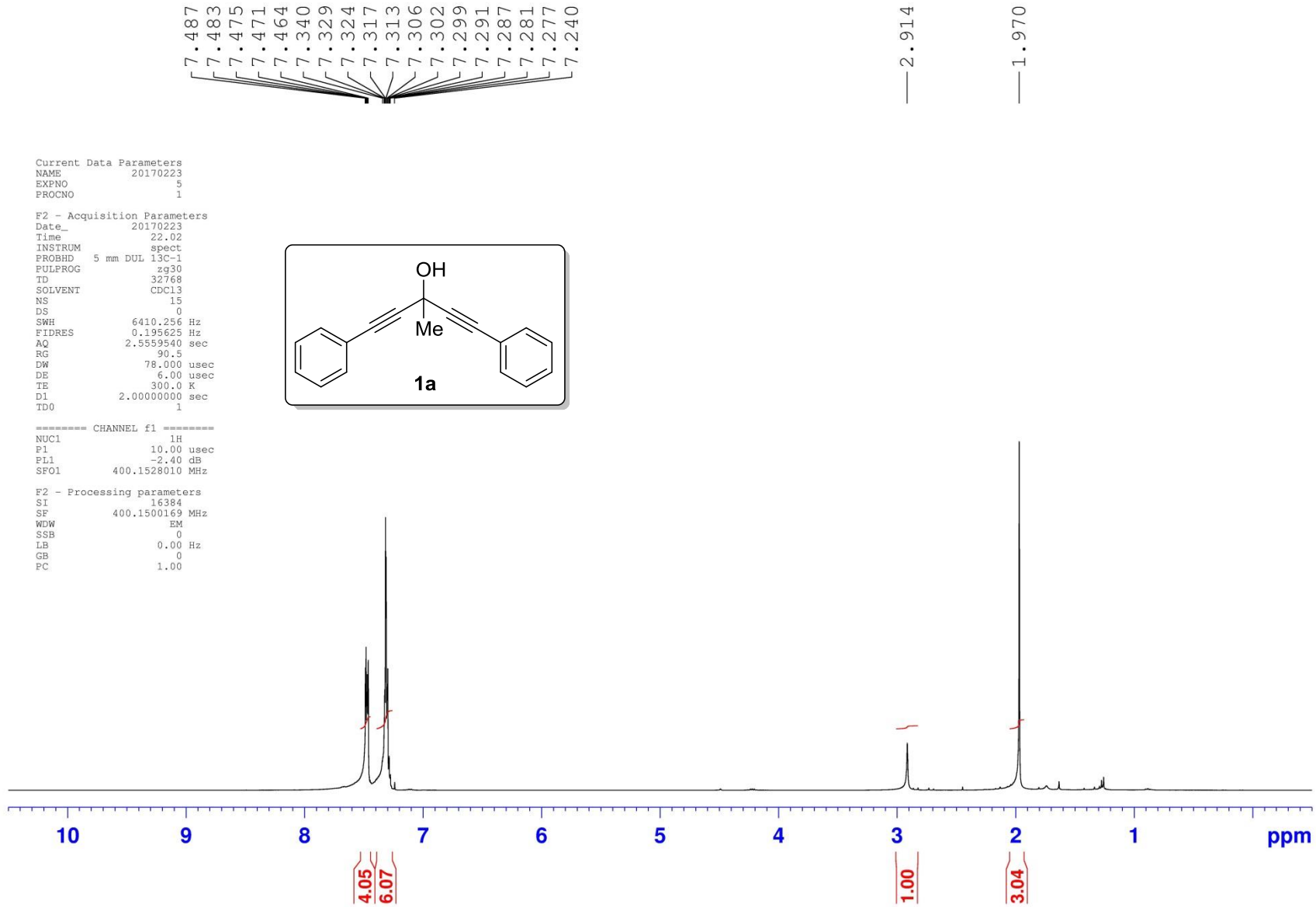
Table 6. Torsion angles [°] for 170328LT.

C(12)-C(1)-C(2)-C(3)	-0.8(4)
C(1)-C(2)-C(3)-C(4)	0.6(4)
C(2)-C(3)-C(4)-C(13)	0.4(3)
C(2)-C(3)-C(4)-C(5)	176.5(2)
C(13)-C(4)-C(5)-O(1)	32.3(3)
C(3)-C(4)-C(5)-O(1)	-143.8(2)
C(13)-C(4)-C(5)-C(6)	-146.8(2)
C(3)-C(4)-C(5)-C(6)	37.1(3)
C(7)-N(1)-C(6)-C(15)	-1.5(2)
C(19)-N(1)-C(6)-C(15)	-179.37(16)

C(7)-N(1)-C(6)-C(5)	-172.33(17)
C(19)-N(1)-C(6)-C(5)	9.9(3)
O(1)-C(5)-C(6)-C(15)	-140.2(2)
C(4)-C(5)-C(6)-C(15)	38.9(3)
O(1)-C(5)-C(6)-N(1)	28.1(3)
C(4)-C(5)-C(6)-N(1)	-152.75(17)
C(6)-N(1)-C(7)-C(14)	1.8(2)
C(19)-N(1)-C(7)-C(14)	179.55(17)
C(6)-N(1)-C(7)-C(8)	-174.25(17)
C(19)-N(1)-C(7)-C(8)	3.5(3)
N(1)-C(7)-C(8)-C(18)	-153.69(19)
C(14)-C(7)-C(8)-C(18)	31.0(3)
N(1)-C(7)-C(8)-C(9)	29.8(3)
C(14)-C(7)-C(8)-C(9)	-145.5(2)
C(18)-C(8)-C(9)-C(10)	0.3(3)
C(7)-C(8)-C(9)-C(10)	176.90(19)
C(8)-C(9)-C(10)-C(11)	-0.9(4)
C(9)-C(10)-C(11)-C(17)	0.5(4)
C(2)-C(1)-C(12)-C(13)	0.0(5)
C(1)-C(12)-C(13)-C(4)	1.0(5)
C(3)-C(4)-C(13)-C(12)	-1.3(4)
C(5)-C(4)-C(13)-C(12)	-177.5(2)
N(1)-C(7)-C(14)-C(15)	-1.5(2)
C(8)-C(7)-C(14)-C(15)	174.55(18)
N(1)-C(6)-C(15)-C(14)	0.6(2)
C(5)-C(6)-C(15)-C(14)	170.1(2)
N(1)-C(6)-C(15)-C(16)	-176.6(2)
C(5)-C(6)-C(15)-C(16)	-7.1(4)
C(7)-C(14)-C(15)-C(6)	0.5(2)
C(7)-C(14)-C(15)-C(16)	177.9(2)
C(10)-C(11)-C(17)-C(18)	0.5(4)
C(11)-C(17)-C(18)-C(8)	-1.1(4)
C(9)-C(8)-C(18)-C(17)	0.7(3)
C(7)-C(8)-C(18)-C(17)	-176.1(2)
C(7)-N(1)-C(19)-C(20)	-109.5(2)
C(6)-N(1)-C(19)-C(20)	67.9(2)
C(7)-N(1)-C(19)-C(24)	72.9(2)
C(6)-N(1)-C(19)-C(24)	-109.7(2)

C(24)-C(19)-C(20)-C(21)	0.8(3)
N(1)-C(19)-C(20)-C(21)	-176.81(18)
C(19)-C(20)-C(21)-C(22)	0.5(3)
C(20)-C(21)-C(22)-C(23)	-1.7(3)
C(20)-C(21)-C(22)-Cl(1)	176.87(16)
C(21)-C(22)-C(23)-C(24)	1.6(3)
Cl(1)-C(22)-C(23)-C(24)	-176.94(17)
C(22)-C(23)-C(24)-C(19)	-0.3(3)
C(20)-C(19)-C(24)-C(23)	-0.9(3)
N(1)-C(19)-C(24)-C(23)	176.72(19)

Symmetry transformations used to generate equivalent atoms: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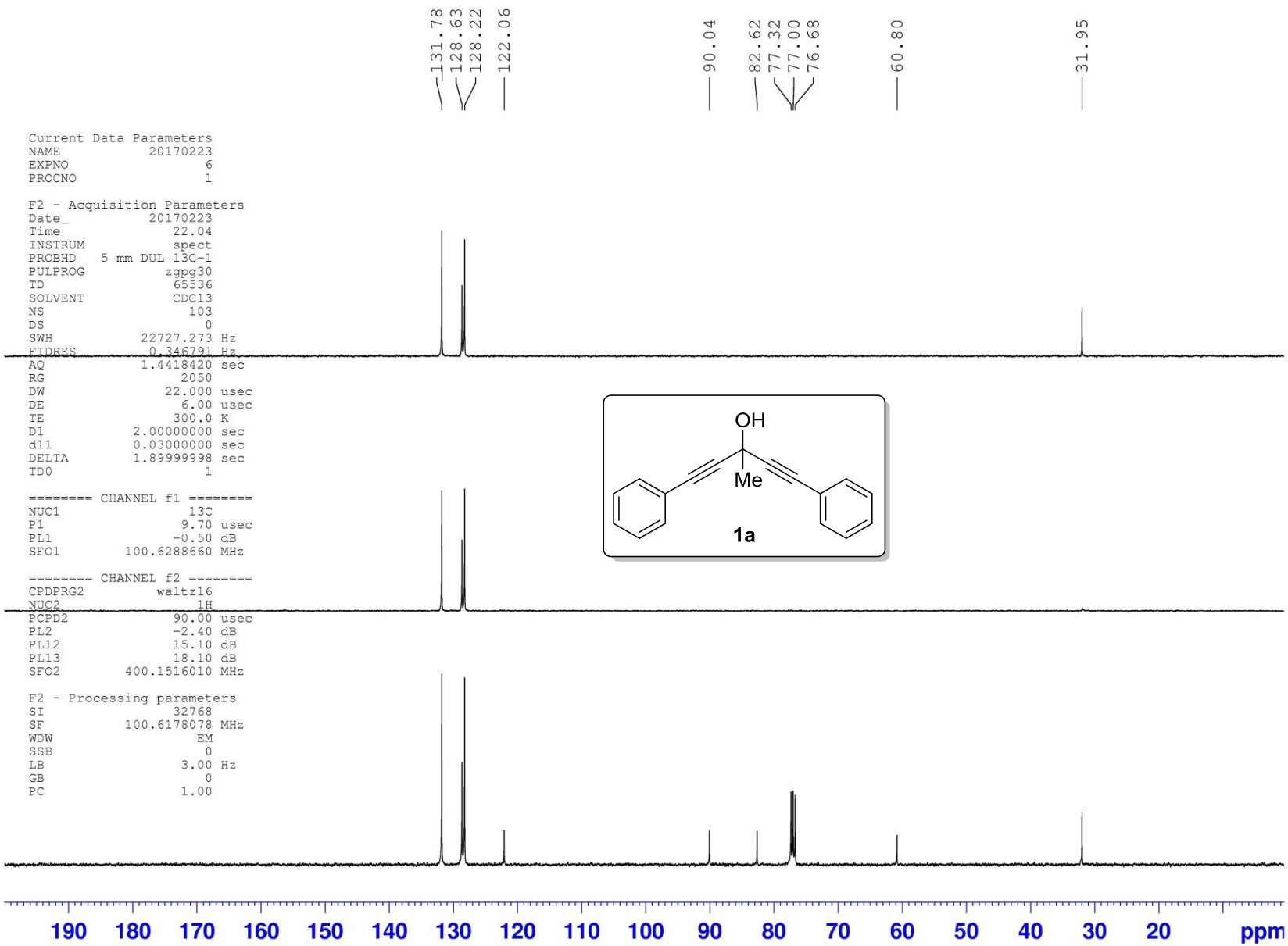
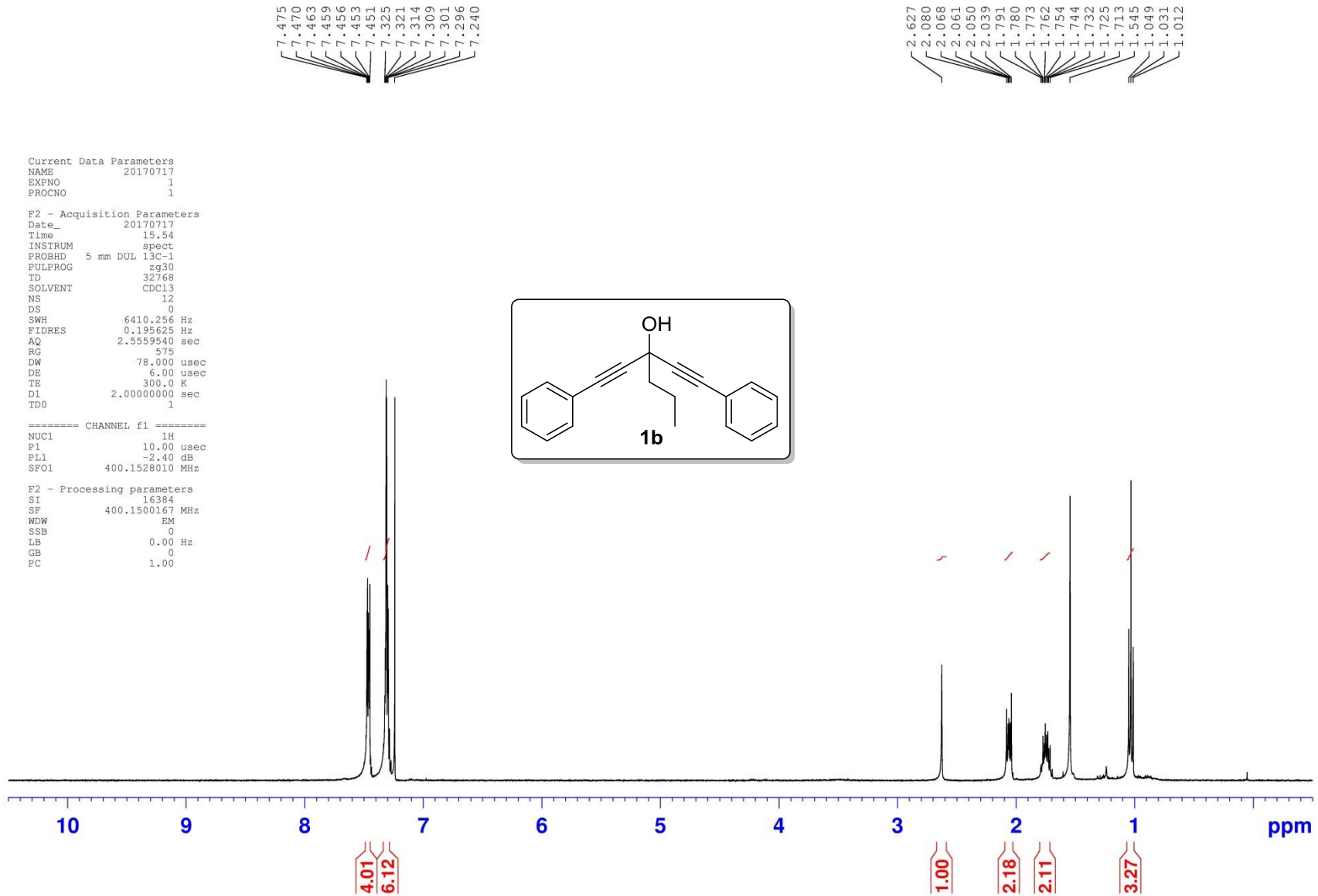
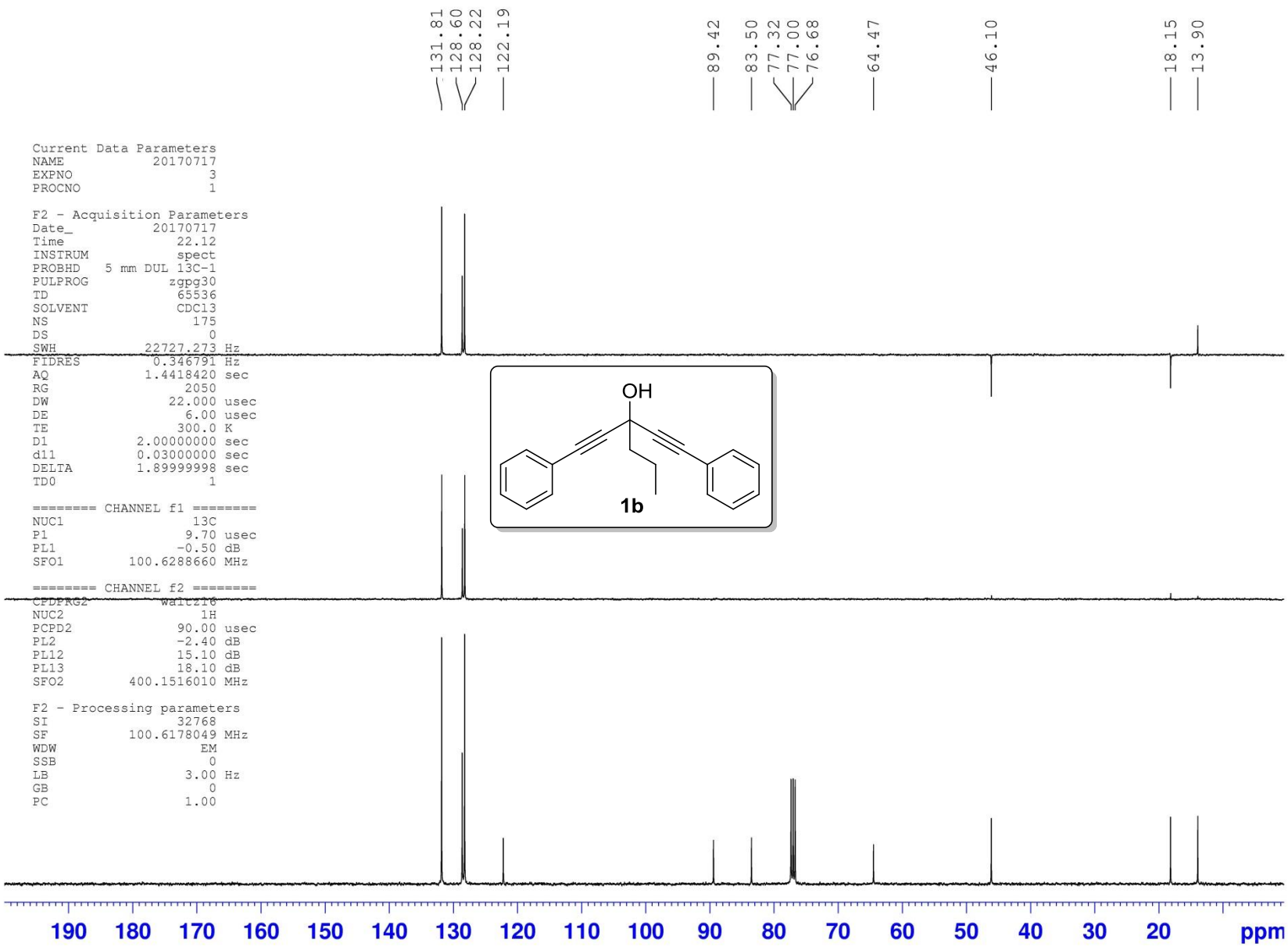
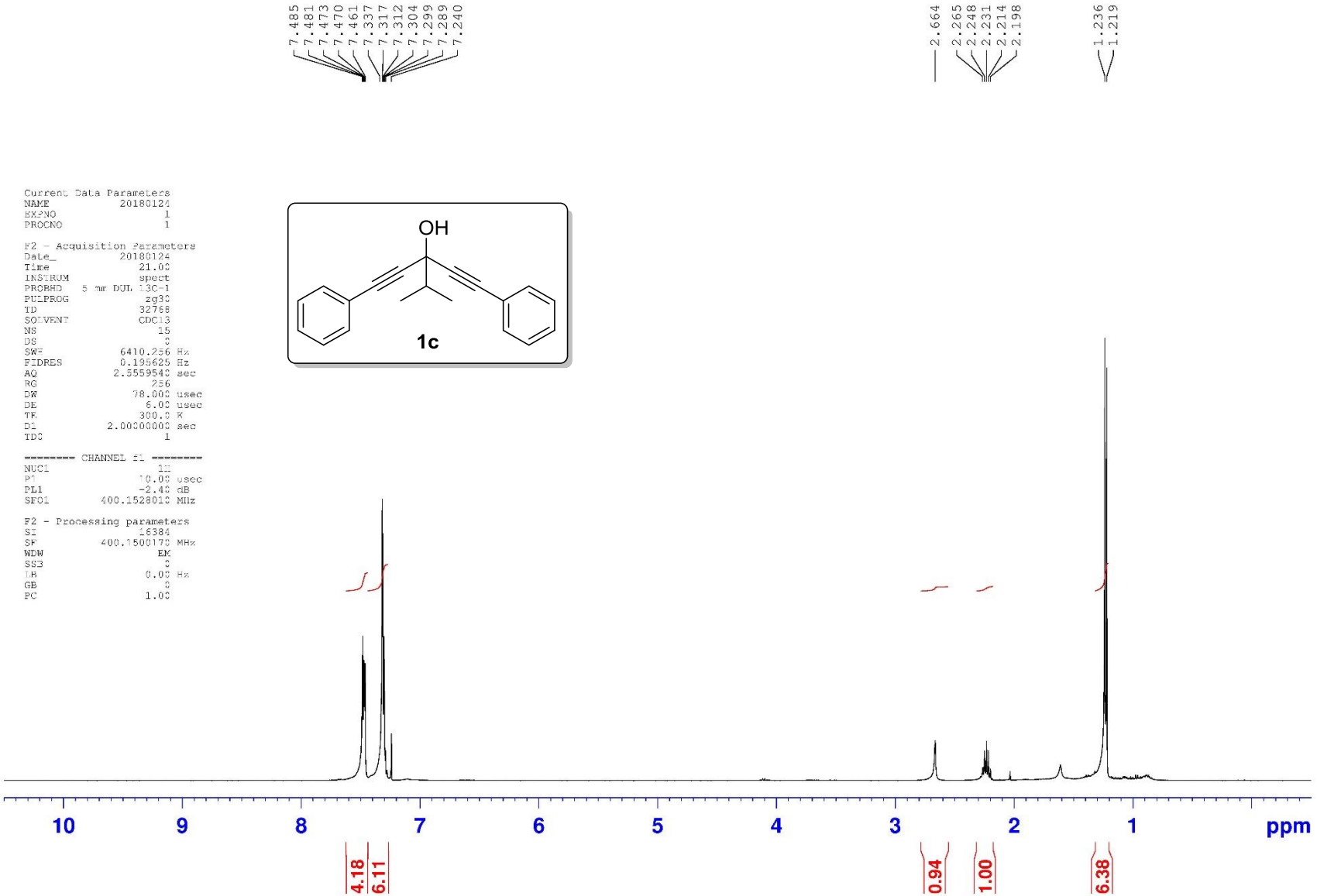
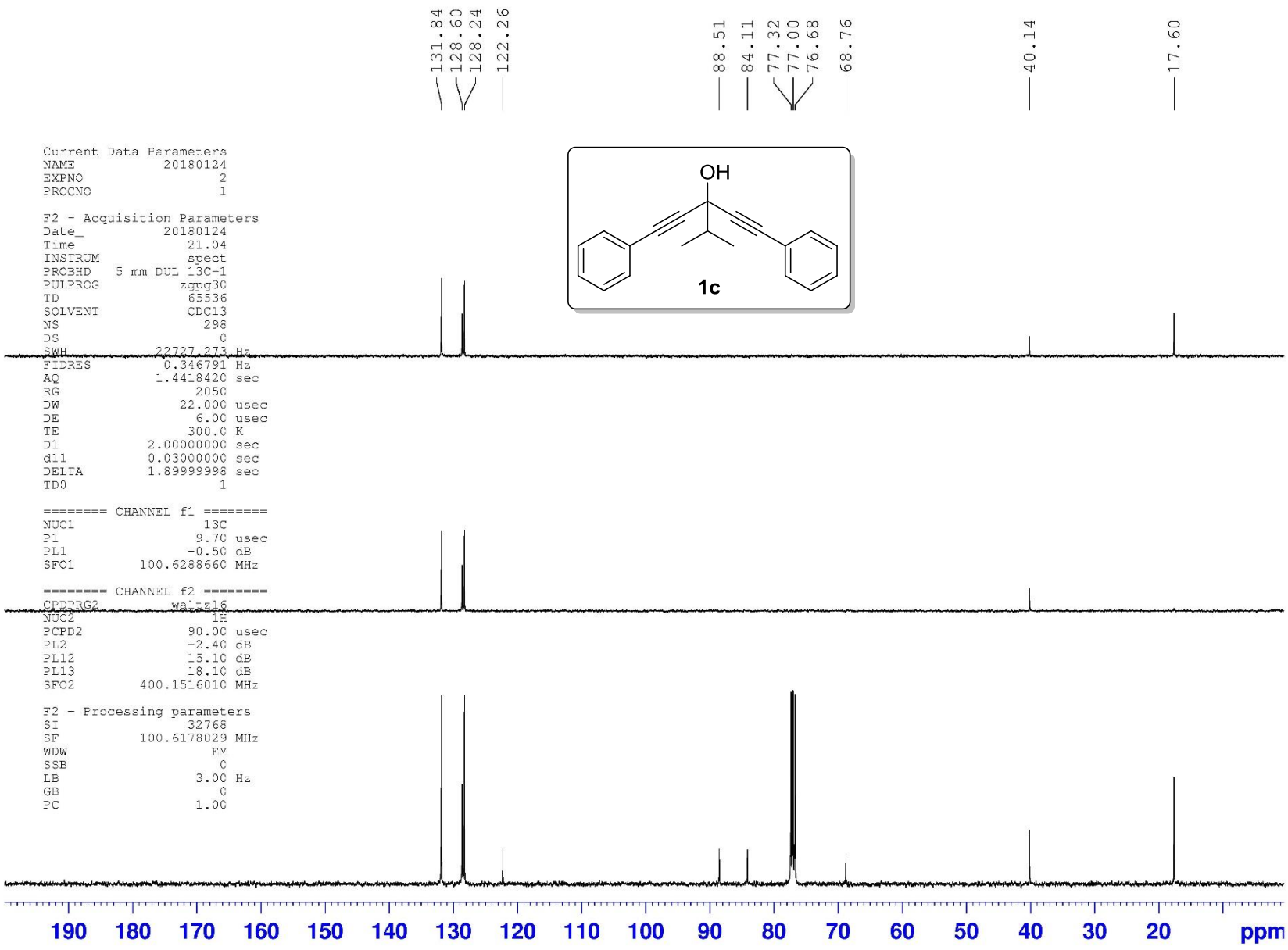
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
Me
1a
10
9
8
7
6
5
4
3
2
1
ppm
4.05
6.07
1.00
3.04

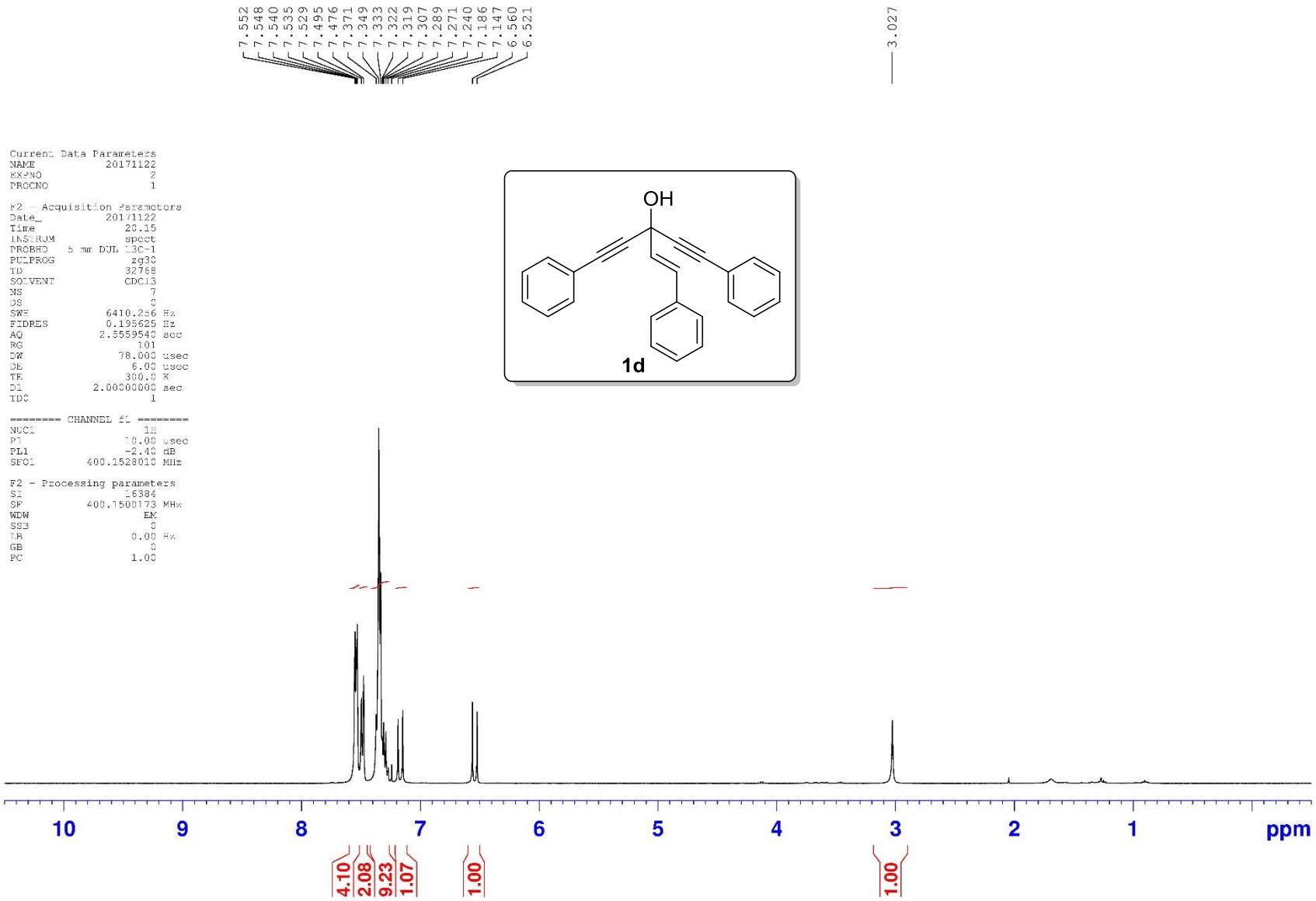

131.78
128.63
128.22
122.06
90.04
82.62
77.32
77.00
76.68
60.80
31.95
Current Data Parameters
NAME 20170223
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170223
Time 22.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 103
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
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 100.6178078 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
1a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

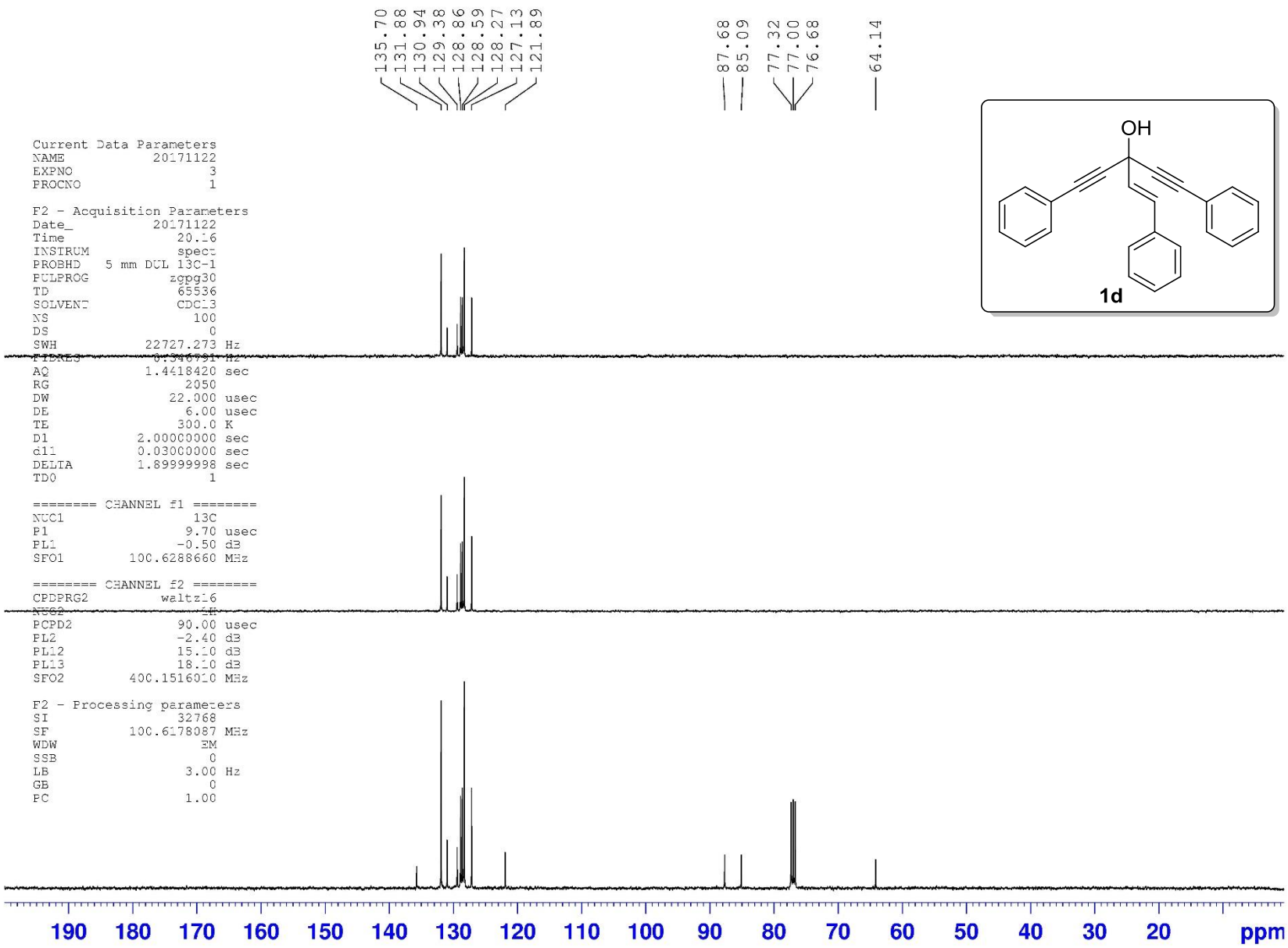

7.475
7.470
7.463
7.459
7.456
7.453
7.451
7.325
7.321
7.314
7.309
7.301
7.296
7.240
2.627
2.080
2.068
2.061
2.050
2.039
1.791
1.780
1.773
1.762
1.754
1.744
1.732
1.725
1.713
1.545
1.049
1.031
1.012
Current Data Parameters
NAME 20170717
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170717
Time 15.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
1b
10
9
8
7
6
5
4
3
2
1
ppm
4.01
6.12
1.00
2.18
2.11
3.27

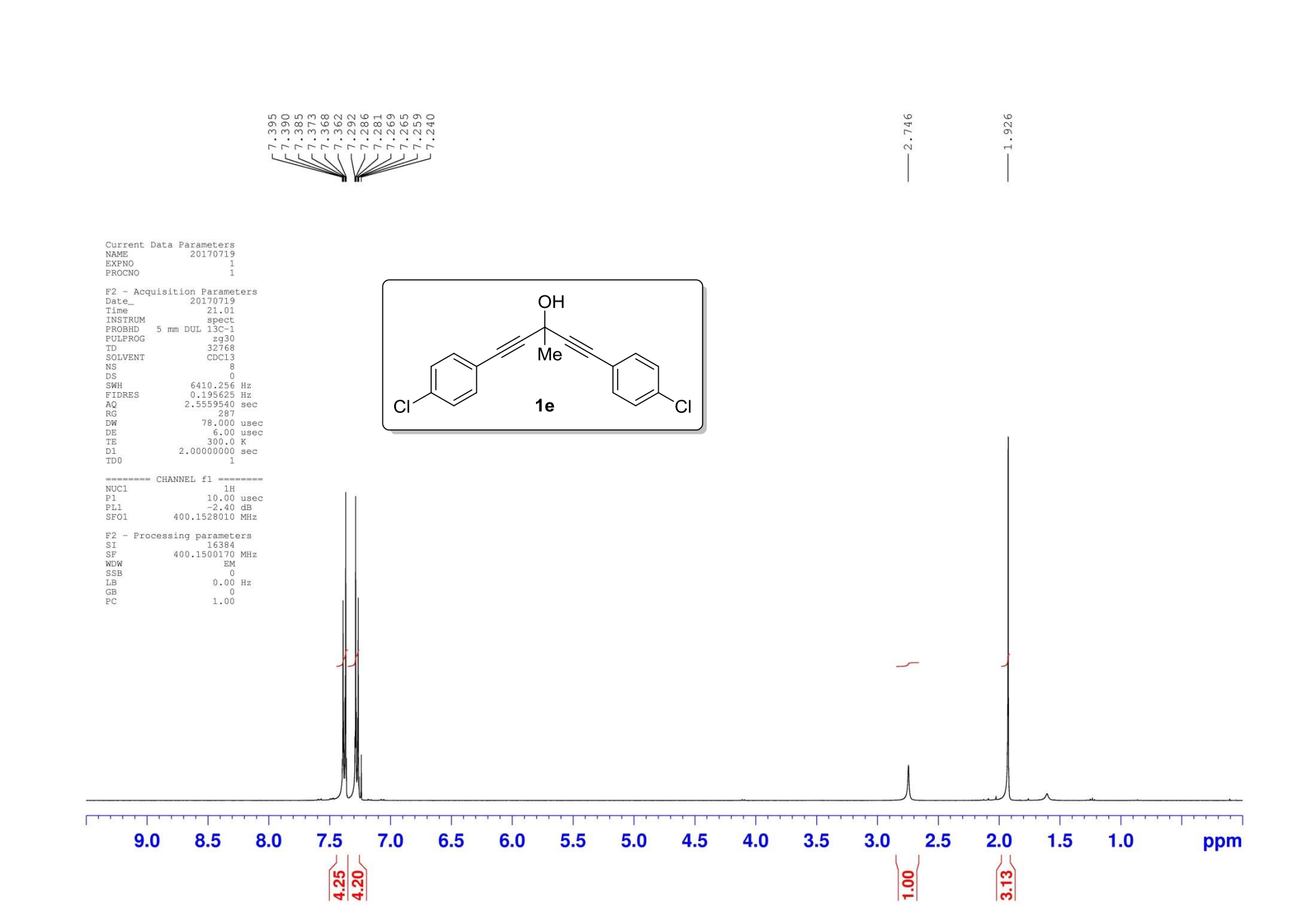

131.81
128.60
128.22
122.19
89.42
83.50
77.32
77.00
76.68
64.47
46.10
18.15
13.90
Current Data Parameters
NAME 20170717
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170717
Time 22.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 175
DS 0
SWH 22727.273 Hz
FIDRES 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 100.6178049 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
1b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

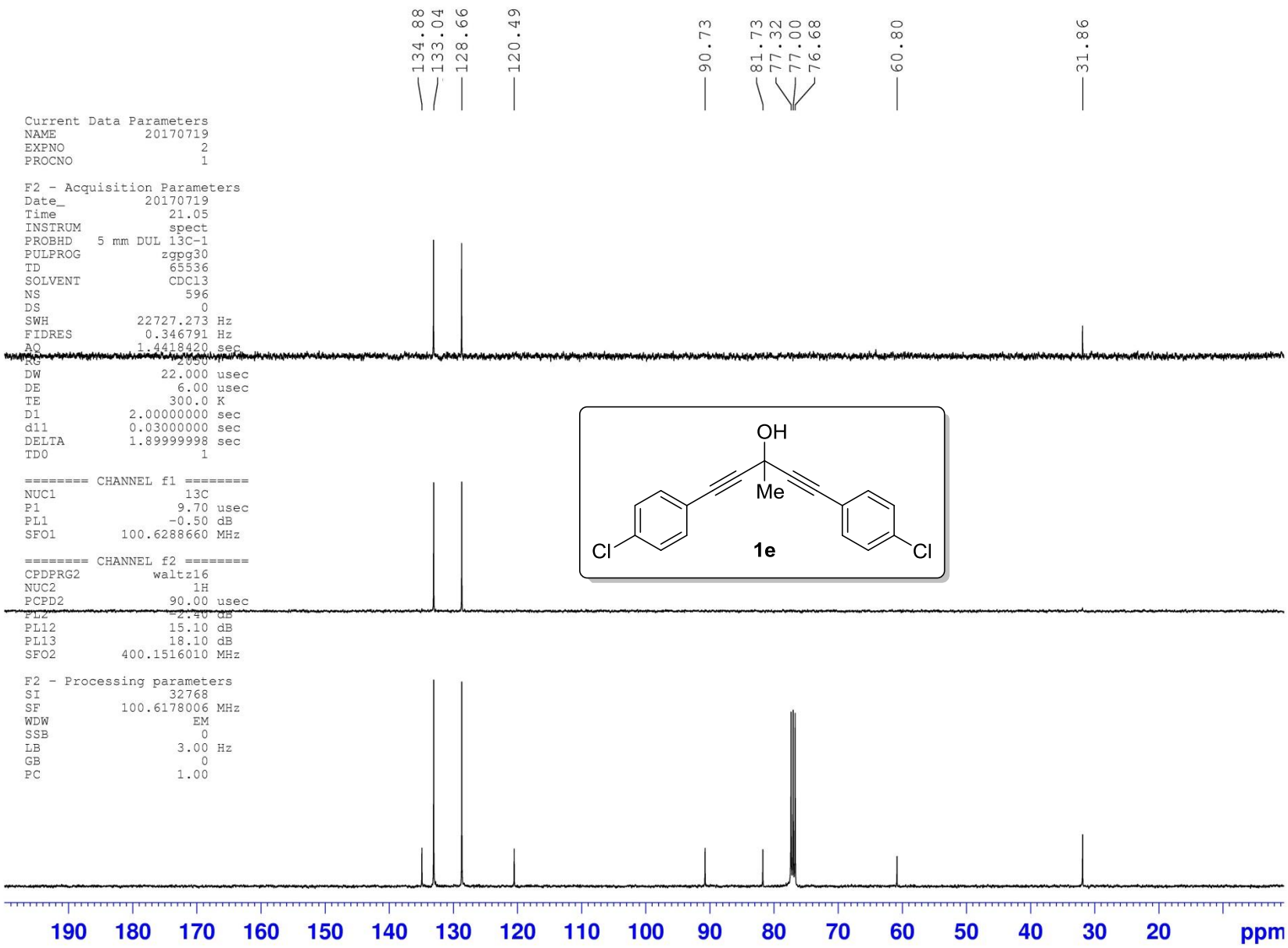

7.485
7.481
7.473
7.470
7.461
7.337
7.317
7.312
7.304
7.299
7.289
7.240
2.664
2.265
2.248
2.231
2.214
2.198
1.236
1.219
Current Data Parameters
NAME 20180124
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180124
Time 21.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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
OH
1c
10
9
8
7
6
5
4
3
2
1
ppm
4.18
6.11
0.94
1.00
6.38

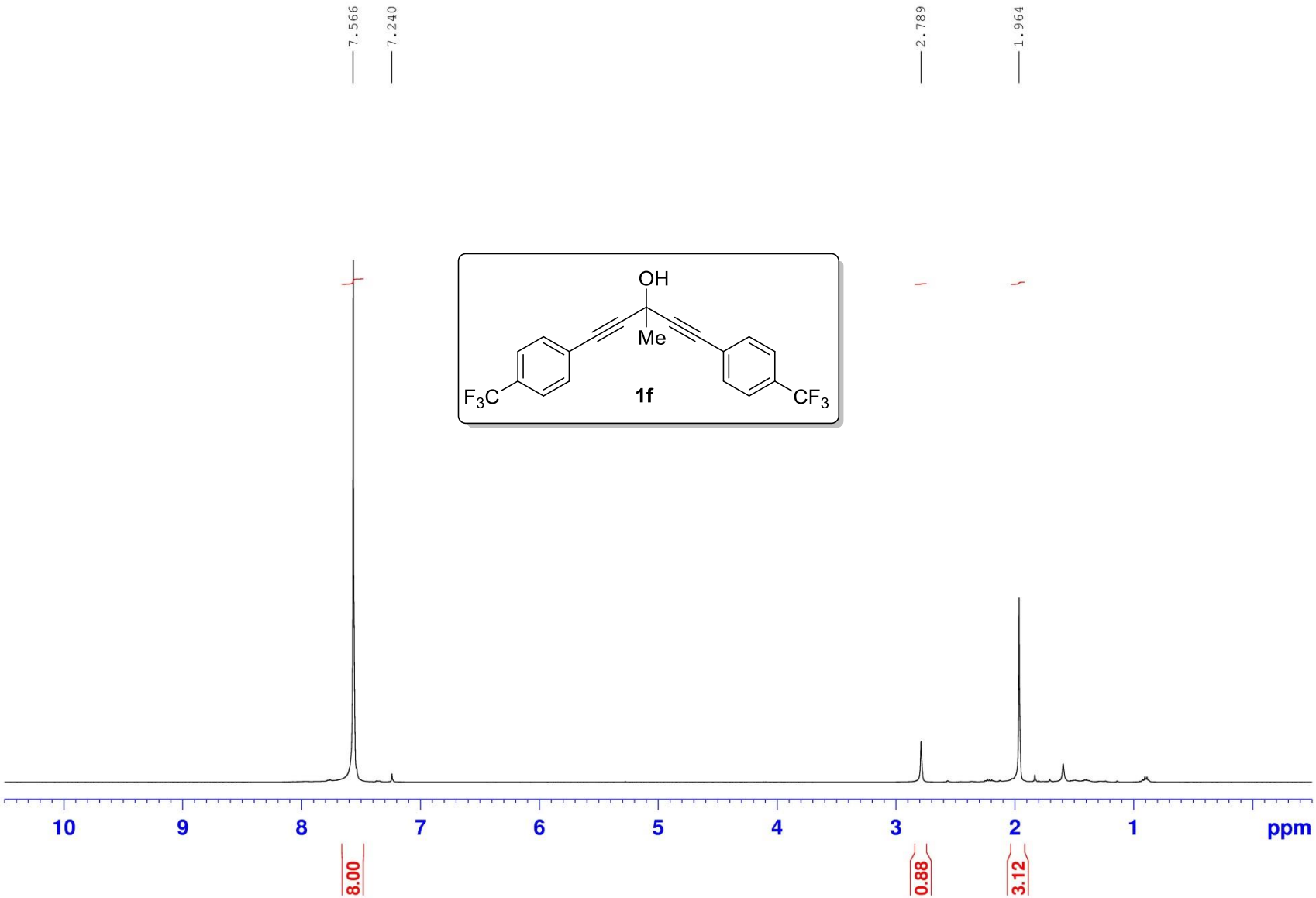

131.84
128.60
128.24
122.26
88.51
84.11
77.32
77.00
76.68
68.76
40.14
17.60
OH
1c
Current Data Parameters
NAME 20180124
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180124
Time 21.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 298
DS 0
SWH 22727.273 Hz
FIDRES 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 100.6178029 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

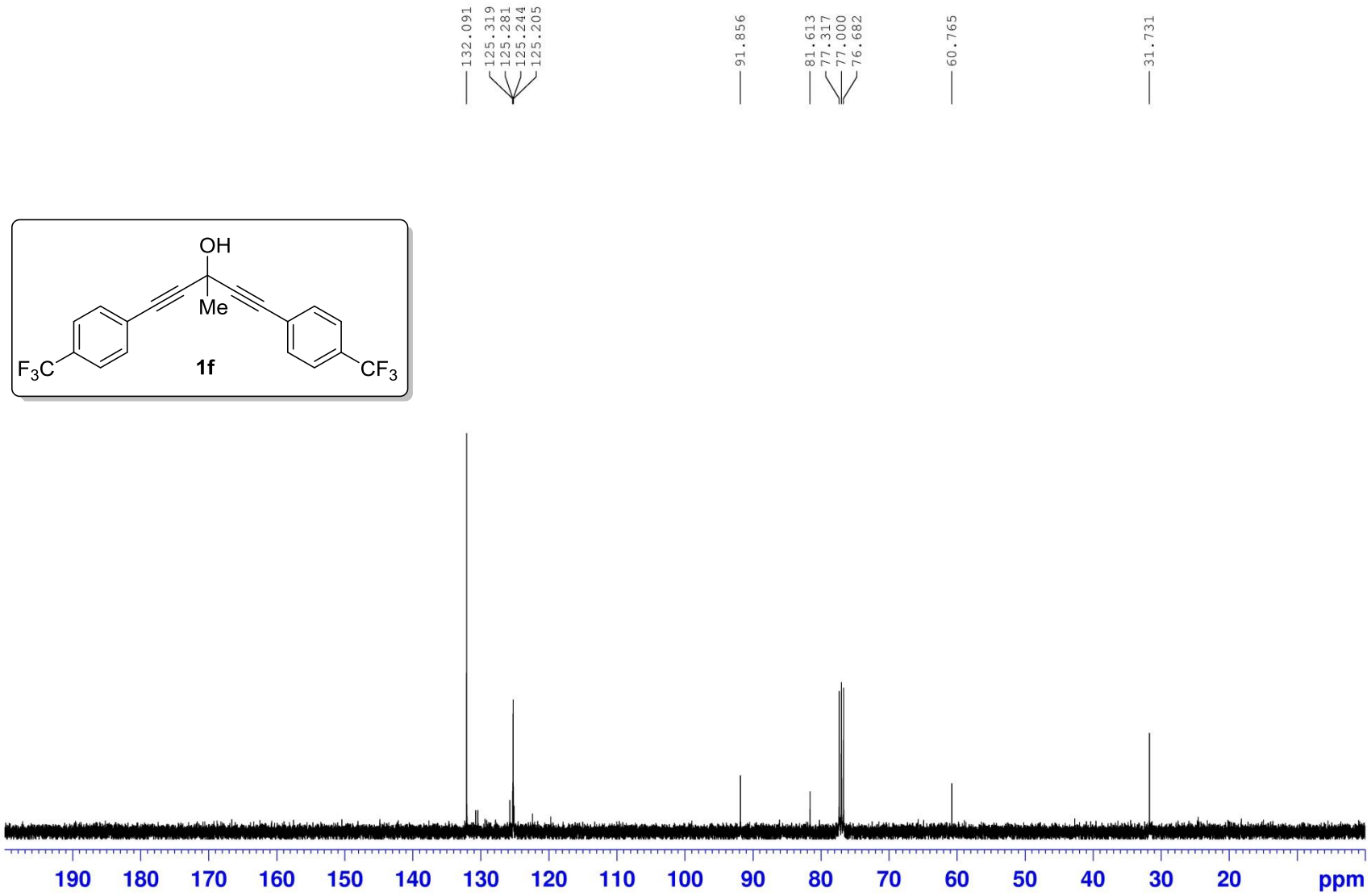

7.552
7.548
7.540
7.535
7.529
7.495
7.476
7.371
7.349
7.333
7.322
7.319
7.307
7.289
7.271
7.240
7.186
7.147
6.560
6.521
3.027
Current Data Parameters
NAME 20171122
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171122
Time 20.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 101
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
1d
10
9
8
7
6
5
4
3
2
1
ppm
4.10
2.08
9.23
1.07
1.00
1.00

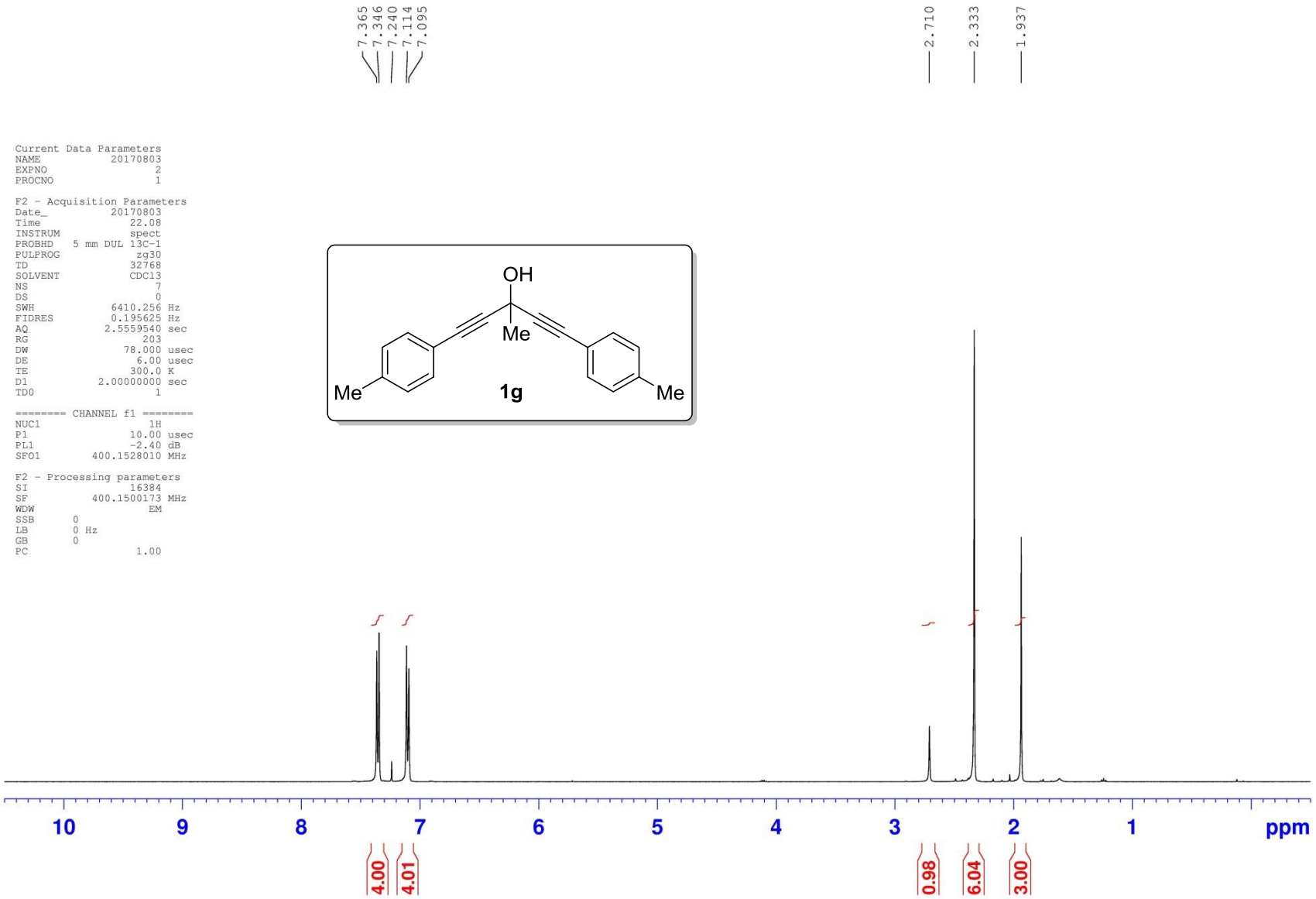

135.70
131.88
130.94
129.38
128.86
128.59
128.27
127.13
121.89
87.68
85.09
77.32
77.00
76.68
64.14
OH
1d
Current Data Parameters
NAME 20171122
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171122
Time 20.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 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 100.6178087 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

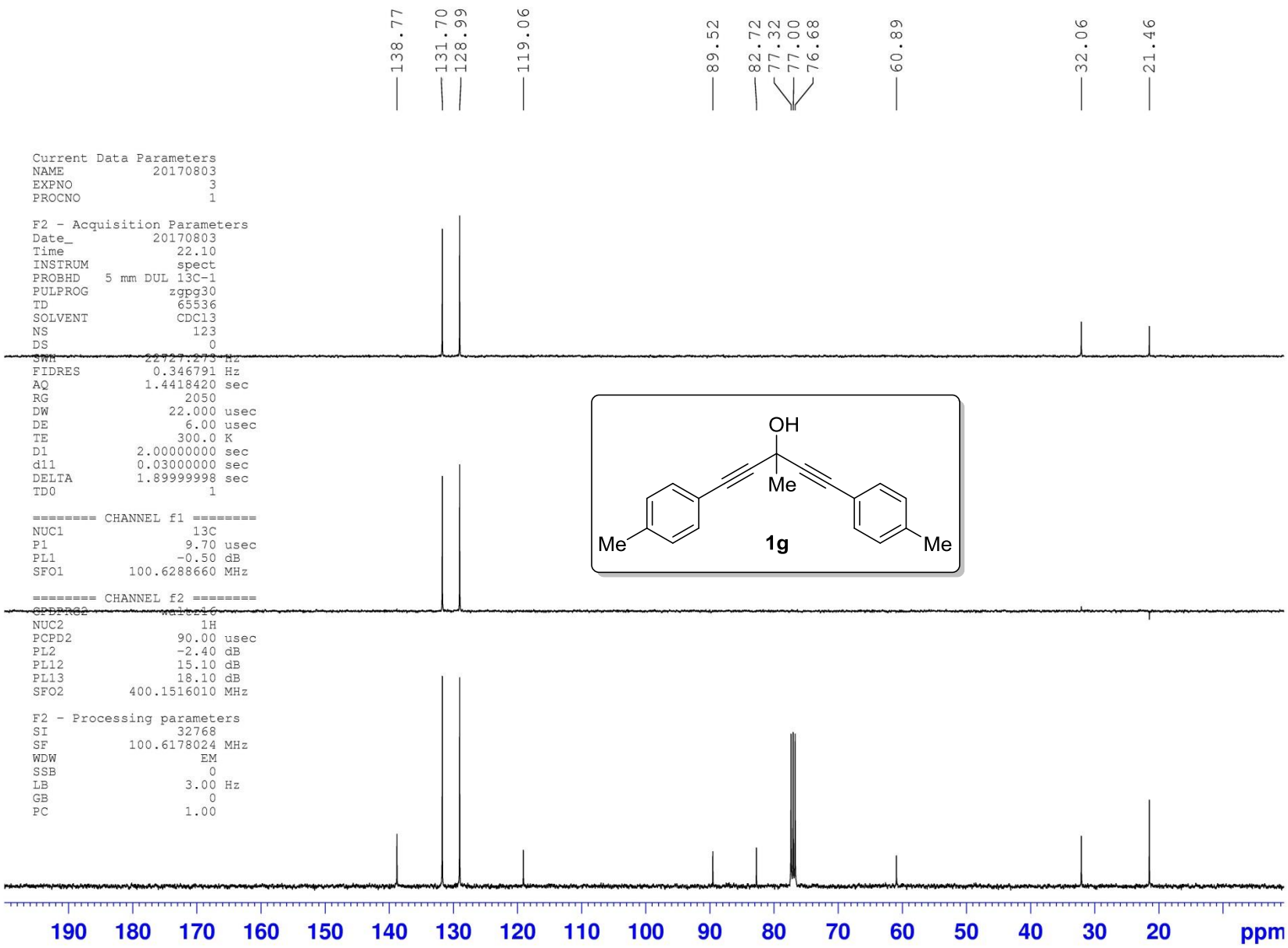

7.395
7.390
7.385
7.373
7.368
7.362
7.292
7.286
7.281
7.269
7.265
7.259
7.240
2.746
1.926
Current Data Parameters
NAME 20170719
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170719
Time 21.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 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 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
Me
Cl
Cl
1e
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
4.25
4.20
1.00
3.13

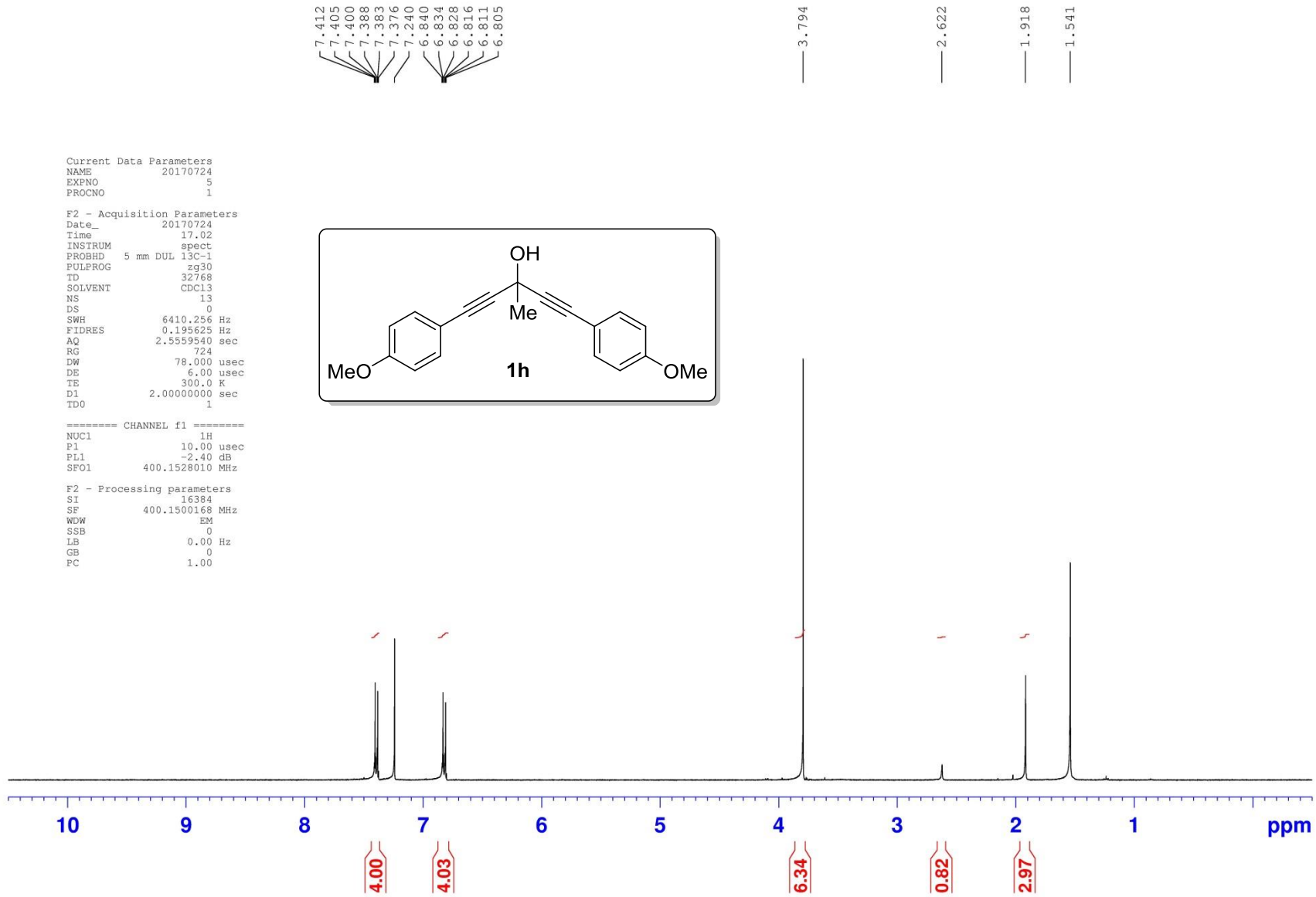

134.88
133.04
128.66
120.49
90.73
81.73
77.32
77.00
76.68
60.80
31.86
Current Data Parameters
NAME 20170719
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170719
Time 21.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 596
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
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
OH
Me
Cl
Cl
1e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

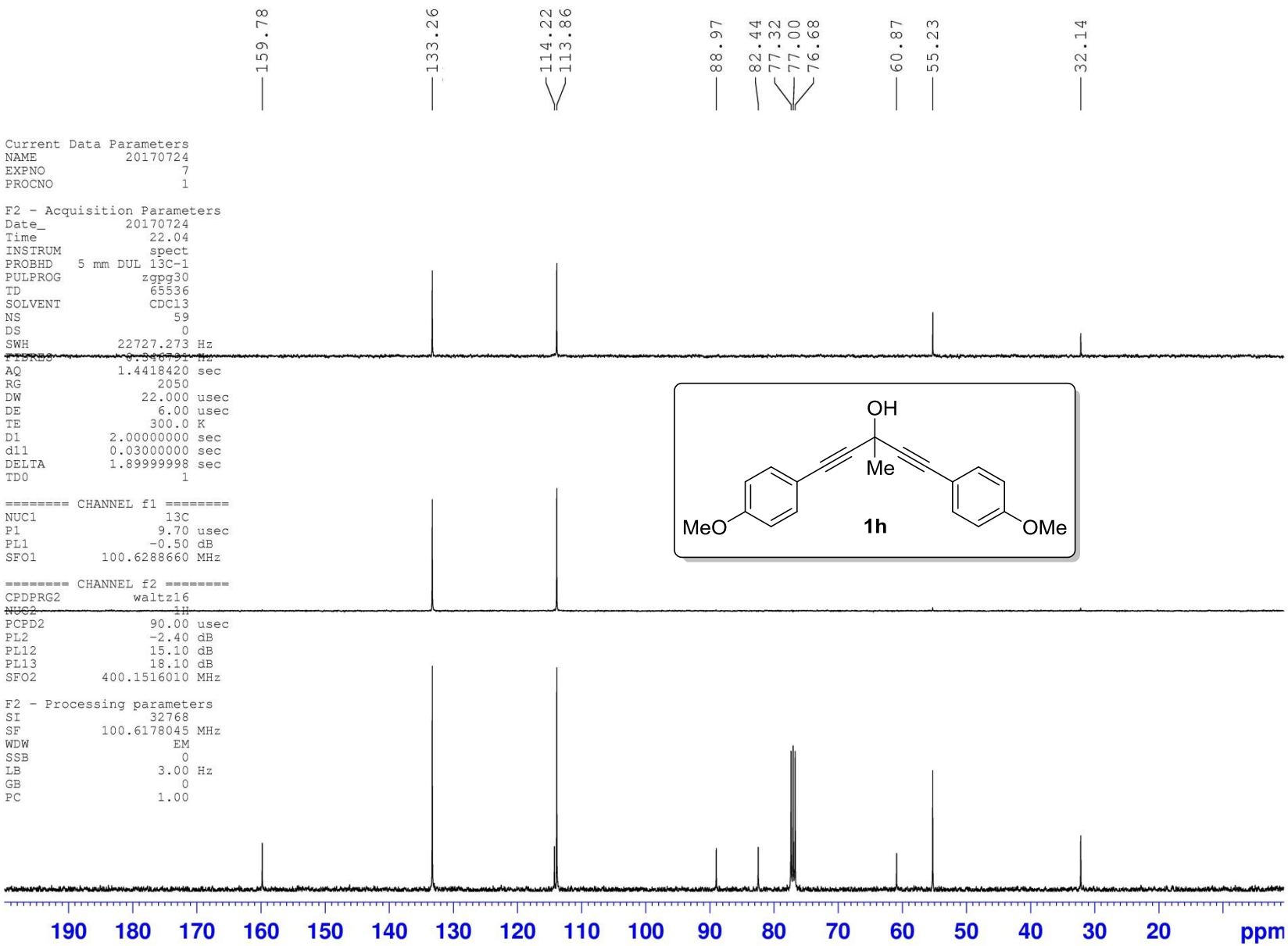

7.566
7.240
2.789
1.964
OH
Me
F3C
CF3
1f
10
9
8
7
6
5
4
3
2
1
ppm
8.00
0.88
3.12

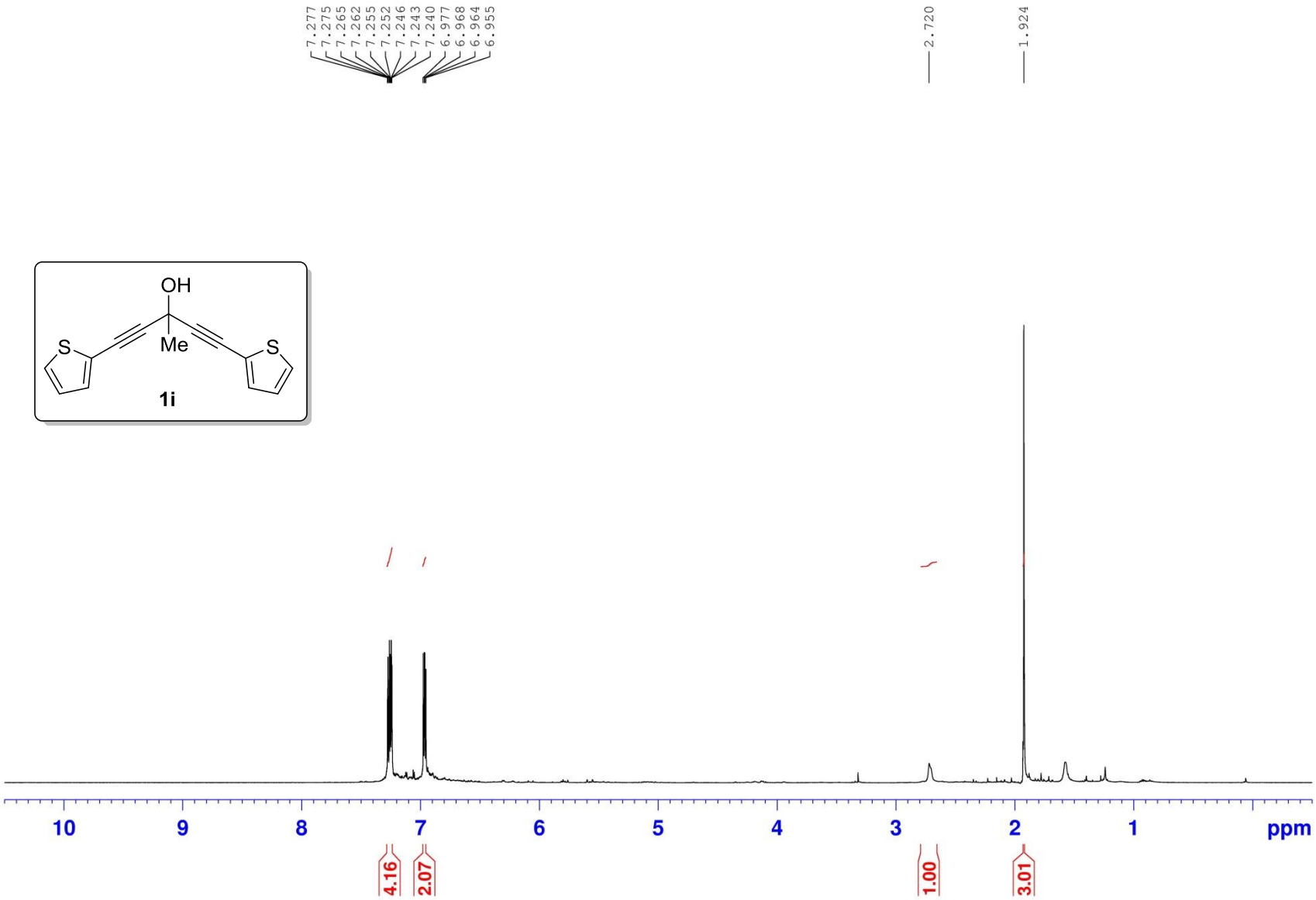

132.091
125.319
125.281
125.244
125.205
91.856
81.613
77.317
77.000
76.682
60.765
31.731
OH
Me
F3C
CF3
1f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

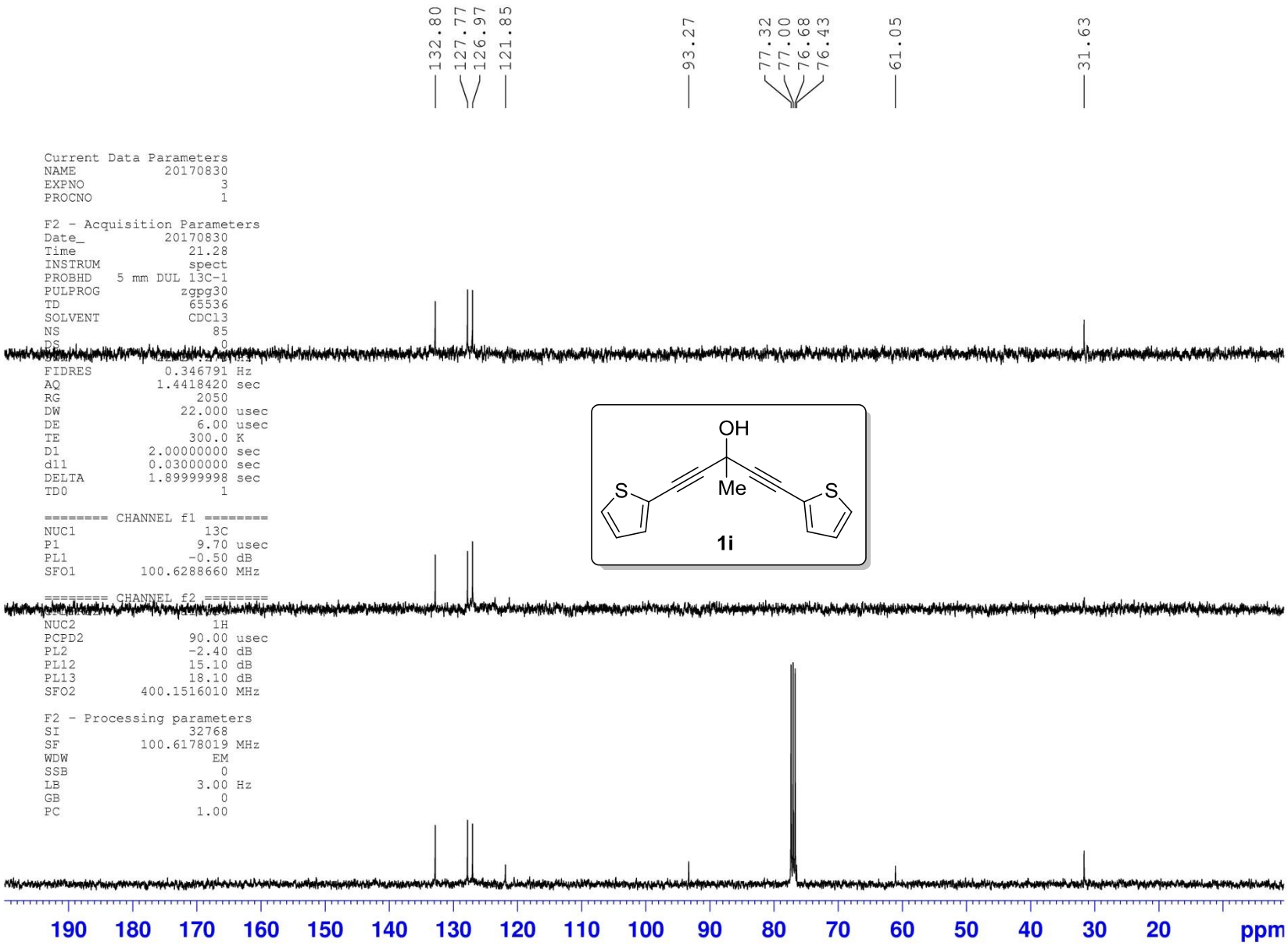

7.365
7.346
7.240
7.114
7.095
2.710
2.333
1.937
Current Data Parameters
NAME 20170803
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170803
Time 22.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 203
DW 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 Hz
GB 0
PC 1.00
OH
Me
Me
Me
1g
10
9
8
7
6
5
4
3
2
1
ppm
4.00
4.01
0.98
6.04
3.00

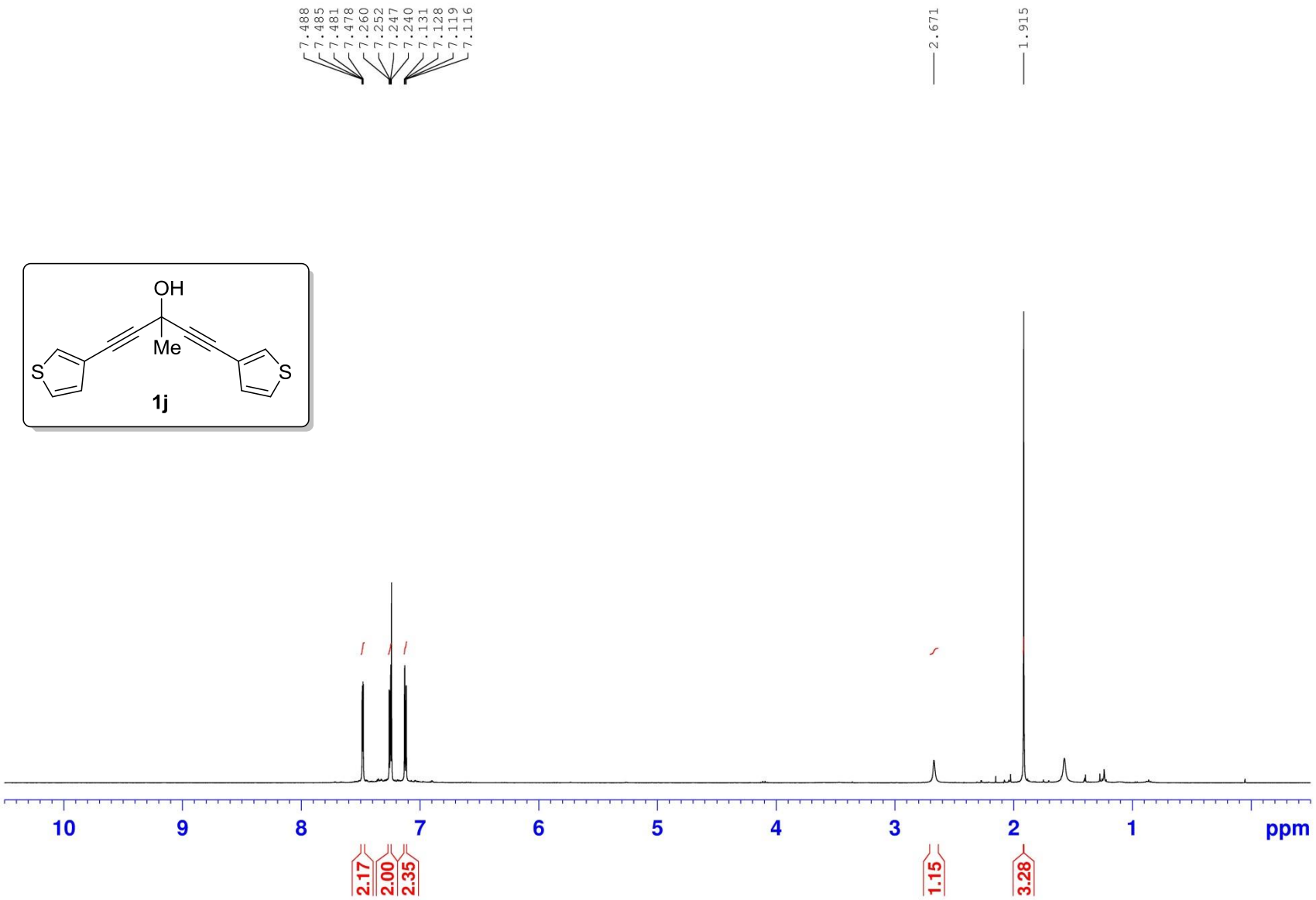

138.77
131.70
128.99
119.06
89.52
82.72
77.32
77.00
76.68
60.89
32.06
21.46
Current Data Parameters
NAME 20170803
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170803
Time 22.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 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 100.6178024 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
Me
Me
1g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

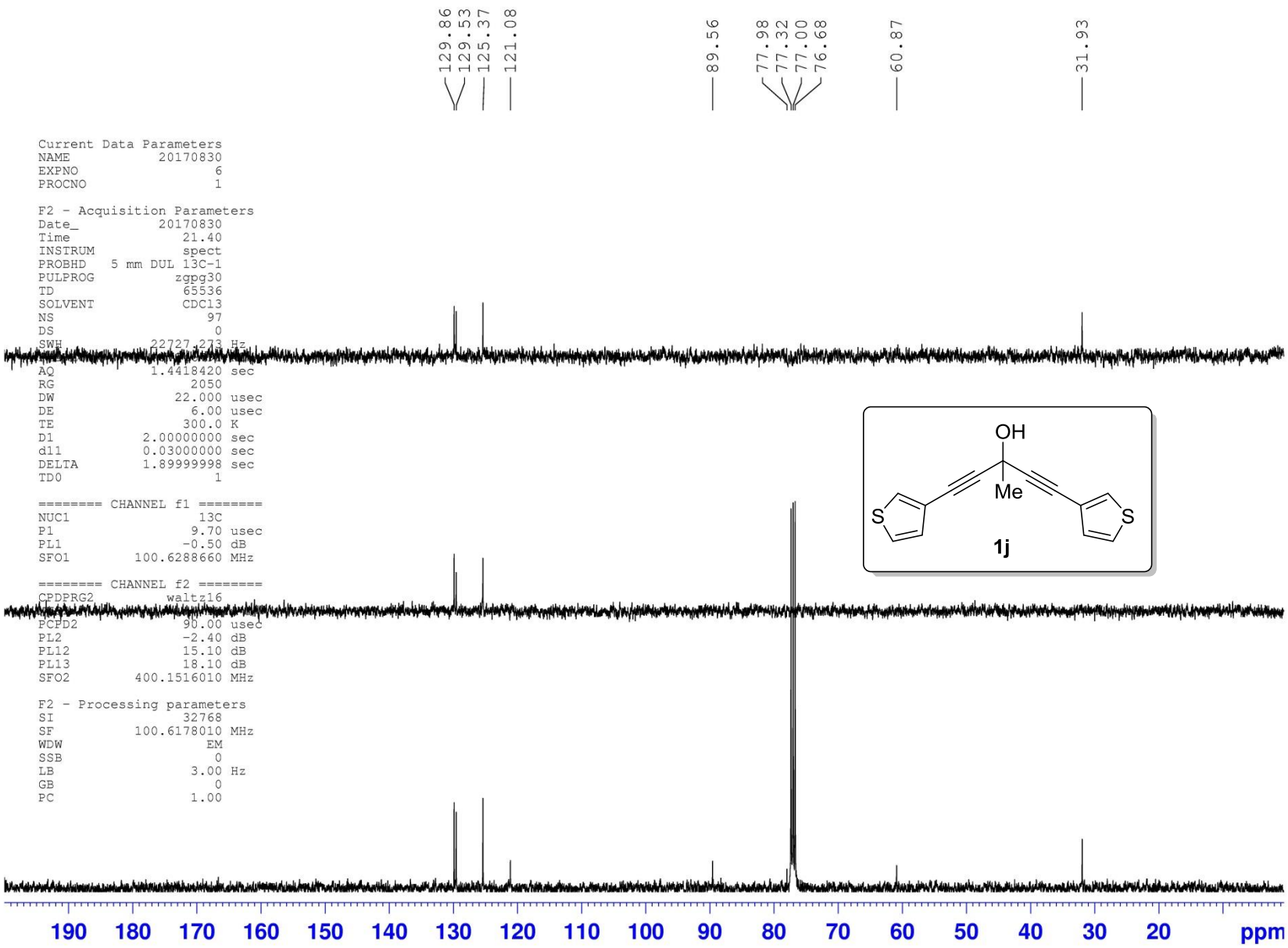

7.412
7.405
7.400
7.388
7.383
7.376
7.240
6.840
6.834
6.828
6.816
6.811
6.805
3.794
2.622
1.918
1.541
Current Data Parameters
NAME 20170724
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170724
Time 17.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 13
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 724
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
OH
Me
MeO
OMe
1h
10
9
8
7
6
5
4
3
2
1
ppm
4.00
4.03
6.34
0.82
2.97

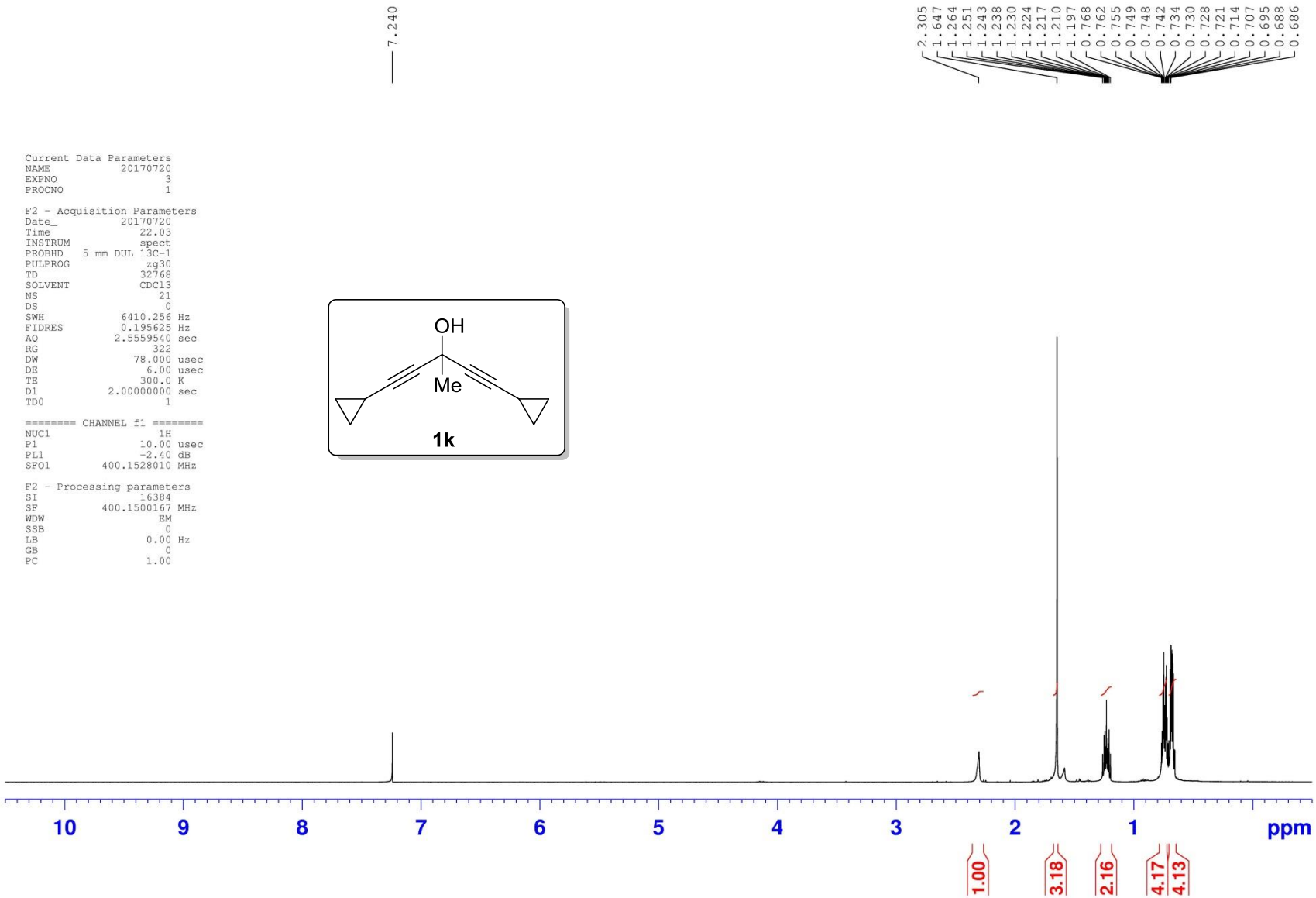

159.78
133.26
114.22
113.86
88.97
82.44
77.32
77.00
76.68
60.87
55.23
32.14
Current Data Parameters
NAME 20170724
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170724
Time 22.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 59
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 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 100.6178045 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
MeO
OMe
1h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

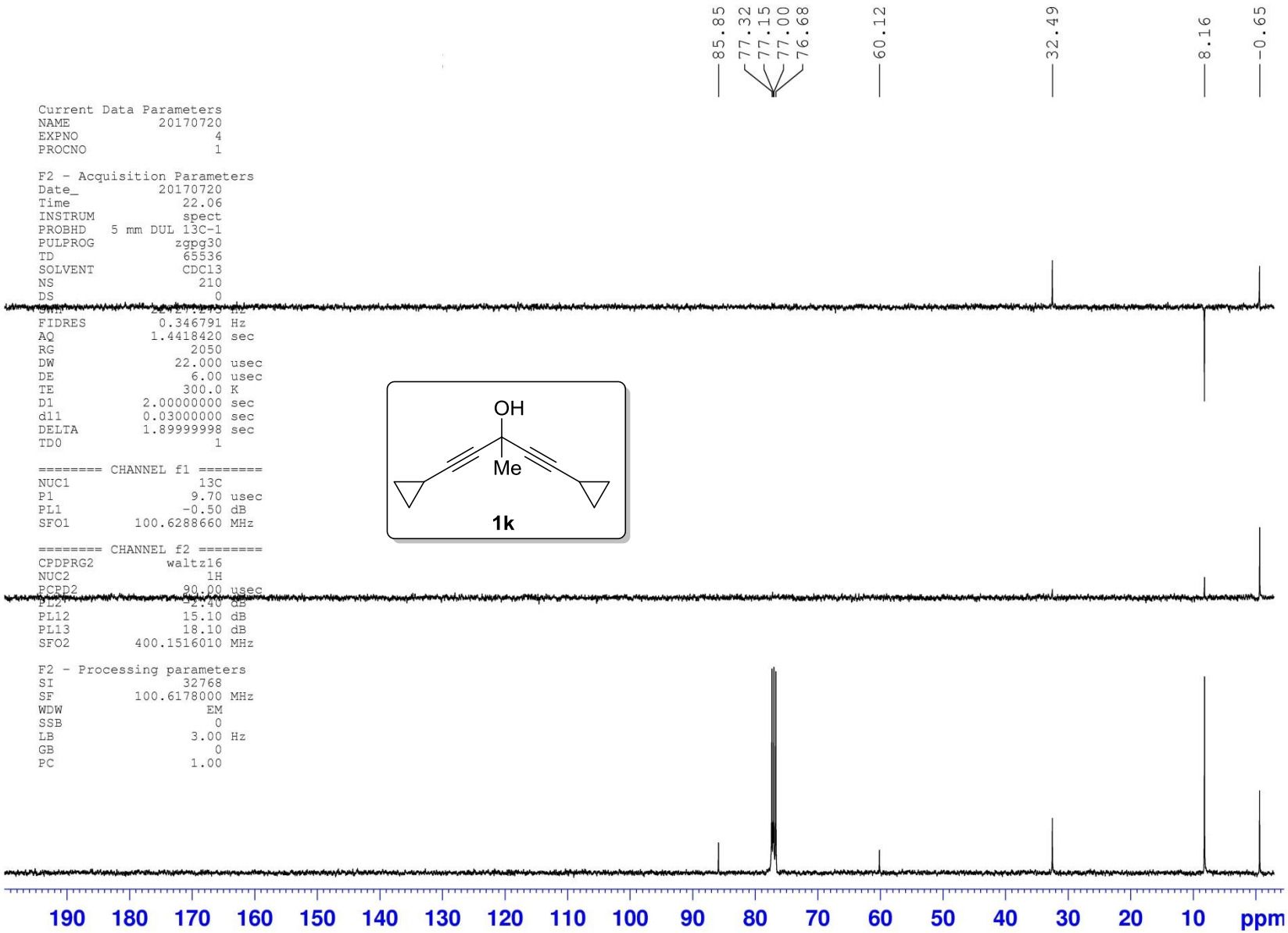

7.277
7.275
7.265
7.262
7.255
7.252
7.246
7.243
7.240
6.977
6.968
6.964
6.955
2.720
1.924
OH
Me
S
S
1i
10
9
8
7
6
5
4
3
2
1
ppm
4.16
2.07
1.00
3.01

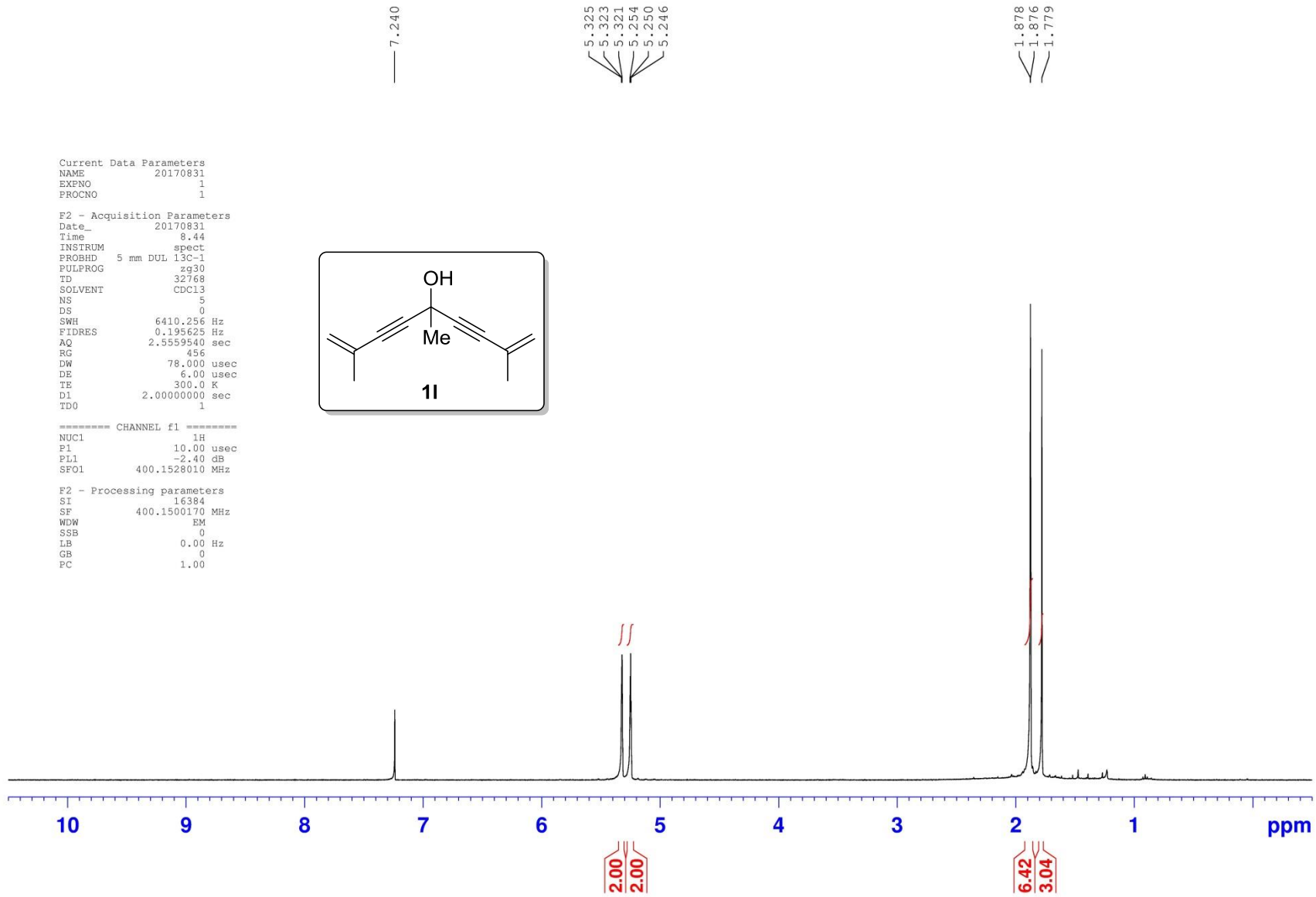

132.80
127.77
126.97
121.85
93.27
77.32
77.00
76.68
76.43
61.05
31.63
Current Data Parameters
NAME 20170830
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170830
Time 21.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 85
DS 0
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178019 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
S
Me
S
1i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

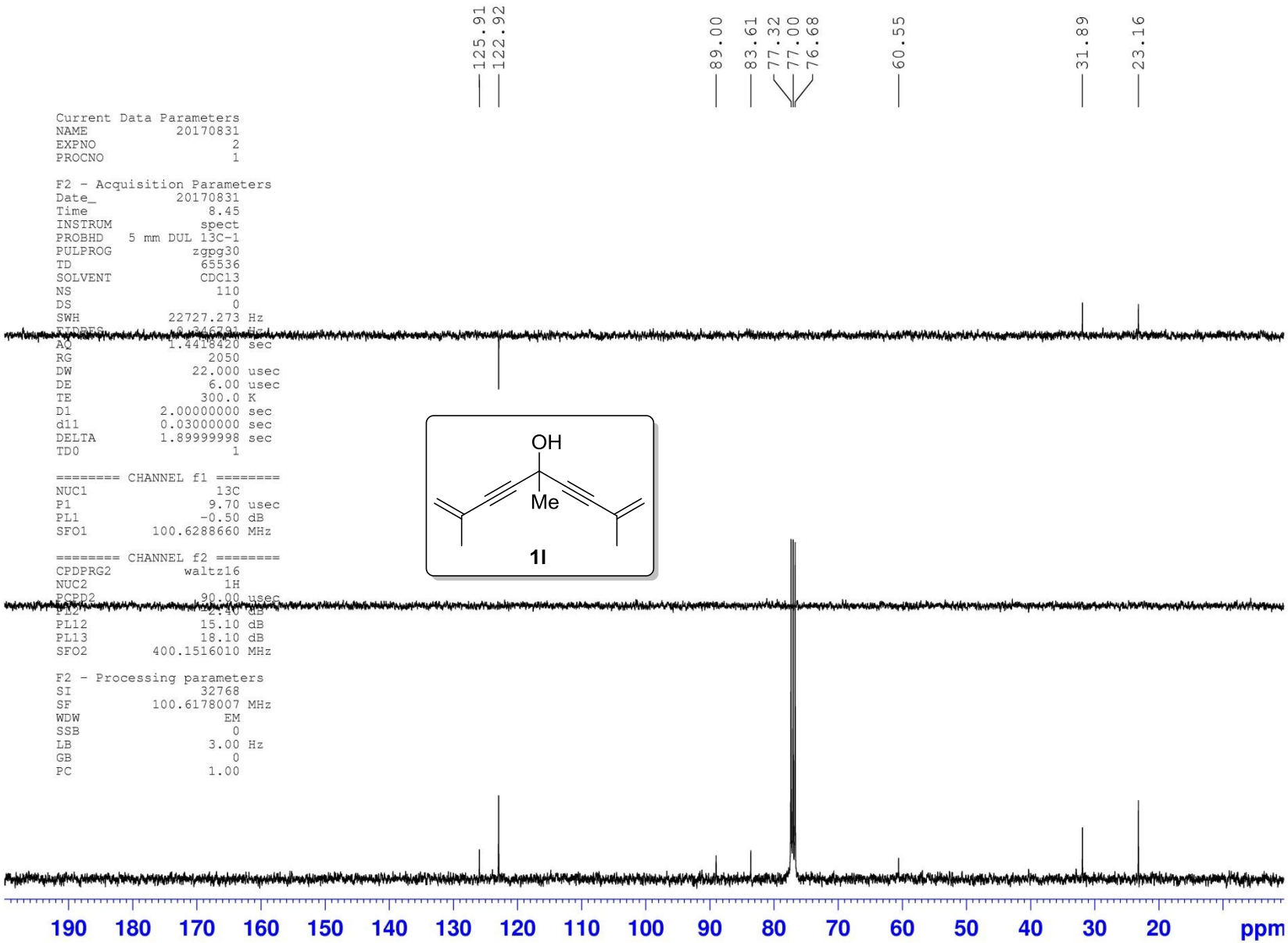

7.488
7.485
7.481
7.478
7.260
7.252
7.247
7.240
7.131
7.128
7.119
7.116
2.671
1.915
OH
Me
S
S
1j
10
9
8
7
6
5
4
3
2
1
ppm
2.17
2.00
2.35
1.15
3.28

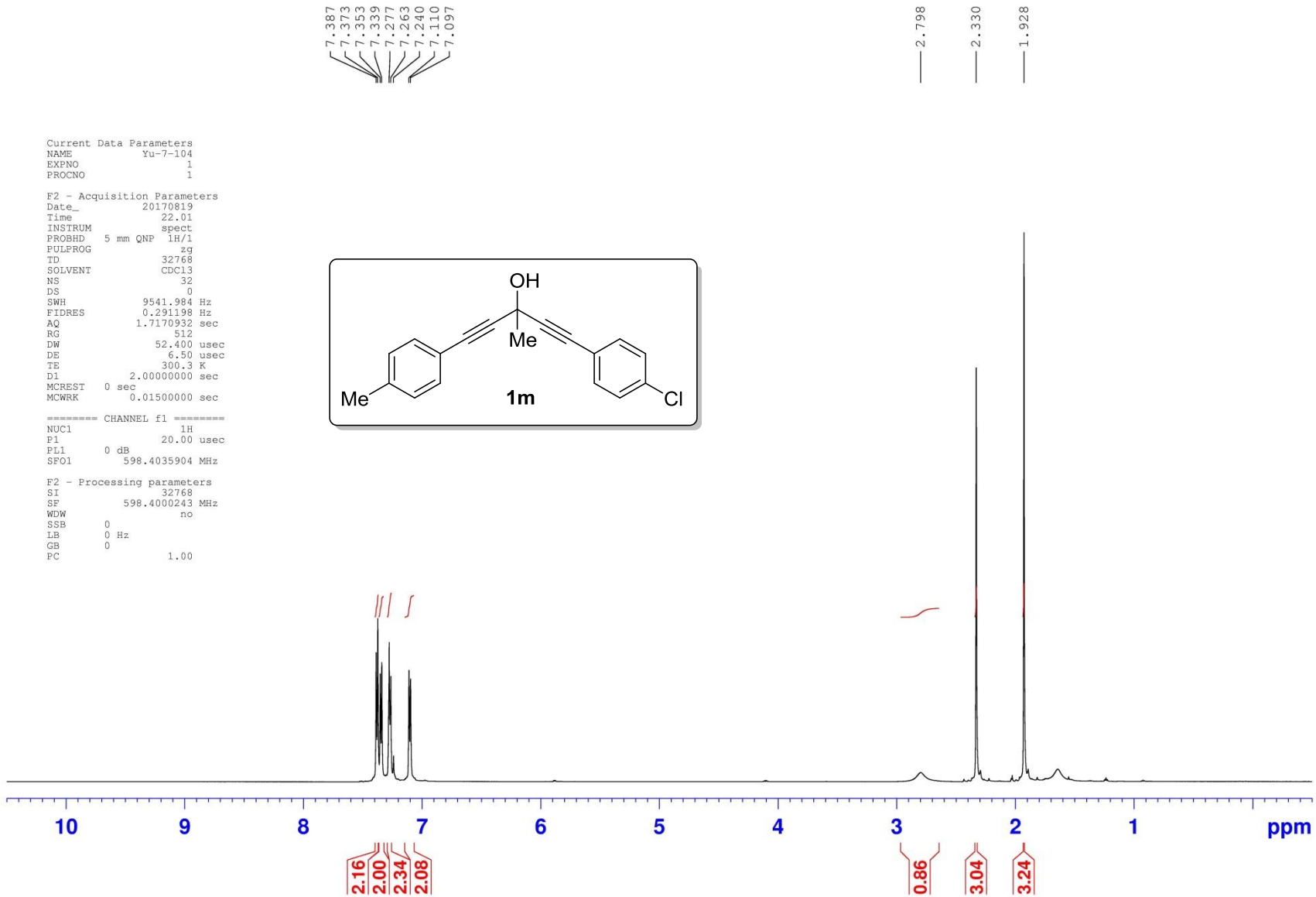

129.86
129.53
125.37
121.08
89.56
77.98
77.32
77.00
76.68
60.87
31.93
Current Data Parameters
NAME 20170830
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170830
Time 21.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 97
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 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
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 100.6178010 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
S
S
1j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

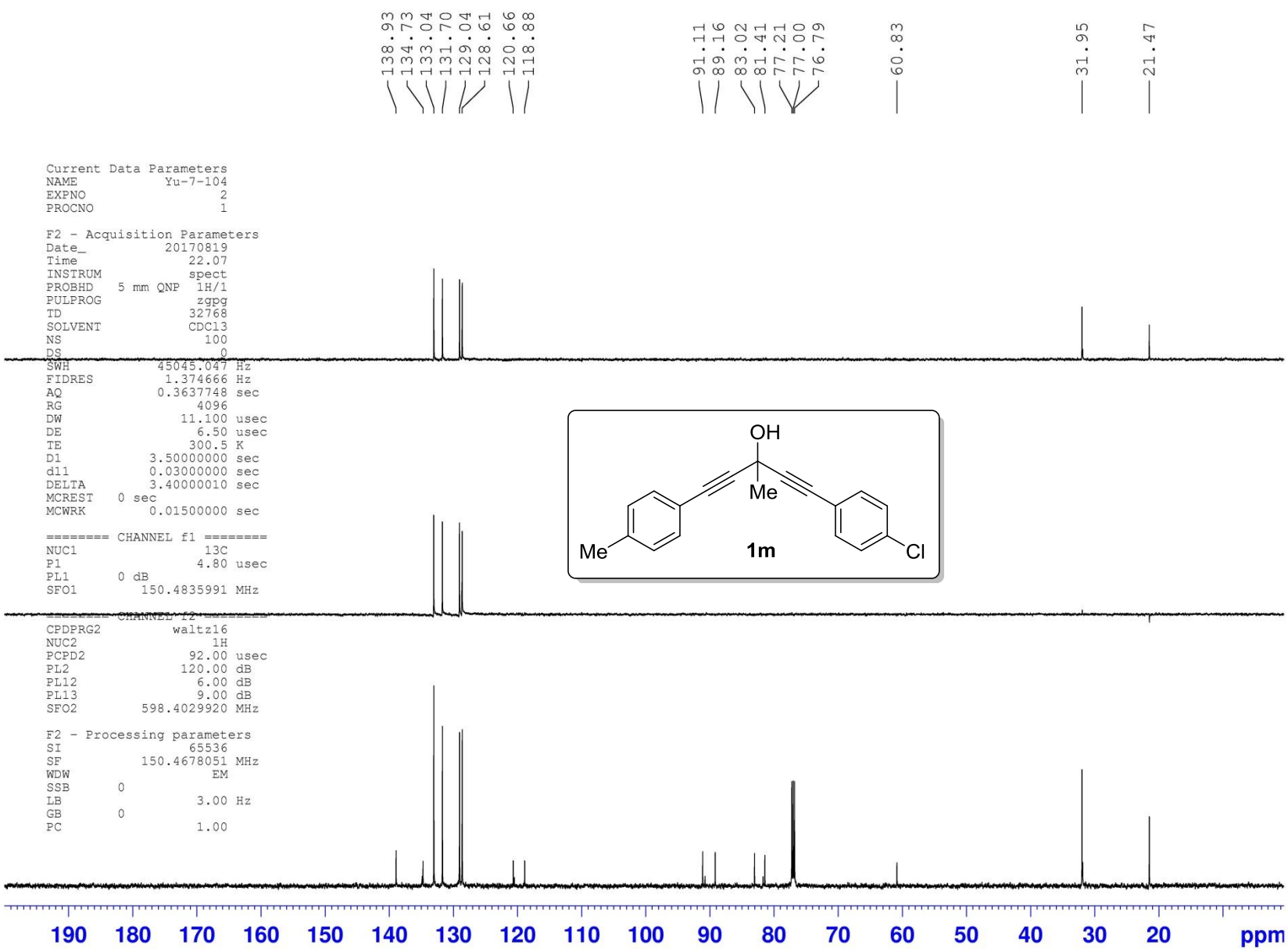

7.240
2.305
1.647
1.264
1.251
1.243
1.238
1.230
1.224
1.217
1.210
1.197
0.768
0.762
0.755
0.749
0.748
0.742
0.734
0.730
0.728
0.721
0.714
0.707
0.695
0.688
0.686
Current Data Parameters
NAME 20170720
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170720
Time 22.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 21
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
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
OH
Me
1k
10
9
8
7
6
5
4
3
2
1
ppm
1.00
3.18
2.16
4.17
4.13

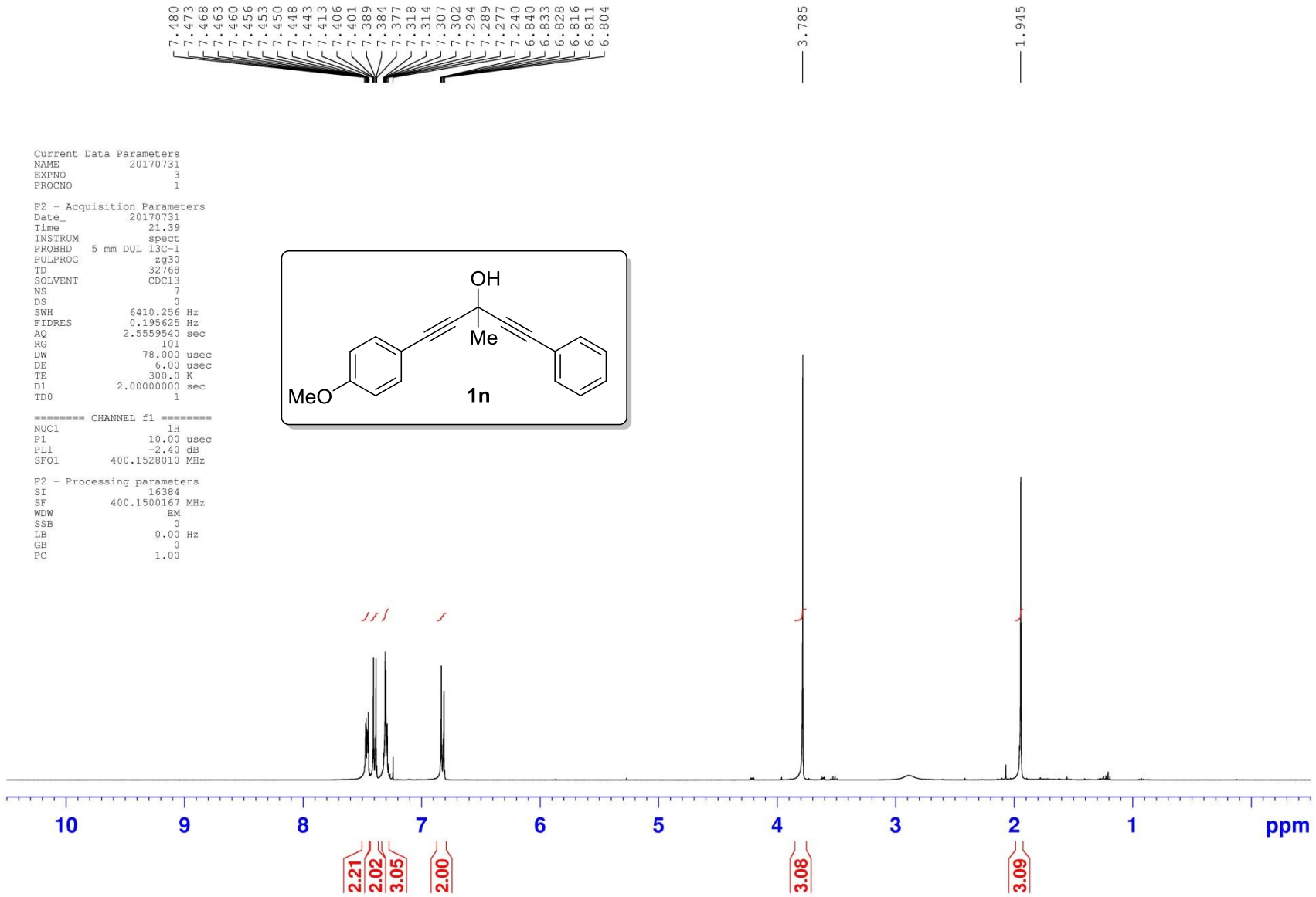

85.85
77.32
77.15
77.00
76.68
60.12
32.49
8.16
0.65
Current Data Parameters
NAME 20170720
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170720
Time 22.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 210
DS 0
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 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 100.6178000 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
1k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

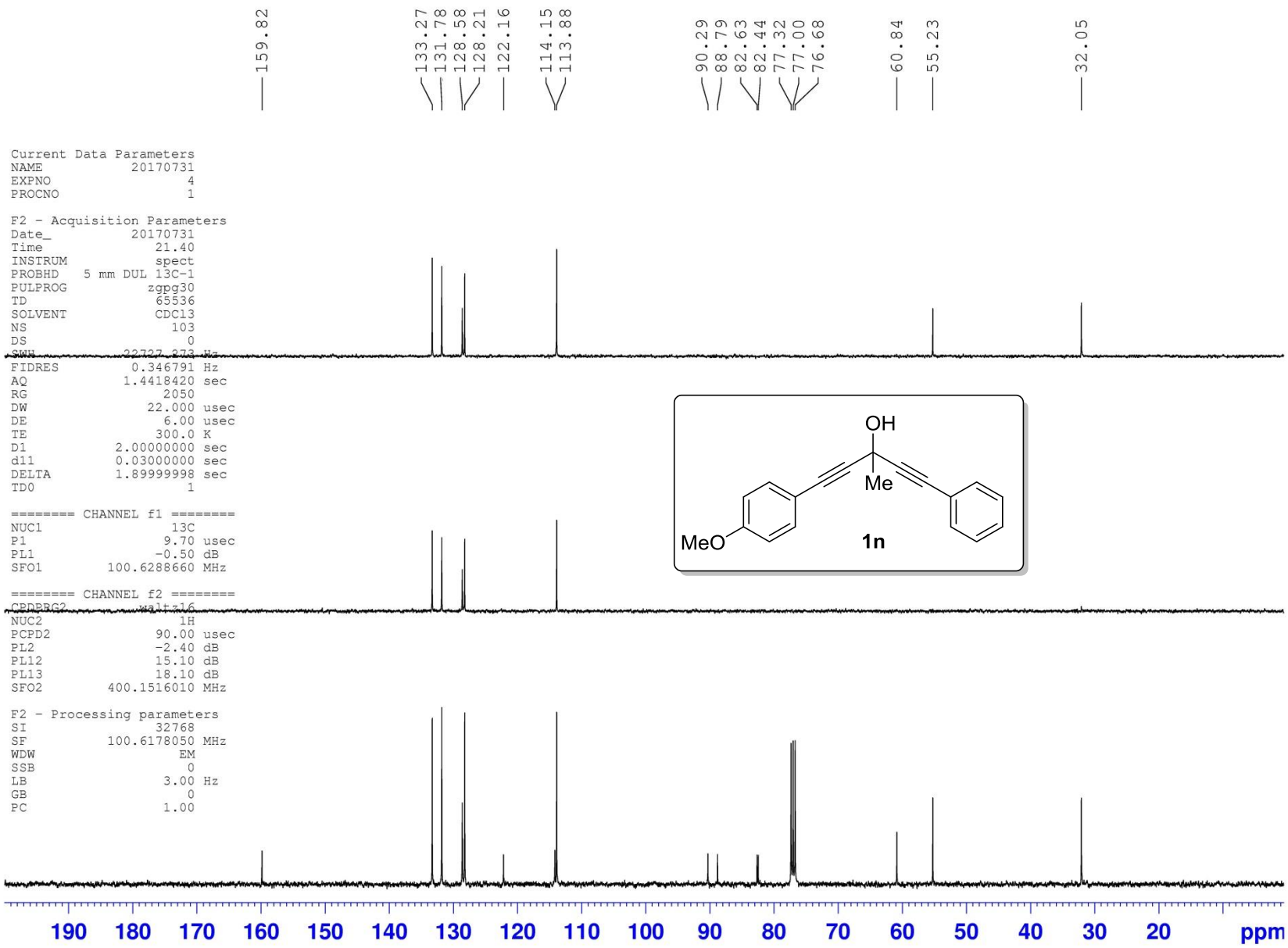

7.240
5.325
5.323
5.321
5.254
5.250
5.246
1.878
1.876
1.779
Current Data Parameters
NAME 20170831
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170831
Time 8.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
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 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
Me
1l
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
6.42
3.04

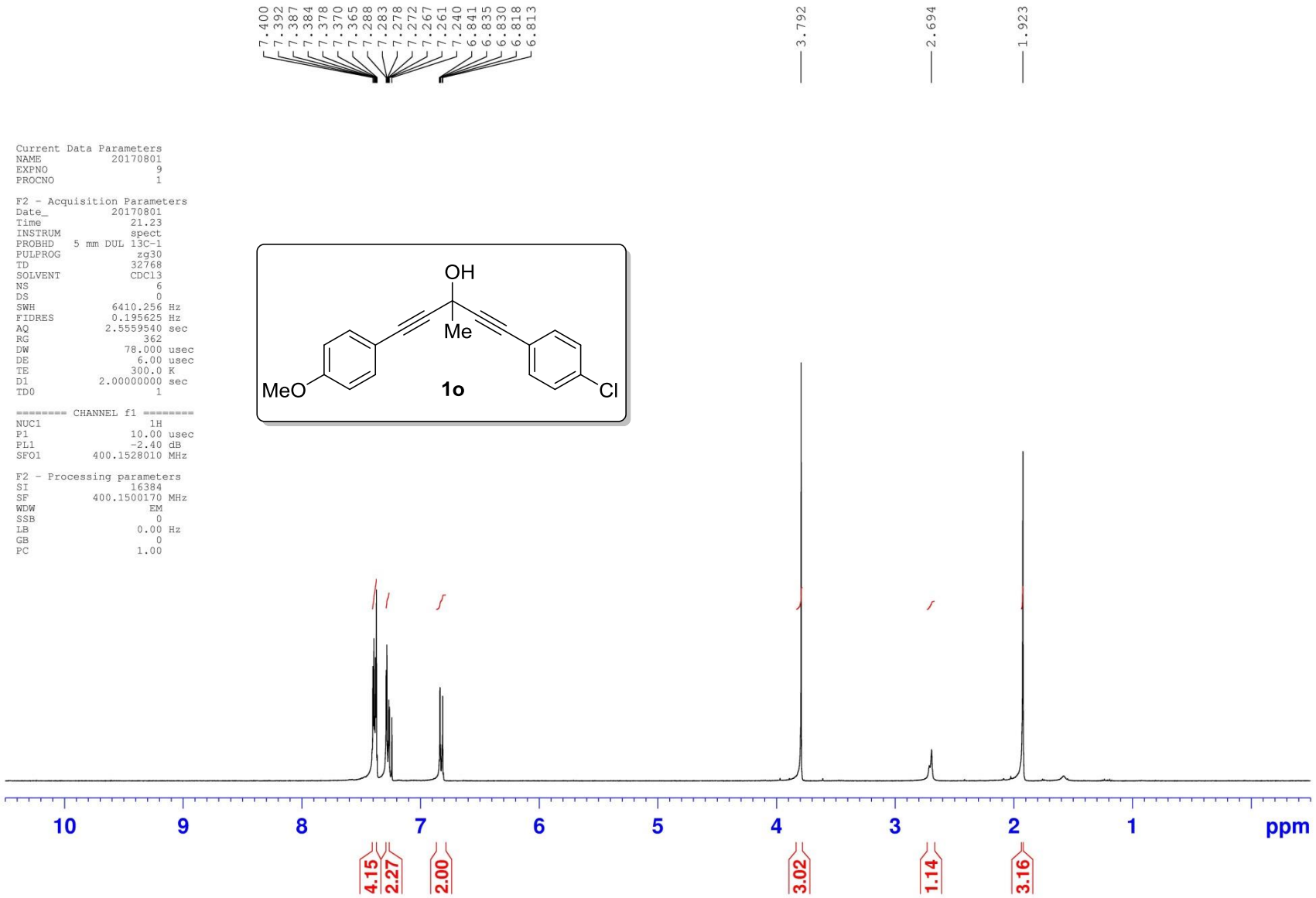

125.91
122.92
89.00
83.61
77.32
77.00
76.68
60.55
31.89
23.16
Current Data Parameters
NAME 20170831
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170831
Time 8.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 110
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 2050
DW 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
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178007 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
1l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

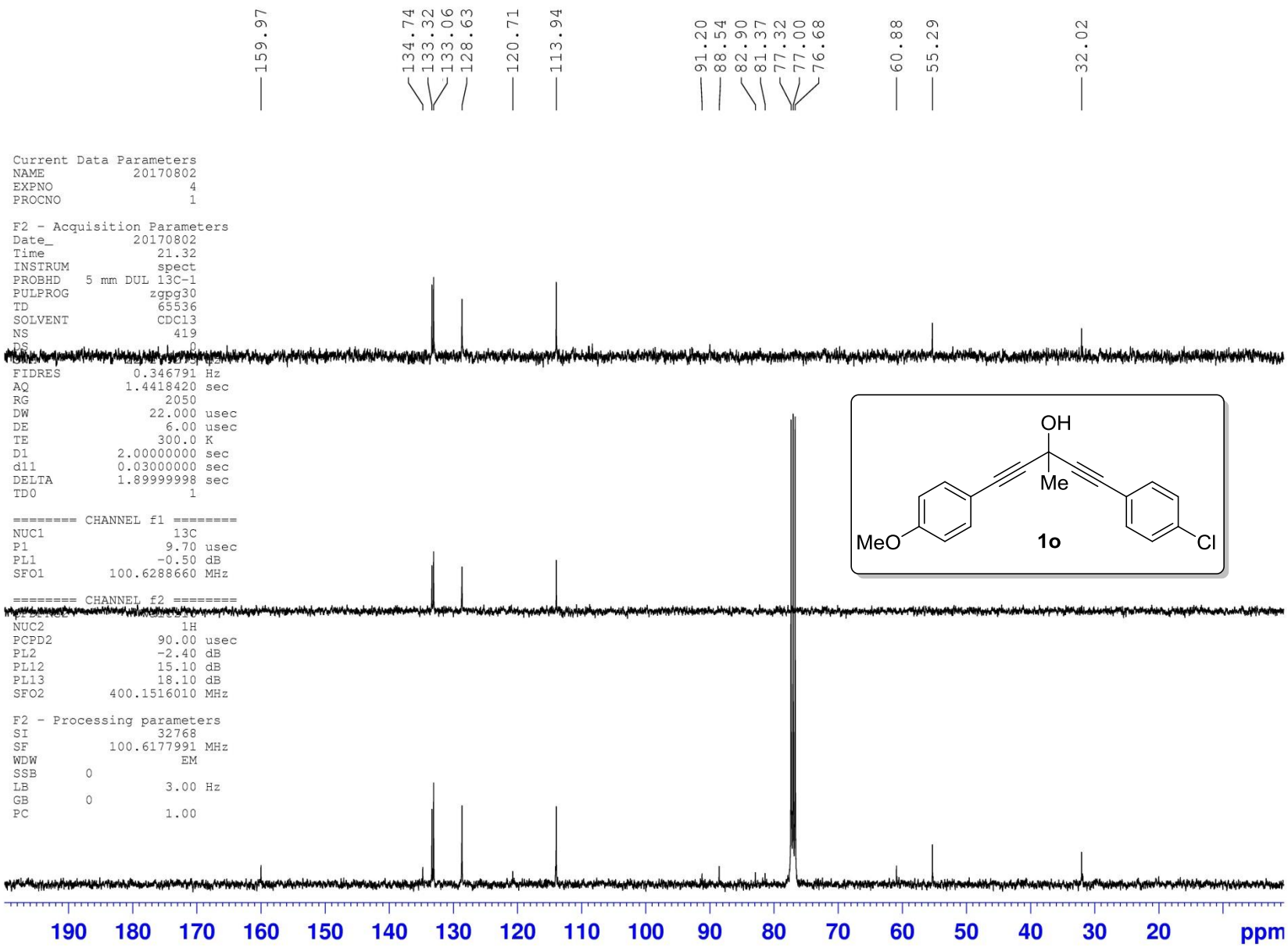

7.387
7.373
7.353
7.339
7.277
7.263
7.240
7.110
7.097
2.798
2.330
1.928
Current Data Parameters
NAME Yu-7-104
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170819
Time 22.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 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 20.00 usec
PL1 0 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000243 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
OH
Me
Me
Cl
1m
10
9
8
7
6
5
4
3
2
1
ppm
2.16
2.00
2.34
2.08
0.86
3.04
3.24

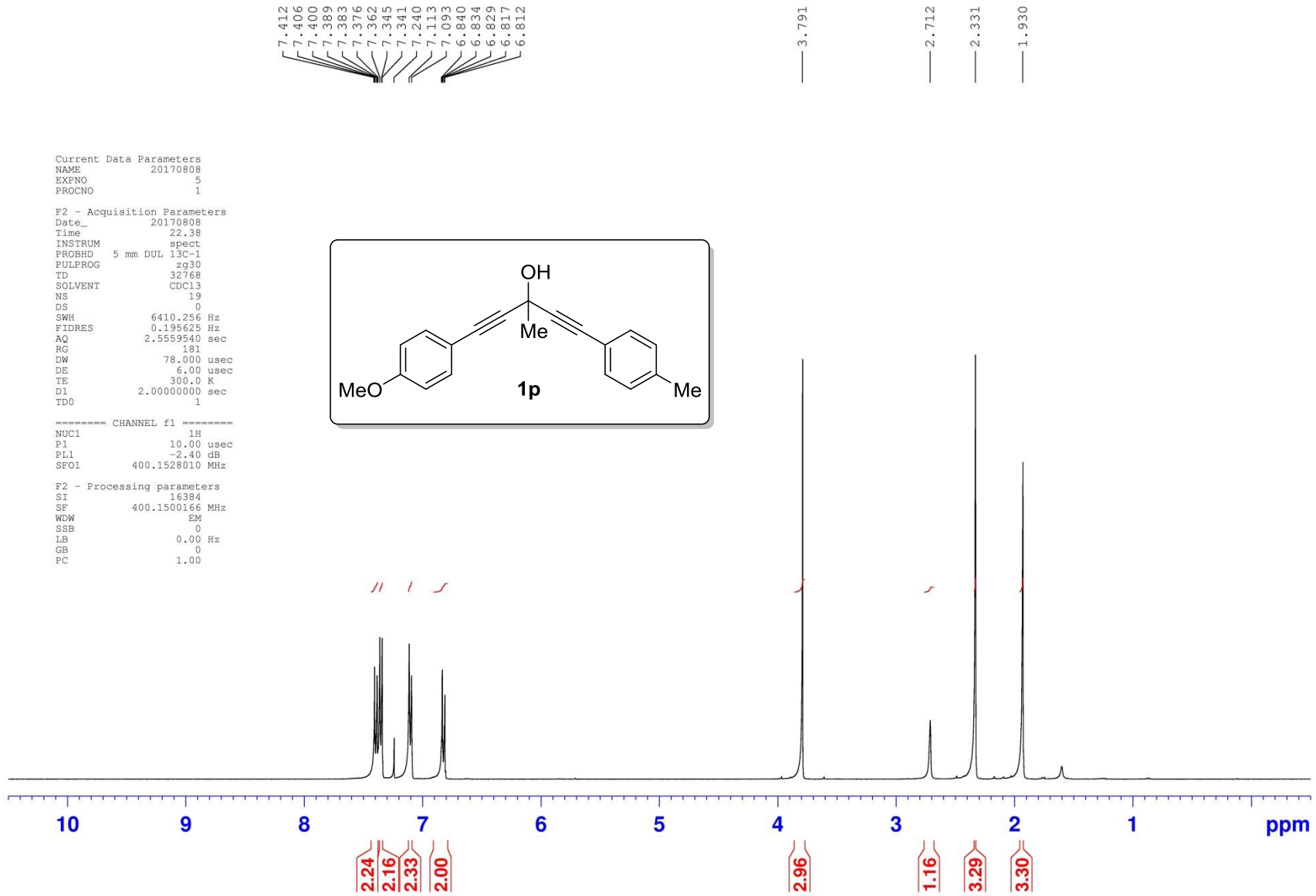

138.93
134.73
133.04
131.70
129.04
128.61
120.66
118.88
91.11
89.16
83.02
81.41
77.21
77.00
76.79
60.83
31.95
21.47
Current Data Parameters
NAME Yu-7-104
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170819
Time 22.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
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 300.5 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 150.4835991 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678051 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
Me
Cl
1m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

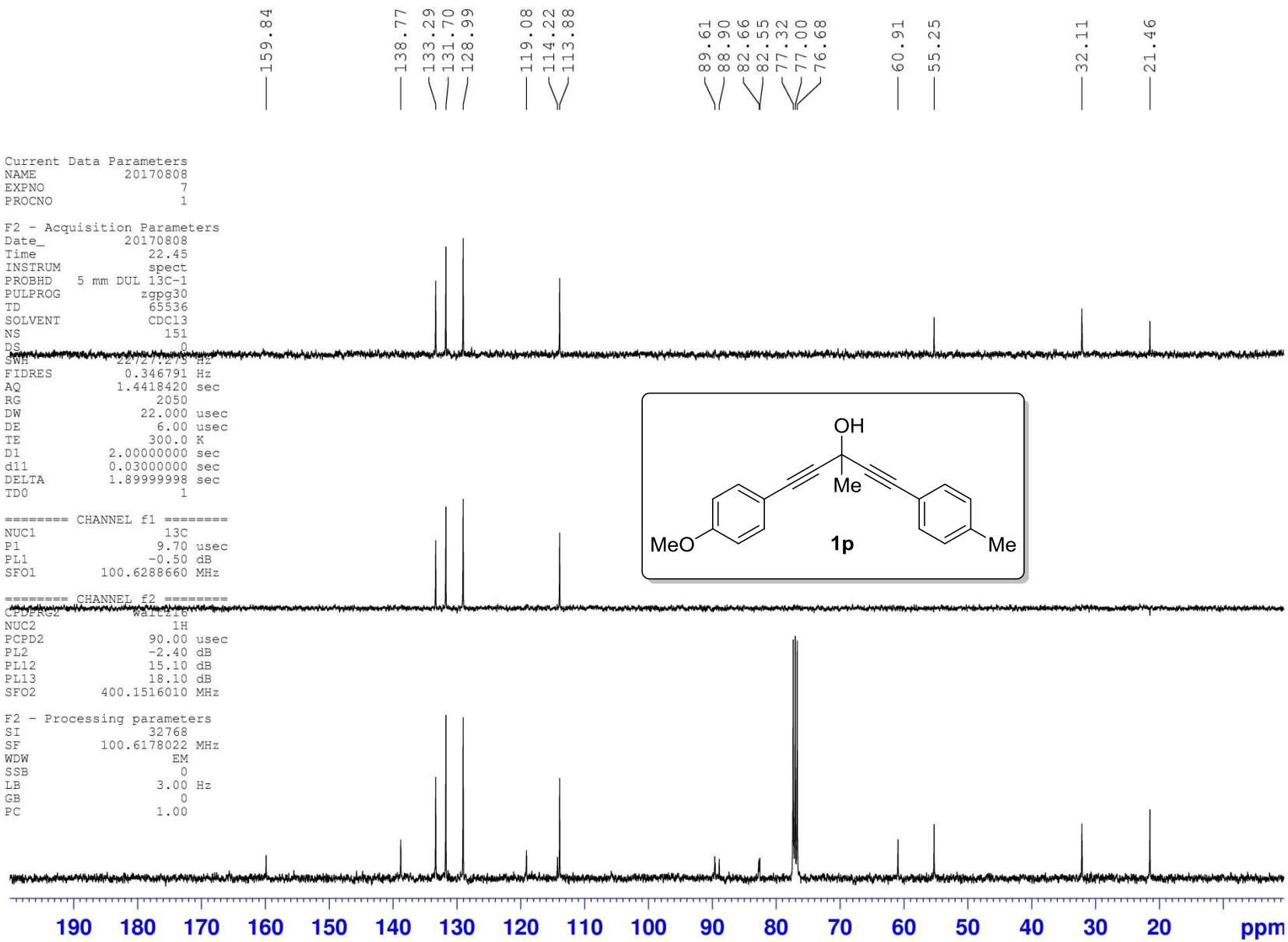

7.480
7.473
7.468
7.463
7.460
7.456
7.453
7.450
7.448
7.443
7.413
7.406
7.401
7.389
7.384
7.377
7.318
7.314
7.307
7.302
7.294
7.289
7.277
7.240
6.840
6.833
6.828
6.816
6.811
6.804
3.785
1.945
Current Data Parameters
NAME 20170731
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170731
Time 21.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 101
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
Me
MeO
1n
10
9
8
7
6
5
4
3
2
1
ppm
2.21
2.02
3.05
2.00
3.08
3.09

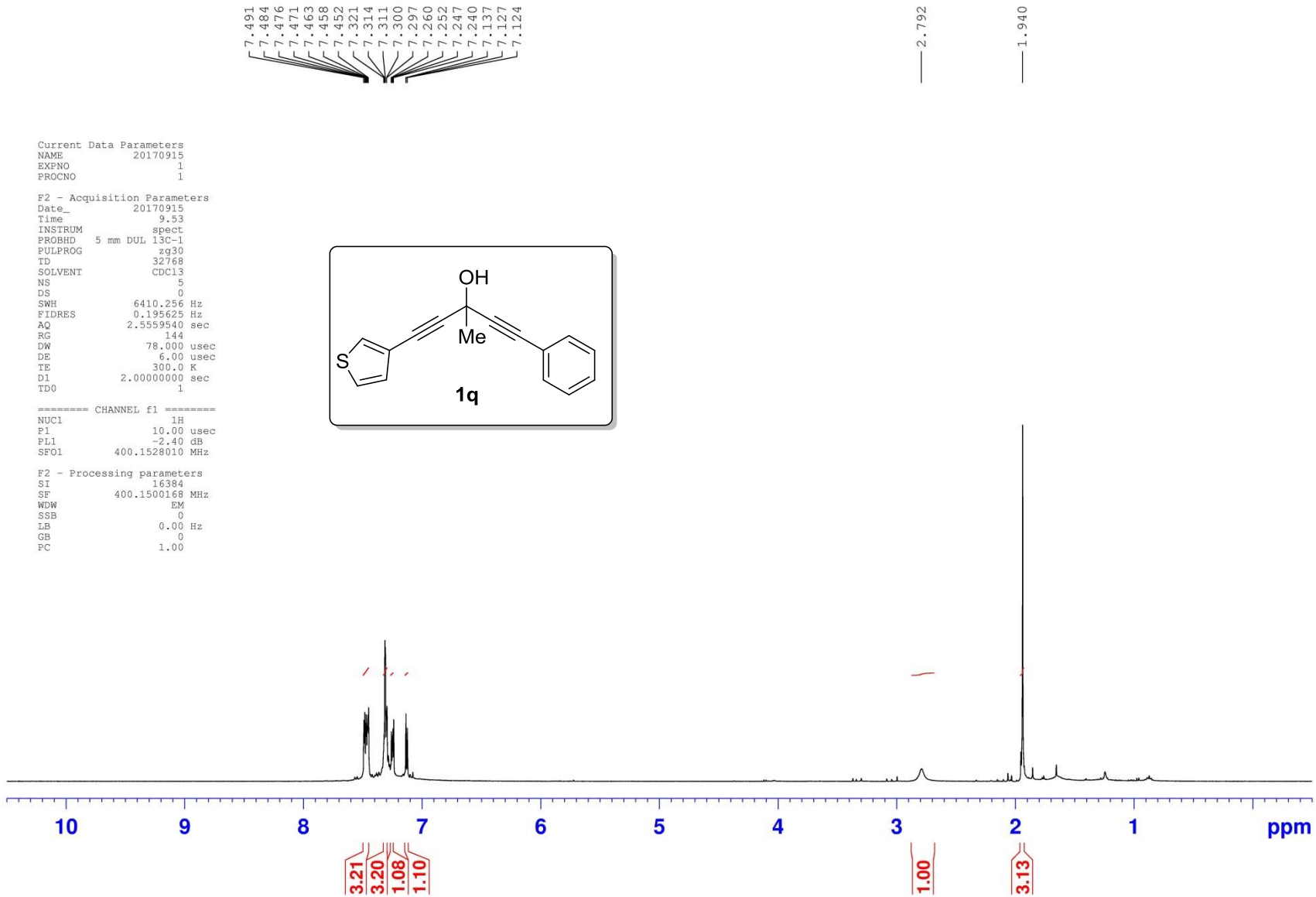

159.82
133.27
131.78
128.58
128.21
122.16
114.15
113.88
90.29
88.79
82.63
82.44
77.32
77.00
76.68
60.84
55.23
32.05
Current Data Parameters
NAME 20170731
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170731
Time 21.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 103
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 100.6178050 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
MeO
1n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

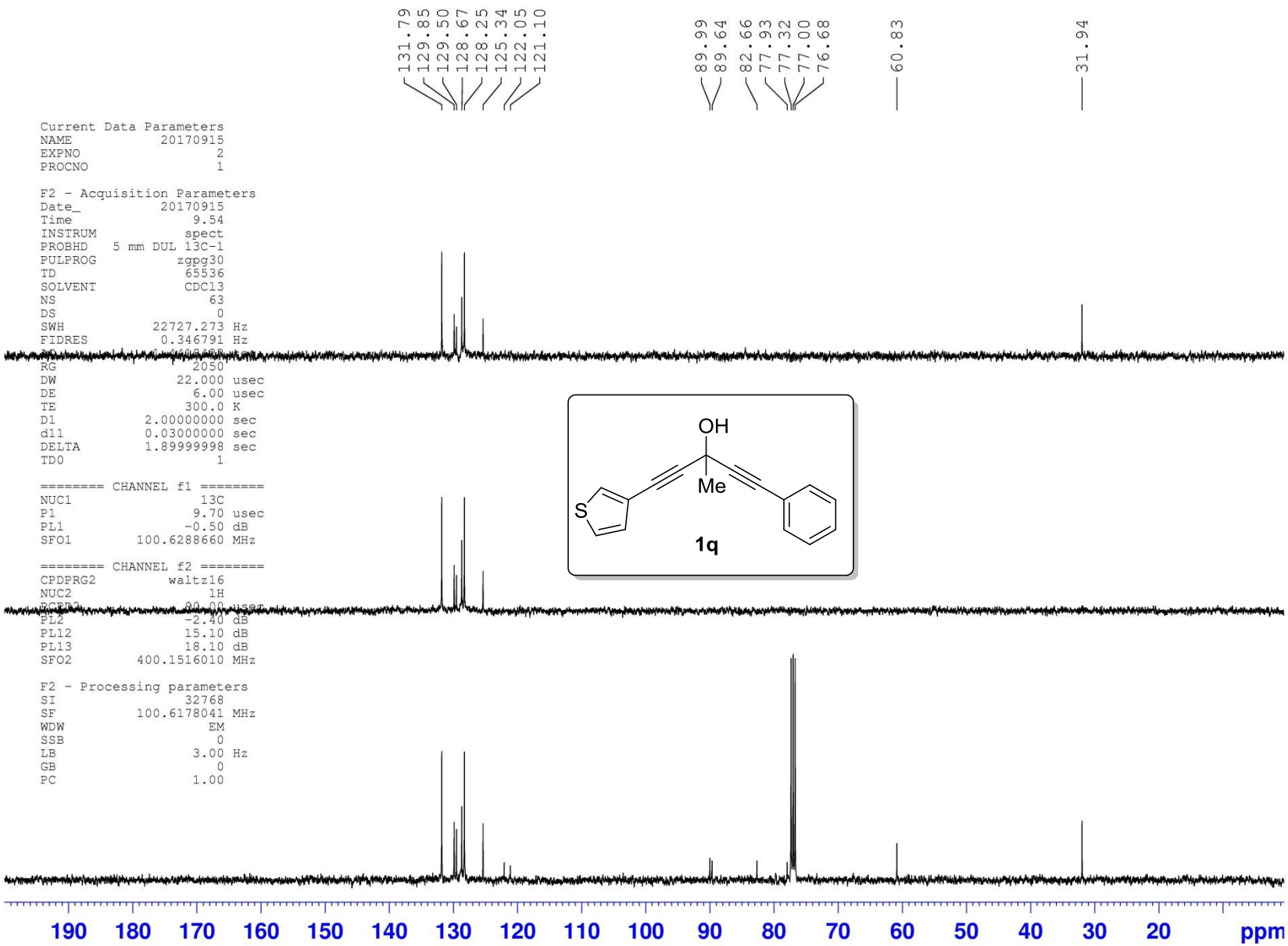

7.400
7.392
7.387
7.384
7.378
7.370
7.365
7.288
7.283
7.278
7.272
7.267
7.261
7.240
6.841
6.835
6.830
6.818
6.813
3.792
2.694
1.923
Current Data Parameters
NAME 20170801
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170801
Time 21.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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
OH
Me
MeO
Cl
1o
10
9
8
7
6
5
4
3
2
1
ppm
4.15
2.27
2.00
3.02
1.14
3.16

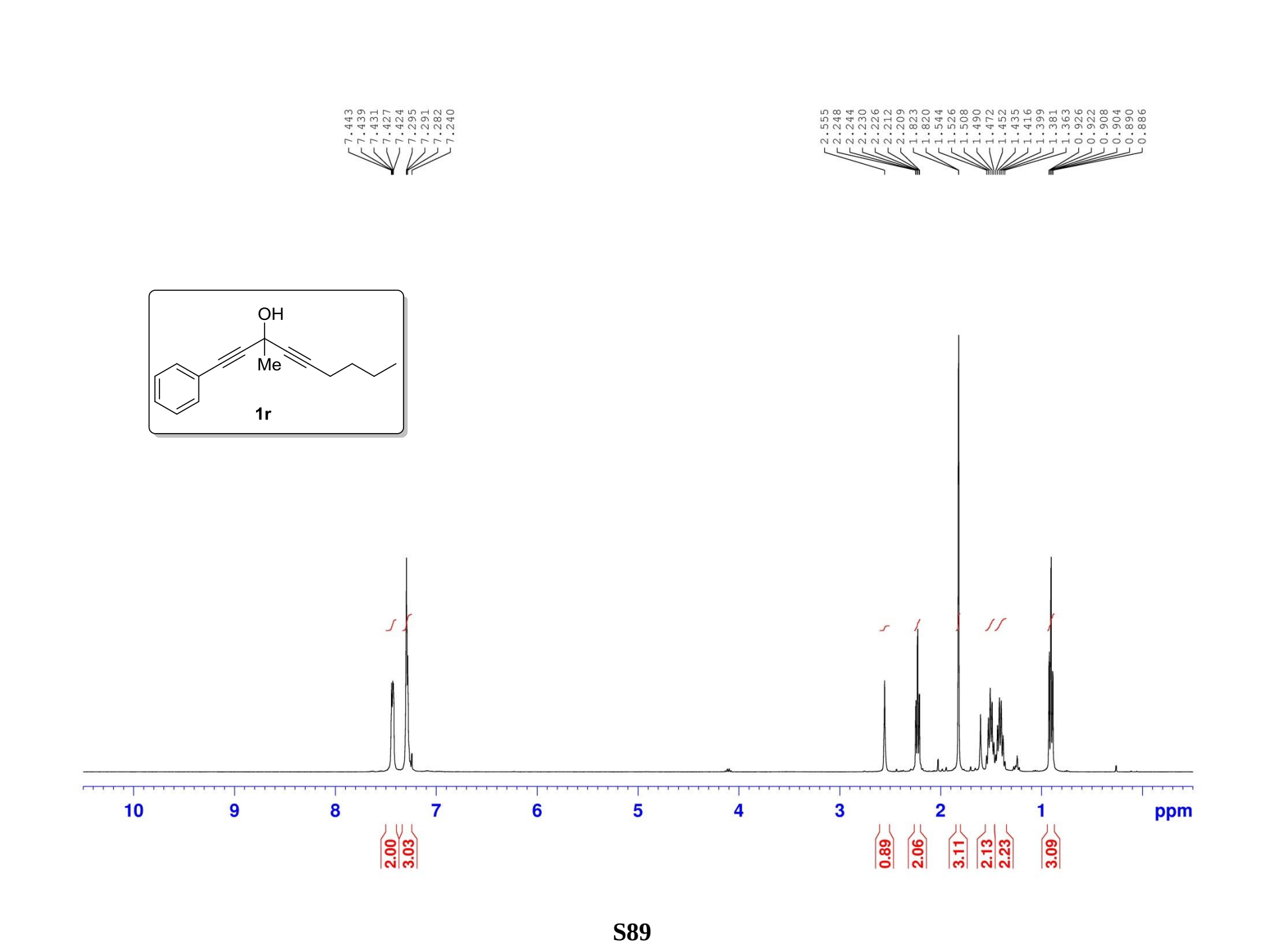

159.97
134.74
133.32
133.06
128.63
120.71
113.94
91.20
88.54
82.90
81.37
77.32
77.00
76.68
60.88
55.29
32.02
Current Data Parameters
NAME 20170802
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170802
Time 21.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 419
DS 0
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177991 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
MeO
Cl
1o
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

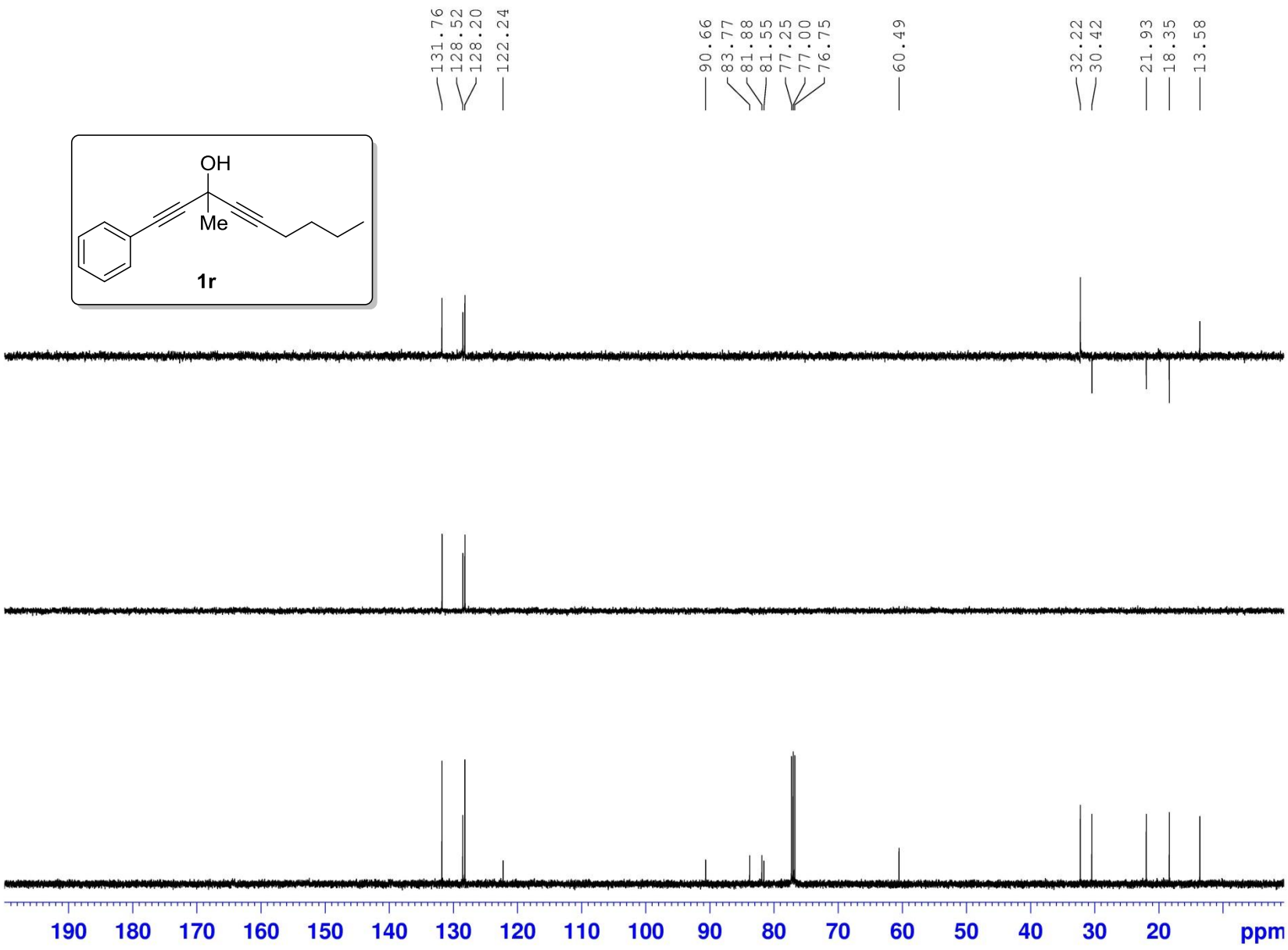

7.412
7.406
7.400
7.389
7.383
7.376
7.362
7.345
7.341
7.240
7.113
7.093
6.840
6.834
6.829
6.817
6.812
3.791
2.712
2.331
1.930
Current Data Parameters
NAME 20170808
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170808
Time 22.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 19
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 181
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 400.1500166 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
Me
MeO
1p
Me
10
9
8
7
6
5
4
3
2
1
ppm
2.24
2.16
2.33
2.00
2.96
1.16
3.29
3.30

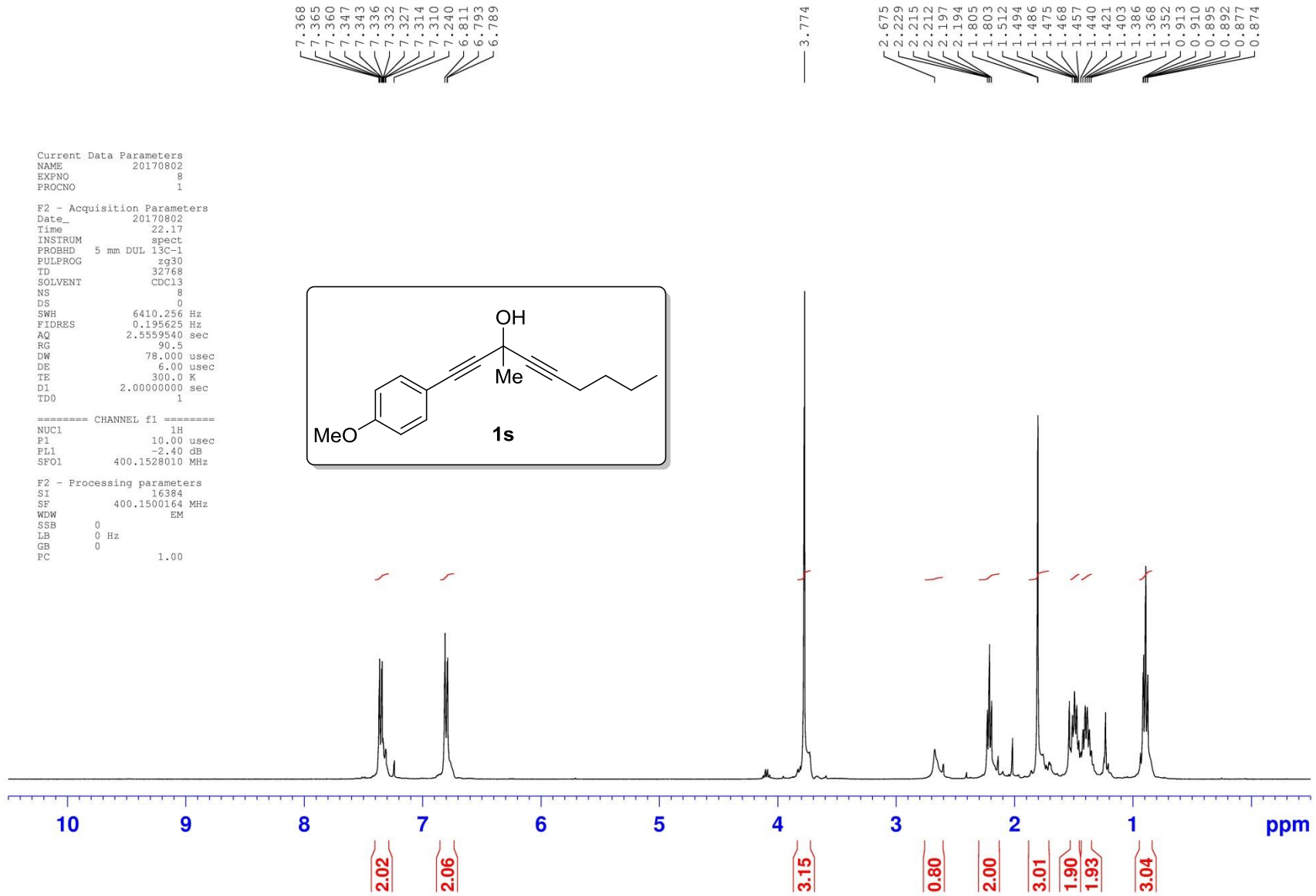

159.84
138.77
133.29
131.70
128.99
119.08
114.22
113.88
89.61
88.90
82.66
82.55
77.32
77.00
76.68
60.91
55.25
32.11
21.46
Current Data Parameters
NAME 20170808
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170808
Time 22.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 0
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178022 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
MeO
1p
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

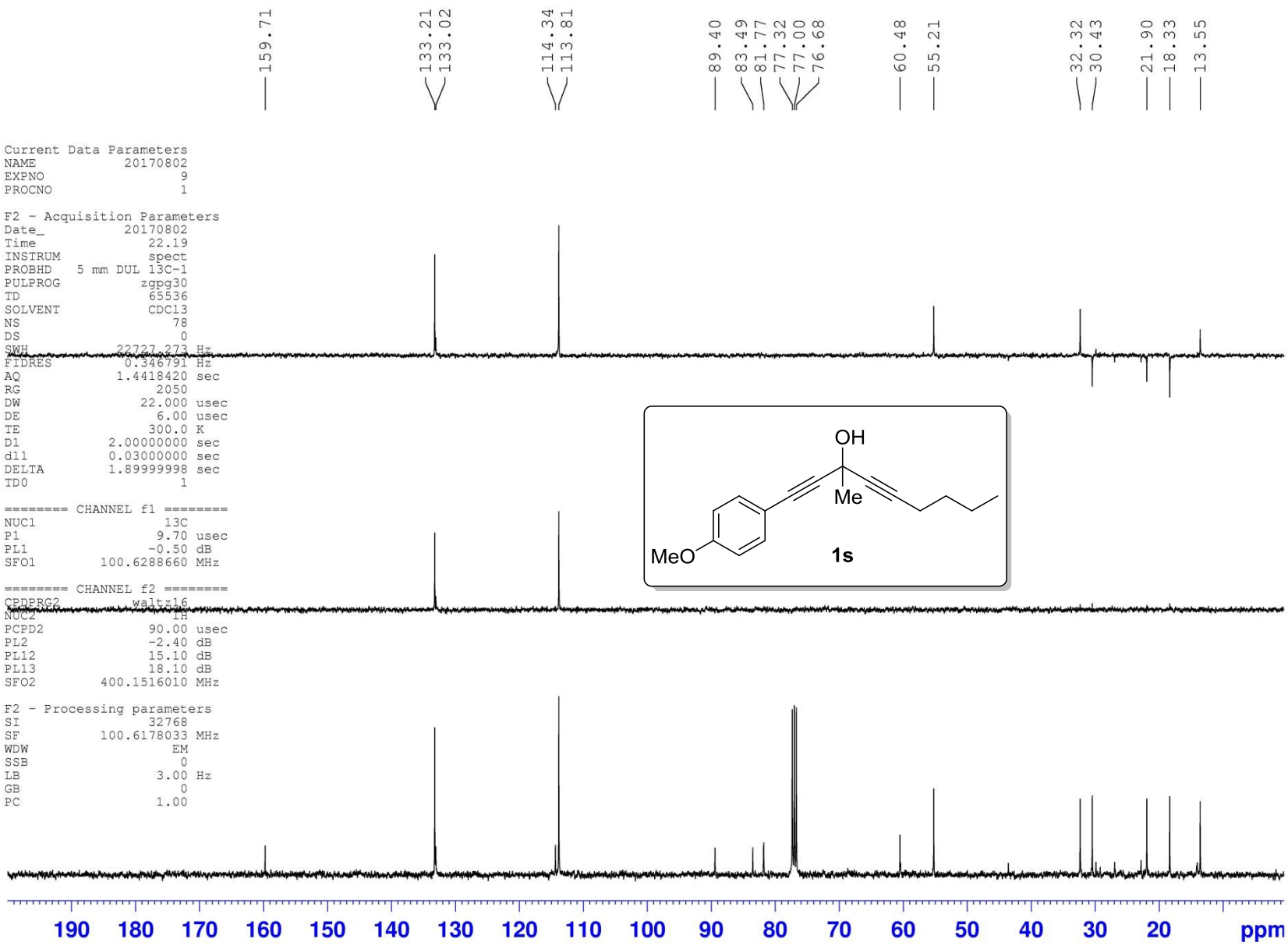

7.491
7.484
7.476
7.471
7.463
7.458
7.452
7.321
7.314
7.311
7.300
7.297
7.260
7.252
7.247
7.240
7.137
7.127
7.124
2.792
1.940
Current Data Parameters
NAME 20170915
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170915
Time 9.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 144
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
Me
S
1q
10
9
8
7
6
5
4
3
2
1
ppm
3.21
3.20
1.08
1.10
1.00
3.13

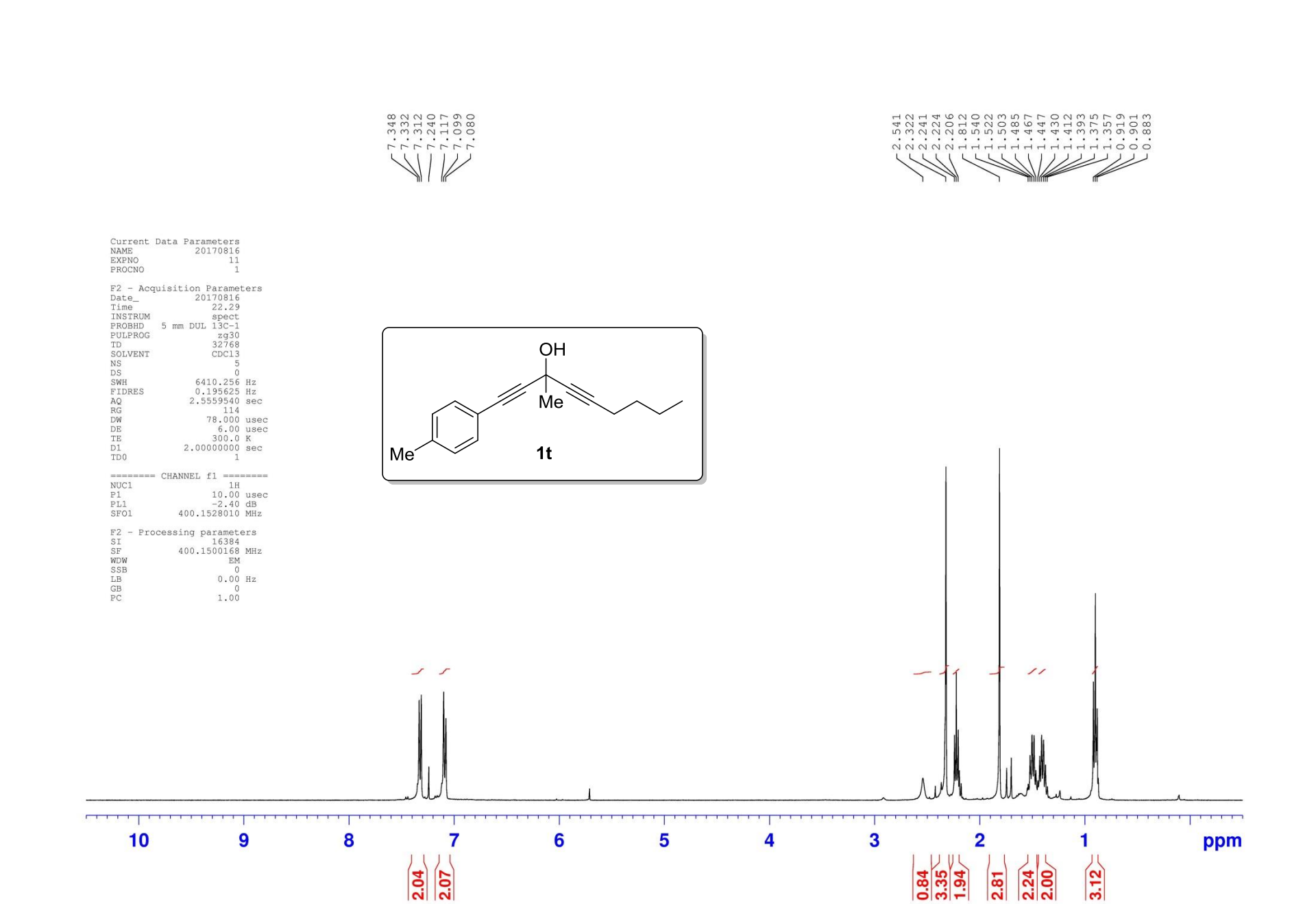

131.79
129.85
129.50
128.67
128.25
125.34
122.05
121.10
89.99
89.64
82.66
77.93
77.32
77.00
76.68
60.83
31.94
Current Data Parameters
NAME 20170915
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170915
Time 9.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 63
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
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 100.6178041 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
S
1q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

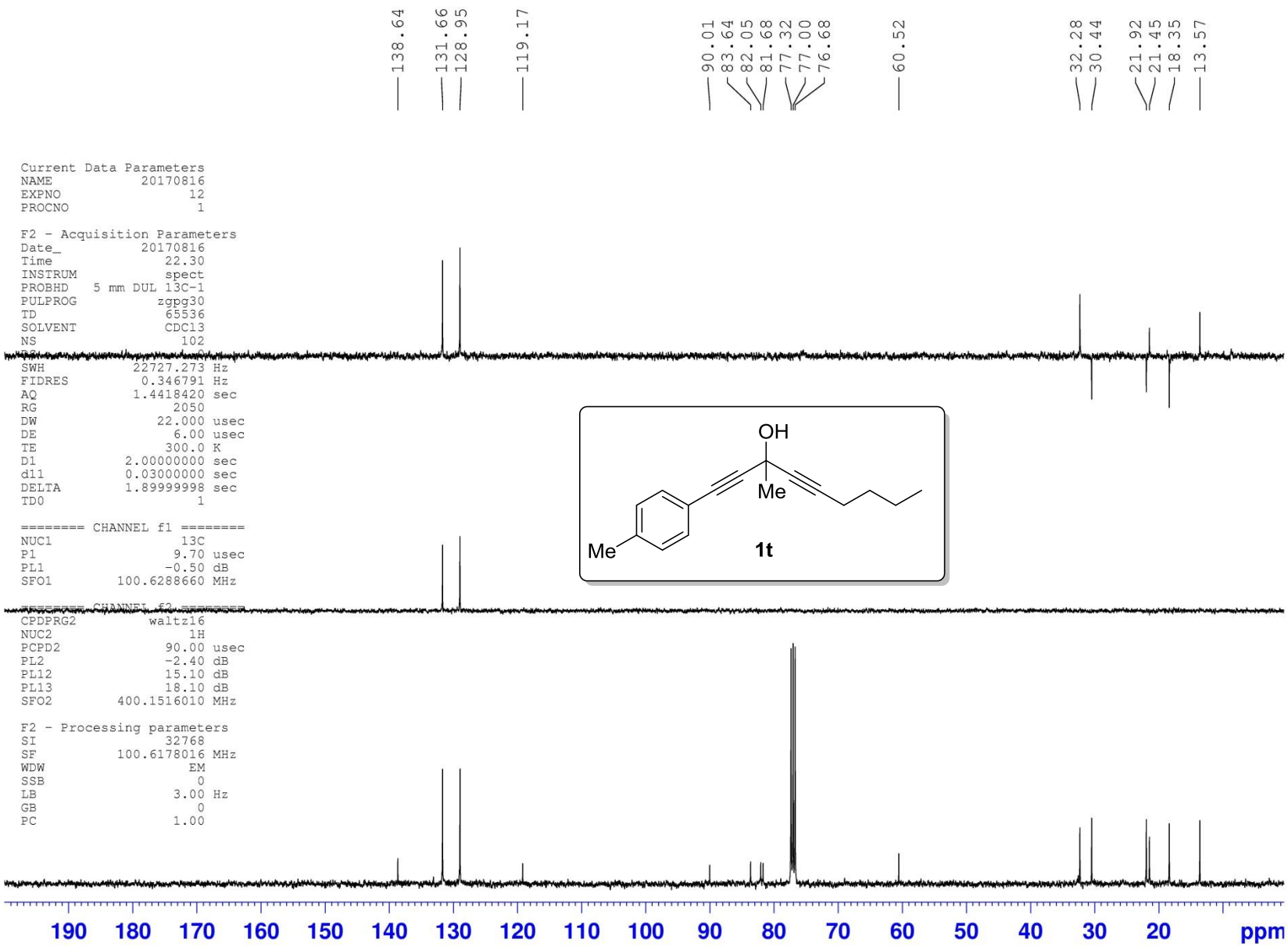

7.443
7.439
7.431
7.427
7.424
7.295
7.291
7.282
7.240
2.555
2.248
2.244
2.230
2.226
2.212
2.209
1.823
1.820
1.544
1.526
1.508
1.490
1.472
1.452
1.435
1.416
1.399
1.381
1.363
0.926
0.922
0.908
0.904
0.890
0.886
OH
Me
1r
10
9
8
7
6
5
4
3
2
1
ppm
2.00
3.03
0.89
2.06
3.11
2.13
2.23
3.09

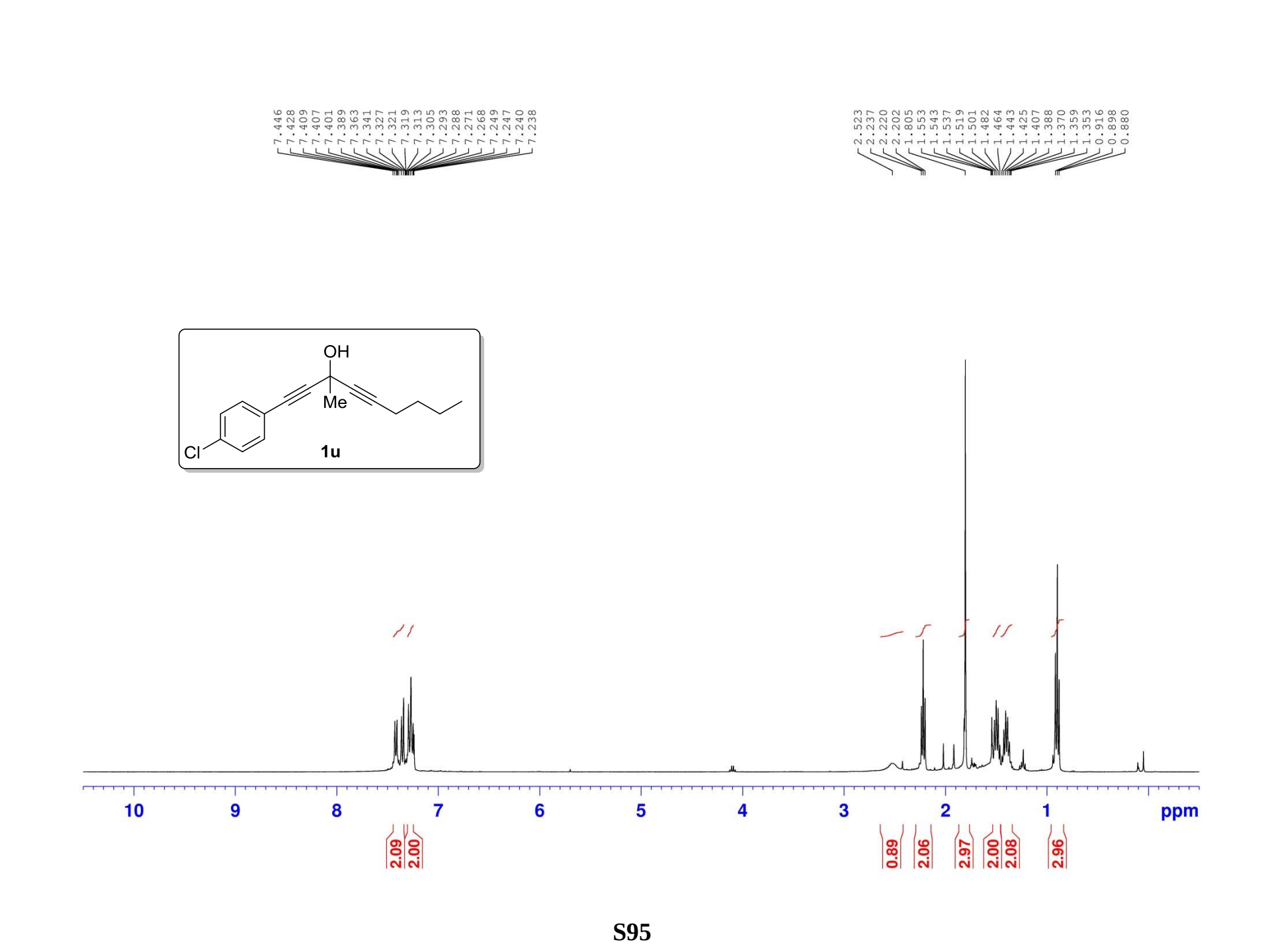

131.76
128.52
128.20
122.24
90.66
83.77
81.88
81.55
77.25
77.00
76.75
60.49
32.22
30.42
21.93
18.35
13.58
OH
Me
1r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

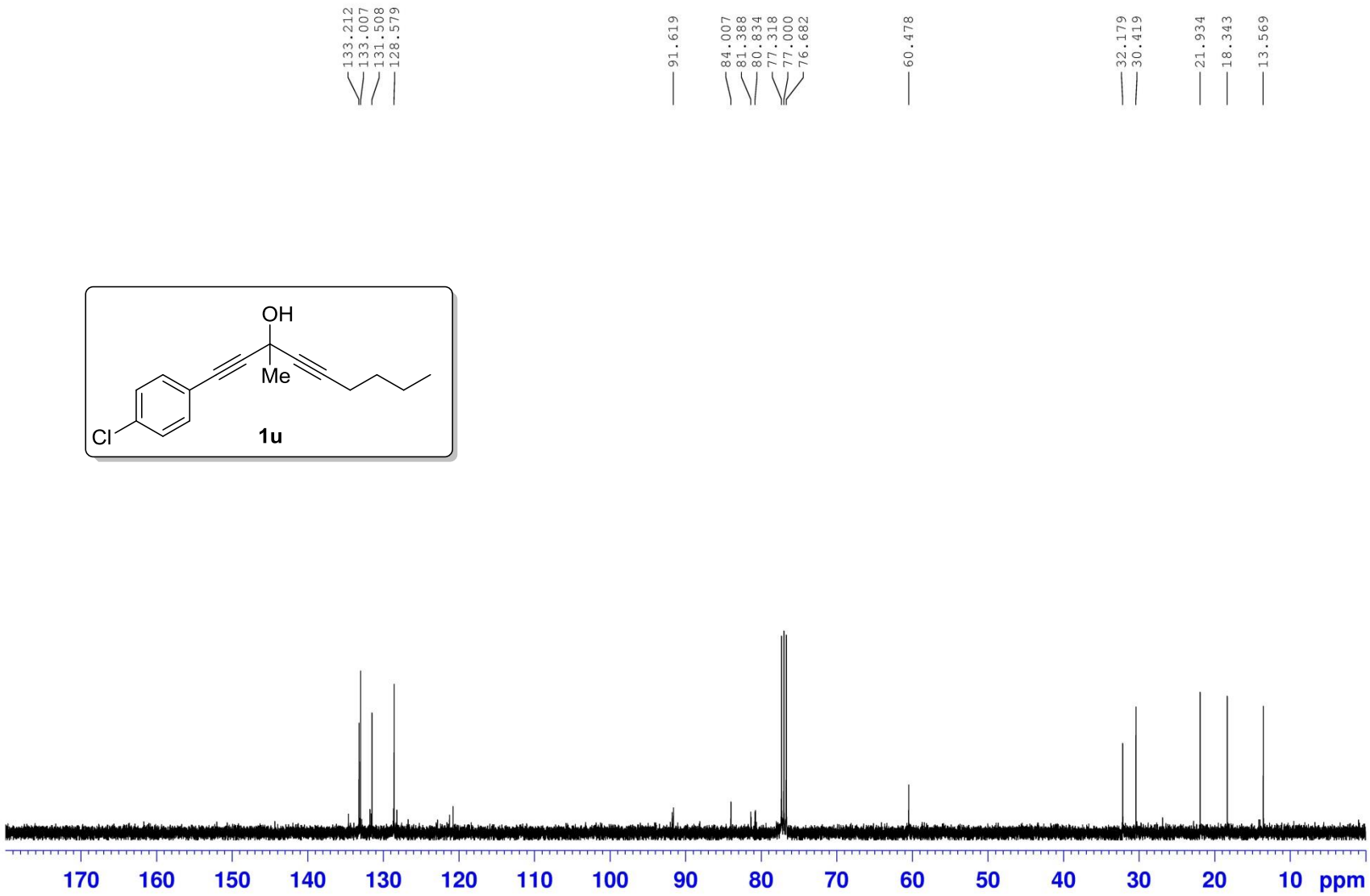

7.368
7.365
7.360
7.347
7.343
7.336
7.332
7.327
7.314
7.310
7.240
6.811
6.793
6.789
3.774
2.675
2.229
2.215
2.212
2.197
2.194
1.805
1.803
1.512
1.494
1.486
1.475
1.468
1.457
1.440
1.421
1.403
1.386
1.368
1.352
0.913
0.910
0.895
0.892
0.877
0.874
Current Data Parameters
NAME 20170802
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170802
Time 22.17
INSTRUM spect
PROBHD 5 mm DUL 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 90.5
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500164 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
OH
Me
MeO
1s
10
9
8
7
6
5
4
3
2
1
ppm
2.02
2.06
3.15
0.80
2.00
3.01
1.90
1.93
3.04

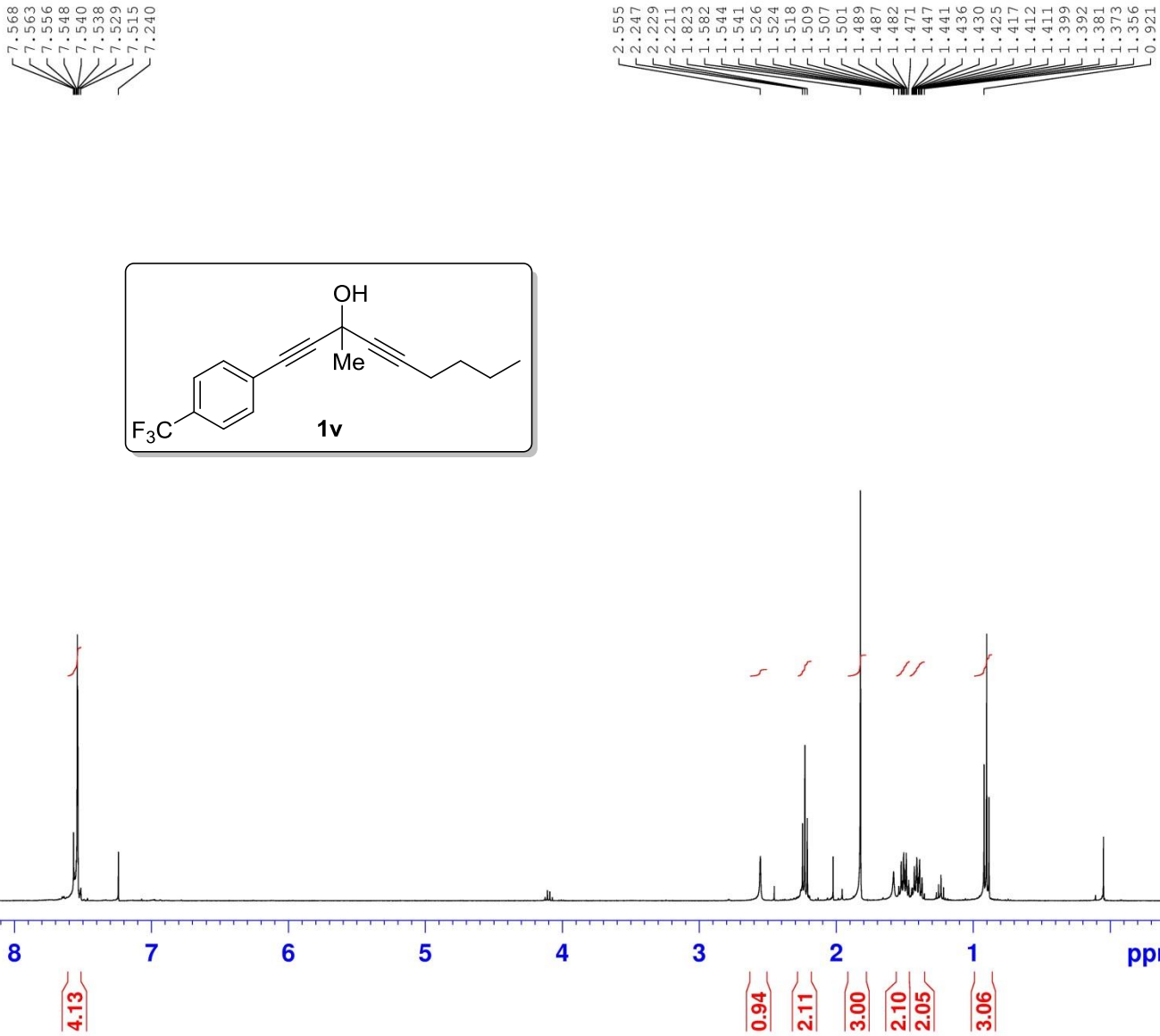

159.71
133.21
133.02
114.34
113.81
89.40
83.49
81.77
77.32
77.00
76.68
60.48
55.21
32.32
30.43
21.90
18.33
13.55
Current Data Parameters
NAME 20170802
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170802
Time 22.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 78
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 100.6178033 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
MeO
1s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

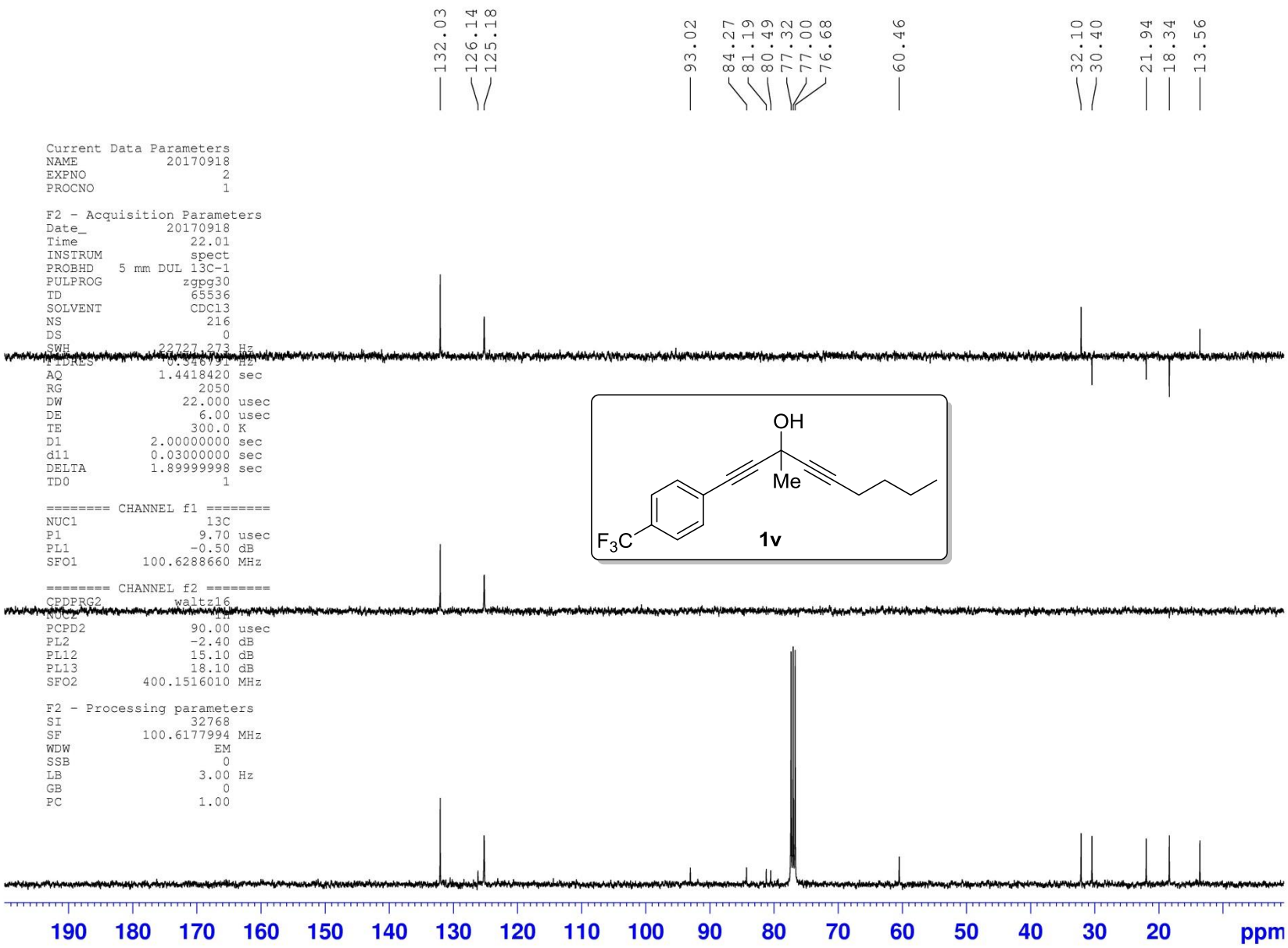

7.348
7.332
7.312
7.240
7.117
7.099
7.080
2.541
2.322
2.241
2.224
2.206
1.812
1.540
1.522
1.503
1.485
1.467
1.447
1.430
1.412
1.393
1.375
1.357
0.919
0.901
0.883
Current Data Parameters
NAME 20170816
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170816
Time 22.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 114
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
OH
Me
Me
1t
10
9
8
7
6
5
4
3
2
1
ppm
2.04
2.07
0.84
3.35
1.94
2.81
2.24
2.00
3.12

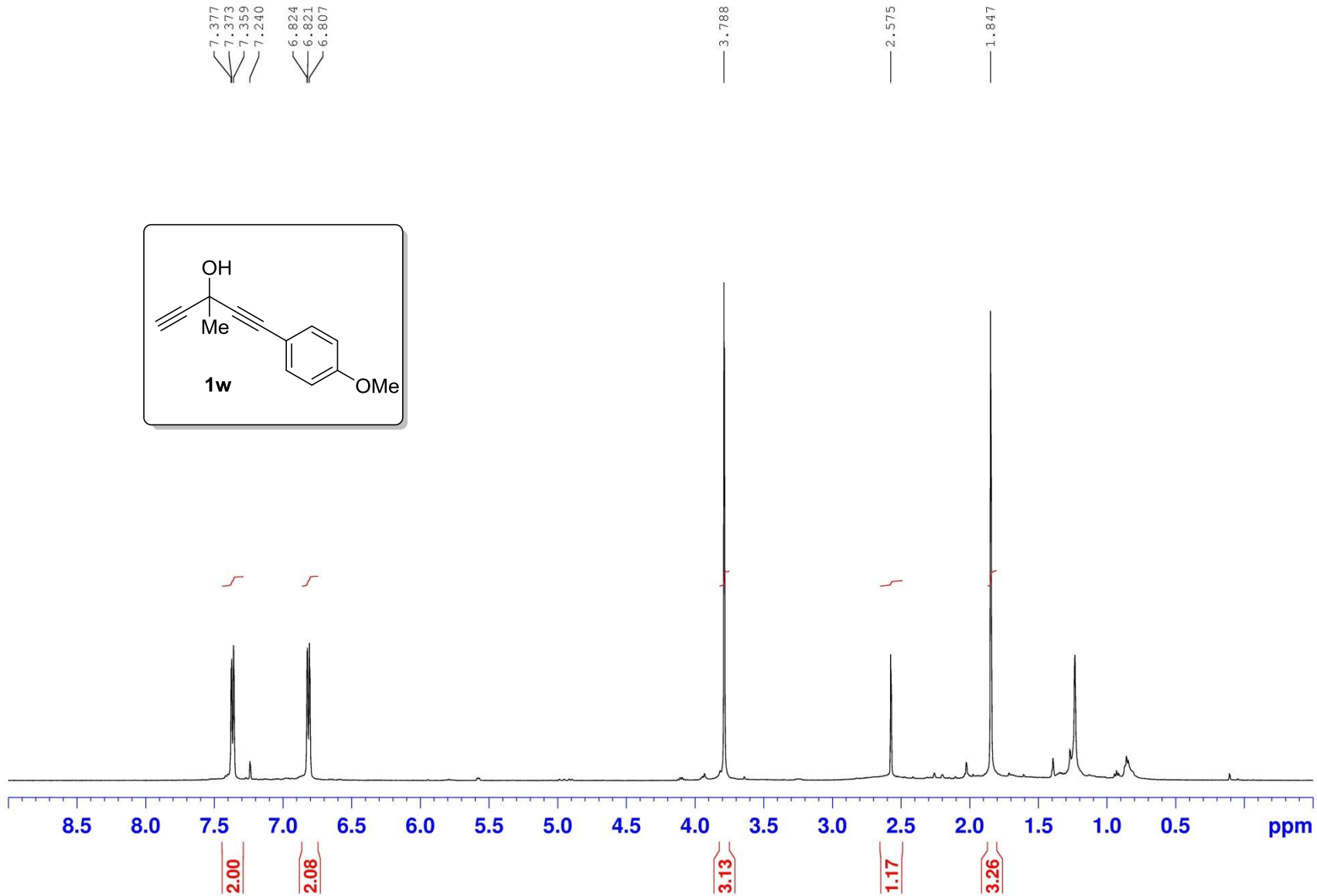

138.64
131.66
128.95
119.17
90.01
83.64
82.05
81.68
77.32
77.00
76.68
60.52
32.28
30.44
21.92
21.45
18.35
13.57
Current Data Parameters
NAME 20170816
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170816
Time 22.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
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
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 100.6178016 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
Me
1t
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

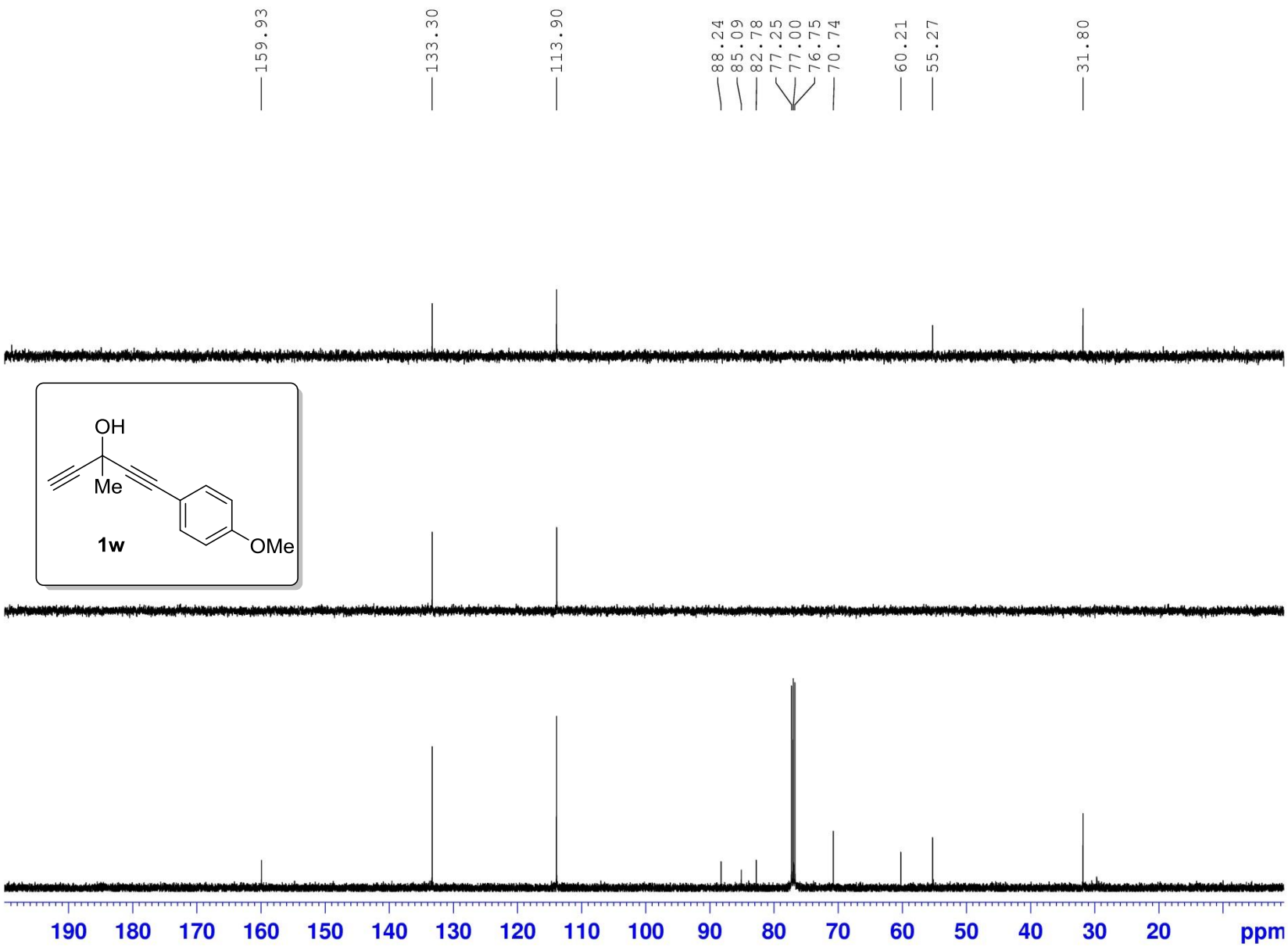

7.446
7.428
7.409
7.407
7.401
7.389
7.363
7.341
7.327
7.321
7.319
7.313
7.305
7.293
7.288
7.271
7.268
7.249
7.247
7.240
7.238
2.523
2.237
2.220
2.202
1.805
1.553
1.543
1.537
1.519
1.501
1.482
1.464
1.443
1.425
1.407
1.388
1.370
1.359
1.353
0.916
0.898
0.880
OH
Me
Cl
1u
10
9
8
7
6
5
4
3
2
1
ppm
2.09
2.00
0.89
2.06
2.97
2.00
2.08
2.96

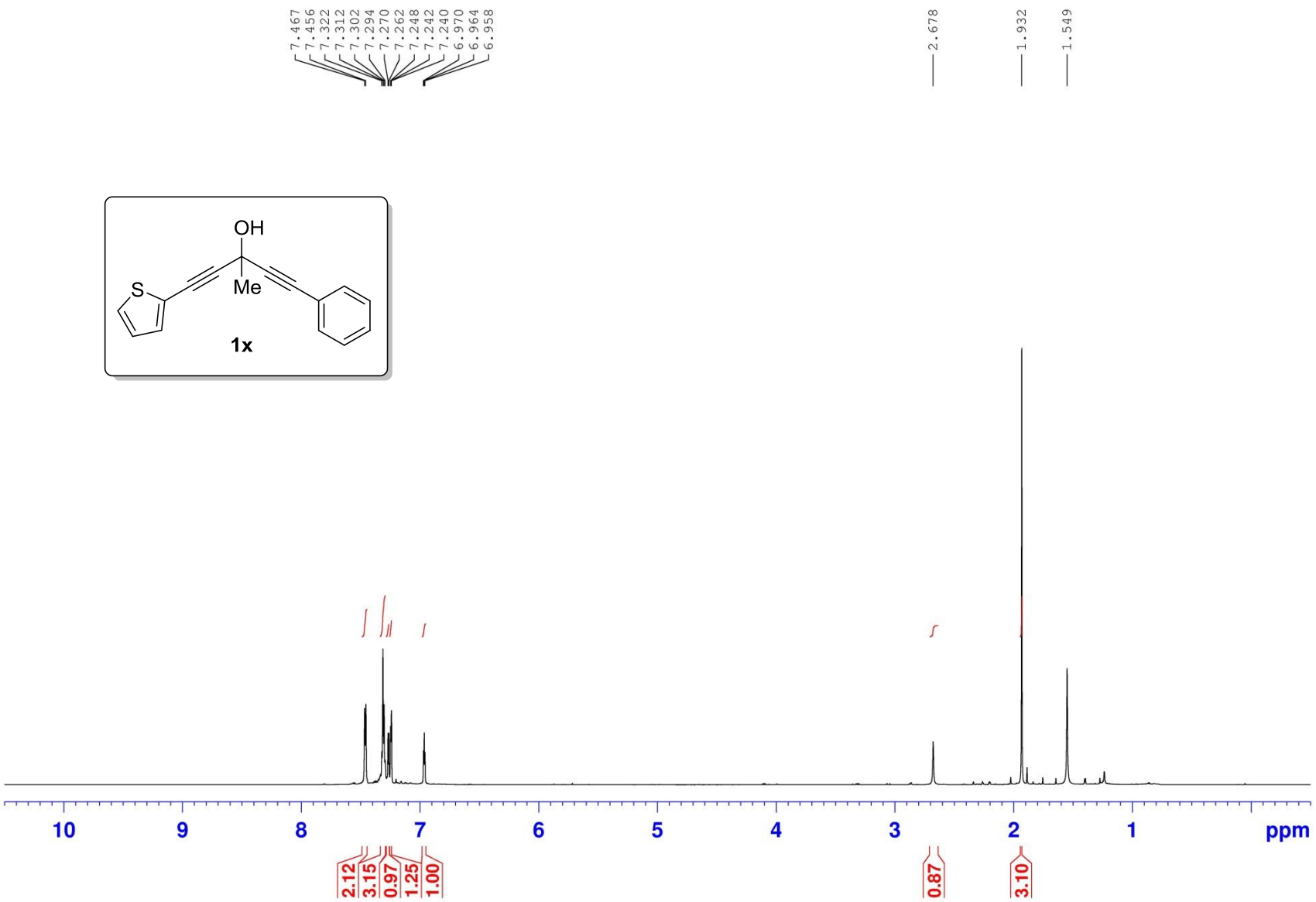

133.212
133.007
131.508
128.579
91.619
84.007
81.388
80.834
77.318
77.000
76.682
60.478
32.179
30.419
21.934
18.343
13.569
OH
Me
Cl
1u
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

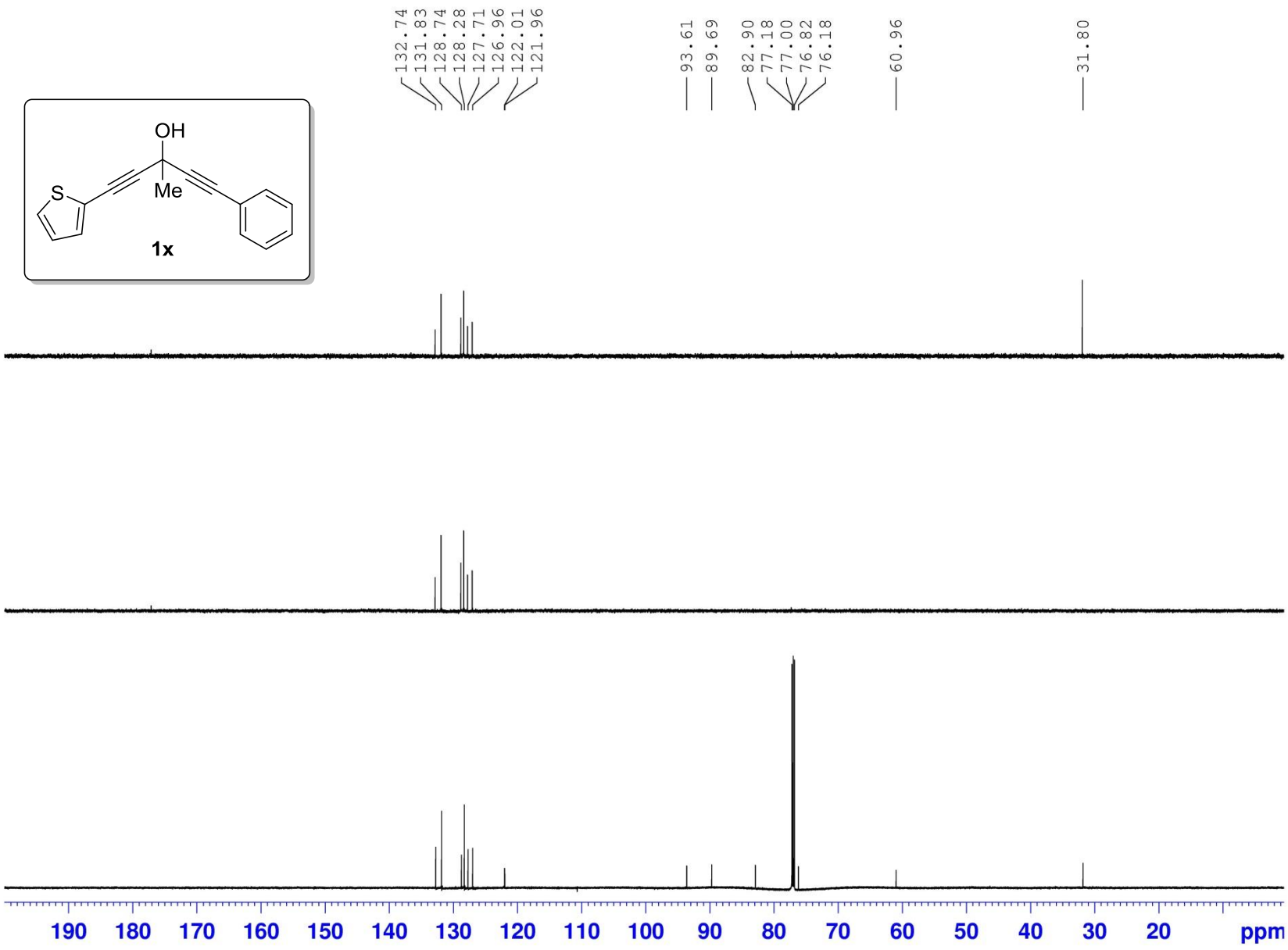

7.568
7.563
7.556
7.548
7.540
7.538
7.529
7.515
7.240
2.555
2.247
2.229
2.211
1.823
1.582
1.544
1.541
1.526
1.524
1.518
1.509
1.507
1.501
1.489
1.487
1.482
1.471
1.447
1.441
1.436
1.430
1.425
1.417
1.412
1.411
1.399
1.392
1.381
1.373
1.356
0.921
Current Data Parameters
NAME 20170918
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170918
Time 22.00
INSTRUM spect
PROBHD 5 mm DUL 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 322
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
Me
F3C
1v
10
9
8
7
6
5
4
3
2
1
ppm
4.13
0.94
2.11
3.00
2.10
2.05
3.06

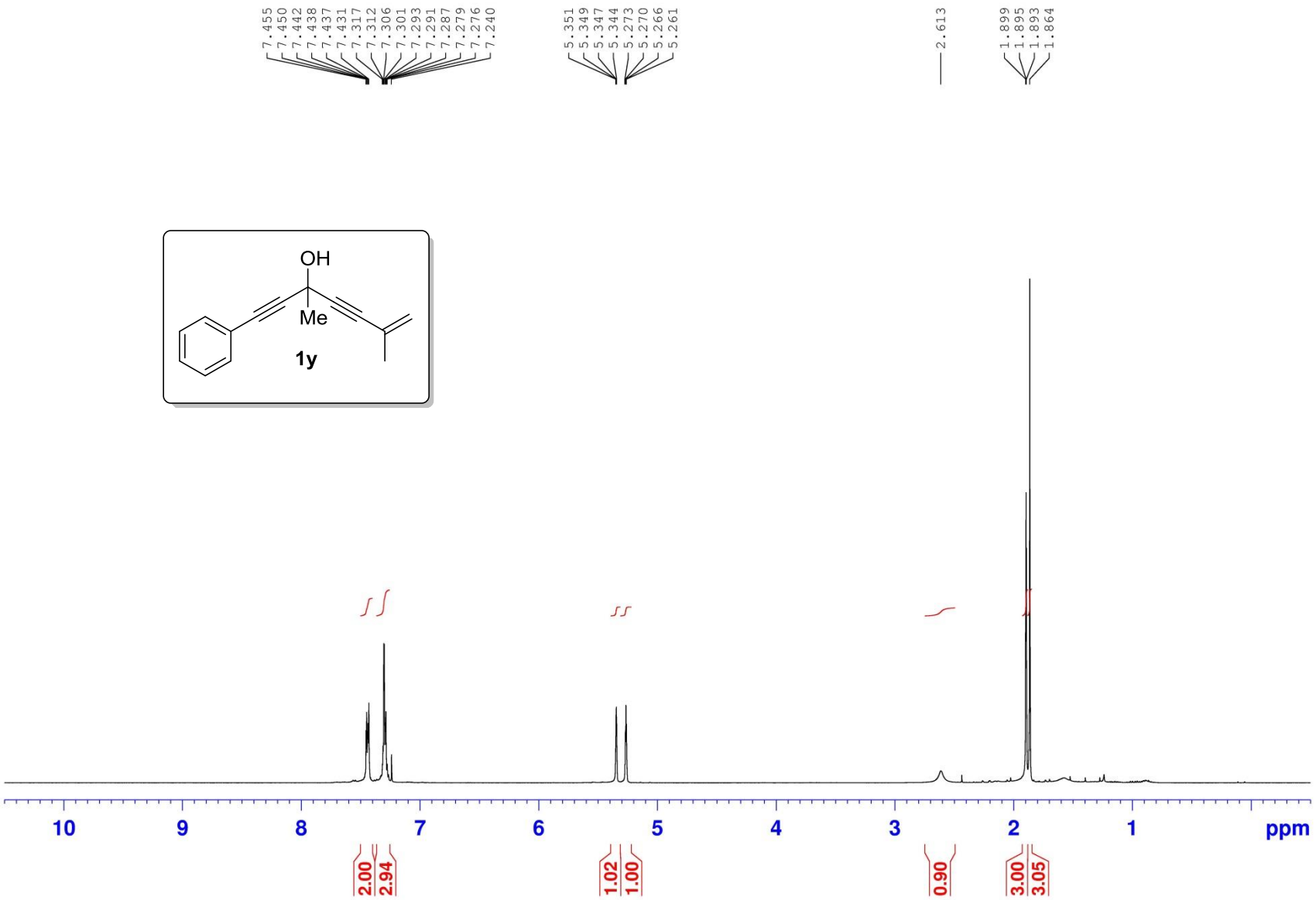

132.03
126.14
125.18
93.02
84.27
81.19
80.49
77.32
77.00
76.68
60.46
32.10
30.40
21.94
18.34
13.56
Current Data Parameters
NAME 20170918
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170918
Time 22.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 216
DS 0
SWH 22727.273 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
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 100.6177994 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
Me
F3C
1v
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

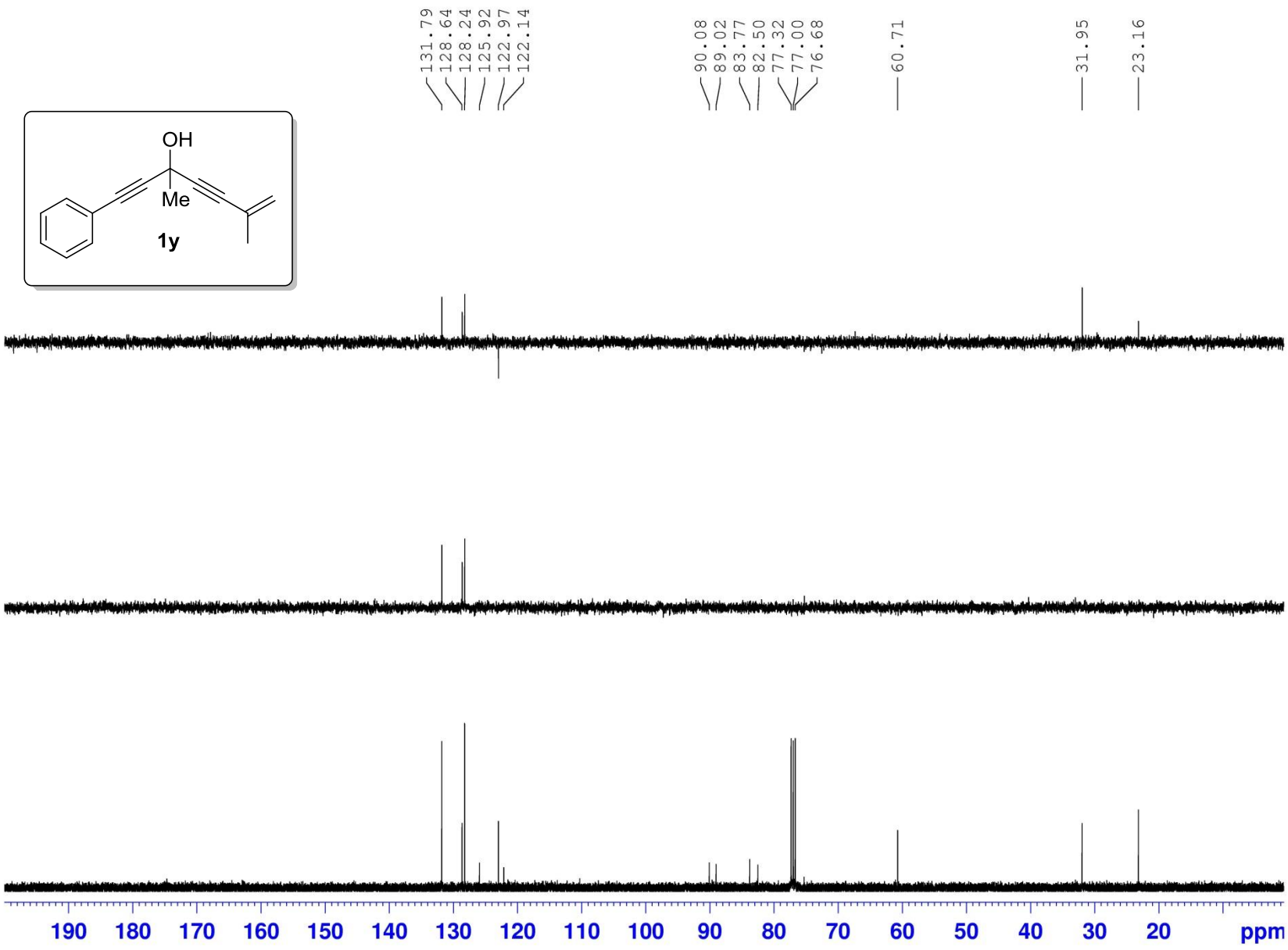

7.377
7.373
7.359
7.240
6.824
6.821
6.807
3.788
2.575
1.847
OH
Me
1w
OMe
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
2.08
3.13
1.17
3.26

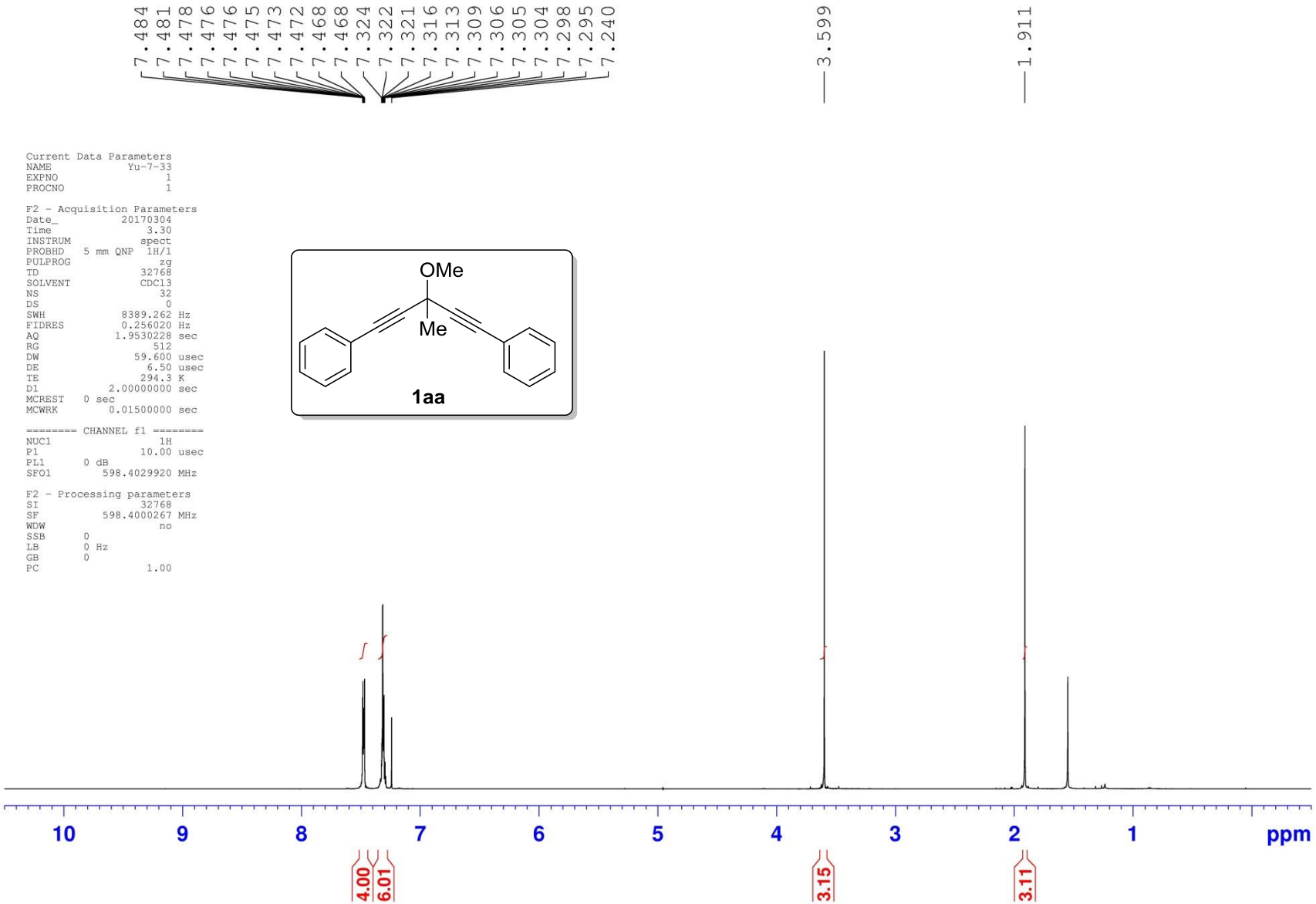

159.93
133.30
113.90
88.24
85.09
82.78
77.25
77.00
76.75
70.74
60.21
55.27
31.80
OH
Me
1w
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

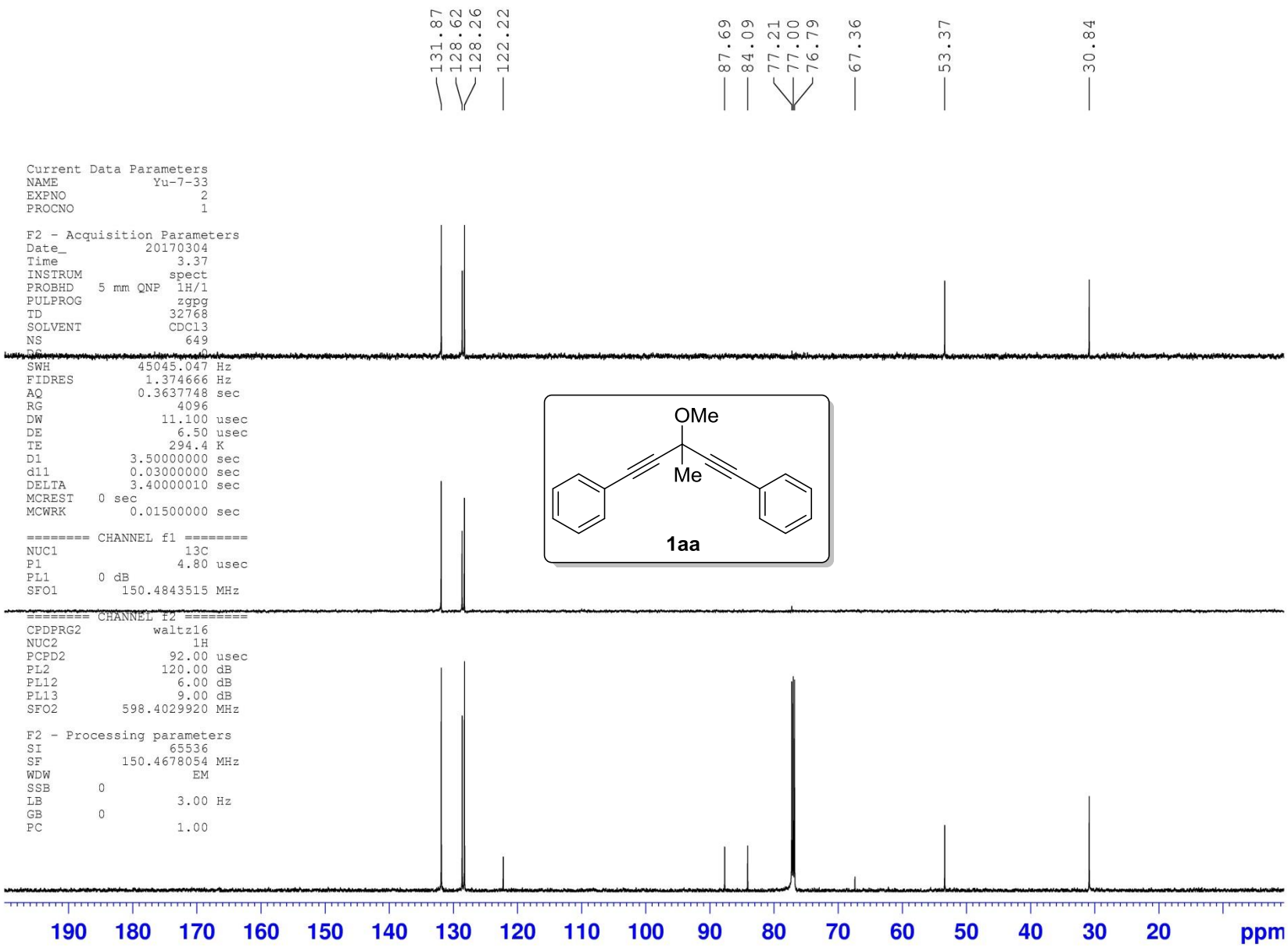

7.467
7.456
7.322
7.312
7.302
7.294
7.270
7.262
7.248
7.242
7.240
6.970
6.964
6.958
2.678
1.932
1.549
OH
Me
S
1x
10
9
8
7
6
5
4
3
2
1
ppm
2.12
3.15
0.97
1.25
1.00
0.87
3.10

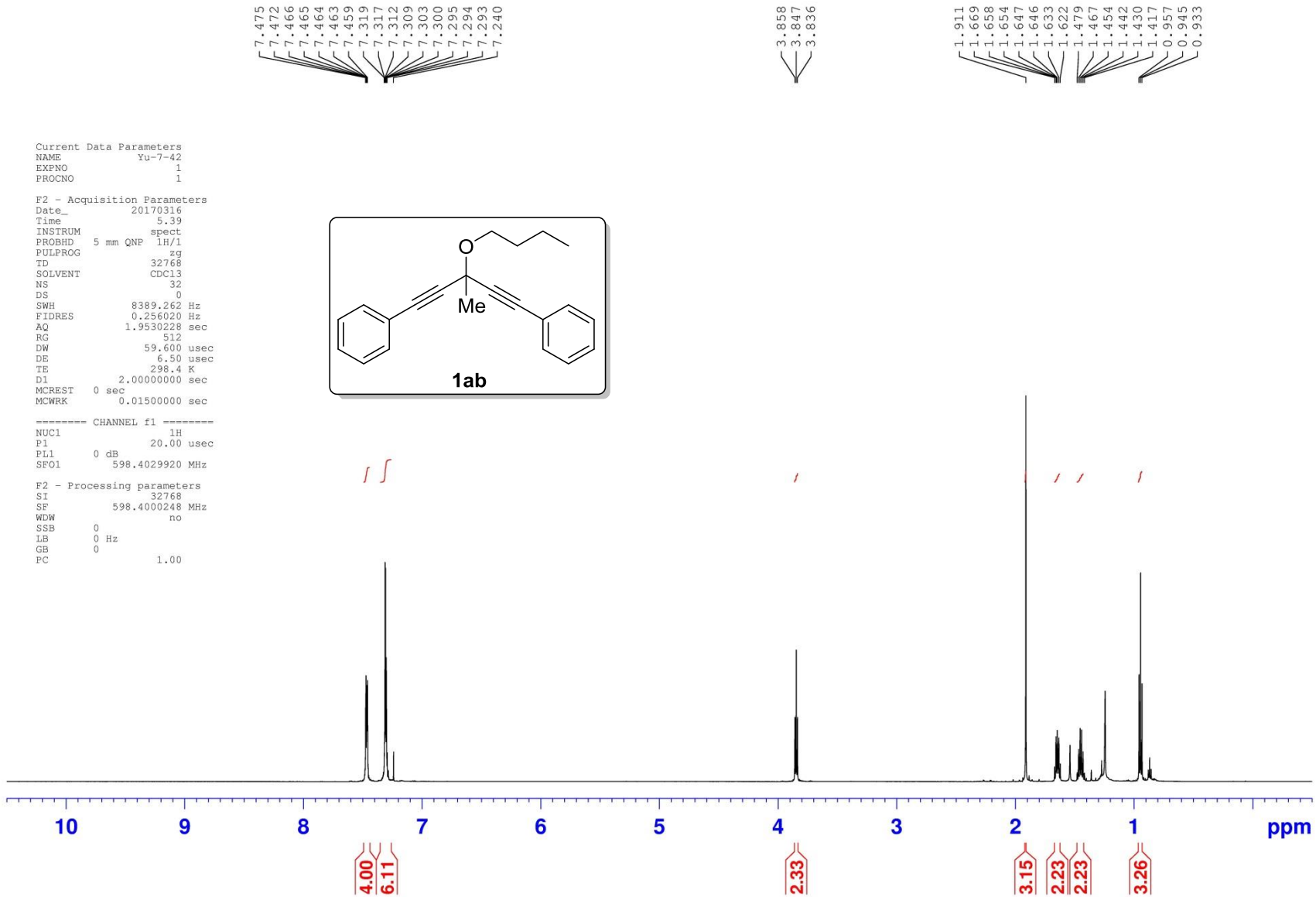

132.74
131.83
128.74
128.28
127.71
126.96
122.01
121.96
93.61
89.69
82.90
77.18
77.00
76.82
76.18
60.96
31.80
OH
Me
S
1x
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

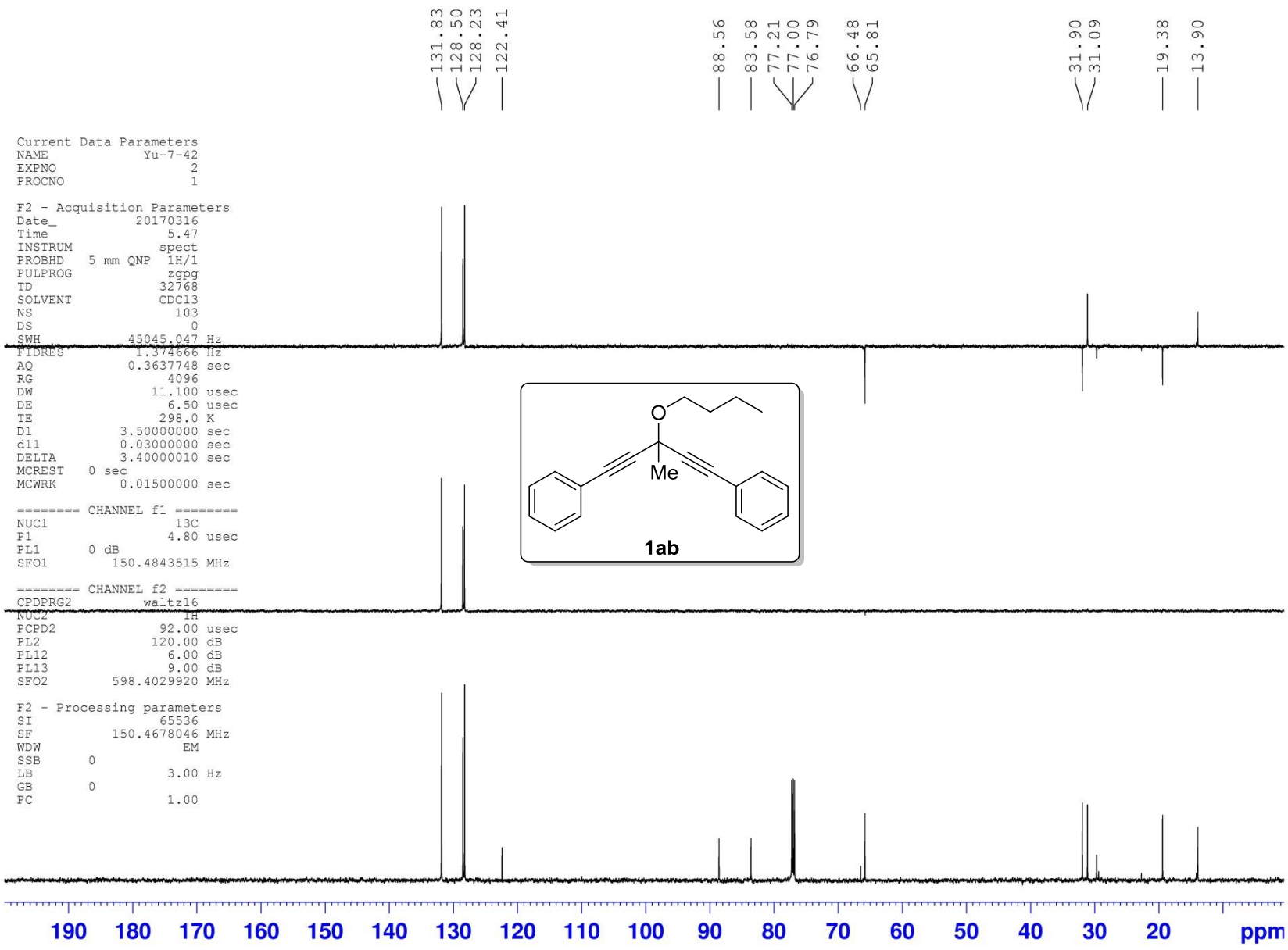

7.455
7.450
7.442
7.438
7.437
7.431
7.317
7.312
7.306
7.301
7.293
7.291
7.287
7.279
7.276
7.240
5.351
5.349
5.347
5.344
5.273
5.270
5.266
5.261
2.613
1.899
1.895
1.893
1.864
OH
Me
1y
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.94
1.02
1.00
0.90
3.00
3.05

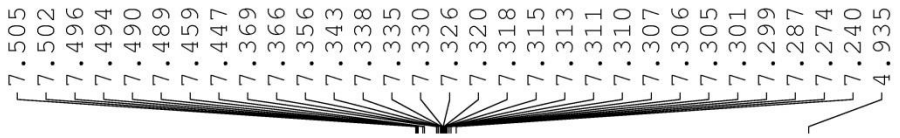

131.79
128.64
128.24
125.92
122.97
122.14
90.08
89.02
83.77
82.50
77.32
77.00
76.68
60.71
31.95
23.16
OH
Me
1y
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

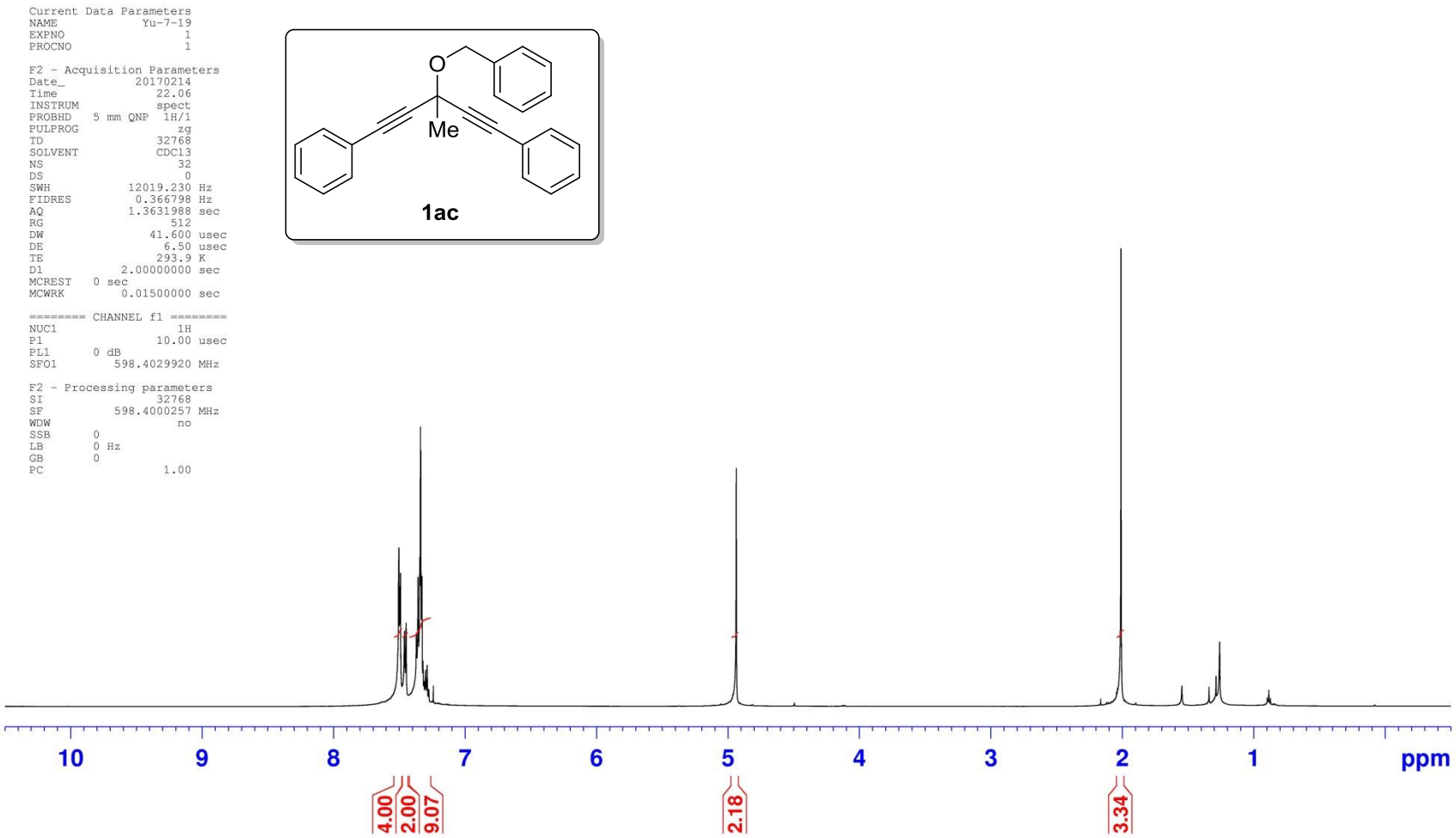

7.484
7.481
7.478
7.476
7.476
7.475
7.473
7.472
7.468
7.468
7.324
7.322
7.321
7.316
7.313
7.309
7.306
7.305
7.304
7.298
7.295
7.240
3.599
1.911
Current Data Parameters
NAME Yu-7-33
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170304
Time 3.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000267 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
OMe
Me
1aa
10
9
8
7
6
5
4
3
2
1
ppm
4.00
6.01
3.15
3.11

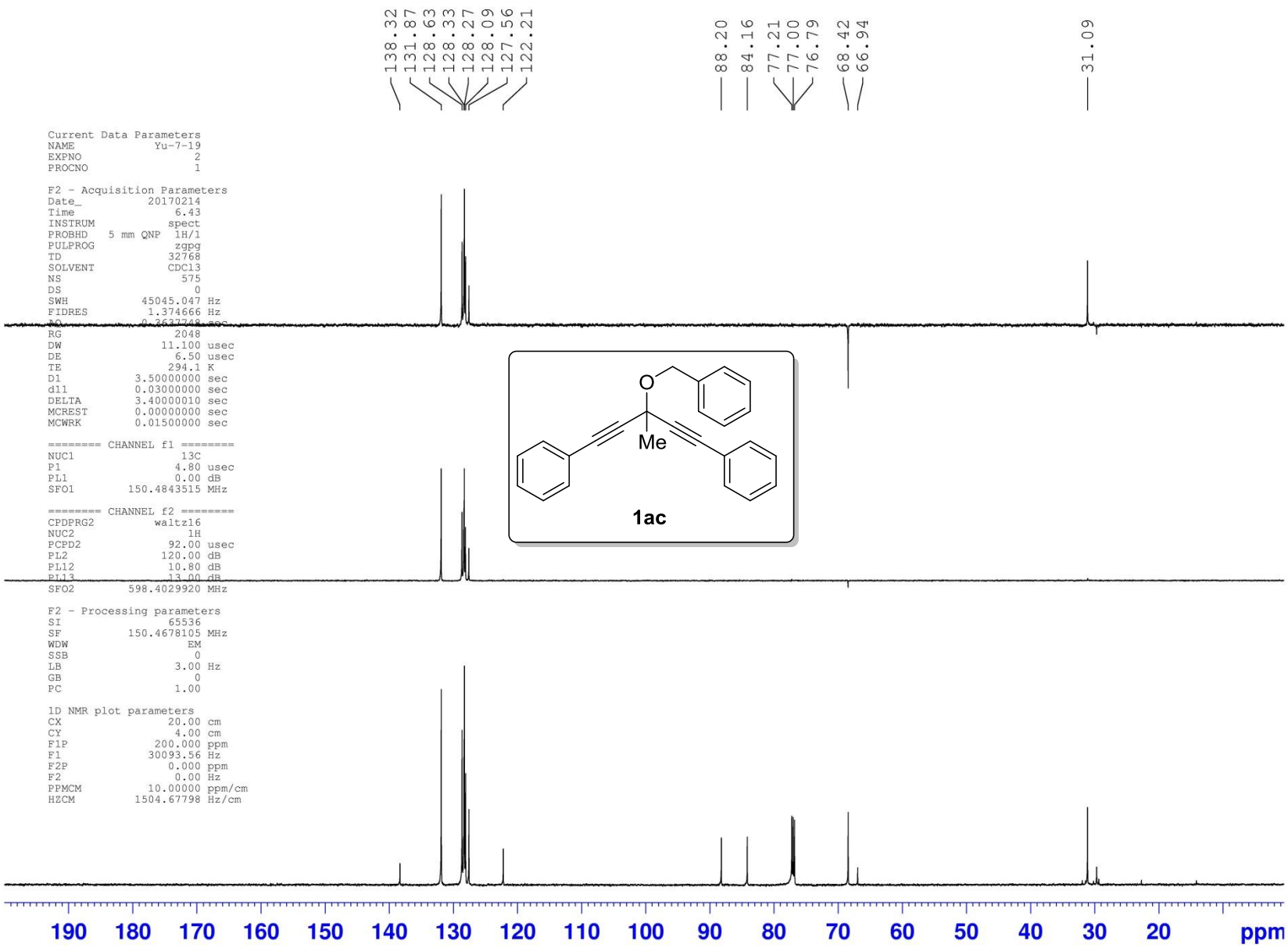

131.87
128.62
128.26
122.22
87.69
84.09
77.21
77.00
76.79
67.36
53.37
30.84
Current Data Parameters
NAME Yu-7-33
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170304
Time 3.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 649
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 294.4 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
Me
1aa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

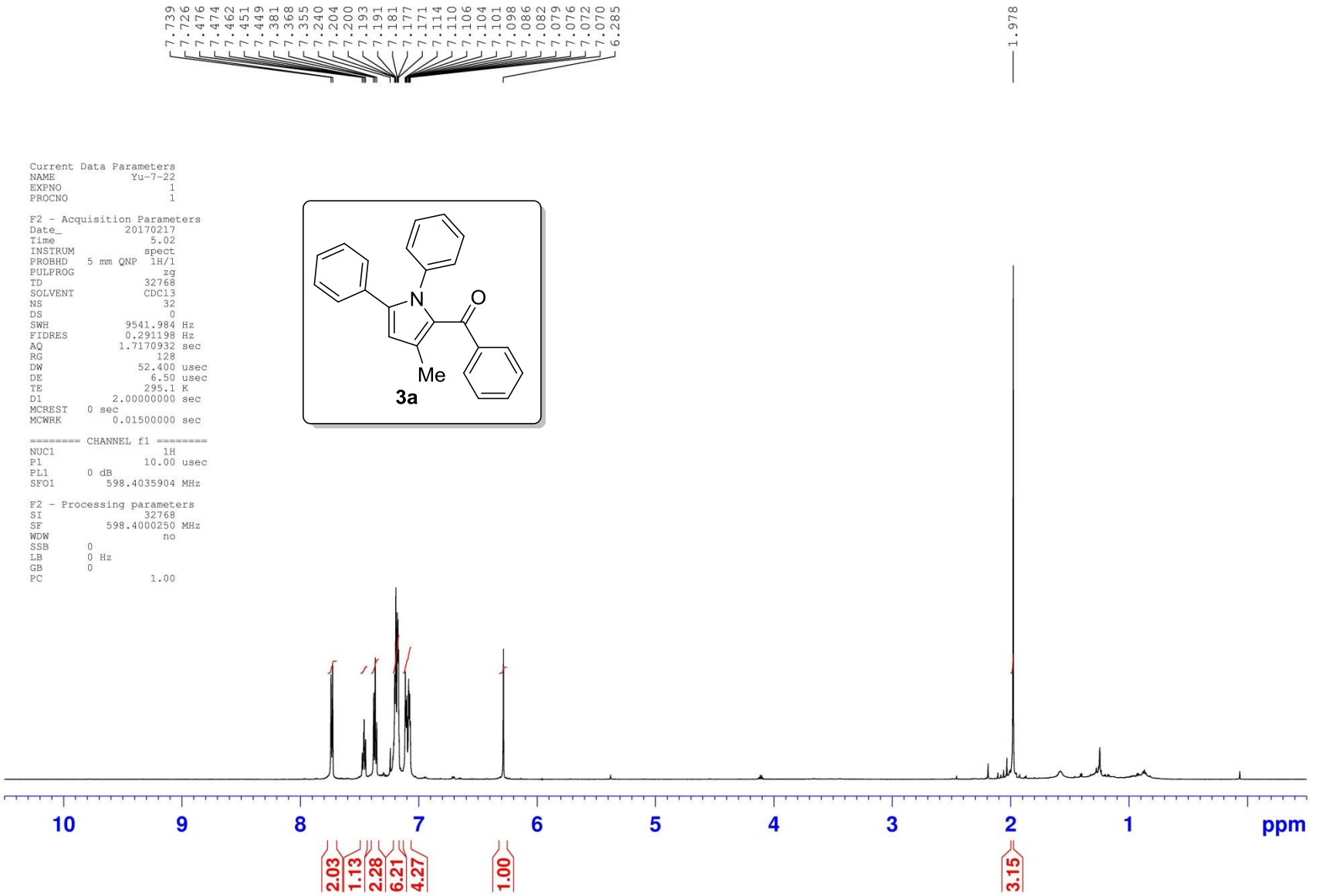

7.475
7.472
7.466
7.465
7.464
7.463
7.459
7.319
7.317
7.312
7.309
7.303
7.300
7.295
7.294
7.293
7.240
3.858
3.847
3.836
1.911
1.669
1.658
1.654
1.647
1.646
1.633
1.622
1.479
1.467
1.454
1.442
1.430
1.417
0.957
0.945
0.933
Current Data Parameters
NAME Yu-7-42
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170316
Time 5.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
Me
1ab
10
9
8
7
6
5
4
3
2
1
ppm
4.00
6.11
2.33
3.15
2.23
2.23
3.26

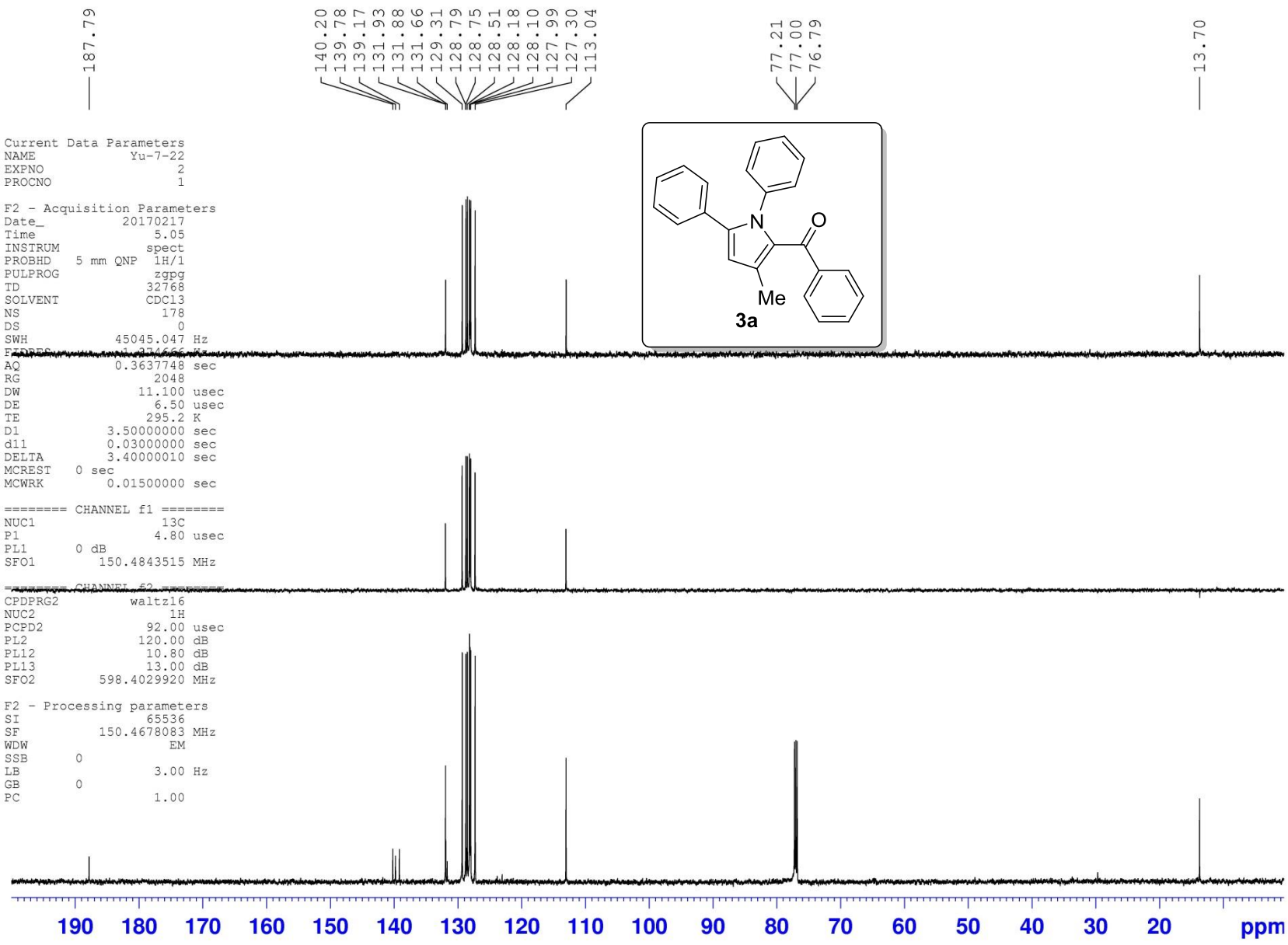

131.83
128.50
128.23
122.41
88.56
83.58
77.21
77.00
76.79
66.48
65.81
31.90
31.09
19.38
13.90
Current Data Parameters
NAME Yu-7-42
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170316
Time 5.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 103
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 298.0 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678046 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
Me
1ab
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

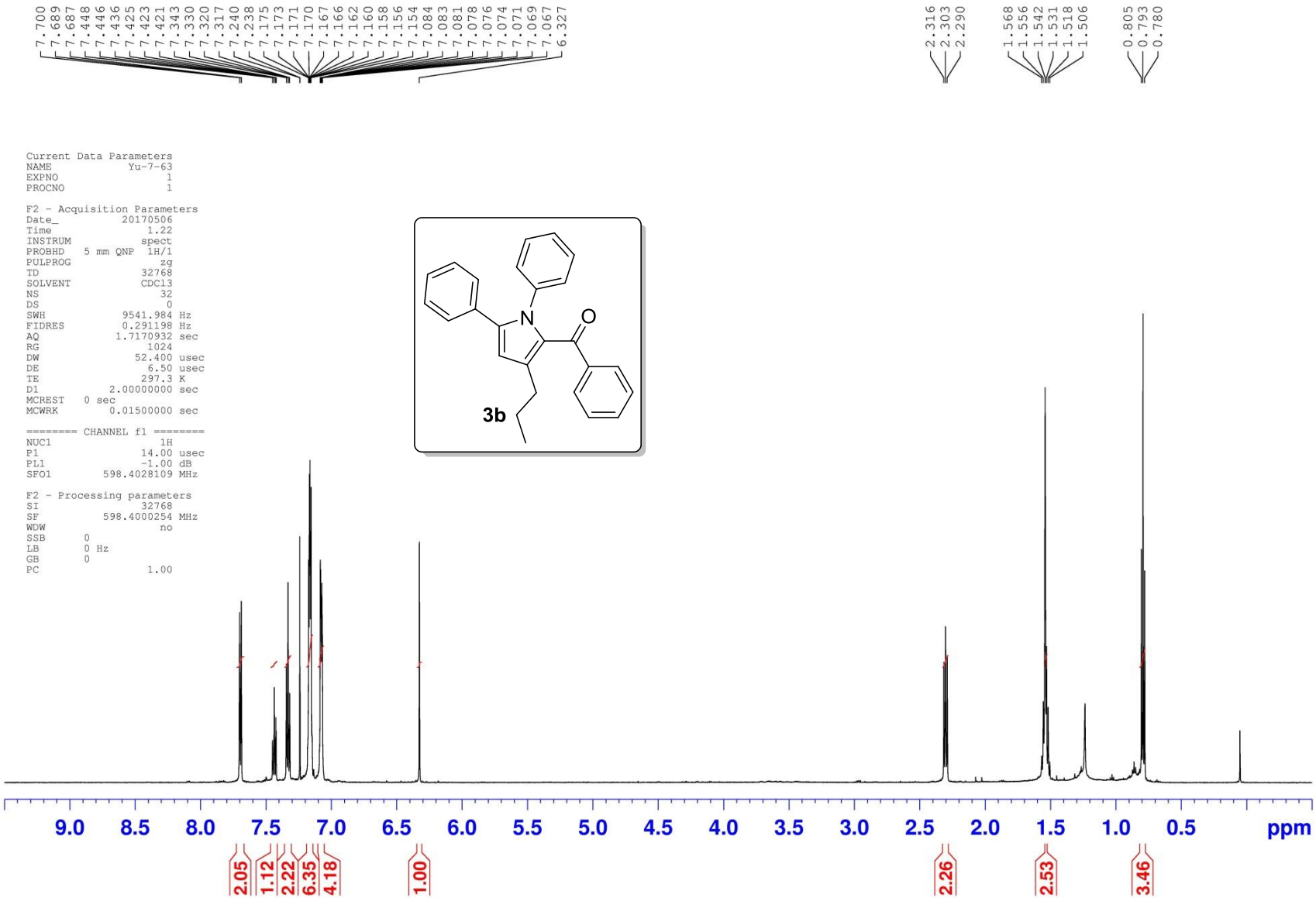

7.505
7.502
7.496
7.494
7.490
7.489
7.459
7.447
7.369
7.366
7.356
7.343
7.338
7.335
7.330
7.326
7.320
7.318
7.315
7.313
7.311
7.310
7.307
7.306
7.305
7.301
7.299
7.287
7.274
7.240
4.935
2.008

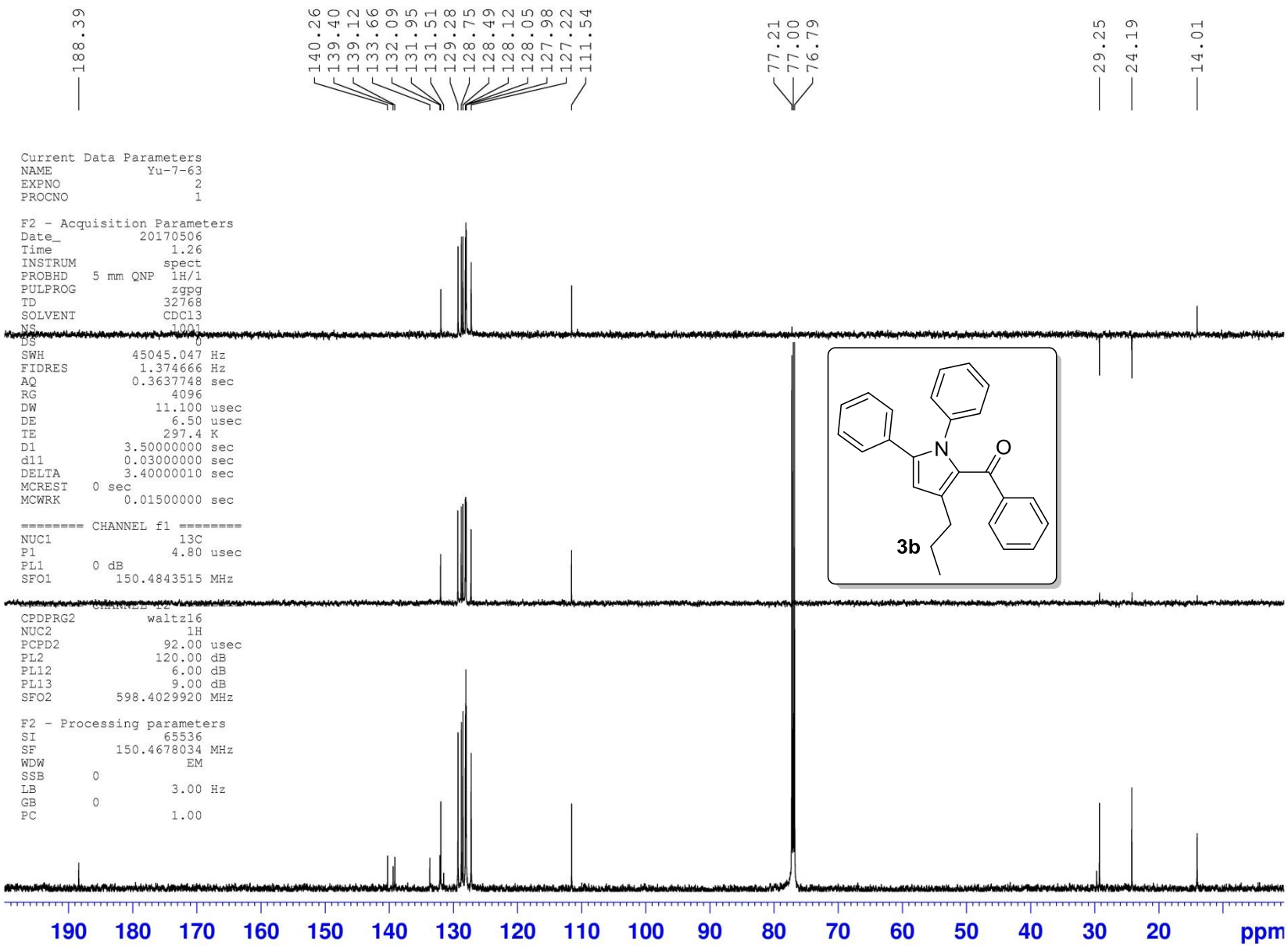

Current Data Parameters
NAME Yu-7-19
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170214
Time 22.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000257 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
Me
1ac
10
9
8
7
6
5
4
3
2
1
ppm
4.00
2.00
9.07
2.18
3.34

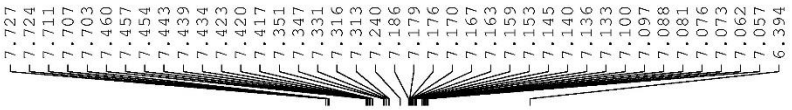

138.32
131.87
128.63
128.33
128.27
128.09
127.56
122.21
88.20
84.16
77.21
77.00
76.79
68.42
66.94
31.09
Current Data Parameters
NAME Yu-7-19
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170214
Time 6.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 575
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 294.1 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 10.80 dB
PL13 13.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678105 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30093.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1504.67798 Hz/cm
O
Me
1ac
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

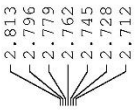

7.739
7.726
7.476
7.474
7.462
7.451
7.449
7.381
7.368
7.355
7.240
7.204
7.200
7.193
7.191
7.181
7.177
7.171
7.114
7.110
7.106
7.104
7.101
7.098
7.086
7.082
7.079
7.076
7.072
7.070
6.285
1.978
Current Data Parameters
NAME Yu-7-22
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170217
Time 5.02
INSTRUM 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 128
DW 52.400 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000250 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
O
Me
3a
10
9
8
7
6
5
4
3
2
1
ppm
2.03
1.13
2.28
6.21
4.27
1.00
3.15


187.79
140.20
139.78
139.17
131.93
131.88
131.66
129.31
128.79
128.75
128.51
128.18
128.10
127.99
127.30
113.04
77.21
77.00
76.79
13.70
Current Data Parameters
NAME Yu-7-22
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170217
Time 5.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 178
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.2 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 150.4843515 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 10.80 dB
PL13 13.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678083 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
O
Me
3a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

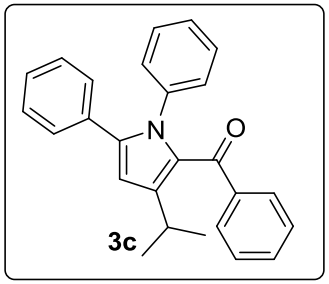

7.700
7.689
7.687
7.448
7.446
7.436
7.425
7.423
7.421
7.343
7.330
7.320
7.317
7.240
7.238
7.175
7.173
7.171
7.170
7.167
7.166
7.162
7.160
7.158
7.156
7.154
7.084
7.083
7.081
7.078
7.076
7.074
7.071
7.069
7.067
6.327
2.316
2.303
2.290
1.568
1.556
1.542
1.531
1.518
1.506
0.805
0.793
0.780
Current Data Parameters
NAME Yu-7-63
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170506
Time 1.22
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 1024
DW 52.400 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 -1.00 dB
SFO1 598.4028109 MHz
F2 - Processing parameters
SI 32768
SF 598.4000254 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
O
3b
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.05
1.12
2.22
6.35
4.18
1.00
2.26
2.53
3.46

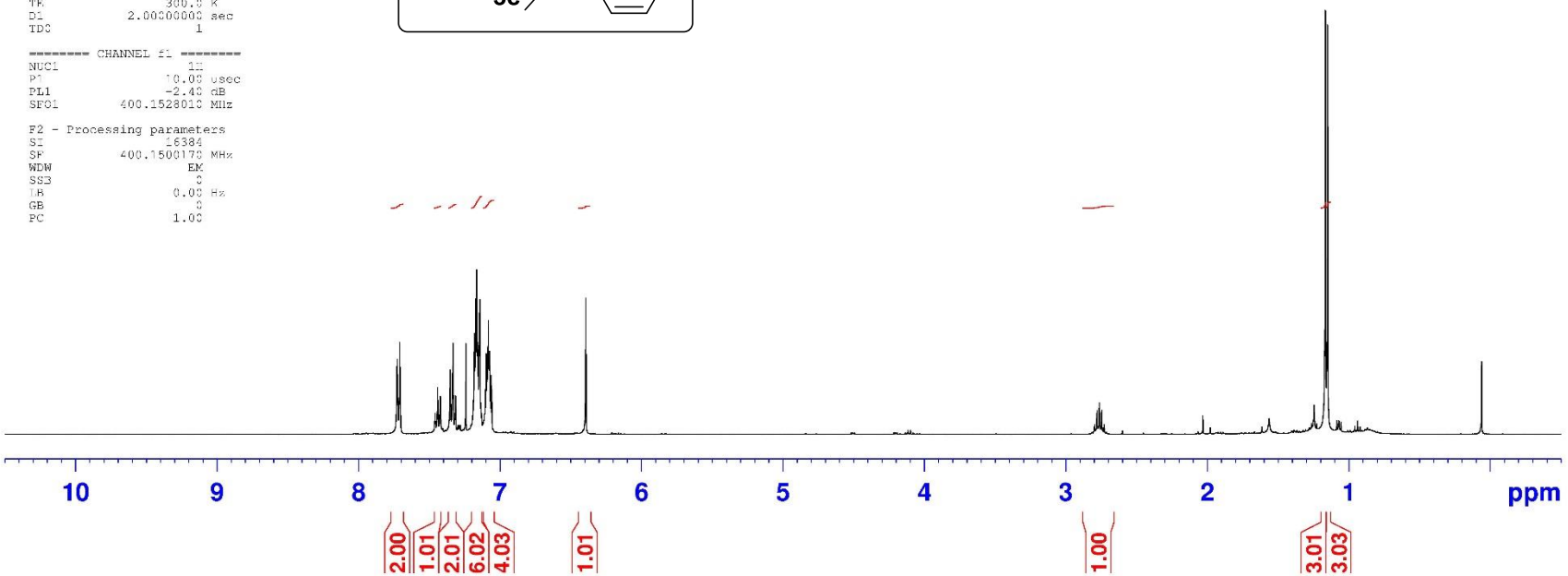

188.39
140.26
139.40
139.12
133.66
132.09
131.95
131.51
129.28
128.75
128.49
128.12
128.05
127.98
127.22
111.54
77.21
77.00
76.79
29.25
24.19
14.01
Current Data Parameters
NAME Yu-7-63
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170506
Time 1.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1001
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.4 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 150.4843515 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678034 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
O
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

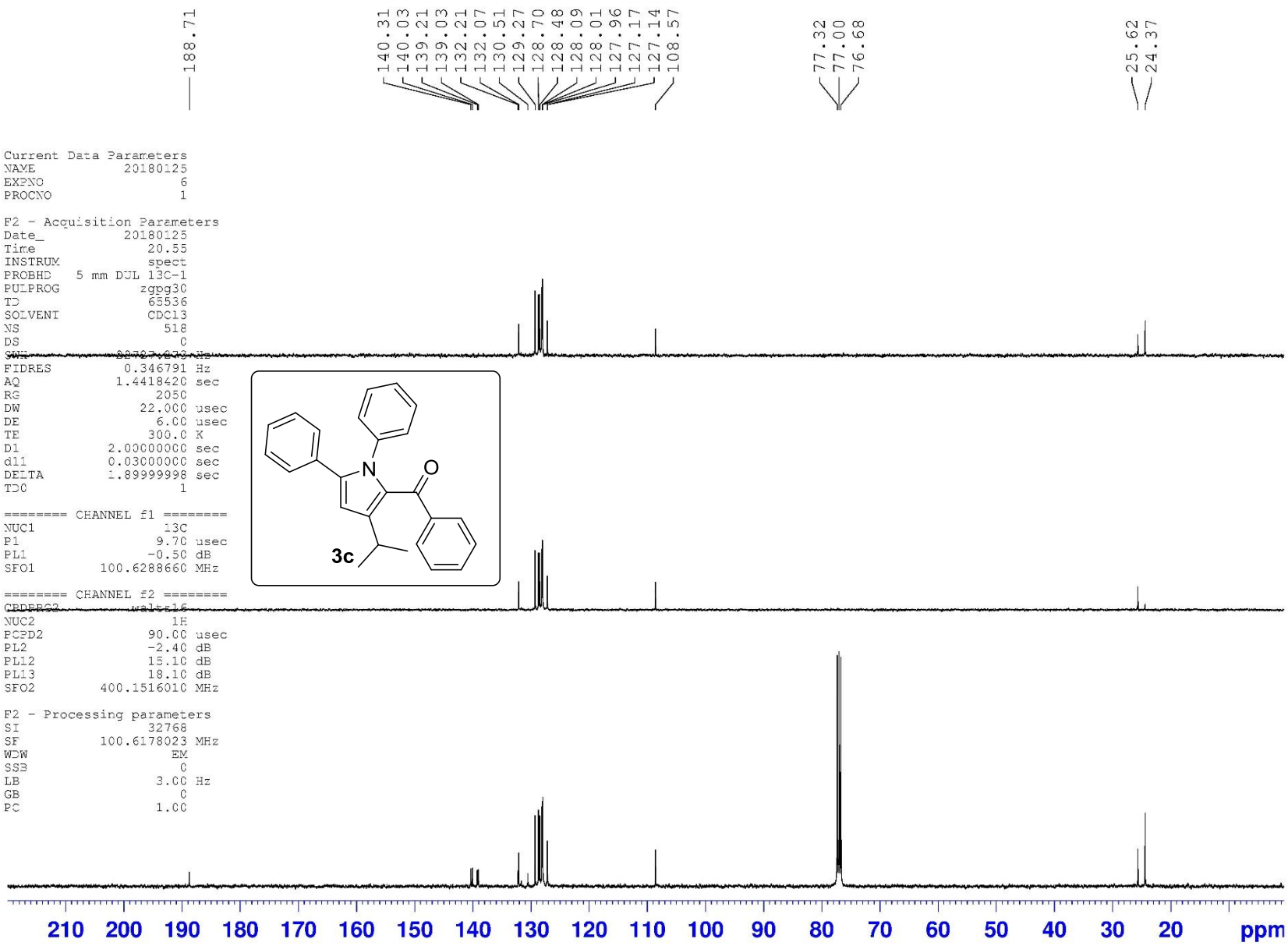


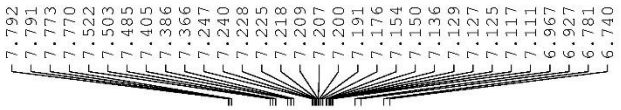



```
Current Data Parameters
NAME                  20180125
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180125
Time                      20.52
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                         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                400.1500170 MHz
WDW                         EM
SSB                          0
LB                       0.00 Hz
GB                           0
PC                       1.00
```

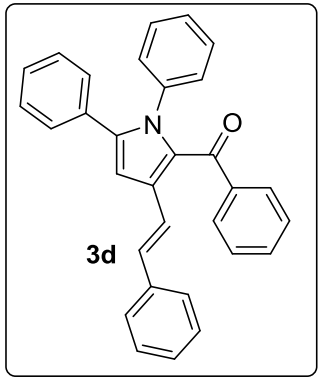


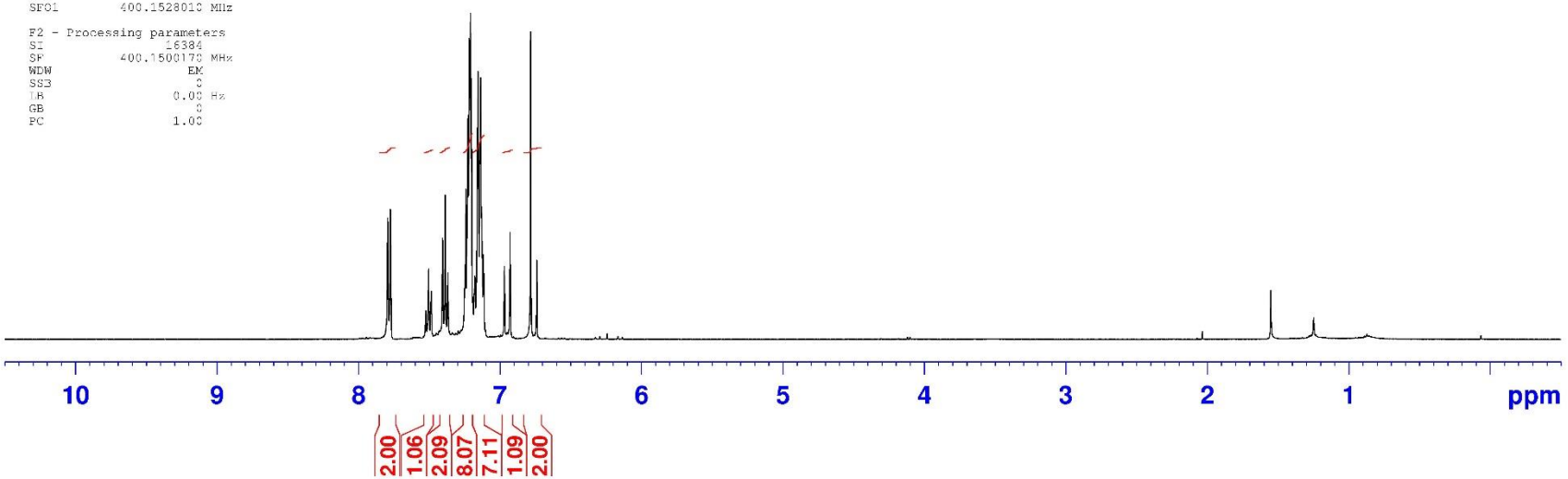


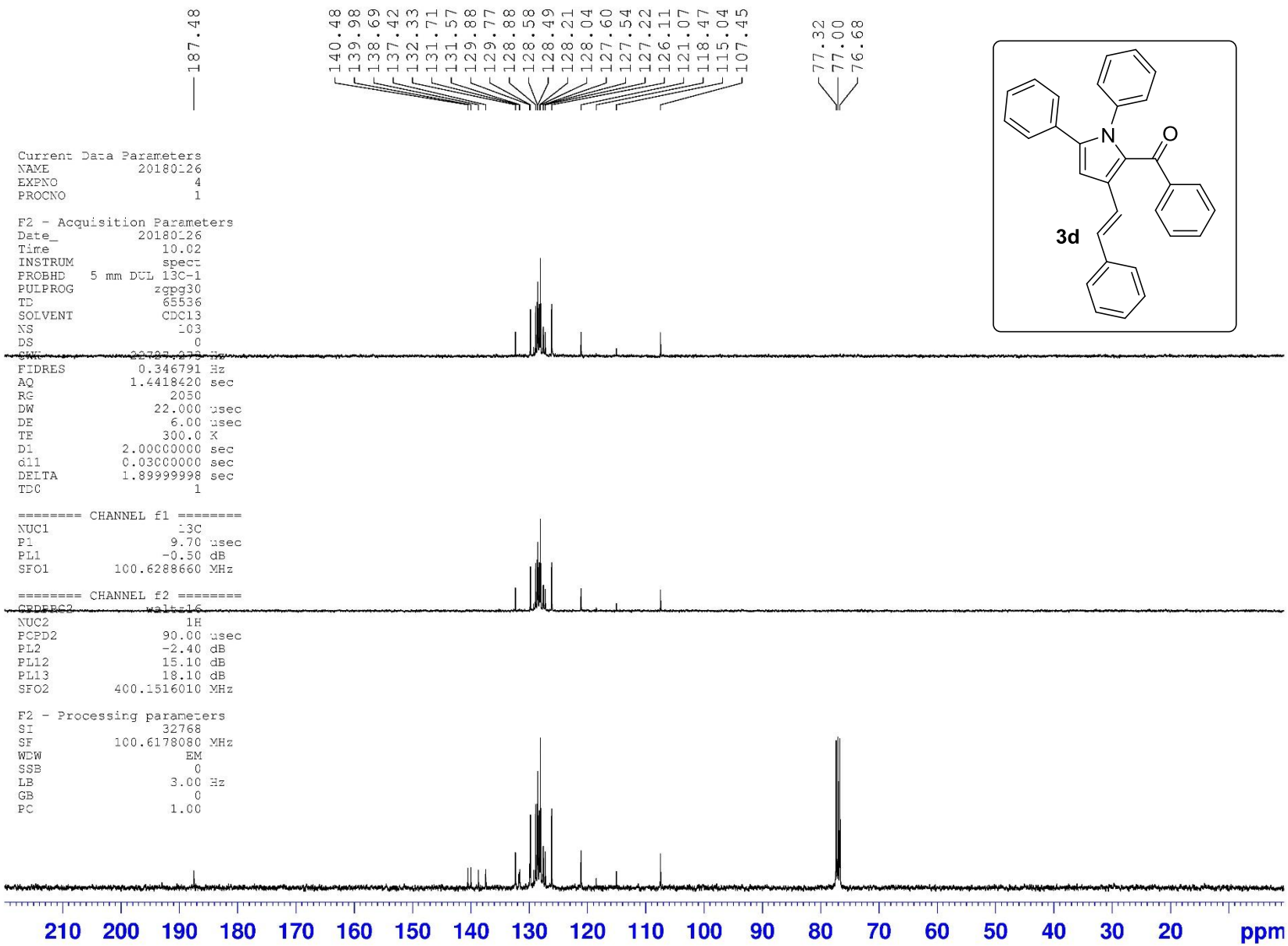

188.71
140.31
140.03
139.21
139.03
132.21
132.07
130.51
129.27
128.70
128.48
128.09
128.01
127.96
127.17
127.14
108.57
77.32
77.00
76.68
25.62
24.37
Current Data Parameters
NAME 20180125
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180125
Time 20.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 518
DS 0
SWH 24038.462 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 100.6178023 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
O
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

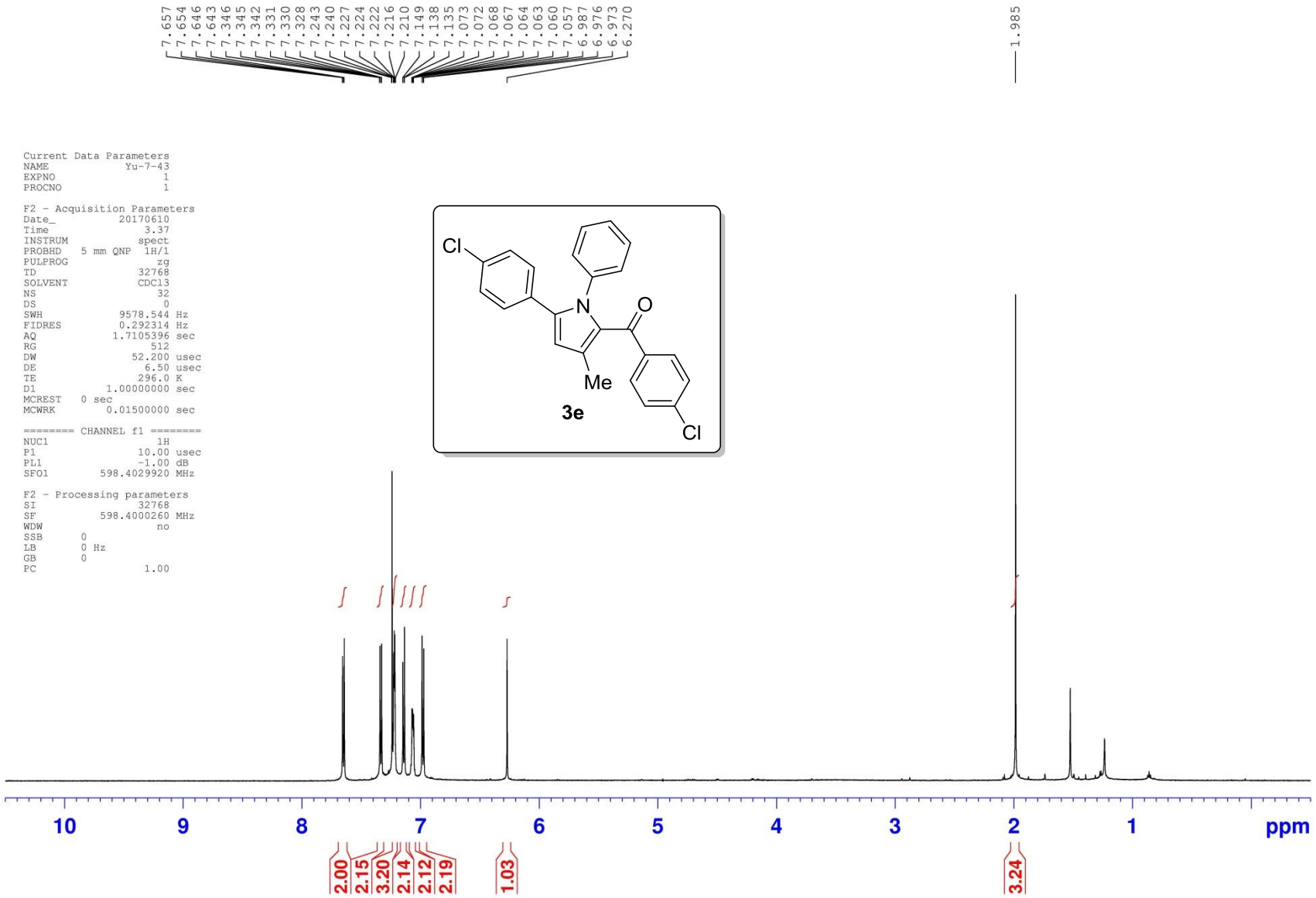


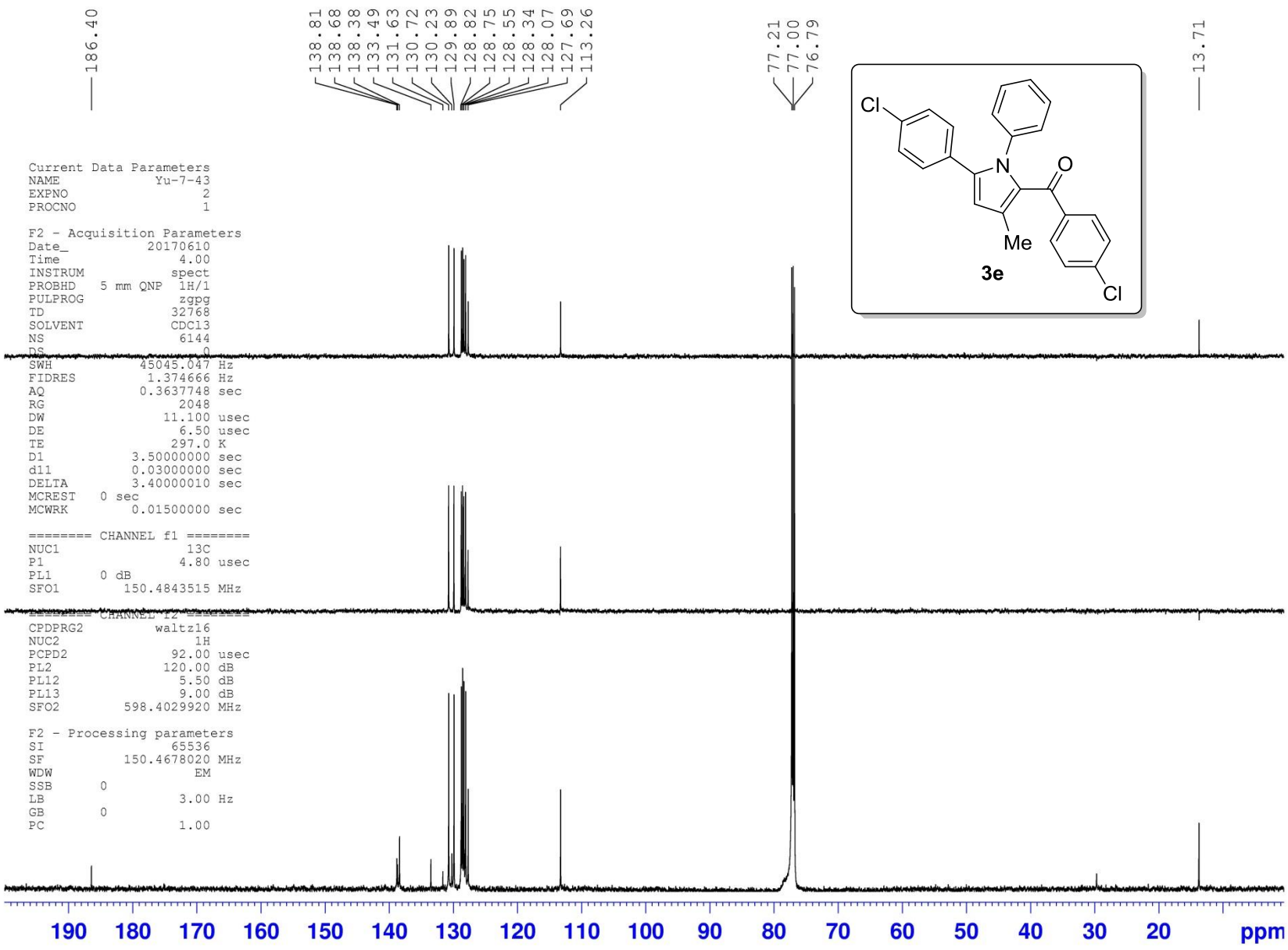

```
Current Data Parameters
NAME                  20180126
EXPNO                        8
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180126
Time                   16.06
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       21
DS                        0
SWH                6410.256 Hz
FIDRES            0.195625 Hz
AQ                2.5559540 sec
RG                      322
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
```

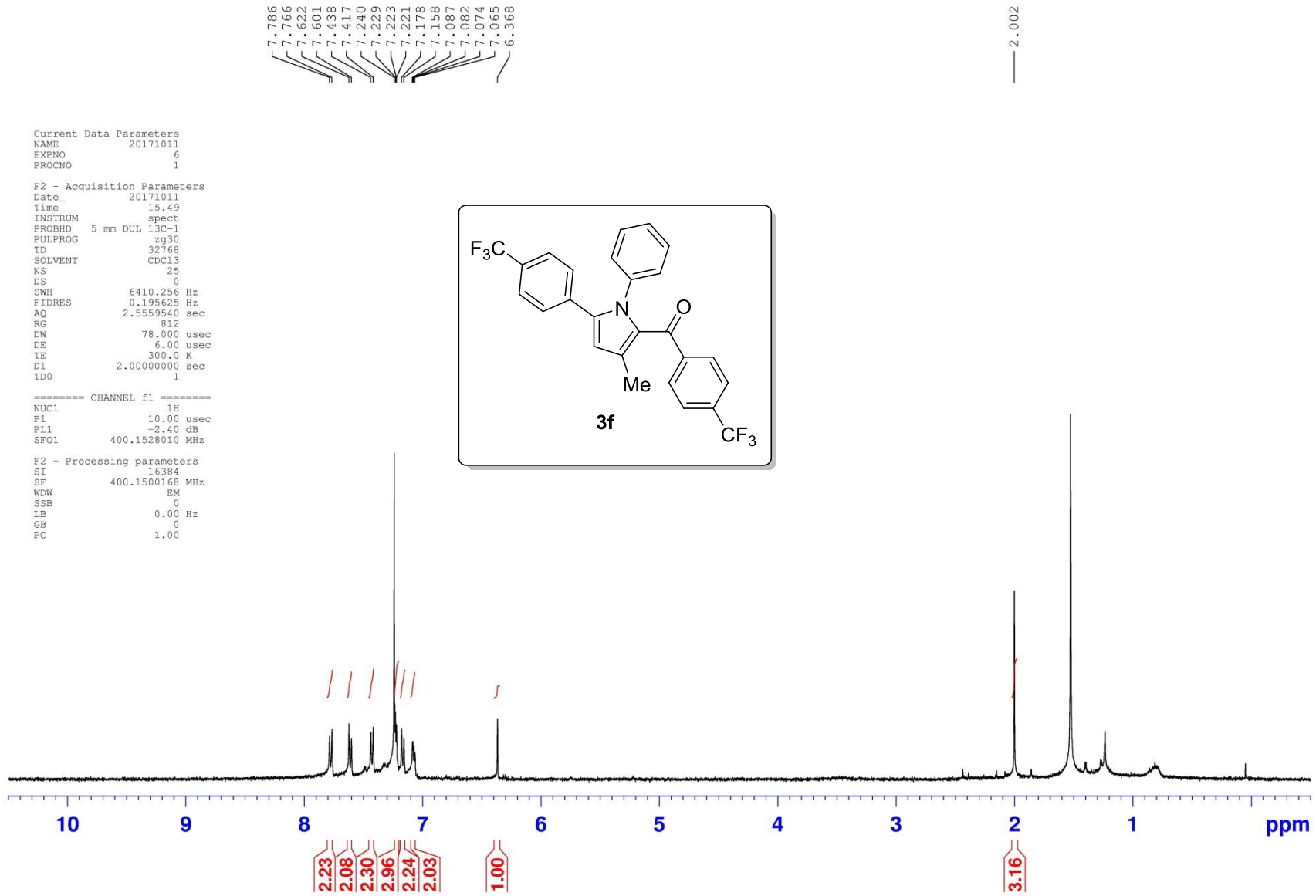


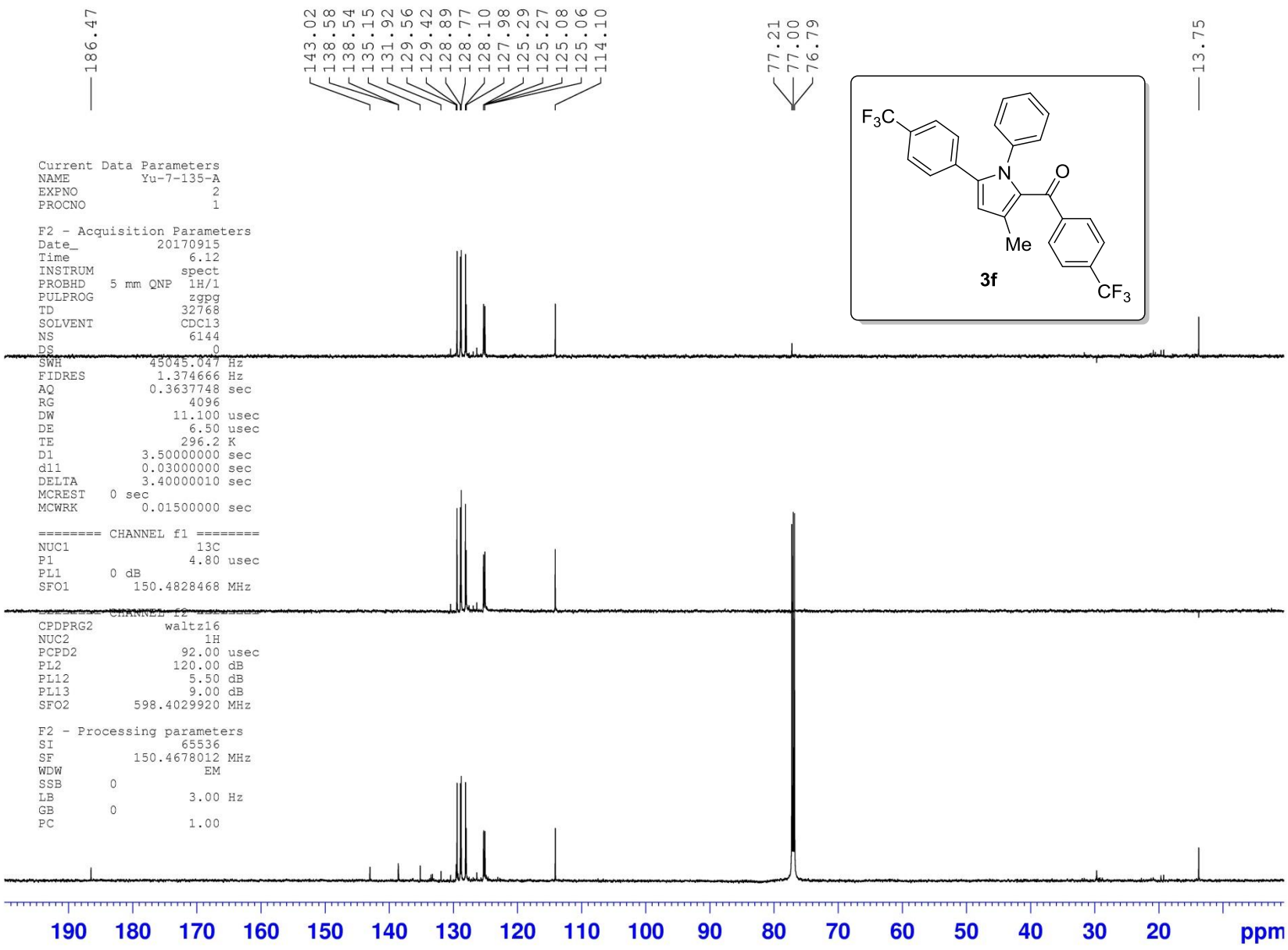


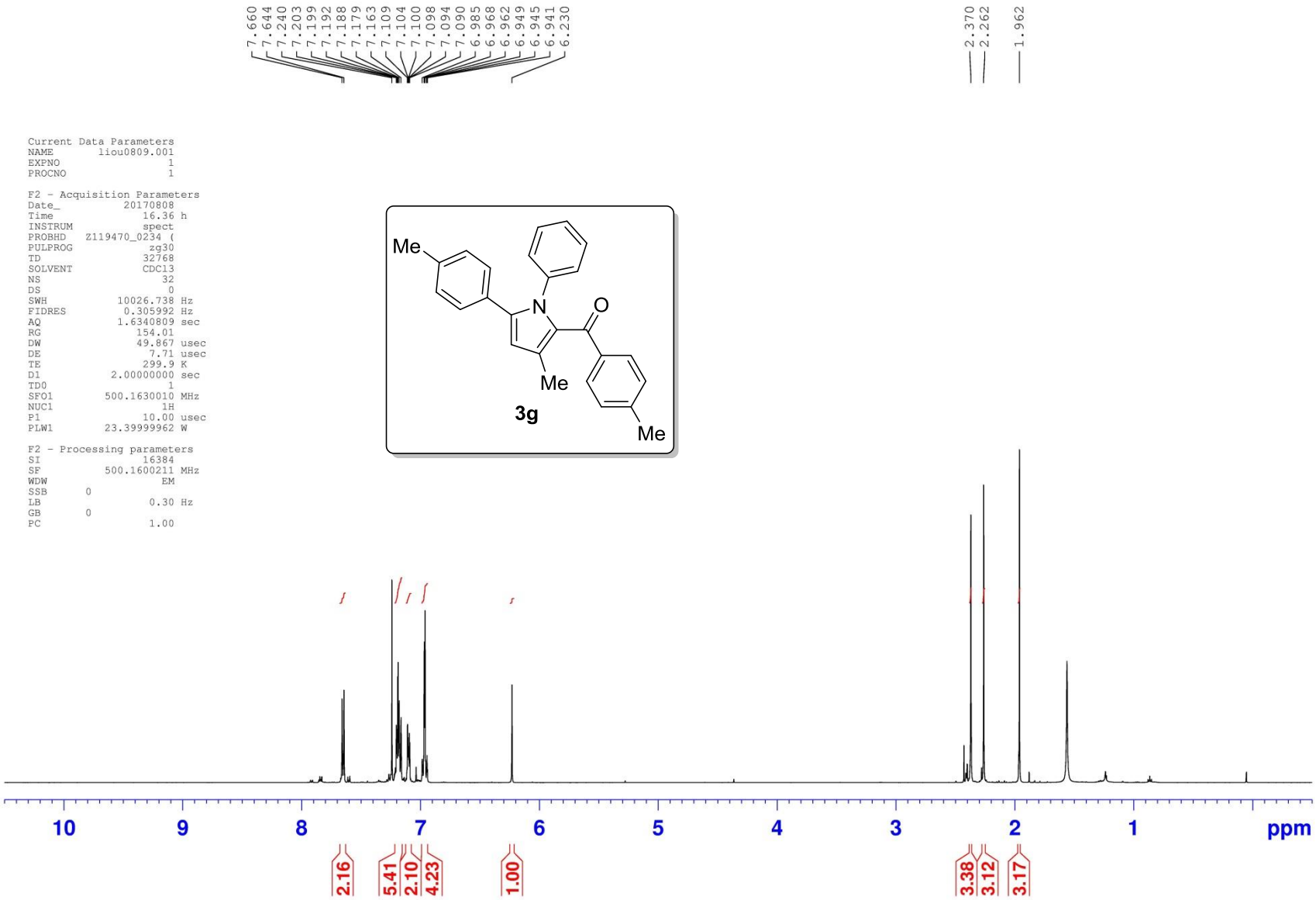

187.48
140.48
139.98
138.69
137.42
132.33
131.71
131.57
129.88
129.77
128.88
128.58
128.49
128.21
128.04
127.60
127.54
127.22
126.11
121.07
118.47
115.04
107.45
77.32
77.00
76.68
N
O
3d
Current Data Parameters
NAME 20180126
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180126
Time 10.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 103
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 100.6178080 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.657
7.654
7.646
7.643
7.346
7.345
7.342
7.331
7.330
7.328
7.243
7.240
7.227
7.224
7.222
7.216
7.210
7.149
7.138
7.135
7.073
7.072
7.068
7.067
7.064
7.063
7.060
7.057
6.987
6.976
6.973
6.270
1.985
Current Data Parameters
NAME Yu-7-43
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170610
Time 3.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9578.544 Hz
FIDRES 0.292314 Hz
AQ 1.7105396 sec
RG 512
DW 52.200 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Cl
N
O
Me
Cl
3e
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.15
3.20
2.14
2.12
2.19
1.03
3.24


186.40
138.81
138.68
138.38
133.49
131.63
130.72
130.23
129.89
128.82
128.75
128.55
128.34
128.07
127.69
113.26
77.21
77.00
76.79
13.71
Cl
N
O
Me
3e
Cl
Current Data Parameters
NAME Yu-7-43
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170610
Time 4.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 297.0 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 150.4843515 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678020 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.786
7.766
7.622
7.601
7.438
7.417
7.240
7.229
7.223
7.221
7.178
7.158
7.087
7.082
7.074
7.065
6.368
2.002
Current Data Parameters
NAME 20171011
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171011
Time 15.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 25
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 812
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
F3C
N
O
Me
CF3
3f
10
9
8
7
6
5
4
3
2
1
ppm
2.23
2.08
2.30
2.96
2.24
2.03
1.00
3.16


186.47
143.02
138.58
138.54
135.15
131.92
129.56
129.42
128.89
128.77
128.10
127.98
125.29
125.27
125.08
125.06
114.10
77.21
77.00
76.79
13.75
F3C
N
O
Me
3f
CF3
Current Data Parameters
NAME Yu-7-135-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170915
Time 6.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.2 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 150.4828468 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678012 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.660
7.644
7.240
7.203
7.199
7.192
7.188
7.179
7.163
7.109
7.104
7.100
7.098
7.094
7.090
6.985
6.968
6.962
6.949
6.945
6.941
6.230
2.370
2.262
1.962
Current Data Parameters
NAME liou0809.001
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170808
Time 16.36 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340809 sec
RG 154.01
DW 49.867 usec
DE 7.71 usec
TE 299.9 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.39999962 W
F2 - Processing parameters
SI 16384
SF 500.1600211 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
N
O
Me
3g
Me
10
9
8
7
6
5
4
3
2
1
ppm
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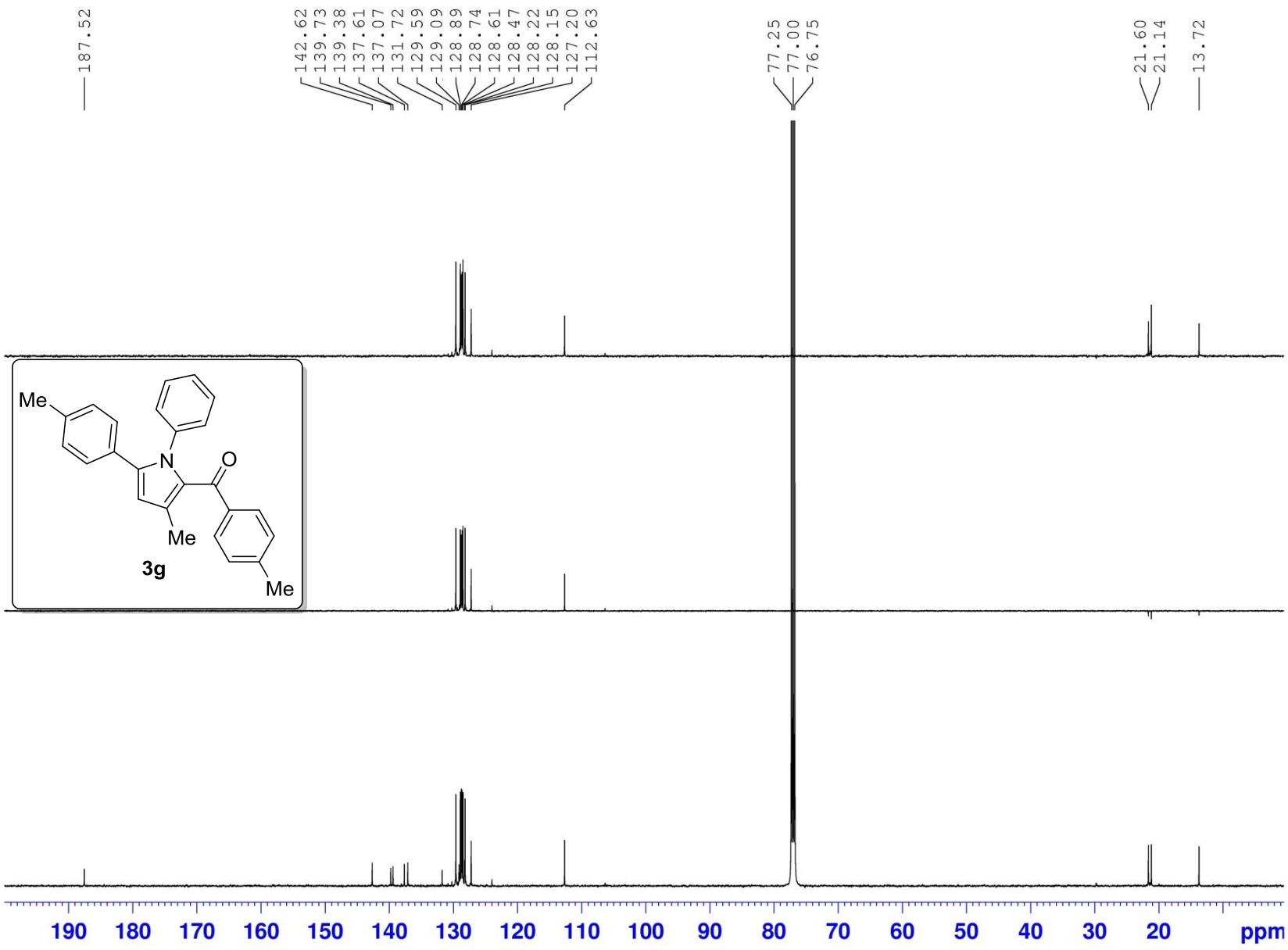
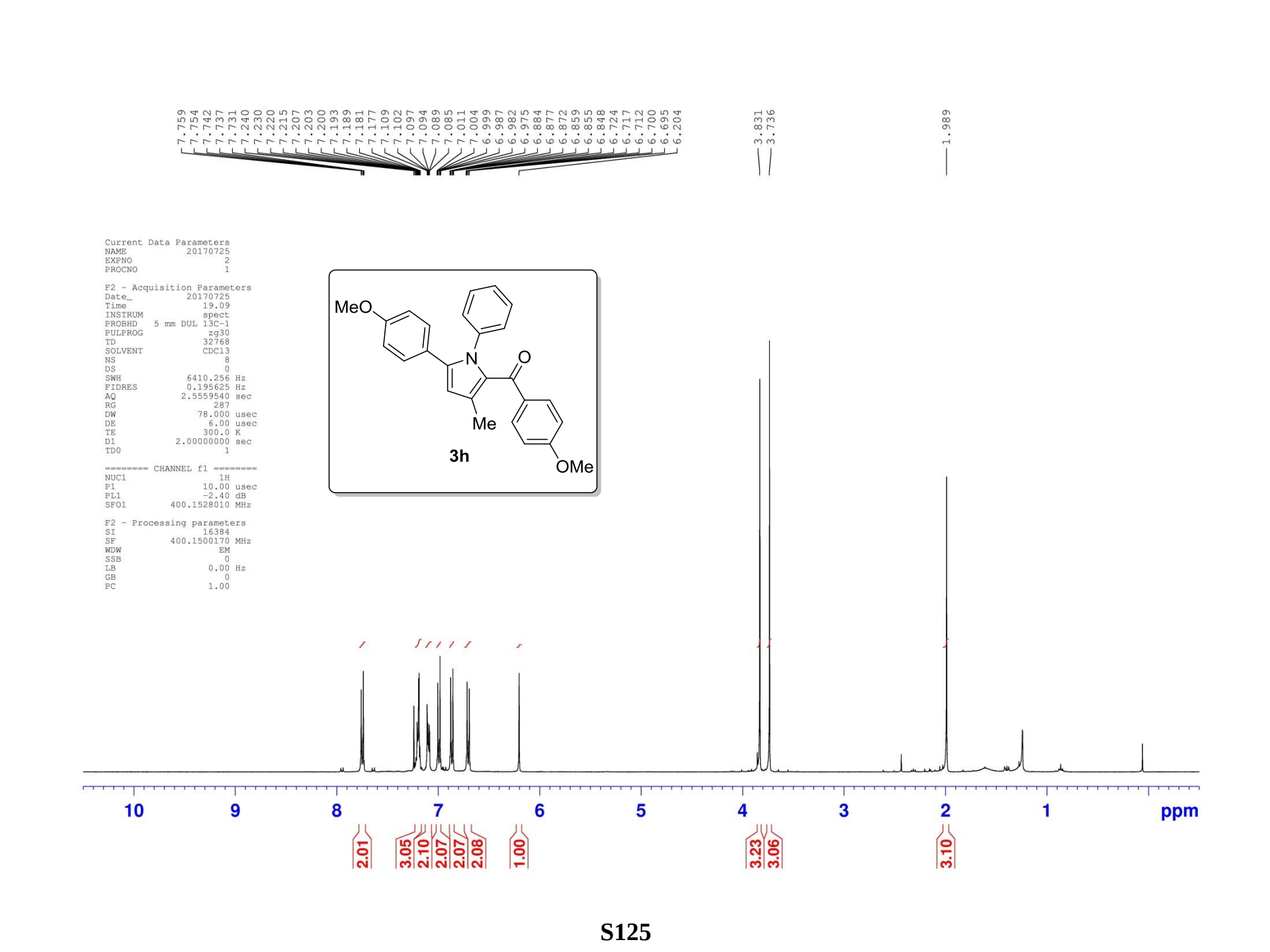
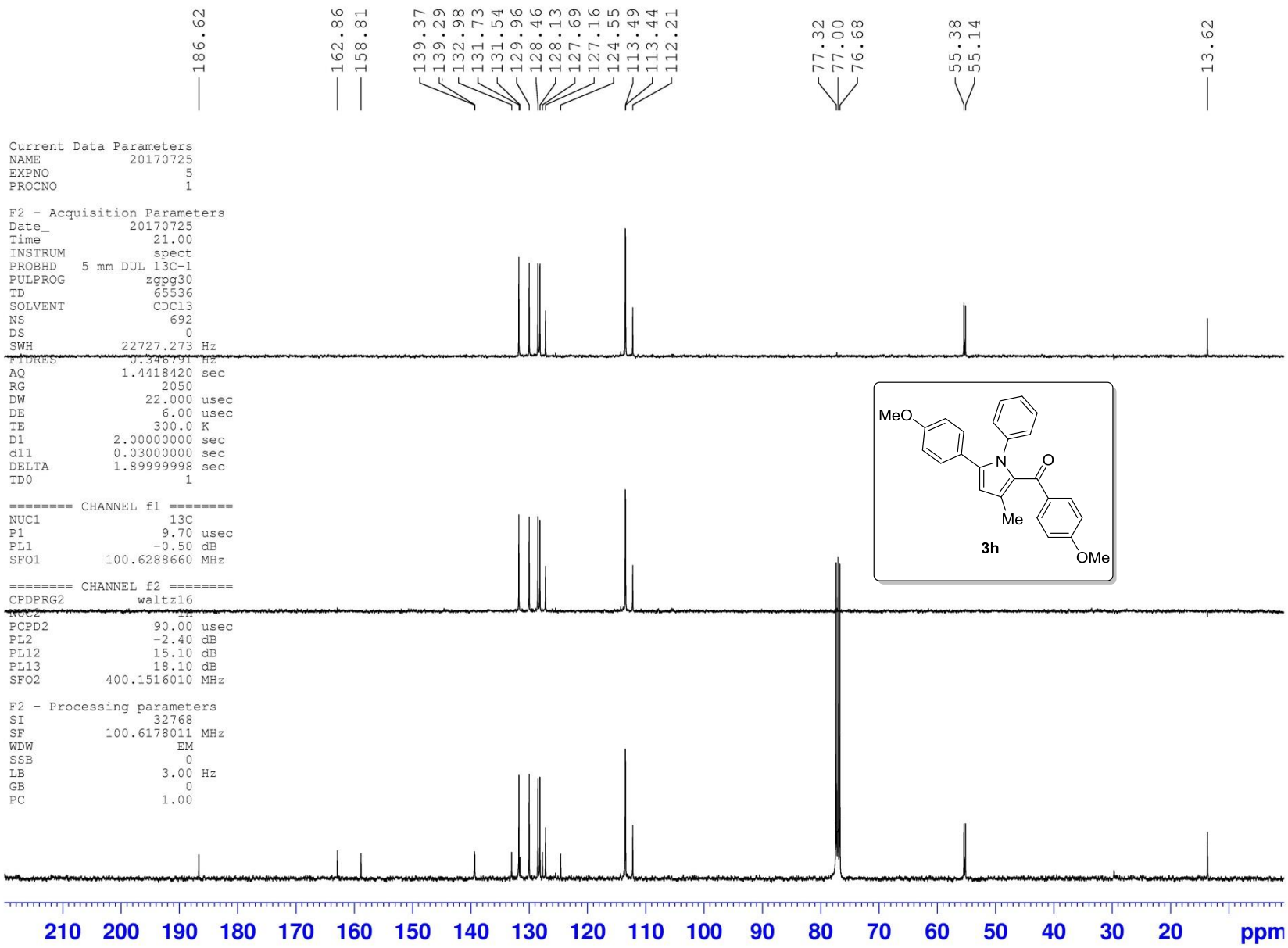
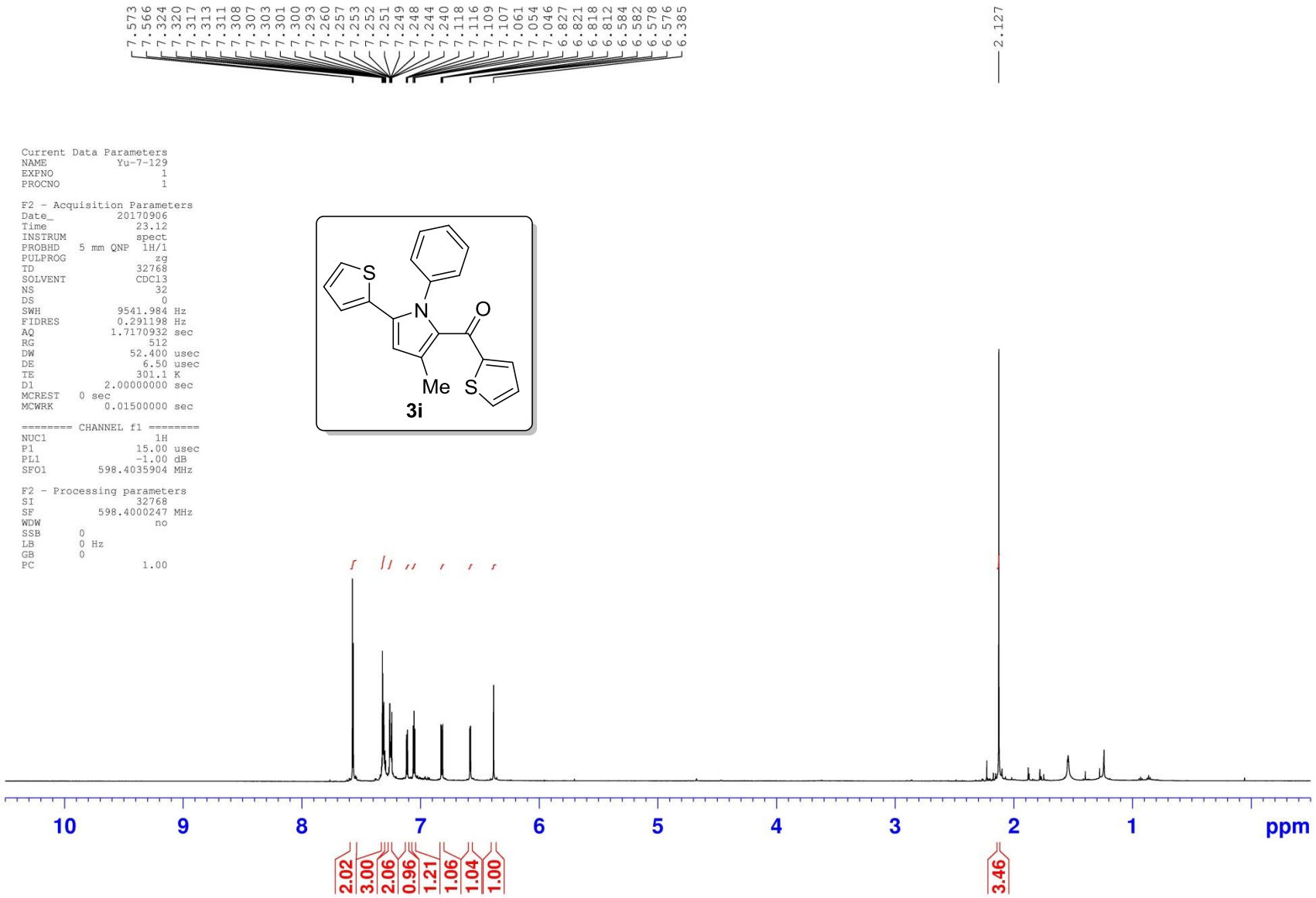
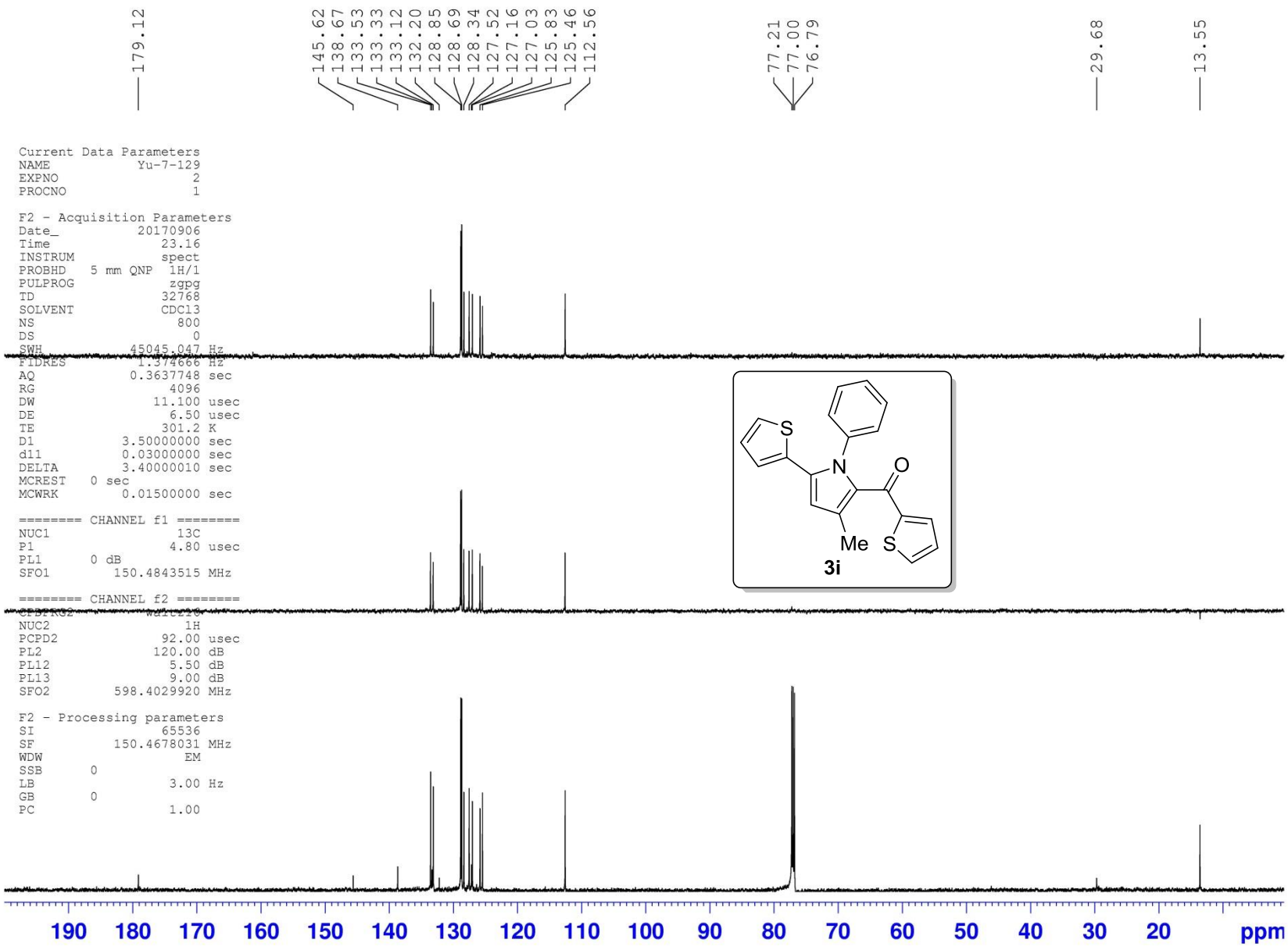
5.41
2.10
4.23
1.00
3.38
3.12
3.17

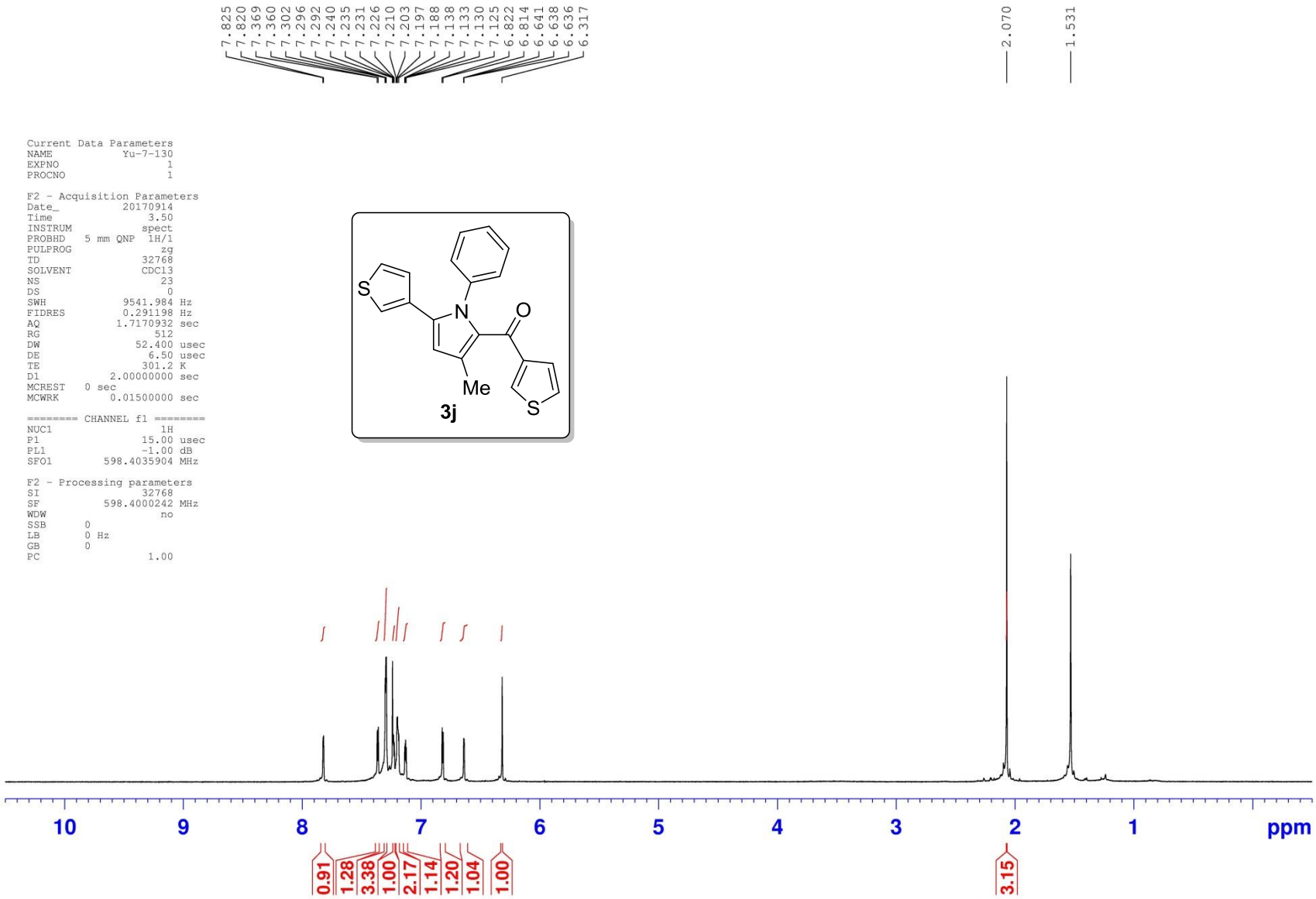

187.52
142.62
139.73
139.38
137.61
137.07
131.72
129.59
129.09
128.89
128.74
128.61
128.47
128.22
128.15
127.20
112.63
77.25
77.00
76.75
21.60
21.14
13.72
Me
N
O
Me
Me
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

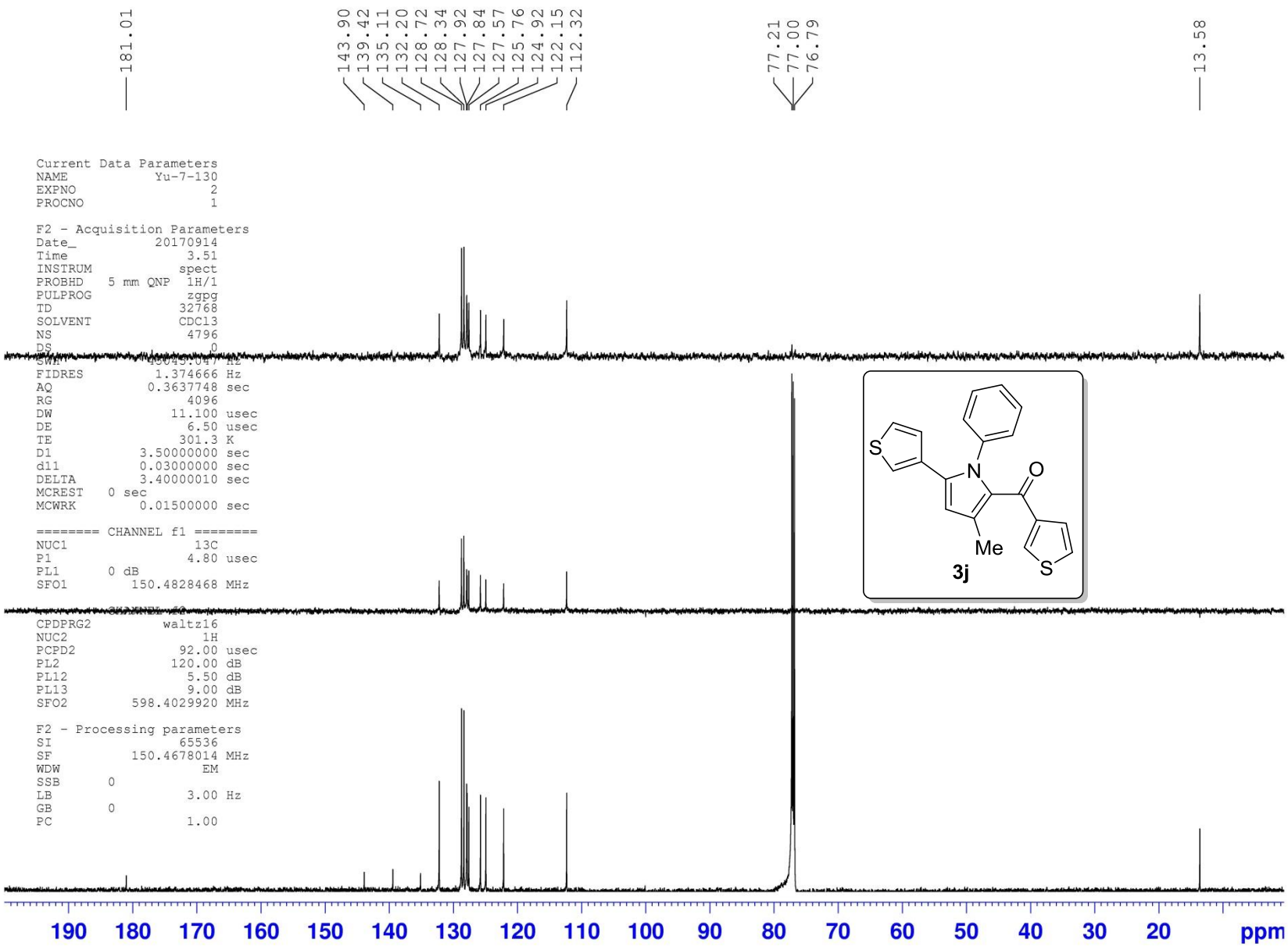

7.759
7.754
7.742
7.737
7.731
7.240
7.230
7.220
7.215
7.207
7.203
7.200
7.193
7.189
7.181
7.177
7.109
7.102
7.097
7.094
7.089
7.085
7.011
7.004
6.999
6.987
6.982
6.975
6.884
6.877
6.872
6.859
6.855
6.848
6.724
6.717
6.712
6.700
6.695
6.204
3.831
3.736
1.989
Current Data Parameters
NAME 20170725
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 19.09
INSTRUM spect
PROBHD 5 mm DUL 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 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
MeO
N
O
Me
OMe
3h
10
9
8
7
6
5
4
3
2
1
ppm
2.01
3.05
2.10
2.07
2.07
2.08
1.00
3.23
3.06
3.10

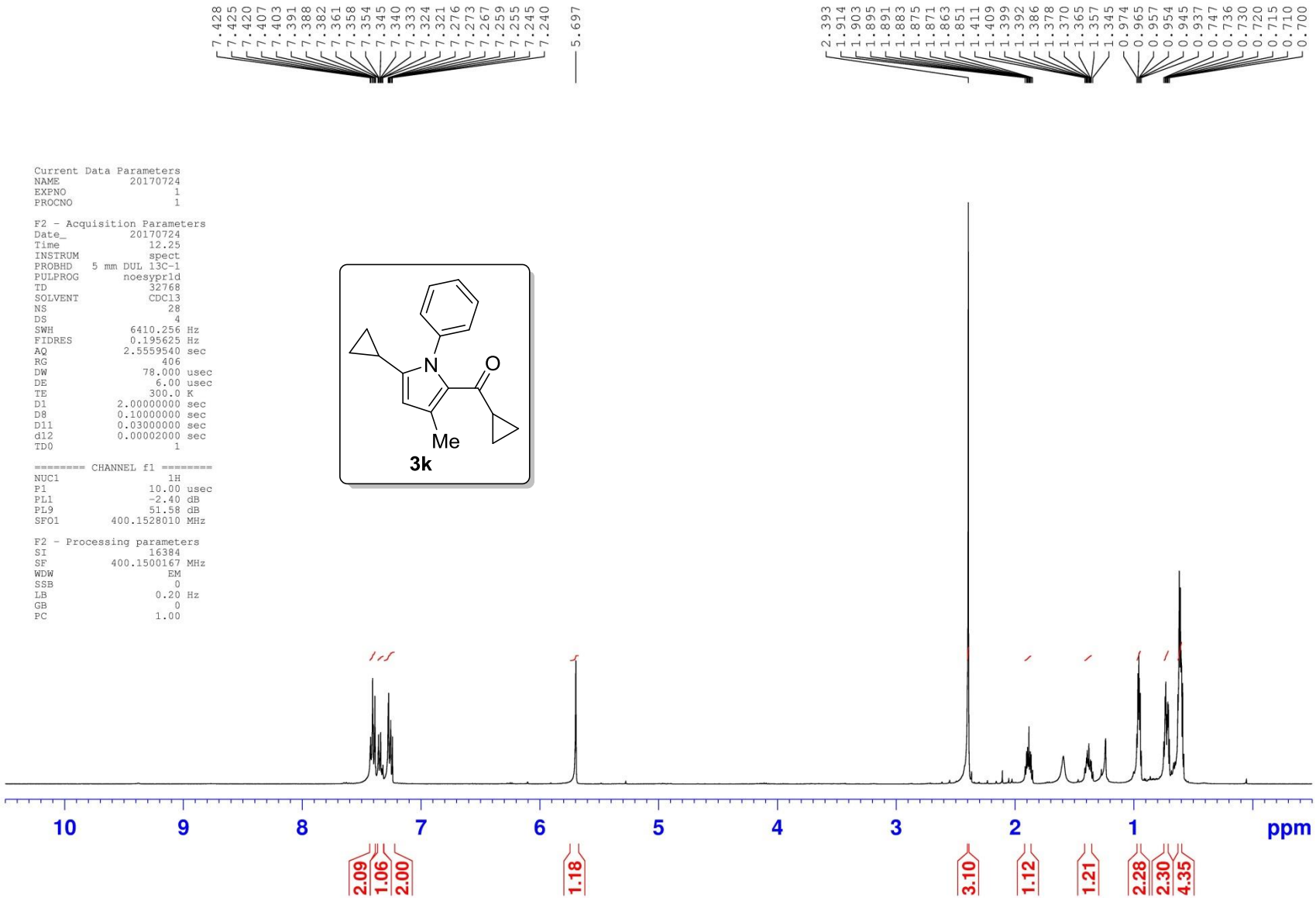

186.62
162.86
158.81
139.37
139.29
132.98
131.73
131.54
129.96
128.46
128.13
127.69
127.16
124.55
113.49
113.44
112.21
77.32
77.00
76.68
55.38
55.14
13.62
Current Data Parameters
NAME 20170725
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 21.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 692
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 100.6178011 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
MeO
N
O
Me
OMe
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

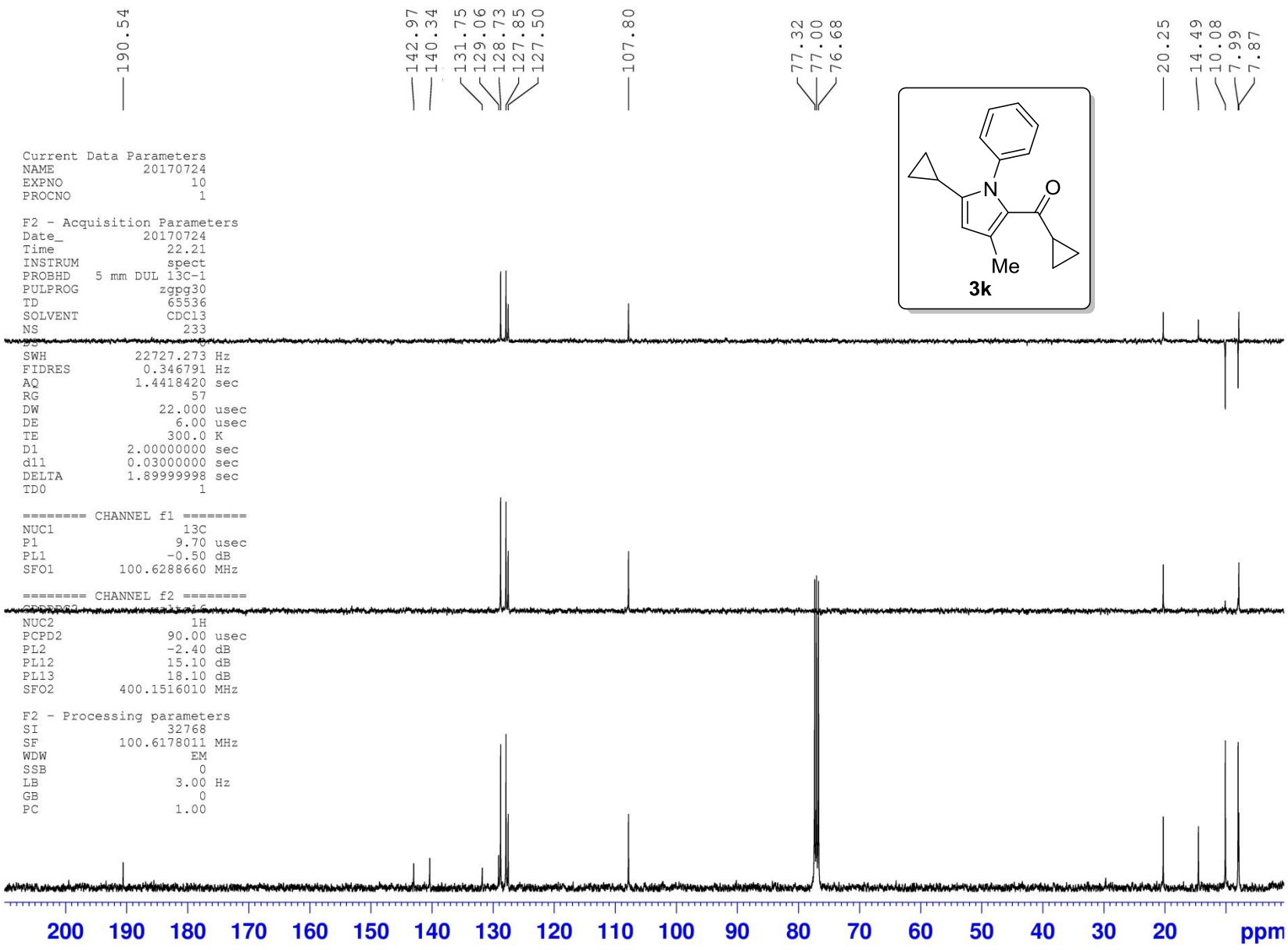

7.573
7.566
7.324
7.320
7.317
7.313
7.311
7.308
7.307
7.303
7.301
7.300
7.293
7.260
7.257
7.253
7.252
7.251
7.249
7.248
7.244
7.240
7.118
7.116
7.109
7.107
7.061
7.054
7.046
6.827
6.821
6.818
6.812
6.584
6.582
6.578
6.576
6.385
2.127
Current Data Parameters
NAME Yu-7-129
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170906
Time 23.12
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 301.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000247 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
S
N
O
Me
S
3i
10
9
8
7
6
5
4
3
2
1
ppm
2.02
3.00
2.06
0.96
1.21
1.06
1.04
1.00
3.46

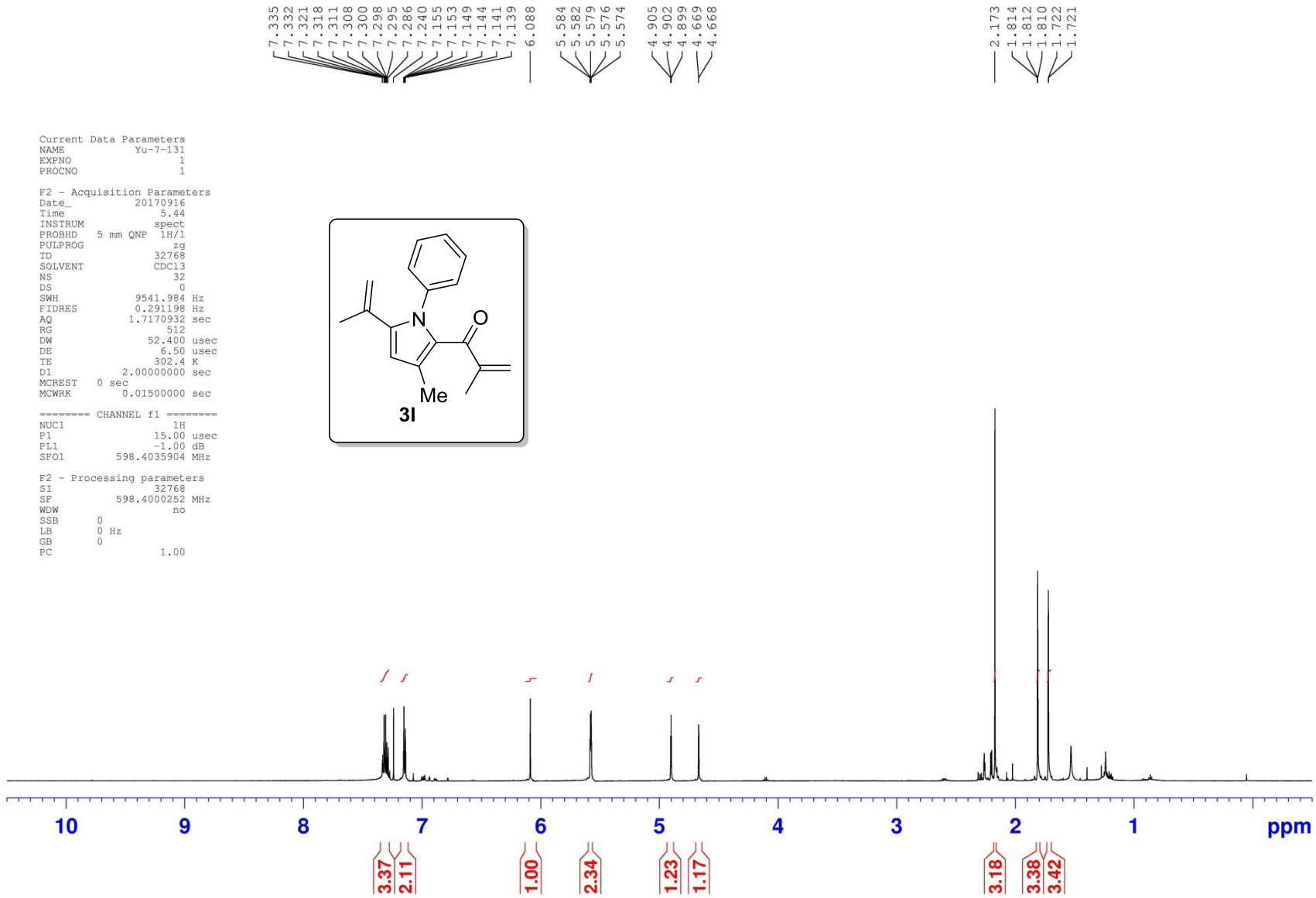

179.12
145.62
138.67
133.53
133.33
133.12
132.20
128.85
128.69
128.34
127.52
127.16
127.03
125.83
125.46
112.56
77.21
77.00
76.79
29.68
13.55
Current Data Parameters
NAME Yu-7-129
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170906
Time 23.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 800
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.2 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 150.4843515 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678031 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
S
N
O
Me
S
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

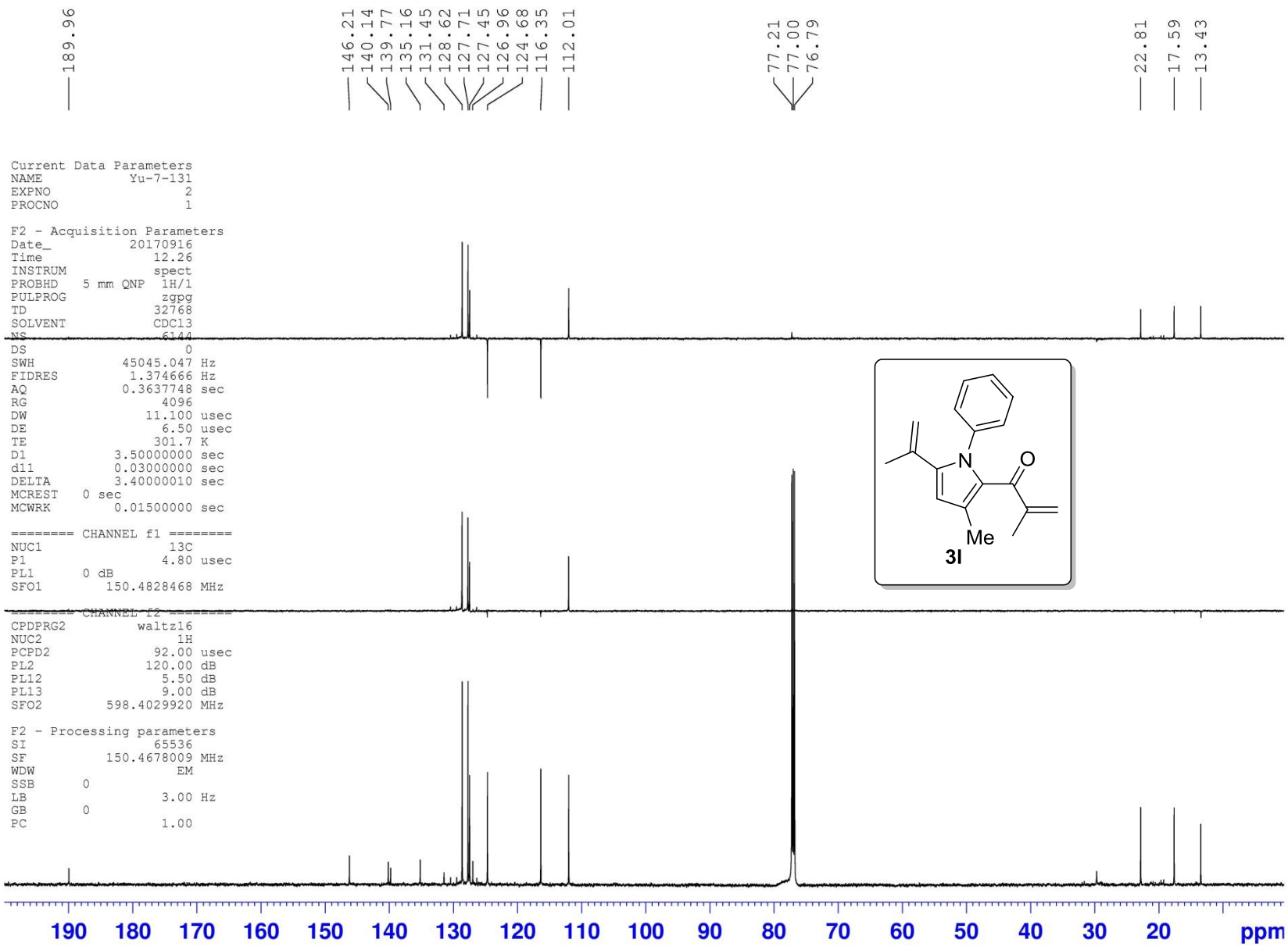

7.825
7.820
7.369
7.360
7.302
7.296
7.292
7.240
7.235
7.231
7.226
7.210
7.203
7.197
7.188
7.138
7.133
7.130
7.125
6.822
6.814
6.641
6.638
6.636
6.317
2.070
1.531
Current Data Parameters
NAME Yu-7-130
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170914
Time 3.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 23
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 301.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000242 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
S
N
O
Me
S
3j
10
9
8
7
6
5
4
3
2
1
ppm
0.91
1.28
3.38
1.00
2.17
1.14
1.20
1.04
1.00
3.15

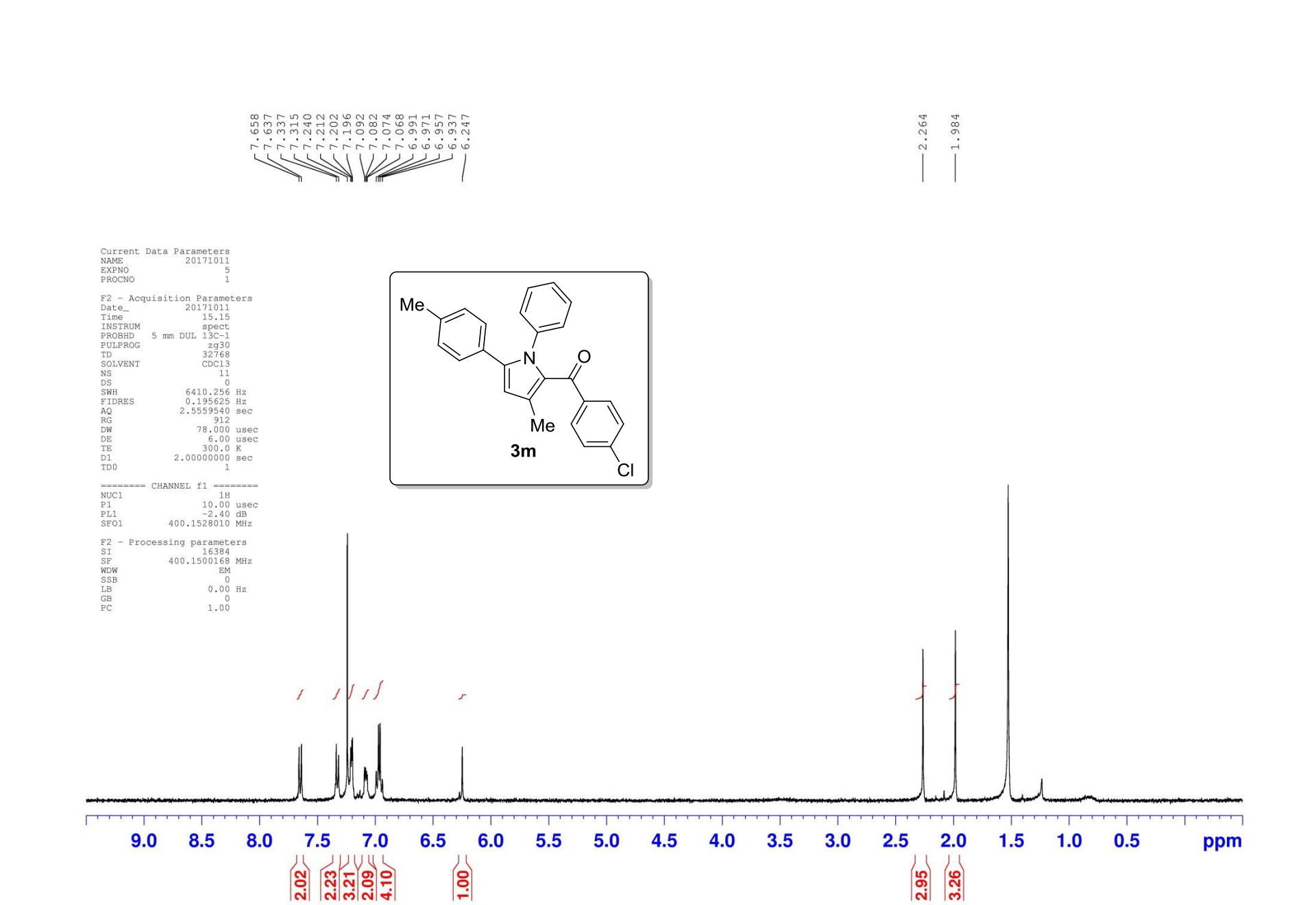

181.01
143.90
139.42
135.11
132.20
128.72
128.34
127.92
127.84
127.57
125.76
124.92
122.15
112.32
77.21
77.00
76.79
13.58
Current Data Parameters
NAME Yu-7-130
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170914
Time 3.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 4796
DS 0
SWH 40045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4828468 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678014 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
S
N
O
Me
S
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

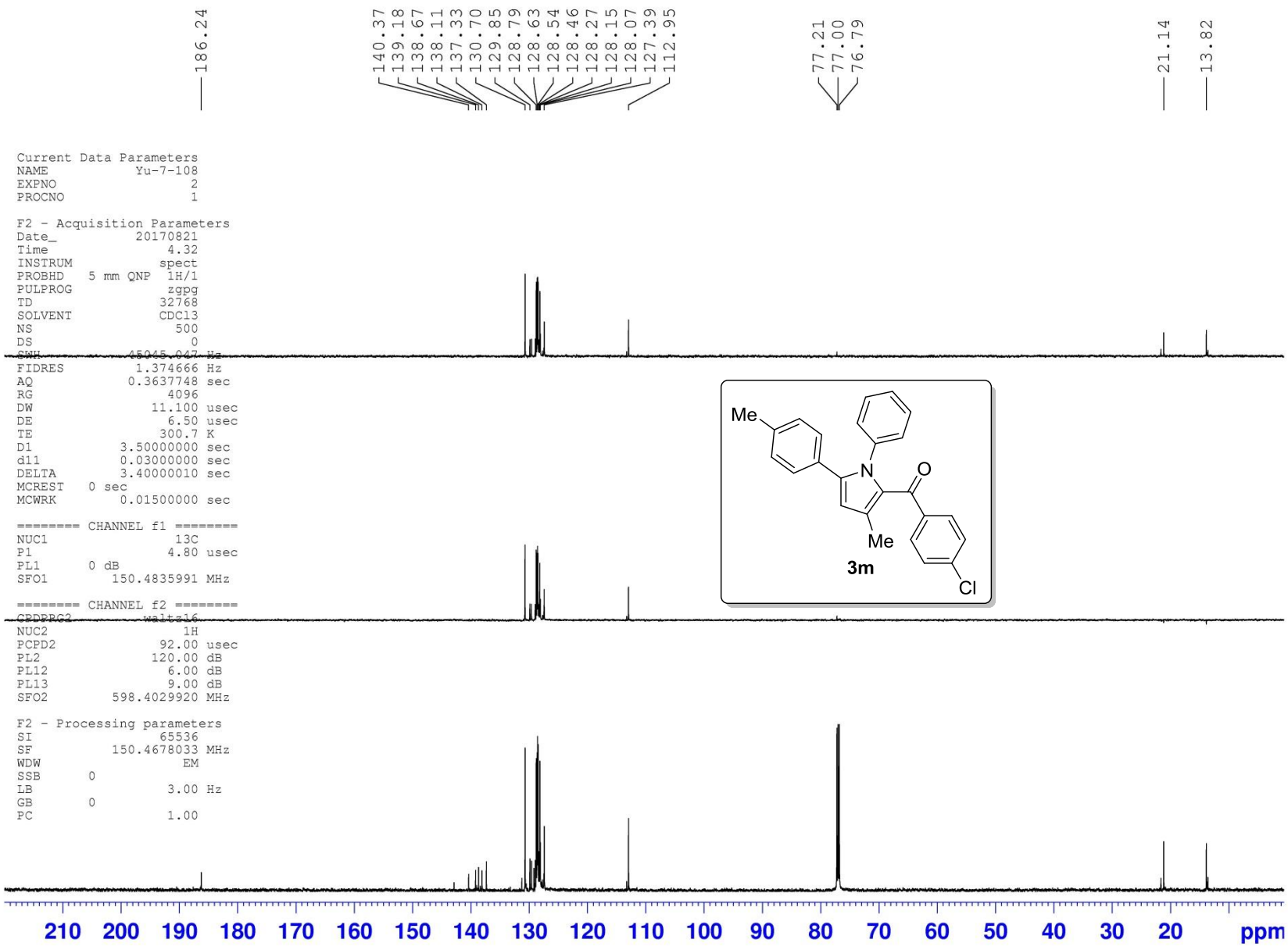

7.428
7.425
7.420
7.407
7.403
7.391
7.388
7.382
7.361
7.358
7.354
7.345
7.340
7.333
7.324
7.321
7.276
7.273
7.267
7.259
7.255
7.245
7.240
5.697
2.393
1.914
1.903
1.895
1.891
1.883
1.875
1.871
1.863
1.851
1.411
1.409
1.399
1.392
1.386
1.378
1.370
1.365
1.357
1.345
0.974
0.965
0.957
0.954
0.945
0.937
0.747
0.736
0.730
0.720
0.715
0.710
0.700
Current Data Parameters
NAME 20170724
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170724
Time 12.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG noesypr1d
TD 32768
SOLVENT CDC13
NS 28
DS 4
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
D8 0.10000000 sec
D11 0.03000000 sec
d12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
PL9 51.58 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500167 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
N
O
Me
3k
10
9
8
7
6
5
4
3
2
1
ppm
2.09
1.06
2.00
1.18
3.10
1.12
1.21
2.28
2.30
4.35

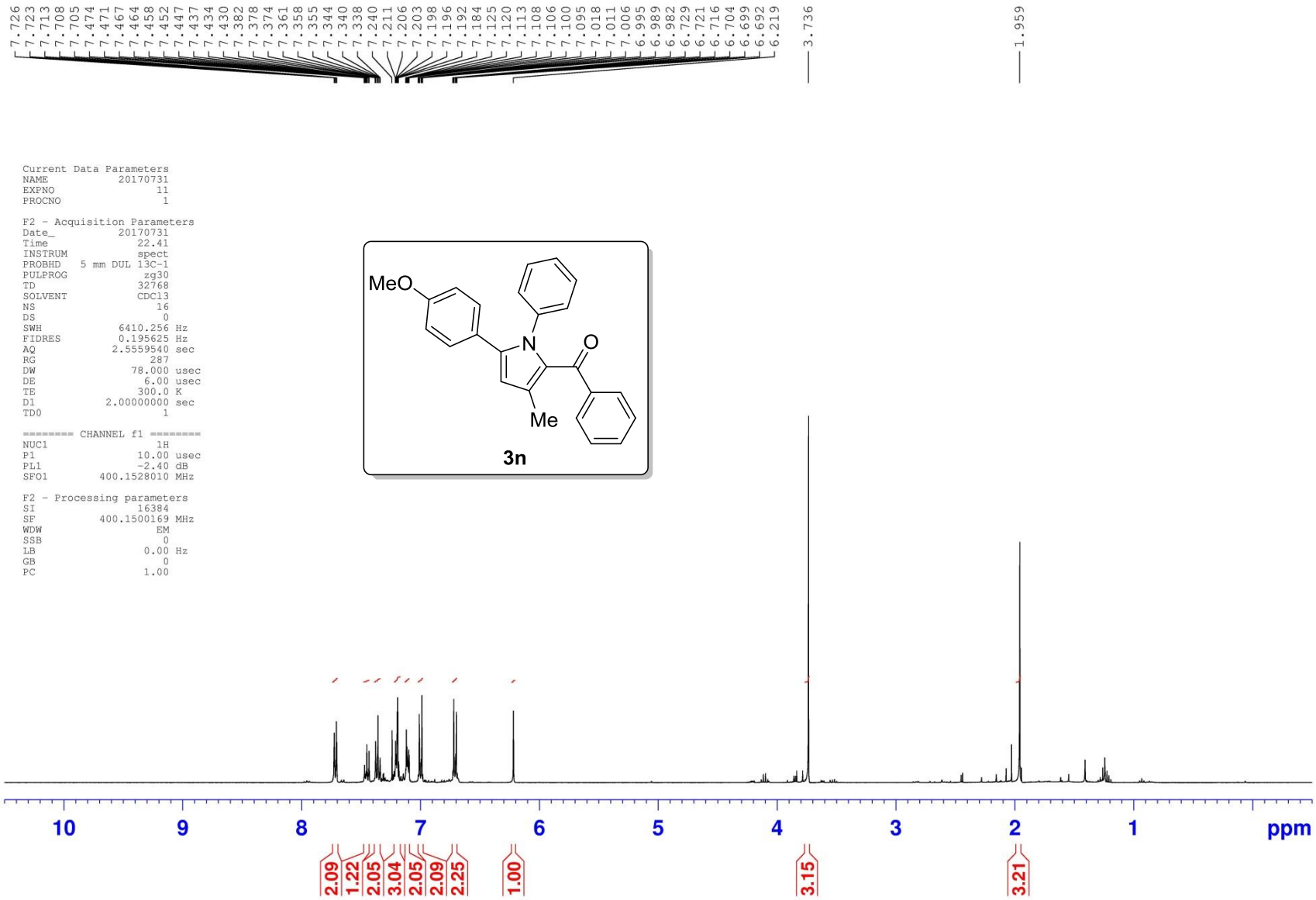

190.54
142.97
140.34
131.75
129.06
128.73
127.85
127.50
107.80
77.32
77.00
76.68
20.25
14.49
10.08
7.99
7.87
N
O
Me
3k
Current Data Parameters
NAME 20170724
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170724
Time 22.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 233
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
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 100.6178011 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

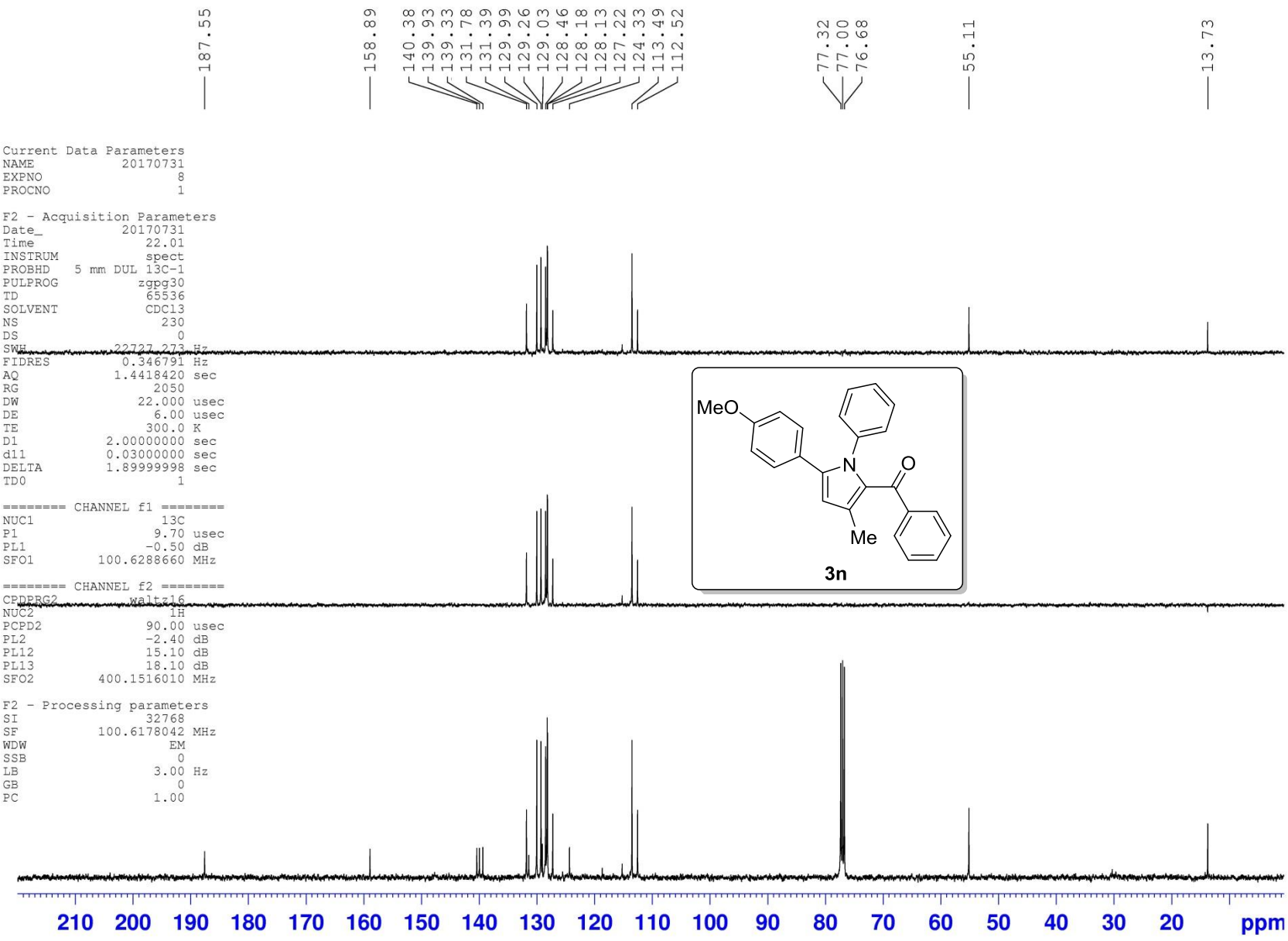

7.335
7.332
7.321
7.318
7.311
7.308
7.300
7.298
7.295
7.286
7.240
7.155
7.153
7.149
7.144
7.141
7.139
6.088
5.584
5.582
5.579
5.576
5.574
4.905
4.902
4.899
4.669
4.668
2.173
1.814
1.812
1.810
1.722
1.721
Current Data Parameters
NAME Yu-7-131
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170916
Time 5.44
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 302.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000252 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
O
Me
3l
10
9
8
7
6
5
4
3
2
1
ppm
3.37
2.11
1.00
2.34
1.23
1.17
3.18
3.38
3.42

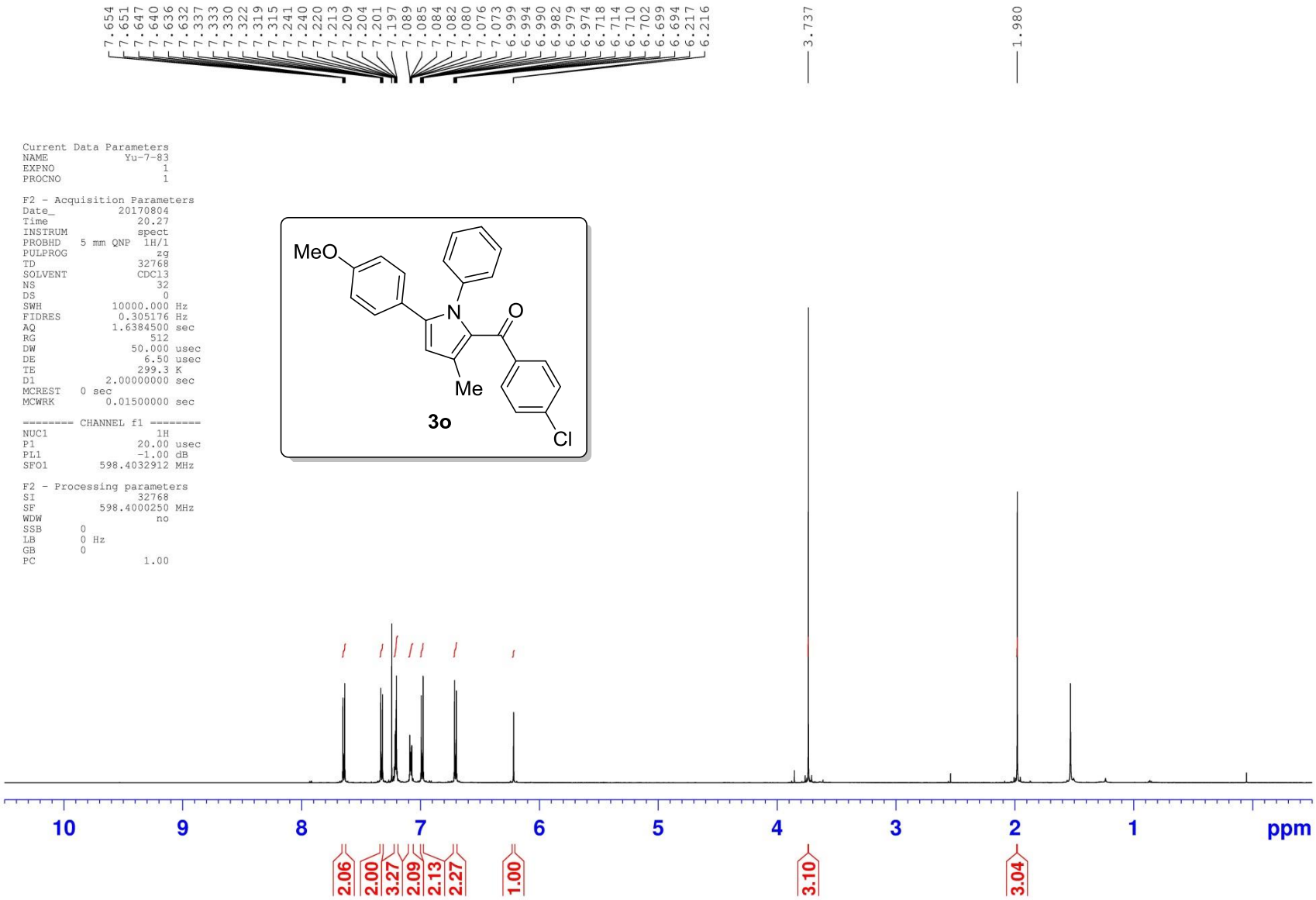

189.96
146.21
140.14
139.77
135.16
131.45
128.62
127.71
127.45
126.96
124.68
116.35
112.01
77.21
77.00
76.79
22.81
17.59
13.43
Current Data Parameters
NAME Yu-7-131
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170916
Time 12.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678009 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
O
Me
3l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.658
7.637
7.337
7.315
7.240
7.212
7.202
7.196
7.092
7.082
7.074
7.068
6.991
6.971
6.957
6.937
6.247
2.264
1.984
Current Data Parameters
NAME 20171011
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171011
Time 15.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 912
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
Me
N
O
Me
3m
Cl
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.02
2.23
3.21
2.09
4.10
1.00
2.95
3.26


186.24
140.37
139.18
138.67
138.11
137.33
130.70
129.85
128.79
128.63
128.54
128.46
128.27
128.15
128.07
127.39
112.95
77.21
77.00
76.79
21.14
13.82
Current Data Parameters
NAME Yu-7-108
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170821
Time 4.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
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 300.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4835991 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678033 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Me
N
O
Me
Cl
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.726
7.723
7.713
7.708
7.705
7.474
7.471
7.467
7.464
7.458
7.452
7.447
7.437
7.434
7.430
7.382
7.378
7.374
7.361
7.358
7.355
7.344
7.340
7.338
7.240
7.211
7.206
7.203
7.198
7.196
7.192
7.184
7.125
7.120
7.113
7.108
7.106
7.100
7.095
7.018
7.011
7.006
6.995
6.989
6.982
6.729
6.721
6.716
6.704
6.699
6.692
6.219
3.736
1.959
Current Data Parameters
NAME 20170731
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170731
Time 22.41
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 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
MeO
N
O
Me
3n
10
9
8
7
6
5
4
3
2
1
ppm
2.09
1.22
2.05
3.04
2.05
2.09
2.25
1.00
3.15
3.21


187.55
158.89
140.38
139.93
139.33
131.78
131.39
129.99
129.26
129.03
128.46
128.18
128.13
127.22
124.33
113.49
112.52
77.32
77.00
76.68
55.11
13.73
Current Data Parameters
NAME 20170731
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170731
Time 22.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 230
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 100.6178042 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
MeO
N
O
Me
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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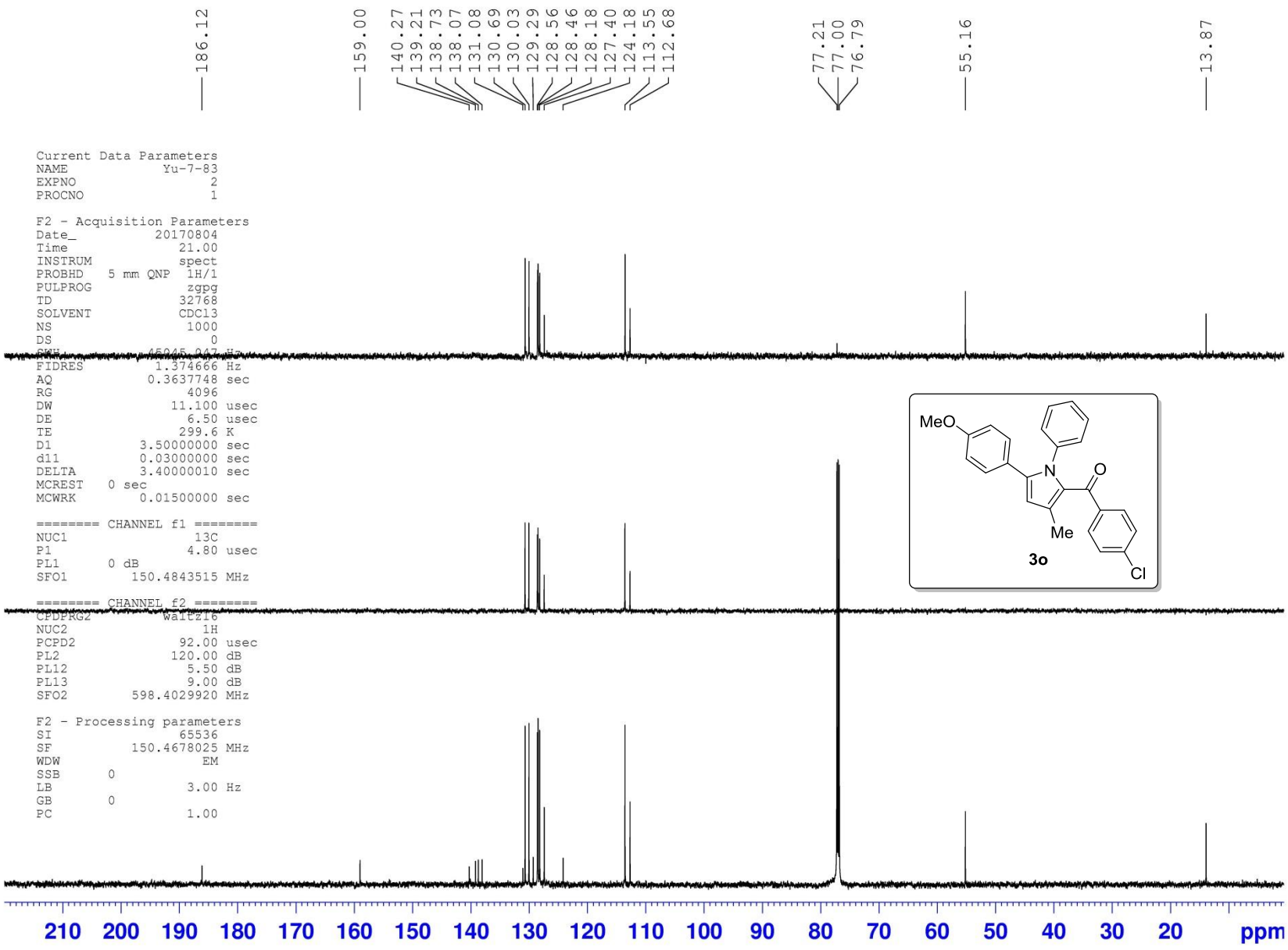
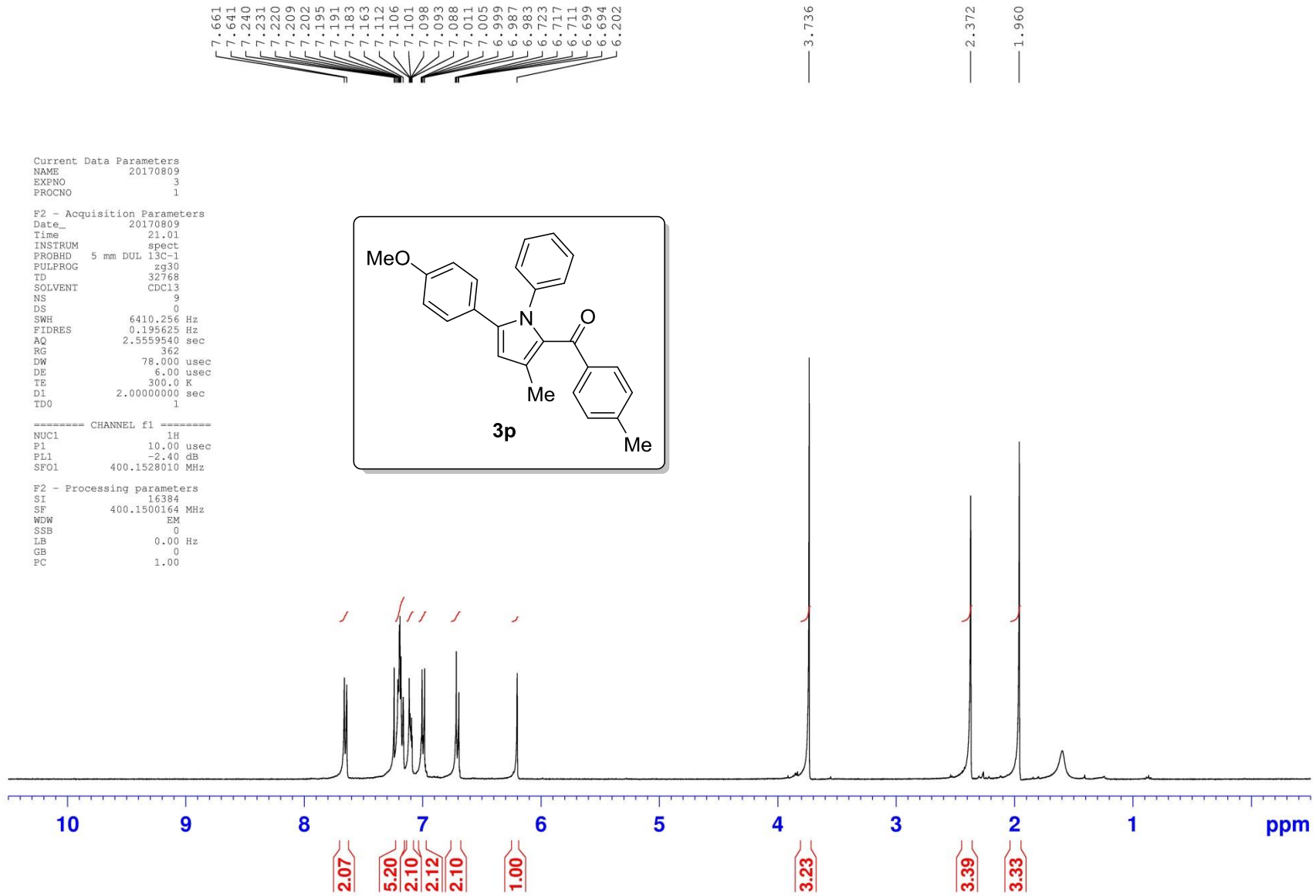
7.647
7.640
7.636
7.632
7.337
7.333
7.330
7.322
7.319
7.315
7.241
7.240
7.220
7.213
7.209
7.204
7.201
7.197
7.089
7.085
7.084
7.082
7.080
7.076
7.073
6.999
6.994
6.990
6.982
6.979
6.974
6.718
6.714
6.710
6.702
6.699
6.694
6.217
6.216
3.737
1.980
Current Data Parameters
NAME Yu-7-83
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170804
Time 20.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 512
DW 50.000 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 -1.00 dB
SFO1 598.4032912 MHz
F2 - Processing parameters
SI 32768
SF 598.4000250 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
MeO
N
O
Me
Cl
3o
10
9
8
7
6
5
4
3
2
1
ppm
2.06
2.00
3.27
2.09
2.13
2.27
1.00
3.10
3.04


186.12
159.00
140.27
139.21
138.73
138.07
131.08
130.69
130.03
129.29
128.56
128.46
128.18
127.40
124.18
113.55
112.68
77.21
77.00
76.79
55.16
13.87
Current Data Parameters
NAME Yu-7-83
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170804
Time 21.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678025 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
MeO
N
O
Me
3o
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.661
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7.231
7.220
7.209
7.202
7.195
7.191
7.183
7.163
7.112
7.106
7.101
7.098
7.093
7.088
7.011
7.005
6.999
6.987
6.983
6.723
6.717
6.711
6.699
6.694
6.202
3.736
2.372
1.960
Current Data Parameters
NAME 20170809
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170809
Time 21.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 9
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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 400.1500164 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
MeO
N
O
Me
3p
Me
10
9
8
7
6
5
4
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2
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ppm
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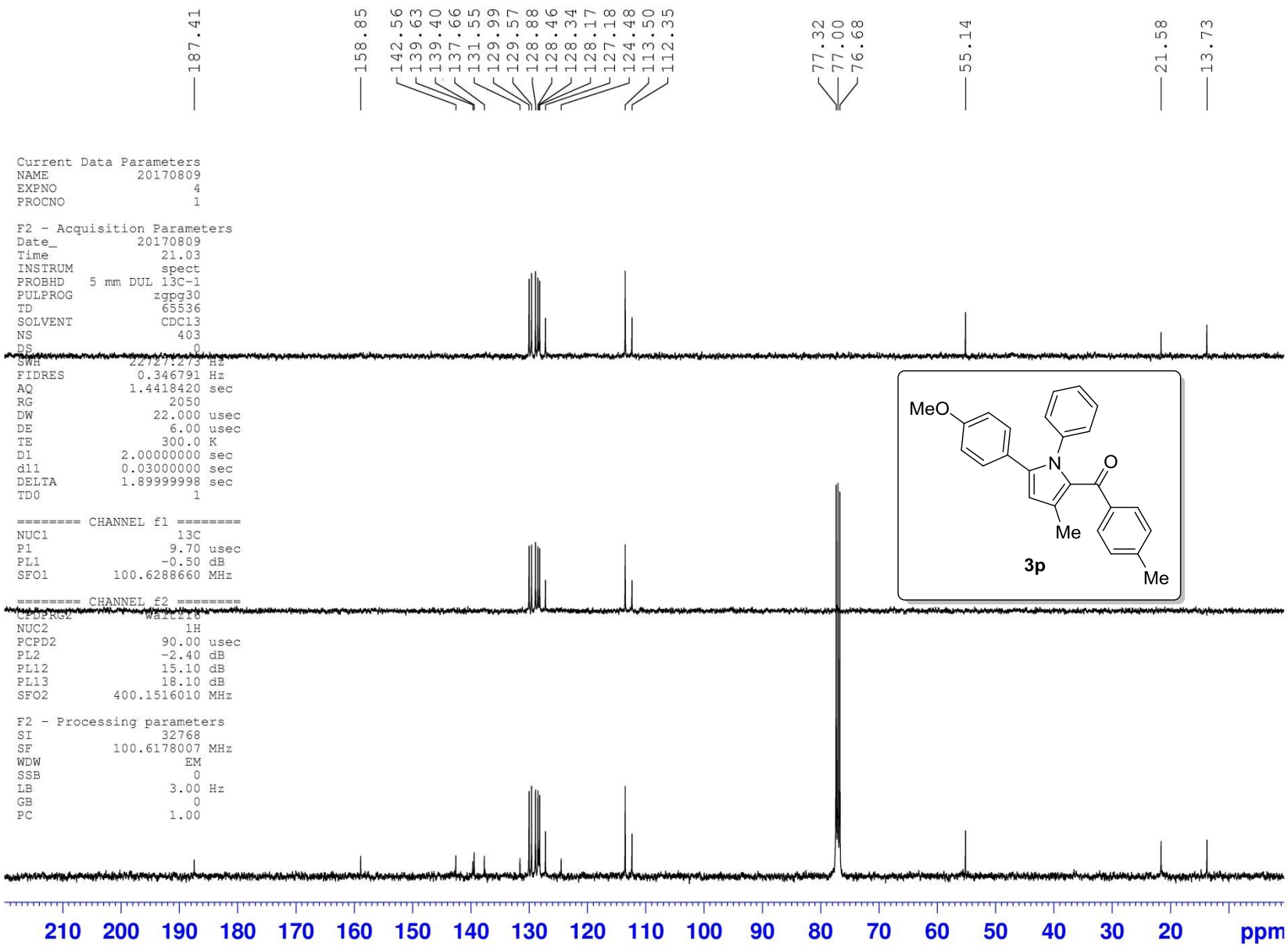
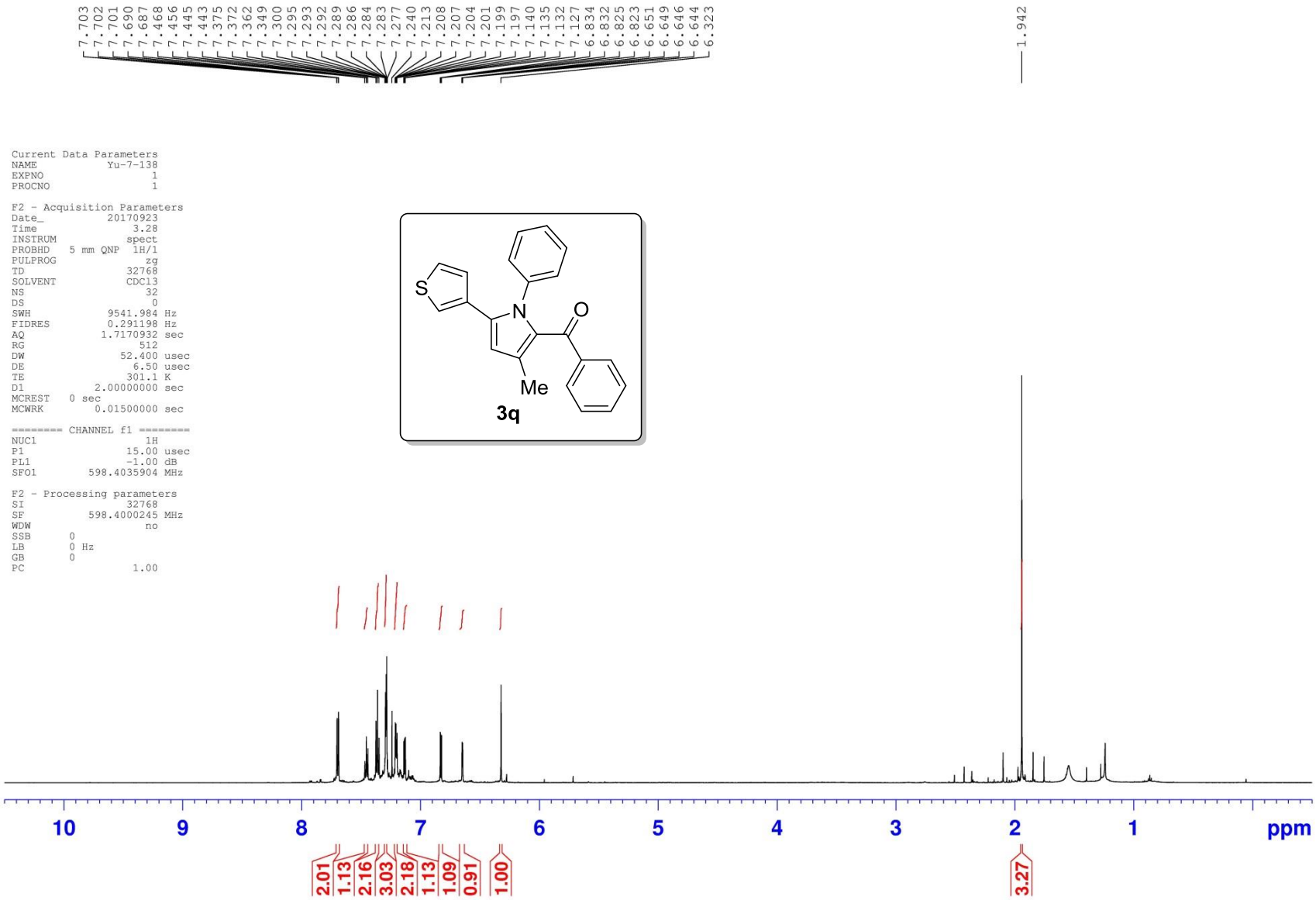
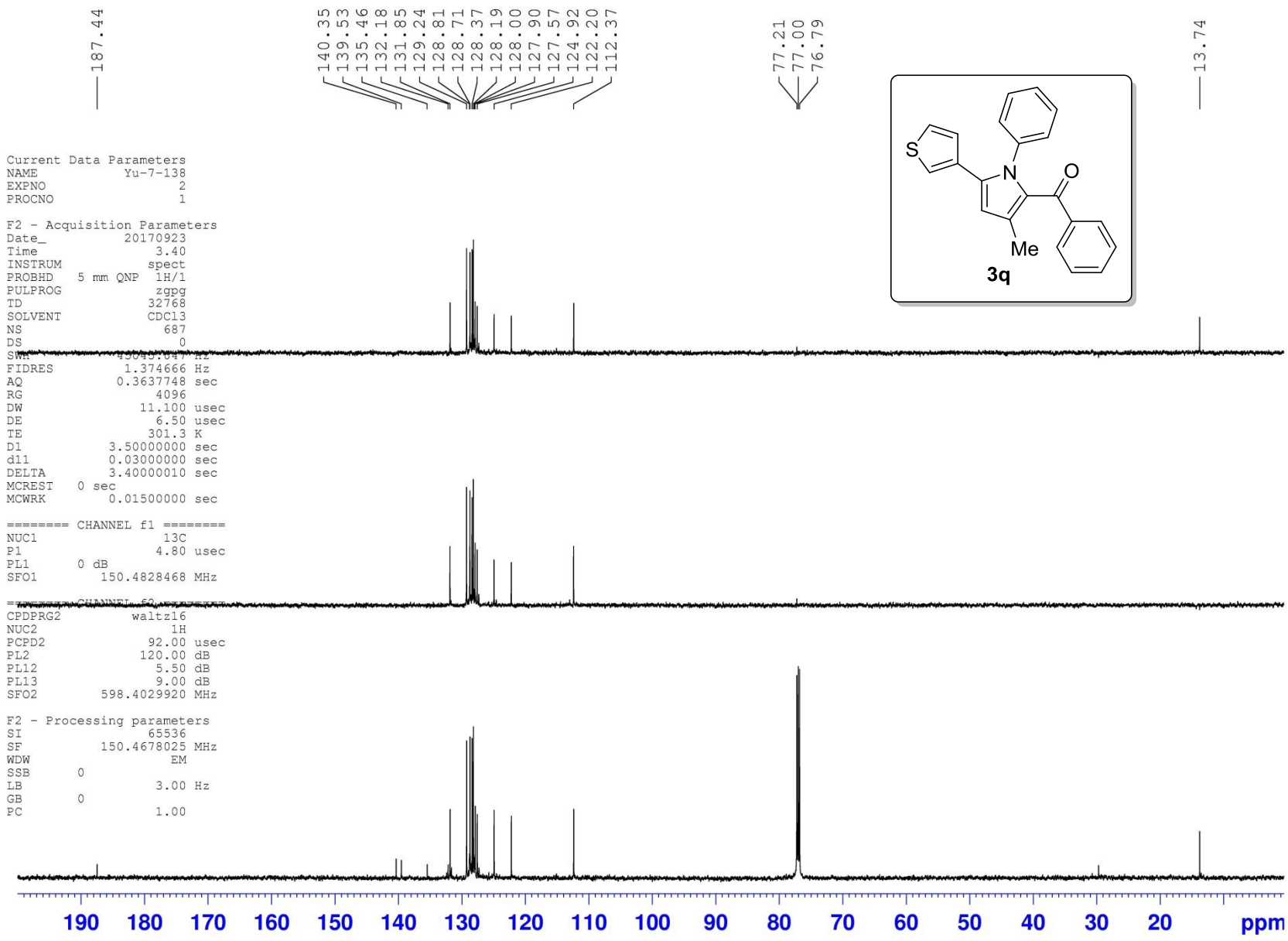
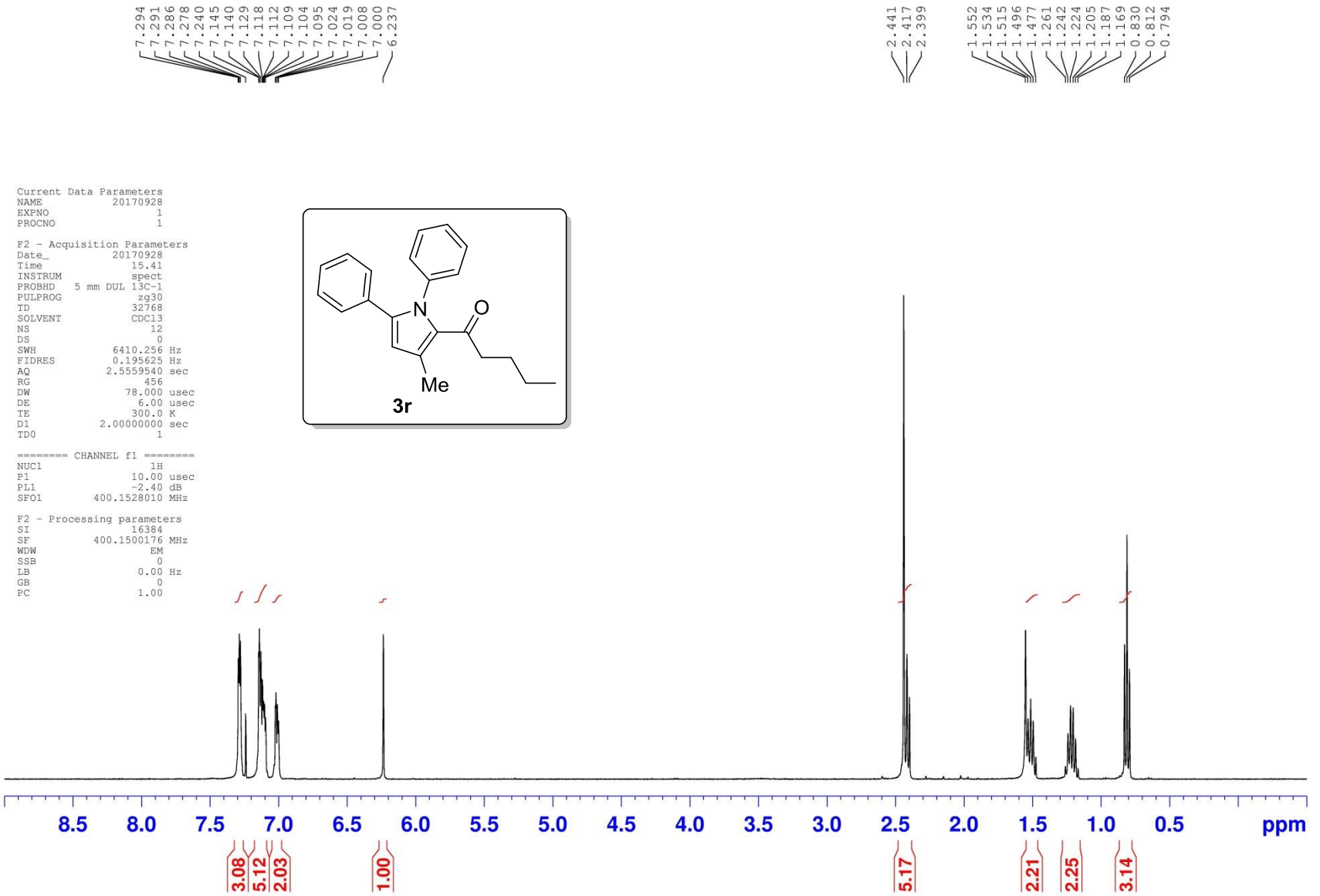
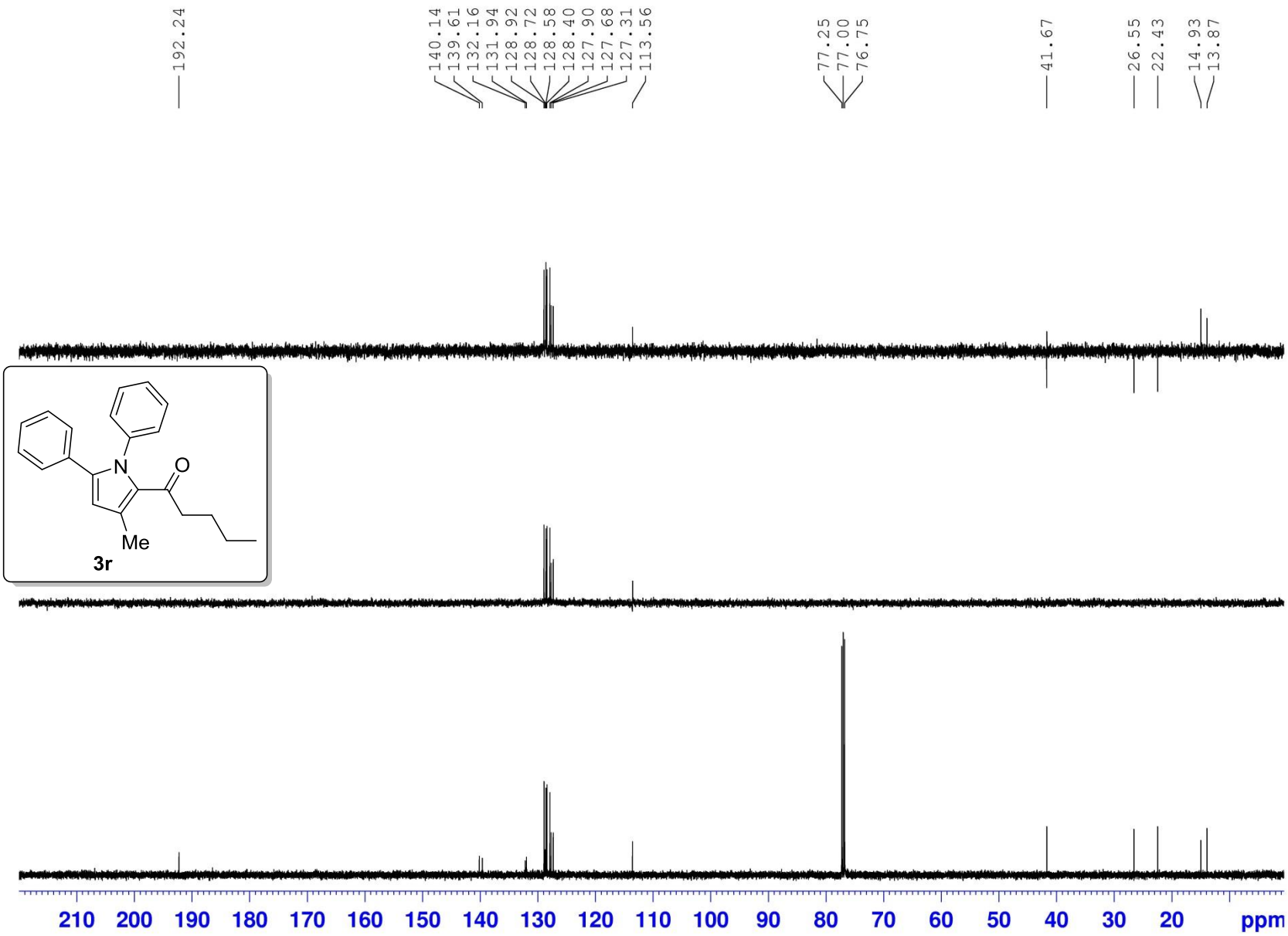
3.23
3.39
3.33

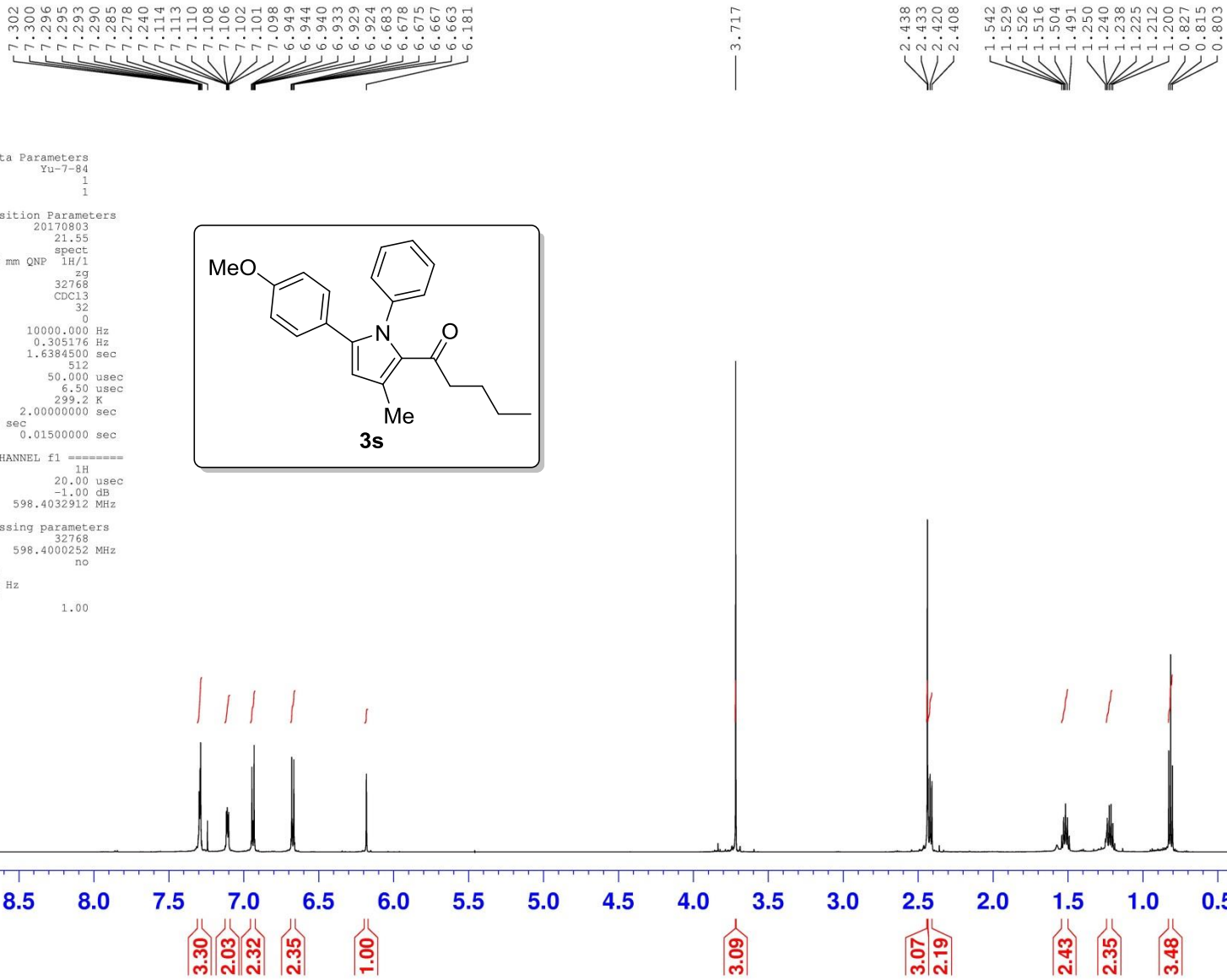

187.41
158.85
142.56
139.63
139.40
137.66
131.55
129.99
129.57
128.88
128.46
128.34
128.17
127.18
124.48
113.50
112.35
77.32
77.00
76.68
55.14
21.58
13.73
Current Data Parameters
NAME 20170809
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170809
Time 21.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 403
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178007 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
MeO
N
O
Me
Me
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

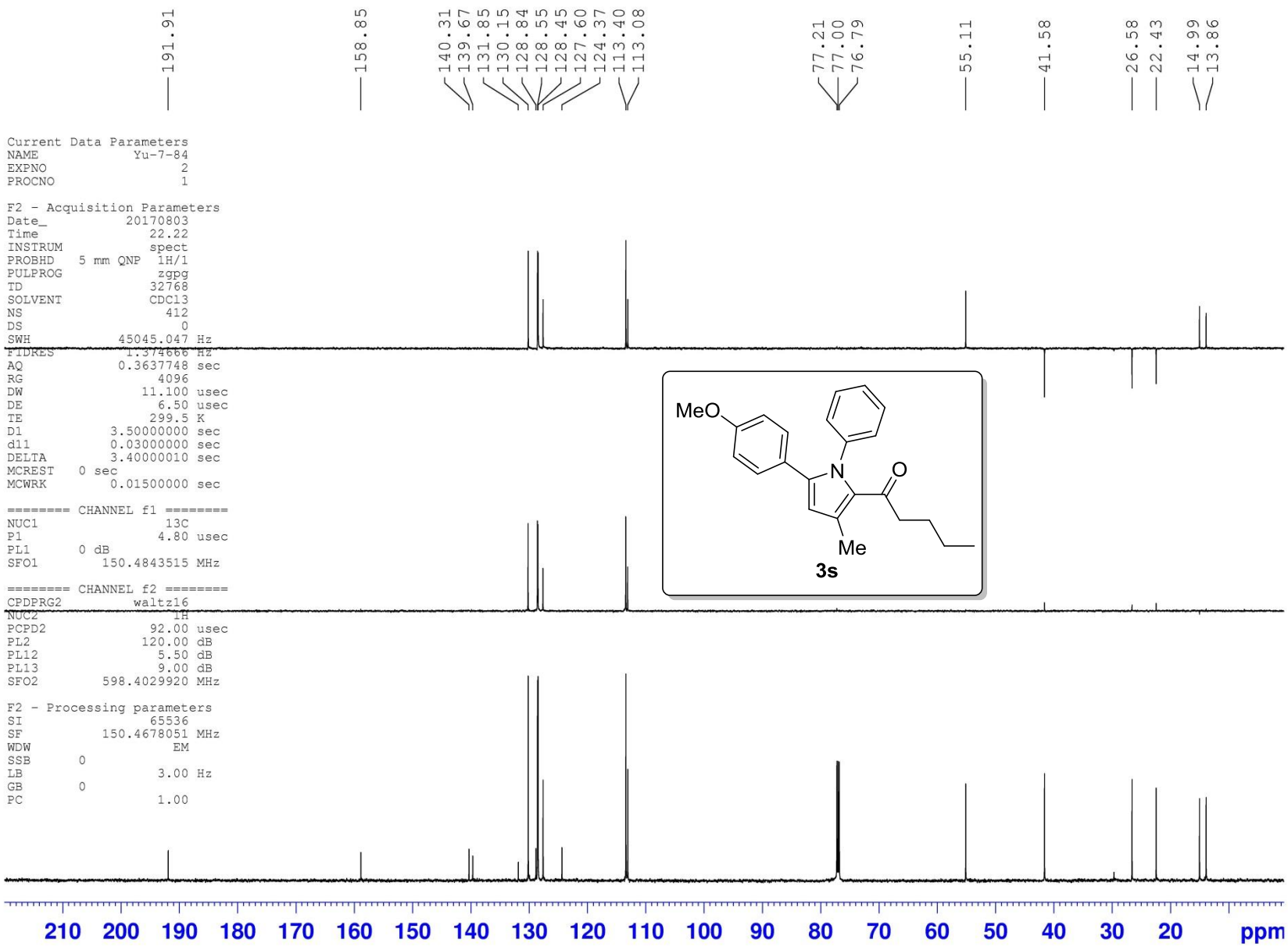

7.703
7.702
7.701
7.690
7.687
7.468
7.456
7.445
7.443
7.375
7.372
7.362
7.349
7.300
7.295
7.293
7.292
7.289
7.286
7.284
7.283
7.277
7.240
7.213
7.208
7.207
7.204
7.201
7.199
7.197
7.140
7.135
7.132
7.127
6.834
6.832
6.825
6.823
6.651
6.649
6.646
6.644
6.323
1.942
Current Data Parameters
NAME Yu-7-138
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170923
Time 3.28
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 301.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000245 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
S
N
O
Me
3q
10
9
8
7
6
5
4
3
2
1
ppm
2.01
1.13
2.16
3.03
2.18
1.13
1.09
0.91
1.00
3.27

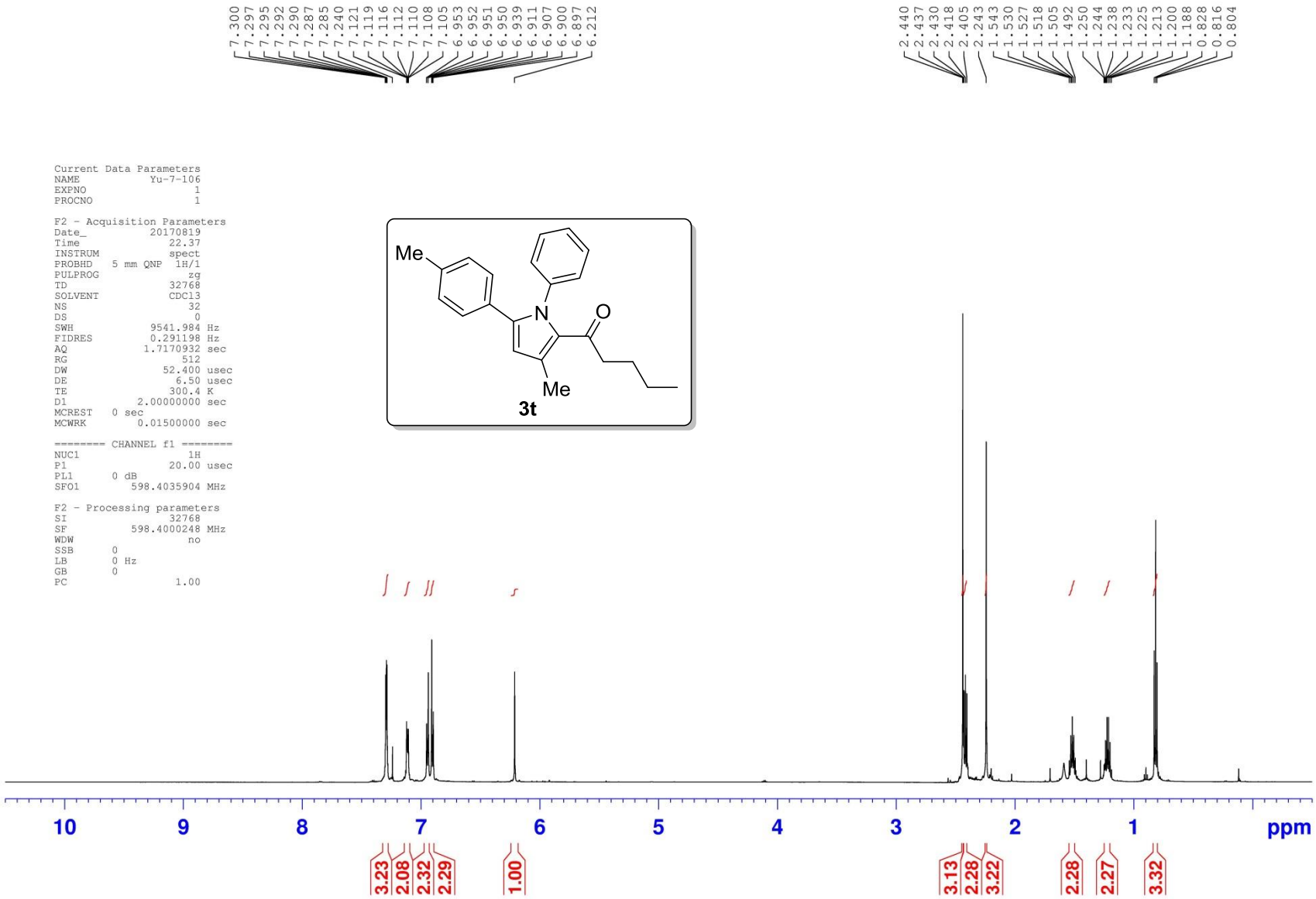

187.44
140.35
139.53
135.46
132.18
131.85
129.24
128.81
128.71
128.37
128.19
128.00
127.90
127.57
124.92
122.20
112.37
77.21
77.00
76.79
13.74
S
N
O
Me
3q
Current Data Parameters
NAME Yu-7-138
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170923
Time 3.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 687
DS 0
SWH 45045.045 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4828468 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678025 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

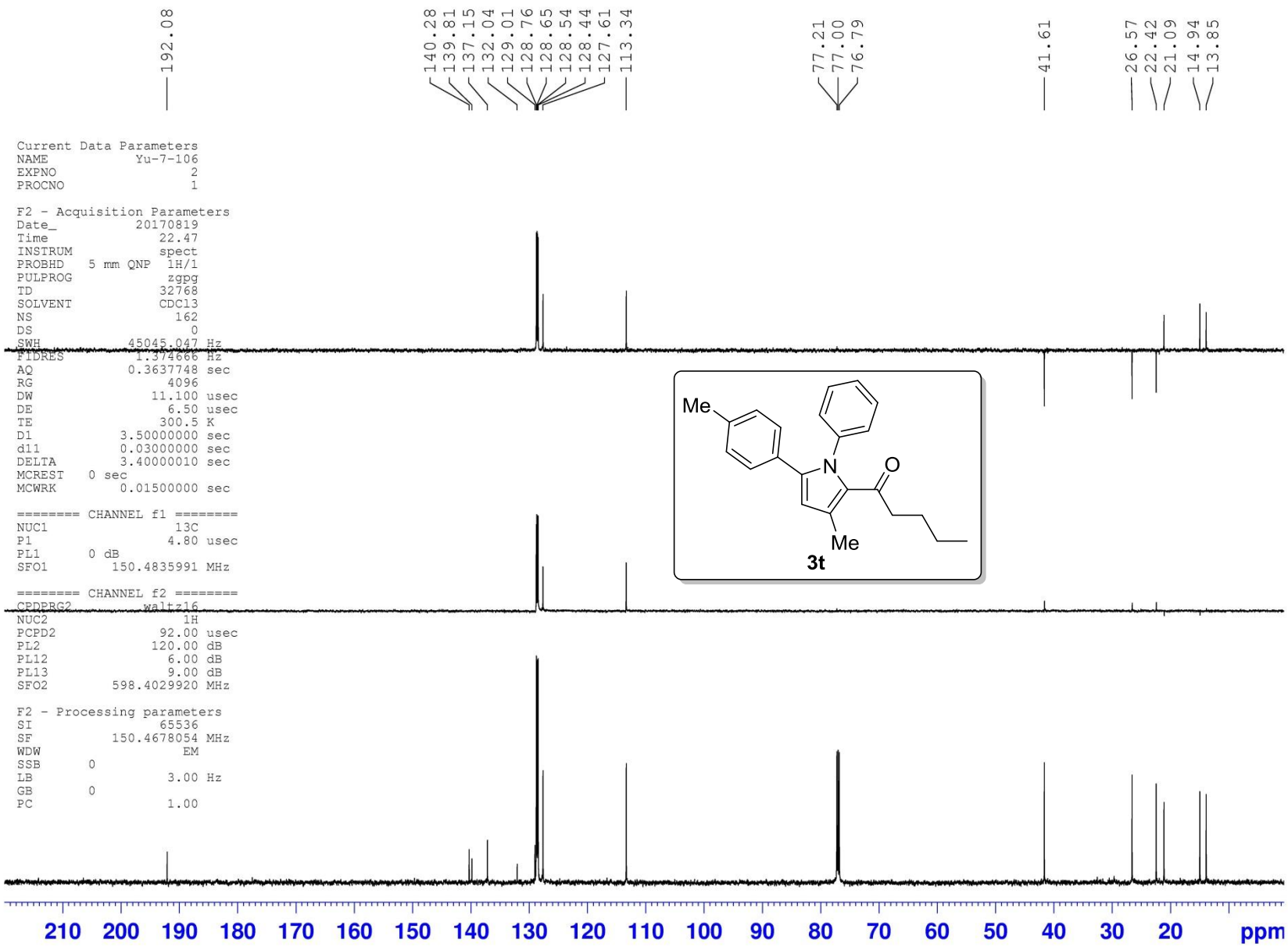

7.294
7.291
7.286
7.278
7.240
7.145
7.140
7.129
7.118
7.112
7.109
7.104
7.095
7.024
7.019
7.008
7.000
6.237
2.441
2.417
2.399
1.552
1.534
1.515
1.496
1.477
1.261
1.242
1.224
1.205
1.187
1.169
0.830
0.812
0.794
Current Data Parameters
NAME 20170928
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170928
Time 15.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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 400.1500176 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
O
Me
3r
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.08
5.12
2.03
1.00
5.17
2.21
2.25
3.14

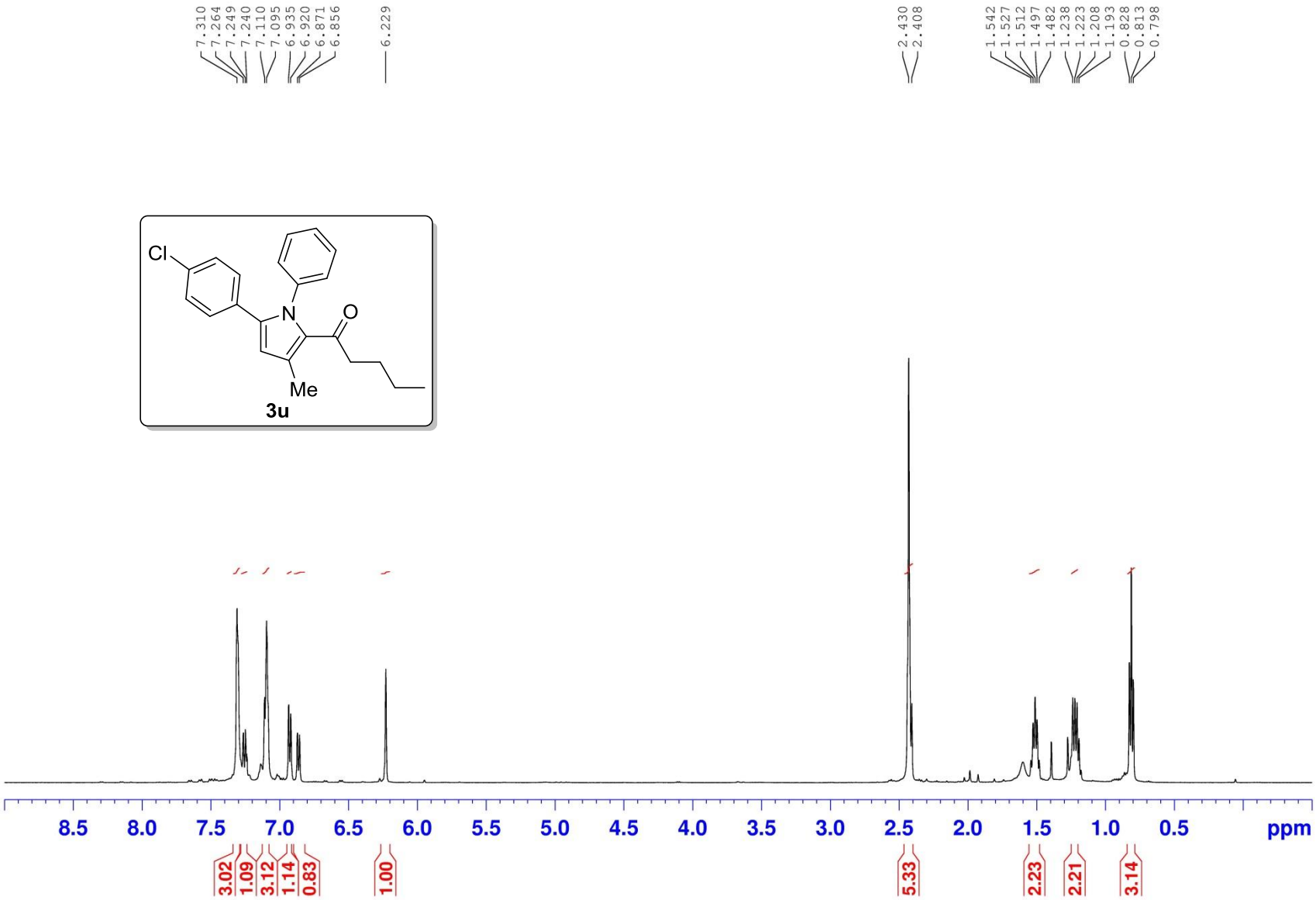

192.24
140.14
139.61
132.16
131.94
128.92
128.72
128.58
128.40
127.90
127.68
127.31
113.56
77.25
77.00
76.75
41.67
26.55
22.43
14.93
13.87
N
O
Me
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

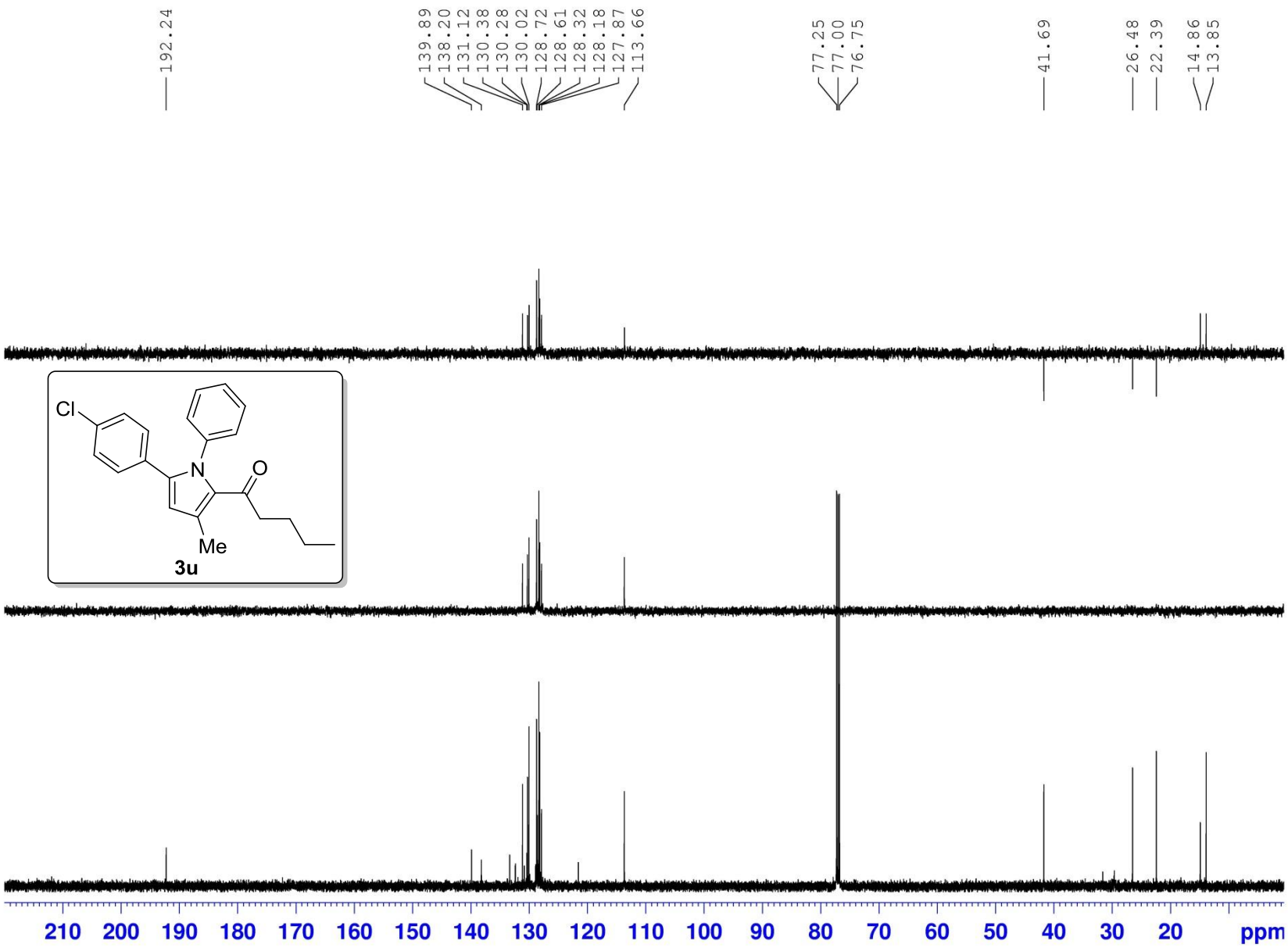

7.302
7.300
7.296
7.295
7.293
7.290
7.285
7.278
7.240
7.114
7.113
7.110
7.108
7.106
7.102
7.101
7.098
6.949
6.944
6.940
6.933
6.929
6.924
6.683
6.678
6.675
6.667
6.663
6.181
3.717
2.438
2.433
2.420
2.408
1.542
1.529
1.526
1.516
1.504
1.491
1.250
1.240
1.238
1.225
1.212
1.200
0.827
0.815
0.803
Current Data Parameters
NAME Yu-7-84
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170803
Time 21.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 512
DW 50.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 -1.00 dB
SFO1 598.4032912 MHz
F2 - Processing parameters
SI 32768
SF 598.4000252 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
MeO
N
O
Me
3s
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.30
2.03
2.32
2.35
1.00
3.09
3.07
2.19
2.43
2.35
3.48

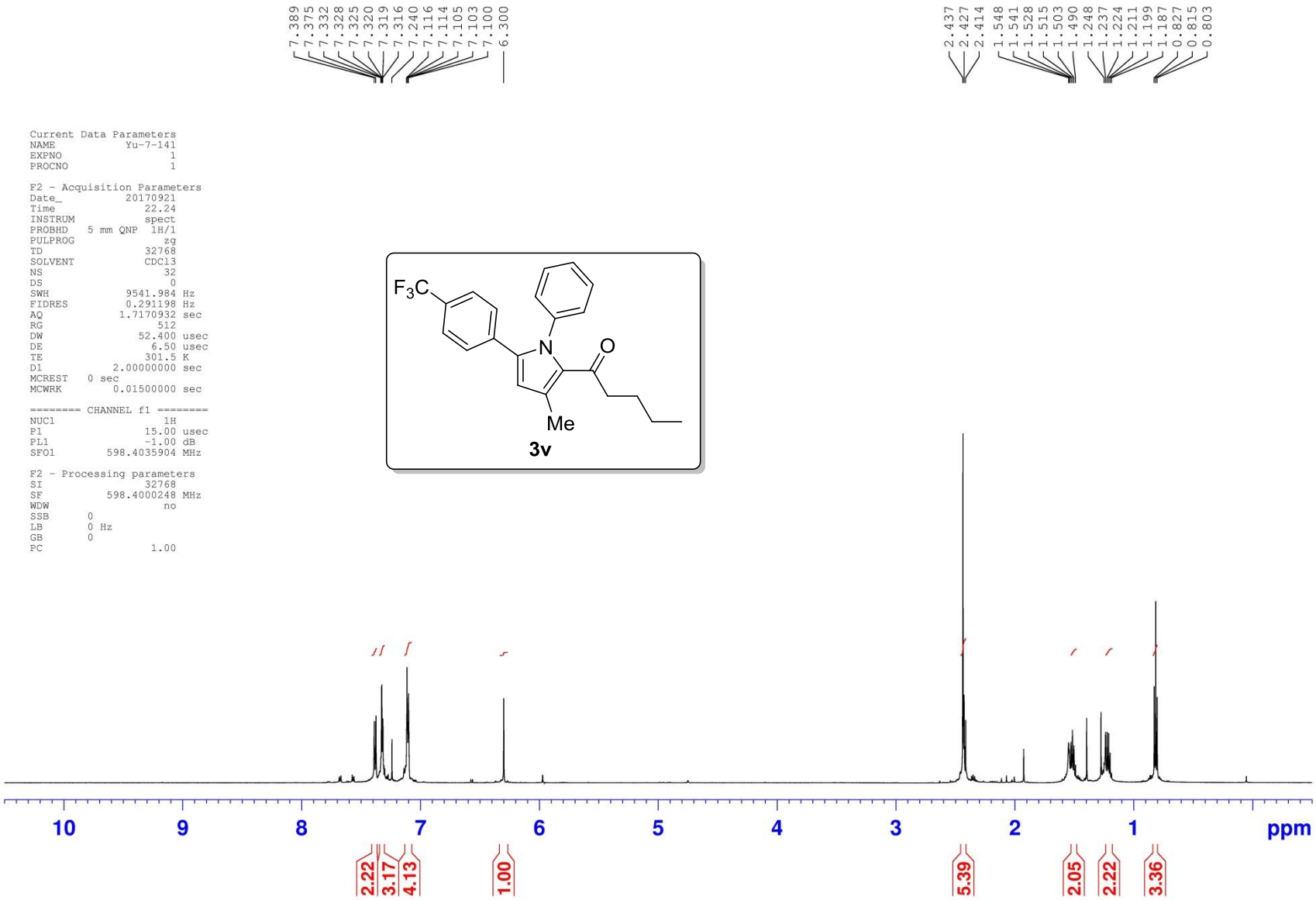

191.91
158.85
140.31
139.67
131.85
130.15
128.84
128.55
128.45
127.60
124.37
113.40
113.08
77.21
77.00
76.79
55.11
41.58
26.58
22.43
14.99
13.86
Current Data Parameters
NAME Yu-7-84
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170803
Time 22.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 412
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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678051 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
MeO
N
O
Me
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

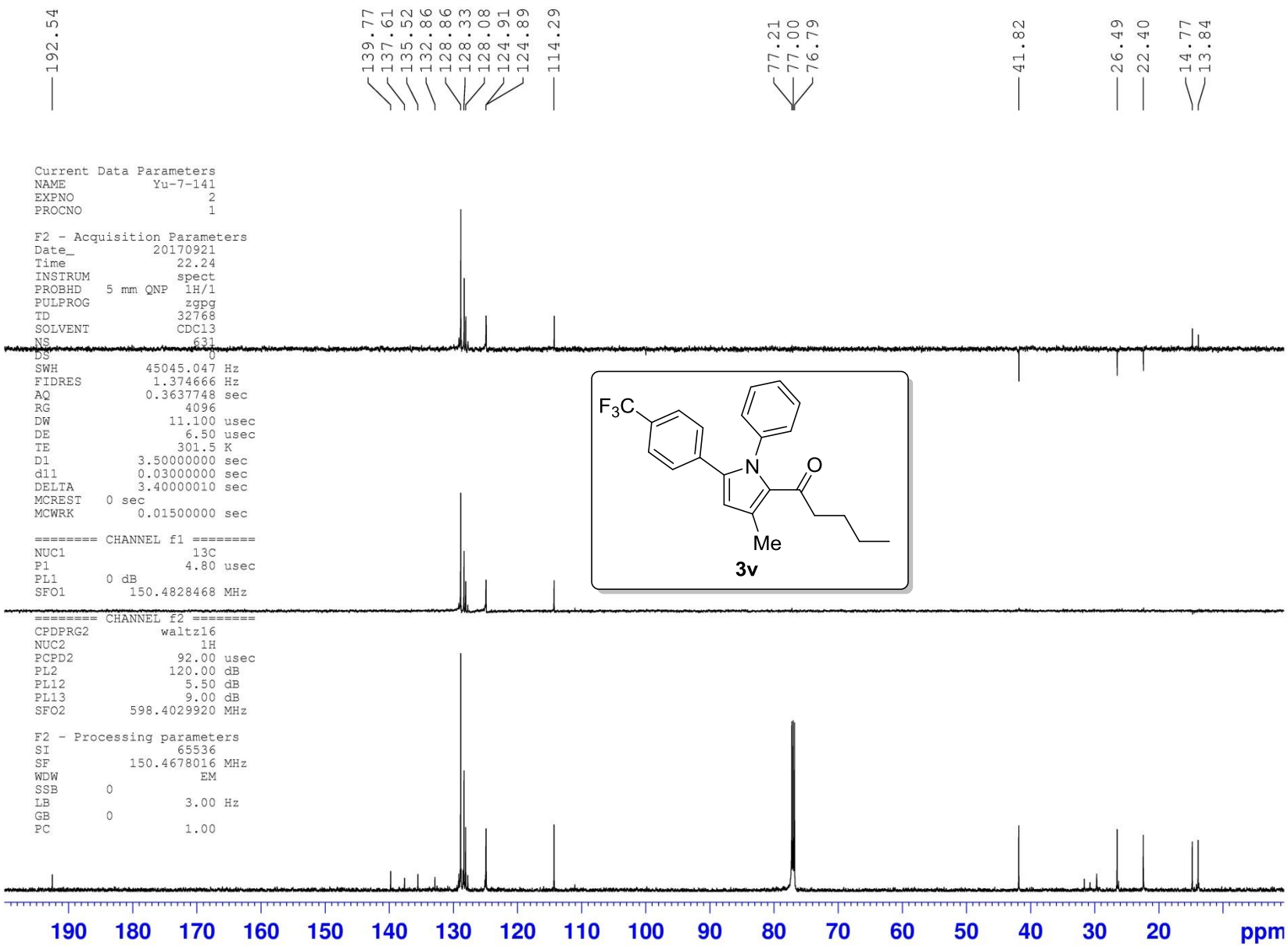

7.300
7.297
7.295
7.292
7.290
7.287
7.285
7.240
7.121
7.119
7.116
7.112
7.110
7.108
7.105
6.953
6.952
6.951
6.950
6.939
6.911
6.907
6.900
6.897
6.212
2.440
2.437
2.430
2.418
2.405
2.243
1.543
1.530
1.527
1.518
1.505
1.492
1.250
1.244
1.238
1.233
1.225
1.213
1.200
1.188
0.828
0.816
0.804
Current Data Parameters
NAME Yu-7-106
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170819
Time 22.37
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 20.00 usec
PL1 0 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Me
N
O
Me
3t
10
9
8
7
6
5
4
3
2
1
ppm
3.23
2.08
2.32
2.29
1.00
3.13
2.28
3.22
2.28
2.27
3.32

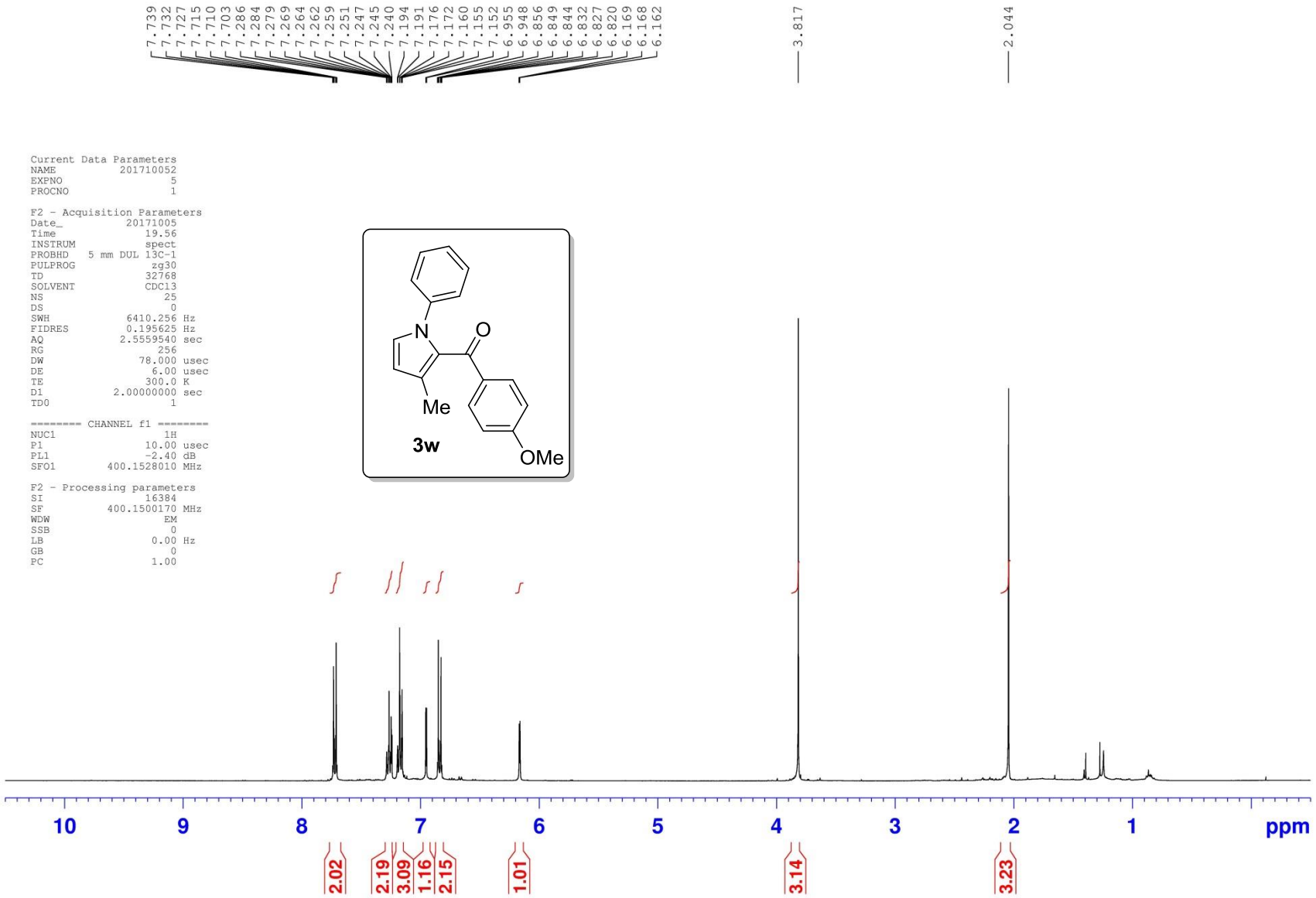

192.08
140.28
139.81
137.15
132.04
129.01
128.76
128.65
128.54
128.44
127.61
113.34
77.21
77.00
76.79
41.61
26.57
22.42
21.09
14.94
13.85
Current Data Parameters
NAME Yu-7-106
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170819
Time 22.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 162
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 300.5 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 150.4835991 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Me
N
O
Me
3t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

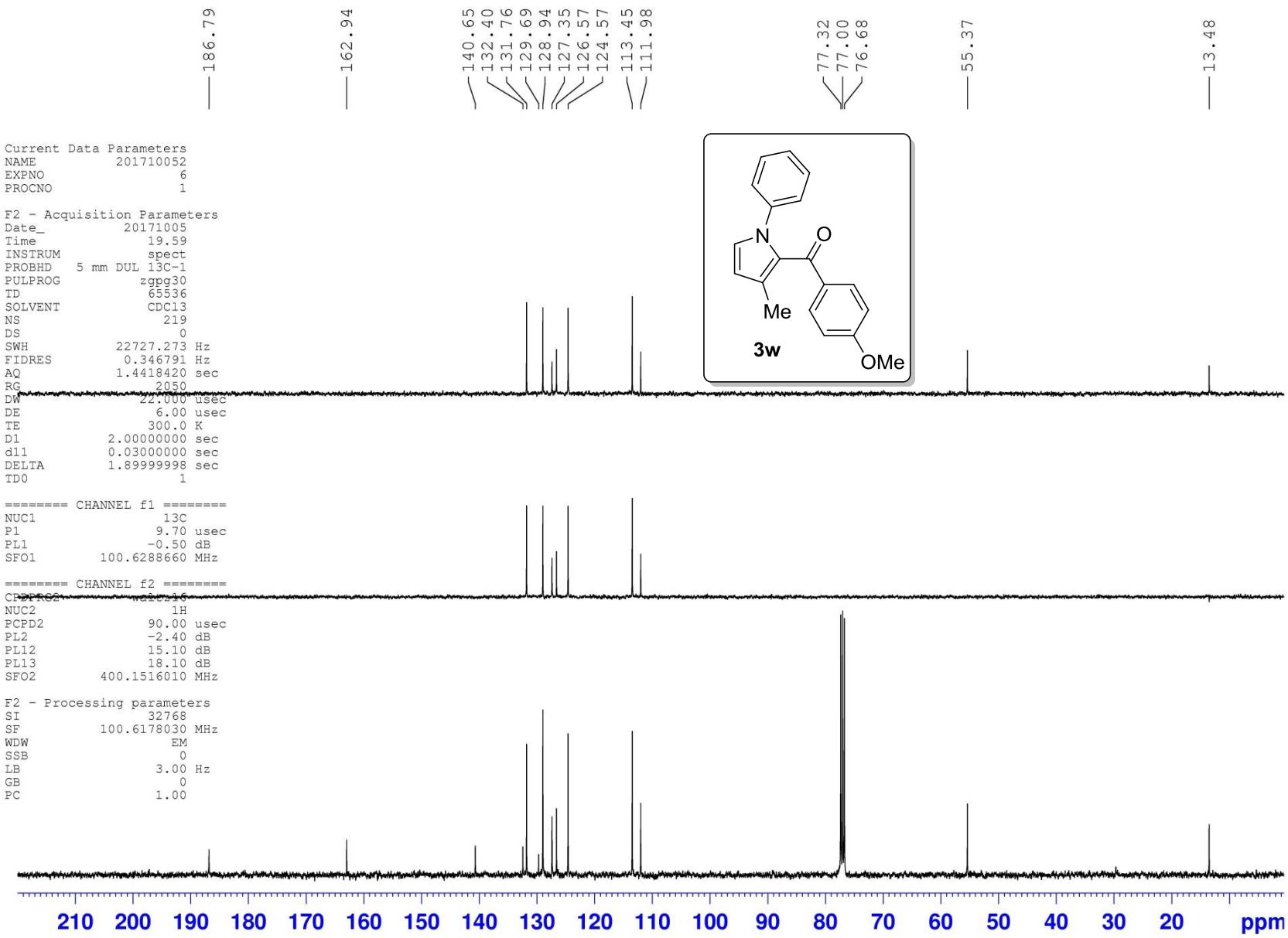

7.310
7.264
7.249
7.240
7.110
7.095
6.935
6.920
6.871
6.856
6.229
2.430
2.408
1.542
1.527
1.512
1.497
1.482
1.238
1.223
1.208
1.193
0.828
0.813
0.798
Cl
N
O
Me
3u
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.02
1.09
3.12
1.14
0.83
1.00
5.33
2.23
2.21
3.14

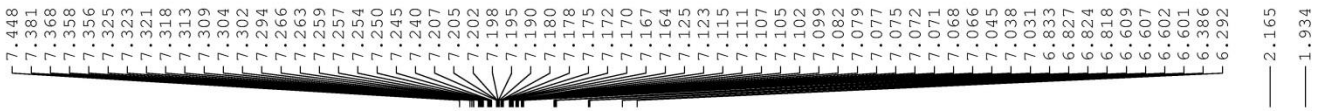

192.24
139.89
138.20
131.12
130.38
130.28
130.02
128.72
128.61
128.32
128.18
127.87
113.66
77.25
77.00
76.75
41.69
26.48
22.39
14.86
13.85
Cl
N
O
Me
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.389
7.375
7.332
7.328
7.325
7.320
7.319
7.316
7.240
7.116
7.114
7.105
7.103
7.100
6.300
2.437
2.427
2.414
1.548
1.541
1.528
1.515
1.503
1.490
1.248
1.237
1.224
1.211
1.199
1.187
0.827
0.815
0.803
Current Data Parameters
NAME Yu-7-141
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170921
Time 22.24
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 301.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000248 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
F3C
N
O
Me
3v
10
9
8
7
6
5
4
3
2
1
ppm
2.22
3.17
4.13
1.00
5.39
2.05
2.22
3.36

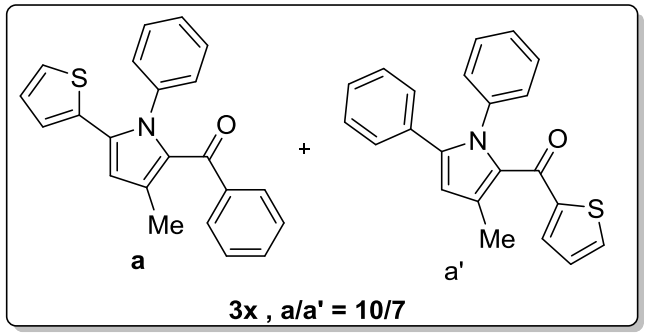

192.54
139.77
137.61
135.52
132.86
128.86
128.33
128.08
124.91
124.89
114.29
77.21
77.00
76.79
41.82
26.49
22.40
14.77
13.84
Current Data Parameters
NAME Yu-7-141
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170921
Time 22.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 631
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 301.5 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 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678016 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
F3C
N
O
Me
3v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

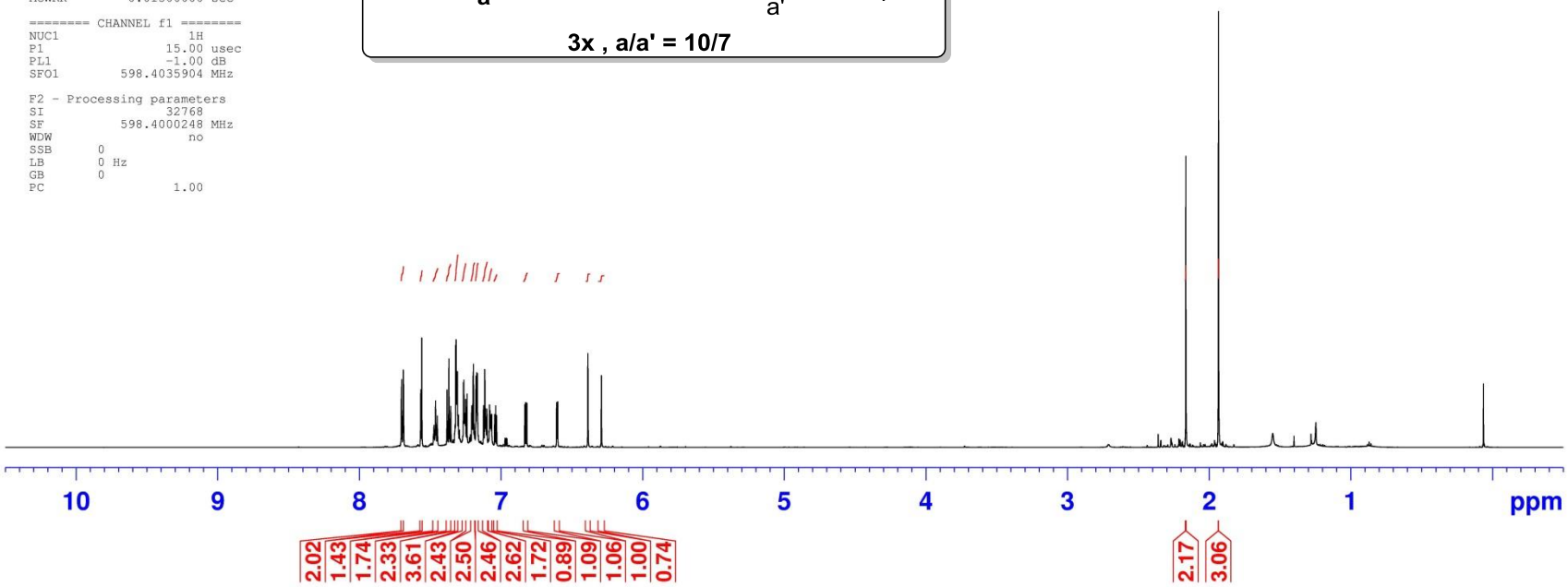

7.739
7.732
7.727
7.715
7.710
7.703
7.286
7.284
7.279
7.269
7.264
7.262
7.259
7.251
7.247
7.245
7.240
7.194
7.191
7.176
7.172
7.160
7.155
7.152
6.955
6.948
6.856
6.849
6.844
6.832
6.827
6.820
6.169
6.168
6.162
3.817
2.044
Current Data Parameters
NAME 201710052
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171005
Time 19.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 25
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
N
O
Me
3w
OMe
10
9
8
7
6
5
4
3
2
1
ppm
2.02
2.19
3.09
1.16
2.15
1.01
3.14
3.23

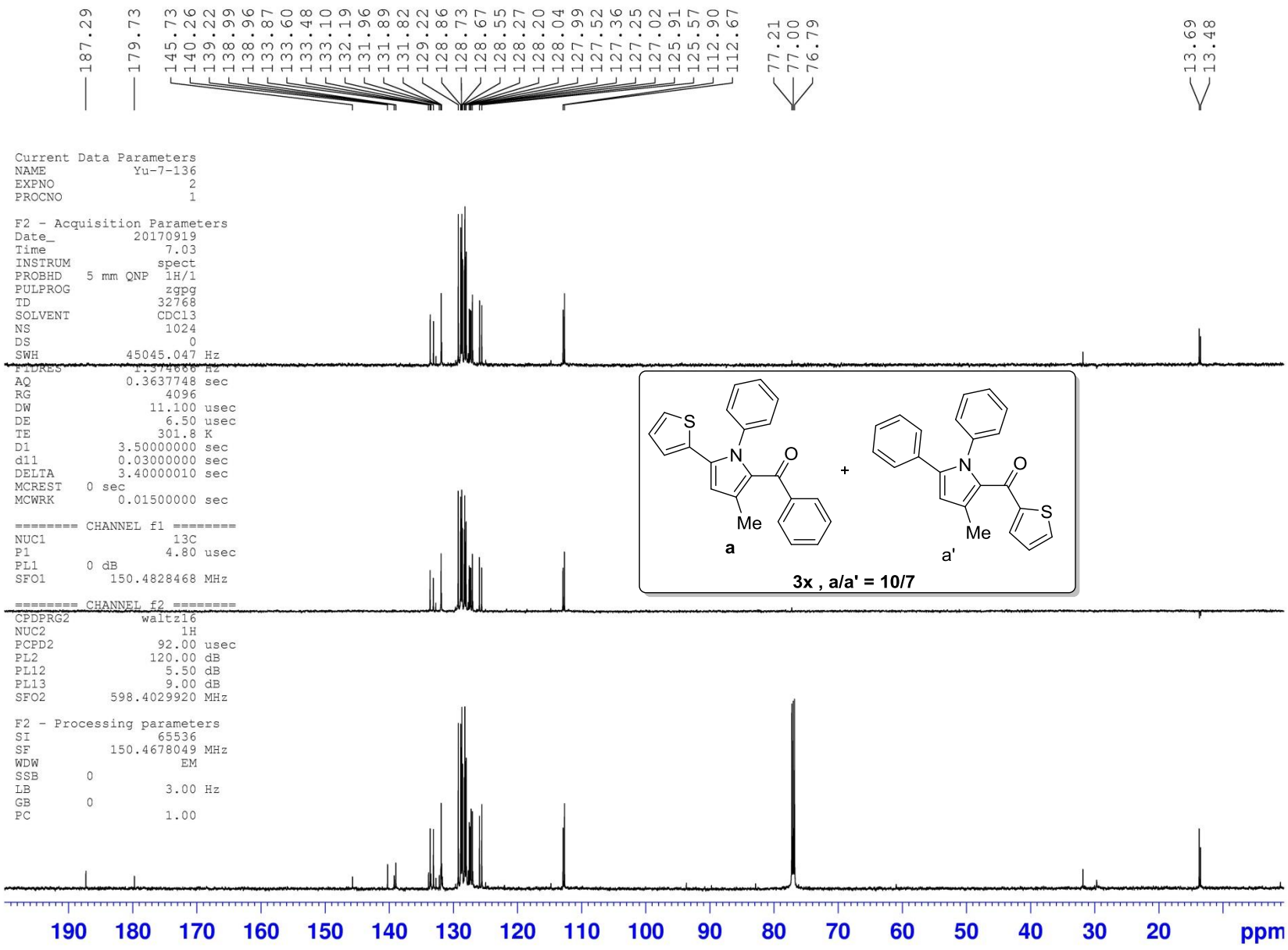

186.79
162.94
140.65
132.40
131.76
129.69
128.94
127.35
126.57
124.57
113.45
111.98
77.32
77.00
76.68
55.37
13.48
Current Data Parameters
NAME 201710052
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171005
Time 19.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 219
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178030 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
O
Me
3w
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

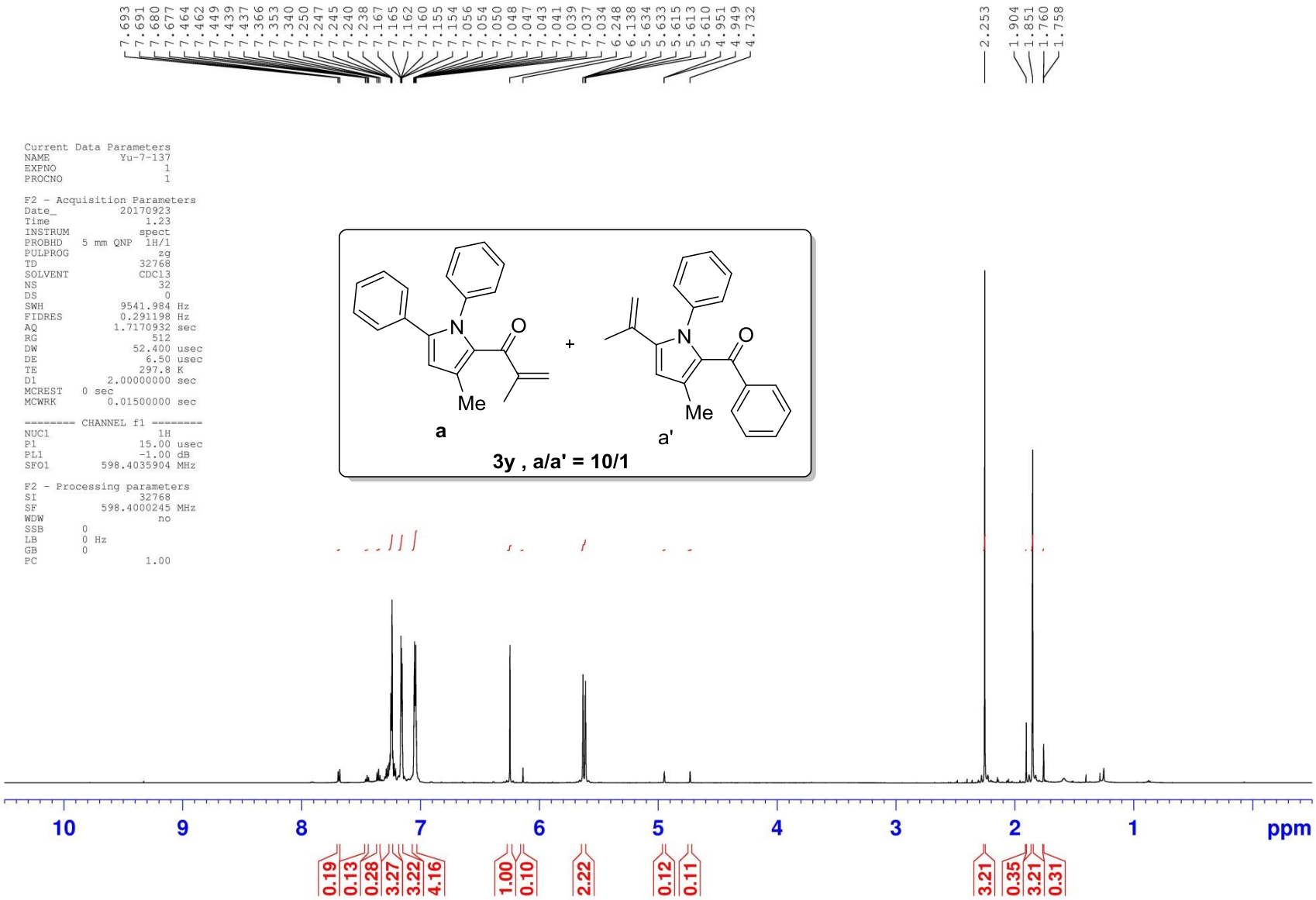


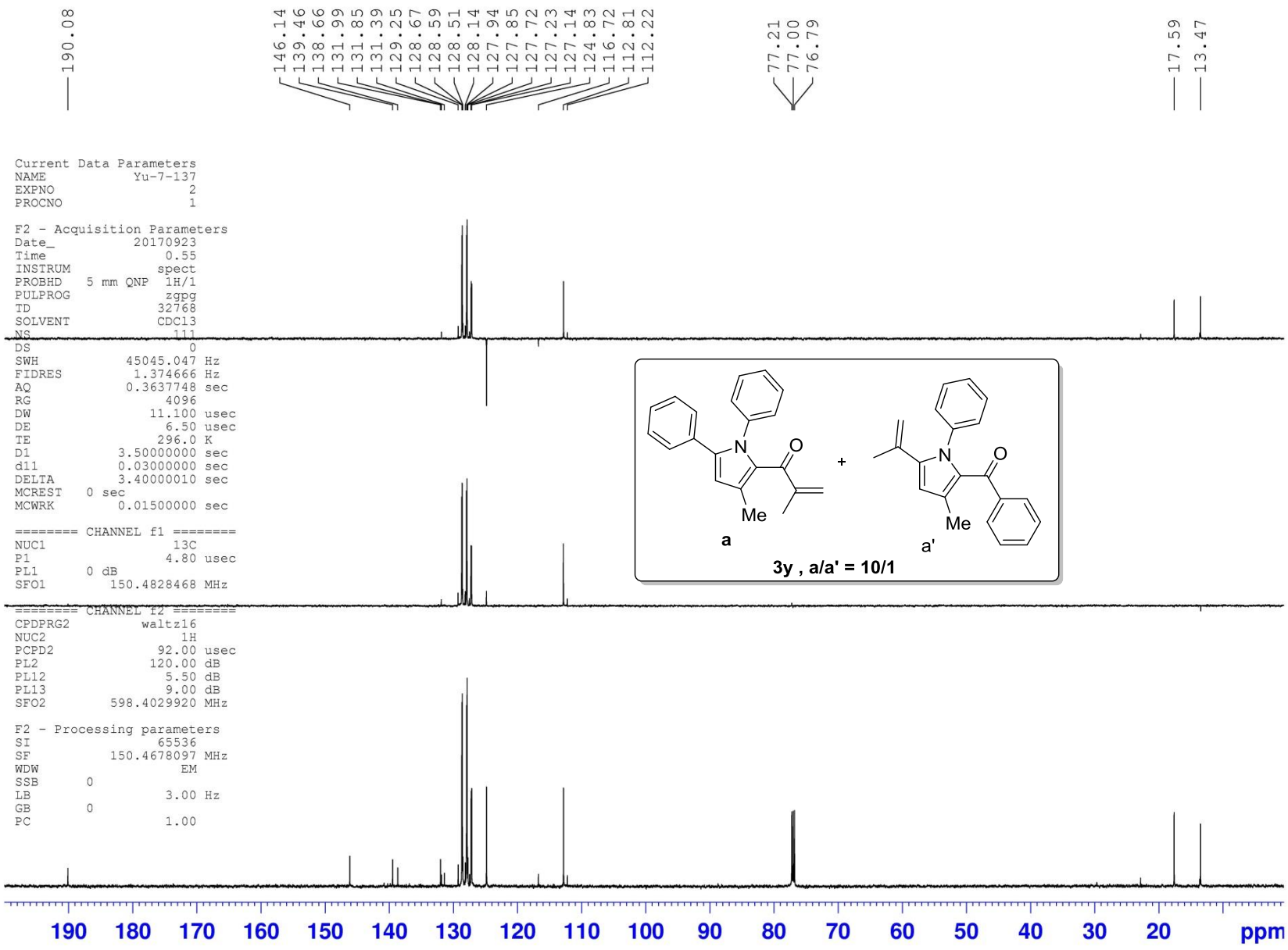

```
Current Data Parameters
NAME            Yu-7-136
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170919
Time                5.39
INSTRUM            spect
PROBHD    5 mm QNP  1H/1
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             9541.984 Hz
FIDRES             0.291198 Hz
AQ              1.7170932 sec
RG                   512
DW                52.400 usec
DE                 6.50 usec
TE                301.7 K
D1             2.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                -1.00 dB
SFO1          598.4035904 MHz

F2 - Processing parameters
SI                 32768
SF            598.4000248 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

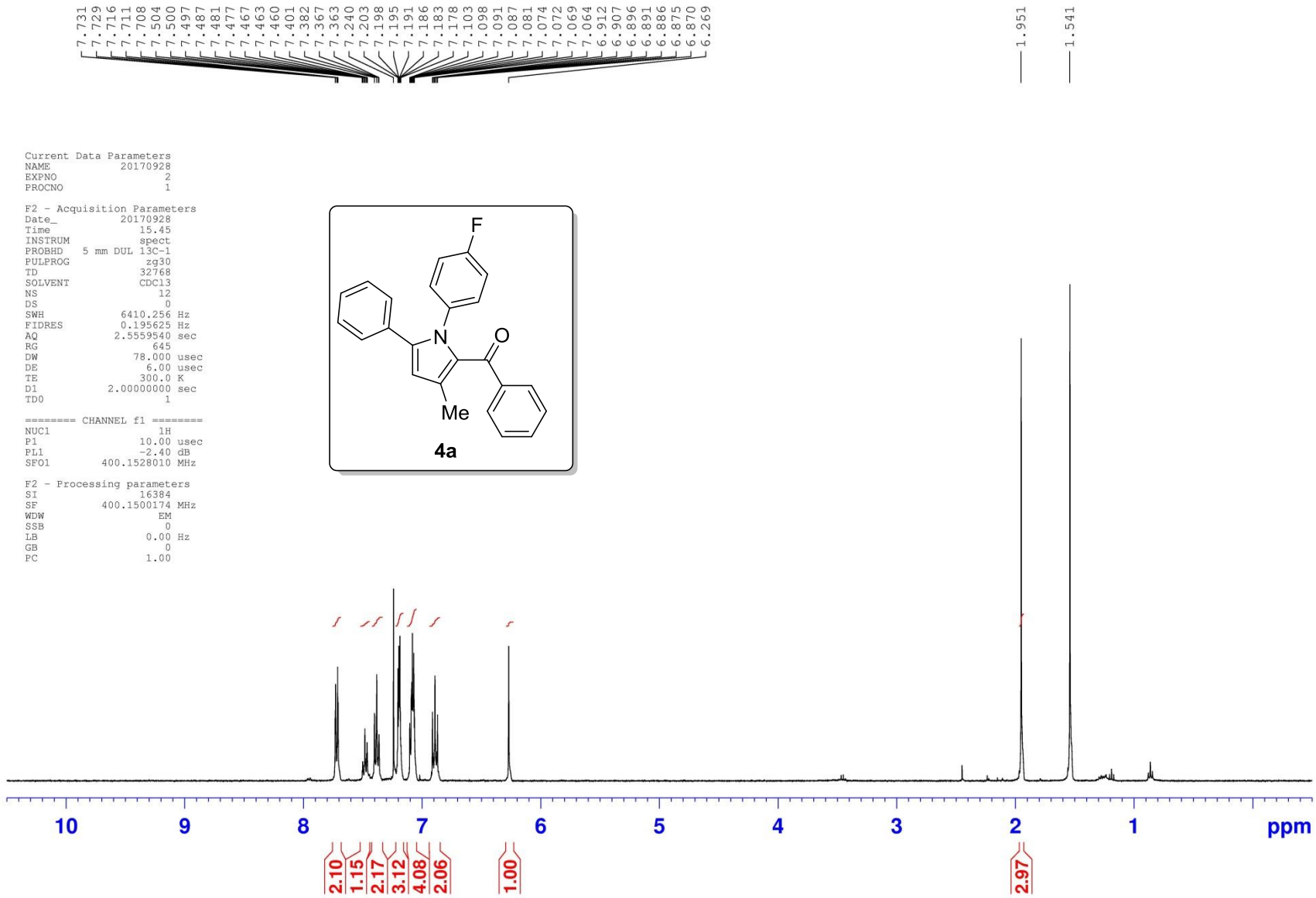


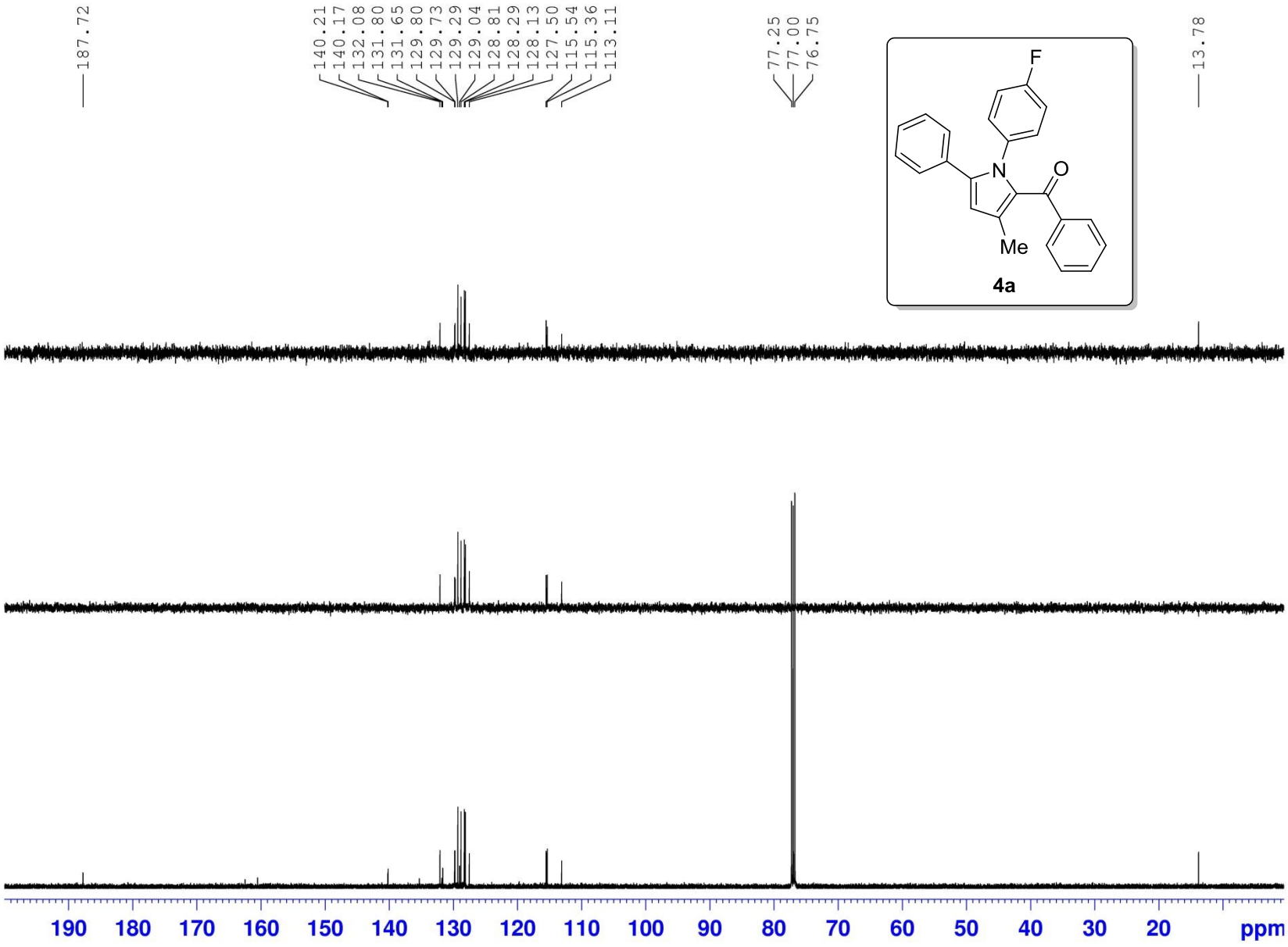


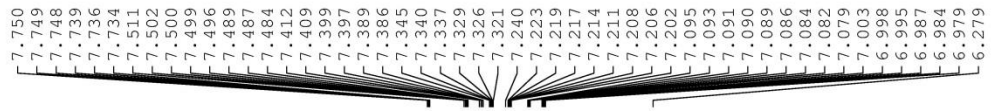

187.29
179.73
145.73
140.26
139.22
138.99
138.96
133.87
133.60
133.48
133.10
132.19
131.96
131.89
131.82
129.22
128.86
128.73
128.67
128.55
128.27
128.20
128.04
127.99
127.52
127.36
127.25
127.02
125.91
125.57
112.90
112.67
77.21
77.00
76.79
13.69
13.48
Current Data Parameters
NAME Yu-7-136
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170919
Time 7.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDC13
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 301.8 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 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678049 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
S
N
O
Me
a
+
N
O
S
Me
a'
3x , a/a' = 10/7
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.693
7.691
7.680
7.677
7.464
7.462
7.449
7.439
7.437
7.366
7.353
7.340
7.250
7.247
7.245
7.240
7.238
7.167
7.165
7.162
7.160
7.155
7.154
7.056
7.054
7.050
7.048
7.047
7.043
7.041
7.039
7.037
7.034
6.248
6.138
5.634
5.633
5.615
5.613
5.610
4.951
4.949
4.732
2.253
1.904
1.851
1.760
1.758
Current Data Parameters
NAME Yu-7-137
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170923
Time 1.23
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 297.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -1.00 dB
SFO1 598.4035904 MHz
F2 - Processing parameters
SI 32768
SF 598.4000245 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
O
Me
a
+
N
O
Me
a'
3y , a/a' = 10/1
10
9
8
7
6
5
4
3
2
1
ppm
0.19
0.13
0.28
3.27
3.22
4.16
1.00
0.10
2.22
0.12
0.11
3.21
0.35
3.21
0.31

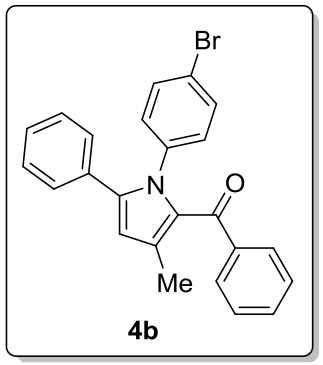

190.08
146.14
139.46
138.66
131.99
131.85
131.39
129.25
128.67
128.59
128.51
128.14
127.94
127.85
127.72
127.23
127.14
124.83
116.72
112.81
112.22
77.21
77.00
76.79
17.59
13.47
Current Data Parameters
NAME Yu-7-137
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170923
Time 0.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 111
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 296.0 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 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678097 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
N
O
Me
a
+
N
O
Me
a'
3y , a/a' = 10/1
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

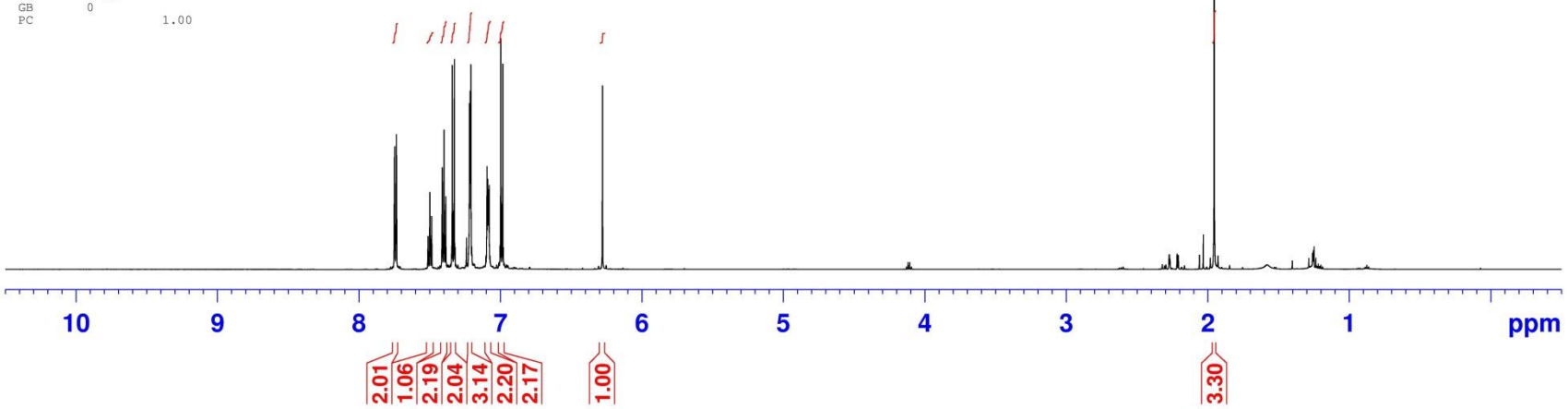

7.731
7.729
7.716
7.711
7.708
7.504
7.500
7.497
7.487
7.481
7.477
7.467
7.463
7.460
7.401
7.382
7.367
7.363
7.240
7.203
7.198
7.195
7.191
7.186
7.183
7.178
7.103
7.098
7.091
7.087
7.081
7.074
7.072
7.069
7.064
6.912
6.907
6.896
6.891
6.886
6.875
6.870
6.269
1.951
1.541
Current Data Parameters
NAME 20170928
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170928
Time 15.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 645
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
F
N
O
Me
4a
10
9
8
7
6
5
4
3
2
1
ppm
2.10
1.15
2.17
3.12
4.08
2.06
1.00
2.97

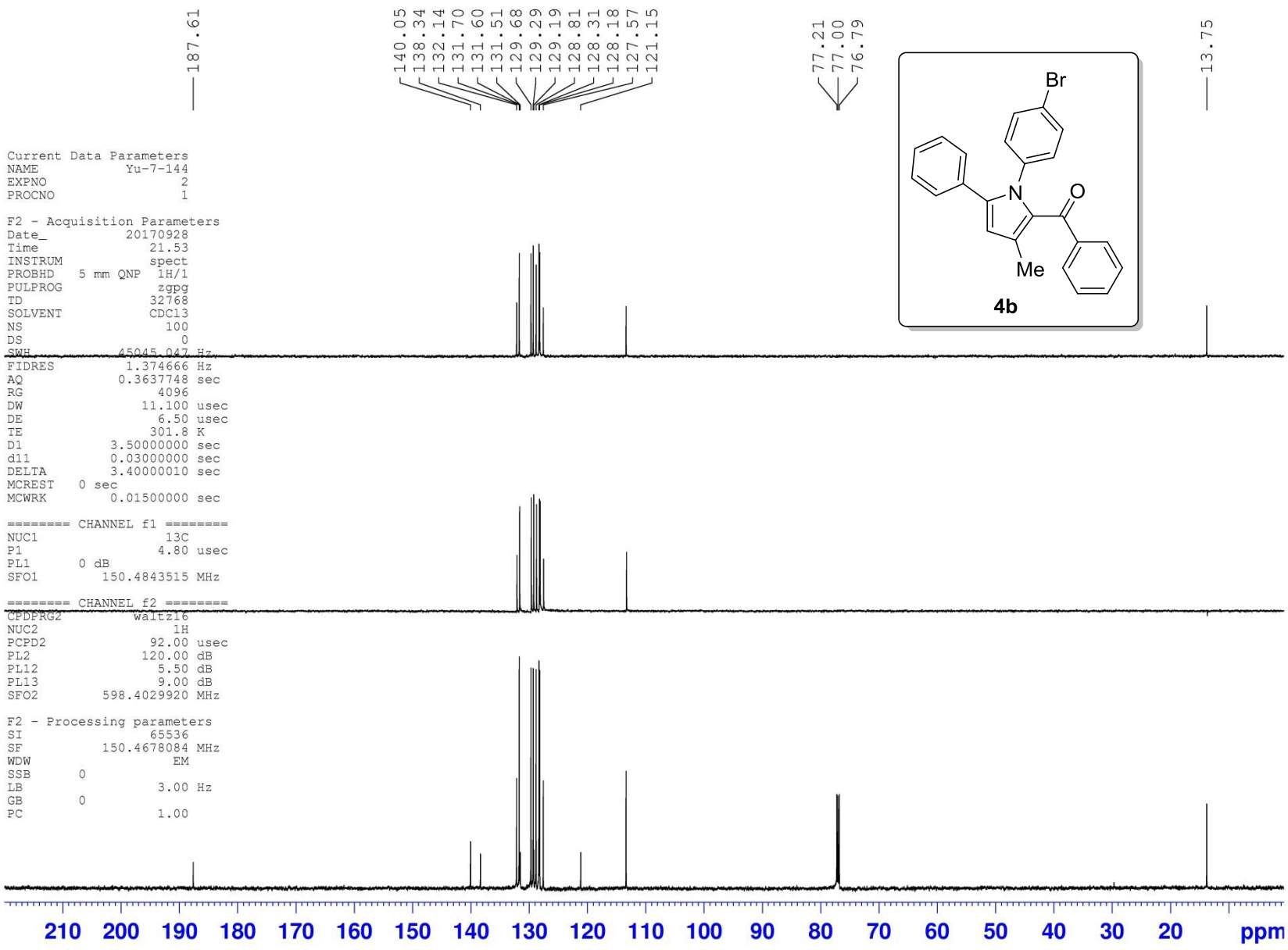

187.72
140.21
140.17
132.08
131.80
131.65
129.80
129.73
129.29
129.04
128.81
128.29
128.13
127.50
115.54
115.36
113.11
77.25
77.00
76.75
13.78
F
N
O
Me
4a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

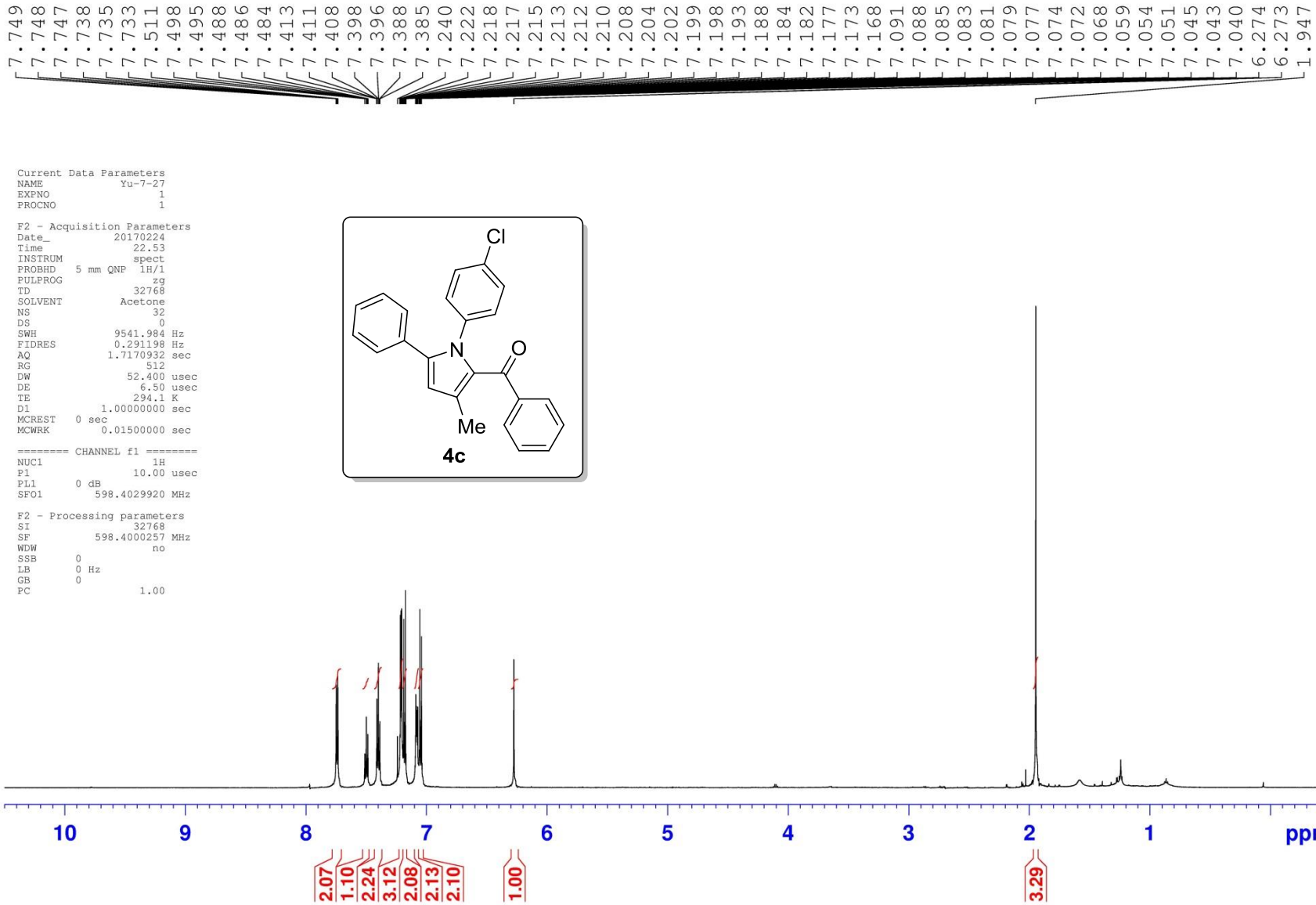


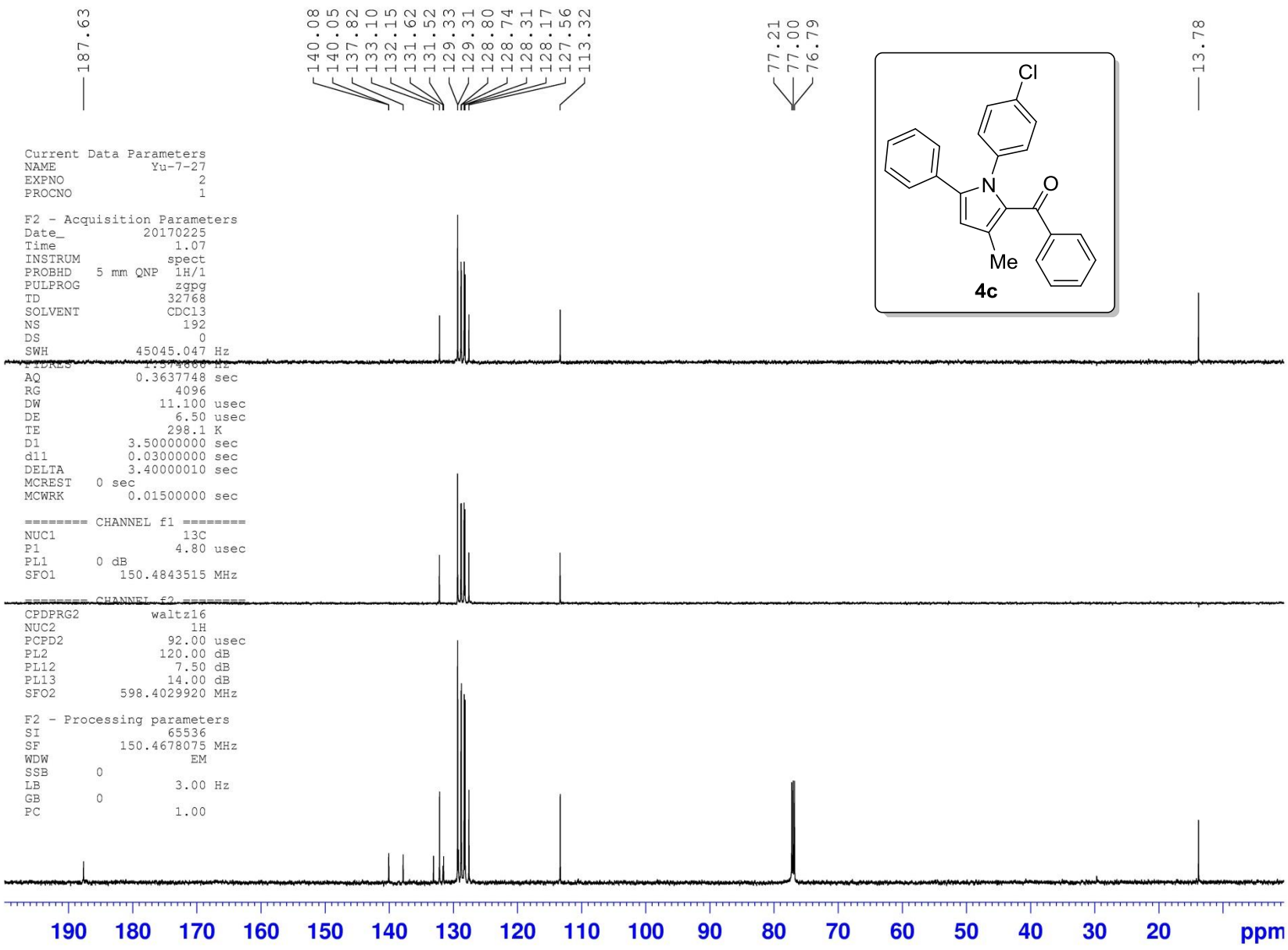

```
Current Data Parameters
NAME            Yu-7-144
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170928
Time              21.52
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG              zg
TD                32768
SOLVENT            C6D6
NS                   32
DS                    0
SWH            8389.262 Hz
FIDRES         0.256020 Hz
AQ             1.9530228 sec
RG                  256
DW                59.600 usec
DE                 6.50 usec
TE                301.8 K
D1             2.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               -1.00 dB
SFO1         598.4029920 MHz

F2 - Processing parameters
SI                32768
SF           598.4000244 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

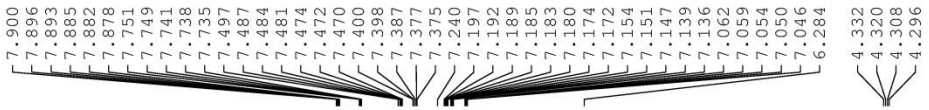




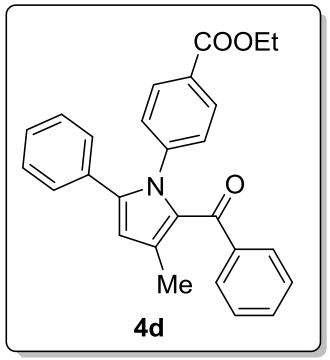

187.61
140.05
138.34
132.14
131.70
131.60
131.51
129.68
129.29
129.19
128.81
128.31
128.18
127.57
121.15
77.21
77.00
76.79
13.75
Br
N
O
Me
4b
Current Data Parameters
NAME Yu-7-144
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170928
Time 21.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.8 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 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678084 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.749 7.748 7.747 7.738 7.735 7.733 7.511 7.498 7.495 7.488 7.486 7.484 7.413 7.411 7.408 7.398 7.396 7.388 7.385 7.240 7.222 7.218 7.217 7.215 7.213 7.212 7.210 7.208 7.204 7.202 7.199 7.198 7.193 7.188 7.184 7.182 7.177 7.173 7.168 7.091 7.088 7.085 7.083 7.081 7.079 7.077 7.074 7.072 7.068 7.059 7.054 7.051 7.045 7.043 7.040 6.274 6.273 1.947
Current Data Parameters
NAME Yu-7-27
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170224
Time 22.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT Acetone
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 294.1 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.4029920 MHz
F2 - Processing parameters
SI 32768
SF 598.4000257 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Cl
N
O
Me
4c
10 9 8 7 6 5 4 3 2 1 ppm
2.07 1.10 2.24 3.12 2.08 2.13 2.10 1.00 3.29

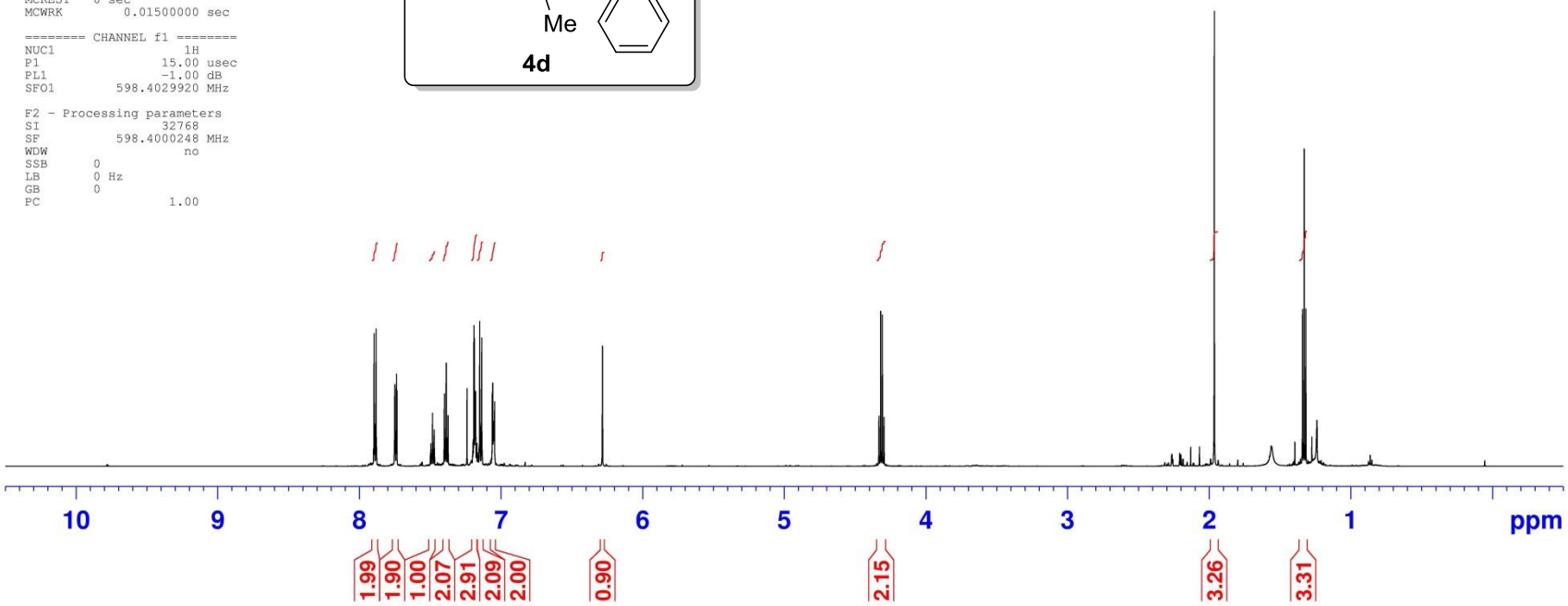

187.63
140.08
140.05
137.82
133.10
132.15
131.62
131.52
129.33
129.31
128.80
128.74
128.31
128.17
127.56
113.32
77.21
77.00
76.79
13.78
Cl
N
O
Me
4c
Current Data Parameters
NAME Yu-7-27
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170225
Time 1.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 192
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 298.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.50 dB
PL13 14.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678075 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

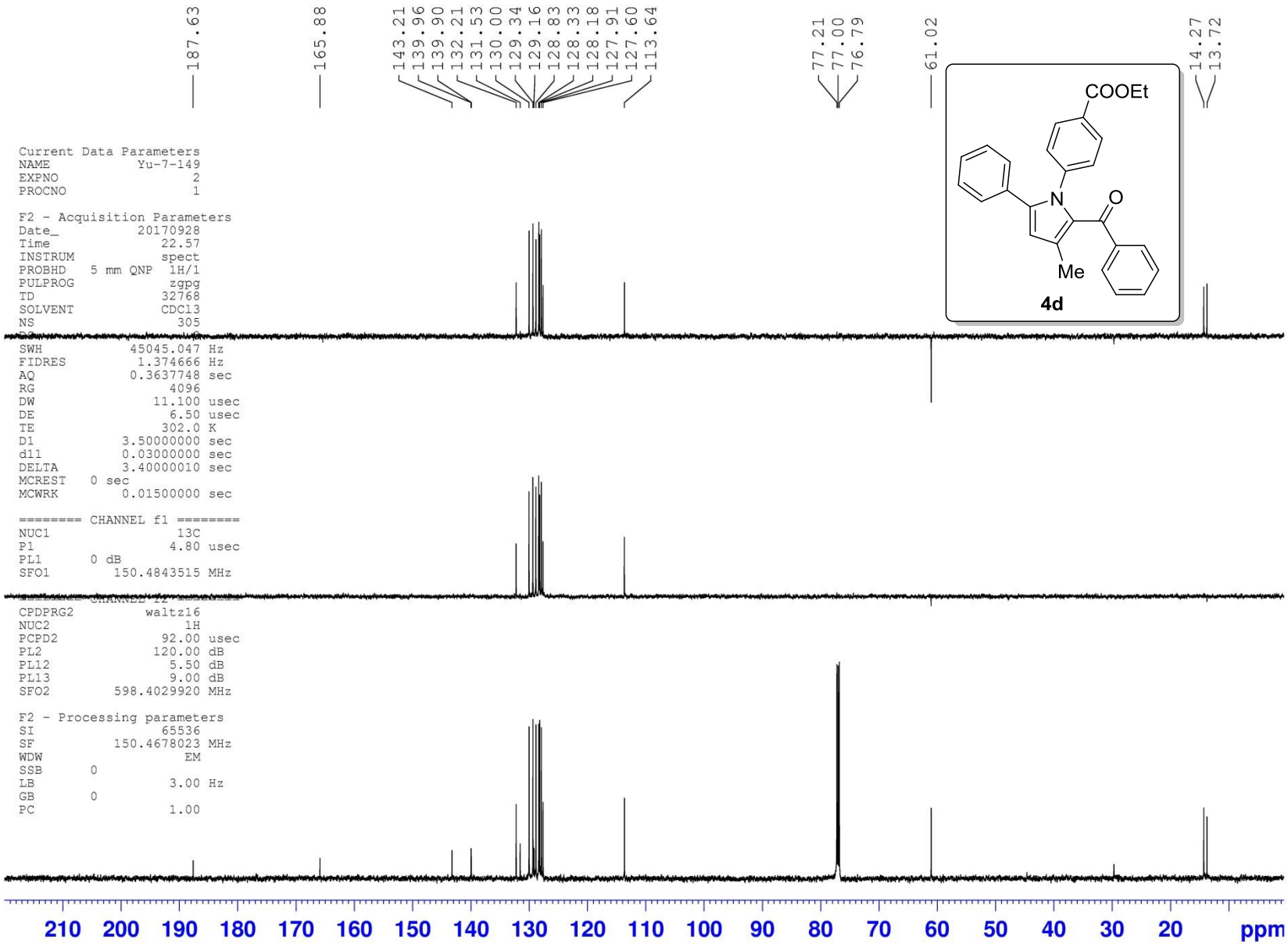


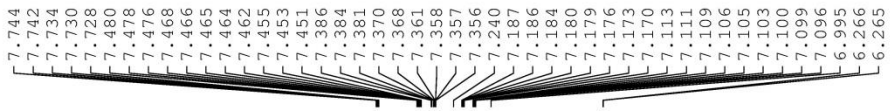

```
Current Data Parameters
NAME                  Yu-7-149
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20170928
Time                     22.49
INSTRUM                  spect
PROBHD    5 mm QNP  1H/1
PULPROG                     zg
TD                       32768
SOLVENT                  C6D6
NS                         32
DS                          0
SWH                   8389.262 Hz
FIDRES                0.256020 Hz
AQ                    1.9530228 sec
RG                         512
DW                      59.600 usec
DE                       6.50 usec
TE                      301.9 K
D1                    2.00000000 sec
MCREST    0 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.00 usec
PL1                      -1.00 dB
SFO1                598.4029920 MHz

F2 - Processing parameters
SI                       32768
SF                  598.4000248 MHz
WDW                         no
SSB                0
LB                 0 Hz
GB                 0
PC                          1.00
```

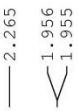


4d

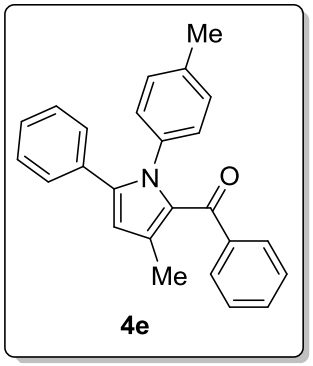


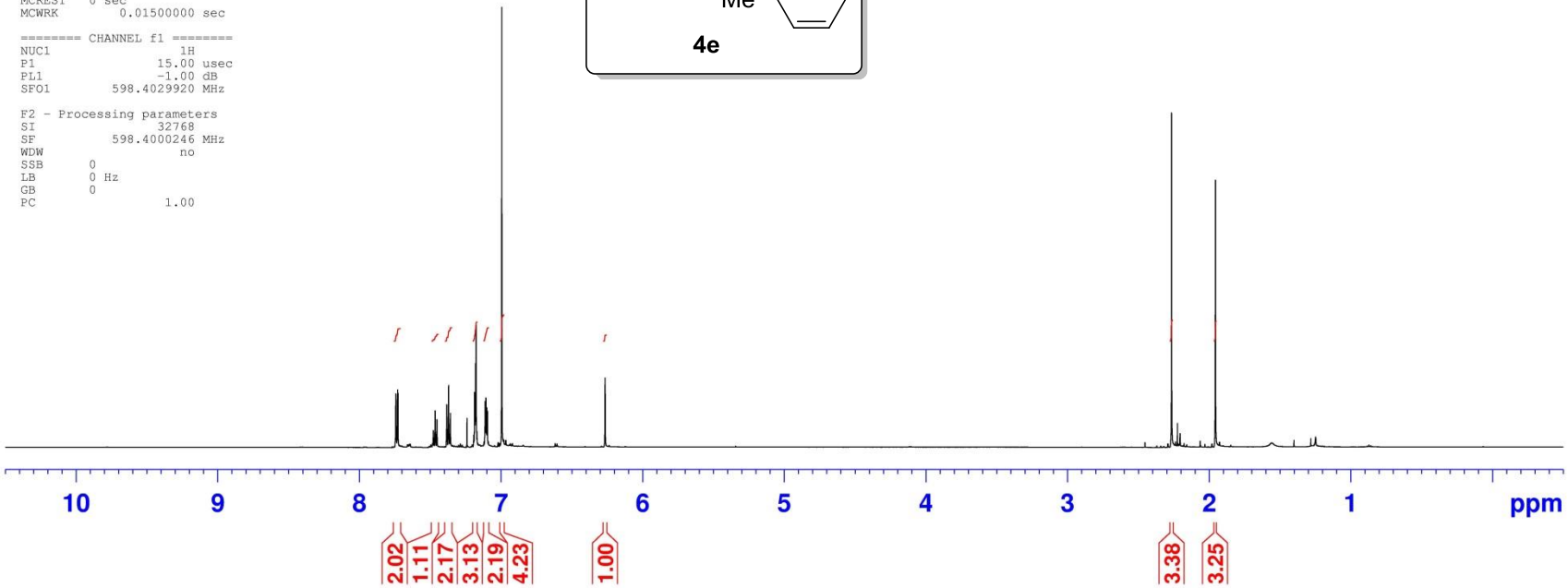

187.63
165.88
143.21
139.96
139.90
132.21
131.53
130.00
129.34
129.16
128.83
128.33
128.18
127.91
127.60
113.64
77.21
77.00
76.79
61.02
14.27
13.72
COOEt
N
O
Me
4d
Current Data Parameters
NAME Yu-7-149
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170928
Time 22.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 305
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 302.0 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 150.4843515 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678023 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

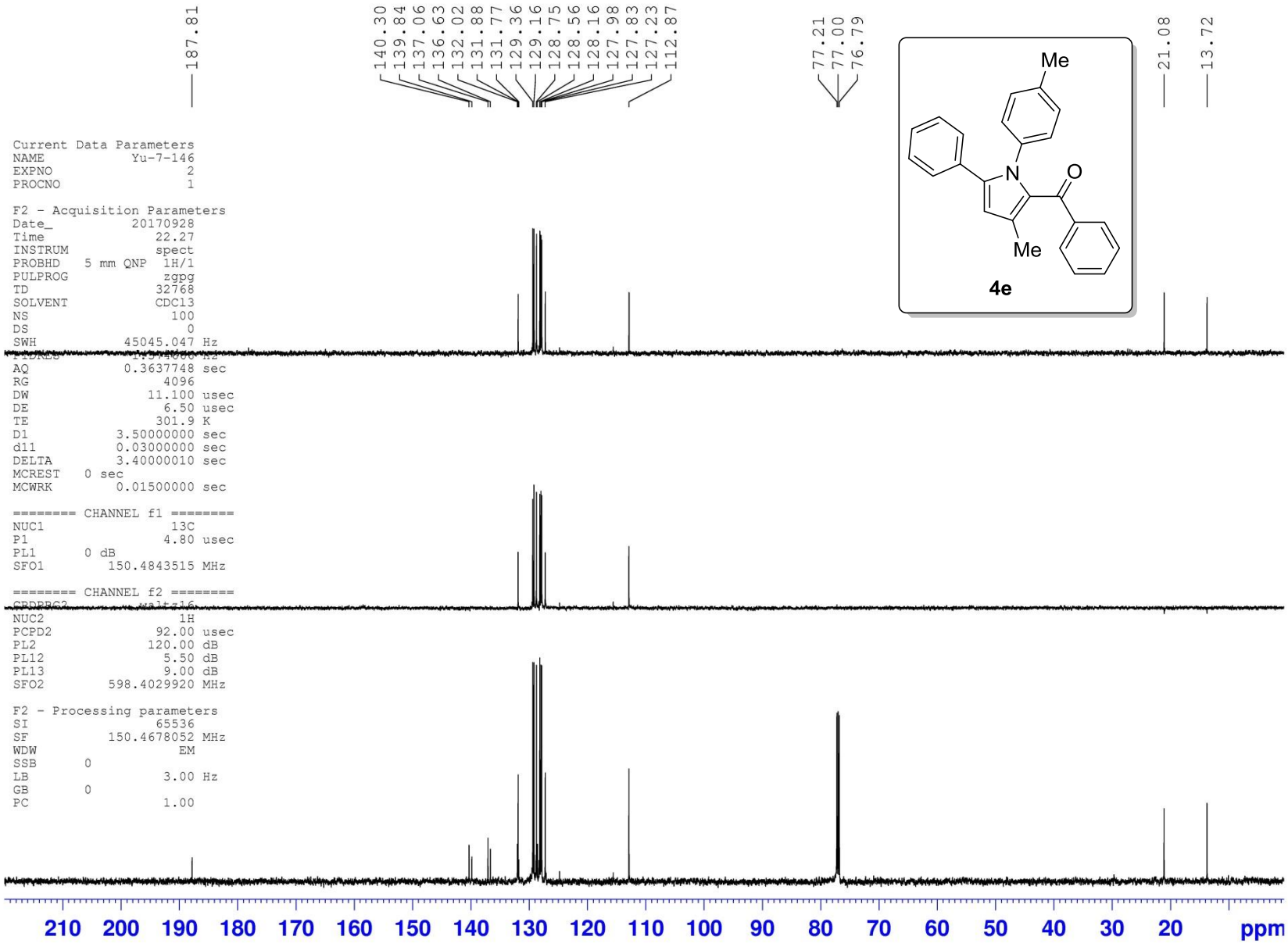


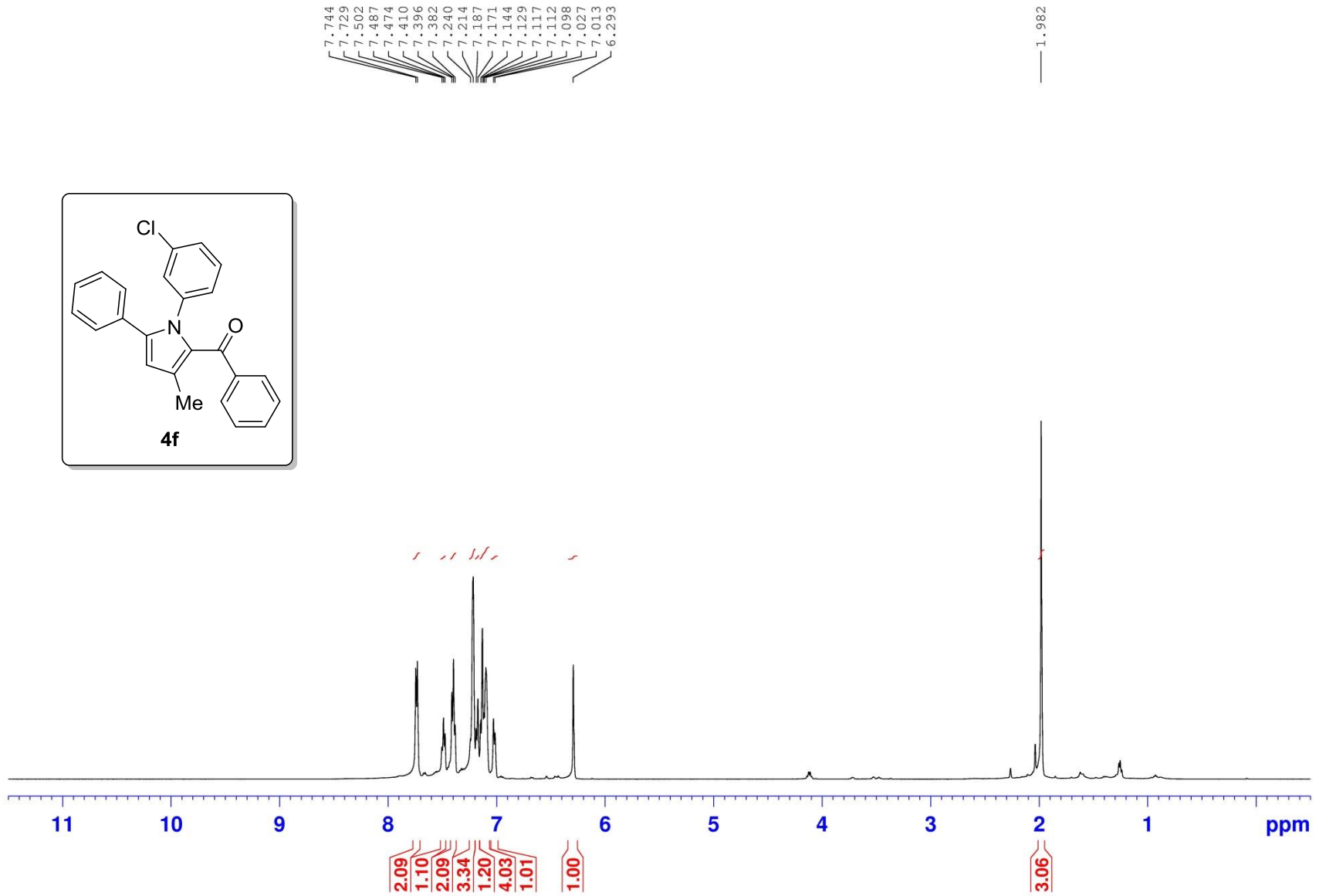


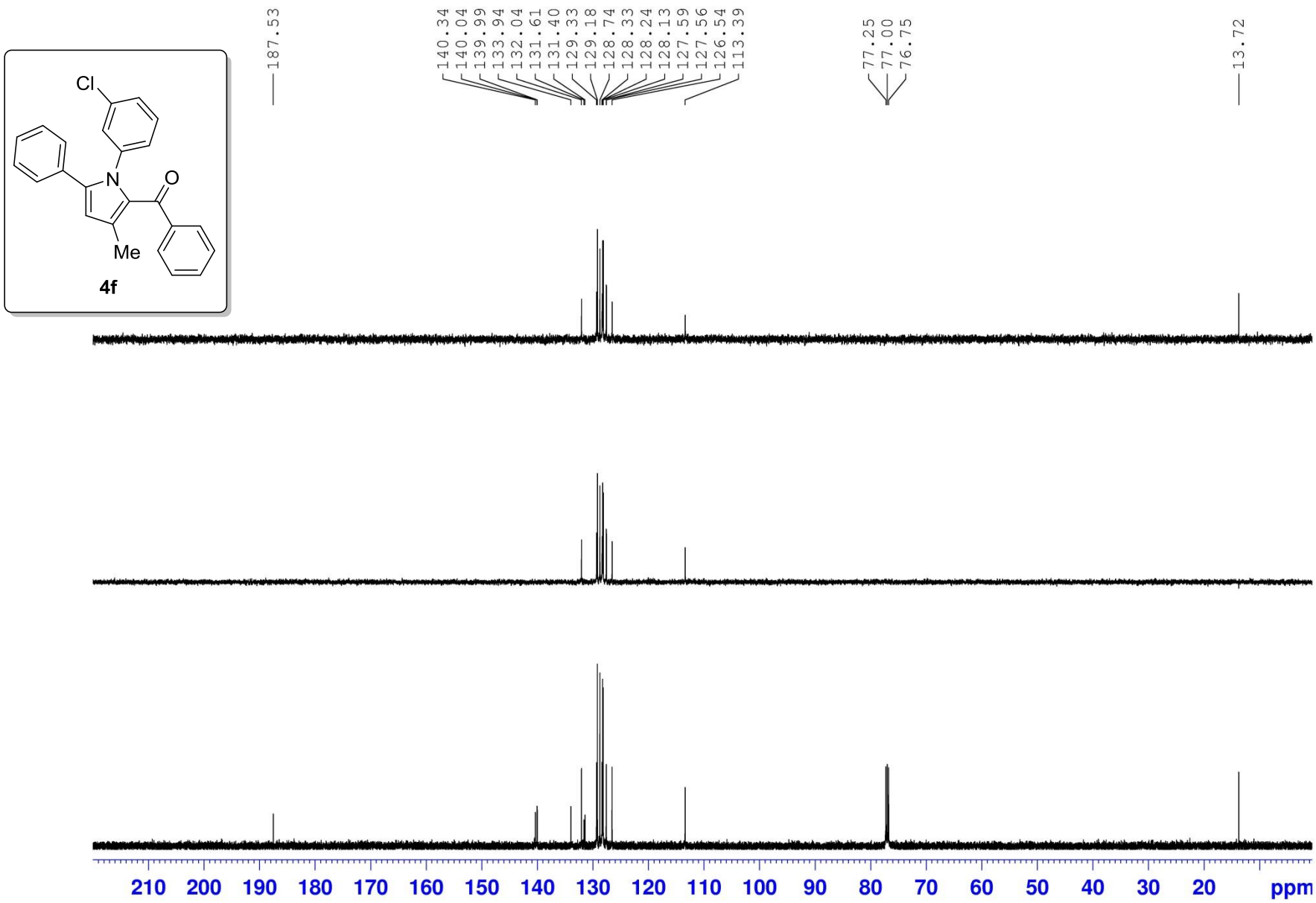

```
Current Data Parameters
NAME            Yu-7-146
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170928
Time               22.22
INSTRUM            spect
PROBHD   5 mm QNP  1H/1
PULPROG              zg
TD                32768
SOLVENT            C6D6
NS                   32
DS                    0
SWH            8389.262 Hz
FIDRES         0.256020 Hz
AQ             1.9530228 sec
RG                   256
DW                59.600 usec
DE                 6.50 usec
TE                301.9 K
D1            2.00000000 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PL1               -1.00 dB
SFO1        598.4029920 MHz

F2 - Processing parameters
SI                32768
SF          598.4000246 MHz
WDW                  no
SSB      0
LB       0 Hz
GB       0
PC                1.00
```

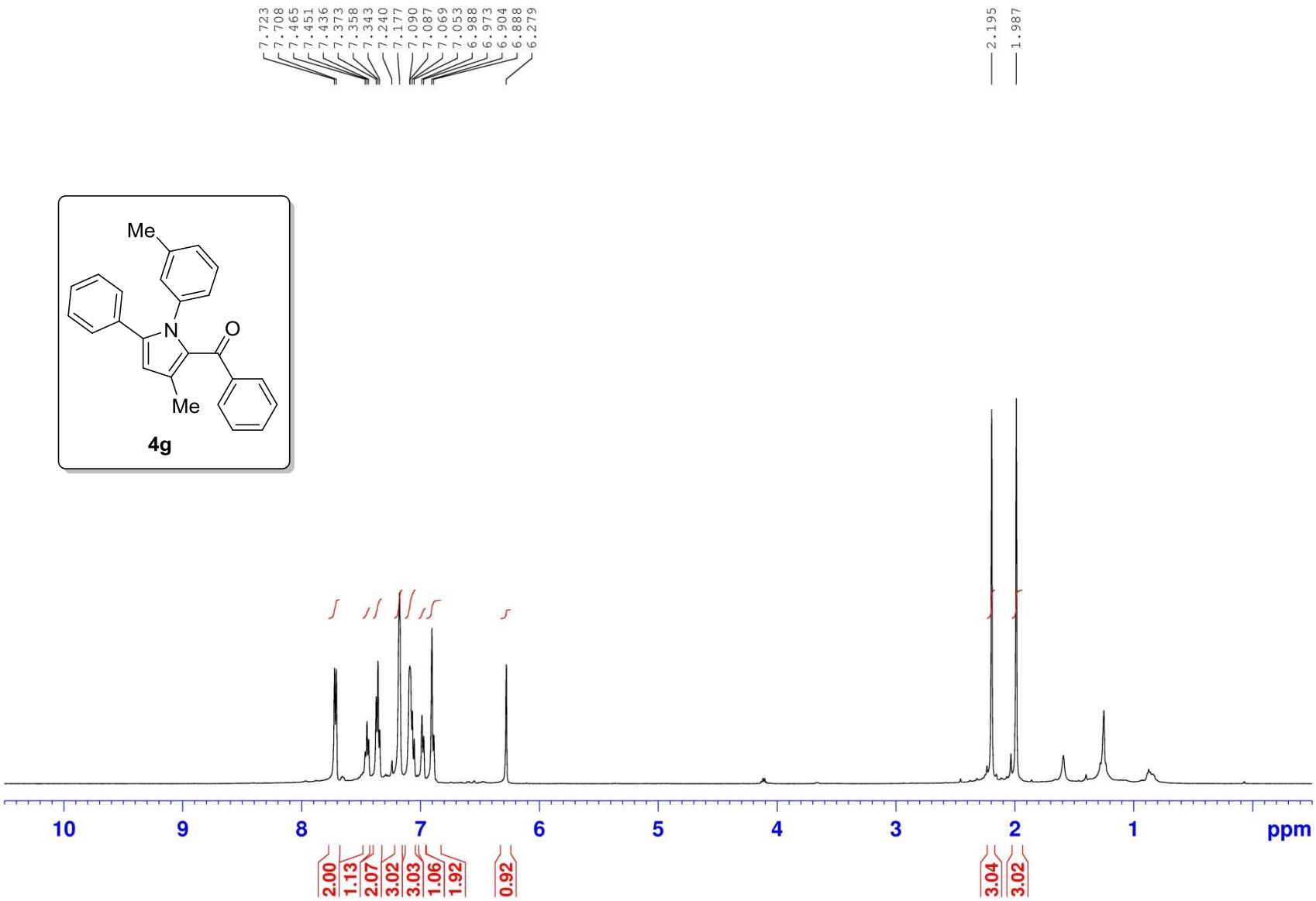


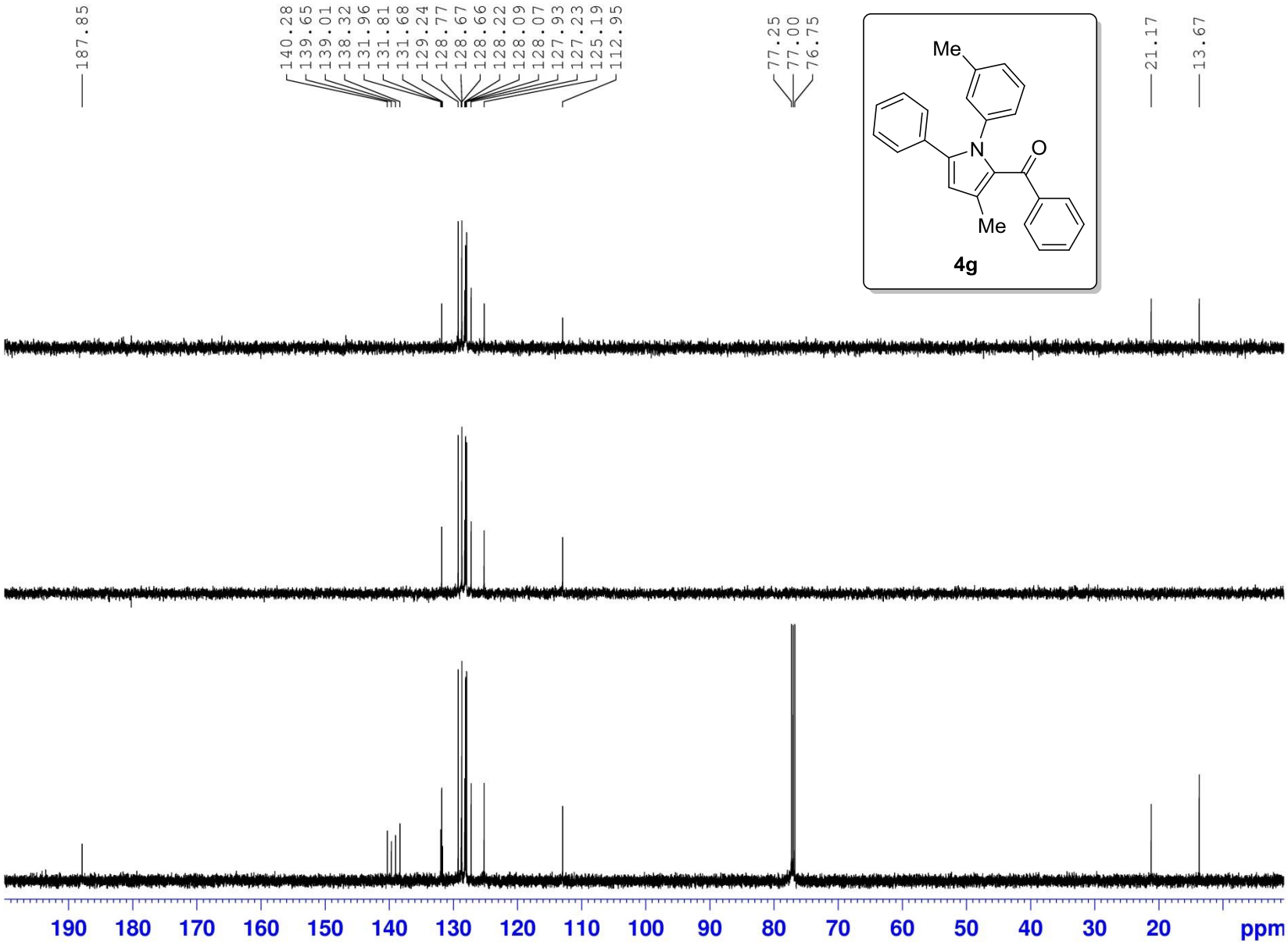


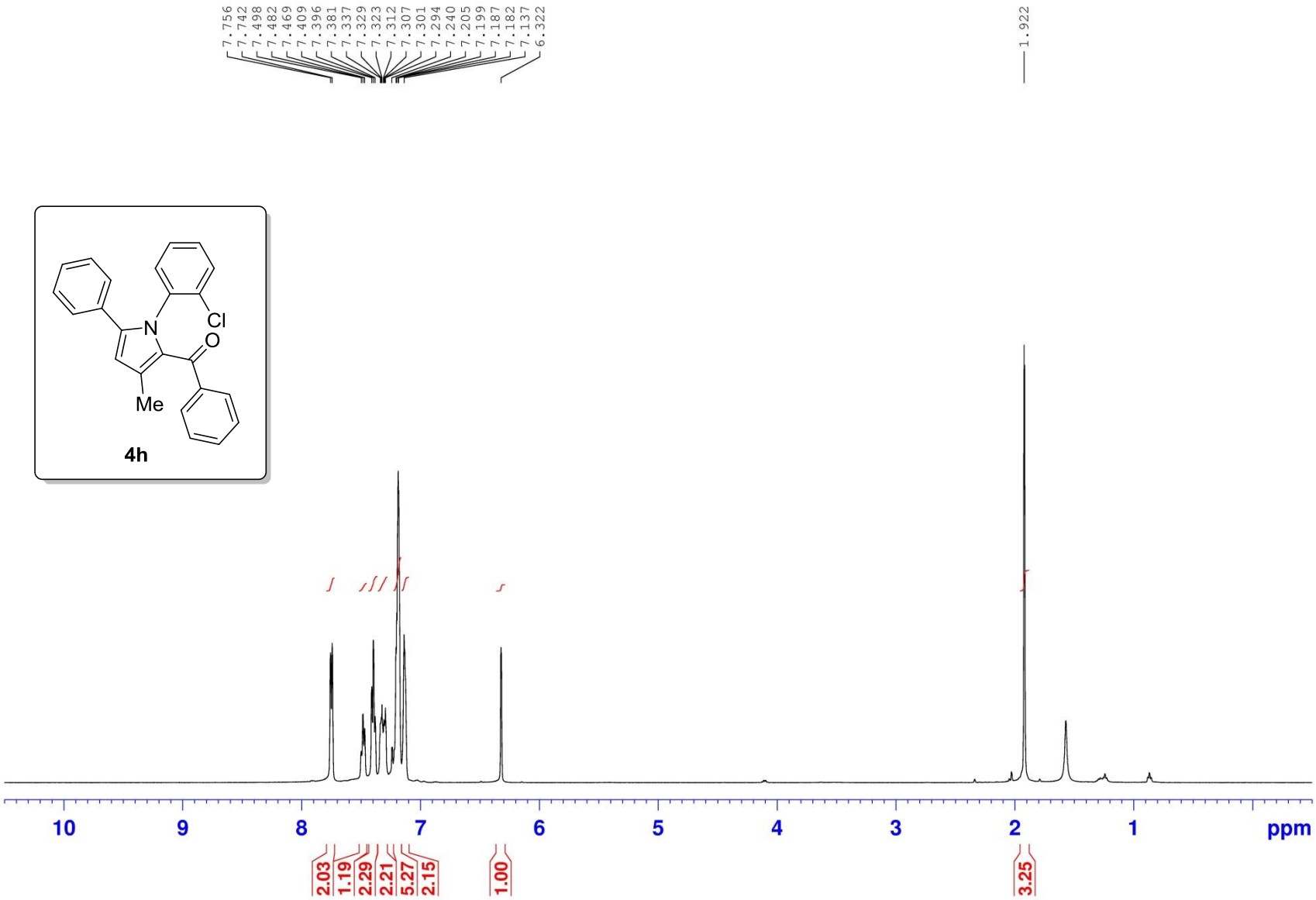

187.81
140.30
139.84
137.06
136.63
132.02
131.88
131.77
129.36
129.16
128.75
128.56
128.16
127.98
127.83
127.23
112.87
77.21
77.00
76.79
21.08
13.72
Me
N
O
Me
4e
Current Data Parameters
NAME Yu-7-146
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170928
Time 22.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4843515 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678052 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

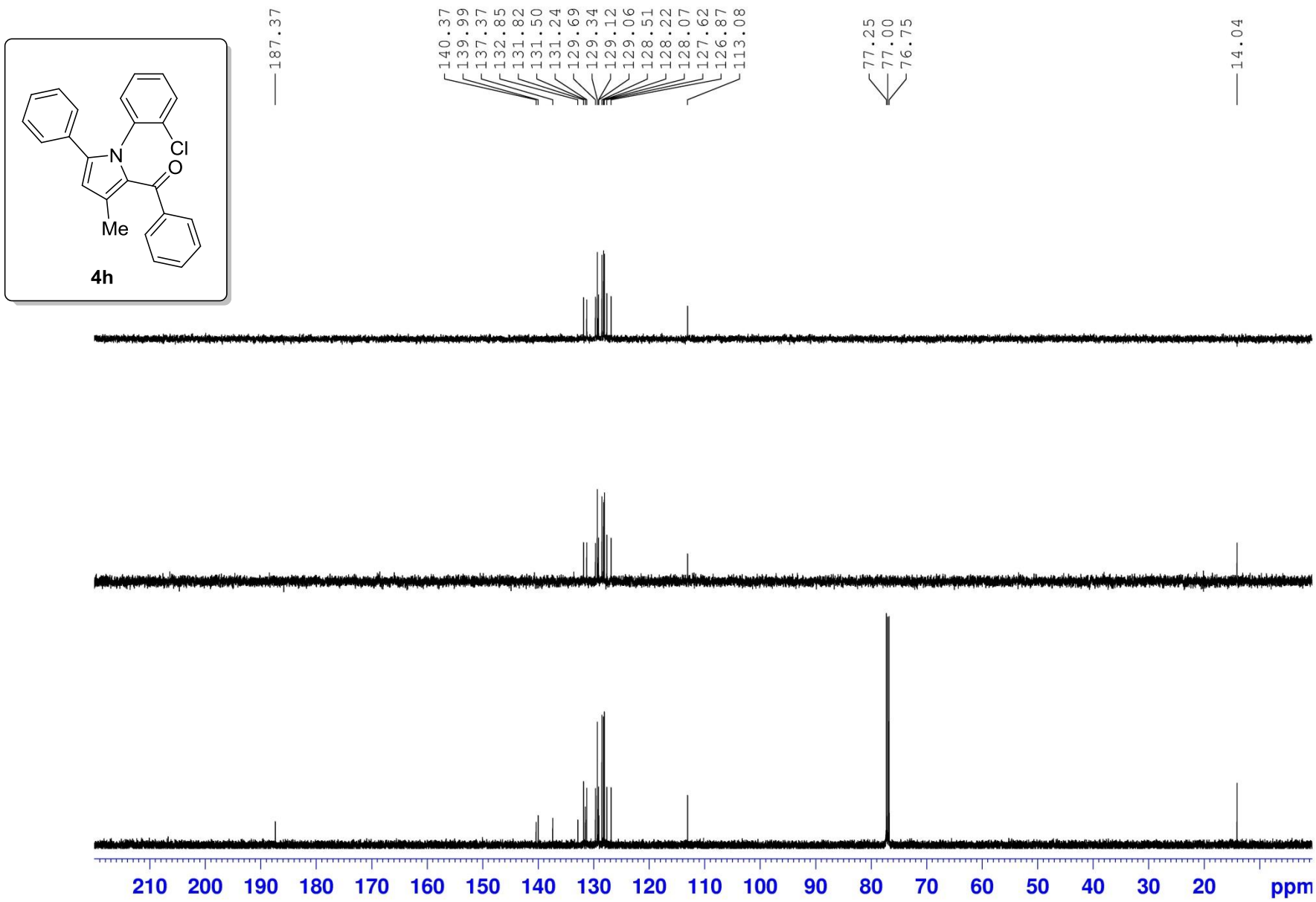

7.744
7.729
7.502
7.487
7.474
7.410
7.396
7.382
7.240
7.214
7.187
7.171
7.144
7.129
7.117
7.112
7.098
7.027
7.013
6.293
1.982
Cl
N
O
Me
4f
11
10
9
8
7
6
5
4
3
2
1
ppm
2.09
1.10
2.09
3.34
1.20
4.03
1.01
1.00
3.06

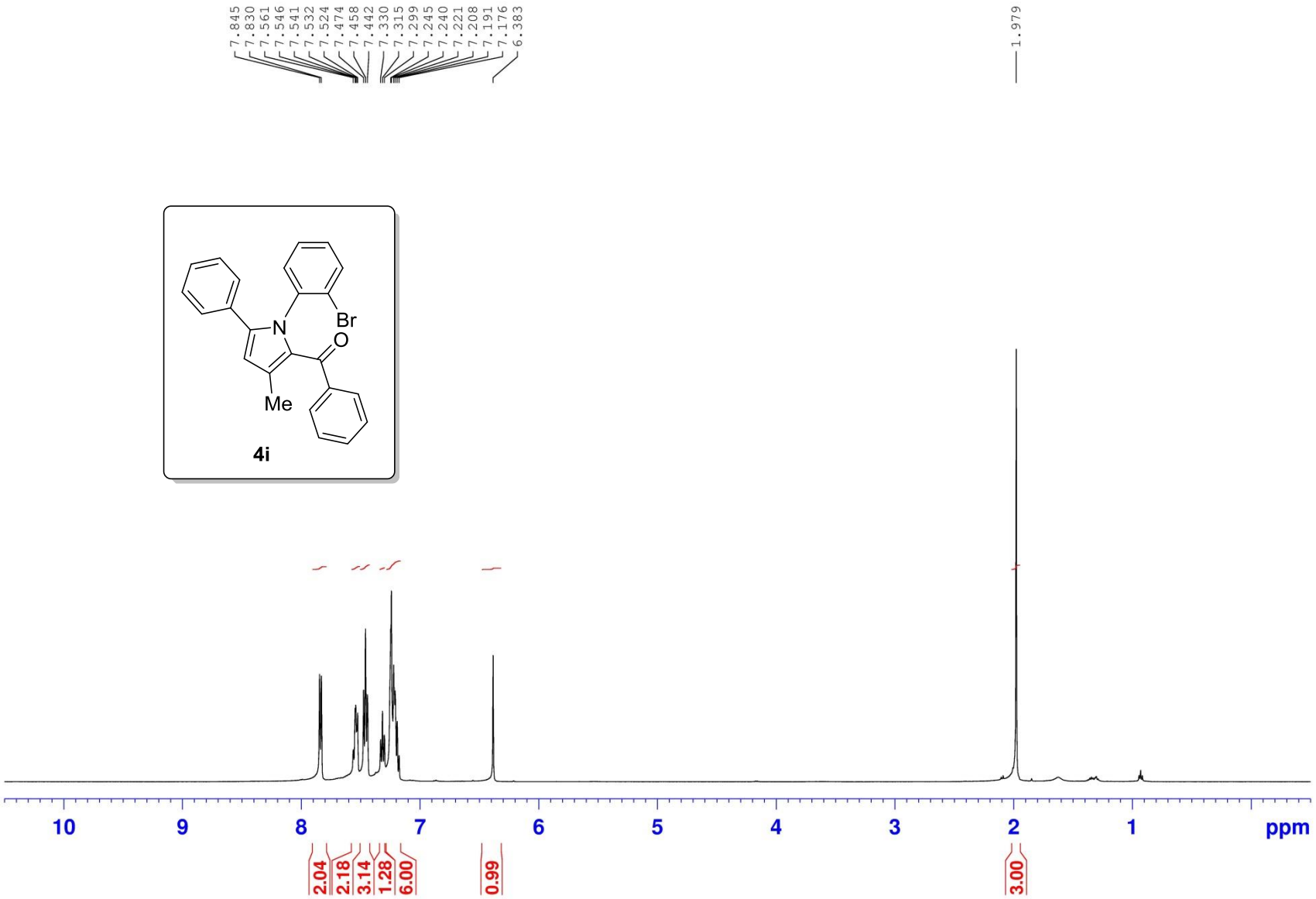

187.53
140.34
140.04
139.99
133.94
132.04
131.61
131.40
129.33
129.18
128.74
128.33
128.24
128.13
127.59
127.56
126.54
113.39
77.25
77.00
76.75
13.72
Cl
N
O
Me
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

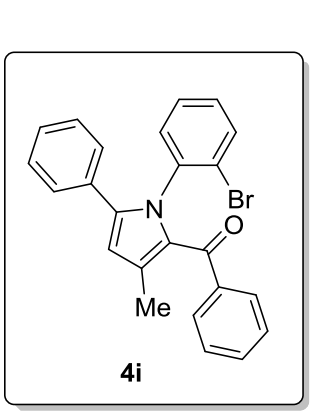

7.723
7.708
7.465
7.451
7.436
7.373
7.358
7.343
7.240
7.177
7.090
7.087
7.069
7.053
6.988
6.973
6.904
6.888
6.279
2.195
1.987
Me
N
O
Me
4g
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.13
2.07
3.02
3.03
1.06
1.92
0.92
3.04
3.02


187.85
140.28
139.65
139.01
138.32
131.96
131.81
131.68
129.24
128.77
128.67
128.66
128.22
128.09
128.07
127.93
127.23
125.19
112.95
77.25
77.00
76.75
21.17
13.67
Me
N
O
Me
4g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

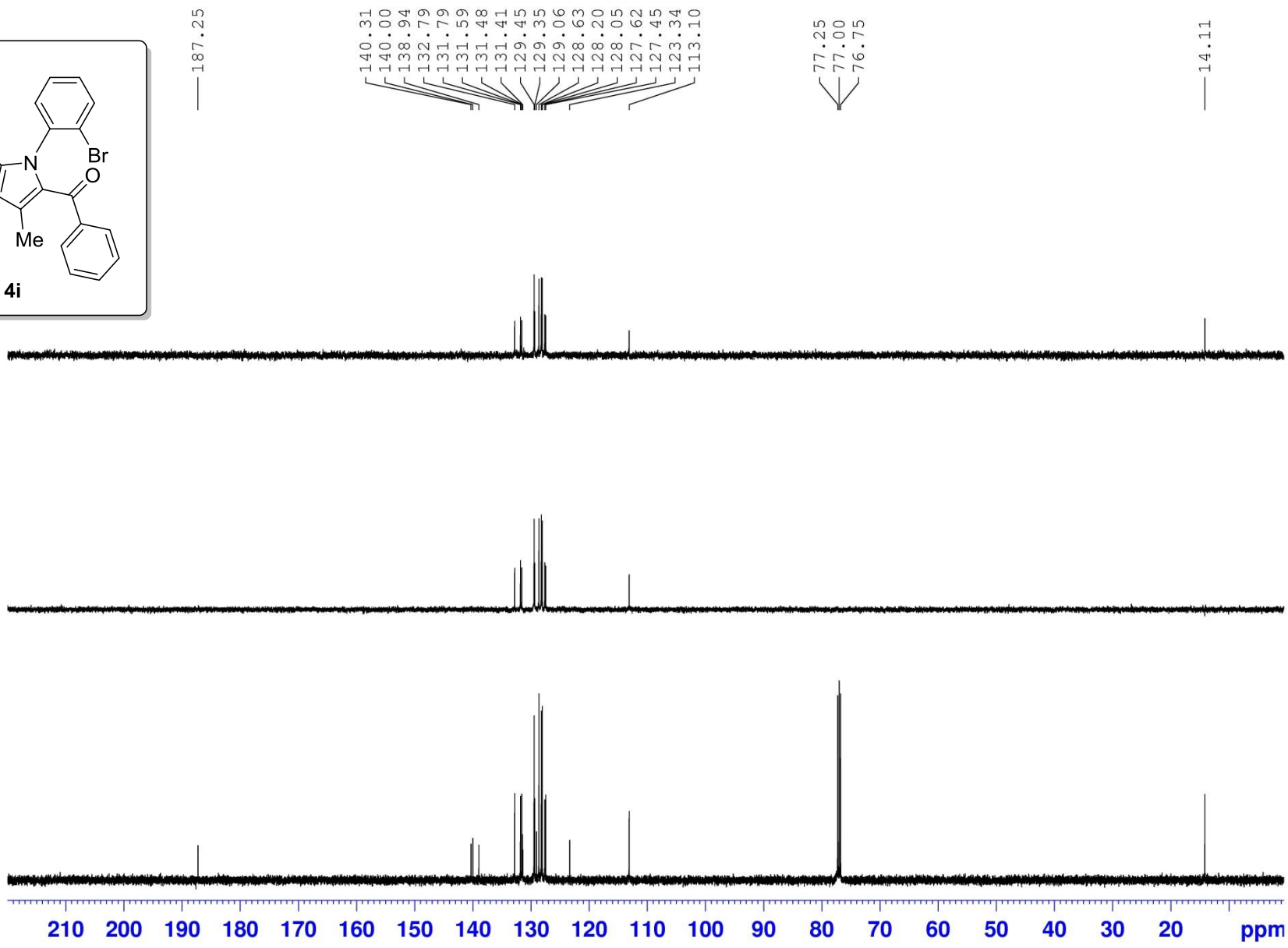

7.756
7.742
7.498
7.482
7.469
7.409
7.396
7.381
7.337
7.329
7.323
7.312
7.307
7.301
7.294
7.240
7.205
7.199
7.187
7.182
7.137
6.322
1.922
Cl
O
N
Me
4h
10
9
8
7
6
5
4
3
2
1
ppm
2.03
1.19
2.29
2.21
5.27
2.15
1.00
3.25

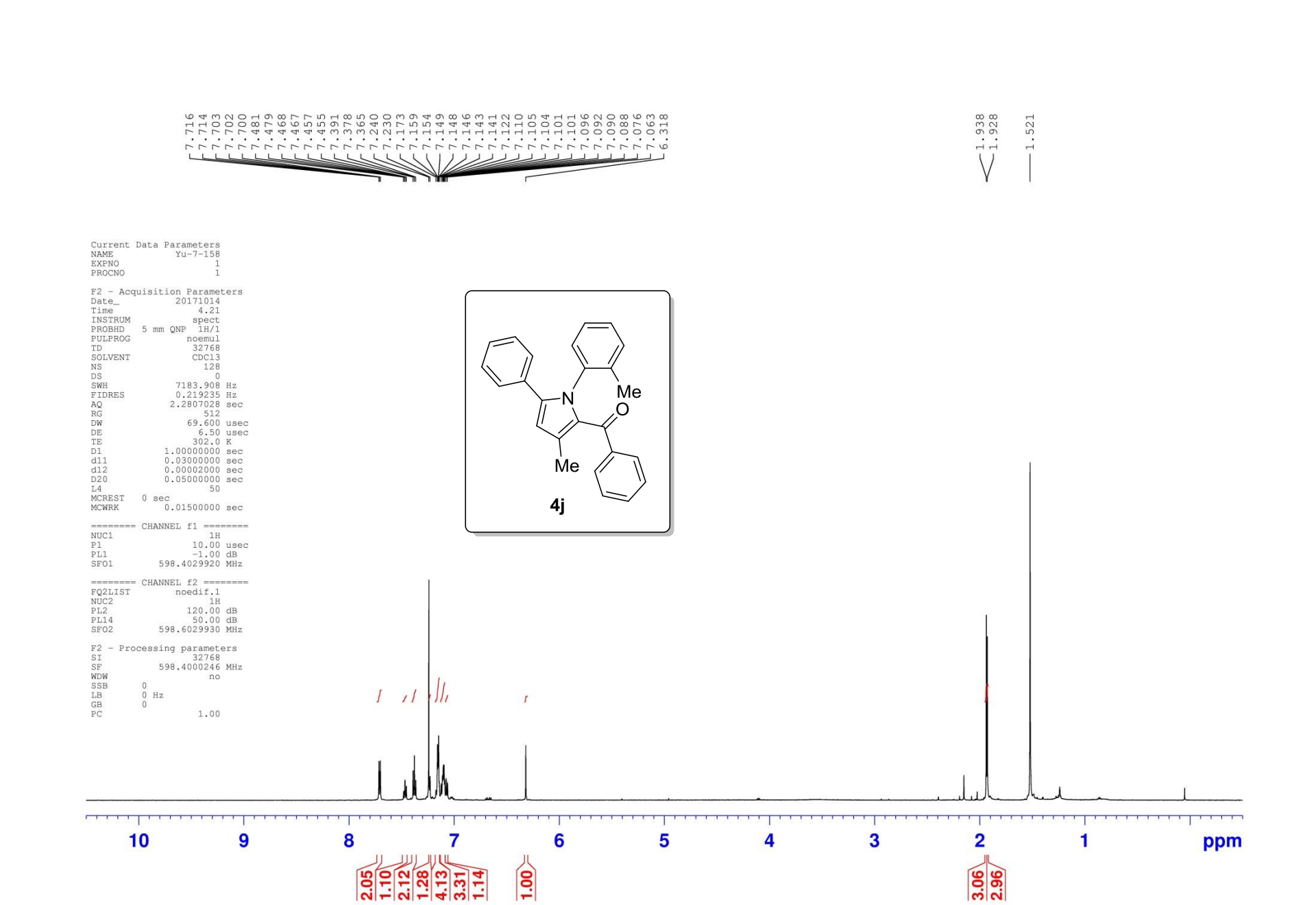

187.37
140.37
139.99
137.37
132.85
131.82
131.50
131.24
129.69
129.34
129.12
129.06
128.51
128.22
128.07
127.62
126.87
113.08
77.25
77.00
76.75
14.04
N
Cl
O
Me
4h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

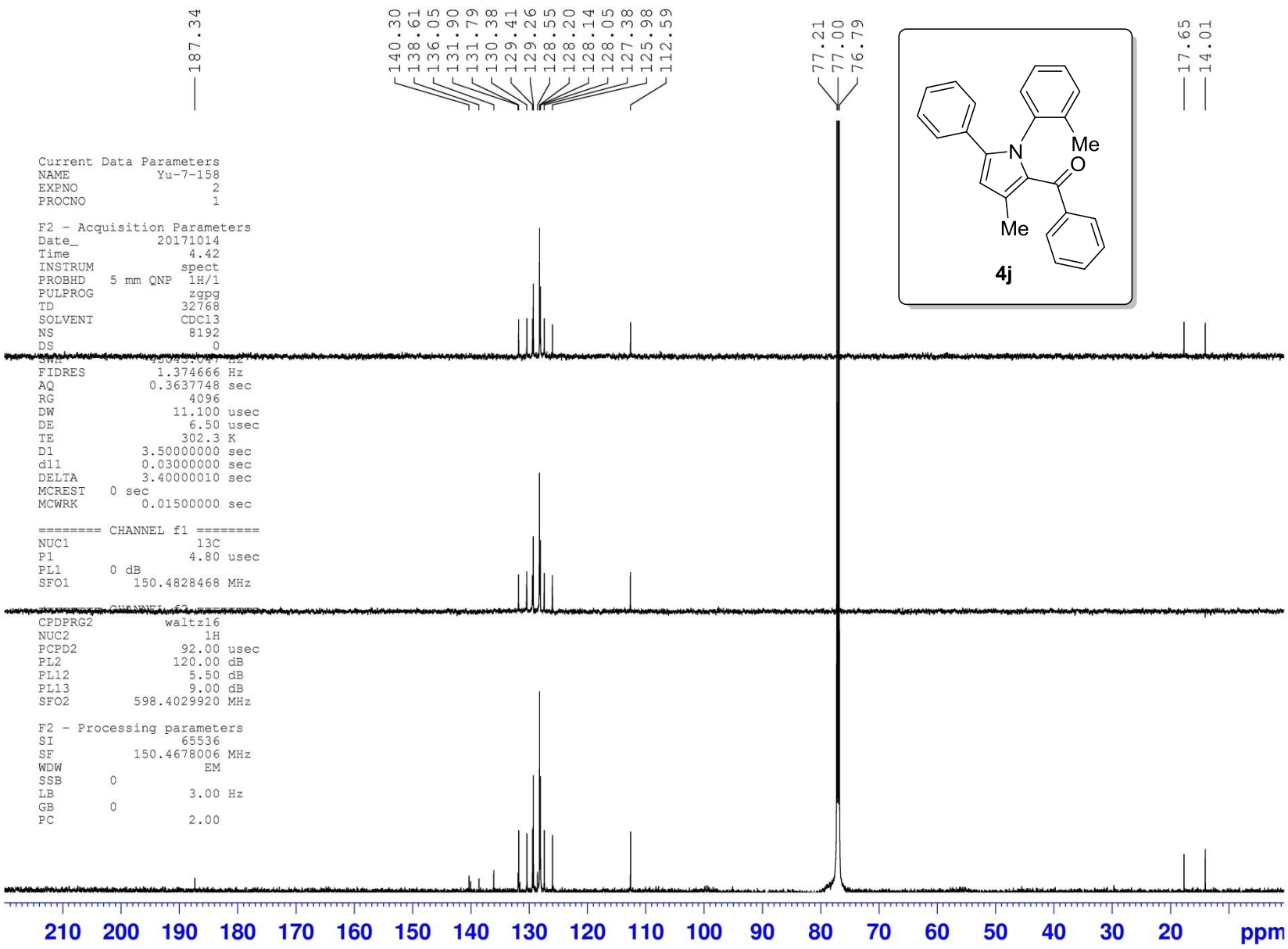

7.845
7.830
7.561
7.546
7.541
7.532
7.524
7.474
7.458
7.442
7.330
7.315
7.299
7.245
7.240
7.221
7.208
7.191
7.176
6.383
1.979
Br
N
O
Me
4i
10
9
8
7
6
5
4
3
2
1
ppm
2.04
2.18
3.14
1.28
6.00
0.99
3.00


N
Br
O
Me

4i


187.25
140.31
140.00
138.94
132.79
131.79
131.59
131.48
131.41
129.45
129.35
129.06
128.63
128.20
128.05
127.62
127.45
123.34
113.10
77.25
77.00
76.75
14.11
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.716
7.714
7.703
7.702
7.700
7.481
7.479
7.468
7.467
7.457
7.455
7.391
7.378
7.365
7.240
7.230
7.173
7.159
7.154
7.149
7.148
7.146
7.143
7.141
7.122
7.110
7.105
7.104
7.101
7.101
7.096
7.092
7.090
7.088
7.076
7.063
6.318
1.938
1.928
1.521
Current Data Parameters
NAME Yu-7-158
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171014
Time 4.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG noemul
TD 32768
SOLVENT CDC13
NS 128
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 512
DW 69.600 usec
DE 6.50 usec
TE 302.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
D20 0.05000000 sec
L4 50
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.4029920 MHz
======== CHANNEL f2 ========
FQ2LIST noedif.1
NUC2 1H
PL2 120.00 dB
PL14 50.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.4000246 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
Me
O
Me
4j
10
9
8
7
6
5
4
3
2
1
ppm
2.05
1.10
2.12
1.28
4.13
3.31
1.14
1.00
3.06
2.96


187.34
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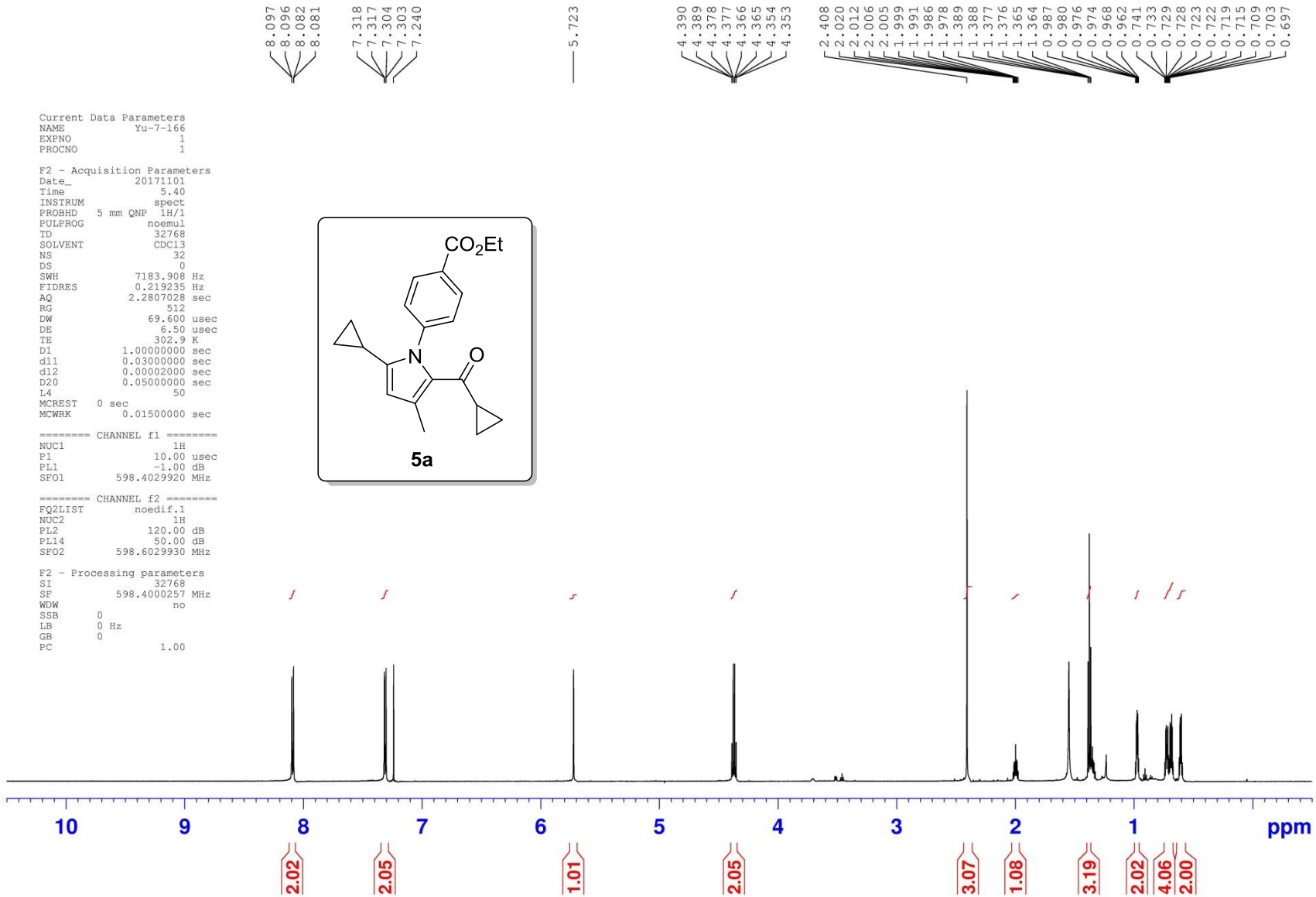
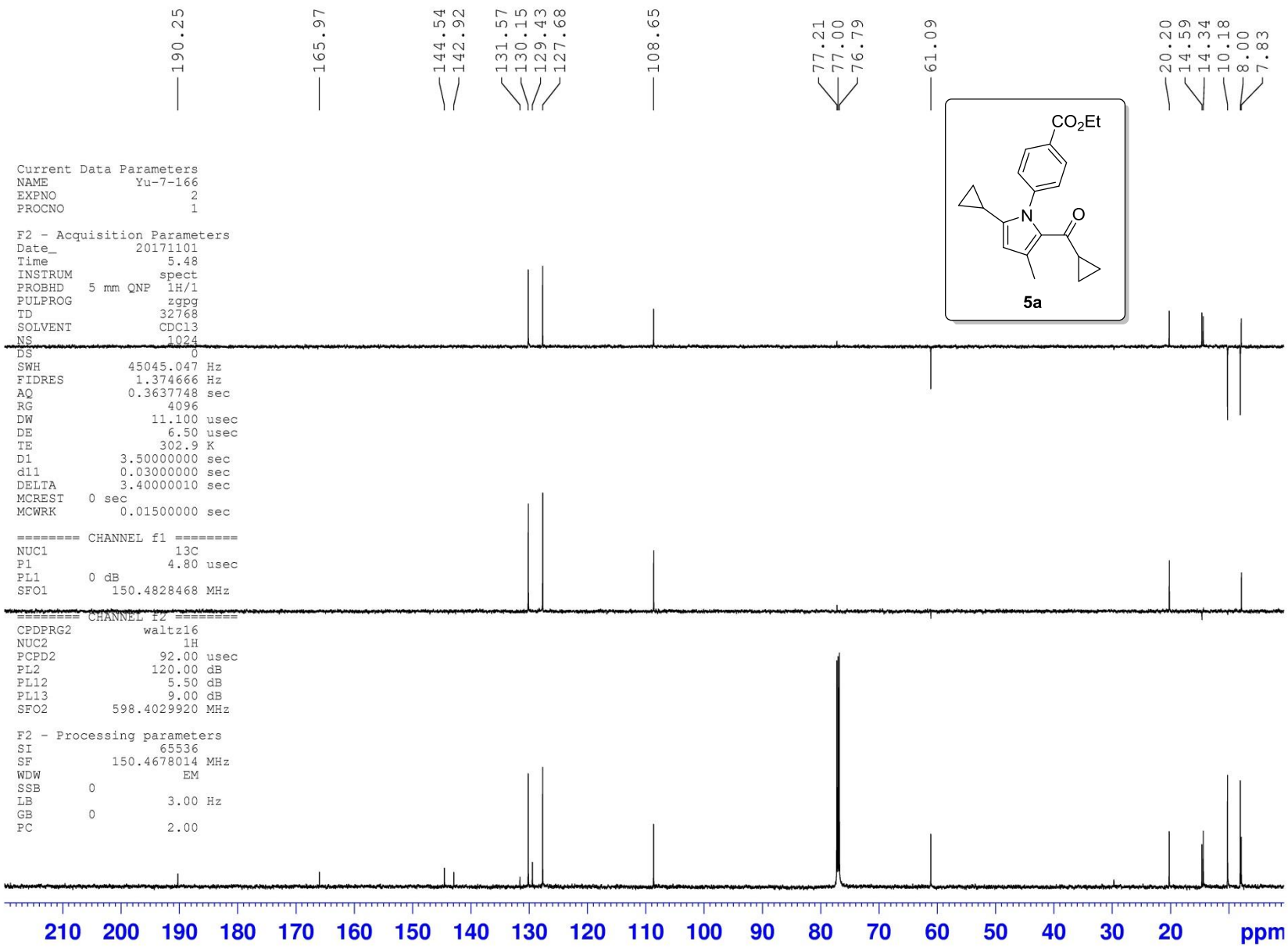
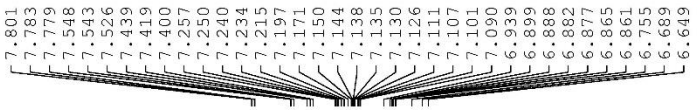
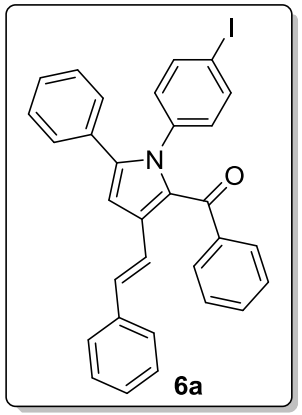
138.61
136.05
131.90
131.79
130.38
129.41
129.26
128.55
128.20
128.14
128.05
127.38
125.98
112.59
77.21
77.00
76.79
17.65
14.01
Me
N
O
Me
4j
Current Data Parameters
NAME Yu-7-158
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171014
Time 4.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 8192
DS 0
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 302.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4828468 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678006 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

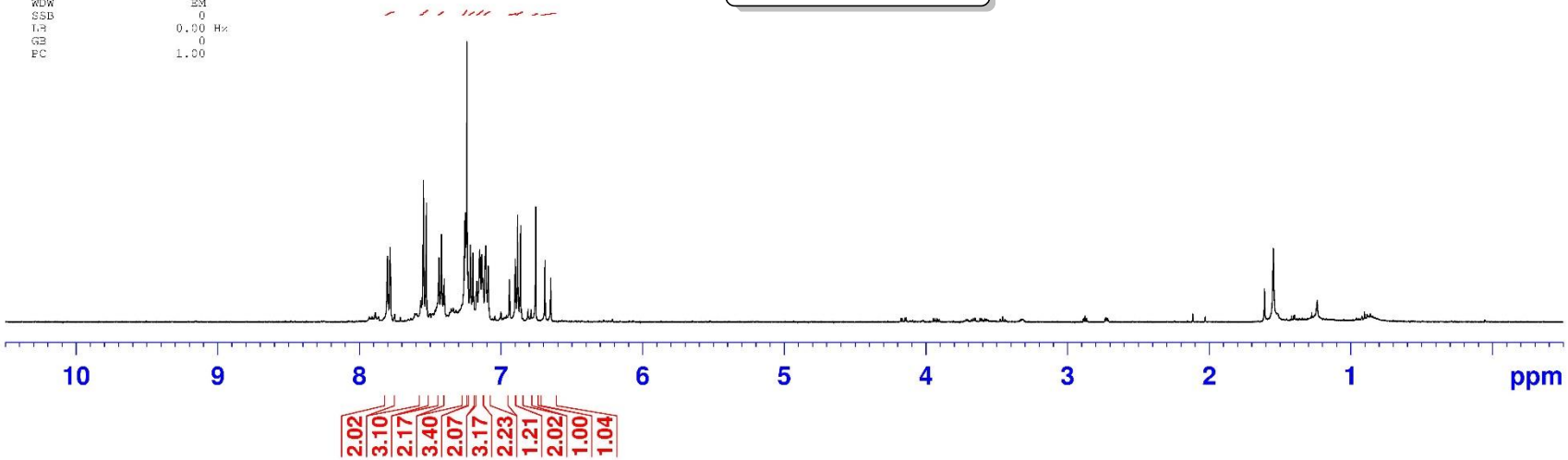

8.097
8.096
8.082
8.081
7.318
7.317
7.304
7.303
7.240
5.723
4.390
4.389
4.378
4.377
4.366
4.365
4.354
4.353
2.408
2.020
2.012
2.006
2.005
1.999
1.991
1.986
1.978
1.389
1.388
1.377
1.376
1.365
1.364
0.987
0.980
0.976
0.974
0.968
0.962
0.741
0.733
0.729
0.728
0.723
0.722
0.719
0.715
0.709
0.703
0.697
Current Data Parameters
NAME Yu-7-166
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171101
Time 5.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG noemul
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 512
DW 69.600 usec
DE 6.50 usec
TE 302.9 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
D20 0.05000000 sec
L4 50
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.4029920 MHz
======== CHANNEL f2 ========
FQ2LIST noedif.1
NUC2 1H
PL2 120.00 dB
PL14 50.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.4000257 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
CO2Et
N
O
5a
10
9
8
7
6
5
4
3
2
1
ppm
2.02
2.05
1.01
2.05
3.07
1.08
3.19
2.02
4.06
2.00

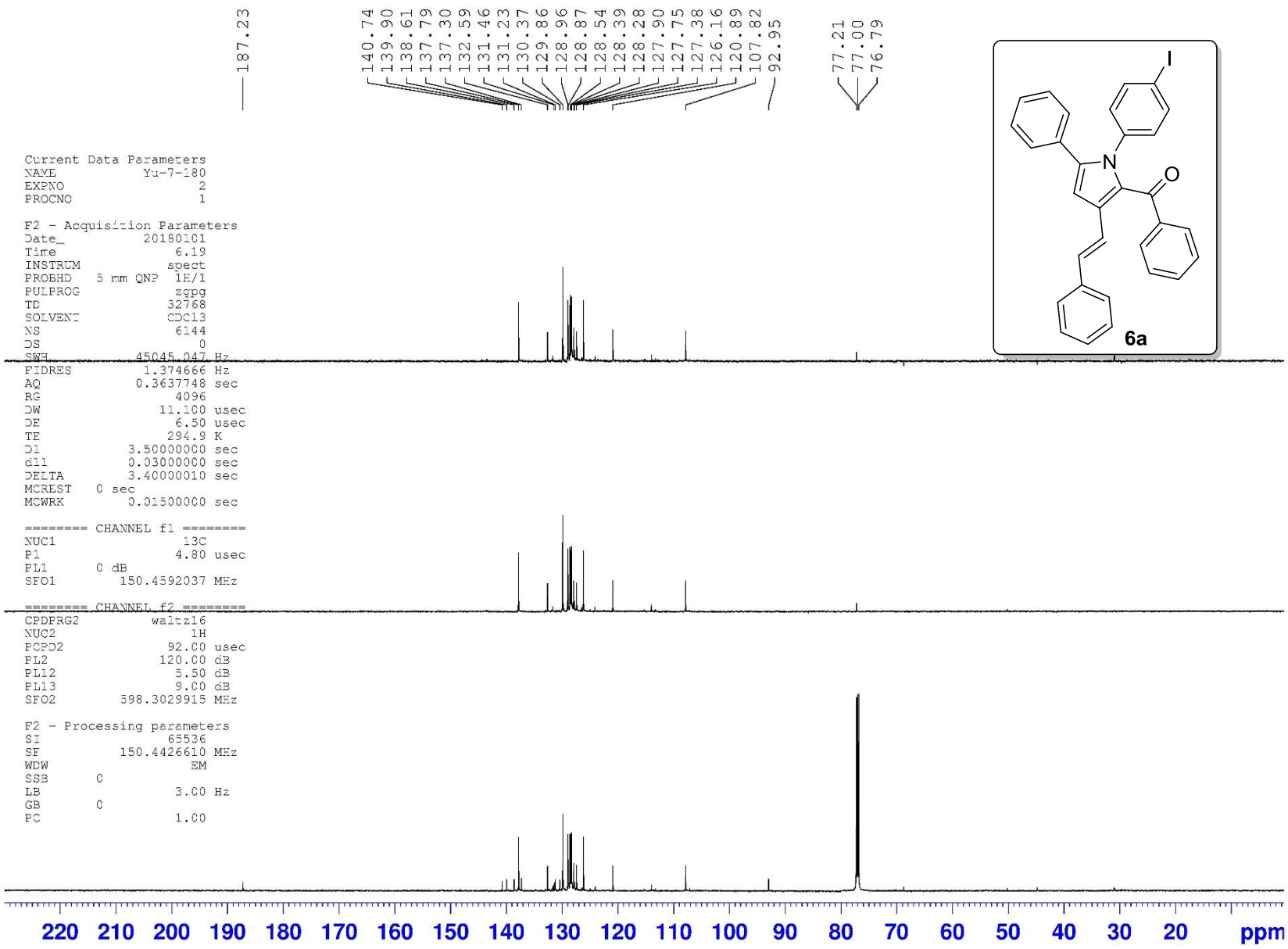

190.25
165.97
144.54
142.92
131.57
130.15
129.43
127.68
108.65
77.21
77.00
76.79
61.09
20.20
14.59
14.34
10.18
8.00
7.83
CO2Et
N
O
5a
Current Data Parameters
NAME Yu-7-166
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171101
Time 5.48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT 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 302.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4828468 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.4029920 MHz
F2 - Processing parameters
SI 65536
SF 150.4678014 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

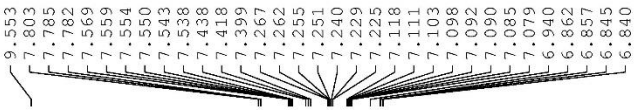



```
Current Data Parameters
NAME              20171229
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171229
Time                 16.21
INSTRUM              spect
PROBHD    5 mm DUL 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                    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           400.1500172 MHz
WDW                    EM
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

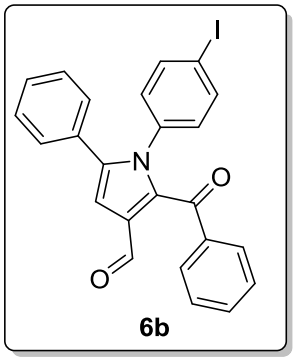


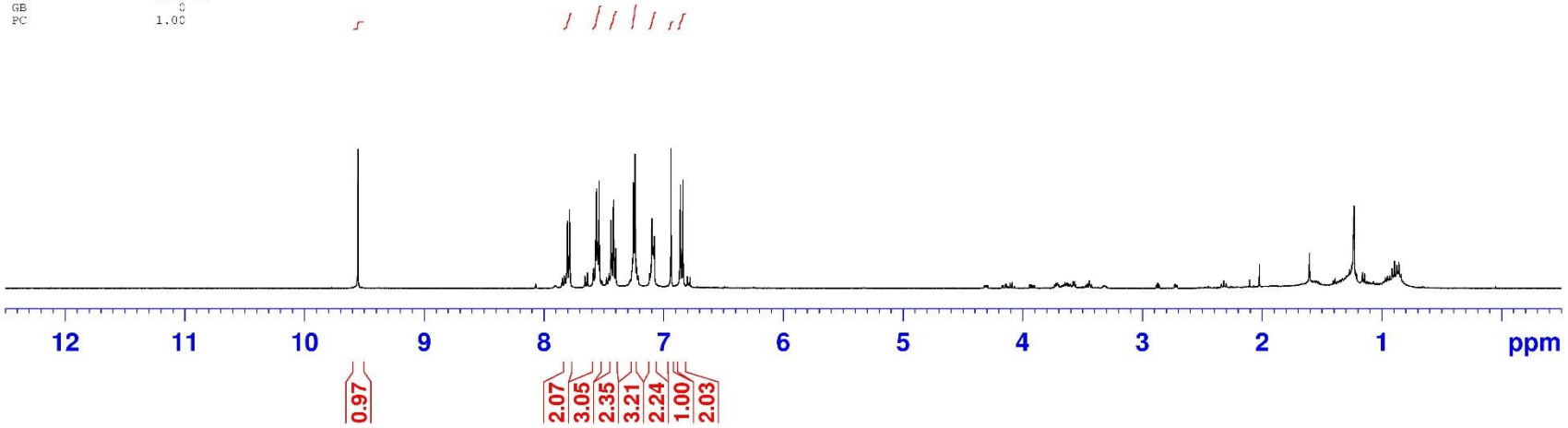


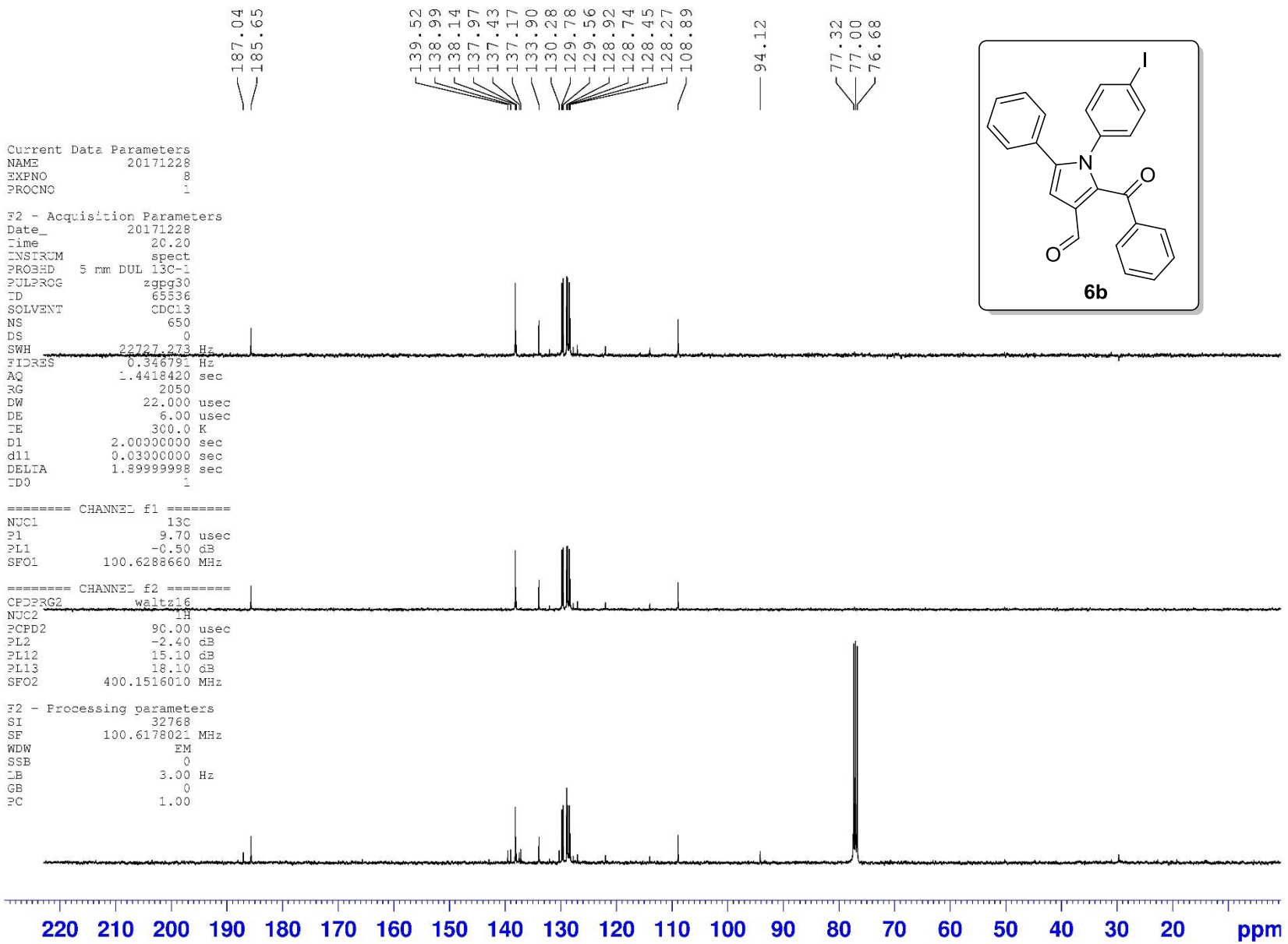

187.23
140.74
139.90
138.61
137.79
137.30
132.59
131.46
131.23
130.37
129.86
128.96
128.87
128.54
128.39
128.28
127.90
127.75
127.38
126.16
120.89
107.82
92.95
77.21
77.00
76.79
I
N
O
6a
Current Data Parameters
NAME Yu-7-180
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180101
Time 6.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 294.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 398.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426610 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

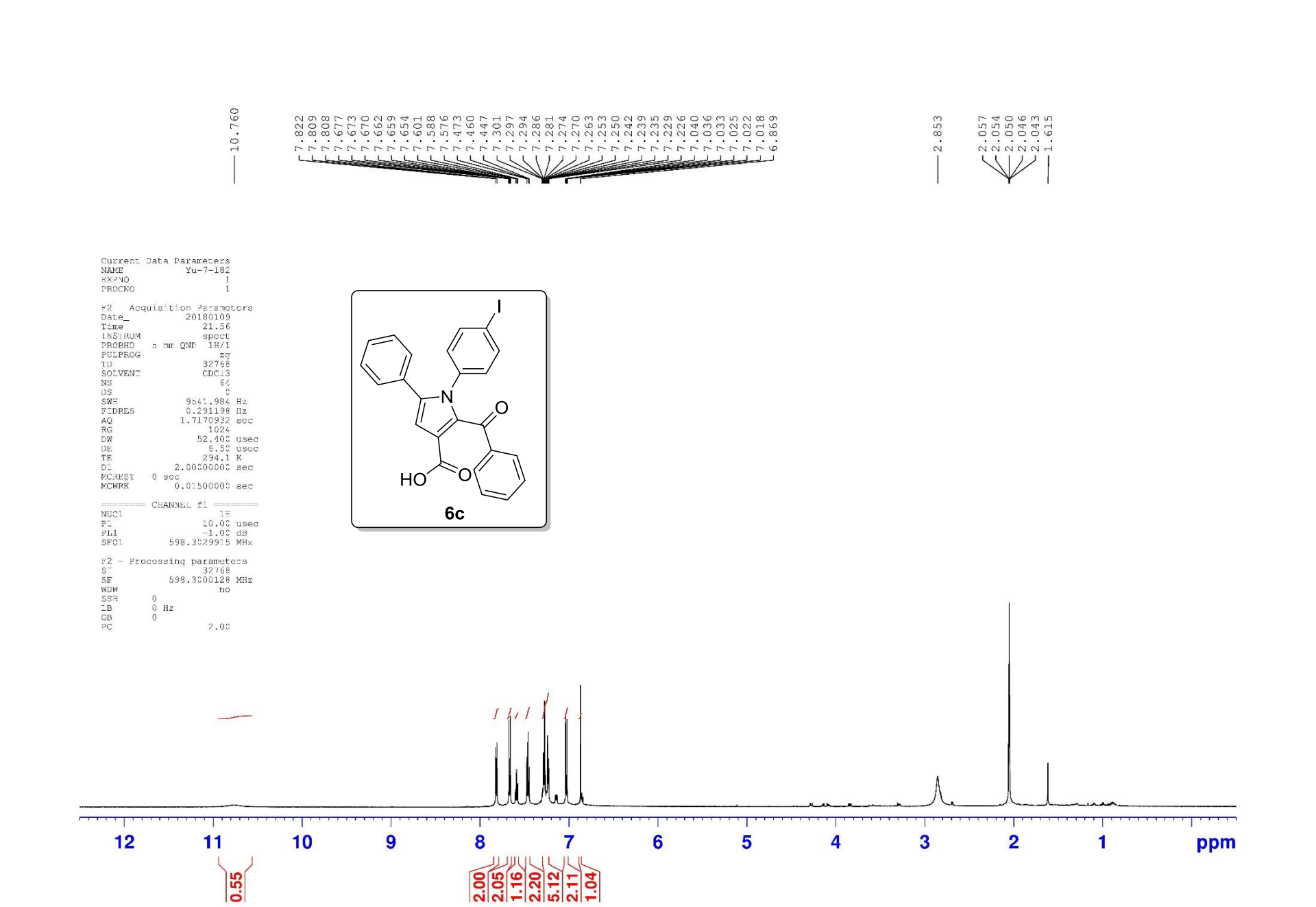


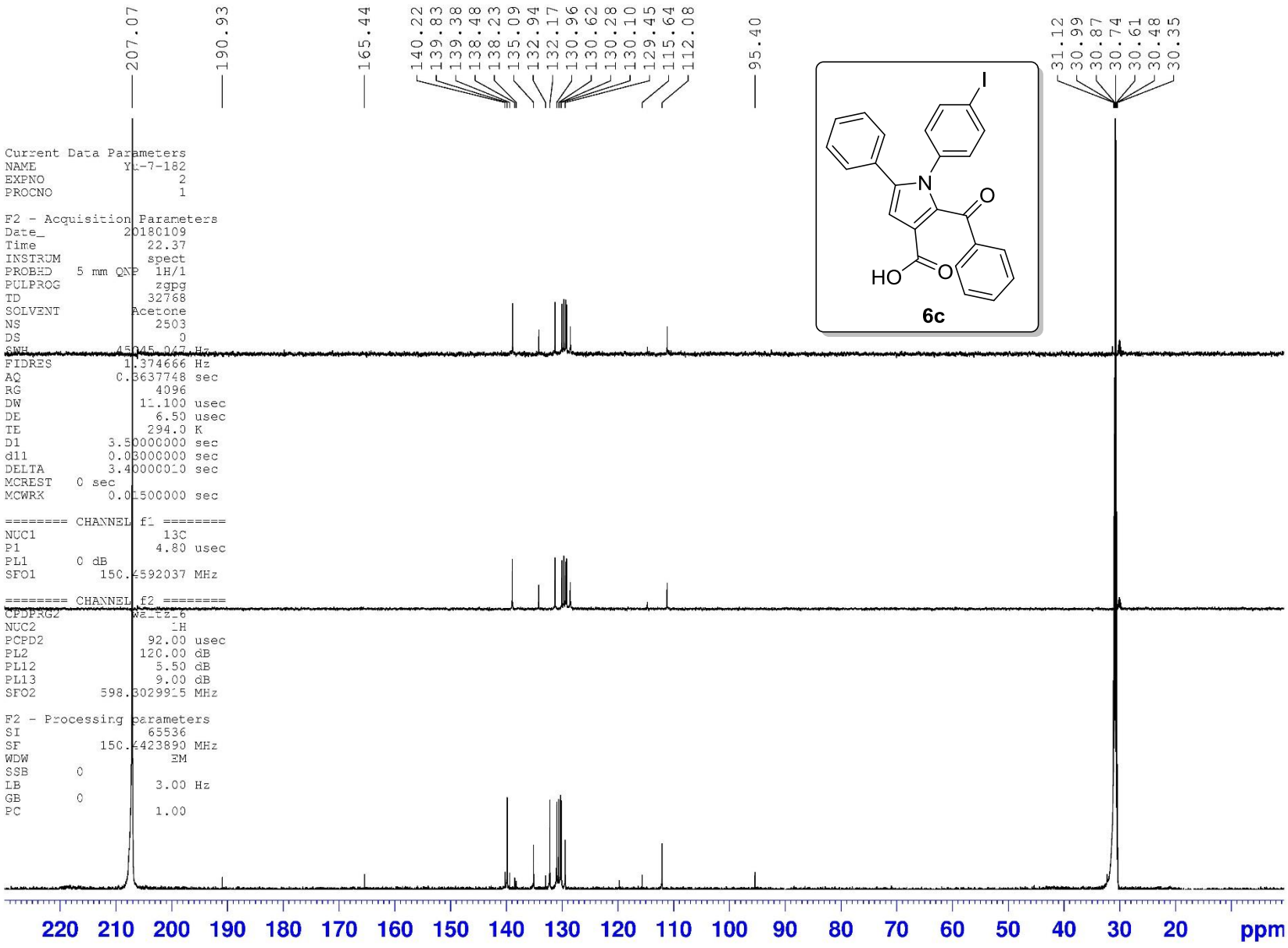

```
Current Data Parameters
NAME                  20171228
EXPNO                        7
PROCNO                       1

F2 - Acquisition Parameters
Date_              20171228
Time                   20.18
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                           5
DS                           0
SWH                6410.256 Hz
FIDRES             0.195625 Hz
AQ                 2.5559540 sec
RG                         322
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
```

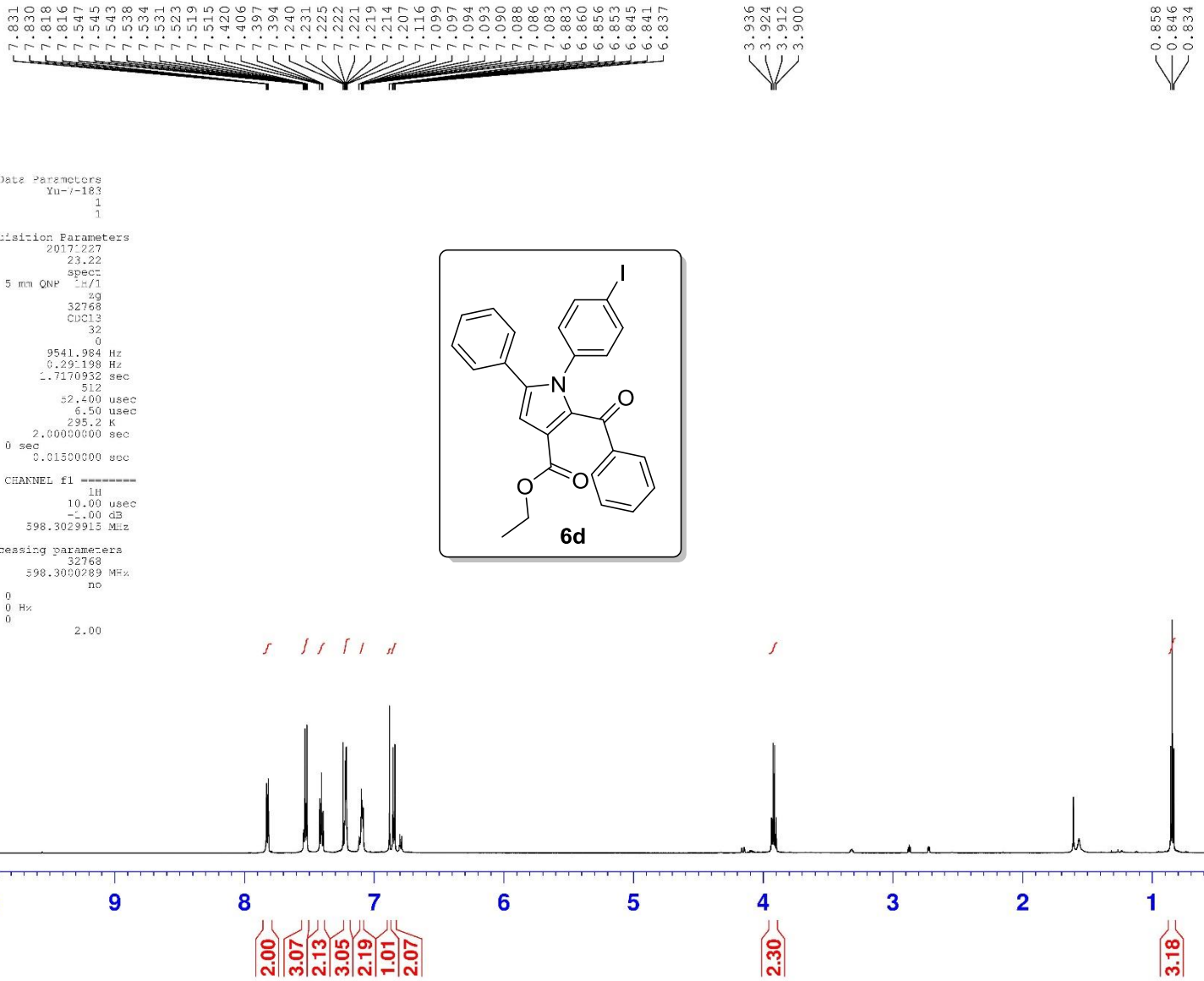


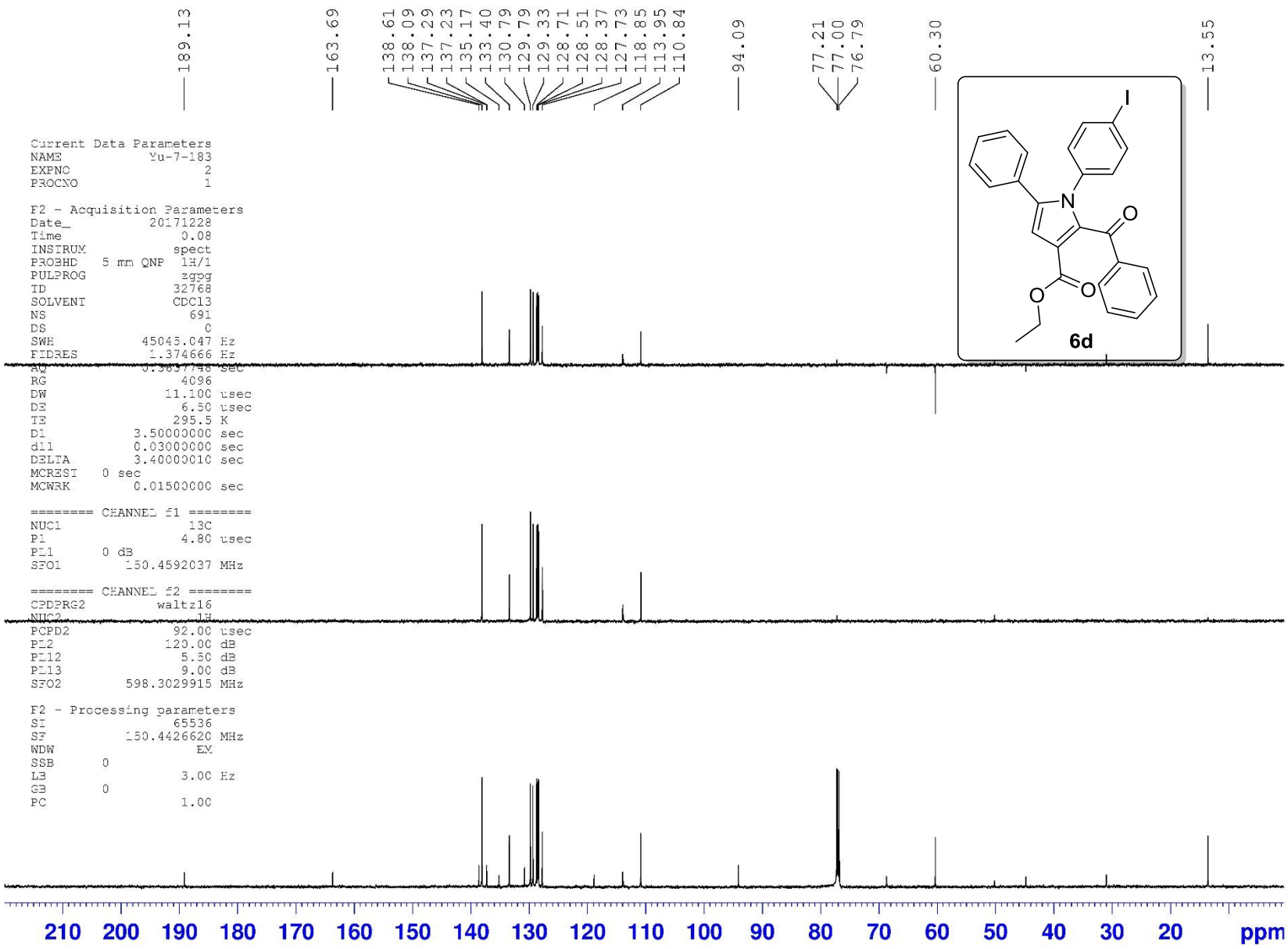



187.04
185.65
139.52
138.99
138.14
137.97
137.43
137.17
133.90
130.28
129.78
129.56
128.92
128.74
128.45
128.27
108.89
94.12
77.32
77.00
76.68
I
N
O
O
6b
Current Data Parameters
NAME 20171228
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171228
Time 20.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 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 100.6178021 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


10.760
7.822
7.809
7.808
7.677
7.673
7.670
7.662
7.659
7.654
7.601
7.588
7.576
7.473
7.460
7.447
7.301
7.297
7.294
7.286
7.281
7.274
7.270
7.263
7.253
7.250
7.242
7.239
7.235
7.229
7.226
7.040
7.036
7.033
7.025
7.022
7.018
6.869
2.853
2.057
2.054
2.050
2.046
2.043
1.615
Current Data Parameters
NAME Yu-7-182
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180109
Time 21.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 1024
DW 52.400 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.3029915 MHz
F2 - Processing parameters
SI 32768
SF 598.3000128 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
I
N
O
HO
O
6c
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.55
2.00
2.05
1.16
2.20
5.12
2.11
1.04


207.07
190.93
165.44
140.22
139.83
139.38
138.48
138.23
135.09
132.94
132.17
130.96
130.62
130.28
130.10
129.45
115.64
112.08
95.40
31.12
30.99
30.87
30.74
30.61
30.48
30.35
I
N
O
HO
O
6c
Current Data Parameters
NAME YL-7-182
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180109
Time 22.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT Acetone
NS 2503
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 294.0 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 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4423890 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.831
7.830
7.818
7.816
7.547
7.545
7.543
7.538
7.534
7.531
7.523
7.519
7.515
7.420
7.406
7.397
7.394
7.240
7.231
7.225
7.222
7.221
7.219
7.214
7.207
7.116
7.099
7.097
7.094
7.093
7.090
7.088
7.086
7.083
6.883
6.860
6.856
6.853
6.845
6.841
6.837
3.936
3.924
3.912
3.900
0.858
0.846
0.834
Current Data Parameters
NAME Yu-Y-183
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20171227
Time 23.22
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 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.3029915 MHz
F2 - Processing parameters
SI 32768
SF 598.3000289 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
I
N
O
O
O
O
6d
10
9
8
7
6
5
4
3
2
1
ppm
2.00
3.07
2.13
3.05
2.19
1.01
2.07
2.30
3.18


189.13
163.69
138.61
138.09
137.29
137.23
135.17
133.40
130.79
129.79
129.33
128.71
128.51
128.37
127.73
118.85
113.95
110.84
94.09
77.21
77.00
76.79
60.30
13.55
I
N
O
O
O
O
6d
Current Data Parameters
NAME Yu-7-183
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171228
Time 0.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 691
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 295.5 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
PL2 120.00 dB
PL12 5.50 dB
PL13 9.00 dB
SFO2 598.3029915 MHz
F2 - Processing parameters
SI 65536
SF 150.4426620 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm