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Supporting Information

Gold-Catalyzed Annulations of *N*-Aryl Ynamides with Benzisoxazoles to Construct 6*H*-Indolo[2,3-b]quinoline Cores

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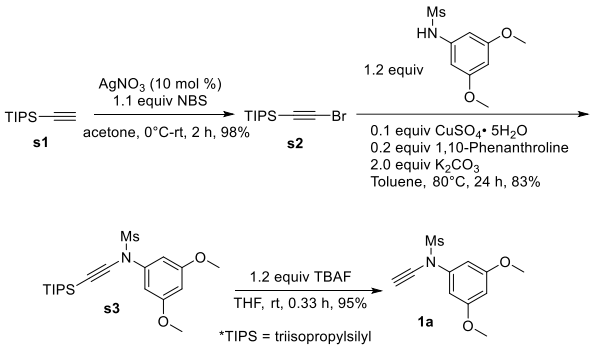
Contents:

(1) General procedure:

Unless otherwise noted, the reactions were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. Tetrahydrofuran (THF) and hexane were dried with sodium, benzophenone and distilled before use. Dichloromethane (DCM), ether and 1,2-dichloroethane (DCE) were dried over CaH_2 and distilled before use. Reagents from commercial sources were used without purifications. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz, 600MHz, Varian 400 MHz, 500MHz and 700 MHz. Spectrometers using chloroform-*d* ($CDCl_3$) and Dimethyl sulfoxide-*d* (DMSO) as the internal standards.

(2) Representative synthetic procedures:

(A) Synthesis of *N*-(3,5-dimethoxyphenyl)-*N*-ethynylmethanesulfonamide (1a)



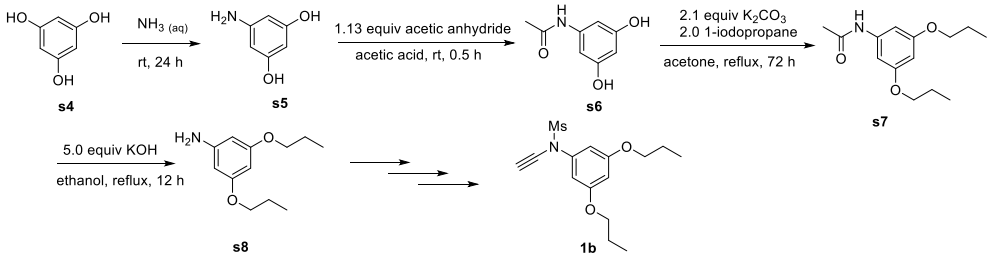
To an acetone solution (50 mL) of triisopropylsilylacetylene (**s1**) (500 mg, 2.74 mmol) was added NBS (536 mg, 3.01 mmol) and $AgNO_3$ (46.5 mg, 0.274 mmol) at 0 °C; the mixture was stirred under N_2 for 2 h at 25 °C before it was quenched with water. The organic layer was extracted with pentane (30 mL×3), washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure to yield 1-(2-bromoethynyl)triisopropylsilane (**s2**) as a colorless oil (637 mg, 2.44 mmol, 89%).

To a dried flask was added *N*-(3,5-dimethoxyphenyl)methanesulfonamide (676 mg, 2.92 mmol), $CuSO_4 \cdot 5H_2O$ (60.8 mg, 0.24 mmol), 1,10-phenanthroline (87.9 mg, 0.488 mmol) and K_2CO_3 (674 mg, 4.87 mmol), and this mixture was subsequently

treated with anhydrous toluene (3 mL) and (bromoethynyl)triisopropylsilane (**s2**) (637 mg, 2.44 mmol). The reaction mixture was caped under a blanket of nitrogen, and heated in an oil bath at 70-80 °C for 24h. After completion, the crude reaction mixture was cooled to room temperature, filtered through a celite bed, and concentrated in vacuo. The residue was purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford 1-silylynamide (**s3**) as brown yellow oil (837 mg, 2.03 mmol, 83%).

To a THF (10 mL) solution of 1-silylynamide (**s3**) (500 mg, 1.21 mmol) was added *N*-tetrabutylammonium fluoride (1.0 M in THF, 1.58 mL, 1.58 mmol) at 0 °C; the resulting mixture was stirred at 25 °C for 0.33 h and evaporated to dryness. The residues were washed with pentane at 0 °C to afford *N*-(3,5-dimethoxyphenyl) -*N*-ethynylmethanesulfonamide (**1a)** as light yellow solid (291 mg, 1.14 mmol, 94%).

(B) Preparation of *N*-(3,5-dipropoxyphenyl)-*N*-ethynylmethanesulfon amide (1b)



To a dried flask with phloroglucinol (4.00 g, 31.7 mmol) was added 30% ammonium hydroxide (40 mL) and stir at 25 °C for 24 h under argon atmosphere. The solution was concentrated under reduced pressure to afford 5-aminobenzene-1,3-diol (**s5**) as black solid (3.94 g, 31.5 mmol, 99%).

To a dried flask was added 5-aminobenzene-1,3-diol (**s5**) (1.00 g, 8.00 mmol) in acetic acid (3.4 mL), and to this mixture was added acetic anhydride (0.85 mL, 9 mmol) dropwise. The resulting mixture was stirred at 25 °C for 0.5 h before it was quenched with 10% NaOH(aq) (7 mL). The solution was extracted with EtOAc (3 × 10 mL); the organic layer was washed with brine, dried over $MgSO_4$, and

concentrated under reduced pressure to afford *N*-(3,5-dipropoxyphenyl)acetamide (**s6**) as brown solid (550 mg, 42%).[s1]

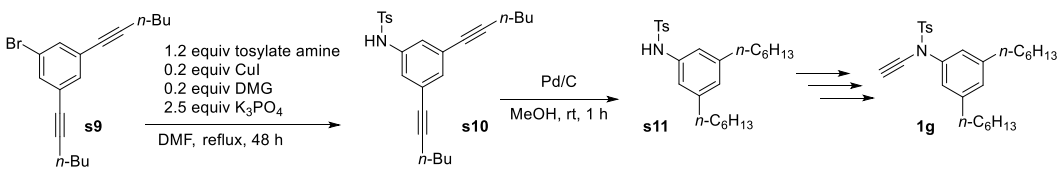
[s1]: Beale, T. M.; Allwood, D. M.; Bender, A.; Bond, P. J.; Brenton, J. D.; Charnock-Jones, D. S.; Ley, S. V.; Myers, R. M.; Shearman, J. W.; Temple, J.; Unger, J.; Watts, C. A.; Xian, J. *ACS Med. Chem. Lett.* **2012**, *3*, 177.

To a dried flask was added *N*-(3,5-dipropoxyphenyl)acetamide (**s6**) (250 mg, 1.5 mmol) and K_2CO_3 (403 mg, 3.1mmol) in acetone (30 mL), and to this mixture was added 1-iodopropane (0.29 mL, 2.99 mmol). The mixture was heated to reflux for 27 h. After cooling, the solution was filtered over a short celite bed, and evaporated to dryness under reduced pressure. The residue was purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford *N*-(3,5-dipropoxyphenyl)acetamide (**s7**) as yellow oil (361 mg, 1.4 mmol, 96%).

To a dried flask was added *N*-(3,5-dipropoxyphenyl)acetamide (**s7**) (100 mg, 0.4 mmol) in ethanol (25mL) and KOH (111 mg, 2.0 mmol), and the mixture was heated under reflux for 12 h. After cooling, the reaction mixture was neutralized with 10% HCl (1 mL), and extracted with EtOAc (3 × 10 mL). The organic layer was dried over $MgSO_4$, and evaporated to dryness to afford 3,5-dipropoxyaniline (**s8**) (80 mg, 0.38 mmol 96%).

3,5-dipropoxyaniline (**s8**) was used to prepare *N*-(3,5-dipropoxyphenyl)-*N*-ethynylmethanesulfonamide (**1b**) according to the procedure to prepare compound **1a**.

(c) Preparation of *N*-(3,5-dihexylphenyl)-*N*-ethynyl-4-methylbenzene sulfonamide (1g)



To a dried flask was added 1-bromo-3,5-di(hex-1-yn-1-yl)benzene[s2] (300 mg,

0.95 mmol), tosylate amine (174 mg, 1.13 mmol), CuI (36.1 mg, 0.19 mmol), DMG (*N*,*N*-dimethylglycine) (20 mg, 0.19 mmol), K_3PO_4 (502 mg, 2.36 mmol) and DMF (*N*,*N*-Dimethylformamide) (25 mL), and the resulting mixture was heated under reflux for 48 h. After cooling, the mixture was filtered over a short celite bed. The solvent was evaporated under reduced pressure, and the residues were purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford *N*-(3,5-di(hex-1-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**s10**) as yellow oil (265 mg, 0.65 mmol, 69%).

[s2]: Deng, W.; Liu, L.; Zhang, C.; Liu, M.; Guo, Q.-X. *Tetrahedron Lett.* **2005**, *46*, 7295

To a dried flask was added a methanol solution (15 mL) of *N*-(3,5-di(hex-1-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**s10**) (265 mg, 0.65 mmol) and 10% Pd/C (1 g), the mixture was purges with N_2 for 5 min. To this flask was fitted with a H_2 balloon, and the mixture was stirred for 1 h. The resulting solution was filtered and concentrated under reduced pressure to afford *N*-(3,5-dihexylphenyl)-4-methylbenzenesulfonamid (**s11**) as yellow oil (266 mg, 0.64 mmol, 98%).

N-(3,5-dihexylphenyl)-4-methylbenzenesulfonamid (**s11**) was used to prepare *N*-(3,5-dihexylphenyl)-*N*-ethynyl-4-methylbenzenesulfonamide (**1g**) according to the preceding procedure..

(D) Preparation of benzisoxazoles (2a-2m)

Benzisoxazoles (**2a-2m**) were prepared according to literature procedure.[s3-s4]

[s3]: Sahani, R. L.; Liu, R.-S. *Angew. Chem. Int. Ed*. **2017**, *56,* 1026.

[s4]: Chauhana, J.; Fletcher, S. *Tetrahedron Lett.* **2012**, *53*, 4951.

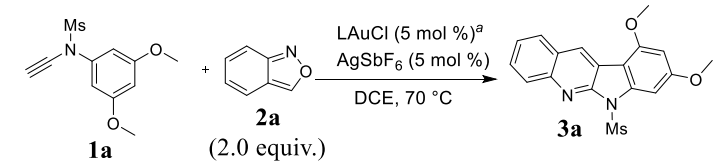
(E) Preparation of 1-(ethynyloxy)-3,5-dimethylbenzene

The preparations of 1-(ethynyloxy)-3,5-dimethylbenzene (**6**) were prepared according

to literature procedure.[s5]

[s5]: Tomita, R.; Al-Maharik, N.; Rodil, A.; Bühl, M.; O'Hagan, D. *Org. Biomol. Chem.* **2018**, *16*, 1113

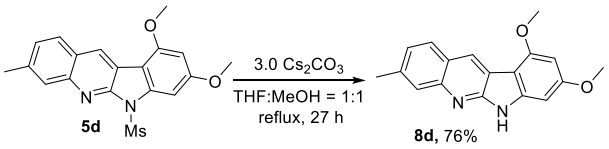
(F) Standard procedures for catalytic operations



1a (0.1 M, 1.0 equiv) [a]L = P(*t*-Bu)$_2$(*o*-biphenyl).

A suspension of chloro[(1,1'-biphenyl-2-yl)di-tert-butylphosphine] gold(I) (11.4 mg, 0.02 mmol) and silver hexafluoroantimonate (6.7g, 0.02) in dry DCE (0.5 mL) was fitted with N_2 balloon, and the mixture was stirred for 5 min. The solution was added a DCE (1.5 mL) solution of *N*-(3,5-dimethoxyphenyl)-*N*-ethynylmethane sulfonamide (**1a**) (100 mg, 0.39 mmol) and benzisoxazole (**2a**) (93 mg, 0.78 mmol) at room temperature. The resulting solution was placed in an oil bath at 70 °C, and the mixture was stirred for 0.25 h. The solution was filtered over a short celite bed, and evaporated under reduced pressure. The residues were purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford the desired 8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-b]quinoline (**3a**) as white solid (61 mg, 0.17 mmol, 88%).

(G) Deprotection of Indoloquinoline

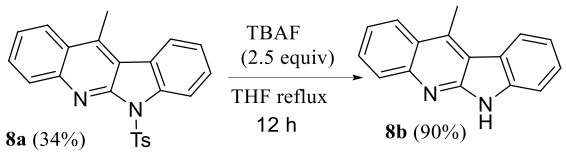


A THF/MeOH (1:1) mixture of 8,10-dimethoxy-3-methyl-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*] quinolone (**5d**) (50 mg, 0.14 mmol) was heated under reflux for 27 h. The resulting mixture was extracted with CH_2Cl_2 (20 mL) and H_2O (10 mL). The organic layer was washed with brine and dried over $MgSO_4$, and concentrated under

reduced pressure. The residues were purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford 8,10-dimethoxy-3-methyl-6*H*-indolo[2,3-*b*]quinoline (**8d**) as light yellow solid (30mg, 0.1mmol, 76%).[s6]

[s6]: Monguchi, Y.; Okami, H.; Ichikawa, T.; Nozaki, K.; Maejima, T.; Oumi, Y.; Sawama, Y.; Sajikia, H. *Adv. Synth. Catal.* **2016**, *358*, 3145

(H) Detosylation



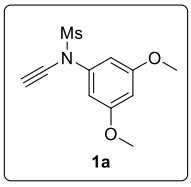
8a (34%) **8b** (90%)

11-methyl-6-tosyl-6*H*-indolo[2,3-*b*]quinoline

A dry THF solution (25 mL) of 11-methyl-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (**8a**) (200 mg, 0.52 mmol) was refluxed for 10 min, and to this mixture was added slowly a THF solution (1.3 mL, 1 M, 1.3 mmol) of TBAF under N_2. The resulting mixture was stirred under reflux for 6 h. The resulting mixture was extracted with CH_2Cl_2 (30 mL) and H_2O (20 mL). The organic layer was washed with brine and dried over $MgSO_4$, and concentrated under reduced pressure. The residues were purified by column chromatography (SiO_2, eluent: EtOAc/hexane) to afford 11-methyl-6*H*-indolo[2,3-*b*]quinoline (**8b**) as light yellow solid (108 mg, 0.45 mmol, 90%).

(3) Spectral data for compounds:

Spectral data for *N*-(3,5-dimethoxyphenyl)-*N*-ethynylmethanesulfonamide (1a)

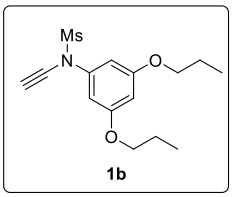


1a

Light yellow solid; mp 96.1 - 96.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.65 (d, J = 2.0 Hz, 2H), 6.42 (t, J = 2.0 Hz, 1H), 3.78 (s, 6H), 3.1 (s, 3H), 2.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 139.5, 103.7, 100.3, 75.4, 60.0, 55.6, 36.7; HRMS (ESI,

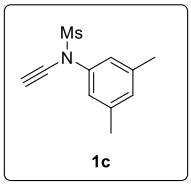
m/z) calcd for $C_{11}H_{14}NO_4S$ $[M+H]^+$: 256.06435, found: 256.06287.

Spectral data for *N*-(3,5-dipropoxyphenyl)-*N*-ethynylmethanesulfonamide (1b)



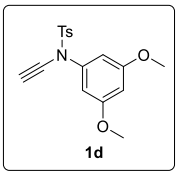
Light yellow solid; mp 43.9 - 44.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.63 (d, J = 2.0 Hz, 2H), 6.42 (t, J = 2.0 Hz, 1H), 3.88 (t, J = 6.6 Hz, 4H), 3.1 (s, 3H), 2.93 (s, 1H), 1.82~1.73 (m, 4H), 1.01 (t, J = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ160.6, 139.4, 104.2, 101.3, 69.9, 59.9, 36.7, 22.4, 10.5; HRMS (ESI, m/z) calcd for $C_{15}H_{21}NNaO_4S$ $[M+Na]^+$: 334.10890, found: 334.10918.

Spectral data for *N*-(3,5-dimethylphenyl)-*N*-ethynylmethanesulfonamide (1c)



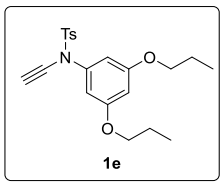
Light yellow solid; mp 79.8 - 80.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.09 (s, 2H), 6.98 (s, 1H), 3.1 (s, 3H), 2.92 (s, 1H), 2.32 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 137.6, 130.3, 123.3, 75.9, 59.3, 35.7, 21.1; HRMS (ESI, m/z) calcd for $C_{11}H_{13}NNaO_2S$ $[M+Na]^+$: 246.05647, found: 246.05725.

Spectral data for *N*-(3,5-dimethoxyphenyl)-*N*-ethynyl-4-methylbenzene sulfonamide (1d)



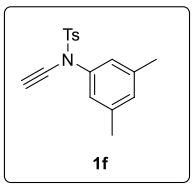
Light yellow solid; mp 97.4 – 97.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 8.4 Hz, 2H), 6.40~6.37 (m, 2H), 6.38 (d, J = 2.0 Hz, 1H), 3.7 (s, 6H), 2.83 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.7, 145.1, 139.8, 133.0, 129.5, 128.2, 104.4, 100.6, 59.2, 55.5, 21.7; HRMS (ESI, m/z) calcd for $C_{17}H_{18}NO_4S$ $[M+H]^+$: 332.09565, found: 332.09460.

Spectral data for *N*-(3,5-dipropoxyphenyl)-*N*-ethynyl-4-methylbenzene sulfonamide (1e)



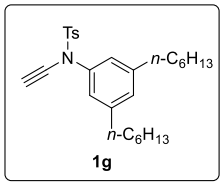
Light yellow solid; mp 79.8 - 80.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.37 (s, 3H), 3.79 (t, *J* = 6.4 Hz, 4H), 2.82 (s, 1H), 2.41 (s, 3H), 1.77~1.68 (m, 4H), 0.97 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.2, 145.0, 139.6, 133.0, 129.5, 128.3, 104.8, 101.6, 76.4, 69.7, 59.1, 22.3, 21.6, 10.4; HRMS (ESI, m/z) calcd for $C_{21}H_{26}NO_4S$ $[M+H]^+$: 388.15825, found: 388.15789.

Spectral data for *N*-(3,5-dimethylphenyl)-*N*-ethynyl-4-methylbenzenesulfon amide (1f)



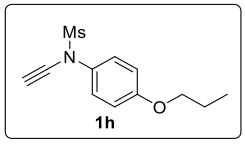
Light yellow solid; mp 98.3 – 98.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.92 (s, 1H), 6.83 (s, 2H), 2.79 (s, 1H), 2.43 (s, 3H), 2.24 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.9, 138.9, 138.0, 133.1, 130.1, 129.4, 128.3, 123.9, 58.6, 21.6, 21.1; HRMS (ESI, m/z) calcd for $C_{17}H_{17}NNaO_2S$ $[M+Na]^+$: 322.08777,found: 322.08688.

Spectral data for *N*-(3,5-dihexylphenyl)-*N*-ethynyl-4-methylbenzenesulfonamide (1g)



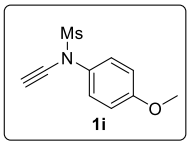
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ7.55 (d, *J* = 6.8 Hz, 2H), 7.25 (d, *J* = 6.8 Hz, 2H), 6.9 (s, 1H), 6.81 (s, 1H), 6.80 (s, 1H), 2.79 (s, 1H), 2.49 (t, *J* = 7.6 Hz, 4H), 2.42 (s, 3H), 1.50~1.44 (m, 4H), 1.28~1.25 (m, 12H), 0.87 (t, *J* = 4.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.8, 143.9, 137.9, 133.0, 129.4, 129.2, 128.9, 128.3, 123.6, 58.5, 35.6, 31.6, 31.2, 28.8, 22.5, 21.6, 14.1; HRMS (ESI, m/z) calcd for $C_{27}H_{37}NNaO_2S$ $[M+Na]^+$: 462.24427,found: 462.24449.

Spectral data for *N*-ethynyl-*N*-(4-propoxyphenyl)methanesulfonamide (1h)



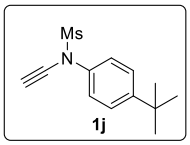
Light yellow solid; mp 51.2 – 51.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39~7.35 (m, 2H), 6.91~6.88 (m, 2H), 3.90 (t, *J* = 6.4 Hz, 2H), 3.08 (s, 3H), 2.89 (s, 1H), 1.83~1.74 (m, 2H), 1.01 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.9, 132.8, 130.5, 129.5, 128.7, 128.3, 127.9, 69.7, 58.2, 22.4, 21.7, 10.4; HRMS (ESI, m/z) calcd for $C_{12}H_{15}NNaO_3S$ $[M+Na]^+$: 276.06703, found: 276.06586.

Spectral data for *N*-ethynyl-*N*-(4-methoxyphenyl)methanesulfonamide (1i)



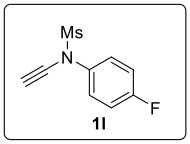
Light yellow solid; mp 98.1 – 98.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 3.08 (s, 3H), 2.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 130.5, 127.4, 114.6, 76.1, 58.9, 55.5, 36.3; HRMS (ESI, m/z) calcd for $C_{10}H_{11}NNaO_3S$ $[M+Na]^+$: 250.03249, found: 250.03031.

Spectral data for *N*-(4-(tert-butyl)phenyl)-*N*-ethynylmethanesulfonamide (1j)



Light yellow solid; mp 100.8 – 101.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (s, 4H), 3.1 (s, 3H), 2.91 (s, 1H), 1.3 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.9, 135.2, 126.5, 125.3, 76.0, 59.3, 36.6, 34.7, 31.2; HRMS (ESI, m/z): calcd for $C_{13}H_{17}NNaO_2S$ $[M+Na]^+$: 274.08777, found: 274.08737.

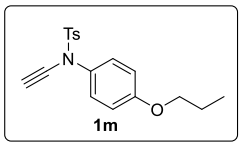
Spectral data for *N*-ethynyl-*N*-(4-fluorophenyl)methanesulfonamide (1l)



Light yellow solid; mp 94.3 – 95.7 °C;^{1}H NMR (600 MHz, $CDCl_3$): δ7.49~7.46 (m, 2H), 7.10 (t, *J* = 8.4Hz, 2H), 3.1 (s, 3H), 2.94 (s, 1H); ^{13}C NMR (600 MHz, $CDCl_3$): δ127.8, 127.7, 116.6, 116.4, 75.6, 59.8, 36.6 ; HRMS (ESI, m/z): calcd for

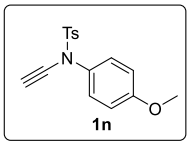
$C_9H_8FNNaO_2S$ [M+Na] $^+$: 236.0157, found: 236.01564

Spectral data for *N*-ethynyl-4-methyl-*N*-(4-propoxyphenyl)benzenesulfonamide (1m)



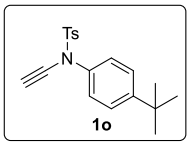
Light yellow solid; mp 91.5 – 91.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 9.2 Hz, 2H), 6.78 (d, *J* = 9.2 Hz, 2H), 3.87 (t, *J* = 6.6 Hz, 2H), 2.77 (s, 1H), 2.42 (s, 3H), 1.82~1.73 (m, 2H), 1.03~0.98 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 144.9, 132.8, 130.5, 129.5, 128.7, 128.3, 127.9, 114.7, 69.7, 58.2, 22.4, 21.7, 10.4; HRMS (ESI, m/z) calcd for $C_{13}H_{19}NNaO_3S$ [M+Na]$^+$: 352.09833, found: 352.09631.

Spectral data for *N*-ethynyl-*N*-(4-methoxyphenyl)-4-methylbenzenesulfonamide (1n)



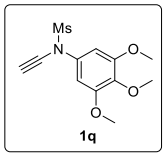
Light yellow solid; mp 113.0 – 113.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 9.2 Hz, 2H), 6.80 (d, *J* = 9.2 Hz, 2H), 3.77 (s, 3H), 2.78 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.0, 132.9, 130.8, 129.5, 128.3, 127.9, 114.3, 58.2, 55.5, 21.7; HRMS (ESI, m/z): calcd for $C_{16}H_{15}NNaO_3S$ [M+Na]$^+$: 324.06703, found: 324.06581.

Spectral data for *N*-(4-(tert-butyl)phenyl)-*N*-ethynyl-4-methylbenzene sulfonamide (1o).



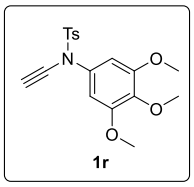
Light yellow solid; mp 95.8 – 96.3 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.31 (dt, *J* = 9.3 Hz & 2.5 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.13 (dt, *J* = 9.3 Hz & 2.5 Hz, 2H), 2.78 (s, 1H), 2.43 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.7, 144.9, 135.5, 133.2, 129.5, 128.3, 126.1, 125.9, 55.5, 34.7, 31.2, 21.7; HRMS (ESI, m/z): calcd for $C_{19}H_{22}NO_2S$ [M+H]$^+$: 328.13712, found: 328.13732.

Spectral data for *N*-ethynyl-*N*-(3,4,5-trimethoxyphenyl)methanesulfonamide (1q)



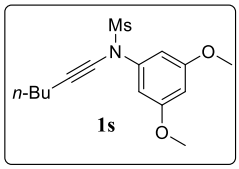
Light yellow solid; mp 155.7 – 156.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.72 (s, 2H), 3.85 (s, 6H), 3.83 (s, 3H), 3.12 (s, 3H), 2.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.5, 138.3, 133.3, 103.4, 75.8, 60.9, 59.8, 56.4, 36.7; HRMS (ESI, m/z) calcd for $C_{12}H_{15}NNaO_5S$ $[M+H]^+$: 310.051106, found :310.05427.

Spectral data for *N*-ethynyl-4-methyl-*N*-(3,4,5-trimethoxyphenyl)benzene sulfonamide (1r)



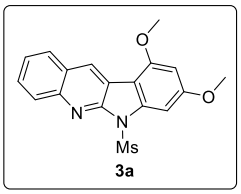
Light yellow solid; mp 122.8 – 123.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 6.4 (s, 2H), 3.8 (s, 3H), 3.71 (s, 6H), 2.83 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 145.1, 138.1, 133.6, 132.8, 129.5, 128.4, 104.1, 60.9, 58.9, 56.2, 21.7; HRMS (ESI, m/z) calcd for $C_{18}H_{19}NNaO_5S$ $[M+Na]^+$: 384.08816, found : 384.08767.

Spectral data for *N*-(3,5-dimethoxyphenyl)-*N*-(hex-1-yn-1-yl) methanesulfonamide (1s)



Light yellow solid; mp 116.3 - 117.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ6.47 (d, *J* = 2.4Hz, 2H), 6.36 (t, *J* = 1.7Hz, 1H), 3.74 (s, 6H), 3.01 (s, 3H), 2.30 (t, *J* = 7.0Hz, 2H), 1.51~1.45 (m, 2H), 1.41~1.35 (m, 2H), 0.87 (t, *J* = 7.3Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ160.8, 140.5, 103.4, 99.7, 72.7, 71.2, 55.4, 35.9, 30.7, 21.8, 18.0, 13.4; HRMS (ESI, m/z) calcd for $C_{15}H_{22}NO_4S$ $[M]^+$: 312.1270, found: 312.1271

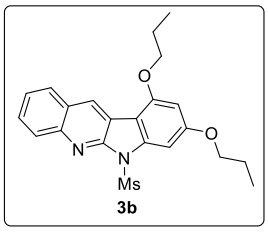
Spectral data for 8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3a)



3a

White solid; mp 170.0 – 170.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.52~7.47 (m, 2H), 6.44 (s, 1H), 4.04 (s, 3H), 3.9 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0, 156.9, 150.9, 144.6, 141.1, 128.6, 128.5, 128.3, 127.9, 126.1, 125.0, 118.3, 104.9, 94.7, 91.6, 55.8, 55.7, 42.1; HRMS (ESI, m/z) calcd for $C_{18}H_{17}N_2O_4S$ $[M+H]^+$: 357.0904, found: 357.0908

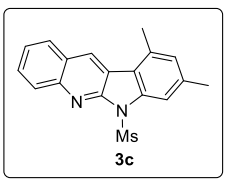
Spectral data for 6-(methylsulfonyl)-8,10-dipropoxy-6*H*-indolo[2,3-*b*]quinoline (3b)



3b

White solid; mp 170.0 – 170.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.49~7.42 (m, 2H), 6.4 (s, 1H), 4.10 (t, *J* = 6.4 Hz, 2H), 3.99 (t, *J* = 6.4 Hz, 2H), 3.7 (s, 3H), 1.99 (q, *J* = 6.9 Hz, 2H), 1.84 (q, *J* = 6.9 Hz, 2H), 1.17 (t, *J* = 7.2 Hz, 3H), 1.07 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 156.3, 150.9, 144.5, 144.1, 128.5, 128.3, 128.0, 127.9, 126.0, 124.9, 118.5, 104.7, 95.4, 92.1, 70.0, 69.8, 42.0, 22.5, 10.6, 10.5; HRMS (ESI, m/z) calcd for $C_{22}H_{25}N_2O_4S$ $[M+H]^+$: 413.15350, found: 413.15314.

Spectral data for 8,10-dimethyl-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3c)

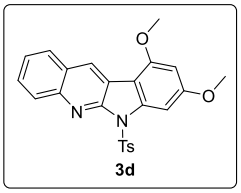


3c

White solid; mp 194.7 – 195.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62 (s, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.74~7.70 (m, 1H),

7.55~7.51 (m, 1H), 7.02 (s, 1H), 3.72 (s, 3H), 2.81 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.3, 139.8, 139.5, 134.1, 129.2, 129.2, 128.6, 128.2, 126.7, 125.6, 125.2, 119.9, 118.3, 112.7, 42.2, 22.2, 20.7; HRMS (ESI, m/z) calcd for $C_{18}H_{17}N_2O_2S$ $[M+H]^+$: 325.1005, found: 325.1005.

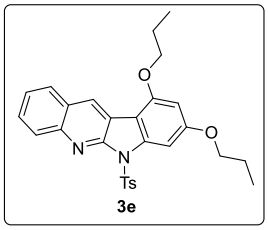
Spectral data for 8,10-dimethoxy-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3d)



3d

White solid; mp 190.8 – 191.5 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 1.8 Hz, 1H), 7.66~7.63 (m, 1H), 7.47~7.44 (m, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.47 (d, *J* = 1.8 Hz, 1H), 4.03 (s, 3H), 3.98 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ162.3, 157.1, 151.0, 145.0, 144.8, 141.6, 136.1, 129.3, 129.0, 128.3, 128.2, 128.0, 127.8, 126.3, 124.9, 118.5, 105.7, 94.9, 92.4, 56.0, 55.7, 21.5; HRMS (ESI, m/z) calcd for $C_{24}H_{21}N_2O_4S$ $[M+H]^+$: 433.1217, found: 433.1226.

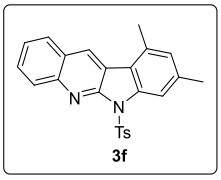
Spectral data for 8,10-dipropoxy-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3e)



3e

White solid; mp 185.7 – 186.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.67~7.63 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.45 (s, 1H), 4.13~4.08 (m, 4H), 2.25 (s, 3H), 2.01~1.96 (m, 2H), 1.92~1.69 (m, 2H), 1.17~1.09 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 156.4, 150.9, 144.8, 144.8, 141.4, 135.7, 129.2, 128.9, 128.2, 128.1, 127.8, 127.7, 126.1, 12.8, 118.7, 105.4, 95.7, 92.6, 70.2, 69.9, 22.6, 21.5, 10.7, 10.6; HRMS (ESI, m/z) calcd for $C_{28}H_{29}N_2O_4S$ $[M+H]^+$: 489.18480, found: 489.18603

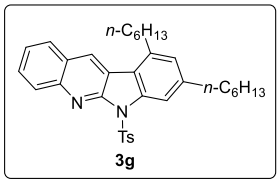
Spectral data for 8,10-dimethyl-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3f)



3f

White solid; mp 254.8 – 255.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.19~8.17 (m, 2H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.70~7.66 (m, 1H), 7.48~7.44 (m, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.98 (s, 1H), 2.73 (s, 3H), 2.52 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.0, 145.3, 144.8, 139.8, 139.3, 135.8, 134.0, 129.2, 128.9, 128.8, 128.7, 128.1, 128.0, 126.8, 125.6, 124.9, 119.8, 118.6, 112.8, 22.3, 21.5, 20.7; HRMS (ESI, m/z) calcd for $C_{24}H_{21}N_2O_2S$ $[M+H]^+$: 401.13237, found: 401.13110.

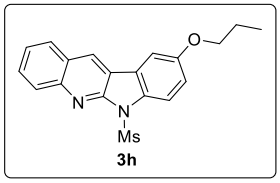
Spectral data for 8,10-dihexyl-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3g)



3g

White solid; mp 129.7 – 130.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.22 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.72~7.69 (m, 1H), 7.51~7.49 (m, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.02 (s, 1H), 3.10 (t, *J* = 7.8 Hz, 2H), 2.79 (t, *J* = 7.8 Hz, 2H), 2.27 (s, 3H), 1.79~1.70 (m, 4H), 1.52~1.48 (m, 2H), 1.41~1.32 (m, 12H), 0.89 (q, *J* = 4.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ151.1, 145.3, 144.8, 144.7, 140.2, 139.1, 135.9, 129.2, 129.0, 128.8, 128.2, 128.1, 125.6, 125.2, 125.0, 119.4, 118.3, 112.3, 36.8, 34.2, 31.9, 31.8, 31.7, 29.4, 29.1, 29.0, 22.7, 22.6, 21.6, 14.1, 14.0; HRMS (ESI, m/z) calcd for $C_{34}H_{41}N_2O_2S$ $[M+H]^+$: 541.28887, found: 541.288876.

Spectral data for 6-(methylsulfonyl)-9-propoxy-6*H*-indolo[2,3-*b*]quinoline (3h)

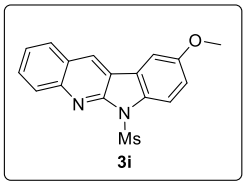


3h

White solid; mp 192.7 – 193.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.12 (t, *J* = 8.0 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.71~7.67 (m, 1H), 7.51~7.45 (m, 2H), 7.05 (d, *J* = 8.0 Hz, 1H), 4.00 (t, *J* = 6.6 Hz, 2H), 3.67 (s, 3H), 1.84 (q, *J* = 7.1 Hz, 2H), 1.08 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ156.0, 151.4, 146.2, 133.3, 129.5, 128.7, 128.1, 127.6, 125.3, 125.2, 123.1, 119.2, 117.0, 115.7, 105.5,

70.1, 41.9, 22.6, 10.5; HRMS (ESI, m/z) calcd for $C_{19}H_{19}N_2O_3S$ $[M+H]^+$: 355.1116, found: 355.11095.

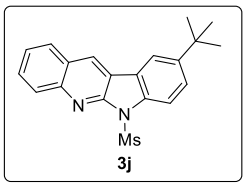
Spectral data for 9-methoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3i)



3i

White solid; mp 189.4 – 189.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.16~8.12 (m, 2H), 7.93~7.91 (m, 1H), 7.73~7.69 (m, 1H), 7.52~7.48 (m, 1H), 7.47 (d, *J* = 2.7 Hz, 1H), 7.05 (dd, *J* = 9.2 Hz & 2.7 Hz, 1H), 3.9 (s, 3H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.5, 151.4, 146.2, 133.4, 129.5, 128.7, 128.2, 127.7, 125.3, 125.2, 123.1, 119.1, 116.4, 115.8, 104.8, 55.8, 42.0; HRMS (ESI, m/z) calcd for $C_{17}H_{15}N_2O_3S$ $[M+H]^+$: 327.0802, found: 327.0798.

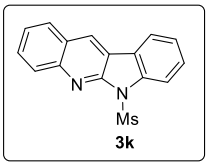
Spectral data for 9-(tert-butyl)-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3j)



3j

White solid; mp 167.6 – 168.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (s, 1H), 8.20 (t, *J* = 9.0 Hz, 2H), 8.07 (d, *J* = 2.0 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.75~7.71 (m, 1H), 7.60 (dd, *J* = 9.0 & 2.0 Hz, 1H), 7.56~7.52 (m, 1H), 3.69 (s, 3H), 1.44 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.5, 147.1, 146.2, 137.3, 129.4, 128.8, 128.1, 127.5, 126.9, 125.5, 125.3, 122.0, 119.5, 117.5, 114.5, 42.1, 34.8, 31.6; HRMS (ESI, m/z) calcd for $C_{20}H_{21}N_2O_2S$ $[M+H]^+$: 353.13237, found: 353.13259.

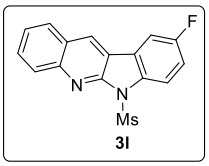
Spectral data for 6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3k)



3k

White solid; mp 167.6 – 168.4 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.57 (s, 1H), 8.30 (d, *J* = 8.3 Hz, 1H), 8.20~8.19 (m, 1H), 8.06~8.05 (m, 1H), 7.99~7.97 (m, 1H), 7.76~7.73 (m, 1H), 7.55~7.52 (m, 2H), 7.42~7.39 (m, 1H), 3.74 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.2, 146.3, 139.4, 129.6, 129.2, 128.8, 128.2, 127.7, 125.5, 125.4, 123.8, 122.3, 121.1, 119.1, 114.9, 42.3; HRMS (ESI, m/z) calcd for $C_{16}H_{13}N_2O_2S$ $[M+H]^+$: 297.06977, found: 297.06950.

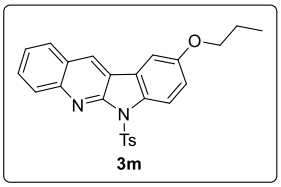
Spectral data for 9-fluoro-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3l)



3l

^{1}H NMR (600 MHz, $CDCl_3$): δ8.67 (s, 1H), 8.28 (dd, *J* = 9.2Hz & 4.4Hz, 1H), 8.21 (d, *J* = 8.2Hz, 1H), 8.01 (d, *J* = 8.2Hz, 1H), 7.79~7.77 (m, 1H), 7.74 (dd, *J* = 7.9Hz & 2.7Hz, 1H), 7.59~7.57 (m, 1H), 7.28~7.25 (m, 1H), 3.75 (s, 3H); ^{13}C NMR (160.426 MHz, $CDCl_3$): δ158.8, 151.5, 146.7, 135.5, 130.1, 128.9, 128.4, 128.3, 125.6, 116.5, 116.3, 116.3, 107.6, 107.5, 42.3; HRMS (ESI, m/z) calcd for $C_{16}H_{11}FN_2O_2S$ $[M+H]^+$: 315.0525, found: 315.05274.

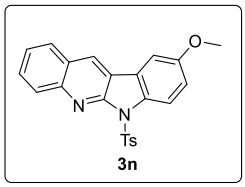
Spectral data for 9-propoxy-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3m)



3m

White solid; mp 173.2 – 174.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (s, 1H), 8.35 (d, *J* = 9.2 Hz, 1H), 8.22 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 7.1 Hz, 1H), 7.49 (t, *J* = 7.1 Hz, 1H), 7.45 (d, *J* = 2.6 Hz, 1H), 7.15~7.11 (m, 3H), 4.01 (t, *J* = 6.6 Hz, 2H), 2.24 (s, 3H), 1.89~1.83 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.2, 151.4, 146.4, 144.8, 135.6, 133.5, 129.3, 129.1, 128.0, 127.9, 127.2, 125.4, 125.1, 123.7, 119.4, 117.0, 116.1, 105.5, 70.2, 29.7, 22.6, 21.5, 10.6; HRMS (ESI, m/z) calcd for $C_{25}H_{23}N_2O_3S$ $[M+H]^+$: 431.14294, found: 431.14308.

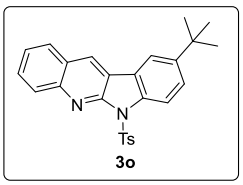
Spectral data for 9-methoxy-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3n)



3n

White solid; mp 205.4 – 206.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.35 (d, *J* = 8.4 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.72~7.68 (m, 1H), 7.49~7.45 (m, 1H), 7.43 (d, *J* = 2.0 Hz, 1H), 7.14~7.11 (m, 3H), 3.9 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.6, 151.3, 146.4, 144.8, 135.5, 133.5, 129.3, 129.0, 128.0, 127.9, 127.3, 125.4, 125.1, 123.7, 119.3, 116.5, 116.1, 104.7, 55.8, 21.5; HRMS (ESI, m/z) calcd for $C_{23}H_{19}N_2O_3S$ $[M+H]^+$: 403.11164 , found: 403.11104.

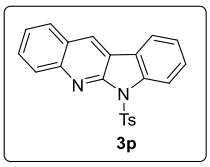
Spectral data for 9-(tert-butyl)-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3o)



3o

White solid; mp 220.9 – 221.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.39 (d, *J* = 8.8 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 2H), 8.01 (s, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.25 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.2, 147.0, 146.2, 144.8, 137.4, 135.7, 129.3, 129.1, 129.0, 128.0, 127.0, 126.8, 125.5, 125.1, 122.4, 119.5, 117.5, 1114.6, 34.7, 31.6, 21.5; HRMS (ESI, m/z) calcd for $C_{26}H_{25}N_2O_2S$ $[M+H]^+$: 429.16367 , found: 429.16289.

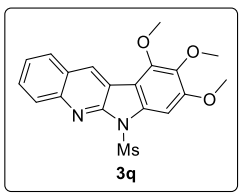
Spectral data for 6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3p)



3p

White solid; mp 172.2 – 172.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.49 (d, *J* = 8.5 Hz, 1H), 8.21 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.73~7.70 (m, 1H), 7.58~7.55 (m, 1H), 7.51~7.48 (m, 1H), 7.40~7.37 (m, 1H), 7.16 (d, *J* = 8.6Hz, 2H), 2.63 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.1, 146.6, 144.9, 139.7, 136.1, 129.3, 129.1, 129.1, 128.2, 128.0, 127.2, 125.6, 125.2, 123.8, 122.8, 121.0, 119.2, 115.2, 21.5; HRMS (ESI, m/z) calcd for $C_{22}H_{17}N_2O_2S$ $[M+H]^+$: 373.10107 , found: 373.10025.

Spectral data for 8,9,10-trimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (3q)

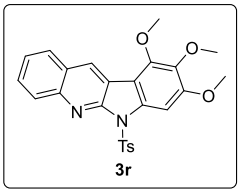


3q

White solid; mp 185.3 – 185.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.71 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.68~7.66 (m, 2H), 7.49 (t, *J* = 8.4 Hz, 1H), 4.22 (s, 3H), 3.98 (s, 3H), 3.92 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 155.4, 151.0, 149.3, 145.1, 138.3, 135.9, 128.8, 128.6, 128.5, 128.0, 126.0,

125.1, 118.4, 108.7, 94.6, 61.3, 60.7, 56.5, 42.2; HRMS (ESI, m/z) calcd for $C_{19}H_{19}N_2O_5S$ $[M+H]^+$: 387.10147 , found: 387.10061.

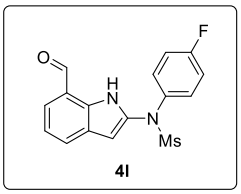
Spectral data for 8,9,10-trimethoxy-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (3r)



3r

White solid; mp 204.0 – 204.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.86 (s, 1H), 7.69~7.65 (m, 1H), 7.49~7.45 (m, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 4.18 (s, 3H), 4.06 (s, 3H), 3.93 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.3, 150.7, 149.5, 145.1, 144.9, 138.2, 135.9, 135.5, 129.3, 128.9, 128.6, 128.2, 128.1, 127.9, 125.9, 125.0, 118.3, 109.0, 94.5, 61.3, 60.8, 56.5, 21.5; HRMS (ESI, m/z) calcd for $C_{25}H_{23}N_2O_5S$ $[M+H]^+$: 463.13277, found: 463.13198.

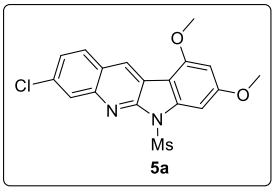
Spectral data for
***N*-(4-fluorophenyl)-*N*-(7-formyl-1*H*-indol-2-yl)methanesulfonamide (4l)**



4l

^{1}H NMR (600 MHz, $CDCl_3$): δ10.36 (s, 1H), 10.07 (s, 1H), 7.77 (d, *J* = 7.9Hz, 1H), 7.62 (dd, *J* = 7.4Hz & 1.0Hz, 1H), 7.49~7.46 (m, 2H), 7.24 (t, *J* = 7.6Hz, 1H), 7.13 (t, *J* = 7.6Hz, 2H), 6.23 (d, *J* = 2.4Hz, 1H), 3.18 (s, 3H); ^{13}C NMR (193.086 MHz, $CDCl_3$): δ136.6, 135.0, 131.4, 130.2, 130.2, 128.7, 128.2, 127.3, 120.2, 116.9, 116.8, 95.4, 39.0; HRMS (ESI, m/z) calcd for $C_{16}H_{13}FN_2O_3S$ $[M+H]^+$: 333.0631, found: 333.06297.

Spectral data for
3-chloro-8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5a)

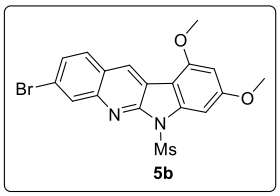


5a

White solid; mp 248 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.67 (s, 1H), 8.16 (s, 1H),

7.87 (d, *J* = 7.8 Hz, 1H), 7.47-7.49 (m, 2H), 6.47 (s, 1H), 4.06 (s, 3H), 3.92 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.4, 157.0, 151.6, 145.0, 141.4, 134.3, 129.0, 128.1, 127.7, 126.1, 124.5, 118.7, 104.7, 95.0, 91.7, 56.0, 55.8, 42.3; HRMS (ESI, m/z) calcd for $C_{18}H_{16}ClN_2O_4S$ $[M+H]^+$: 391.0519,found : 391.0512.

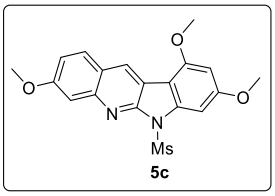
Spectral data for
3-bromo-8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5b)



5b

White solid; mp 252 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.66 (s, 1H), 8.34 (s, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.59 (d, *J* = 8.6 Hz, 1H), 7.48 (s, 1H), 6.47 (s, 1H), 4.06 (s, 3H), 3.92 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.4, 157.1, 151.4, 145.2, 141.4, 131.0, 129.1, 128.6, 128.2, 124.7, 122.5, 118.8, 104.7, 95.0, 91.7, 56.0, 55.8, 42.3; HRMS (ESI, m/z) calcd for $C_{18}H_{17}BrN_2O_4S$ $[M+H]^+$: 435.0014,found : 435.0000.

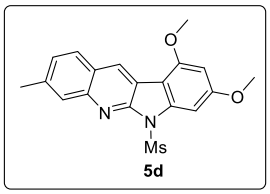
Spectral data for 3,8,10-trimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5c)



5c

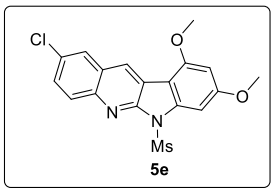
Light yellow solid; mp 223 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.47 (s, 2H), 7.15-7.17 (m, 1H), 6.46 (s, 1H), 4.04 (s, 3H), 3.96 (s, 3H), 3.91 (s, 3H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.6, 160.3, 156.5, 151.3, 146.6, 140.6, 128.9, 128.4, 121.3, 118.2, 116.4, 107.2, 105.3, 94.8, 91.6, 55.9, 55.7, 55.6, 42.0; HRMS (ESI, m/z) calcd for $C_{19}H_{19}N_2O_5S$ $[M+H]^+$: 387.1015, found: 387.1009.

Spectral data for
8,10-dimethoxy-3-methyl-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5d)



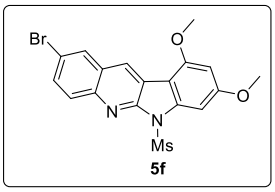
Light yellow solid; mp 223 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.65 (s, 1H), 7.94 (s, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 2.0 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 6.46 (d, *J* = 2.0 Hz, 1H), 4.05 (s, 3H), 3.91 (s, 3H), 3.71 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.9, 156.8, 151.1, 145.0, 141.0, 138.9, 128.2, 127.8, 127.6, 127.3, 124.2, 117.7, 105.2, 94.8, 91.7, 55.9, 55.7, 42.1, 21.8; HRMS (ESI, m/z) calcd for $C_{19}H_{19}N_2O_4S$ $[M+H]^+$: 371.1066, found: 371.1057.

Spectral data for 2-chloro-8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo [2,3-*b*]quinoline (5e)



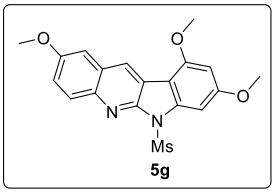
White solid; mp 248.2 – 248.6 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.6 (s, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 2.4 Hz, 1H), 7.60 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.50 (d, *J* = 2.4 Hz, 1H), 6.48 (s, 1H), 4.07 (s, 3H), 3.93 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ162.8, 157.3, 151.3, 143.2, 141.7, 130.8, 130.2, 129.3, 127.2, 126.9, 126.5, 119.4, 104.9, 95.1, 92.1, 56.0, 55.8, 42.4; HRMS (ESI, m/z) calcd for $C_{18}H_{16}ClN_2O_4S$ $[M+H]^+$: 391.05193 , found: 391.05215.

Spectral data for 2-bromo-8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5f)



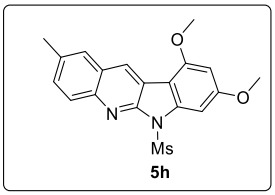
White solid; mp 220.9 – 222.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.61 (s, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.73 (dd, J = 9.0Hz & 2.0 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 6.49 (d, J = 2.0 Hz, 1H), 4.07 (s, 3H), 3.93 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.8, 157.3, 151.3, 143.4, 141.7, 131.8, 130.4, 129.9, 127.5, 127.2, 119.4, 118.7, 104.9, 95.1, 92.1, 56.0, 55.8, 42.4; HRMS (ESI, m/z) calcd for $C_{18}H_{16}BrN_2O_4S$ $[M+H]^+$: 436.99937 , found: 437.00043.

Spectral data for 2,8,10-trimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5g)



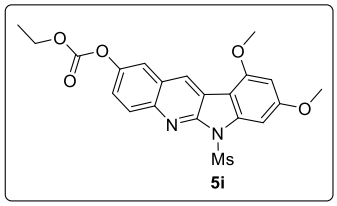
Light blue solid; mp 196 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (s, 1H), 8.00 (d, *J* = 9.2 Hz, 1H), 7.43 (d, *J* = 9.2 Hz, 1H), 7.31 (dd, *J* = 9.2 & 2.0 Hz, 1H), 7.16 (d, *J* = 2.0 Hz, 1H), 6.40 (d, *J* = 2.0 Hz, 1H), 4.01 (s, 3H), 3.91 (s, 3H), 3.88(s, 3H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.8, 156.9, 156.7, 149.6, 141.1, 140.5, 129.8, 127.1, 127.0, 121.0, 118.5, 105.6, 105.5, 94.6, 91.6, 55.8, 55.7, 55.4, 42.0; HRMS (ESI, m/z) calcd for $C_{19}H_{19}N_2O_5S$ $[M+H]^+$: 387.1015, found: 387.1012.

Spectral data for 8,10-dimethoxy-2-methyl-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*] quinoline (5h)



White solid; mp 221 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (s, 1H), 8.01 (d, *J* = 8.6 Hz, 1H), 7.66 (s, 1H), 7.49 (d, *J* = 8.6 Hz, 1H), 7.45 (s, 1H), 6.42 (s, 1H), 4.02 (s, 3H), 3.89 (s, 3H), 3.69 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9, 156.9, 150.5, 143.2, 141.1, 134.7, 130.8, 128.3, 127.7, 126.8, 126.1, 118.3, 105.1, 94.7, 91.6, 55.8, 55.7, 42.1, 21.5; HRMS (ESI, m/z) calcd for $C_{19}H_{19}N_2O_4S$ $[M+H]^+$: 371.1066, found: 371.1070.

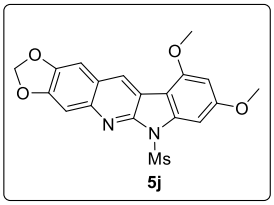
Spectral data for 8,10-dimethoxy-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinolin-2-yl ethyl carbonate (5i)



White solid; mp 233 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62 (s, 1H), 8.13 (d, *J* = 9.2 Hz, 1H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.50 (dd, *J* = 9.2 & 2.0 Hz, 1H), 7.46 (d, *J* = 2.0 Hz,

1H), 6.43 (d, *J* = 2.0 Hz, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.03 (s, 3H), 3.90 (s, 3H), 3.69 (s, 3H), 1.41 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 157.1, 153.6, 151.0, 147.8, 142.5, 141.4, 130.0, 127.9, 126.2, 123.0, 110.0, 118.0, 104.7, 94.8, 91.6, 65.0, 55.9, 55.8, 42.1, 14.2; HRMS (ESI, m/z) calcd for $C_{21}H_{21}N_2O_7S$ $[M+H]^+$: 445.1069,found : 445.1057.

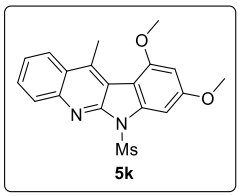
Spectral data for
8,10-dimethoxy-6-(methylsulfonyl)-6*H*-[1,3]dioxolo[4,5-*g*]indolo[2,3-*b*]quinoline (5j)



5j

White solid; mp 267.5 – 267.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54 (s, 1H), 7.47 (d, *J* = 2.0 Hz, 1H), 7.45 (s, 1H), 7.19 (s, 1H), 6.46 (d, *J* = 2.0 Hz, 1H), 6.1 (s, 2H), 4.05 (s, 3H), 3.91 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.8, 156.7, 150.3, 150.0, 147.0, 143.0, 140.8, 127.6, 122.9, 116.7, 105.7, 103.1, 101.7, 95.0, 92.0, 55.9, 55.8, 42.3; HRMS (ESI, m/z) calcd for $C_{19}H_{17}N_2O_6S$ $[M+H]^+$: 401.08073 , found: 401.08047.

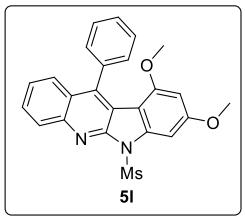
Spectral data for
8,10-dimethoxy-11-methyl-6-(methylsulfonyl)-6*H*-indolo[2,3-*b*]quinoline (5k)



5k

White solid; mp 211.8 – 212.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.22~8.21 (m, 1H), 8.10~8.09 (m, 1H), 7.68~7.65 (m, 2H), 7.53~7.50 (m, 1H), 6.48 (d, *J* = 2.0 Hz, 1H), 4.0 (s, 3H), 3.93 (s, 3H), 3.77 (s, 3H), 3.28 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.8, 155.7, 150.9, 144.5, 141.9, 138.7, 128.9, 128.5, 126.6, 124.8, 124.3, 117.7, 106.3, 95.3, 91.8, 55.8, 55.4, 42.7, 17.8; HRMS (ESI, m/z): calcd for $C_{19}H_{19}N_2O_4S$ $[M+H]^+$: 371.10655 , found: 371.10627.

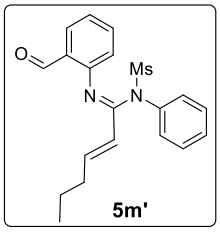
Spectral data for 8,10-dimethoxy-6-(methylsulfonyl)-11-phenyl-6*H*-indolo [2,3-*b*]quinoline (5l)



5l

Yellow solid; mp 232 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.57 (s, 1H), 7.47-7.53 (m, 4H), 7.33-7.37 (m, 3H), 6.18 (s, 1H), 3.88 (s, 3H), 3.83 (s, 3H), 3.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0, 156.2, 150.7, 144.2, 141.8, 141.5, 139.6, 129.8, 128.5, 128.3, 127.2, 126.9, 126.8, 126.3, 124.8, 116.9, 105.1, 94.4, 91.0, 55.7, 55.3, 42.6; HRMS (ESI, m/z) calcd for $C_{24}H_{21}N_2O_4S$ $[M+H]^+$: 433.1222, found: 433.1210.

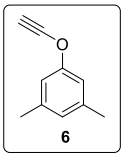
Spectral data for (1Z,2E)-*N′*-(2-formylphenyl)-*N*-(methylsulfonyl)-*N*-phenylhex-2-enimidamide (5m')



5m'

Yellow liquid; ^{1}H NMR (400 MHz, acetone-d_6): δ10.28 (s, 1H), 7.88 (d, *J* = 7.4Hz, 1H), 7.64 (t, *J* = 7.4Hz, 1H), 7.31 (t, *J* = 7.4Hz, 1H), 6.96 (d, *J* = 7.4Hz, 1H), 6.86 (s, 2H), 6.68~6.60 (m, 1H), 6.53 (s, 1H), 5.60 (d, *J* = 14.9Hz, 1H), 3.84 (s, 6H), 3.38 (s, 3H), 1.91 (q, *J* = 6.9Hz, 2H), 1.23~1.14 (m, 2H), 0.60 (t, *J* = 7.3Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ190.9, 160.9, 155.6, 149.4, 148.4, 140.1, 134.7, 130.4, 126.4, 124.3, 121.2, 119.8, 106.6, 100.4, 55.5, 39.8, 34.3, 21.1, 13.0.

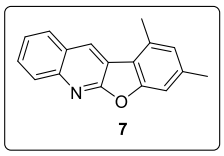
Spectral data for 1-(ethynyloxy)-3,5-dimethylbenzene (6)



6

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.9 (s, 2H), 6.78-6.77 (m, 1H), 2.32 (s, 6H), 2.06 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.4, 139.7, 126.3, 112.5, 84.8, 33.1, 21.3; HRMS (ESI, m/z) calcd. for $C_{10}H_{11}O$ $[M+Na]^+$: 169.0629, found: 169.0524.

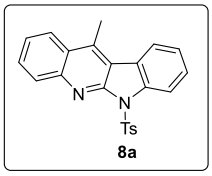
Spectral data for 1,3-dimethylbenzofuro[2,3-*b*]quinoline (7)



7

Light yellow solid; mp 184 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (s, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 1H), 7.63-7.67 (m, 1H), 7.42-7.46 (m, 1H), 7.13 (s, 1H), 6.85 (s, 1H), 2.66 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 155.9, 144.9, 139.8, 134.1, 129.2, 129.0, 128.1, 127.9, 126.0, 125.7, 124.7, 118.2, 118.1, 109.4, 21.9, 19.6; HRMS (ESI, m/z) calcd. for $C_{17}H_{14}NO$ $[M+H]^+$: 248.1075, found: 248.1081.

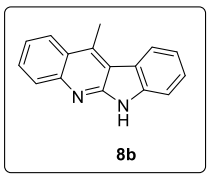
Spectral data for 11-methyl-6-tosyl-6*H*-indolo[2,3-*b*]quinoline (8a)



8a

White solid; mp 191.2 – 191.8 °C; ^{1}H NMR (600 MHz, d_6-DMSO): δ 8.45 (d, *J* = 8.4 Hz, 1H), 8.36 (t, *J* = 8.4 Hz, 2H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 2H), 7.82 (t, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.8 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 2H), 3.1 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (150 MHz, d_6-DMSO): δ 149.8, 145.5, 145.2, 140.5, 138.4, 134.9, 129.7, 128.8, 128.7, 127.6, 125.2, 125.1, 124.6, 124.3, 124.2, 123.2, 116.2, 114.2, 21.0, 14.9; HRMS (ESI, m/z) calcd for $C_{23}H_{19}N_2O_2S$ $[M+H]^+$: 387.11672 , found: 387.11719

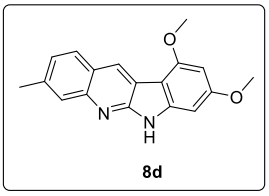
Spectral data for 11-methyl-6*H*-indolo[2,3-*b*]quinoline (8b)



8b

White yellow solid; mp 270.0 – 270.3 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.95 (s, 1H), 8.27 (d, *J* = 8.4 Hz, 2H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.76~7.73 (m, 1H), 7.53~7.50 (m, 3H), 7.32~7.24 (m, 1H), 3.22 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.7, 146.1, 140.8, 139.6, 128.8, 127.5, 127.3, 124.2, 124.2, 123.7, 122.9, 122.1, 120.2, 117.0, 110.8, 15.2; HRMS (ESI, m/z) calcd for $C_{16}H_{13}N_2$ $[M+H]^+$: 233.10787 , found: 233.10769.

Spectral data for 8,10-dimethoxy-3-methyl-6*H*-indolo[2,3-*b*]quinoline (8d)

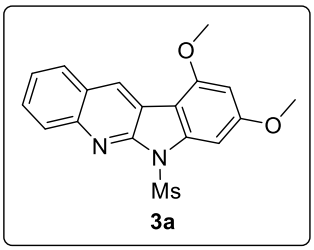


8d

Light yellow solid; mp 315 °C; ^{1}H NMR (600 MHz, d_6-DMSO): δ 11.58 (s, 1H), 8.62 (s, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 7.69 (s, 1H), 7.26 (d, *J* = 8.3 Hz, 1H), 6.58 (d, *J* = 1.7 Hz, 1H), 6.41 (d, *J* = 1.7 Hz, 1H), 4.03 (s, 3H), 3.86 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.5, 156.9, 152.8, 145.1, 143.5, 137.4, 128.0, 126.3, 126.0, 124.9, 122.2, 116.5, 102.7, 91.2, 87.9, 55.7, 55.6, 21.5; HRMS (ESI, m/z) calcd for $C_{18}H_{17}N_2O_2$ $[M+H]^+$: 293.1290, found: 293.1299.

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

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



3a

(CCDC 1840927)

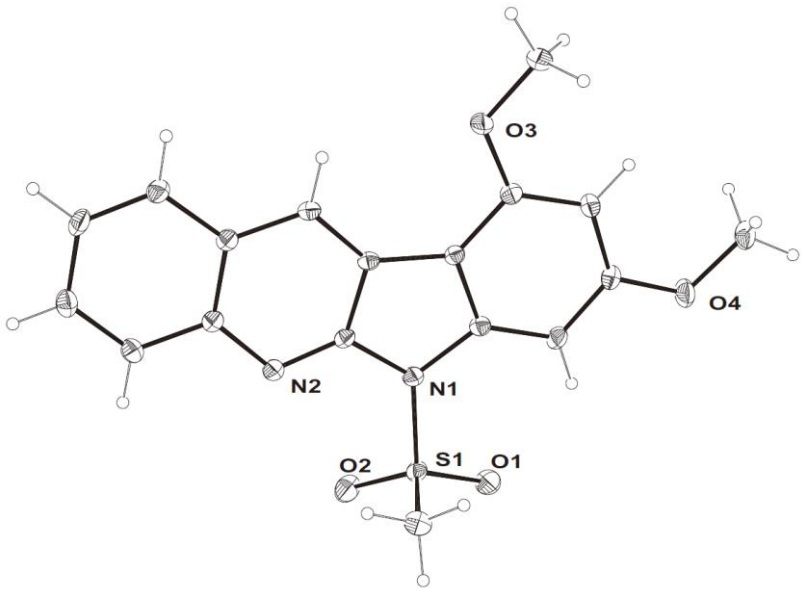


Table 1. Crystal data and structure refinement for d20007.

Identification code	d20007	
Empirical formula	C18 H16 N2 O4 S	
Formula weight	356.39	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 5.1019(5) Å	α= 90°.
	b = 33.051(3) Å	β= 92.525(4)°.
	c = 9.4100(10) Å	γ = 90°.
Volume	1585.2(3) Å ^{3}	
Z	4	
Density (calculated)	1.493 Mg/m^3	
Absorption coefficient	0.232 mm^{-1}	
F(000)	744	
Crystal size	0.72 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.25 to 25.09°.	
Index ranges	-6<=h<=6, -38<=k<=39, -11<=l<=11	
Reflections collected	25241	
Independent reflections	2800 [R(int) = 0.0730]	
Completeness to theta = 25.09°	99.7 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9977 and 0.8509	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2800 / 0 / 229	
Goodness-of-fit on F^2	1.159	
Final R indices [I>2sigma(I)]	R1 = 0.0632, wR2 = 0.1114	
R indices (all data)	R1 = 0.0821, wR2 = 0.1177	
Largest diff. peak and hole	0.213 and -0.340 e.Å $^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for d20007. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2566(8)	3226(1)	5855(4)	52(1)
C(2)	5439(6)	3567(1)	2985(3)	27(1)

C(3)	8195(6)	3124(1)	2017(3)	30(1)
C(4)	10183(6)	2832(1)	2179(4)	36(1)
C(5)	11271(7)	2662(1)	1025(4)	41(1)
C(6)	10408(7)	2776(1)	-347(4)	41(1)
C(7)	8490(7)	3056(1)	-549(4)	38(1)
C(8)	7315(6)	3240(1)	618(3)	30(1)
C(9)	5302(6)	3532(1)	462(3)	29(1)
C(10)	4350(6)	3700(1)	1656(3)	27(1)
C(11)	2360(6)	3996(1)	1949(3)	27(1)
C(12)	639(6)	4220(1)	1068(3)	31(1)
C(13)	-1081(7)	4334(1)	-1298(4)	44(1)
C(14)	-1085(6)	4487(1)	1658(3)	34(1)
C(15)	-1092(6)	4529(1)	3129(3)	35(1)
C(16)	-4522(7)	5022(1)	2967(4)	49(1)
C(17)	587(6)	4312(1)	4039(3)	36(1)
C(18)	2280(6)	4046(1)	3422(3)	30(1)
N(1)	4219(5)	3788(1)	4077(3)	33(1)
N(2)	7225(5)	3292(1)	3221(3)	33(1)
O(1)	3198(5)	3977(1)	6543(2)	52(1)
O(2)	7068(4)	3569(1)	6153(3)	57(1)
O(3)	817(4)	4151(1)	-347(2)	42(1)
O(4)	-2721(5)	4786(1)	3799(3)	52(1)
S(1)	4425(2)	3664(1)	5793(1)	34(1)

Table 3. Bond lengths [Å] and angles [°] for d20007.

C(1)-S(1)	1.733(4)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-N(2)	1.300(4)
C(2)-C(10)	1.415(4)
C(2)-N(1)	1.426(4)
C(3)-N(2)	1.373(4)
C(3)-C(4)	1.403(4)
C(3)-C(8)	1.424(4)
C(4)-C(5)	1.362(5)
C(4)-H(4)	0.9300

C(5)-C(6)	1.398(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.352(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.412(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.414(4)
C(9)-C(10)	1.362(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.445(4)
C(11)-C(12)	1.393(4)
C(11)-C(18)	1.398(4)
C(12)-O(3)	1.358(4)
C(12)-C(14)	1.381(4)
C(13)-O(3)	1.424(4)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.390(4)
C(14)-H(14)	0.9300
C(15)-O(4)	1.363(4)
C(15)-C(17)	1.384(5)
C(16)-O(4)	1.414(4)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(18)	1.379(4)
C(17)-H(17)	0.9300
C(18)-N(1)	1.425(4)
N(1)-S(1)	1.665(3)
O(1)-S(1)	1.413(2)
O(2)-S(1)	1.411(2)

S(1)-C(1)-H(1A)	109.5
S(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
S(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5

H(1B)-C(1)-H(1C)	109.5
N(2)-C(2)-C(10)	127.8(3)
N(2)-C(2)-N(1)	124.1(3)
C(10)-C(2)-N(1)	108.1(3)
N(2)-C(3)-C(4)	118.3(3)
N(2)-C(3)-C(8)	122.9(3)
C(4)-C(3)-C(8)	118.8(3)
C(5)-C(4)-C(3)	121.0(3)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	120.2(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(7)-C(6)-C(5)	120.7(3)
C(7)-C(6)-H(6)	119.7
C(5)-C(6)-H(6)	119.7
C(6)-C(7)-C(8)	121.0(3)
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-H(7)	119.5
C(7)-C(8)-C(9)	123.1(3)
C(7)-C(8)-C(3)	118.4(3)
C(9)-C(8)-C(3)	118.5(3)
C(10)-C(9)-C(8)	118.5(3)
C(10)-C(9)-H(9)	120.8
C(8)-C(9)-H(9)	120.8
C(9)-C(10)-C(2)	117.5(3)
C(9)-C(10)-C(11)	135.4(3)
C(2)-C(10)-C(11)	107.1(3)
C(12)-C(11)-C(18)	118.9(3)
C(12)-C(11)-C(10)	132.5(3)
C(18)-C(11)-C(10)	108.7(3)
O(3)-C(12)-C(14)	125.0(3)
O(3)-C(12)-C(11)	115.3(3)
C(14)-C(12)-C(11)	119.7(3)
O(3)-C(13)-H(13A)	109.5
O(3)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(3)-C(13)-H(13C)	109.5

H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-C(15)	119.6(3)
C(12)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
O(4)-C(15)-C(17)	114.2(3)
O(4)-C(15)-C(14)	123.4(3)
C(17)-C(15)-C(14)	122.4(3)
O(4)-C(16)-H(16A)	109.5
O(4)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(15)	116.9(3)
C(18)-C(17)-H(17)	121.6
C(15)-C(17)-H(17)	121.6
C(17)-C(18)-C(11)	122.6(3)
C(17)-C(18)-N(1)	129.5(3)
C(11)-C(18)-N(1)	107.9(3)
C(18)-N(1)-C(2)	108.2(2)
C(18)-N(1)-S(1)	125.4(2)
C(2)-N(1)-S(1)	124.2(2)
C(2)-N(2)-C(3)	114.7(3)
C(12)-O(3)-C(13)	118.2(2)
C(15)-O(4)-C(16)	118.8(3)
O(2)-S(1)-O(1)	118.84(16)
O(2)-S(1)-N(1)	107.82(14)
O(1)-S(1)-N(1)	107.11(14)
O(2)-S(1)-C(1)	108.96(19)
O(1)-S(1)-C(1)	109.80(18)
N(1)-S(1)-C(1)	103.14(17)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for d20007. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

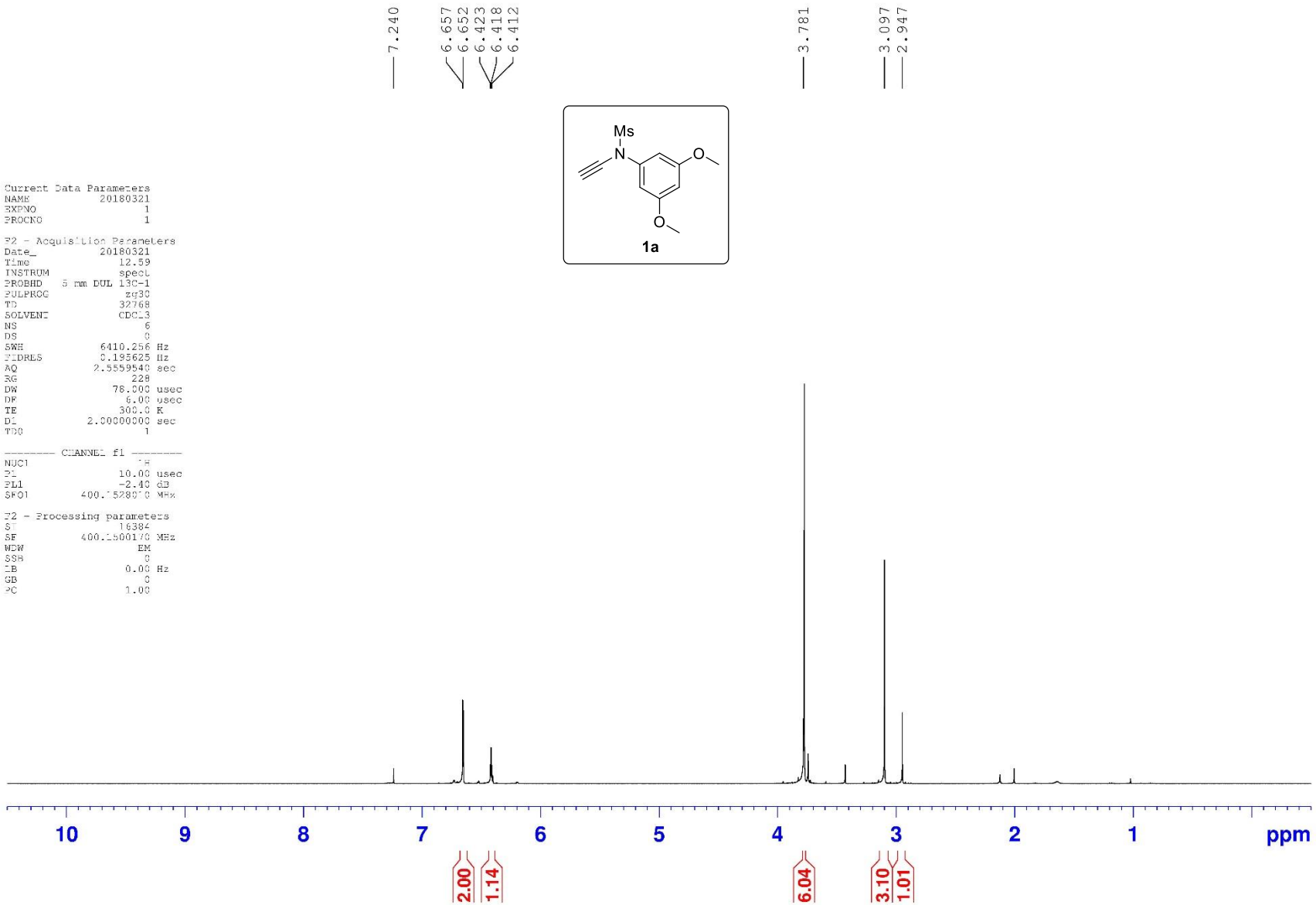
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	57(2)	48(2)	51(2)	11(2)	6(2)	5(2)
C(2)	31(2)	26(2)	25(2)	-2(1)	6(1)	-3(1)
C(3)	31(2)	28(2)	31(2)	-2(1)	4(1)	-3(1)
C(4)	38(2)	29(2)	42(2)	1(2)	0(2)	2(2)
C(5)	37(2)	31(2)	54(2)	-2(2)	7(2)	4(2)
C(6)	44(2)	40(2)	41(2)	-9(2)	16(2)	5(2)
C(7)	46(2)	36(2)	32(2)	-3(2)	7(2)	4(2)
C(8)	33(2)	26(2)	31(2)	-1(1)	5(1)	-3(1)
C(9)	35(2)	28(2)	24(2)	2(1)	2(1)	-3(1)
C(10)	30(2)	26(2)	24(2)	1(1)	2(1)	-4(1)
C(11)	29(2)	26(2)	26(2)	0(1)	4(1)	-1(1)
C(12)	32(2)	32(2)	30(2)	-1(1)	2(1)	-2(2)
C(13)	43(2)	54(2)	33(2)	6(2)	-4(2)	5(2)
C(14)	28(2)	35(2)	38(2)	0(2)	-1(1)	4(1)
C(15)	31(2)	35(2)	38(2)	-6(2)	6(2)	4(2)
C(16)	44(2)	46(2)	59(2)	-3(2)	11(2)	16(2)
C(17)	38(2)	40(2)	29(2)	-7(2)	7(1)	5(2)
C(18)	32(2)	29(2)	29(2)	1(1)	3(1)	-2(1)
N(1)	41(2)	35(2)	25(1)	1(1)	3(1)	7(1)
N(2)	36(2)	33(2)	30(2)	0(1)	2(1)	3(1)
O(1)	73(2)	54(2)	30(1)	-10(1)	4(1)	17(1)
O(2)	32(1)	104(2)	34(1)	-2(1)	-6(1)	10(1)
O(3)	47(1)	54(2)	25(1)	-1(1)	-3(1)	17(1)
O(4)	48(2)	60(2)	46(2)	-11(1)	2(1)	25(1)
S(1)	34(1)	46(1)	22(1)	-2(1)	1(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d20007.

	x	y	z	U(eq)
H(1A)	825	3279	5472	77
H(1B)	2483	3138	6824	77
H(1C)	3361	3019	5304	77
H(4)	10766	2753	3087	44

H(5)	12592	2470	1151	49
H(6)	11161	2659	-1130	50
H(7)	7937	3127	-1469	45
H(9)	4643	3608	-435	35
H(13A)	-840	4238	-2246	65
H(13B)	-873	4622	-1271	65
H(13C)	-2811	4264	-1018	65
H(14)	-2234	4638	1077	40
H(16A)	-3580	5196	2351	74
H(16B)	-5555	5183	3580	74
H(16C)	-5653	4846	2405	74
H(17)	574	4345	5020	43

(5) $^{1}H,^{13}C$ Spectral of key compound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6.652
6.423
6.418
6.412
3.781
3.097
2.947
Ms
N
O
O
1a
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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180321
Time 12.59
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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 228
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
10
9
8
7
6
5
4
3
2
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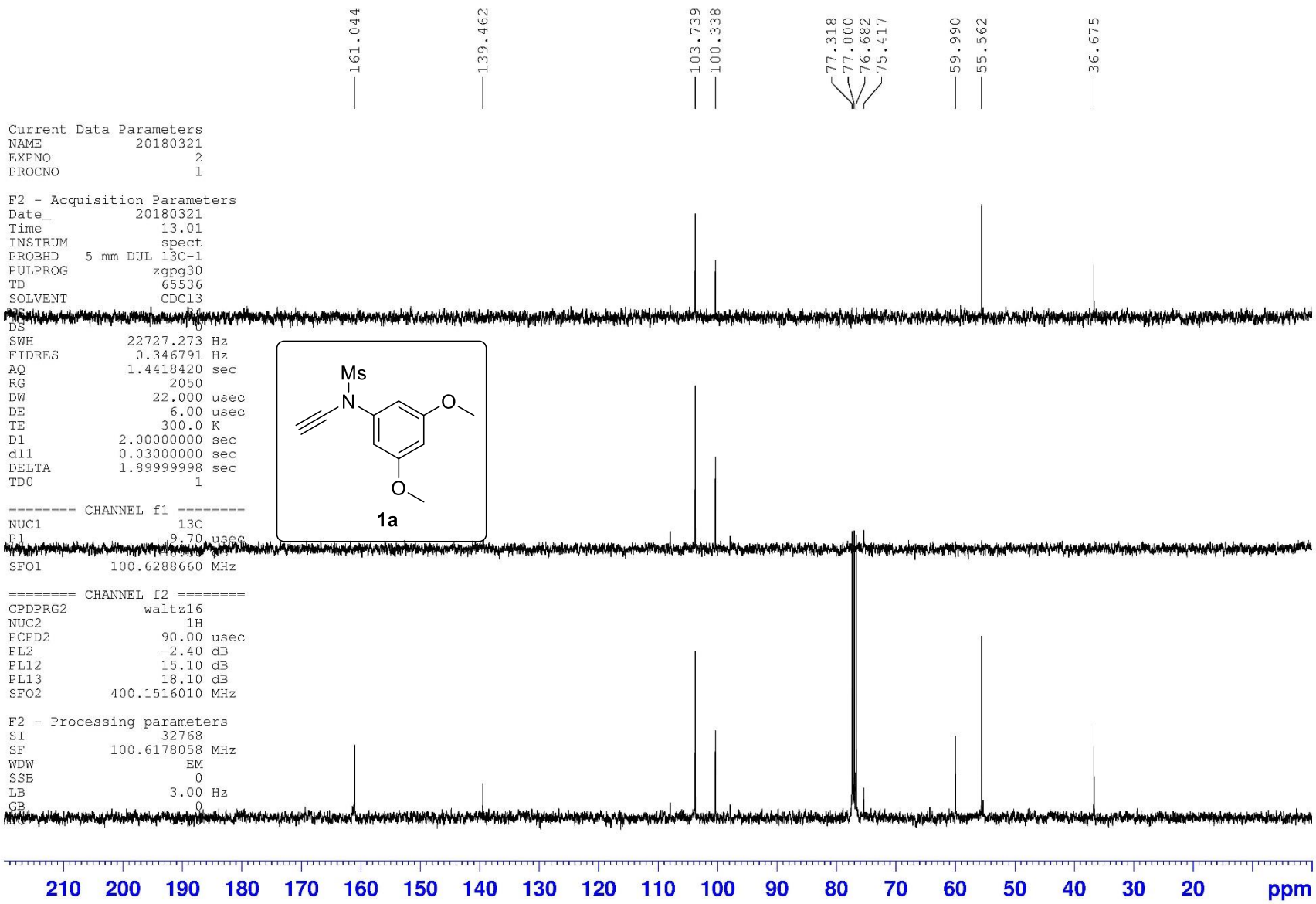
ppm
2.00
1.14
6.04
3.10
1.01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103.739
100.338
77.318
77.000
76.682
75.417
59.990
55.562
36.675
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EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
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Time 13.01
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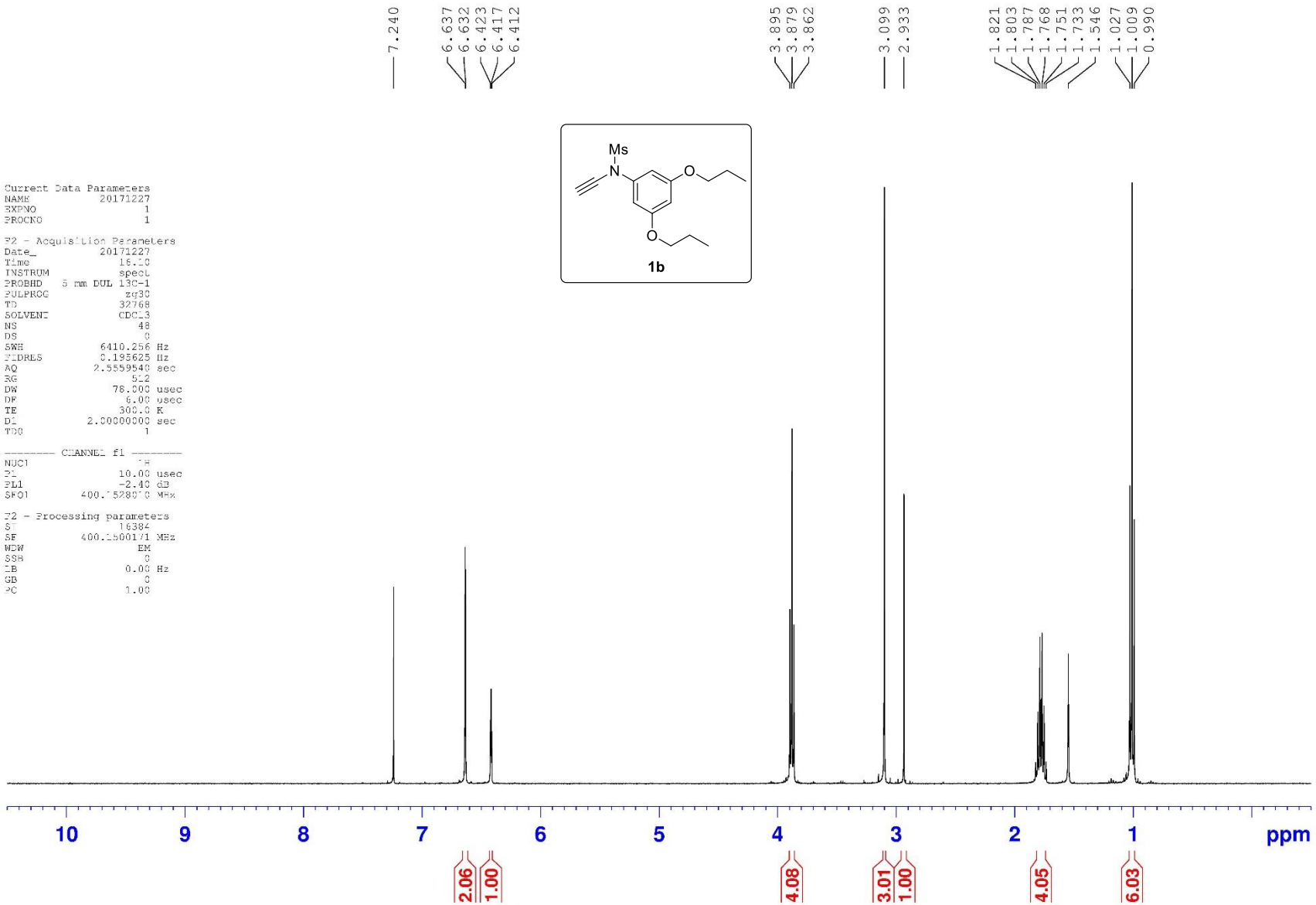
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
DS 16
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
SFO1 100.6288660 MHz
======== 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 100.6178058 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
Ms
N
O
O
1a
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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1.821
1.803
1.787
1.768
1.751
1.733
1.546
1.027
1.009
0.990
Ms
N
O
O
1b
Current Data Parameters
NAME 20171227
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171227
Time 16.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 48
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
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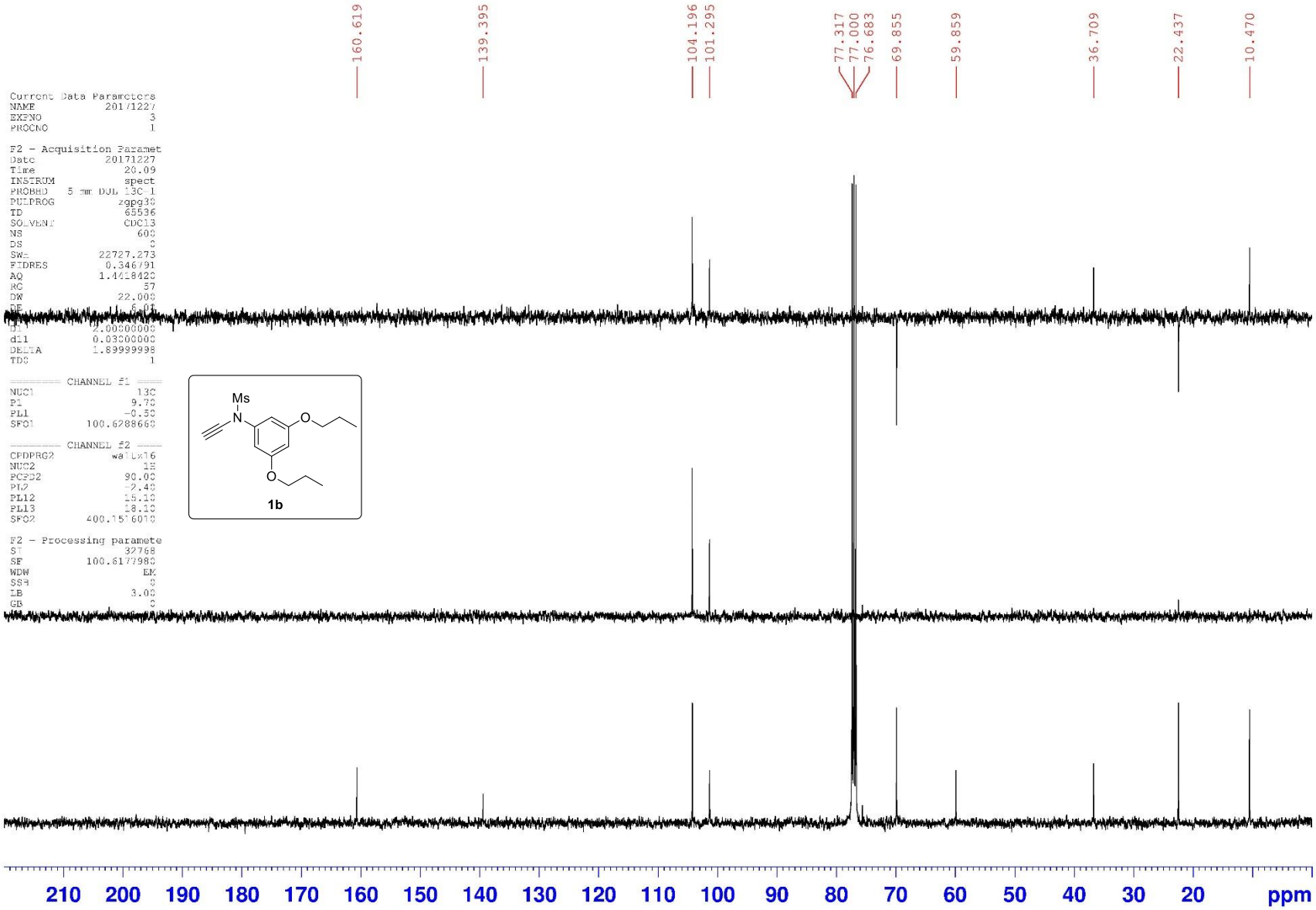
1.00
4.08
3.01
1.00
4.05
6.03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104.196
101.295
77.317
77.000
76.683
69.855
59.859
36.709
22.437
10.470
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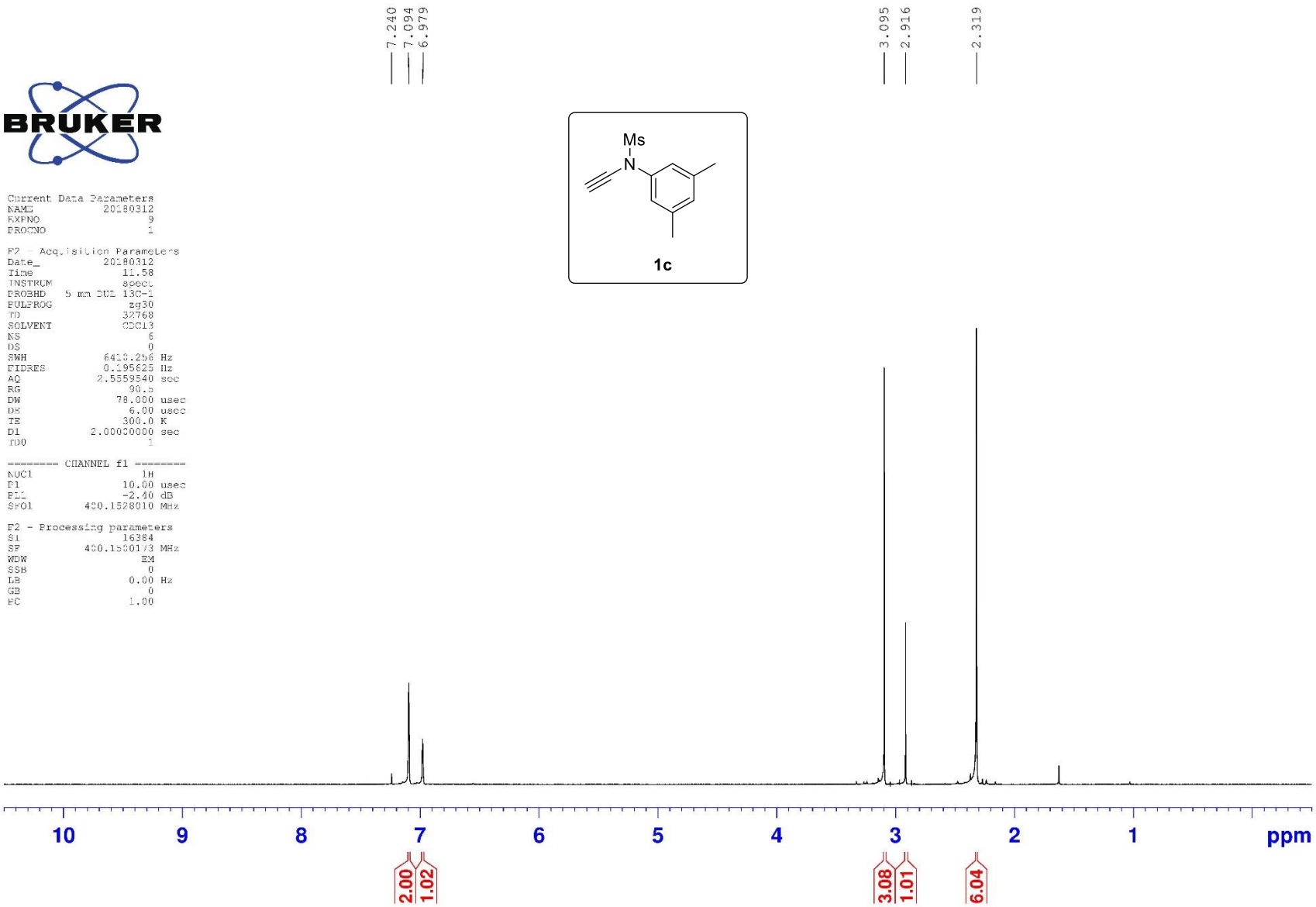
NAME 201/1227
EXPNO 3
PROCNO 1
F2 - Acquisition Paramet
Date 20171227
Time 20.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 57
DW 22.000
DE 6.00
TE 298.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6177980
WDW EM
SSB 0
LB 3.00
GB 0
Ms
N
O
O
1b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.240
7.094
6.979
3.095
2.916
2.319
Ms
N
1c
Current Data Parameters
NAME 20180312
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180312
Time 11.58
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 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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
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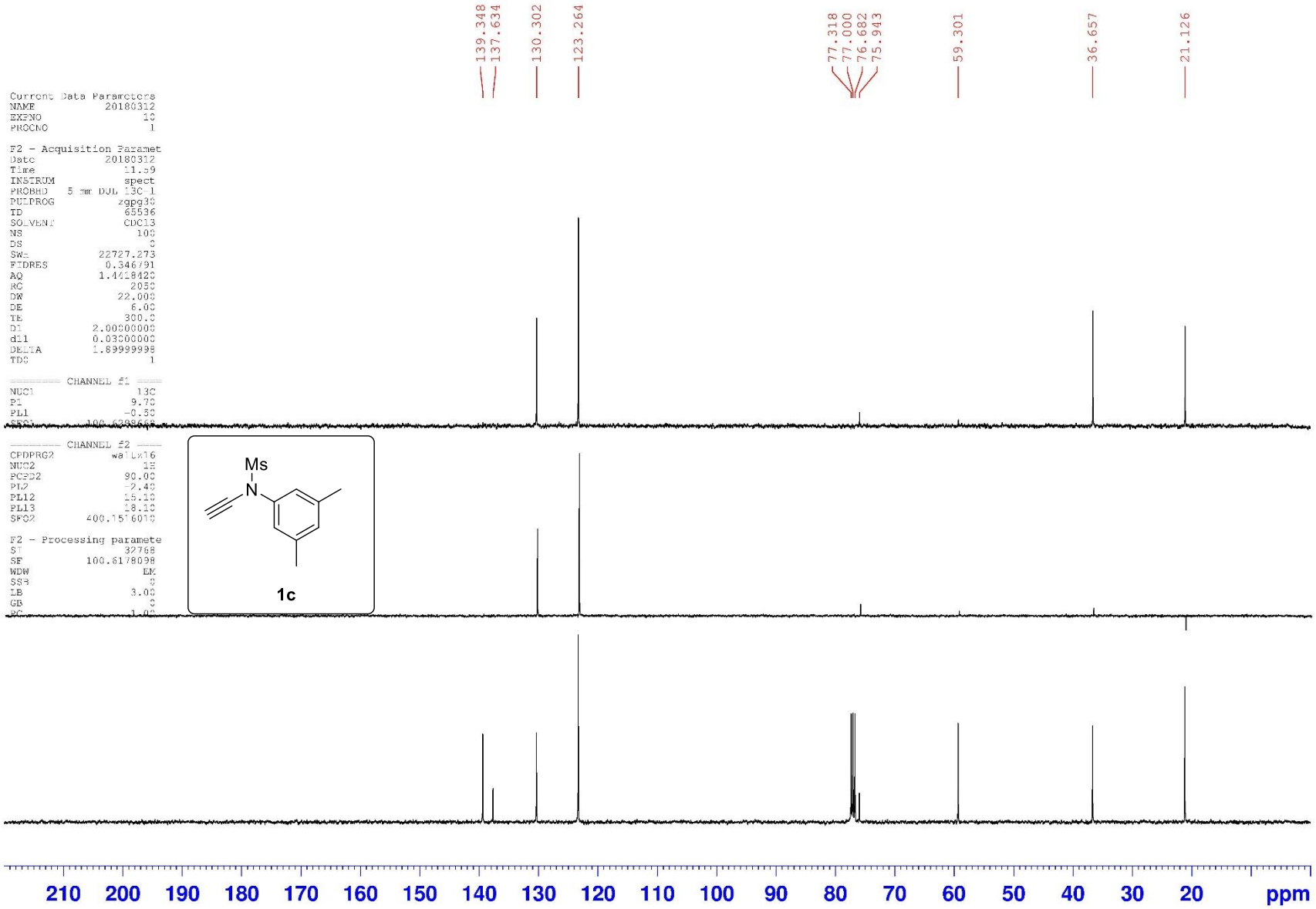
ppm
2.00
1.02
3.08
1.01
6.04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137.634
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77.318
77.000
76.682
75.943
59.301
36.657
21.126
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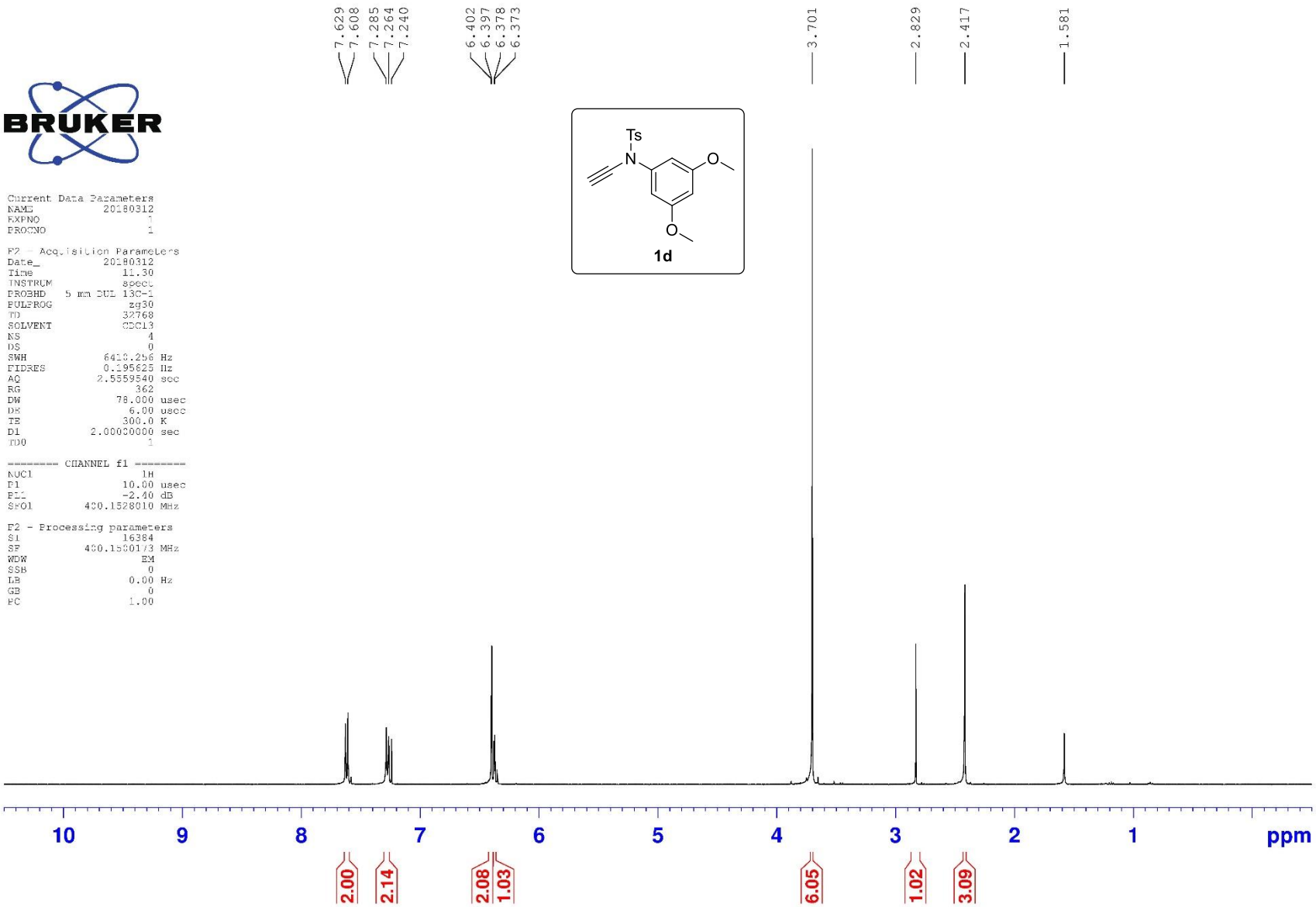
NAME 20180312
EXPNO 10
PROCNO 1
F2 - Acquisition Paramet
Date 20180312
Time 11.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178098
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ms
N
1c
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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7.608
7.285
7.264
7.240
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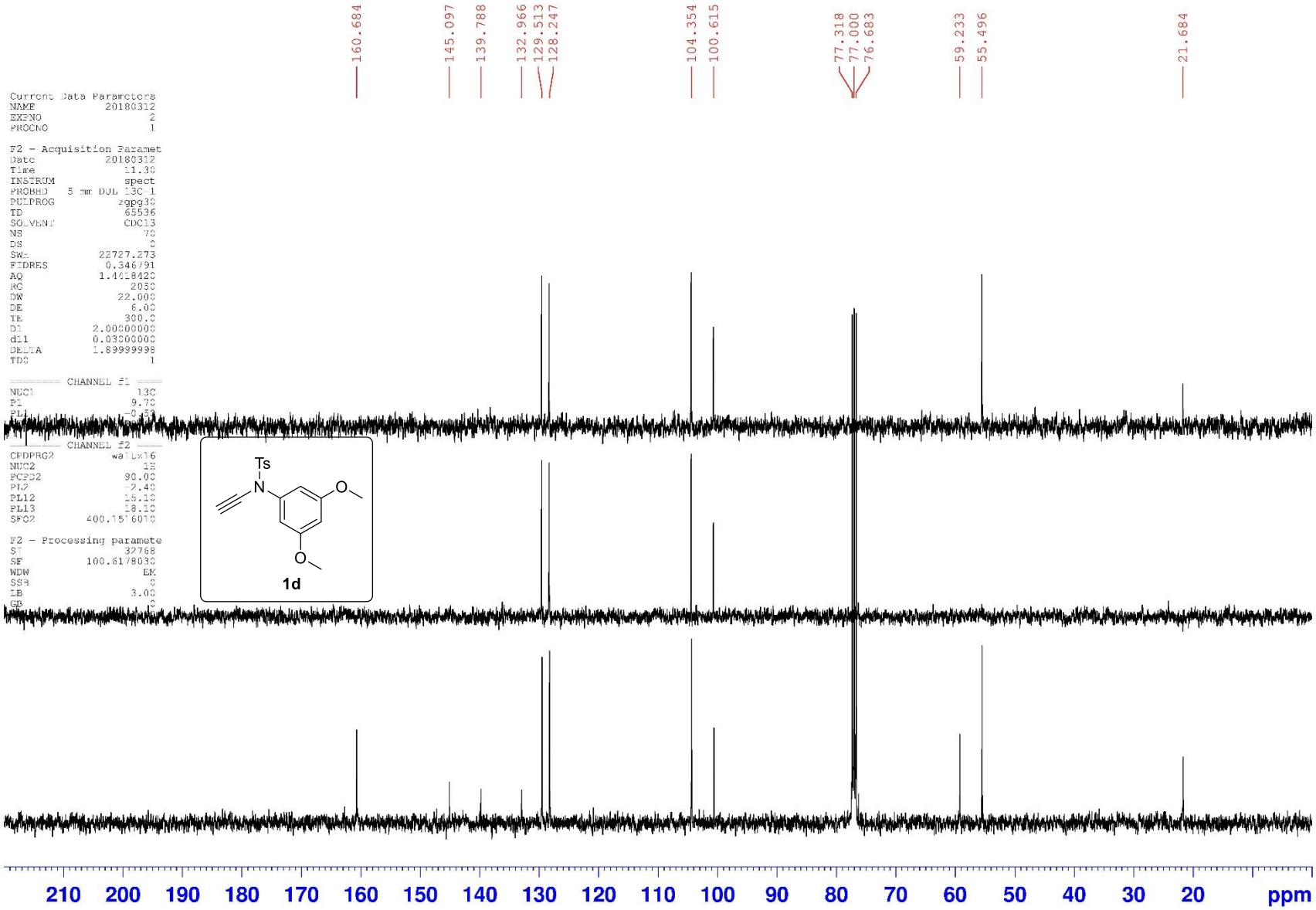
6.378
6.373
3.701
2.829
2.417
1.581
Ts
N
O
O
1d
Current Data Parameters
NAME 20180312
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180312
Time 11.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 362
DW 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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.14
2.08
1.03
6.05
1.02
3.09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55.496
21.684
Current Data Parameters
NAME 20180312
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180312
Time 11.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 78
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178030
WDW EM
SSB 0
LB 3.00
GB 0
Ts
N
O
O
1d
210
200
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180
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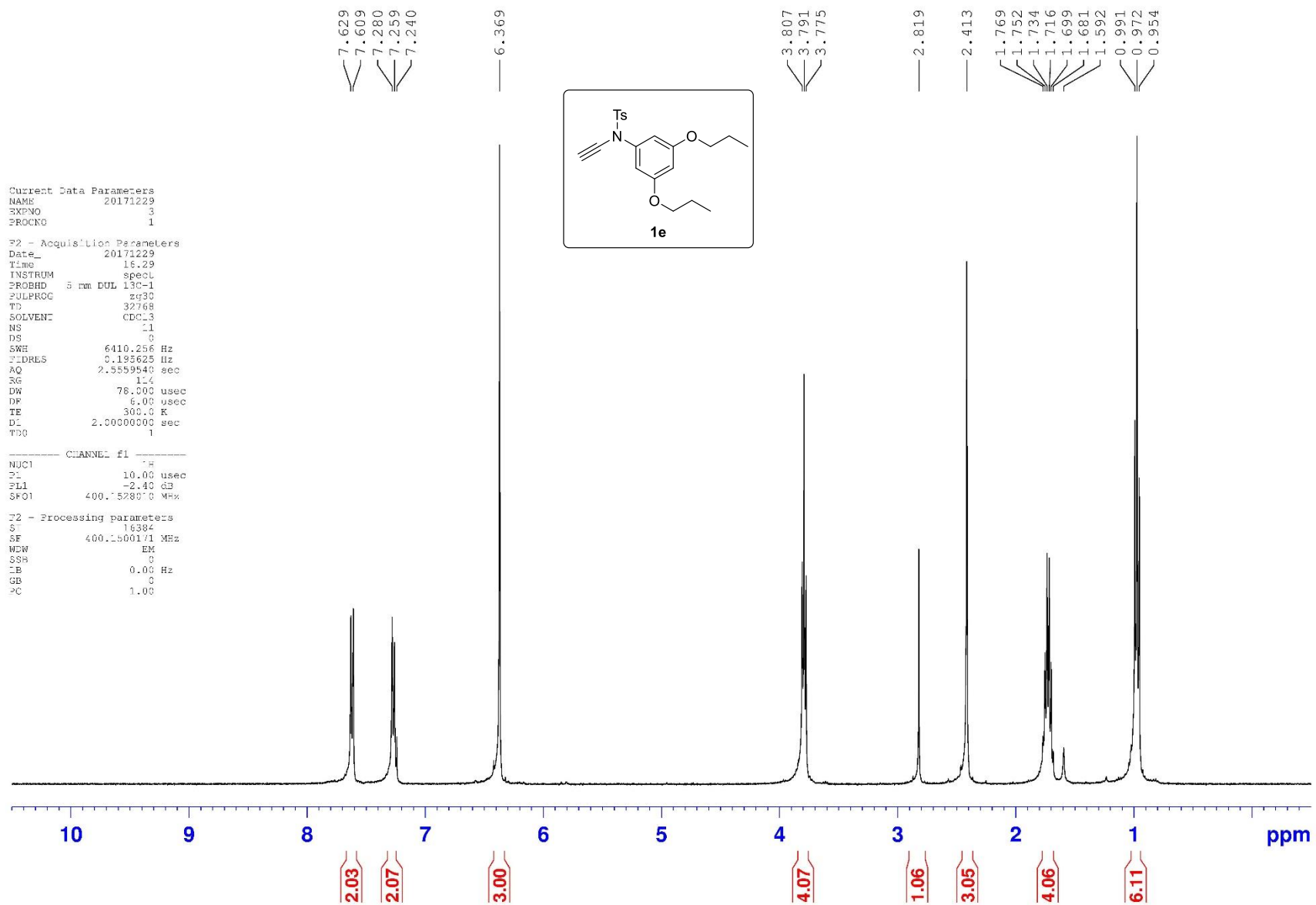
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.259
7.240
6.369
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3.791
3.775
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2.413
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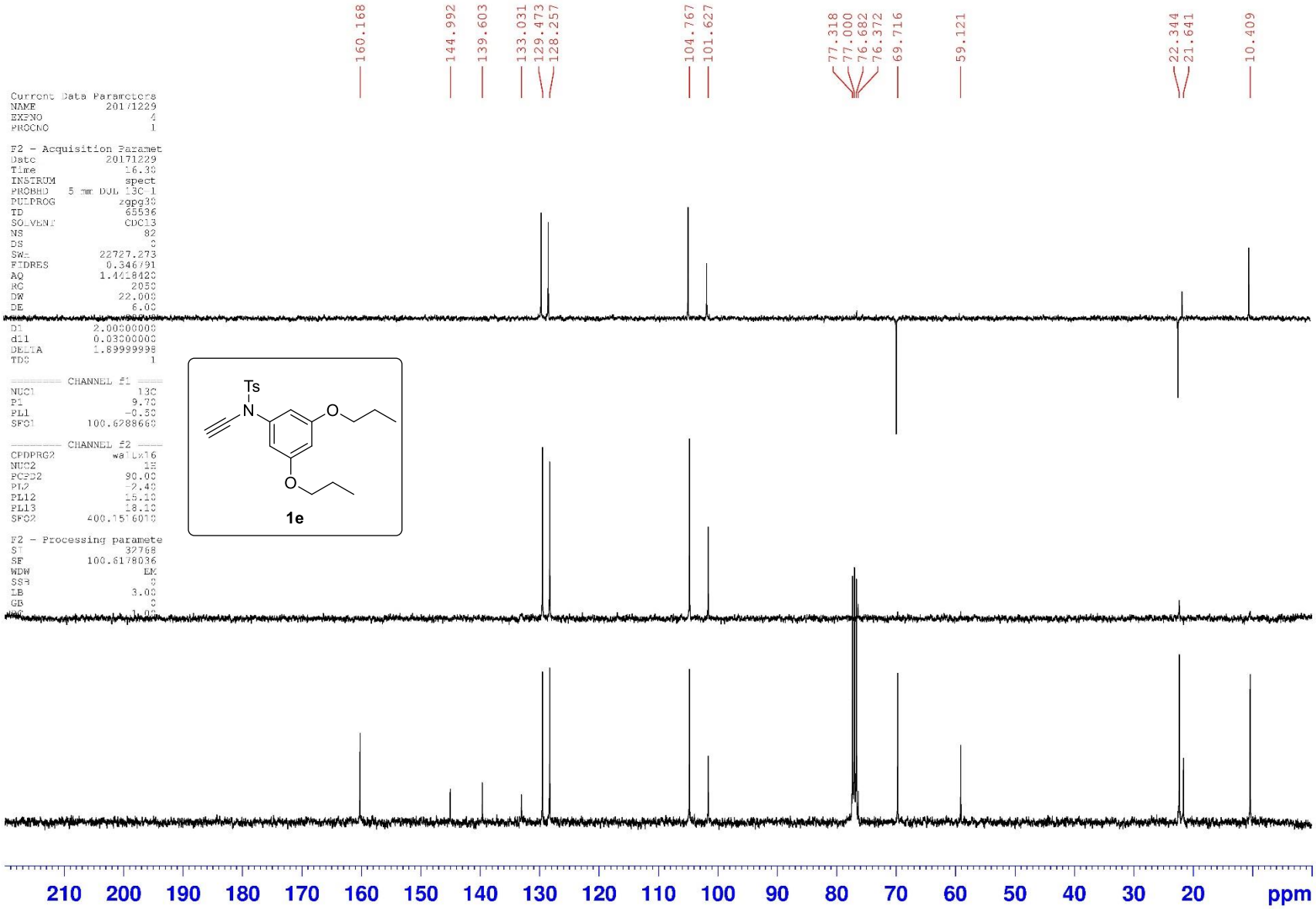
1.752
1.734
1.716
1.699
1.681
1.592
0.991
0.972
0.954
Ts
N
O
O
1e
Current Data Parameters
NAME 20171229
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171229
Time 16.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 21
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.03
2.07
3.00
4.07
1.06
3.05
4.06
6.11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69.716
59.121
22.344
21.641
10.409
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NAME 201712229
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171229
Time 16.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 82
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178036
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ts
N
O
O
1e
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200
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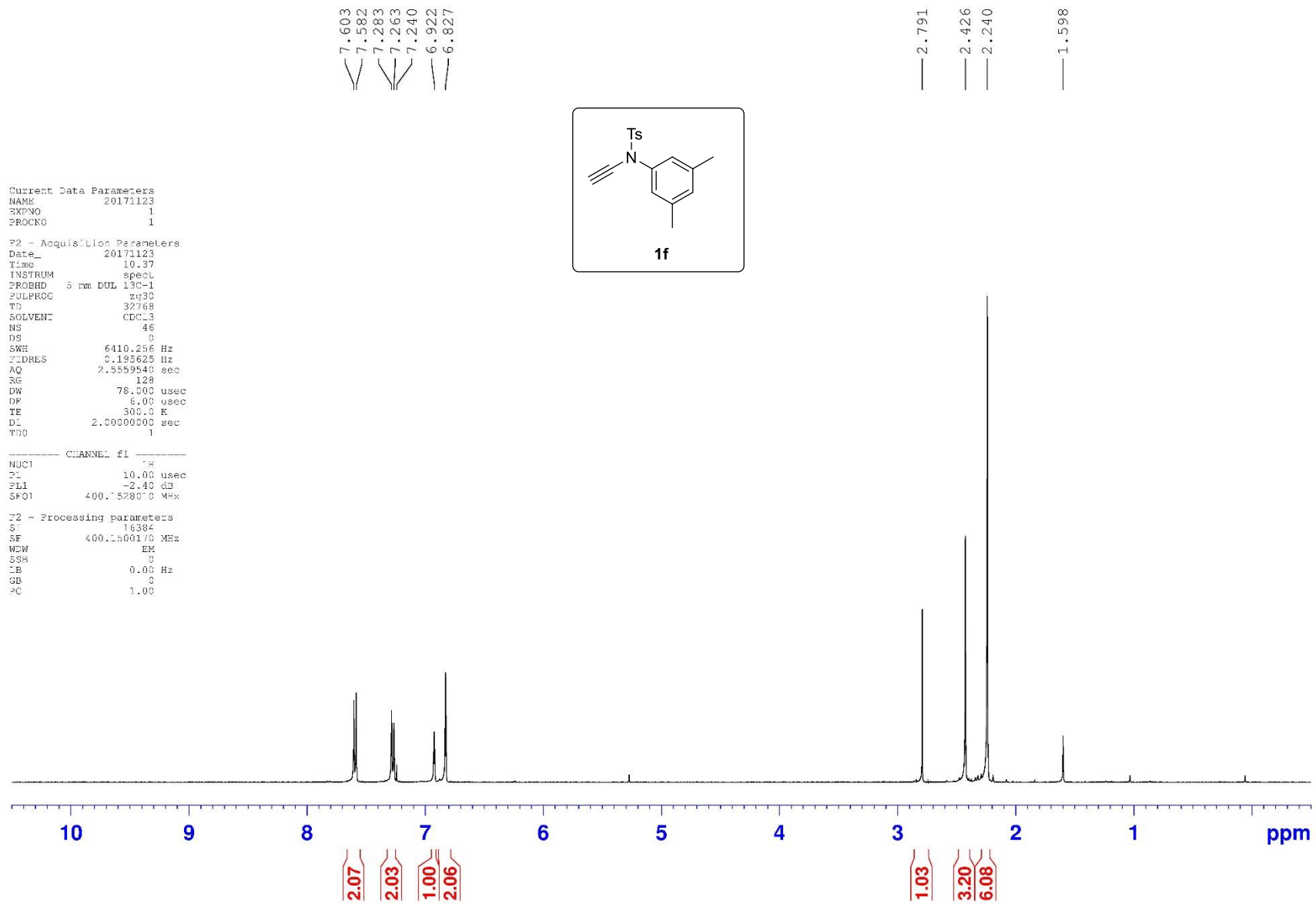
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.240
6.922
6.827
2.791
2.426
2.240
1.598
Ts
N
1f
Current Data Parameters
NAME 20171123
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171123
Time 10.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 46
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
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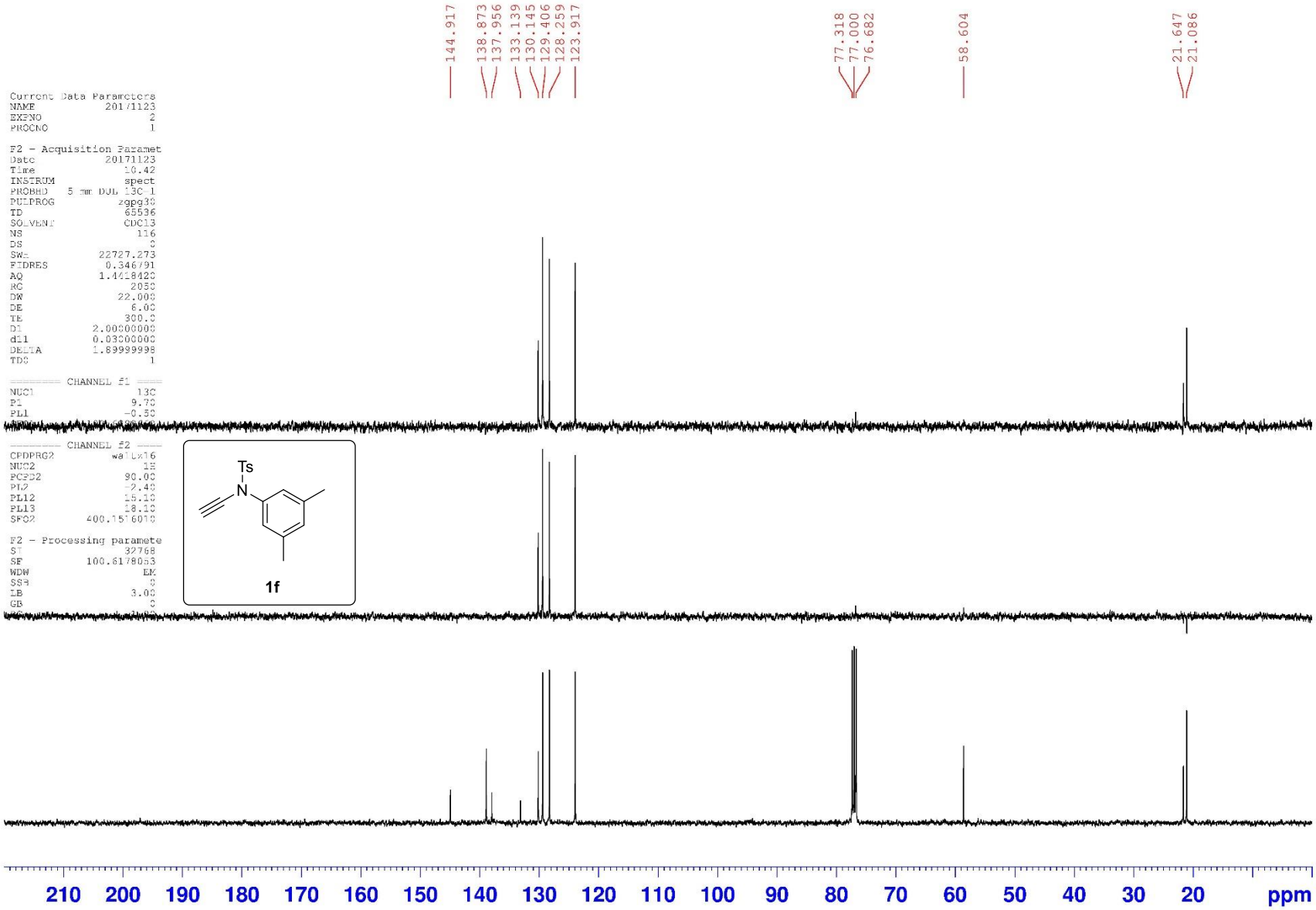
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.07
2.03
1.00
2.06
1.03
3.20
6.08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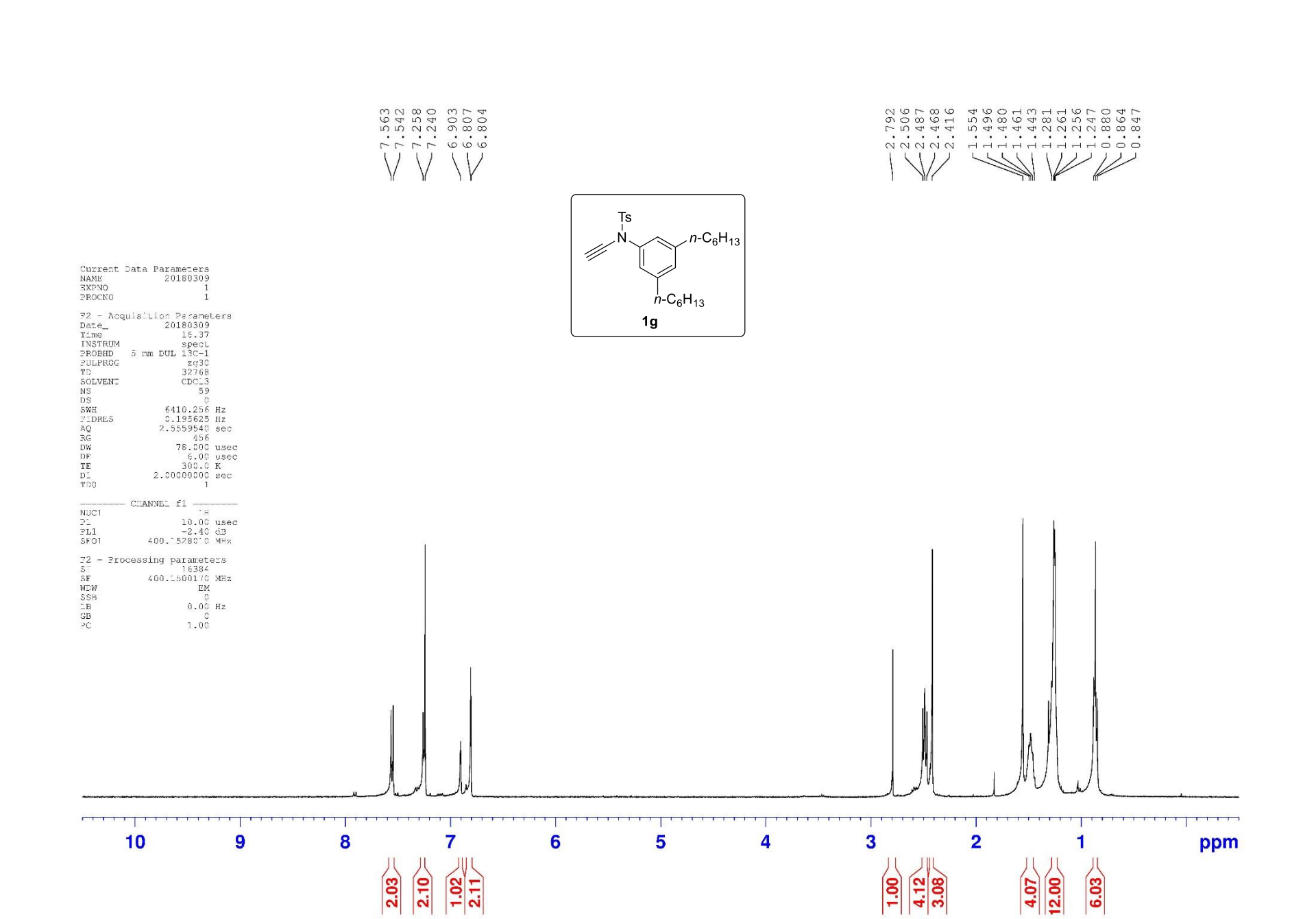
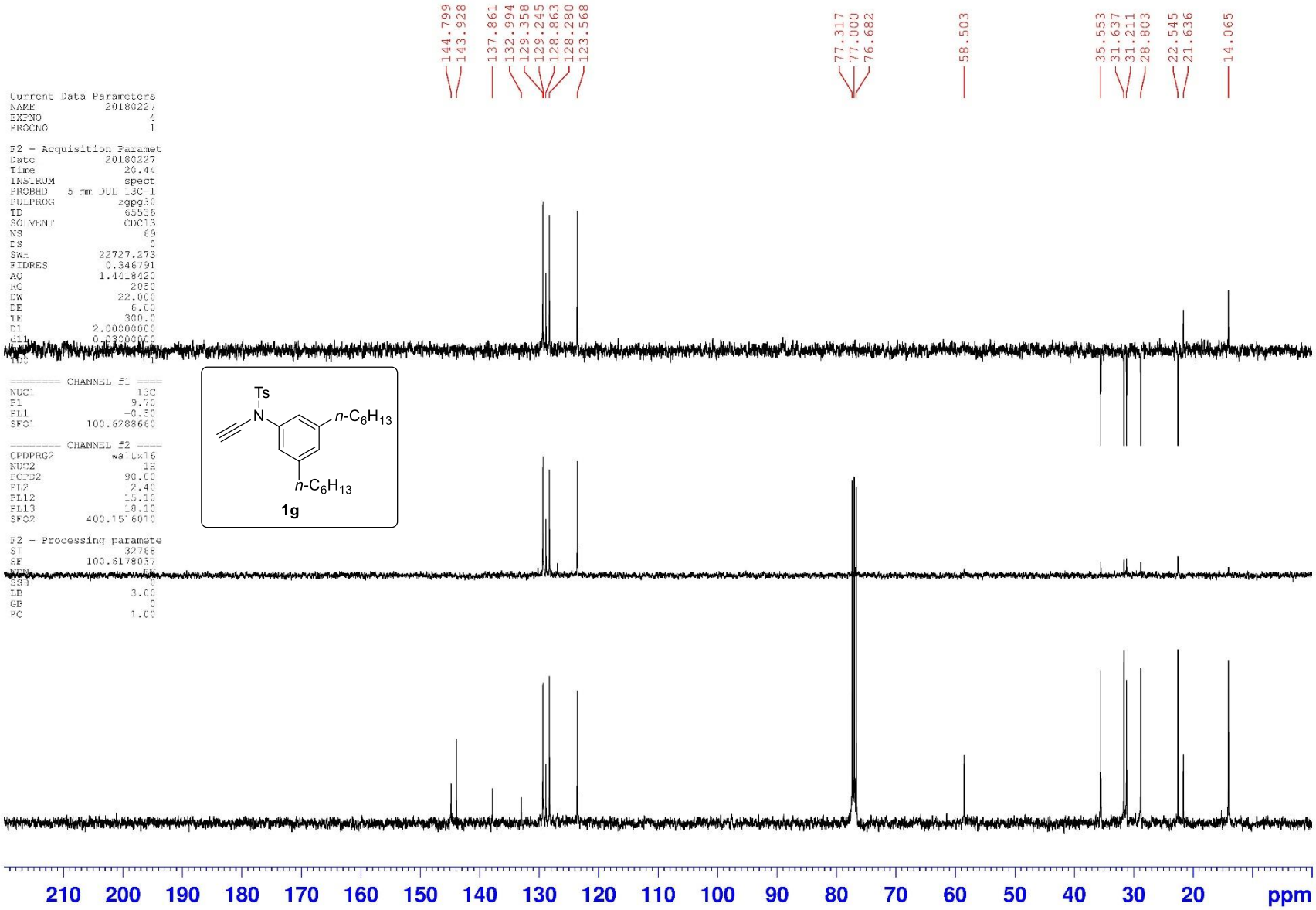
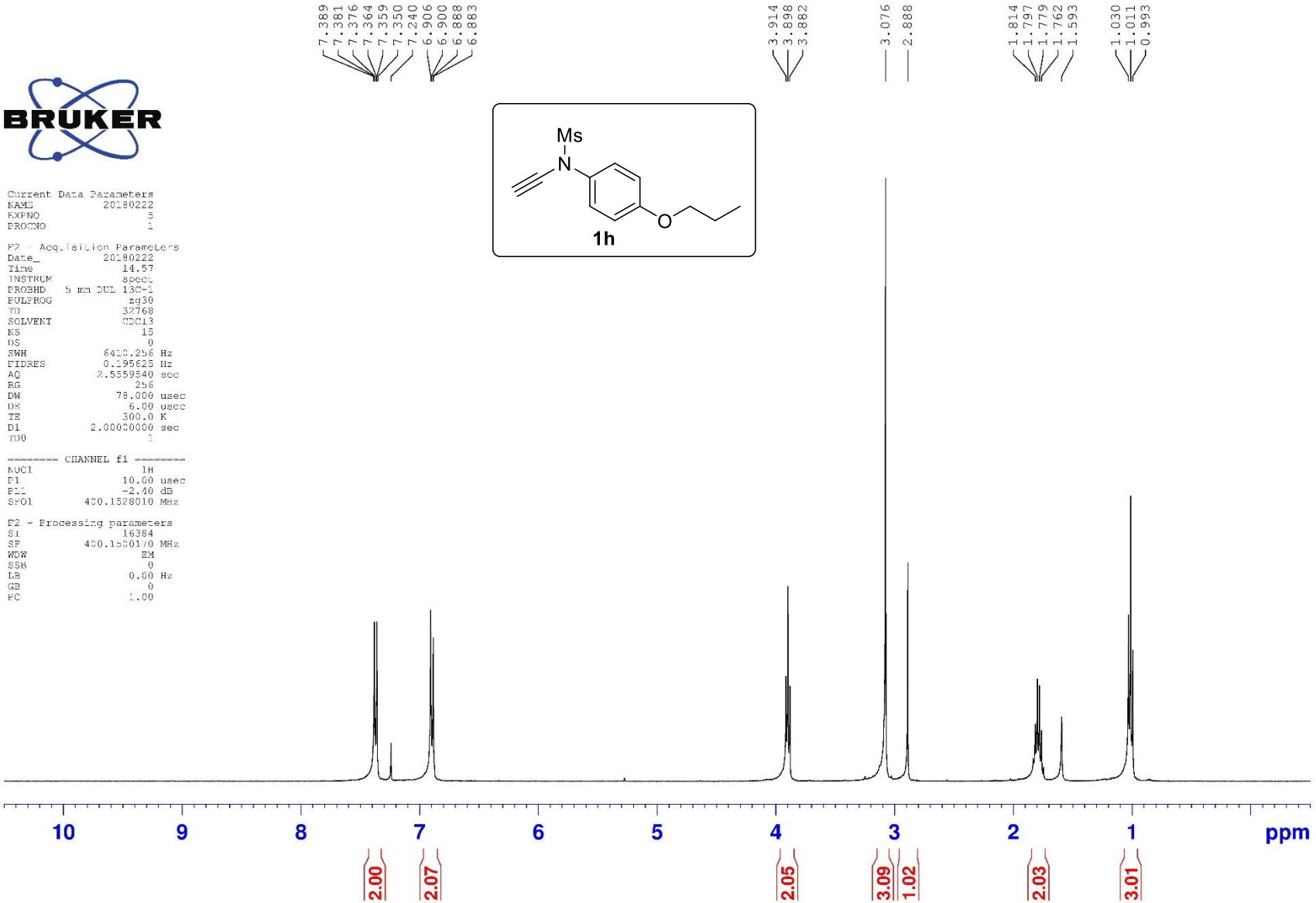
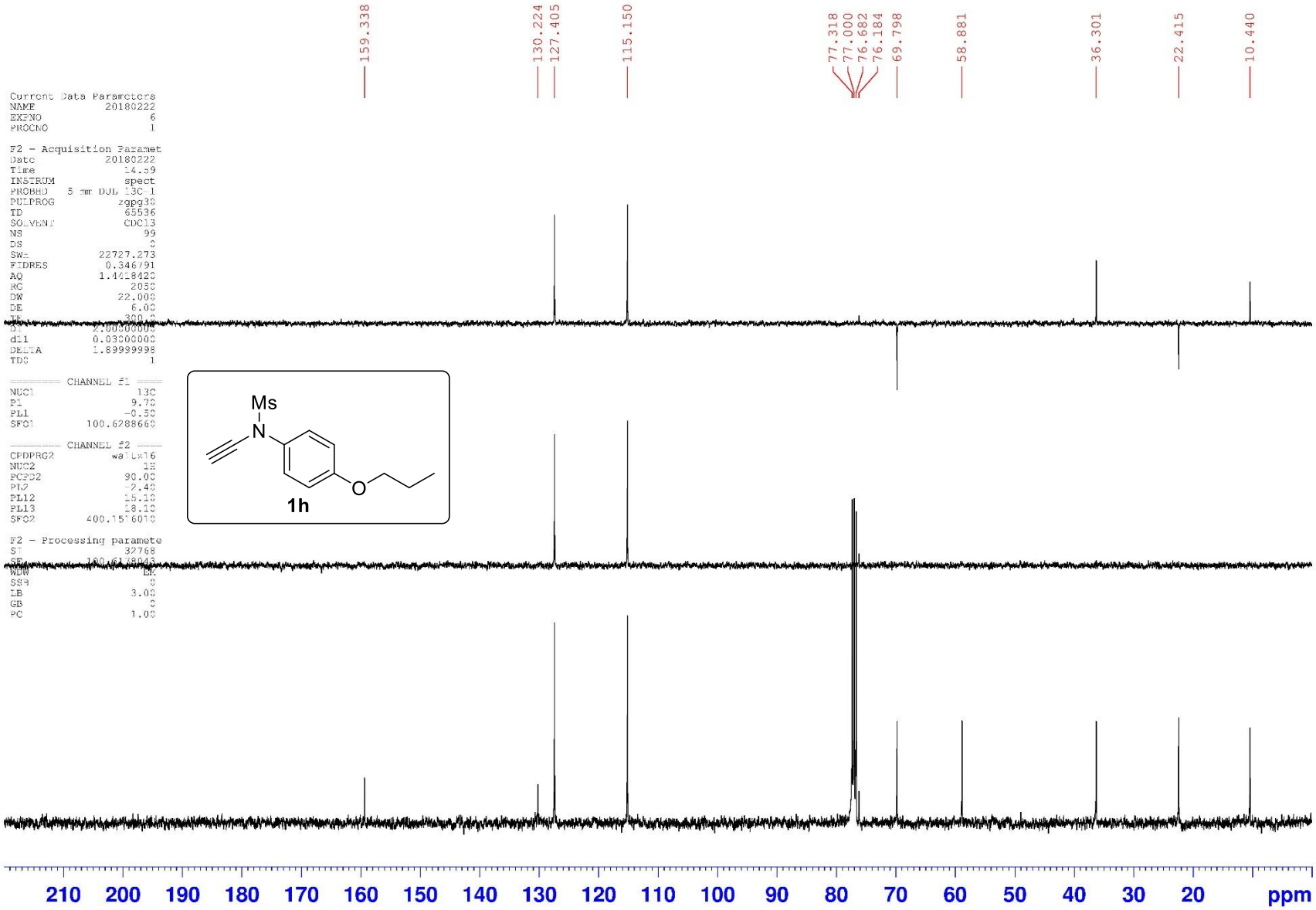
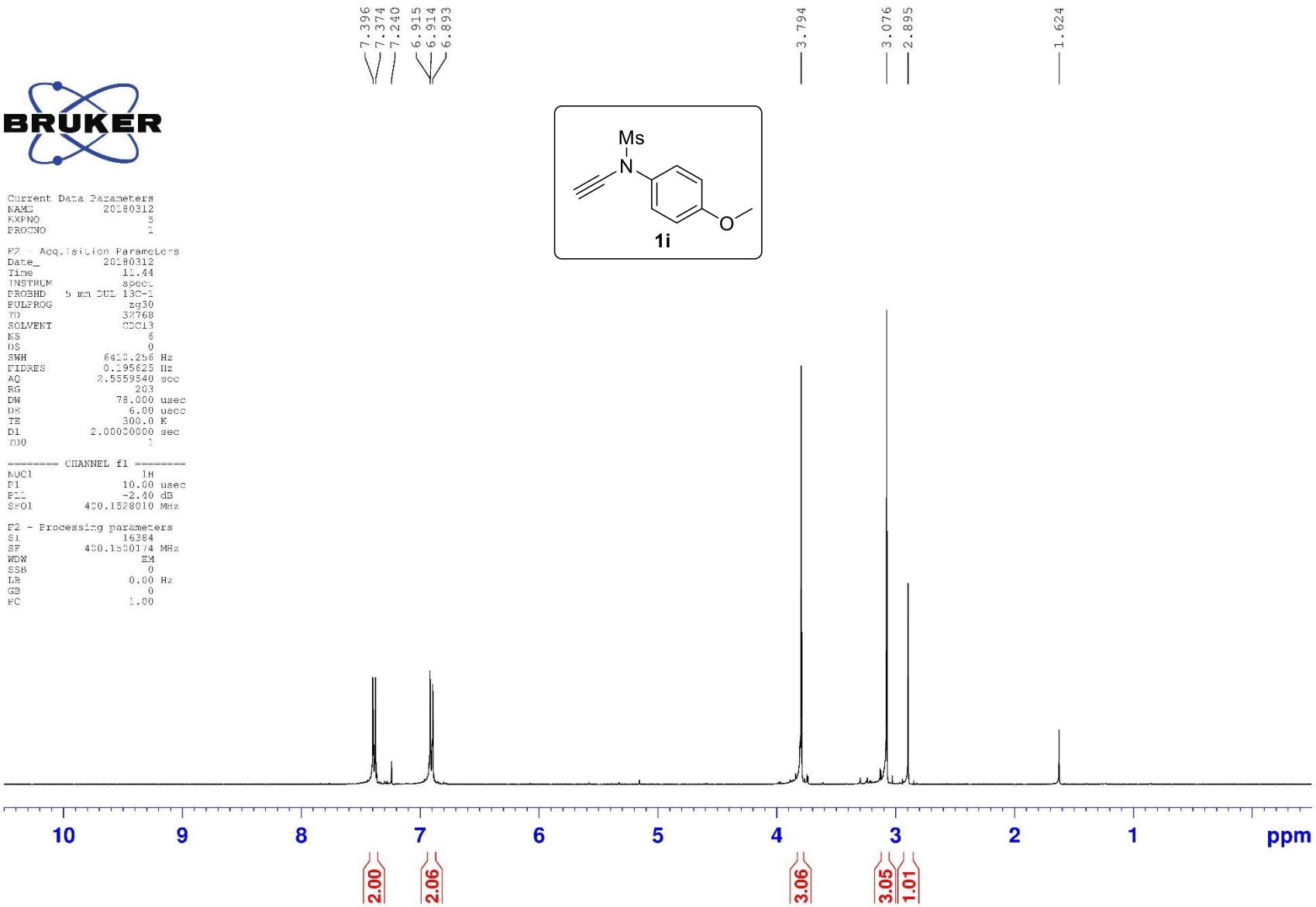
130.145
129.406
128.259
123.917
77.318
77.000
76.682
58.604
21.647
21.086
Current Data Parameters
NAME 201/1123
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171123
Time 10.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 116
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
CHANNEL f2
CPDPRG2 wa
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178053
WDW EM
SSB 0
LB 3.00
GB 0
Ts
N
1f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

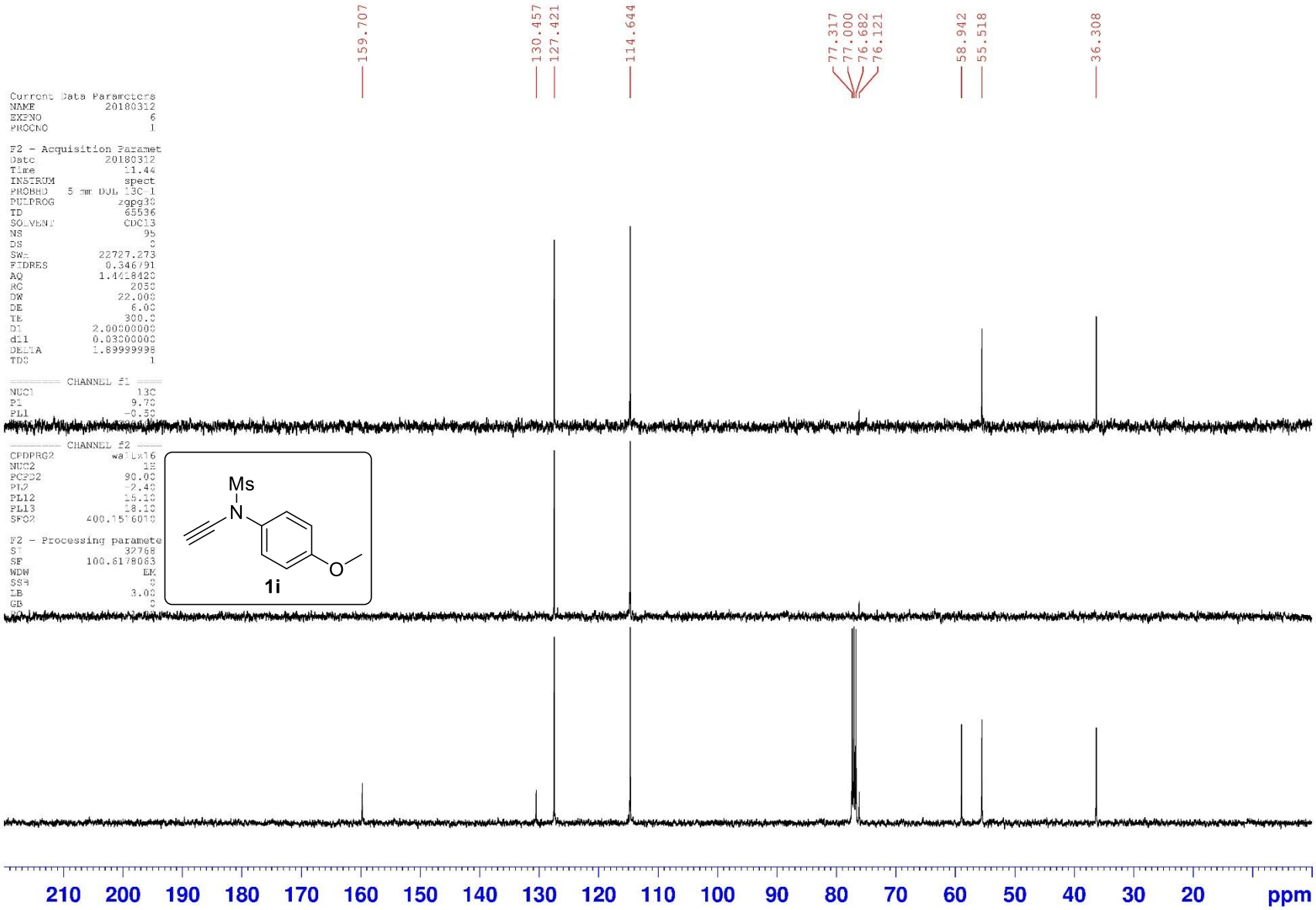

7.563
7.542
7.258
7.240
6.903
6.807
6.804
2.792
2.506
2.487
2.468
2.416
1.554
1.496
1.480
1.461
1.443
1.281
1.261
1.256
1.247
0.880
0.864
0.847
Ts
N
n-C6H13
n-C6H13
1g
Current Data Parameters
NAME 20180309
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180309
Time 16.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 59
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 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.03
2.10
1.02
2.11
1.00
4.12
3.08
4.07
12.00
6.03


144.799
143.928
137.861
132.994
129.358
129.245
128.863
128.280
123.568
77.317
77.000
76.682
58.503
35.553
31.637
31.211
28.803
22.545
21.636
14.065
Current Data Parameters
NAME 20180227
EXPNO 4
PROCNO 1
F2 - Acquisition Paramet
Date 20180227
Time 20.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 69
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
D11 0.03000000
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178037
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ts
N
n-C6H13
n-C6H13
1g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.389
7.381
7.376
7.364
7.359
7.350
7.240
6.906
6.900
6.888
6.883
3.914
3.898
3.882
3.076
2.888
1.814
1.797
1.779
1.762
1.593
1.030
1.011
0.993
Ms
N
O
1h
Current Data Parameters
NAME 20180222
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180222
Time 14.57
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
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.07
2.05
3.09
1.02
2.03
3.01


159.338
130.224
127.405
115.150
77.318
77.000
76.682
76.184
69.798
58.881
36.301
22.415
10.440
Current Data Parameters
NAME 20180222
EXPNO 6
PROCNO 1
F2 - Acquisition Paramet
Date 20180222
Time 14.59
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 99
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.2
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6128045
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ms
N
O
1h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.396
7.374
7.240
6.915
6.914
6.893
3.794
3.076
2.895
1.624
Ms
N
O
1i
Current Data Parameters
NAME 20180312
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180312
Time 11.44
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 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 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.06
3.06
3.05
1.01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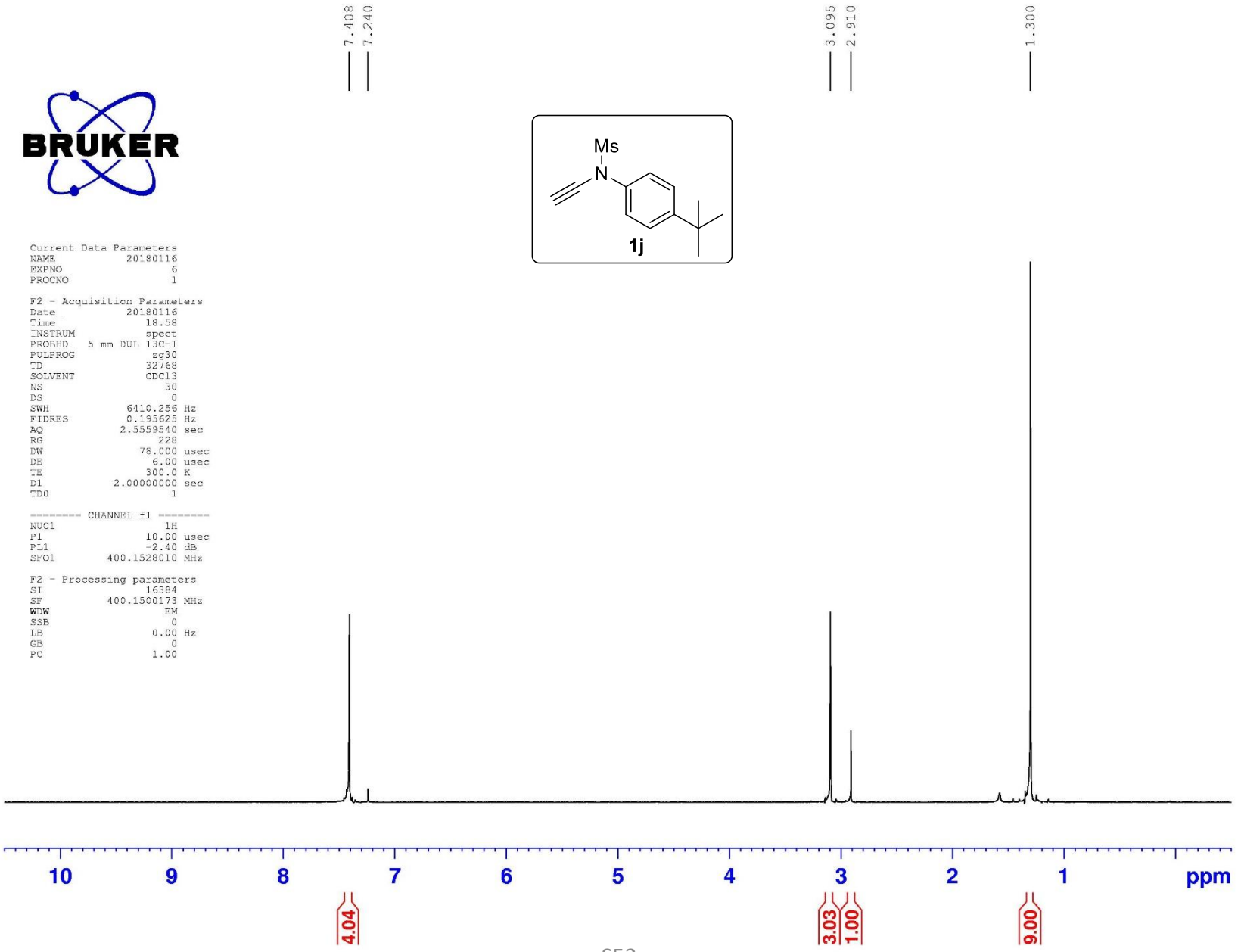
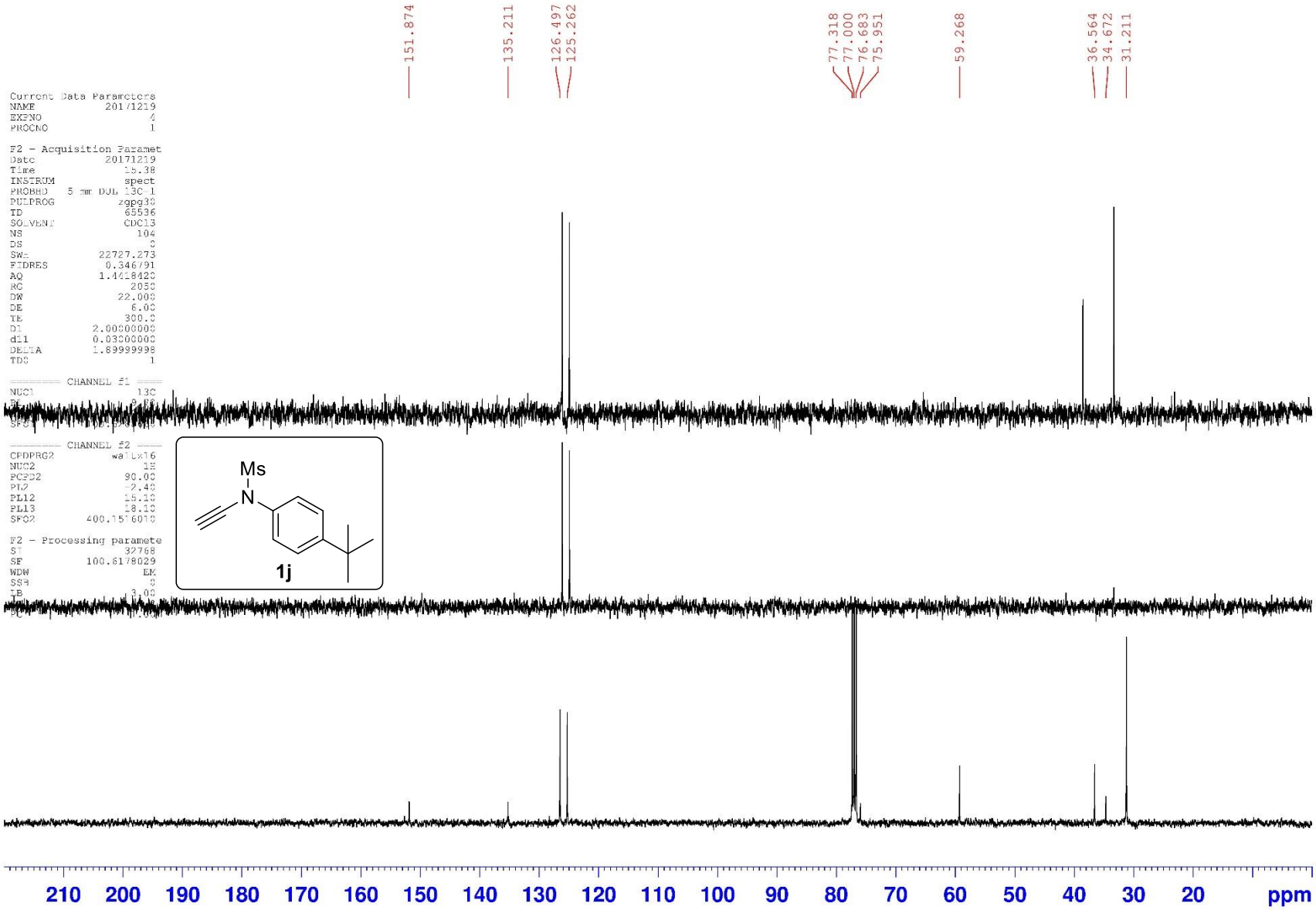
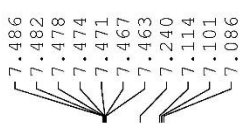
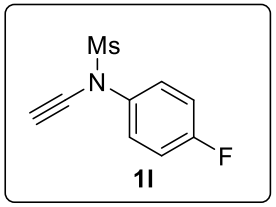
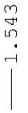
130.457
127.421
114.644
77.317
77.000
76.682
76.121
58.942
55.518
36.308
Current Data Parameters
NAME 20180312
EXPNO 6
PROCNO 1
F2 - Acquisition Paramet
Date 20180312
Time 11.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178063
WDW EM
SSB 0
LB 3.00
GB 0
Ms
N
O
1i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.408
7.240
3.095
2.910
1.300
Ms
N
1j
Current Data Parameters
NAME 20180116
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180116
Time 18.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 228
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
10
9
8
7
6
5
4
3
2
1
ppm
4.04
3.03
1.00
9.00

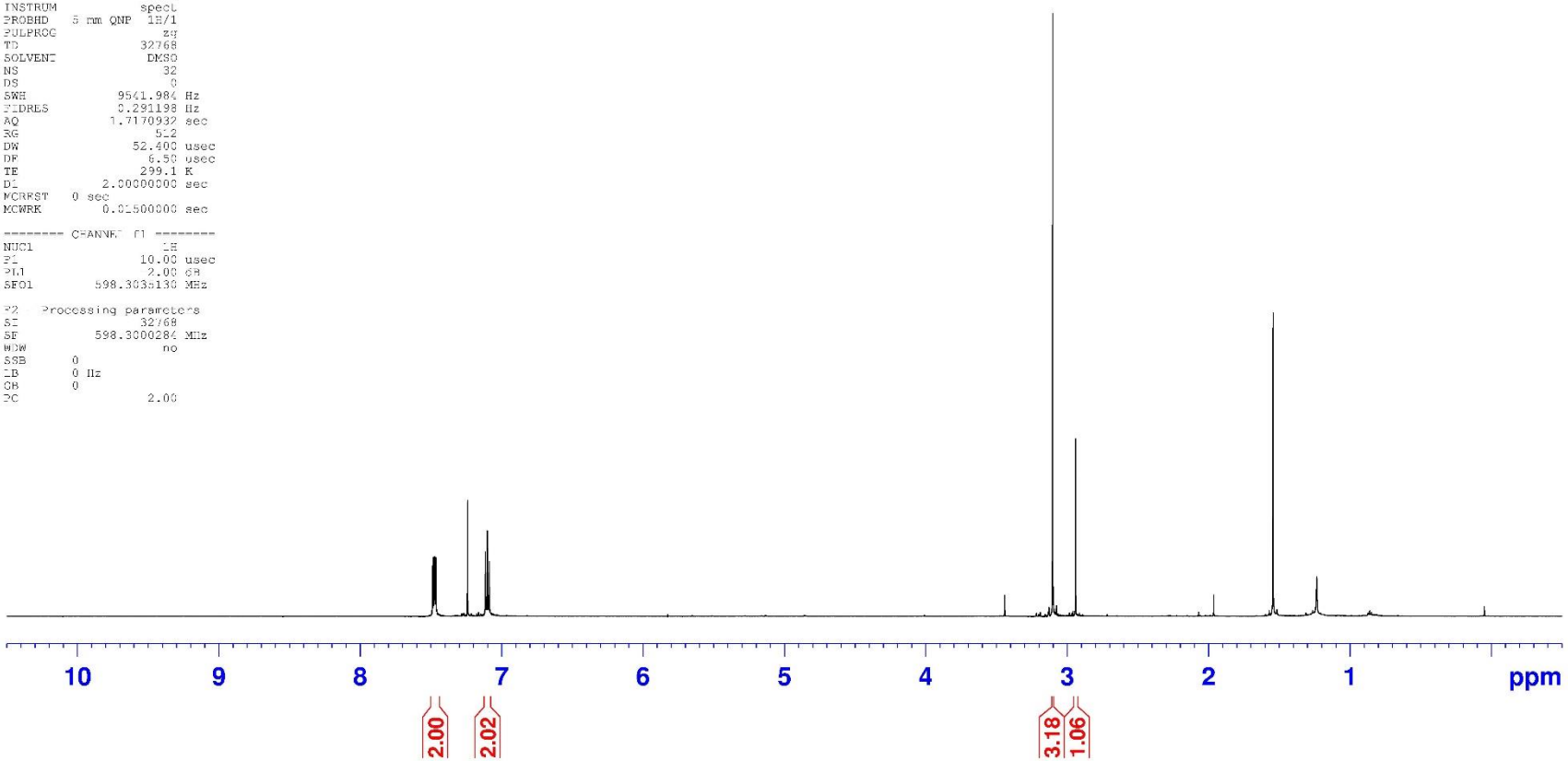

151.874
135.211
126.497
125.262
77.318
77.000
76.683
75.951
59.268
36.564
34.672
31.211
Current Data Parameters
NAME 201/1219
EXPNO 4
PROCNO 1
F2 - Acquisition Paramet
Date 20171219
Time 15.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 104
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178029
WDW EM
SSB 0
LB 3.00
Ms
N
1j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

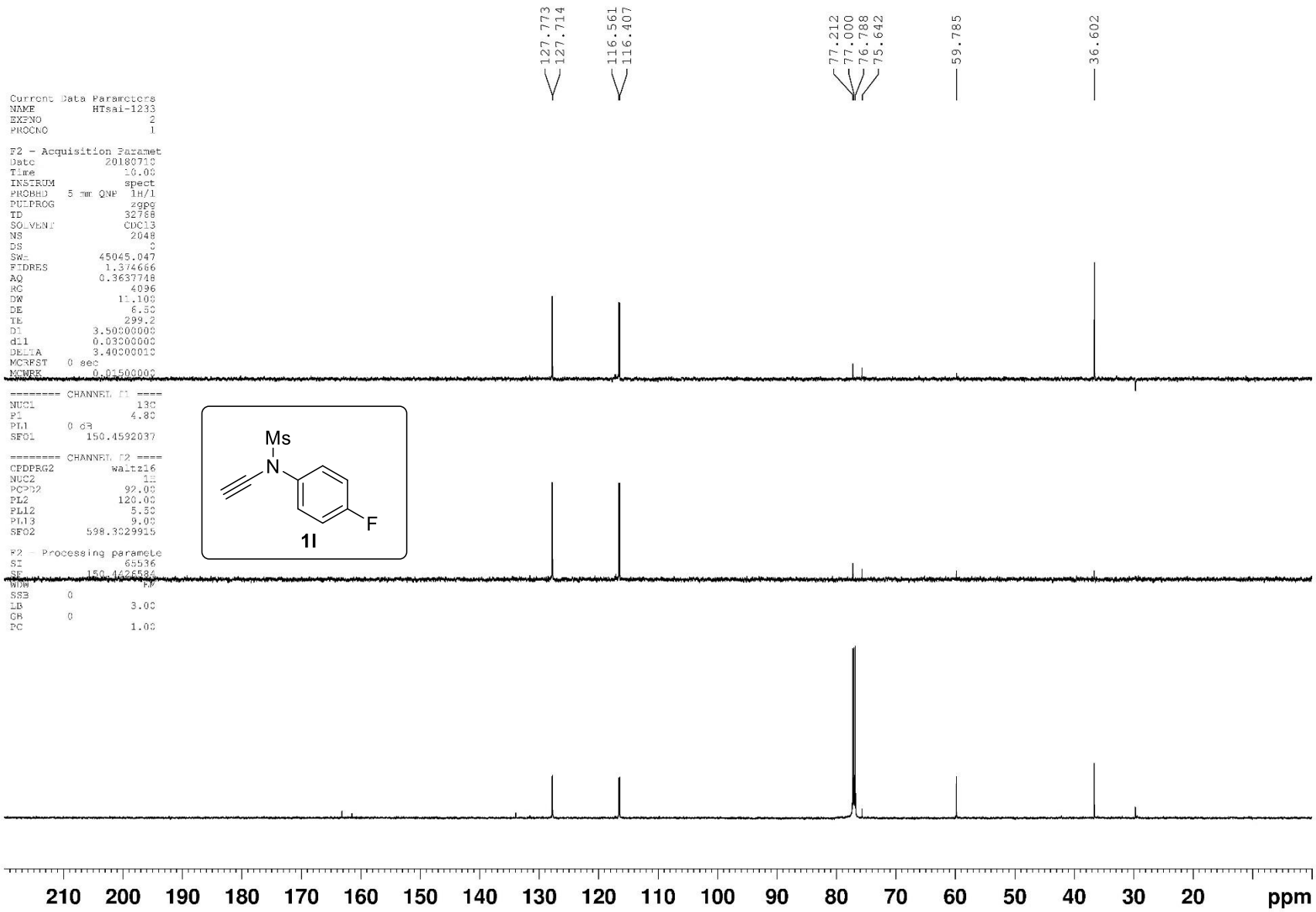


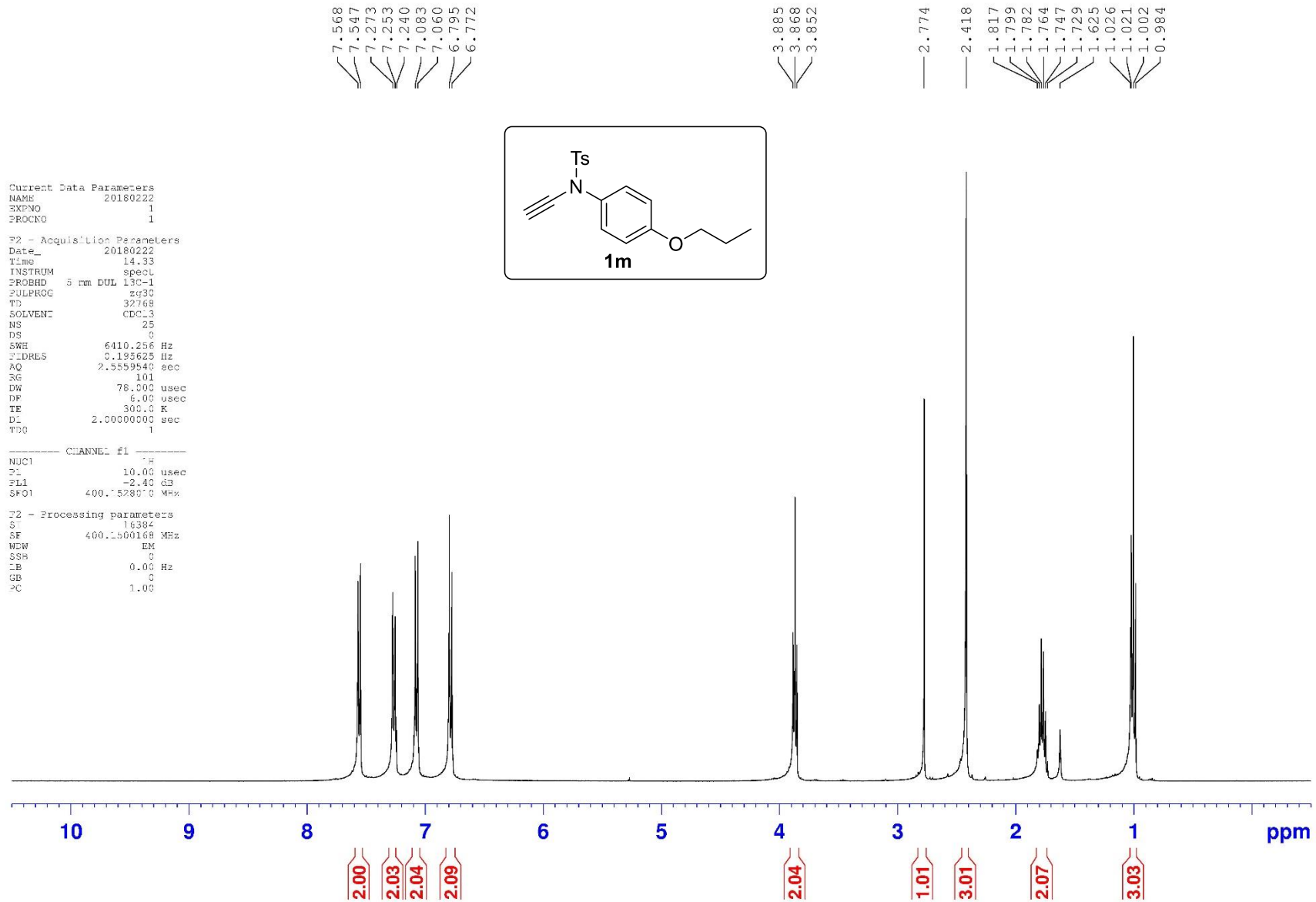





```
Current Data Parameters
NAME          HFsai-1233
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180710
Time               9.45
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG              zg
TD                32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH             9541.984 Hz
FIDRES          0.291198 Hz
AQ              1.7170932 sec
RG                   512
DW                52.400 usec
DE                 6.50 usec
TE                299.1 K
D1             2.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                10.00 usec
PL1                2.00 dB
SFO1         598.3035130 MHz

F2 - Processing parameters
SI                 32768
SF           598.3000284 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                  2.00
```




127.773
127.714
116.561
116.407
77.212
77.000
76.788
75.642
59.785
36.602
Current Data Parameters
NAME HTsai-1233
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180710
Time 10.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 299.2
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4592037
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426582
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ms
N
F
1l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.568
7.547
7.273
7.253
7.240
7.083
7.060
6.795
6.772
3.885
3.868
3.852
2.774
2.418
1.817
1.799
1.782
1.764
1.747
1.729
1.625
1.026
1.021
1.002
0.984
Ts
N
O
1m
Current Data Parameters
NAME 20180222
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180222
Time 14.33
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 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 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
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ppm
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2.03
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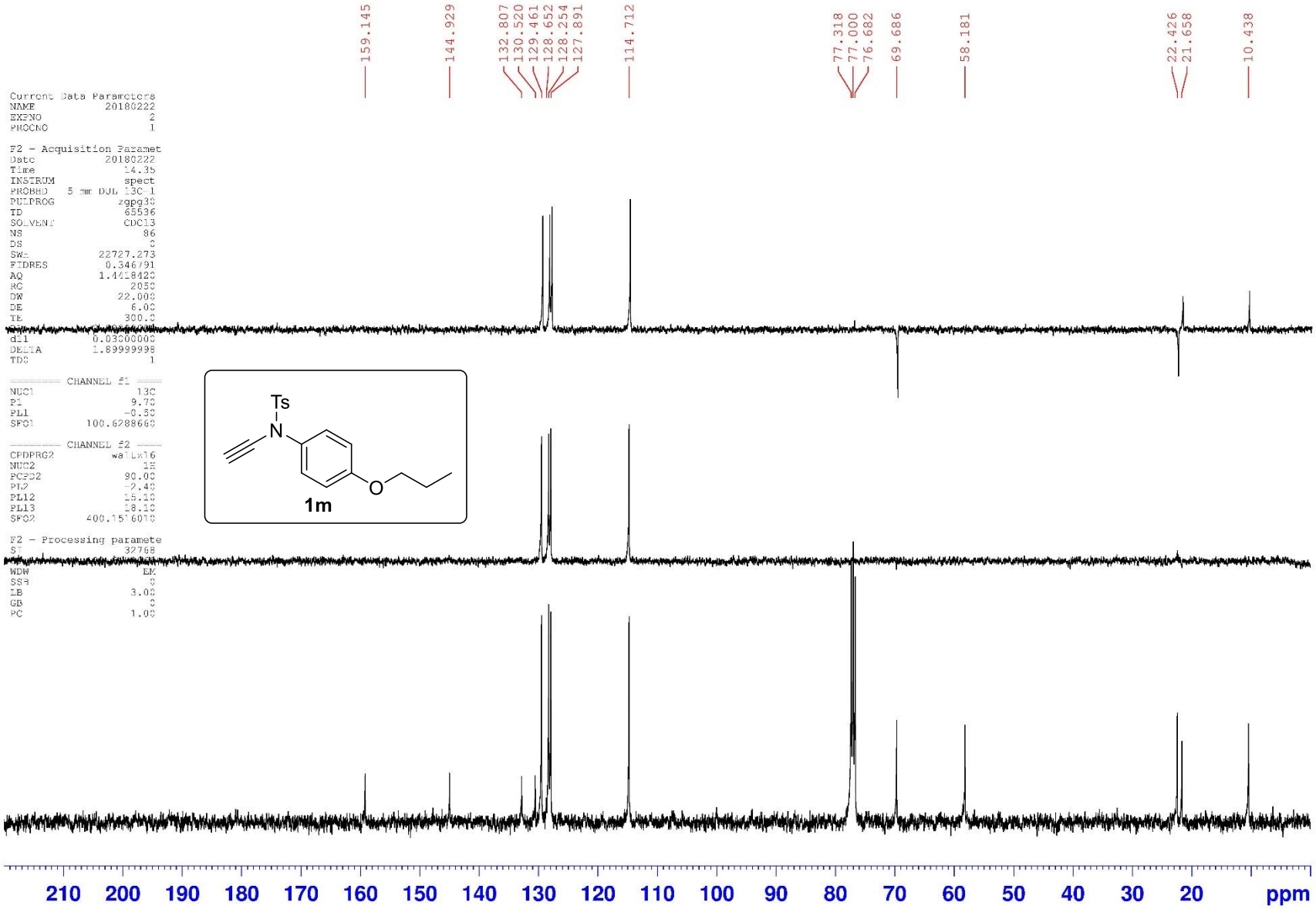
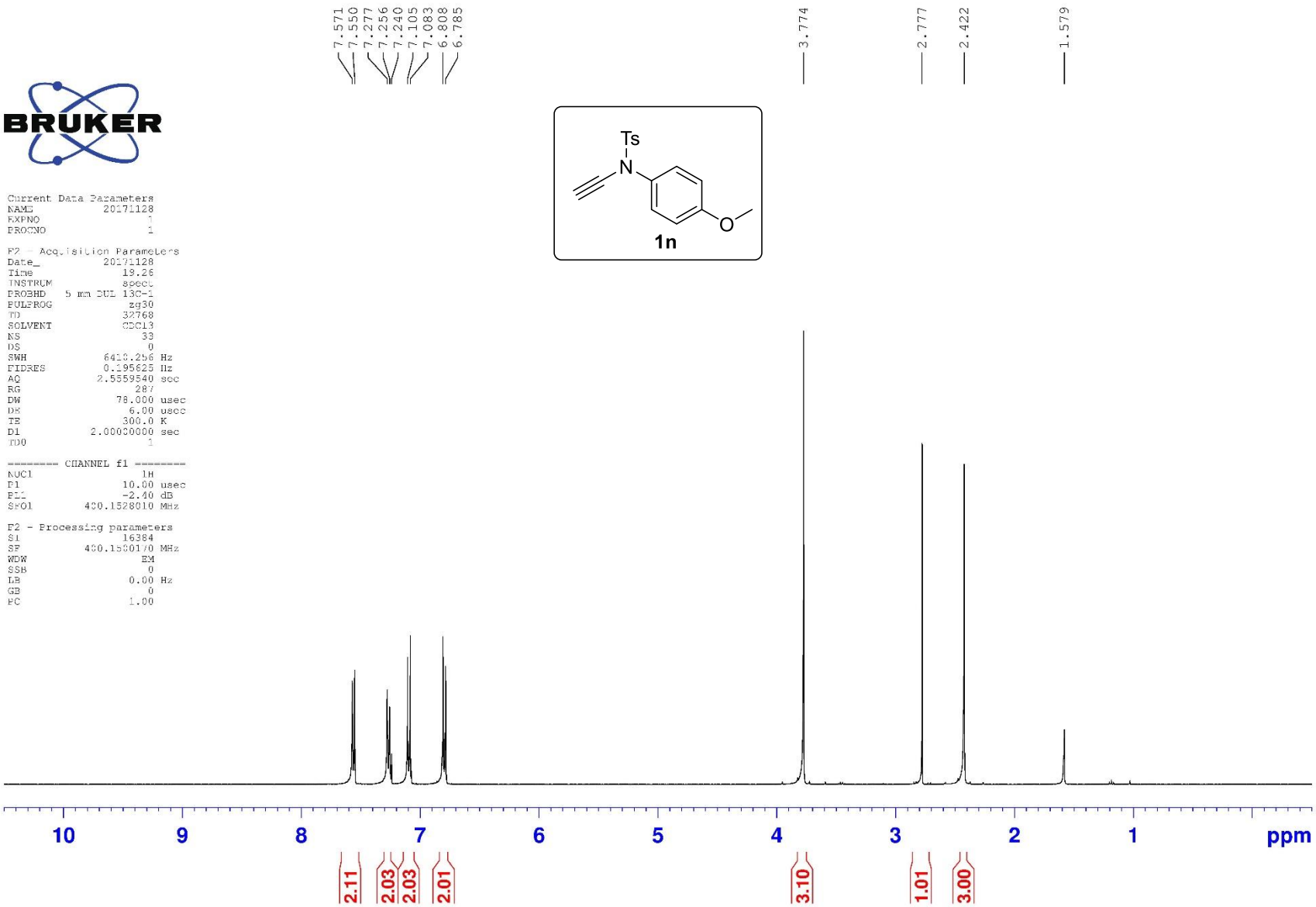
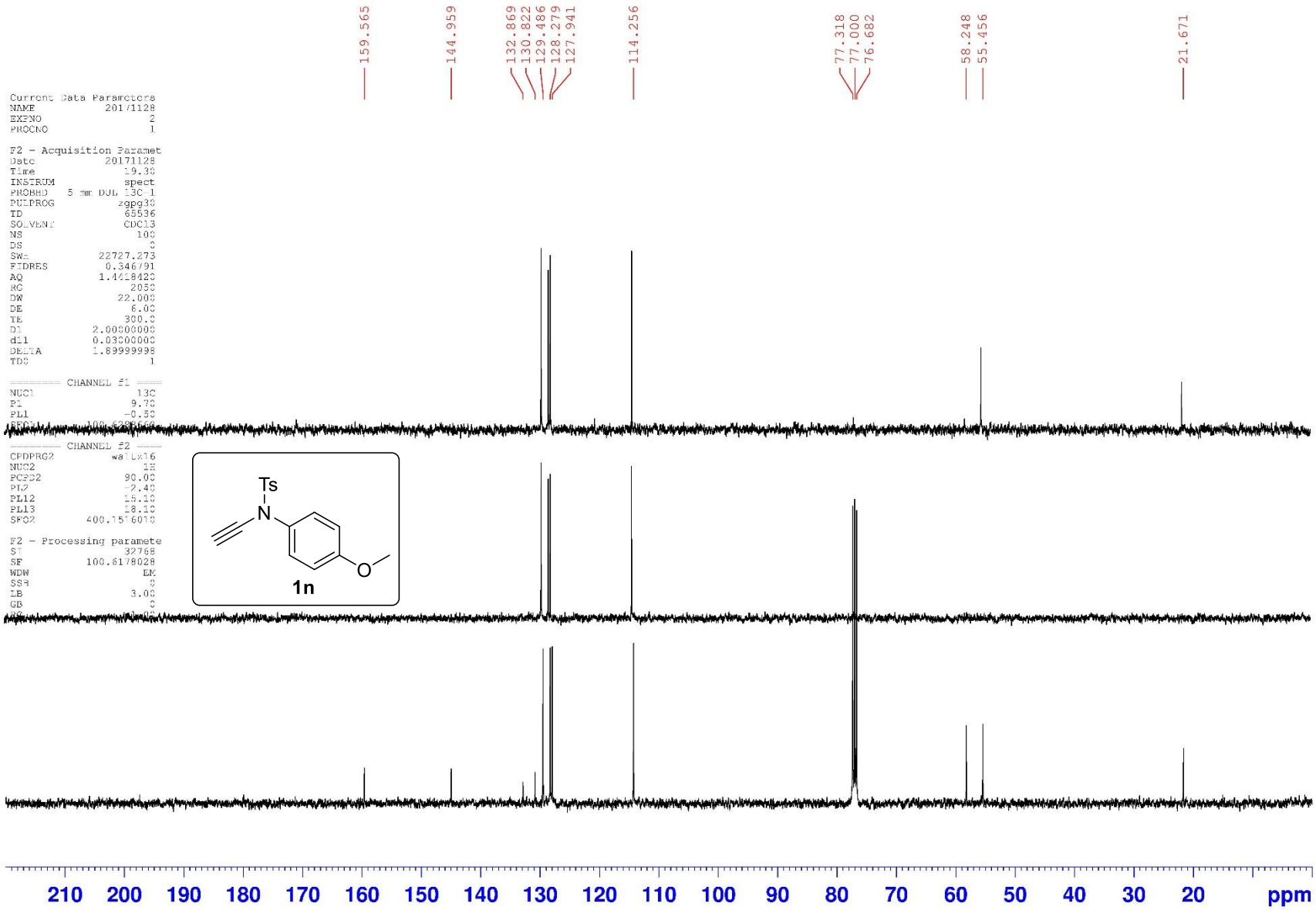
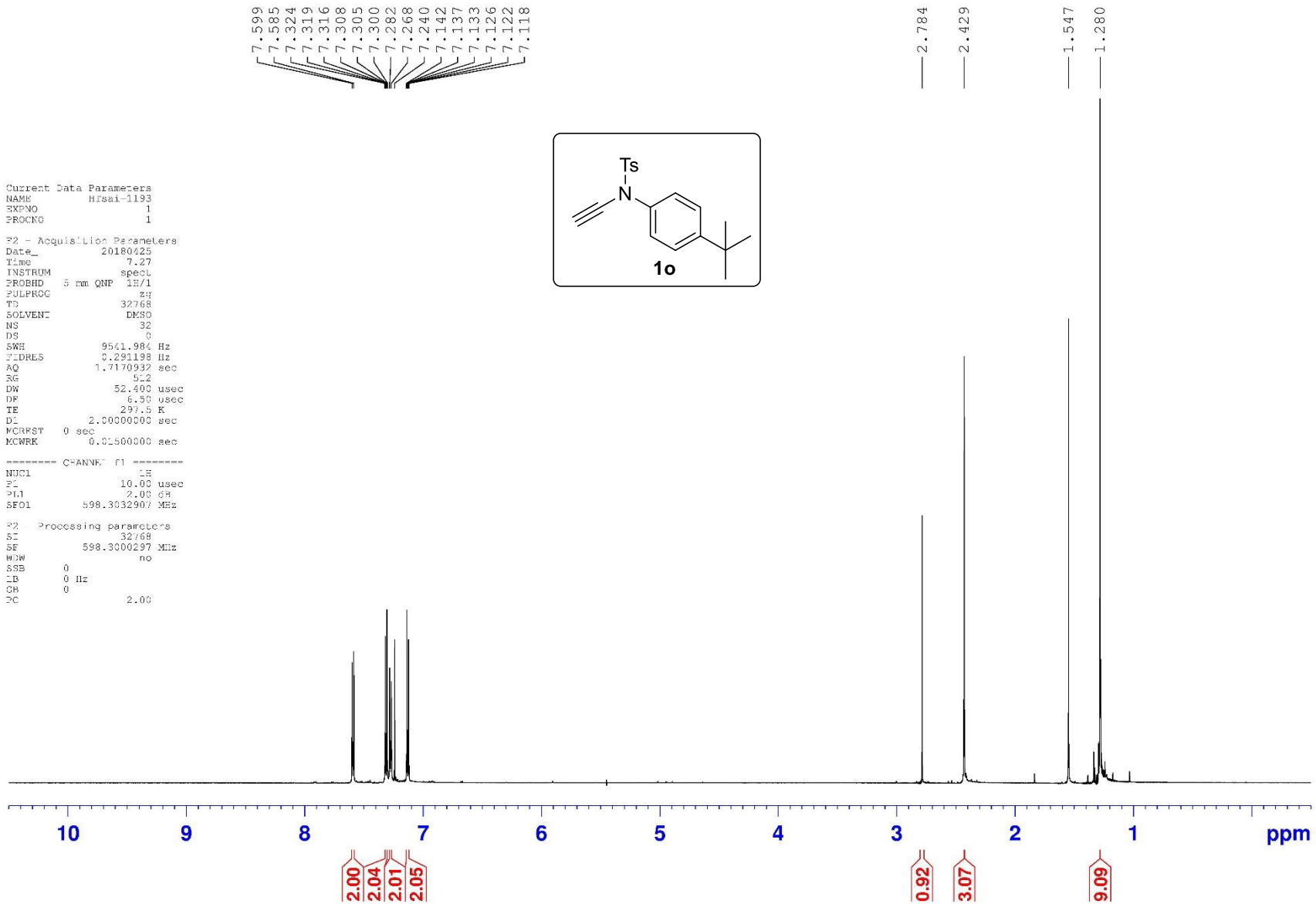
2.09
2.04
1.01
3.01
2.07
3.03


159.145
144.929
132.807
130.520
129.461
128.652
128.254
127.891
114.712
77.318
77.000
76.682
69.686
58.181
22.426
21.658
10.438
Current Data Parameters
NAME 20180222
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180222
Time 14.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 86
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
Ts
N
O
1m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.571
7.550
7.277
7.256
7.240
7.105
7.083
6.808
6.785
3.774
2.777
2.422
1.579
Ts
N
O
1n
Current Data Parameters
NAME 20171128
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171128
Time 18.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
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
10
9
8
7
6
5
4
3
2
1
ppm
2.11
2.03
2.03
2.01
3.10
1.01
3.00


159.565
144.959
132.869
130.822
129.486
128.279
127.941
114.256
77.318
77.000
76.682
58.248
55.456
21.671
Current Data Parameters
NAME 201/1128
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171128
Time 19.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178028
WDW EM
SSB 0
LB 3.00
GB 0
Ts
N
O
1n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.599
7.585
7.324
7.319
7.316
7.308
7.305
7.300
7.282
7.268
7.240
7.142
7.137
7.133
7.126
7.122
7.118
2.784
2.429
1.547
1.280
Ts
N
1o
Current Data Parameters
NAME HFsai-1193
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20180425
Time 7.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT DMSO
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 297.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 2.00 dB
SFO1 598.3032907 MHz
P2 - Processing parameters
SI 32768
SF 598.3000297 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
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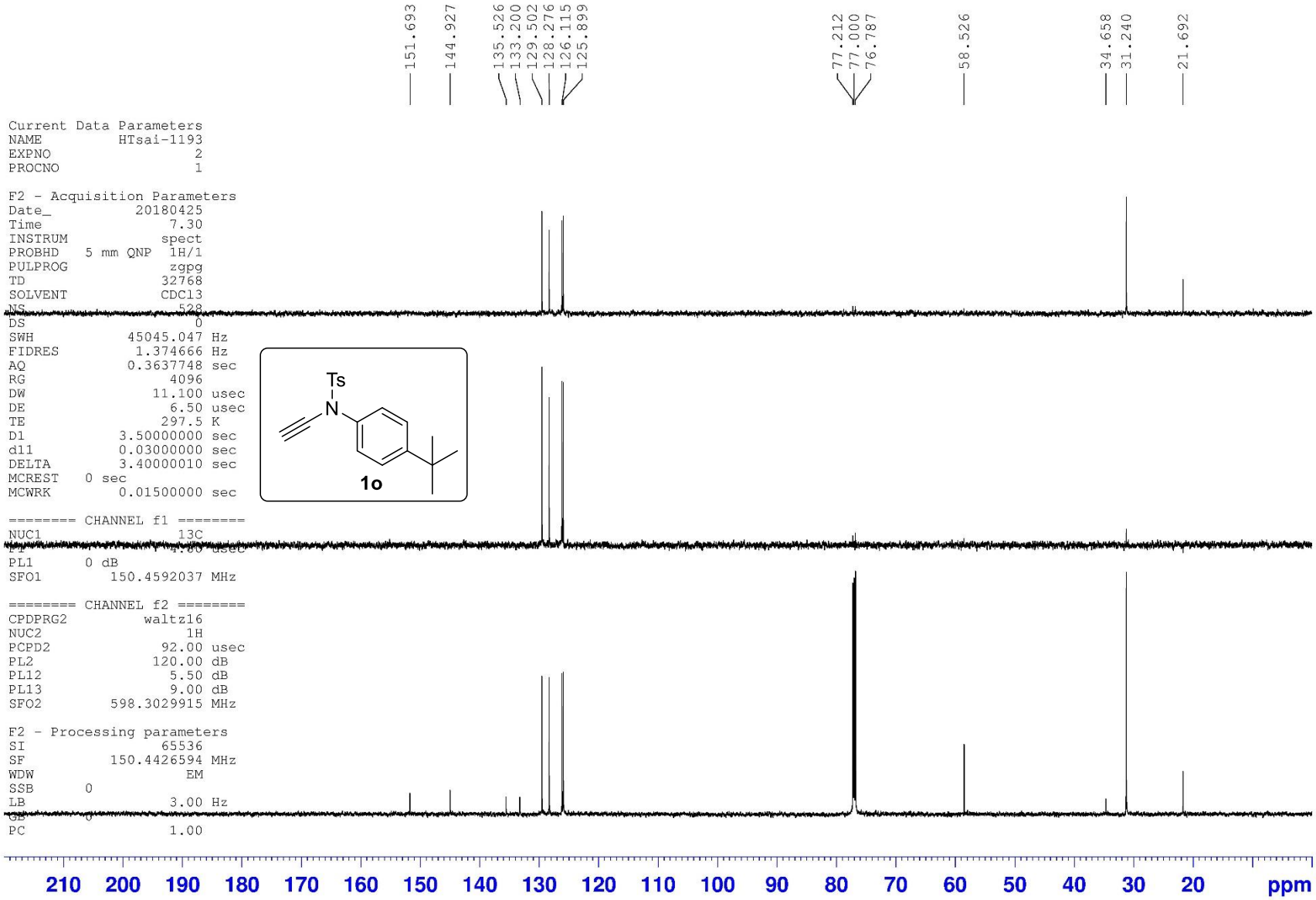
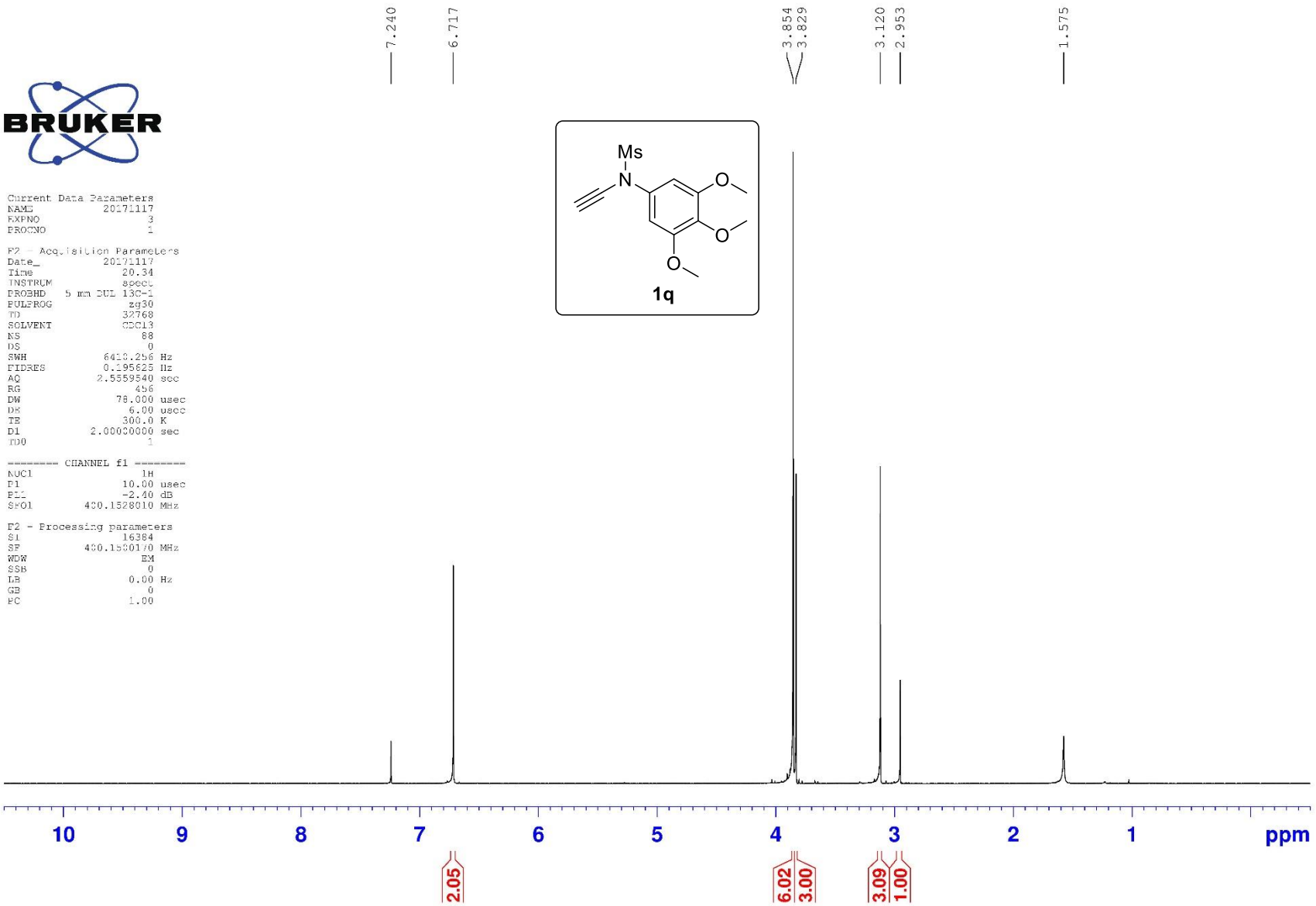
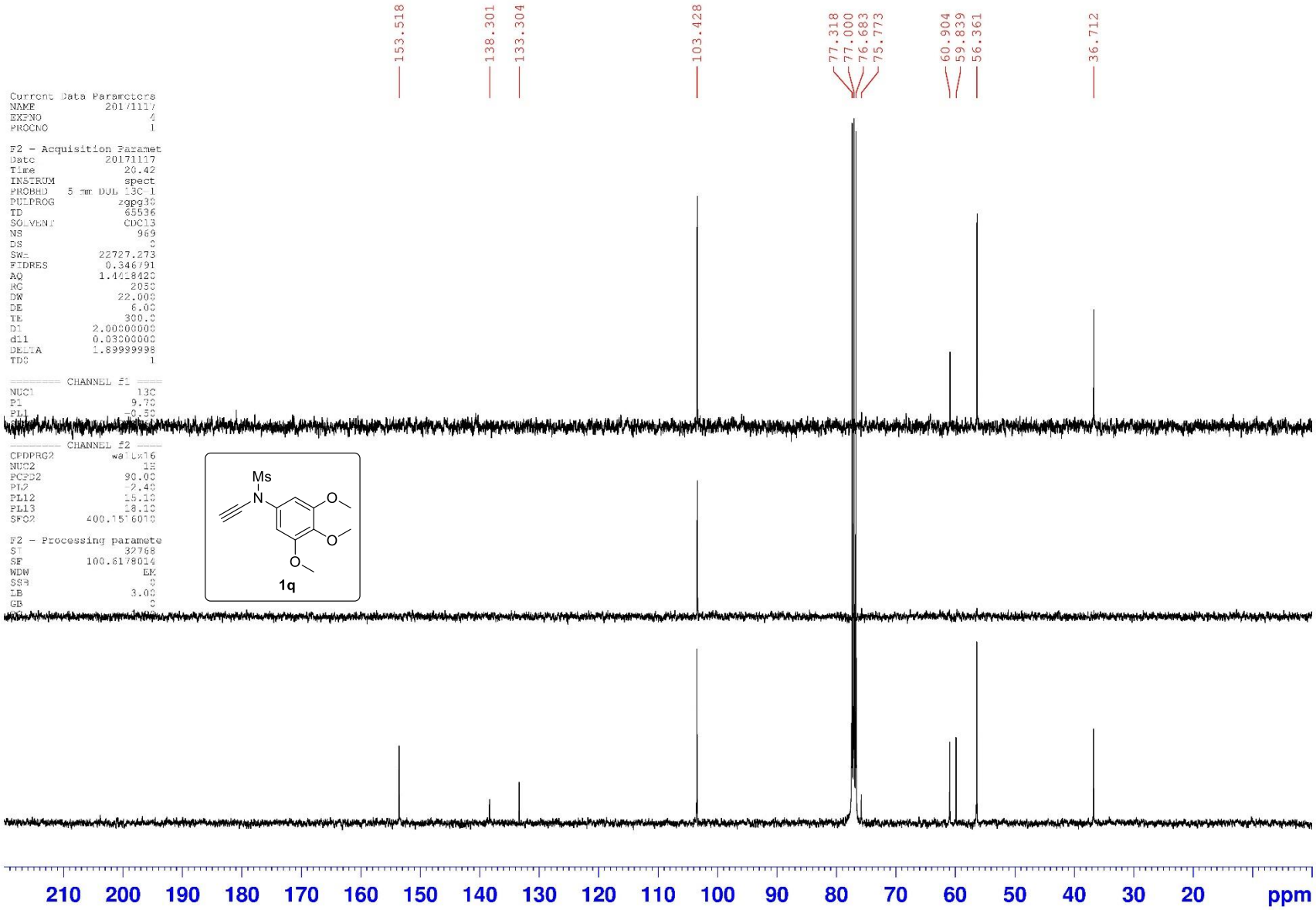
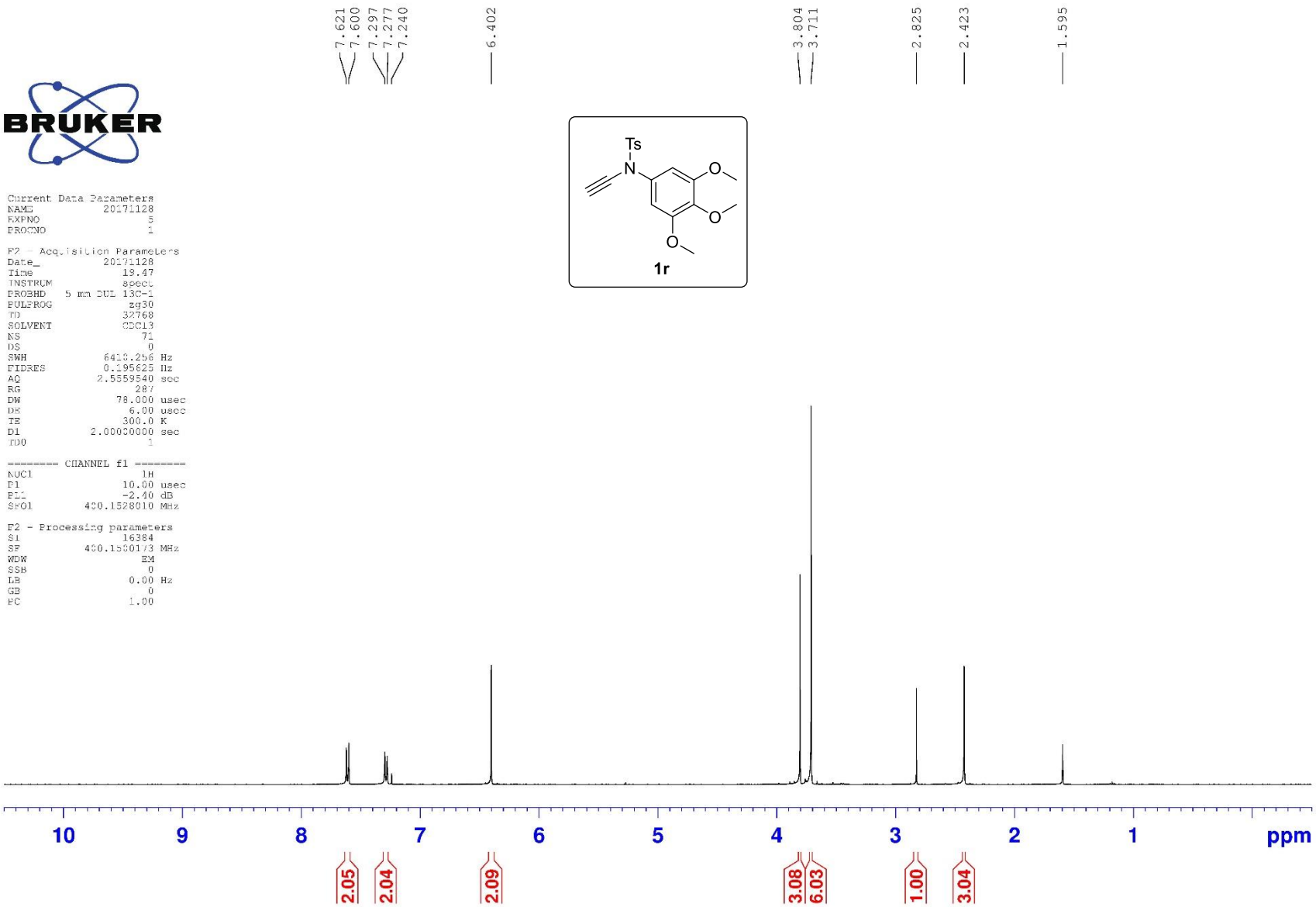
2.04
2.01
2.05
0.92
3.07
9.09

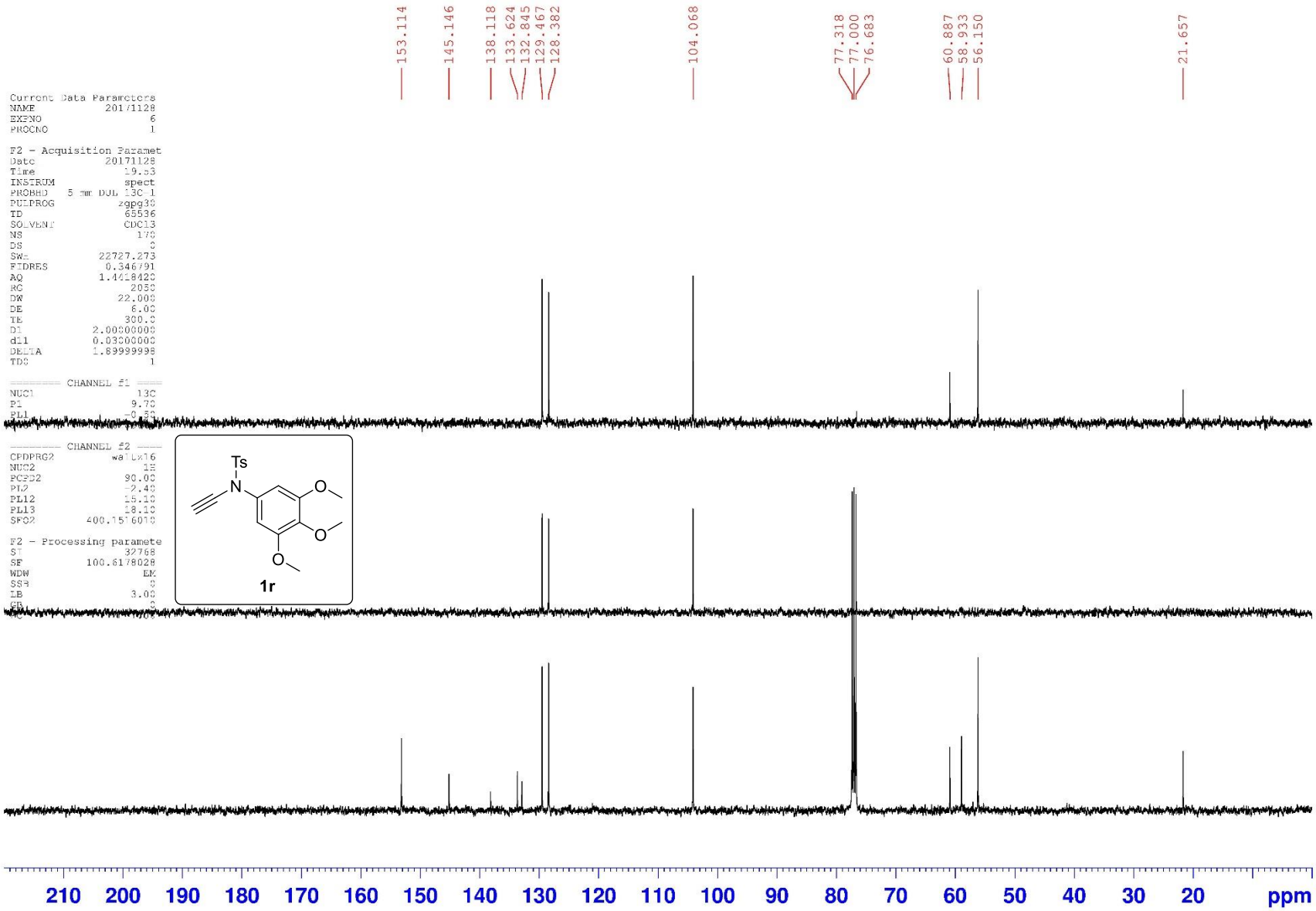

151.693
144.927
135.526
133.200
129.502
128.276
126.115
125.899
77.212
77.000
76.787
58.526
34.658
31.240
21.692
Current Data Parameters
NAME HTsai-1193
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180425
Time 7.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 528
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 297.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
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 150.4426594 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
1o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

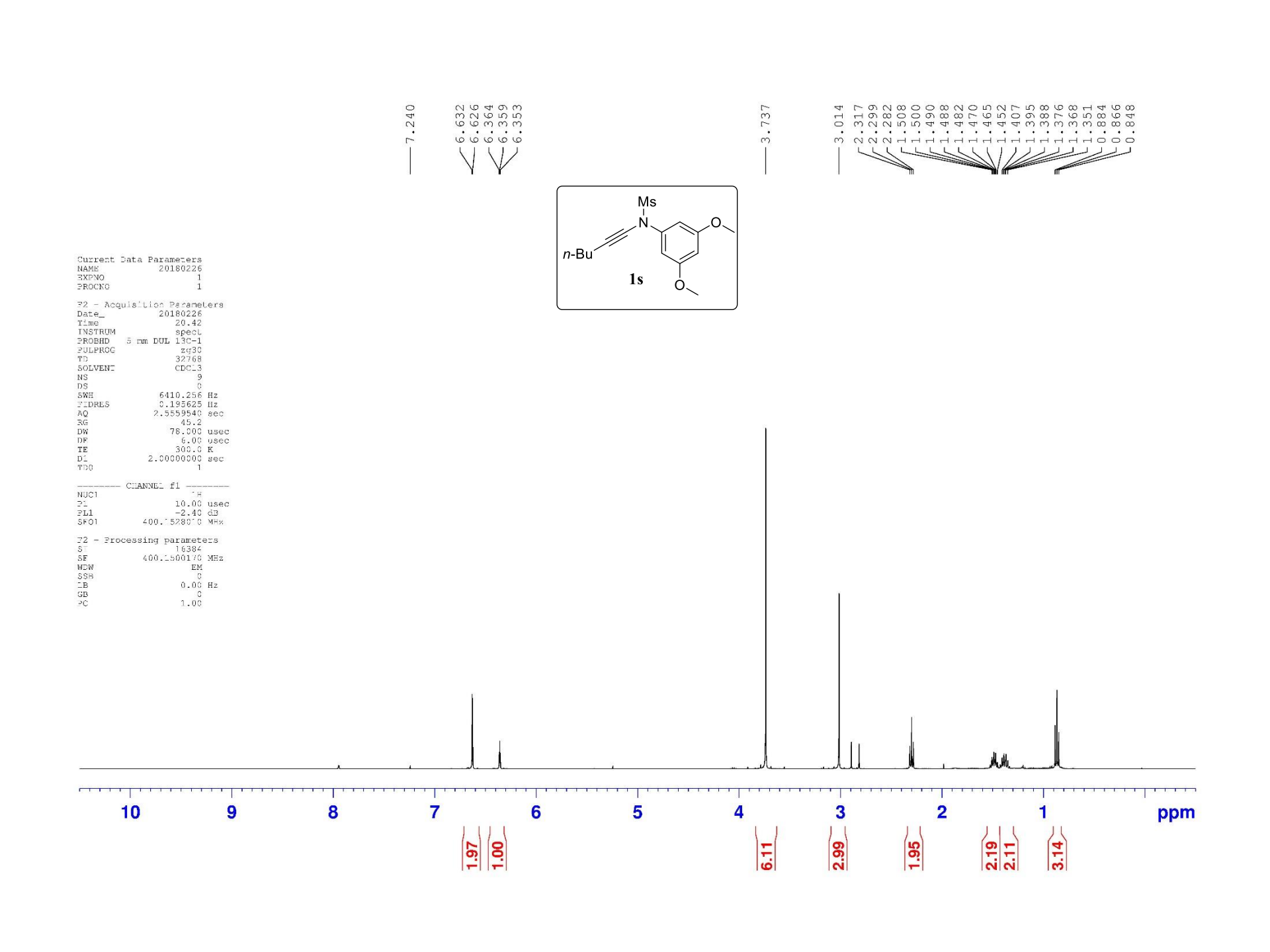


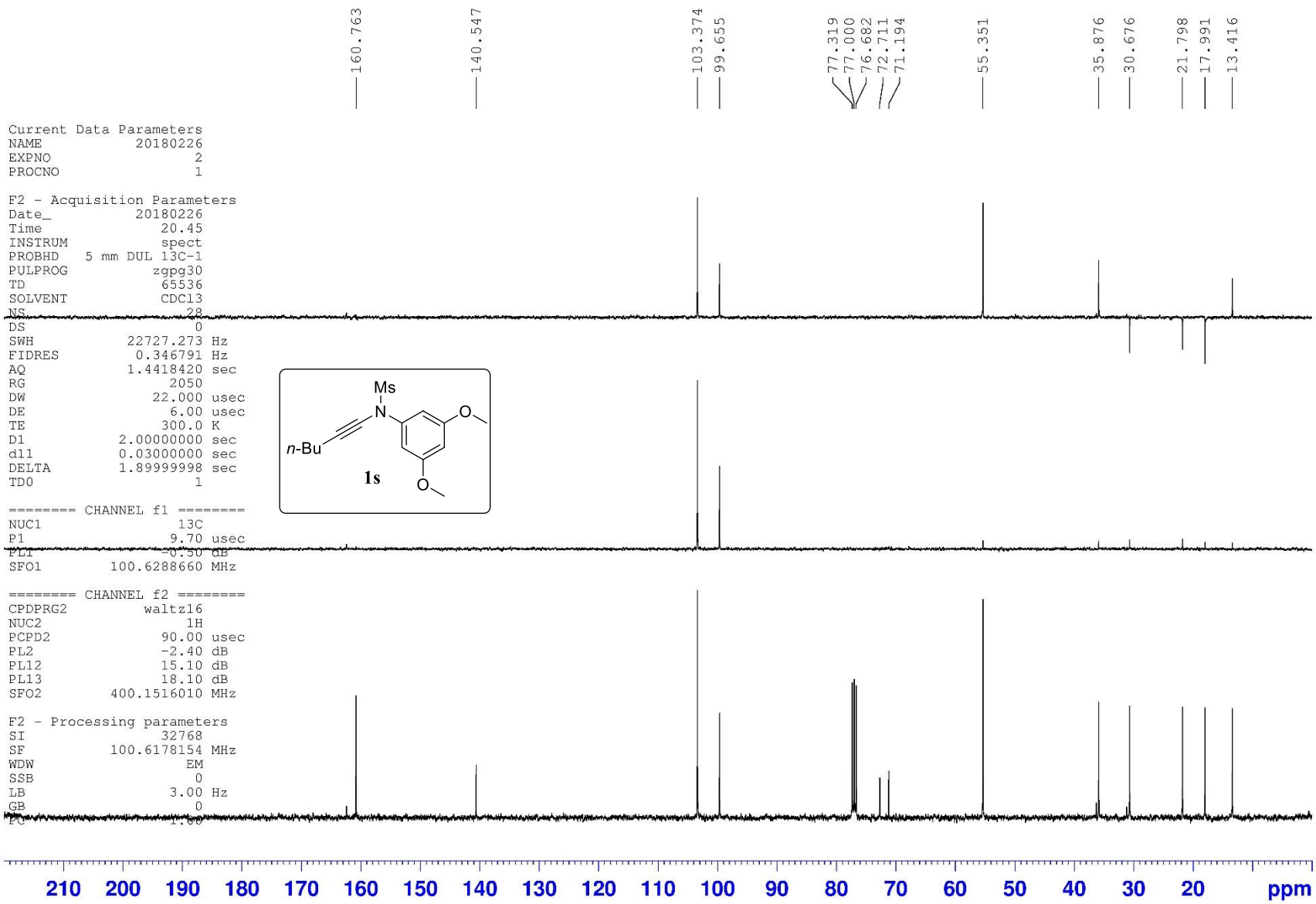

```
Current Data Parameters
NAME                  20171117
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20171117
Time                   20.34
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       88
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
```

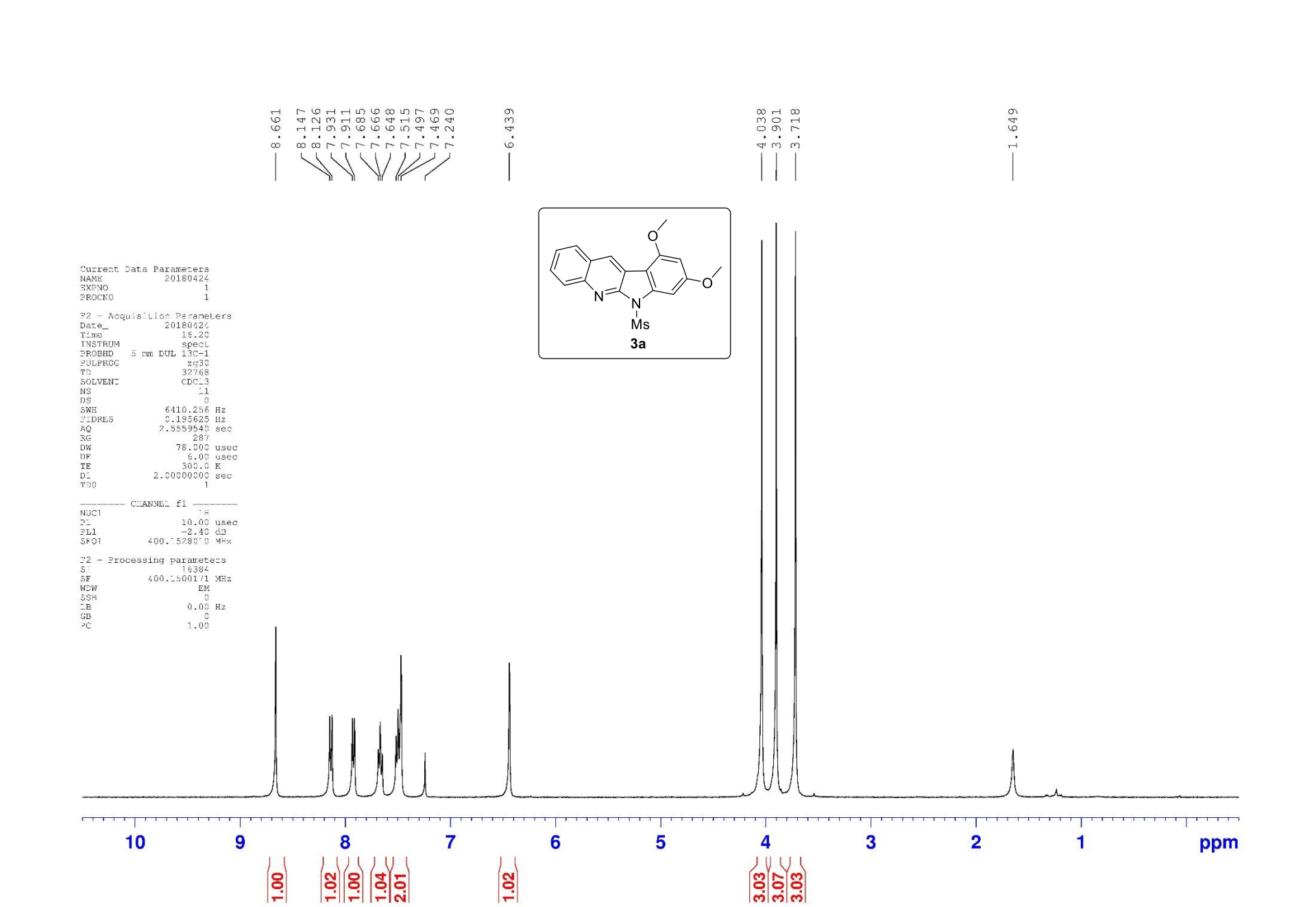

153.518
138.301
133.304
103.428
77.318
77.000
76.683
75.773
60.904
59.839
56.361
36.712
Current Data Parameters
NAME 201711l7
EXPNO 4
PROCNO 1
F2 - Acquisition Paramet
Date 20171117
Time 20.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 969
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.38
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.18
PL13 18.18
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178014
WDW EM
SSB 0
LB 3.00
GB 0
Ms
N
O
O
O
1q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

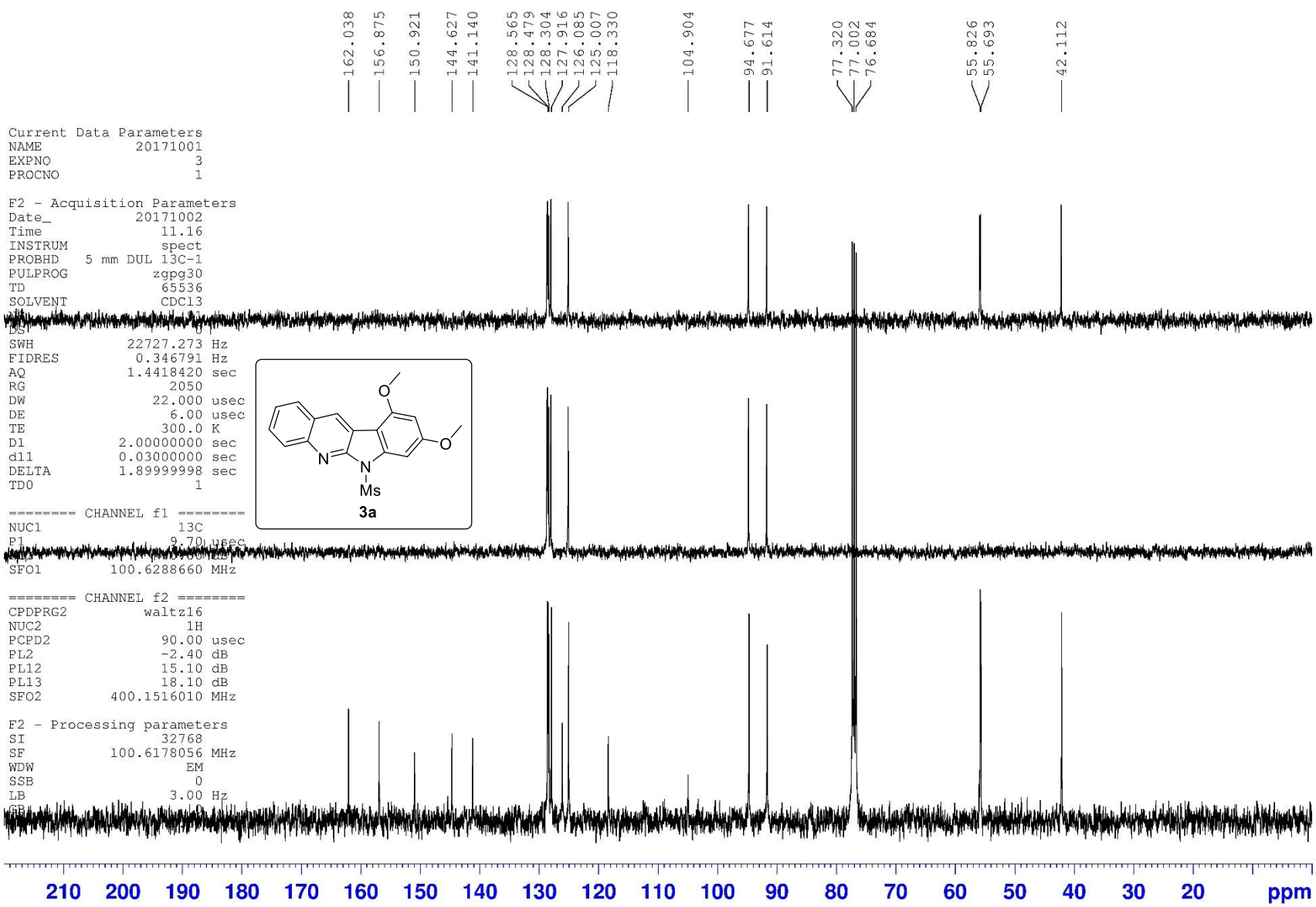

7.621
7.600
7.297
7.277
7.240
6.402
3.804
3.711
2.825
2.423
1.595
Ts
N
O
O
O
1r
Current Data Parameters
NAME 20171128
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171128
Time 18.47
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 71
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.05
2.04
2.09
3.08
6.03
1.00
3.04

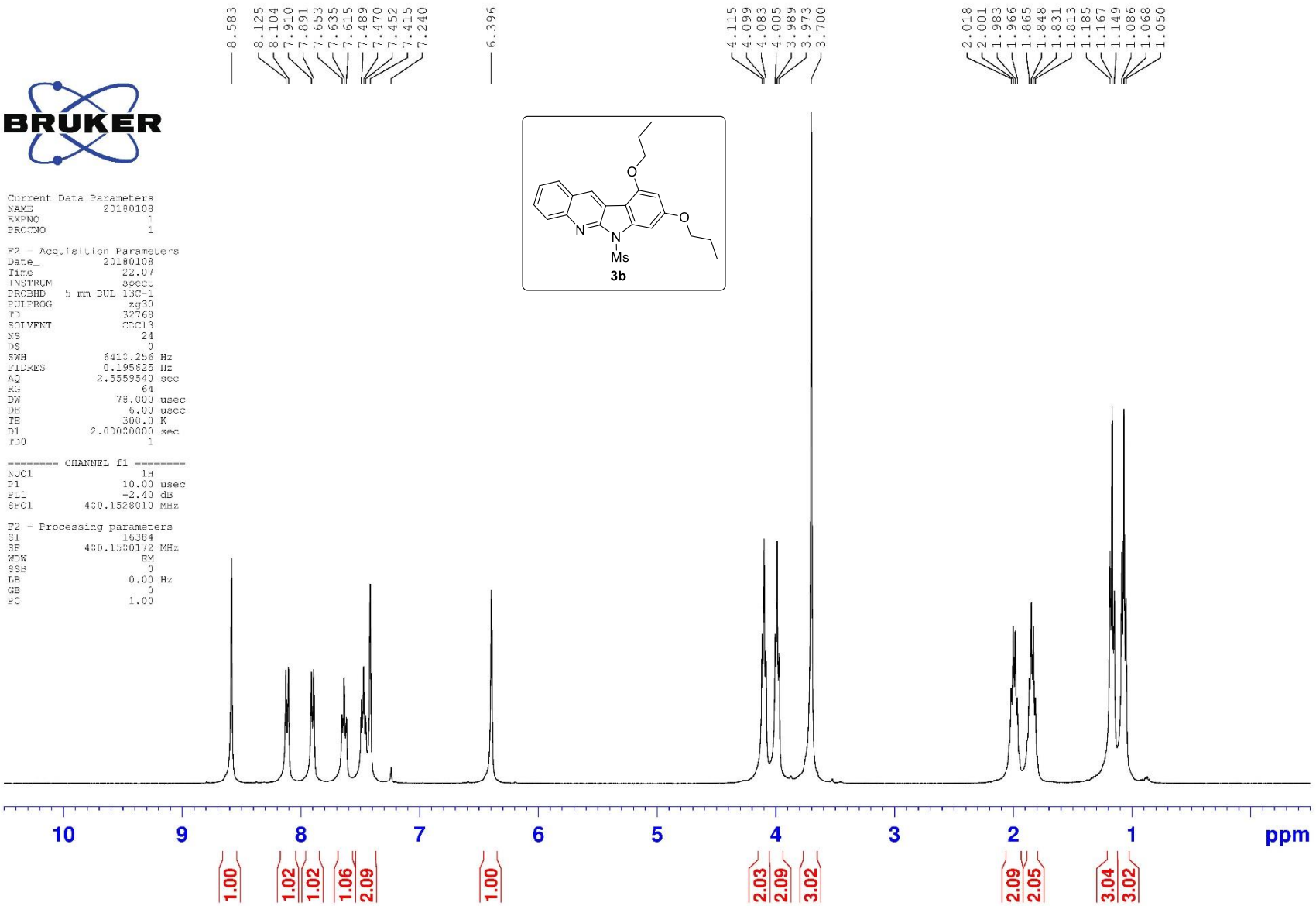

153.114
145.146
138.118
133.624
132.845
129.467
128.382
104.068
77.318
77.000
76.683
60.887
58.933
56.150
21.657
Current Data Parameters
NAME 201/1128
EXPNO 6
PROCNO 1
F2 - Acquisition Paramet
Date 20171128
Time 19.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 176
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.50
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178028
WDW EM
SSB 0
LB 3.00
GB 0
Ts
N
O
O
O
1r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.240
6.632
6.626
6.364
6.359
6.353
3.737
3.014
2.317
2.299
2.282
1.508
1.500
1.490
1.488
1.482
1.470
1.465
1.452
1.407
1.395
1.388
1.376
1.368
1.351
0.884
0.866
0.848
Ms
N
O
O
n-Bu
1s
Current Data Parameters
NAME 20180226
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180226
Time 20.42
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 45.2
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 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.97
1.00
6.11
2.99
1.95
2.19
2.11
3.14


160.763
140.547
103.374
99.655
77.319
77.000
76.682
72.711
71.194
55.351
35.876
30.676
21.798
17.991
13.416
Current Data Parameters
NAME 20180226
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180226
Time 20.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 28
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 100.6178154 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
Ms
N
O
O
n-Bu
1s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.661
8.147
8.126
7.931
7.911
7.685
7.666
7.648
7.515
7.497
7.469
7.240
6.439
4.038
3.901
3.718
1.649
Current Data Parameters
NAME 20180424
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180424
Time 16.20
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 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 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
O
N
N
Ms
3a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
1.00
1.04
2.01
1.02
3.03
3.07
3.03


162.038
156.875
150.921
144.627
141.140
128.565
128.479
128.304
127.916
126.085
125.007
118.330
104.904
94.677
91.614
77.320
77.002
76.684
55.826
55.693
42.112
Current Data Parameters
NAME 20171001
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171002
Time 11.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
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
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 100.6178056 MHz
WDW EM
SSB 0
LB 3.00 Hz
O
O
N
N
Ms
3a
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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8.125
8.104
7.910
7.891
7.653
7.635
7.615
7.489
7.470
7.452
7.415
7.240
6.396
4.115
4.099
4.083
4.005
3.989
3.973
3.700
2.018
2.001
1.983
1.966
1.865
1.848
1.831
1.813
1.185
1.167
1.149
1.086
1.068
1.050
BRUKER
Current Data Parameters
NAME 20180108
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180108
Time 22.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 64
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
O
N
N
Ms
O
3b
10
9
8
7
6
5
4
3
2
1
ppm
1.00
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2.09
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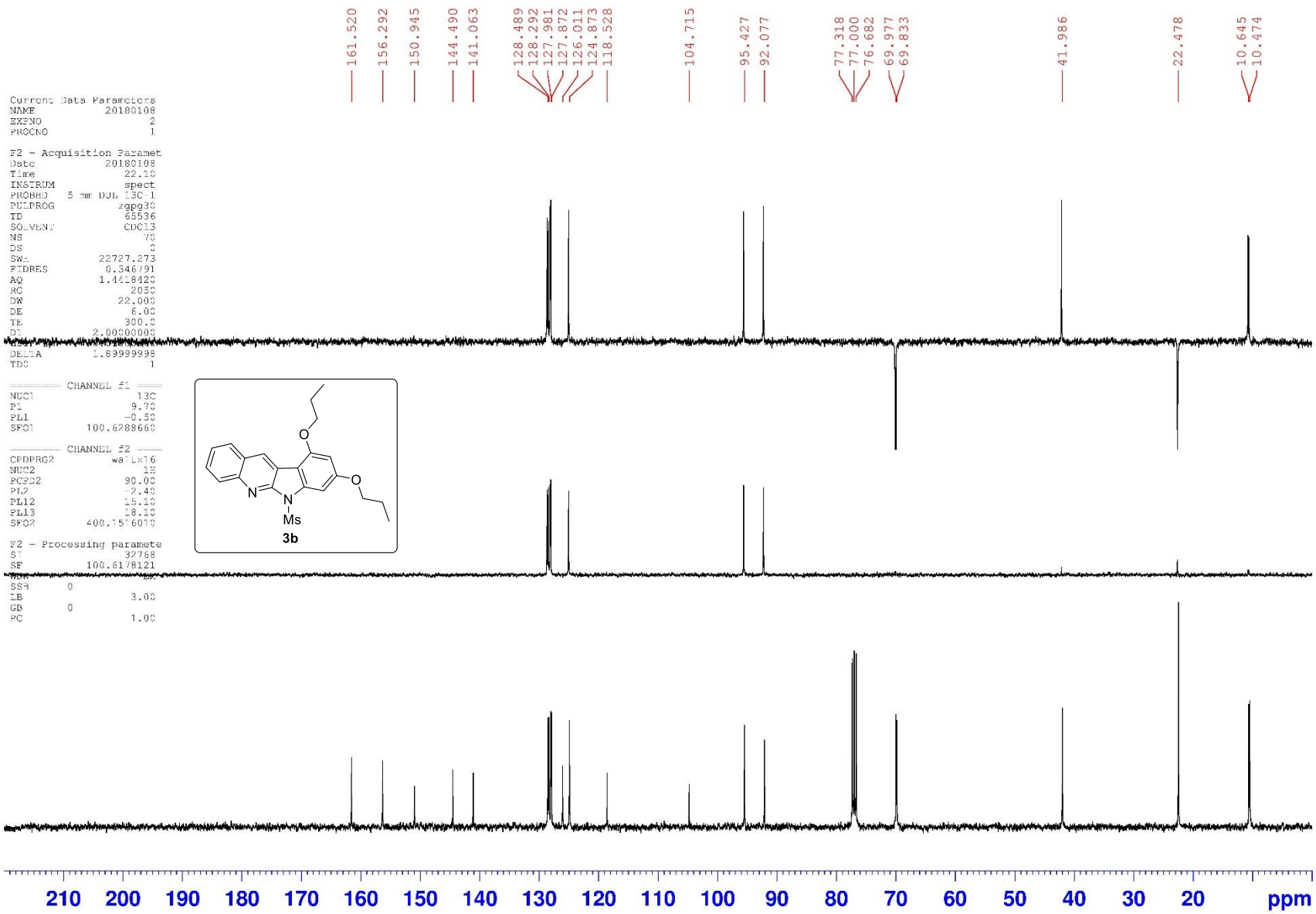
2.09
3.02
2.09
2.05
3.04
3.02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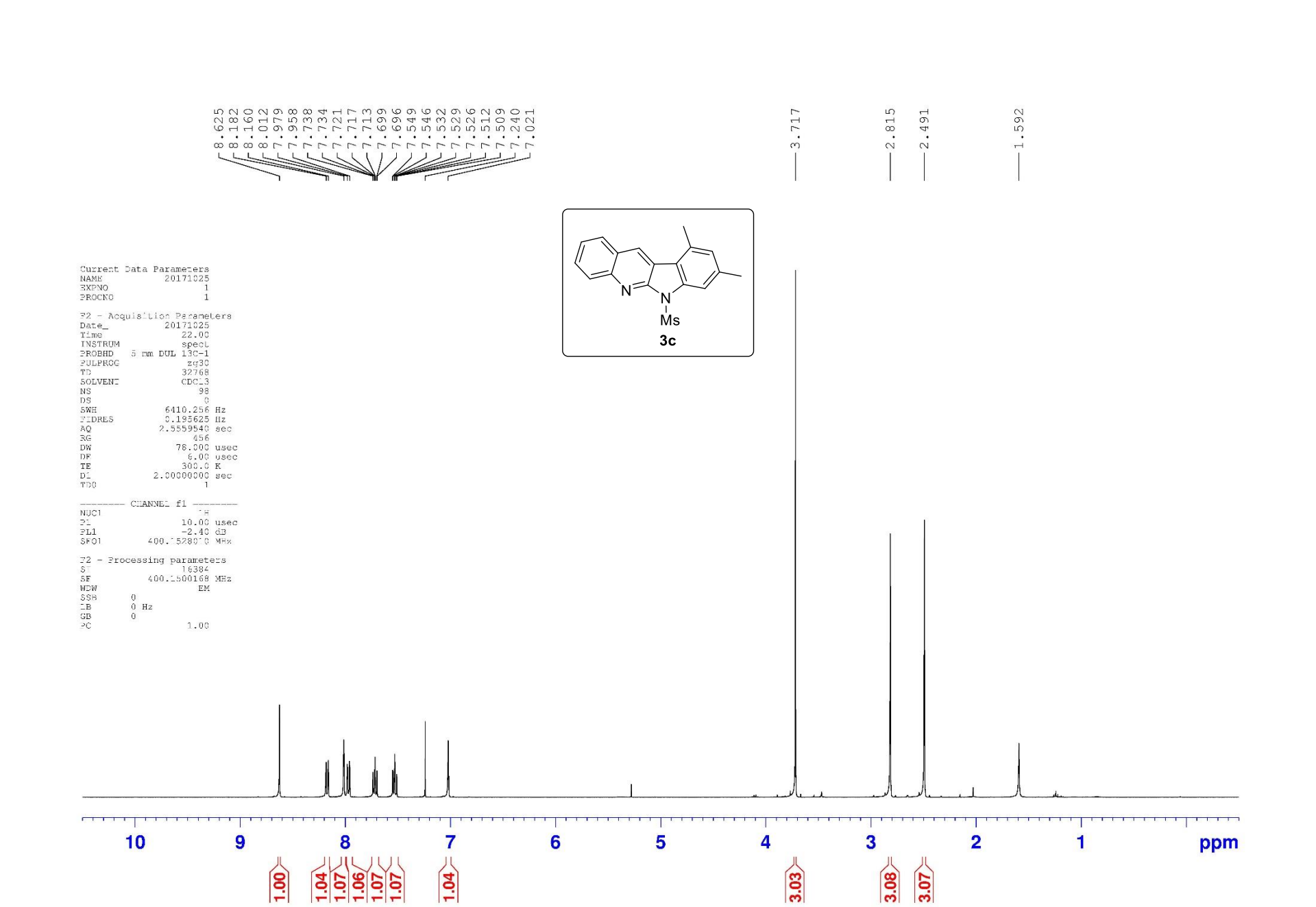
156.292
150.945
144.490
141.063
128.489
128.292
127.981
127.872
126.011
124.873
118.528
104.715
95.427
92.077
77.318
77.000
76.682
69.977
69.833
41.986
22.478
10.645
10.474
Current Data Parameters
NAME 20180108
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180108
Time 22.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 70
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178121
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
O
N
N
Ms
O
3b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.625
8.182
8.160
8.012
7.979
7.958
7.738
7.734
7.721
7.717
7.713
7.699
7.696
7.549
7.546
7.532
7.529
7.526
7.512
7.509
7.240
7.021
3.717
2.815
2.491
1.592
N
N
Ms
3c
Current Data Parameters
NAME 20171025
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171025
Time 22.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 98
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 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
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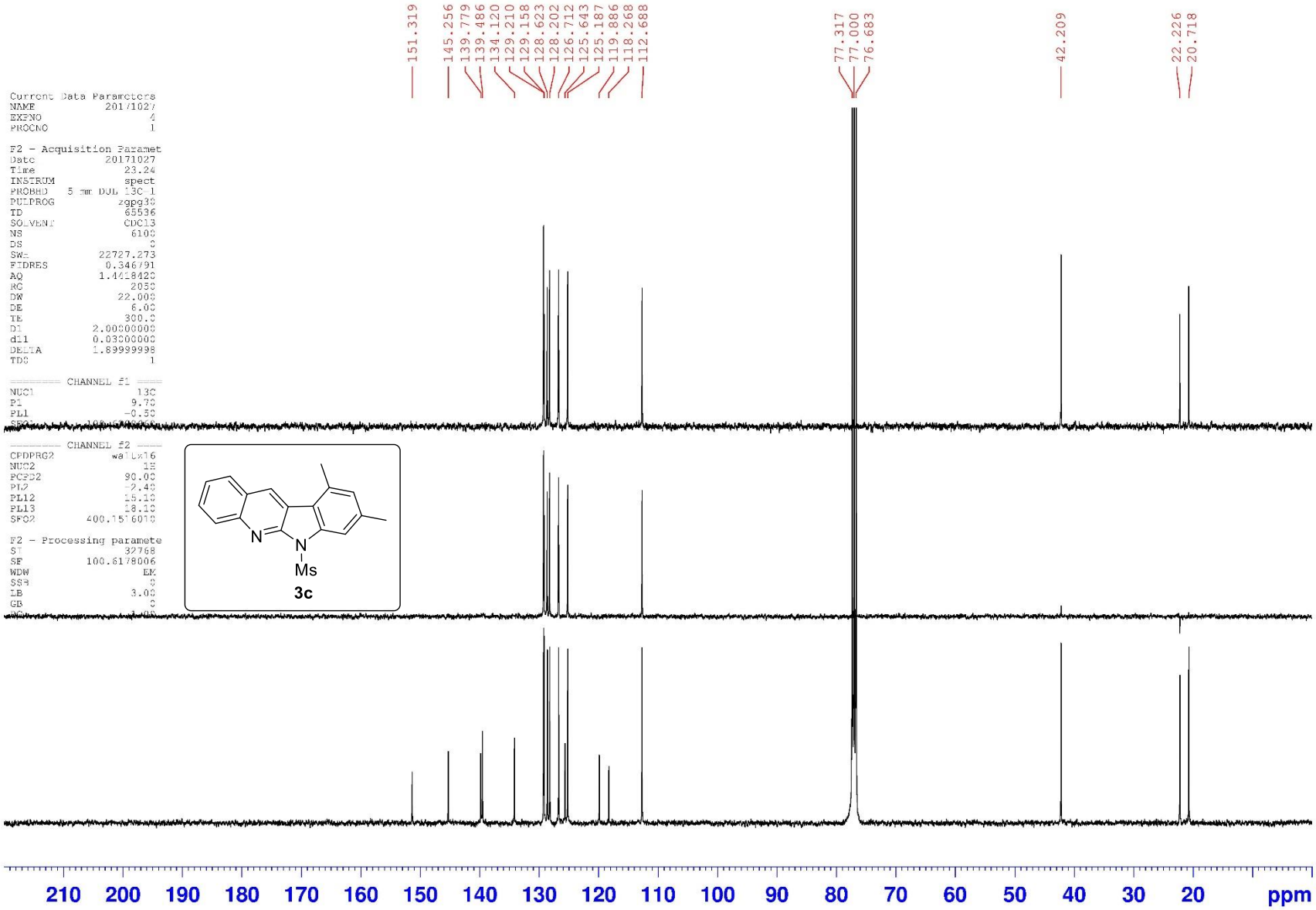
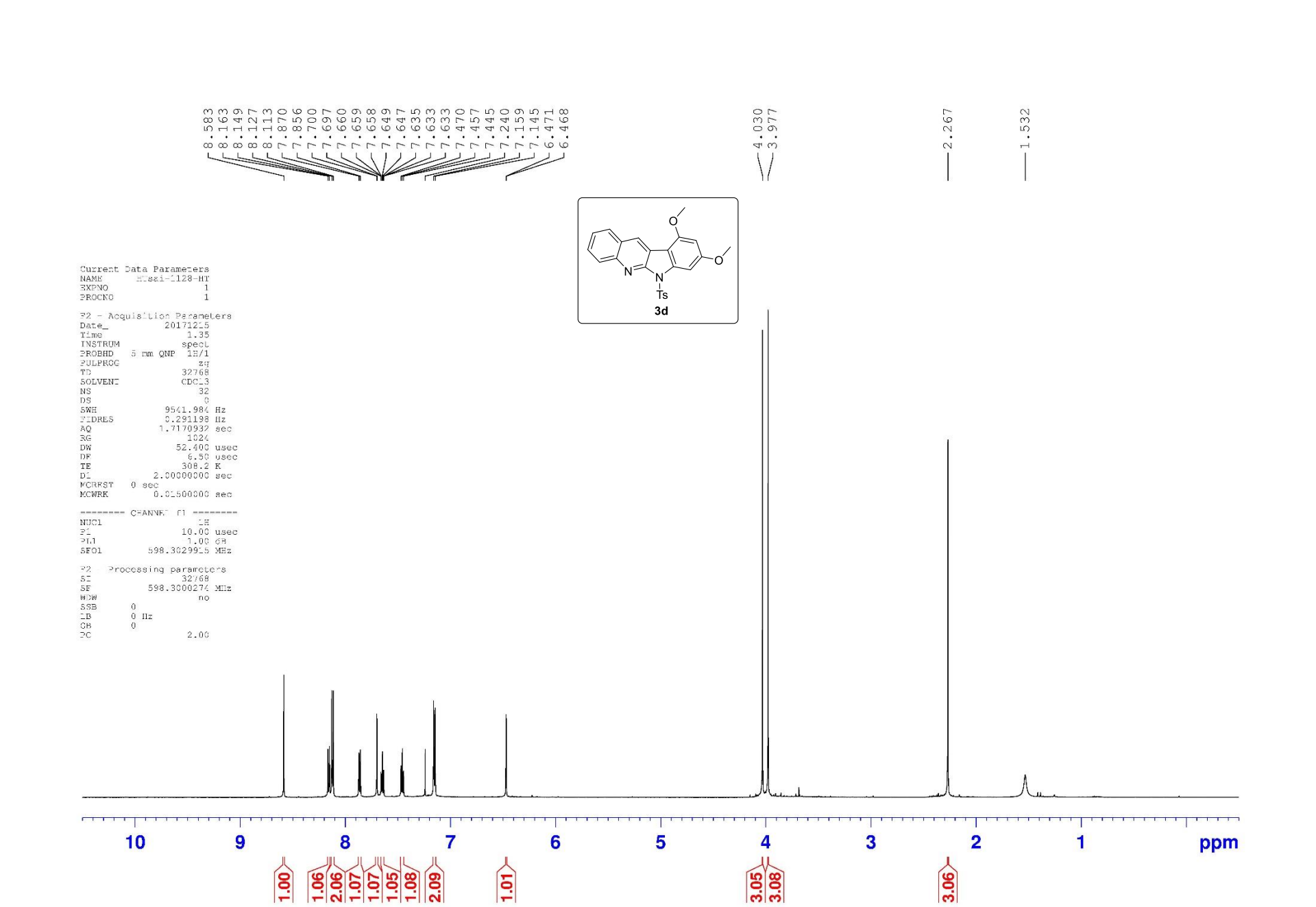
1.04
1.07
1.06
1.07
1.07
1.04
3.03
3.08
3.07


151.319
145.256
139.779
139.486
134.120
129.210
129.158
128.623
128.202
126.712
125.643
125.187
119.886
118.268
112.688
77.317
77.000
76.683
42.209
22.226
20.718
Current Data Parameters
NAME 201/1027
EXPNO 4
PROCNO 1
F2 - Acquisition Paramet
Date 20171027
Time 23.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6100
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178006
WDW EM
SSB 0
LB 3.00
GB 0
N
N
Ms
3c
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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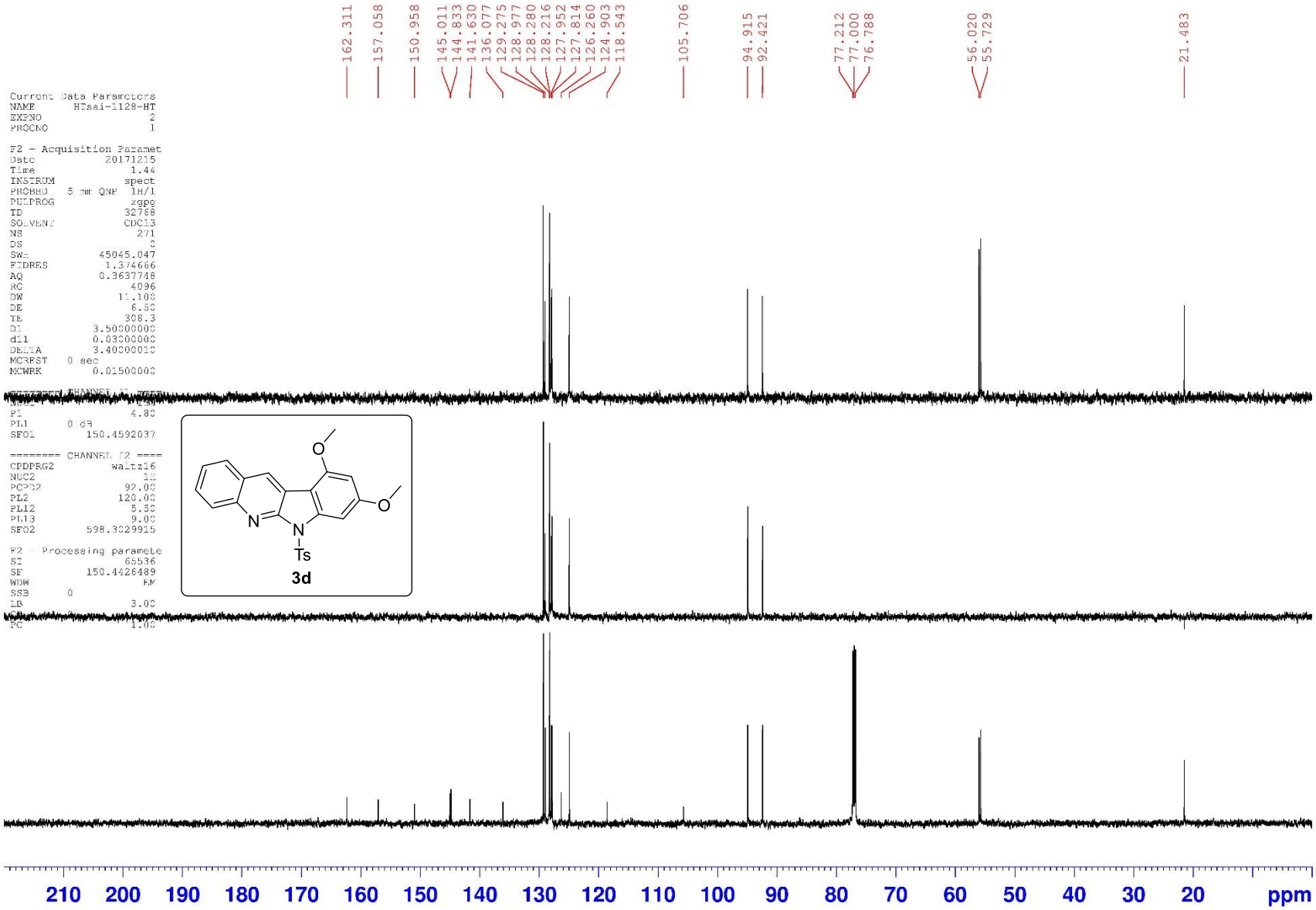
8.163
8.149
8.127
8.113
7.870
7.856
7.700
7.697
7.660
7.659
7.658
7.649
7.647
7.635
7.633
7.633
7.470
7.457
7.445
7.240
7.159
7.145
6.471
6.468
4.030
3.977
2.267
1.532
Current Data Parameters
NAME Hisai-1128-HT
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171215
Time 1.35
INSTRUM spect
PROBHD 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 308.2 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 598.3000274 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
O
O
N
N
Ts
3d
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
2.06
1.07
1.07
1.05
1.08
2.09
1.01
3.05
3.08
3.06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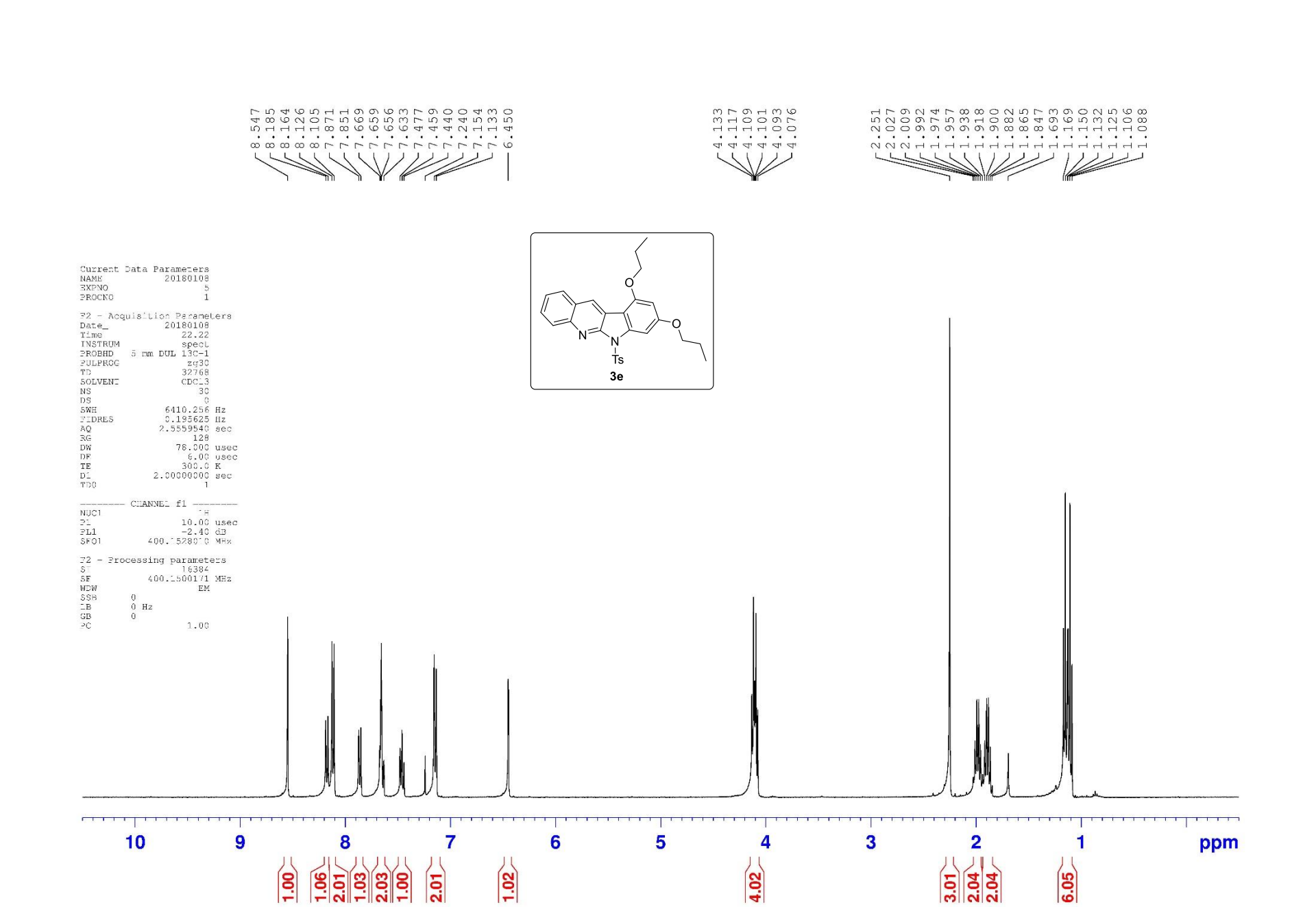
150.958
145.011
144.833
141.630
136.077
129.275
128.977
128.280
128.216
127.952
127.814
126.260
124.903
118.543
105.706
94.915
92.421
77.212
77.000
76.788
56.020
55.729
21.483
Current Data Parameters
NAME HIsai-1128-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171215
Time 1.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 271
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 308.3
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
P1 4.80
PL1 0 dB
SFO1 150.4592037
======== CHANNEL F2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426489
WDW EM
SSB 0
LB 3.00
PC 1.00
O
O
N
N
Ts
3d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.547
8.185
8.164
8.126
8.105
7.871
7.851
7.669
7.659
7.656
7.633
7.477
7.459
7.440
7.240
7.154
7.133
6.450
4.133
4.117
4.109
4.101
4.093
4.076
2.251
2.027
2.009
1.992
1.974
1.957
1.938
1.918
1.900
1.882
1.865
1.847
1.693
1.169
1.150
1.132
1.125
1.106
1.088
Current Data Parameters
NAME 20180108
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180108
Time 22.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O
N
N
Ts
3e
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
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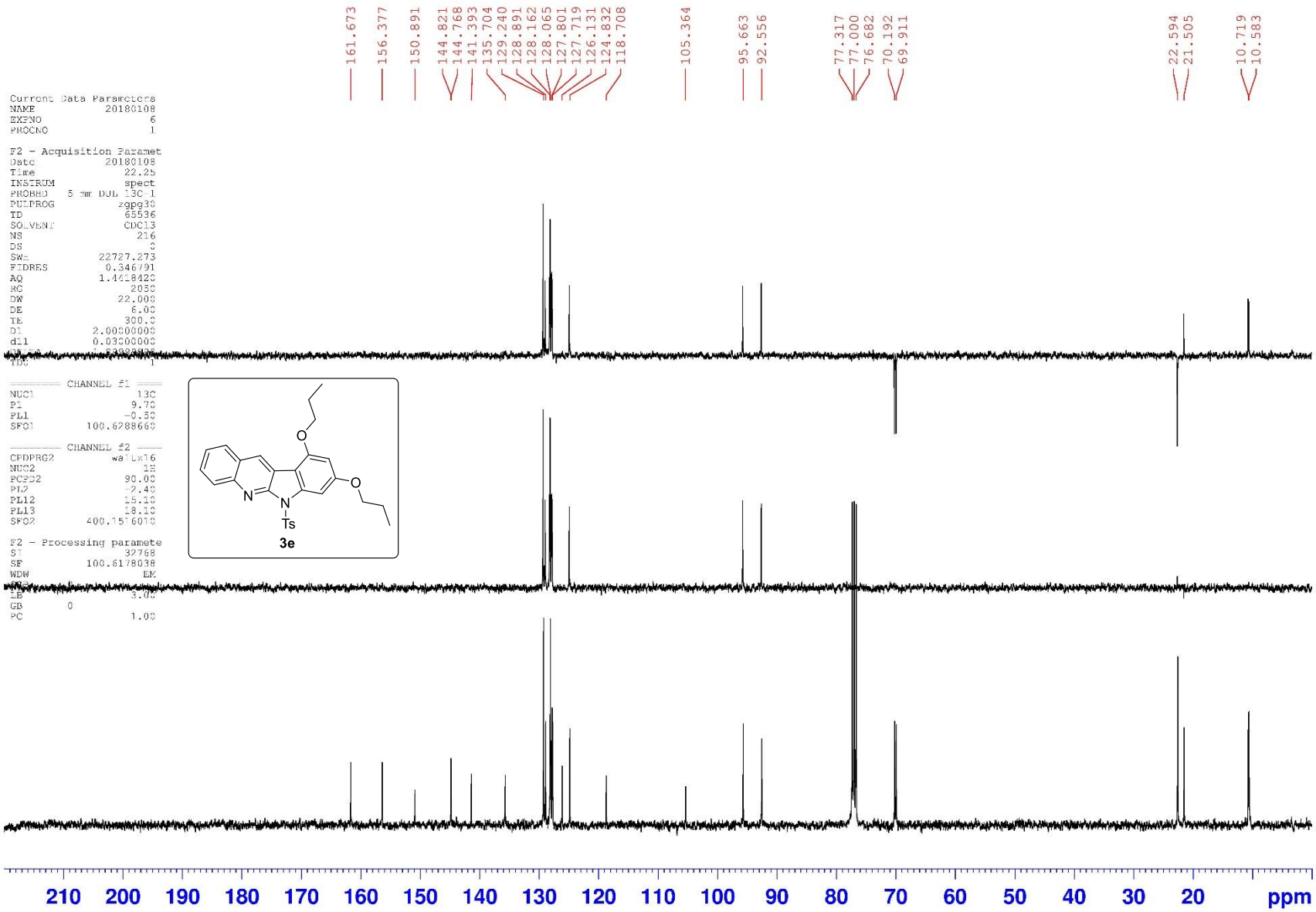
1.02
4.02
3.01
2.04
2.04
6.05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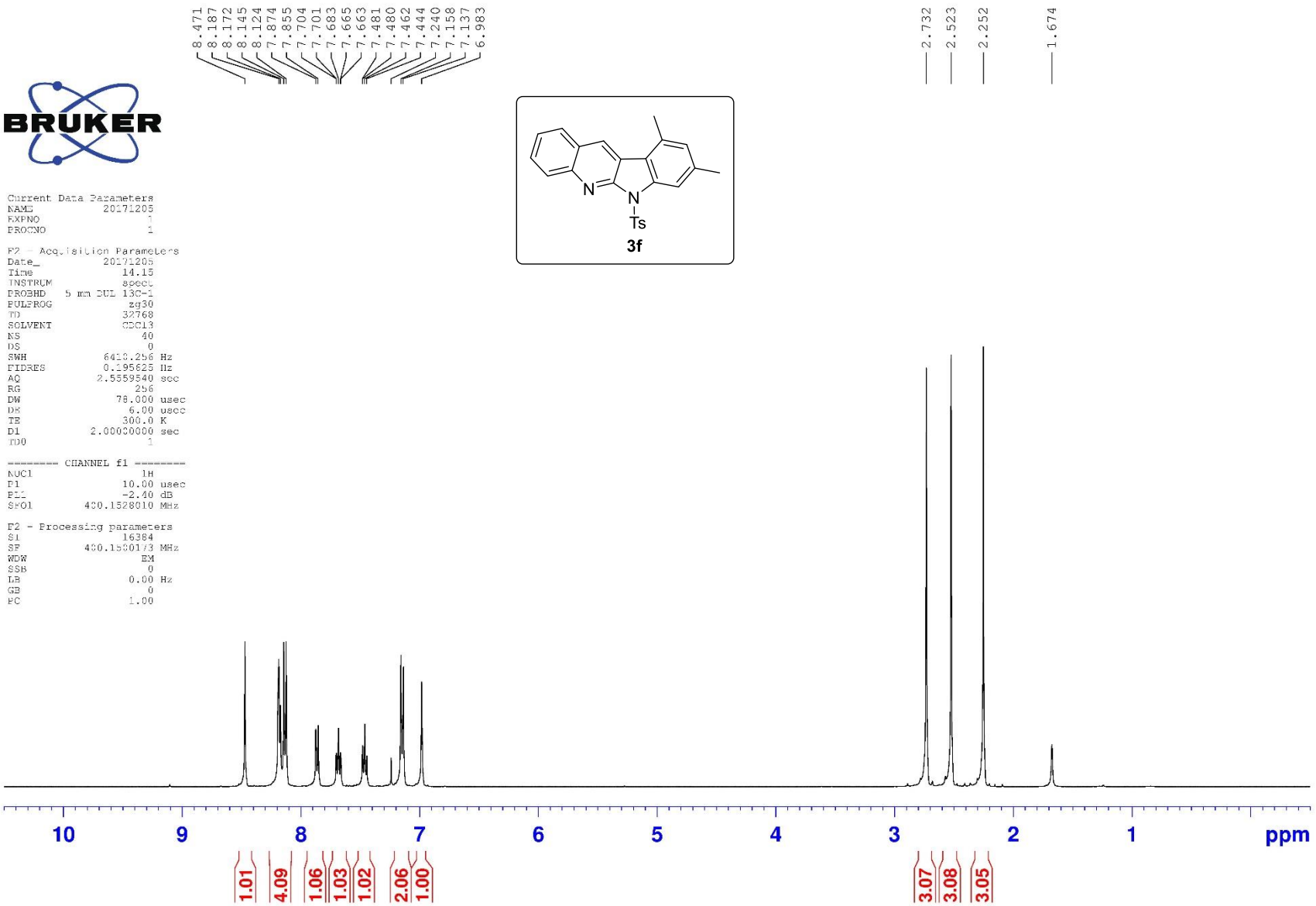
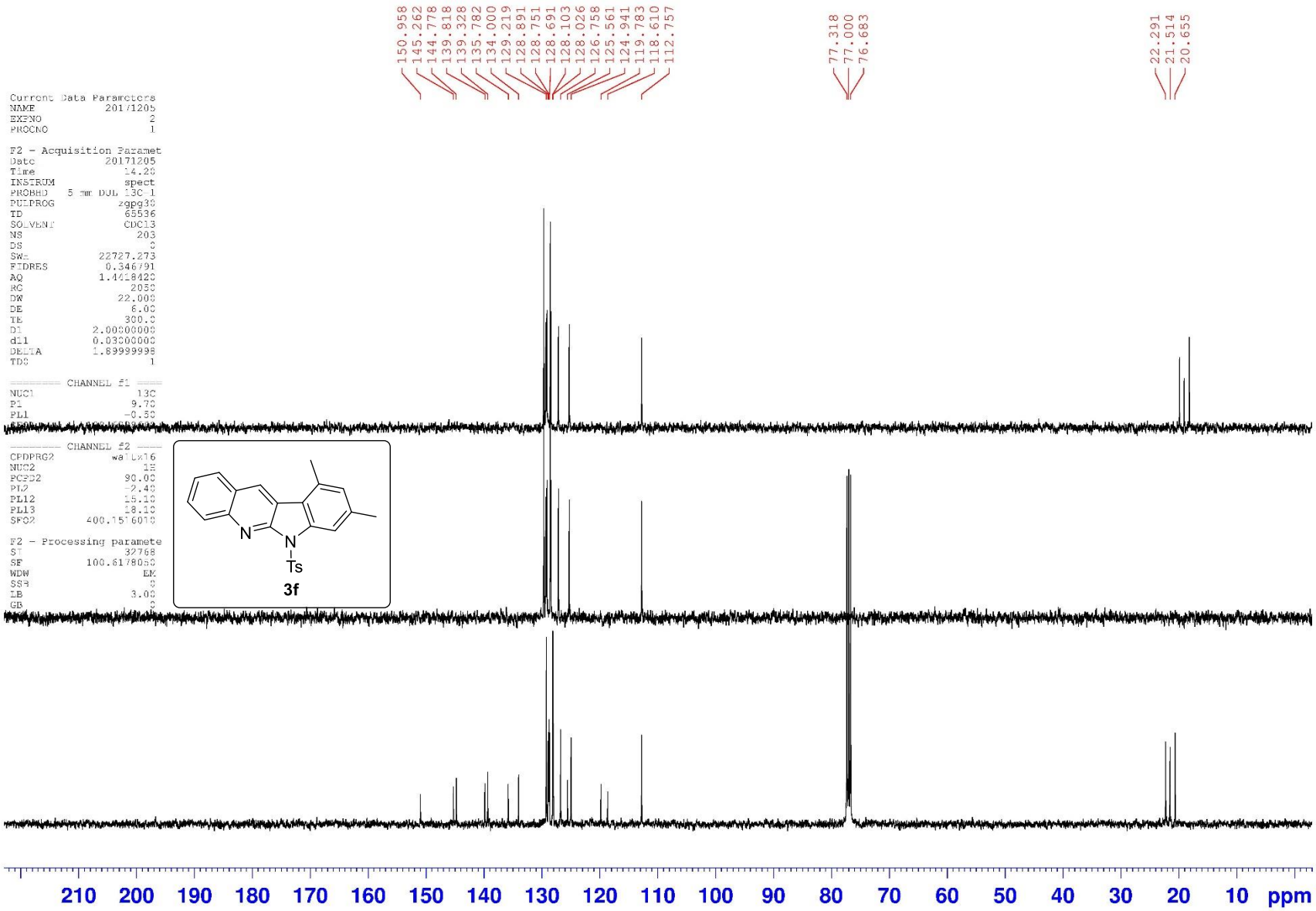
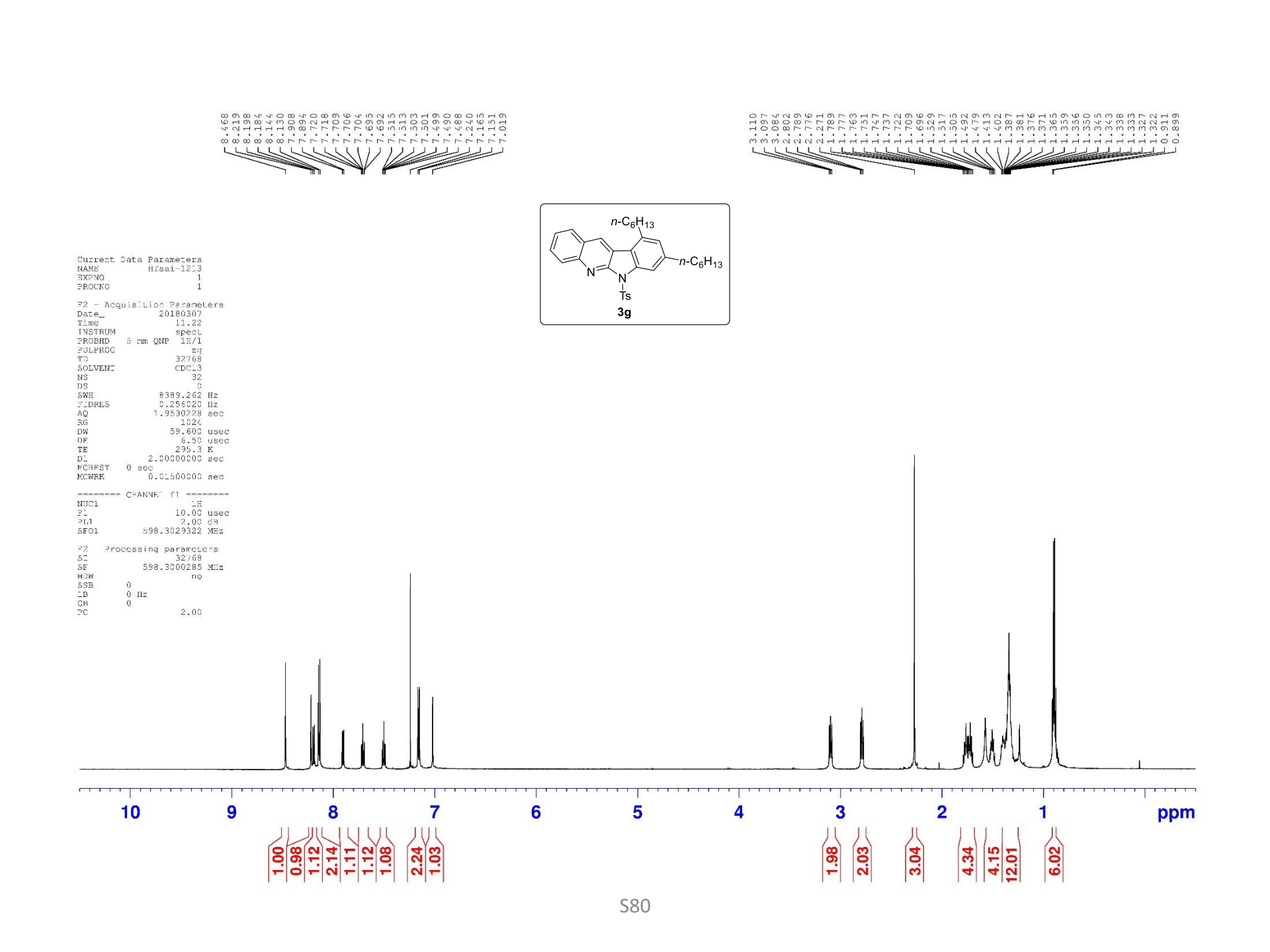
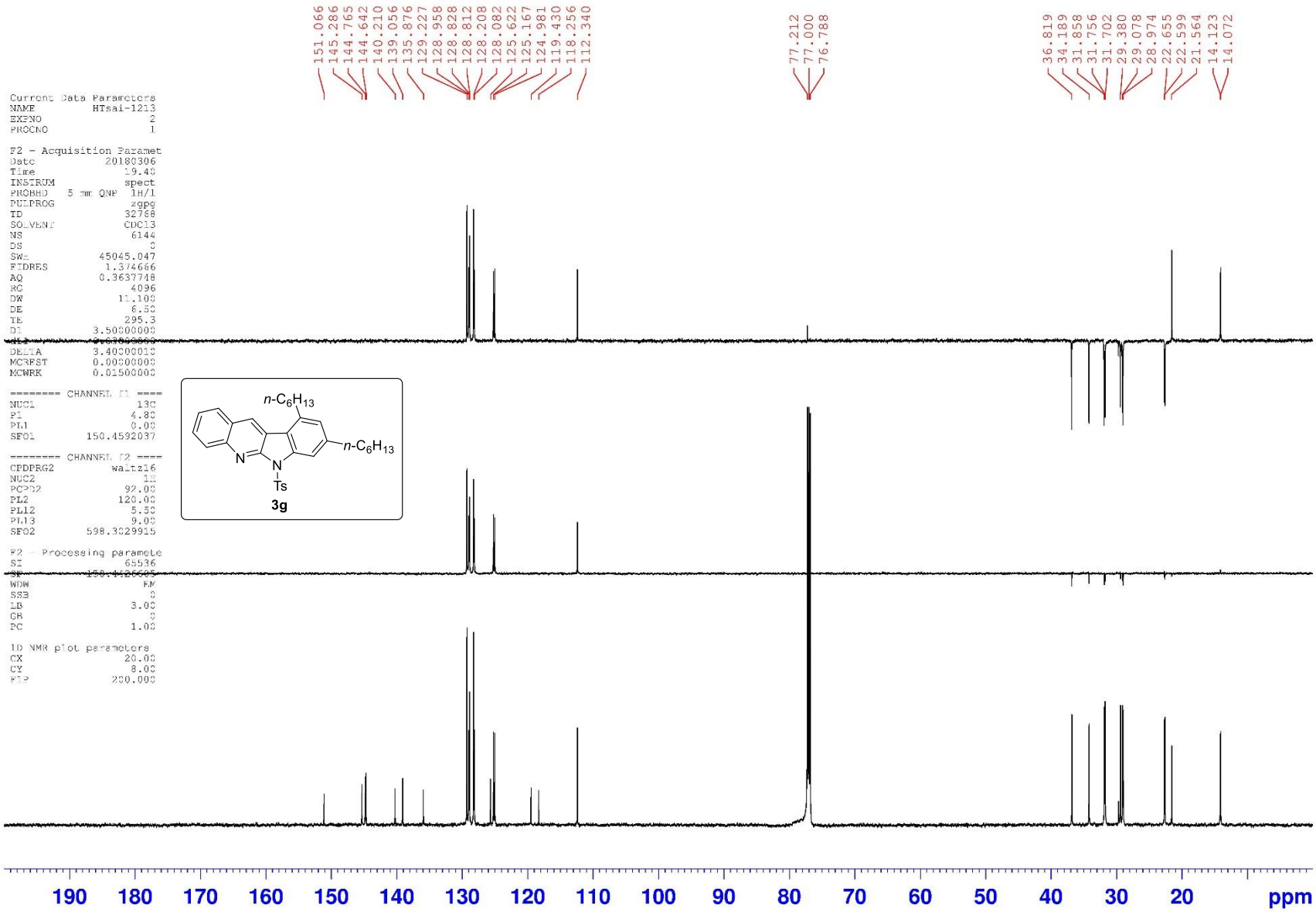
156.377
150.891
144.821
144.768
141.393
135.704
129.240
128.891
128.162
128.065
127.801
127.719
126.131
124.832
118.708
105.364
95.663
92.556
77.317
77.000
76.682
70.192
69.911
22.594
21.505
10.719
10.583
Current Data Parameters
NAME 20180108
EXPNO 6
PROCNO 1
F2 - Acquisition Paramet
Date 20180108
Time 22.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 216
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178038
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
N
N
O
O
Ts
3e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.471
8.187
8.172
8.145
8.124
7.874
7.855
7.704
7.701
7.683
7.665
7.663
7.481
7.480
7.462
7.444
7.240
7.158
7.137
6.983
2.732
2.523
2.252
1.674
BRUKER
Current Data Parameters
NAME 20171205
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171205
Time 14.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 40
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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
Ts
3f
10
9
8
7
6
5
4
3
2
1
ppm
1.01
4.09
1.06
1.03
1.02
2.06
1.00
3.07
3.08
3.05


150.958
145.262
144.778
139.818
139.328
135.782
134.000
129.219
128.891
128.751
128.691
128.103
128.026
126.758
125.561
124.941
119.783
118.610
112.757
77.318
77.000
76.683
22.291
21.514
20.655
Current Data Parameters
NAME 201120
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171205
Time 14.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178053
WDW EM
SSB 0
LB 3.00
GB 0
N
N
Ts
3f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.468
8.219
8.198
8.184
8.144
8.130
7.908
7.894
7.720
7.718
7.709
7.706
7.704
7.695
7.692
7.515
7.313
7.303
7.501
7.499
7.490
7.488
7.240
7.165
7.151
7.019
3.110
3.097
3.084
2.802
2.789
2.776
2.271
1.789
1.777
1.763
1.751
1.747
1.737
1.722
1.709
1.696
1.529
1.517
1.505
1.492
1.479
1.413
1.402
1.387
1.381
1.376
1.371
1.365
1.359
1.356
1.350
1.345
1.343
1.338
1.333
1.327
1.322
0.911
0.899
n-C6H13
n-C6H13
N
N
Ts
3g
Current Data Parameters
NAME HFsai-1213
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180307
Time 11.22
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 1.9530728 sec
RG 1024
DW 59.600 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 2.00 dB
SFO1 598.3029322 MHz
F2 - Processing parameters
SI 32768
SF 598.3000285 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.98
1.12
2.14
1.11
1.12
1.08
2.24
1.03
1.98
2.03
3.04
4.34
4.15
12.01
6.02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140.210
139.056
135.876
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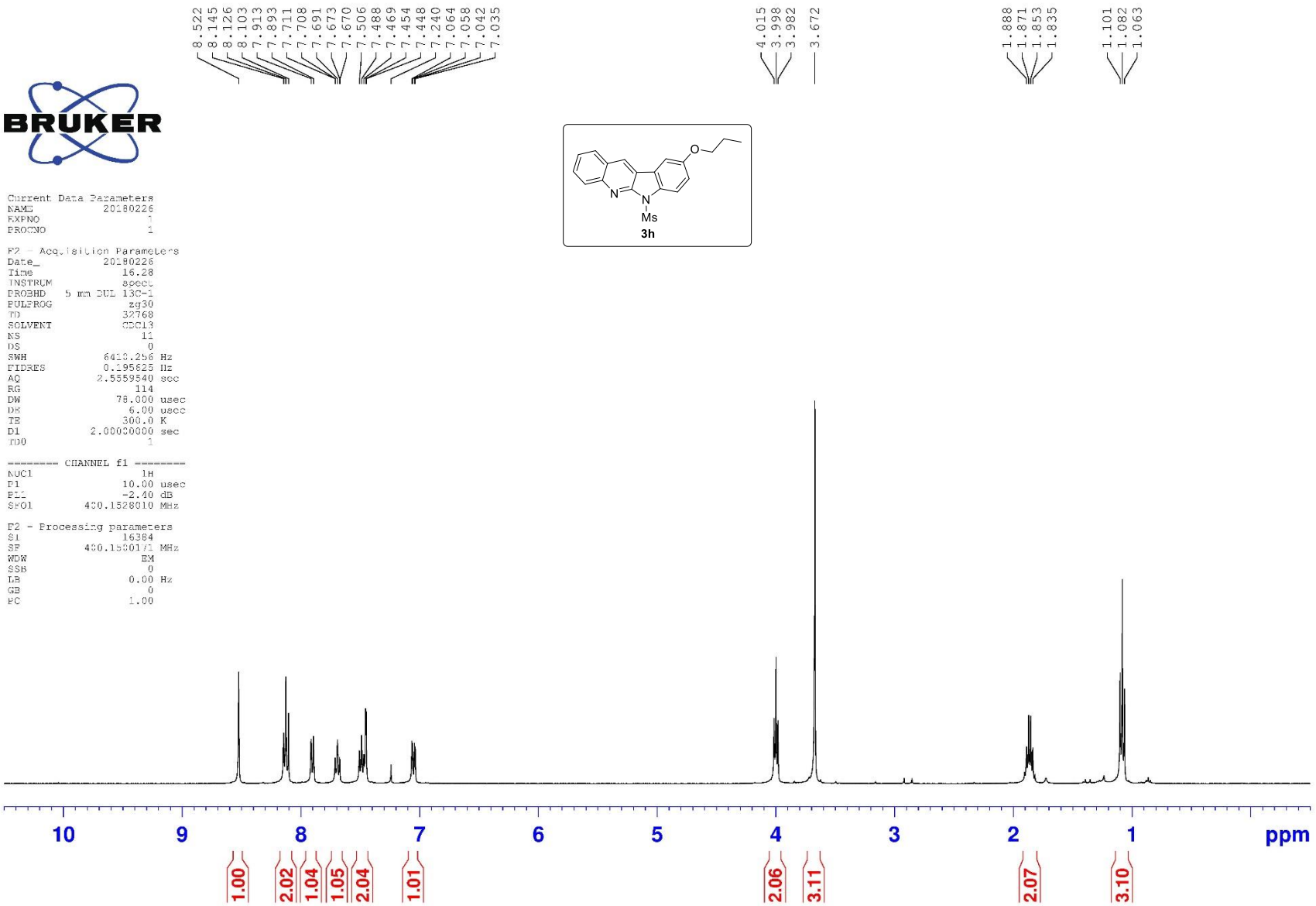
128.828
128.812
128.208
128.082
125.622
125.167
124.981
119.430
118.256
112.340
77.212
77.000
76.788
36.819
34.189
31.858
31.756
31.702
29.380
29.078
28.974
22.655
22.599
21.564
14.123
14.072
Current Data Parameters
NAME HTsai-1213
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180306
Time 19.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 295.3
D1 3.50000000
D11 0.03000000
DELTA 3.40000010
MCREST 0.00000000
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0.00
SFO1 150.4592037
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426005
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00
CY 8.00
F1P 200.000
n-C6H13
n-C6H13
N
N
Ts
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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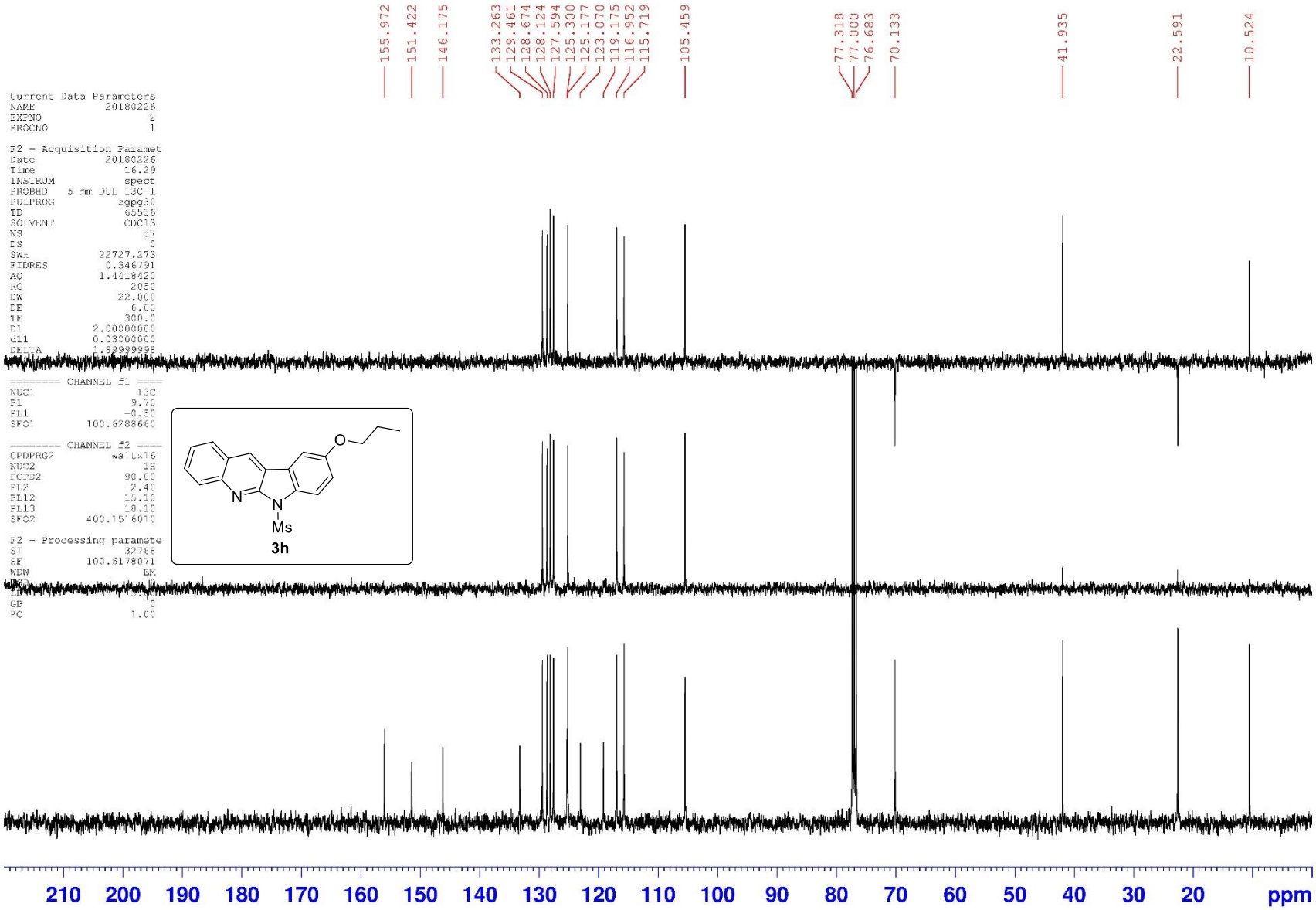
8.103
7.913
7.893
7.711
7.708
7.691
7.673
7.670
7.506
7.488
7.469
7.454
7.448
7.240
7.064
7.058
7.042
7.035
4.015
3.998
3.982
3.672
1.888
1.871
1.853
1.835
1.101
1.082
1.063
BRUKER
Current Data Parameters
NAME 20180226
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180226
Time 16.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
N
Ms
3h
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.02
1.04
1.05
2.04
1.01
2.06
3.11
2.07
3.10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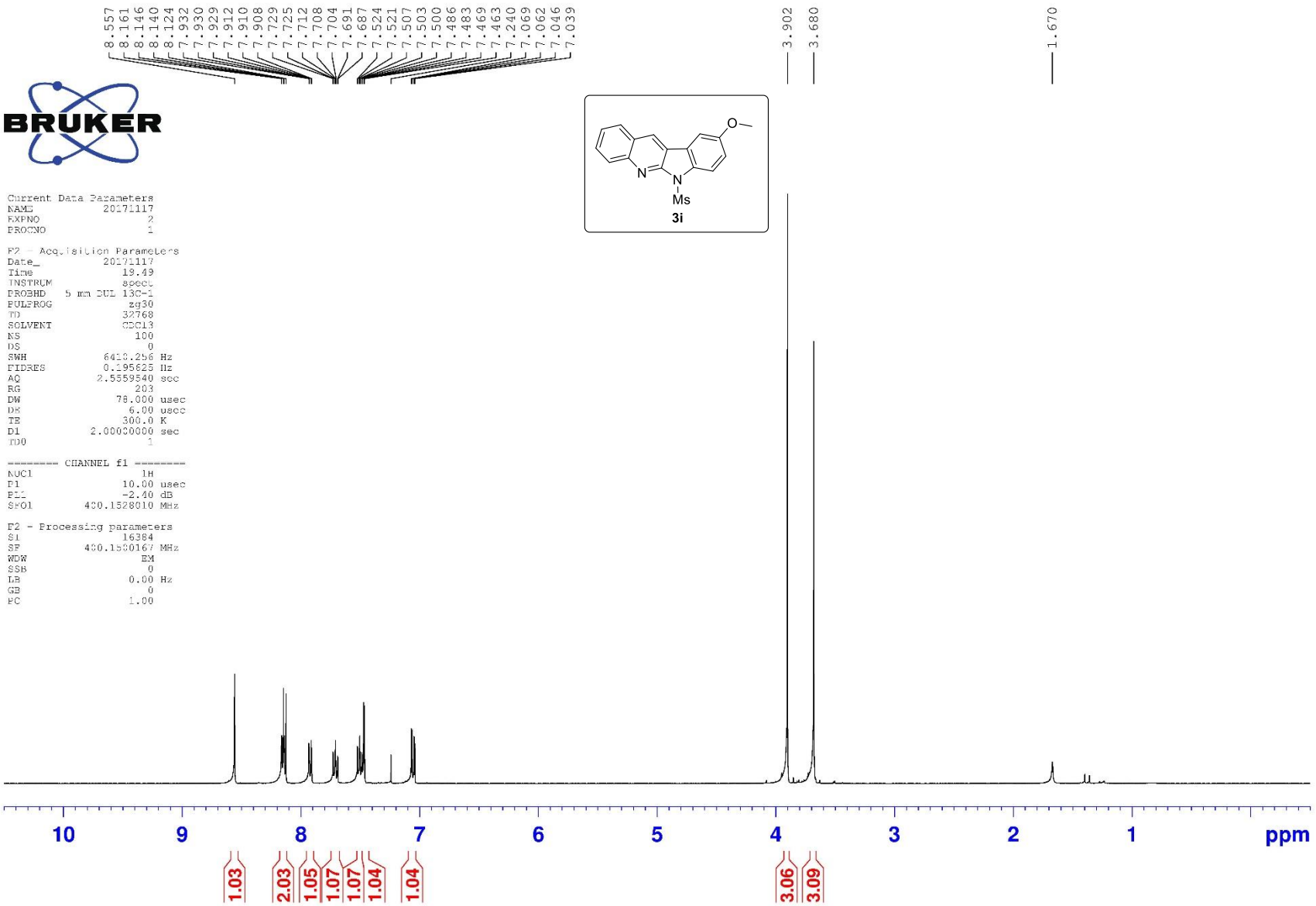
146.175
133.263
129.461
128.674
128.124
127.594
125.300
125.177
123.070
119.175
116.952
115.719
105.459
77.318
77.000
76.683
70.133
41.935
22.591
10.524
Current Data Parameters
NAME 20180226
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180226
Time 16.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 57
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178071
WDW EM
GB 0
PC 1.00
N
N
Ms
O
3h
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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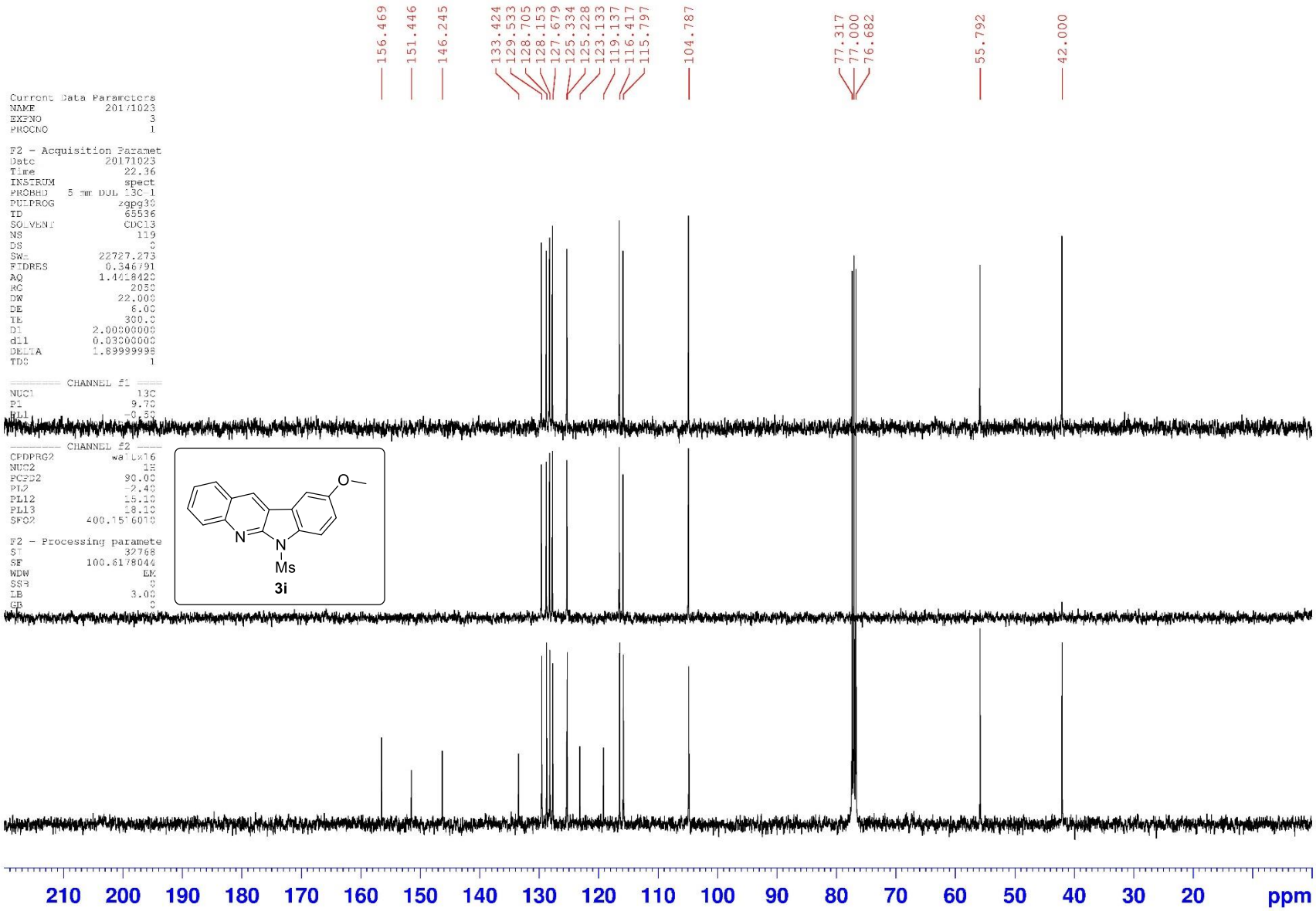
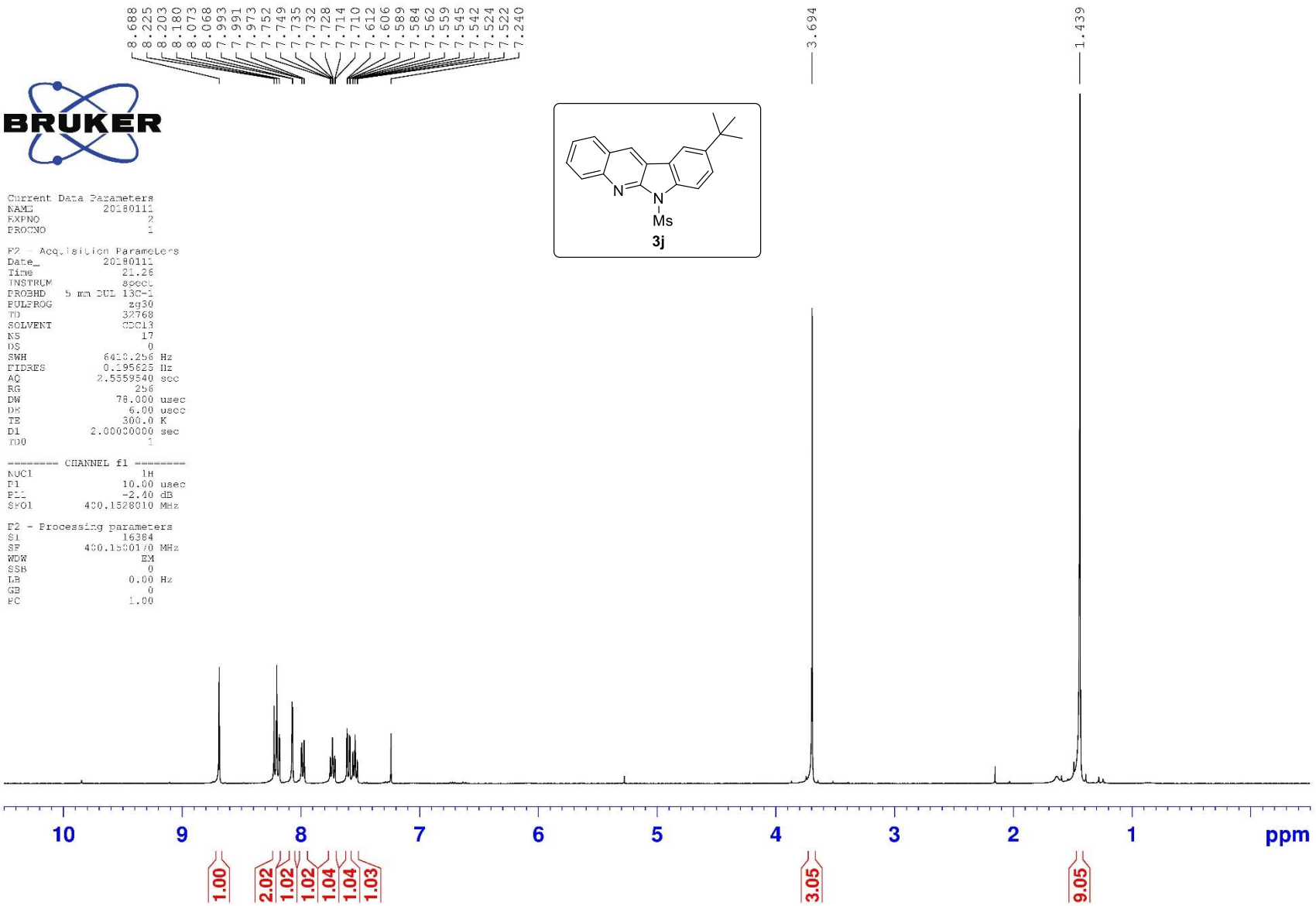
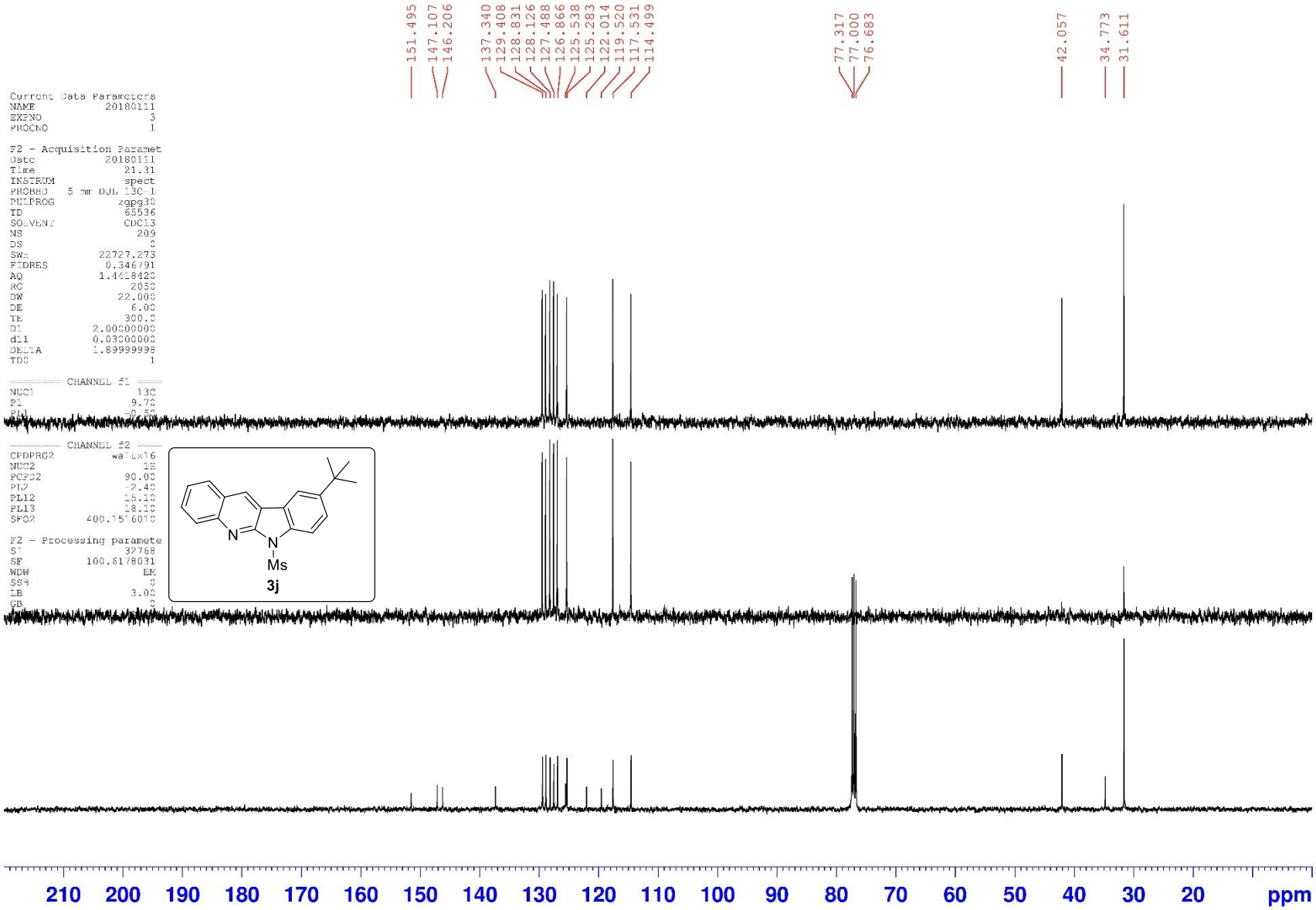
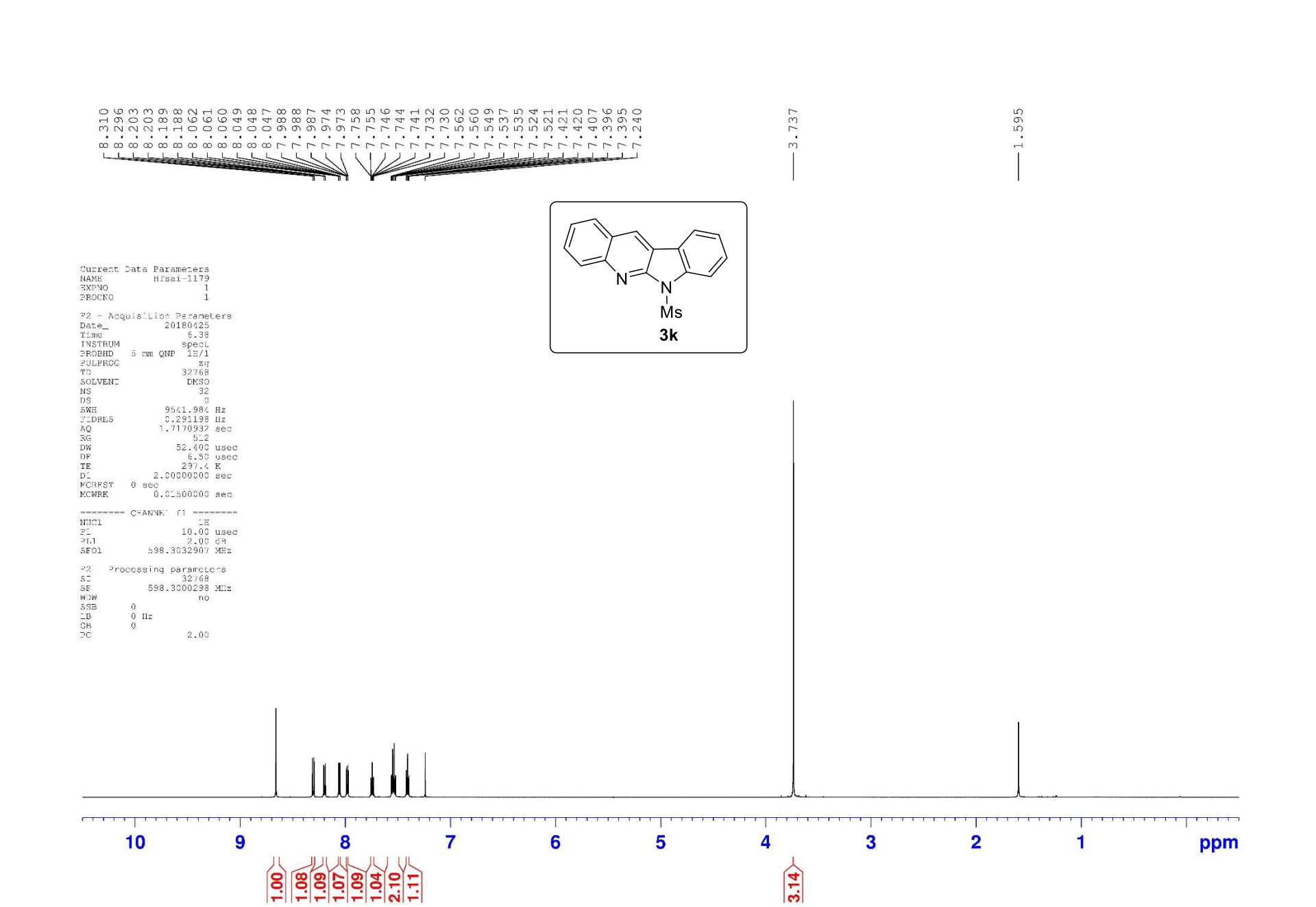
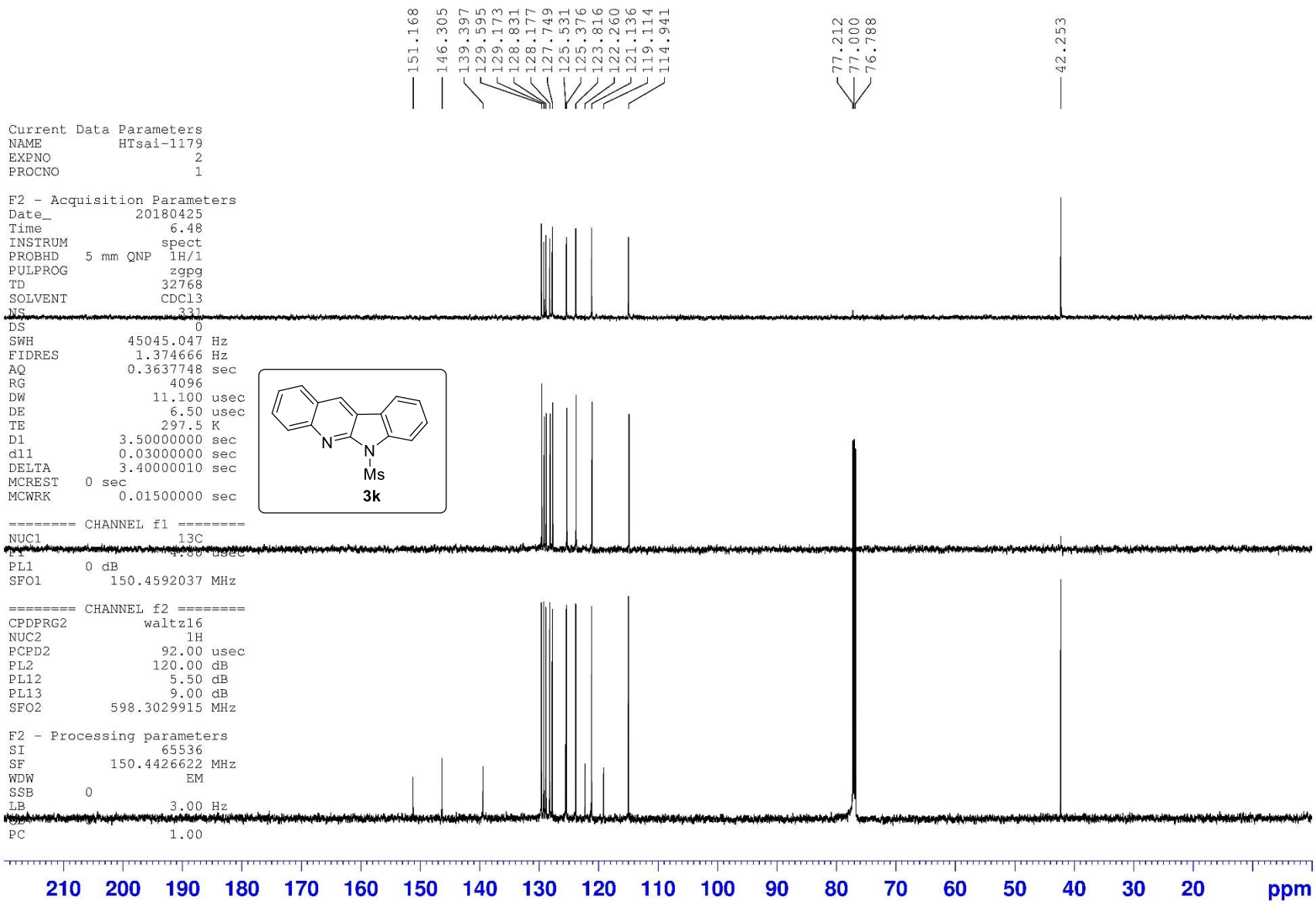
8.140
8.124
7.932
7.930
7.929
7.912
7.910
7.908
7.729
7.725
7.712
7.708
7.704
7.691
7.687
7.524
7.521
7.507
7.503
7.500
7.486
7.483
7.469
7.463
7.240
7.069
7.062
7.046
7.039
3.902
3.680
1.670
BRUKER
Current Data Parameters
NAME 20171117
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171117
Time 18.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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 400.1500167 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
N
Ms
3i
10
9
8
7
6
5
4
3
2
1
ppm
1.03
2.03
1.05
1.07
1.07
1.04
1.04
3.06
3.09

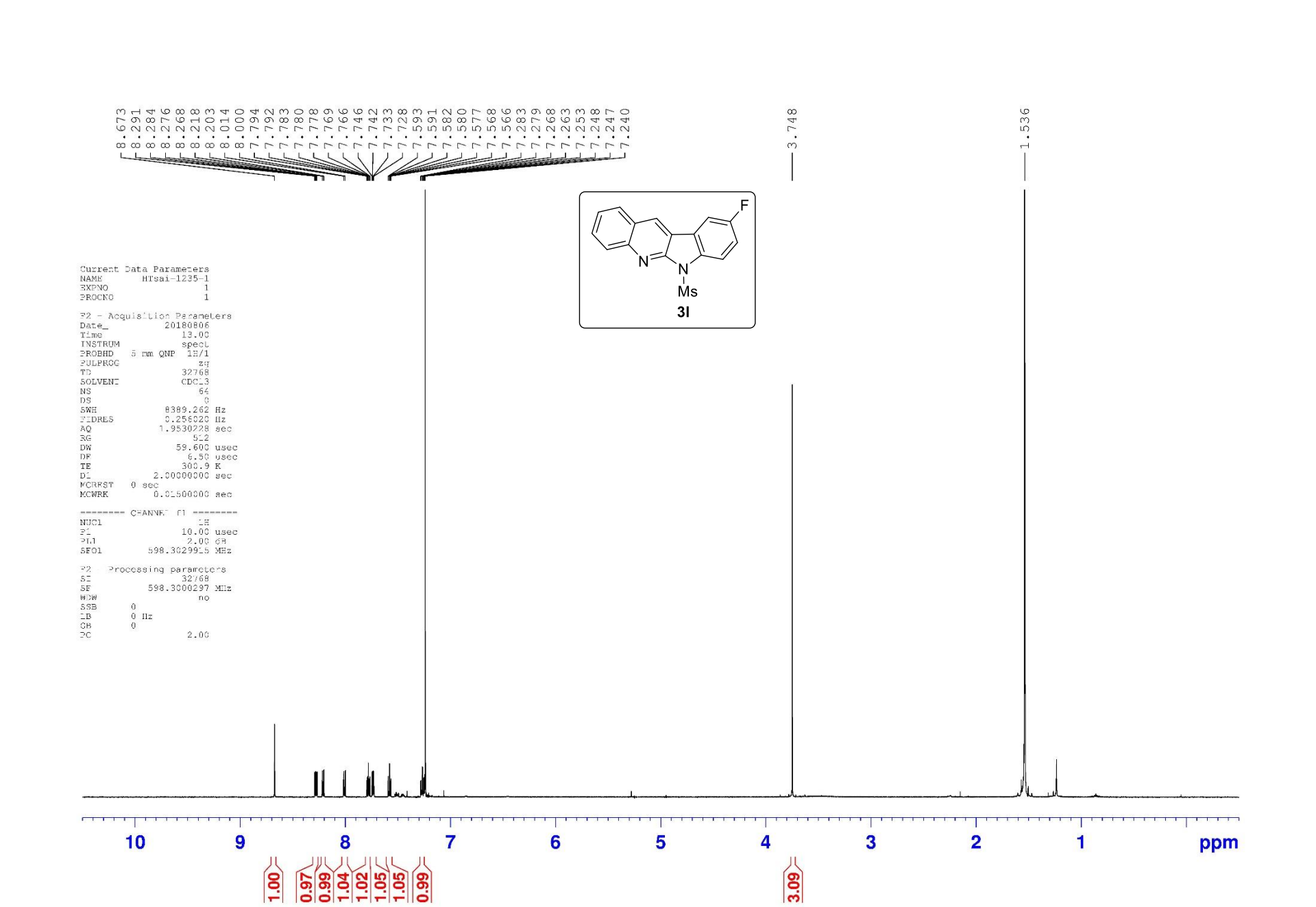

156.469
151.446
146.245
133.424
129.533
128.705
128.153
127.679
125.334
125.228
123.133
119.137
116.417
115.797
104.787
77.317
77.000
76.682
55.792
42.000
Current Data Parameters
NAME 201/1023
EXPNO 3
PROCNO 1
F2 - Acquisition Paramet
Date 20171023
Time 22.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 119
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.33
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178044
WDW EM
SSB 0
LB 3.00
GB 0
O
N
N
Ms
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.688
8.225
8.203
8.180
8.073
8.068
7.993
7.991
7.973
7.752
7.749
7.735
7.732
7.728
7.714
7.710
7.612
7.606
7.589
7.584
7.562
7.559
7.545
7.542
7.524
7.522
7.240
3.694
1.439
BRUKER
Current Data Parameters
NAME 20180111
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180111
Time 21.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 17
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 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
N
Ms
3j
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.02
1.02
1.02
1.04
1.04
1.03
3.05
9.05


151.495
147.107
146.206
137.340
129.408
128.831
128.126
127.488
126.866
125.538
125.283
122.014
119.520
117.531
114.499
77.317
77.000
76.683
42.057
34.773
31.611
Current Data Parameters
NAME 20180111
EXPNO 3
PROCNO 1
F2 - Acquisition Paramet
Date 20180111
Time 21.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 209
DS 2
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178031
WDW EM
SSB 0
LB 3.00
GB 0
N
N
Ms
3j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.310
8.296
8.203
8.203
8.189
8.188
8.062
8.061
8.060
8.049
8.048
8.047
7.988
7.988
7.987
7.974
7.973
7.758
7.755
7.746
7.744
7.741
7.732
7.730
7.562
7.560
7.549
7.537
7.535
7.524
7.521
7.421
7.420
7.407
7.396
7.395
7.240
3.737
1.595
N
N
Ms
3k
Current Data Parameters
NAME HFsai-1179
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180425
Time 6.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT DMSO
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 297.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 2.00 dB
SFO1 598.3032907 MHz
F2 - Processing parameters
SI 32768
SF 598.3000298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.08
1.09
1.07
1.09
1.04
2.10
1.11
3.14


151.168
146.305
139.397
129.595
129.173
128.831
128.177
127.749
125.531
125.376
123.816
122.260
121.136
119.114
114.941
77.212
77.000
76.788
42.253
Current Data Parameters
NAME HTsai-1179
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180425
Time 6.48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 331
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 297.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
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 150.4426622 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
N
N
Ms
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.673
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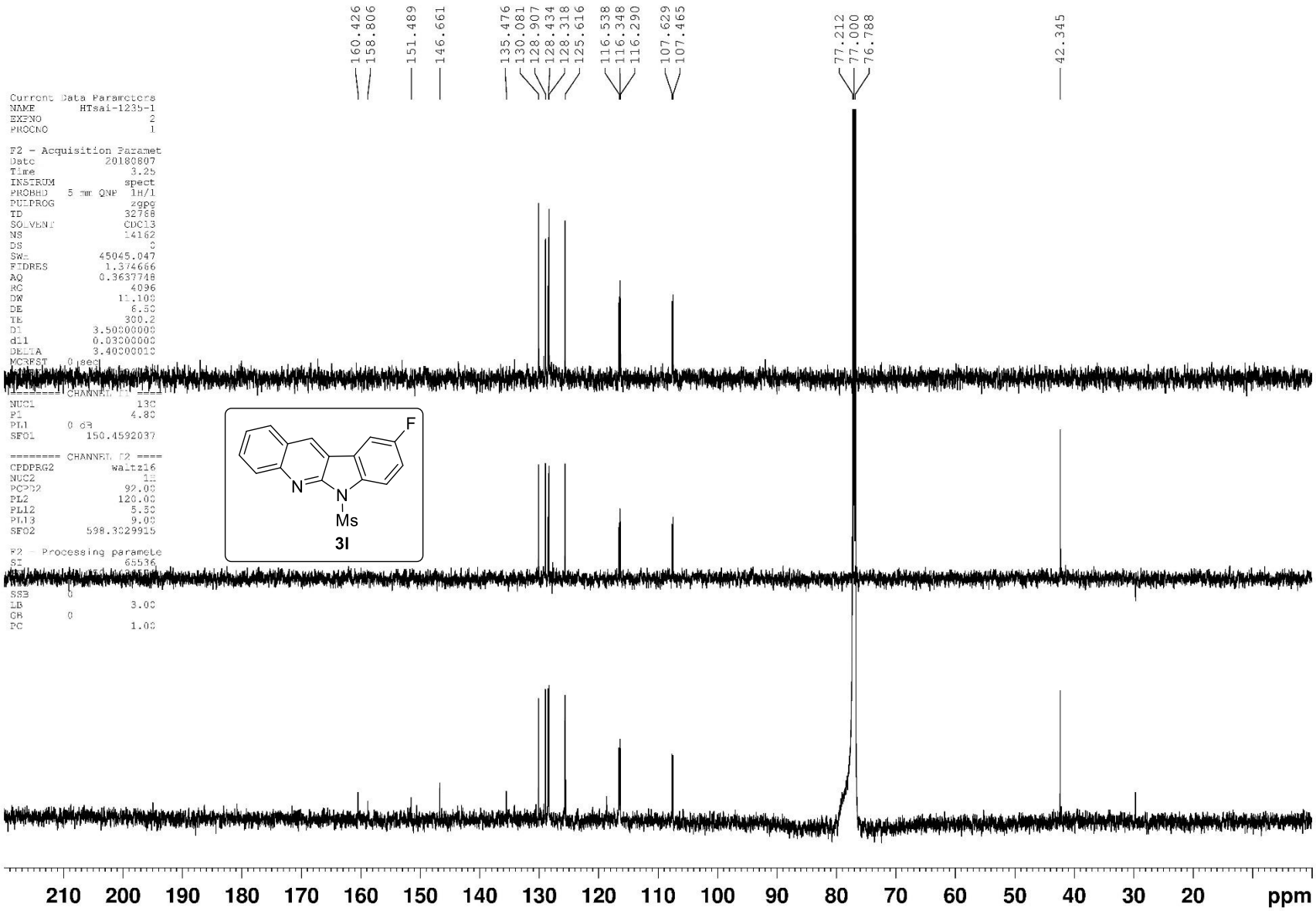
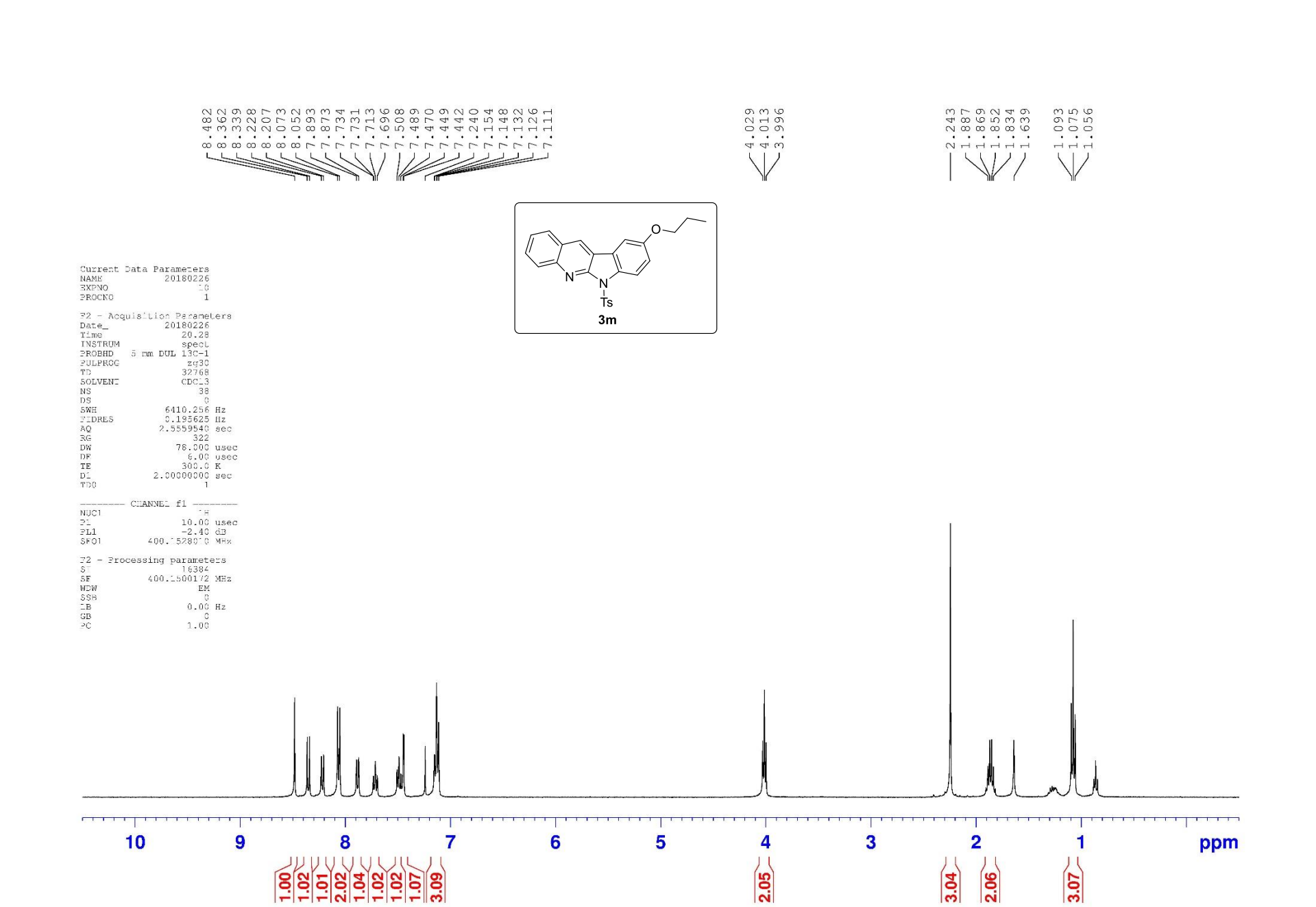
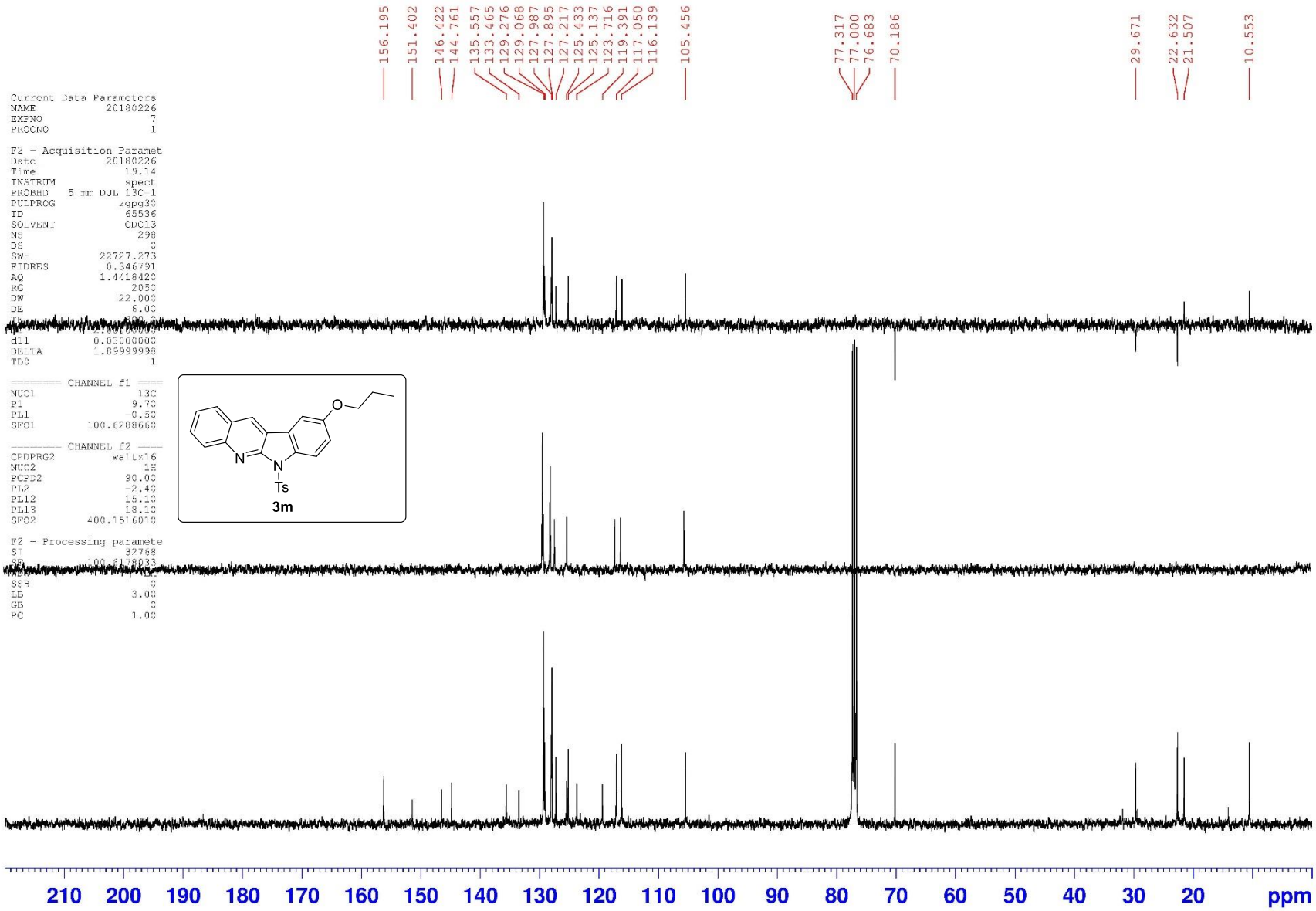
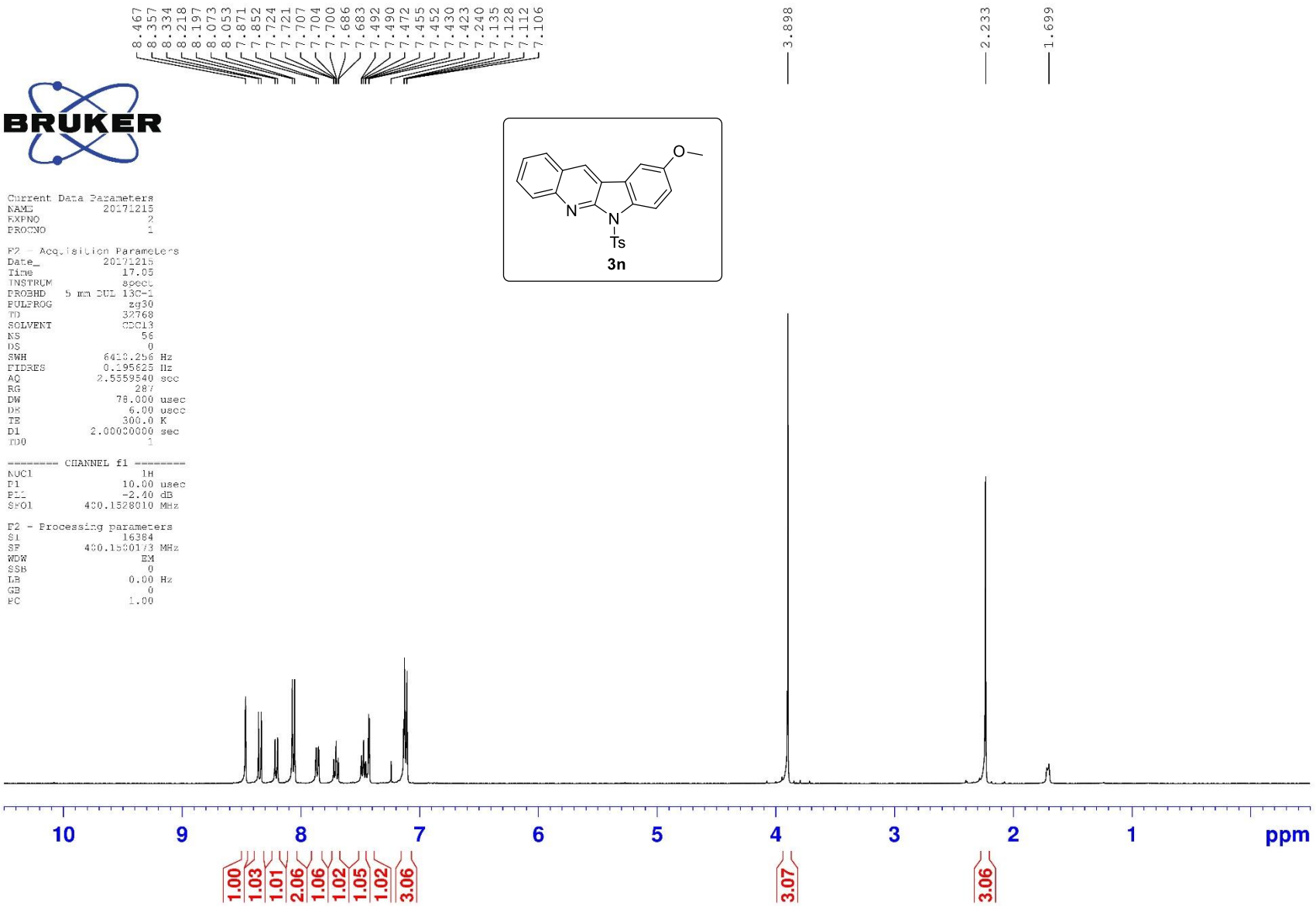
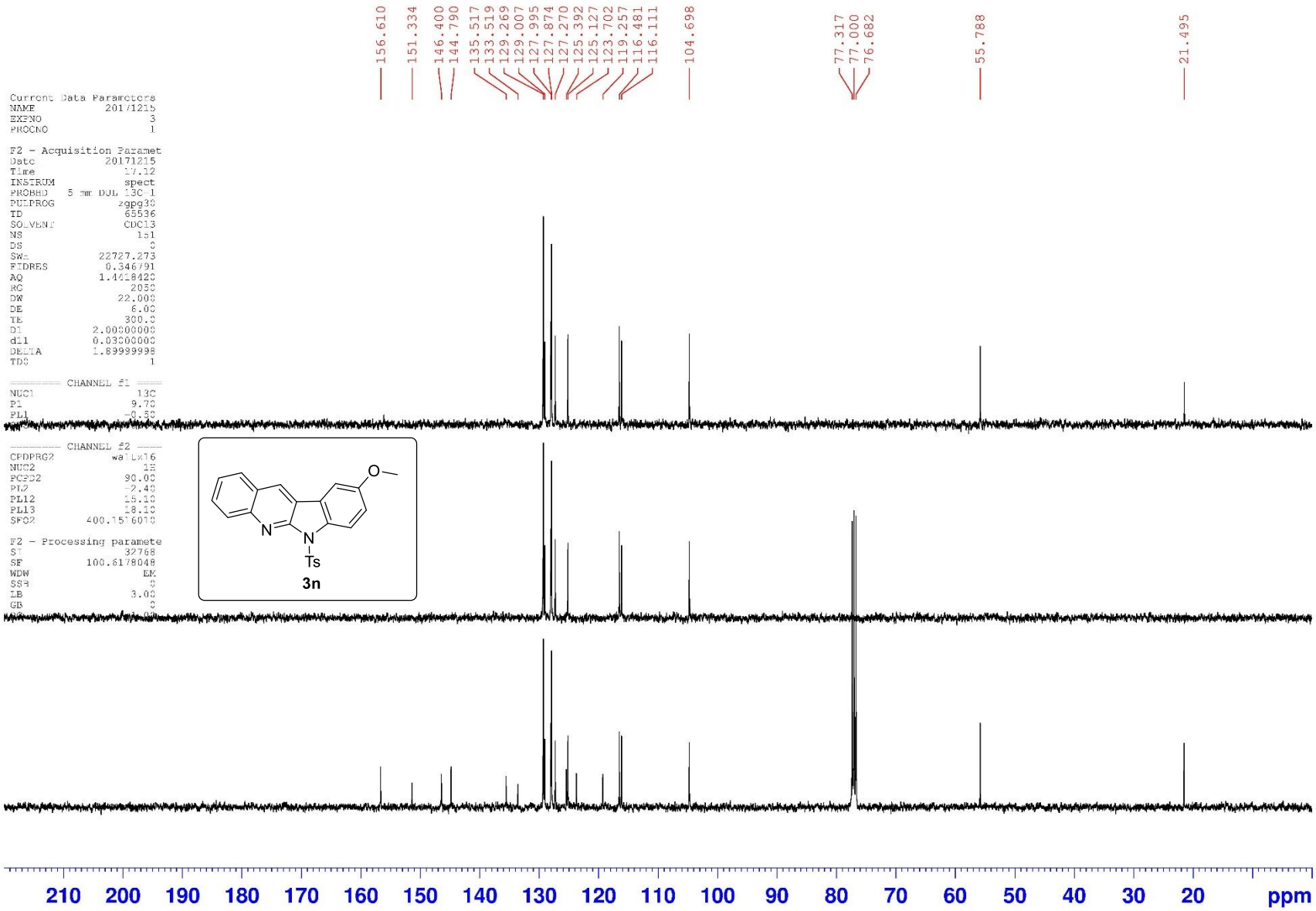
8.284
8.276
8.268
8.218
8.203
8.014
8.000
7.794
7.792
7.783
7.780
7.778
7.769
7.766
7.746
7.742
7.733
7.728
7.593
7.591
7.582
7.580
7.577
7.568
7.566
7.283
7.279
7.268
7.263
7.253
7.248
7.247
7.240
3.748
1.536
F
N
N
Ms
3l
Current Data Parameters
NAME HIsai-1235-1
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20180806
Time 13.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 64
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 300.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 2.00 dB
SFO1 598.3029915 MHz
P2 Processing parameters
SI 32768
SF 598.3000297 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.97
0.99
1.04
1.02
1.05
1.05
0.99
3.09


160.426
158.806
151.489
146.661
135.476
130.081
128.907
128.434
128.318
125.616
116.538
116.348
116.290
107.629
107.465
77.212
77.000
76.788
42.345
Current Data Parameters
NAME HTsai-1235-1
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180807
Time 3.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 14162
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 300.2
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
CHANNEL f1
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4592037
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SSB 0
LB 3.00
GB 0
PC 1.00
F
N
N
Ms
3l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.482
8.362
8.339
8.228
8.207
8.073
8.052
7.893
7.873
7.734
7.731
7.713
7.696
7.508
7.489
7.470
7.449
7.442
7.240
7.154
7.148
7.132
7.126
7.111
4.029
4.013
3.996
2.243
1.887
1.869
1.852
1.834
1.639
1.093
1.075
1.056
O
N
N
Ts
3m
Current Data Parameters
NAME 20180226
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180226
Time 20.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 38
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 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
1.01
2.02
1.04
1.02
1.02
1.07
3.09
2.05
3.04
2.06
3.07


156.195
151.402
146.422
144.761
135.557
133.465
129.276
129.068
127.987
127.895
127.217
125.433
125.137
123.716
119.391
117.050
116.139
105.456
77.317
77.000
76.683
70.186
29.671
22.632
21.507
10.553
Current Data Parameters
NAME 20180226
EXPNO 7
PROCNO 1
F2 - Acquisition Paramet
Date 20180226
Time 19.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 298
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288660
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6128033
SSB 0
LB 3.00
GB 0
PC 1.00
O
N
N
Ts
3m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.467
8.357
8.334
8.218
8.197
8.073
8.053
7.871
7.852
7.724
7.721
7.707
7.704
7.700
7.686
7.683
7.492
7.490
7.472
7.455
7.452
7.430
7.423
7.240
7.135
7.128
7.112
7.106
3.898
2.233
1.699
BRUKER
Current Data Parameters
NAME 20171215
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171215
Time 17.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 56
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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
N
Ts
3n
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.01
2.06
1.06
1.02
1.05
1.02
3.06
3.07
3.06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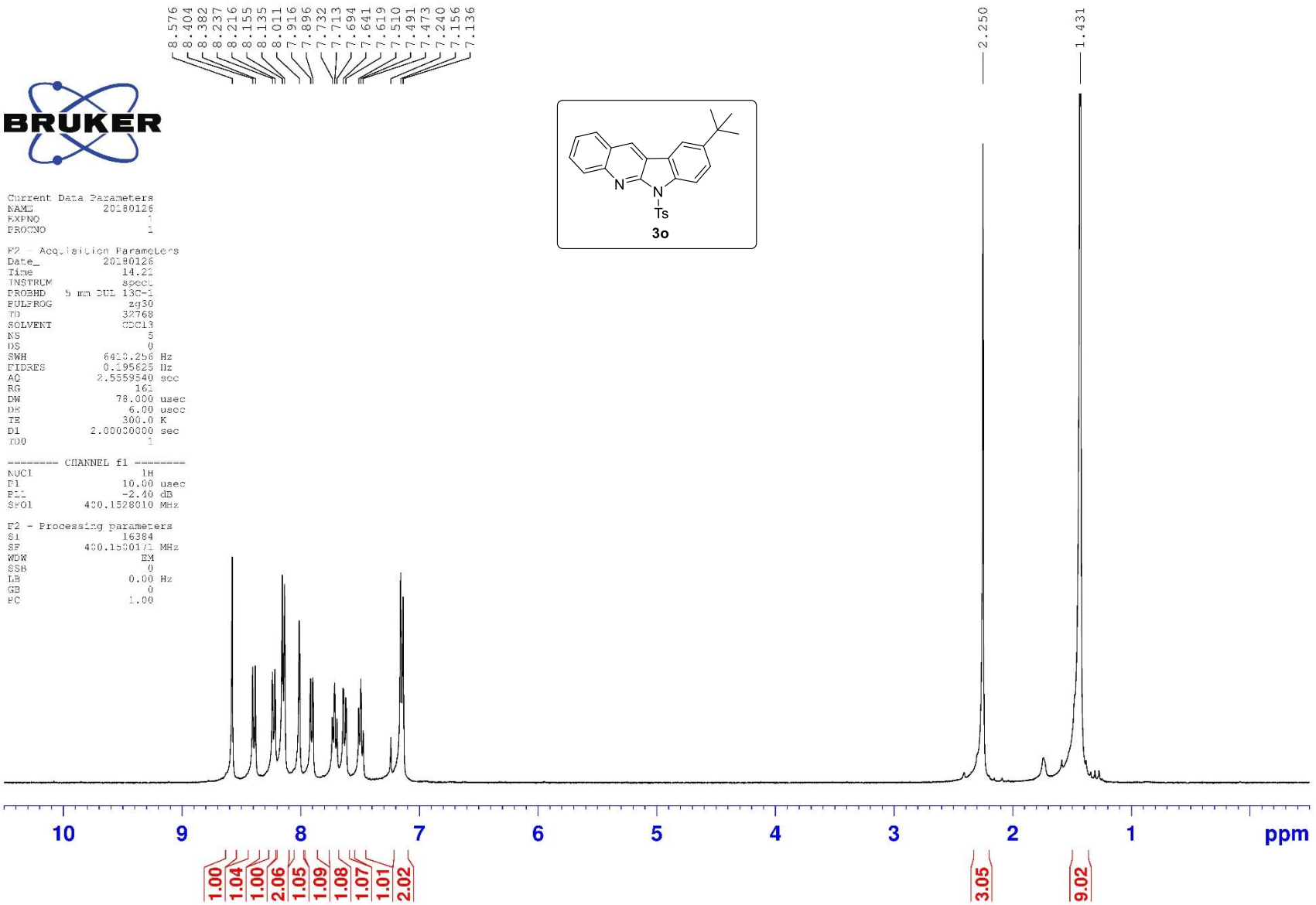
151.334
146.400
144.790
135.517
133.519
129.269
129.007
127.995
127.874
127.270
125.392
125.127
123.702
119.257
116.481
116.111
104.698
77.317
77.000
76.682
55.788
21.495
Current Data Parameters
NAME 201712l5
EXPNO 3
PROCNO 1
F2 - Acquisition Paramet
Date 20171215
Time 17.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178048
WDW EM
SSB 0
LB 3.00
GB 0
N
N
Ts
O
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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8.237
8.216
8.155
8.135
8.011
7.916
7.896
7.732
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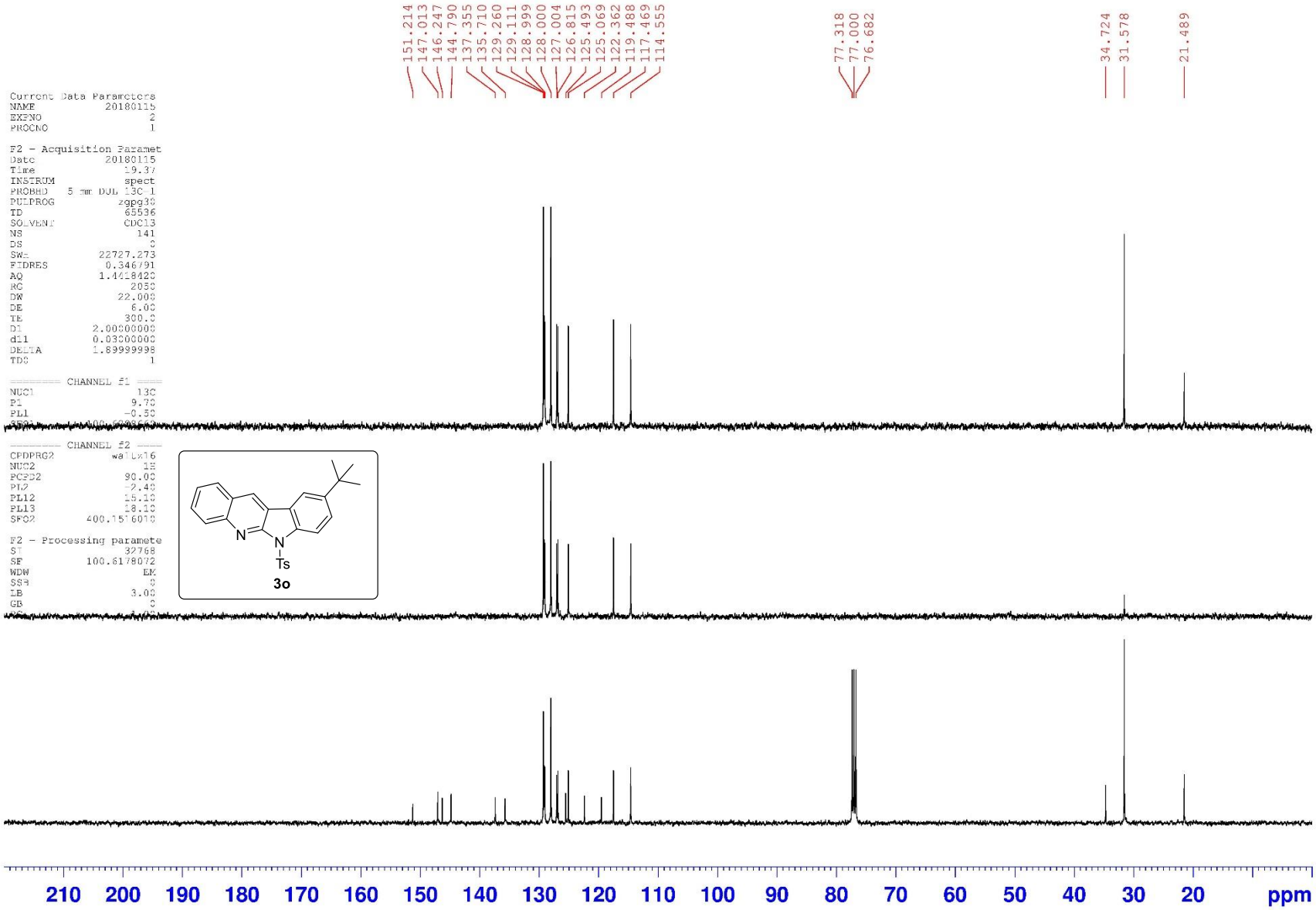
7.694
7.641
7.619
7.510
7.491
7.473
7.240
7.156
7.136
2.250
1.431
BRUKER
Current Data Parameters
NAME 20180126
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180126
Time 14.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 161
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
Ts
3o
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.00
2.06
1.05
1.09
1.08
1.07
1.01
2.02
3.05
9.02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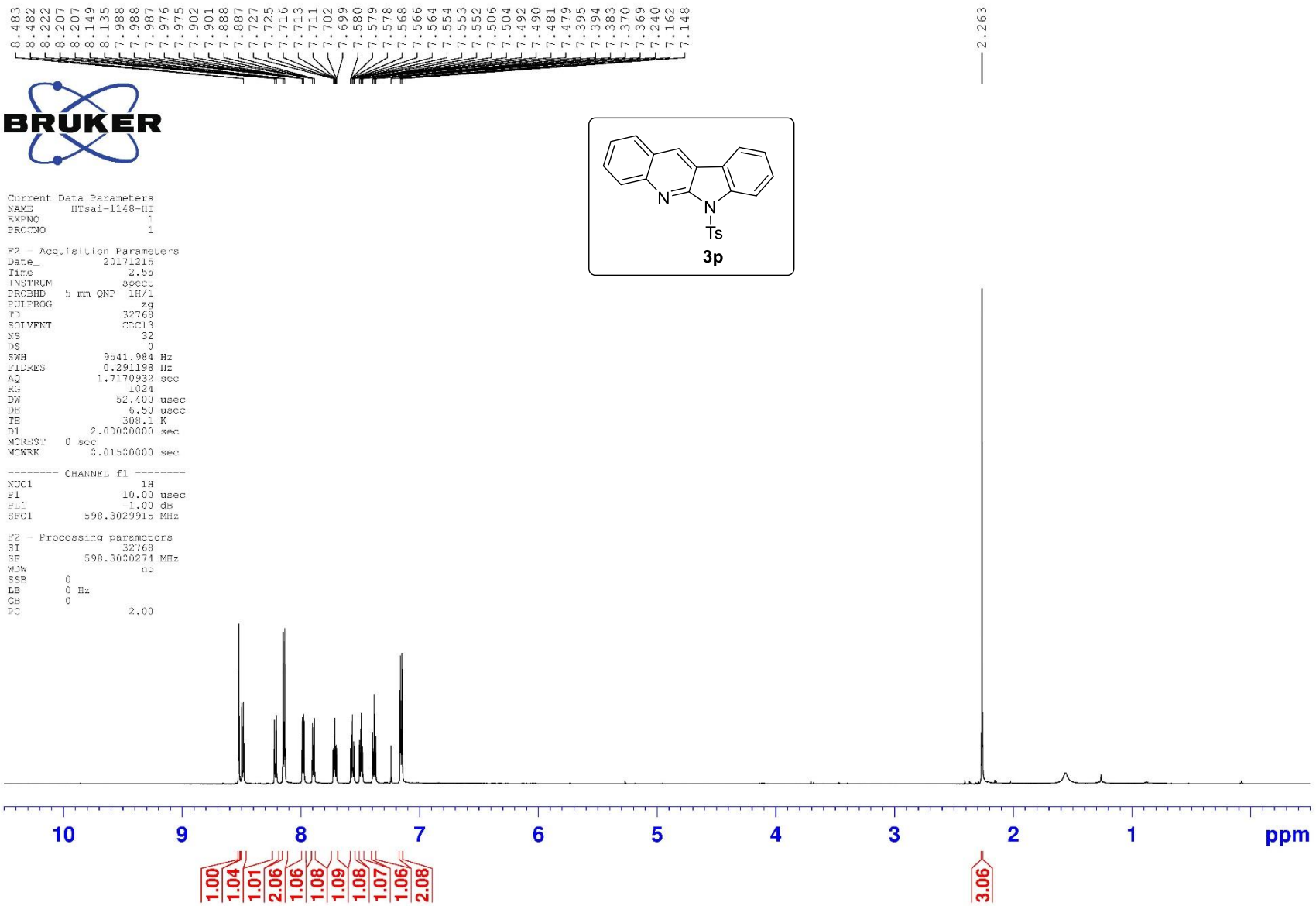
137.355
135.710
129.260
129.111
128.999
128.000
127.004
126.815
125.493
125.069
122.362
119.488
117.469
114.555
77.318
77.000
76.682
34.724
31.578
21.489
Current Data Parameters
NAME 20180115
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180115
Time 19.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 141
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70
PL1 -0.30
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.19
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178072
WDW EM
SSB 0
LB 3.00
GB 0
N
N
Ts
3o
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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8.222
8.207
8.207
8.149
8.135
7.988
7.988
7.987
7.976
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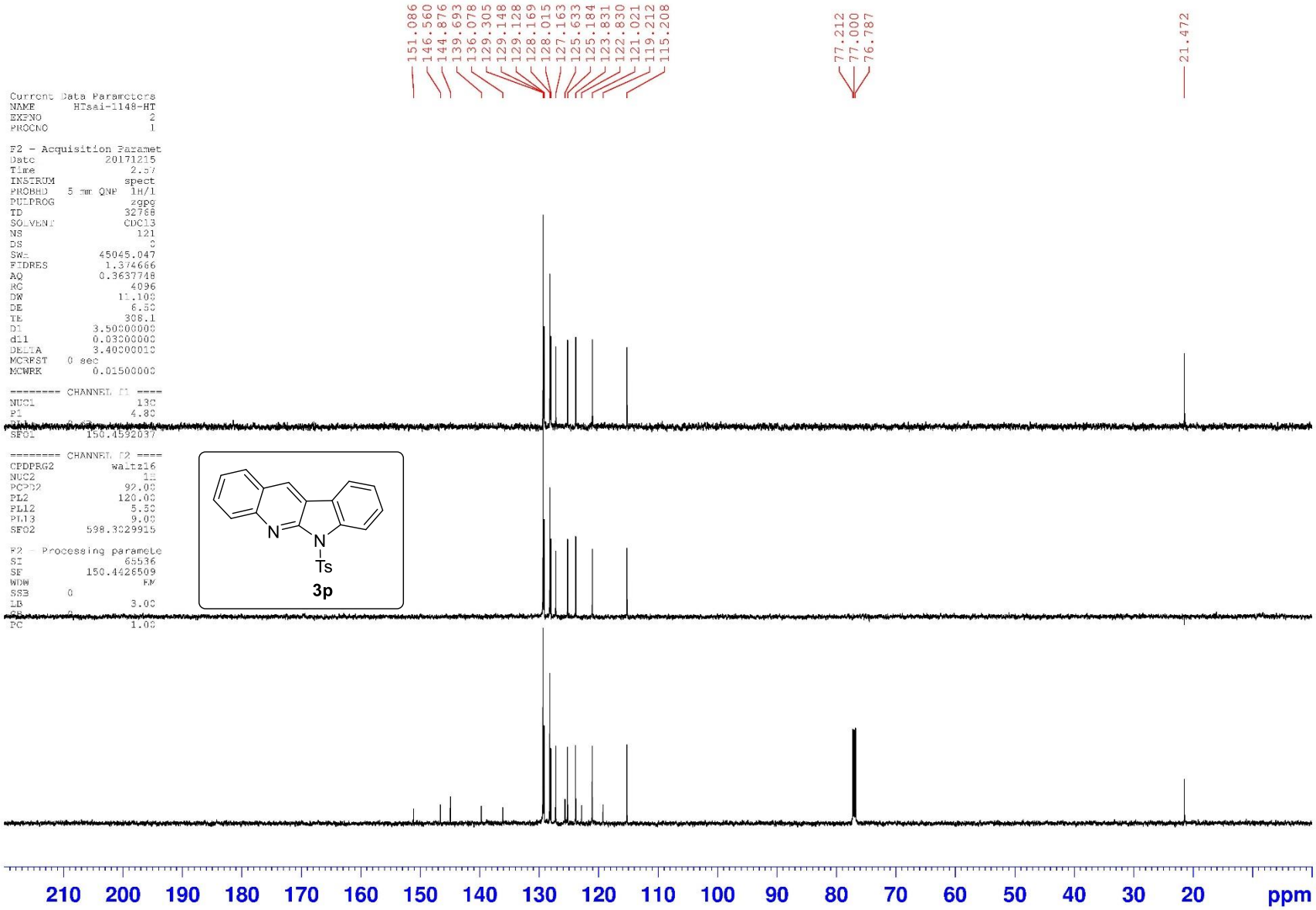
7.901
7.888
7.887
7.727
7.725
7.716
7.713
7.711
7.702
7.699
7.580
7.579
7.578
7.568
7.566
7.564
7.554
7.553
7.552
7.506
7.504
7.492
7.490
7.481
7.479
7.395
7.394
7.383
7.370
7.369
7.240
7.162
7.148
2.263
BRUKER
Current Data Parameters
NAME HTsai-1248-HZ
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171215
Time 2.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 1024
DW 52.400 usec
DE 6.50 usec
TE 308.1 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 598.3000274 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
N
N
Ts
3p
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.01
2.06
1.06
1.08
1.09
1.08
1.07
1.06
2.08
3.06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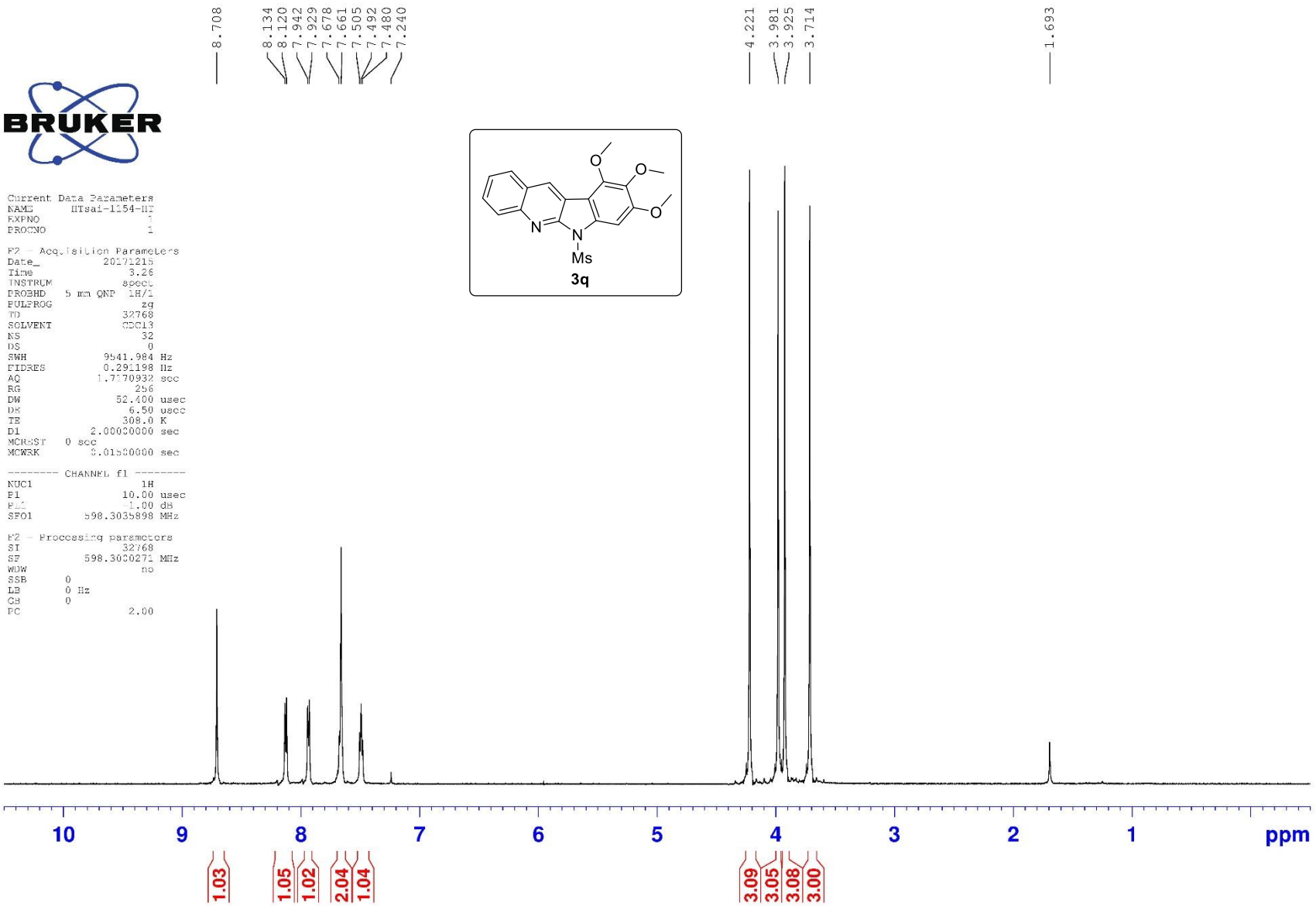
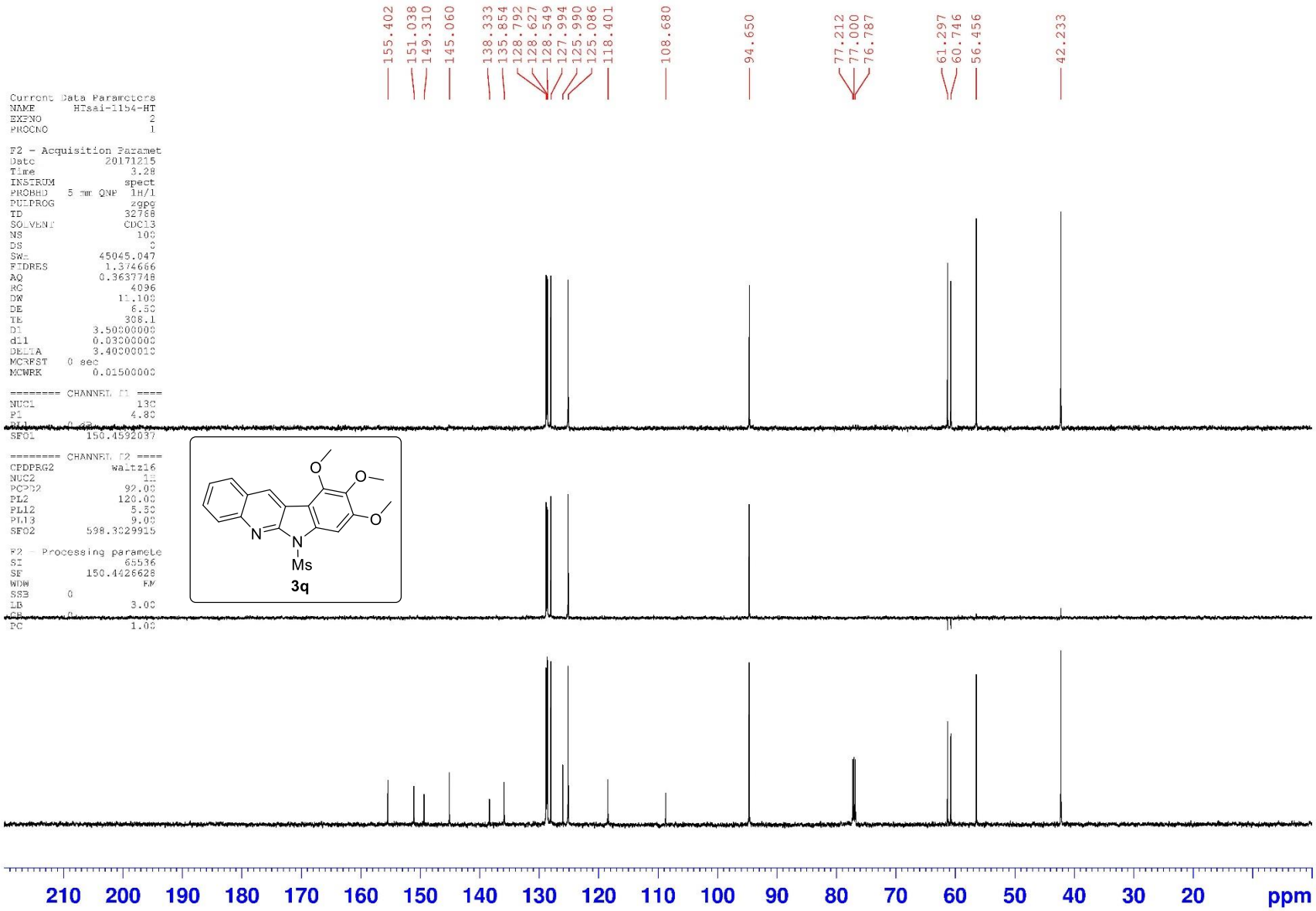
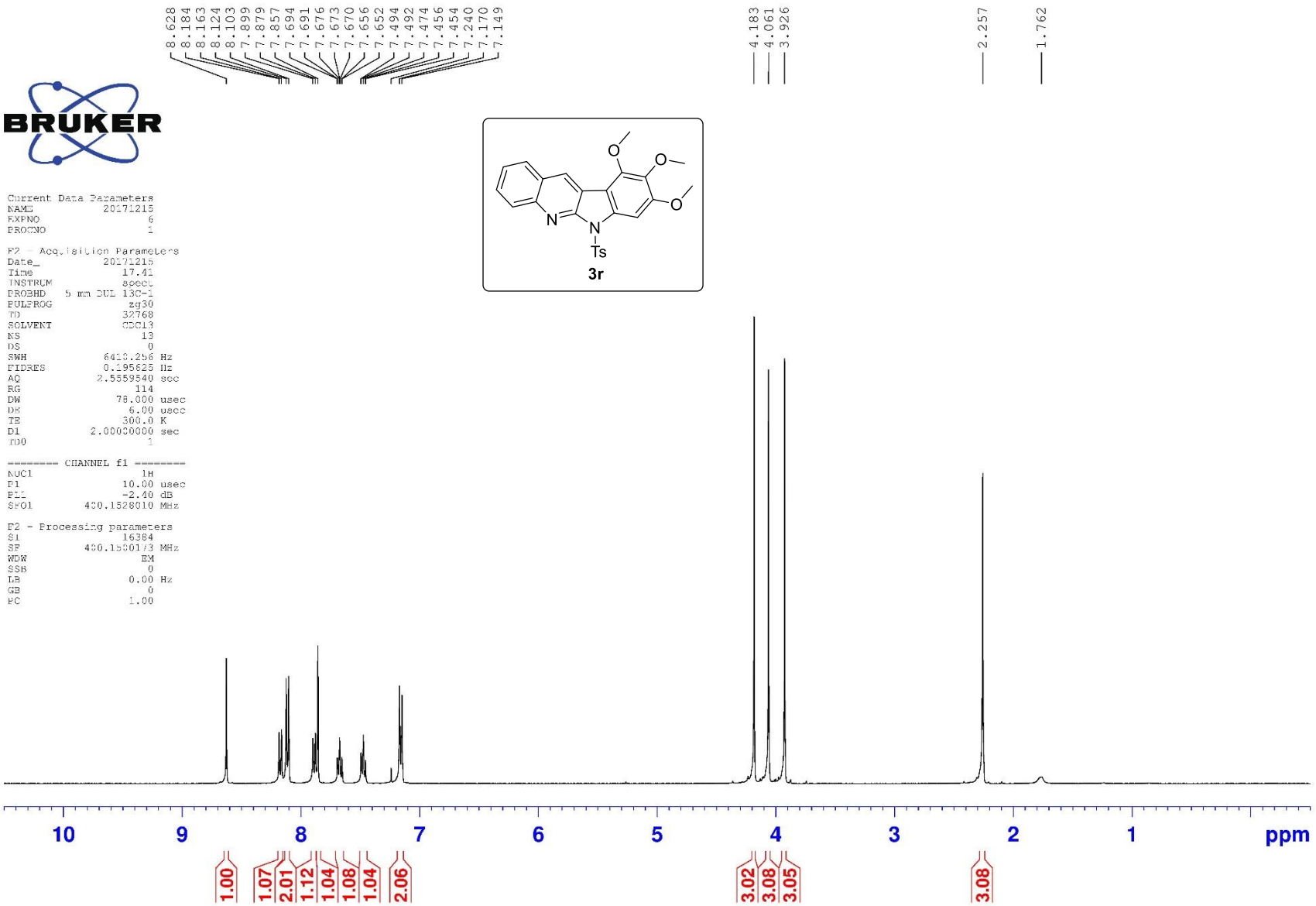
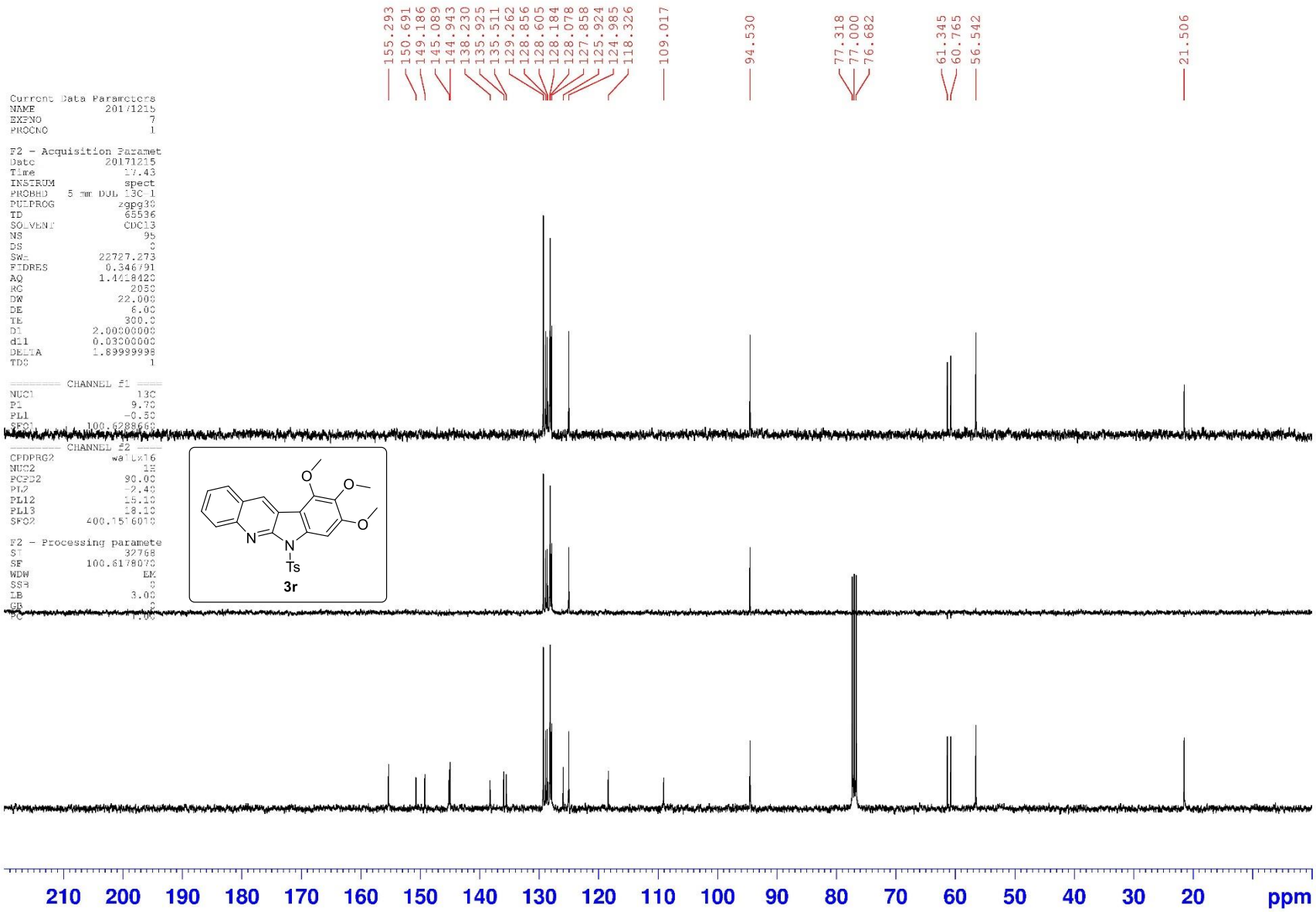
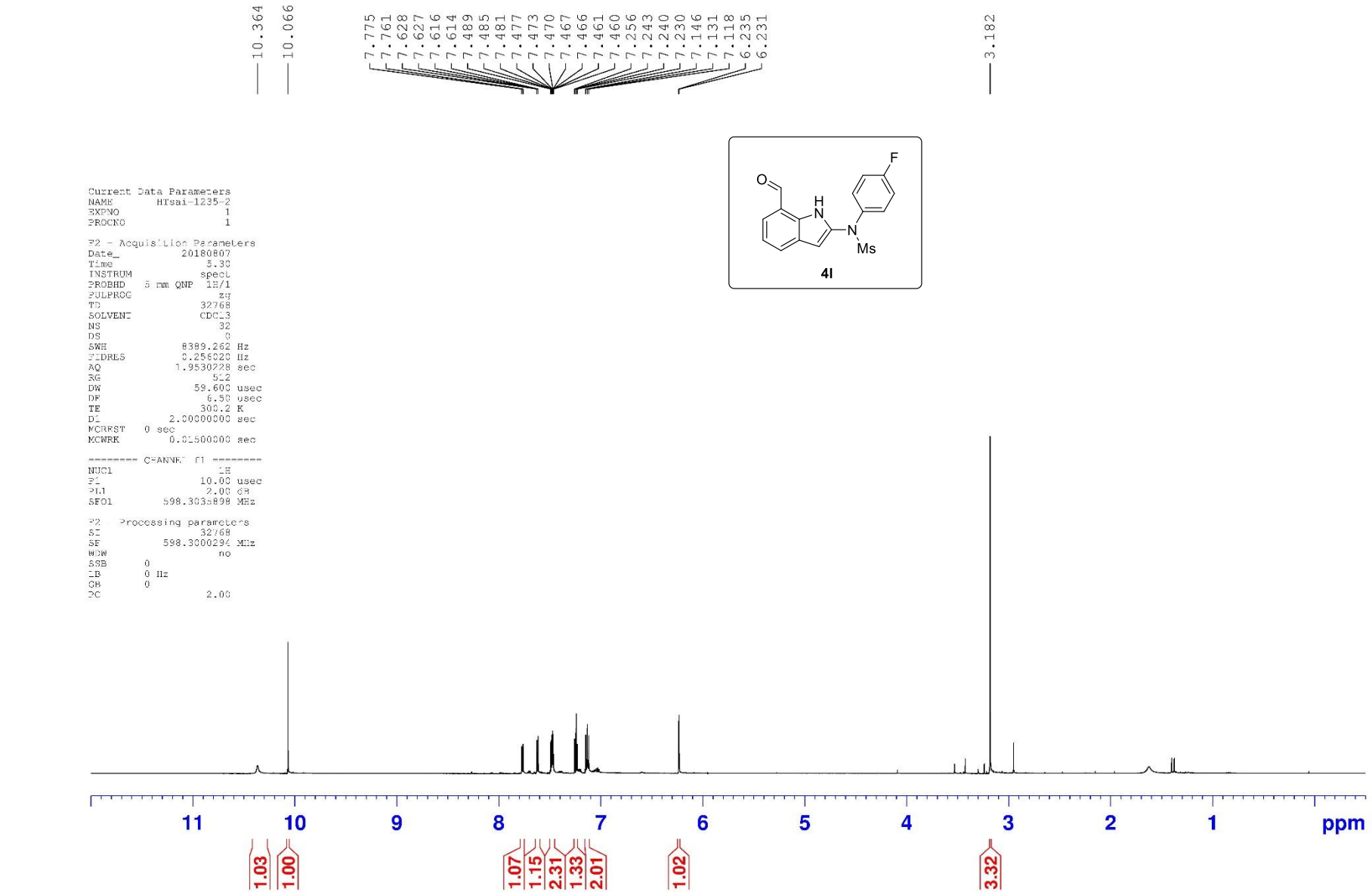
146.560
144.876
139.693
136.078
129.305
129.148
129.128
128.169
128.015
127.163
125.633
125.184
123.831
122.830
121.021
119.212
115.208
77.212
77.000
76.787
21.472
Current Data Parameters
NAME HIsai-1148-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171215
Time 2.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 121
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 308.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
SFO1 150.4592037
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426509
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
N
N
Ts
3p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

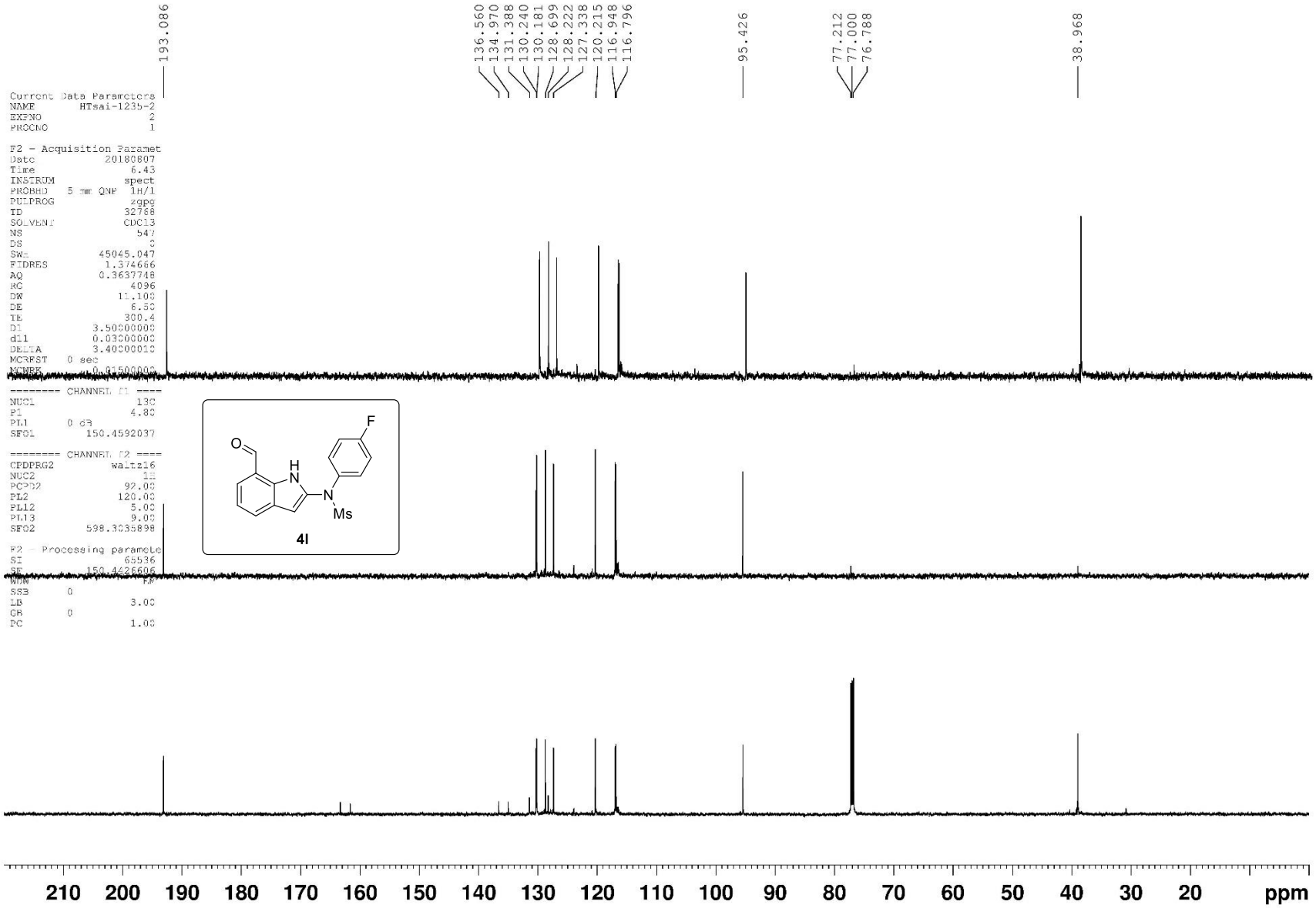

8.708
8.134
8.120
7.942
7.929
7.678
7.661
7.505
7.492
7.480
7.240
4.221
3.981
3.925
3.714
1.693
BRUKER
Current Data Parameters
NAME HTsai-1154-HZ
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171215
Time 3.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 308.0 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 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000271 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
O
O
O
N
N
Ms
3q
10
9
8
7
6
5
4
3
2
1
ppm
1.03
1.05
1.02
2.04
1.04
3.09
3.05
3.08
3.00

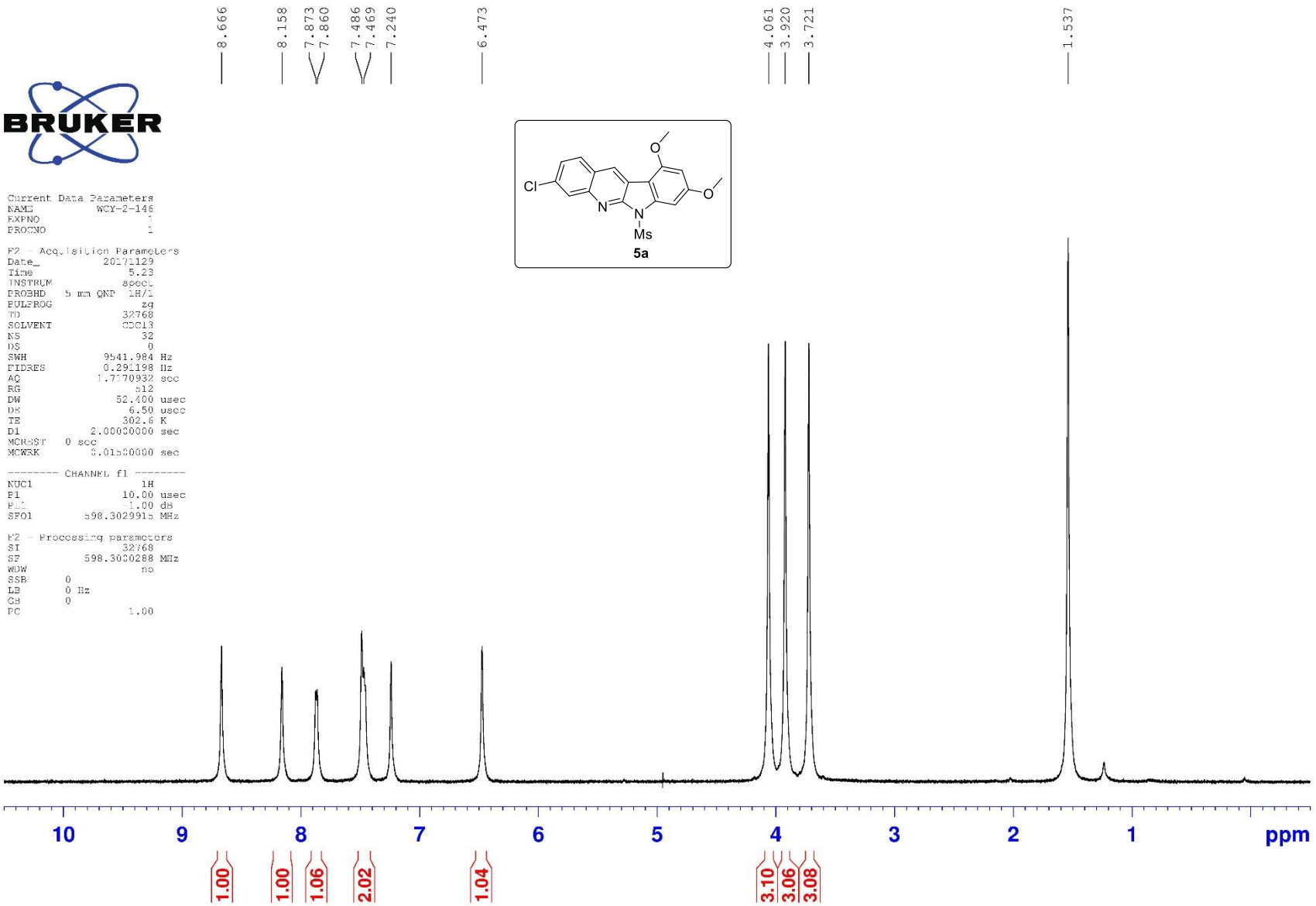

155.402
151.038
149.310
145.060
138.333
135.854
128.792
128.627
128.549
127.994
125.990
125.086
118.401
108.680
94.650
77.212
77.000
76.787
61.297
60.746
56.456
42.233
Current Data Parameters
NAME HIsai-1154-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171215
Time 3.28
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 308.1
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4592037
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426628
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
O
O
O
N
N
Ms
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

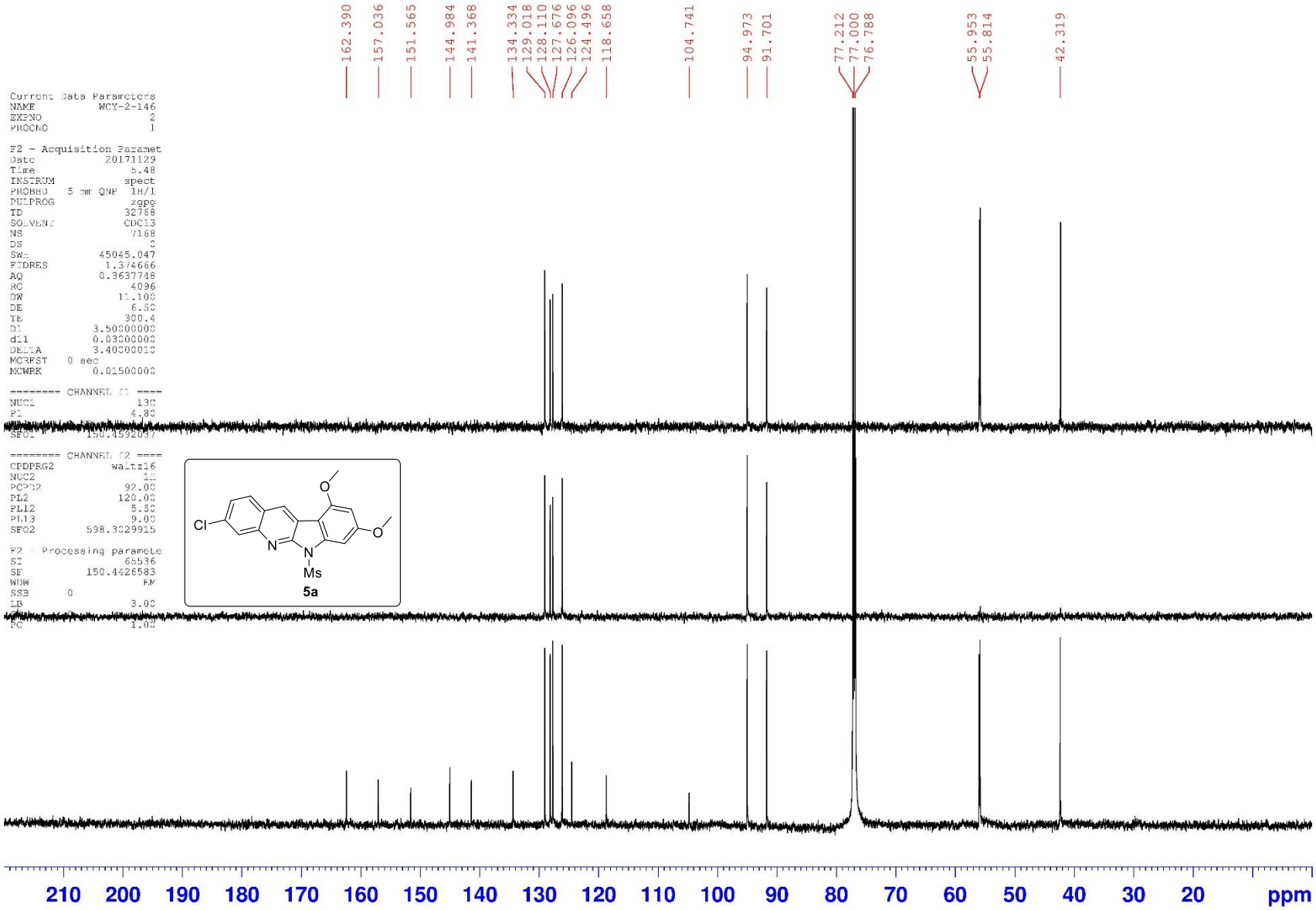

8.628
8.184
8.163
8.124
8.103
7.899
7.879
7.857
7.694
7.691
7.676
7.673
7.670
7.656
7.652
7.494
7.492
7.474
7.456
7.454
7.240
7.170
7.149
4.183
4.061
3.926
2.257
1.762
BRUKER
Current Data Parameters
NAME 20171215
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171215
Time 17.41
INSTRUM spect
PROBHD 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 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 400.1500173 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
O
O
N
N
Ts
3r
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.07
2.01
1.12
1.04
1.08
1.04
2.06
3.02
3.08
3.05
3.08

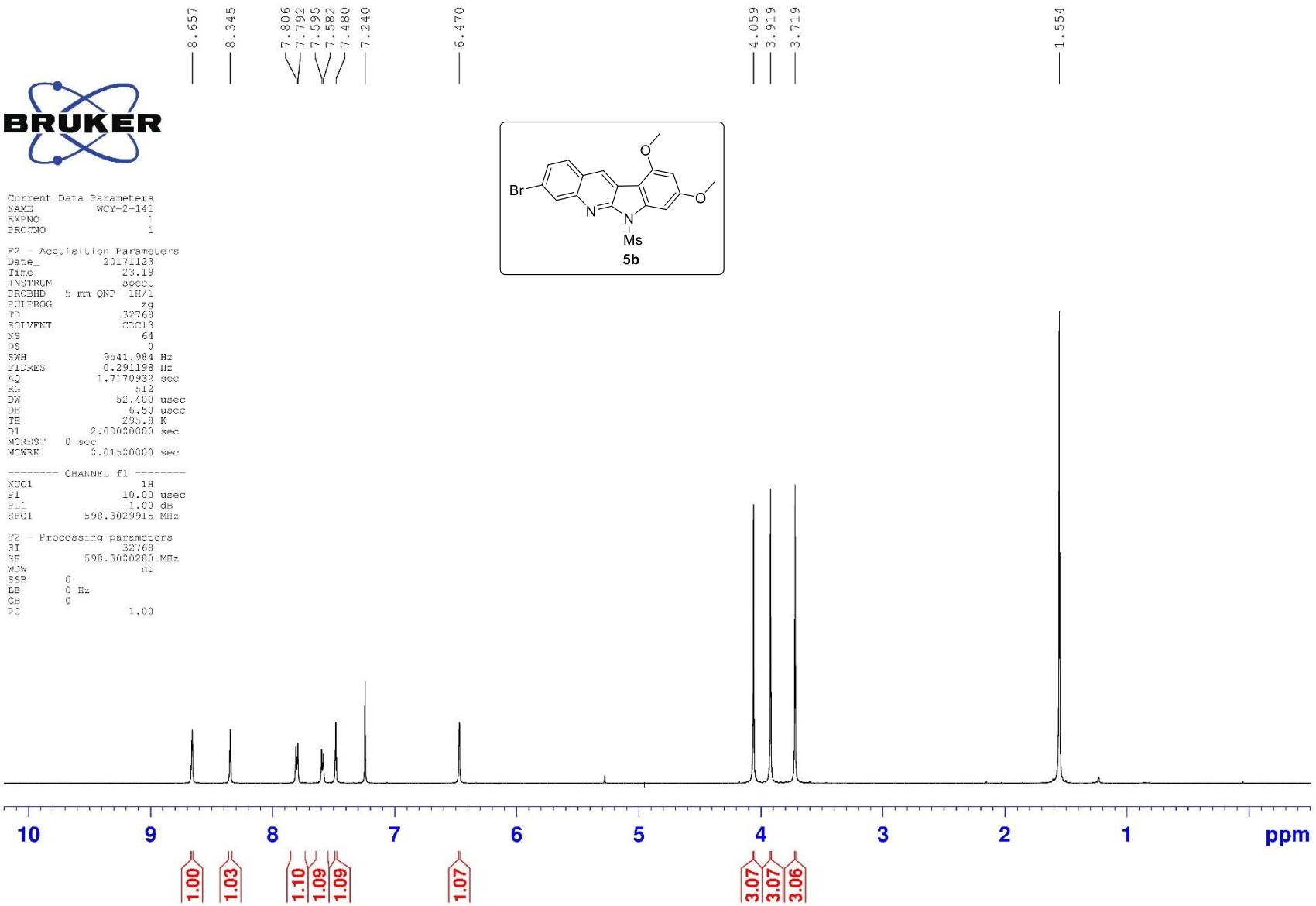

155.293
150.691
149.186
145.089
144.943
138.230
135.925
135.511
129.262
128.856
128.605
128.184
128.078
127.858
125.924
124.985
118.326
109.017
94.530
77.318
77.000
76.682
61.345
60.765
56.542
21.506
Current Data Parameters
NAME 201712l5
EXPNO 7
PROCNO 1
F2 - Acquisition Paramet
Date 20171215
Time 17.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 95
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4418420
RG 2050
DW 22.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1
======== CHANNEL f1 ====
NUC1 13C
P1 9.70
PL1 -0.30
SFO1 100.6288665
======== CHANNEL f2 ====
CPDPRG2 wa l pl6
NUC2 1H
PCPD2 90.00
PL2 -2.40
PL12 15.10
PL13 18.10
SFO2 400.1516010
F2 - Processing paramete
SI 32768
SF 100.6178078
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
O
O
O
N
N
Ts
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

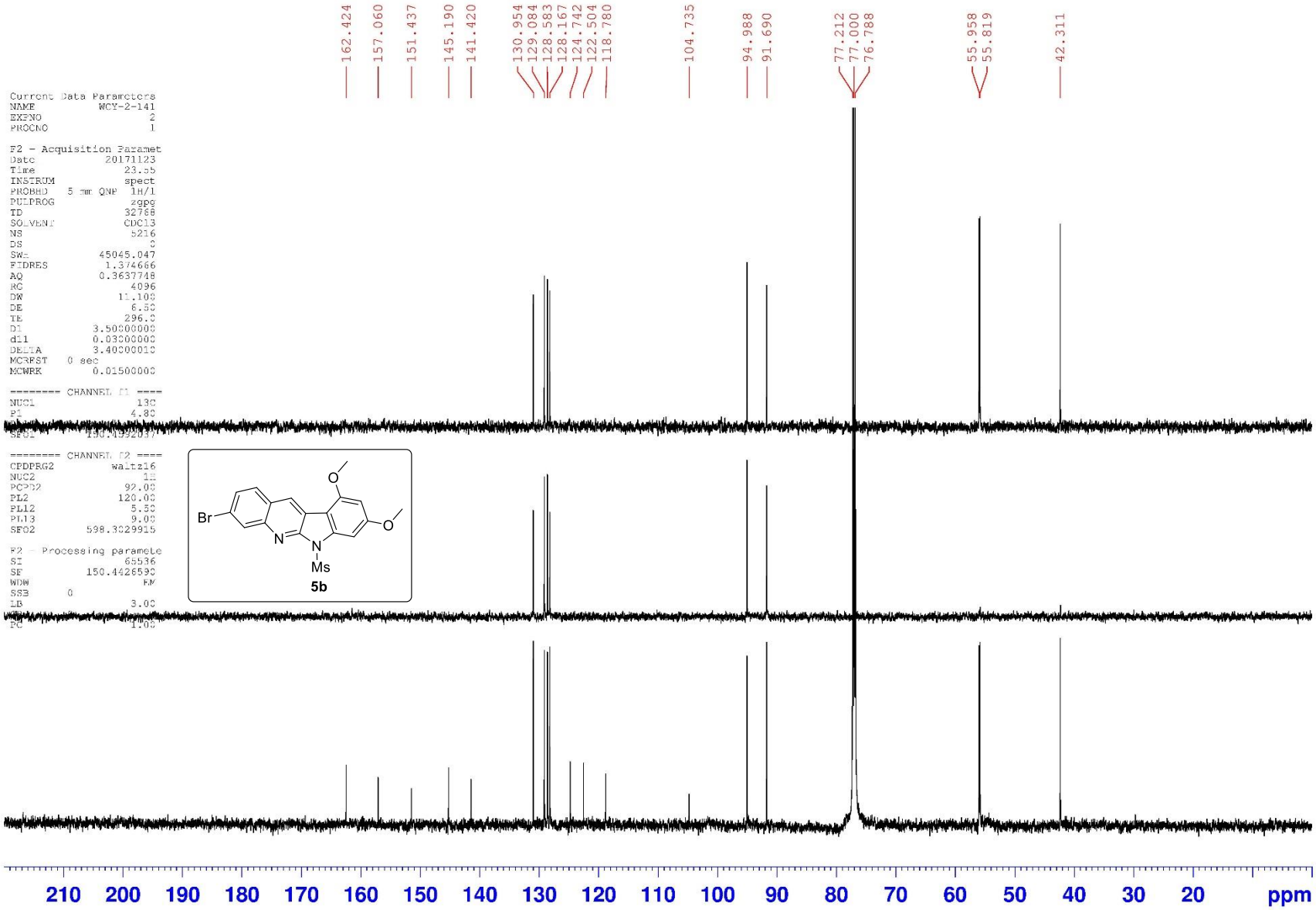

10.364
10.066
7.775
7.761
7.628
7.627
7.616
7.614
7.489
7.485
7.481
7.477
7.473
7.470
7.467
7.466
7.461
7.460
7.256
7.243
7.240
7.230
7.146
7.131
7.118
6.235
6.231
3.182
Current Data Parameters
NAME HIsai-1235-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180807
Time 5.30
INSTRUM spect
PROBHD 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 300.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 2.00 dB
SFO1 598.3035898 MHz
F2 - Processing parameters
SI 32768
SF 598.3000294 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
F
O
H
N
N
Ms
4l
11
10
9
8
7
6
5
4
3
2
1
ppm
1.03
1.00
1.07
1.15
2.31
1.33
2.01
1.02
3.32

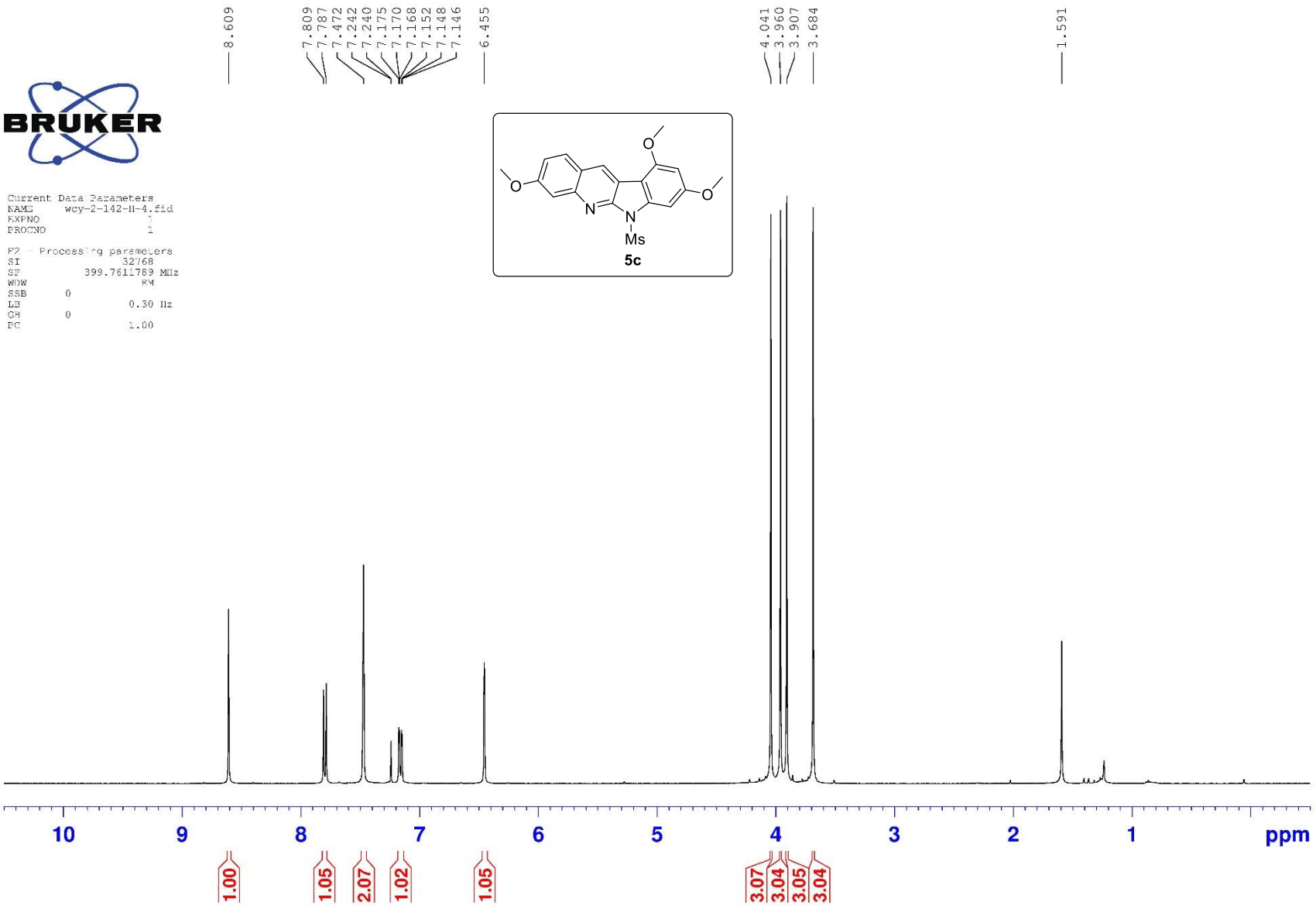

193.086
136.560
134.970
131.388
130.240
130.181
128.699
128.222
127.338
120.215
116.948
116.796
95.426
77.212
77.000
76.788
38.968
Current Data Parameters
NAME HTsai-1235-2
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20180807
Time 6.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 547
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 300.4
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.07500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
PL1 0 dB
SFO1 150.4592037
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.00
PL13 9.00
SFO2 598.3035898
F2 - Processing parameter
SI 65536
SF 150.4426606
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
O
H
N
F
N
Ms
4l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

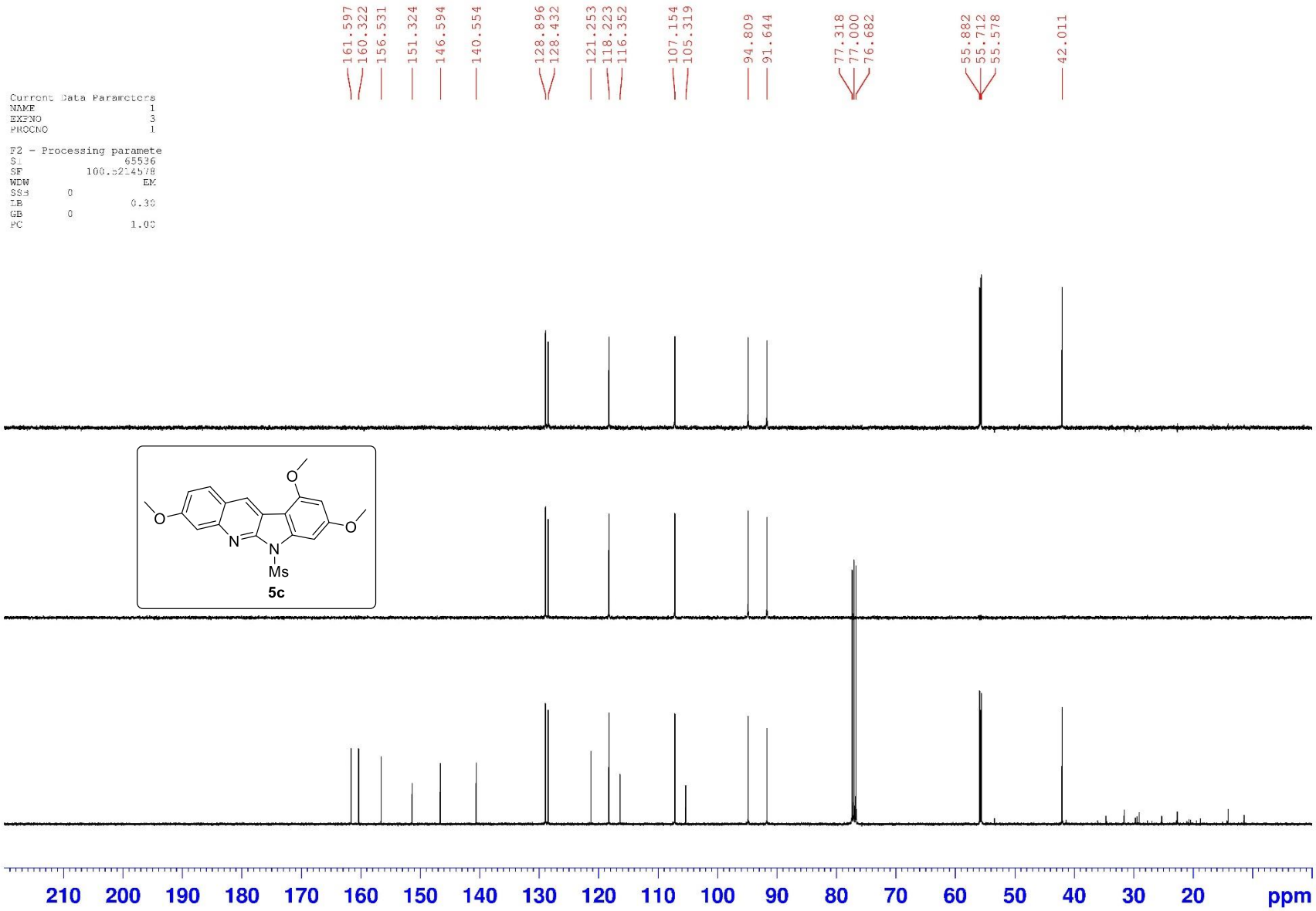

8.666
8.158
7.873
7.860
7.486
7.469
7.240
6.473
4.061
3.920
3.721
1.537
Current Data Parameters
NAME WCY-2-146
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171129
Time 5.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 302.6 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 598.3000288 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Cl
O
O
N
N
Ms
5a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.06
2.02
1.04
3.10
3.06
3.08

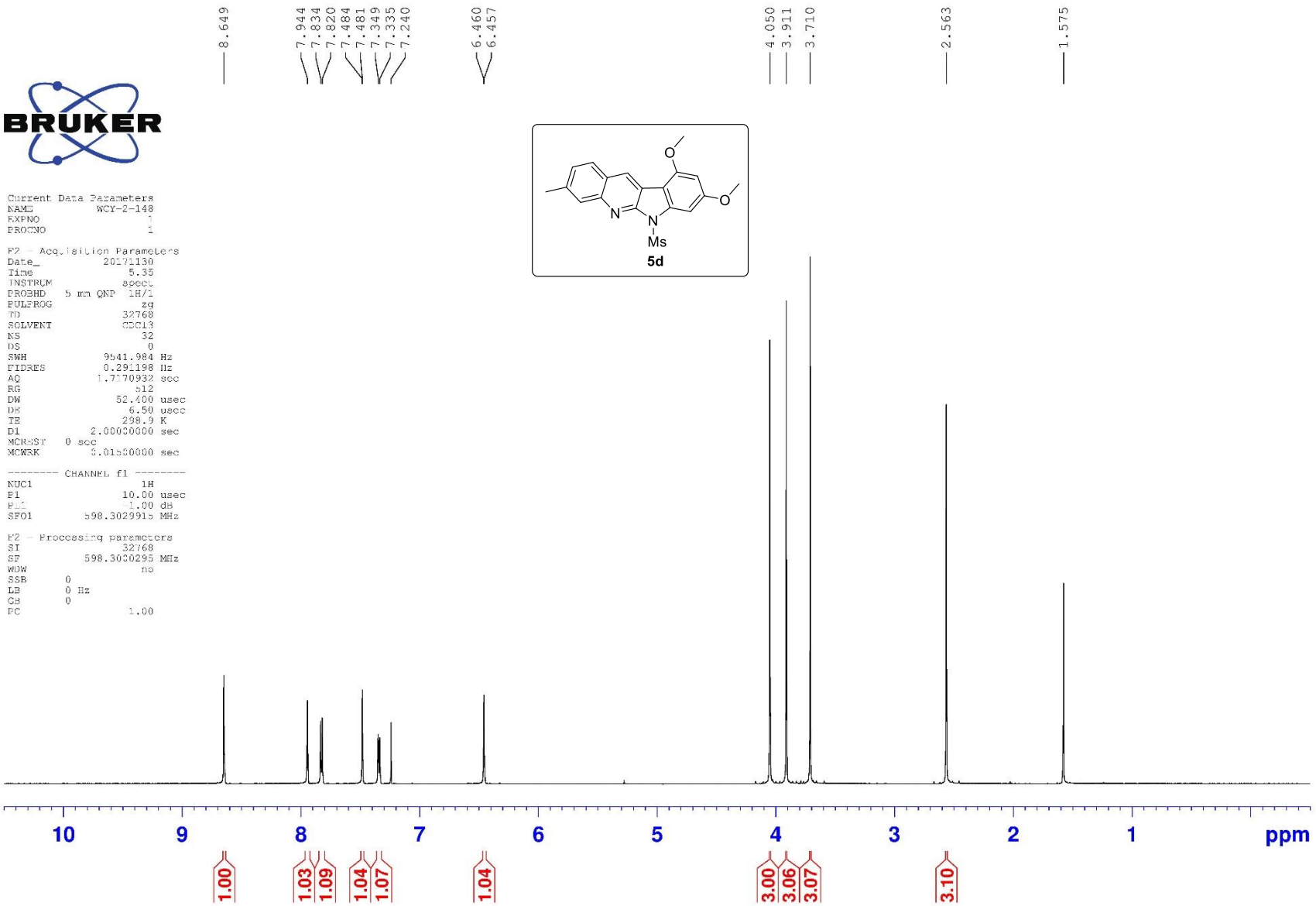

162.390
157.036
151.565
144.984
141.368
134.334
129.018
128.110
127.676
126.096
124.496
118.658
104.741
94.973
91.701
77.212
77.000
76.788
55.953
55.814
42.319
Current Data Parameters
NAME WCY-2-146
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171129
Time 5.48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 7168
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 300.4
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
SFO1 150.1992057
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426583
WDW EM
SSB 0
LB 3.00
PC 1.00
Cl
O
O
N
N
Ms
5a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

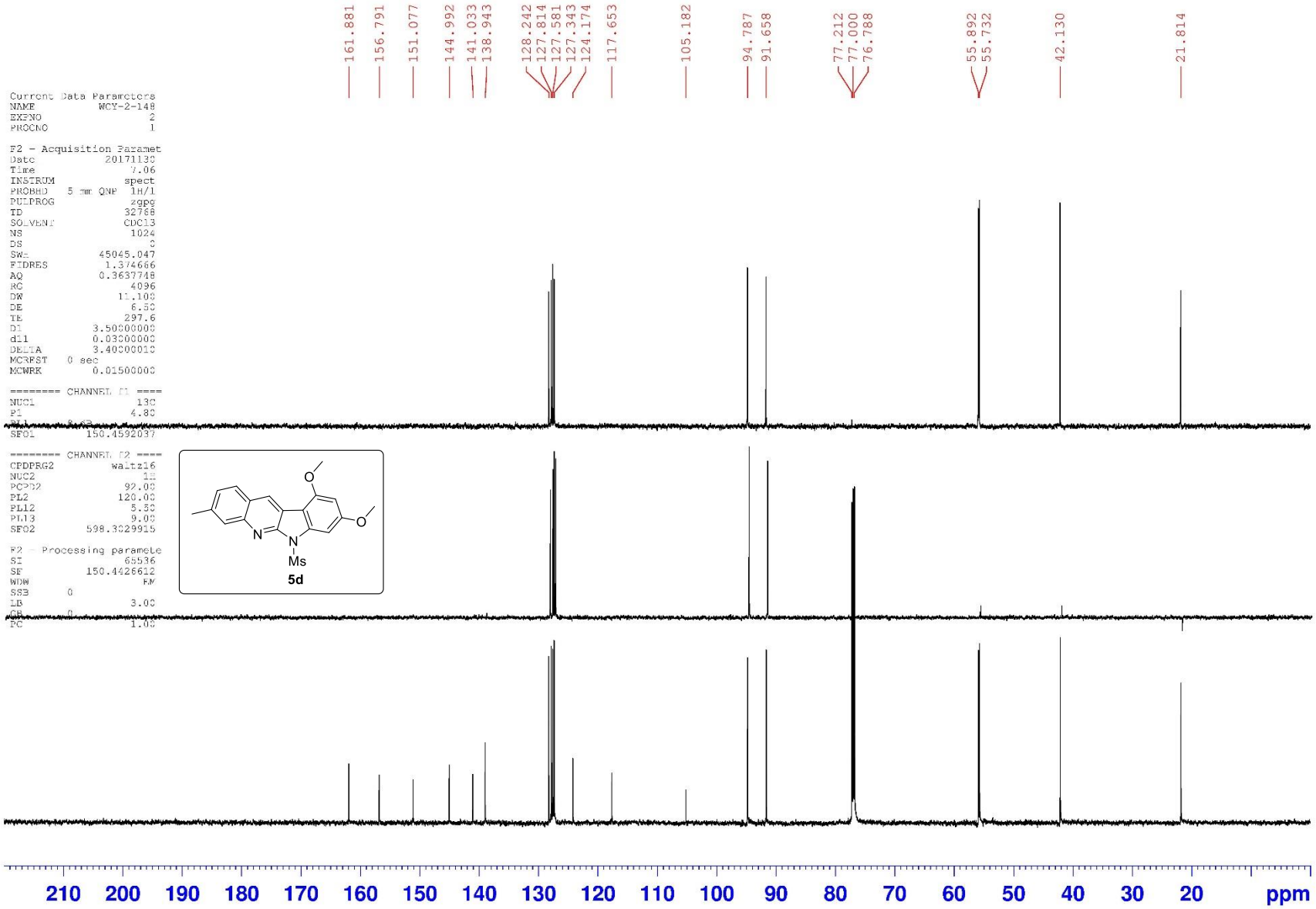

8.657
8.345
7.806
7.792
7.595
7.582
7.480
7.240
6.470
4.059
3.919
3.719
1.554
BRUKER
Current Data Parameters
NAME WCY-2-141
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171123
Time 23.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 295.8 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 598.3000280 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Br
O
O
N
N
Ms
5b
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.10
1.09
1.09
1.07
3.07
3.07
3.06

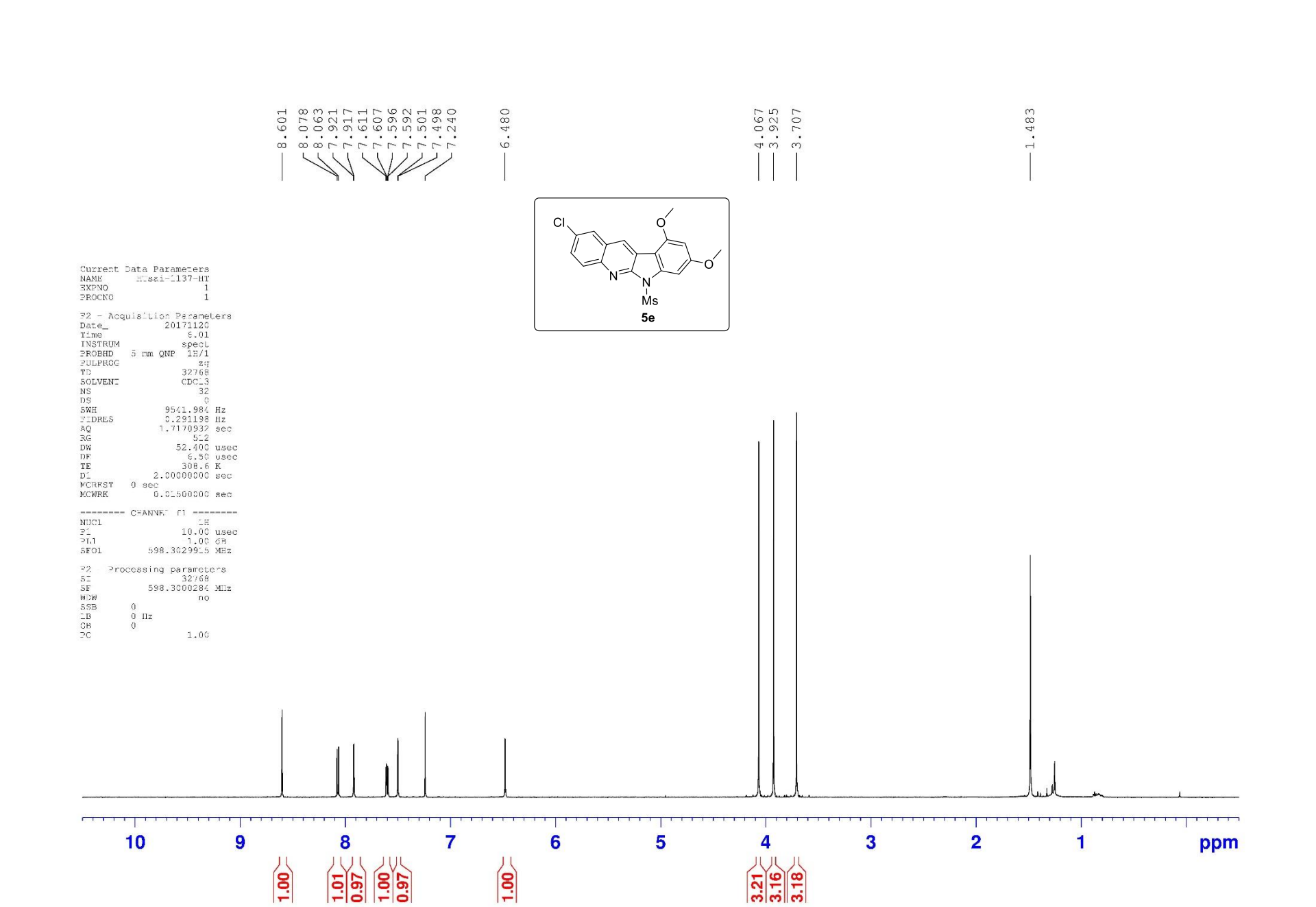

162.424
157.060
151.437
145.190
141.420
130.954
129.084
128.583
128.167
124.742
122.504
118.780
104.735
94.988
91.690
77.212
77.000
76.788
55.958
55.819
42.311
Current Data Parameters
NAME WCY-2-141
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171123
Time 23.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 5216
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 296.0
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
SFO1 150.4992077
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426590
WDW EM
SSB 0
LB 3.00
GB
PC 1.00
Br
O
O
N
N
Ms
5b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

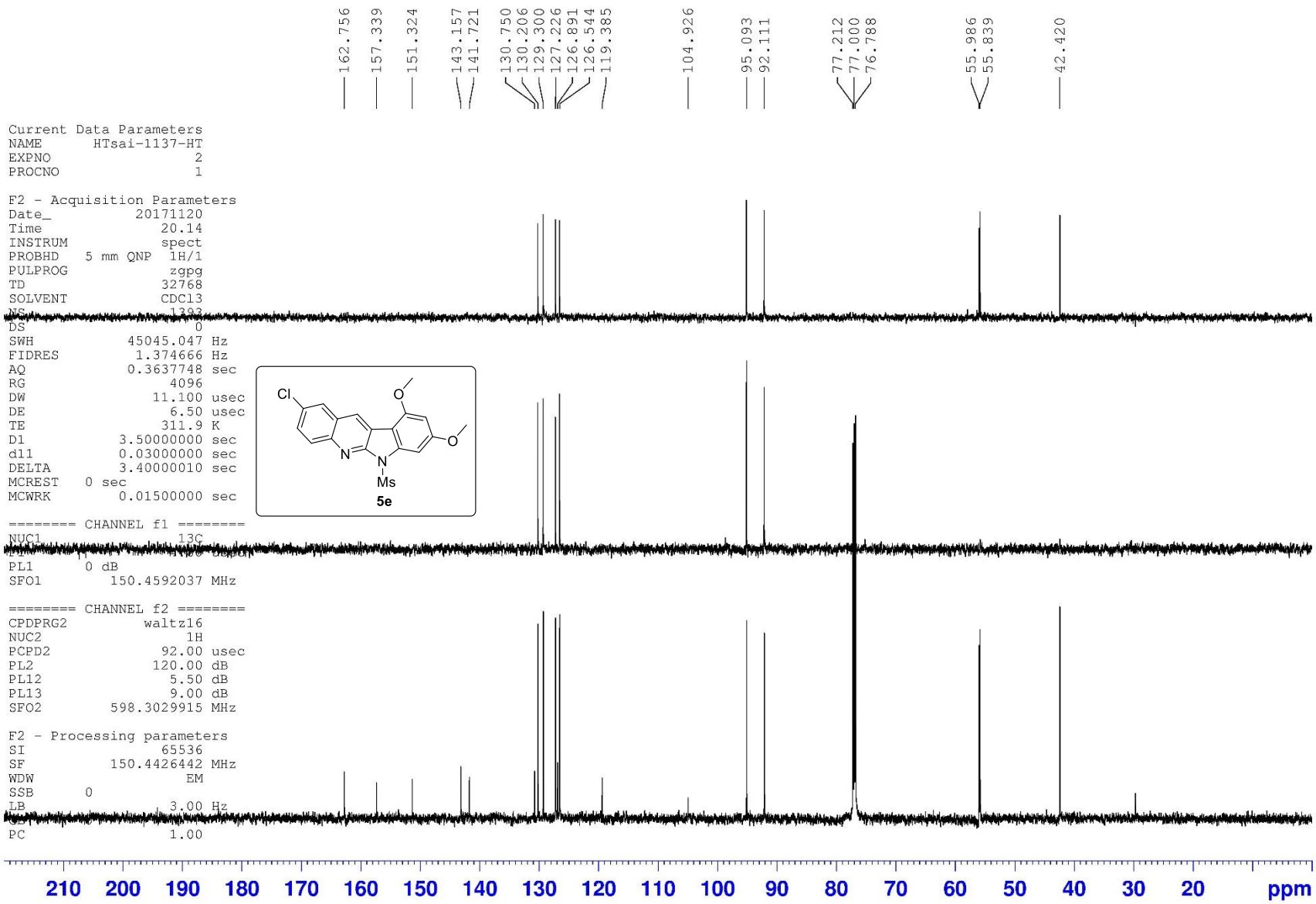

8.609
7.809
7.787
7.472
7.242
7.240
7.175
7.170
7.168
7.152
7.148
7.146
6.455
4.041
3.960
3.907
3.684
1.591
Current Data Parameters
NAME wcy-2-142-H-4.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611789 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
O
N
N
Ms
5c
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.05
2.07
1.02
1.05
3.07
3.04
3.05
3.04

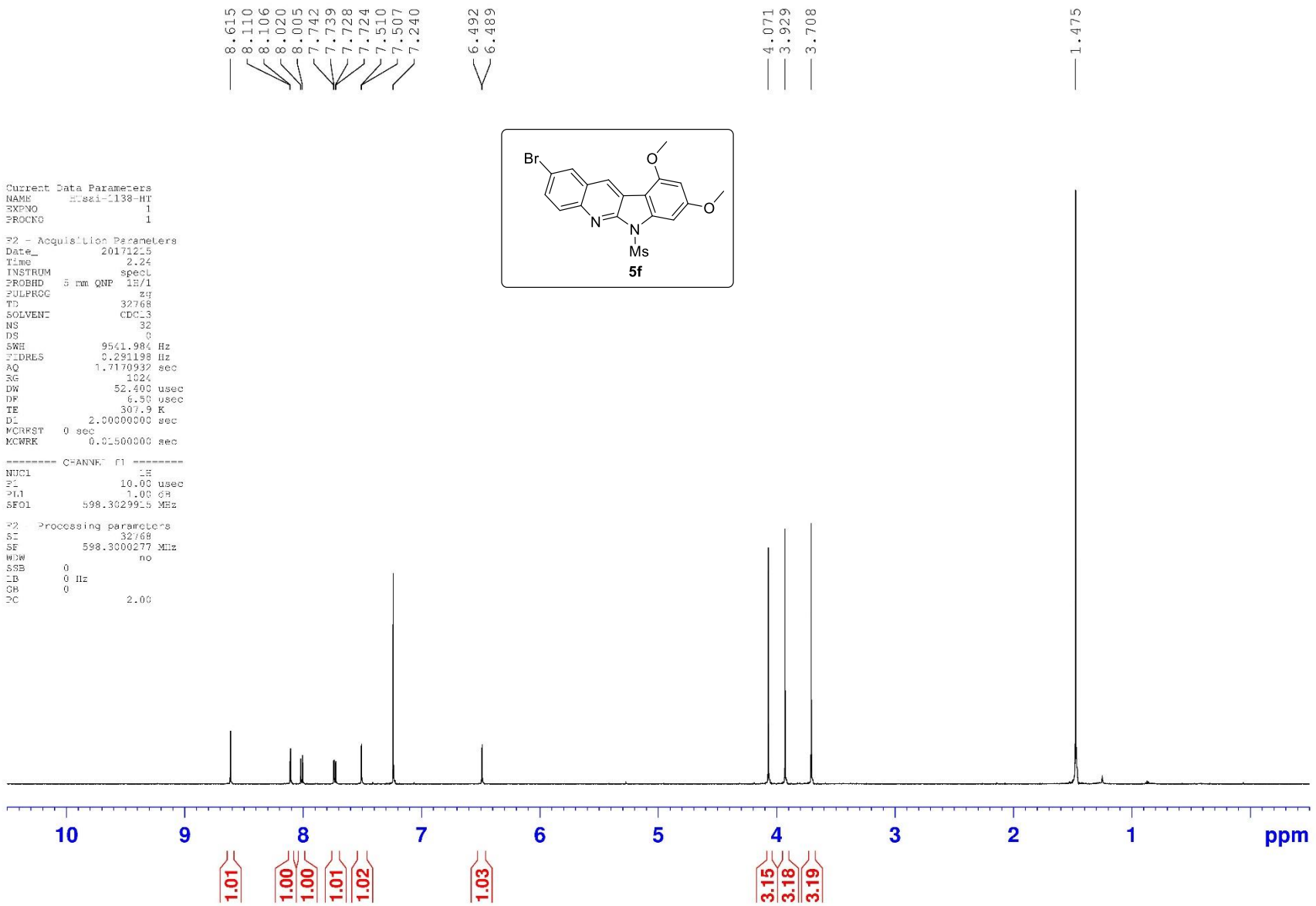

161.597
160.322
156.531
151.324
146.594
140.554
128.896
128.432
121.253
118.223
116.352
107.154
105.319
94.809
91.644
77.318
77.000
76.682
55.882
55.712
55.578
42.011
Current Data Parameters
NAME 1
EXPNO 3
PROCNO 1
F2 - Processing paramete
SI 65536
SF 100.6214578
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
O
O
O
N
N
Ms
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

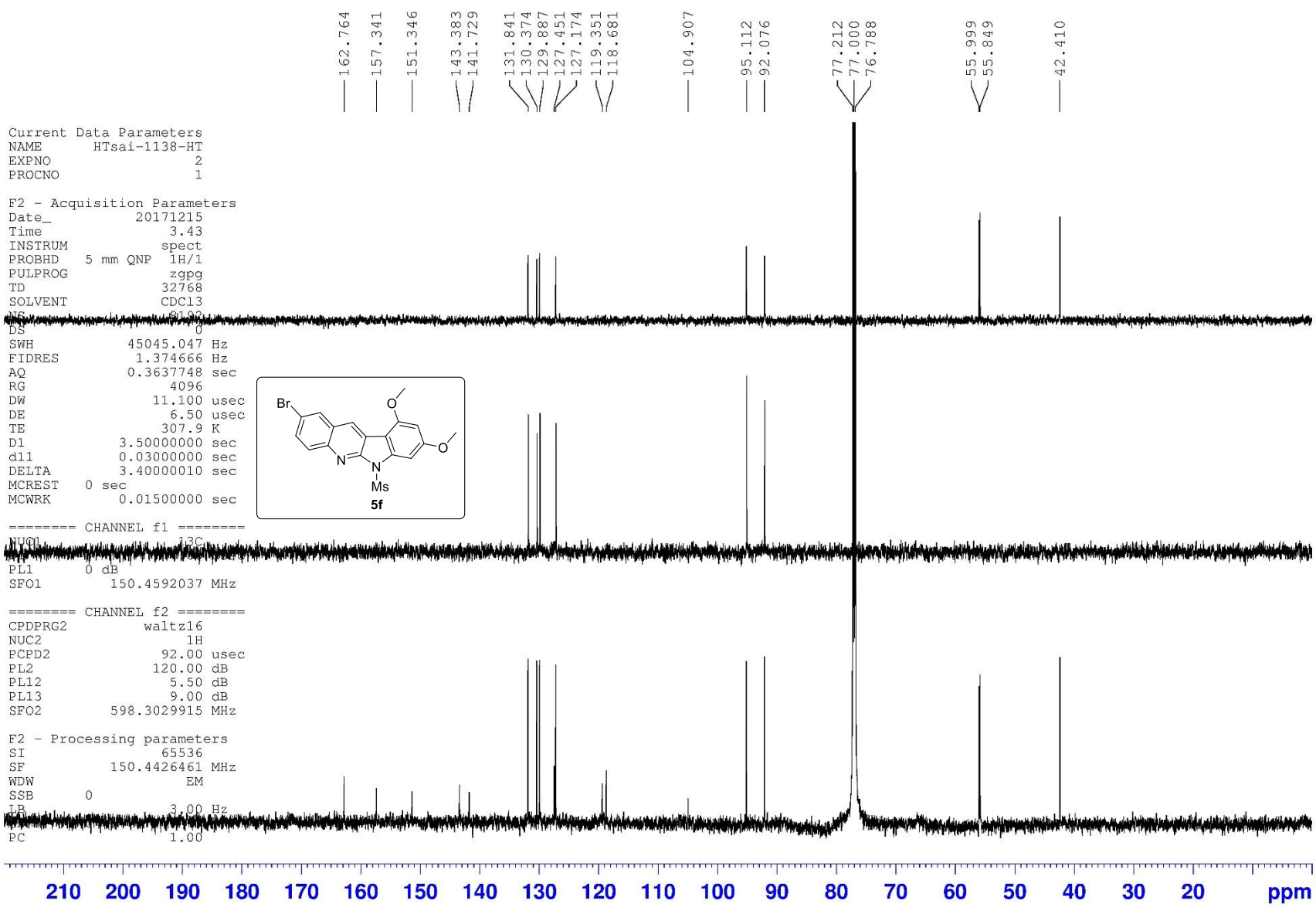

8.649
7.944
7.834
7.820
7.484
7.481
7.349
7.335
7.240
6.460
6.457
4.050
3.911
3.710
2.563
1.575
Ms
5d
Current Data Parameters
NAME WCY-2-148
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171130
Time 5.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 -1.00 dB
SFO1 598.3029915 MHz
F2 - Processing parameters
SI 32768
SF 598.3000295 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.09
1.04
1.07
1.04
3.00
3.06
3.07
3.10

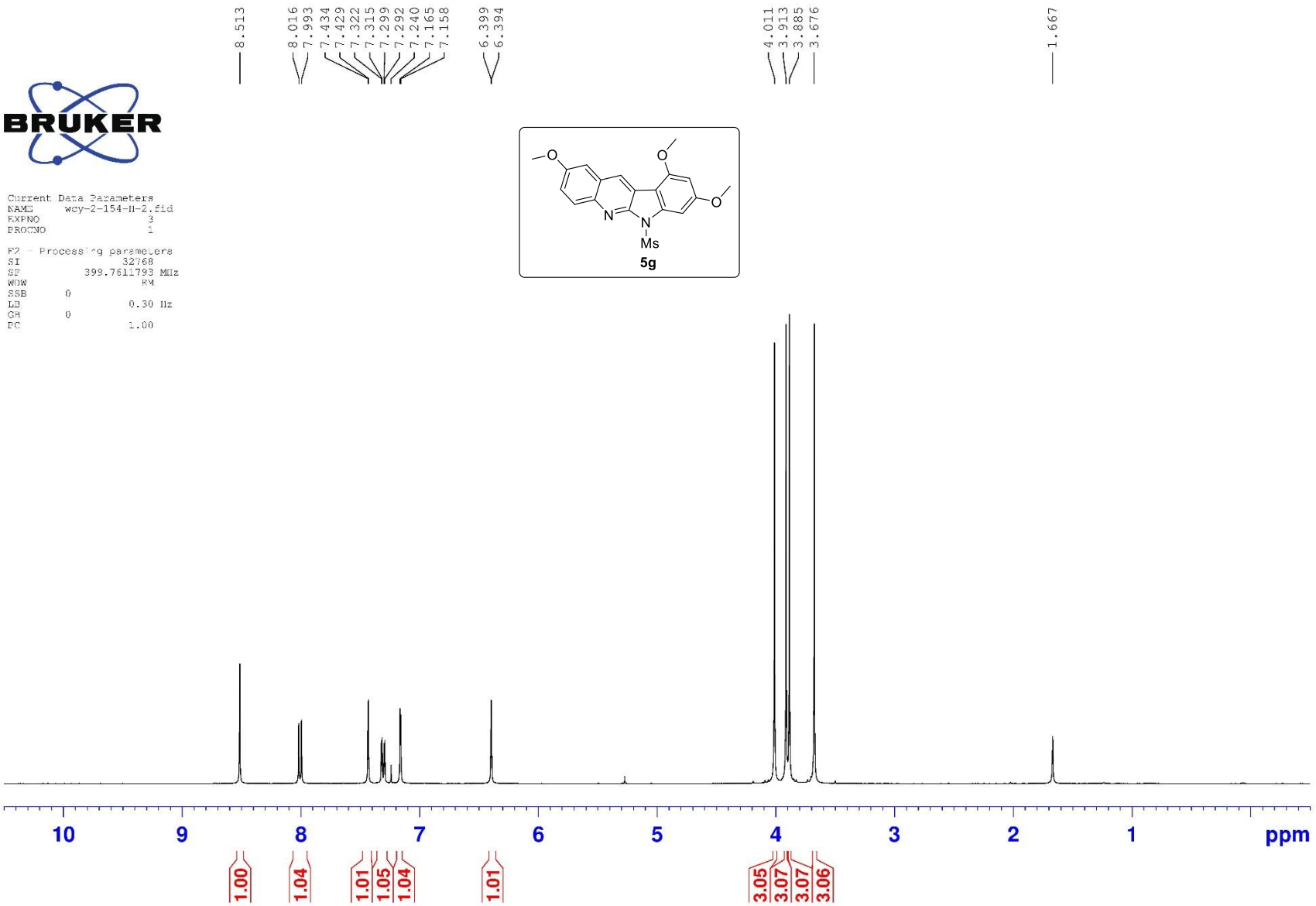

161.881
156.791
151.077
144.992
141.033
138.943
128.242
127.814
127.581
127.343
124.174
117.653
105.182
94.787
91.658
77.212
77.000
76.788
55.892
55.732
42.130
21.814
Current Data Parameters
NAME WCY-2-148
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171130
Time 7.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1024
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 297.6
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
SFO1 150.4592037
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4426612
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.00
O
O
N
N
Ms
5d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

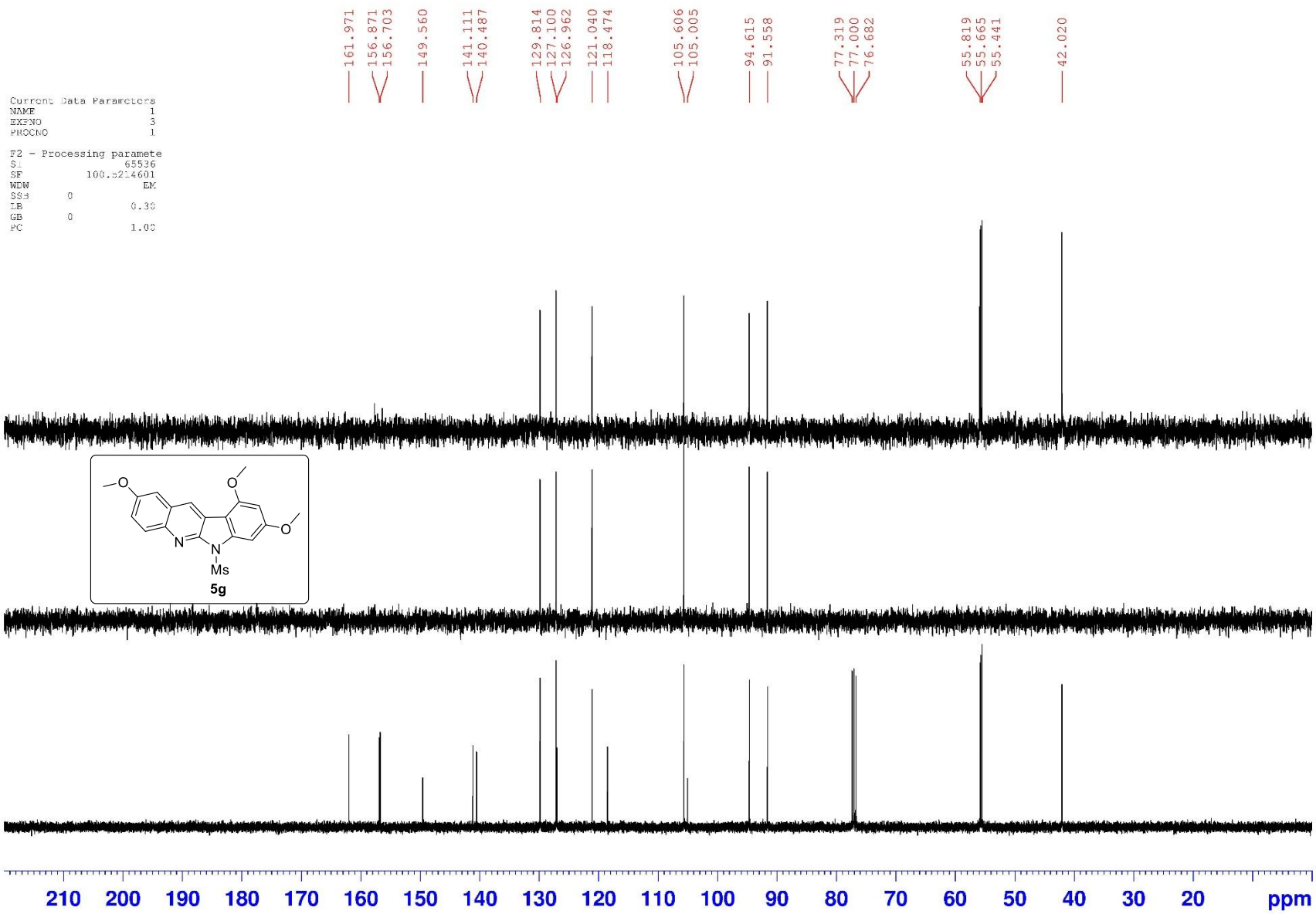

8.601
8.078
8.063
7.921
7.917
7.611
7.607
7.596
7.592
7.501
7.498
7.240
6.480
4.067
3.925
3.707
1.483
Cl
O
O
N
N
Ms
5e
Current Data Parameters
NAME Hisai-1137-HT
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171120
Time 6.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
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 308.6 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 598.3000284 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
0.97
1.00
0.97
1.00
3.21
3.16
3.18

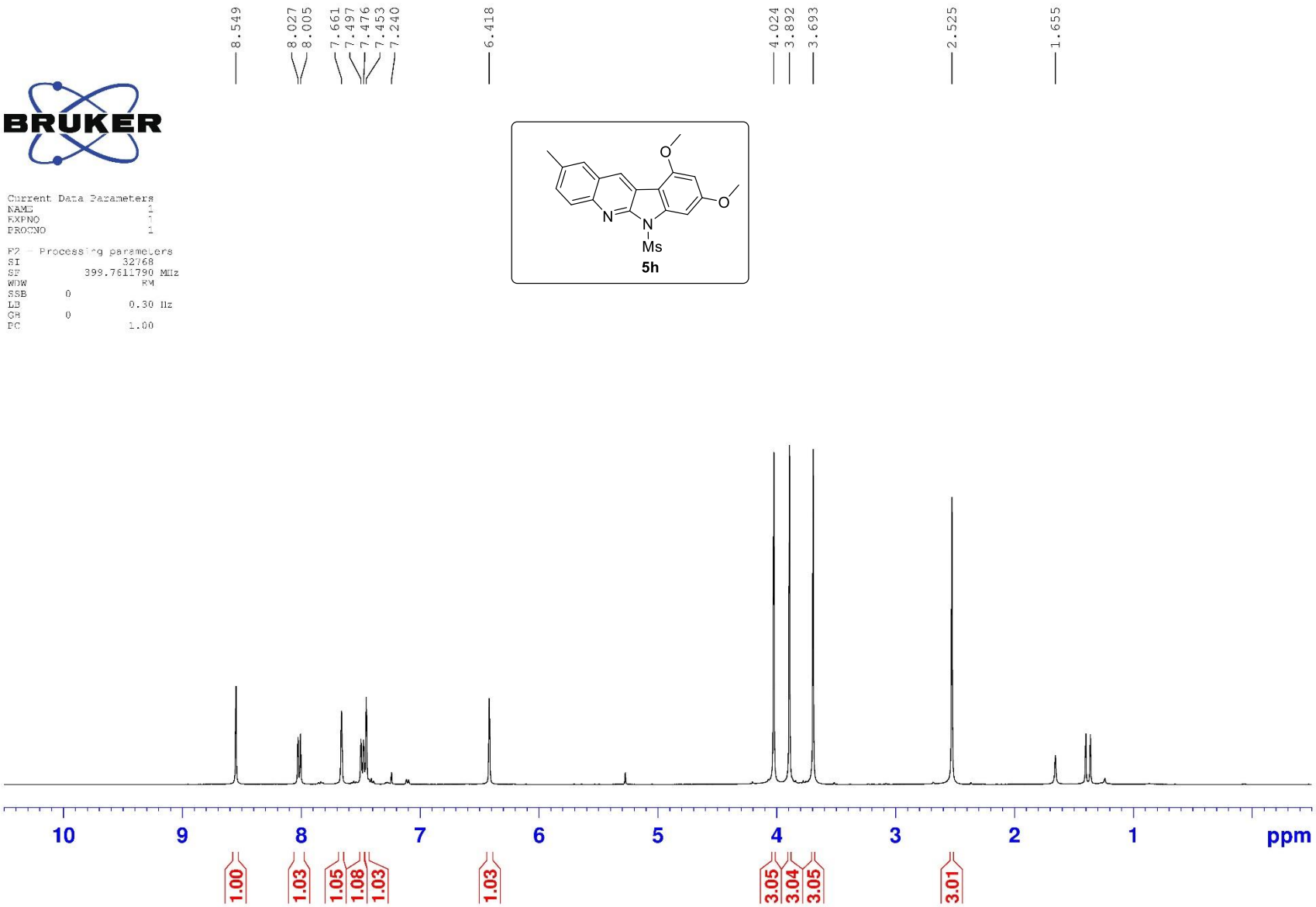

162.756
157.339
151.324
143.157
141.721
130.750
130.206
129.300
127.226
126.891
126.544
119.385
104.926
95.093
92.111
77.212
77.000
76.788
55.986
55.839
42.420
Current Data Parameters
NAME HTsai-1137-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171120
Time 20.14
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1393
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 311.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
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 150.4426442 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
Cl
O
O
N
N
Ms
5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

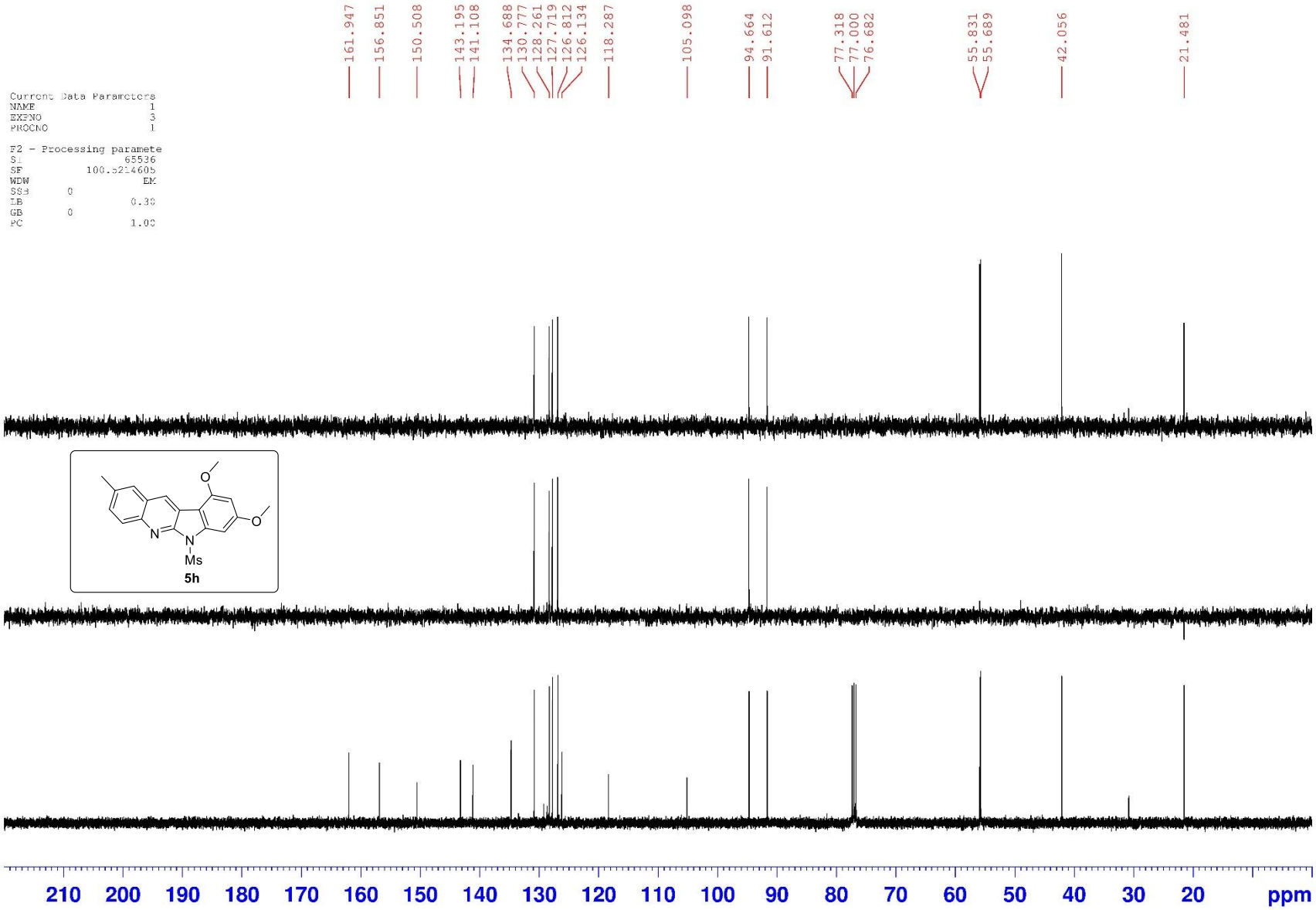

8.615
8.110
8.106
8.020
8.005
7.742
7.739
7.728
7.724
7.510
7.507
7.240
6.492
6.489
4.071
3.929
3.708
1.475
Br
O
O
N
N
Ms
5f
Current Data Parameters
NAME Hisai-2138-HT
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20171225
Time 2.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 1024
DW 52.400 usec
DE 6.50 usec
TE 307.9 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
P2 - Processing parameters
SI 32768
SF 598.3000277 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
1.01
1.00
1.00
1.01
1.02
1.03
3.15
3.18
3.19

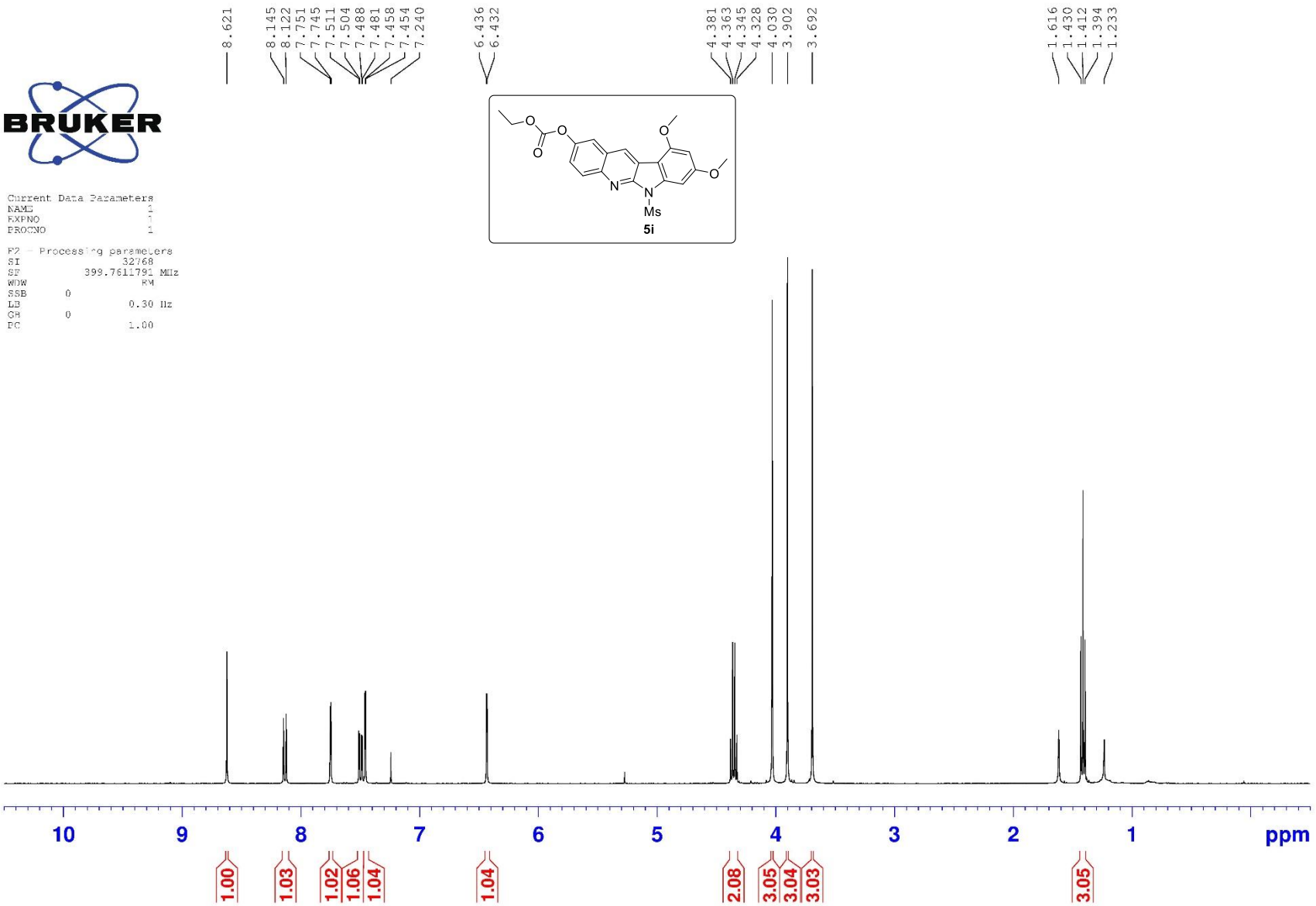

162.764
157.341
151.346
143.383
141.729
131.841
130.374
129.887
127.451
127.174
119.351
118.681
104.907
95.112
92.076
77.212
77.000
76.788
55.999
55.849
42.410
Current Data Parameters
NAME HTsai-1138-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171215
Time 3.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
DS
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 307.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
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 150.4426461 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
Br
O
O
N
N
Ms
5f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

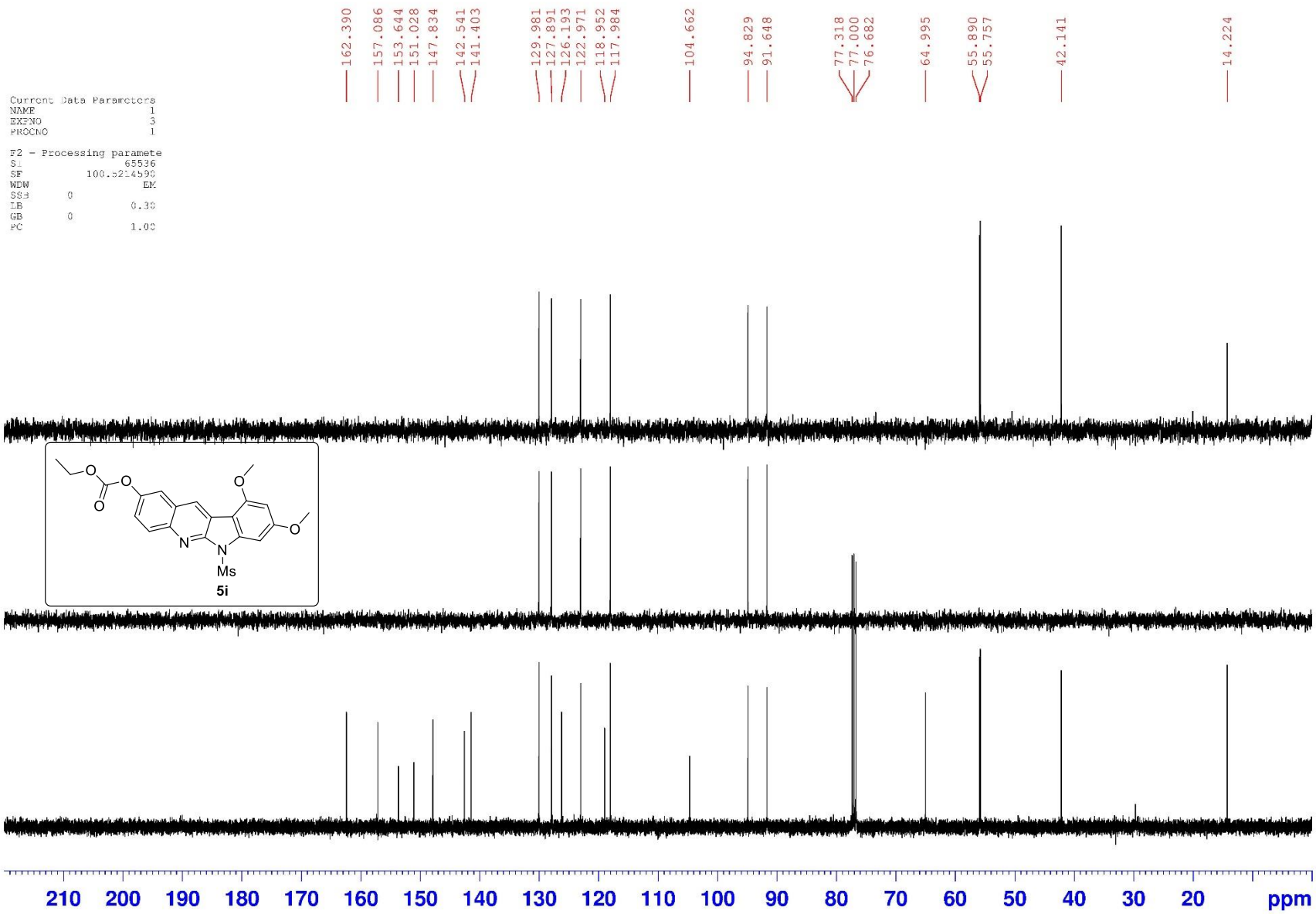

8.513
8.016
7.993
7.434
7.429
7.322
7.315
7.299
7.292
7.240
7.165
7.158
6.399
6.394
4.011
3.913
3.885
3.676
1.667
BRUKER
Current Data Parameters
NAME wcy-2-154-H-2.fid
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611793 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
O
N
N
Ms
5g
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.01
1.05
1.04
1.01
3.05
3.07
3.07
3.06

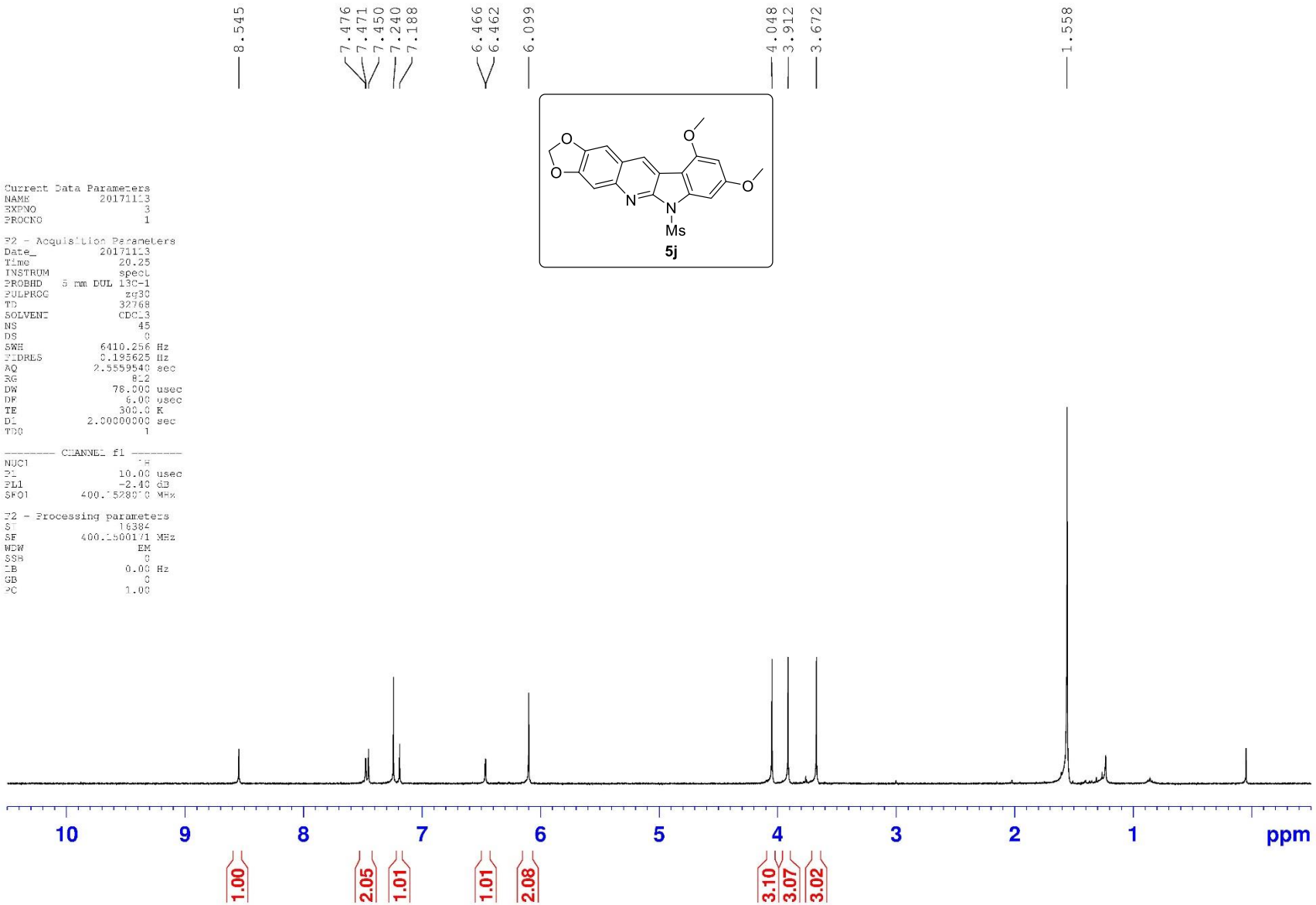

161.971
156.871
156.703
149.560
141.111
140.487
129.814
127.100
126.962
121.040
118.474
105.606
105.005
94.615
91.558
77.319
77.000
76.682
55.819
55.665
55.441
42.020
Current Data Parameters
NAME 1
EXPNO 3
PROCNO 1
F2 - Processing paramete
SI 65536
SF 100.6214601
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
O
O
O
N
N
Ms
5g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

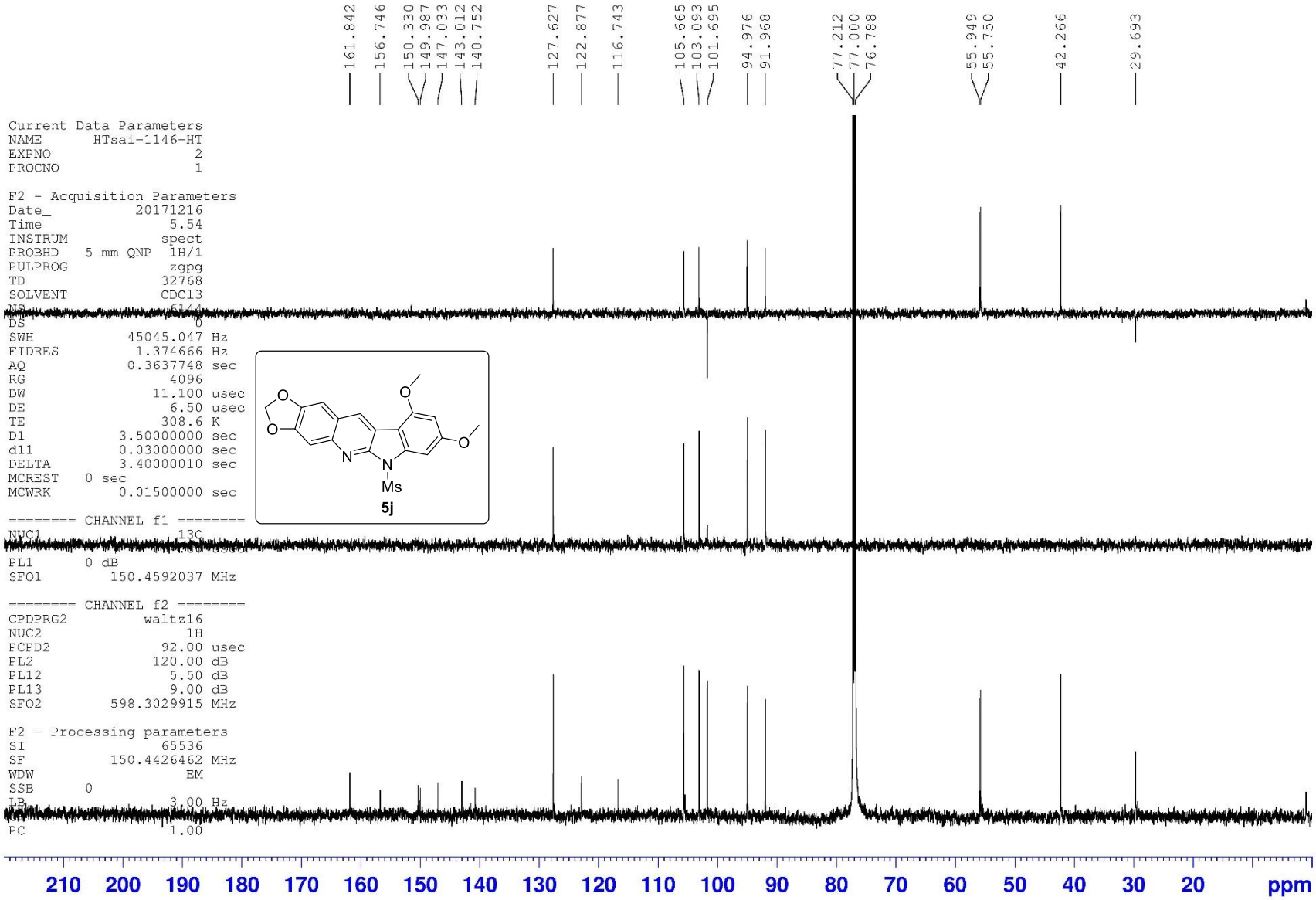

8.549
8.027
8.005
7.661
7.497
7.476
7.453
7.240
6.418
4.024
3.892
3.693
2.525
1.655
BRUKER
Current Data Parameters
NAME 2
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611790 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
N
Ms
5h
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.05
1.08
1.03
1.03
3.05
3.04
3.05
3.01


161.947
156.851
150.508
143.195
141.108
134.688
130.777
128.261
127.719
126.812
126.134
118.287
105.098
94.664
91.612
77.318
77.000
76.682
55.831
55.689
42.056
21.481
Current Data Parameters
NAME 1
EXPNO 3
PROCNO 1
F2 - Processing paramete
SI 65536
SF 100.6214605
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
O
O
N
N
Ms
5h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.621
8.145
8.122
7.751
7.745
7.511
7.504
7.488
7.481
7.458
7.454
7.240
6.436
6.432
4.381
4.363
4.345
4.328
4.030
3.902
3.692
1.616
1.430
1.412
1.394
1.233
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Processing parameters
SI 32768
SF 399.7611791 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ms
5i
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.02
1.06
1.04
1.04
2.08
3.05
3.04
3.03
3.05


162.390
157.086
153.644
151.028
147.834
142.541
141.403
129.981
127.891
126.193
122.971
118.952
117.984
104.662
94.829
91.648
77.318
77.000
76.682
64.995
55.890
55.757
42.141
14.224
Current Data Parameters
NAME 1
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.6214590
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
O
O
O
O
N
N
Ms
5i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.545
7.476
7.471
7.450
7.240
7.188
6.466
6.462
6.099
4.048
3.912
3.672
1.558
Current Data Parameters
NAME 20171113
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171113
Time 20.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 45
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 400.1328710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
O
O
O
N
N
Ms
5j
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.05
1.01
1.01
2.08
3.10
3.07
3.02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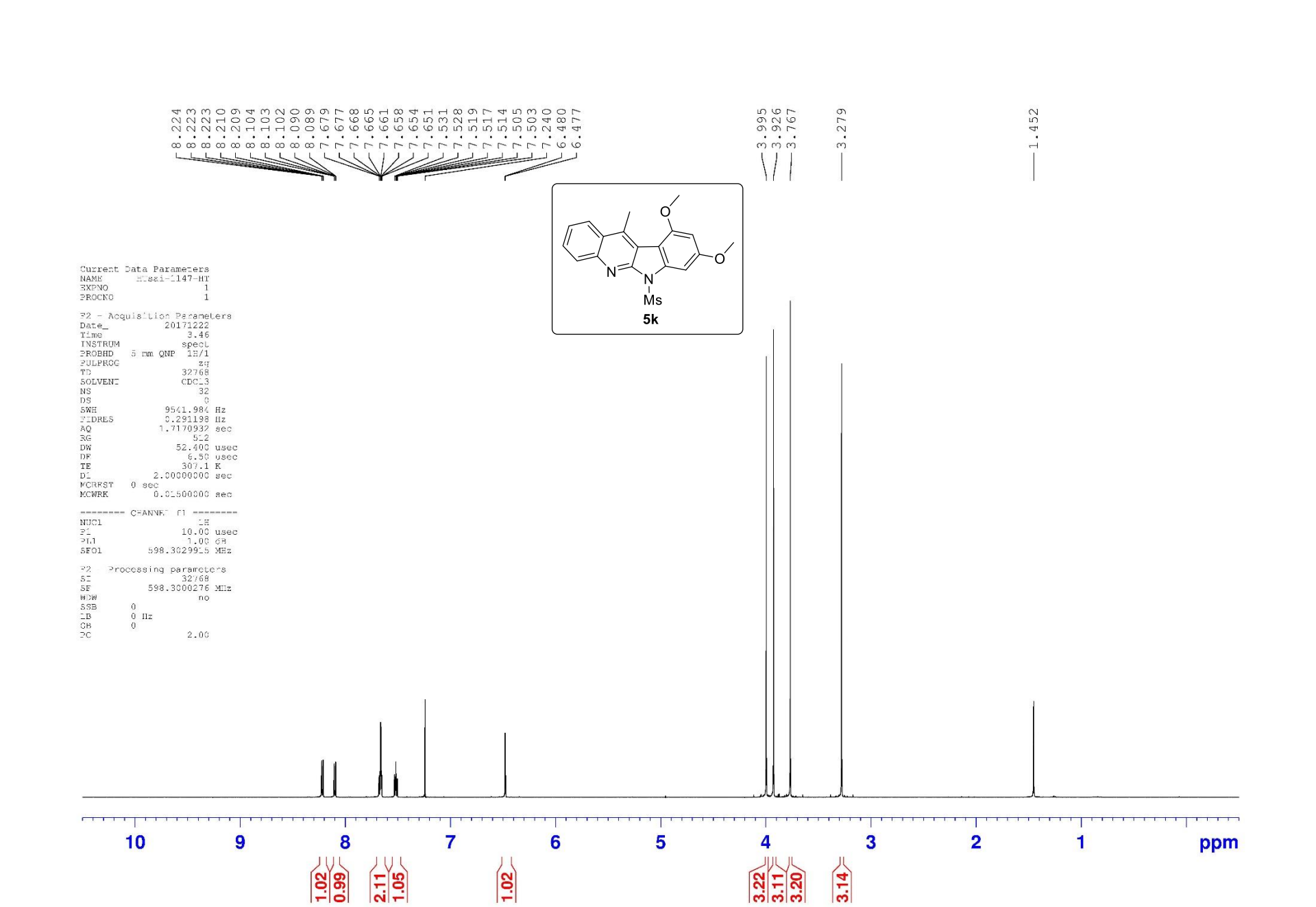
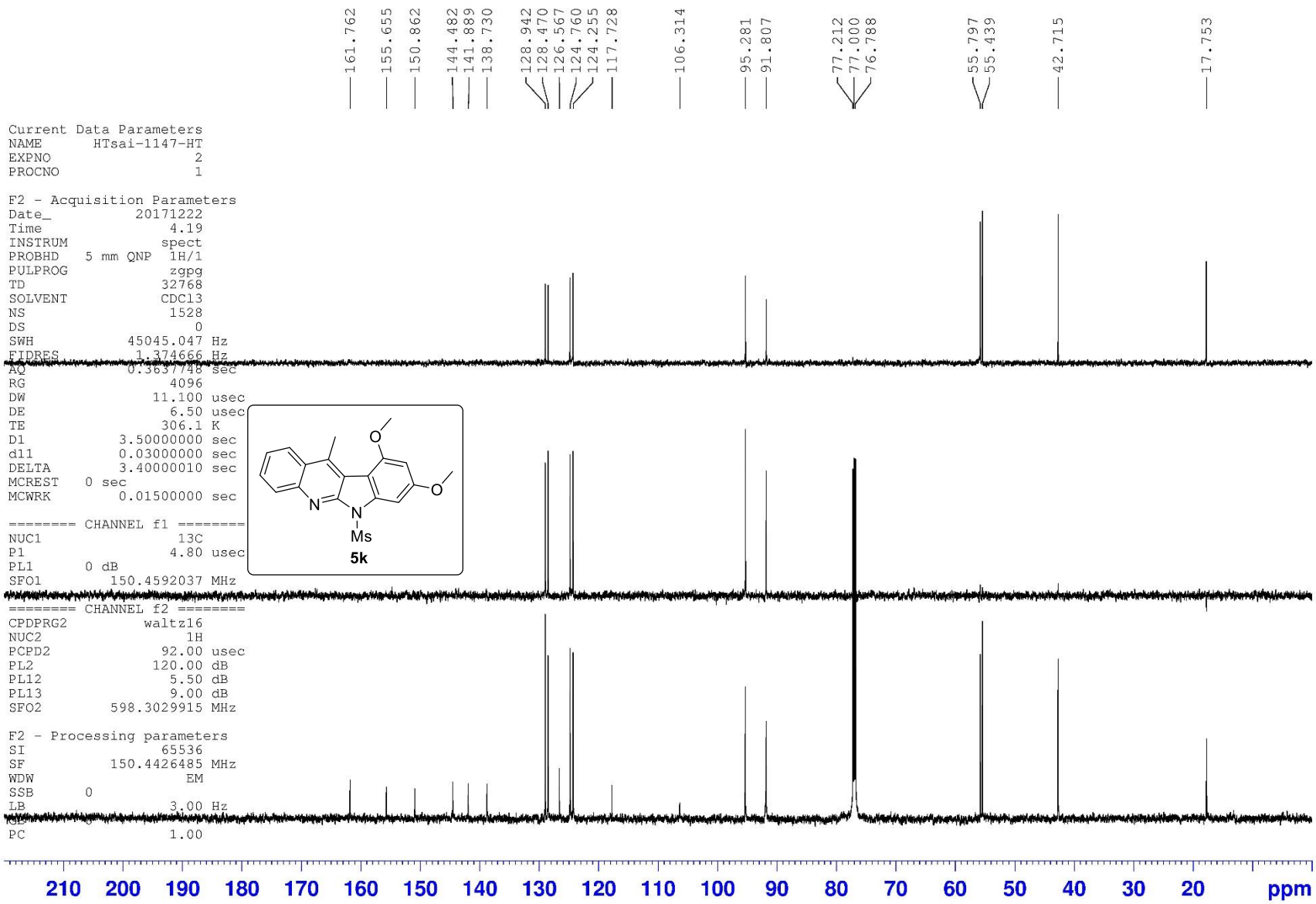
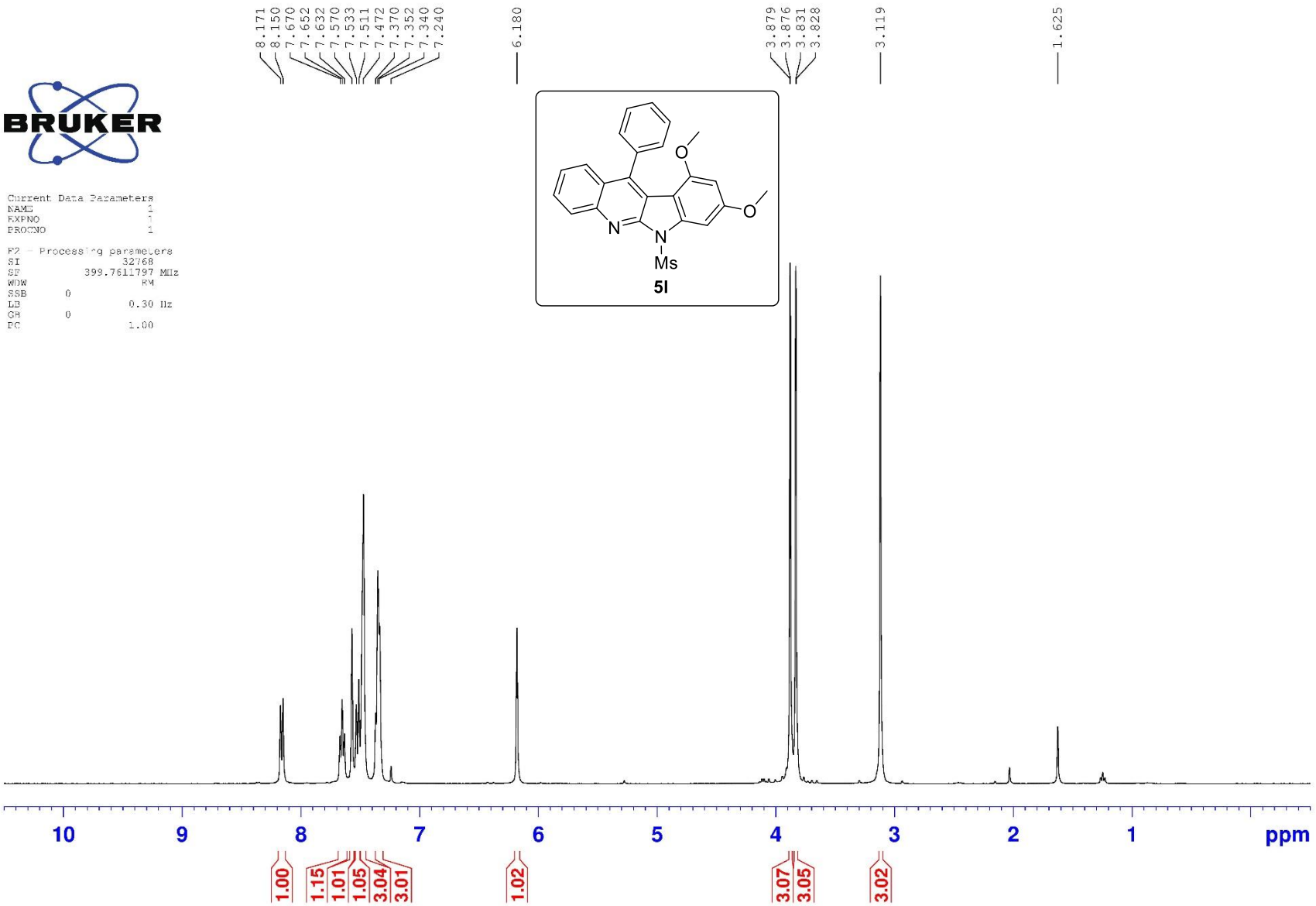
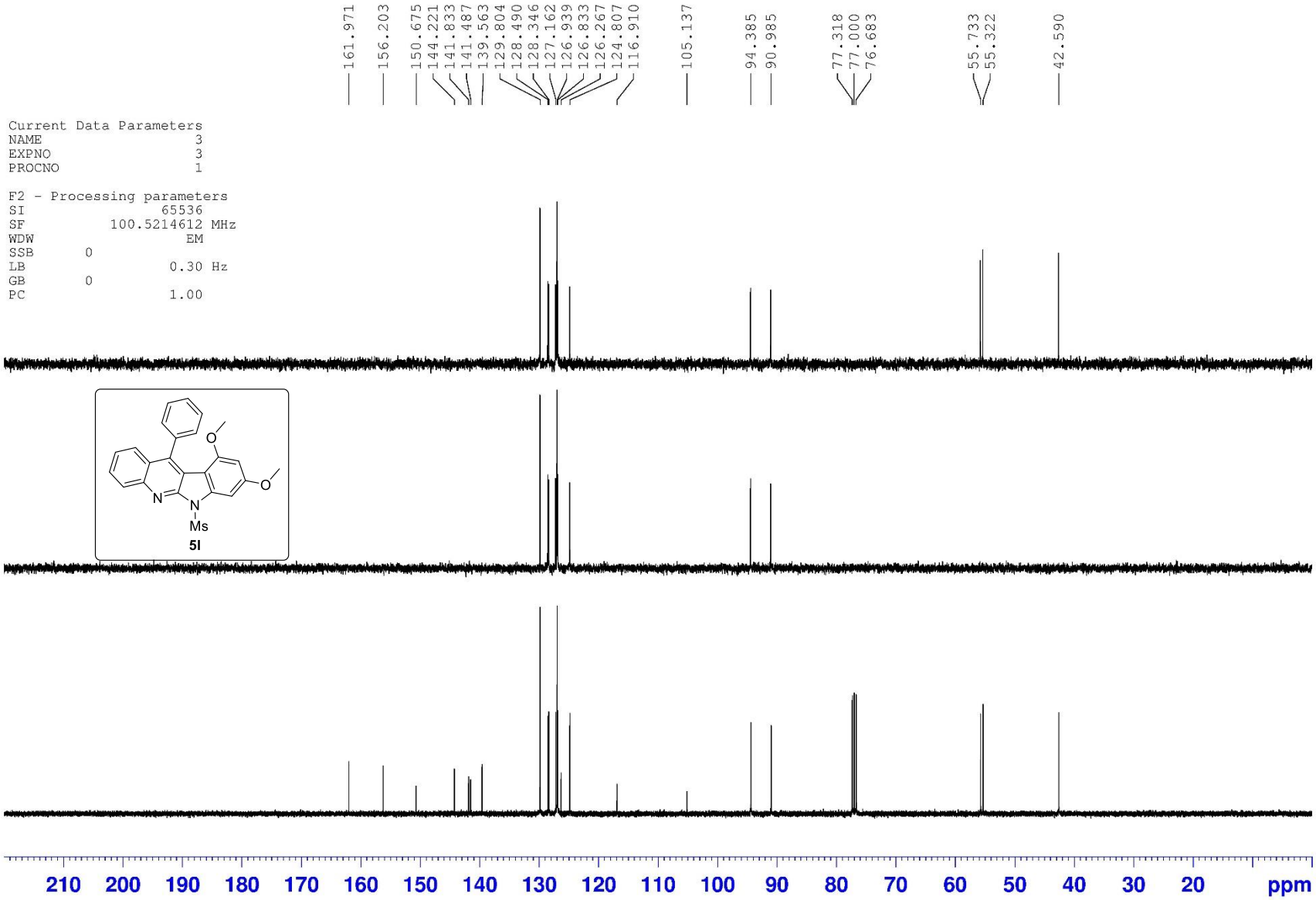
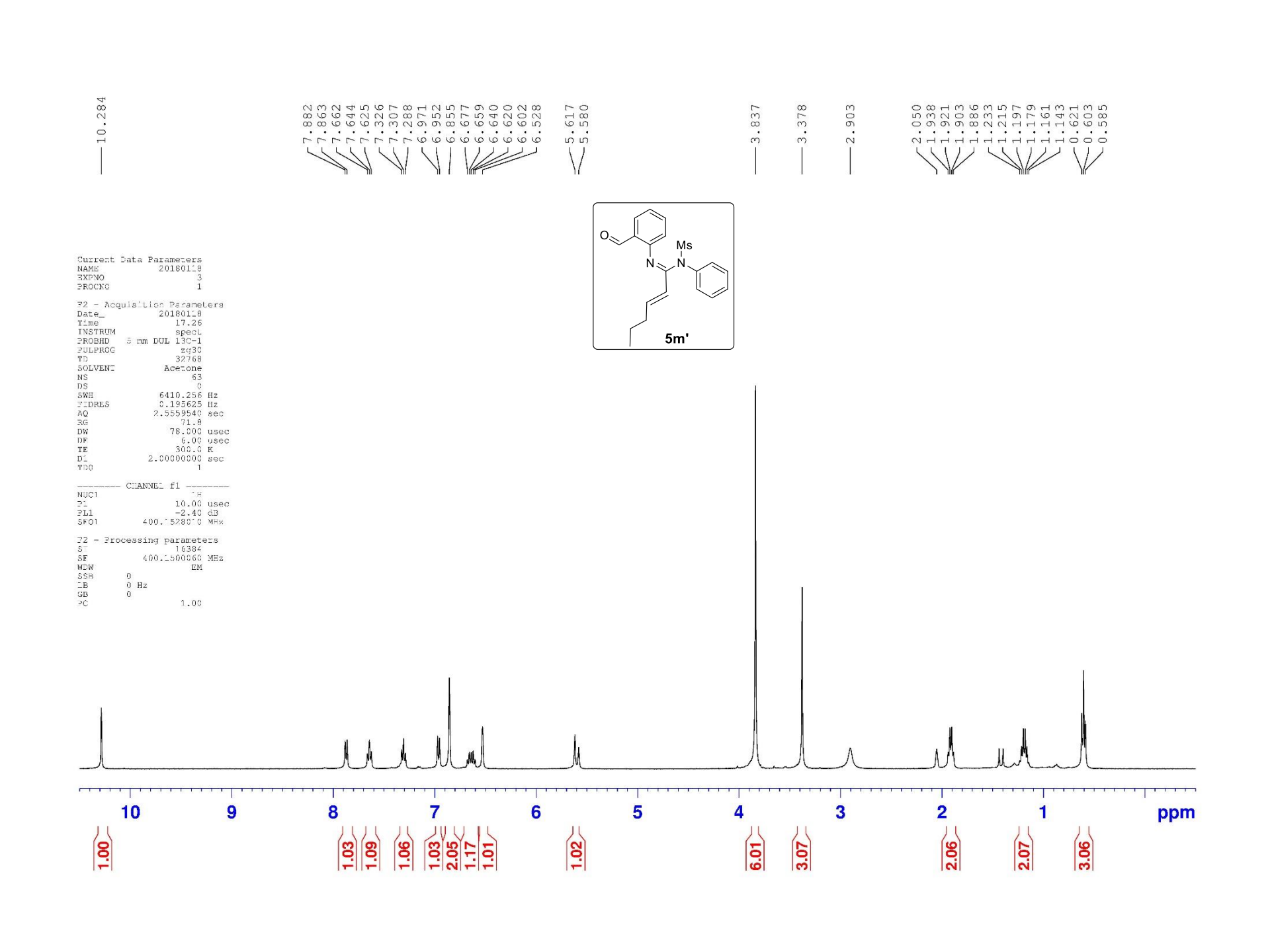
150.330
149.987
147.033
143.012
140.752
127.627
122.877
116.743
105.665
103.093
101.695
94.976
91.968
77.212
77.000
76.788
55.949
55.750
42.266
29.693
Current Data Parameters
NAME HTsai-1146-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171216
Time 5.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 308.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
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 150.4426462 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
O
O
O
O
N
N
Ms
5j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

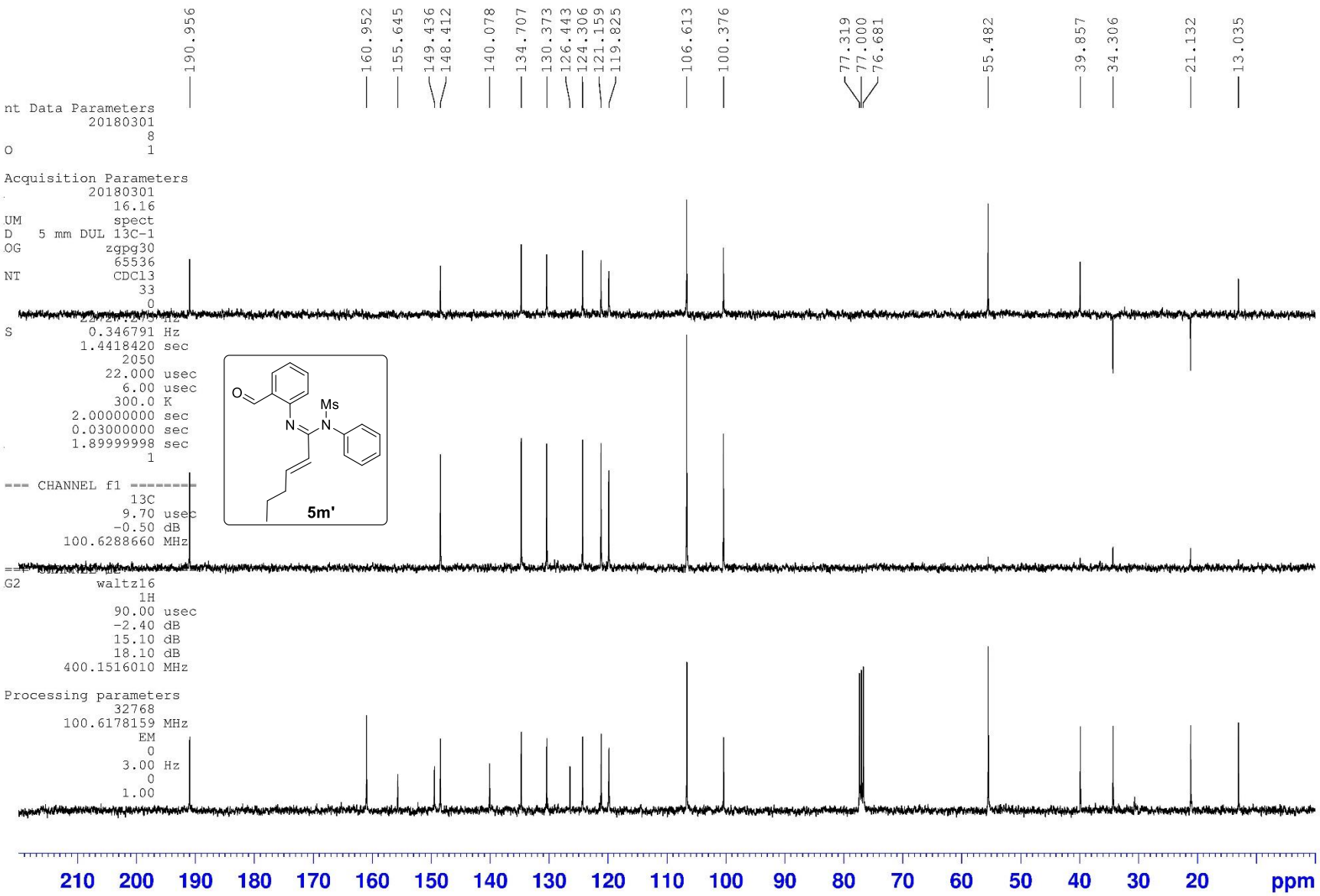

8.224
8.223
8.223
8.210
8.209
8.104
8.103
8.102
8.090
8.089
7.679
7.677
7.668
7.665
7.661
7.658
7.654
7.651
7.531
7.528
7.519
7.517
7.514
7.505
7.503
7.240
6.480
6.477
3.995
3.926
3.767
3.279
1.452
O
O
N
N
Ms
5k
Current Data Parameters
NAME Hisai-2147-HT
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171222
Time 3.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 307.1 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 598.3000276 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
1.02
0.99
2.11
1.05
1.02
3.22
3.11
3.20
3.14

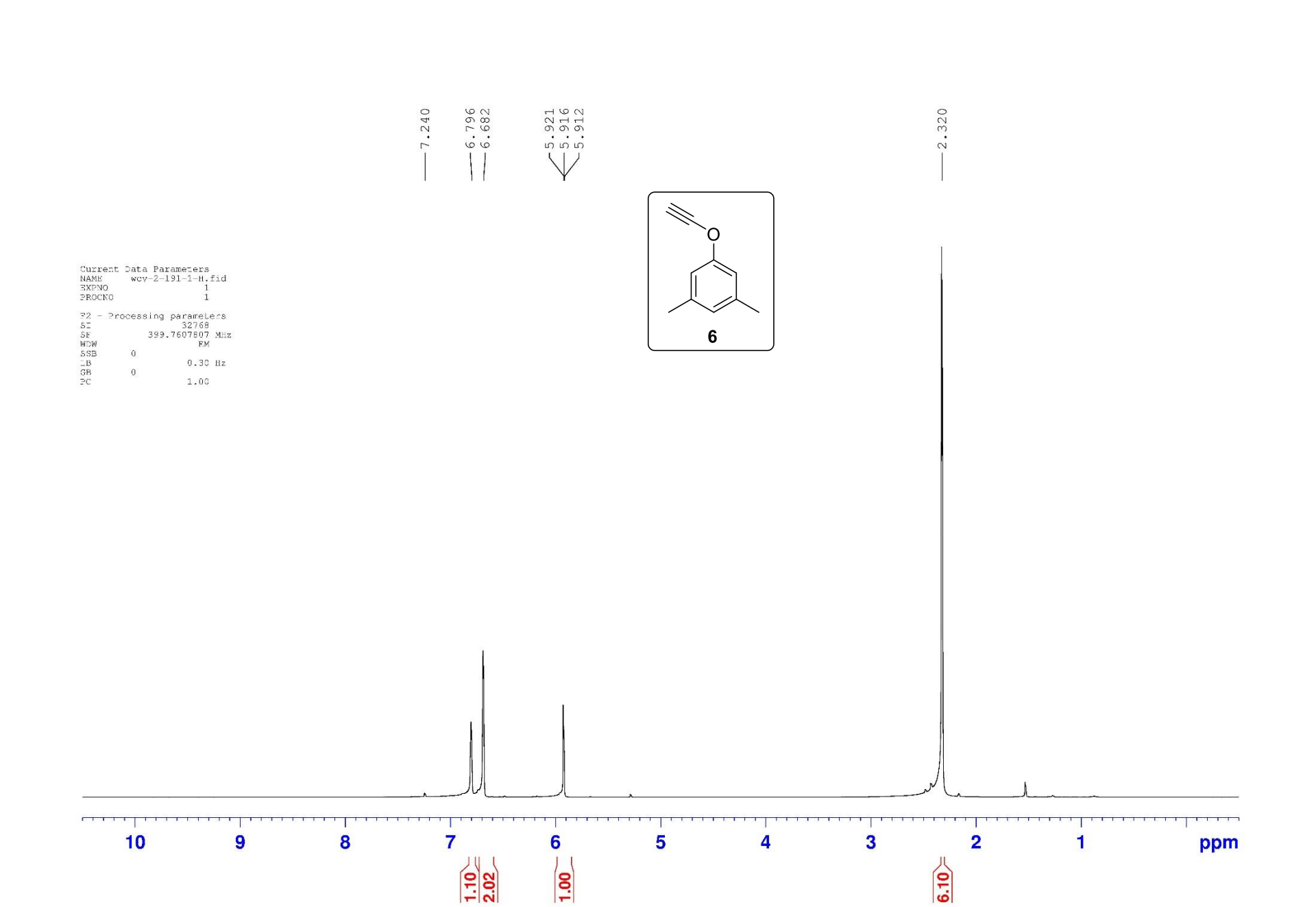

161.762
155.655
150.862
144.482
141.889
138.730
128.942
128.470
126.567
124.760
124.255
117.728
106.314
95.281
91.807
77.212
77.000
76.788
55.797
55.439
42.715
17.753
Current Data Parameters
NAME HTsai-1147-HT
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171222
Time 4.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1528
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 306.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4592037 MHz
======== CHANNEL f2 ========
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 150.4426485 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
O
O
N
N
Ms
5k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

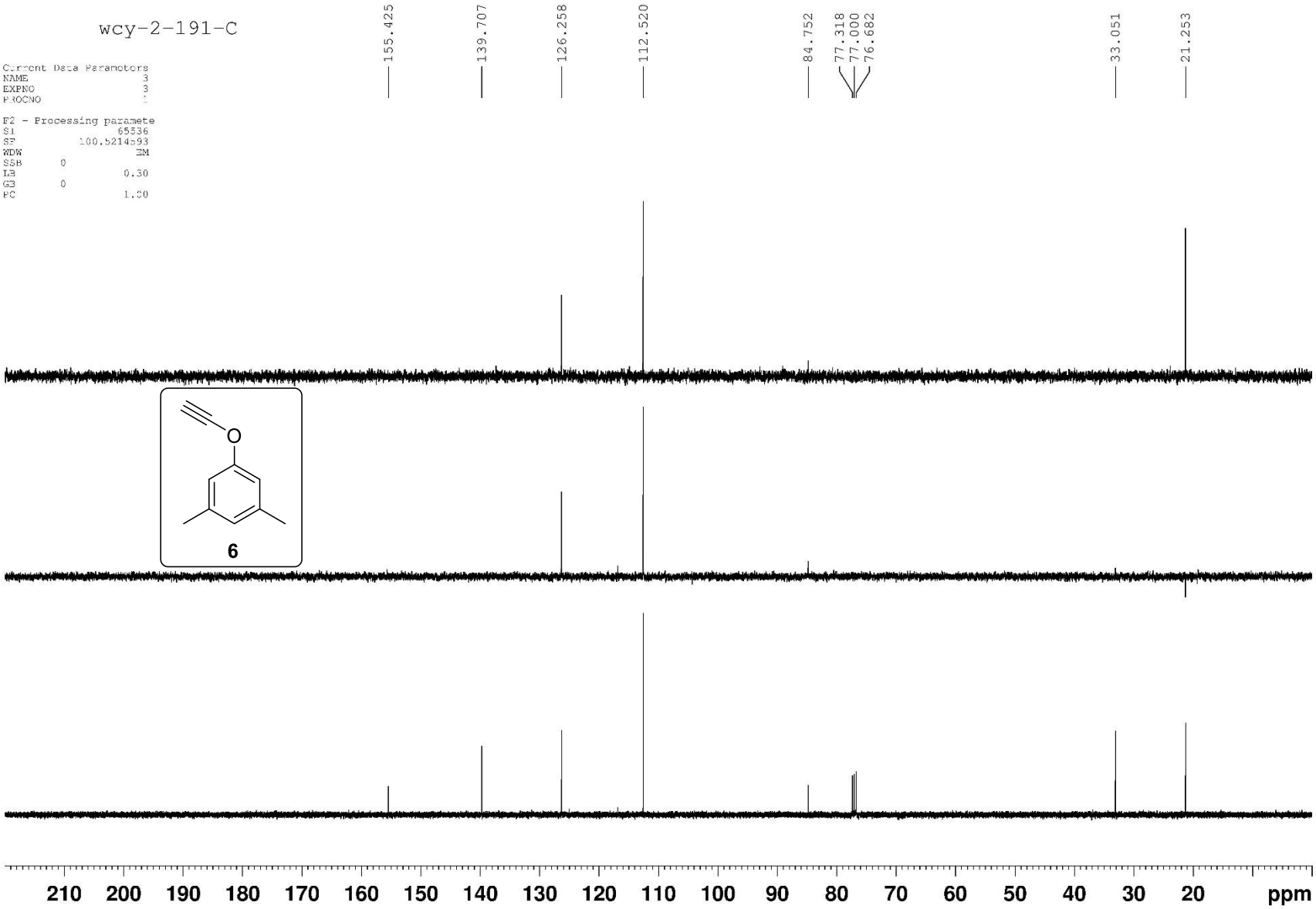

8.171
8.150
7.670
7.652
7.632
7.570
7.533
7.511
7.472
7.370
7.352
7.340
7.240
6.180
3.879
3.876
3.831
3.828
3.119
1.625
Current Data Parameters
NAME 2
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611797 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
N
Ms
5l
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.15
1.01
1.05
3.04
3.01
1.02
3.07
3.05
3.02

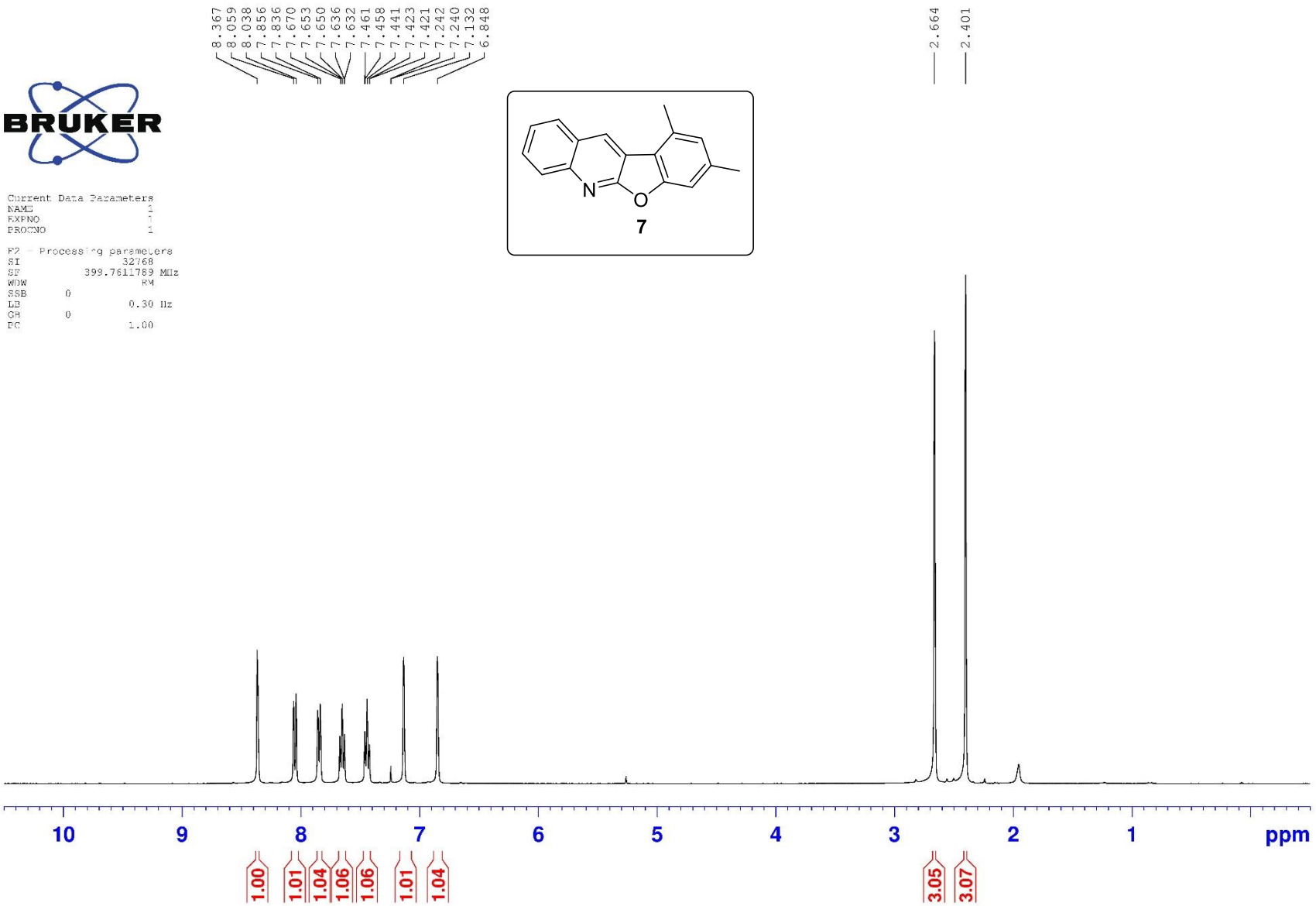

161.971
156.203
150.675
144.221
141.833
141.487
139.563
129.804
128.490
128.346
127.162
126.939
126.833
126.267
124.807
116.910
105.137
94.385
90.985
77.318
77.000
76.683
55.733
55.322
42.590
Current Data Parameters
NAME 3
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214612 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
N
Ms
5l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

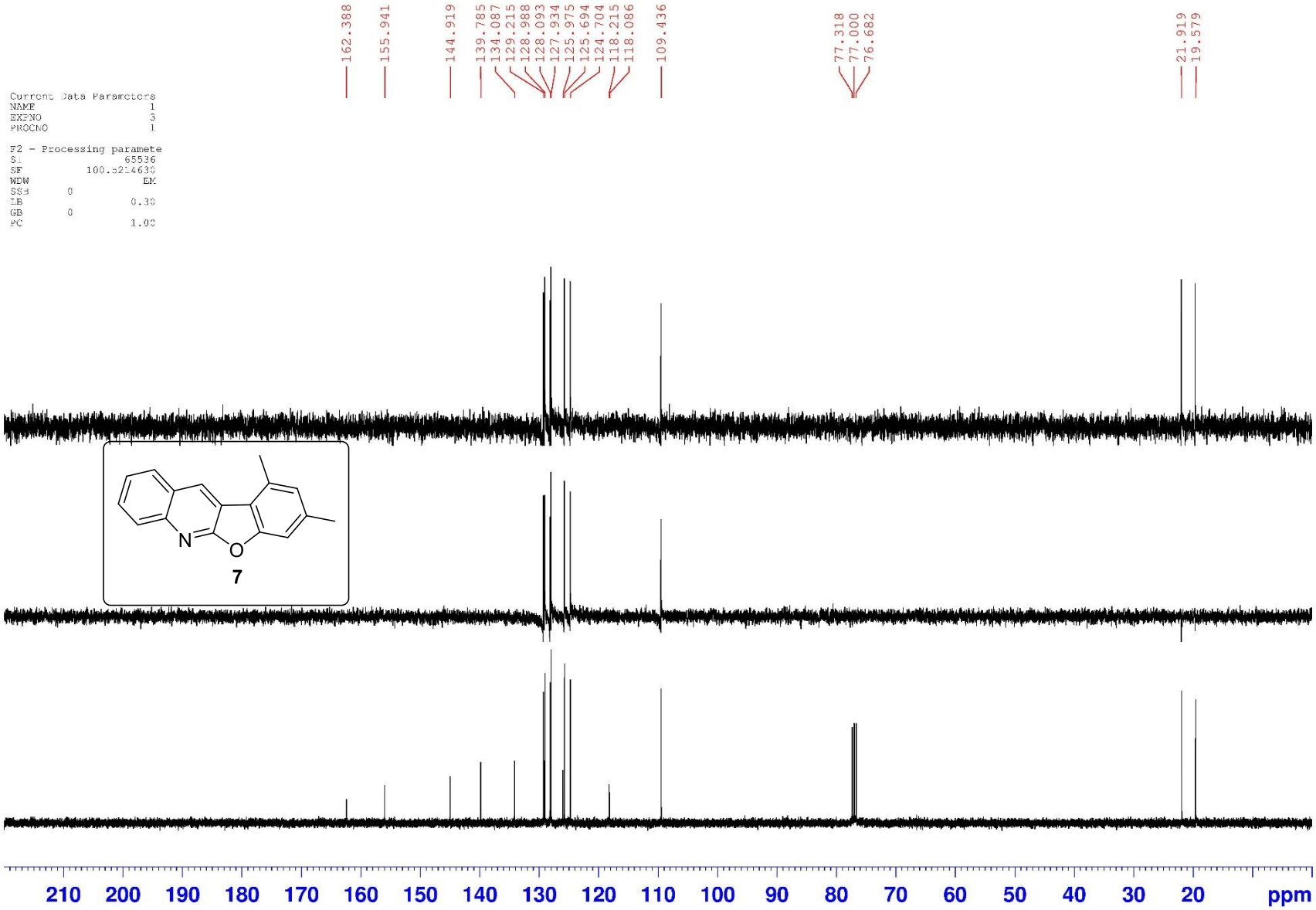

10.284
7.882
7.863
7.662
7.644
7.625
7.326
7.307
7.288
6.971
6.952
6.855
6.677
6.659
6.640
6.620
6.602
6.528
5.617
5.580
3.837
3.378
2.903
2.050
1.938
1.921
1.903
1.886
1.233
1.215
1.197
1.179
1.161
1.143
0.621
0.603
0.585
O
N
Ms
N
5m'
Current Data Parameters
NAME 20180118
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180118
Time 17.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 63
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 71.8
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.7528710 MHz
F2 - Processing parameters
SI 16384
SF 400.1500060 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.09
1.06
1.03
2.05
1.17
1.01
1.02
6.01
3.07
2.06
2.07
3.06

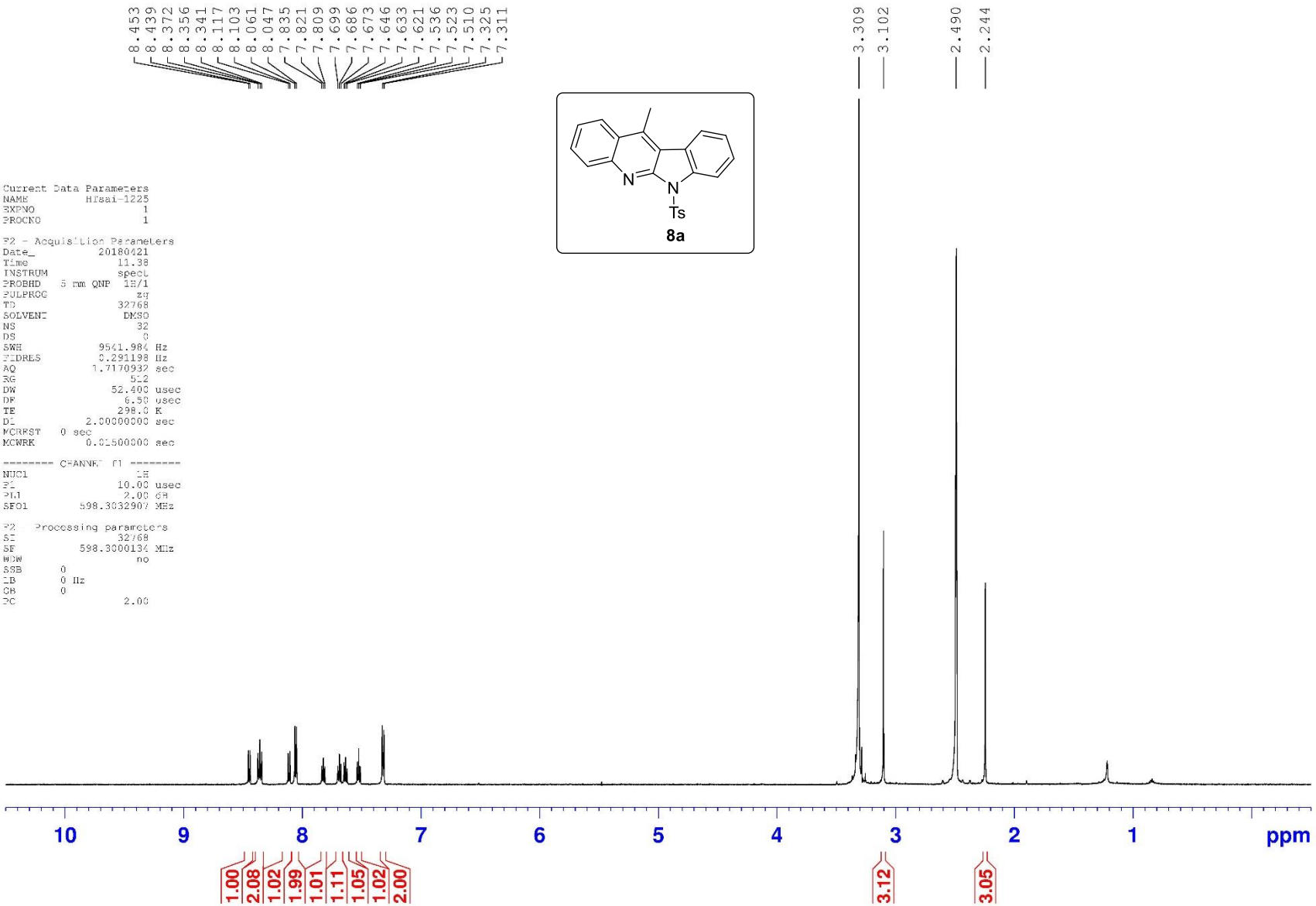

190.956
160.952
155.645
149.436
148.412
140.078
134.707
130.373
126.443
124.306
121.159
119.825
106.613
100.376
77.319
77.000
76.681
55.482
39.857
34.306
21.132
13.035
nt Data Parameters
20180301
8
O 1
Acquisition Parameters
20180301
16.16
UM spect
D 5 mm DUL 13C-1
OG zgpg30
65536
NT CDCl3
33
0
S 0.346791 Hz
1.4418420 sec
2050
22.000 usec
6.00 usec
300.0 K
2.00000000 sec
0.03000000 sec
1.89999998 sec
1
=== CHANNEL f1 ========
13C
9.70 usec
-0.50 dB
100.6288660 MHz
G2 waltz16
1H
90.00 usec
-2.40 dB
15.10 dB
18.10 dB
400.1516010 MHz
Processing parameters
32768
100.6178159 MHz
EM
0
3.00 Hz
0
1.00
O
N
Ms
N
5m'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

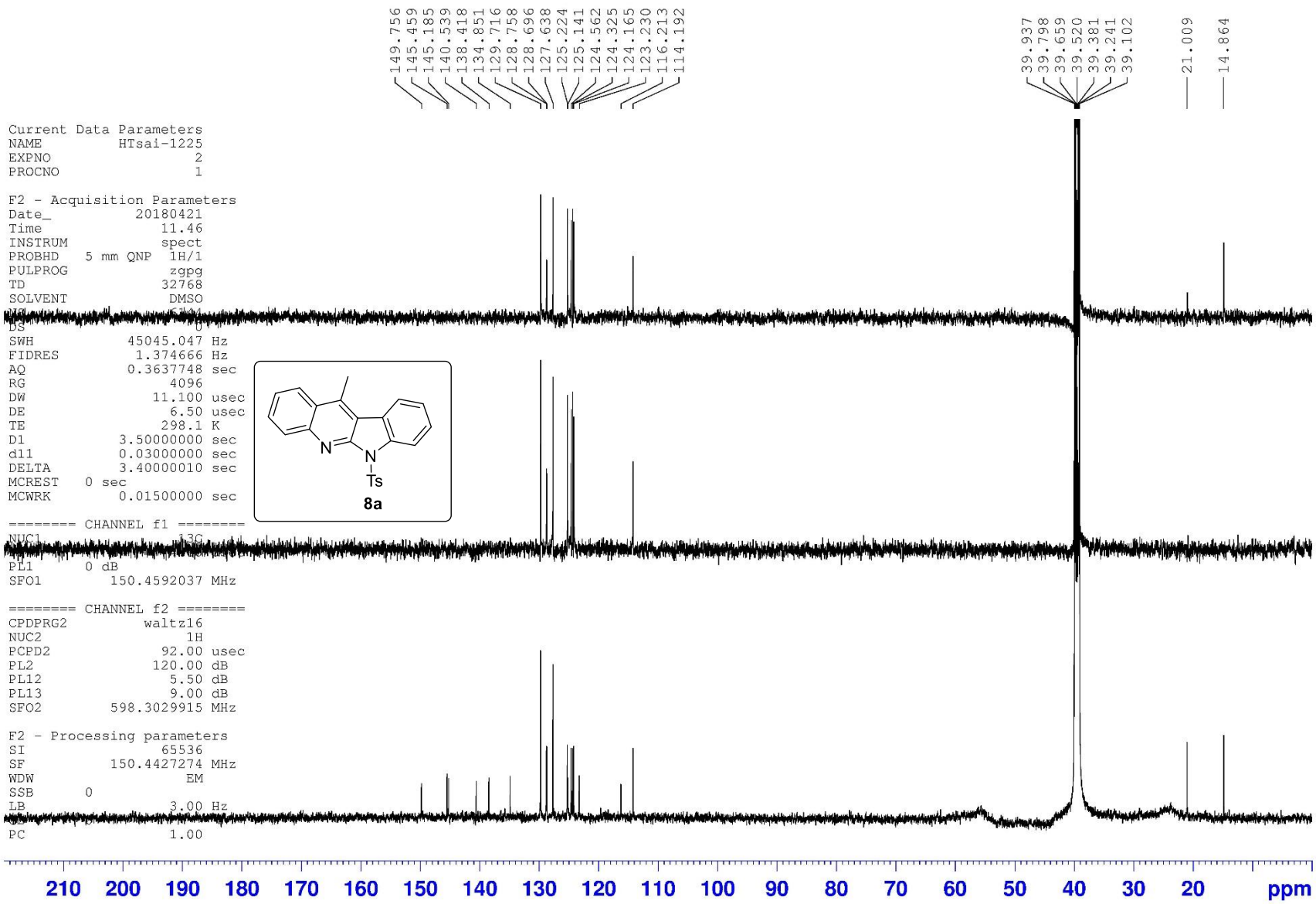

7.240
6.796
6.682
5.921
5.916
5.912
2.320
Current Data Parameters
NAME wcy-2-191-1-H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7607807 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
6
10
9
8
7
6
5
4
3
2
1
ppm
1.10
2.02
1.00
6.10

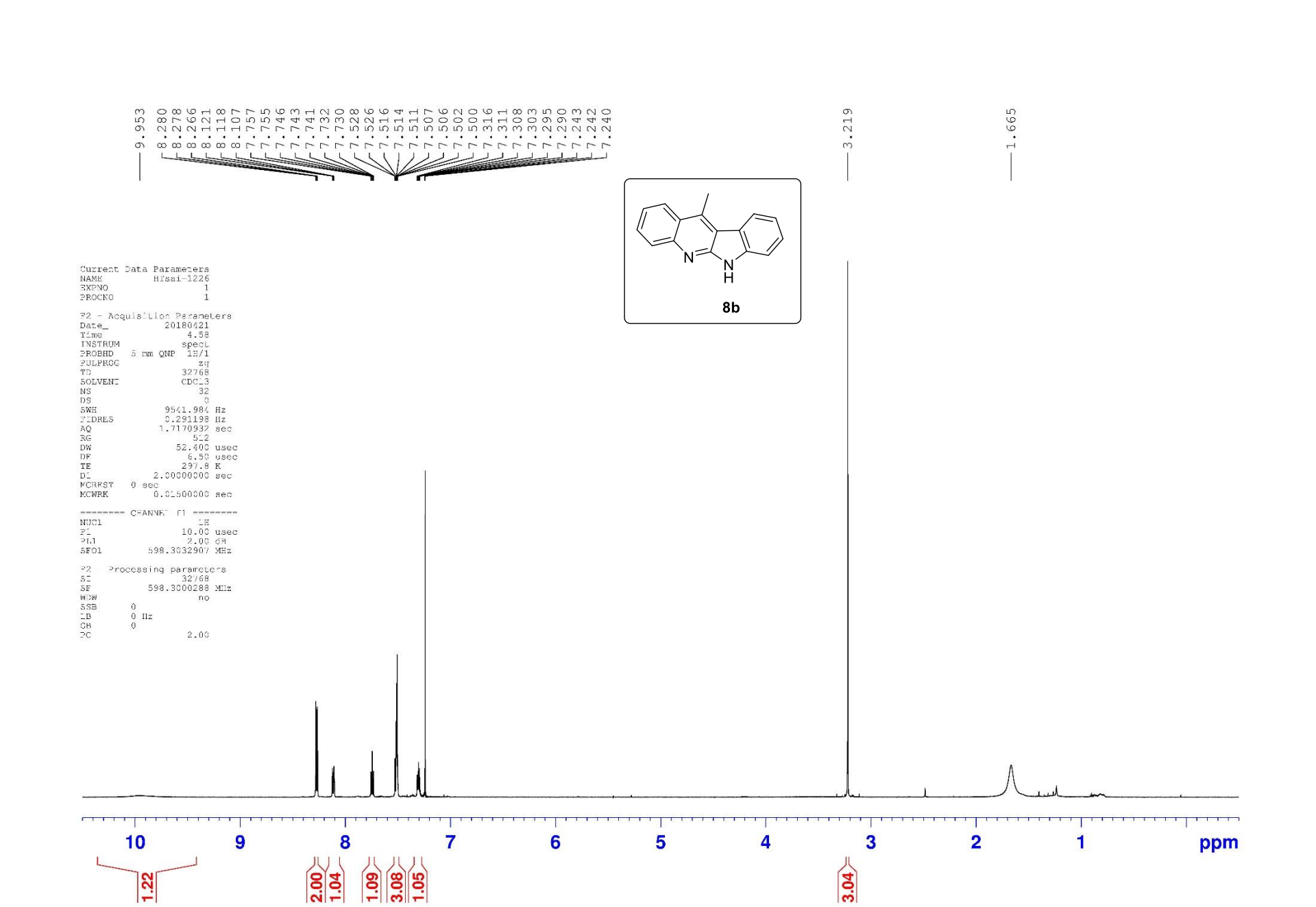

wcy-2-191-C
Current Data Parameters
NAME 3
EXPNO 3
PROCNO 1
F2 - Processing paramete
SI 65536
SF 100.5214893
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
155.425
139.707
126.258
112.520
84.752
77.318
77.000
76.682
33.051
21.253
O
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

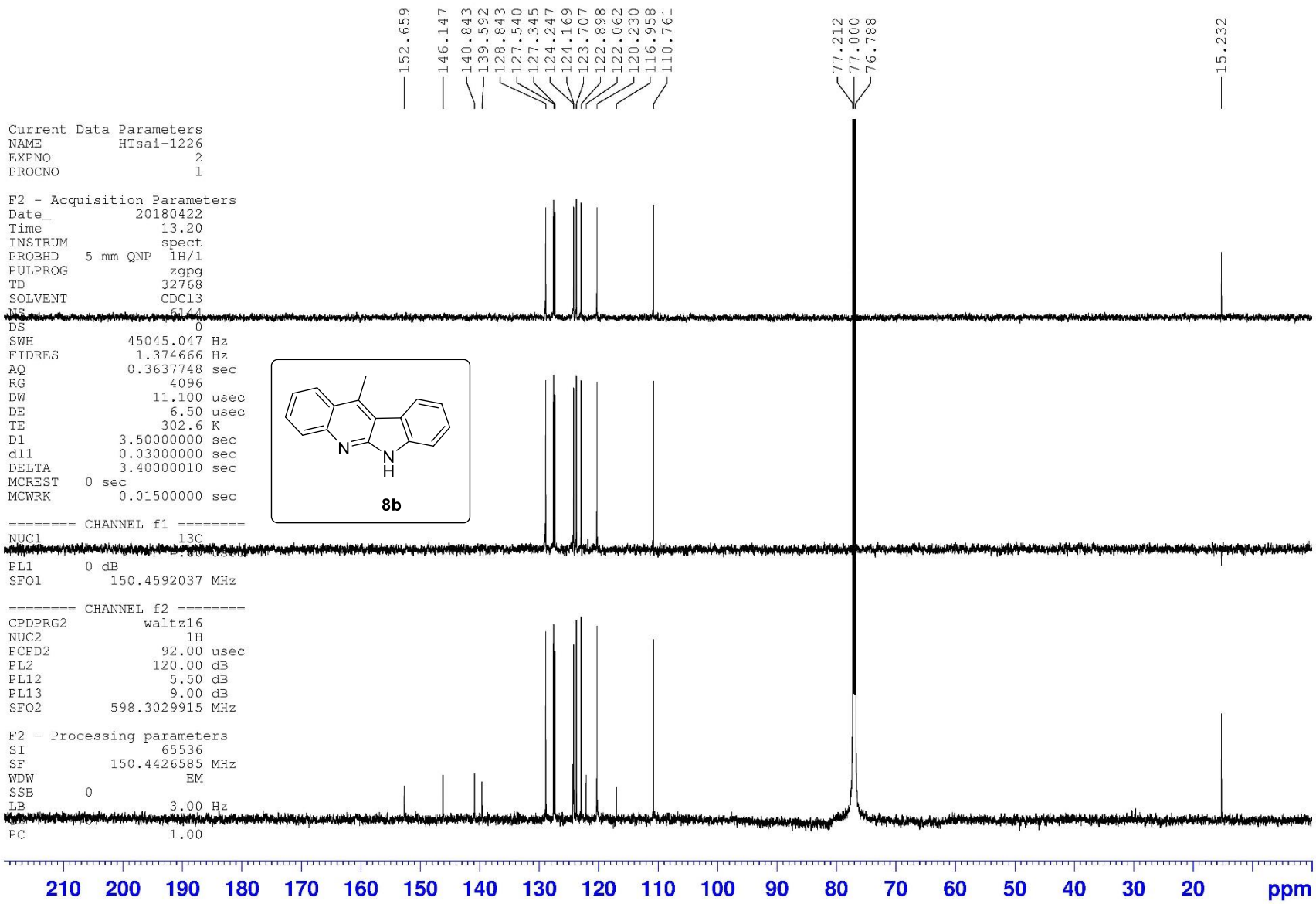

8.367
8.059
8.038
7.856
7.836
7.670
7.653
7.650
7.636
7.632
7.461
7.458
7.441
7.423
7.421
7.242
7.240
7.132
6.848
2.664
2.401
BRUKER
Current Data Parameters
NAME 2
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611789 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
O
7
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.04
1.06
1.06
1.01
1.04
3.05
3.07

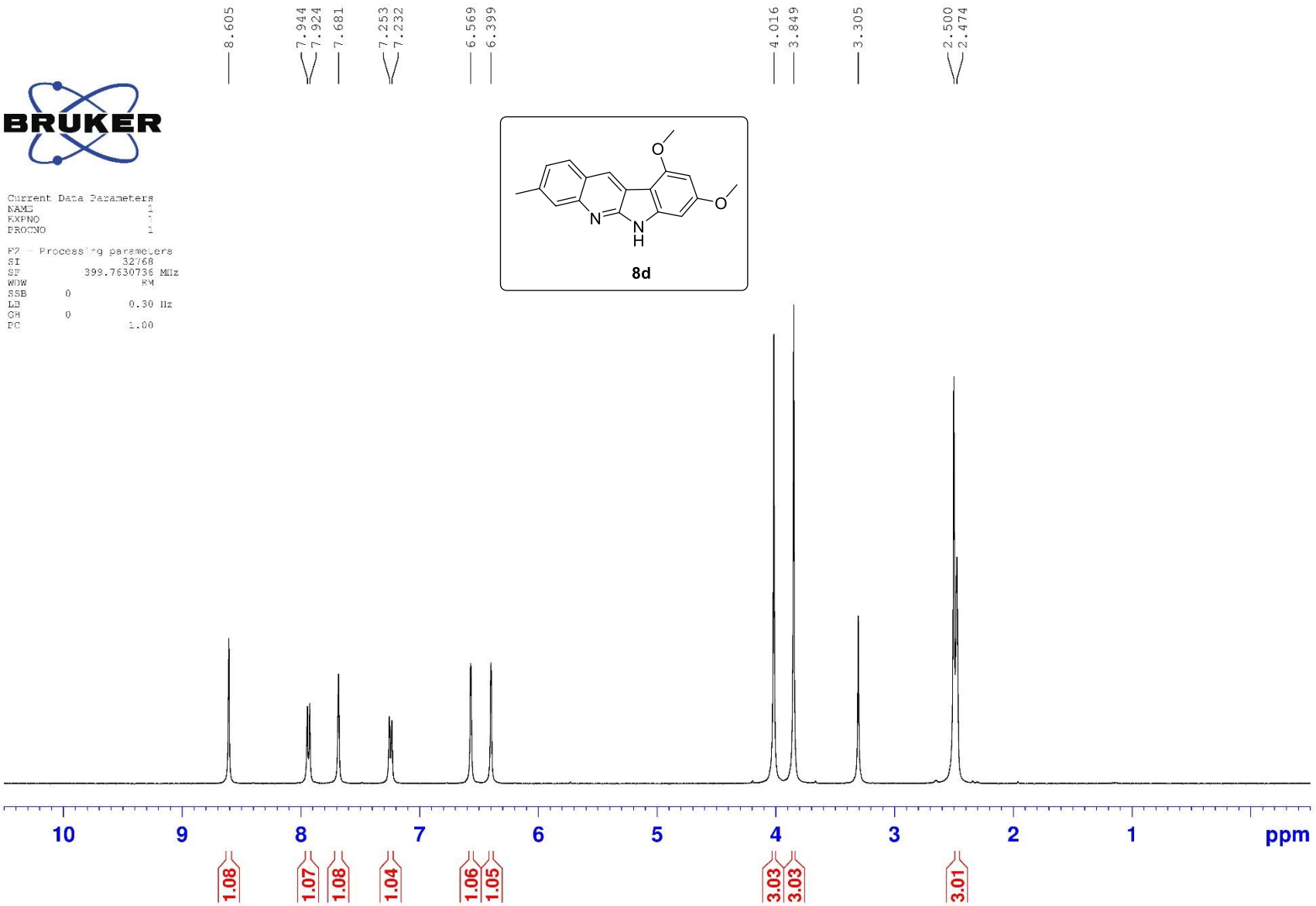

162.388
155.941
144.919
139.785
134.087
129.215
128.988
128.093
127.934
125.975
125.694
124.704
118.215
118.086
109.436
77.318
77.000
76.682
21.919
19.579
Current Data Parameters
NAME 1
EXPNO 3
PROCNO 1
F2 - Processing paramete
SI 65536
SF 100.6214630
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
N
O
7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

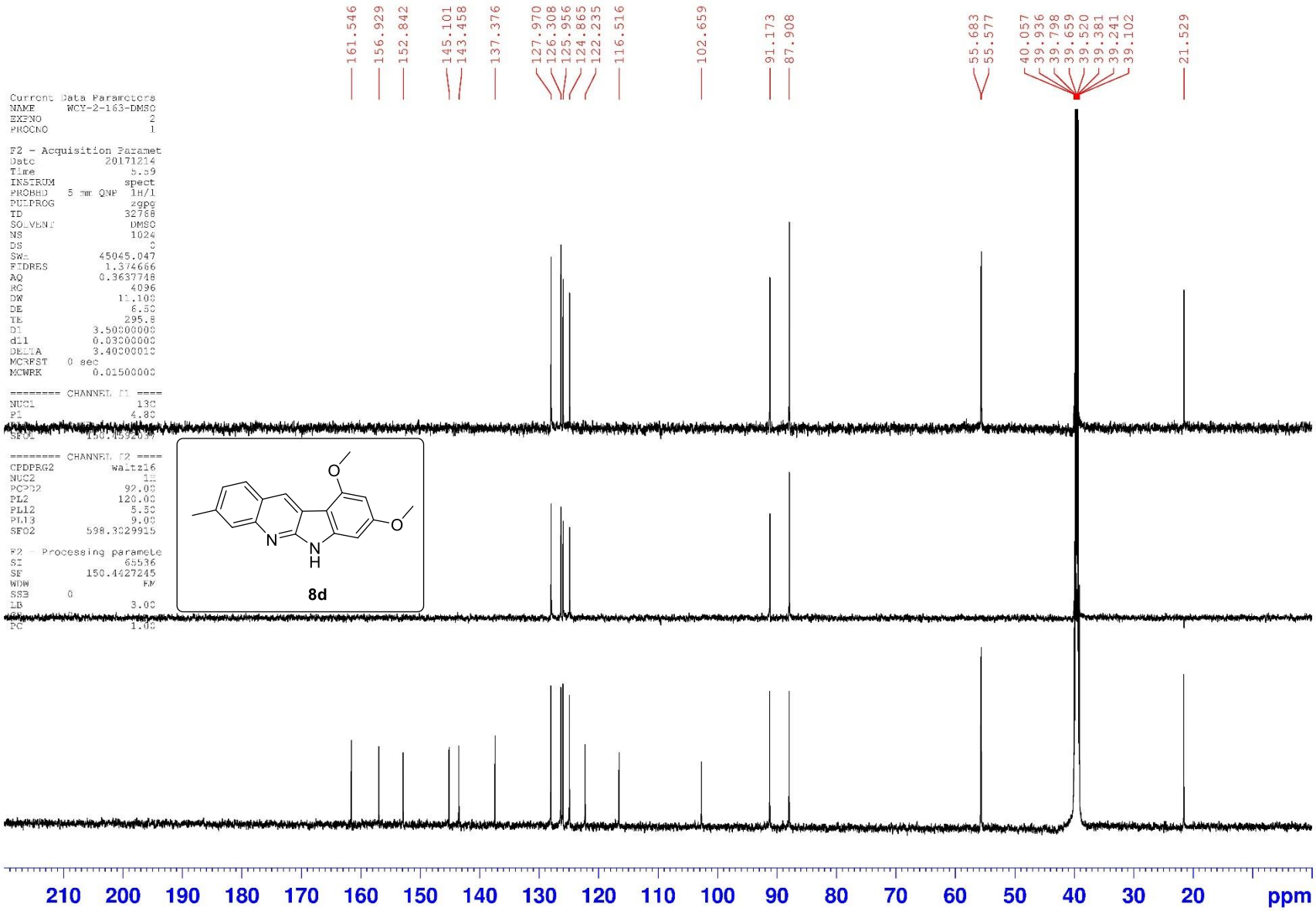

8.453
8.439
8.372
8.356
8.341
8.117
8.103
8.061
8.047
7.835
7.821
7.809
7.699
7.686
7.673
7.646
7.633
7.621
7.536
7.523
7.510
7.325
7.311
3.309
3.102
2.490
2.244
Current Data Parameters
NAME HFsai-1225
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20180421
Time 11.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 2.00 dB
SFO1 598.3032907 MHz
P2 - Processing parameters
SI 32768
SF 598.3000134 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
N
N
Ts
8a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.08
1.02
1.99
1.01
1.11
1.05
1.02
2.00
3.12
3.05


149.756
145.459
145.185
140.539
138.418
134.851
129.716
128.758
128.696
127.638
125.224
125.141
124.562
124.325
124.165
123.230
116.213
114.192
39.937
39.798
39.659
39.520
39.381
39.241
39.102
21.009
14.864
Current Data Parameters
NAME HTsai-1225
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180421
Time 11.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
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 298.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
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 150.4427274 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
N
N
Ts
8a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


9.953
8.280
8.278
8.266
8.121
8.118
8.107
7.757
7.755
7.746
7.743
7.741
7.732
7.730
7.528
7.526
7.516
7.514
7.511
7.507
7.506
7.502
7.500
7.316
7.311
7.308
7.303
7.295
7.290
7.243
7.242
7.240
3.219
1.665
N
N
H
8b
Current Data Parameters
NAME HIsai-1226
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20180421
Time 4.58
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 10.00 usec
PL1 2.00 dB
SFO1 598.3032907 MHz
P2 - Processing parameters
SI 32768
SF 598.3000288 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
10
9
8
7
6
5
4
3
2
1
ppm
1.22
2.00
1.04
1.09
3.08
1.05
3.04


152.659
146.147
140.843
139.592
128.843
127.540
127.345
124.247
124.169
123.707
122.898
122.062
120.230
116.958
110.761
77.212
77.000
76.788
15.232
Current Data Parameters
NAME HTsai-1226
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180422
Time 13.20
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 302.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
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 150.4426585 MHz
WDW EM
SSB 0
LB 3.00 Hz
PC 1.00
N
N
H
8b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.605
7.944
7.924
7.681
7.253
7.232
6.569
6.399
4.016
3.849
3.305
2.500
2.474
Current Data Parameters
NAME 2
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7630736 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8d
10
9
8
7
6
5
4
3
2
1
ppm
1.08
1.07
1.08
1.04
1.06
1.05
3.03
3.03
3.01


161.546
156.929
152.842
145.101
143.458
137.376
127.970
126.308
125.956
124.865
122.235
116.516
102.659
91.173
87.908
55.683
55.577
40.057
39.936
39.798
39.659
39.520
39.381
39.241
39.102
21.529
Current Data Parameters
NAME MCY-2-163-DMSO
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date 20171214
Time 5.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 1024
DS 0
SWH 45045.047
FIDRES 1.374666
AQ 0.3637748
RG 4096
DW 11.100
DE 6.50
TE 295.8
D1 3.50000000
d11 0.03000000
DELTA 3.40000010
MCREST 0 sec
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 4.80
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00
PL2 120.00
PL12 5.50
PL13 9.00
SFO2 598.3029915
F2 - Processing parameter
SI 65536
SF 150.4427245
WDW EM
SSB 0
LB 3.00
PC 1.00
O
N
H
O
8d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm