Supporting Information

Cp*Ir(III) Complexes Catalyzed solvent free synthesis of Quinolines, Pyrroles and pyridines via ADC strategy

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1. General Information:

All the reagents were purchased commercially and used without further purification. ^{1}H NMR and ^{13}C NMR were recorded with Bruker 400 MHz.^{1}H NMR (400MHz) and ^{13}C NMR (100MHz) spectra were recorded in $CDCl_3$, CD_3OD or DMSO-d6 with tetramethylsilane as the internal standard. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, sep = septet, br = broad resonance. All the NMR spectra were acquired at ambient temperature. Analytical thin layer chromatography (TLC) was performed using Silica Gel 60 Å F254 pre-coated plates (0.25 mm thickness). Visualization of I_2 stained TLC plate was accomplished by a UV lamp and single-crystal data were collected from a Bruker-APEX-II CCD X-ray diffractometer.

2.A. General experimental procedure for preparation of Ir-catalyzed product [*7A1-7A33, 9A1-9A21, 12AA-12CH, 14AA-14AG*]:

Amino alcohol (1mmol), ketone or secondary alcohol (1.1 mmol), Ir(III) complex (0.003 mmol), KOH (0.2 mmol) without any solvent were placed in a 5 ml screw-capped vial and allowed to react at 90°C for 2 h. The progress of the reaction was monitored by TLC. After completion of starting material, the reaction mass was evaporated, and the residue was purified with column chromatography over silica gel where hexane/ethyl acetate mixture was used as eluent.

2.B. General experimental procedure for preparation of Ir (III) catalyzed product [*17AA-17GA, 20AA-20CQ and 23AA-23BR*]:

Amino alcohol (1 mmol), ketone or secondary alcohol (1.1 mmol), Ir(III) complex (0.003 mmol), KOH (0.2 mmol) without any solvent were placed in a 5 ml screw-capped vial and allowed to react at 110°C for 2-8 h. The progress of the reaction was monitored by TLC. After

completion of starting material, the reaction mass was evaporated, and the residue was purified with column chromatography over silica gel where hexane/ethyl acetate mixture was used as eluent.

General experimental procedure for preparation of ligands (1.A.):

In a round bottom flask to a stirred solution of picolinic acid (500 mg, 4.065 mmol,1.0 eq) and TEA (0.571 mL, 4.065 mmol,1.0eq) in THF (4 mL/mmol) at 0°C under argon atmosphere was added ClCOOEt (0.435 mL, 4.065 mmol, 1.0eq). The reaction mixture was stirred at 0°C to 10°C for 1h, followed by naphthalene-1- amine (581 mg, 4.065 mmol, 1.0 eq) was added to the reaction mixture by dissolving in THF (2 mL). The reaction mixture was heated at 80°C under stirring for 2-3h. The completion of the reaction was monitored by silica TLC. The reaction mixture was cooled to rt and diluted with ethyl acetate (10 mL) solid formed which was filtered out, The Filtrate was evaporated under reduced pressure to get the crude, which was purified by silica gel column chromatography using MeOH in DCM. Yield 852 mg (85%).

Following this general procedure (A) prepared all three ligands (3a-3c).

#General experimental procedure for preparation of Ir (III)-Complexes (1.B.):

In a round bottom flask to a stirred solution of $[Cp^*IrCl_2]_2$ (2.0 mmol) [Cp* = 1,2,3,4,5-pentamethylcyclopentadienyl] and picolinamide **3** (4.0 mmol) in DCM (25 mL) was added Et3N (4.0 mmol) under argon atmosphere. The resulting solution was stirred at room temperature for 16h. The progress of the reaction was monitored by silica TLC. After completion, the reaction mixture was diluted with DCM (50 mL) and combined organic layer was washed with water (2×30 mL). The organic layer was separated and dried over anhydrous sodium sulphate, filtered and removed under reduced pressure to get the crude compound. The crude was washed with di ethyl ether (25x2) filtered and collected solid, which was dried under reduced pressure to get the desired Ir(III)-complex. Yield: 85-90%.

(Following this general procedure prepared all three-iridium complex 4a-Ir-4c-Ir).

3. *Characterization data of Ir catalysed compounds (7A1-7A33, 12AA-12CH, 9A1-9A21, 14AA-14AG, 7A20-H-7A28-Me, 17AA-17GA, 20AA-20CQ and 23AA-23BR).*

All the reactions were carried out in 1 mmol scale of amino alcohol and according to the general procedure 2.A.

***2-phenylquinoline(7A1)[1]*:** *Yield 199 mg, 97%*

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.46 (d, *J* = 8.6 Hz, 1H), 8.27 (d, *J* = 7.4 Hz, 2H), 8.15 (d, *J* = 8.6 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.78 (t, *J* = 7.3 Hz, 1H), 7.62-7.50 (m, 4H).

2-(o-tolyl) quinoline(7A2)[2]: *Yield202 mg,92%*

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.20 (d,*J* = 8.8 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.57-7.48 (m, 3H), 7.32 (m, 3H), 2.40 (s, 3H).

2-(m-tolyl) quinoline(7A3)[3]: *Yield195 mg, 89%*

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.22-8.18 (m, 2H), 8.00 (br, 1H), 7.91 (d, *J* = 7.3 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 7.72 Hz, 1H), 7.72 (t, *J* = 7.3 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.28-7.24 (m, 1H), 2.47 (s, 3H).

2-(2-methoxyphenyl) quinoline(7A4)[3]: *Yield 205 mg, 87%*

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.18-8.13 (m, 2H), 7.88-7.81 (m, 3H), 7.70 (t, *J* = 7.08 Hz, 1H), 7.52 (t, *J* = 7.48 Hz, 1H), 7.43-7.39 (m, 1H), 7.12 (t, *J* = 7.36 Hz, 1H), 7.03 (d, *J* = 8.28 Hz, 1H), 3.90 (s, 3H).

2-(3-methoxyphenyl) quinoline(7A5)[3]: Yield207 mg, 88%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.23 (d, *J* = 8.5 Hz, 2H), 7.87-7.82 (m, 2H), 7.77-7.29 (m, 3H), 7.53 (t, *J* = 7.32 Hz, 1H), 7.43 (t, *J* = 7.96 Hz, 1H), 7.03-7.01 (m, 1H), 3.93 (s, 3H).

2-(2-fluorophenyl) quinoline(7A6)[3]: yield182 mg, 81%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.39 (d, *J* = 8.56 Hz, 1H), 8.10 (d, *J* = 8.52 Hz, 1H), 7.97-7.91 (m, 2H), 7.87-7.84 (dd, J_1 = 2.52 Hz, J_2 = 8.52 Hz, 1H),7.78 (t, *J* = 7.44 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.54-7.49 (m, 1H), 7.36 (t, J = 7.48 Hz, 1H), 7.30-7.25 (m, 1H).

2-(3-fluorophenyl) quinoline(7A7)[2]: Yield 204 mg,92%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.24 (d, *J* = 8.8 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.92 (d, J = 8.0 Hz, 2H), 7.86-7.82 (m, 2H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.54 (t, J = 7.4 Hz, 1H), 7.48-7.45 (m, 1H), 7.15 (t, *J* =7.6 Hz, 1H).

2-(4-fluorophenyl) quinoline (7A8)[2]: Yield190 mg, 85%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.22 (d, *J* = 8.6 Hz, 1H), 8.17-8.14 (m, 3H), 7.84-7.82 (m, 2H), 7.74-7.71 (m, 1H), 7.54-7.51 (m, 1H), 7.23-7.18 (m, 2H).

2-(4-(trifluoromethyl) phenyl) quinoline(7A9)[3]: Yield, 210 mg,77%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.29-8.27 (m, 3H), 8.19 (d, *J* = 8 Hz, 1H), 7.90-7.84 (m, 2H), 7.78-7.73 (m, 3H), 7.58-7.50 (m, 1H),

2-(3,5-difluorophenyl) quinoline(7A10)[4]: Yield, 205 mg,85%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.26 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 8.52 Hz, 1H),7.85-7.80 (m, 2H), 7.77-7.71 (m, 3H), 7.56 (d, *J* = 7.2 Hz, 1H), 6.90 (t, *J* = 8.6 Hz, 1H).

2-(2-chlorophenyl) quinoline(7A11)[5]: Yield, 198 mg,83%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.26-8.20 (m, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.78-7.71 (m, 3H), 7.60 (d, *J* = 6.8 Hz, 1H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.43-7.40 (m, 2H).

2-(2-bromophenyl) quinoline (7A12)[6]:Yield,216 mg,76%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.22-8.16 (m, 2H), 7.87(d, *J* = 8.0 Hz, 1H), 7.76-7.69 (m, 3H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.59-7.56 (m, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.31-7.27(m, 1H).

2-(3-bromophenyl) quinoline (7A13)[2]: Yield 242 mg, 85%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.35 (br,1H), 8.23 (d,*J* = 8.6 Hz, 1H), 8.17 (d, *J* = 8.48 Hz, 1H), 8.07 (d, *J* = 7.8Hz, 1H), 7.76-7.72 (m, 1H), 7.83 (d, J = 8.56 Hz, 2H), 7.59-7.52(m, 2H), 7.38 (t, *J* = 7.84 Hz, 1H).

2-(4-bromophenyl) quinoline (7A14)[2]: Yield 202 mg, 71%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.23 (d, *J* = 8.6 Hz, 1H), 8.16 (d, *J* = 8.32 Hz, 1H),8.05 (d, *J* = 8.52 Hz, 2H), 7.85-7.81(m, 2H), 7.73(t, J = 6.8 Hz, 1H),7.64(d, *J* = 8.32 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H).

4-(quinolin-2-yl) benzonitrile (7A15)[7]: Yield120 mg,52%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.54(d, *J* = 8.48 Hz, 1H), 8.48 (d, *J* = 7.2 Hz, 2H), 8.26 (d, *J* = 8.56 Hz, 1H), 8.12 (d, *J* = 8.48 Hz,1H), 8.04-8.02 (m, 3H),7.83 (t, *J* = 7.36 Hz, 1H), 7.65 (t, *J* = 7.24 Hz, 1H).

4-(quinolin-2-yl) benzamide(7A15')[8]: Yield95 mg,38%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.50 (d, *J* = 8.56 Hz, 1H), 8.36 (d, *J* = 8.2 Hz, 2H), 8.23 (d, *J* = 8.64 Hz, 1H), 8.10 (d, *J* = 7.92 Hz, 2H), 8.06-8.01 (m, 3H), 7.80 (t, *J* = 7.76 Hz, 1H), 7.62 (t, *J* = 7.72 Hz, 1H), 7.46 (br, 1H).

^{1}H NMR (400 MHz, DMSO-d6, D_2O exchange): δ (ppm) = 8.48 (d, *J* = 8.64 Hz, 1H), 8.31 (d, *J* = 8.36 Hz, 2H), 8.17 (d, *J* = 8.64 Hz, 1H), 8.09 (d, *J* = 8.48 Hz, 2H), 8.02-7.99 (m, 3H), 7.80 (t, *J* = 8.28 Hz, 1H), 7.61 (t, *J* = 7.88 Hz, 1H),

2-(2-nitrophenyl) quinoline(7A16)[9]: Yield153 mg,61%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.53 (d, *J* = 8.52 Hz, 1H), 8.05 (t, *J* = 6.56 Hz, 2H), 7.94-7.89 (m, 2H), 7.87-7.80 (m, 2H), 7.78-7.74 (m, 1H) 7.72-7.68 (m, 1H) 7.68-7.64(m,1H).

2-(3-nitrophenyl) quinoline(7A17)[5]: Yield160 mg, 64%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 9.10 (br, 1H), 8.73 (d, *J* = 7.48 Hz, 1H), 8.56 (d, *J* = 8.48 Hz, 1H), 8.37-8.31 (m, 2H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 7.88 Hz, 1H), 7.89-7.82 (m, 2H), 7.66 (t, *J* = 7.28 Hz, 1H).

2-(naphthalen-1-yl) quinoline(7A18)[6]: Yield 227 mg, 90%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.31-8.25 (m, 2H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.96-7.90 (m, 3H), 7.80-7.70(m,3H), 7.61-7.58 (m, 2H), 7.53-7.44 (m, 2H).

2-phenethylquinoline (7A19)[1]: Yield 215 mg, 92%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.25 (d, *J* = 8.44 Hz, 1H), 7.96 (d, *J* = 8.48 Hz, 1H), 7.92 (d, *J* = 8.04 Hz, 1H), 7.74-7.70 (m, 1H), 7.56-7.52 (m, 1H), 7.45 (d, *J* = 6.24 Hz, 1H), 7.27-7.24 (m, 4H), 7.18-7.16 (m, 1H), 3.24-3.20 (m, 2H), 3.12-3.08 (m, 2H).

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.21 (br, 1H), 8.11 (d, *J* = 7.92 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.74 (t, *J* = 6.88 Hz, 1H), 7.53 (t, *J* = 7.04 Hz, 1H), 7.25-7.18 (m, 6H) 3.37-3.35 (m, 2H), 3.17 (t, *J* = 8.32 Hz, 2H).

2-(3,4-dimethoxyphenethyl) quinoline(7A20)[1]: Yield 261 mg,89%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.25 (d, *J* = 8.44 Hz, 1H), 7.97-7.91 (m, 2H), 7.74-7.70 (m, 1H), 7.55-7.53 (m, 1H), 7.45 (d,*J* = 8.44 Hz, 1H), 6.87-6.86 (m, 1H), 6.82 (d, *J* = 8.16 Hz, 1H),6.77-6.75 (m, 1H) 3.69 (s, 6H), 3.22-3.18 (m, 2H), 3.05-3.01 (m, 2H).

2-(pyridin-2-yl) quinoline(7A21)[2]: Yield 165 mg,80%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.74-8.72 (m, 1H), 8.64 (d, *J* = 7.92 Hz, 1H), 8.56-8.53 (m, 1H), 8.29-8.25 (m, 1H), 8.17 (d, *J* = 8.56 Hz, 1H), 7.89-7.83 (m, 2H), 7.74-7.69 (m, 1H), 7.56-7.52 (m, 1H), 7.37-7.32 (m, 1H).

2-(pyridin-3-yl) quinoline (7A22)[5]: Yield157 mg,76%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 9.334-9.33 (m, 1H), 8.65-8.63 (m, 1H), 8.62-8.59 (m, 1H), 8.44 (d, *J* = 8.64 Hz, 1H), 8.13 (d, *J* = 8.48 Hz, 1H), 8.06 (d, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 8.16 Hz, 1H), 7.81-7.77 (m, 1H), 7.63-7.60 (m, 2H).

2-(pyridin-4-yl) quinoline(7A23)[10]: Yield151 mg, 73%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.79-8.77 (m, 2H), 8.29 (d, *J* = 8.52 Hz,1H), 8.19 (d, *J* = 8.48 Hz, 1H), 8.07 (d, *J* = 4.68 Hz, 2H), 7.92-7.85 (m, 2H), 7.77 (t, *J* = 7.32 Hz, 1H), 7.59 (t,*J* = 7.56 Hz, 1H).

2-(4-(1H-imidazol-1-yl) phenyl) quinoline (7A24): Yield 221 mg, 81%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.41 (d, *J* = 8.6 Hz,1H), 8.33 (d, *J* = 8.56 Hz,2H), 8.27(br,1H), 8.12 (d, *J* = 8.52 Hz, 1H), 8.04 (d, *J* = 8.64 Hz, 1H), 7.95 (d, *J* = 8.12 Hz, 1H), 7.80-7.75 (m, 3H), 7.69 (br, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.19 (br,1H).

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.31 (d, *J* = 9.2 Hz, 2H), 8.26 (d, *J* = 8.68 Hz, 1H), 8.17(d, *J* = 8.6 Hz, 1H), 8.02 (br 1H), 7.89 (d, *J* = 8.6 Hz, 1H), 7.85 (d, *J* = 8.56 Hz, 1H), 7.75 (t, J = 6.72 Hz, 1H), 7.56-7.54 (m, 3H), 7.40 (br, 1H), 7.29 (m, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) =155.56, 148.19, 138.64,137.90, 136.95, 135.43, 130.60, 130.22, 129.84, 129.64, 129.25, 128.96, 127.43, 127.19, 126.53, 121.33, 118.41, 117.97; HRMS (ESI) m/z: [M+ H] − Calcd for C18H14N3 272.1188; Found 272.1184

2-methylquinoline (7A25)[1]: Yield 106 mg, 74%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.07-8.03 (m, 2H), 7.77(d, *J* = 8.0 Hz, 1H), 7.68 (t, *J* = 7.84 Hz, 1H),7.48 (t, *J* = 7.60 Hz, 1H), 7.29 (d, *J* = 8.36 Hz, 1H), 2.75 (s, 3H).

2-isopropylquinoline(7A26)[1]: Yield 142 mg, 81%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.09-8.03 (m, 2H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.68-7.64 (m,1H), 7.46 (d, *J* = 7.28 Hz, 1H), 7.33 (d, *J* = 8.44 Hz, 1H), 3.33-3.21 (m, 1H), 1.39-1.38 (m, 6H).

2-(tert-butyl) quinoline (7A27)[2]: Yield135 mg,73%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = = 8.05 (br, 2H), 7.75 (d, *J* = 7.88 Hz, 1H), 7.67-7.64 (m, 1H), 7.52 (d, *J* = 8.76 Hz, 1H), 7.48-7.44 (m, 1H), 1.46 (s, 9H).

2-pentylquinoline (7A28)[1]: Yield187 mg, 94%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.07 (d, *J* = 8.32Hz, 2H), 7.77 (d, *J* = 8.04 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H),7.48 (t, *J* = 7.48 Hz, 1H), 7.30 (d, *J* = 8.4 Hz,1H), 2.97 (t, *J* = 7.8 Hz, 2H), 1.85 (m, 2H), 1.43-1.37 (m, 4H), 0.9-0.85 (m, 3H).

3-methyl-2-phenylquinoline (7A29)[5]: Yield172 mg,78%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.26 (br,1H), 7.97-7.92 (m,2H), 7.72-7.69 (m,1H), 7.63-7.56 (m,3H), 7.51-7.47 (m, 3H), 2.44 (s, 3H).

3-ethyl-2-phenylquinoline (7A30)[2]: Yield178 mg,76%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.18-8.07(br, 2H), 7.81(d, *J* = 8.12 Hz,1H), 7.67 (t, J = 7.44 Hz, 1H), 7.55-7.41(m, 6H), 2.82-2.76(q,*J* = 7.46 Hz,2H), 1.23-1.12(m,3H).

3-butyl-2-phenylquinoline (7A31)[11]: Yield187 mg,72%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.24(s,1H), 7.99(d, *J* = 8.44 Hz, 1H),7.91(d, *J* = 8.12 Hz, 1H),7.70 (t, *J* = 7.92 Hz,1H), 7.57(t, *J* = 7.6 Hz, 1H), 7.51-7.49 (m, 5H), 2.77(t, *J* = 7.76 Hz, 2H), 1.53-1.45 (m, 2H), 1.27-1.19 (m, 2H), 0.79(t, *J* = 7.36 Hz, 3H).

3-pentyl-2-phenylquinoline (7A32)[12]: Yield 201 mg,73%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.14 (br, 1H), 8.04 (s, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.54-7.52 (m, 6H), 2.75 (t, *J* = 8.0 Hz, 2H), 1.55-1.53 (m, 2H), 1.24-1.21 (m, 4H), 0.87-0.80 (m, 3H).

2-(4-chlorophenyl)-3-methylquinoline (7A33)[13]: Yield208 mg,82%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.19-8.17 (m, 1H), 8.06 (s,1H), 7.79 (d, *J* = 8.48 Hz, 1H), 7.72-7.62 (m, 1H), 7.56-7.54 (m, 3H), 7.48-7.45 (m, 2H), 2.46 (s, 3H).

2,7-diphenylquinoline(12AA)[14]: 256 mg, 91%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.40 (d, *J* = 8.56 Hz, 1H), 8.32 (br, 1H), 8.14-8.12 (m,2H), 8.02-7.96 (m, 2H), 7.90-7.87 (dd, J_1= 1.76Hz,J_2= 8.48 Hz, 1H), 7.82-7.80 (m, 2H), 7.57-7.48 (m,5H), 7.41(t, t, *J* = 7.36 Hz, 1H).

7-phenyl-2-(o-tolyl) quinoline (12AB): 260mg, 88%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.48 (d, *J* = 8.44 Hz, 1H), 8.26 (br, 1H), 8.07 (d, *J* = 8.52 Hz, 1H), 7.95-7.93 (dd, J_1= 1.6 Hz, J_2= 8.48 Hz, 1H), 7.82-7.80 (m, 2H), 7.60 (d, *J* = 8.44 Hz, 1H), 7.51(t, *J* = 7.44 Hz, 2H), 7.46-7.41 (m, 2H), 7.39-7.34 (m, 3H), 2.35 (s, 3H);^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 160.63, 147.97, 142.43, 140.28, 153.98, 153.91, 130.86, 129.66, 128.96, 128.57, 127.89, 127.85, 127.43, 127.06, 126.09, 126.0, 125.81, 20.33. HRMS (ESI) m/z: [M+ H] − Calcd for C22H18N 296.1439; Found 296.1436

2-pentyl-7-phenylquinoline(12AC): 212 mg, 77%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.27 (d, *J* = 8.4 Hz, 1H), 8.18 (br, 1H), 7.96 (d, *J* = 8.44 Hz, 1H), 7.86-7.83 (dd, J_1= 1.68 Hz, J_2= 8.44 Hz, 1H), 7.78-7.76 (m, 2H), 7.50 (t, *J* = 7.36 Hz, 2H), 7.45-7.38(m, 2H), 2.97 (t,*J* = 7.68 Hz,2H), 1.86-1.78 (m, 2H),1.44-1.39 (m, 4H), 0.93-0.89 (m, 3H);^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 163.43, 128.90, 127.84, 127.79, 127.41, 121.26, 31.68, 29.68, 22.51, 13.95. HRMS (ESI) m/z: [M+ H] − Calcd for C20H22N 276.1752; Found 276.1748

2-(4-chlorophenyl)-3-methyl-7-phenylquinoline (12AD): 280 mg, 85%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.28 (br, 1H), 8.24 (br, 1H), 8.00 (d, *J* = 8.52 Hz, 1H), 7.93-7.91 (dd, J_1= 1.72 Hz, J_2= 8.52 Hz, 1H), 7.81-7.79 (m, 2H), 7.63-7.61 (m,2H), 7.58-7.56 (m, 2H), 7.52 (t,*J* = 7.36 Hz, 2H), 7.43-7.40 (m, 1H), 2.48 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 159.52, 146.75, 141.64, 140.26, 139.03, 136.80, 134.38, 130.30, 128.93, 128.50, 127.31, 127.12, 126.69, 126.27, 20.52. HRMS (ESI) m/z: [M+ H] − Calcd for C22H17ClN 330.1050; Found 330.1044

7-phenyl-2-(pyridin-2-yl) quinoline(12AE)[49]: 234 mg, 83%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.74 (m, 1H), 8.67 (d, *J* = 9.48 Hz, 1H), 8.55 (d, *J* = 8.68 Hz, 1H), 8.41 (br, 1H), 8.30 (d, *J* = 8.6 Hz, 1H), 7.91 (t,*J* = 8.72 Hz, 2H), 7.86-7.78 (m, 3H), 7.51 (t, *J* = 7.76 Hz, 2H), 7.43-7.35 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 156.38, 156.03, 149.07, 148.03, 142.35, 140.26, 137.03, 136.62, 128.93, 127.98, 127.83, 127.43, 127.27, 126.48, 124.08, 121.92, 118.93. HRMS (ESI) m/z: [M+ H] − Calcd for C20H15N2 283.1235; Found 283.1227

7-bromo-2-phenylquinoline(12BA)[5]: 262 mg, 92%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.39 (d, *J* = 8.52 Hz, 1H), 8.28 (s, 1H), 8.14 (d, *J* = 7.16 Hz, 1H), 8.03 (d, *J* = 8.68 Hz, 1H), 7.86 (d, *J* = 8.64 Hz, 1H), 7.68 (d, *J* = 8.76 Hz, 1H), 7.56-7.50 (m, 3H).

7-cyclopropyl-2-phenylquinoline (12CA): 218mg, 89%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.33 (d, *J* = 8.56 Hz, 1H), 8.09 (d, *J* = 7.04 Hz, 2H), 7.88 (d, *J* = 8.56 Hz, 1H), 7.83 (d, *J* = 8.48 Hz, 1H), 7.80 (br, 1H), 7.57-7.50 (m, 3H), 7.34-7.32 (m, 1H), 2.25-2.16 (m,1H), 1.14-1.11 (m, 2H), 0.92-0.88(M, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 157.41, 148.43, 146.32, 139.77, 136.43, 129.18, 128.77, 127.52, 127.12, 126.46, 125.62, 125.36, 124.66, 118.06, 15.81, 9.93. HRMS (ESI) m/z: [M+ H] − Calcd for C18H16N 246.1283; Found 246.1273

7-cyclopentyl-2-phenylquinoline (12DA)[50]: 238 mg, 87%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.32 (d, *J* = 8.56 Hz, 1H), 8.08-8.06 (m, 2H), 7.94 (br, 1H), 7.89 (d, *J* = 8.52 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.55-7.43 (m, 4H), 3.29-3.25 (m, 1H), 2.19-2.15 (m, 2H), 1.92-1.85 (m, 2H), 1.83-1.72 (m, 4H).

7-(4-methoxyphenyl)-2-phenylquinoline (12EA): 280 mg, 90%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.39 (d, *J* = 8.72 Hz, 1H), 8.27 (s,1H), 8.13-8.11 (m, 2H), 7.99-7.94 (m, 2H), 7.88-7.86 (dd, J_1 = 1.72 Hz, J_2 = 8.6 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 2H), 7.57-7.50 (m, 3H), 7.08 (d,*J* = 8.76 Hz, 2H), 3.86 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 159.58, 157.69, 148.55, 141.97, 139.60, 136.49, 132.76, 129.32, 128.81, 128.48, 127.75, 127.55, 126.40, 125.90, 125.71, 118.67, 114.38, 55.33. HRMS (ESI) m/z: [M+ H] − Calcd for C22H18NO 312.1388 Found 312.1396

2-(4-chlorophenyl)-3-methyl-7-(naphthalen-1-yl) quinoline (12FD): 349 mg, 92%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.35 (br, 1H), 8.11 (br, 1H), 8.04(d, *J* = 8.72 Hz, 1H), 7.95 (t,*J* = 8.16 Hz, 2H), 7.86 (d, *J* = 8.12 Hz, 1H), 7.72 (d, *J* = 6.96 Hz, 1H), 7.62-7.52 (m, 6H), 7.49-7.44 (m, 2H), 2.50 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 159.54, 146.51, 141.70, 139.43, 139.02, 136.98, 134.46, 133.82, 131.39, 130.37, 129.80, 129.42, 129.11, 128.53, 128.33, 128.14, 128.05, 127.33, 126.71, 126.42, 126.22, 125.88, 125.43, 20.59. HRMS (ESI) m/z: [M+ H] − Calcd for C26H19ClN 380.1206; Found 380.1194

3-ethyl-7-(naphthalen-1-yl)-2-phenylquinoline (12FF): 294 mg, 82%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.37 (br, 1H), 8.10 (br, 1H), 8.07 (d, *J* = 8.36 Hz, 1H), 7.94 (t, *J* = 8.0 Hz, 2H), 7.86 (d, *J* = 8.48 Hz, 1H), 7.73-7.71 (dd, J_1 = 1.52 Hz, J_2= 8.44Hz, 1H), 7.60-7.49 (m, 8H), 7.46-7.44 (m, 1H), 2.84(q, *J* = 7.52 Hz, 2H), 1.21 (t, *J* = 7.48 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 160.79, 141.83, 139.45, 135.57, 133.82, 131.39, 129.34, 128.80, 128.33, 128.17, 128.04, 127.36,

127.22, 126.84, 126.61, 126.47, 126.21, 125.92, 125.86, 125.44, 26.01, 14.78. HRMS (ESI) m/z: [M+ H] − Calcd for C27H22N 360.1752; Found 360.1751

7-(naphthalen-1-yl)-2-(pyridin-2-yl) quinoline(12FE): 279 mg, 84%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.76-8.75 (m, 1H), 8.68-8.62 (m, 2H), 8.36-8.34 (m,2H), 7.99-7.91 (m,4H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.16 Hz, 1H), 7.60-7.57 (m, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.72 Hz, 1H), 7.36-7.33 (m,1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 156-53, 156.23, 149.12, 147.91, 142.23, 139.42, 136.93, 136.59, 133.79, 131.44, 130.47, 129.40, 128.32, 128.07, 127.29, 127.26, 126.25, 125.89, 125.39, 124.03, 121.81, 119.04. HRMS (ESI) m/z: [M+ H] − Calcd for C24H17N2 333.1392; Found 333.1388

2-(tert-butyl)-7-(3,5-difluorophenyl) quinoline (12GH): 259 mg, 87%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.27 (br, 1H), 8.24 (d, *J* = 8.68 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.44 Hz, 1H), 7.67 (d, *J* = 8.68 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 2H), 6.98 (t, *J* = 8.96 Hz, 1H), 1.48 (s,9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 170.21, 164.64, 164.51, 162.18, 162.05, 147.50, 144.09, 144.00, 143.90, 139.25, 139.22, 139.20, 135.54, 128.02, 127.57, 126.14, 124.50, 118.76, 110.36, 110.29, 110.17, 110.10, 103.06, 102.80, 102.55, 38.21, 30.07. HRMS (ESI) m/z: [M+ H] − Calcd for C19H18F2N 298.1407; Found 298.1400

7-bromo-2-(tert-butyl) quinoline(12BH)[15]: 247 mg, 93%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.21-8.19 (m, 2H), 7.76 (d, *J* = 8.64 Hz, 1H), 7.66 (d, *J* = 8.72 Hz, 1H), 7.62-7.59(m, 1H), 1.44 (s, 9H).

2-(tert-butyl)-7-(naphthalen-1-yl) quinoline (12FH): 236 mg, 76%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.30 (d,*J* = 8.72 Hz, 1H), 8.12 (br, 1H), 7.98-7.92 (m,3H), 7.88 (d, *J* = 8.44 Hz, 1H), 7.70 (d, *J* = 8.76 Hz, 1H), 7.65-7.62 (dd, J_1 = 1.48 Hz, J_2= 8.20 Hz, 1H), 7.58 (t, *J* = 7.12 Hz, 1H), 7.53-7.49 (m, 2H), 7.46-7.42 (m,1H), 1.49 (s,9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 169.65, 147.42, 141.88, 139.65, 135.78, 131.50, 130.02, 128.30, 127.98, 127.34, 126.82, 126.15, 125.99, 125.82, 125.57, 125.39, 118.34, 38.19, 30.13. HRMS (ESI) m/z: [M+ H] − Calcd for C23H22N 312.1752; Found 312.1754.

2-(tert-butyl)-7-cyclopropylquinoline (12CH): 185 mg, 82%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.11 (d,*J* = 8.68 Hz, 1H), 7.71-7.69 (m, 2H), 7.52 (d, *J* = 8.64 Hz, 1H), 7.25-7.23 (dd, J_1 = 1.52 Hz, J_2= 8.36 Hz, 1H), 2.12-2.08 (m, 1H), 1.44 (s, 9H), 1.10-1.05 (m, 2H), 0.85-0.81 (m,2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 169.27,

147.55, 145.52, 135.60, 126.92, 124.95, 124.62, 124.52, 117.18, 38.02, 29.95, 15.77, , 14.10, 9.63. HRMS (ESI) m/z: [M+ H] − Calcd for C16H20N 226.1596; Found 226.1593

2-phenylquinoline (9A1)[11]: Yield190 mg,92%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.39 (d, *J* = 8.6 Hz, 1H), 8.12-8.10 (m, 3H), 7.98 (d, *J* = 8.6 Hz, 1H), 7.94 (d, *J* = 6.24 Hz, 1H), 7.79-7.74 (m, 1H), 7.60-7.47 (m, 4H).

2-(o-tolyl) quinoline(9A2)[2]: Yield 193 mg, 88%

^{1}H NMR (400 MHz, MeOD): δ (ppm) =8.41 (d, *J* = 6.8 Hz, 1H), 8.04(d, *J* = 8.52 Hz, 1H), 7.98(d, *J* = 8.12 Hz, 1H), 7.80-7.76 (m, 1H), 7.64-7.59 (m, 2H), 7.43-7.59 (m, 1H), 7.37-7.30 (m, 3H), 2.32 (s3H).

2-(m-tolyl) quinoline (9A3)[3]: Yield 184 mg, 84%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.45(d, *J* = 8.6 Hz, 1H), 8.14 (d, *J*= 8.16 Hz, 1H), 8.11 (br,1H), 8.06 (t, *J* = 8.2 Hz,2H), 8.0 (d, J = 9.6 Hz, 1H),7.80-7.76 (m, 1H), 7.61-7.57 (m,1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.44 Hz, 1H), 2.44 (s, 3H).

2-(p-tolyl) quinoline (9A4)[5]: Yield 178 mg, 81%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.36 (d, *J* = 8.64 Hz, 1H), 8.08 (d, *J* = 8.56 Hz, 1H),8.00 (d, *J* = 8.04 Hz, 2H), 7.96-7.91 (m, 2H), 7.75 (t, *J* = 7.16 Hz, 1H), 7.56(t, *J* = 7.2 Hz, 1H), 7.35 (d, *J* = 7.88 Hz, 2H), 2.42 (s, 3H).

2-(2-methoxyphenyl) quinoline(9A5)[3]: Yield 193 mg, 82%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.29 (d, *J* = 8.52 Hz, 1H), 8.06 (d, *J* = 8.48 Hz, 1H), 7.93 (d, *J* = 8.12 Hz, 1H), 7.83 (d, J = 8.56 Hz, 1H), 7.77-7.72 (m, 1H), 7.65-7.57 (m, 2H), 7.49-7.44 (m, 1H), 7.17-7.09 (m, 2H), 3.86 (s, 3H).

2-(3-methoxyphenyl) quinoline (9A6)[3]: Yield 201 mg, 85%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.46 (d, *J* = 8.64 Hz, 1H), 8.16 (d, *J* = 8.64 Hz, 1H), 8.08 (d, *J* = 8.44 Hz, 1H), 8.00 (d, *J* = 7.56 Hz, 1H), 7.85-7.83 (m, 2H), 7.80-7.76(m, 1H), 7.62-7.58(m, 1H), 7.47 (t, *J* = 7.92 Hz, 1H), 7.09-7.07 (dd, J_1 = 2.16 Hz, J_2 = 7.72 Hz, 1H), 3.88 (s, 3H);

2-(4-methoxyphenyl) quinoline (9A7)[5]: Yield 205 mg, 87%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.33 (d, *J* = 8.56 Hz, 1H), 8.08-8.05 (m,3H), 7.96-7.89 (m,2H), 7.73 (t, *J* = 7.28 Hz, 1H), 7.54 (t, *J* = 7.68 Hz, 1H), 7.08 (d, *J* = 8.68 Hz, 2H), 3.87 (s, 3H).

2-(2-chlorophenyl) quinoline (9A8)[5]: Yield 180 mg, 75%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.48 (d, *J* = 8.48 Hz, 1H), 8.09 (d, *J* = 8.52 Hz, 1H), 8.04-8.01 (m,1H), 7.85-7.81 (m,1H), 7.76 (d, *J* = 8.48 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.64-7.62 (m, 1H), 7.60-7.58 (m,1H), 7.50-7.48 (m, 2H).

2-(3-fluorophenyl) quinoline (9A9)[2]: Yield 198 mg, 89%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.39 (d, *J* = 8.64 Hz, 1H), 8.11 (d, *J* = 8.48 Hz, 1H), 8.0-7.90 (m,4H), 7.75 (t, *J* = 7.04 Hz,1H), 7.61-7.52 (m,2H), 7.24-7.18 (m,1H).

2-(2-fluorophenyl) quinoline (9A10)[3]: Yield 172 mg, 77%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.40 (d, *J* = 8.56 Hz, 1H), 8.10 (d, *J* = 8.52 Hz, 1H), 7.98-7.93 (m, 2H), 7.87-7.84 (dd, J_1 = 2.68 Hz, J_2 = 5.88 Hz, 1H),7.81-7.77 (m, 1H), 7.62 (t, *J* = 7.16 Hz, 1H), 7.53-7.49 (m,1H), 7.38-7.34 (m, 1H), 7.30-7.25(m, 1H).

2-(4-fluorophenyl) quinoline (9A11)[2]: Yield 187 mg, 83%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.37 (d, *J* = 8.6 Hz, 1H), 8.19-8.15 (m, 2H), 8.08 (d, *J* = 8.52 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.92 (d, *J* = 8.24 Hz, 1H), 7.78-7.74 (m, 1H), 7.59-7.55 (m, 1H), 7.28-7.24(m, 2H).

2-(4-(trifluoromethyl) phenyl) quinoline (9A12)[3]: Yield 202 mg, 74%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.43 (d,*J* = 8.52 Hz, 1H), 8.35 (d, *J* = 7.84 Hz, 2H), 8.15 (d,*J* = 8.2 Hz, 1H), 8.06 (d, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 7.92 Hz, 1H), 7.85-7.77 (m,3H), 7.61 (t, *J* = 7.44 Hz, 1H).

2-(2-bromophenyl) quinoline (9A13)[6]: Yield 215 mg, 76%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.40 (d, *J* = 8.56 Hz, 1H), 8.35-8.34 (m, 1H), 8.12-8.08 (m, 2H), 7.98 (d, *J* = 8.6 Hz, 1H), 7-94 (d, *J* = 8.08 Hz, 1H), 7.80-7.75 (m, 1H), 7.65-7.63 (m, 1H), 7.61-7.57 (m, 1H), 7.46 (t, *J* = 7.88 Hz, 1H).

2-(3-bromophenyl) quinoline(9A14)[2]: Yield 227 mg, 80%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.41 (d, *J* = 8.48 Hz, 1H), 8.06 (d,*J* = 8.48 Hz, 1H), 7.99 (d, *J* = 8.2 Hz,1H), 7.82-7.76 (m, 1H), 7.75-7.74(m, 1H), 7.69-7.63 (m, 2H), 7.60-7.54 (m, 1H), 7.53-7.49 (m, 1H), 7.41-7.37 (m, 1H).

2-(4-bromophenyl) quinoline(9A15)[2]: Yield 224 mg, 79%

^{1}H NMR (400 MHz, CD_3OD): δ (ppm) = 8.39 (d, *J* = 8.64 Hz,1H), 8.10-8.06 (m, 3H), 7.98 (d, *J* = 8.6 Hz,1H), 7.94-7.92 (m, 1H),7.77-7.74 (m, 1H), 7.71-7.69 (m, 2H), 7.61-7.59 (m, 1H).

2-(naphthalen-1-yl) quinoline (9A16)[6]: Yield 230 mg, 90%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.49 (d, *J* = 8.4 Hz, 1H), 8.10 (d, *J* = 8.44 Hz, 1H), 8.05-7.95 (m, 3H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.82(t, *J* = 7.44 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.69-7.61 (m,3H), 7.56-7.52 (m,1H), 7.50-7.46(m, 1H).

2-(pyridin-2-yl) quinoline (9A17)[2]: Yield 158mg, 76%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.70 (d, *J* = 4.56 Hz, 1H), 8.54 (d, *J* = 7.96 Hz, 1H), 8.45-8.40 (m, 2H), 8.14 (d, *J* = 8.52 Hz, 1H), 8.01-7.94 (m, 2H), 7.80-7.94 (m, 1H), 7.62-7.58 (m, 1H), 7.50-7.46(m,1H).

2-(pyridin-3-yl) quinoline (9A18)[5]: Yield 152 mg, 74%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 9.32 (br, 1H), 8.65-8.63 (m, 1H), 8.61-8.59 (m, 1H), 8.43 (d, *J* = 8.56 Hz, 1H),8.13 (d, *J* = 8.48 Hz, 1H), 8.05 (d, *J* = 8.56 Hz,1H), 7.95 (d, *J* = 8.12 Hz, 1H), 7.81-7.77 (m, 1H), 7.63-7.59 (m, 2H).

2-(pyridin-4-yl) quinoline (9A19)[10]: Yield 160 mg, 77%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.73 (d, *J* = 5.64 Hz, 2H), 8.48 (d, *J* = 8.56 Hz, 1H), 8.24 (d, *J* = 5.92 Hz, 2H), 8.18-8.12 (m, 2H), 7.83 (t, *J* = 7.32 Hz, 1H), 7.66 (t,*J* = 7.36 Hz, 1H), 8.00 (d, *J* = 8.16 Hz, 1H).

3-ethyl-2-phenylquinoline (9A20)[2]: Yield 184 mg, 79%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.26 (br, 1H), 7.99 (d, *J* = 8.52 Hz, 1H), 7.93 (d, *J* = 8.12 Hz, 1H), 7.72-7.68 (m, 1H), 7.60-7.55 (m,1H), 7.53-7.48 (m,5H), 2.81-2.76 (m, 2H), 1.16(t, *J* = 7.52 Hz, 3H).

3-butyl-2-phenylquinoline (9A21)[11]:Yield 202 mg, 77%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.24 (br, 1H), 7.99 (d,*J* = 8.52 Hz, 1H), 7.92 (d, *J* = 8.04 Hz,1H), 7.79-7.69 (m, 1H), 7.60-7.58 (m, 1H), 7.53-7.51 (s, 5H), 2.78 (t, *J* = 7.76 Hz, 2H), 1.51-1.47 (m, 2H), 1.27-1.20 (m,2H), 0.77 (t, *J* = 7.36 Hz, 3H).

11H-indeno[1,2-b] quinoline (14AA)[16]: Yield 163mg, 75%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 8.46 (s,1H), 8.16-8.14 (m,1H), 8.10 (d, *J* = 8.4 Hz, 1H), 8.00 (d,*J* = 8.0 Hz,1H), 7.76-7.71(m, 2H), 7.59-5.58 (m, 1H), 7.56-7.53 (m, 2H), 4.14 (s, 2H).

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.33 (br, 1H), 8.22-8.20 (m, 2H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.70 (t, *J* = 7.2 Hz, 1H), 7.62-7.60 (m, 1H), 7.53-7.47 (m, 3H), 4.05 (s, 2H).

5,6-dihydrobenzo[b] [1,10] phenanthroline (14AB)[16]: Yield 183 mg, 78%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.80 (m,1H), 8.39-8.37 (m, 1H), 8.00 (br,1H), 7.83-7.76 (m, 1H), 7.67-7.62 (m, 2H), 7.55-7.52 (m, 1H), 7.34-7.29 (m, 1H), 32.5-3.07 (m, 4H).

5,6-dihydrobenzo[c]acridine (14AC)[2]: Yield 190 mg, 82%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.58 (d,*J* = 6.12 Hz, 1H), 8.13 (br,1H), 7.92 (br, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.64 (t,*J* = 7.28 Hz, 1H), 7.49-7.35 (m,3H), 7.28-7.24 (m, 1H) 3.13 (t, *J* = 5.88 Hz, 2H), 3.00 (t, *J* = 7.28 Hz, 2H),

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.42 (m, 1H), 8.09 (br, 1H), 8.06 (d, J = 8.6 Hz, 1H), 7.84 (d, *J* = 8.16 Hz, 1H), 7.67 (t, *J* = 7.68 Hz, 1H), 7.51 (t, J = 7.44 Hz, 1H), 7.40-7.37 (m, 2H), 7.33-7.32 (m, 1H), 3.12 (t, *J* = 6.16 Hz, 2H), 3.00 (t, *J* = 7.3 Hz, 2H),

2,3-dihydro-1H-cyclopenta[b]quinoline (14AD)[17]: Yield 156 mg, 92%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.06 (br, 1H), 7.90 (d,*J* = 8.4 Hz,1H), 7.83 (d,*J* = 8.08 Hz, 1H), 7.64 (t, *J* = 7.72 Hz, 1H), 7.49 (t, *J* = 7.52 Hz, 1H), 3.12 (t, *J* = 7.64 Hz, 4H), 2.22 (t, *J* = 7.48 Hz, 2H).

1,2,3,4-tetrahydroacridine (14AE)[18]: Yield 165 mg, 90%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.99 (br, 1H), 7.88 (d, *J* = 8.48 Hz, 1H), 7.79 (d, *J* = 8.08 Hz, 1H), 7.63 (t, *J* = 7.92 Hz, 1H), 7.47 (t, *J* = 7.56 Hz, 1H), 3.08 (t, *J* = 6.36 Hz, 2H), 3.01 (t, *J* = 6.32 Hz, 2H), 2.01-1.97 (m, 2H), 1.93-1.89 (m, 2H);

7,8,9,10-tetrahydro-6H-cyclohepta[b]quinoline (14AF)[18]:Yield172 mg, 77%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.01 (br, 1H), 7.93 (d, *J* = 8.48 Hz, 1H), 7.82 (d, *J* = 8.04 Hz, 1H), 7-81-7.64 (m, 1H), 7.54-7.52(m, 1H), 3.22-3.20 (m, 2H), 3.03-3.00 (m, 2H), 1.95-1.94 (m, 2H), 1.81-1.77 (m, 4H).

6,7,8,9,10,11-hexahydrocycloocta[b]quinoline (14AG)[17]: Yield 178 mg,84%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.04 (br, 1H), 7.94 (d, *J* = 8.48 Hz, 1H), 7.83 (d, *J* = 8.16 Hz, 1H), 7.65 (t, *J* = 7.96 Hz, 1H), 7.50 (t, *J* = 7.64 Hz, 1H), 3.18-3.15 (m, 2H), 3.04-3.00 (m, 2H), 1.88 (br, 2H), 1.80 (br, 2H), 1.42 (br, 4H);

All the reactions were carried out in a 1.0 mmol scale of amino alcohol and according to the general procedure 2.B.

1-methyl-2-phenyl-1H-pyrrole (17BA)[19]: Yield 105 mg,67%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.39-7.36 (m, 4H), 7.30-7.28 (m, 1H), 6.70 (br, 1H), 6.20 (d, *J* = 7.88 Hz, 2H), 3.66 (s, 3H).

1-methyl-2-(o-tolyl)-1H-pyrrole (17BF)[20]: Yield 118 mg,69%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.25-7.20 (m, 4H), 6.69 (br, 1H), 6.20 (br, 1H), 6.05 (br, 1H), 3.39 (s, 3H), 2.18 (s, 3H).

1-methyl-2-(m-tolyl)-1H-pyrrole (17BG)[20]: Yield 112 mg,65%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.29-7.17 (m, 3H), 7.10 (d, *J* = 6.96 Hz, 1H), 6.69 (br, 1H), 6.18 (br, 2H), 3.65 (s, 3H), 2.37 (s, 3H).

2-(2-fluorophenyl)-1-methyl-1H-pyrrole (17BH)[19]: Yield 117 mg,67%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.35-7.29 (m, 2H), 7.18-7.10 (m, 2H), 6.75 (br, 1H), 6.21 (br, 2H), 3.56 (s, 3H).

2-(4-fluorophenyl)-1-methyl-1H-pyrrole (17BI)[19]: Yield 123 mg,70%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.35-7.32 (m, 2H), 7.07 (t, *J* = 8.56 Hz, 2H), 6.69 (br, 1H), 6.17 (br, 2H), 3.51 (s,3H).

2-(2-methoxyphenyl)-1-methyl-1H-pyrrole (17BJ)[20]: Yield 135 mg,72%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.33 (t, *J* = 7.28 Hz, 1H), 7.28-7.24 (m, 1H), 7.00-6.93 (m,2H), 6.71 (br, 1H), 6.209-6.023- (m, 1H), 6.13-6.12 (m, 1H), 3.80 (s, 3H), 3.47 (s, 3H).

2-(3-methoxyphenyl)-1-methyl-1H-pyrrole (17BC)[21]: Yield 122 mg,65%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.31-7.27 (m, 1H), 6.97 (d, *J* = 7.28 Hz, 1H), 6.93 (s, 1H), 6.84 (d, *J* = 6.6 Hz, 1H), 6.69 (br, 1H), 6.21 (d, *J* = 13.52 Hz, 2H), 3.82 (s, 3H), 3.62 (s, 3H).

2-(4-methoxyphenyl)-1-methyl-1H-pyrrole (17BK)[20]: Yield 133 mg,71%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.31 (d, J = 8.44 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.67 (br, 1H), 6.16 (d, *J* = 10.32 Hz, 2H), 3.8 (s, 3H), 3.61 (s, 3H).

1-methyl-2-(naphthalen-1-yl)-1H-pyrrole (17BL)[19]: Yield 151 mg,73%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.87 (t,*J* = 7.36 Hz, 2H), 7.70 (d, *J* = 8.24, Hz, 1H), 7.52-7.43 (m, 4H), 6.80 (br, 1H), 6.30-6.25 (m, 2H), 3.38 (s, 3H).

2-(1-methyl-1H-pyrrol-2-yl) pyridine (17BM)[22]: Yield 97 mg,61%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.55 (br, 1H), 7.63-7.62 (m, 1H), 7.52 (d, *J* = 8.36 Hz, 1H), 7.07 (m, 1H), 6.72 (br,1H), 6.56 (br,1H), 6.17 (br, 1H), 3.98 (s, 3H).

1,3-dimethyl-2-phenyl-1H-pyrrole (17BD)[23]: Yield 113 mg,66%

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.40 (t, *J* = 7.6 Hz, 2H), 7.32-7.28 (m, 3H), 6.61 (br, 1H), 6.06 (br, 1H), 3.47 (s, 3H), 2.06 (s, 3H).

***3-ethyl-1-methyl-2-phenyl-1H-pyrrole (17BN)*: Yield 115 mg, 62%**

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.40 (t,*J* = 7.48 Hz,2H), 7.33-7.24 (m, 3H), 7.639-7.633 (m, 1H), 6.129-6.124 (m, 1H), 3.49(s, 3H), 2.45-2.40 (m, 2H),1.13 (t, *J* = 7.56 Hz, 3H);^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 132.77, 130.43, 128.13, 126.89, 124.07, 121.58, 107.07, 34.66, 29.68, 19.55, 15.95

***3-butyl-1-methyl-2-phenyl-1H-pyrrole (17BO)*: Yield 128 mg, 60%**

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.40 (t, *J* = 7.32 Hz, 2H), 7.33-7.27 (m, 3H), 6.62-6.61 (m, 1H), 6.094-6.090 (m, 1H), 3.47 (s, 3H), 2.38(t, *J* = 7.64 Hz, 2H), 1.54-1.45 (m, 2H), 1.32-1.23 (m, 2H), 0.83 (t, *J* = 7.28 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 132.84, 130.75, 130.48, 128.11, 126.87, 121.46, 107.57, 34.66, 33.75 29.68, 26.07, 22.57, 13.94

***1-methyl-3-pentyl-2-phenyl-1H-pyrrole (17BP)*: Yield 141 mg, 62%**

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.40 (t, *J* = 8.72 Hz, 2H), 7.33-7.25 (m, 3H), 6.62 (br, 1H), 6.09 (s, 1H), 3.47 (s, 3H), 2.37 (t, *J* = 7.6 Hz, 2H), 1.53-1.47 (m, 2H), 1.26-1.24 (m, 4H), 0.83 (t, *J* = 6.8 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 132.83, 130.73, 130.47, 128.11, 126.87, 122.61, 121.47, 34.67, 31.74, 31.26, 29.68, 26.33, 22.51, 14.02.

***2-(4-chlorophenyl)-1,3-dimethyl-1H-pyrrole (17BE)*[24]: Yield 137 mg, 67%**

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.38 (d, *J* = 8.32 Hz, 2H), 7.22 (t, *J* = 8.4 Hz, 2H), 6.61 (s, 1H), 6.05 (s, 1H), 3.84 (s, 3H), 2.04 (s, 3H).

***1-butyl-2-phenyl-1H-pyrrole (17CA)*[25]: Yield 116 mg, 58%**

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.39-7.32 (m, 4H), 7.28-7.25 (m, 1H), 6.76 (br, 1H), 6.09-6.05 (m, 2H), 3.95 (t, *J* = 7.2 Hz, 2H), 1.57-1.50 (m, 2H), 1.16-1.11 (m, 2H), 0.77 (t, *J* = 7.36 Hz, 3H).

***1-benzyl-2-phenyl-1H-pyrrole (17DA)*[25]: Yield 142 mg, 61%**

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.36-7.30 (m, 4H), 7.26 (t, *J* = 7.44 Hz, 3H), 7.21-7.18 (m, 1H), 6.93-6.89 (m, 3H), 6.21-6.20 (m, 1H), 6.16-6.15 (m, 1H), 5.21 (s, 2H).

***1-(2-chloro-6-fluorobenzyl)-2-phenyl-1H-pyrrole (17EA)*: Yield 160 mg, 56%**

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.46-7.37 (m, 4H), 7.34-7.30 (m, 2H), 7.22 (d, *J* = 8.04 Hz, 1H), 7.07 (t, *J* = 9.08 Hz, 1H), 6.48 (br, 1H), 6.066-6.061(m,2H), 5.25 (s, 2H);^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 162.15, 136.13, 135.14, 135.04, 134.7, 130.83, 130.78, 130.14, 129.96, 129.60, 128.41, 128.28, 126.84, 126.70, 125.89, 125.85, 124.44, 116.98, 116.73, 110.52, 109.73, 45.29, 45.24. HRMS (ESI) m/z: [M+ H] − Calcd for C17H14ClFN 286.0799 Found 286.0797.

***1-(2-chloro-6-fluorobenzyl)-2-phenyl-1H-pyrrole (17FA)*: Yield 148 mg, 52%**

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.38-7.27 (m, 6H), 7.19 (d, *J* = 6.8 Hz, 1H), 6.939-6.934 (m, 1H), 6.60 (t, *J* = 8.28 Hz, 1H), 6.21-6.17 (m, 2H), 5.24 (s, 2H).

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.33-7.29 (m, 2H), 7.26 (d, *J* = 7.16 Hz, 3H), 7.09 (d, J = 10.2 Hz, 1H), 7.04 (d, *J* = 8.28 Hz, 1H), 6.81 (br, 1H), 7.599(t, J = 8.2 Hz, 1H), 6.19-6.18 (m, 2H), 5.19 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 160.61, 134.95, 134.01, 133.91, 132.92, 129.27, 129.22, 128.80, 128.47, 127.32, 127.20, 124.80, 124.77, 122.77, 116.09, 115.85, 109.32, 108.90, 44.24, 44.20. HRMS (ESI) m/z: [M+ H] − Calcd for C17H14ClFN 286.0799; Found 286.0785

***1-(4-chloro-2-fluorobenzyl)-2-phenyl-1H-pyrrole (17GA)*: Yield 163 mg, 55%**

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.82-7.80 (m, 1H), 7.78-7.75 (m, 2H), 7.60 (d, *J* = 7.84 Hz, 2H), 7.48 (t, *J* = 7.56 Hz, 2H), 7.39-7.33 (m, 4H), 6.14 (br, 1H), 6.11 (br, 1H), 7.94 (br, 1H), 5.54 (s, 2H), 2.40 (s, 3H).

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.82-7.80 (m, 1H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 7.36 Hz, 2H), 7.50 (t, *J* = 7.04 Hz, 2H), 7.43-7.34 (m, 4H), 6.28 (br, 1H), 6.22 (br, 1H), 6.05 (br, 1H), 5.53 (s, 2H), 2.45 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 135-84, 134.51, 133.65, 132.73, 132.43,129.23, 129.16, 129.03, 128.65, 128.50, 127.01, 126.83, 124.95, 123.01, 120.81, 44.62, 19.93, HRMS (ESI) m/z: [M+ H] − Calcd for C22H20N 298.1596; Found 298.1583.

***2,5-diphenyl-1H-pyrrole (20AA)[26]*: Yield 158 mg, 72%**

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.60-8.57 (br, 1H), 7.52 (d, *J* = 7.68 Hz, 4H), 7.38 (t, *J* = 7.64 Hz, 4H), 7.24-7.20 (m,2H), 6.57 (s, 2H).

***2-phenyl-5-(o-tolyl)-1H-pyrrole (20AB)[27]*: Yield 152 mg, 65%**

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.61 (d, *J* = 7.04 Hz,2H), 7.41 (d, *J* = 7.04 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.23-7.11 (m,4H), 6.53 (d, *J* = 3.48 Hz, 1H), 6.23 (d, *J* = 3.52 Hz, 1H), 2.42 (s, 3H).

2-phenyl-5-(m-tolyl)-1H-pyrrole (20AC)[27]: Yield 145 mg, 62%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.19 (br, 1H), 7.76 (d, *J* = 7.64 Hz, 2H), 7.60(s, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.64 Hz, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.32 Hz, 1H), 7.00 (d, *J* = 7.44 Hz, 1H), 6.59-6.56 (m, 2H), 2.34 (s, 3H).

2-(3-fluorophenyl)-5-phenyl-1H-pyrrole (20AD)[27]: Yield 169 mg, 67%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.67-7.65 (m, 2H), 7.48-7.46 (m, 1H), 7.44-7.40 (m, 1H), 7.36-7.29 (m, 3H), 7.18-7.15 (m, 1H) 6.88-6.83 (m, 1H), 6.57 (d, *J* = 3.76 Hz, 1H), 6.52 (d, J = 3.6 Hz, 1H).

2-phenyl-5-(4-(trifluoromethyl) phenyl)-1H-pyrrole (20AE)[27]:Yield 213 mg, 74%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.46 (br, 1H), 7.98 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 7.56 Hz, 2H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 7.56 Hz, 2H), 7.22 (t,*J* = 7.24 Hz, 2H), 6.80 (br, 1H), 6.66 (br, 1H).

2-(2-bromophenyl)-5-phenyl-1H-pyrrole (20AF)[27]: Yield 188 mg, 63%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.34 (br, 1H), 7.74-7.69 (m, 3H), 7.61-7.59 (dd, J_1 = 1.48 Hz, J_2 = 7.72 Hz, 1H), 7.46-7.42 (m, 1H), 7.36 (t, *J* = 7.56 Hz, 2H), 7.23-7.16 (m, 2H), 6.62-6.60 (m, 1H), 6.55-6.53 (m, 1H).

2-(3-bromophenyl)-5-phenyl-1H-pyrrole(20AG)[27]: Yield 194 mg, 65%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.32 (br, 1H), 8.04 (br, 1H), 7.78-7.76 (m, 3H), 7.40-7.29 (m,4H), 7.20 (t, *J* = 7.24 Hz, 1H), 6.70 (br, 1H), 6.61 (br, 1H).

2-(naphthalen-1-yl)-5-phenyl-1H-pyrrole (20AH)[28]: Yield 197 mg, 73%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.56 (br, 1H), 8.31-8.30 (m, 1H), 7.97 (m, 1H), 7.89 (d, *J* = 7.36 Hz, 2H), 7.77 (d, *J* = 7.36 Hz, 1H), 7.63-7.55 (m, 4H), 7.36 (t, J = 7.44 Hz, 2H), 7.17 (t, *J* = 6.6 Hz, 1H), 6.72 (br, 1H), 6.43 (br, 1H).

2-phenethyl-5-phenyl-1H-pyrrole (20AI)[29]: Yield 158 mg, 64%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.96 (br, 1H), 7.57 (d, *J* = 7.32 Hz, 2H), 7.32 (d, *J* = 7.64 Hz, 2H), 7.29-7.28 (m, 1H), 7.27-7.24 (m, 3H), 7.19-7.18 (m, 1H), 7.09 (t,*J* = 7.36 Hz, 1H), 6.36 (t, *J* = 2.92 Hz, 1H), 5.84-5.82 (m, 1H),2.94-2.90 (m, 2H), 2.87-2.83 (m, 2H).

3-(5-phenyl-1H-pyrrol-2-yl) pyridine (20AJ)[30]: Yield 123 mg, 56%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.41 (br, 1H), 9.00 (br, 1H), 8.37-8.36 (m, 1H), 8.12 (d, *J* = 7.04 Hz, 1H), 7.77 (d, *J* = 7.28 Hz, 2H), 7.40-7.37 (m, 3H), 7.22-7.20 (m, 1H), 6.73 (br, 1H), 6.64 (br, 1H).

2-isopropyl-5-phenyl-1H-pyrrole (20AK)[26]: Yield 109 mg, 59%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.78 (br, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.30 (t, *J* = 7.56 Hz, 2H), 7.08 (t, *J* = 7.32 Hz, 1H), 7.33 (t, *J* = 3.08 Hz, 1H), 5.79 (t, *J* = 2.68 Hz, 1H), 2.94-2.87 (m, 1H), 1.22 (d, J = 6.88 Hz, 6H).

2-(tert-butyl)-5-phenyl-1H-pyrrole (20AL)[31]: Yield 122 mg, 61%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.54 (br, 1H), 7.62 (d, *J* = 7.44 Hz, 2H), 7.31 (d, *J* = 7.6 Hz, 2H), 7.10 (t, *J* = 7.32 Hz, 1H), 6.29 (t, *J* = 3.0 Hz, 1H), 5.78 (t, *J* = 3.0 Hz, 1H), 1.26 (s, 9H).

2-pentyl-5-phenyl-1H-pyrrole (20AM)[32]: Yield 145mg, 68%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.85 (br, 1H), 7.55 (d, *J* = 7.36 Hz, 2H), 7.29 (t, *J* = 7.56 Hz, 2H), 7.07 (t, *J* = 7.32 Hz, 1H), 6.35 (t, *J* = 2.92 Hz, 1H), 5.79-5.78 (m, 1H), 2.56-2.49 (m, 2H), 1.59 (t, *J* = 7.52 Hz, 2H), 1.32-1.28 (m, 4H), 0.87 (t, *J* = 6.8 Hz, 3H).

3-methyl-2,5-diphenyl-1H-pyrrole (20AN)[33]: Yield 142 mg, 61%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.00 (br, 1H), 7.71 (d, *J* = 7.48 Hz, 2H), 7.55 (d, *J* = 7.48 Hz, 2H), 7.42 (t, *J* = 7.48 Hz, 2H), 7.33 (t, *J* = 7.28 Hz, 2H), 7.23 (t,*J* = 7.44 Hz,1H), 7.14 (t, *J* = 6.96 Hz, 1H), 6.46 (br, 1H), 2.20 (s, 3H).

2-(4-chlorophenyl)-3-methyl-5-phenyl-1H-pyrrole (20AO): Yield 195 mg, 73%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.04 (br, 1H), 7.71 (d, *J* = 7.56 Hz, 2H), 7.58 (d, *J* = 8.32 Hz, 2H), 7.47 (d, *J* = 8.28 Hz, 2H), 7.34 (t, *J* = 7.48 Hz, 2H), 7.16 (t, *J* = 7.12 Hz, 1H), 6.46 (br, 1H), 2.20 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 132.22, 131.78, 131.73, 129.03, 128.89, 128.81, 128.23, 127.32, 126.33, 123.66, 118.59, 110.09, 12.56. HRMS (ESI) m/z: [M+ H] − Calcd for C17H15ClN 268.0893; Found 268.0883

2-(4-chlorophenyl)-5-isopropyl-3-methyl-1H-pyrrole (20BO)[34]: Yield 149 mg, 64%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.51 (br, 1H), 7.45-7.38 (q, *J* = 8.94 Hz, 4H), 5.68-5.67 (m, 1H), 2.88-2.81 (m, 1H), 2.13 (s,3H), 1.19 (d, J = 6.88 Hz,6H).

2-ethyl-5-phenyl-1H-pyrrole (20CA)[26]: Yield 116 mg, 68%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.88 (br, 1H), 7.57-7.55 (m, 2H), 7.30(t, *J* = 7.52 Hz, 2H), 7.08 (t, *J* = 7.32 Hz, 1H), 6.35 (t, *J* = 2.92 Hz, 1H), 5.81-5.79 (m, 1H), 2.61-2.55 (q, *J* = 7.56 Hz, 2H), 1.19 (t, J = 7.56 Hz, 3H).

2-(4-chlorophenyl)-5-ethyl-3-methyl-1H-pyrrole (20CO)[34]: Yield 156 mg, 71%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.59 (br, 1H), 7.44-7.38 (m, 4H), 5.68 (br, 1H), 2.66-2.48 (m, 2H), 2.13 (s, 3H), 1.16 (t, J = 7.48 Hz, 3H).

4-(5-ethyl-1H-pyrrol-2-yl) benzonitrile (20CP): Yield 102 mg, 52%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.20 (br, 1H), 7.72 (s, 4H), 6.63 (t, *J* = 3.04 Hz, 1H), 5.91-5.89 (m, 1H), 2.63-2.57 (q, *J* = 7.56 Hz, 2H), 1.23-1.18 (m, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 138-28, 137.07, 132.93, 129.02, 128.78, 126.87, 126.51, 123.24, 119.55, 109.38, 108.21, 107.65, 21.25, 13.70.

2-ethyl-4,5-dihydro-1H-benzo[g]indole (20CQ)[35]: Yield 134 mg, 68%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 10.79 (br, 1H), 7.33 (d, *J* = 7.32 Hz, 1H), 7.13-7.10 (m, 2H), 6.91 (t, *J* = 7.2 Hz, 1H), 5.66 (br,1H), 2.77 (d, *J* = 7.28 Hz, 2H), 2.59-2.49 (m, 4H), 1.19 (t,*J* = 7.52 Hz,3H).

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.28 (d, *J* = 7.16 Hz, 1H), 7.09 (t, *J* = 7.24 Hz, 2H), 6.90 (t, *J* = 5.88 Hz, 1H), 5.64 (br, 1H), 2.75 (t, *J* = 7.32 Hz, 2H), 2.56-2.50 (m, 3H), 1.17-1.13 (m, 3H).

2-phenyl-1H-pyrrole (20DA)[36]: Yield 106 mg, 74%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.24 (br, 1H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.52 Hz, 2H), 7.13 (t, *J* = 7.32 Hz, 1H), 6.83 (br, 1H), 6.49 (br, 1H), 6.106-6.10 (m, 1H).

2-(3-fluorophenyl)-1H-pyrrole(20DD)[36]: Yield 110 mg, 68%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 11.35 (br, 1H), 7.46-7.42 (m, 2H), 7.38-7.33 (m, 1H), 6.96-6.91 (m, 1H), 6.88-6.87 (m, 1H), 6.60-6.58 (m, 1H), 6.13-6.11 (m, 1H).

2-(3-methoxyphenyl)-1H-pyrrole(20DR)[37]: Yield 121 mg, 70%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 11.25 (br, 1H), 7.25-7.19 (m, 3H), 6.83 (br, 1H), 6.71 (d, *J* = 7.6 Hz, 1H), 7.50 (br, 1H), 6.09 (br, 1H), 3.78 (s, 3H).

3-methyl-2-phenyl-1H-pyrrole (20DN)[23]: Yield 109 mg, 69%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 10.87 (br, 1H), 7.45 (d, *J* = 7.64 Hz, 2H), 7.38 (t, *J* = 7.48 Hz, 2H), 7.17 (t, *J* = 7.24 Hz, 1H), 6.72-6.70 (m, 1H), 5.96-5.95 (m, 1H), 2.19 (s, 3H).

2-(4-chlorophenyl)-3-methyl-1H-pyrrole (20DO)[24]: Yield 136 mg, 71%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 10.96 (br, 1H), 7.47-7.41 (m, 4H), 6.74 (br, 1H), 5.96 (br, 1H), 2.18 (s, 3H).

2,6-diphenylpyridine (23AA)[38]: Yield 187 mg, 81%

^{1}H NMR (400 MHz, CDCl3): δ (ppm) = 8.15 (br, 3H), 7.82-7.79 (m, 1H), 7.71-7.68 (m,2H), 7.50-7.49 (m,3H), 7.43-7.41 (m,2H), 3.18-3.15 (m, 2H), 3.04-3.00 (m, 2H), 1.88 (br, 2H), 1.80 (br, 2H), 1.42 (br, 4H);

2-phenyl-6-(m-tolyl) pyridine (23AB)[38]: Yield 186 mg, 76%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.13-8.11 (m, 2H), 7.95 (br, 1H), 7.89 (d, *J* = 7.72 Hz, 2H), 7.79-7.76 (dd, J_1 = 2.52 Hz,J_2 = 10.28 Hz,2H), 7.49 (t, *J* = 7.08 Hz, 2H), 7.43 (d, *J* = 7.24 Hz, 1H), 7.37 (t,*J* = 7.64 Hz, 1H), 7.25 (d, *J* = 7.44 Hz, 1H), 2.44 (s, 3H).

2-(2-fluorophenyl)-6-phenylpyridine (23AC)[39]: Yield 181 mg, 72%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.10-8.06 (m, 3H), 7.92 (t, *J*= 7.76 Hz, 1H), 7.83 (d, *J* = 7.32 Hz, 1H), 7.75-7.73 (m, 1H), 7.50-7.40 (m, 4H), 7.34-7.30 (m, 1H), 7.25-7.20(m, 1H).

^{1}H NMR (400 MHz, DMSO): δ (ppm) = 8.18 (d, *J* = 7.2 Hz, 2H), 8.10 (t, *J* = 6.6 Hz, 1H), 8.02-7.99 (m, 2H), 7.77-7.76 (m, 1H), 7.54-7.45 (m, 4H), 7.40-7034 (m, 2H).

2-(2-methoxyphenyl)-6-phenylpyridine (23AD)[38]: Yield 191 mg, 73%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.14 (d, *J* = 7.24 Hz, 2H), 7.92-7.89 (m, 3H), 7.83-7.80 (dd, J_1 = 2.22 Hz, J_2 = 6.24 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.46-7.41 (m,2H), 7.18 (t, *J* = 8.2 Hz, 1H), 7.10 (d,*J* = 7.44 Hz, 1H), 3.86 (s, 3H).

2-(4-(1H-imidazol-1-yl) phenyl)-6-phenylpyridine (23AE): Yield 244 mg, 82%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.36 (d, *J* = 8.68 Hz, 2H), 8.25 (br, 1H), 7.8.18 (d, *J* = 7.2 Hz, 2H), 7.96 (t, *J* = 7.76 Hz, 1H), 7.89-7.85 (m,2H), 7.73 (d, *J* = 8.6 Hz, 2H), 7.68 (br, 1H), 7.52 (t,*J* = 7.04 Hz, 2H), 7.47-7.45 (m, 1H), 7.20 (s, 1H);^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 157.02, 155.21, 139.15, 138.72, 137.65, 137.53, 135.43, 130.15, 129.13, 128.71, 128.44, 126.91, 121.39, 119.04, 118.42, 118.15. HRMS (ESI) m/z: [M+ H] − Calcd for C20H16N3 298.1344; Found 298.1337

3-methyl-2,6-diphenylpyridine (23AF)[40]: Yield 179 mg, 73%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.10 (d,*J* = 7.28 Hz,2H), 7.87 (d, *J* = 8.00 Hz, 1H), 7.81 (d, *J* = 8.00 Hz, 1H), 7.64 (d, *J* = 7.08 Hz, 2H), 7.53-7.39 (m,6H), 2.36 (s, 3H).

3-ethyl-2,6-diphenylpyridine (23AG)[41]: Yield 184 mg, 71%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.95 (d, *J* = 7.04 Hz, 2H), 7.82 (d, *J* = 7.96 Hz, 1H), 7.75 (d, *J* = 8.08 Hz, 1H), 7.52-7.36 (m,8H), 2.71-2.66 (m, 2H), 1.14 (t,*J* = 7.6 Hz,3H).

2-(4-chlorophenyl)-3-methyl-6-phenylpyridine (23AH)[38]: Yield 232 mg, 83%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.00 (d, *J* = 7.08 Hz, 2H), 7.80 (d, *J* = 8.04 Hz, 1H), 7.75 (d, *J* = 8.00 Hz, 1H), 7.61 (t, *J* = 8.48 Hz, 2H), 7.51 (d, *J* = 8.52 Hz, 2H), 7.49 (t,*J* = 7.6 Hz, 2H), 7.42-7.40 (m, 1H), 2.38 (s, 3H).

2-phenyl-5,6-dihydrobenzo[h]quinoline (23AI)[42]: Yield 175 mg, 68%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.43-8.41(m, 1H), 8.16-8.13 (m, 2H), 7.70 (q, *J* = 7.05 Hz, 2H), 7.50 (t, *J* = 7.16 Hz, 2H), 7.42 (d, *J* = 7.24 Hz, 1H), 7.40-7.38 (m, 1H), 7.36-7.25 (m, 2H), 2.99 (s, 4H).

2-phenyl-5,6-dihydro-1,10-phenanthroline (23AJ)[43]: Yield 191 mg, 74%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.59-8.58 (m, 1H), 8.22 (d, *J* = 7.36 Hz, 2H), 7.83 (d, *J* = 7.96 Hz,1H), 7.78 (d, *J* = 7.96 Hz, 2H), 7.48 (t, *J* = 7.16 Hz, 2H), 7.43-7.37 (m, 2H), 3.05 (s, 4H).

2-phenyl-5,6-dihydro-1,10-phenanthroline(23AK)[44]: Yield 136 mg, 65%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 7.48 (d,*J* = 9.16 Hz,2H), 7.52 (q, *J* = 8.09 Hz, 2H), 7.46-7.38 (m,3H), 2.94 (t, *J* = 6.12 Hz, 2H), 2.82 (t, *J* = 6.28 Hz, 2H), 1.96-1.91 (m, 2H), 1.87-1.83 (m, 2H).

2-(o-tolyl) pyridine(23BL)[45]: Yield 122 mg, 72%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.58-8.57 (m, 1H), 7.93-7.89 (m, 1H), 7.48 (d, *J* = 7.84 Hz, 1H), 7.41-7.38 (m,1H), 7.32-7.27 (m, 4H), 2.26 (s, 3H).

2-(3-methoxyphenyl) pyridine (23BM)[46]: Yield 130 mg, 70%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.59-8.58 (m, 1H), 7.88 (t, *J* = 7.4 Hz, 1H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.49-7.46 (m,2H), 7.40-7.34 (m, 2H), 7.00 (d,*J* = 7.04 Hz,1H), 3.86 (s, 3H).

2-(4-bromophenyl) pyridine (23BN)[47]: Yield 158 mg, 68%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.60 (br, 1H), 7.88-7.86 (m, 4H), 7.64 (d, *J* = 8.00 Hz, 2H), 7.37 (br, 1H).

2-(4-(trifluoromethyl) phenyl) pyridine(23BO)[45]: Yield 167 mg, 75%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.66-8.65 (m, 1H), 8.15 (d, *J* = 8.16 Hz, 2H), 7.94-7.93 (m, 2H), 7.78 (d, *J* = 8.24 Hz, 2H), 7.43-7.40 (m, 1H).

2-(naphthalen-1-yl) pyridine (23BP)[48]: Yield 146 mg, 71%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.68-8.67 (m, 1H), 8.02-8.00 (dd, J_1 = 1.76 Hz,J_2= 9.48 Hz, 1H), 7.98-7.94 (m, 2H), 7.85 (d, *J* = 8.36 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 7.04 Hz, 1H), 7.56-7.51 (m, 1H), 7.50-7.46 (m, 3H).

3-butyl-2-phenylpyridine (23BQ): Yield 163 mg, 77%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.38-8.37 (m, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.49-7.25 (m, 6H), 2.62 (t, *J* = 7.8 Hz, 2H), 1.48-1.41 (m, 2H), 1.33-1.11 (m, 2H), 0.86-0.71 (m, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 158.81, 146.69, 140.69, 137.24, 135.63, 128.79, 128.18, 128.07, 127.72, 122.13, 33.04, 31.98, 22.35, 13.73. HRMS (ESI) m/z: [M+ H] − Calcd for C15H18N 212.1439; Found 212.1441

3-pentyl-2-phenylpyridine (23BR): Yield 167 mg, 74%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 8.38-8.37 (m, 1H), 7.78 (d, *J* = 7.48 Hz, 1H), 7.49-7.33 (m, 6H), 2.62 (t, *J* = 7.72 Hz, 2H), 1.49-1.44 (m, 2H), 1.28-1.17 (m, 4H), 0.79 (t, J = 5.88 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 158.79, 146.67, 140.67, 137.24, 135.67, 128.77, 128.06, 127.72, 122.13, 32.25, 31.44, 30.52, 29.65, 22.24, 13.85. HRMS (ESI) m/z: [M+ H] − Calcd for C16H20N 226.1596; Found 226.1595.

4. Characterization data of Natural product:

2-pentyl-1,2,3,4-tetrahydroquinoline (7A28-H)[1]: Yield 152 mg, 75%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 6.82-6.79 (m, 2H), 6.46 (d, *J* = 7.92 Hz, 1H), 6.37 (t, *J* = 7.28 Hz, 1H), 5.44 (br, 1H), 3.13 (br, 1H), 2.72-2.56 (m, 2H), 1.89-1.84 (m, 1H), 1.47-1.31 (m, 5H), 1.28-1.17 (m, 4H), 0.89-0.79 (m,3H).

^{1}H NMR (400 MHz, DMSO-d6, D_2O exchange): δ (ppm) = 6.81-6.78 (m, 2H), 6.44 (d, *J* = 8.28 Hz, 1H), 6.38 (t, *J* = 7.16 Hz, 1H), 3.15-3.05 (m, 1H), 2.64-2.58 (m, 2H), 1.85-1.81 (m, 1H), 1.44-1.38 (m, 5H), 1.29-1.19 (m, 4H), 0.85-0.82 (m, 3H).

1-methyl-2-pentyl-1,2,3,4-tetrahydroquinoline (7A28-Me)[1]: Yield 199 mg, 92%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 6.96 (t, *J* = 7.68 Hz, 1H), 6.87 (d, *J* = 7.2 Hz, 1H), 6.49-6.47 (m, 2H), 3.23-3.22 (m, 1H), 2.89 (br, 3H), 2.80-2.72 (m, 1H), 2.62-2.58 (m, 1H), 1.91-1.79 (m, 2H), 1.58-1.55 (m, 1H), 1.38-1.31(m, 7H), 0.90-.85 (m, 3H).

Chiral HPLC data: Column:I CELLULOSE J, Co Solvent 0.5% IPamine_MeOH; Proc. Chnl. Descr.: PDA Spectrum PDA 254.0 nm, temperature 25°C, Run time 10 min, Rt for peak1 = 2.741 min (area% 49.65) and for peak2 = 2.898 min (area% 50.35).

2-(3,4-dimethoxyphenethyl)-1,2,3,4-tetrahydroquinoline (7A20-H)[1]: Yield 237 mg,80%

^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 6.85-6.80 (m, 4H), 6.75-6.72 (dd, J_1= 1.84 Hz,J_2 = 8.08 Hz, 1H), 6.49 (t, *J* = 7.76 Hz, 1H), 6.39(t,*J* = 7.32 Hz, 1H), 5.55 (br, 1H), 3.73 (s, 3H), 3.69 (s, 3H), 3.16-3.15 (m, 1H), 2.68-2.61 (m, 4H), 1.89-1.88 (m, 1H), 1.75-1.67 (m, 2H), 1.50-1.23(m, 1H).

^{1}H NMR (400 MHz, DMSO-d6, D_2O exchange): δ (ppm) 6.84-6.80 (m, 4H), 6.74-6.71 (m, 1H), 6.48 (t, *J* = 7.56 Hz, 1H), 6.41-6.37 (m, 1H), 3.71 (s, 3H), 3.68 (s, 3H), 3.14-3.11 (m, 1H), 2.66-2.58 (m, 4H), 1.90-1.86 (m, 1H), 1.73-1.63 (m, 2H), 1.50-1.48(m, 1H).

2-(3,4-dimethoxyphenethyl)-1-methyl-1,2,3,4-tetrahydroquinoline (7A20-Me)[121]: Yield 289 mg,93%

^{1}H NMR (400 MHz, MeOD): δ (ppm) = 6.97 (t, *J* = 7.48 Hz, 1H), 6.89 (d, *J* = 7.36 Hz, 1H), 6.84 (d, *J* = 8.16 Hz, 1H), 6.80-6.79 (m, 1H), 6.74-6.72 (m, 1H), 6.51-6.48 (, 2H), 3.79-3.78(m, 6H), 3.29-3.23 (m, 1H), 2.87 (s, 3H), 2.83-2.79 (m, 1H), 2.78-2.60 (m, 2H), 2.55-2.50 (m, 1H), 2.01-1.98 (m, 1H), 1.97-1.84(m, 2H), 1.70-1.66 (m, 1H).

Chiral HPLC data: Column: CHIRALCEL OD-H (250X4.6) mm,5µ, M.P.- Hexane/EtOH/IPAmine: 80/20/0.1; PDA Multi 1 254nm,4nm, Flow Rate - 1.0 ml/min, temperature 25°C, Run time 14 min, Rt for peak1 = 6.082 min (area% 50.112) and for peak2 = 6.824 min (area% 49.888).

5. Characterization data of Control experiment:

2-amino-4-bromobenzaldehyde (10C): ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 9.80 (s, 1H), 7.31(d, *J* = 8.24 Hz, 1H), 6.87-6.83 (m, 2H), 6.16 (br, 2H).

1-phenylpent-4-en-1-one (10G): ^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.97 (d,*J* = 7.16 Hz, 2H), 7.65-7.61 (m, 1H), 7.52 (t, *J* = 7.8 Hz, 2H), 5.92-5.82 (m, 1H), 5.09-5.04 (m, 1H), 4.98-4.95 (m, 1H), 3.13 (t,*J* = 7.24 Hz, 2H), 2.39-2.34 (m, 2H).

1-phenylpentan-1-one (10H): ^{1}H NMR (400 MHz, DMSO-d6): δ (ppm) = 7.96 (d, *J* = 7.56 Hz, 2H), 7.62 (t, *J* = 7.36 Hz, 1H), 7.51 (t, *J* = 7.64 Hz, 2H), 3.01 (t, *J* = 7.24Hz, 2H), 1.62-1.55 (m, 2H), 1.38-1.29 (m, 2H), 0.900 (t,*J* = 7.32 Hz,3H); GCMS calculated m/z = 162.10, observed m/z = 162.2

#. *Characterization data of ligands (3a-3c):*

All the reaction was carried out according to the general procedure (1.A.)

N-(naphthalen-1-yl) picolinamide(3a)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 10.75 (s, 1H), 8.71 (d, *J* = 4.6 Hz, 1H), 8.40-8.35 (m, 2H), 8.1 (d, *J* = 8.1 Hz, 1H), 7.95 (t, *J* = 6.2 Hz, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.60-7.52 (m, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) =162.1, 149.9, 148, 137.6, 134, 132.3, 128.7, 126.4, 126.2, 126.1, 125.9, 124.9, 122.3, 120.3, 118.4.

N-(naphthalen-2-yl) picolinamide (3b)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 10.2 (s, 1H), 8.64 (d, *J* = 7.5 Hz, 1H), 8.5 (s, 1H), 8.33 (d, *J* = 7.7 Hz, 1H), 7.94 (t, *J* = 6.4 Hz, 1H), 7.86 (d, *J* = 5.2 Hz, 2H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 6.9 Hz, 1H), 7.51-7.45 (m, 2H), 7.43-7.39 (m, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) =162, 149.7, 147.9, 137.6, 135.1, 133.9, 130.6, 128.7, 127.6, 127.5, 126.44, 126.41, 124.9, 122.3, 119.7, 116.3.

N-(2,5-dimethylphenyl)picolinamide (3c)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 10.03 (s, 1H), 8.61 (d, *J* = 4.4 Hz, 1H), 8.29 (d, *J* = 7.7 Hz, 1H), 8.11 (s, 1H), 7.9 (t, *J* = 7.7 Hz, 1H), 7.48-7.45 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 7.4 Hz, 1H), 2.36 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):δ (ppm) = 161.6, 150, 147.9, 137.4, 136.4, 135.5, 130, 126.2, 125.1, 124.7, 122.1, 121.7, 21.1, 17.1.

Characterization data of Ir(III) complexes (4a-Ir-4c-Ir):

All the reaction was carried out according to the general procedure (1.B.)

[*N*-(naphthalen-1-yl) picolinamide] Cp*Ir(III) chloride (4a-Ir)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.61 (d, *J* = 5.2 Hz, 1H), 8.21 (d, *J* = 7.5 Hz, 1H), 7.96-7.92 (m, 2H), 7.85-7.84 (m, 2H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.52-7.40 (m, 4H), 1.29 (s, 15H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 168.8, 155.1, 149.6, 146, 138.5, 133.6, 130.2, 128.2, 127.5, 127.4, 127.2, 126.6, 126.4, 126.1, 125.8, 125.2, 125.1, 125, 124.1, 122.4, 87.8, 86.7, 86.4, 84.6, 8.7, 8.6, 8.5, 8.

[*N*-(naphthalen-2-yl) picolinamide] Cp*Ir(III) chloride (4b-Ir)

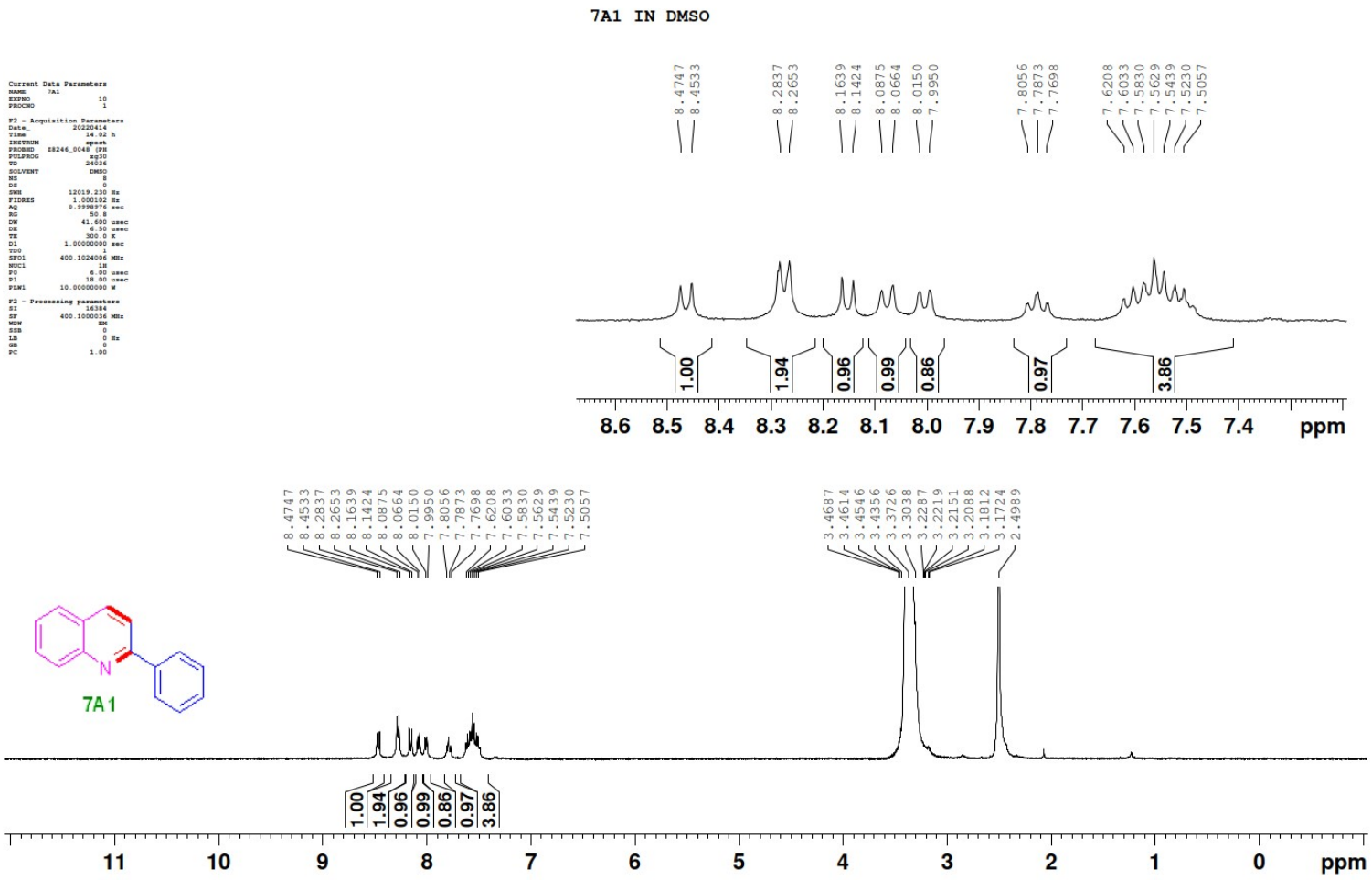
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.62 (d, *J* = 5.2 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 813 (s, 1H), 7.96 (t, *J* = 7.1 Hz, 1H), 7.90-7.87 (m, 1H), 7.84-7.78 (m, 3H), 7.52 (t, *J* = 6.9 Hz, 1H), 7.44-7.37 (m, 2H), 1.40 (s, 15H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 168.7, 155.7, 149.7, 145.9, 138.7, 133.8, 131.1, 127.7, 127.5, 127.1, 126.4, 125.6, 124.6, 123.9, 86.7, 8.5.

[*N*-(2, 5-dimethylphenyl)picolinamide] Cp*Ir(III) chloride (4c-Ir)

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.57 (d, *J* = 5.2 Hz, 1H), 8.17 (d, *J* = 7.7 Hz, 1H), 8.90 (t, *J* = 6.9 Hz, 1H), 7.49 (s, 1H), 7.46 (t, *J* = 6.7 Hz, 1H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 8.1 Hz, 1H), 2.25-2.21(m, 6H), 1.41 (s, 15H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = 167.5, 155.4, 149.1, 146.6, 138.3, 135.3, 131.4, 129, 127, 126.6, 126.5, 125.5, 86.7, 29.5, 29.2, 20.8, 18.5, 8.45, 8.15.

6. Copies of 1H NMR of ^{1}H NMR, ^{13}C NMR Spectra

7A1 IN DMSO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EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220414
Time 14.02 h
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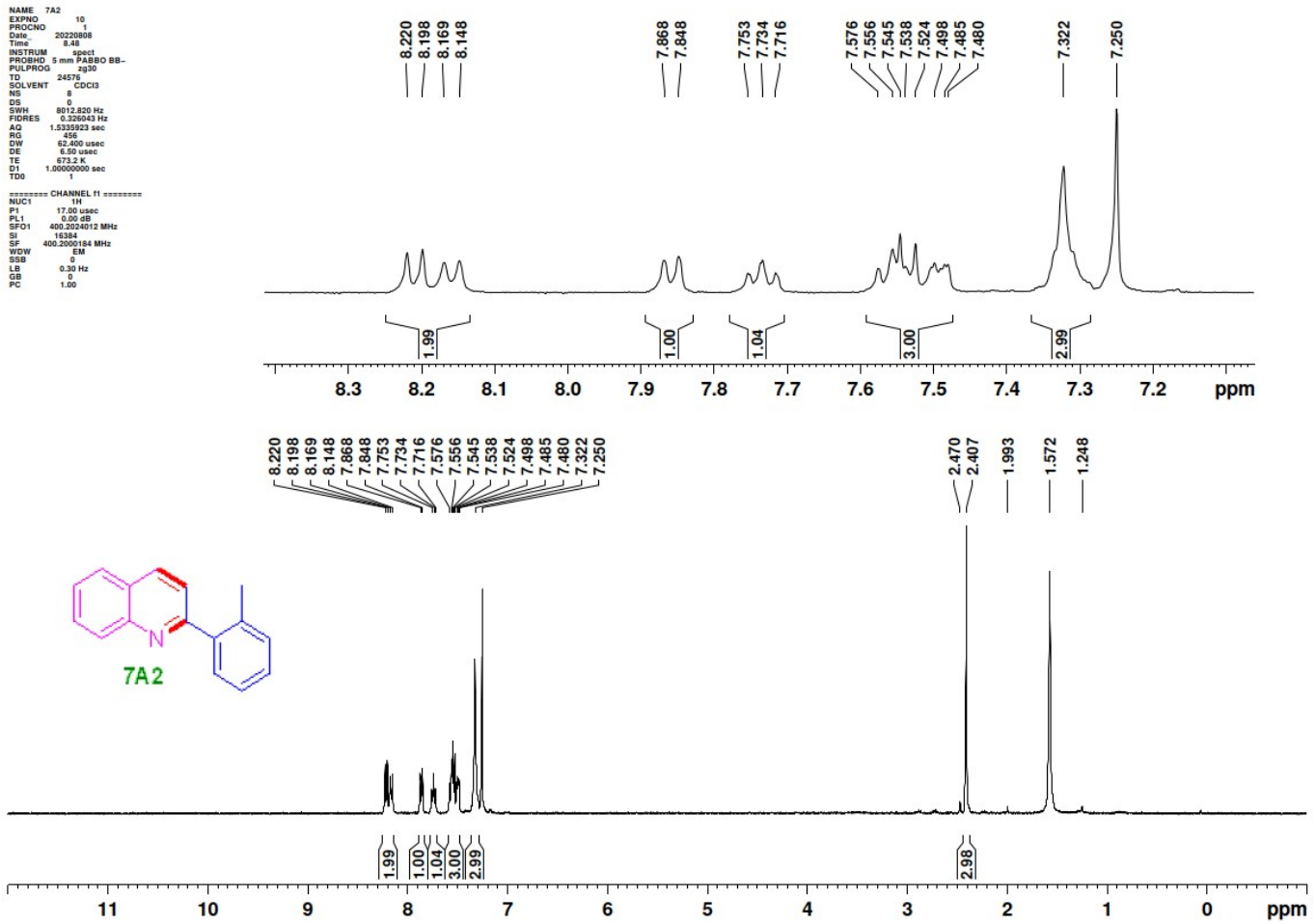
PROBHD Z8246_0048 (PR
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 1.000102 Hz
AQ 0.9998976 sec
RG 50.8
DW 41.600 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1024006 MHz
NUC1 1H
P0 6.00 usec
P1 18.00 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 16384
SF 400.1000036 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
8.4747
8.4533
8.2837
8.2653
8.1639
8.1424
8.0875
8.0664
8.0150
7.9950
7.8056
7.7873
7.7698
7.6208
7.6033
7.5830
7.5629
7.5439
7.5230
7.5057
1.00
1.94
0.96
0.99
0.86
0.97
3.86
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
3.4687
3.4614
3.4546
3.4356
3.3726
3.3038
3.2287
3.2219
3.2151
3.2088
3.1812
3.1724
2.4989
N
7A1
11 10 9 8 7 6 5 4 3 2 1 0 ppm

7A2 IN CDCl3


NAME 7A2
EXPNO 10
PROCNO 1
Date_ 20220808
Time 8.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 24576
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.326043 Hz
AQ 1.5335923 sec
RG 456
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024012 MHz
SI 16384
SF 400.2000184 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.220
8.198
8.169
8.148
7.868
7.848
7.753
7.734
7.716
7.576
7.556
7.545
7.538
7.524
7.498
7.485
7.480
7.322
7.250
1.99
1.00
1.04
3.00
2.99
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
2.470
2.407
1.993
1.572
1.248
2.98
11
10
9
8
7
6
5
4
3
2
1
0
ppm
N
7A2

7A3 IN CDCl3

```
Current Data Parameters
NAME        7A3
EXPNO            10
PROCNO            1

F2 - Acquisition Parameters
Date_      20220603
Time           17.56 h
INSTRUM         spect
PROBHD   Z8246_0048 (PH
PULPROG         zg30
TD             24576
SOLVENT         CDCl3
NS                 8
DS                 0
SWH         8012.820 Hz
FIDRES      0.652085 Hz
AQ          1.5335424 sec
RG               203
DW            62.400 usec
DE             6.50 usec
TE            300.0 K
D1          1.00000000 sec
TD0                1
SFO1      400.1024006 MHz
NUC1              1H
P0             6.00 usec
P1            18.00 usec
PLW1       10.00000000 W

F2 - Processing parameters
SI             16384
SF        400.1000139 MHz
WDW               EM
SSB                0
LB                 0 Hz
GB                 0
PC              1.00
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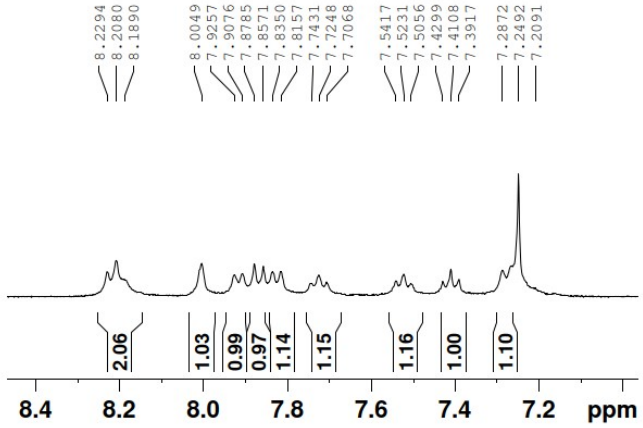
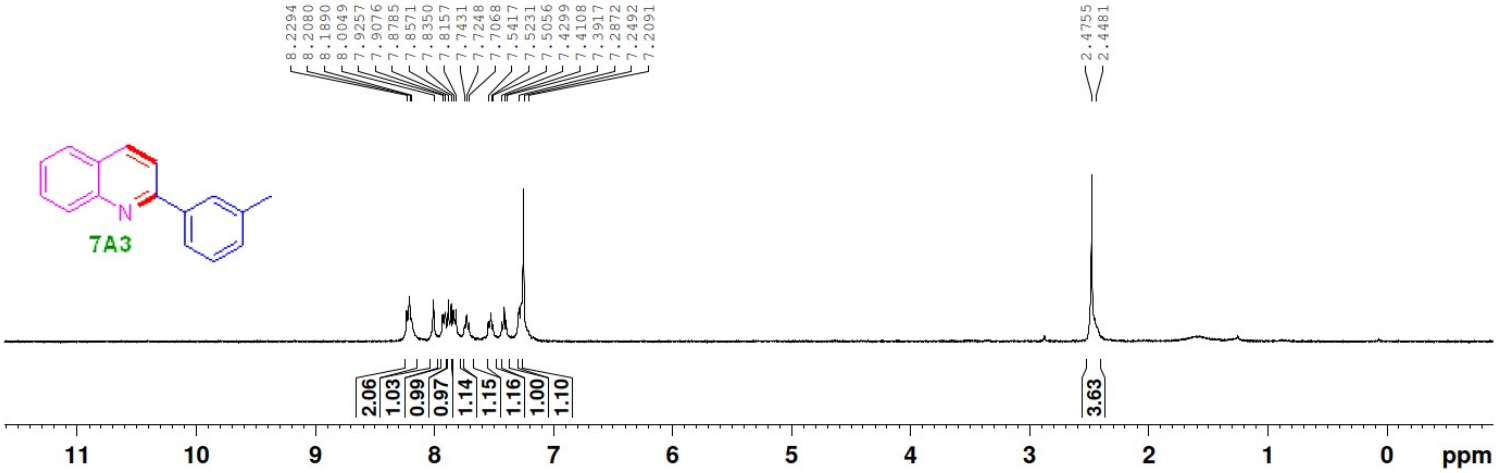
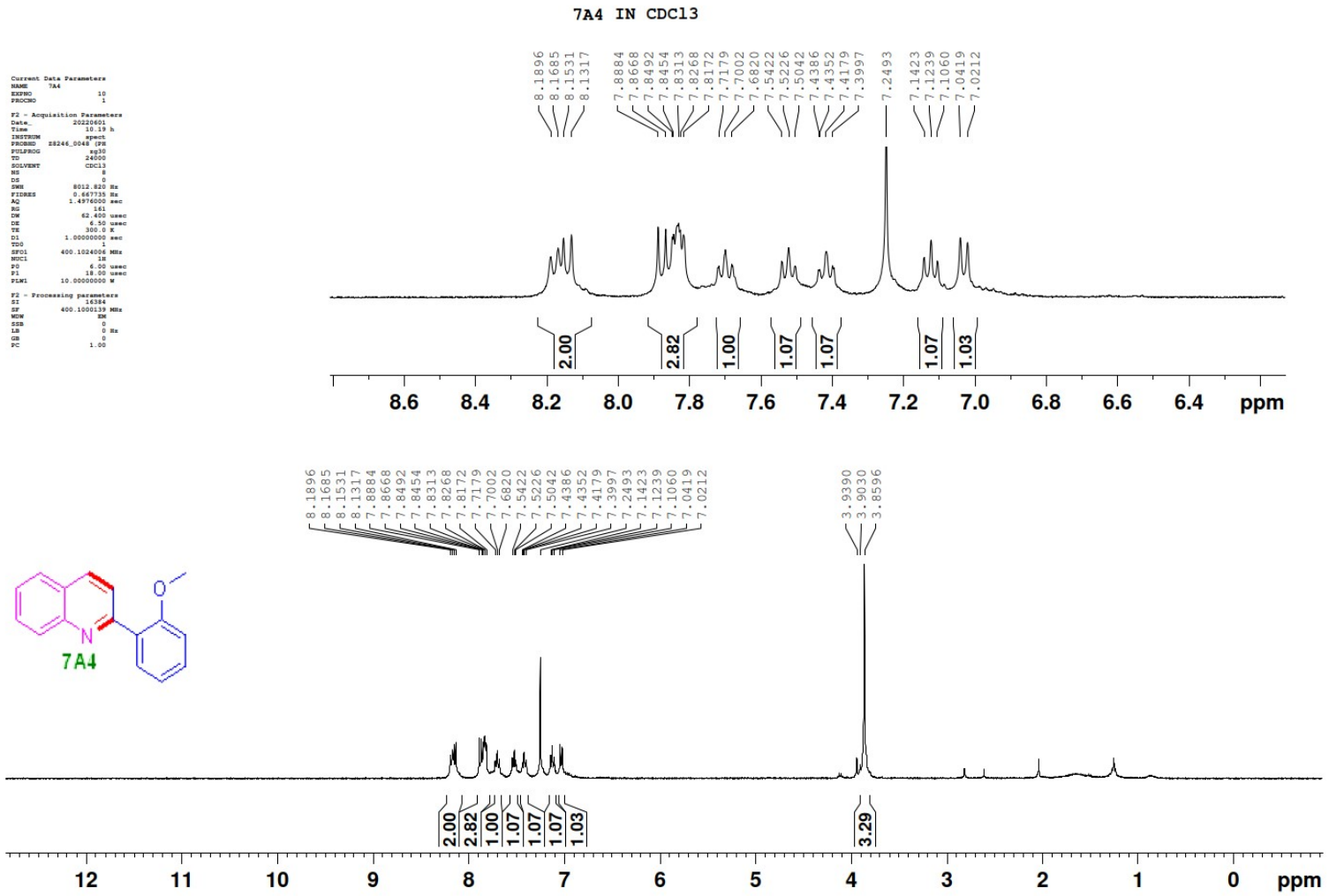
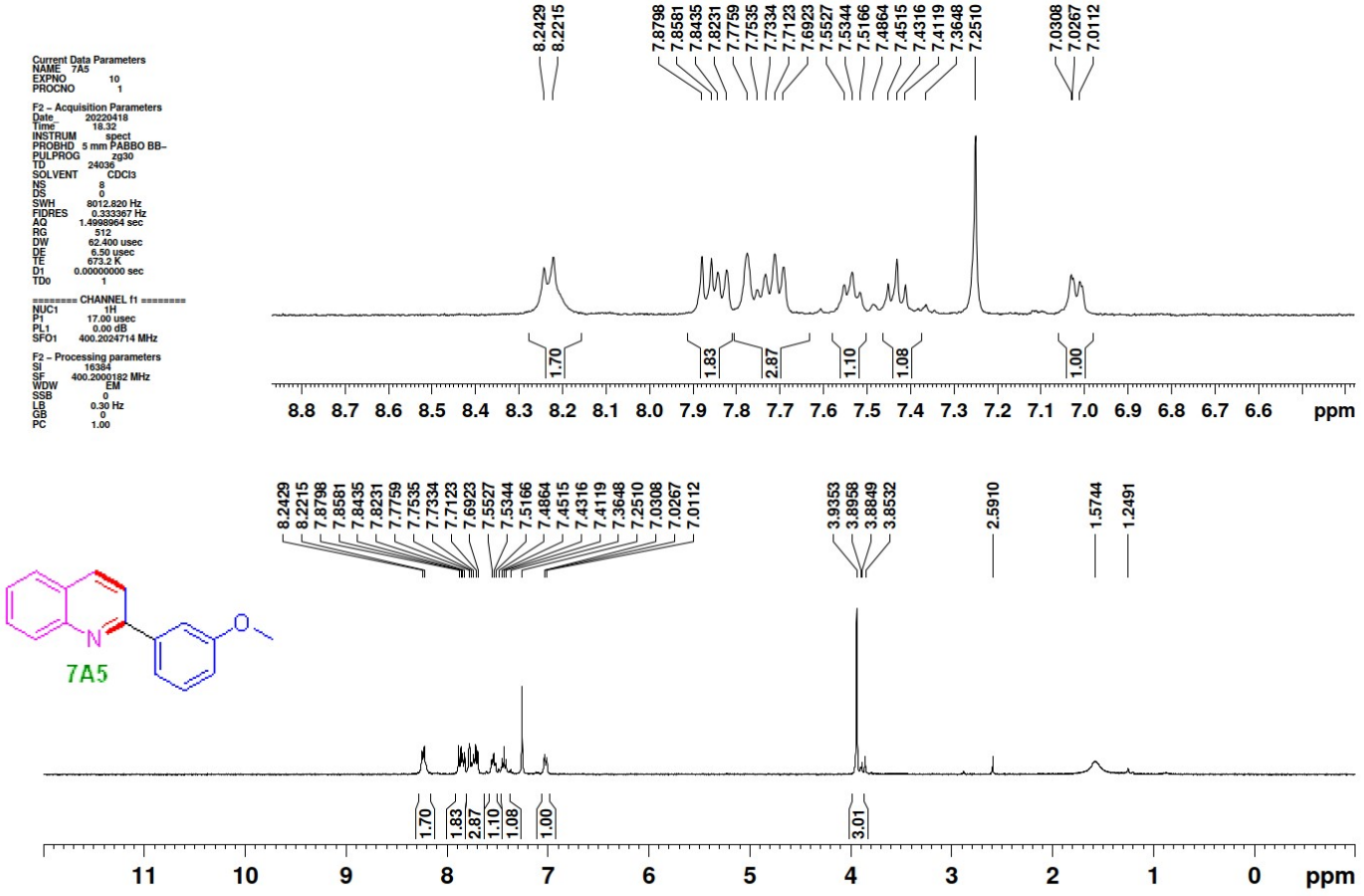





7A4 IN CDCl3
Current Data Parameters
NAME 7A4
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220601
Time 10.19 h
INSTRUM spect
PROBHD Z8246_0048 (PR
PULPROG zg30
TD 24000
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.667735 Hz
AQ 1.4976000 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1024006 MHz
NUC1 1H
P0 6.00 usec
P1 18.00 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 16384
SF 400.1000139 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
8.1896
8.1685
8.1531
8.1317
7.8884
7.8668
7.8492
7.8454
7.8313
7.8268
7.8172
7.7179
7.7002
7.6820
7.5422
7.5226
7.5042
7.4386
7.4352
7.4179
7.3997
7.2493
7.1423
7.1239
7.1060
7.0419
7.0212
2.00
2.82
1.00
1.07
1.07
1.07
1.03
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
ppm
3.9390
3.9030
3.8596
3.29
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
O
N
7A4

7A5 IN CDCl3

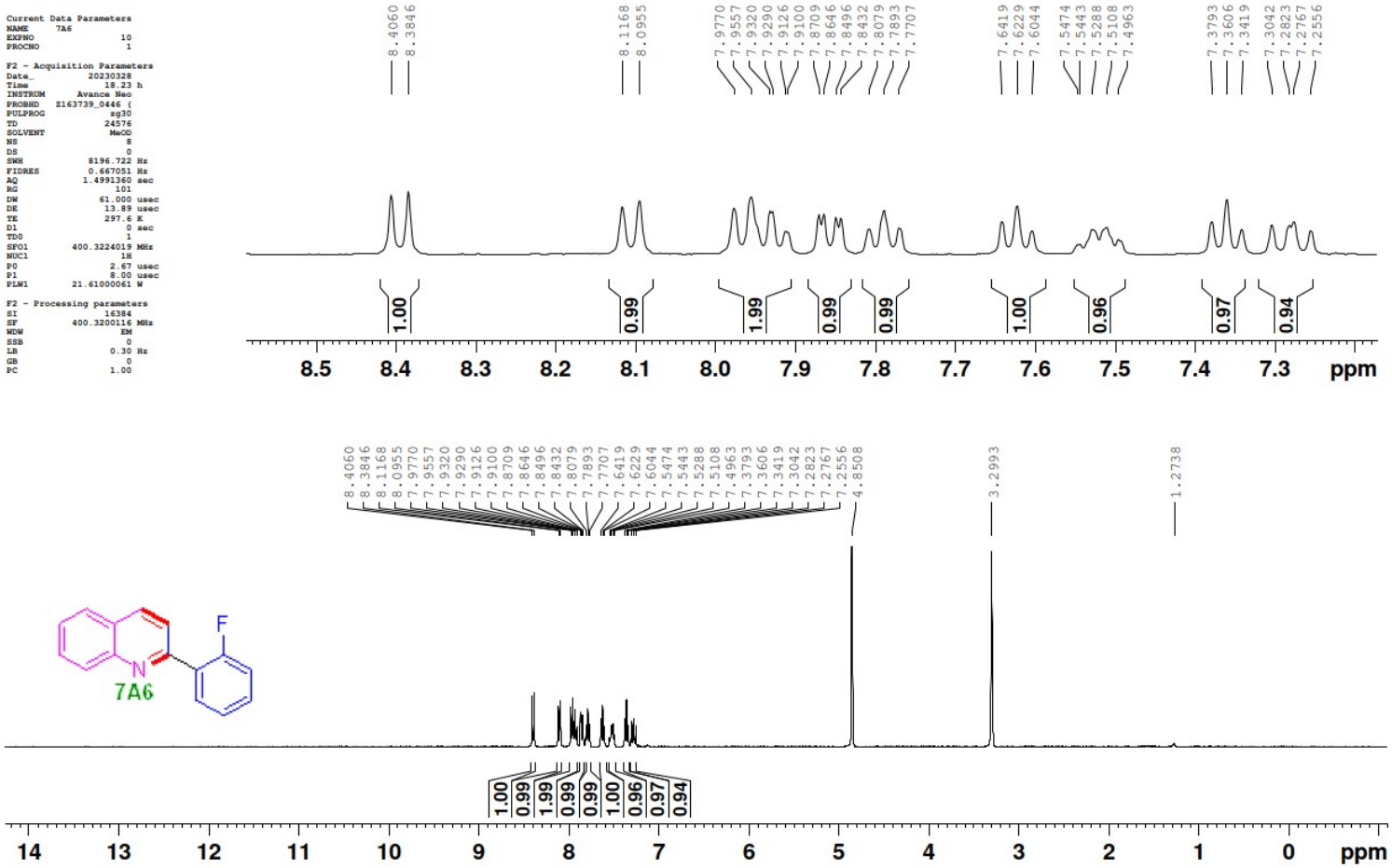

Current Data Parameters
NAME 7A5
EXPNO 10
PROCNO 1
F2 – Acquisition Parameters
Date 20220418
Time 18.32
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.333367 Hz
AQ 1.4998964 sec
RG 512
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 0.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024714 MHz
F2 – Processing parameters
SI 16384
SF 400.2000182 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.2429
8.2215
7.8798
7.8581
7.8435
7.8231
7.7759
7.7535
7.7334
7.7123
7.6923
7.5527
7.5344
7.5166
7.4864
7.4515
7.4316
7.4119
7.3648
7.2510
7.0308
7.0267
7.0112
1.70
1.83
2.87
1.10
1.08
1.00
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
3.9353
3.8958
3.8849
3.8532
2.5910
1.5744
1.2491
3.01
11 10 9 8 7 6 5 4 3 2 1 0 ppm
N
O
7A5

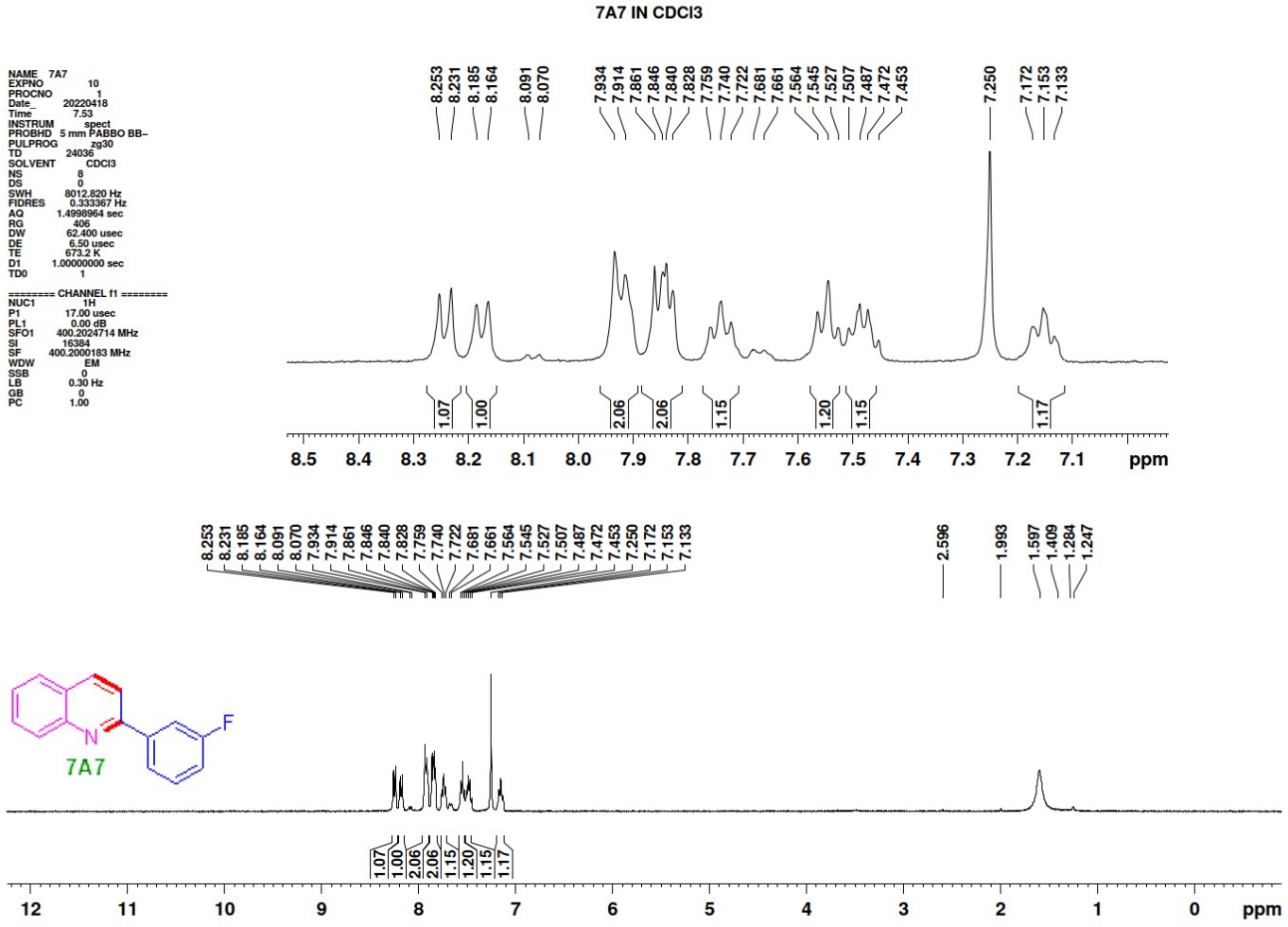
7A6 IN MeOD

```
Current Data Parameters
NAME          7A6
EXPNO          10
PROCNO         1

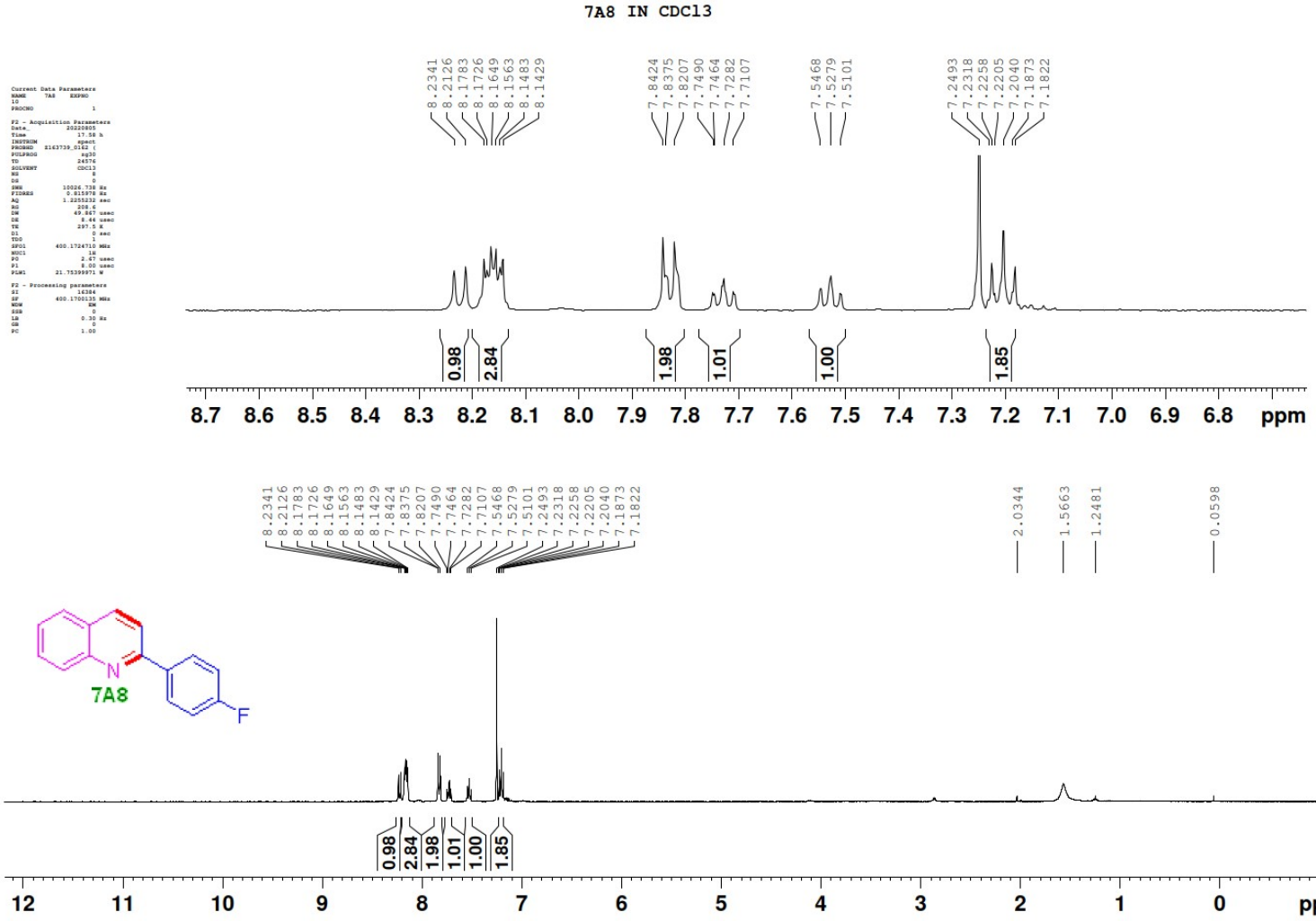
F2 - Acquisition Parameters
Date_          20230328
Time           18.23 h
INSTRUM        Avance Neo
PROBHD    Z163739_0446 (
PULPROG        zg30
TD             24576
SOLVENT        MeOD
NS             8
DS             0
SWH            8196.722 Hz
FIDRES         0.667051 Hz
AQ             1.4991360 sec
RG             101
DW             61.000 usec
DE             13.89 usec
TE             297.6 K
D1             0 sec
TD0            1
SFO1           400.3224019 MHz
NUC1           1H
P0             2.67 usec
P1             8.00 usec
PLW1           21.61000061 W

F2 - Processing parameters
SI             16384
SF             400.3200116 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
```




7A7 IN CDCl3
NAME 7A7
EXPNO 10
PROCNO 1
Date_ 20220418
Time 7.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.333367 Hz
AQ 1.4998964 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024714 MHz
SI 16384
SF 400.2000183 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.253
8.231
8.185
8.164
8.091
8.070
7.934
7.914
7.861
7.846
7.840
7.828
7.759
7.740
7.722
7.681
7.661
7.564
7.545
7.527
7.507
7.487
7.472
7.453
7.250
7.172
7.153
7.133
1.07
1.00
2.06
2.06
1.15
1.20
1.15
1.17
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
2.596
1.993
1.597
1.409
1.284
1.247
N
F
7A7
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

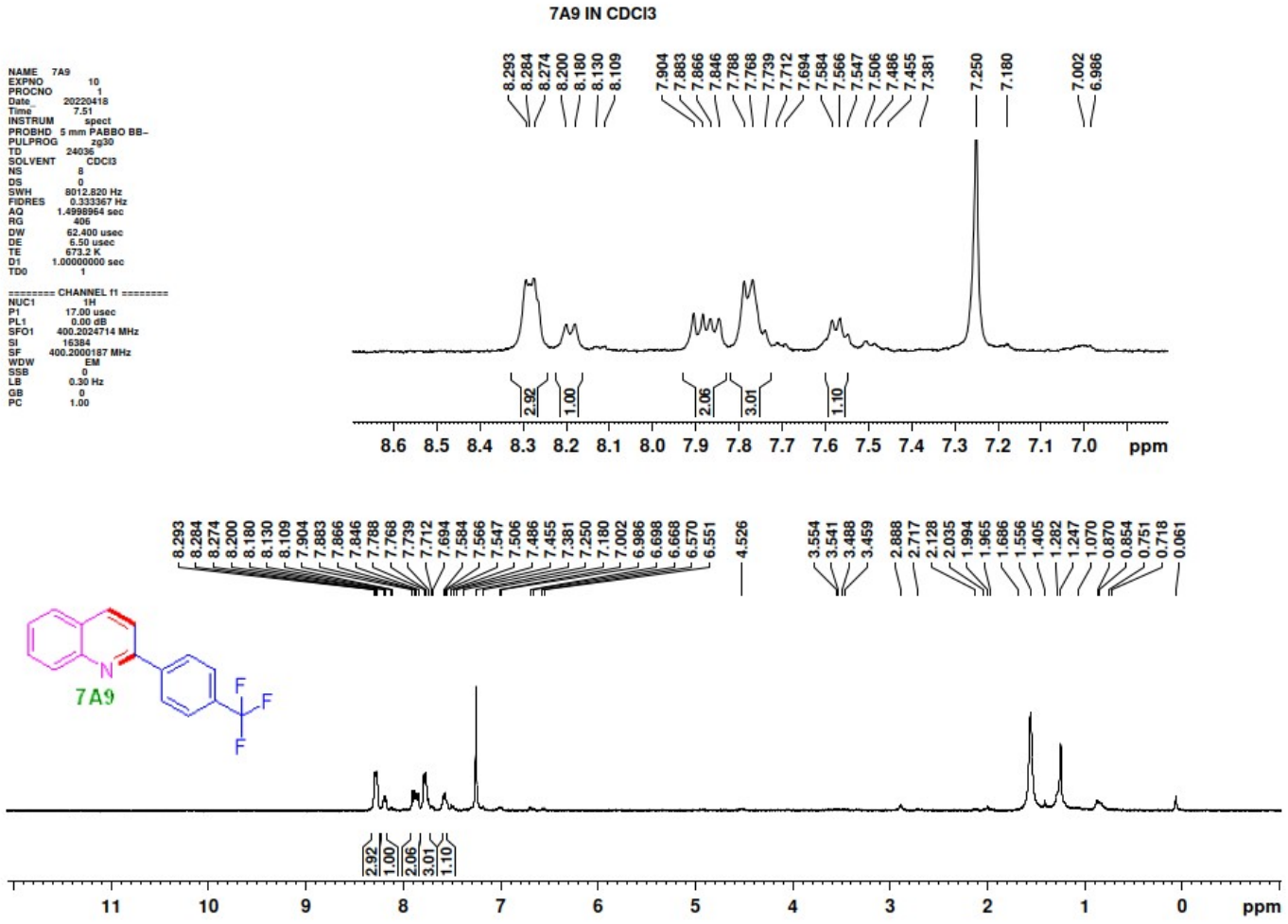
7A8 IN CDCl3




```
Current Data Parameters
NAME       7A8     EXPNO
10
PROCNO                1

F2 - Acquisition Parameters
Date_           20220805
Time               17.56 h
INSTRUM              spect
PROBHD    2163739.0162 (
PULPROG              zg30
TD                  24576
SOLVENT             CDCl3
NS                      8
DS                      0
SWH             10026.736 Hz
FIDRES          0.815978 Hz
AQ              1.2255232 sec
RG                  208.6
DW                 49.847 usec
DE                  6.44 usec
TE                297.5 K
D1                      0 sec
TD0                     1
SFO1         400.1724710 MHz
NUC1                   1H
P0                  2.47 usec
P1                  8.00 usec
PLW1        21.75399971 W

F2 - Processing parameters
SI                  16384
SF           400.1700135 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```


7A9 IN CDCl3
NAME 7A9
EXPNO 10
PROCNO 1
Date 20220418
Time 7.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.333367 Hz
AQ 1.4998964 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024714 MHz
SI 16384
SF 400.2000187 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.293
8.284
8.274
8.200
8.180
8.130
8.109
7.904
7.883
7.866
7.846
7.788
7.768
7.739
7.712
7.694
7.584
7.566
7.547
7.506
7.486
7.455
7.381
7.250
7.180
7.002
6.986
2.92
1.00
2.06
3.01
1.10
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
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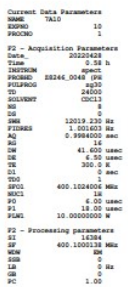
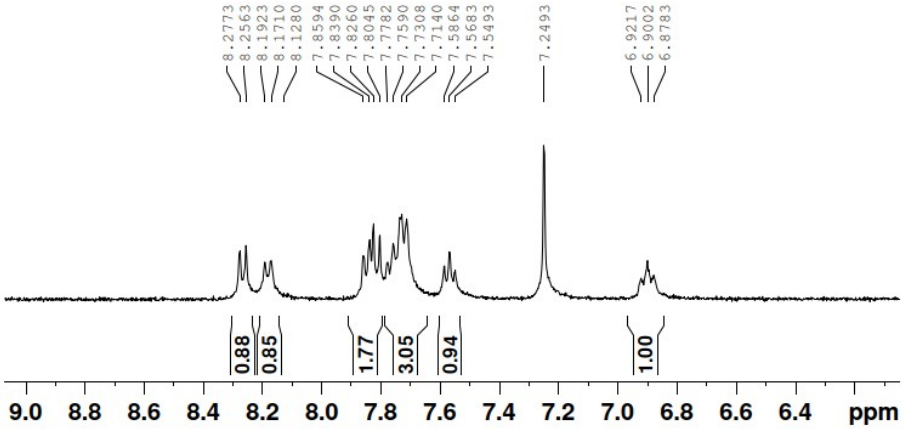
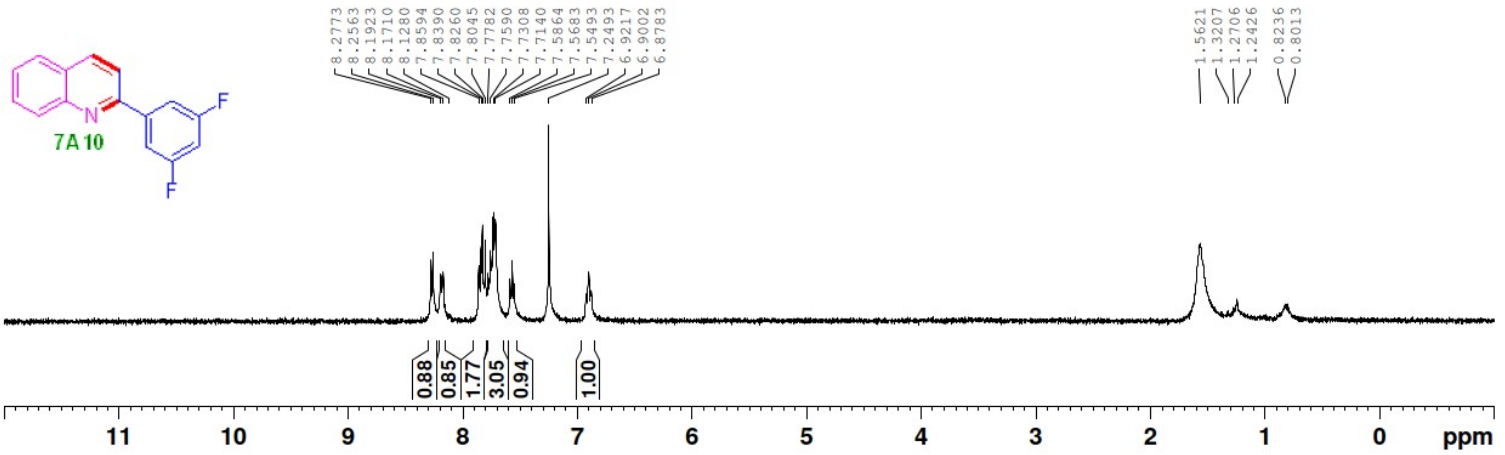
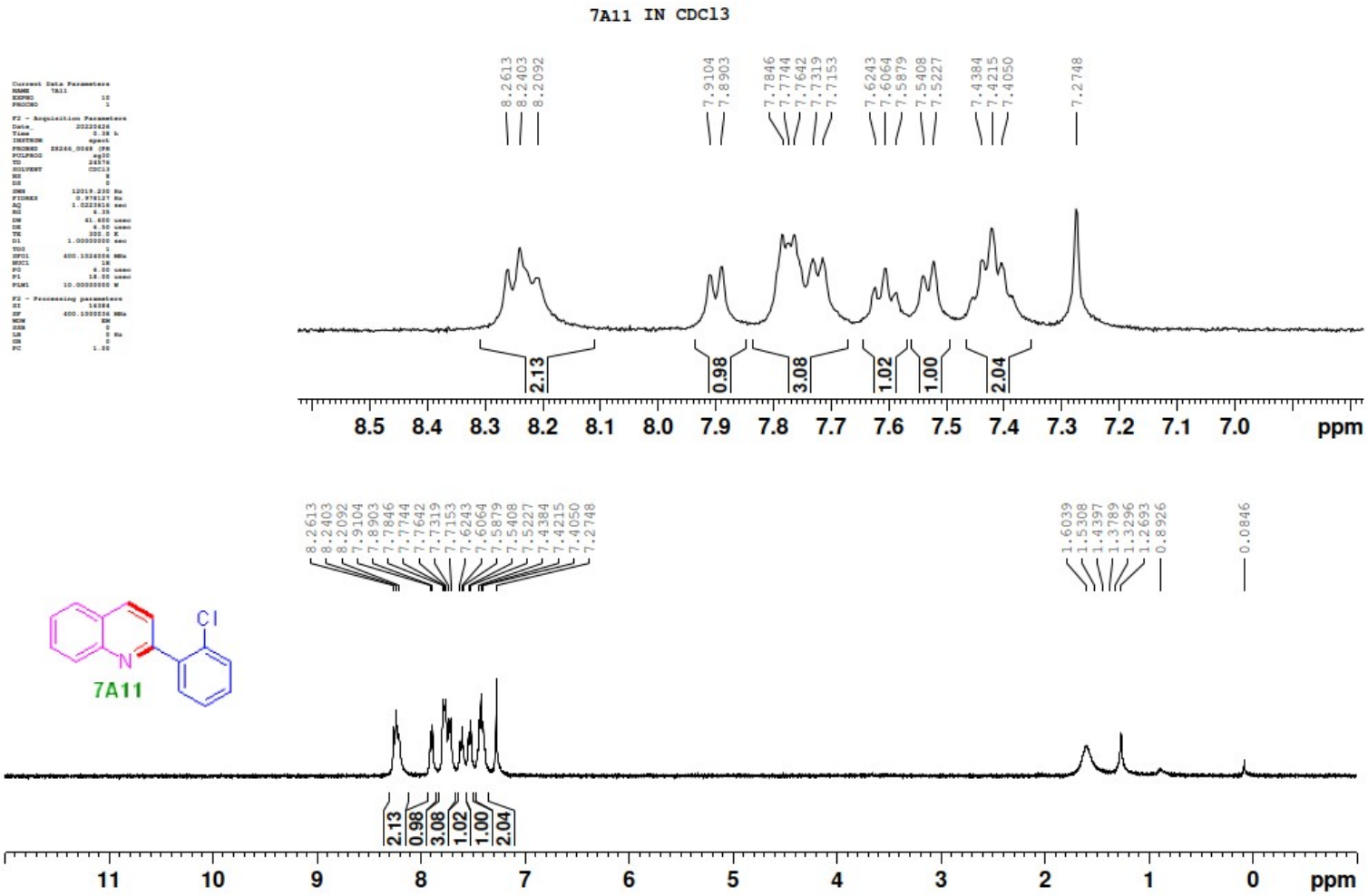
6.668
6.570
6.551
4.526
3.554
3.541
3.488
3.459
2.888
2.717
2.128
2.035
1.994
1.965
1.686
1.556
1.405
1.282
1.247
1.070
0.870
0.854
0.751
0.718
0.061
N
F
F
F
7A9
11 10 9 8 7 6 5 4 3 2 1 0 ppm

7A10 IN CDCl3








7A11 IN CDCl3
8.2613
8.2403
8.2092
7.9104
7.8903
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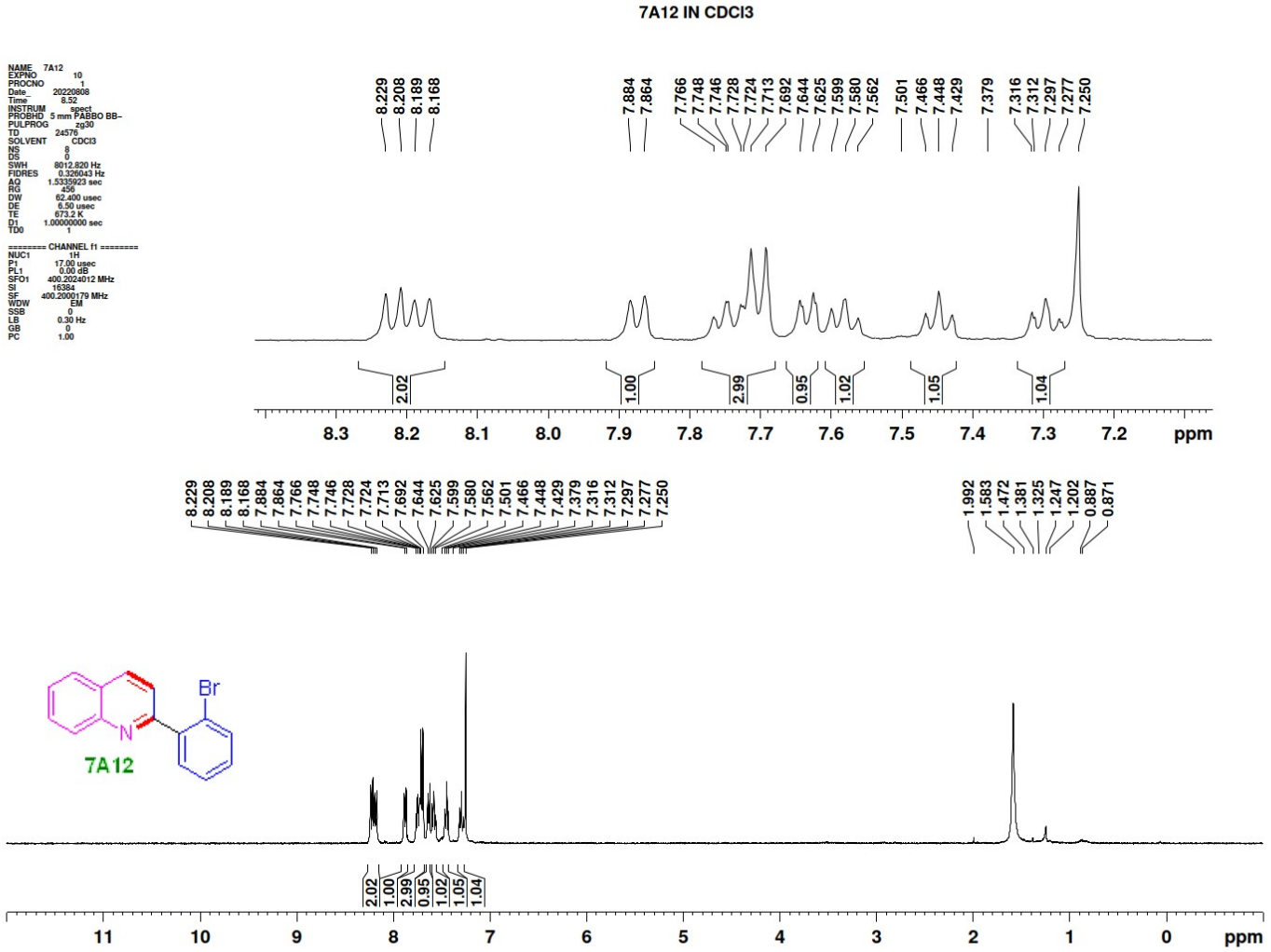
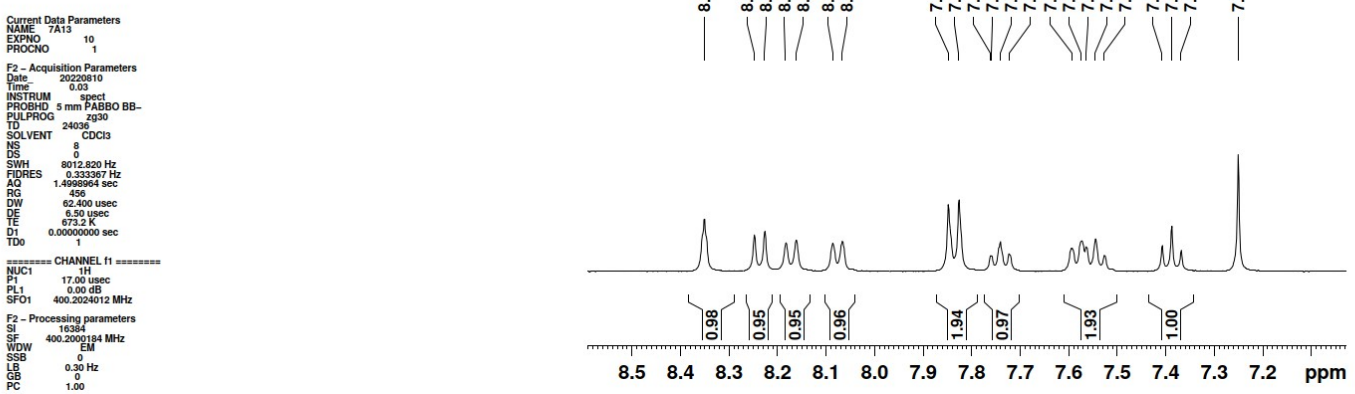
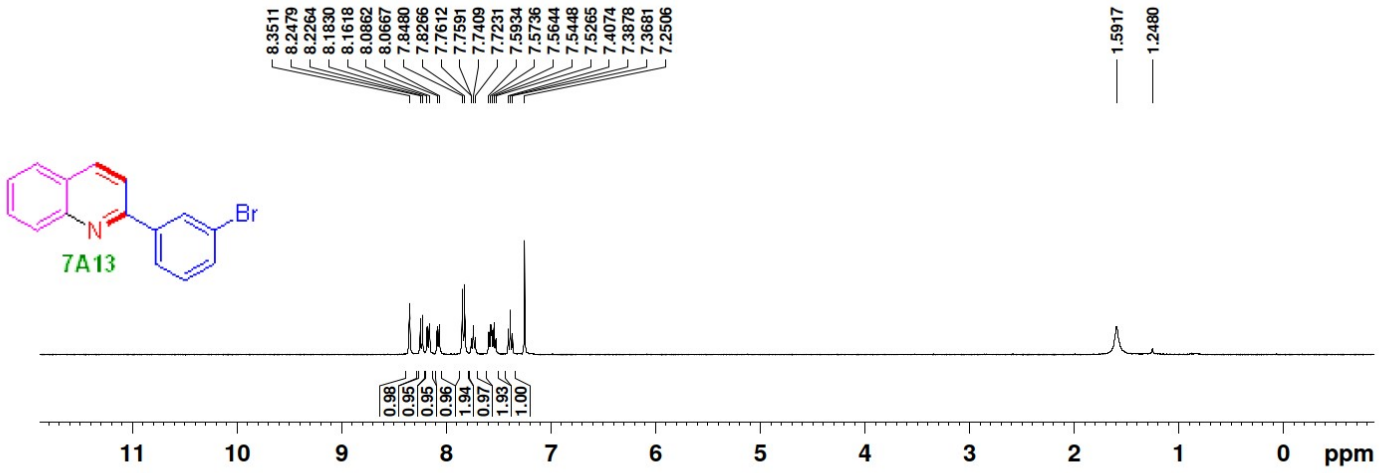
7.7744
7.7642
7.7319
7.7153
7.6243
7.6064
7.5879
7.5408
7.5227
7.4384
7.4215
7.4050
7.2748
2.13
0.98
3.08
1.02
1.00
2.04
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
1.6039
1.5308
1.4397
1.3789
1.3296
1.2693
0.8926
0.0846
Cl
N
7A11
11 10 9 8 7 6 5 4 3 2 1 0 ppm

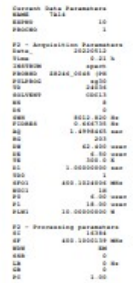

7A12 IN CDCl3
NAME 7A12
EXPNO 10
PROCNO 1
Date_ 20220808
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 24576
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.326043 Hz
AQ 1.5335923 sec
RG 456
DW 62.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024012 MHz
SI 16384
SF 400.2000179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.229
8.208
8.189
8.168
7.884
7.864
7.766
7.748
7.746
7.728
7.724
7.713
7.692
7.644
7.625
7.599
7.580
7.562
7.501
7.466
7.448
7.429
7.379
7.316
7.312
7.297
7.277
7.250
2.02
1.00
2.99
0.95
1.02
1.05
1.04
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
1.992
1.583
1.472
1.381
1.325
1.247
1.202
0.887
0.871
Br
N
7A12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

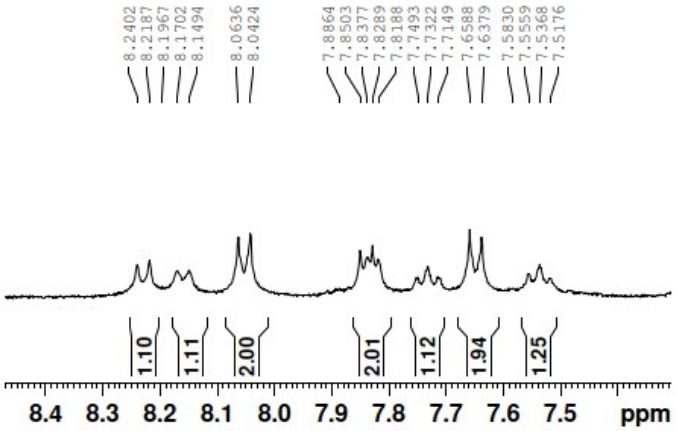
7A13 IN CDCl3

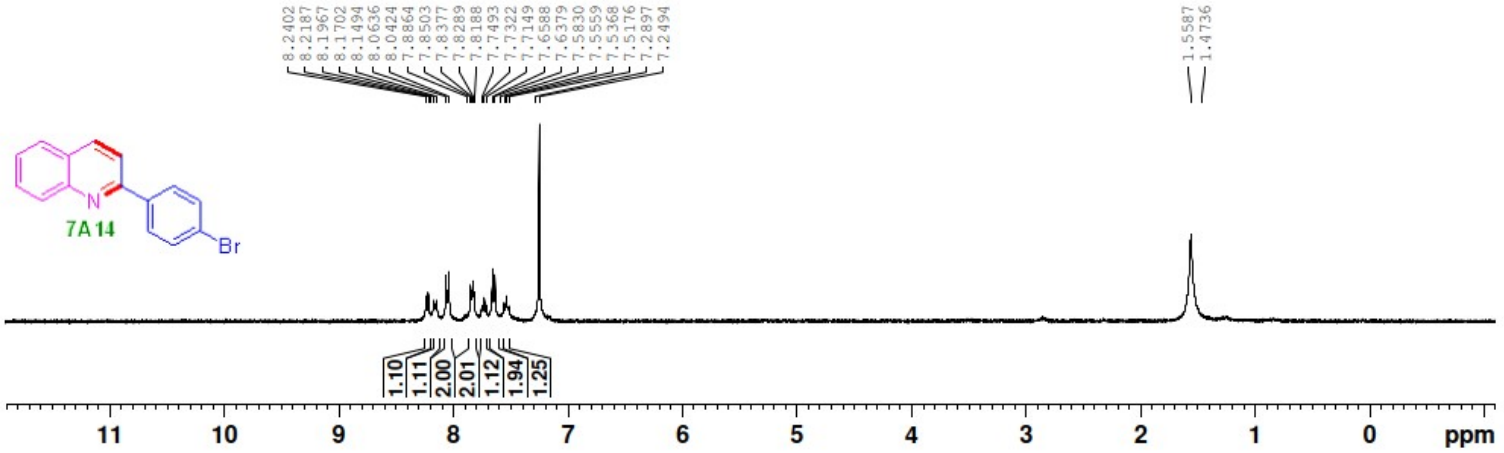


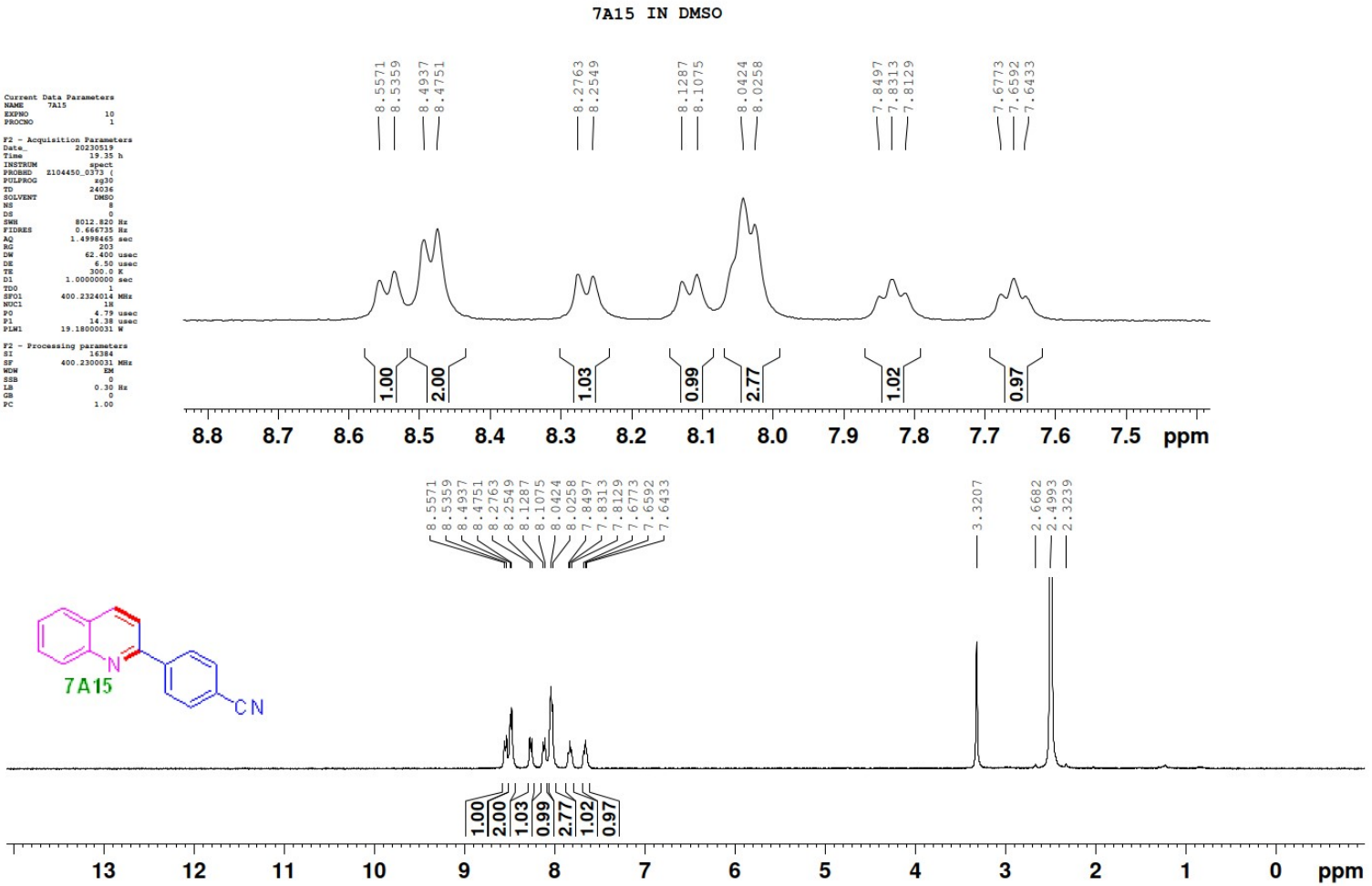


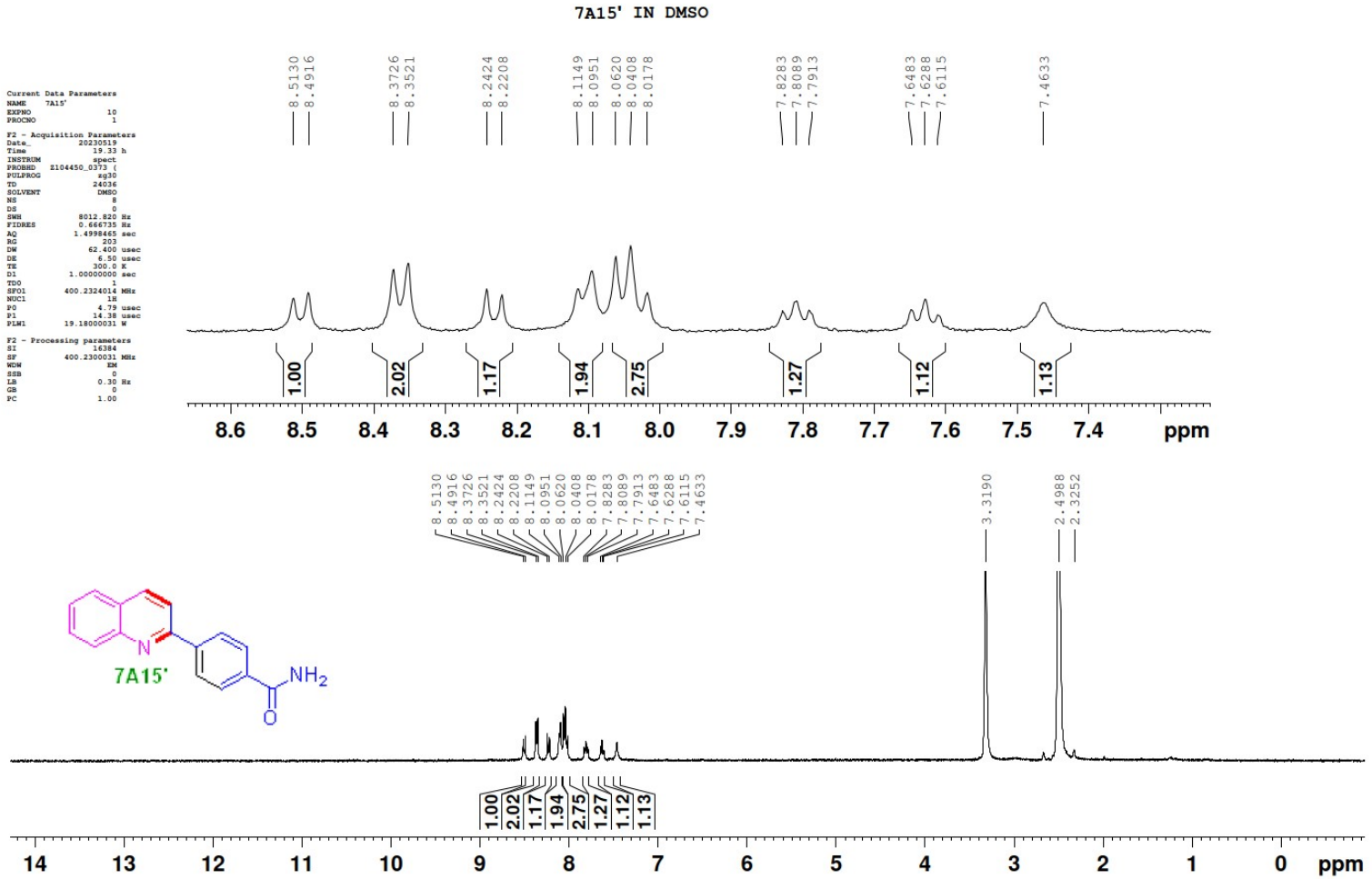
7A14 IN CDCl3



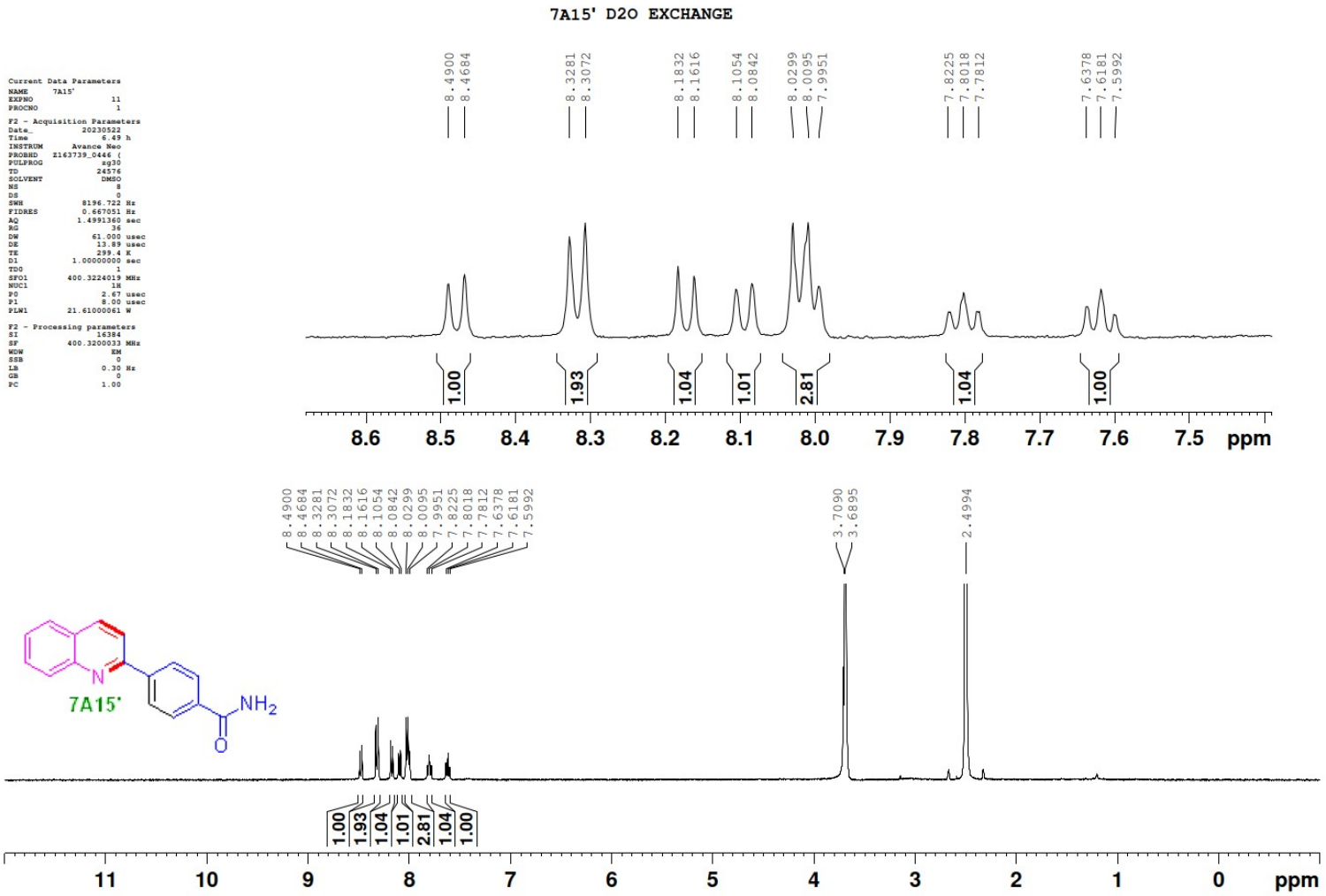





7A15 IN DMSO
Current Data Parameters
NAME 7A15
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230519
Time 19.35 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5571
8.5359
8.4937
8.4751
8.2763
8.2549
8.1287
8.1075
8.0424
8.0258
7.8497
7.8313
7.8129
7.6773
7.6592
7.6433
1.00
2.00
1.03
0.99
2.77
1.02
0.97
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
3.3207
2.6682
2.4993
2.3239
7A15
N
CN
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm


7A15' IN DMSO
Current Data Parameters
NAME 7A15'
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230519
Time 19.33 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5130
8.4916
8.3726
8.3521
8.2424
8.2208
8.1149
8.0951
8.0620
8.0408
8.0178
7.8283
7.8089
7.7913
7.6483
7.6288
7.6115
7.4633
1.00
2.02
1.17
1.94
2.75
1.27
1.12
1.13
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
3.3190
2.4988
2.3252
7A15'
NH2
O
N
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

7A15' D2O EXCHANGE

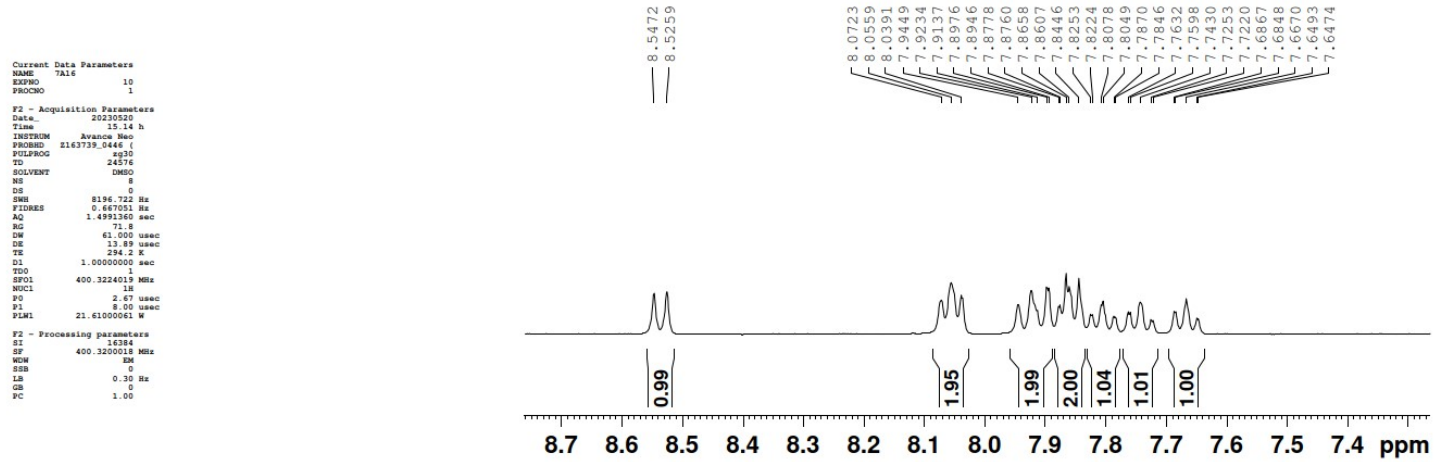


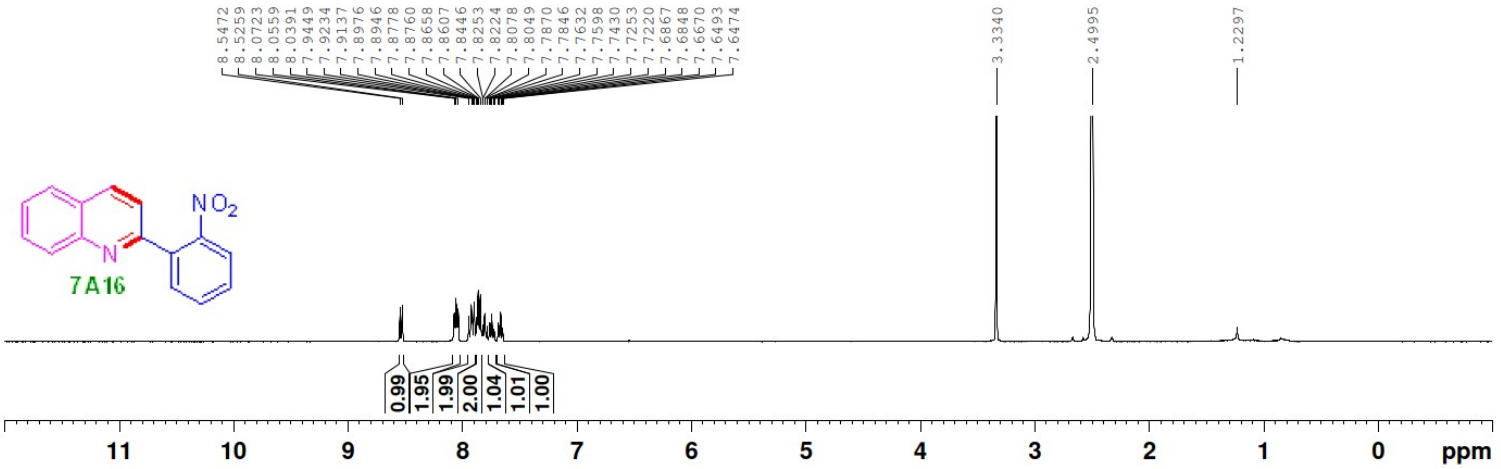
7A16 IN DMSO

```
Current Data Parameters
NAME      7A16
EXPNO       10
PROCNO       1

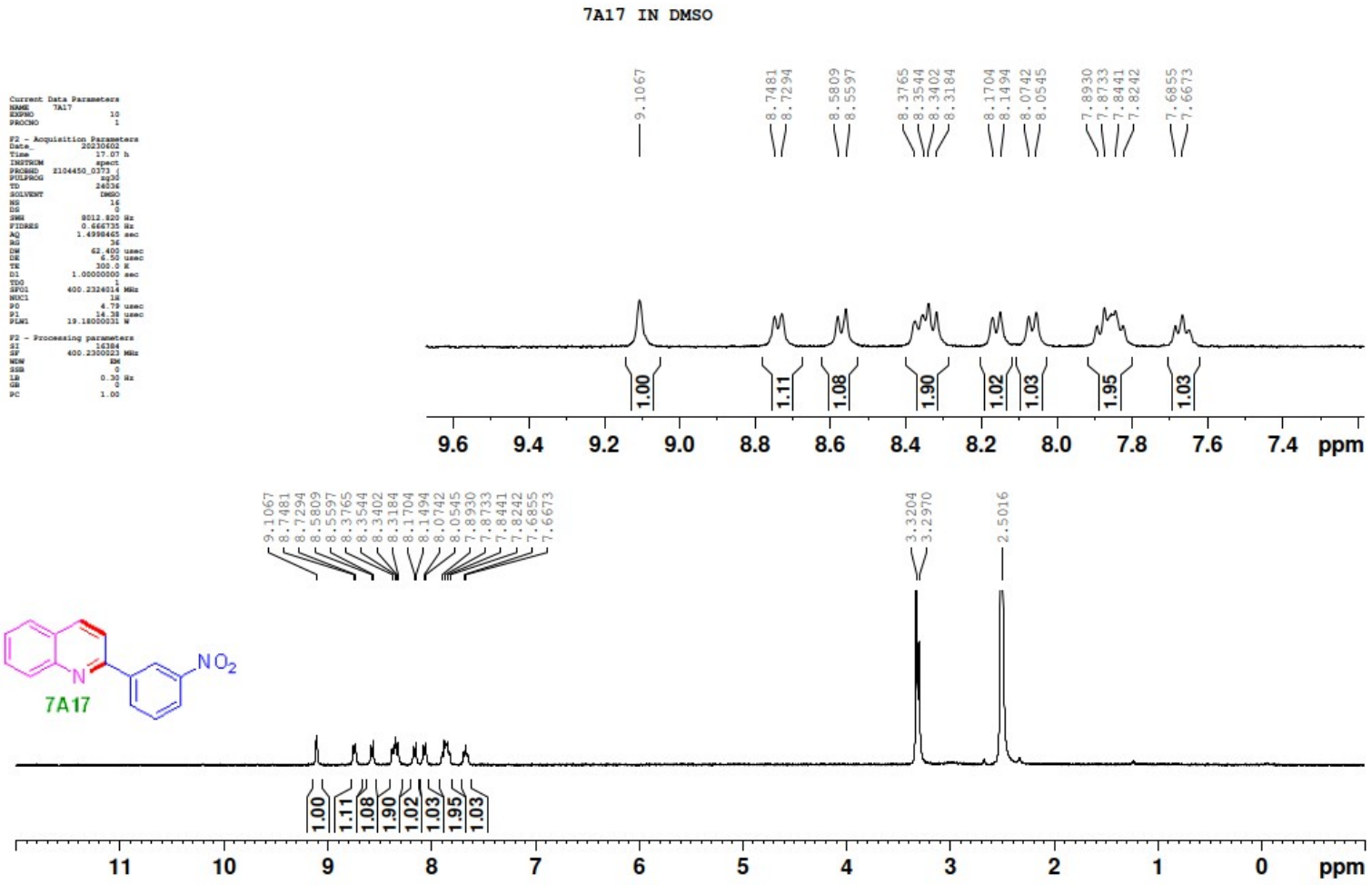
F2 - Acquisition Parameters
Date_     20230520
Time         15.14 h
INSTRUM   Avance Neo
PROBHD    Z163739_0446 (
PULPROG      zg30
TD          24576
SOLVENT      DMSO
NS              8
DS              0
SWH       8196.722 Hz
FIDRES    0.667051 Hz
AQ        1.4991360 sec
RG             71.8
DW            61.000 usec
DE            13.89 usec
TE            294.2 K
D1        1.00000000 sec
TD0             1
SFO1      400.3224019 MHz
NUC1            1H
P0            2.67 usec
P1            8.00 usec
PLW1     21.61000061 W

F2 - Processing parameters
SI          16384
SF        400.3200018 MHz
WDW            EM
SSB             0
LB           0.30 Hz
GB              0
PC           1.00
```

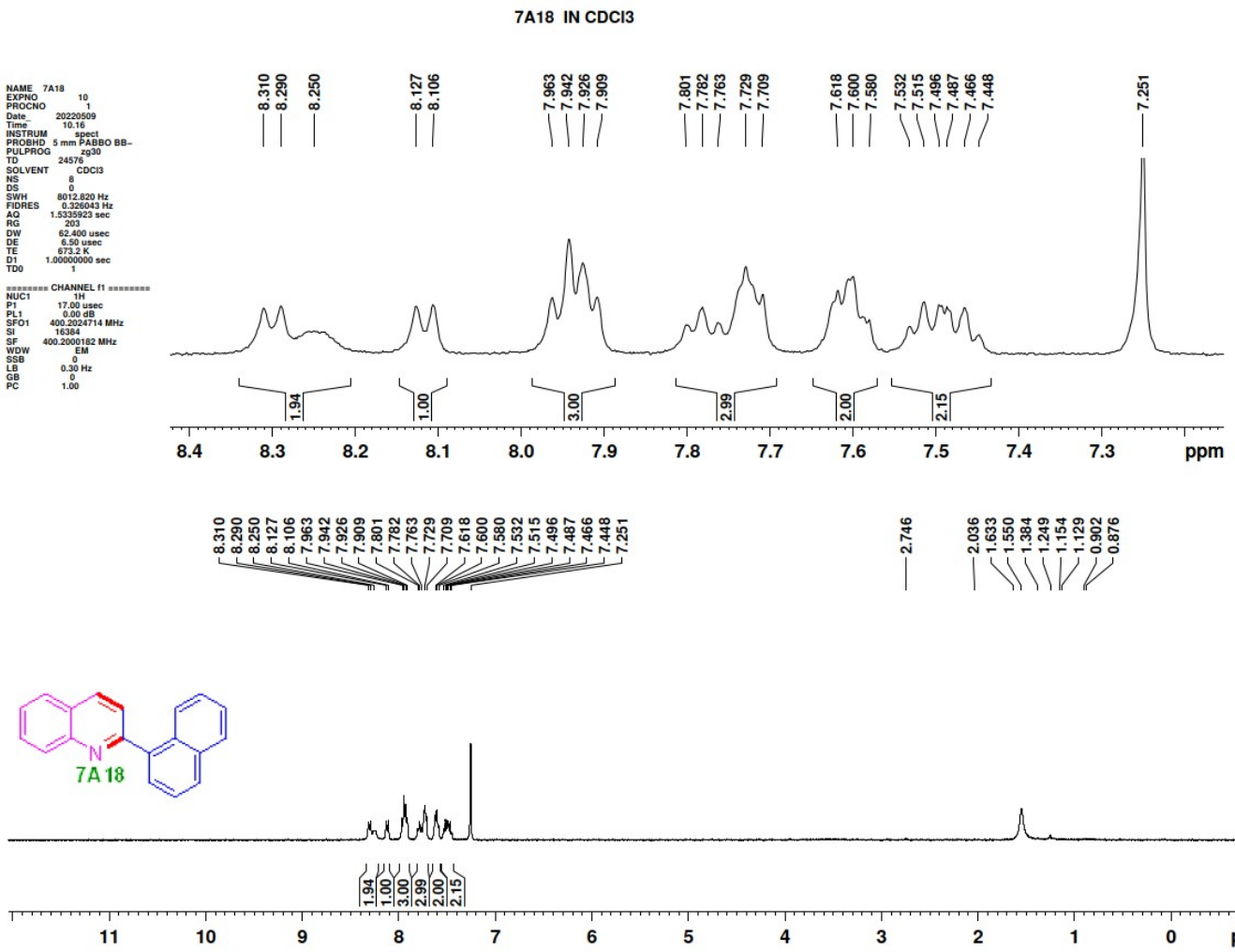




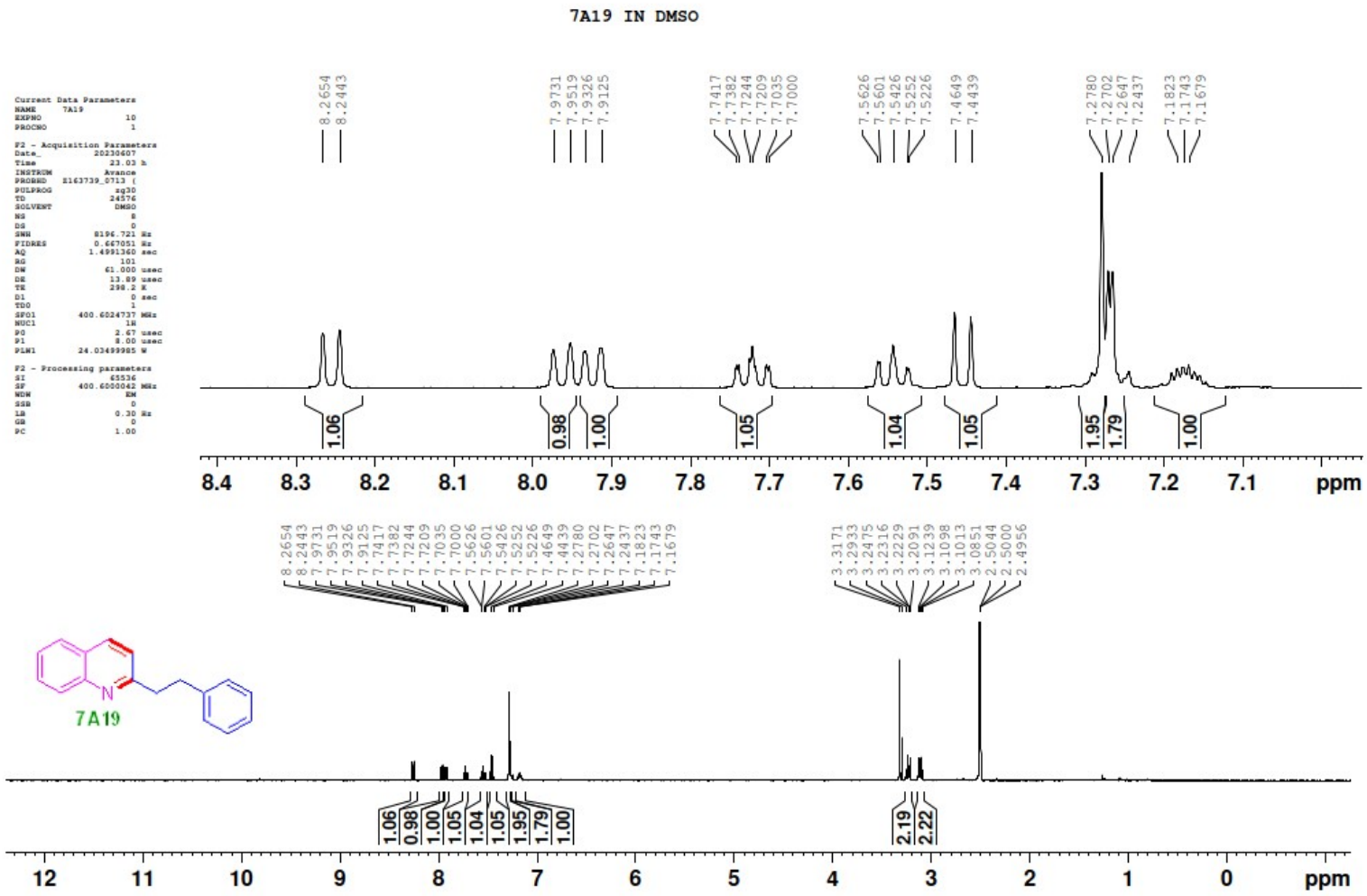
7A17 IN DMSO


Current Data Parameters
NAME 7A17
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230602
Time 17.07 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4996465 sec
RG 36
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.1067
8.7481
8.7294
8.5809
8.5597
8.3765
8.3544
8.3402
8.3184
8.1704
8.1494
8.0742
8.0545
7.8930
7.8733
7.8441
7.8242
7.6855
7.6673
1.00
1.11
1.08
1.90
1.02
1.03
1.95
1.03
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
ppm
3.3204
3.2970
2.5016
N
NO2
7A17
11
10
9
8
7
6
5
4
3
2
1
0
ppm

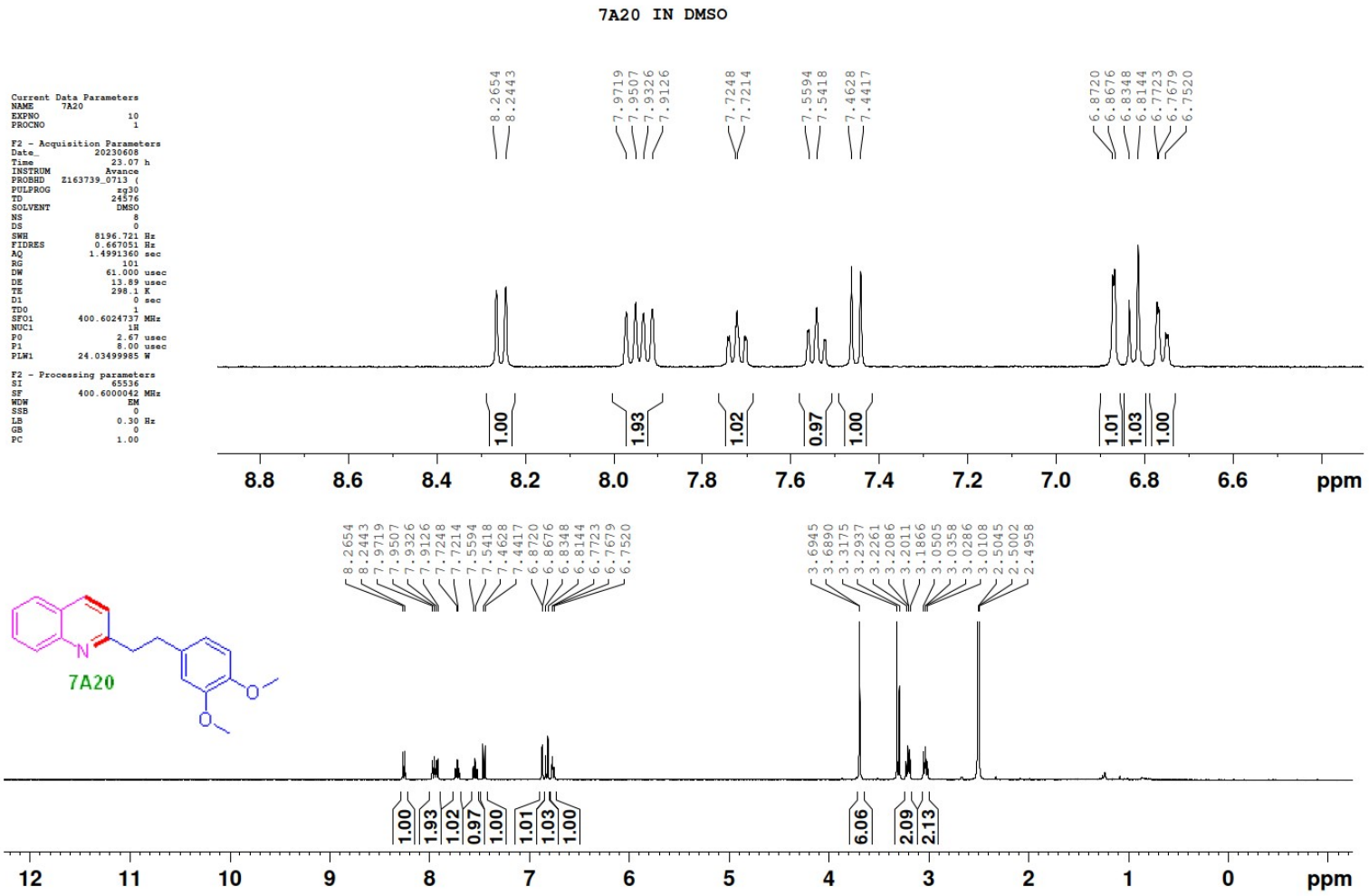
7A18 IN CDCl3



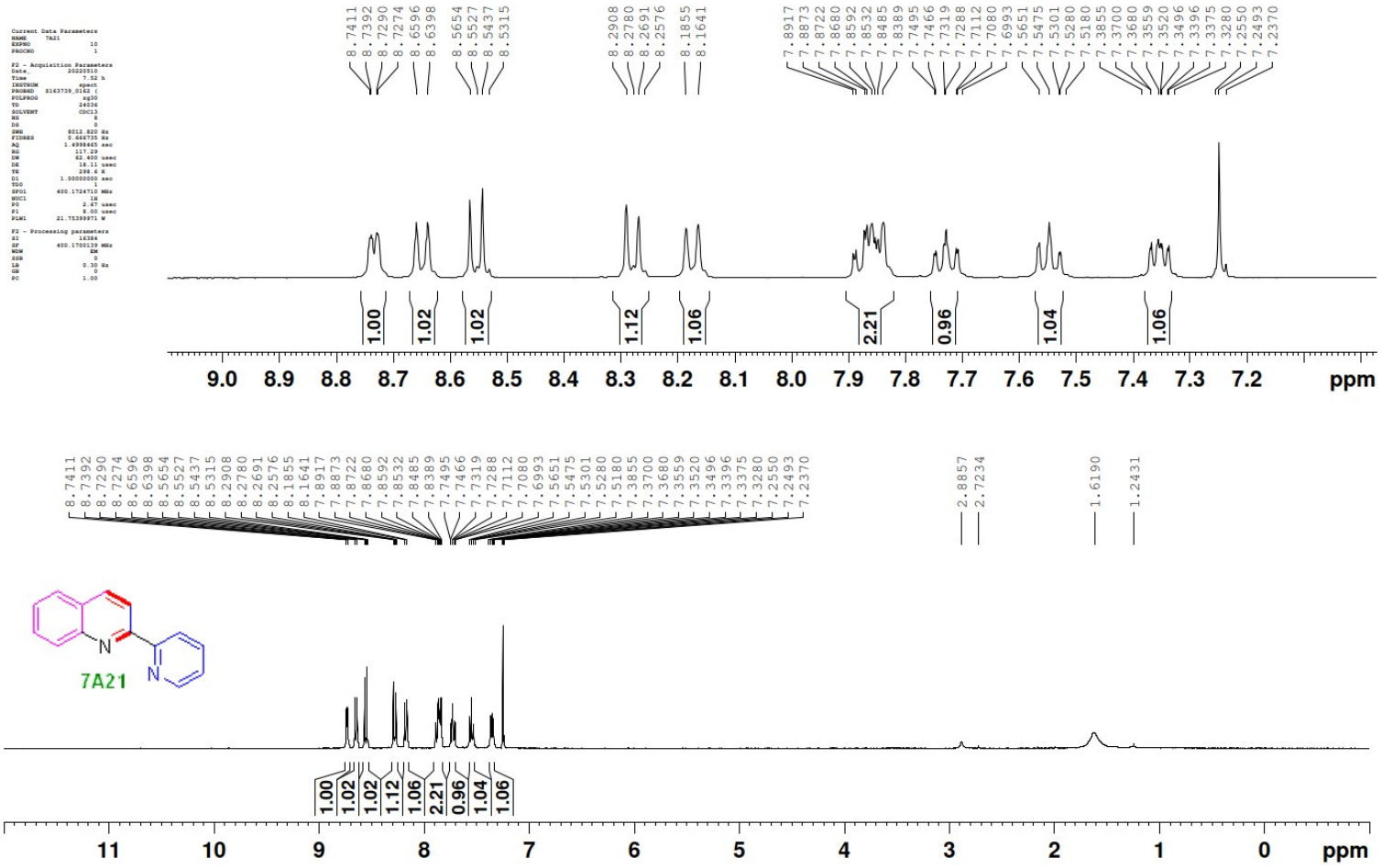
7A19 IN DMSO


Current Data Parameters
NAME 7A19
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230607
Time 23.03 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 0 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.2654
8.2443
7.9731
7.9519
7.9326
7.9125
7.7417
7.7382
7.7244
7.7209
7.7035
7.7000
7.5626
7.5601
7.5426
7.5252
7.5226
7.4649
7.4439
7.2780
7.2702
7.2647
7.2437
7.1823
7.1743
7.1679
1.06
0.98
1.00
1.05
1.04
1.05
1.95
1.79
1.00
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
3.3171
3.2933
3.2475
3.2316
3.2229
3.2091
3.1239
3.1098
3.1013
3.0851
2.5044
2.5000
2.4956
7A19
2.19
2.22
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

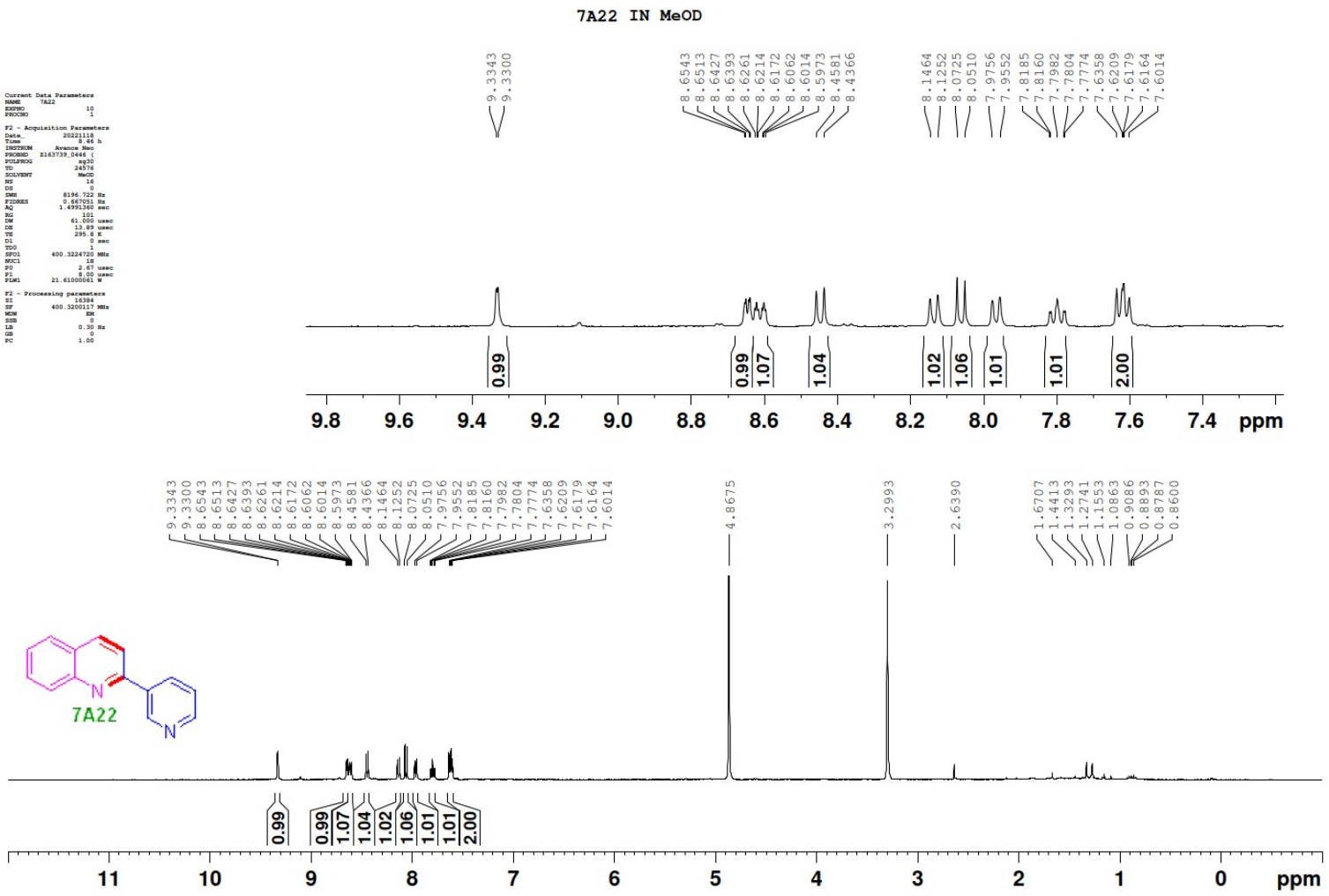
7A20 IN DMSO


Current Data Parameters
NAME 7A20
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230608
Time 23.07 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.1 K
D1 0 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.2654
8.2443
7.9719
7.9507
7.9326
7.9126
7.7248
7.7214
7.5594
7.5418
7.4628
7.4417
6.8720
6.8676
6.8348
6.8144
6.7723
6.7679
6.7520
1.00
1.93
1.02
0.97
1.00
1.01
1.03
1.00
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm
3.6945
3.6890
3.3175
3.2937
3.2261
3.2086
3.2011
3.1866
3.0505
3.0358
3.0286
3.0108
2.5045
2.5002
2.4958
6.06
2.09
2.13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
7A20

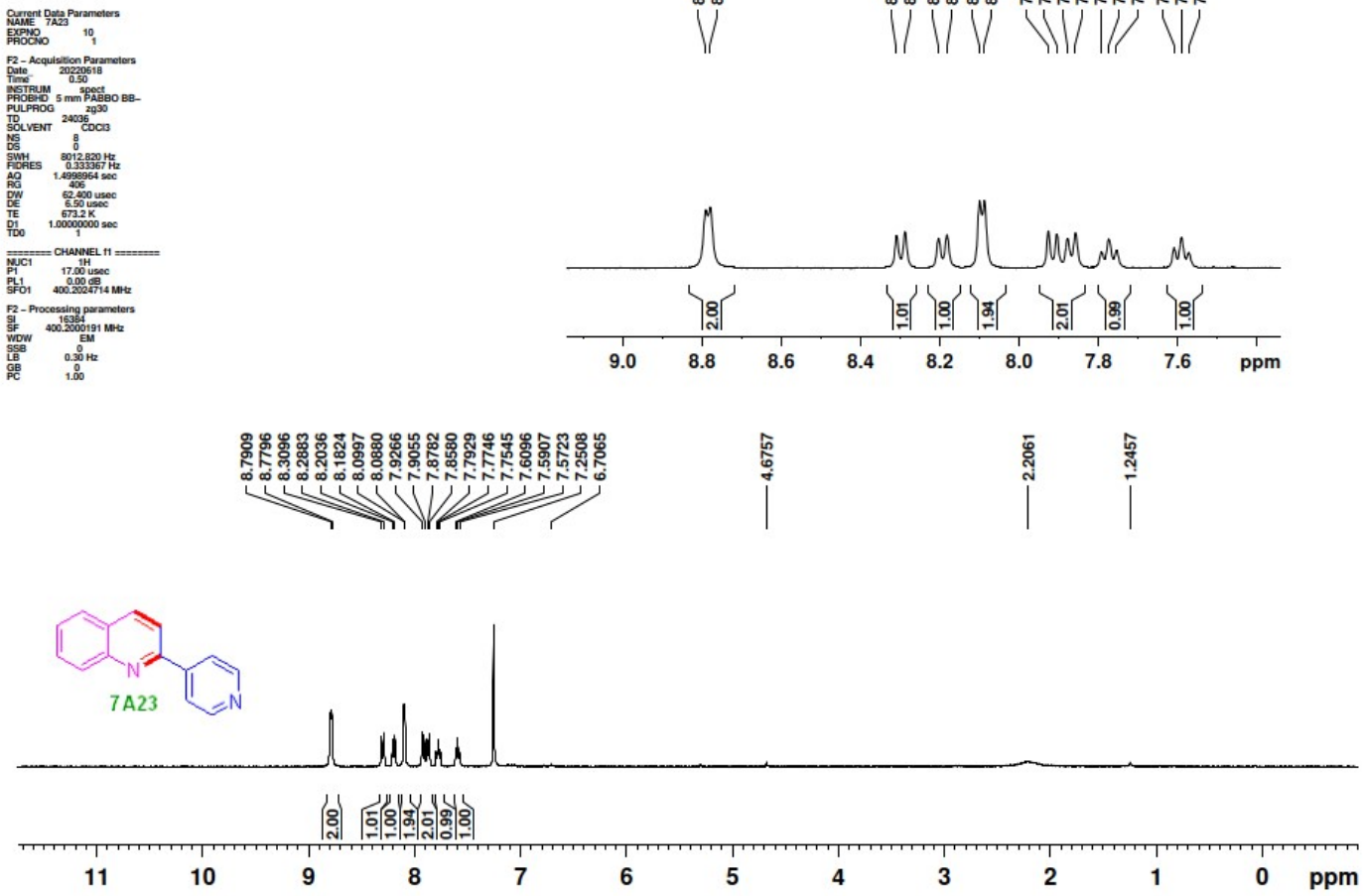
7A21 IN CDCl3



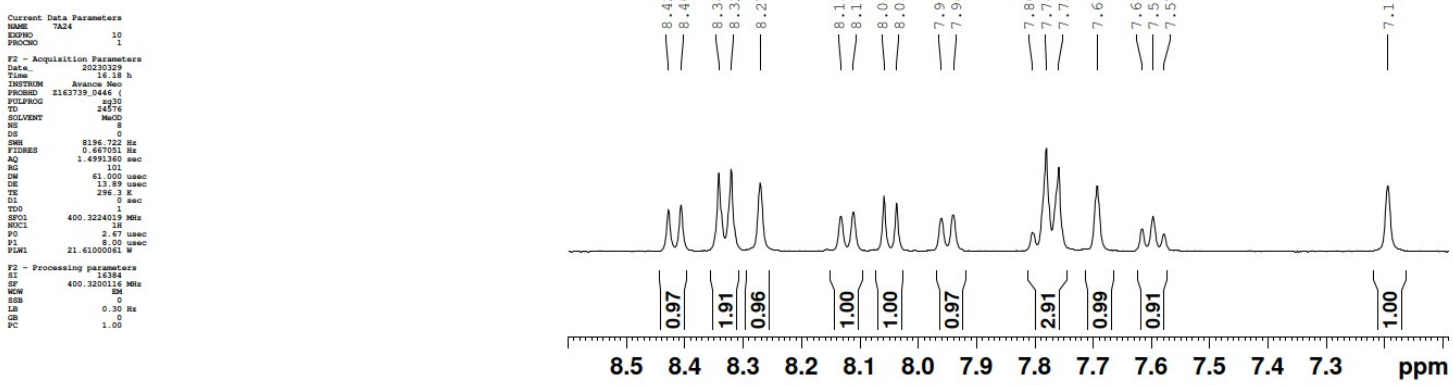
7A22 IN MeOD

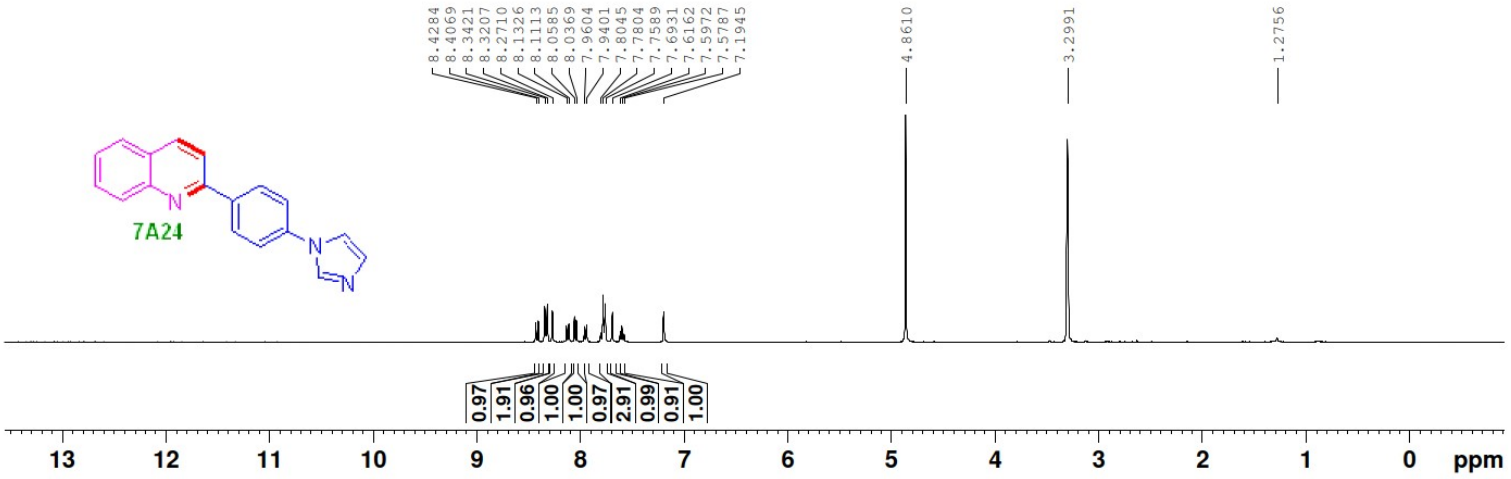

Current Data Parameters
NAME 7A22
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221118
Time 8.46 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 295.8 K
D1 0 sec
TD0 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.3343
9.3300
8.6543
8.6513
8.6427
8.6393
8.6261
8.6214
8.6172
8.6062
8.6014
8.5973
8.4581
8.4366
8.1464
8.1252
8.0725
8.0510
7.9756
7.9552
7.8185
7.8160
7.7982
7.7804
7.7774
7.6358
7.6209
7.6179
7.6164
7.6014
0.99
0.99
1.07
1.04
1.02
1.06
1.01
1.01
2.00
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
ppm
4.8675
3.2993
2.6390
1.6707
1.4413
1.3293
1.2741
1.1553
1.0863
0.9086
0.8893
0.8787
0.8600
N
7A22
N
0.99
0.99
1.07
1.04
1.02
1.06
1.01
1.01
2.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm

7A23 IN CDCl3



7A24 IN MeOD



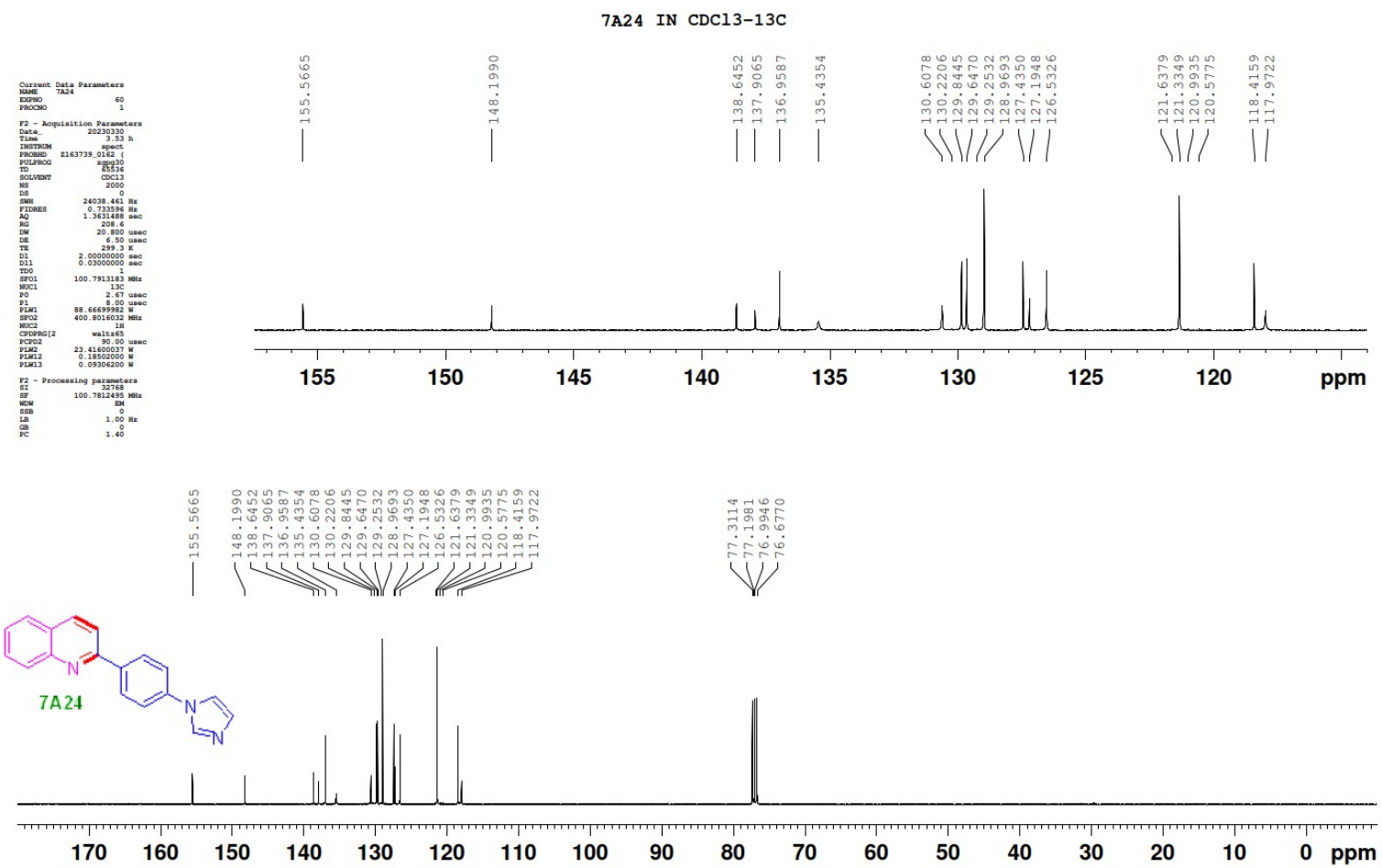


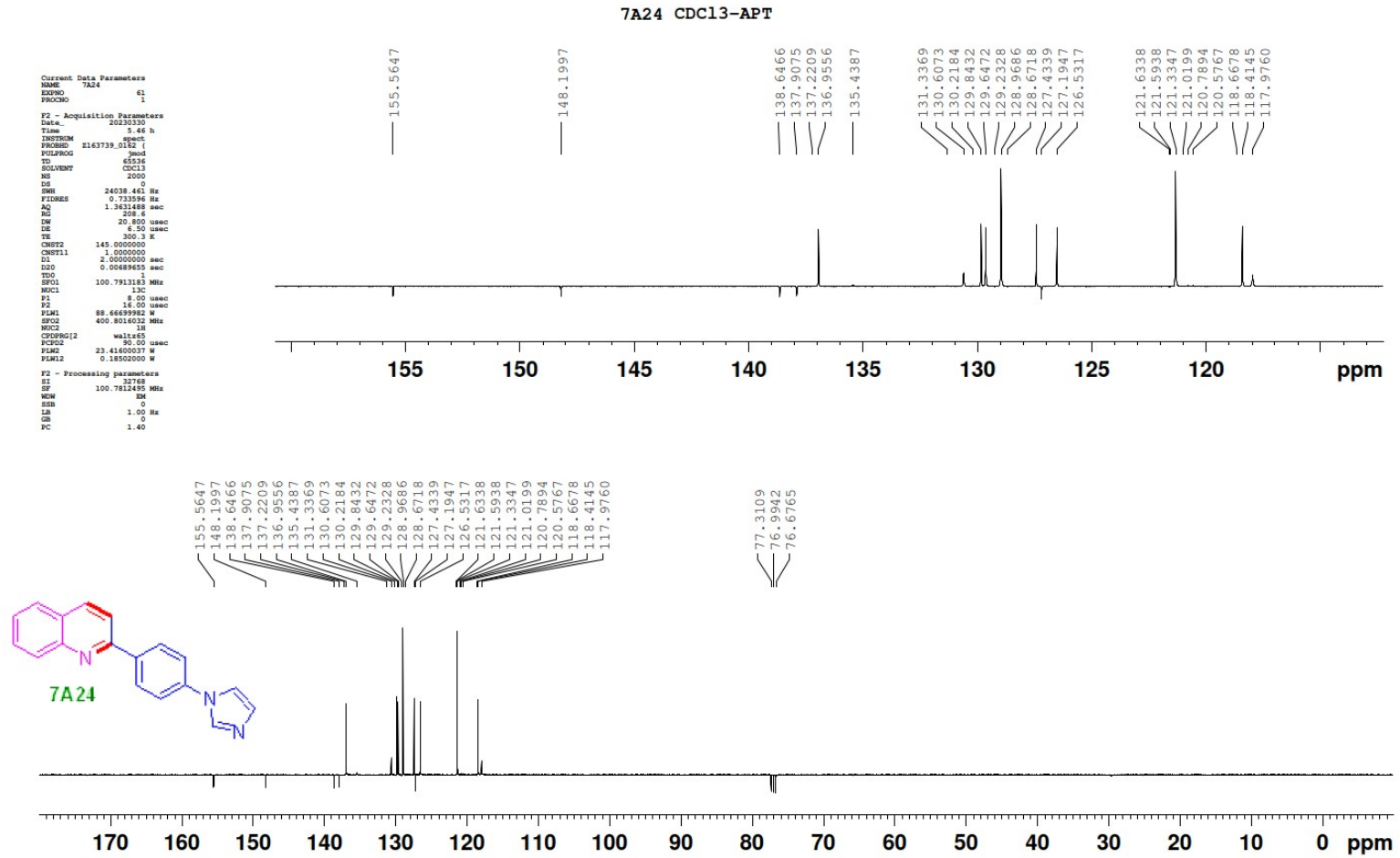

```
Current Data Parameters
NAME       7A24
EXPNO            10
PROCNO            1

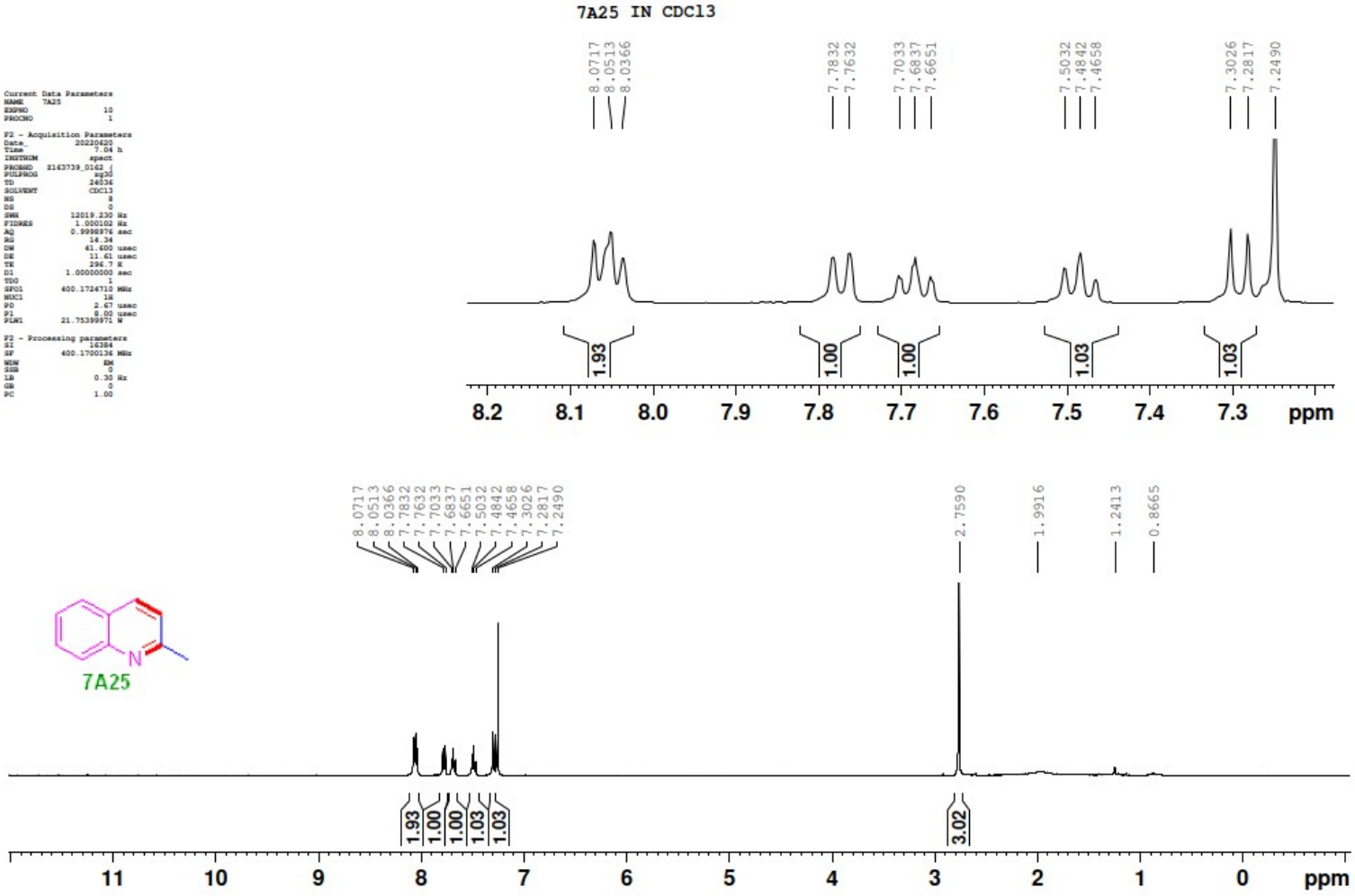
F2 - Acquisition Parameters
Date_      20230329
Time         16.18 h
INSTRUM  Avance Neo
PROBHD   Z163739_0446 (
PULPROG        zg30
TD            24576
SOLVENT        MeOD
NS                8
DS                0
SWH         8196.722 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG              101
DW           61.000 usec
DE           13.89 usec
TE           296.3 K
D1              0 sec
TD0             1
SFO1    400.3224019 MHz
NUC1           1H
P0           2.67 usec
P1           8.00 usec
PLW1    21.61000061 W

F2 - Processing parameters
SI            16384
SF      400.3200116 MHz
WDW            EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```

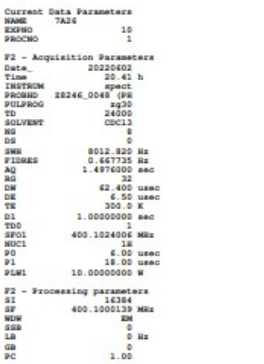
7A24 IN CDCl3-13C

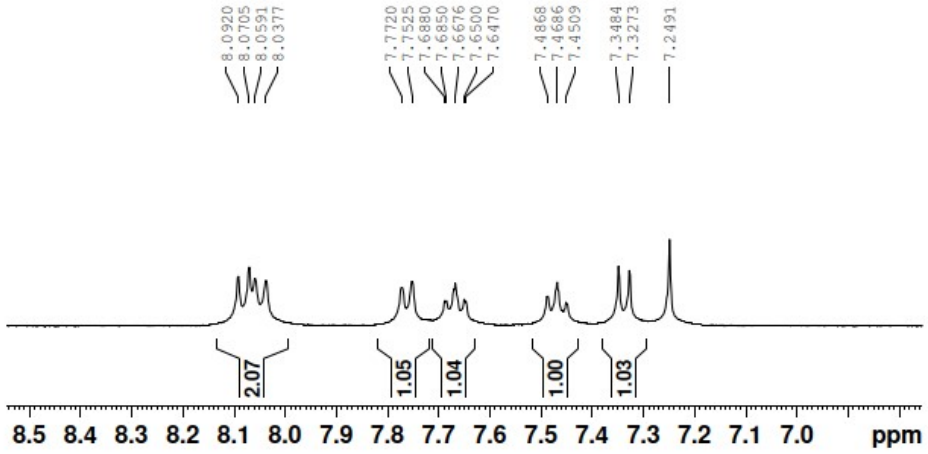


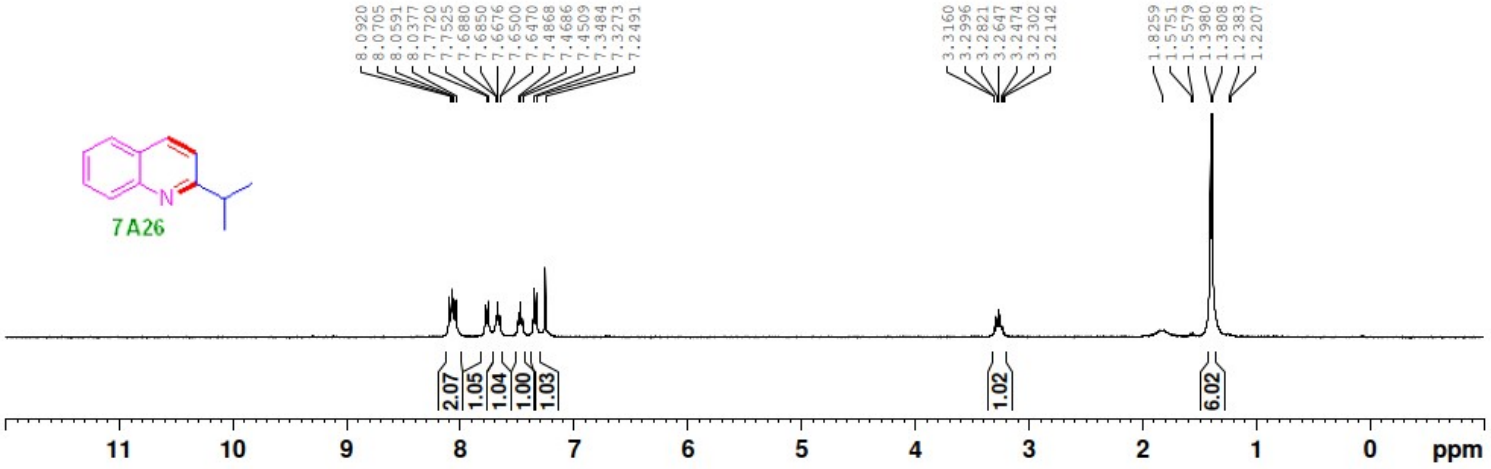

7A24 CDCl3-APT
Current Data Parameters
NAME 7A24
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230330
Time 5.46 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 208.6
DW 20.800 usec
DE 6.50 usec
TE 300.3 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.7913183 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 88.66699982 W
SFO2 400.8016032 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 23.41600037 W
PLW12 0.18502000 W
F2 - Processing parameters
SI 32768
SF 100.7812495 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
155.5647
148.1997
138.6466
137.9075
137.2209
136.9556
135.4387
131.3369
130.6073
130.2184
129.8432
129.6472
129.2328
128.9686
128.6718
127.4339
127.1947
126.5317
121.6338
121.5938
121.3347
121.0199
120.7894
120.5767
118.6678
118.4145
117.9760
155 150 145 140 135 130 125 120 ppm
77.3109
76.9942
76.6765
7A24
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7A25 IN CDCl3
Current Data Parameters
NAME 7A25
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220620
Time 7.04 h
INSTRUM spect
PROBHD Z143739_0162 (
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 1.000102 Hz
AQ 0.9998976 sec
RG 14.34
DW 41.600 usec
DE 11.61 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.75399971 W
F2 - Processing parameters
SI 16384
SF 400.1700136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0717
8.0513
8.0366
7.7832
7.7632
7.7033
7.6837
7.6651
7.5032
7.4842
7.4658
7.3026
7.2817
7.2490
1.93
1.00
1.00
1.03
1.03
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
7A25
2.7590
1.9916
1.2413
0.8665
3.02
11
10
9
8
7
6
5
4
3
2
1
0
ppm

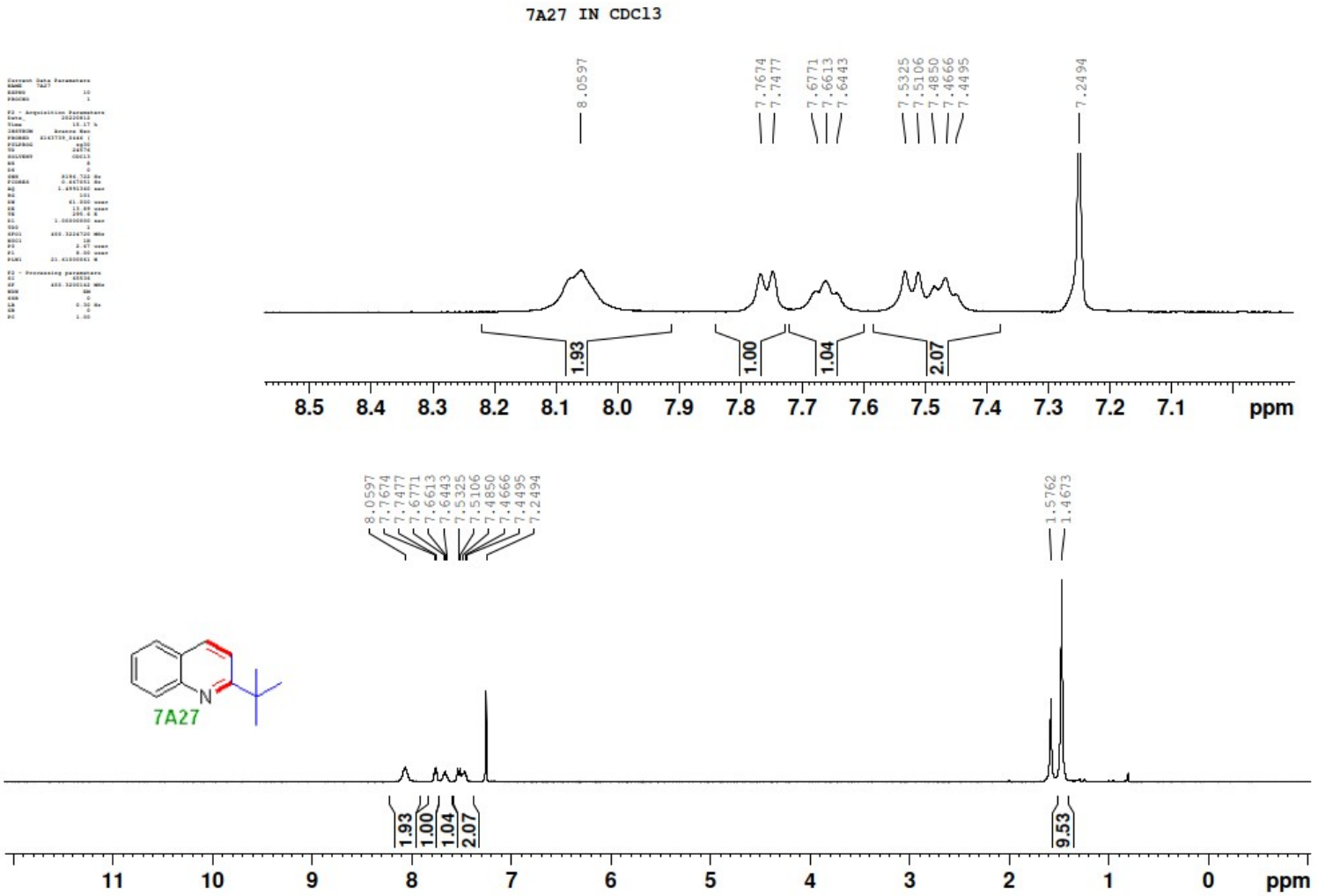
7A26 IN CDCl3



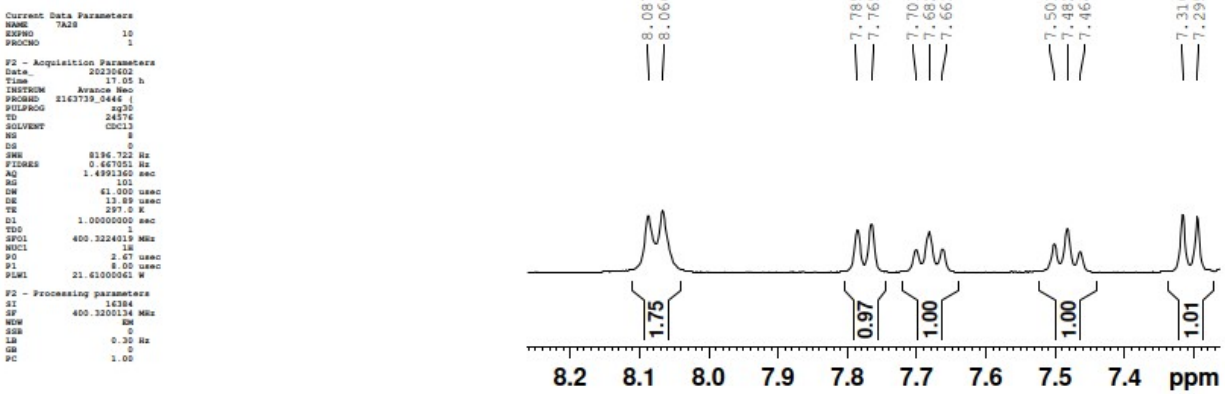


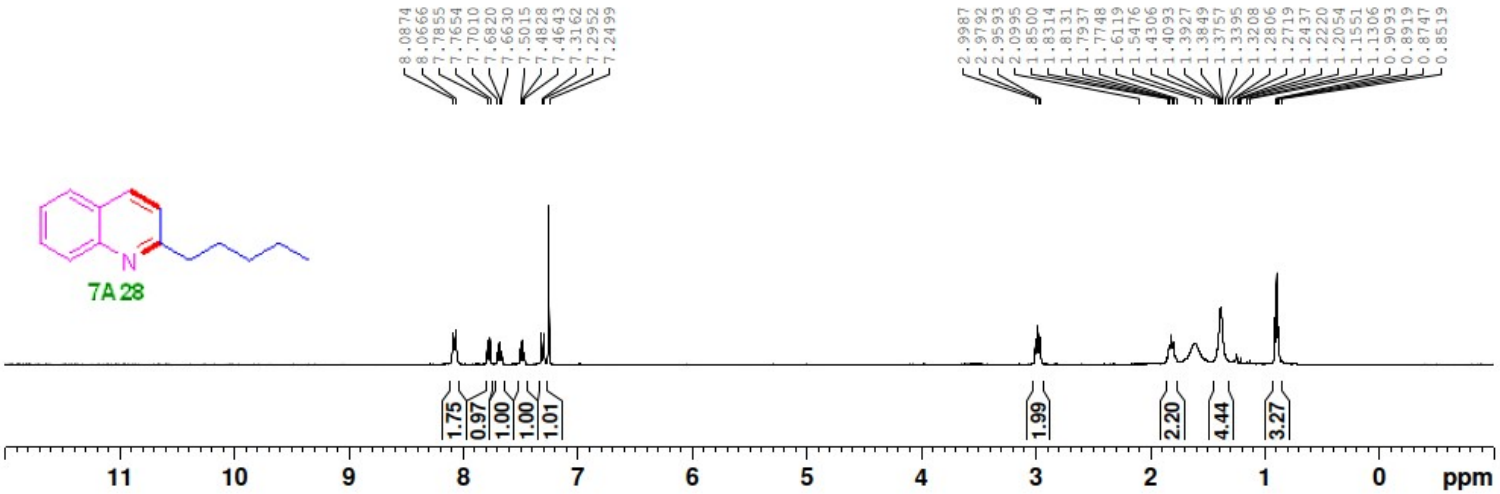


7A27 IN CDCl3



7A28 IN CDCl3

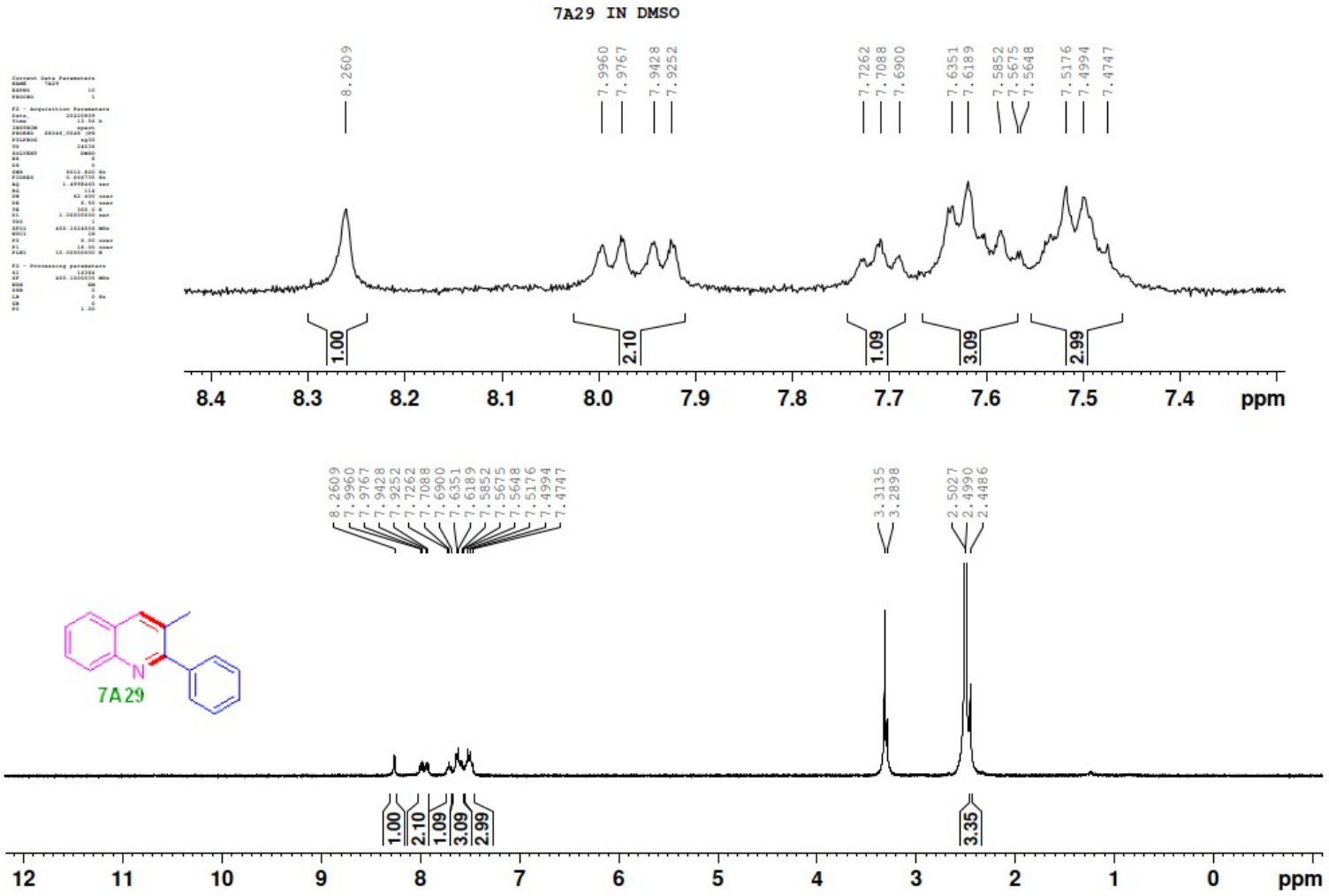




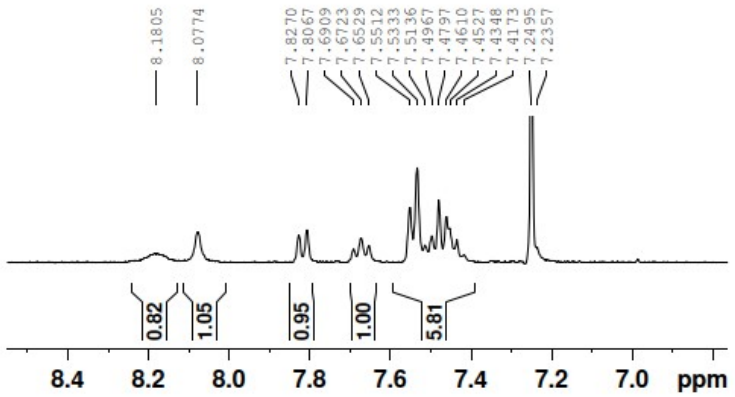
Current Data Parameters
NAME 7A28
EXPNO 10
PROCNO 1

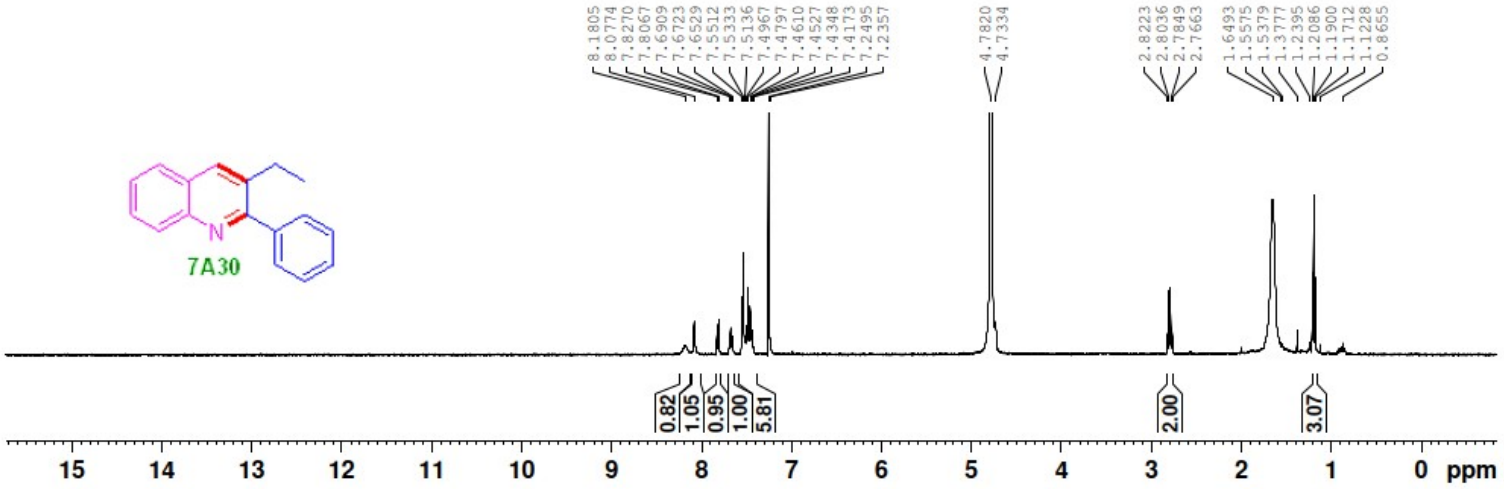
F2 - Acquisition Parameters
Date_ 20230602
Time 17.05 h
INSTRUM Avance Neo
PROBHD 2163739_0446 (
PULPROG zg30
TD 24576
SOLVENT CDCl3
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W

F2 - Processing parameters
SI 16384
SF 400.3200134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

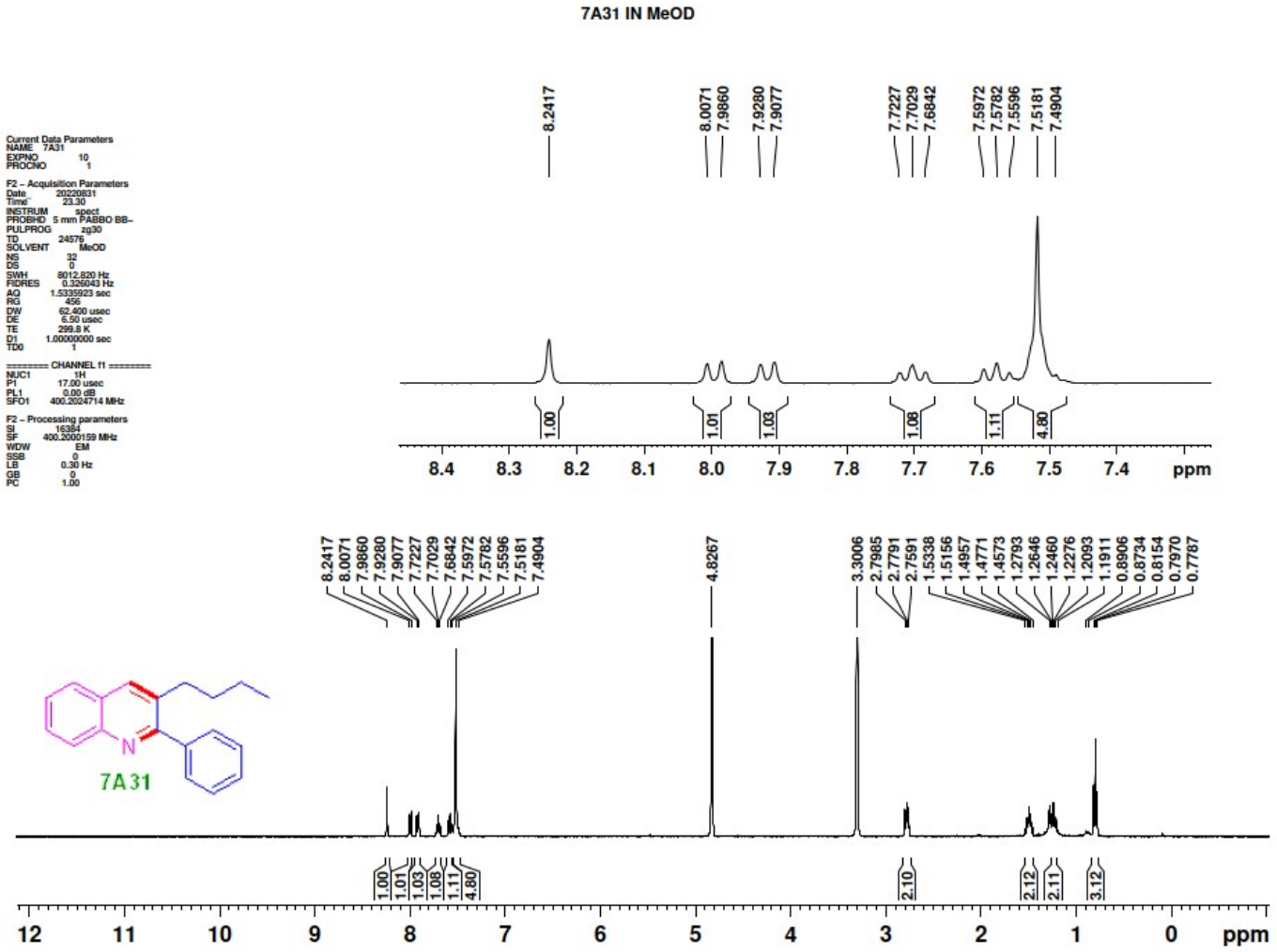

7A29 IN DMSO
8.2609
7.9960
7.9767
7.9428
7.9252
7.7262
7.7088
7.6900
7.6351
7.6189
7.5852
7.5675
7.5648
7.5176
7.4994
7.4747
1.00
2.10
1.09
3.09
2.99
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
3.3135
3.2898
2.5027
2.4990
2.4486
3.35
7A29
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

7A30 IN CDCl3

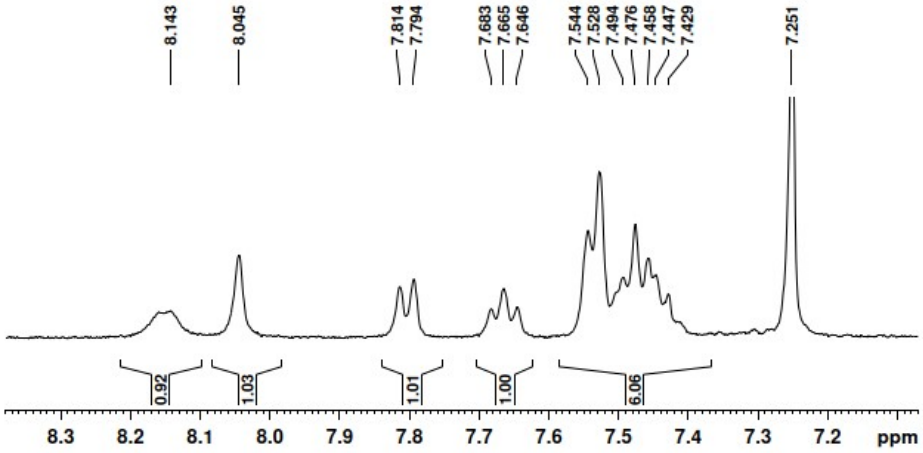


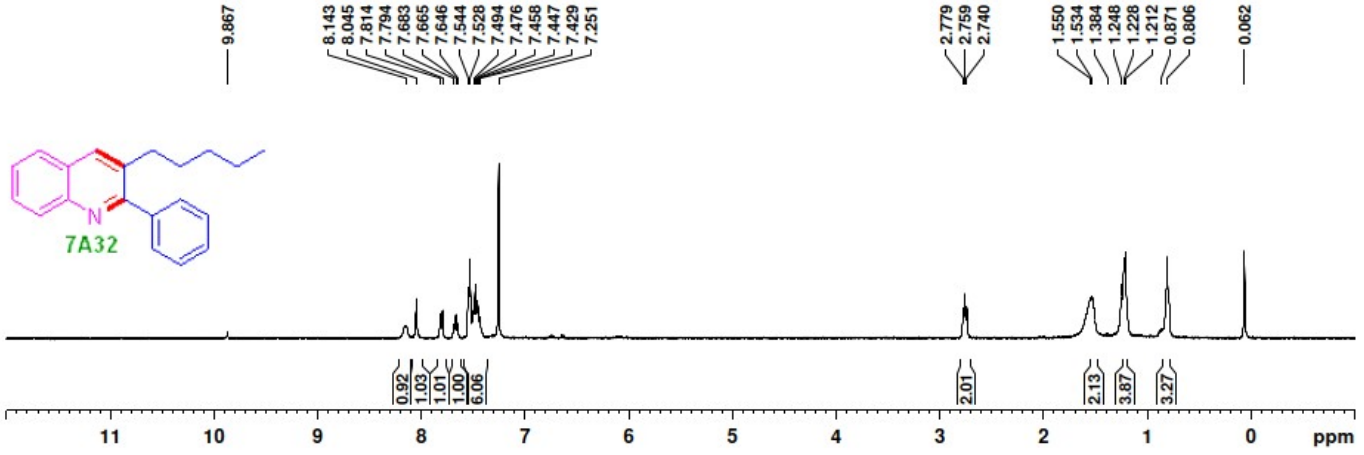


7A31 IN MeOD

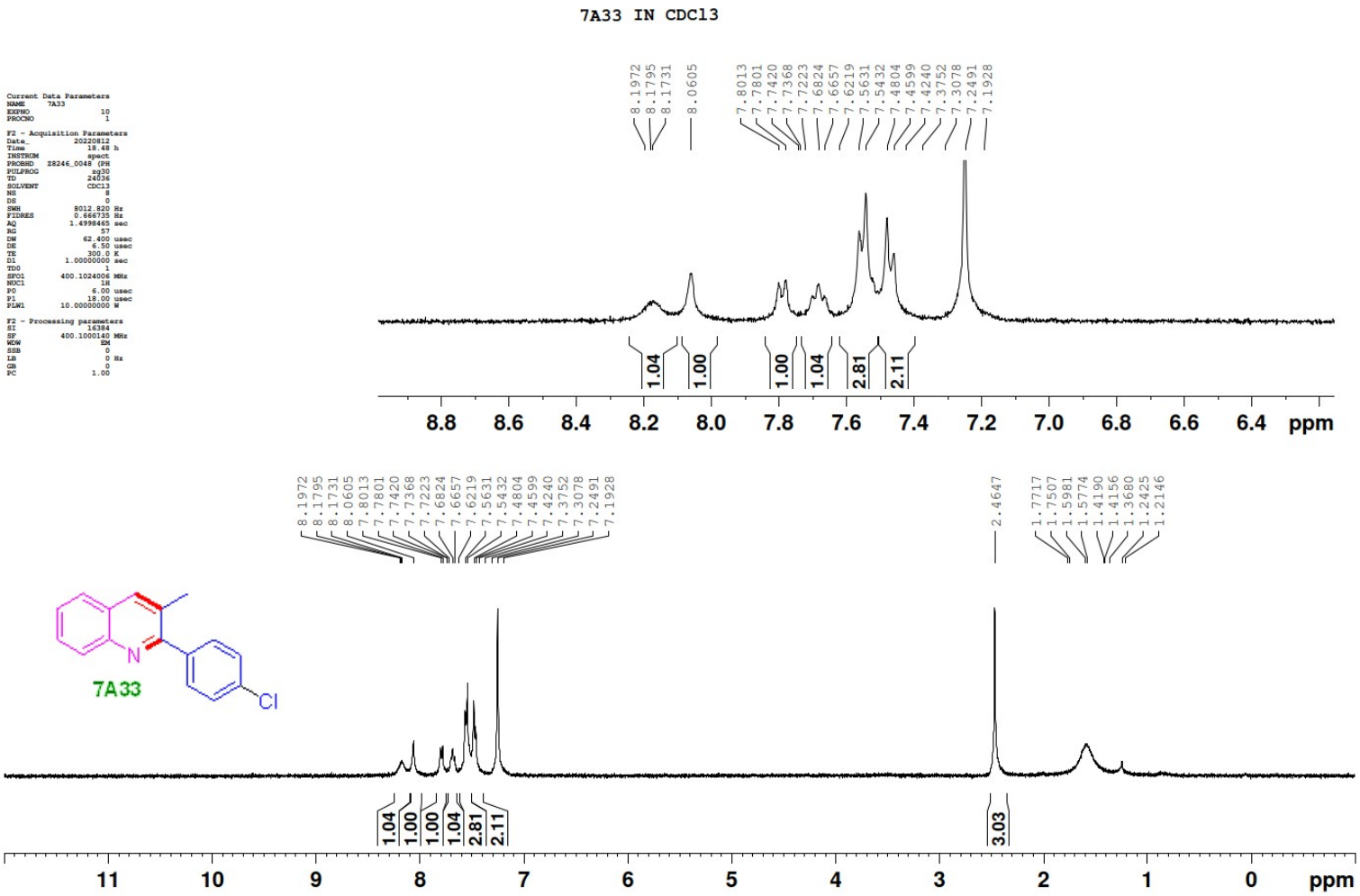

Current Data Parameters
NAME 7A31
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date 20220831
Time 23.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.326043 Hz
AQ 1.5335923 sec
RG 456
DW 62.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024714 MHz
F2 - Processing parameters
SI 16384
SF 400.2000159 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.2417
8.0071
7.9860
7.9280
7.9077
7.7227
7.7029
7.6842
7.5972
7.5782
7.5596
7.5181
7.4904
1.00
1.01
1.03
1.06
1.11
4.80
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
4.8267
3.3006
2.7985
2.7791
2.7591
1.5338
1.5156
1.4957
1.4771
1.4573
1.2793
1.2646
1.2460
1.2276
1.2093
1.1911
0.8906
0.8734
0.8154
0.7970
0.7787
2.10
2.12
2.11
3.12
N
7A31
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

7A32 IN CDCl3

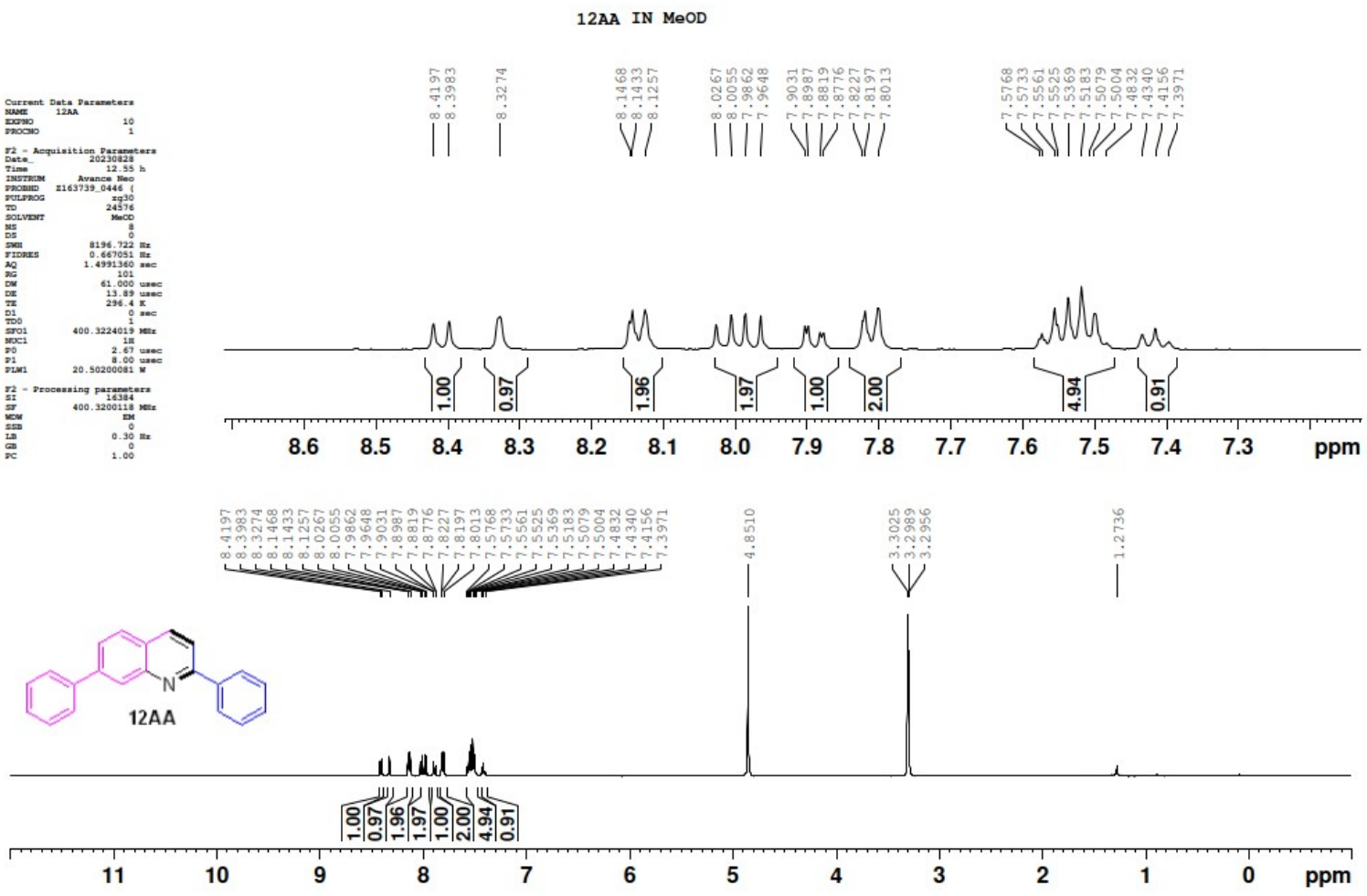




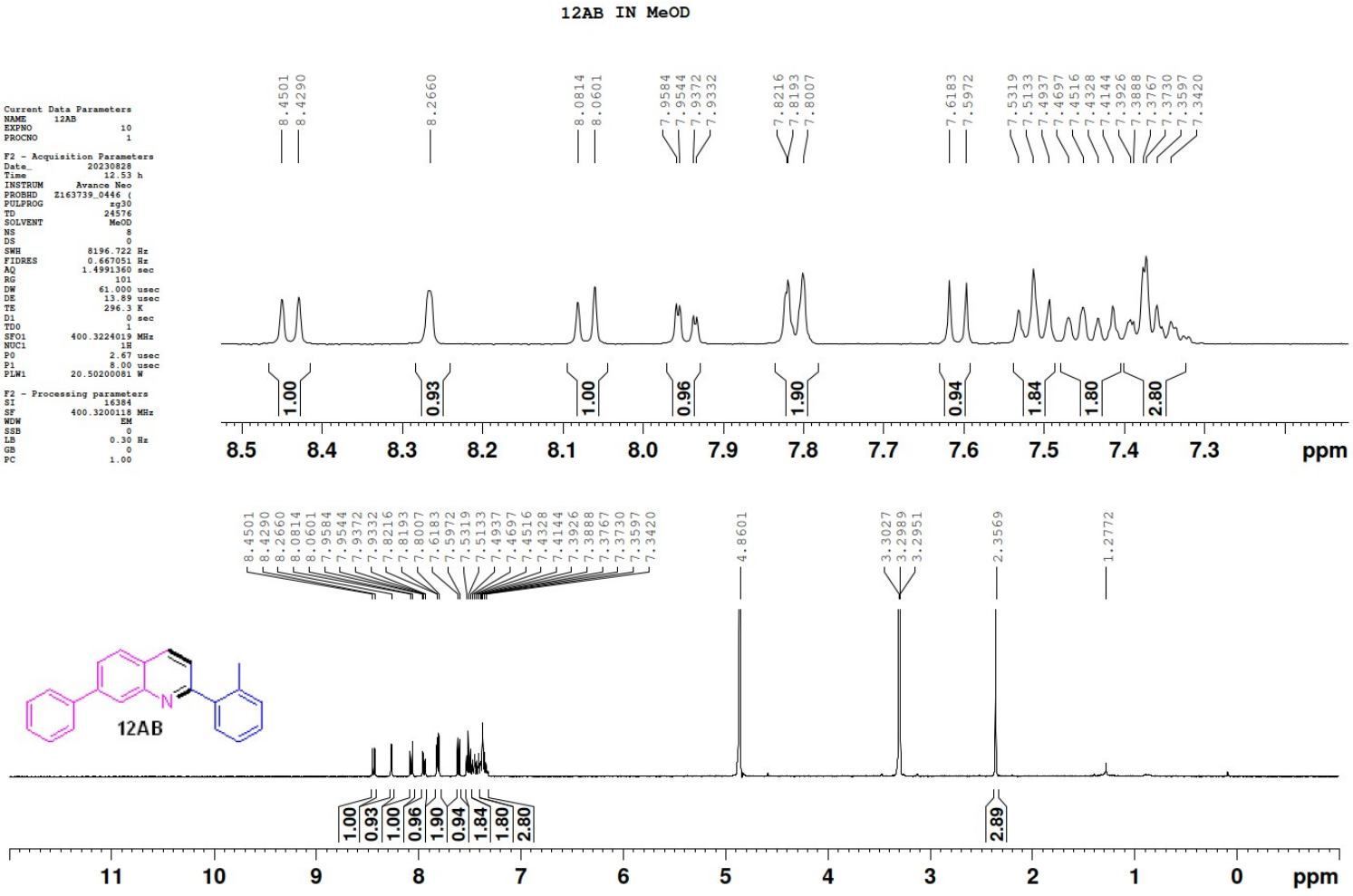
7A33 IN CDCl3



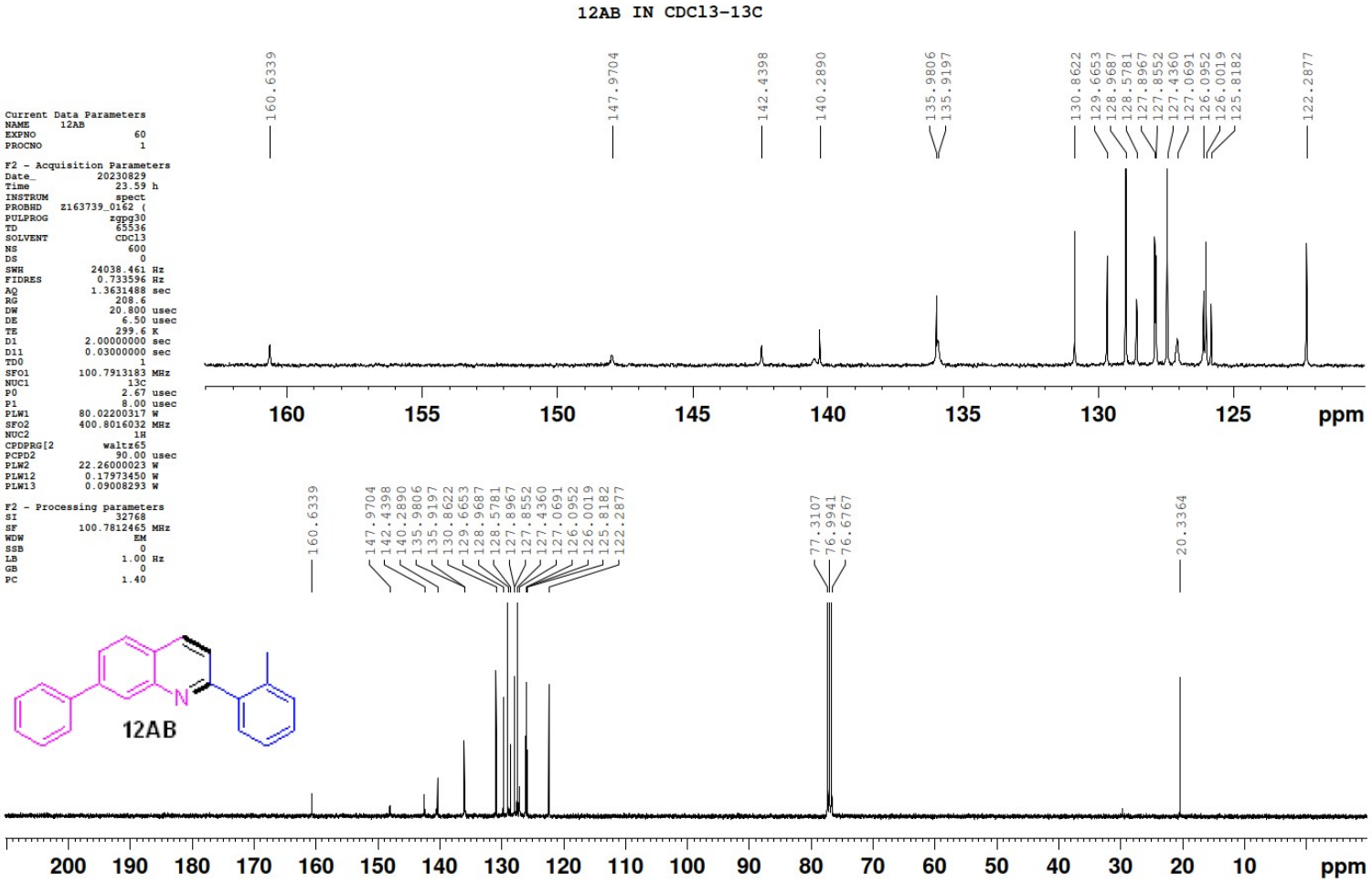
12AA IN MeOD

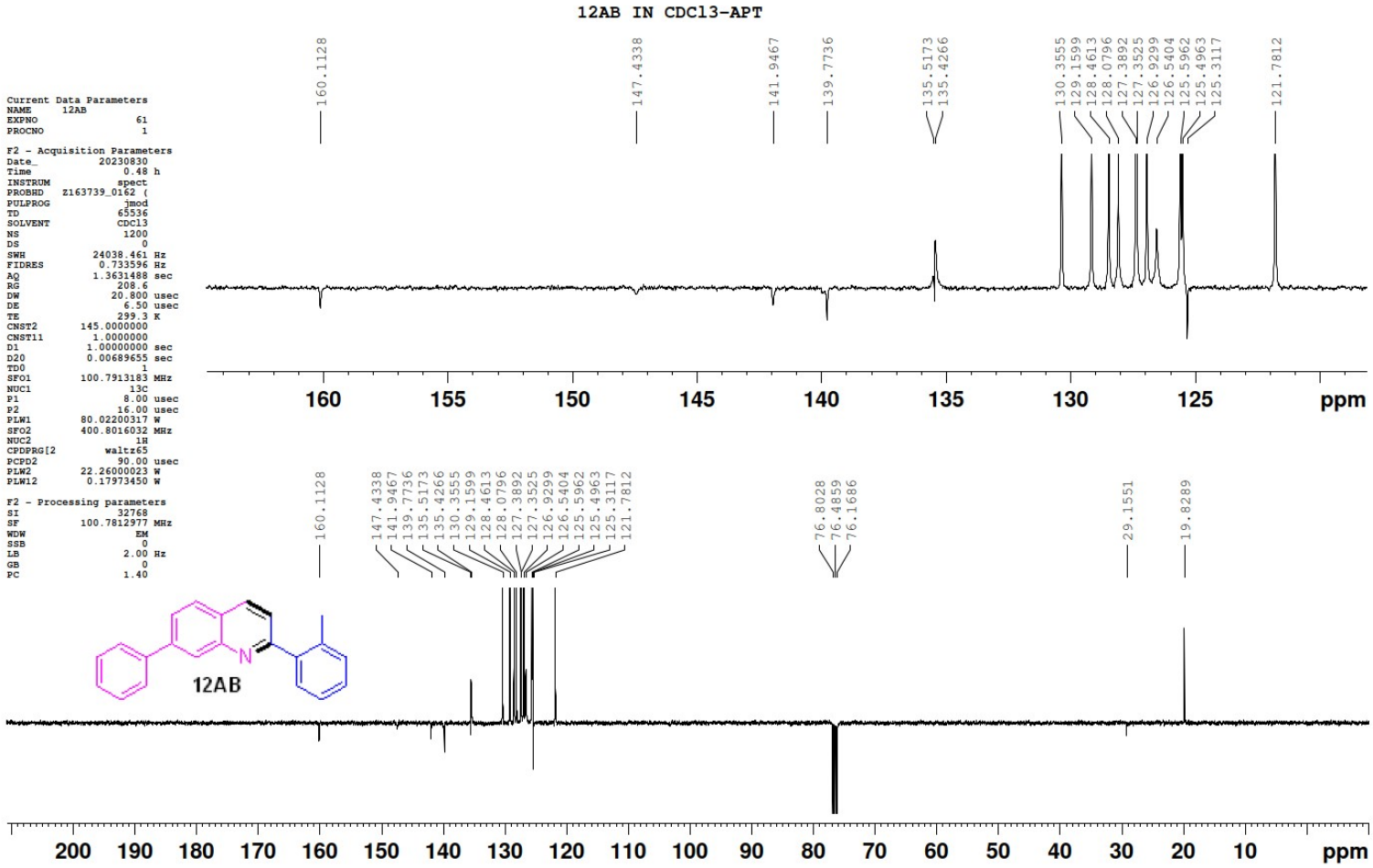

Current Data Parameters
NAME 12AA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230828
Time 12.55 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.4 K
D1 0 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 20.50200081 W
F2 - Processing parameters
SI 16384
SF 400.3200118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4197
8.3983
8.3274
8.1468
8.1433
8.1257
8.0267
8.0055
7.9862
7.9648
7.9031
7.8987
7.8819
7.8776
7.8227
7.8197
7.8013
7.5768
7.5733
7.5561
7.5525
7.5369
7.5183
7.5079
7.5004
7.4832
7.4340
7.4156
7.3971
1.00
0.97
1.96
1.97
1.00
2.00
4.94
0.91
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8510
3.3025
3.2989
3.2956
1.2736
N
12AA
11
10
9
8
7
6
5
4
3
2
1
0
ppm

12AB IN MeOD


Current Data Parameters
NAME 12AB
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230828
Time 12.53 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.3 K
D1 0 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 20.50200081 W
F2 - Processing parameters
SI 16384
SF 400.3200118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4501
8.4290
8.2660
8.0814
8.0601
7.9584
7.9544
7.9372
7.9332
7.8216
7.8193
7.8007
7.6183
7.5972
7.5319
7.5133
7.4937
7.4697
7.4516
7.4328
7.4144
7.3926
7.3888
7.3767
7.3730
7.3597
7.3420
1.00
0.93
1.00
0.96
1.90
0.94
1.84
1.80
2.80
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8601
3.3027
3.2989
3.2951
2.3569
1.2772
2.89
11
10
9
8
7
6
5
4
3
2
1
0
ppm
12AB

12AB IN CDCl3-13C



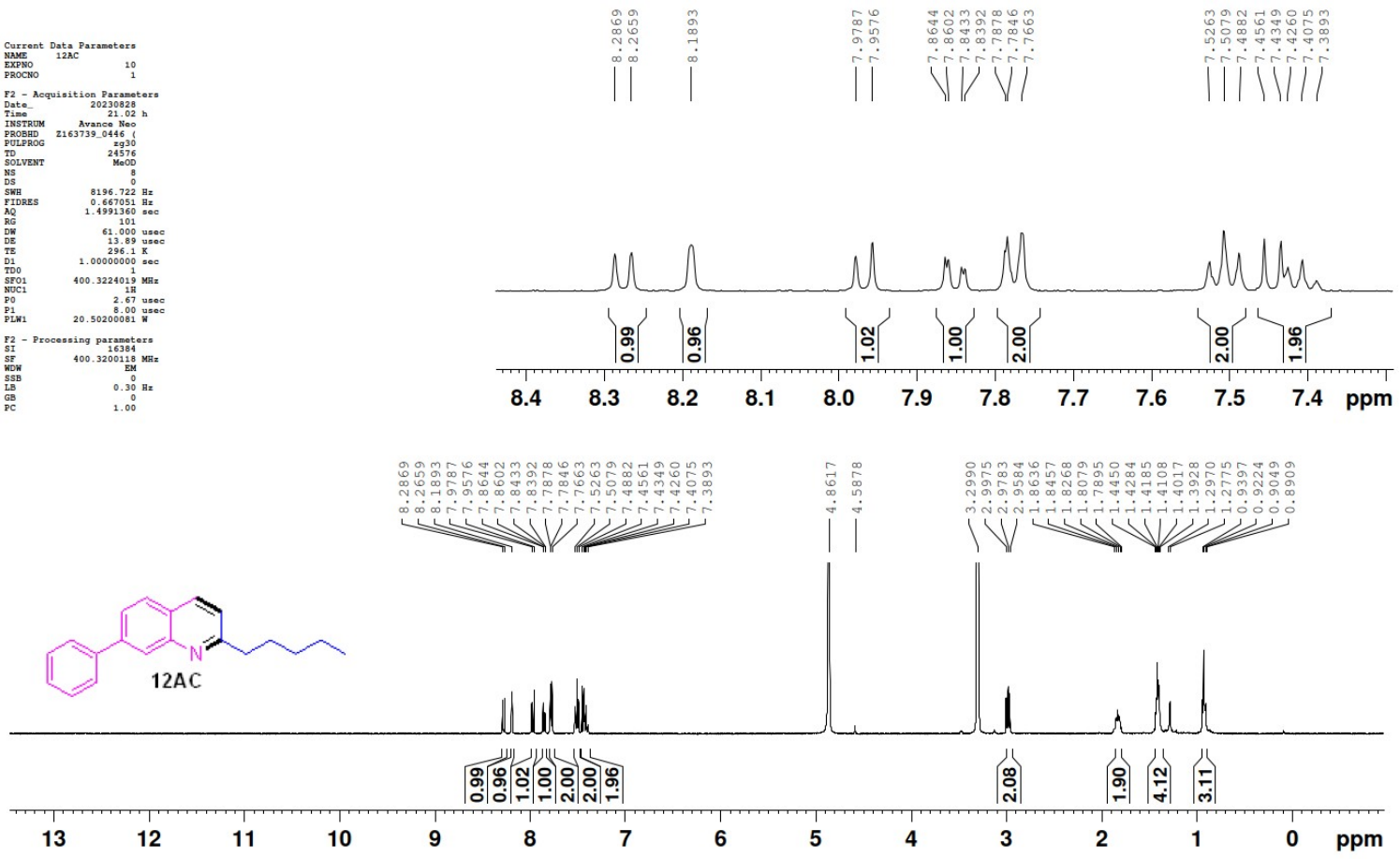

12AB IN CDCl3-APT
Current Data Parameters
NAME 12AB
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230830
Time 0.48 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 208.6
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.7913183 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 80.02200317 W
SFO2 400.8016032 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 22.26000023 W
PLW12 0.17973450 W
F2 - Processing parameters
SI 32768
SF 100.7812977 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
160.1128
147.4338
141.9467
139.7736
135.5173
135.4266
130.3555
129.1599
128.4613
128.0796
127.3892
127.3525
126.9299
126.5404
125.5962
125.4963
125.3117
121.7812
160 155 150 145 140 135 130 125 ppm
76.8028
76.4859
76.1686
29.1551
19.8289
N
12AB
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

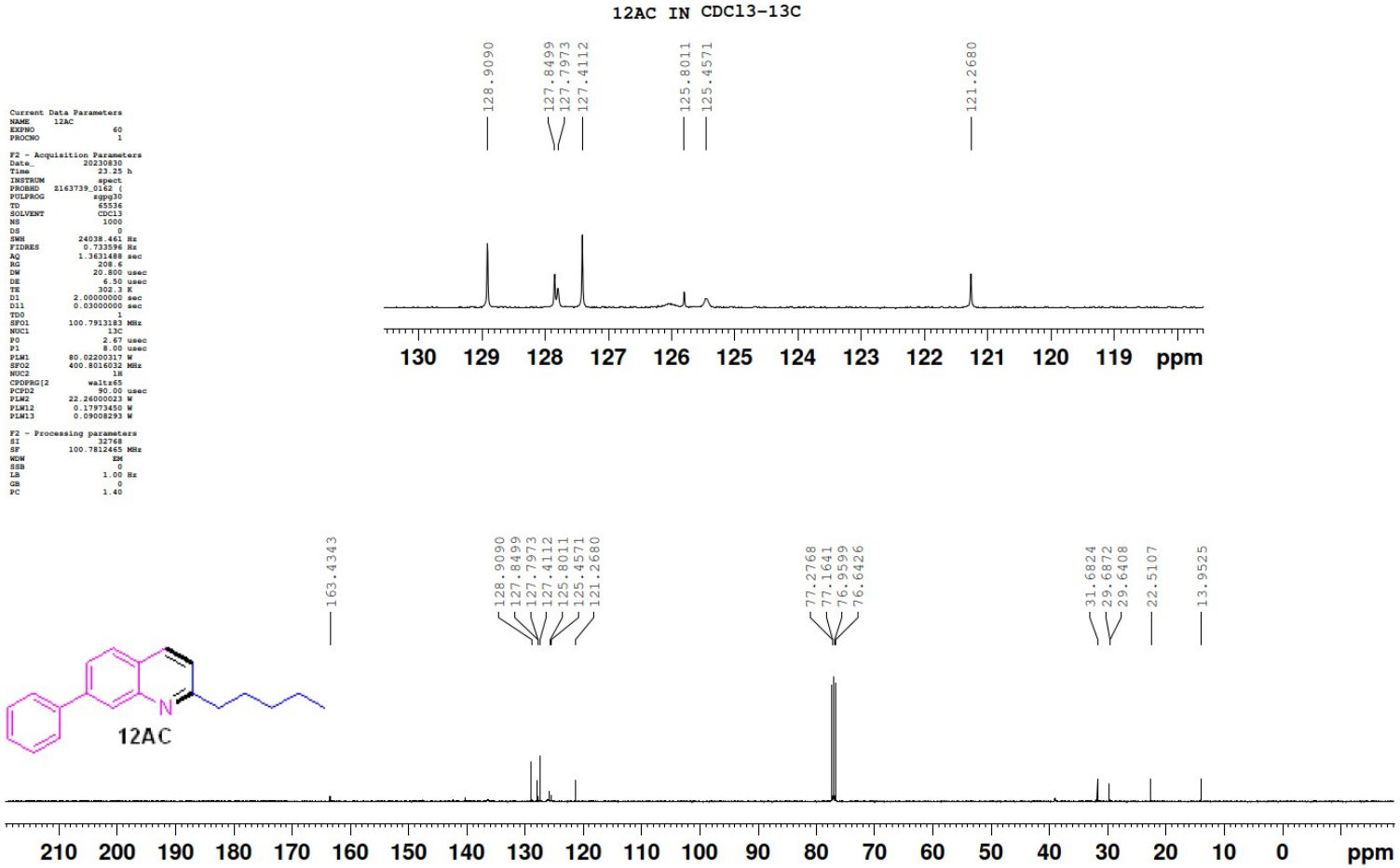
12AC IN MeOD

```
Current Data Parameters
NAME      12AC
EXPNO           10
PROCNO           1

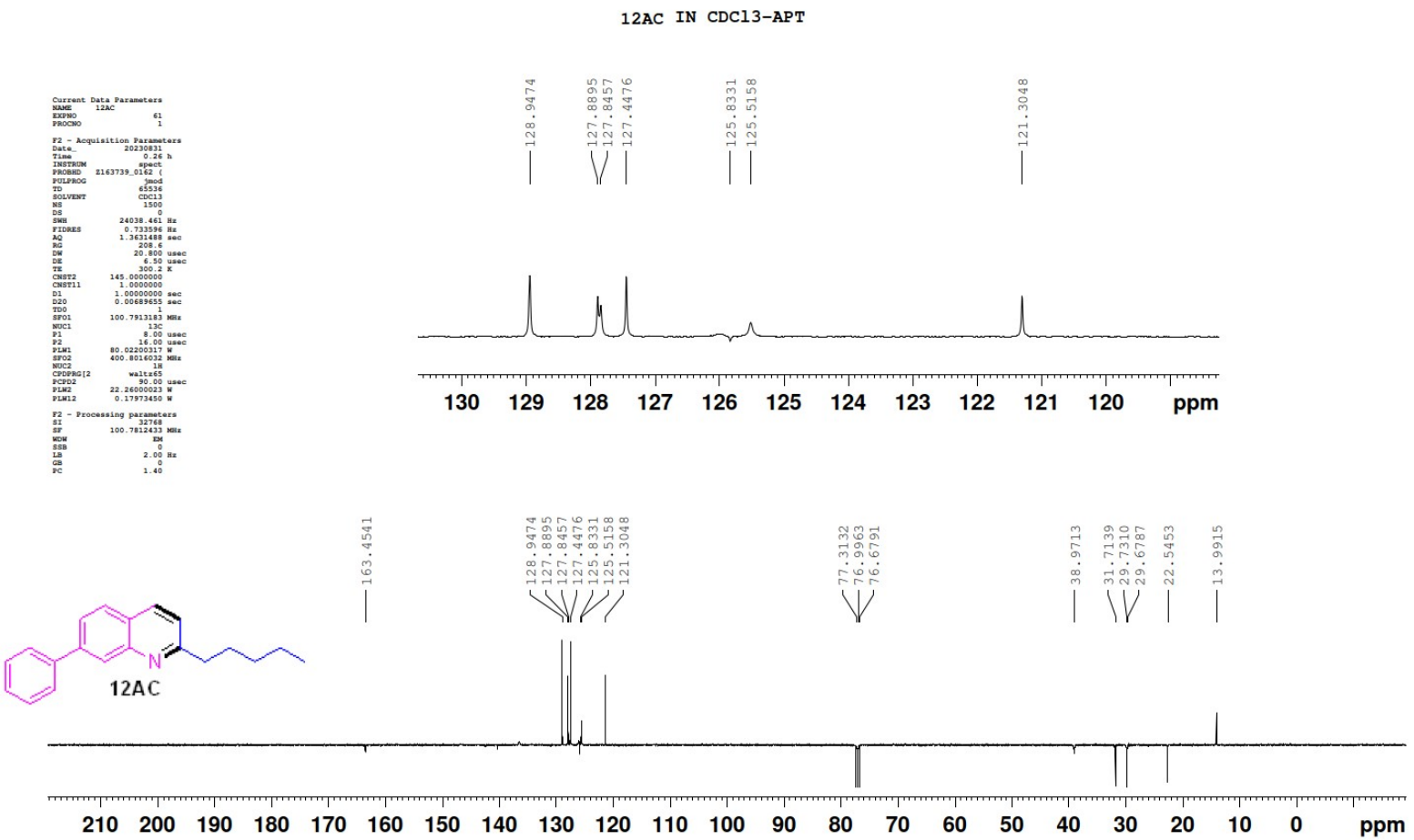
F2 - Acquisition Parameters
Date_      20230828
Time         21.02 h
INSTRUM      Avance Neo
PROBHD   Z163739_0446 (
PULPROG         zg30
TD             24576
SOLVENT          MeOD
NS                8
DS                0
SWH         8196.722 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG              101
DW            61.000 usec
DE            13.89 usec
TE            296.1 K
D1         1.00000000 sec
TD0               1
SFO1      400.3224019 MHz
NUC1             1H
P0             2.67 usec
P1             8.00 usec
PLW1      20.50200081 W

F2 - Processing parameters
SI            16384
SF        400.3200118 MHz
WDW              EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```

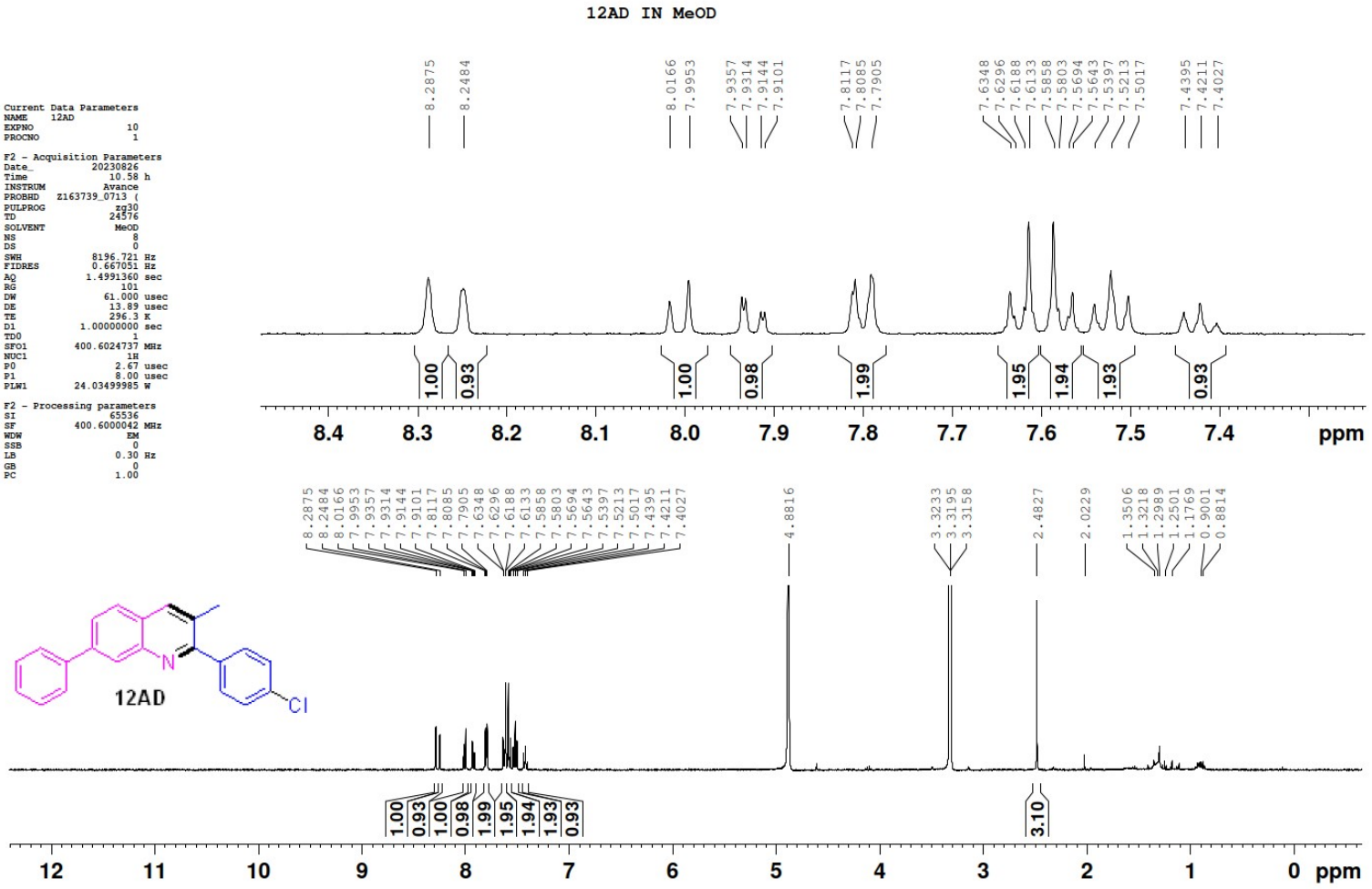



12AC IN CDCl3-13C
Current Data Parameters
NAME 12AC
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230830
Time 23.25 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 208.6
DW 20.800 usec
DE 6.50 usec
TE 302.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.7913183 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 80.02200317 W
SFO2 400.8016032 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 22.26000023 W
PLW12 0.17973450 W
PLW13 0.09008293 W
F2 - Processing parameters
SI 32768
SF 100.7812465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
128.9090
127.8499
127.7973
127.4112
125.8011
125.4571
121.2680
130 129 128 127 126 125 124 123 122 121 120 119 ppm
163.4343
128.9090
127.8499
127.7973
127.4112
125.8011
125.4571
121.2680
77.2768
77.1641
76.9599
76.6426
31.6824
29.6872
29.6408
22.5107
13.9525
N
12AC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

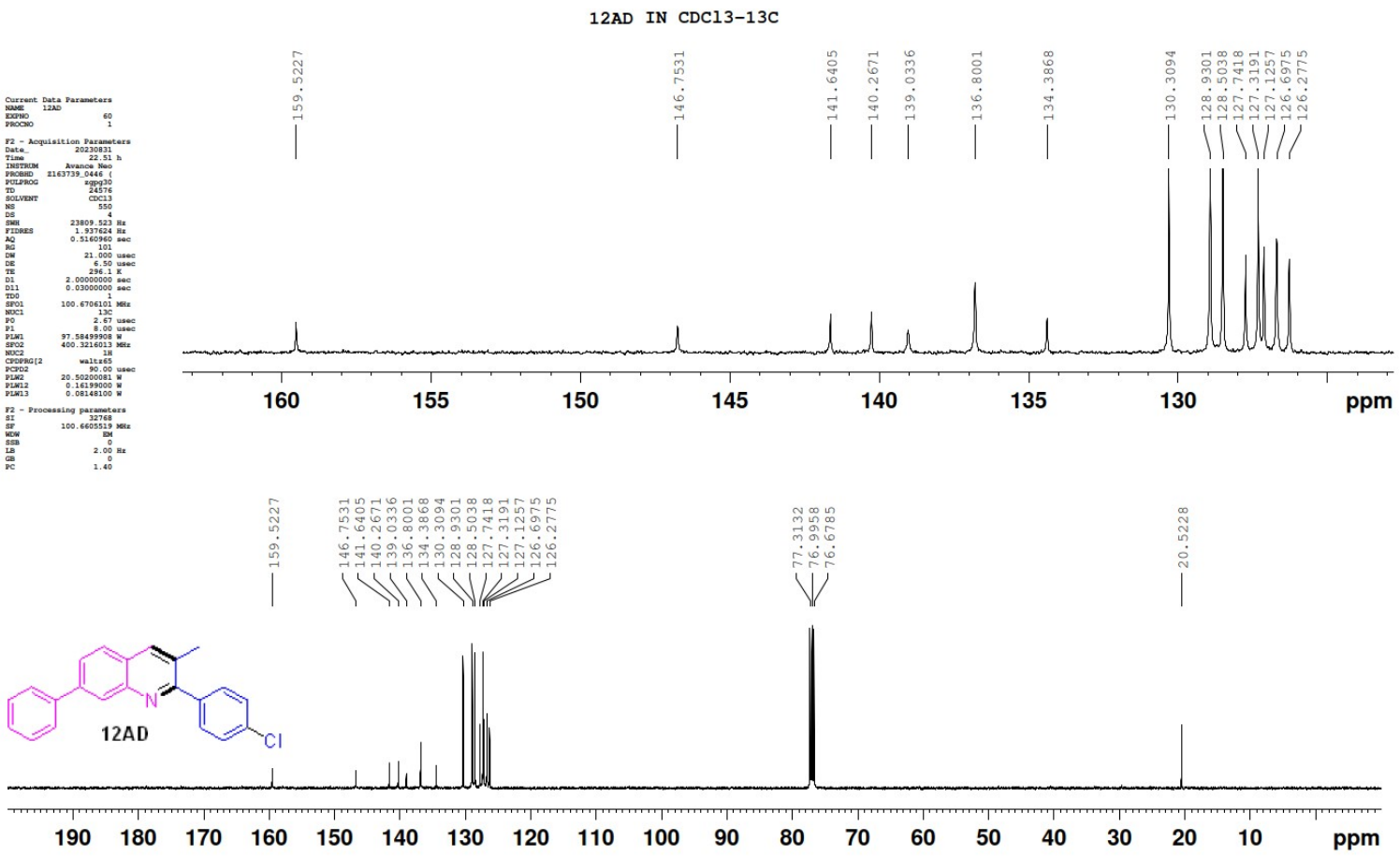
12AC IN CDCl3-APT

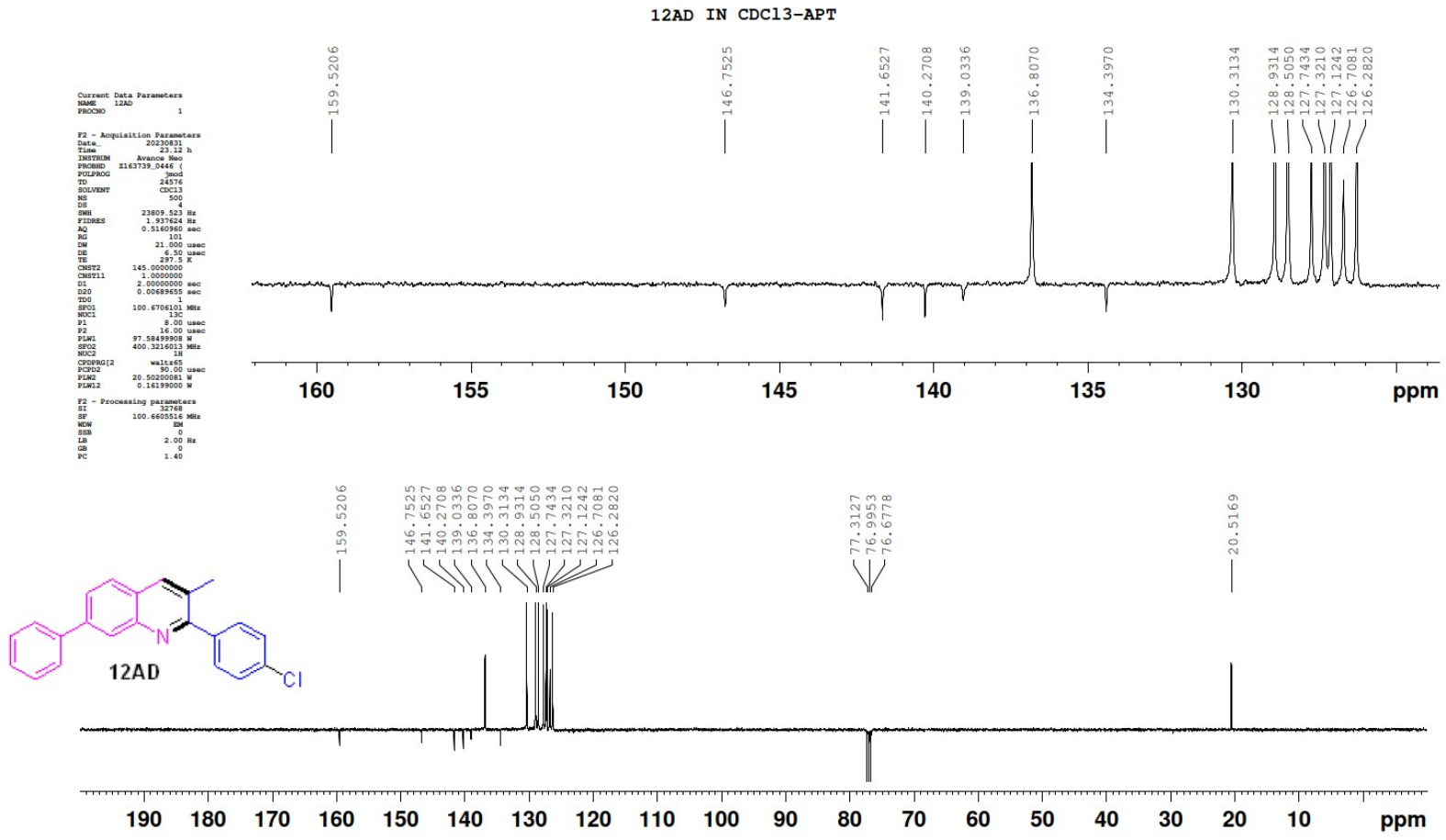


12AD IN MeOD

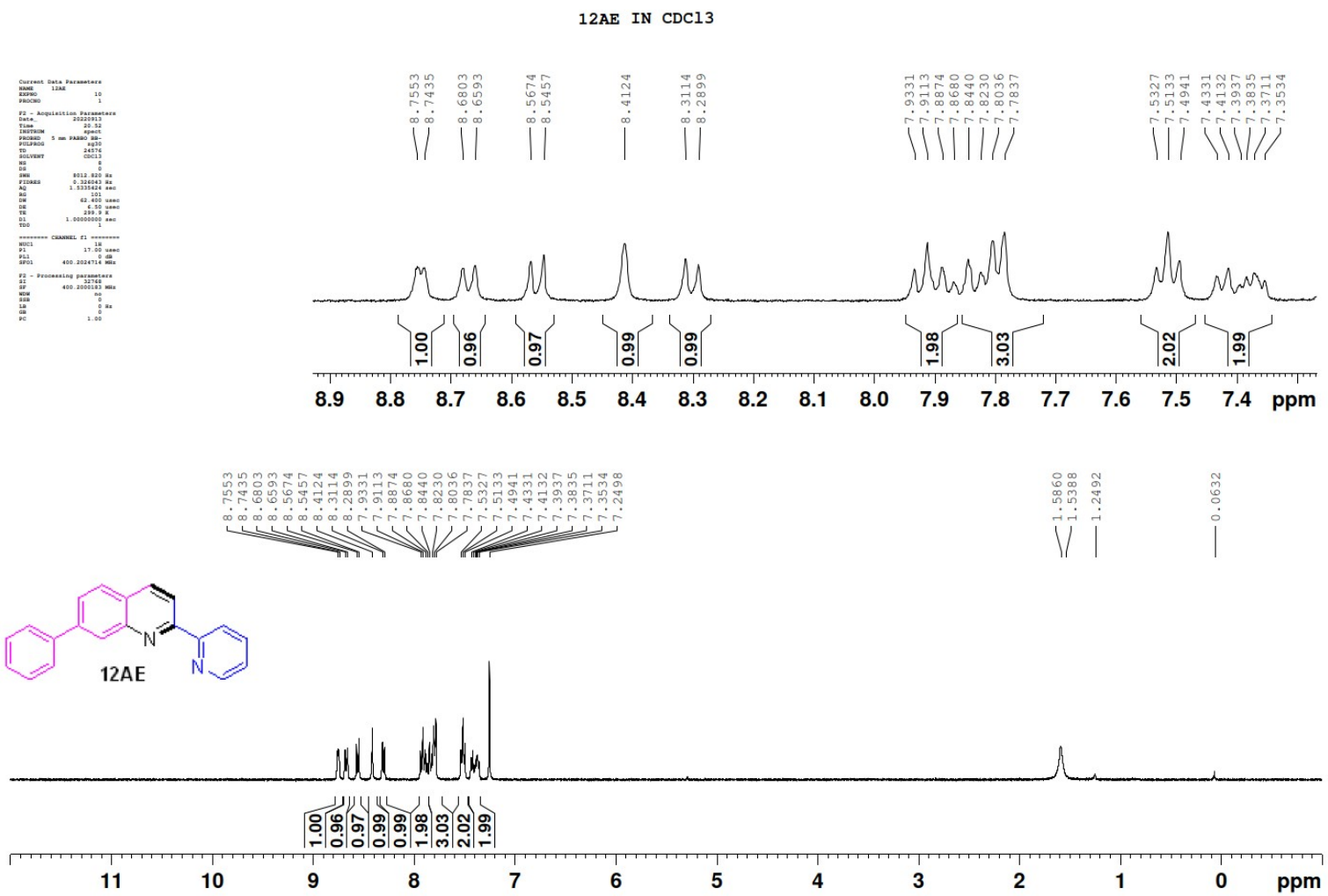

Current Data Parameters
NAME 12AD
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230826
Time 10.58 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.2875
8.2484
8.0166
7.9953
7.9357
7.9314
7.9144
7.9101
7.8117
7.8085
7.7905
7.6348
7.6296
7.6188
7.6133
7.5858
7.5803
7.5694
7.5643
7.5397
7.5213
7.5017
7.4395
7.4211
7.4027
1.00
0.93
1.00
0.98
1.99
1.95
1.94
1.93
0.93
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
4.8816
3.3233
3.3195
3.3158
2.4827
2.0229
1.3506
1.3218
1.2989
1.2501
1.1769
0.9001
0.8814
3.10
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
12AD
N
Cl

12AD IN CDCl3-13C

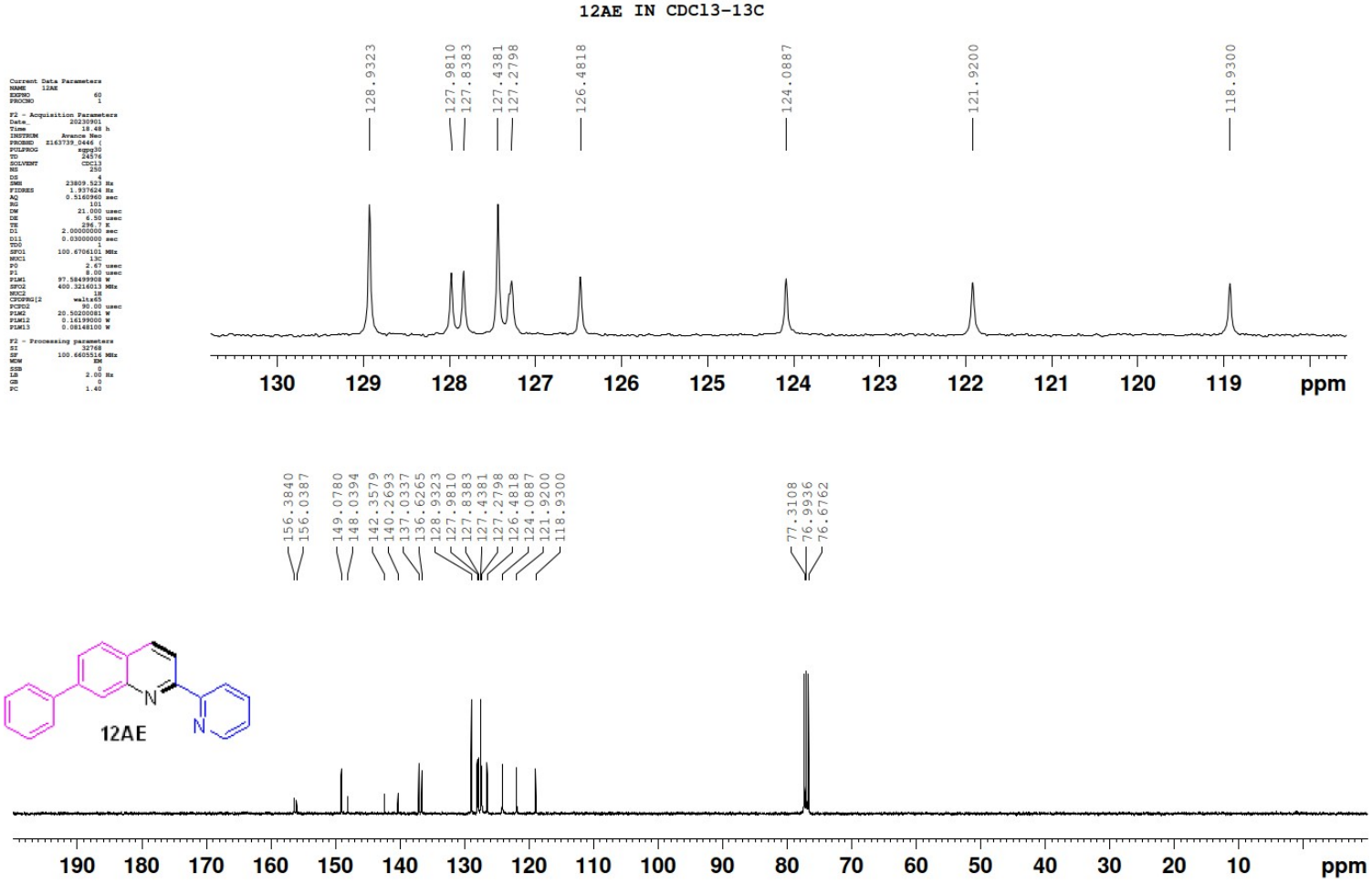



12AD IN CDCl3-APT
Current Data Parameters
NAME 12AD
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230831
Time 23.12 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG jmod
TD 24576
SOLVENT CDCl3
NS 500
DS 4
SWH 23809.523 Hz
FIDRES 1.937624 Hz
AQ 0.5160960 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 297.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 97.58499908 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 20.50200081 W
PLW12 0.16199000 W
F2 - Processing parameters
SI 32768
SF 100.6605516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
159.5206
146.7525
141.6527
140.2708
139.0336
136.8070
134.3970
130.3134
128.9314
128.5050
127.7434
127.3210
127.1242
126.7081
126.2820
160
155
150
145
140
135
130
ppm
159.5206
146.7525
141.6527
140.2708
139.0336
136.8070
134.3970
130.3134
128.9314
128.5050
127.7434
127.3210
127.1242
126.7081
126.2820
77.3127
76.9953
76.6778
20.5169
N
Cl
12AD
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

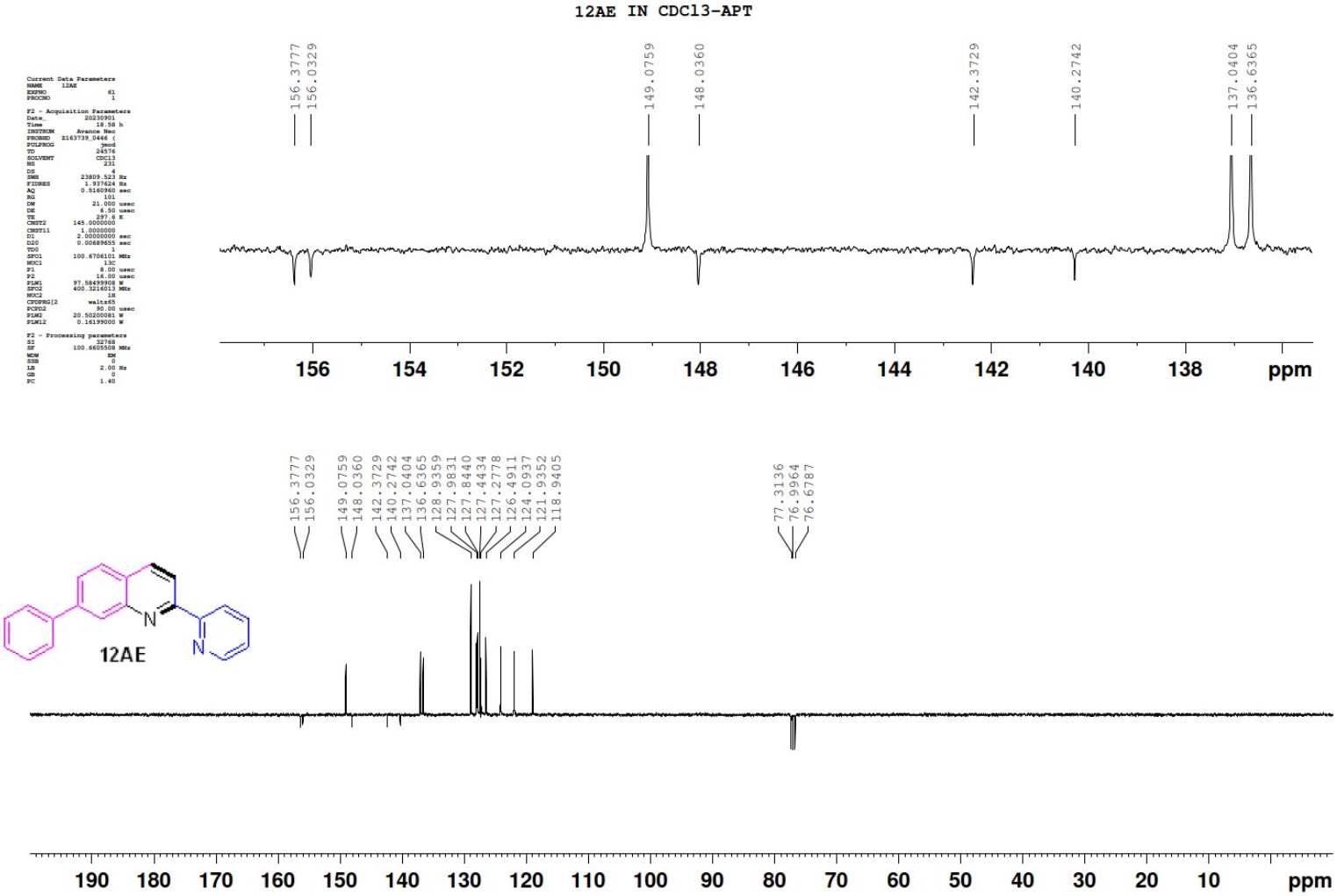
12AE IN CDCl3



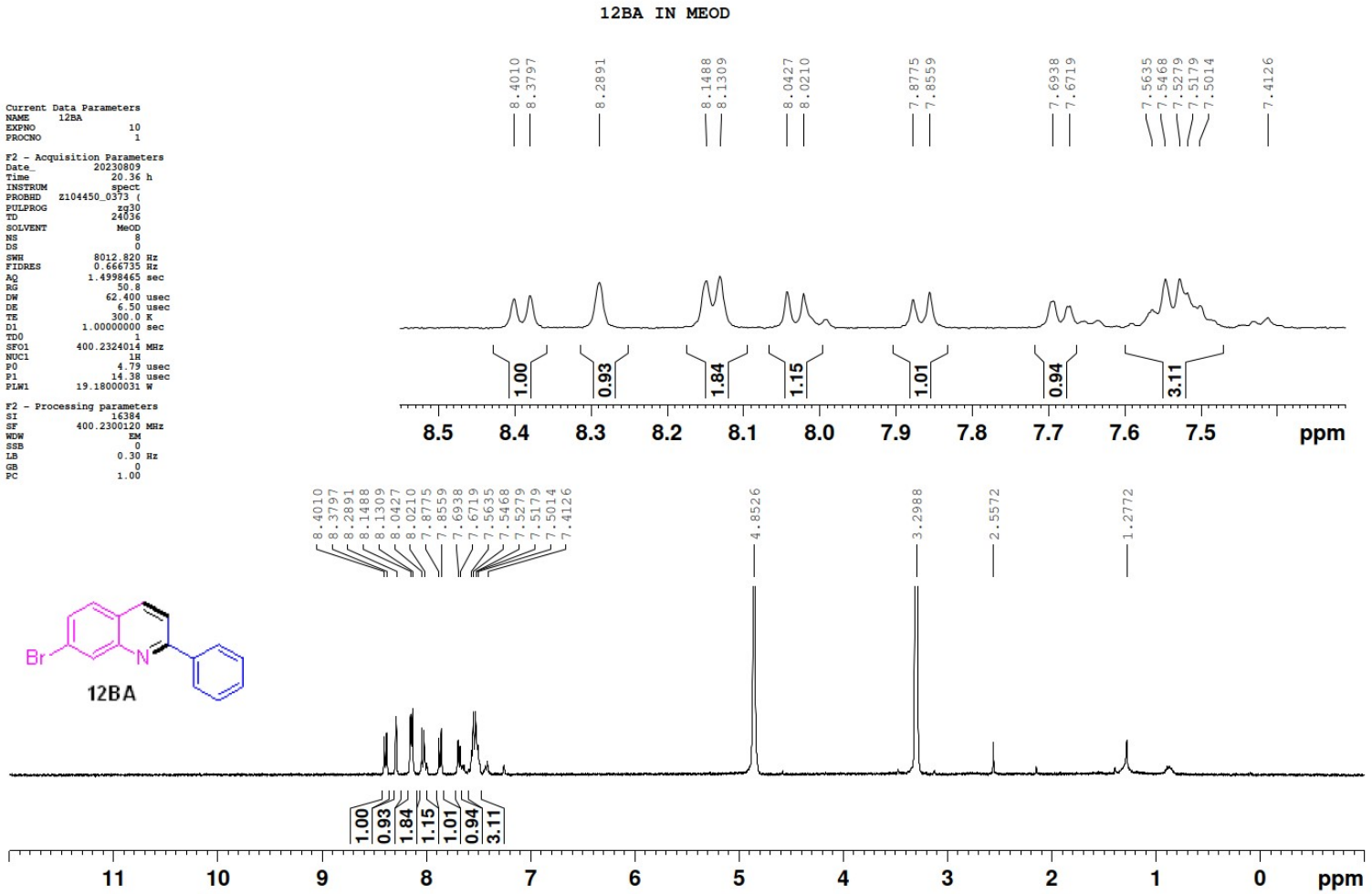
12AE IN CDCl3-13C

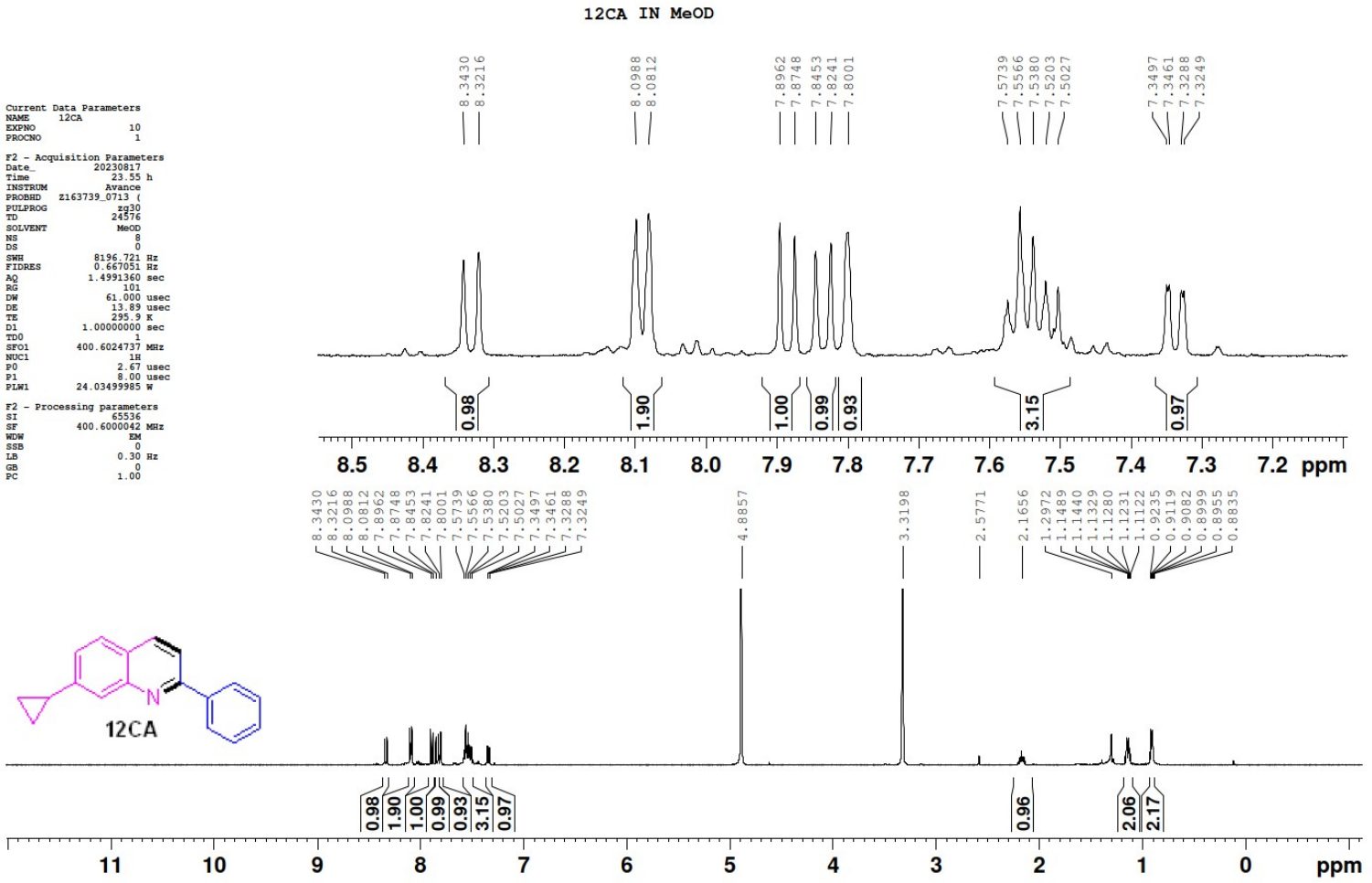


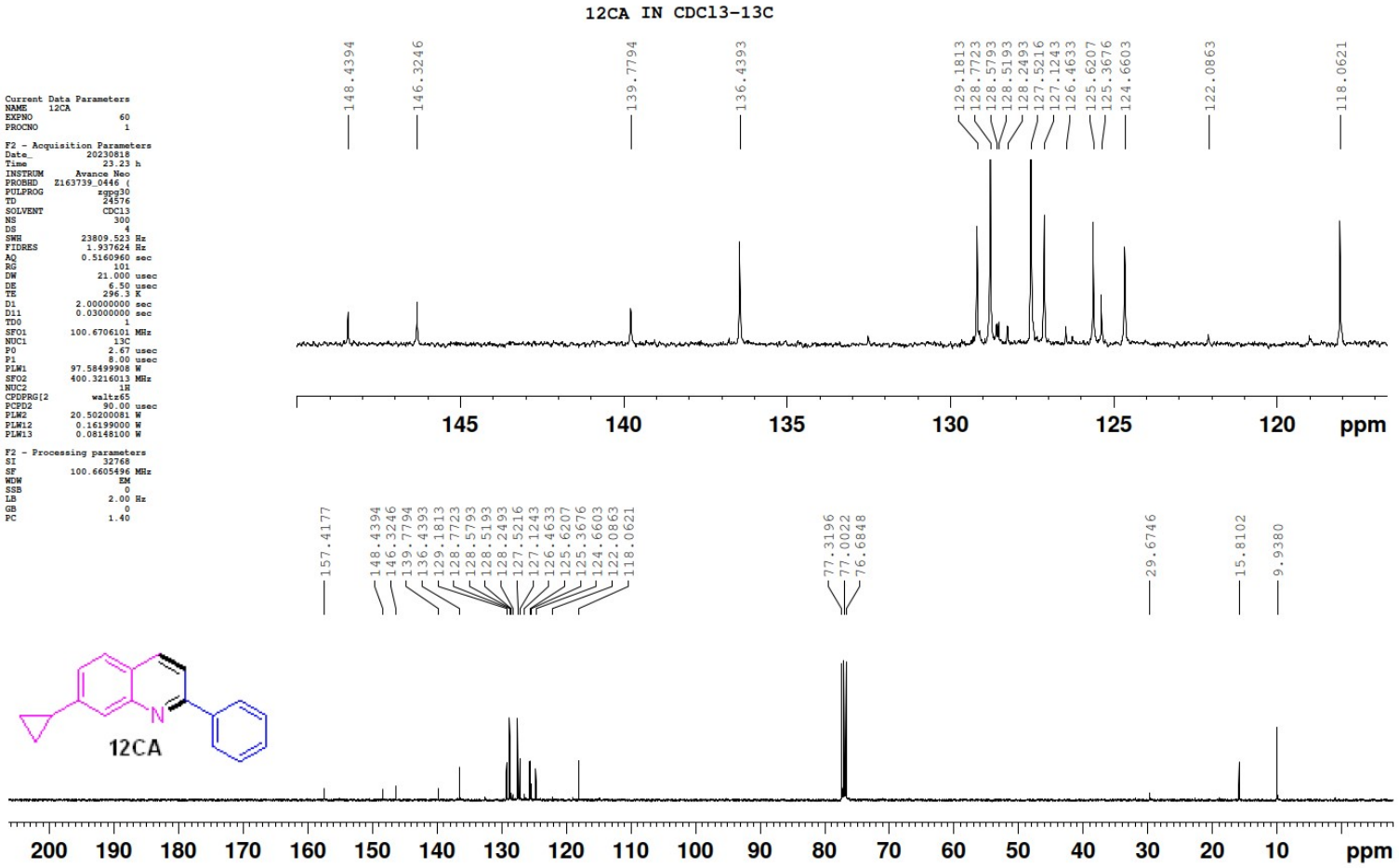
12AE IN CDCl3-APT

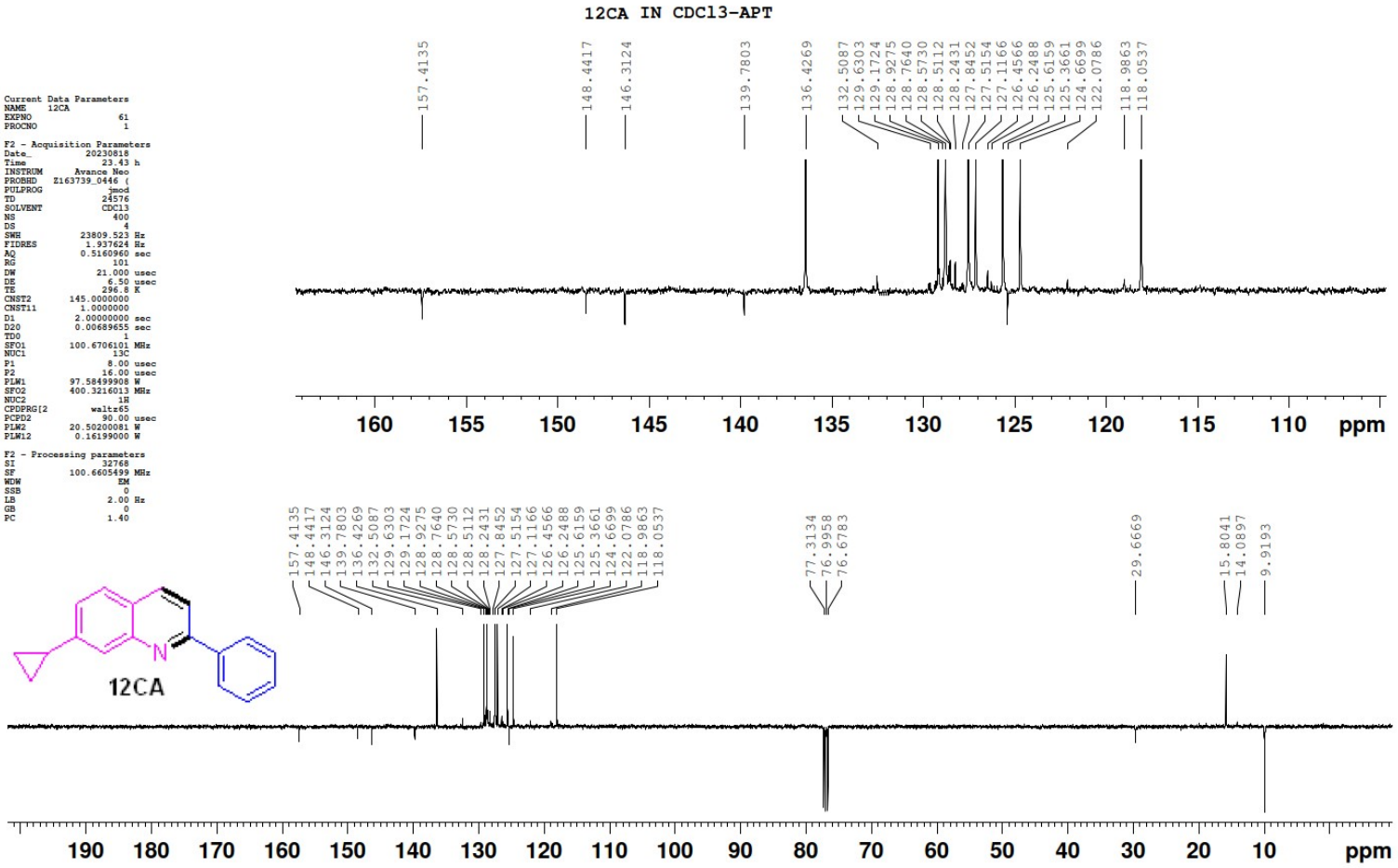


12BA IN MEOD

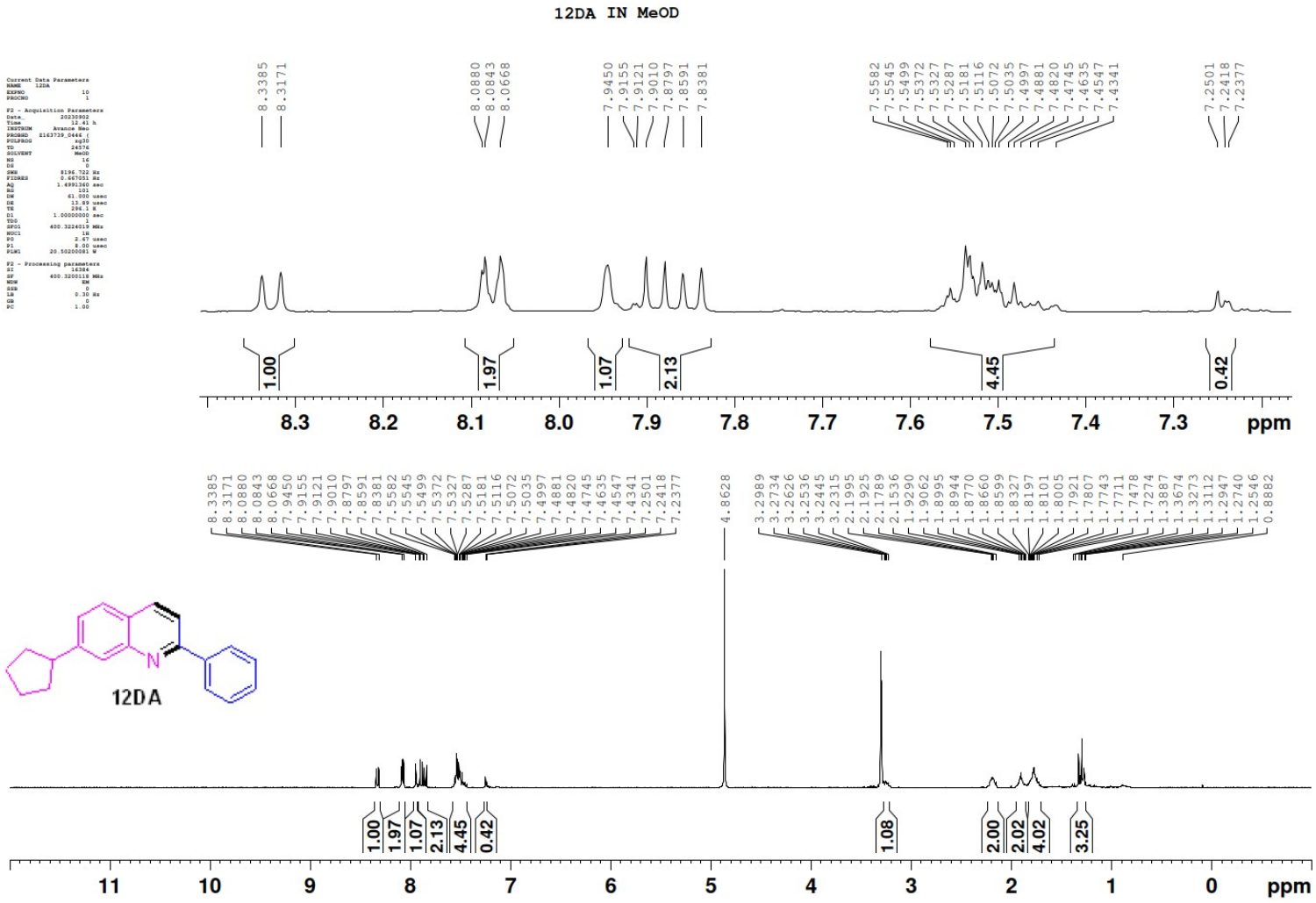

Current Data Parameters
NAME 12BA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230809
Time 20.36 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4010
8.3797
8.2891
8.1488
8.1309
8.0427
8.0210
7.8775
7.8559
7.6938
7.6719
7.5635
7.5468
7.5279
7.5179
7.5014
7.4126
1.00
0.93
1.84
1.15
1.01
0.94
3.11
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
ppm
4.8526
3.2988
2.5572
1.2772
11
10
9
8
7
6
5
4
3
2
1
0
ppm
Br
N
12BA


12CA IN MeOD
Current Data Parameters
NAME 12CA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230817
Time 23.55 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3430
8.3216
8.0988
8.0812
7.8962
7.8748
7.8453
7.8241
7.8001
7.5739
7.5566
7.5380
7.5203
7.5027
7.3497
7.3461
7.3288
7.3249
0.98
1.90
1.00
0.99
0.93
3.15
0.97
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
4.8857
3.3198
2.5771
2.1656
1.2972
1.1489
1.1440
1.1329
1.1280
1.1231
1.1122
0.9235
0.9119
0.9082
0.8999
0.8955
0.8835
0.96
2.06
2.17
11 10 9 8 7 6 5 4 3 2 1 0 ppm
N
12CA

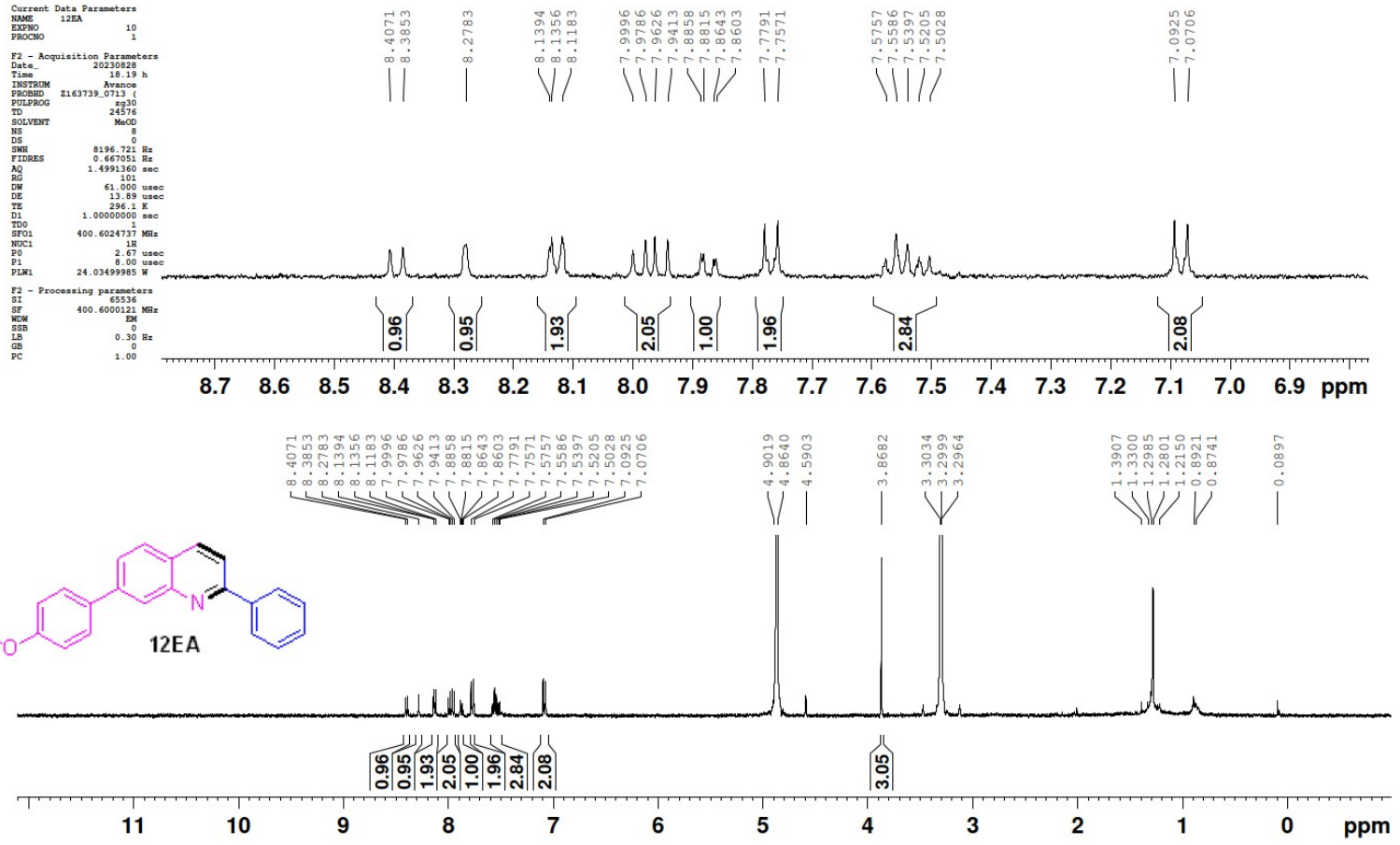

12CA IN CDCl3-13C
Current Data Parameters
NAME 12CA
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230818
Time 23.23 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zgpg30
TD 24576
SOLVENT CDCl3
NS 300
DS 4
SWH 23809.523 Hz
FIDRES 1.937624 Hz
AQ 0.5160960 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 97.58499908 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 20.50200081 W
PLW12 0.16199000 W
PLW13 0.08148100 W
F2 - Processing parameters
SI 32768
SF 100.6605496 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
148.4394
146.3246
139.7794
136.4393
129.1813
128.7723
128.5793
128.5193
128.2493
127.5216
127.1243
126.4633
125.6207
125.3676
124.6603
122.0863
118.0621
145
140
135
130
125
120
ppm
157.4177
148.4394
146.3246
139.7794
136.4393
129.1813
128.7723
128.5793
128.5193
128.2493
127.5216
127.1243
126.4633
125.6207
125.3676
124.6603
122.0863
118.0621
77.3196
77.0022
76.6848
29.6746
15.8102
9.9380
N
12CA
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


12CA IN CDCl3-APT
Current Data Parameters
NAME 12CA
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230818
Time 23.43 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG jmod
TD 24576
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 1.937624 Hz
AQ 0.5160960 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 296.8 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 97.58499908 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 20.50200081 W
PLW12 0.16199000 W
F2 - Processing parameters
SI 32768
SF 100.6605499 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
157.4135
148.4417
146.3124
139.7803
136.4269
132.5087
129.6303
129.1724
128.9275
128.7640
128.5730
128.5112
128.2431
127.8452
127.5154
127.1166
126.4566
126.2488
125.6159
125.3661
124.6699
122.0786
118.9863
118.0537
160 155 150 145 140 135 130 125 120 115 110 ppm
77.3134
76.9958
76.6783
29.6669
15.8041
14.0897
9.9193
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
N
12CA

12DA IN MeOD


8.3385
8.3171
8.0880
8.0843
8.0668
7.9450
7.9155
7.9121
7.9010
7.8797
7.8591
7.8381
7.5582
7.5545
7.5499
7.5372
7.5327
7.5287
7.5181
7.5116
7.5072
7.5035
7.4997
7.4881
7.4820
7.4745
7.4635
7.4547
7.4341
7.2501
7.2418
7.2377
1.00
1.97
1.07
2.13
4.45
0.42
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8628
3.2989
3.2734
3.2626
3.2536
3.2445
3.2315
2.1995
2.1925
2.1789
2.1536
1.9290
1.9062
1.8995
1.8944
1.8770
1.8660
1.8599
1.8327
1.8197
1.8101
1.8005
1.7921
1.7807
1.7743
1.7711
1.7478
1.7274
1.3887
1.3674
1.3273
1.3112
1.2947
1.2740
1.2546
0.8882
1.08
2.00
2.02
4.02
3.25
11
10
9
8
7
6
5
4
3
2
1
0
ppm
12DA

12EA IN MeOD

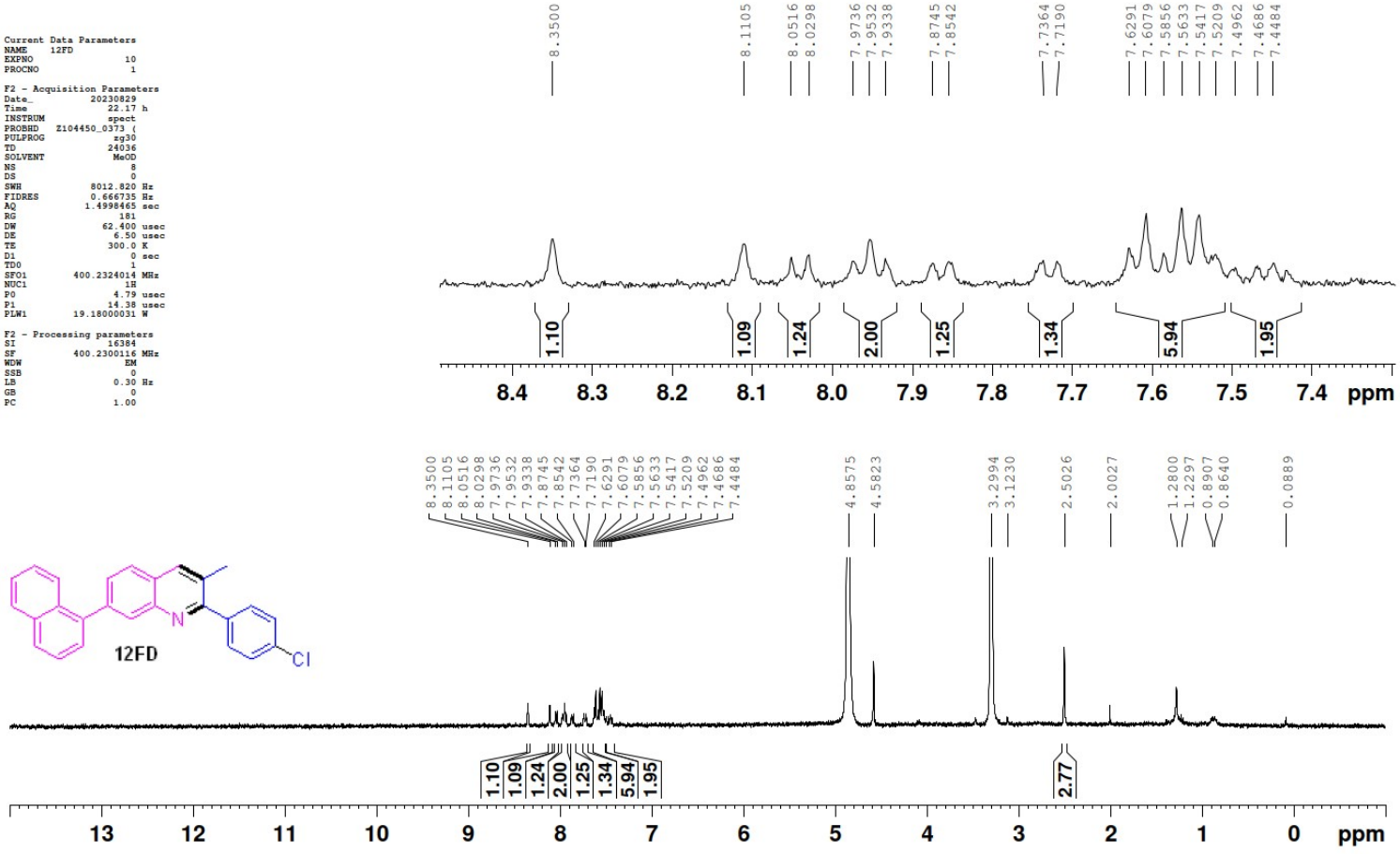

Current Data Parameters
NAME 12EA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230828
Time 18.19 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4071
8.3853
8.2783
8.1394
8.1356
8.1183
7.9996
7.9786
7.9626
7.9413
7.8858
7.8815
7.8643
7.8603
7.7791
7.7571
7.5757
7.5586
7.5397
7.5205
7.5028
7.0925
7.0706
0.96
0.95
1.93
2.05
1.00
1.96
2.84
2.08
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
4.9019
4.8640
4.5903
3.8682
3.3034
3.2999
3.2964
1.3907
1.3300
1.2985
1.2801
1.2150
0.8921
0.8741
0.0897
3.05
11 10 9 8 7 6 5 4 3 2 1 0 ppm
12EA

12FD IN MeOD

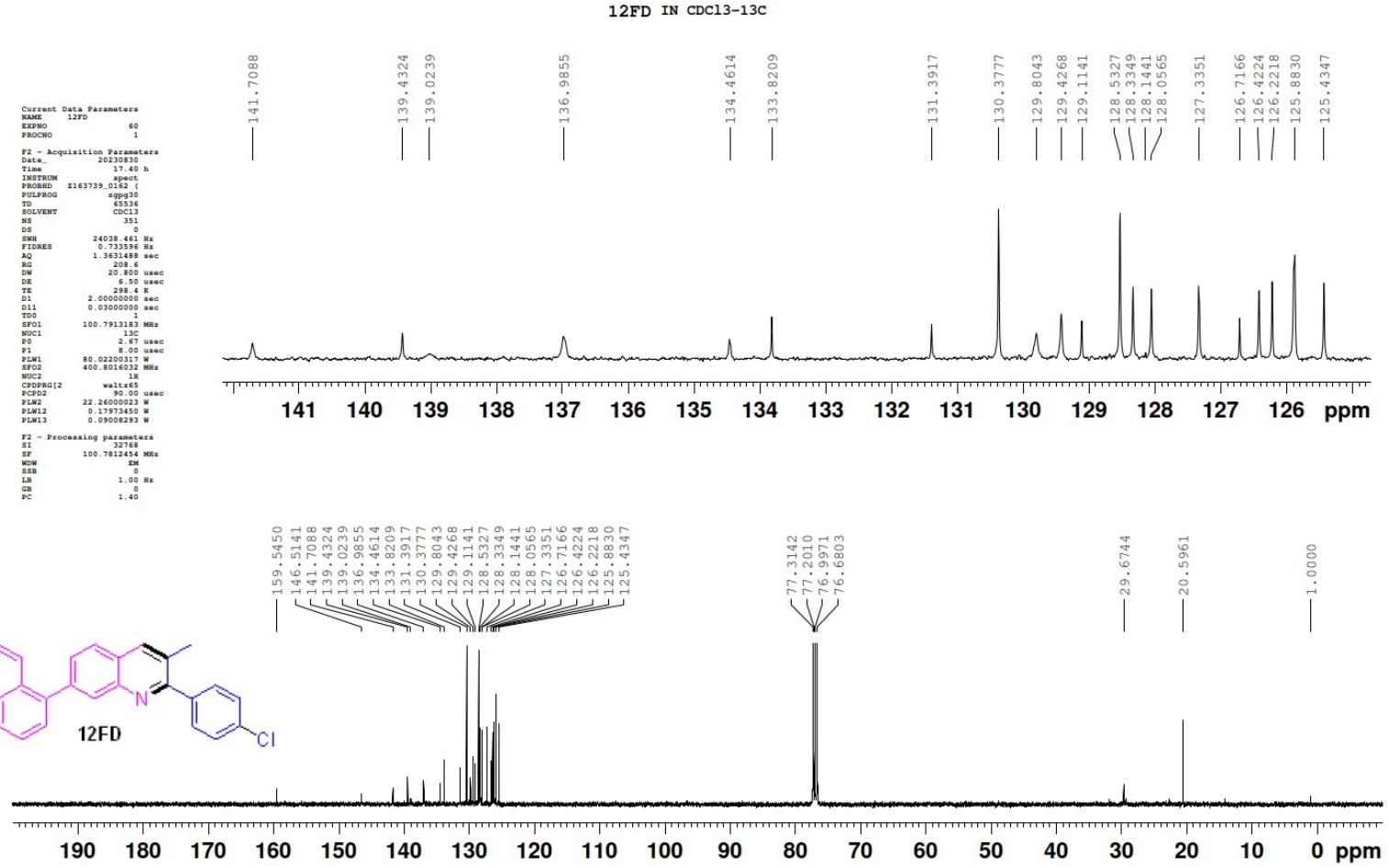
```
Current Data Parameters
NAME      12FD
EXPNO           10
PROCNO           1

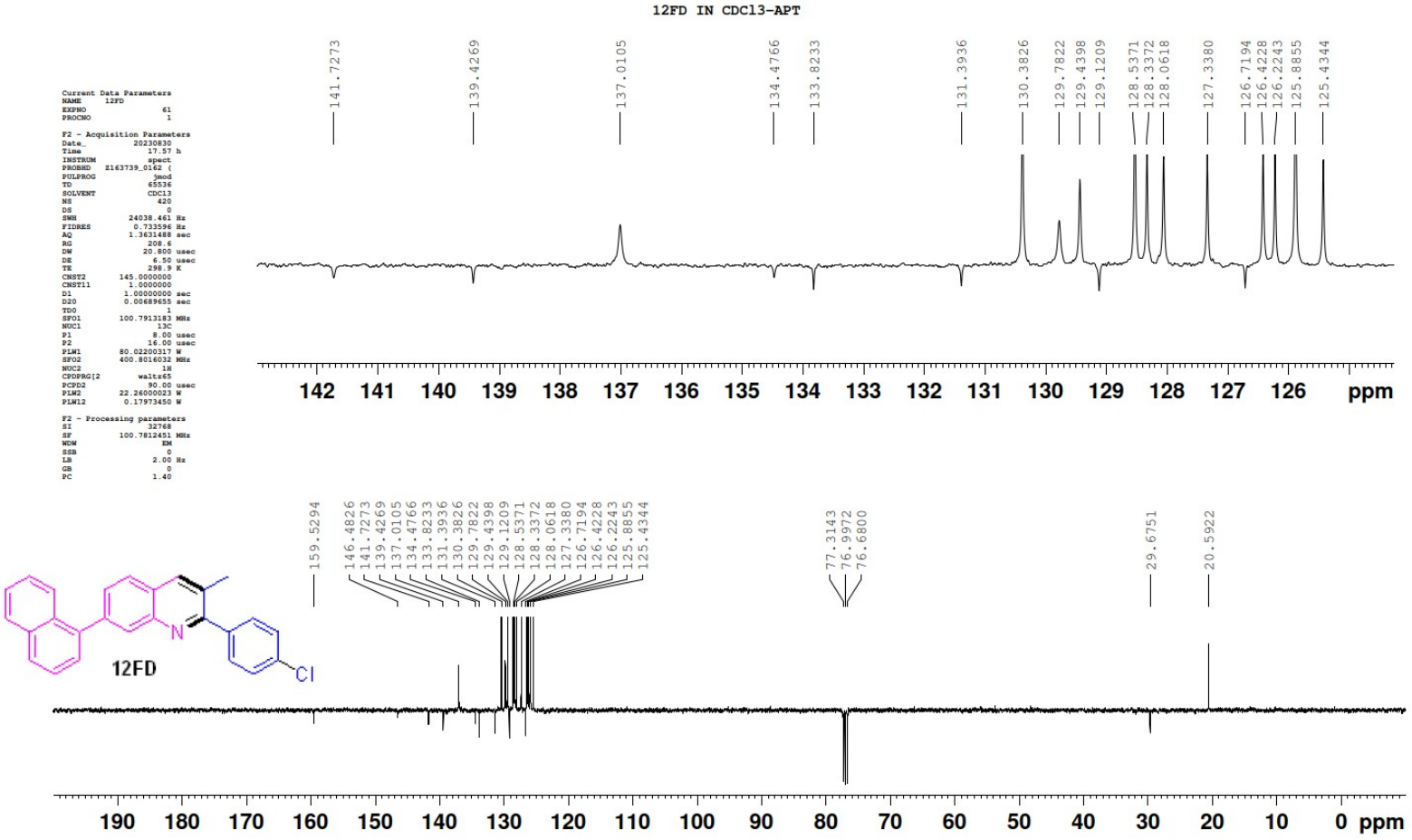
F2 - Acquisition Parameters
Date_      20230829
Time           22.17 h
INSTRUM         spect
PROBHD   Z104450_0373 (
PULPROG         zg30
TD             24036
SOLVENT          MeOD
NS                8
DS                0
SWH         8012.820 Hz
FIDRES      0.666735 Hz
AQ          1.4998465 sec
RG              181
DW           62.400 usec
DE            6.50 usec
TE           300.0 K
D1              0 sec
TD0             1
SFO1    400.2324014 MHz
NUC1            1H
P0            4.79 usec
P1           14.38 usec
PLW1    19.18000031 W

F2 - Processing parameters
SI          16384
SF      400.2300116 MHz
WDW             EM
SSB             0
LB           0.30 Hz
GB              0
PC           1.00
```



12FD IN CDCl3-13C



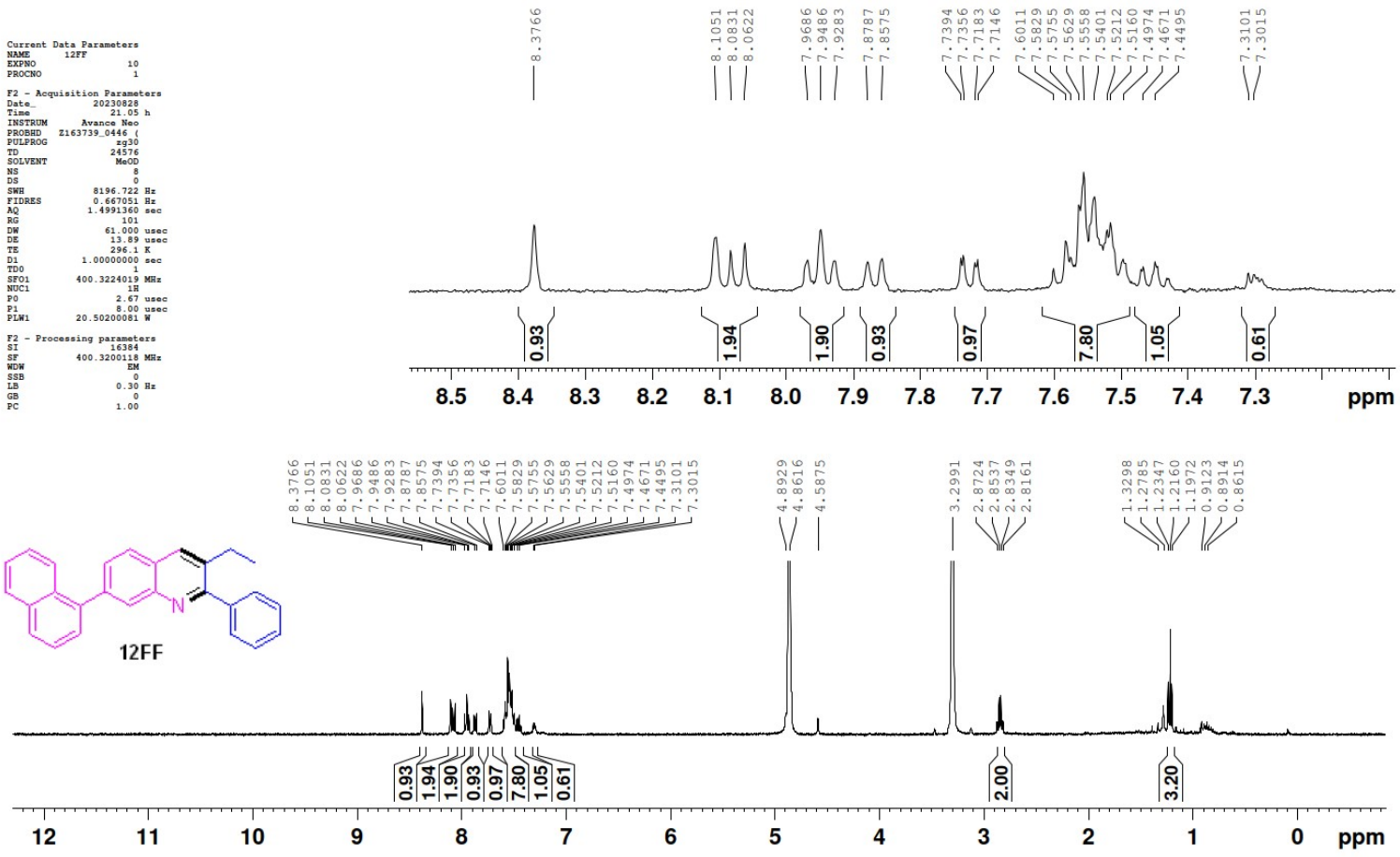

12FD IN CDCl3-APT
Current Data Parameters
NAME 12FD
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230830
Time 17.57 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 420
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 208.6
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.7913183 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 80.02200317 W
SFO2 400.8016032 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 22.26000023 W
PLW12 0.17973450 W
F2 - Processing parameters
SI 32768
SF 100.7812451 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
141.7273
139.4269
137.0105
134.4766
133.8233
131.3936
130.3826
129.7822
129.4398
129.1209
128.5371
128.3372
128.0618
127.3380
126.7194
126.4228
126.2243
125.8855
125.4344
142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 ppm
159.5294
146.4826
141.7273
139.4269
137.0105
134.4766
133.8233
131.3936
130.3826
129.7822
129.4398
129.1209
128.5371
128.3372
128.0618
127.3380
126.7194
126.4228
126.2243
125.8855
125.4344
77.3143
76.9972
76.6800
29.6751
20.5922
N
Cl
12FD
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

12FF IN MeOD

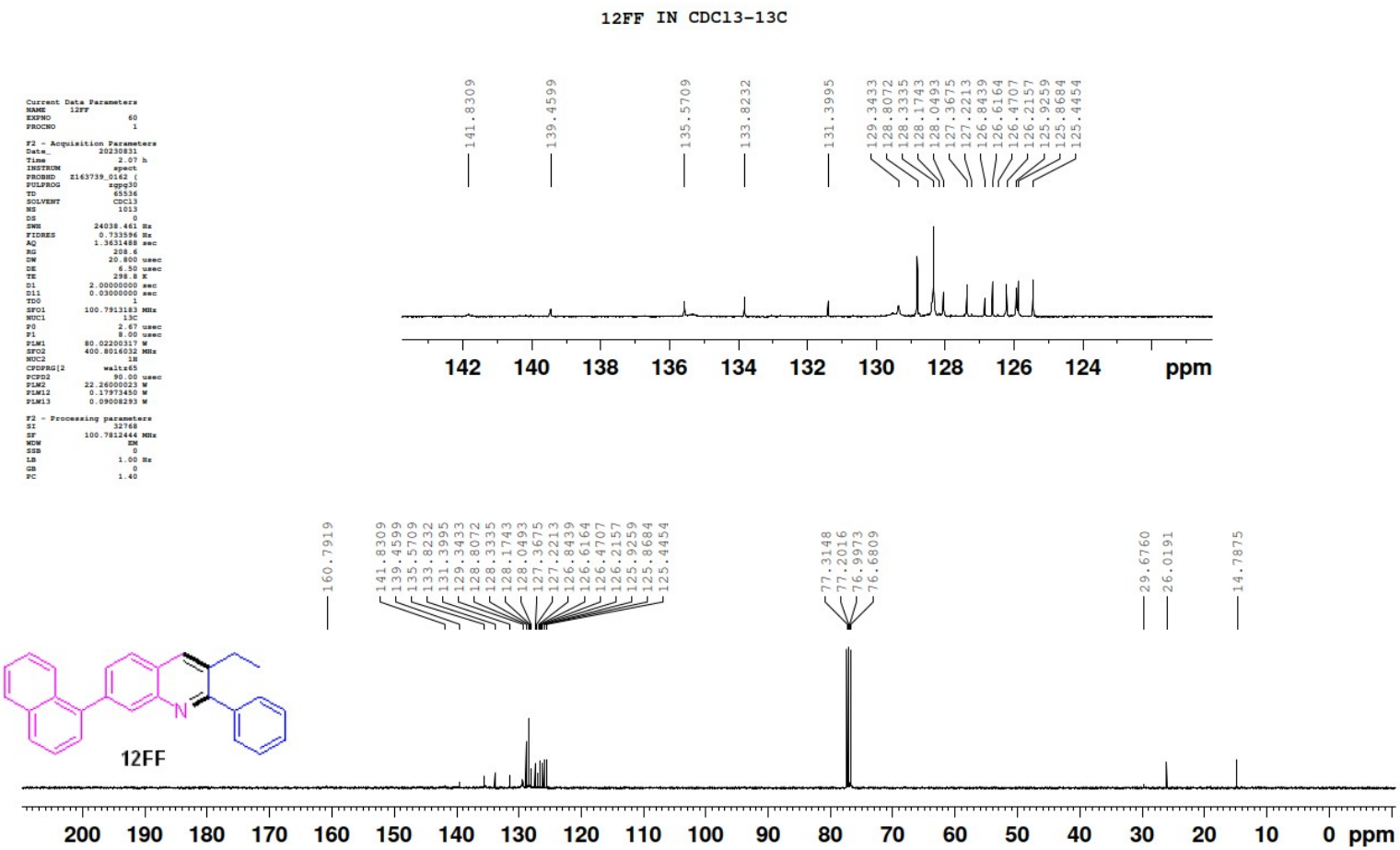
```
Current Data Parameters
NAME        12FF
EXPNO             10
PROCNO             1

F2 - Acquisition Parameters
Date_       20230828
Time            21.05 h
INSTRUM      Avance Neo
PROBHD   Z163739_0446 (
PULPROG          zg30
TD              24576
SOLVENT          MeOD
NS                  8
DS                  0
SWH          8196.722 Hz
FIDRES       0.667051 Hz
AQ           1.4991360 sec
RG                101
DW             61.000 usec
DE             13.89 usec
TE             296.1 K
D1          1.00000000 sec
TD0                 1
SFO1       400.3224019 MHz
NUC1               1H
P0             2.67 usec
P1             8.00 usec
PLW1      20.50200081 W

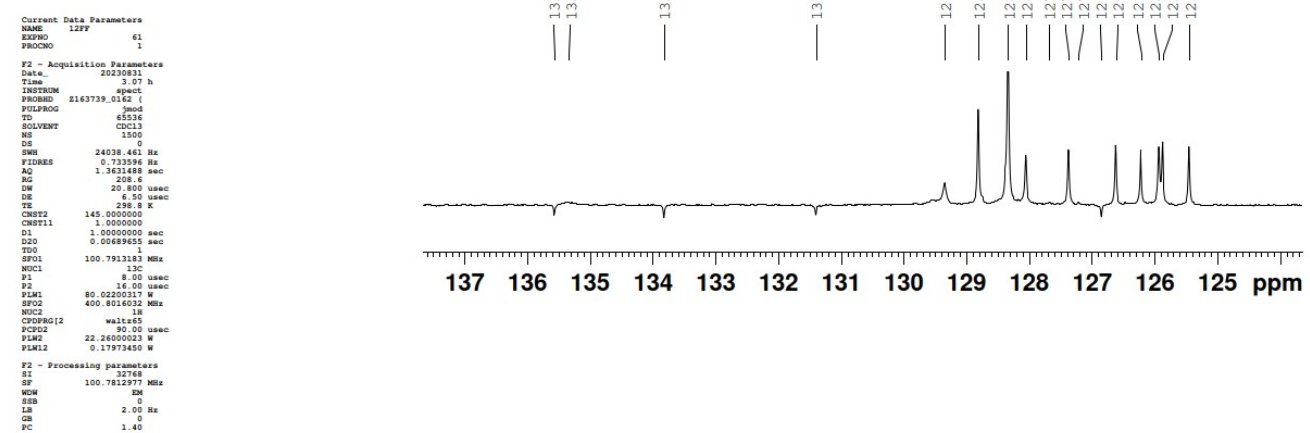
F2 - Processing parameters
SI              16384
SF         400.3200118 MHz
WDW               EM
SSB                 0
LB             0.30 Hz
GB                  0
PC             1.00
```



12FF IN CDC13-13C



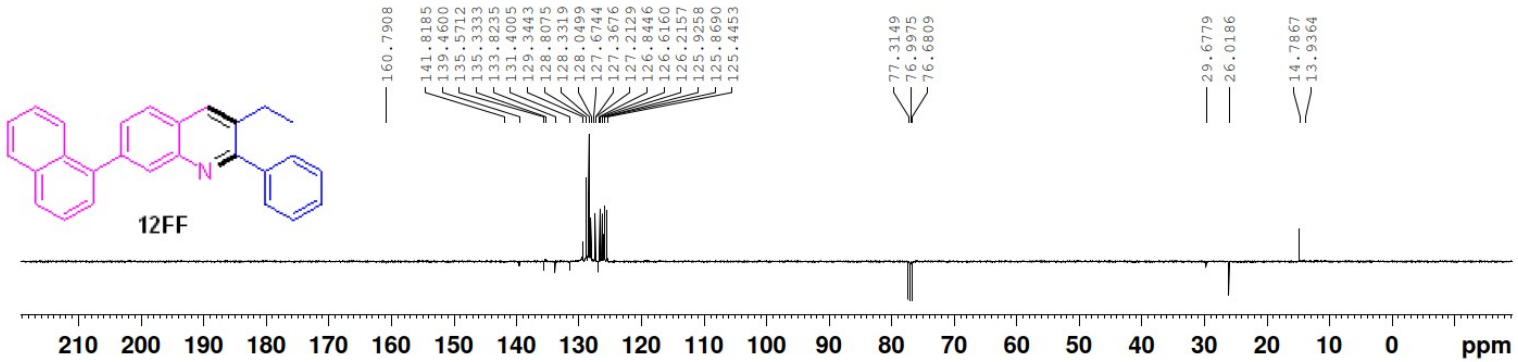
12FF IN CDCl3-APT



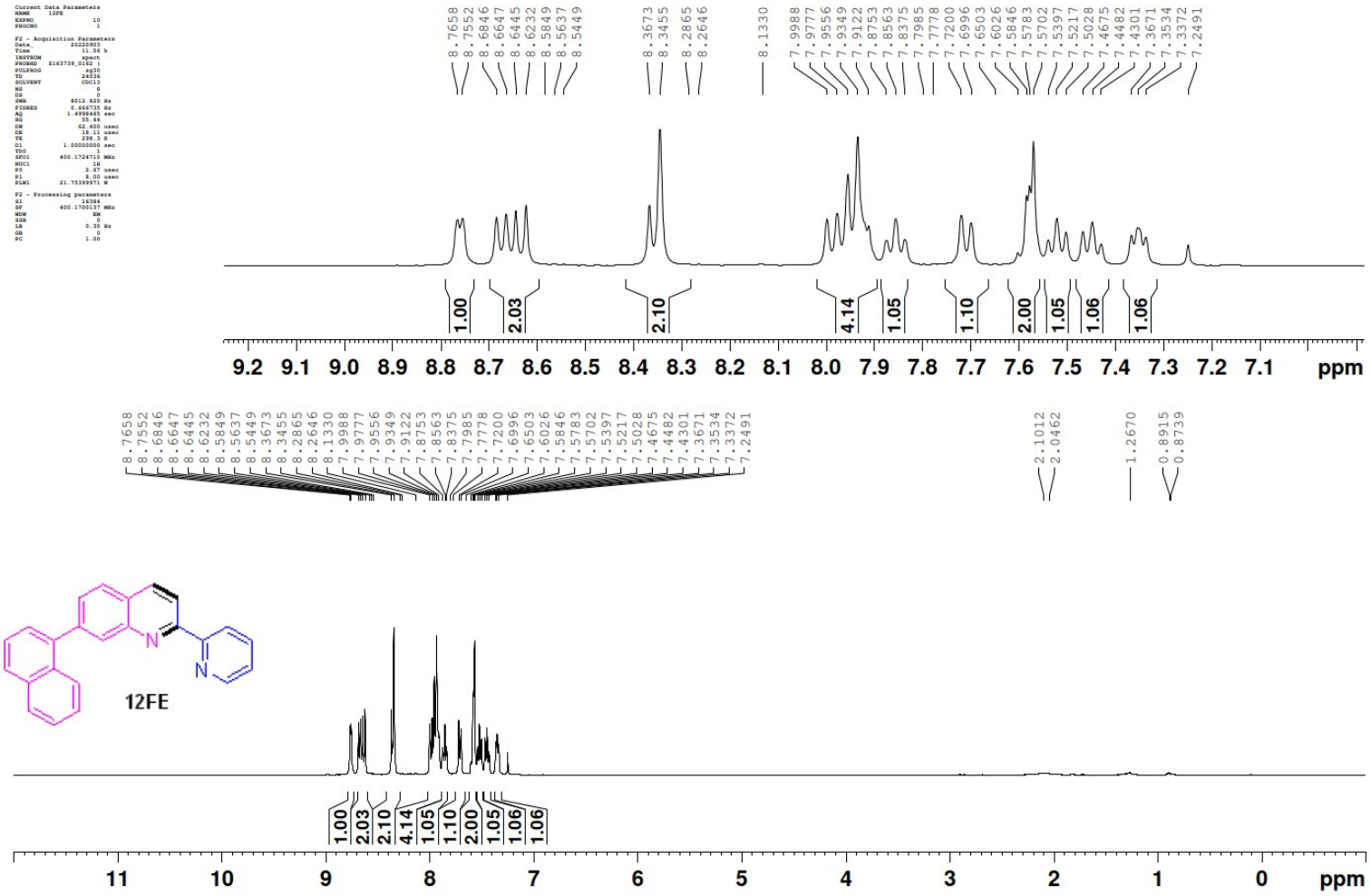
Current Data Parameters
NAME 12FF
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 3.07 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 208.6
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.7913183 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 80.02200317 W
SFO2 400.8016032 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 22.26000023 W
PLW12 0.17973450 W

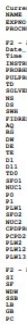
F2 - Processing parameters
SI 32768
SF 100.7812977 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

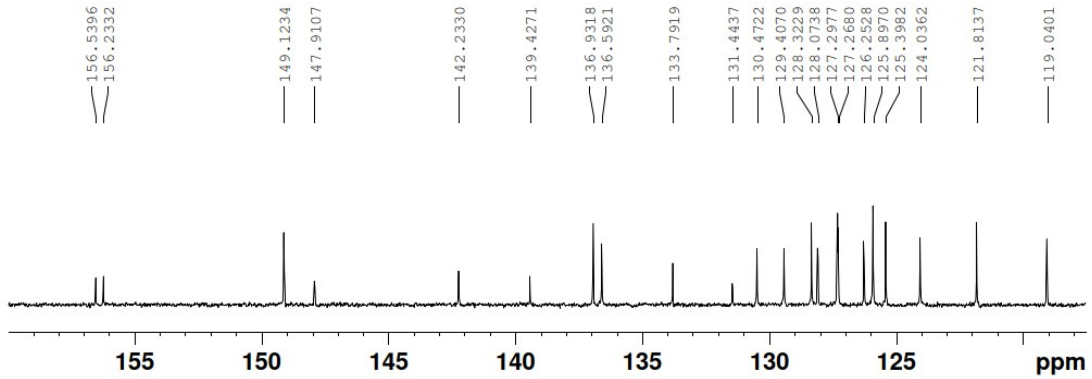


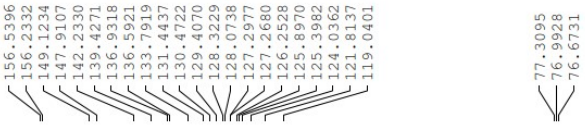
12FE IN CDCl3

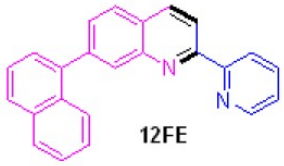


12FE IN CDCl3-13C

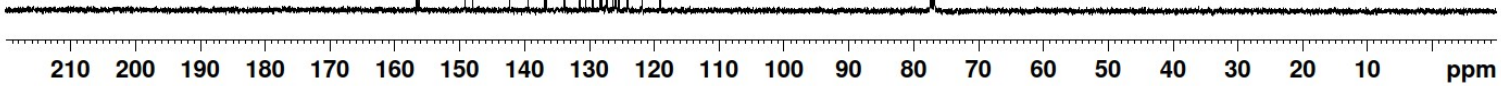




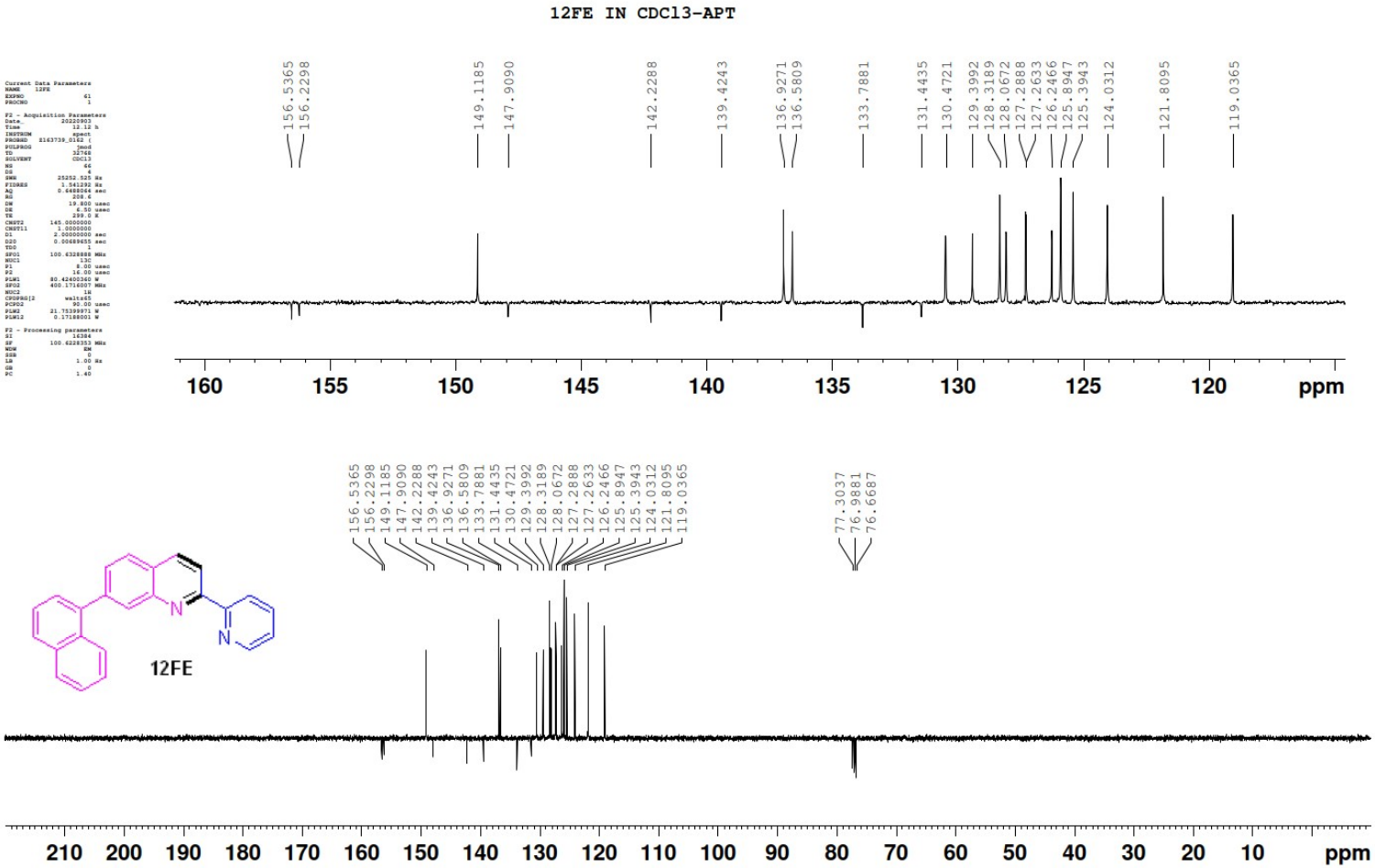


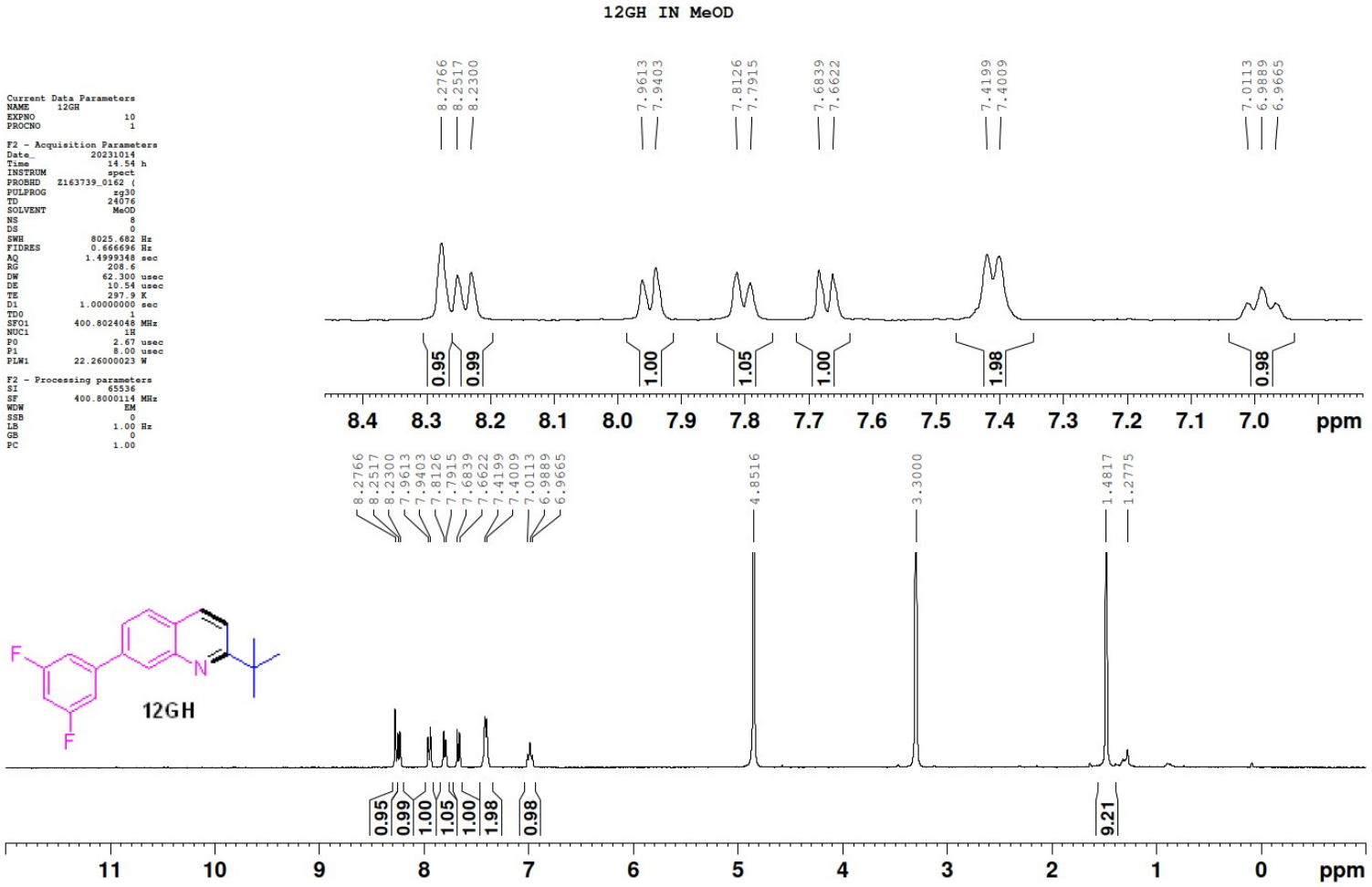


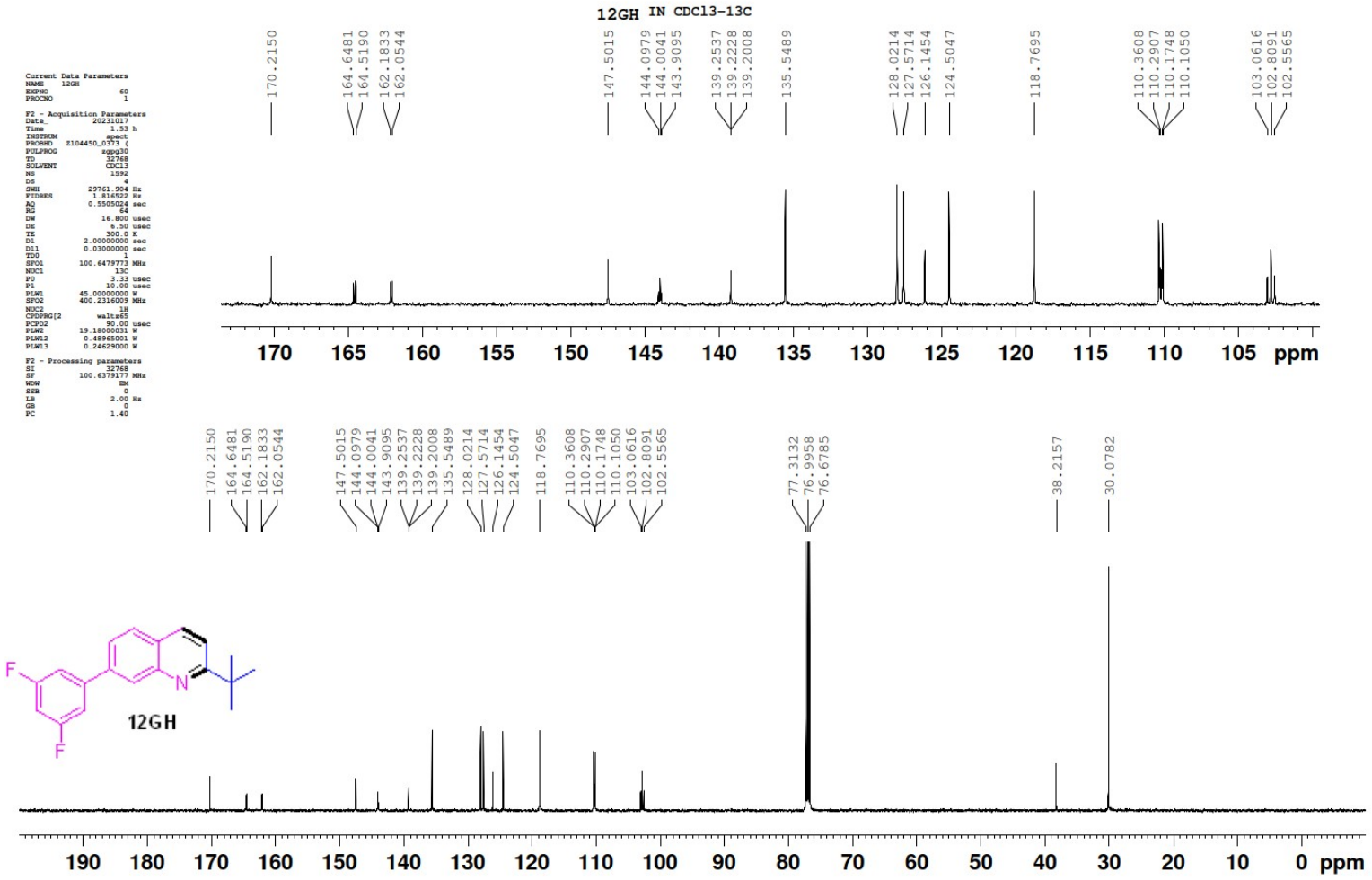
12FE



12FE IN CDCl3-APT



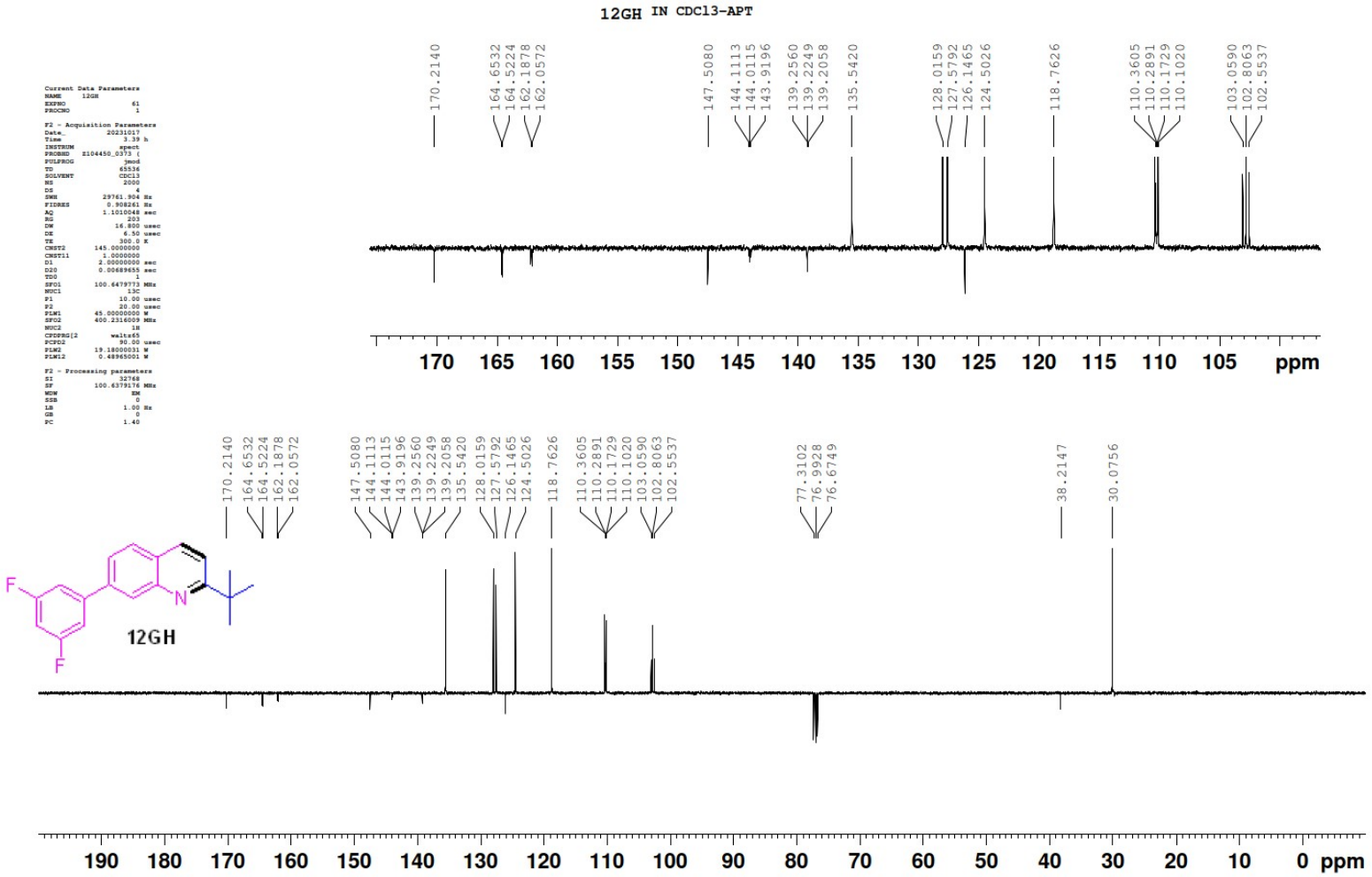

12GH IN MeOD
Current Data Parameters
NAME 12GH
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231014
Time 14.54 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24076
SOLVENT MeOD
NS 8
DS 0
SWH 8025.682 Hz
FIDRES 0.666696 Hz
AQ 1.4999348 sec
RG 208.6
DW 62.300 usec
DE 10.54 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.8024048 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.26000023 W
F2 - Processing parameters
SI 65536
SF 400.8000114 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
8.2766
8.2517
8.2300
7.9613
7.9403
7.8126
7.7915
7.6839
7.6622
7.4199
7.4009
7.0113
6.9889
6.9665
0.95
0.99
1.00
1.05
1.00
1.98
0.98
ppm
4.8516
3.3000
1.4817
1.2775
9.21
F
N
F
12GH



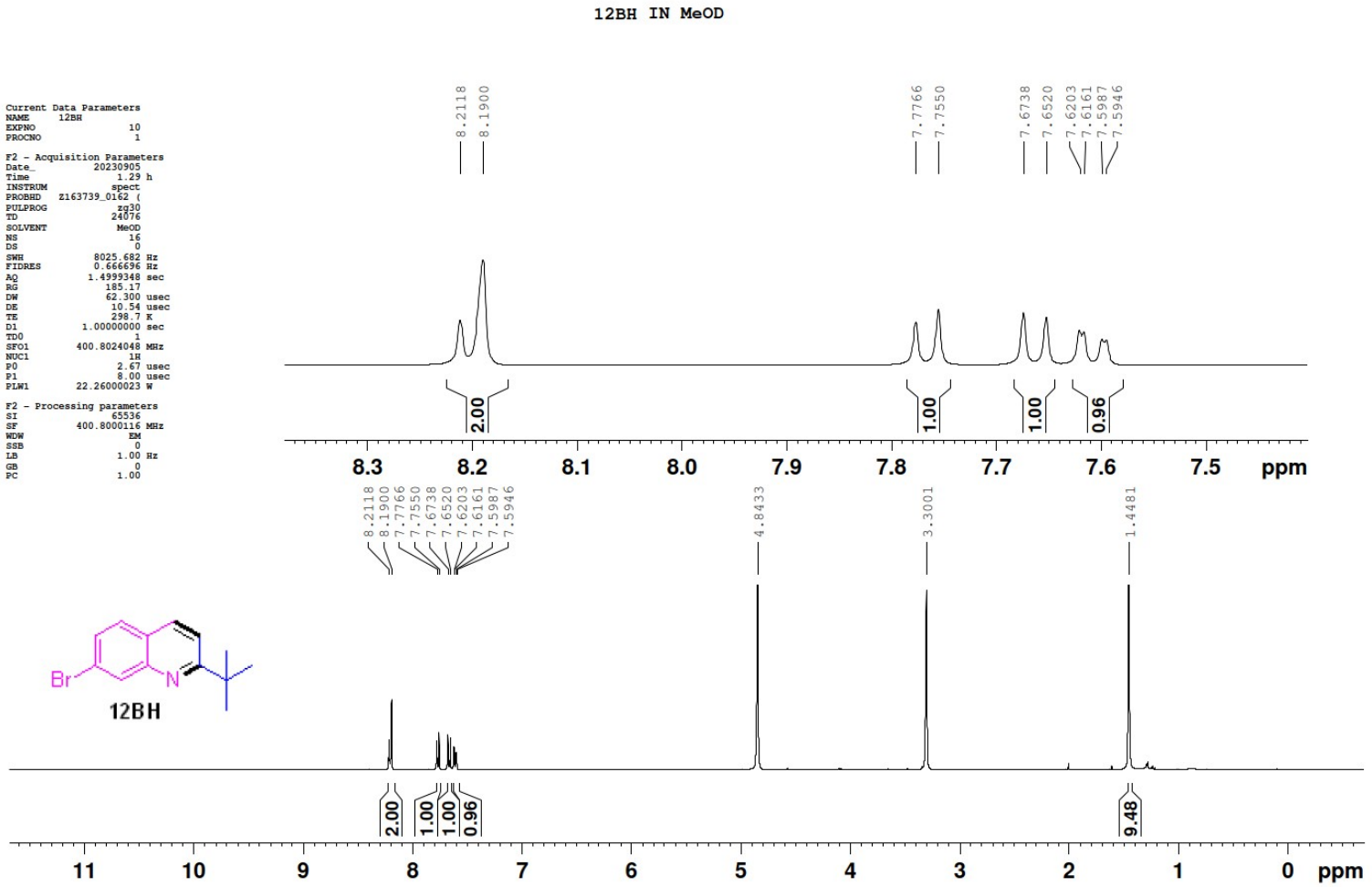
Current Data Parameters
NAME 12GH
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231017
Time 1.53 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1592
DS 4
SWH 29761.904 Hz
FIDRES 1.816522 Hz
AQ 0.5505024 sec
RG 64
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 45.00000000 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 19.18000031 W
PLW12 0.48965001 W
PLW13 0.24629000 W

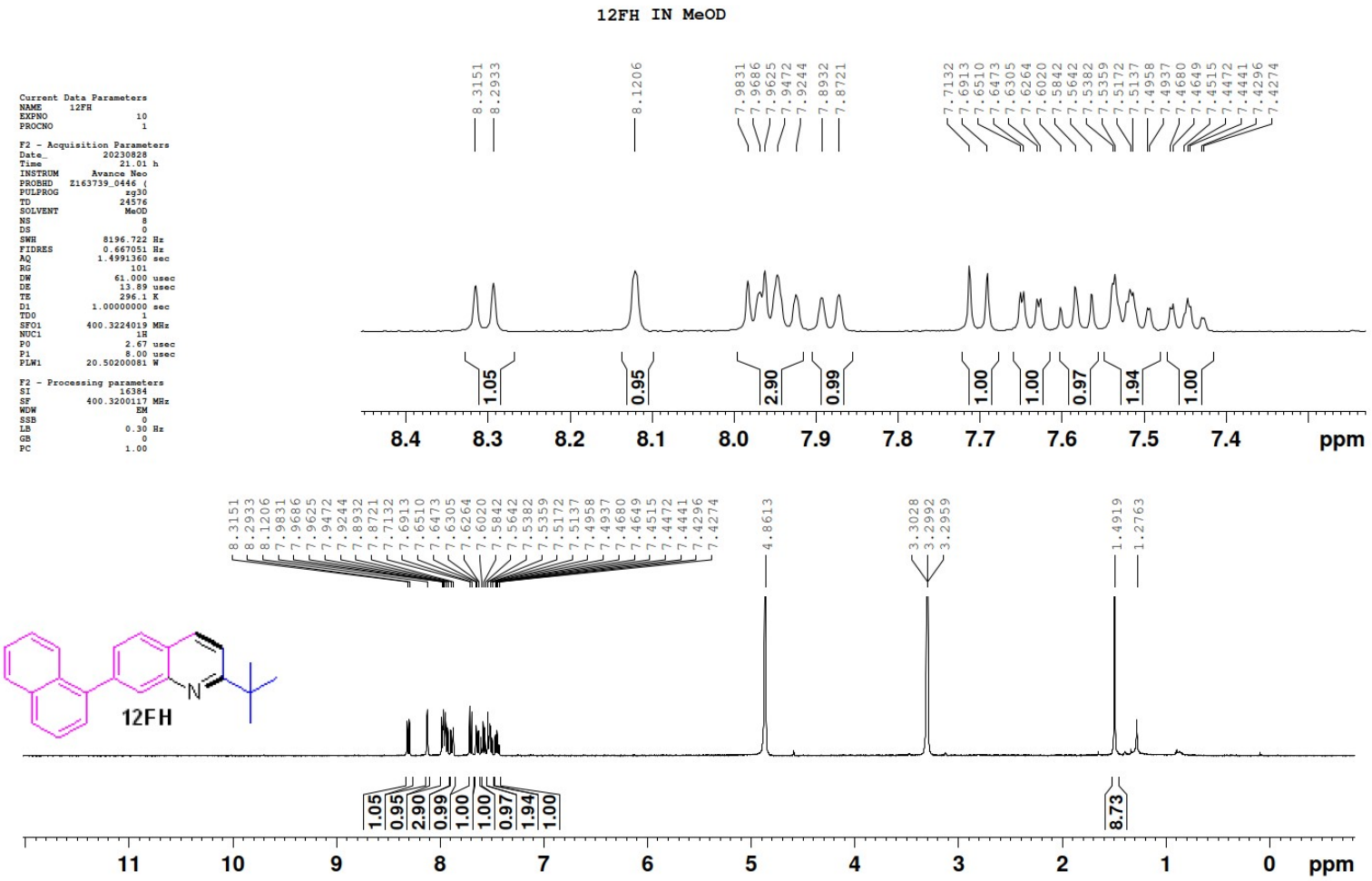
F2 - Processing parameters
SI 32768
SF 100.6379177 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


12GH IN CDCl3-APT
Current Data Parameters
NAME 12GH
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231017
Time 3.39 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 45.00000000 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 19.18000031 W
PLW12 0.48965001 W
F2 - Processing parameters
SI 32768
SF 100.6379176 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170.2140
164.6532
164.5224
162.1878
162.0572
147.5080
144.1113
144.0115
143.9196
139.2560
139.2249
139.2058
135.5420
128.0159
127.5792
126.1465
124.5026
118.7626
110.3605
110.2891
110.1729
110.1020
103.0590
102.8063
102.5537
77.3102
76.9928
76.6749
38.2147
30.0756
F
N
F
12GH
170 165 160 155 150 145 140 135 130 125 120 115 110 105 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

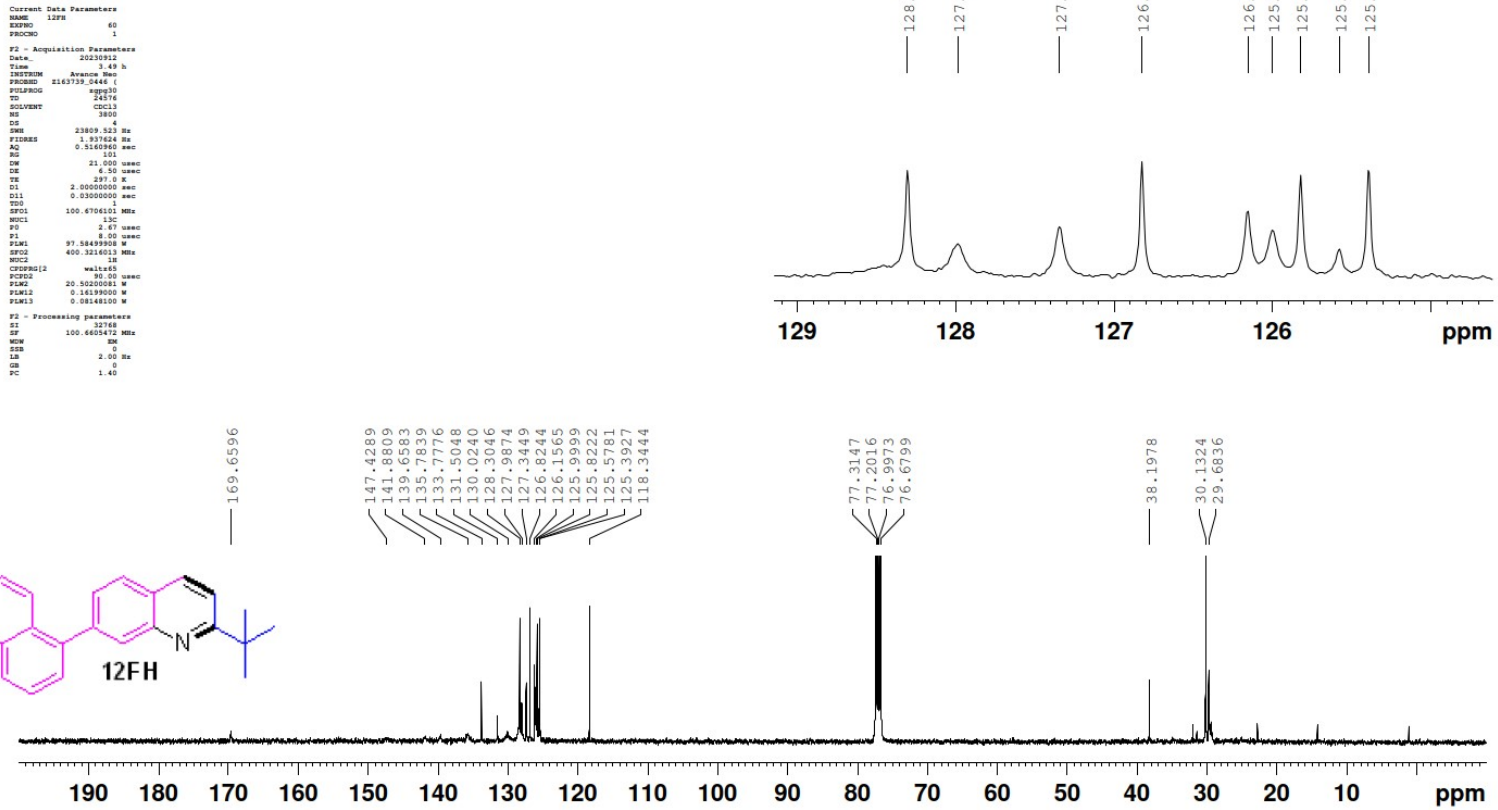
12BH IN MeOD


Current Data Parameters
NAME 12BH
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230905
Time 1.29 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24076
SOLVENT MeOD
NS 16
DS 0
SWH 8025.682 Hz
FIDRES 0.666696 Hz
AQ 1.4999348 sec
RG 185.17
DW 62.300 usec
DE 10.54 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.8024048 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.26000023 W
F2 - Processing parameters
SI 65536
SF 400.8000116 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
8.2118
8.1900
7.7766
7.7550
7.6738
7.6520
7.6203
7.6161
7.5987
7.5946
2.00
1.00
1.00
0.96
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
ppm
4.8433
3.3001
1.4481
Br
N
12BH
2.00
1.00
1.00
0.96
9.48
11
10
9
8
7
6
5
4
3
2
1
0
ppm

12FH IN MeOD


Current Data Parameters
NAME 12FH
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230828
Time 21.01 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 20.50200081 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3151
8.2933
8.1206
7.9831
7.9686
7.9625
7.9472
7.9244
7.8932
7.8721
7.7132
7.6913
7.6510
7.6473
7.6305
7.6264
7.6020
7.5842
7.5642
7.5382
7.5359
7.5172
7.5137
7.4958
7.4937
7.4680
7.4649
7.4515
7.4472
7.4441
7.4296
7.4274
1.05
0.95
2.90
0.99
1.00
1.00
0.97
1.94
1.00
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
4.8613
3.3028
3.2992
3.2959
1.4919
1.2763
8.73
11
10
9
8
7
6
5
4
3
2
1
0
ppm
12FH

12FH IN CDCl3-13C

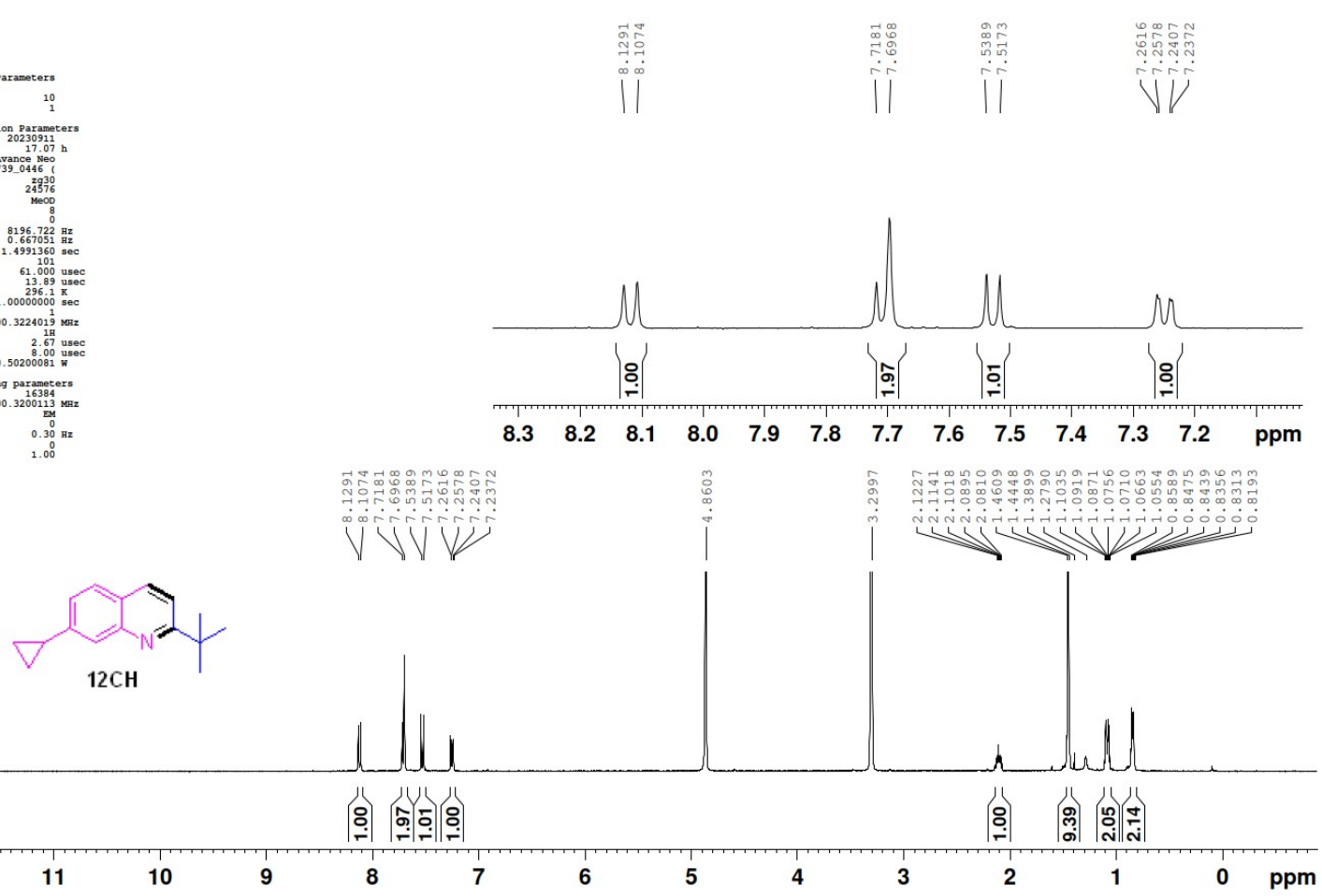


12CH IN MeOD

```
Current Data Parameters
NAME      12CH
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20230911
Time           17.07 h
INSTRUM   Avance Neo
PROBHD  Z163739_0446 (
PULPROG         zg30
TD             24576
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8196.722 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE             296.1 K
D1          1.00000000 sec
TD0                1
SFO1      400.3224019 MHz
NUC1              1H
P0             2.67 usec
P1             8.00 usec
PLW1      20.50200081 W

F2 - Processing parameters
SI             16384
SF        400.3200113 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

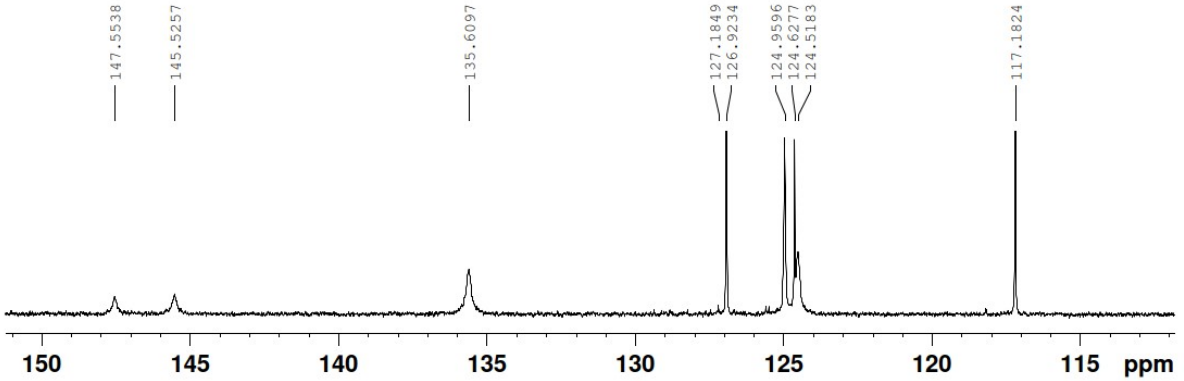


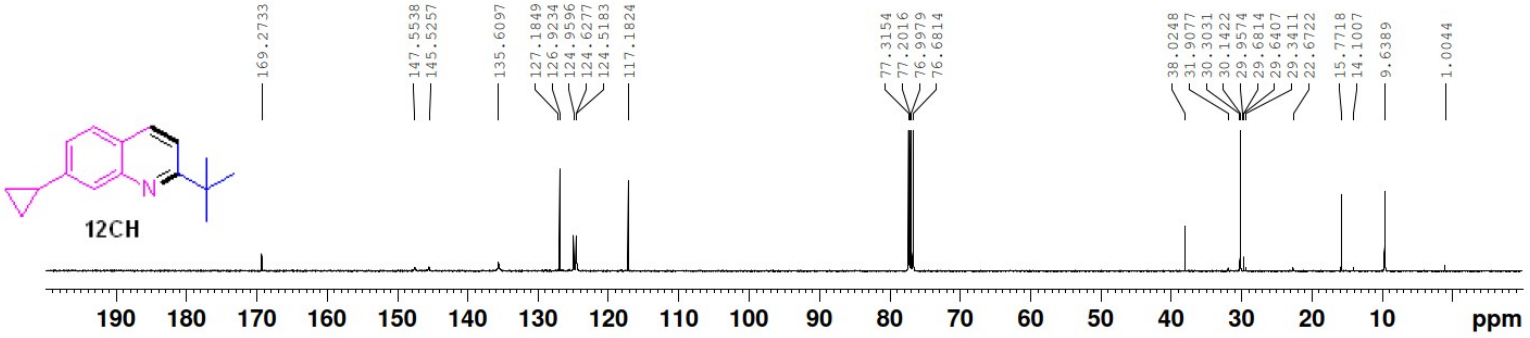
12CH IN CDCI3-13C

```
Current Data Parameters
NAME      12CH
EXPNO           60
PROCNO           1

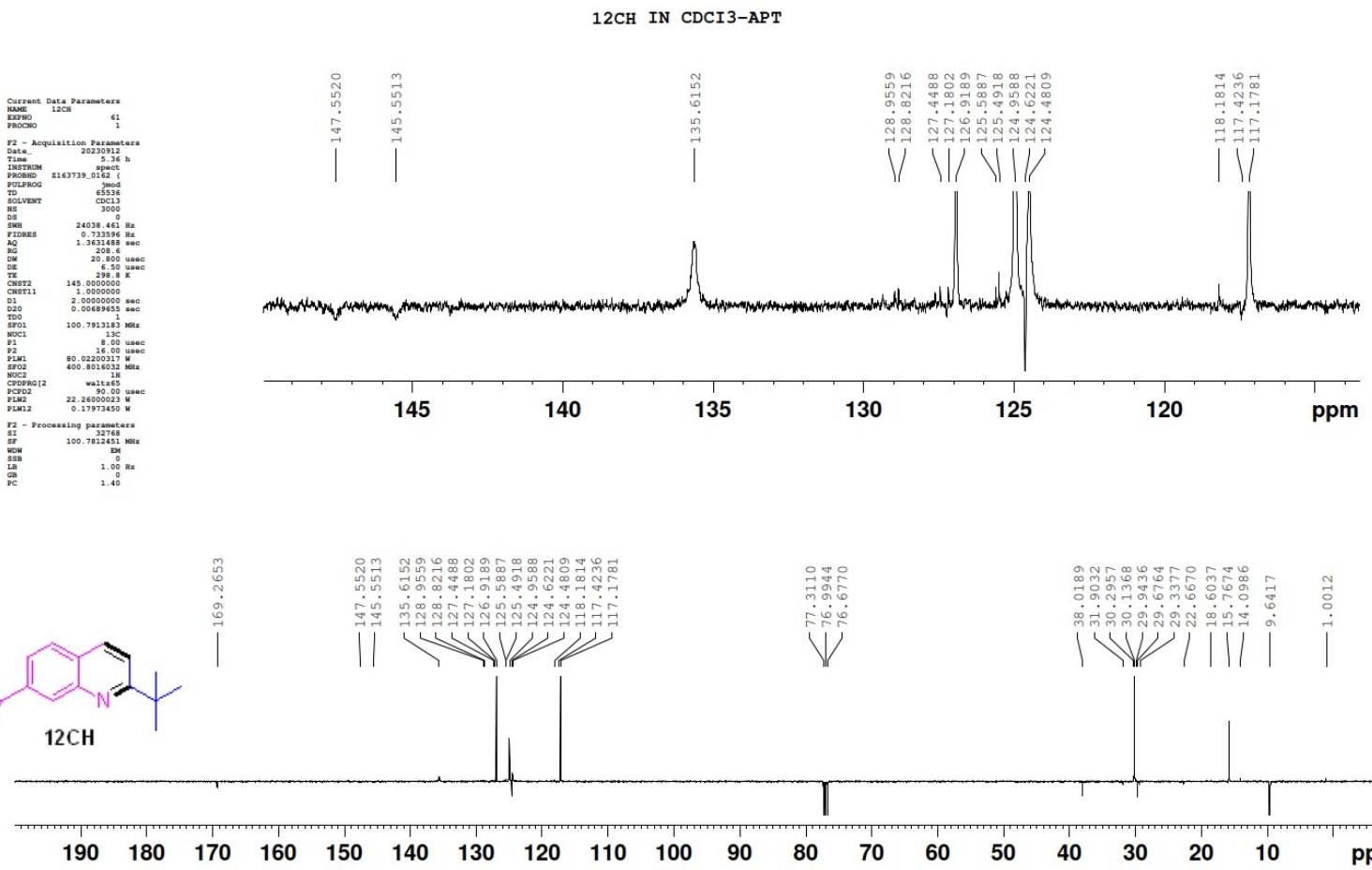
F2 - Acquisition Parameters
Date_      20230912
Time           2.46 h
INSTRUM         spect
PROBHD   Z163739_0162 (
PULPROG      zgpg30
TD            65536
SOLVENT         CDCl3
NS              3000
DS                 0
SWH        24038.461 Hz
FIDRES         0.733596 Hz
AQ          1.3631488 sec
RG             208.6
DW            20.800 usec
DE             6.50 usec
TE            301.3 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0               1
SFO1     100.7913183 MHz
NUC1           13C
P0            2.67 usec
P1            8.00 usec
PLW1     80.02200317 W
SFO2     400.8016032 MHz
NUC2           1H
CPDPRG[2      waltz65
PCPD2         90.00 usec
PLW2     22.26000023 W
PLW12     0.17973450 W
PLW13     0.09008293 W

F2 - Processing parameters
SI              32768
SF       100.7812444 MHz
WDW               EM
SSB               0
LB             1.00 Hz
GB                0
PC             1.40
```

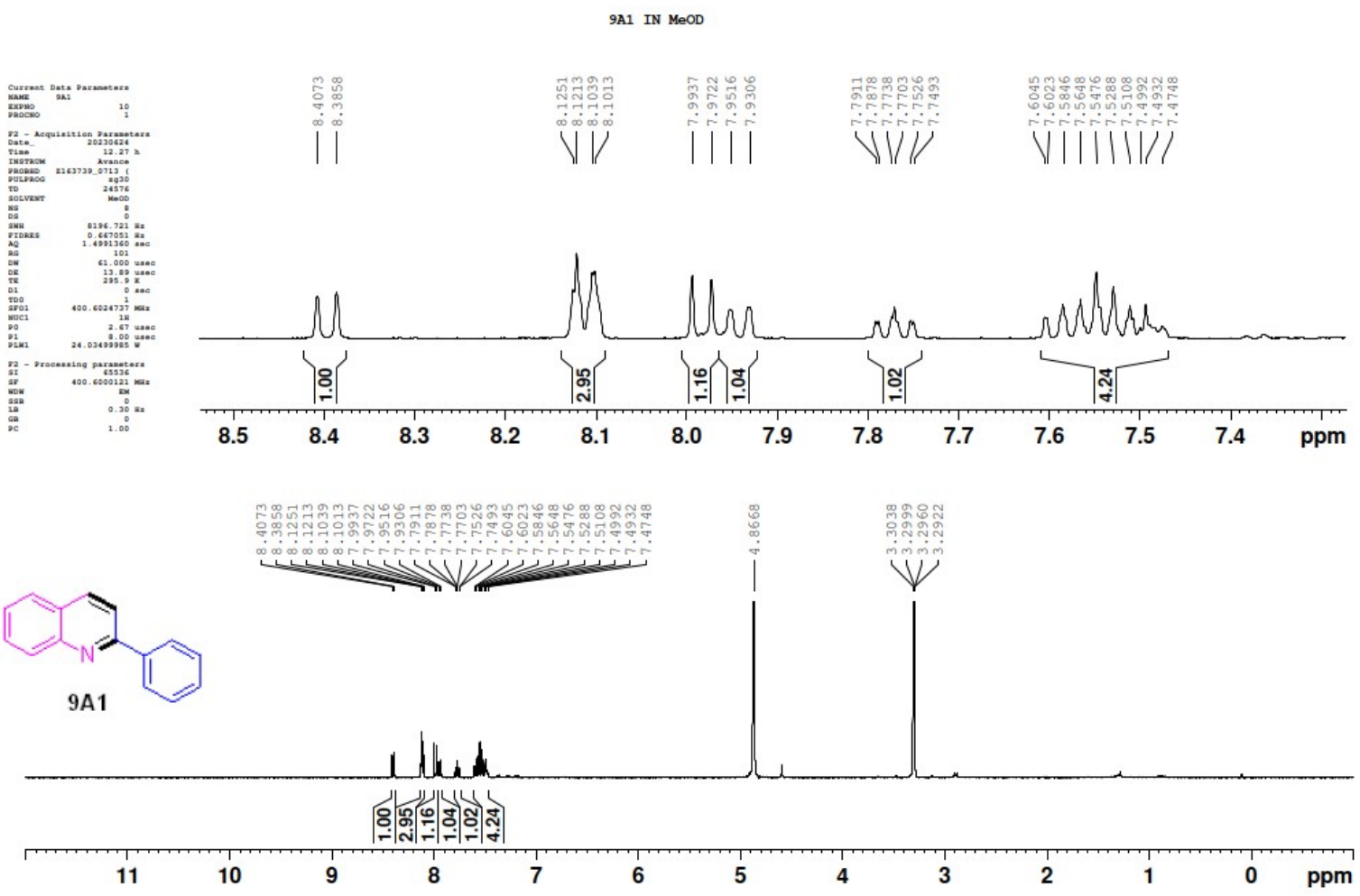




12CH IN CDCI3-APT



9A1 IN MeOD

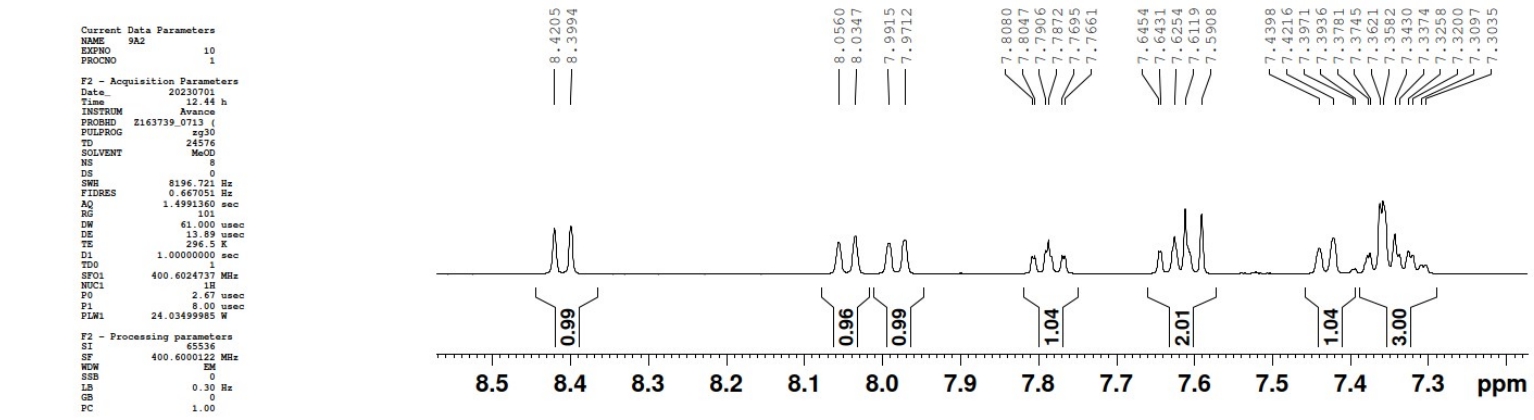

Current Data Parameters
NAME 9A1
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230624
Time 12.27 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 295.9 K
D1 0 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4073
8.3858
8.1251
8.1213
8.1039
8.1013
7.9937
7.9722
7.9516
7.9306
7.7911
7.7878
7.7738
7.7703
7.7526
7.7493
7.6045
7.6023
7.5846
7.5648
7.5476
7.5288
7.5108
7.4992
7.4932
7.4748
1.00
2.95
1.16
1.04
1.02
4.24
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
4.8668
3.3038
3.2999
3.2960
3.2922
N
9A1
11
10
9
8
7
6
5
4
3
2
1
0
ppm

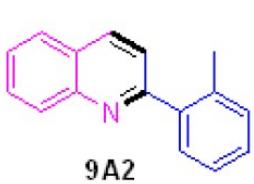
9A2 IN MeOD

```
Current Data Parameters
NAME      9A2
EXPNO          10
PROCNO          1

F2 - Acquisition Parameters
Date_      20230701
Time          12.44 h
INSTRUM       Avance
PROBHD   Z163739_0713 (
PULPROG         zg30
TD             24576
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8196.721 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE            296.5 K
D1          1.00000000 sec
TD0                1
SFO1      400.6024737 MHz
NUC1             1H
P0             2.67 usec
P1             8.00 usec
PLW1     24.03499985 W

F2 - Processing parameters
SI             65536
SF        400.6000122 MHz
WDW              EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```





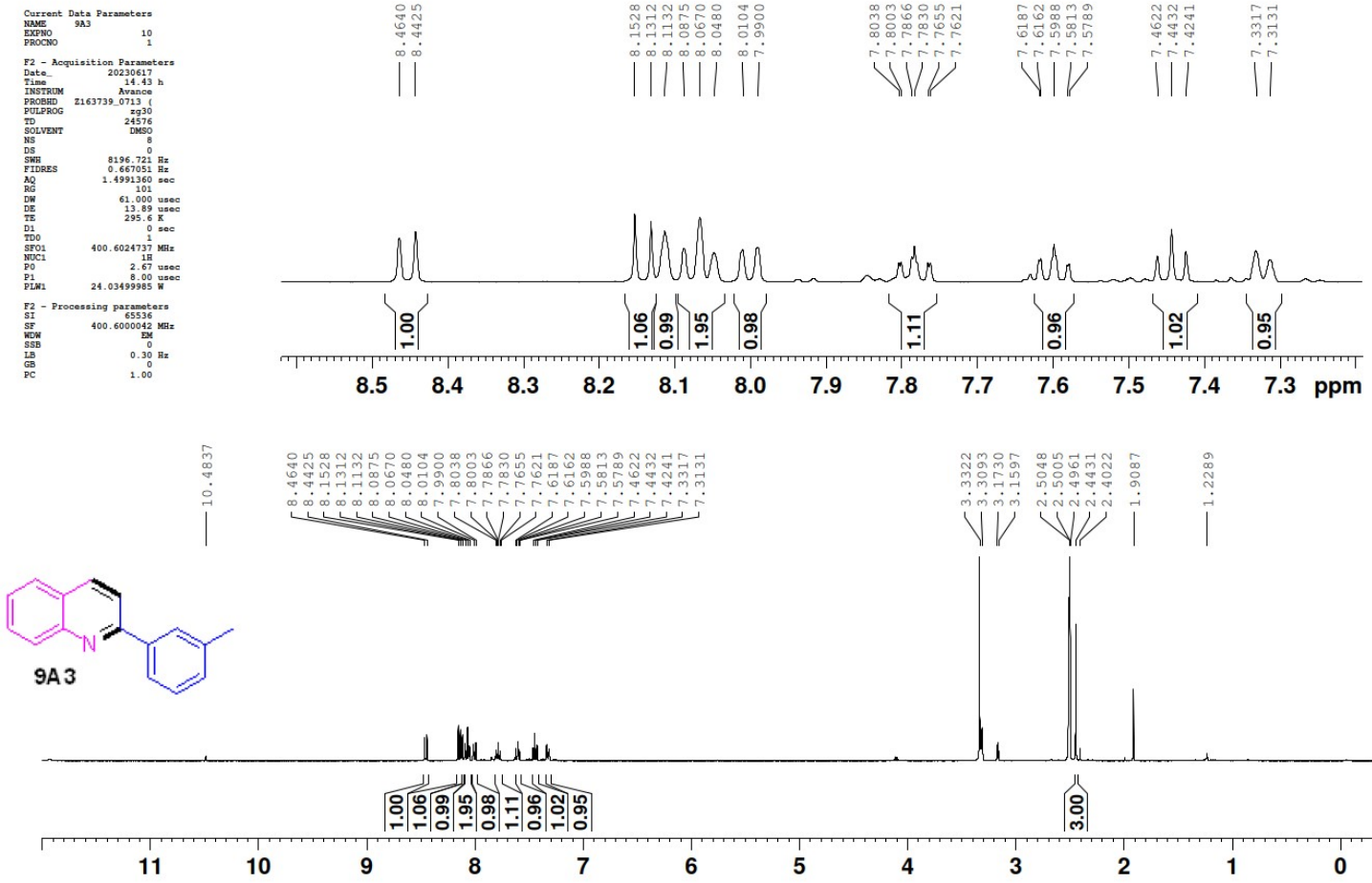
9A2

9A3 IN DMSO

```
Current Data Parameters
NAME          9A3
EXPNO          10
PROCNO          1

F2 - Acquisition Parameters
Date_       20230617
Time          14.43 h
INSTRUM       Avance
PROBHD   Z163739_0713 (
PULPROG         zg30
TD             24576
SOLVENT         DMSO
NS                 8
DS                 0
SWH         8196.721 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE            295.6 K
D1                 0 sec
TD0                1
SFO1      400.6024737 MHz
NUC1             1H
P0             2.67 usec
P1             8.00 usec
PLW1     24.03499985 W

F2 - Processing parameters
SI             65536
SF        400.6000042 MHz
WDW              EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

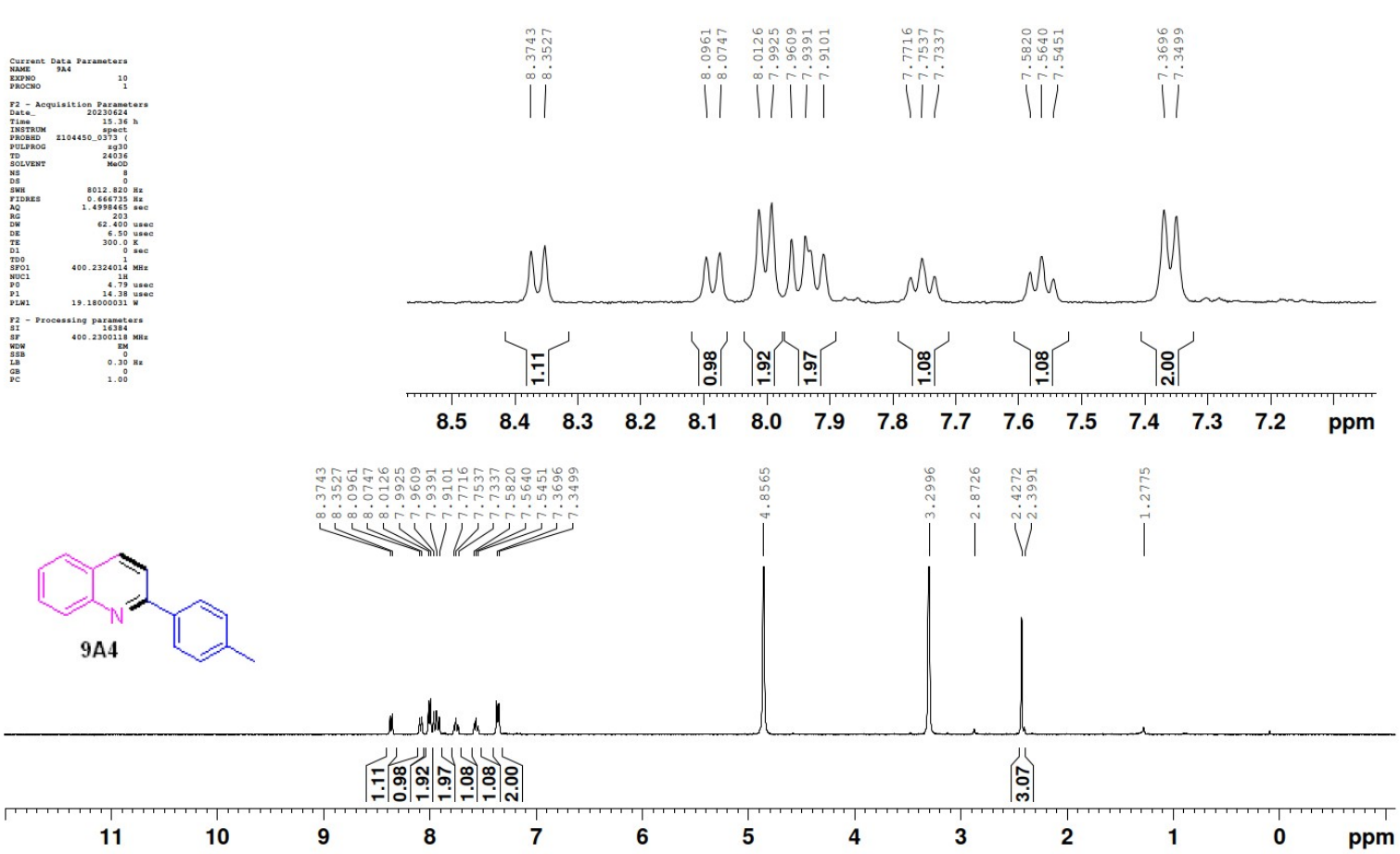


9A4 IN MeOD

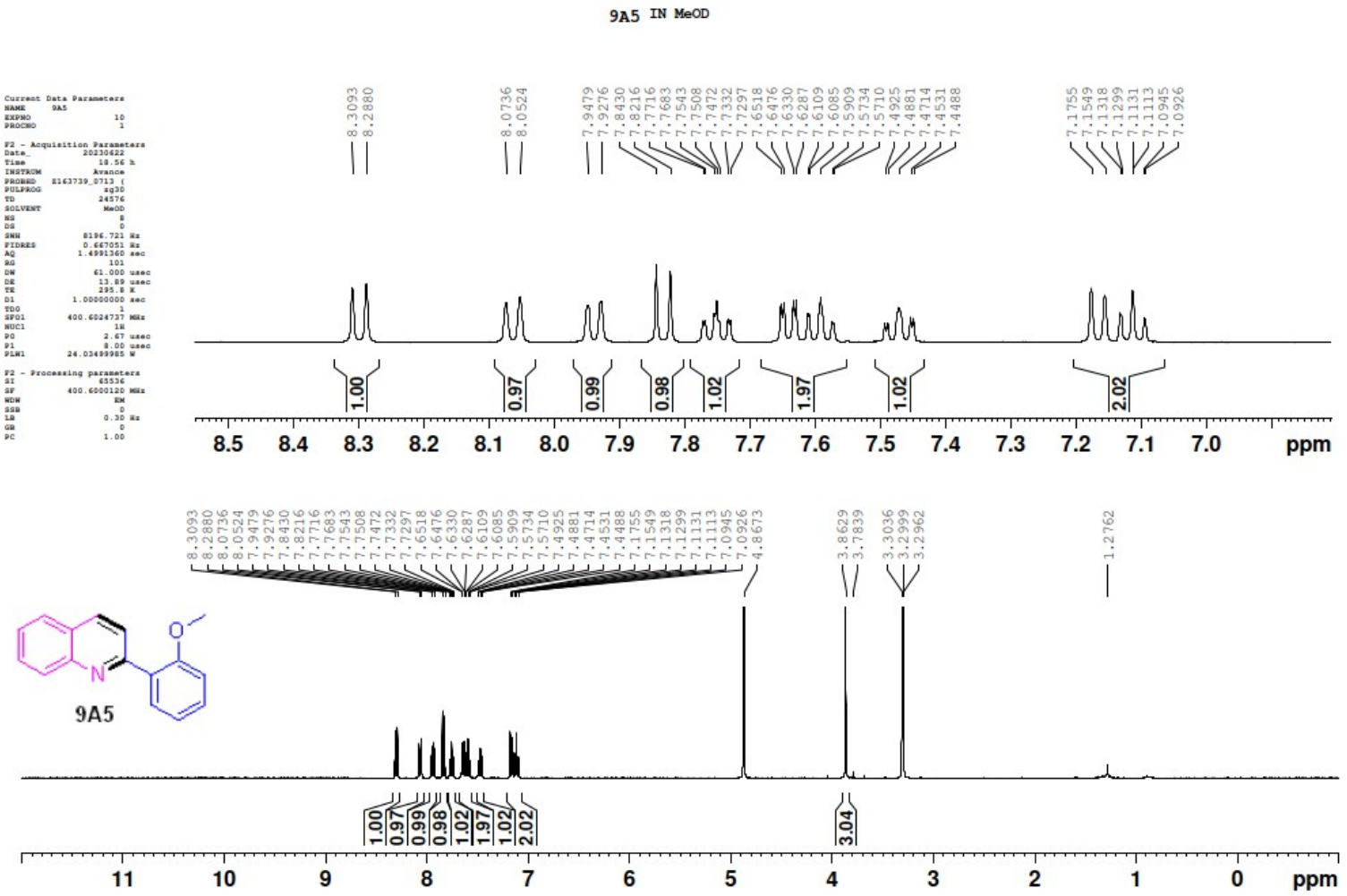
```
Current Data Parameters
NAME        9A4
EXPNO            10
PROCNO            1

F2 - Acquisition Parameters
Date_      20230624
Time           15.36 h
INSTRUM        spect
PROBHD   Z104450_0373 (
PULPROG        zg30
TD            24036
SOLVENT         MeOD
NS                8
DS                0
SWH         8012.820 Hz
FIDRES      0.666735 Hz
AQ          1.4998465 sec
RG              203
DW             62.400 usec
DE              6.50 usec
TE             300.0 K
D1               0 sec
TD0              1
SFO1    400.2324014 MHz
NUC1           1H
P0             4.79 usec
P1            14.38 usec
PLW1    19.18000031 W

F2 - Processing parameters
SI            16384
SF      400.2300118 MHz
WDW            EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```



9A4

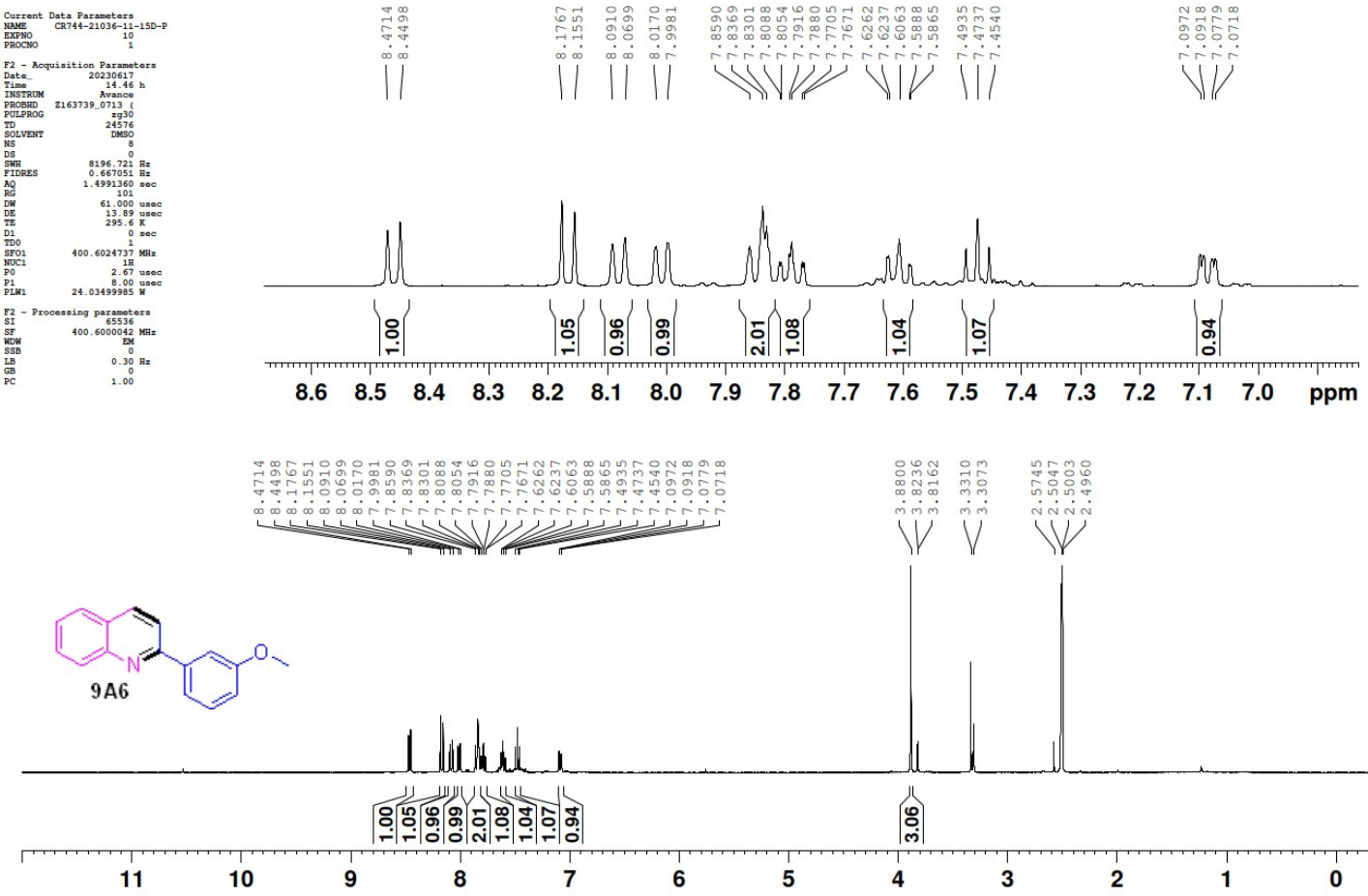

9A5 IN MeOD
Current Data Parameters
NAME 9A5
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230622
Time 18.56 h
INSTRUM Avance
PROBHD B163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3093
8.2880
8.0736
8.0524
7.9479
7.9276
7.8430
7.8216
7.7716
7.7683
7.7543
7.7508
7.7472
7.7332
7.7297
7.6518
7.6476
7.6330
7.6287
7.6109
7.6085
7.5909
7.5734
7.5710
7.4925
7.4881
7.4714
7.4531
7.4488
7.1755
7.1549
7.1318
7.1299
7.1131
7.1113
7.0945
7.0926
1.00
0.97
0.99
0.98
1.02
1.97
1.02
2.02
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
4.8673
3.8629
3.7839
3.3036
3.2999
3.2962
1.2762
3.04
11 10 9 8 7 6 5 4 3 2 1 0 ppm
9A5

9A6 IN DMSO

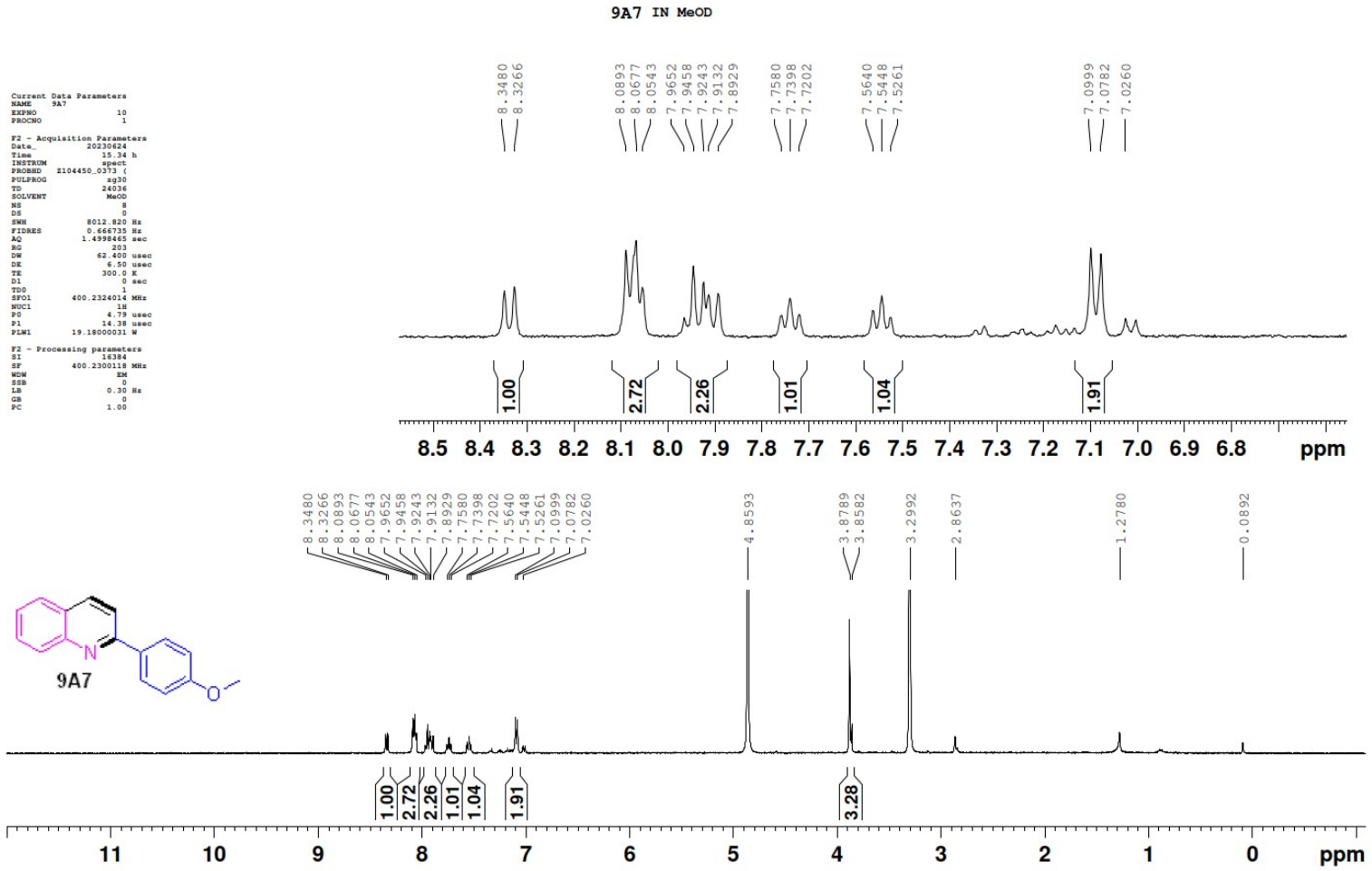
```
Current Data Parameters
NAME      CR744-21036-11-15D-P
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230617
Time                 14.46 h
INSTRUM              Avance
PROBHD    Z163739_0713 (
PULPROG                zg30
TD                    24576
SOLVENT                DMSO
NS                        8
DS                        0
SWH               8196.721 Hz
FIDRES            0.667051 Hz
AQ                1.4991360 sec
RG                      101
DW                 61.000 usec
DE                 13.89 usec
TE                 295.6 K
D1                        0 sec
TD0                       1
SFO1           400.6024737 MHz
NUC1                    1H
P0                  2.67 usec
P1                  8.00 usec
PLW1           24.03499985 W

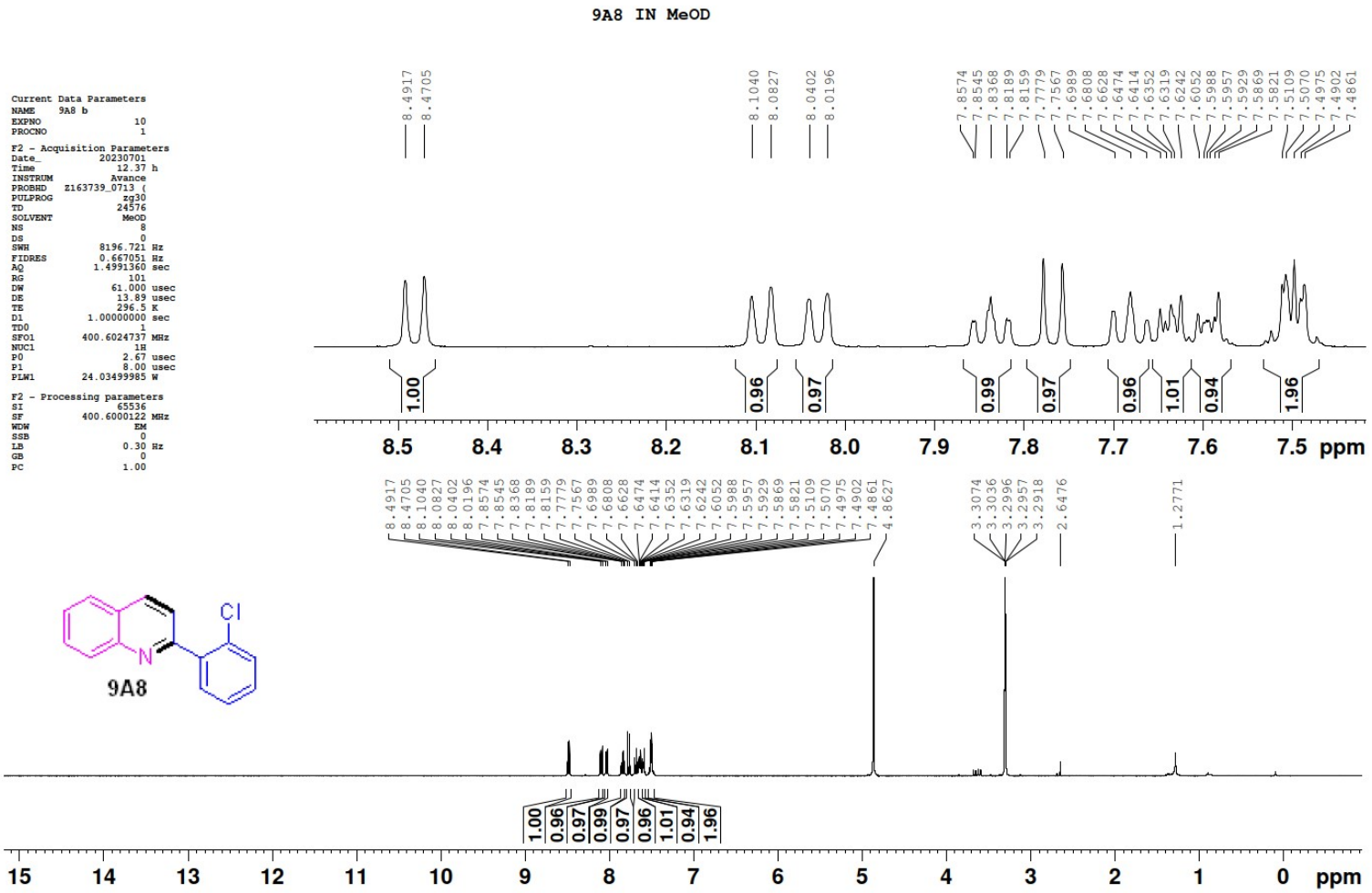
F2 - Processing parameters
SI                    65536
SF             400.6000042 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```

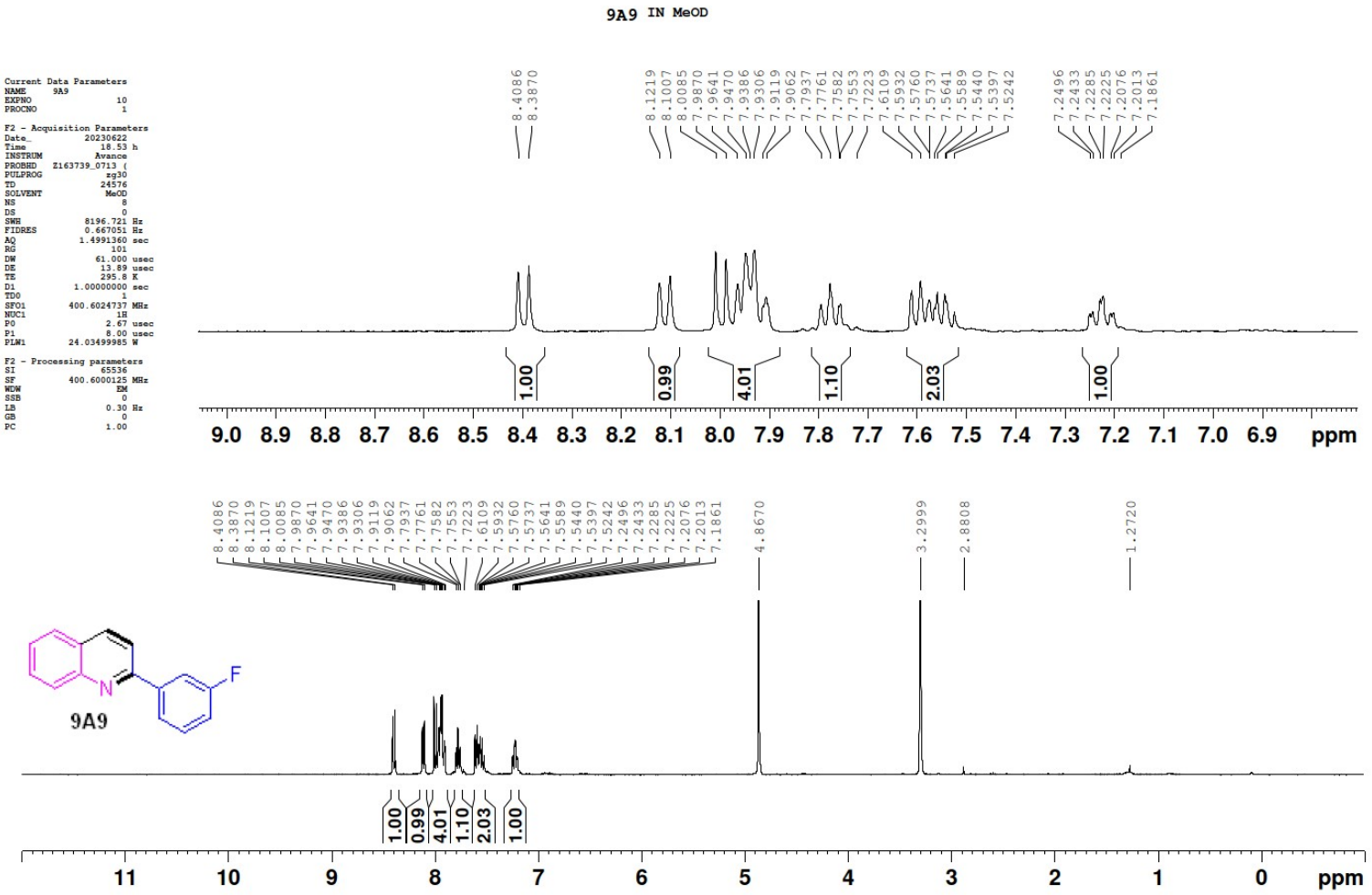


9A6

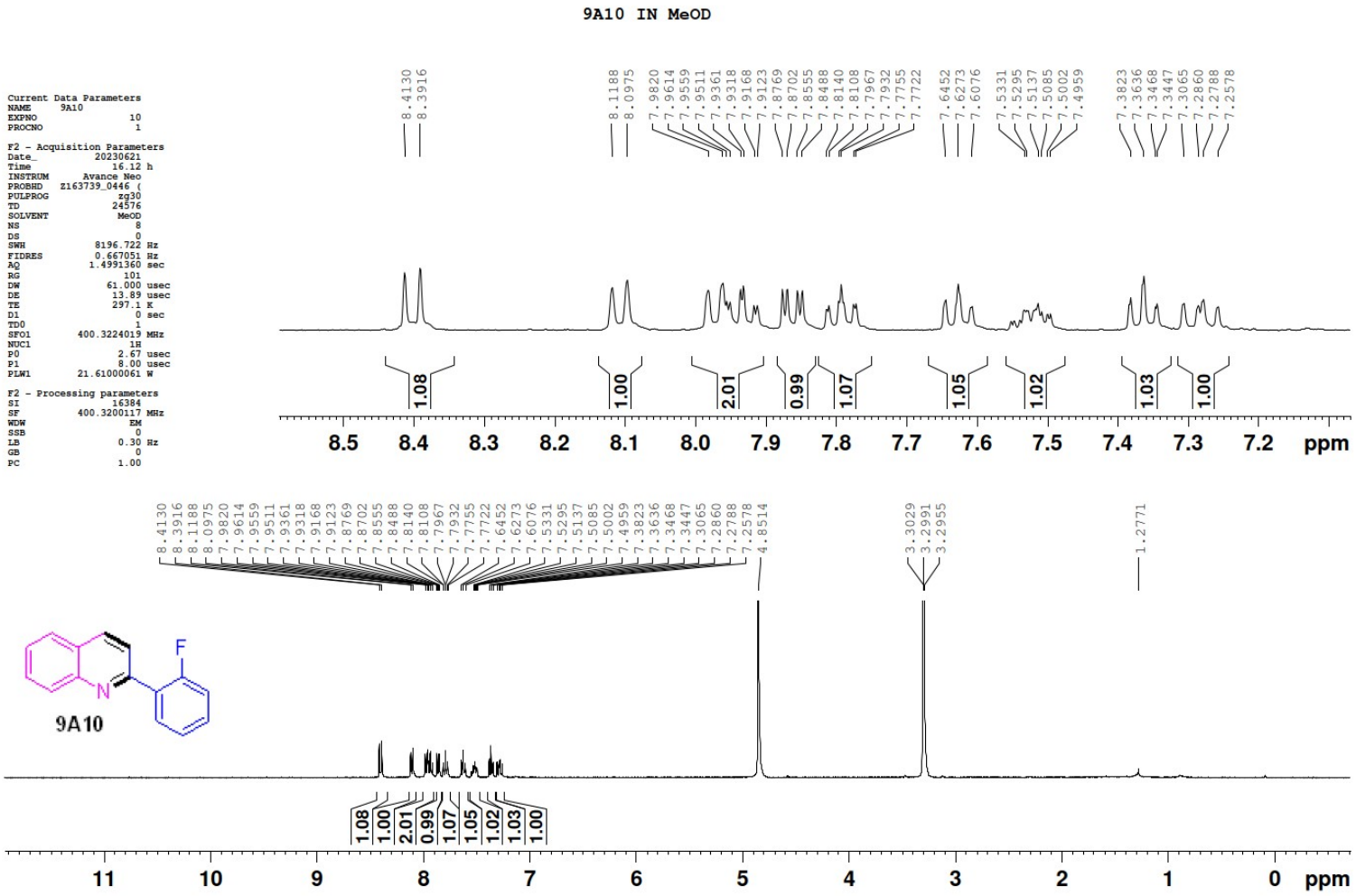

9A7 IN MeOD
Current Data Parameters
NAME 9A7
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230624
Time 15.34 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 0 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3480
8.3266
8.0893
8.0677
8.0543
7.9652
7.9458
7.9243
7.9132
7.8929
7.7580
7.7398
7.7202
7.5640
7.5448
7.5261
7.0999
7.0782
7.0260
1.00
2.72
2.26
1.01
1.04
1.91
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
4.8593
3.8789
3.8582
3.2992
2.8637
1.2780
0.0892
3.28
9A7
11 10 9 8 7 6 5 4 3 2 1 0 ppm

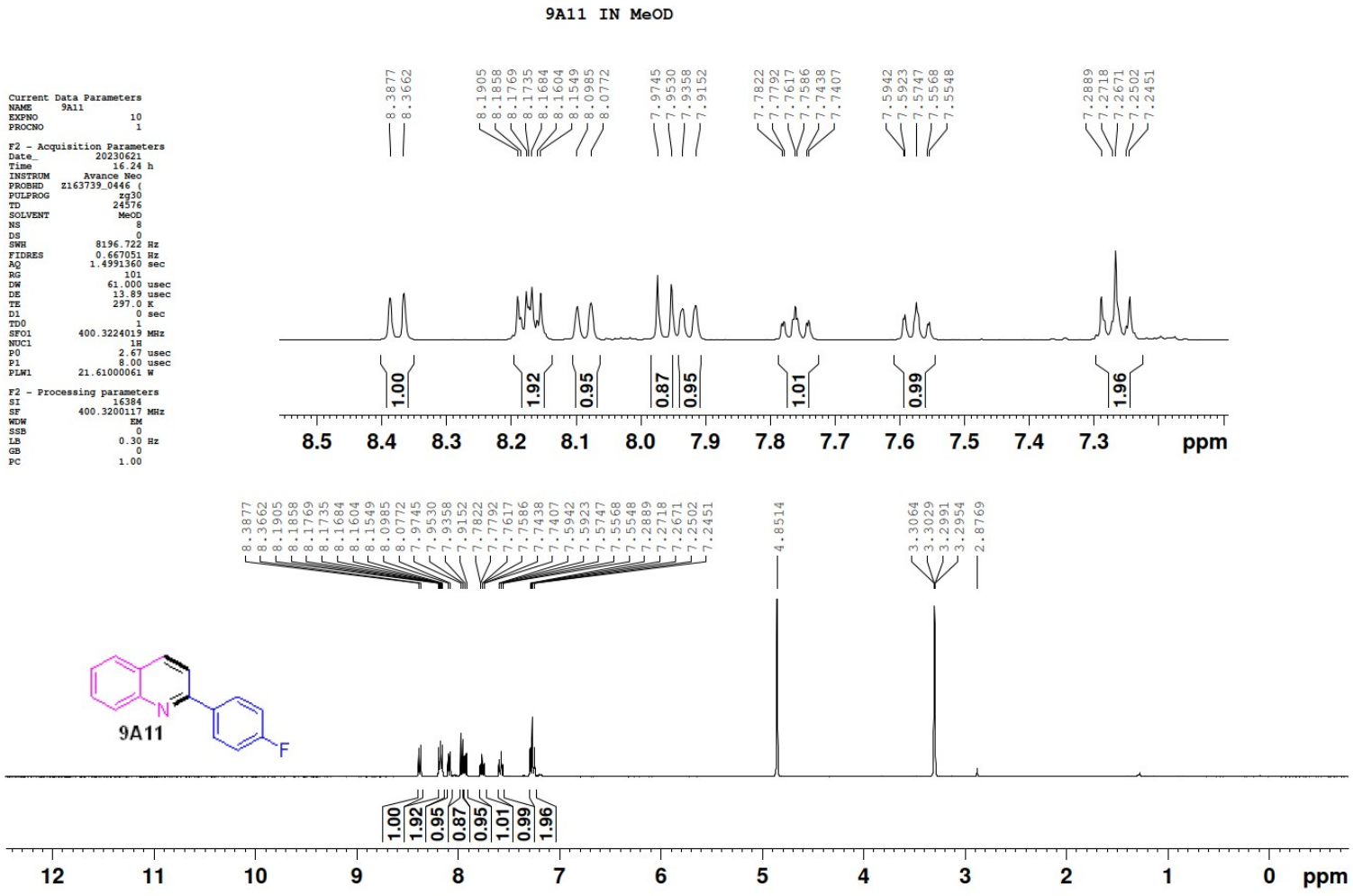
9A8 IN MeOD


Current Data Parameters
NAME 9A8 b
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230701
Time 12.37 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4917
8.4705
8.1040
8.0827
8.0402
8.0196
7.8574
7.8545
7.8368
7.8189
7.8159
7.7779
7.7567
7.6989
7.6808
7.6628
7.6474
7.6414
7.6352
7.6319
7.6242
7.6052
7.5988
7.5957
7.5929
7.5869
7.5821
7.5109
7.5070
7.4975
7.4902
7.4861
1.00
0.96
0.97
0.99
0.97
0.96
1.01
0.94
1.96
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5 ppm
4.8627
3.3074
3.3036
3.2996
3.2957
3.2918
2.6476
1.2771
Cl
N
9A8
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm


9A9 IN MeOD
Current Data Parameters
NAME 9A9
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230622
Time 18.53 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4086
8.3870
8.1219
8.1007
8.0085
7.9870
7.9641
7.9470
7.9386
7.9306
7.9119
7.9062
7.7937
7.7761
7.7582
7.7553
7.7223
7.6109
7.5932
7.5760
7.5737
7.5641
7.5589
7.5440
7.5397
7.5242
7.2496
7.2433
7.2285
7.2225
7.2076
7.2013
7.1861
1.00
0.99
4.01
1.10
2.03
1.00
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
4.8670
3.2999
2.8808
1.2720
N
F
9A9
11 10 9 8 7 6 5 4 3 2 1 0 ppm

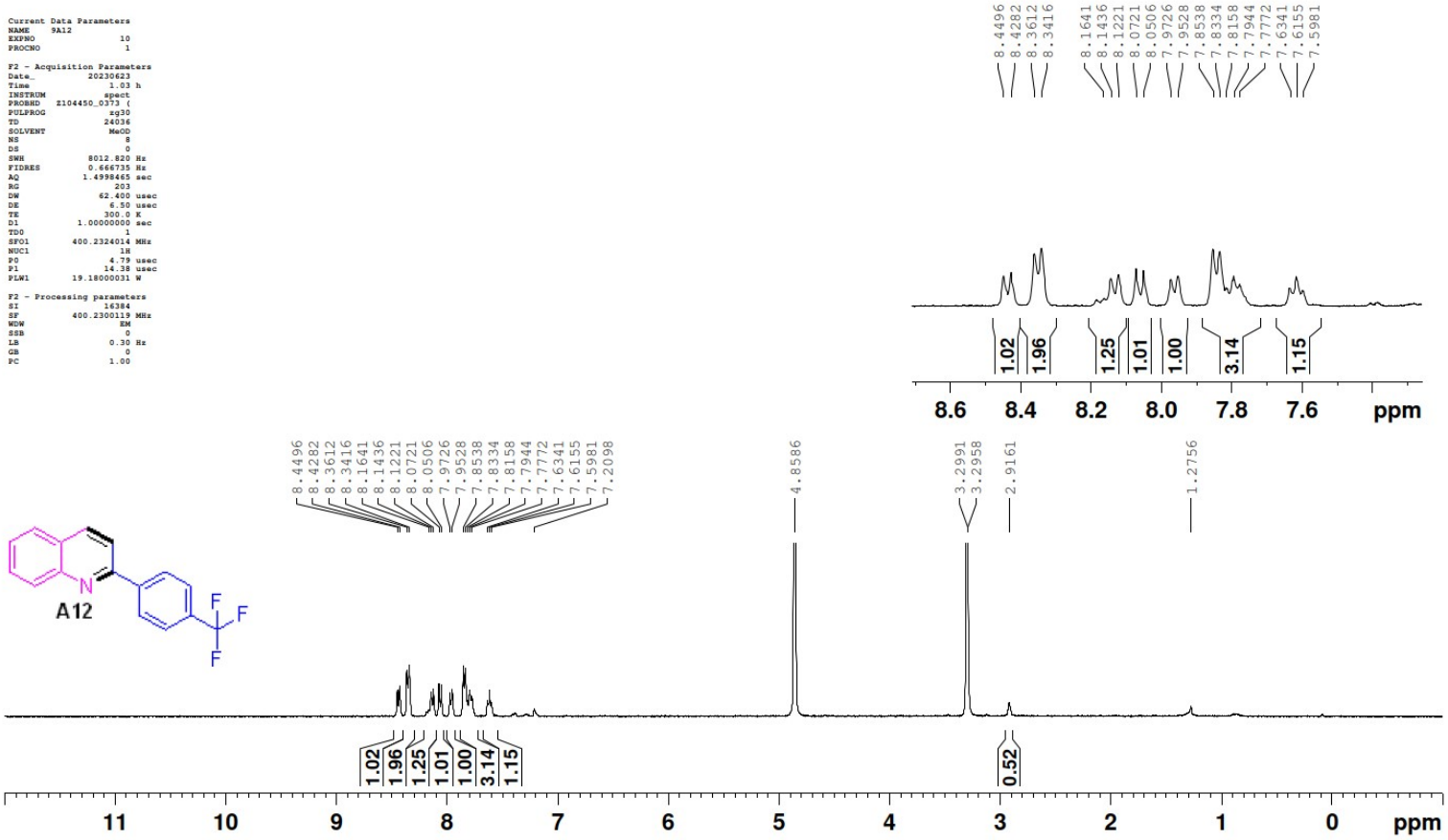
9A10 IN MeOD


Current Data Parameters
NAME 9A10
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230621
Time 16.12 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.1 K
D1 0 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4130
8.3916
8.1188
8.0975
7.9820
7.9614
7.9559
7.9511
7.9361
7.9318
7.9168
7.9123
7.8769
7.8702
7.8555
7.8488
7.8140
7.8108
7.7967
7.7932
7.7755
7.7722
7.6452
7.6273
7.6076
7.5331
7.5295
7.5137
7.5085
7.5002
7.4959
7.3823
7.3636
7.3468
7.3447
7.3065
7.2860
7.2788
7.2578
1.08
1.00
2.01
0.99
1.07
1.05
1.02
1.03
1.00
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
4.8514
3.3029
3.2991
3.2955
1.2771
F
N
9A10
11
10
9
8
7
6
5
4
3
2
1
0
ppm

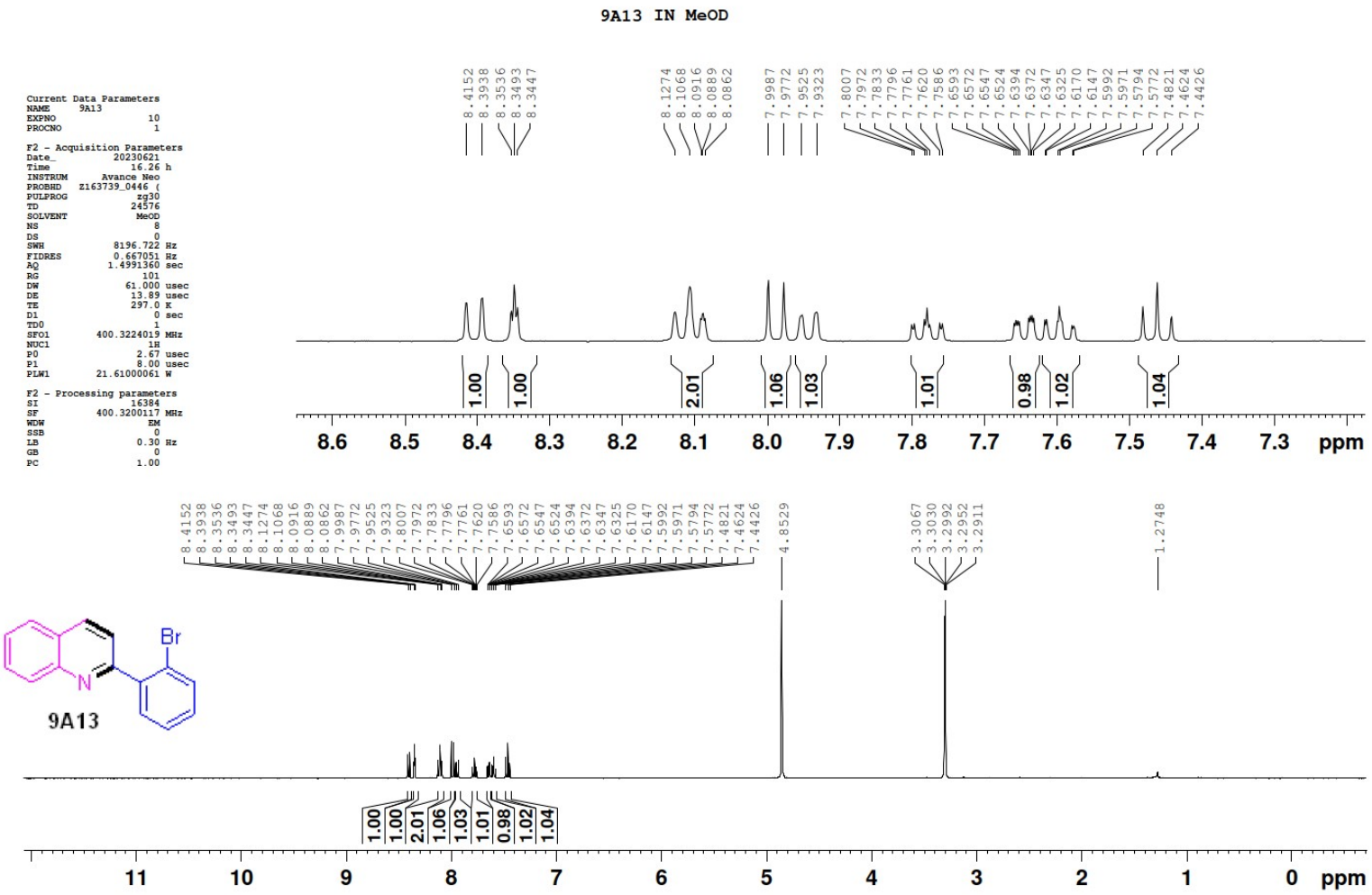

9A11 IN MeOD
Current Data Parameters
NAME 9A11
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230621
Time 16.24 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.0 K
D1 0 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3877
8.3662
8.1905
8.1858
8.1769
8.1735
8.1684
8.1604
8.1549
8.0985
8.0772
7.9745
7.9530
7.9358
7.9152
7.7822
7.7792
7.7617
7.7586
7.7438
7.7407
7.5942
7.5923
7.5747
7.5568
7.5548
7.2889
7.2718
7.2671
7.2502
7.2451
1.00
1.92
0.95
0.87
0.95
1.01
0.99
1.96
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8514
3.3064
3.3029
3.2991
3.2954
2.8769
9A11
N
F
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

9999999999

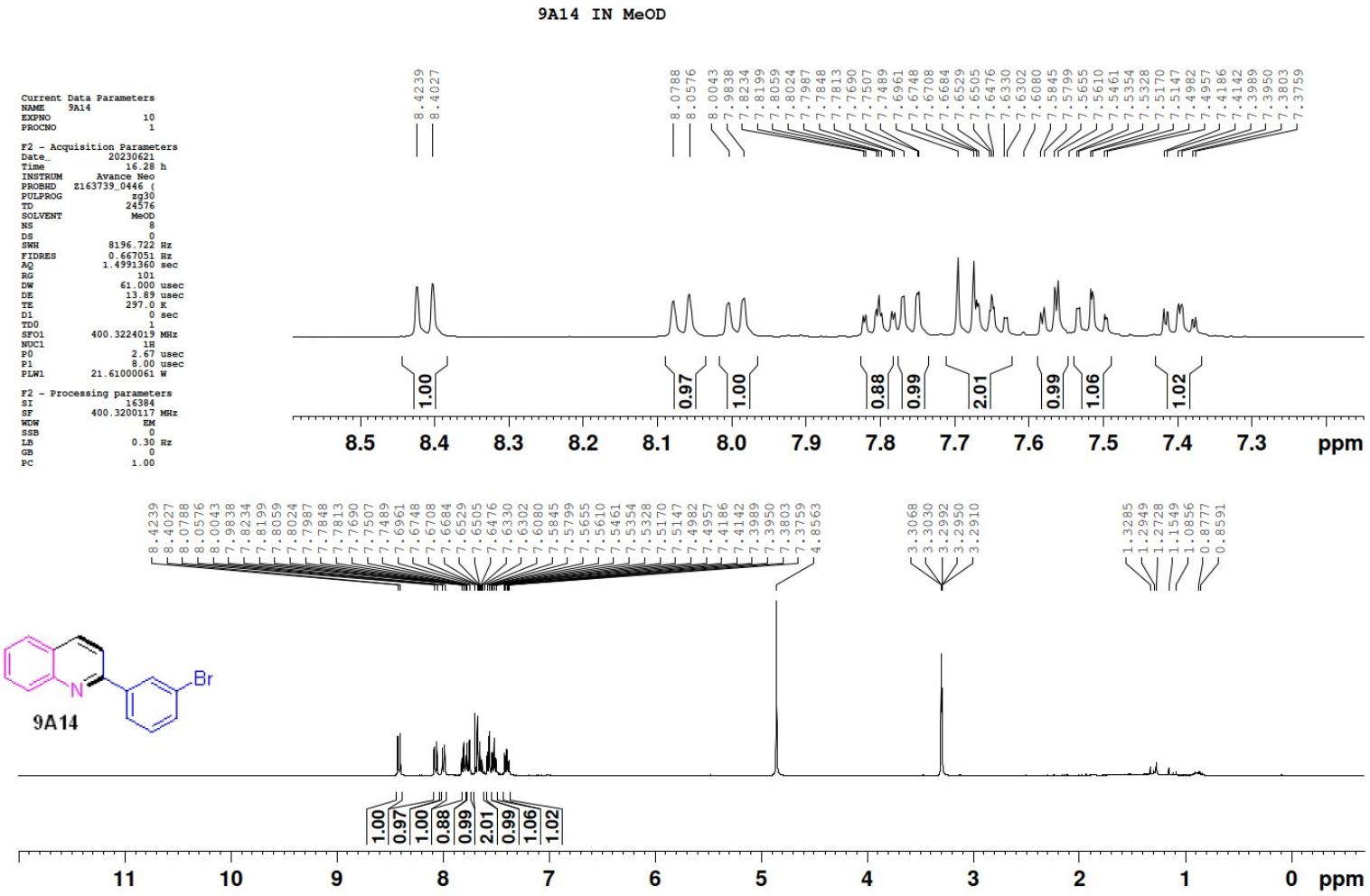
9A12 IN MeOD


Current Data Parameters
NAME 9A12
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230623
Time 1.03 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4496
8.4282
8.3612
8.3416
8.1641
8.1436
8.1221
8.0721
8.0506
7.9726
7.9528
7.8538
7.8334
7.8158
7.7944
7.7772
7.6341
7.6155
7.5981
1.02
1.96
1.25
1.01
1.00
3.14
1.15
8.6
8.4
8.2
8.0
7.8
7.6
ppm
7.2098
4.8586
3.2991
3.2958
2.9161
1.2756
0.52
A12
N
F
F
F
11
10
9
8
7
6
5
4
3
2
1
0

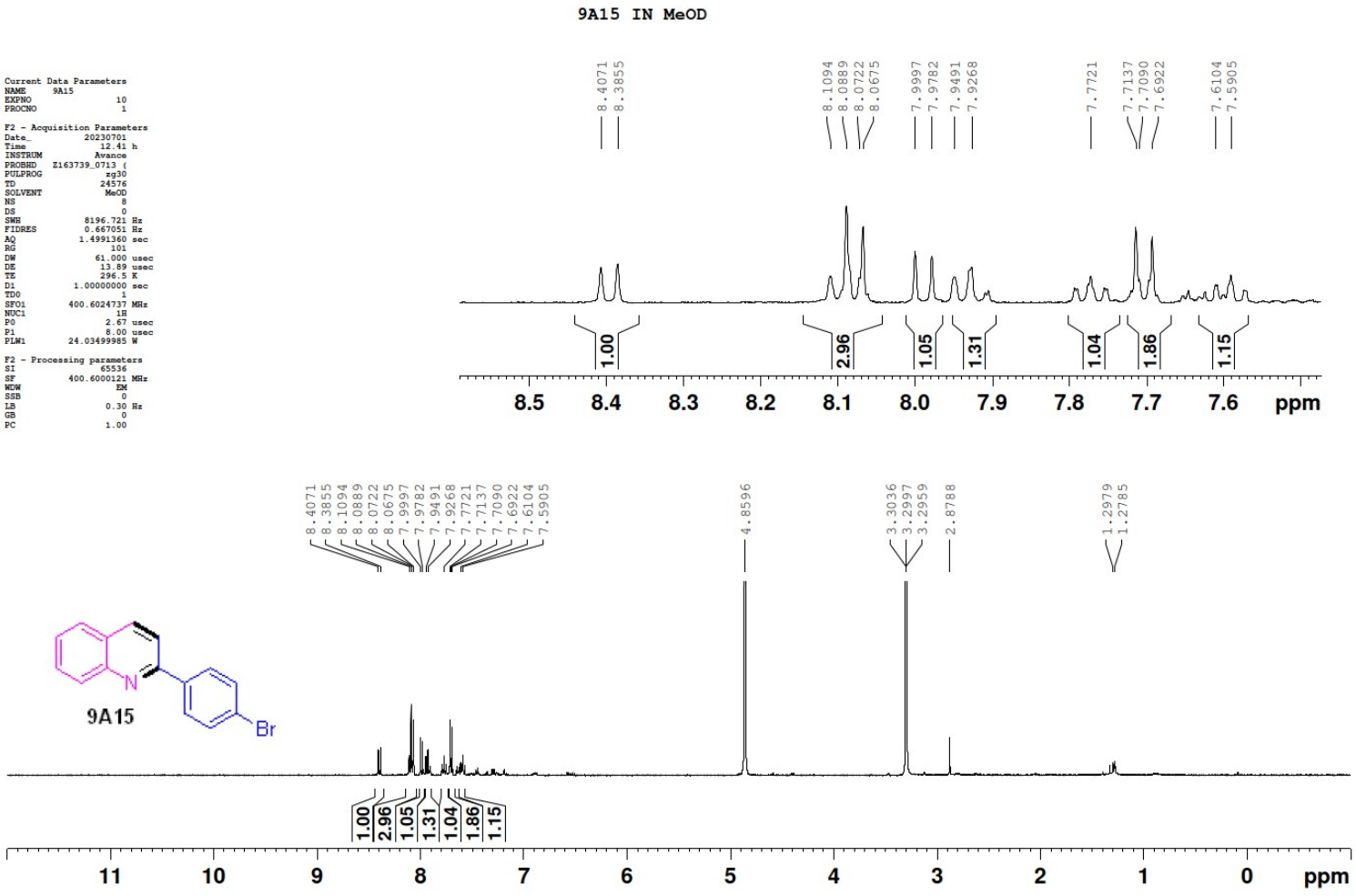
9A13 IN MeOD


Current Data Parameters
NAME 9A13
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230621
Time 16.26 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.0 K
D1 0 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4152
8.3938
8.3536
8.3493
8.3447
8.1274
8.1068
8.0916
8.0889
8.0862
7.9987
7.9772
7.9525
7.9323
7.8007
7.7972
7.7833
7.7796
7.7761
7.7620
7.7586
7.6593
7.6572
7.6547
7.6524
7.6394
7.6372
7.6347
7.6325
7.6170
7.6147
7.5992
7.5971
7.5794
7.5772
7.4821
7.4624
7.4426
1.00
1.00
2.01
1.06
1.03
1.01
0.98
1.02
1.04
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8529
3.3067
3.3030
3.2992
3.2952
3.2911
1.2748
Br
N
9A13
11
10
9
8
7
6
5
4
3
2
1
0
ppm

9A14 IN MeOD


Current Data Parameters
NAME 9A14
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230621
Time 16.28 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.0 K
D1 0 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4239
8.4027
8.0788
8.0576
8.0043
7.9838
7.8234
7.8199
7.8059
7.8024
7.7987
7.7848
7.7813
7.7690
7.7507
7.7489
7.6961
7.6748
7.6708
7.6684
7.6529
7.6505
7.6476
7.6330
7.6302
7.6080
7.5845
7.5799
7.5655
7.5610
7.5461
7.5354
7.5328
7.5170
7.5147
7.4982
7.4957
7.4186
7.4142
7.3989
7.3950
7.3803
7.3759
1.00
0.97
1.00
0.88
0.99
2.01
0.99
1.06
1.02
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8563
3.3068
3.3030
3.2992
3.2950
3.2910
1.3285
1.2949
1.2728
1.1549
1.0856
0.8777
0.8591
N
Br
9A14
11
10
9
8
7
6
5
4
3
2
1
0
ppm

9A15 IN MeOD

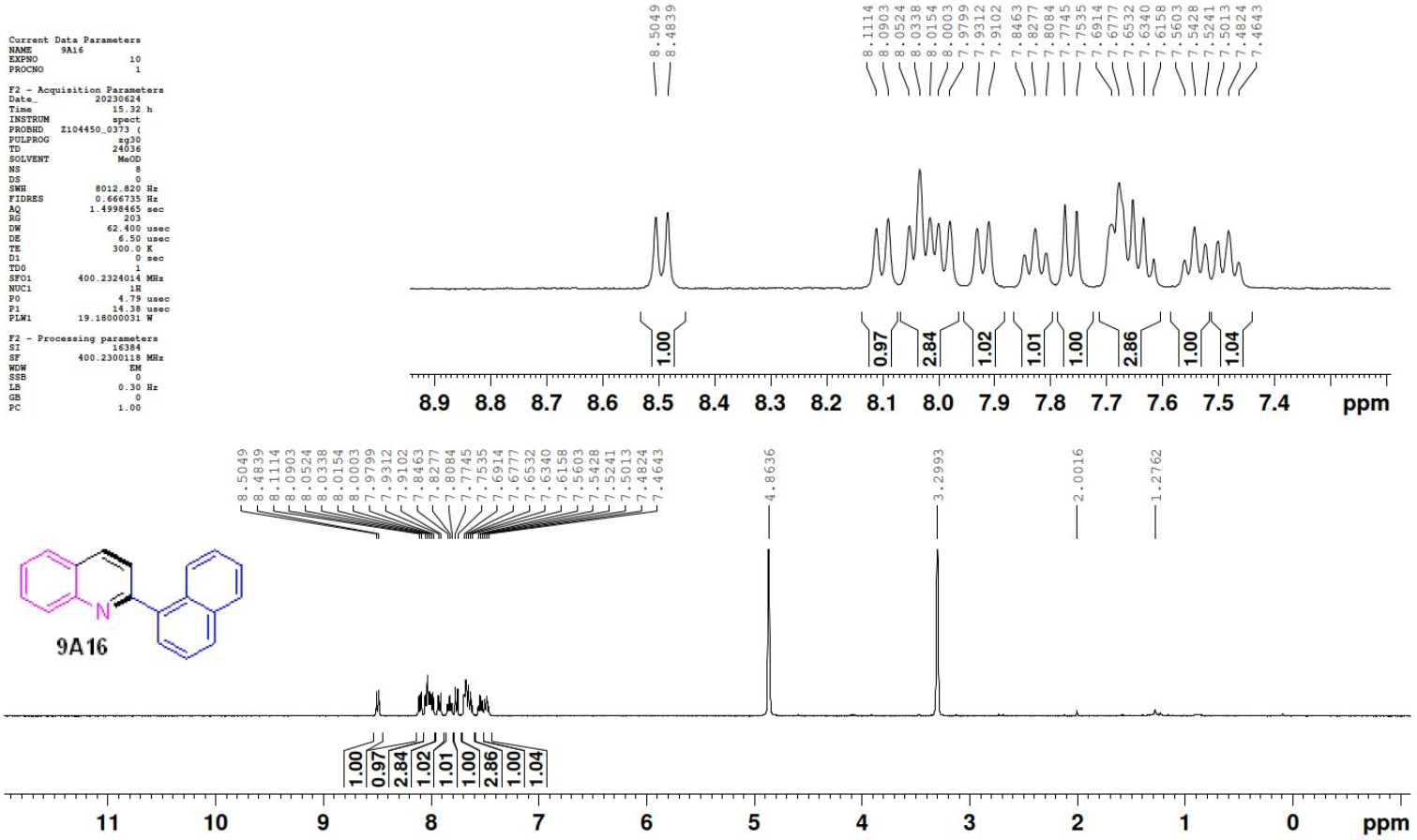

Current Data Parameters
NAME 9A15
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230701
Time 12.41 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4071
8.3855
8.1094
8.0889
8.0722
8.0675
7.9997
7.9782
7.9491
7.9268
7.7721
7.7137
7.7090
7.6922
7.6104
7.5905
1.00
2.96
1.05
1.31
1.04
1.86
1.15
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
ppm
4.8596
3.3036
3.2997
3.2959
2.8788
1.2979
1.2785
9A15
N
Br
11
10
9
8
7
6
5
4
3
2
1
0
ppm

9A16 IN MeOD

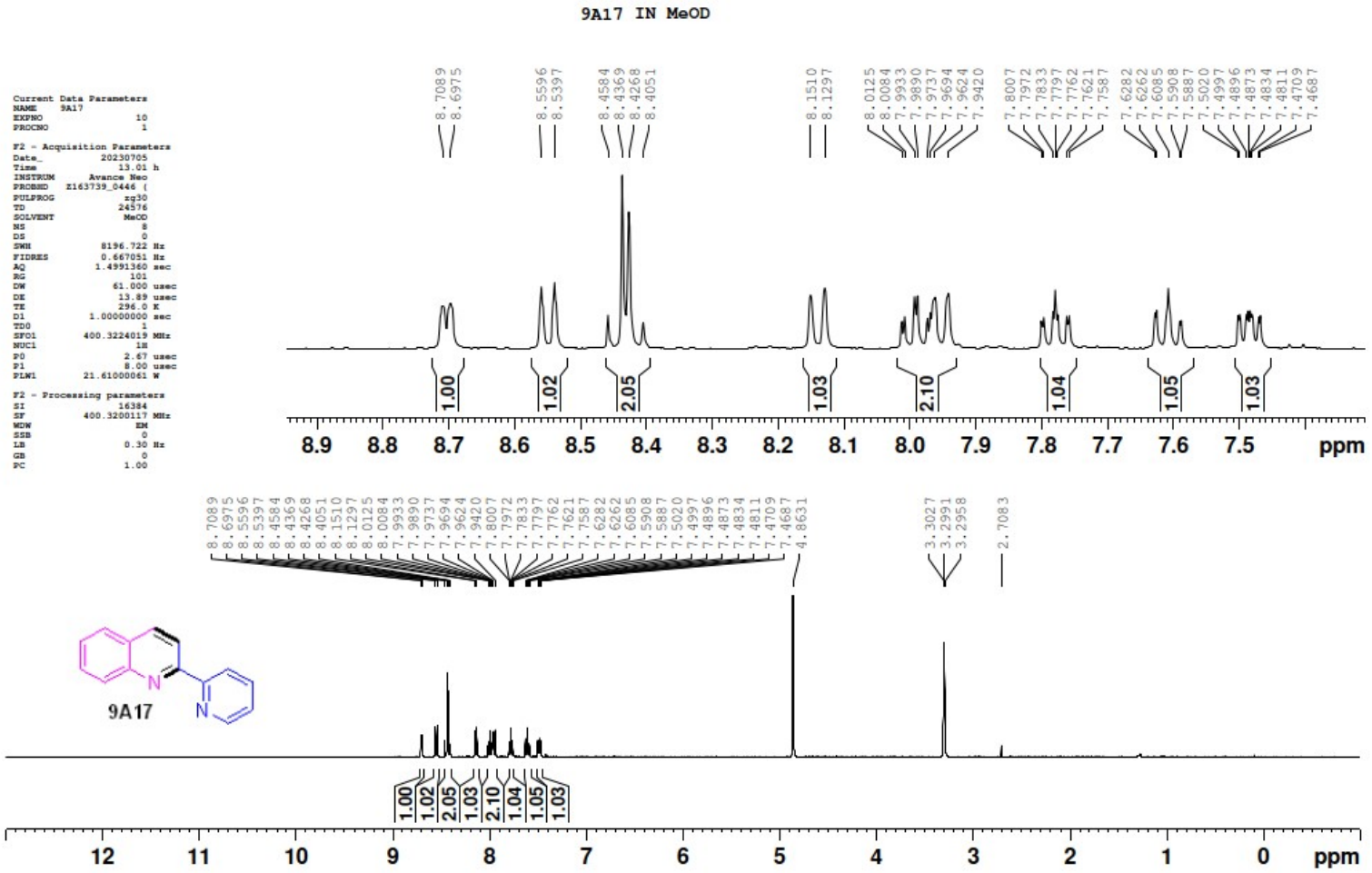
```
Current Data Parameters
NAME      9A16
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20230624
Time           15.32 h
INSTRUM         spect
PROBHD   Z104450_0373 (
PULPROG         zg30
TD             24036
SOLVENT          MeOD
NS                8
DS                0
SWH         8012.820 Hz
FIDRES      0.666735 Hz
AQ          1.4998465 sec
RG              203
DW           62.400 usec
DE            6.50 usec
TE           300.0 K
D1              0 sec
TD0             1
SFO1    400.2324014 MHz
NUC1            1H
P0            4.79 usec
P1           14.38 usec
PLW1    19.18000031 W

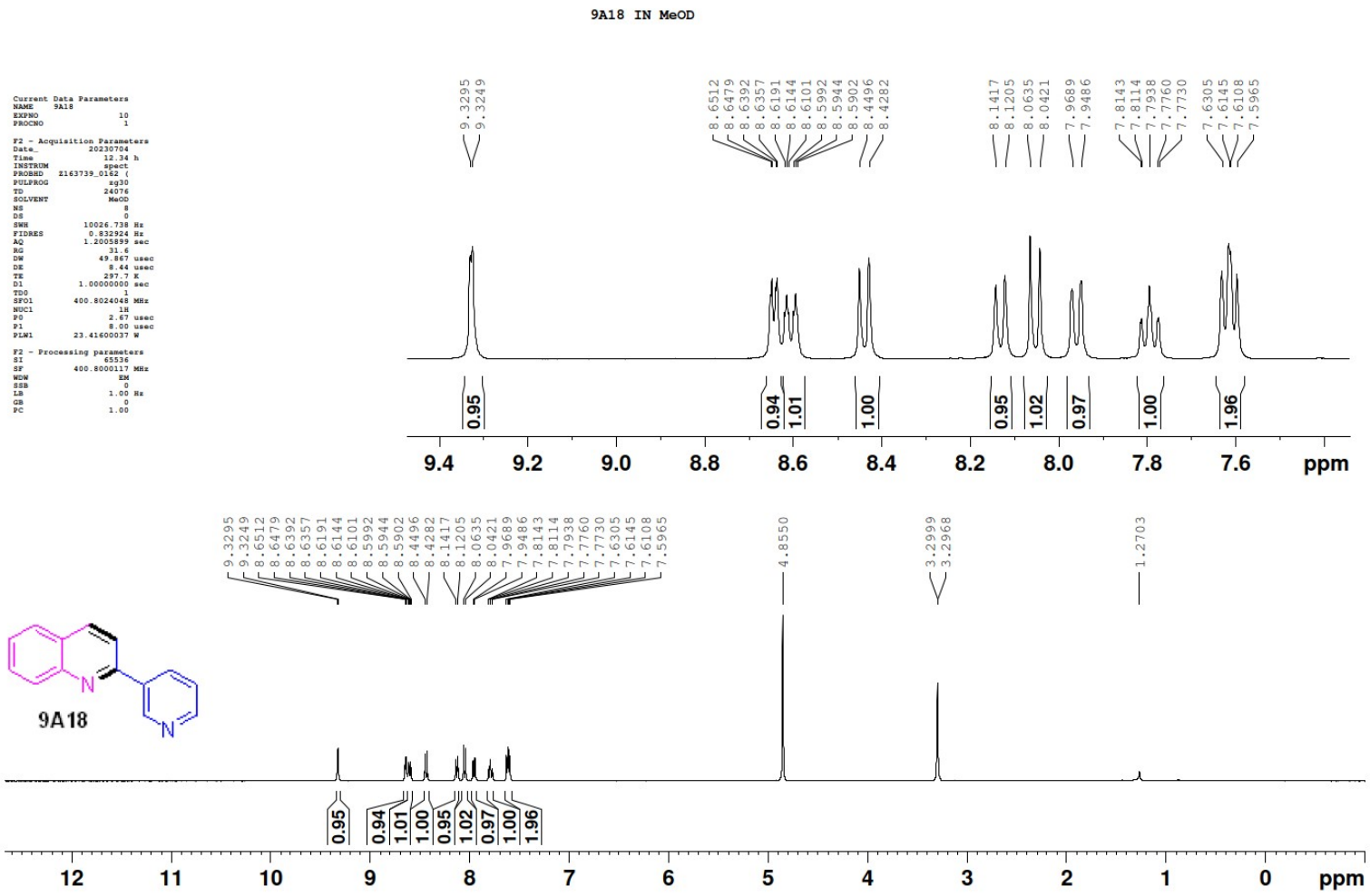
F2 - Processing parameters
SI          16384
SF      400.2300118 MHz
WDW            EM
SSB             0
LB           0.30 Hz
GB              0
PC           1.00
```



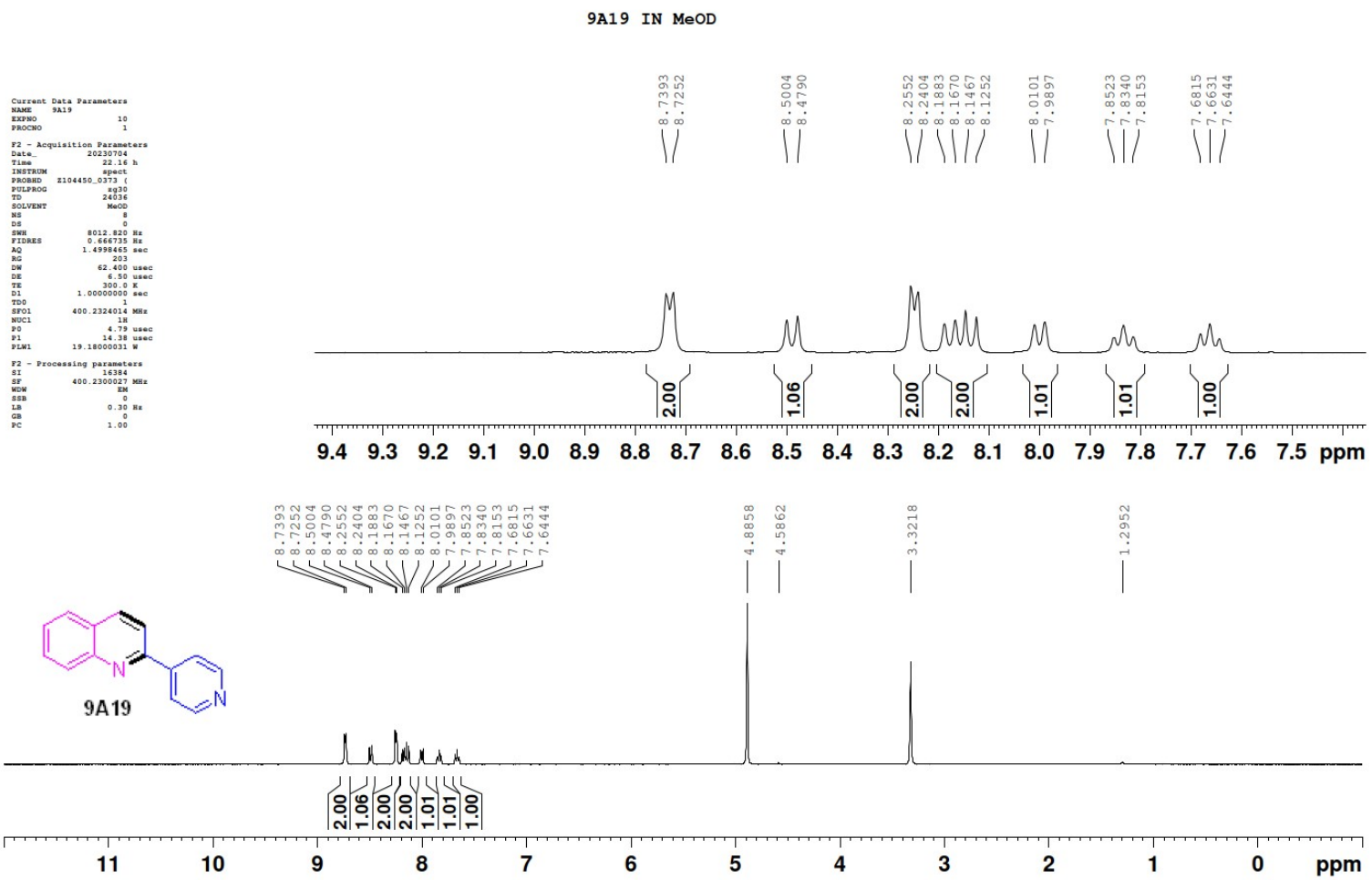
9A16


9A17 IN MeOD
Current Data Parameters
NAME 9A17
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230705
Time 13.01 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.3224019 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.7089
8.6975
8.5596
8.5397
8.4584
8.4369
8.4268
8.4051
8.1510
8.1297
8.0125
8.0084
7.9933
7.9890
7.9737
7.9694
7.9624
7.9420
7.8007
7.7972
7.7833
7.7797
7.7762
7.7621
7.7587
7.6282
7.6262
7.6085
7.5908
7.5887
7.5020
7.4997
7.4896
7.4873
7.4834
7.4811
7.4709
7.4687
1.00
1.02
2.05
1.03
2.10
1.04
1.05
1.03
8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
4.8631
3.3027
3.2991
3.2958
2.7083
9A17
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

9A18 IN MeOD


Current Data Parameters
NAME 9A18
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230704
Time 12.34 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24076
SOLVENT MeOD
NS 8
DS 0
SWH 10026.738 Hz
FIDRES 0.832924 Hz
AQ 1.2005899 sec
RG 31.6
DW 49.867 usec
DE 8.44 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.8024048 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.41600037 W
F2 - Processing parameters
SI 65536
SF 400.8000117 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
9.3295
9.3249
8.6512
8.6479
8.6392
8.6357
8.6191
8.6144
8.6101
8.5992
8.5944
8.5902
8.4496
8.4282
8.1417
8.1205
8.0635
8.0421
7.9689
7.9486
7.8143
7.8114
7.7938
7.7760
7.7730
7.6305
7.6145
7.6108
7.5965
0.95
0.94
1.01
1.00
0.95
1.02
0.97
1.00
1.96
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
ppm
4.8550
3.2999
3.2968
1.2703
9A18
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

9A19 IN MeOD

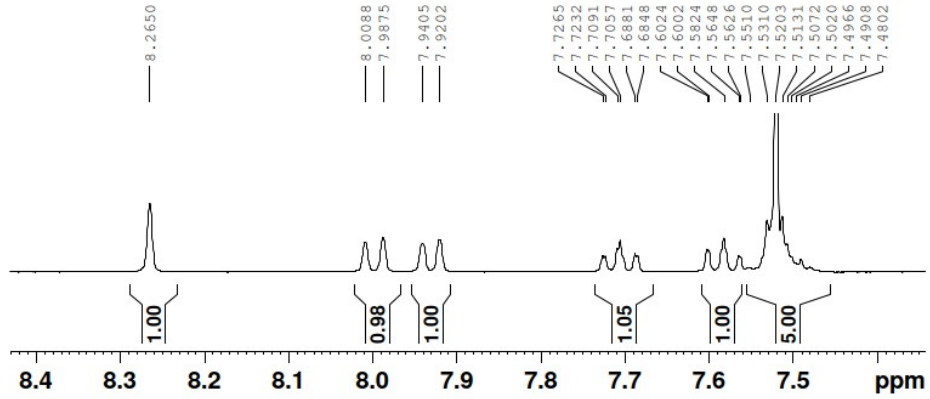

Current Data Parameters
NAME 9A19
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230704
Time 22.16 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.7393
8.7252
8.5004
8.4790
8.2552
8.2404
8.1883
8.1670
8.1467
8.1252
8.0101
7.9897
7.8523
7.8340
7.8153
7.6815
7.6631
7.6444
2.00
1.06
2.00
2.00
1.01
1.01
1.00
9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
4.8858
4.5862
3.3218
1.2952
N
N
9A19
11 10 9 8 7 6 5 4 3 2 1 0 ppm

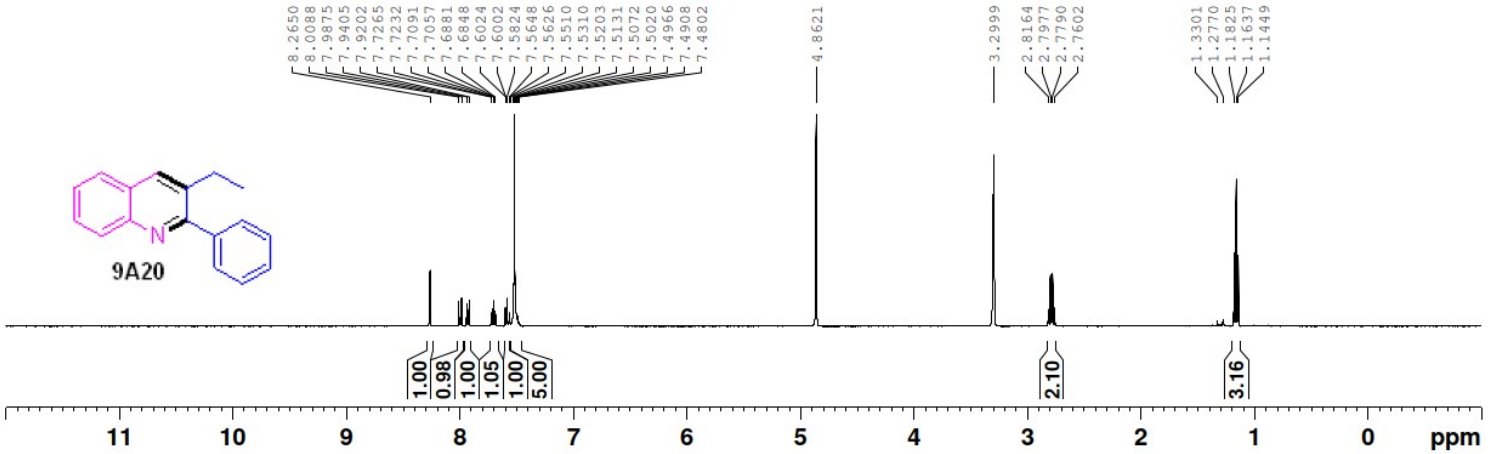
9A20 IN MeOD

```
Current Data Parameters
NAME      9A20
EXPNO       10
PROCNO       1

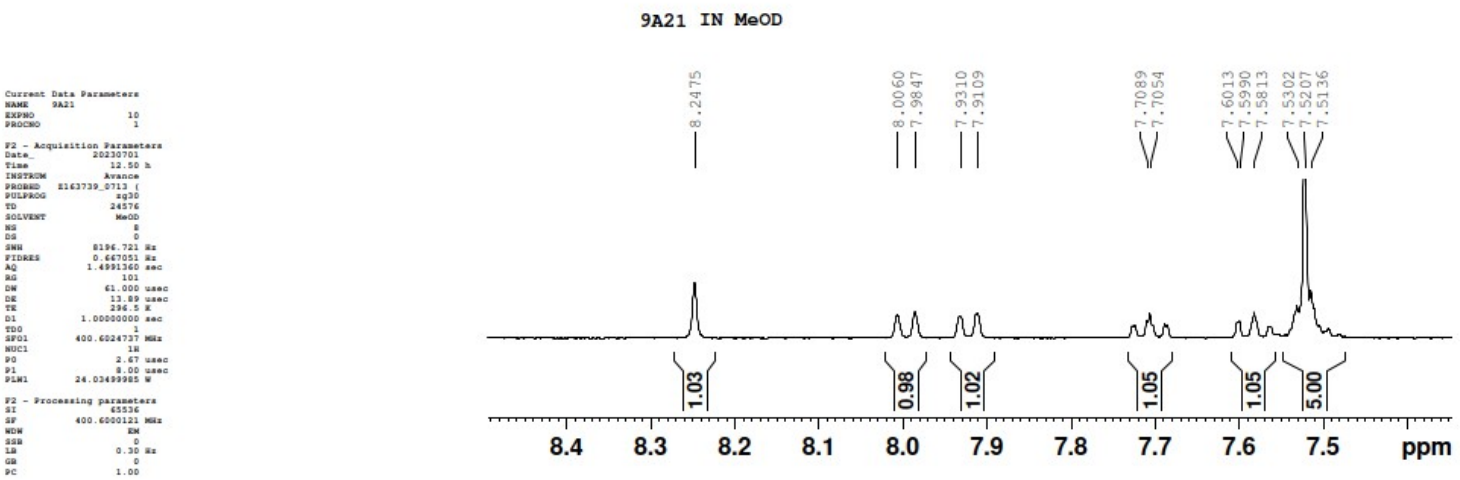
F2 - Acquisition Parameters
Date_     20230701
Time         12.47 h
INSTRUM      Avance
PROBHD   Z163739_0713 (
PULPROG      zg30
TD          24576
SOLVENT      MeOD
NS              8
DS              0
SWH       8196.721 Hz
FIDRES    0.667051 Hz
AQ        1.4991360 sec
RG            101
DW         61.000 usec
DE         13.89 usec
TE          296.5 K
D1        1.00000000 sec
TD0             1
SFO1    400.6024737 MHz
NUC1            1H
P0          2.67 usec
P1          8.00 usec
PLW1   24.03499985 W

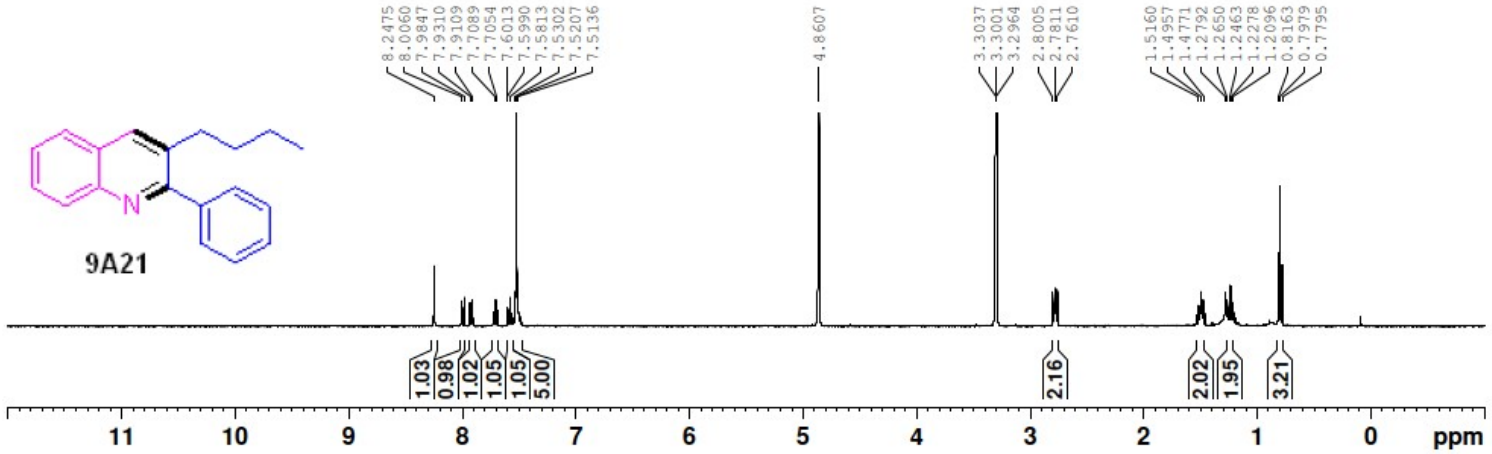
F2 - Processing parameters
SI          65536
SF      400.6000121 MHz
WDW            EM
SSB             0
LB           0.30 Hz
GB              0
PC           1.00
```



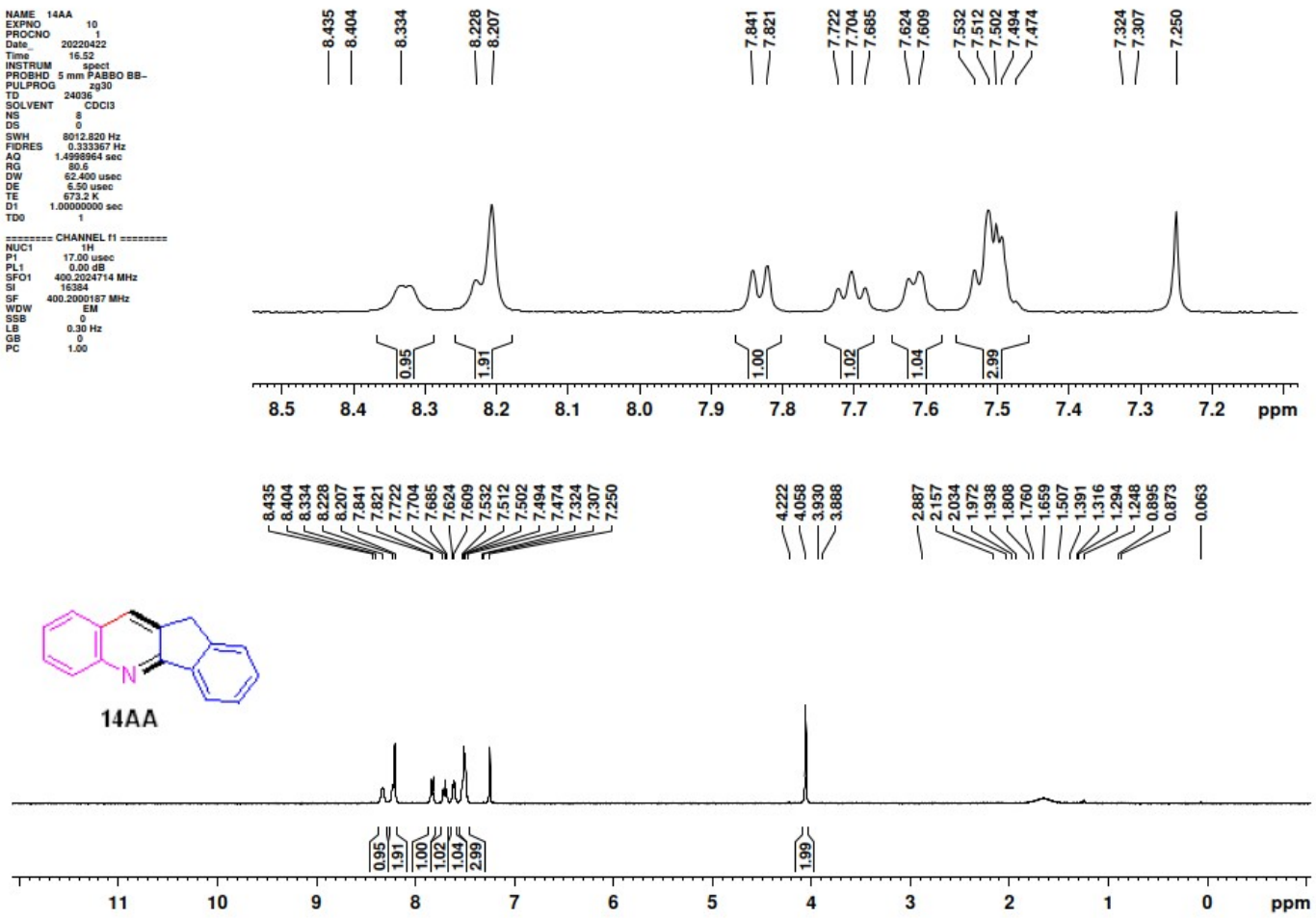


9A21 IN MeOD


Current Data Parameters
NAME 9A21
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230701
Time 12.50 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.2475
8.0060
7.9847
7.9310
7.9109
7.7089
7.7054
7.6013
7.5990
7.5813
7.5302
7.5207
7.5136
1.03
0.98
1.02
1.05
1.05
5.00
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
ppm


9A21
8.2475
8.0060
7.9847
7.9310
7.9109
7.7089
7.7054
7.6013
7.5990
7.5813
7.5302
7.5207
7.5136
4.8607
3.3037
3.3001
3.2964
2.8005
2.7811
2.7610
1.5160
1.4957
1.4771
1.2792
1.2650
1.2463
1.2278
1.2096
0.8163
0.7979
0.7795
1.03
0.98
1.02
1.05
1.05
5.00
2.16
2.02
1.95
3.21
11
10
9
8
7
6
5
4
3
2
1
0
ppm

14AA IN CDCl3

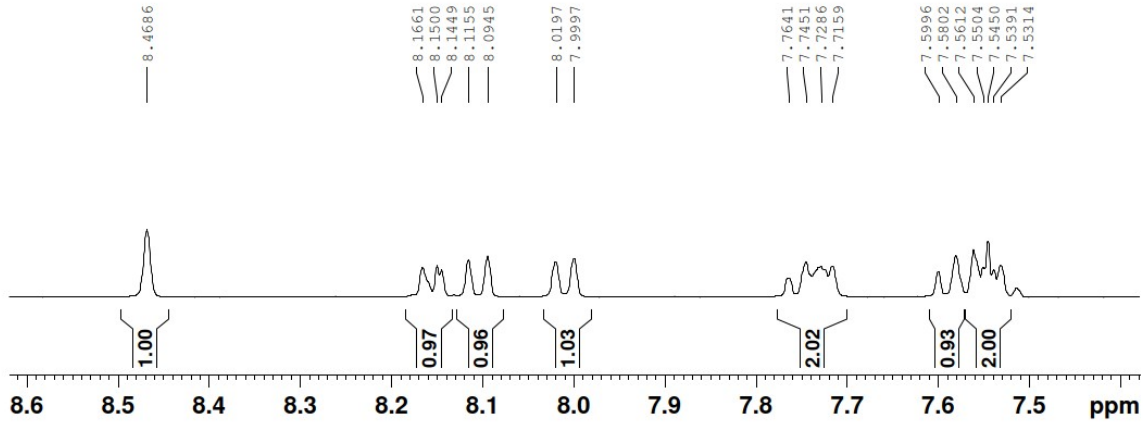


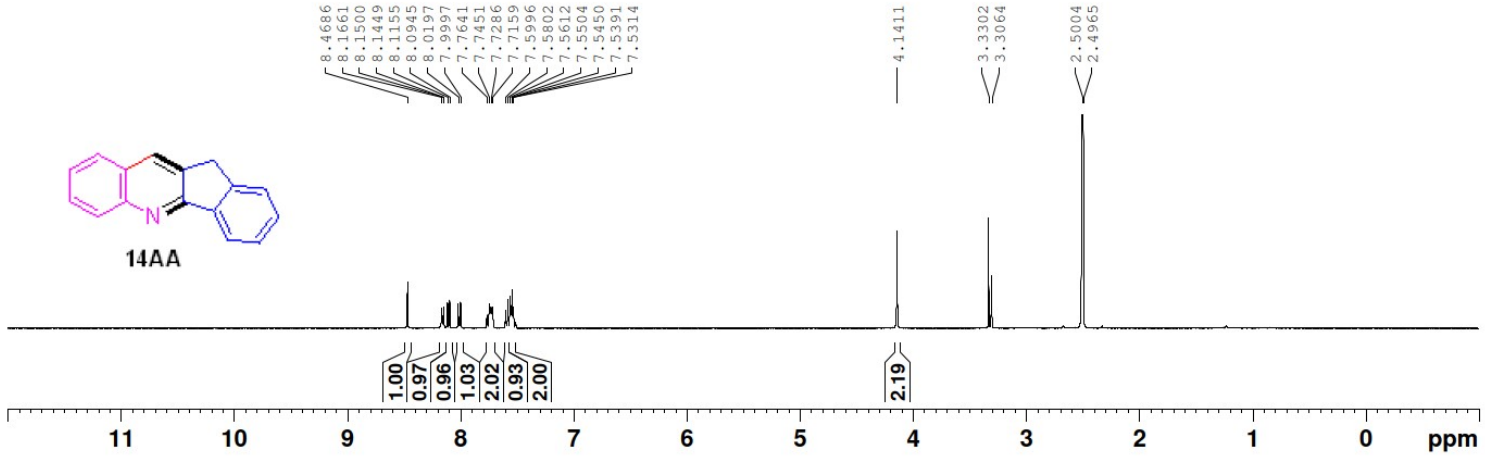
14AA IN DMSO

```
Current Data Parameters
NAME      14AA
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20230617
Time         14.49 h
INSTRUM      Avance
PROBHD   Z163739_0713 (
PULPROG         zg30
TD             24576
SOLVENT         DMSO
NS                 8
DS                 0
SWH         8196.721 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE            295.6 K
D1                 0 sec
TD0                1
SFO1      400.6024737 MHz
NUC1             1H
P0             2.67 usec
P1             8.00 usec
PLW1     24.03499985 W

F2 - Processing parameters
SI             65536
SF        400.6000042 MHz
WDW              EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```



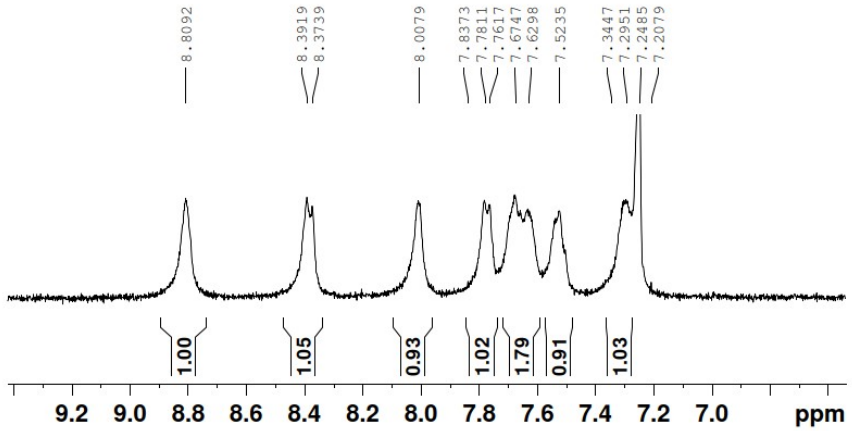


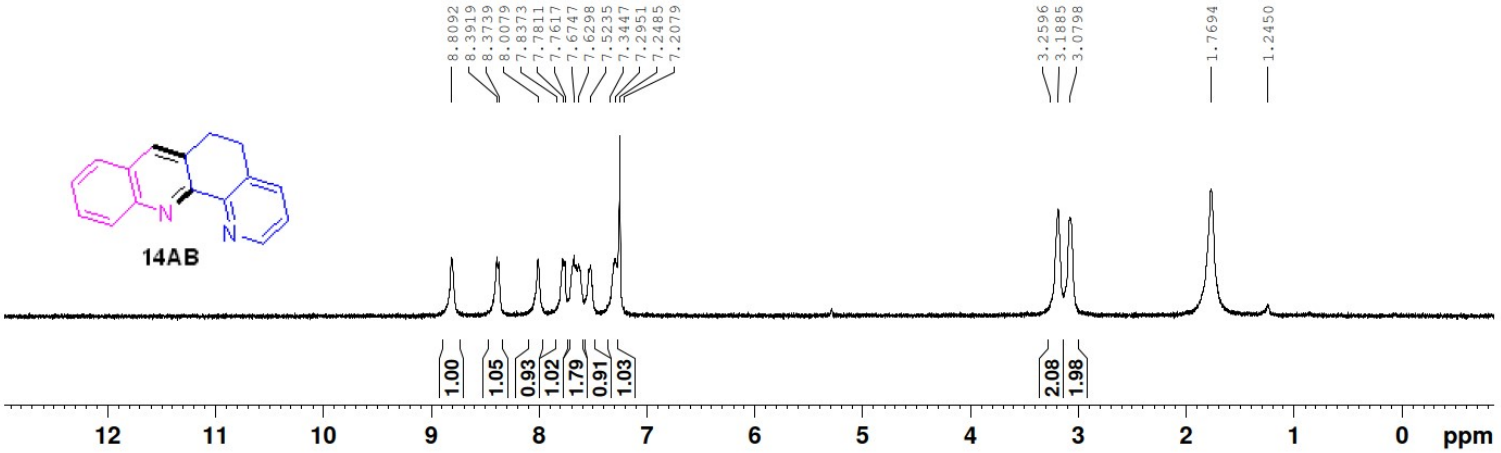
14AB IN CDCl3


```
Current Data Parameters
NAME          14AB
EXPNO             10
PROCNO             1

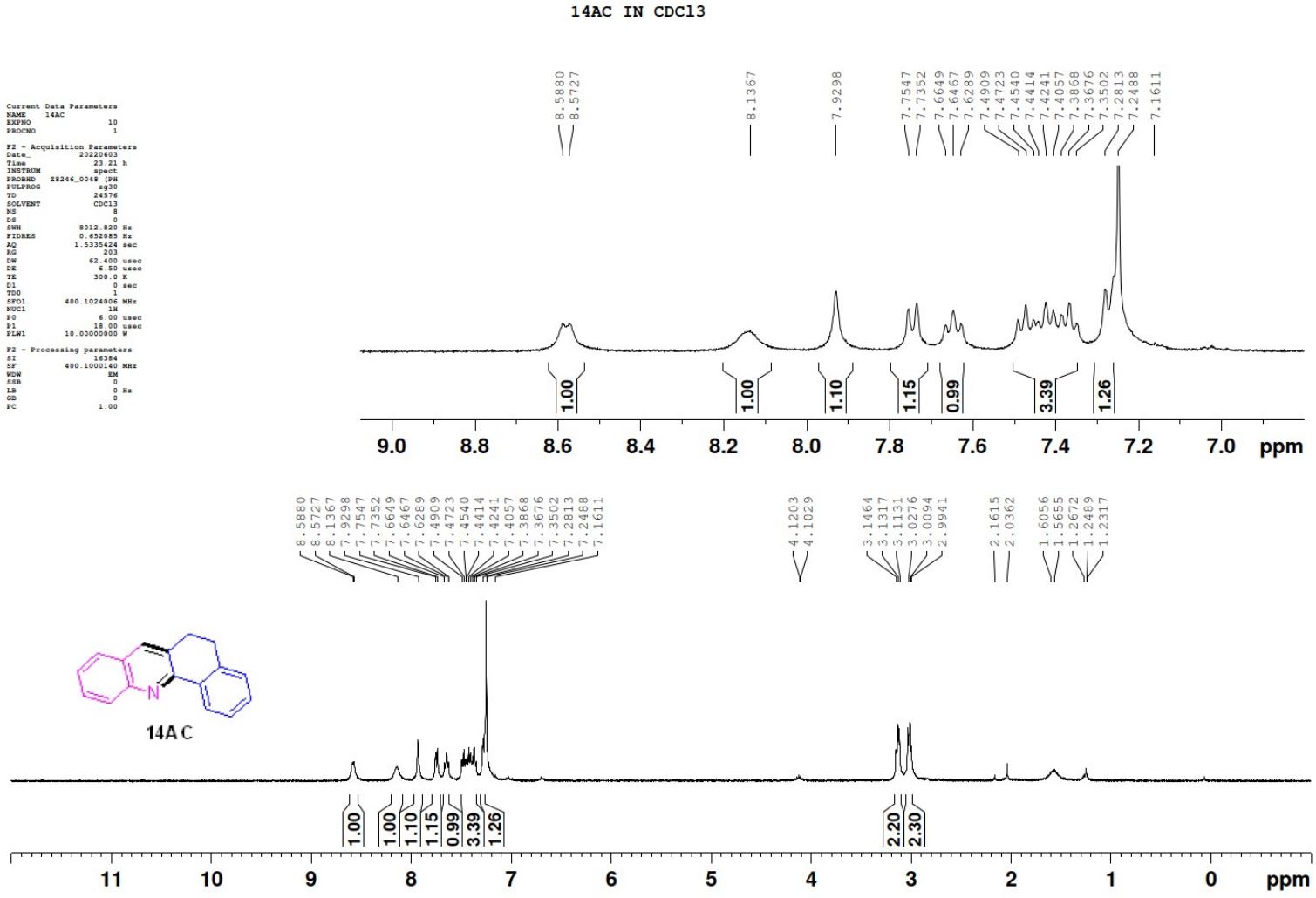
F2 - Acquisition Parameters
Date_        20220505
Time              1.35 h
INSTRUM           spect
PROBHD    Z8246_0048 (PR
PULPROG          zg30
TD              24000
SOLVENT         CDCl3
NS                 8
DS                 0
SWH          8012.820 Hz
FIDRES       0.667735 Hz
AQ           1.4976000 sec
RG               161
DW              62.400 usec
DE               6.50 usec
TE              300.0 K
D1                 0 sec
TD0                1
SFO1       400.1024006 MHz
NUC1               1H
PG              6.00 usec
P1             18.00 usec
PLW1       10.00000000 W

F2 - Processing parameters
SI             16384
SF       400.1000129 MHz
WDW               EM
SSB                0
LB                 0 Hz
GB                 0
PC              1.00
```



14AC IN CDCl3

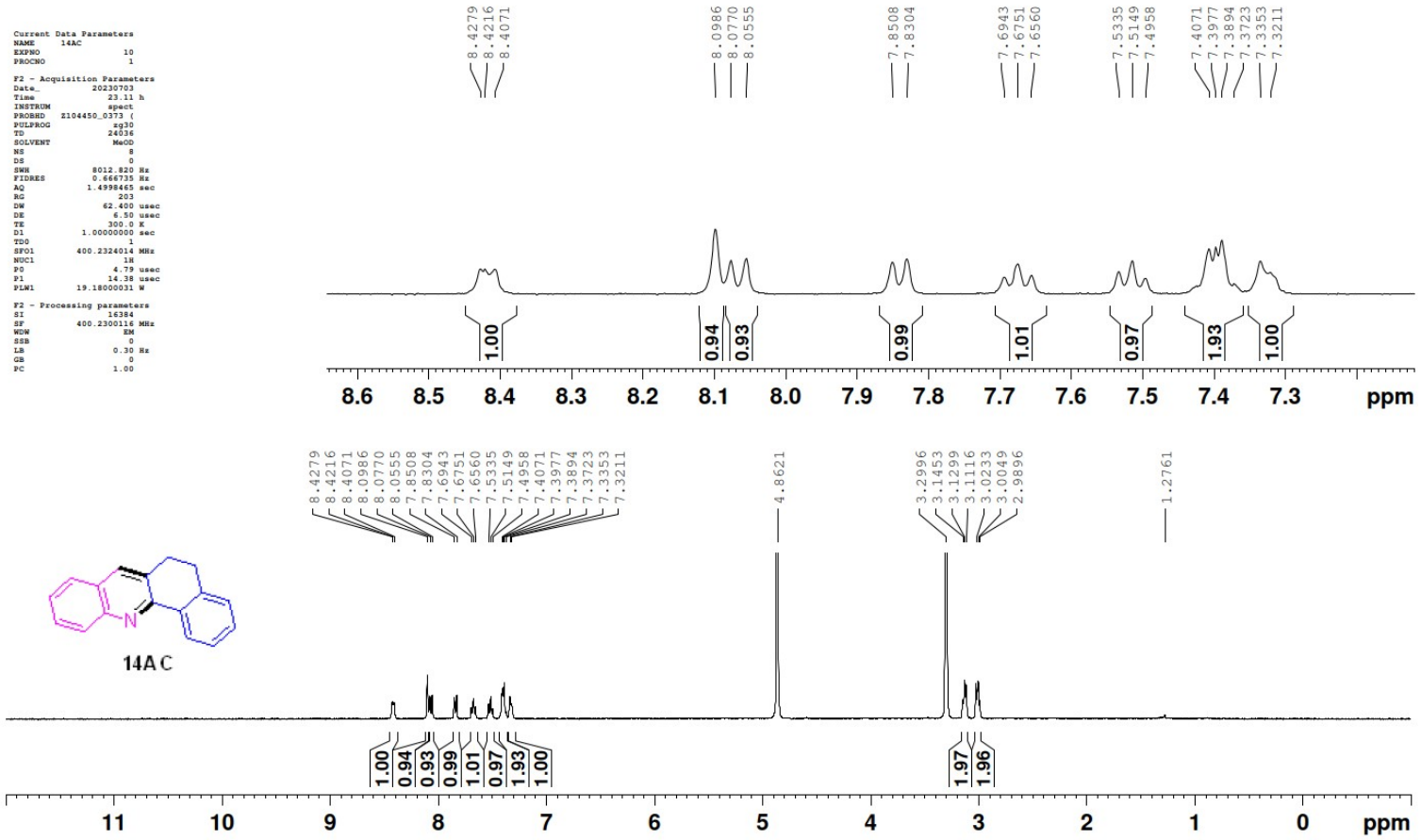


14AC IN MeOD

```
Current Data Parameters
NAME      14AC
EXPNO           10
PROCNO           1

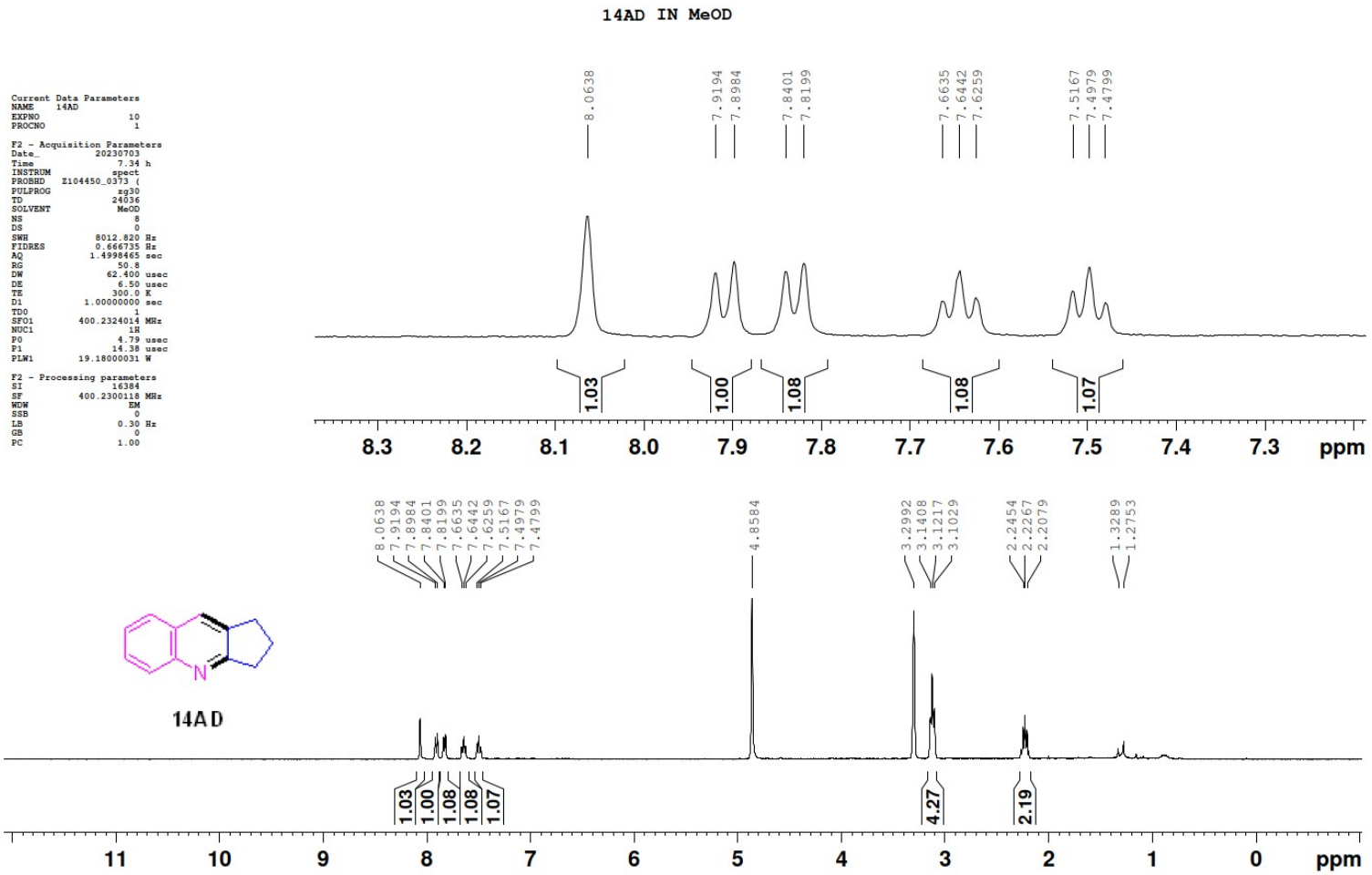
F2 - Acquisition Parameters
Date_        20230703
Time            23.11 h
INSTRUM          spect
PROBHD   Z104450_0373 (
PULPROG          zg30
TD              24036
SOLVENT          MeOD
NS                  8
DS                  0
SWH          8012.820 Hz
FIDRES       0.666735 Hz
AQ           1.4998465 sec
RG                203
DW             62.400 usec
DE              6.50 usec
TE             300.0 K
D1          1.00000000 sec
TD0                 1
SFO1       400.2324014 MHz
NUC1               1H
P0              4.79 usec
P1             14.38 usec
PLW1       19.18000031 W

F2 - Processing parameters
SI              16384
SF         400.2300116 MHz
WDW               EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



14AC

14AD IN MeOD

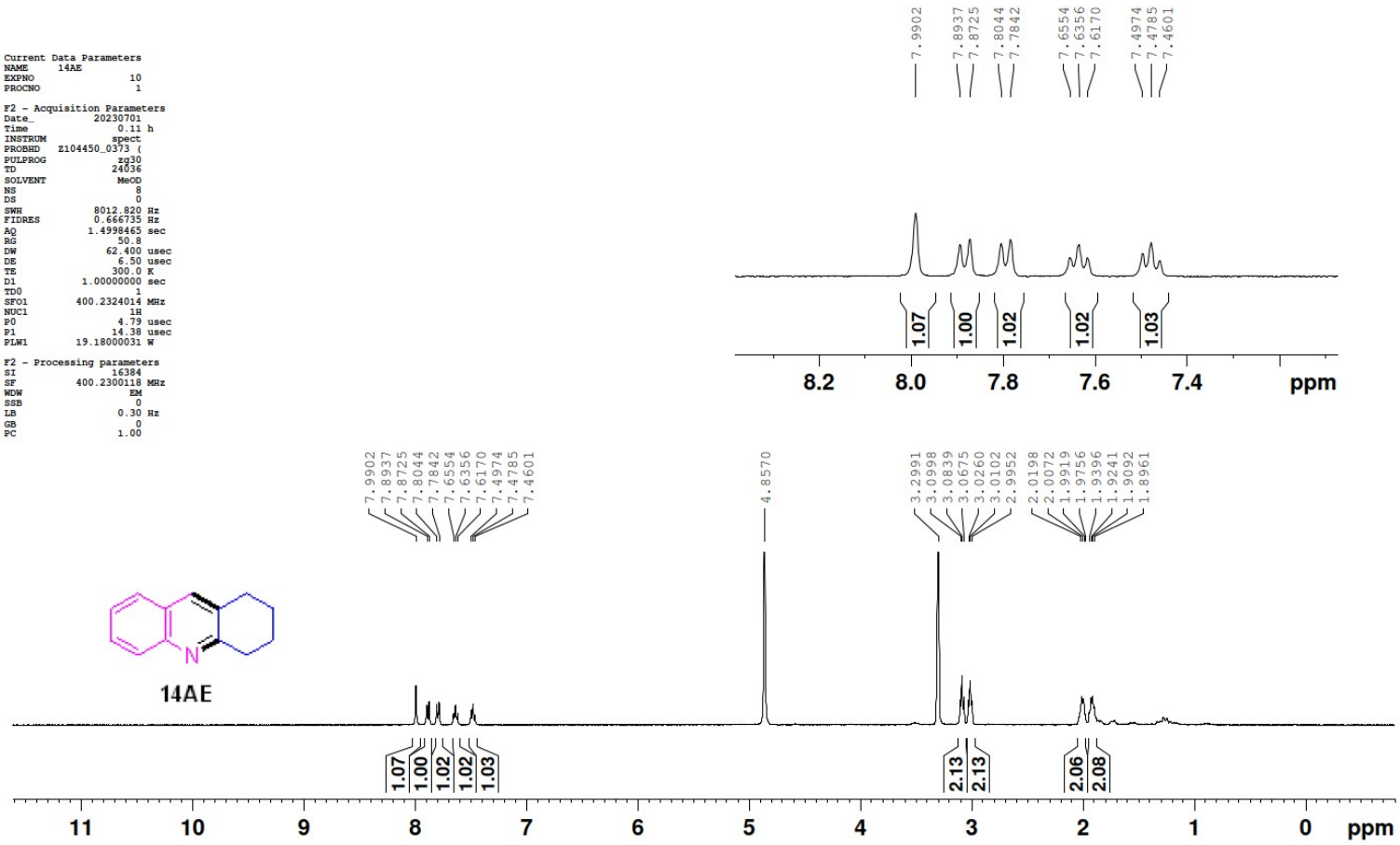

Current Data Parameters
NAME 14AD
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230703
Time 7.34 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0638
7.9194
7.8984
7.8401
7.8199
7.6635
7.6442
7.6259
7.5167
7.4979
7.4799
1.03
1.00
1.08
1.08
1.07
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
4.8584
3.2992
3.1408
3.1217
3.1029
2.2454
2.2267
2.2079
1.3289
1.2753
4.27
2.19
11
10
9
8
7
6
5
4
3
2
1
0
ppm
N
14AD

14AE IN MEOD

```
Current Data Parameters
NAME      14AE
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20230701
Time           0.11 h
INSTRUM       spect
PROBHD   Z104450_0373 (
PULPROG         zg30
TD             24036
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8012.820 Hz
FIDRES      0.666735 Hz
AQ          1.4998465 sec
RG              50.8
DW             62.400 usec
DE              6.50 usec
TE             300.0 K
D1          1.00000000 sec
TD0                1
SFO1      400.2324014 MHz
NUC1              1H
P0              4.79 usec
P1             14.38 usec
PLW1      19.18000031 W

F2 - Processing parameters
SI             16384
SF        400.2300118 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

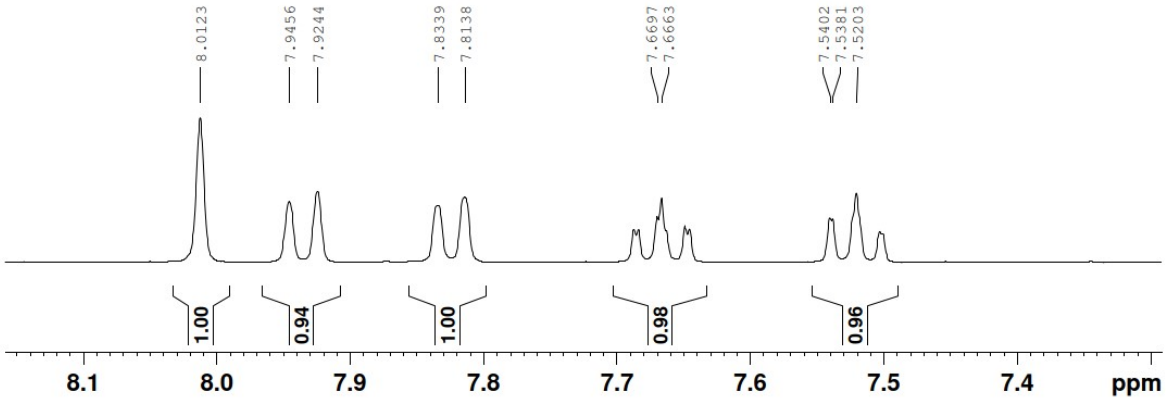


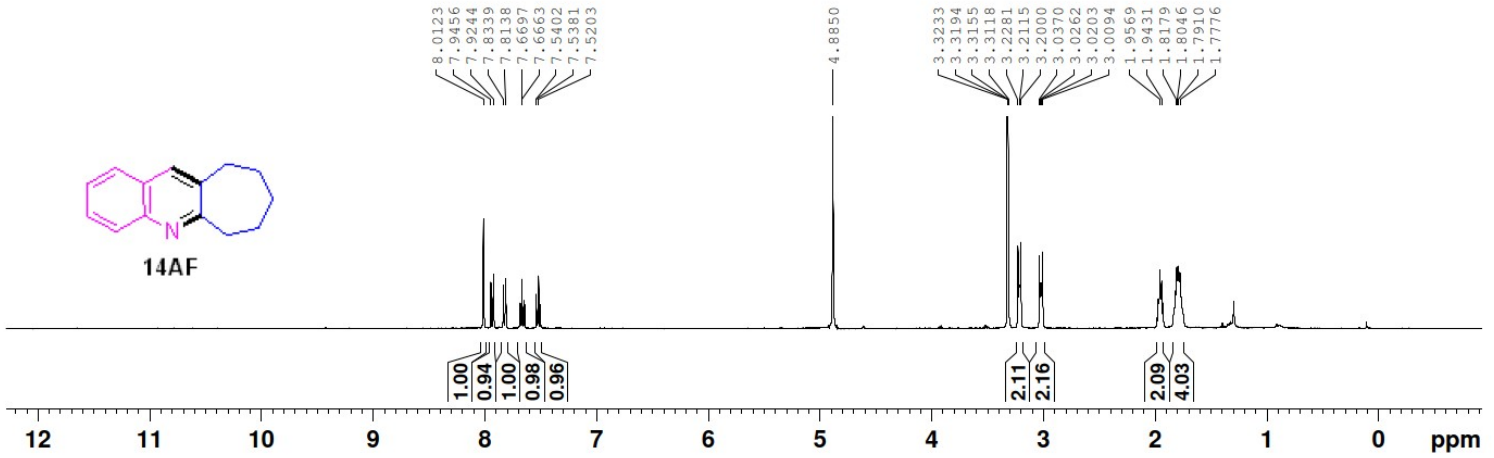
14AF IN MeOD

```
Current Data Parameters
NAME      14AF
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_        20230626
Time            7.35 h
INSTRUM       Avance
PROBHD    Z163739_0713 (
PULPROG          zg30
TD              24576
SOLVENT          MeOD
NS                  8
DS                  0
SWH          8196.721 Hz
FIDRES       0.667051 Hz
AQ           1.4991360 sec
RG                101
DW             61.000 usec
DE             13.89 usec
TE             296.2 K
D1          1.00000000 sec
TD0                 1
SFO1       400.6024737 MHz
NUC1               1H
P0              2.67 usec
P1              8.00 usec
PLW1       24.03499985 W

F2 - Processing parameters
SI              65536
SF       400.6000042 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```





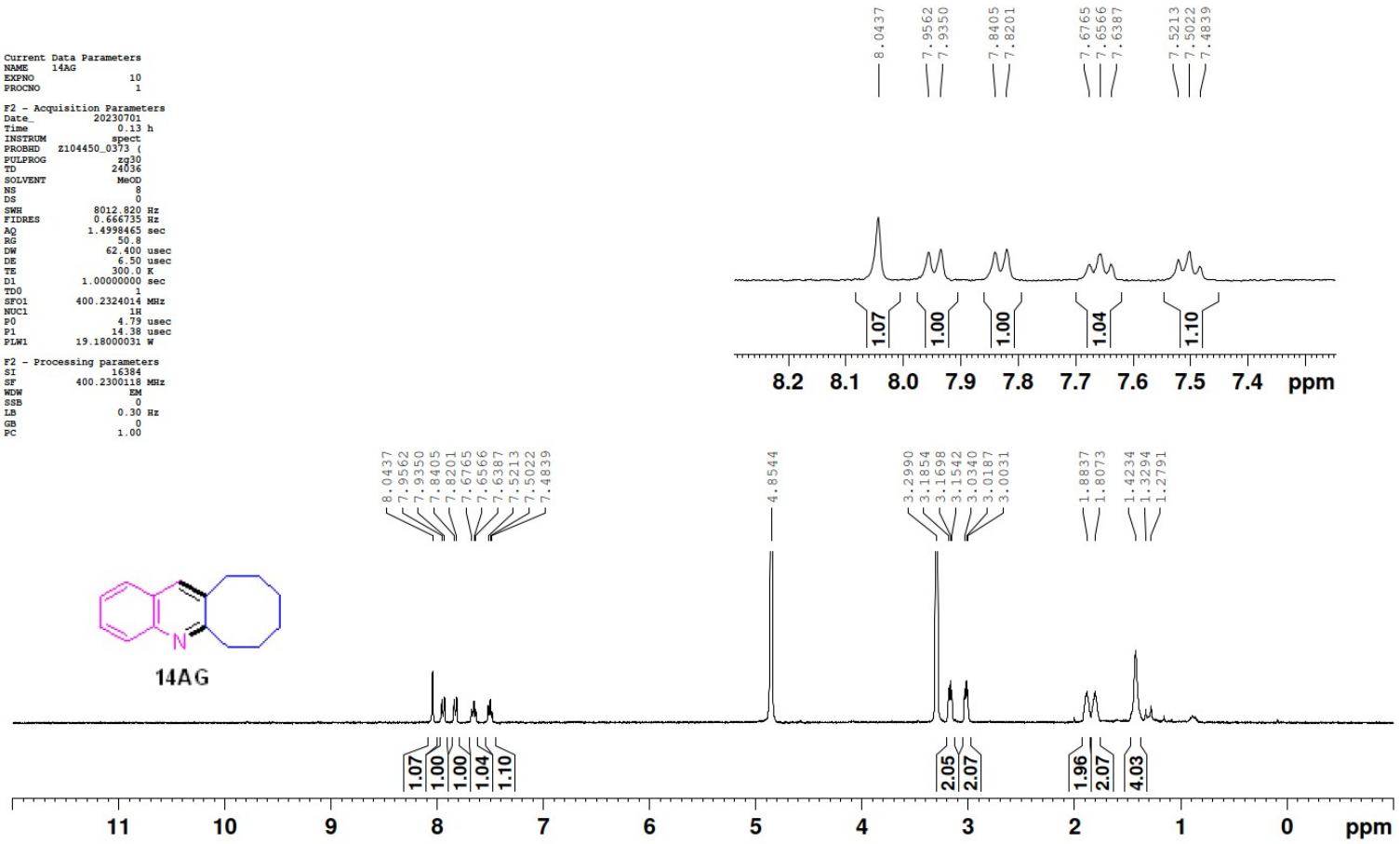
14AF

14AG IN MEOD

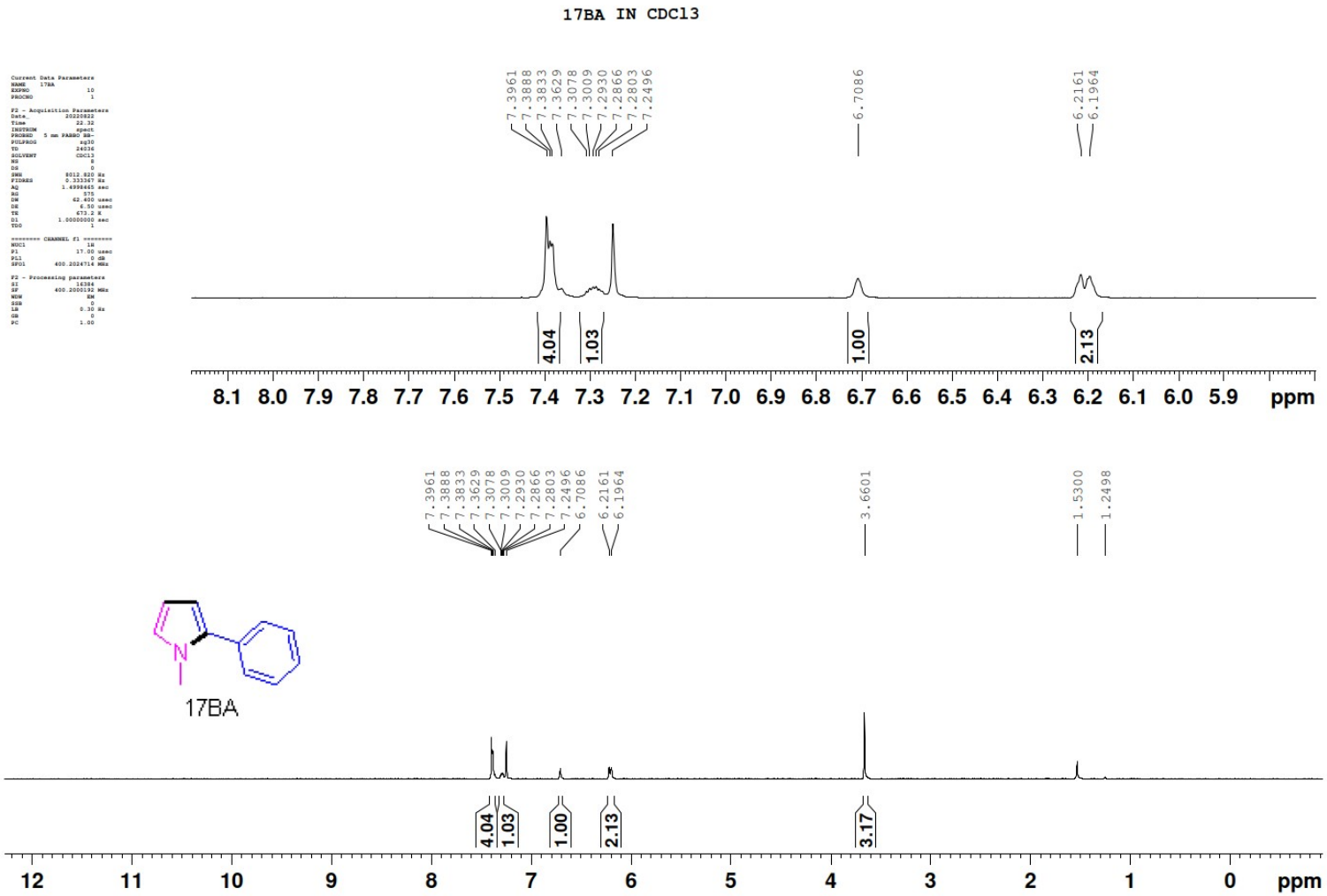
```
Current Data Parameters
NAME     14AG
EXPNO              10
PROCNO              1

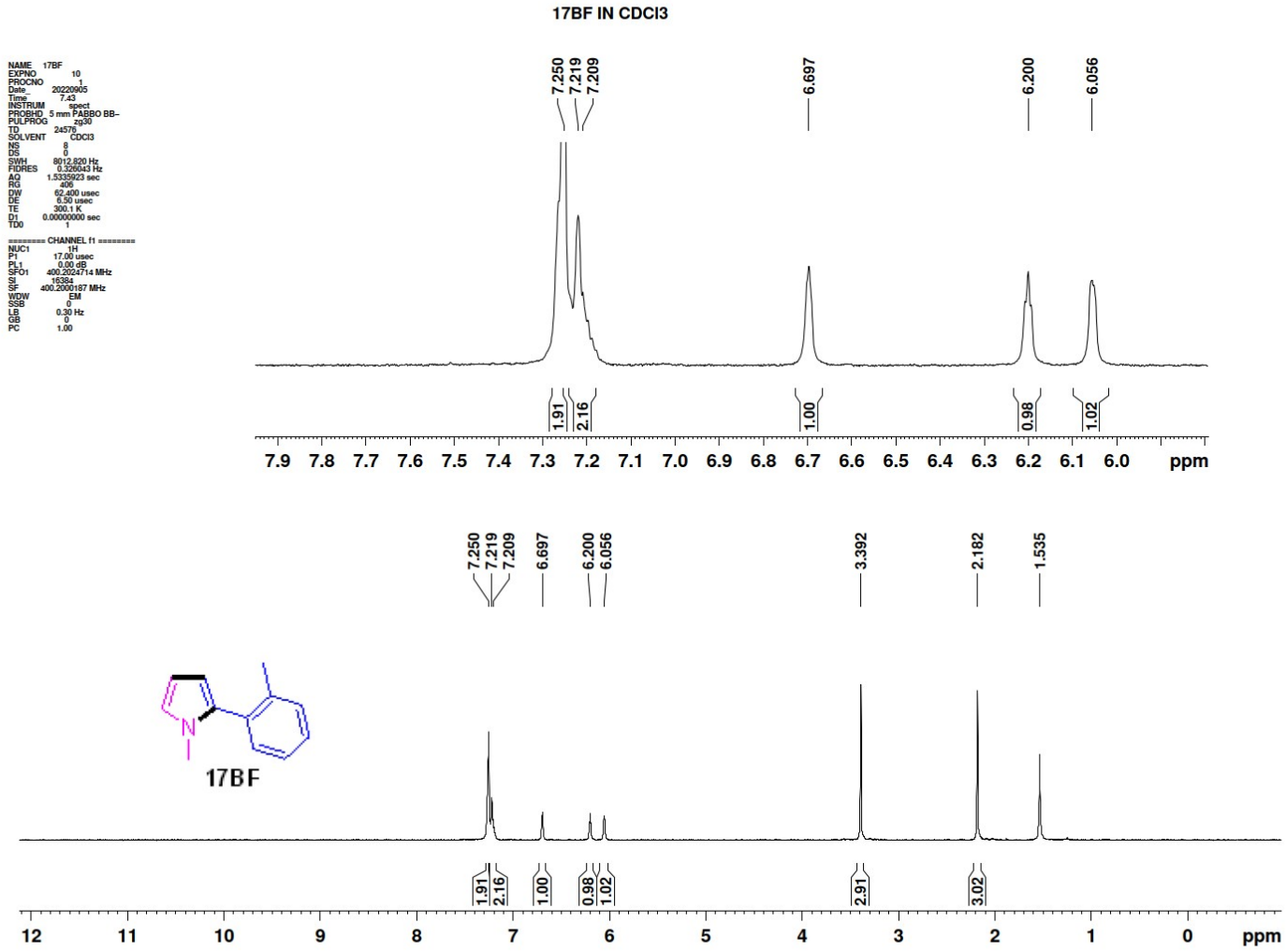
F2 - Acquisition Parameters
Date_          20230701
Time               0.13 h
INSTRUM           spect
PROBHD   Z104450_0373 (
PULPROG           zg30
TD               24036
SOLVENT           MeOD
NS                   8
DS                   0
SWH           8012.820 Hz
FIDRES        0.666735 Hz
AQ            1.4998465 sec
RG                50.8
DW               62.400 usec
DE                6.50 usec
TE               300.0 K
D1            1.00000000 sec
TD0                  1
SFO1        400.2324014 MHz
NUC1                 1H
P0                4.79 usec
P1               14.38 usec
PLW1         19.18000031 W

F2 - Processing parameters
SI               16384
SF          400.2300118 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

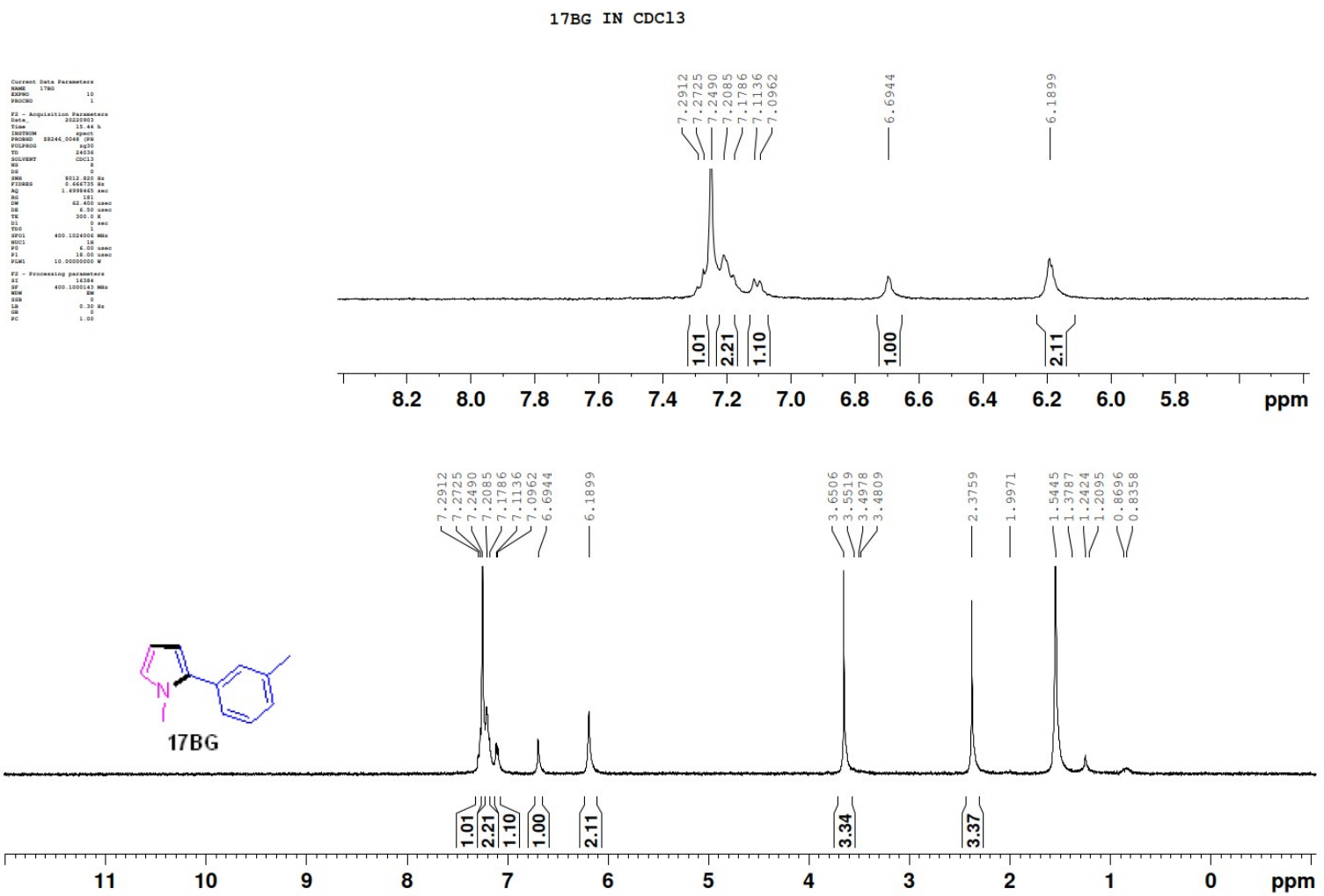


17BA IN CDCl3

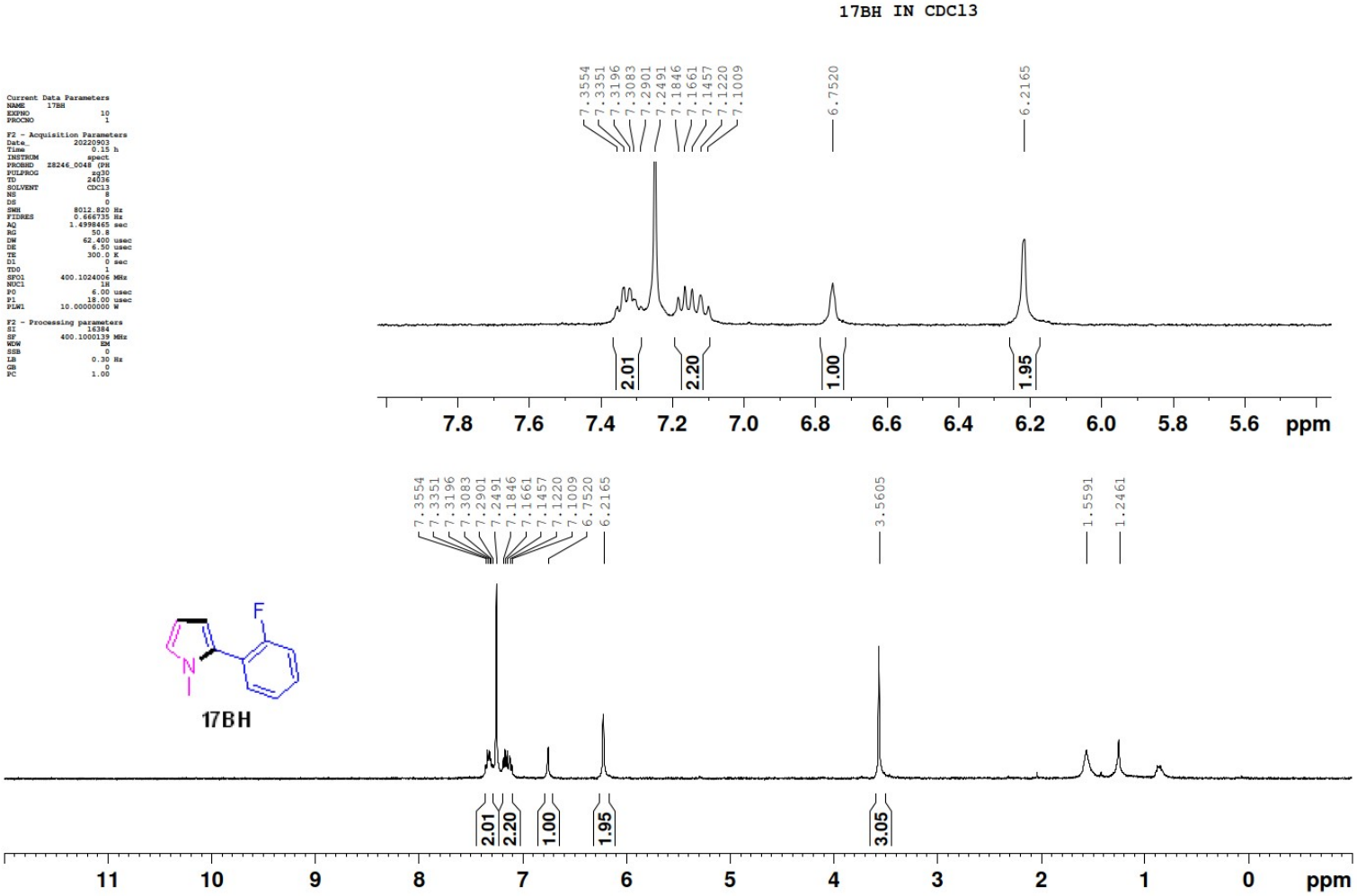



17BF IN CDCl3
NAME 17BF
EXPNO 10
PROCNO 1
Date_ 20220905
Time 7.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 24576
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.326043 Hz
AQ 1.5335923 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 300.1 K
D1 0.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 17.00 usec
PL1 0.00 dB
SFO1 400.2024714 MHz
SI 16384
SF 400.2000187 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.250
7.219
7.209
6.697
6.200
6.056
1.91
2.16
1.00
0.98
1.02
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 ppm
7.250
7.219
7.209
6.697
6.200
6.056
3.392
2.182
1.535
17BF
1.91
2.16
1.00
0.98
1.02
2.91
3.02
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

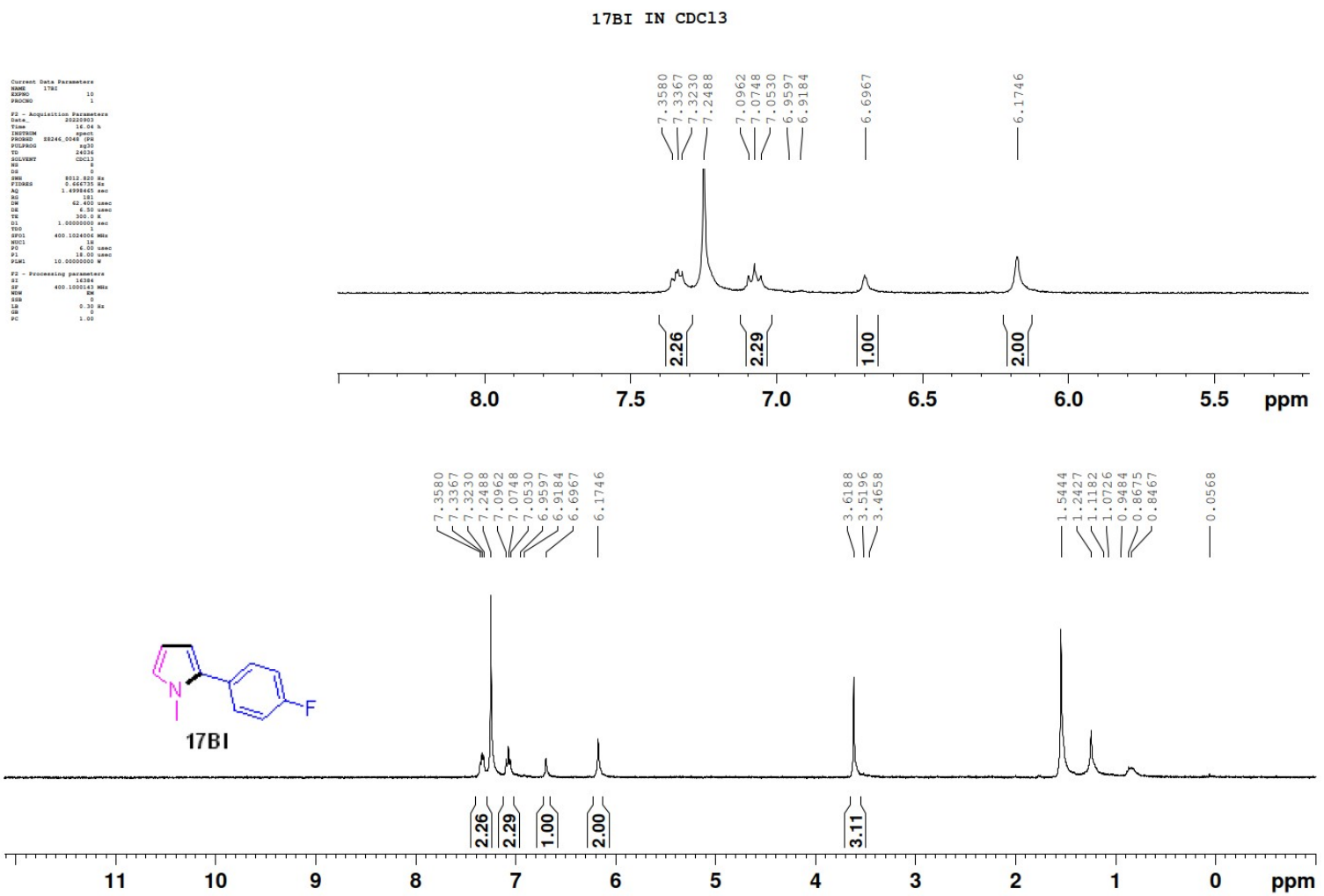
17BG IN CDCl3



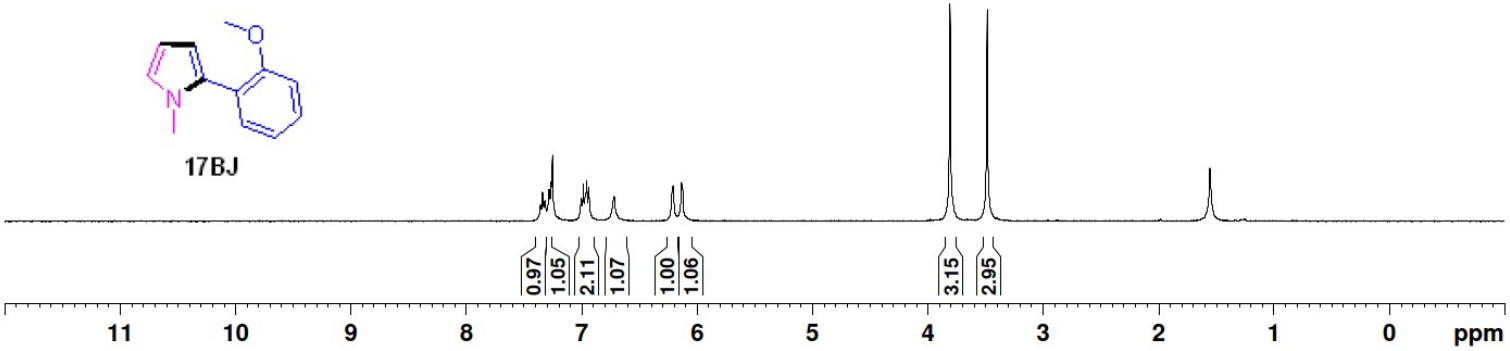
17BH IN CDCl3



17BI IN CDCl3



17BJ IN CDCl3



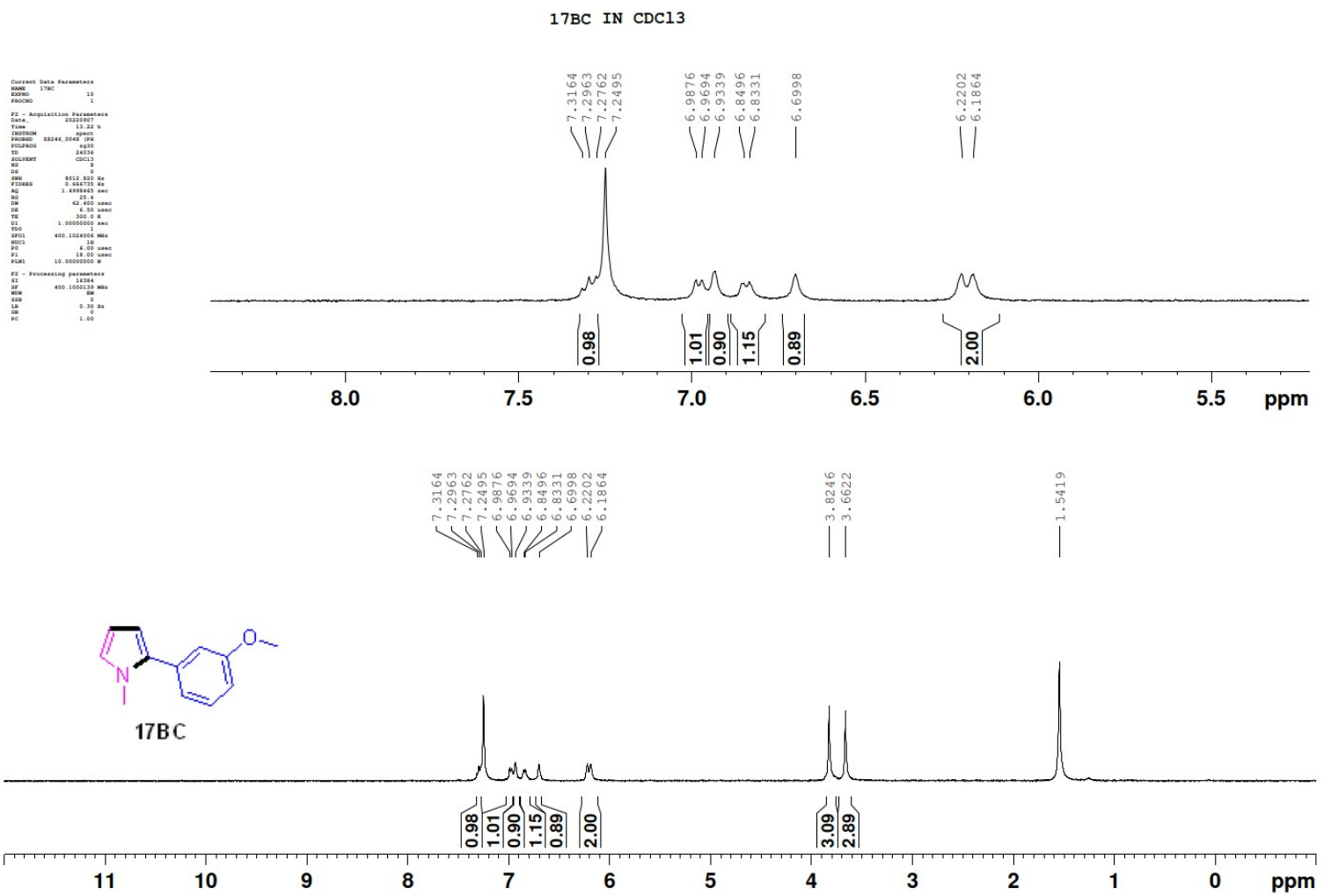
17BJ

Current Data Parameters
NAME 17BJ
EXPNO 10
PROCNO 1

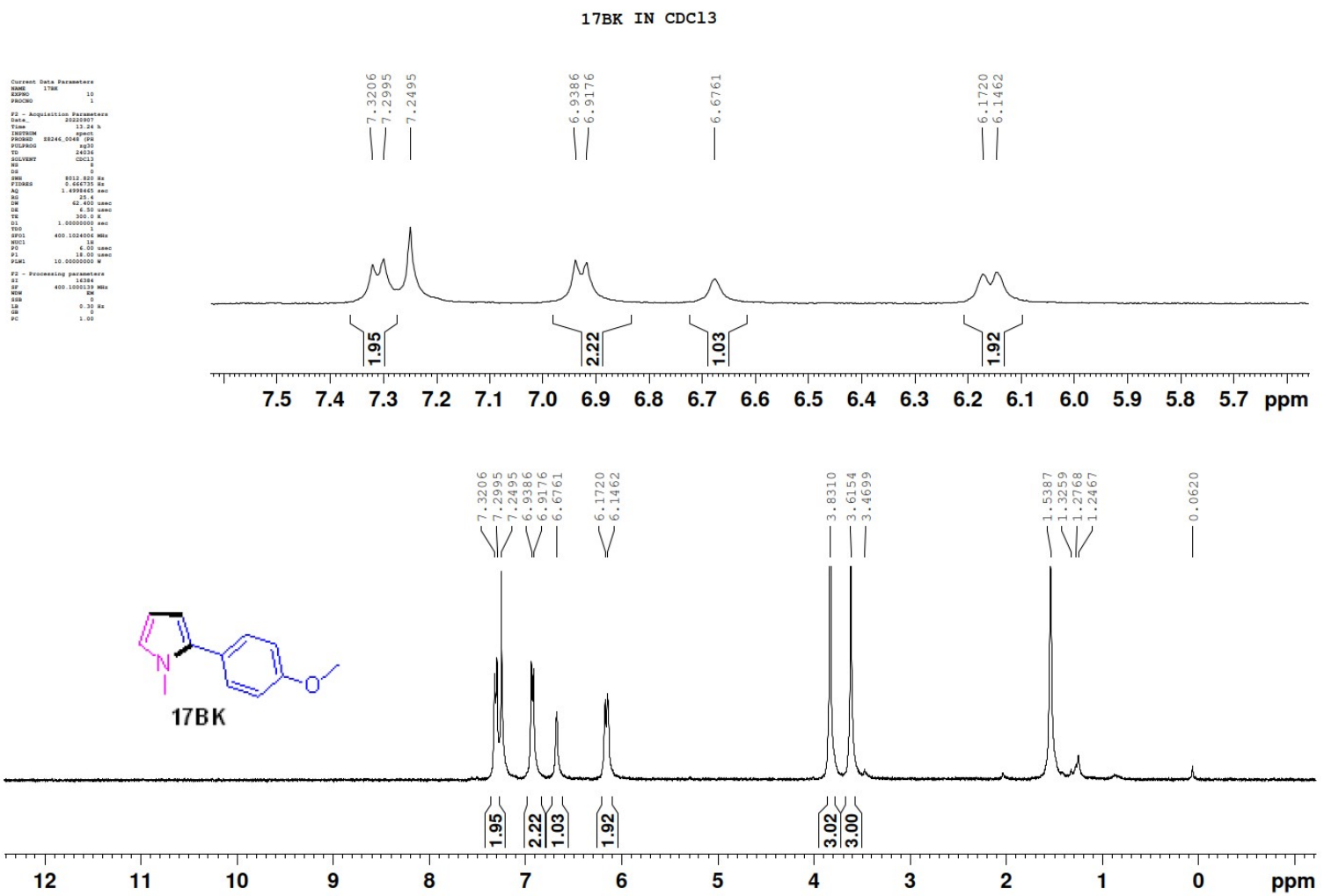
F2 - Acquisition Parameters
Date_ 20220907
Time 18.32 h
INSTRUM spect
PROBHD Z8246_0048 (PH
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 25.4
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 0 sec
TD0 1
SFO1 400.1024006 MHz
NUC1 1H
P0 6.00 usec
P1 18.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1000139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17BC IN CDCl3

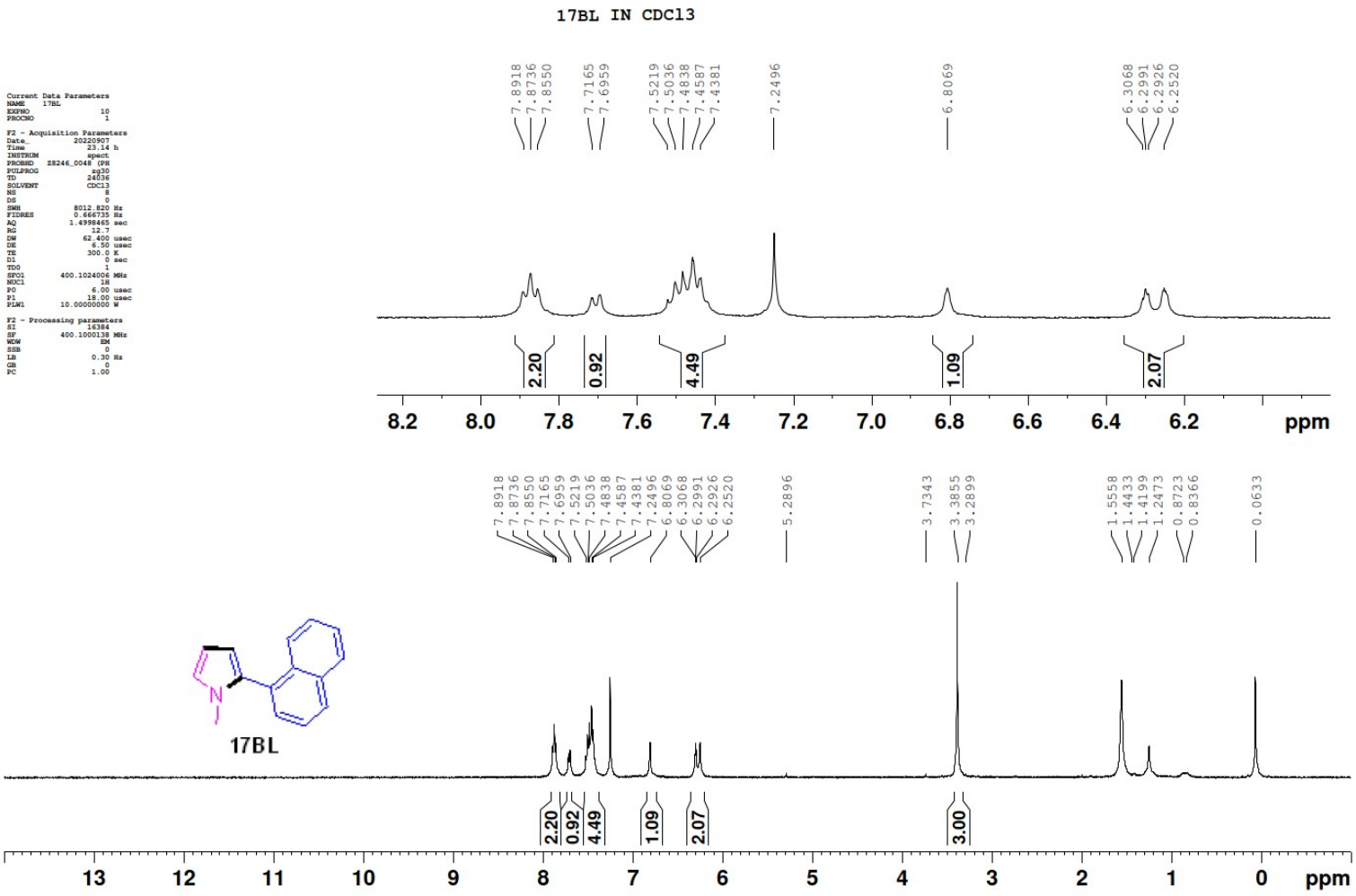


17BK IN CDCl3

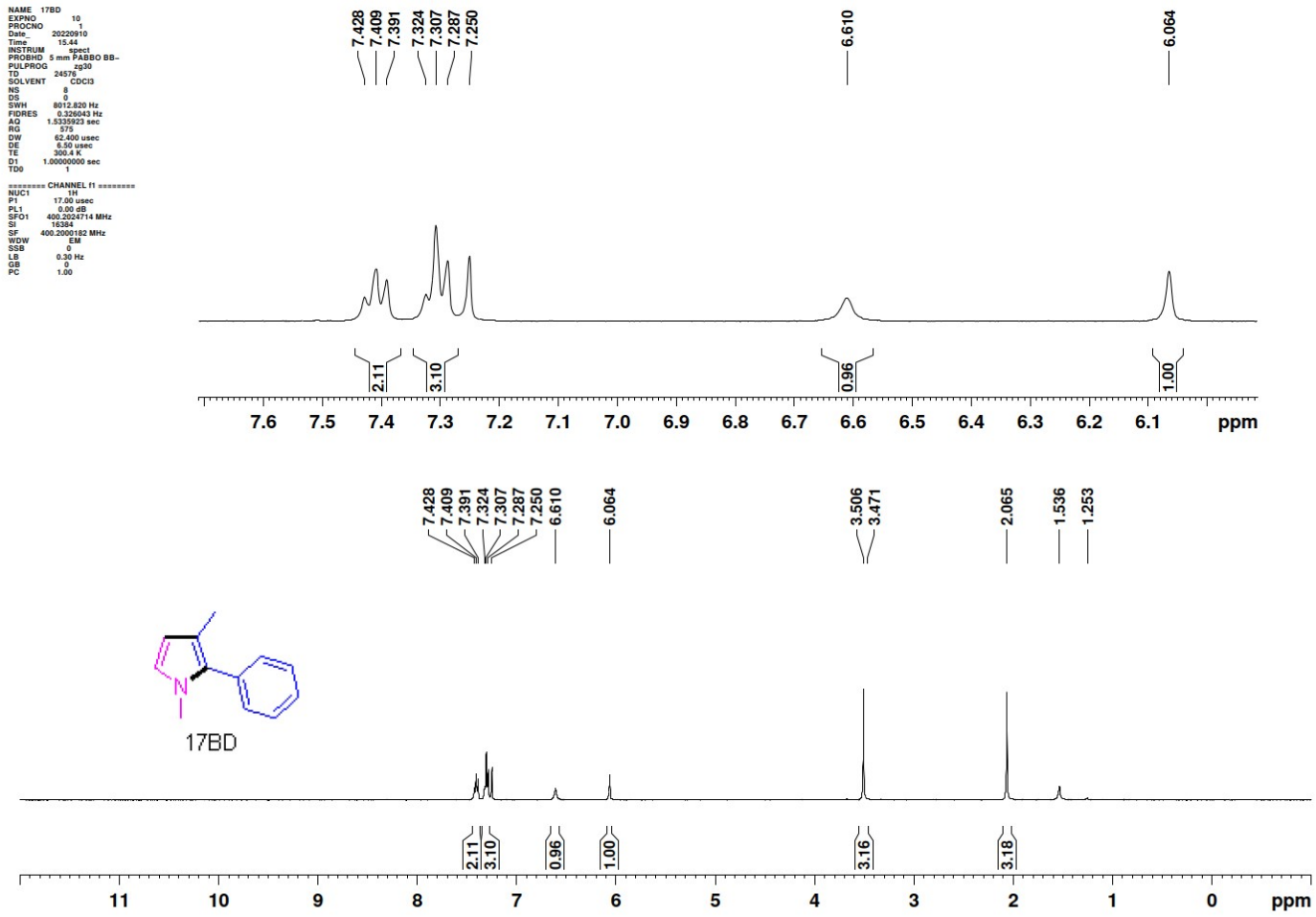


17BK

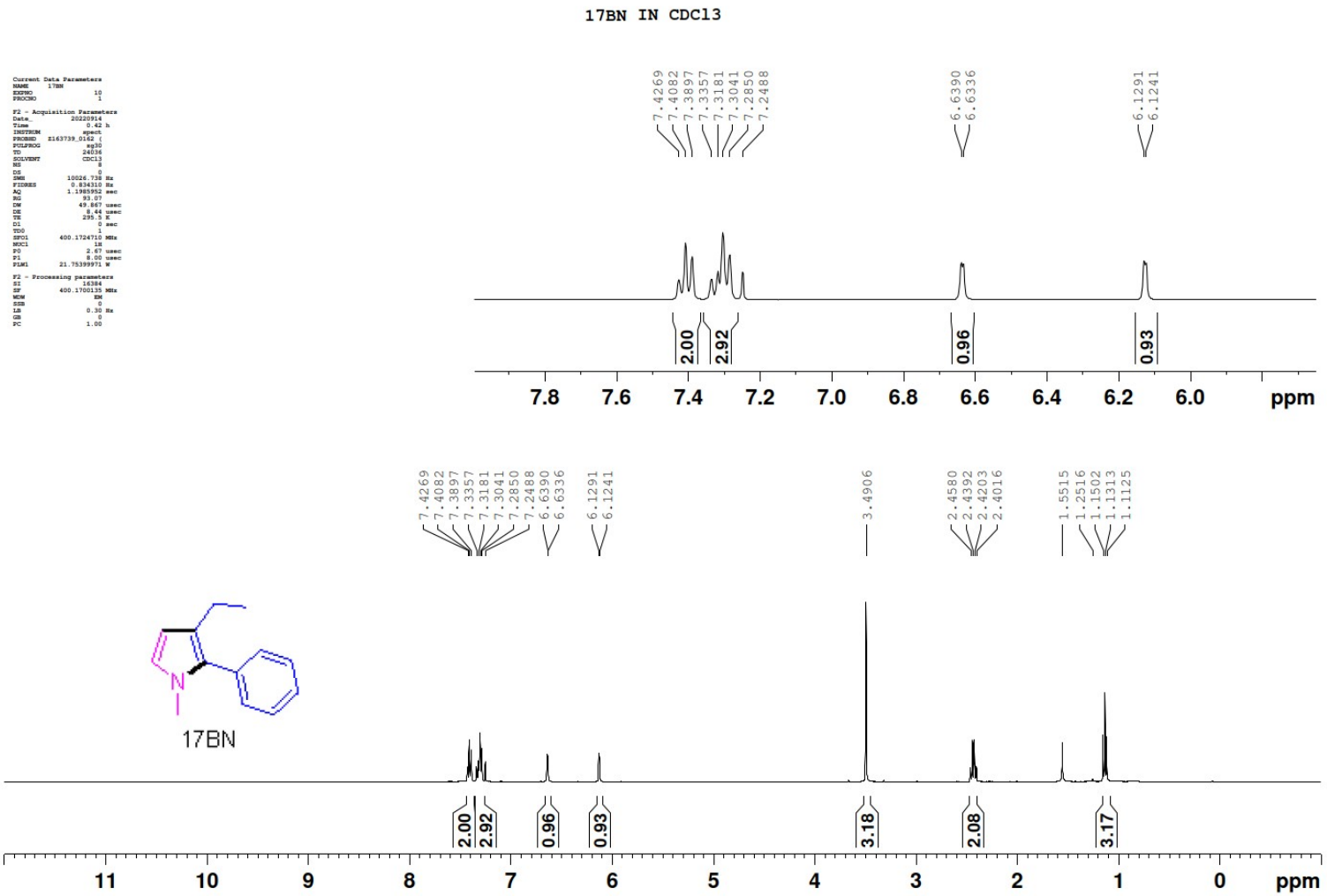
17BL IN CDCl3



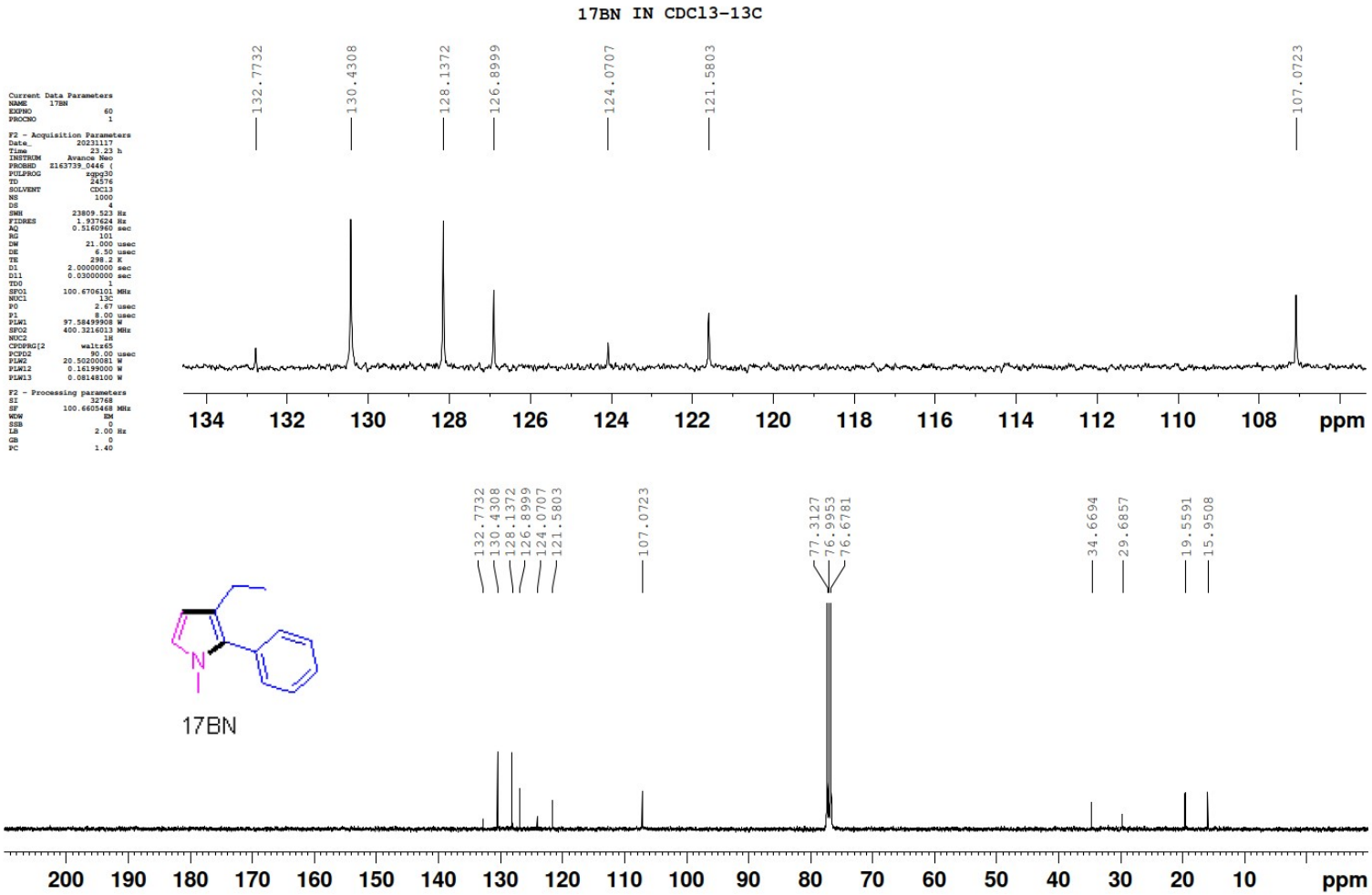
17BD IN CDCl3

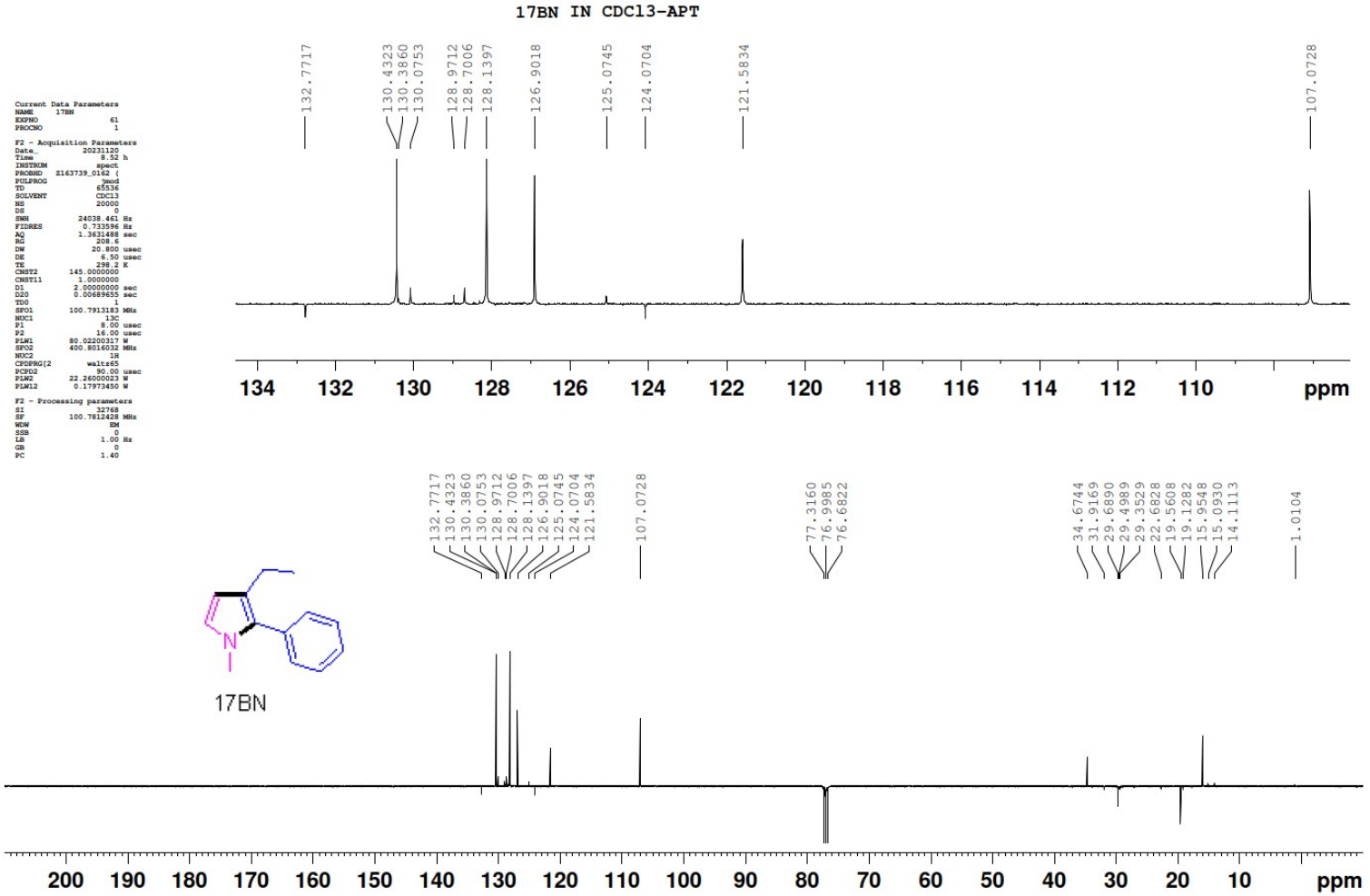


17BN IN CDCl3

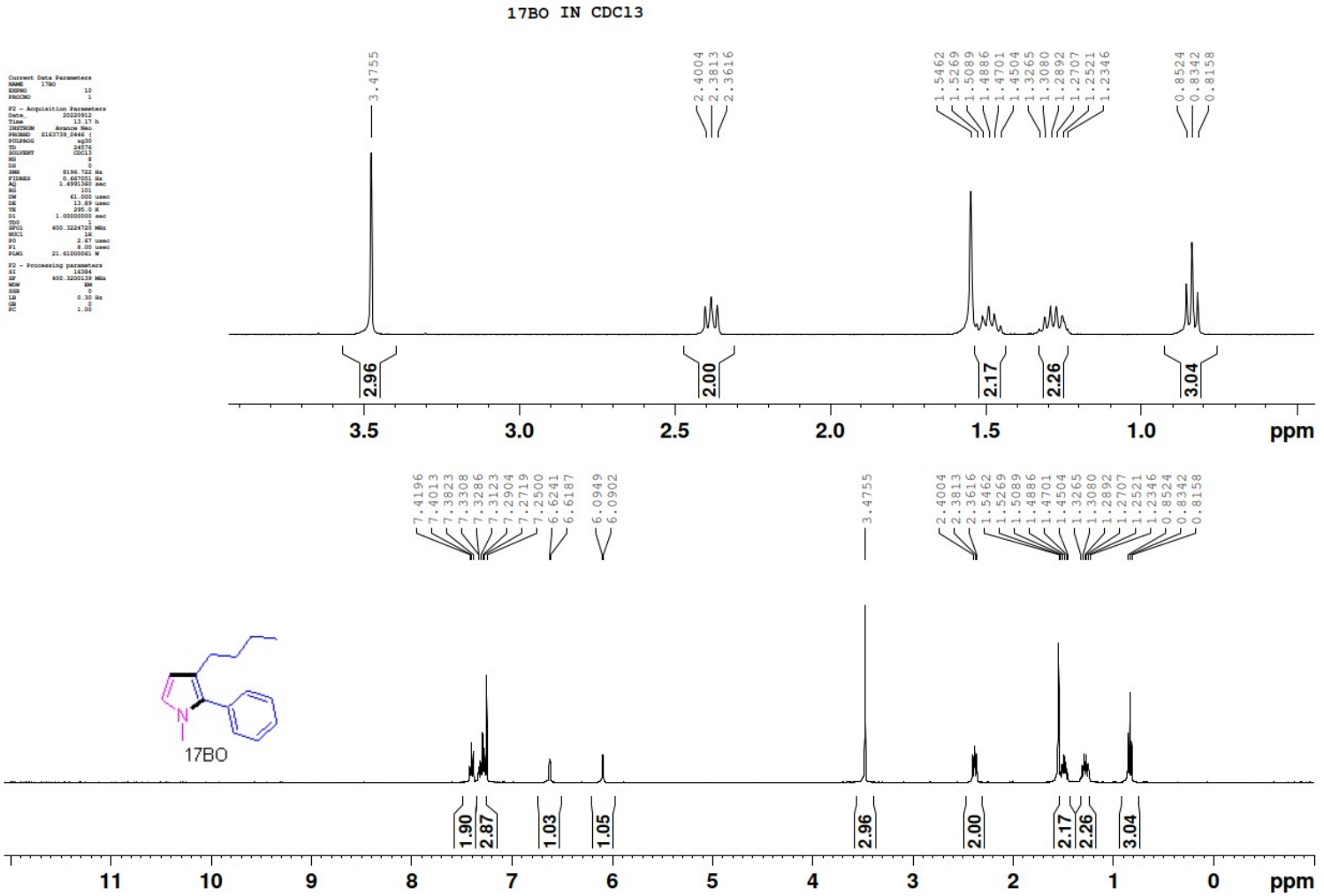


17BN IN CDCl3-13C

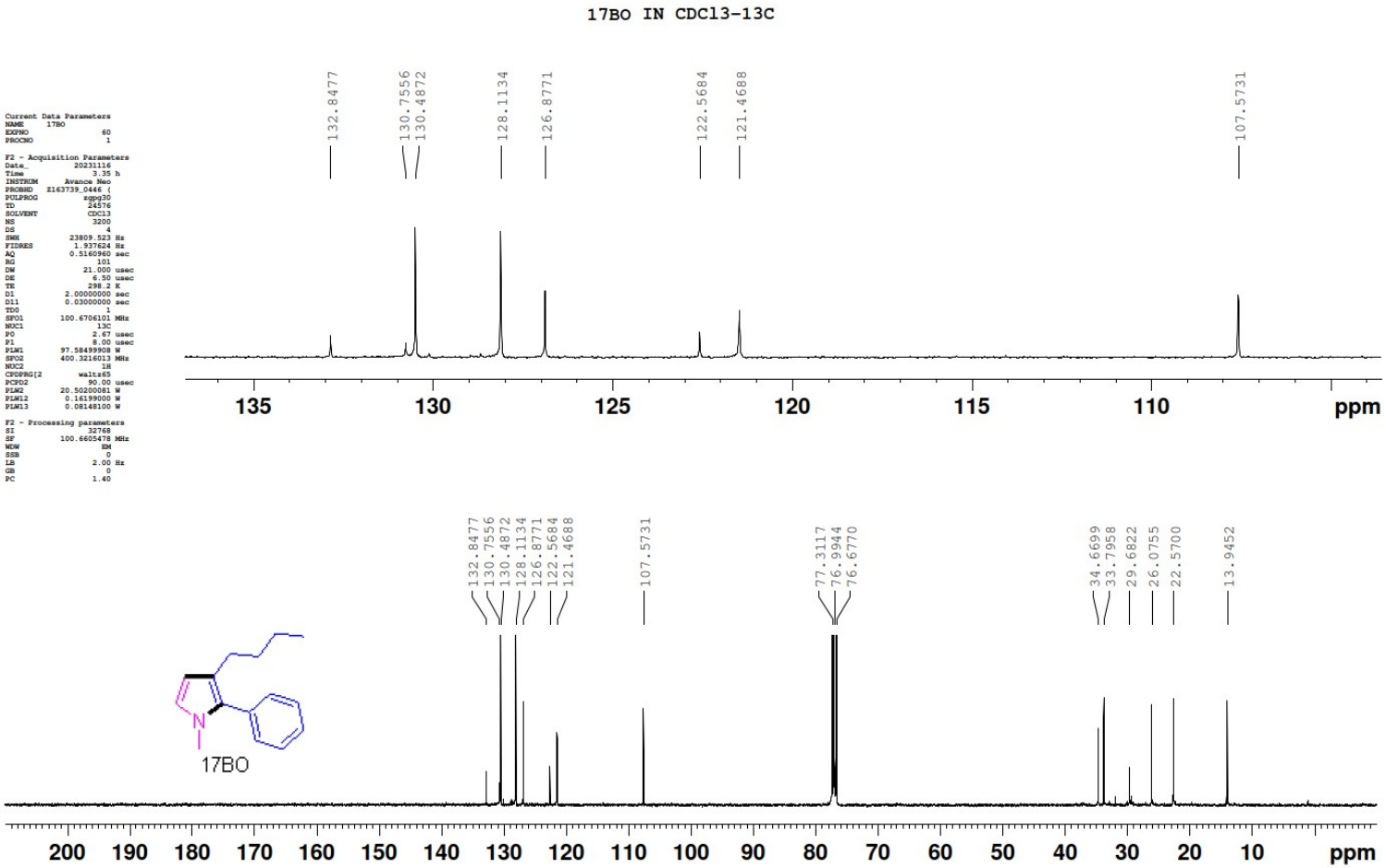



17BN IN CDCl3-APT
Current Data Parameters
NAME 17BN
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231120
Time 8.52 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 20000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.36314888 sec
RG 208.6
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.7913183 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 80.02200317 W
SFO2 400.8016032 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 22.26000023 W
PLW12 0.17973450 W
F2 - Processing parameters
SI 32768
SF 100.7812428 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
132.7717
130.4323
130.3860
130.0753
128.9712
128.7006
128.1397
126.9018
125.0745
124.0704
121.5834
107.0728
134
132
130
128
126
124
122
120
118
116
114
112
110
ppm
77.3160
76.9985
76.6822
34.6744
31.9169
29.6890
29.4989
29.3529
22.6828
19.5608
19.1282
15.9548
15.0930
14.1113
1.0104
17BN
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

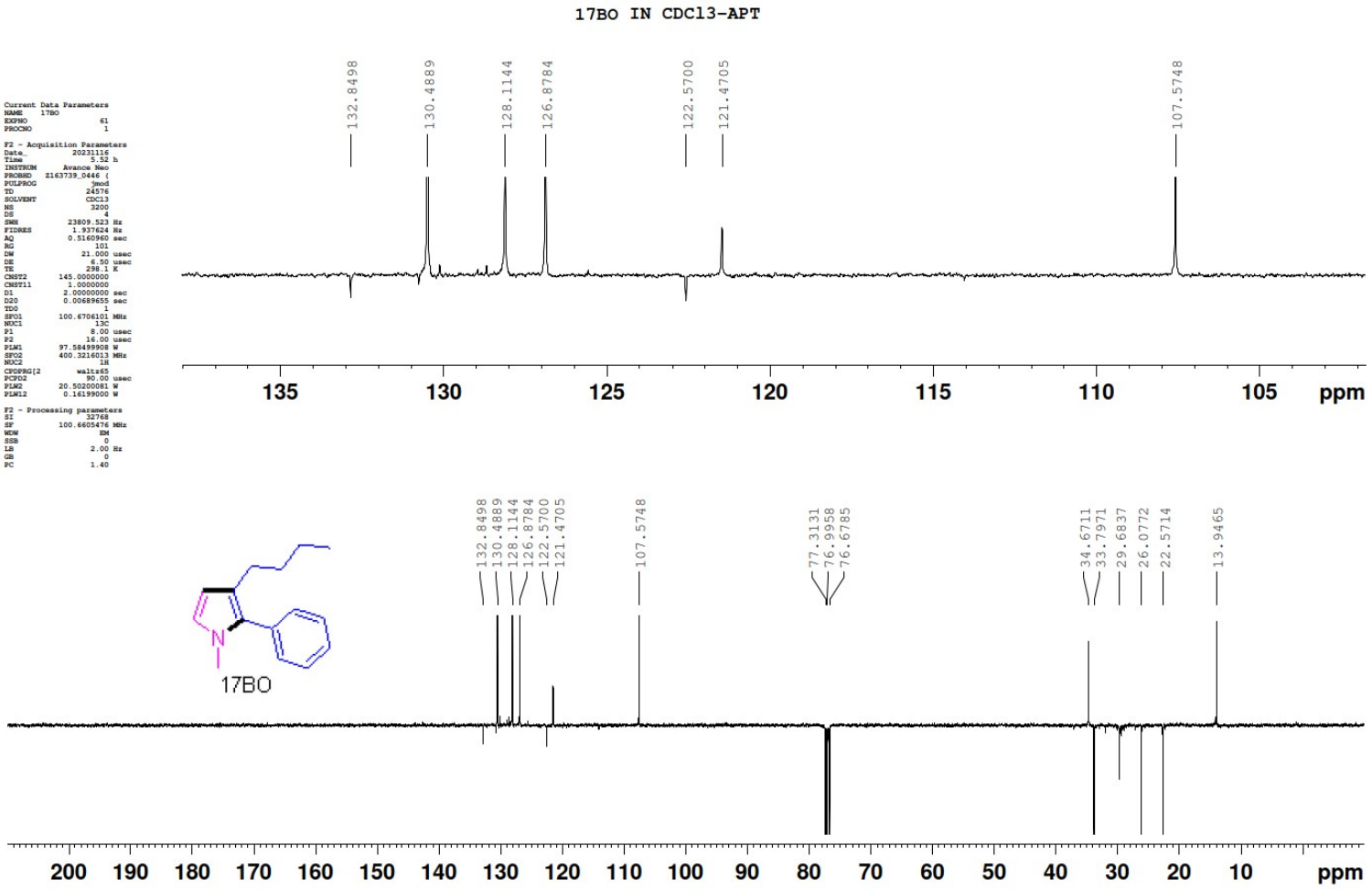
17BO IN CDCl3



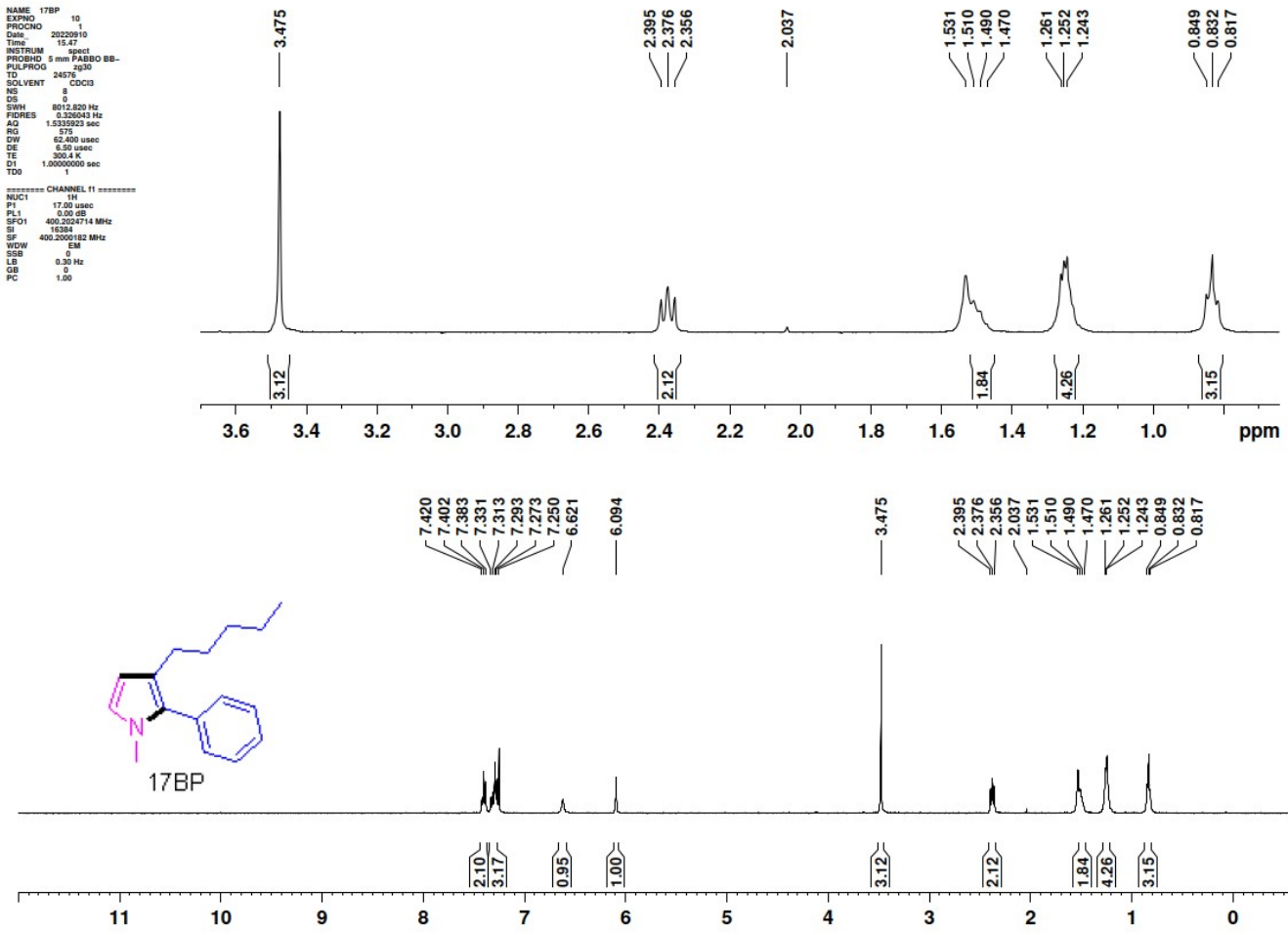
17BO IN CDCl3-13C



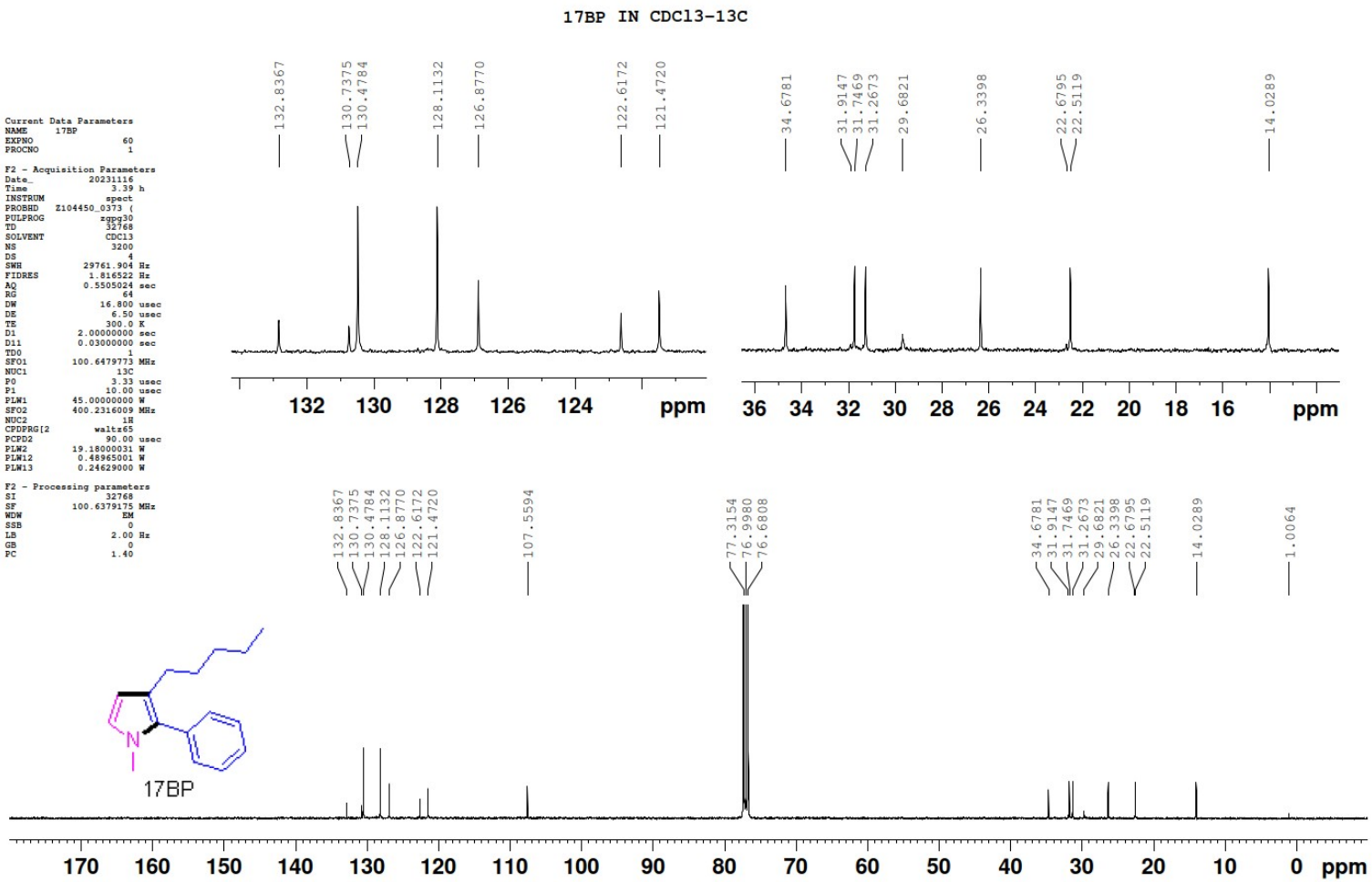
17BO IN CDCl3-APT



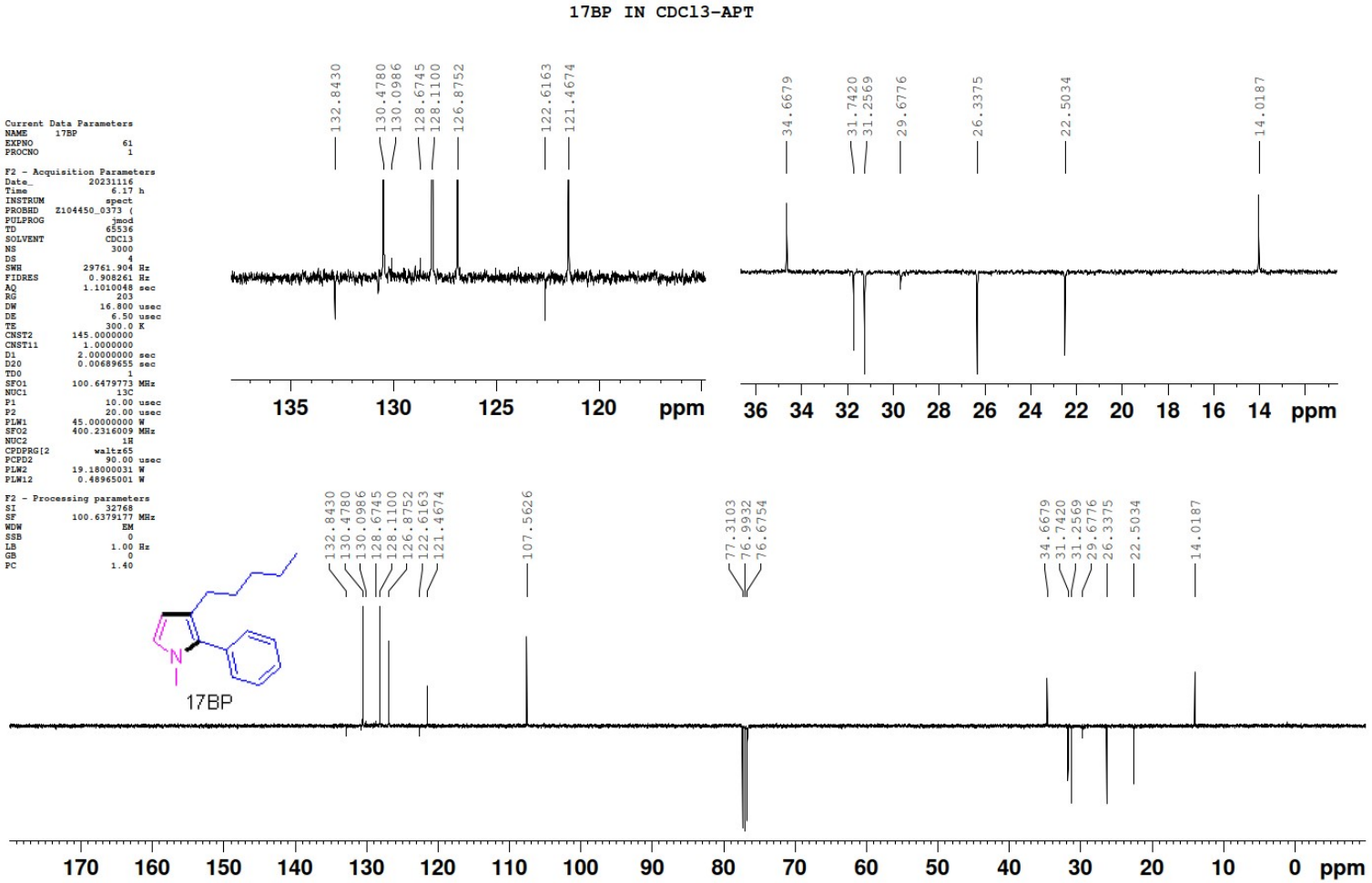
17BP IN CDCl3



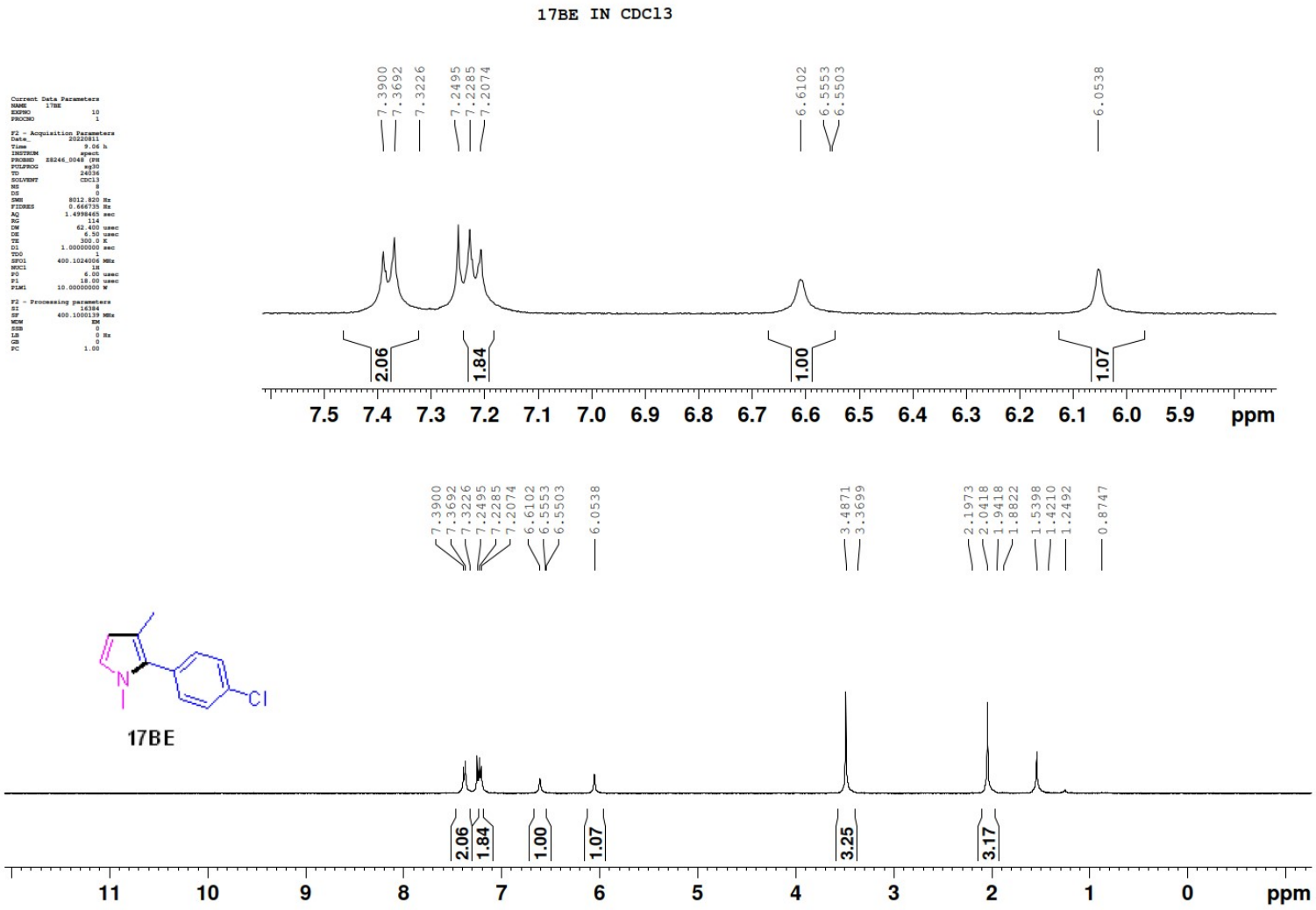
17BP IN CDCl3-13C



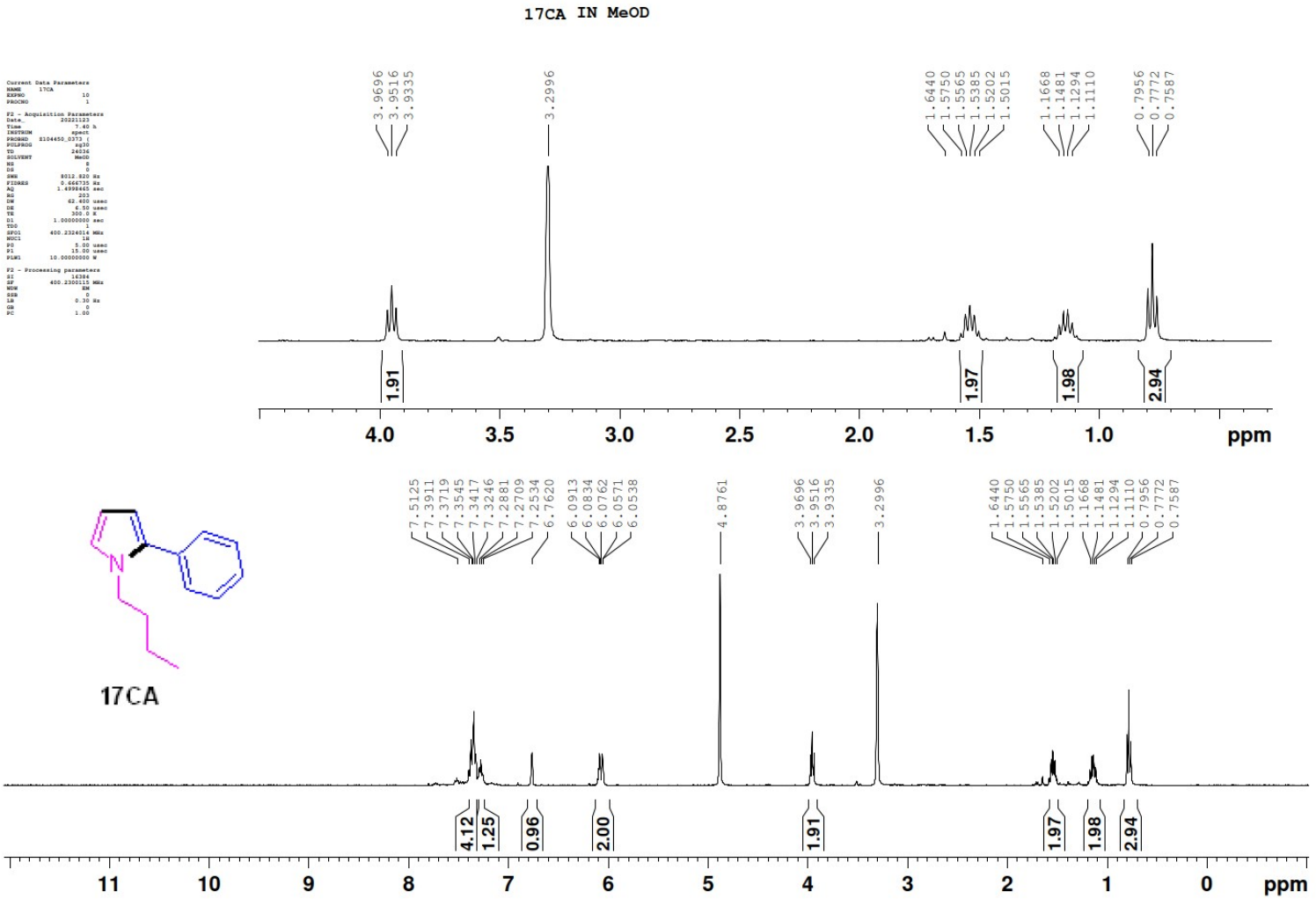
17BP IN CDCl3-APT



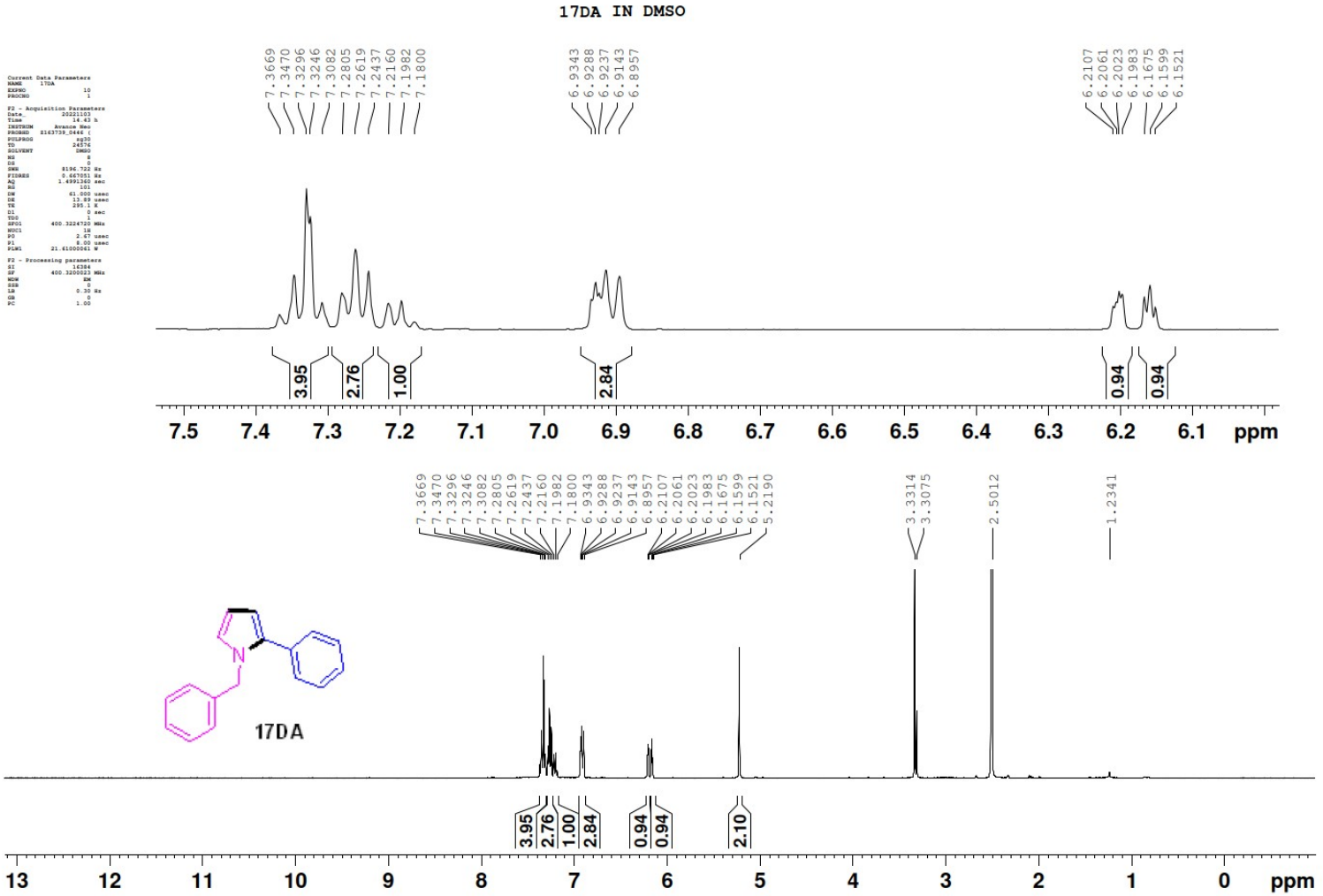
17BE IN CDCl3



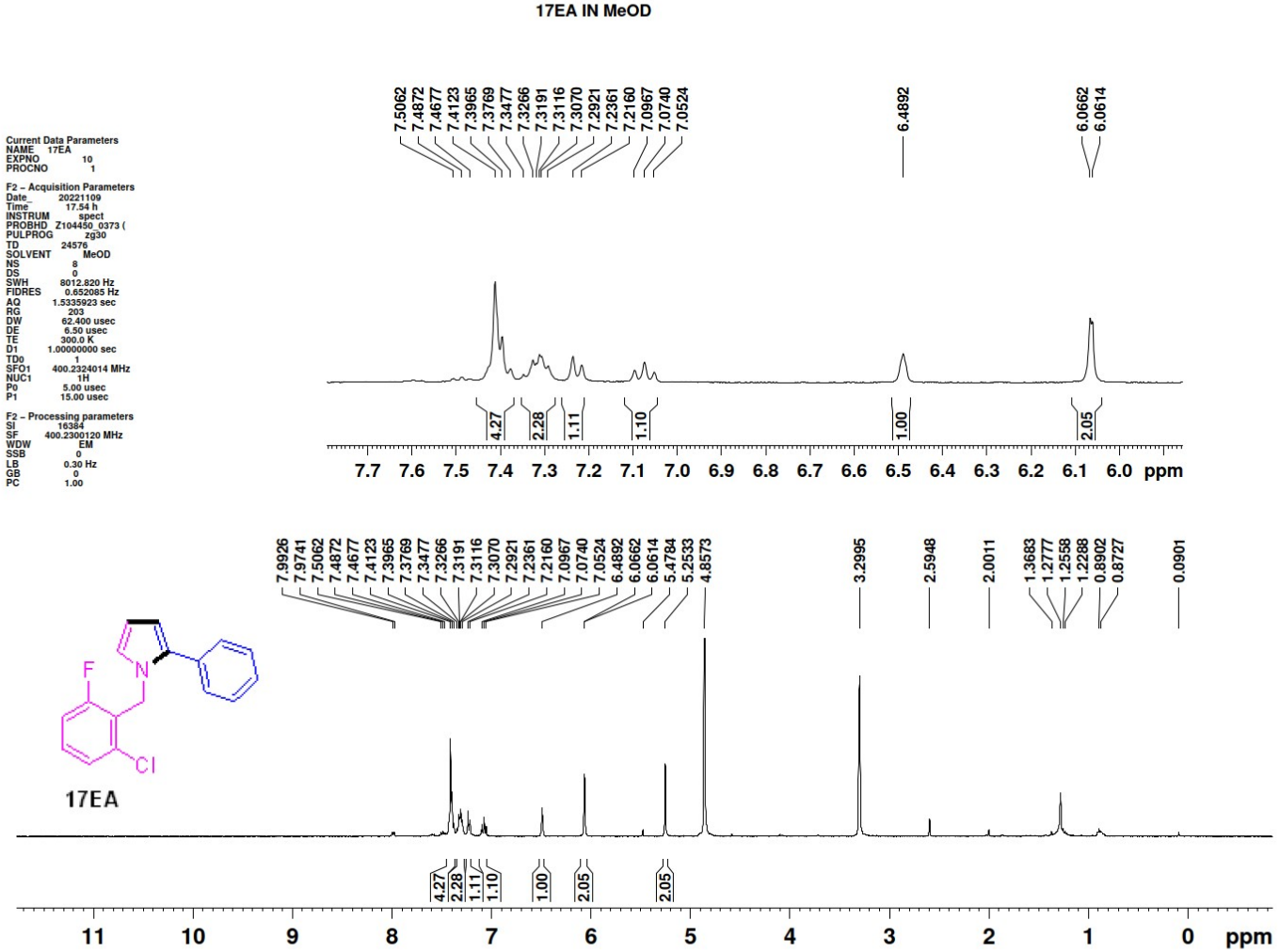
17CA IN MeOD



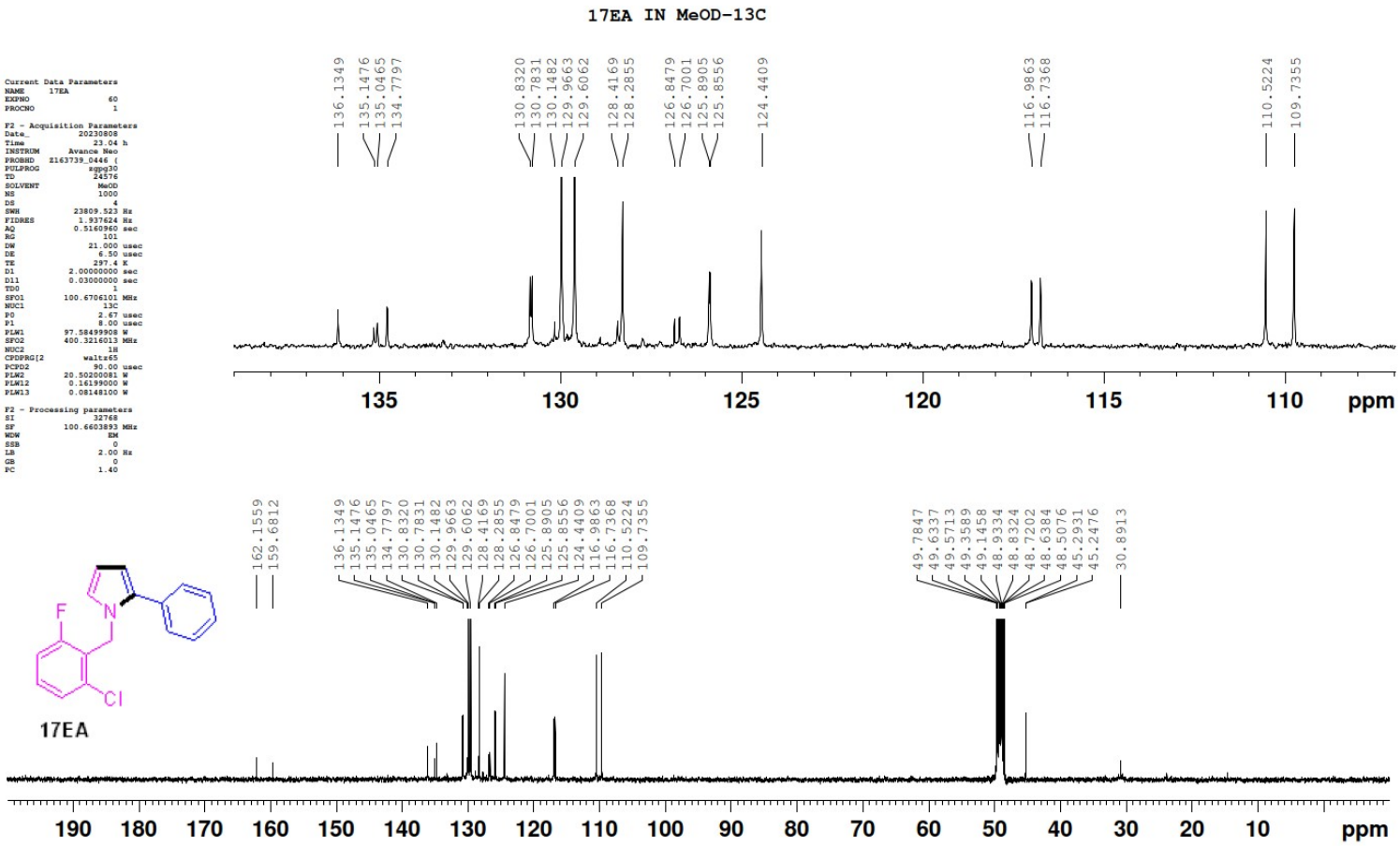
17CA


17DA IN DMSO
7.3669
7.3470
7.3296
7.3246
7.3082
7.2805
7.2619
7.2437
7.2160
7.1982
7.1800
6.9343
6.9288
6.9237
6.9143
6.8957
6.2107
6.2061
6.2023
6.1983
6.1675
6.1599
6.1521
3.95
2.76
1.00
2.84
0.94
0.94
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
ppm
5.2190
3.3314
3.3075
2.5012
1.2341
2.10
13
12
11
10
9
8
7
6
5
4
3
2
1
0
17DA

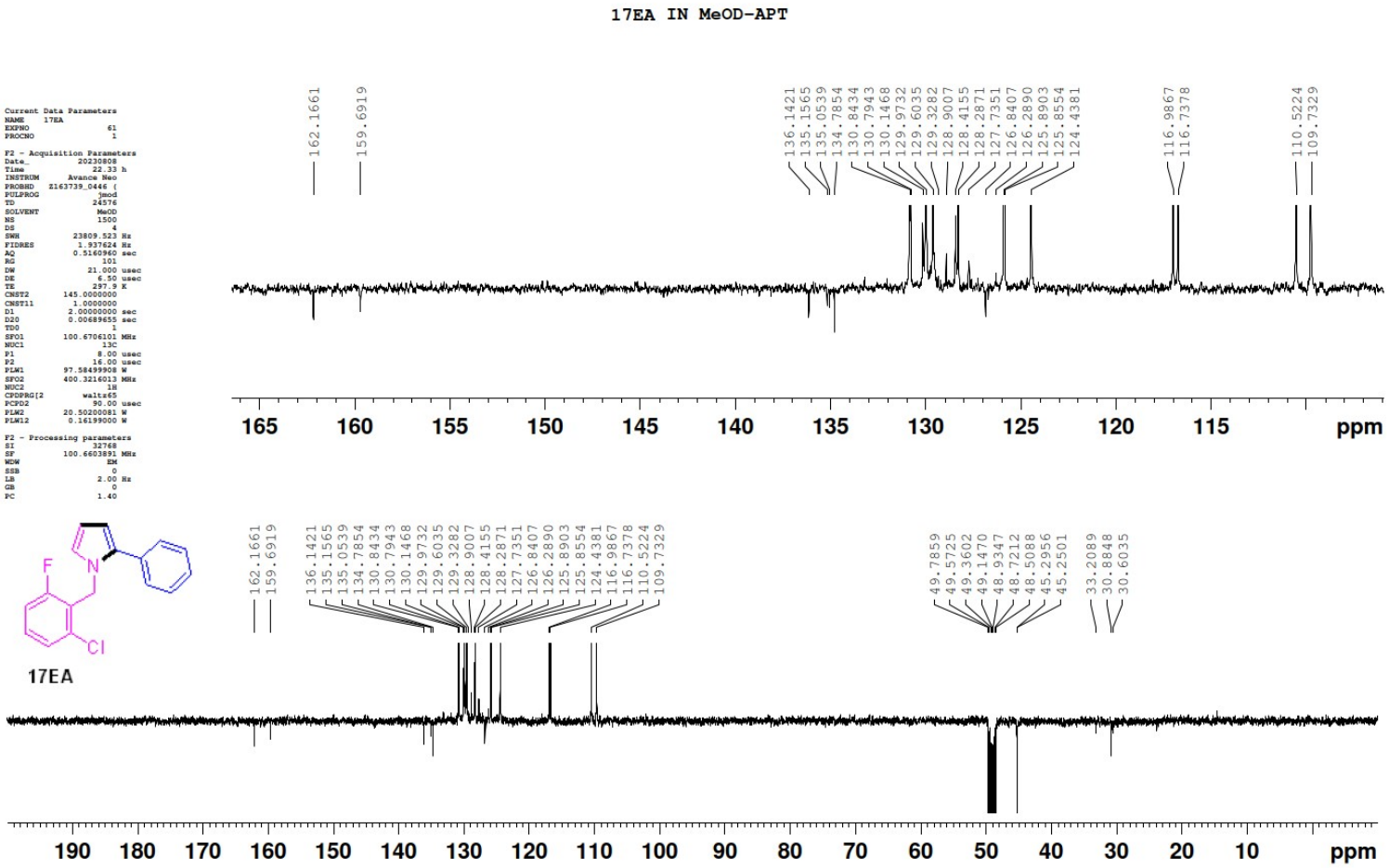
17EA IN MeOD


Current Data Parameters
NAME 17EA
EXPNO 10
PROCNO 1
F2 – Acquisition Parameters
Date_ 20221109
Time 17.54 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.652085 Hz
AQ 1.5335923 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
F2 – Processing parameters
SI 16384
SF 400.2300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5062
7.4872
7.4677
7.4123
7.3965
7.3769
7.3477
7.3266
7.3191
7.3116
7.3070
7.2921
7.2361
7.2160
7.0967
7.0740
7.0524
6.4892
6.0662
6.0614
4.27
2.28
1.11
1.10
1.00
2.05
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 ppm
7.9926
7.9741
7.5062
7.4872
7.4677
7.4123
7.3965
7.3769
7.3477
7.3266
7.3191
7.3116
7.3070
7.2921
7.2361
7.2160
7.0967
7.0740
7.0524
6.4892
6.0662
6.0614
5.4784
5.2533
4.8573
3.2995
2.5948
2.0011
1.3683
1.2777
1.2558
1.2288
0.8902
0.8727
0.0901
F
N
Cl
17EA
4.27
2.28
1.11
1.10
1.00
2.05
2.05
11 10 9 8 7 6 5 4 3 2 1 0 ppm

17EA IN MeOD-13C



17EA IN MeOD-APT

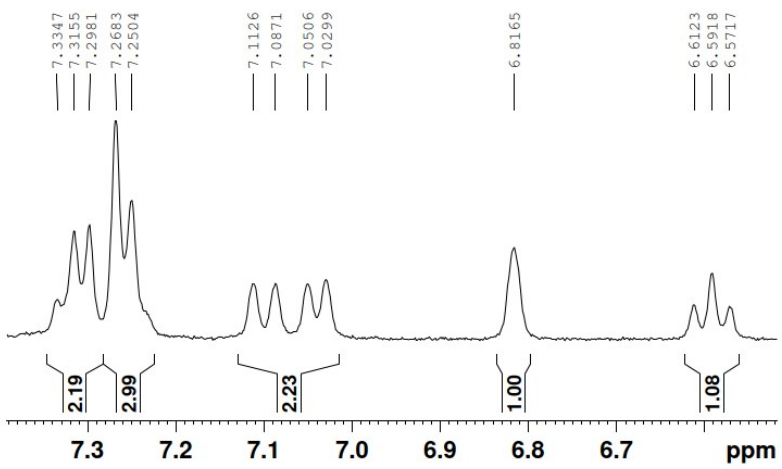


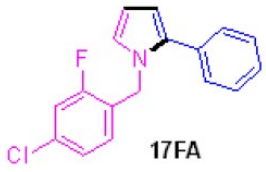
17FA IN MeOD

```
Current Data Parameters
NAME      17FA
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20230802
Time           0.24 h
INSTRUM       spect
PROBHD    Z104450_0373 (
PULPROG         zg30
TD             24036
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8012.820 Hz
FIDRES      0.666735 Hz
AQ          1.4998465 sec
RG              28.5
DW             62.400 usec
DE              6.50 usec
TE             300.0 K
D1          1.00000000 sec
TD0                1
SFO1       400.2324014 MHz
NUC1              1H
P0              4.79 usec
P1             14.38 usec
PLW1       19.18000031 W

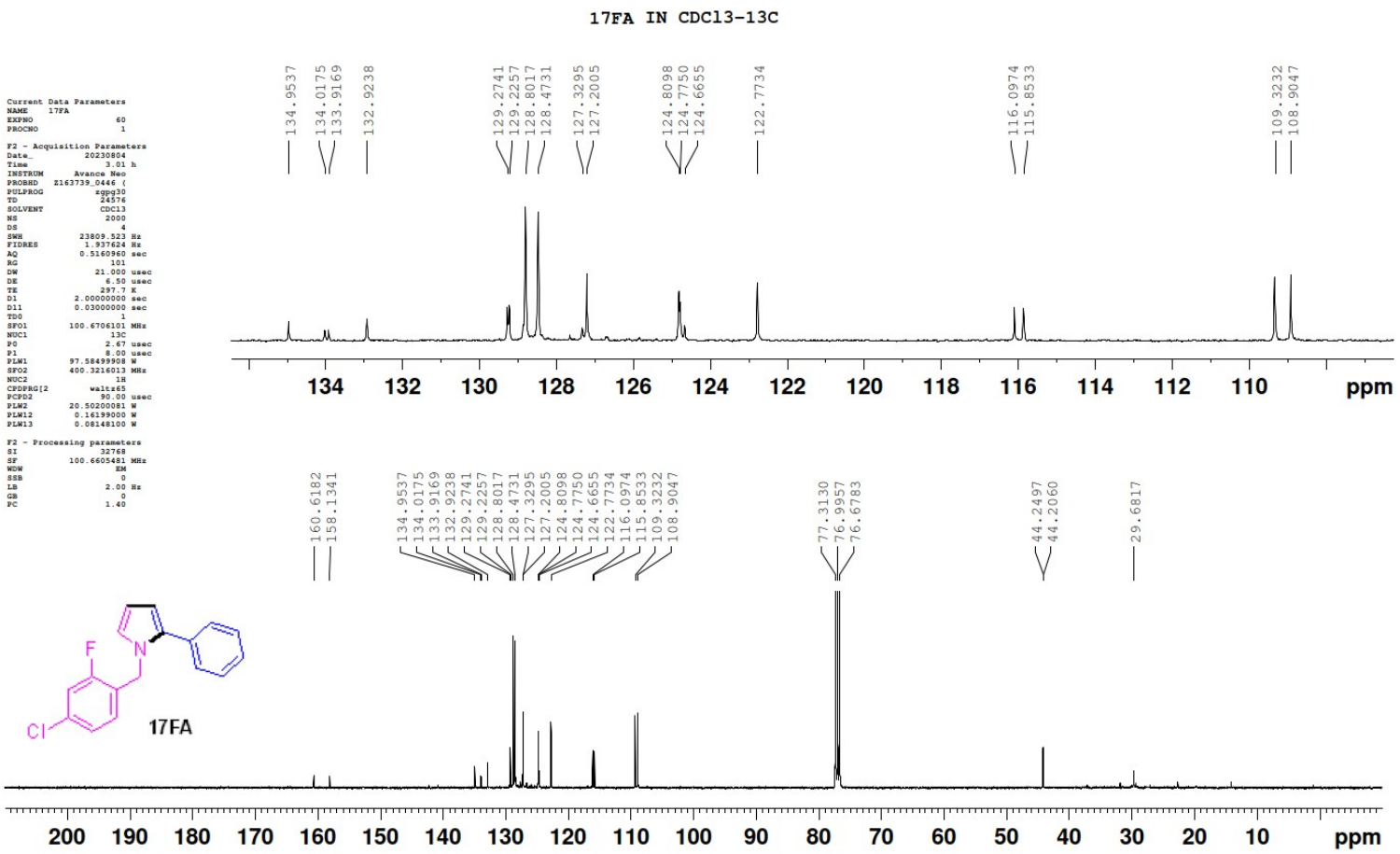
F2 - Processing parameters
SI             16384
SF         400.2300120 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```



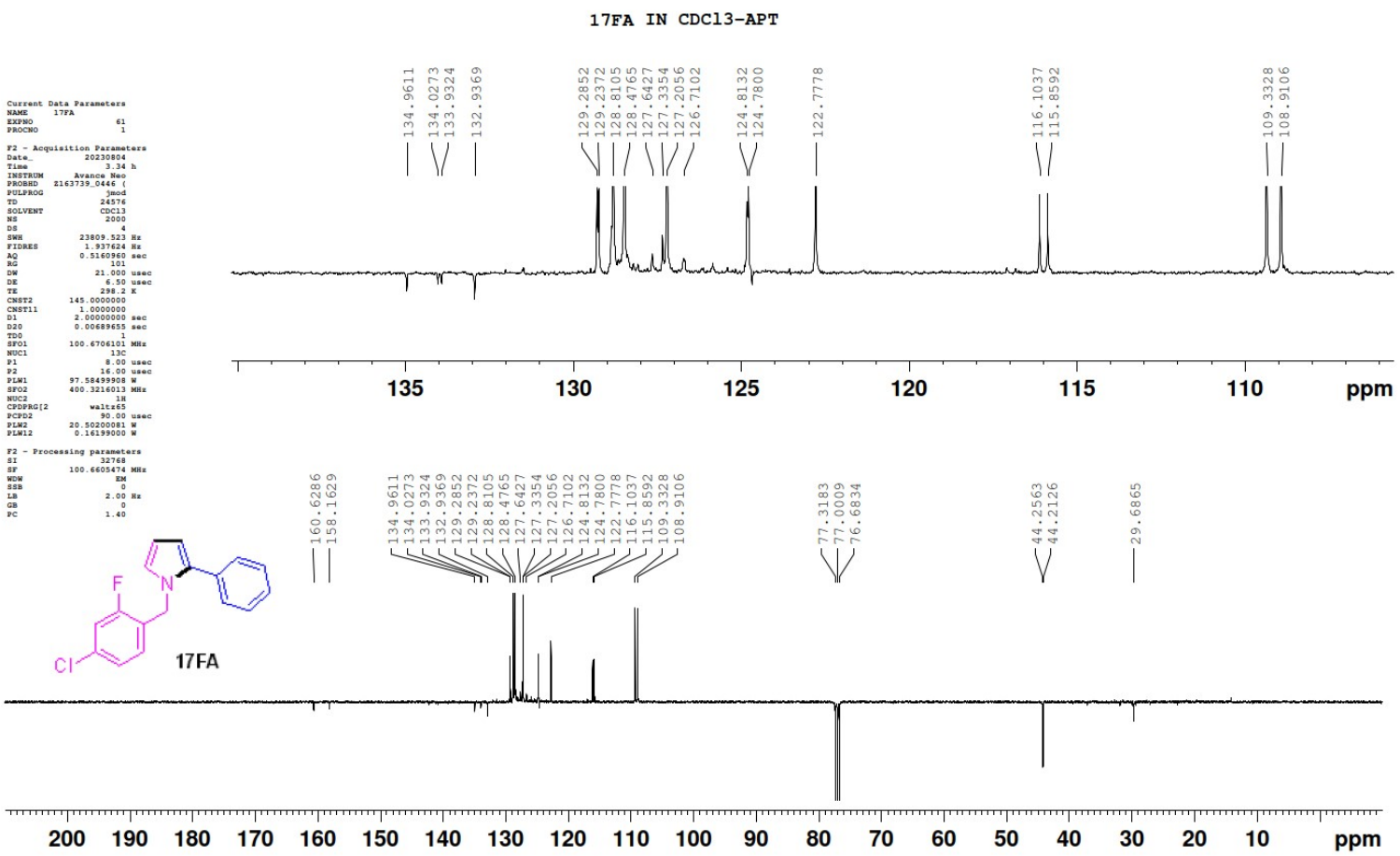


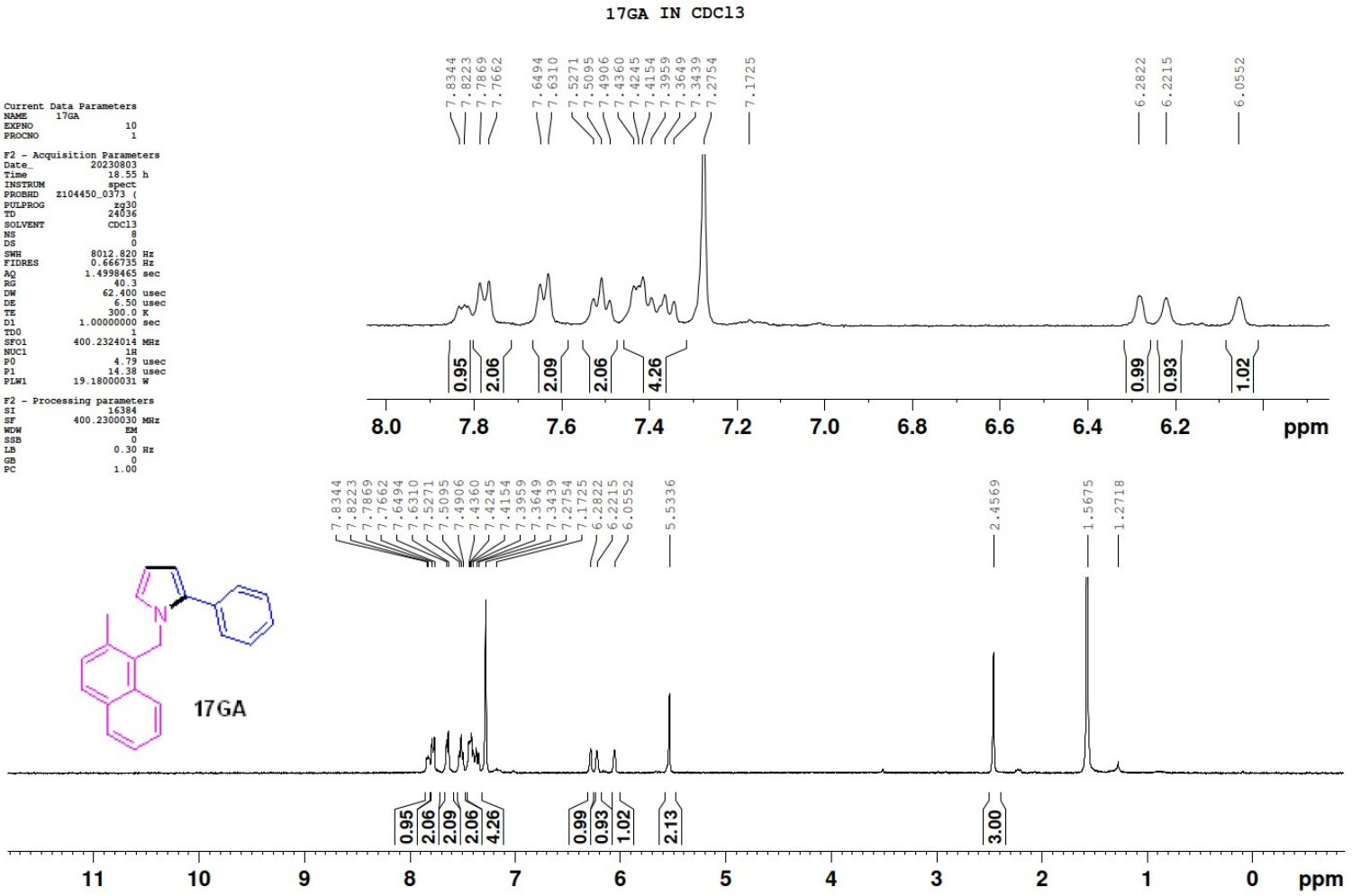
17FA

17FA IN CDCl3-13C

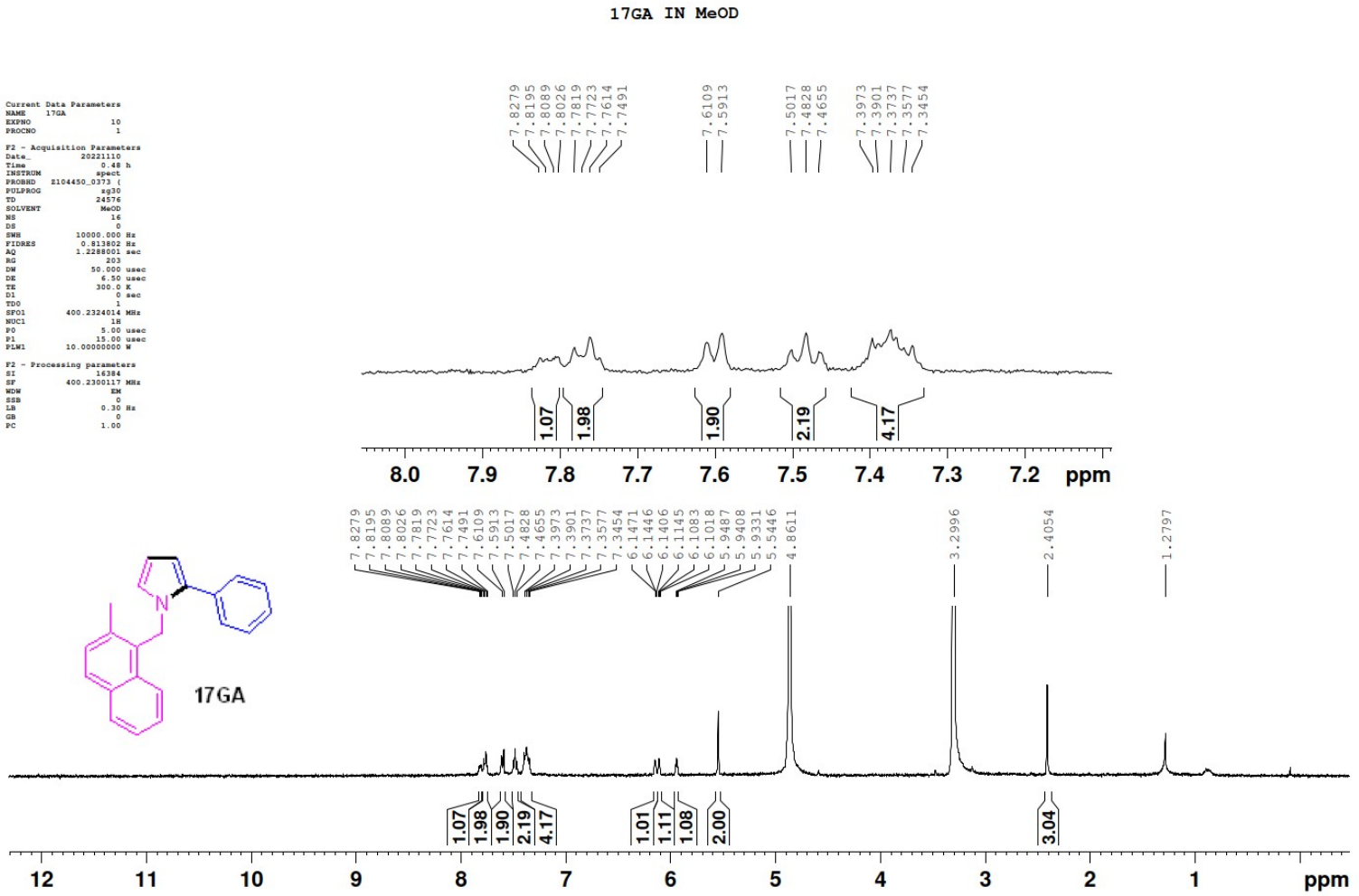


17FA IN CDCl3-APT

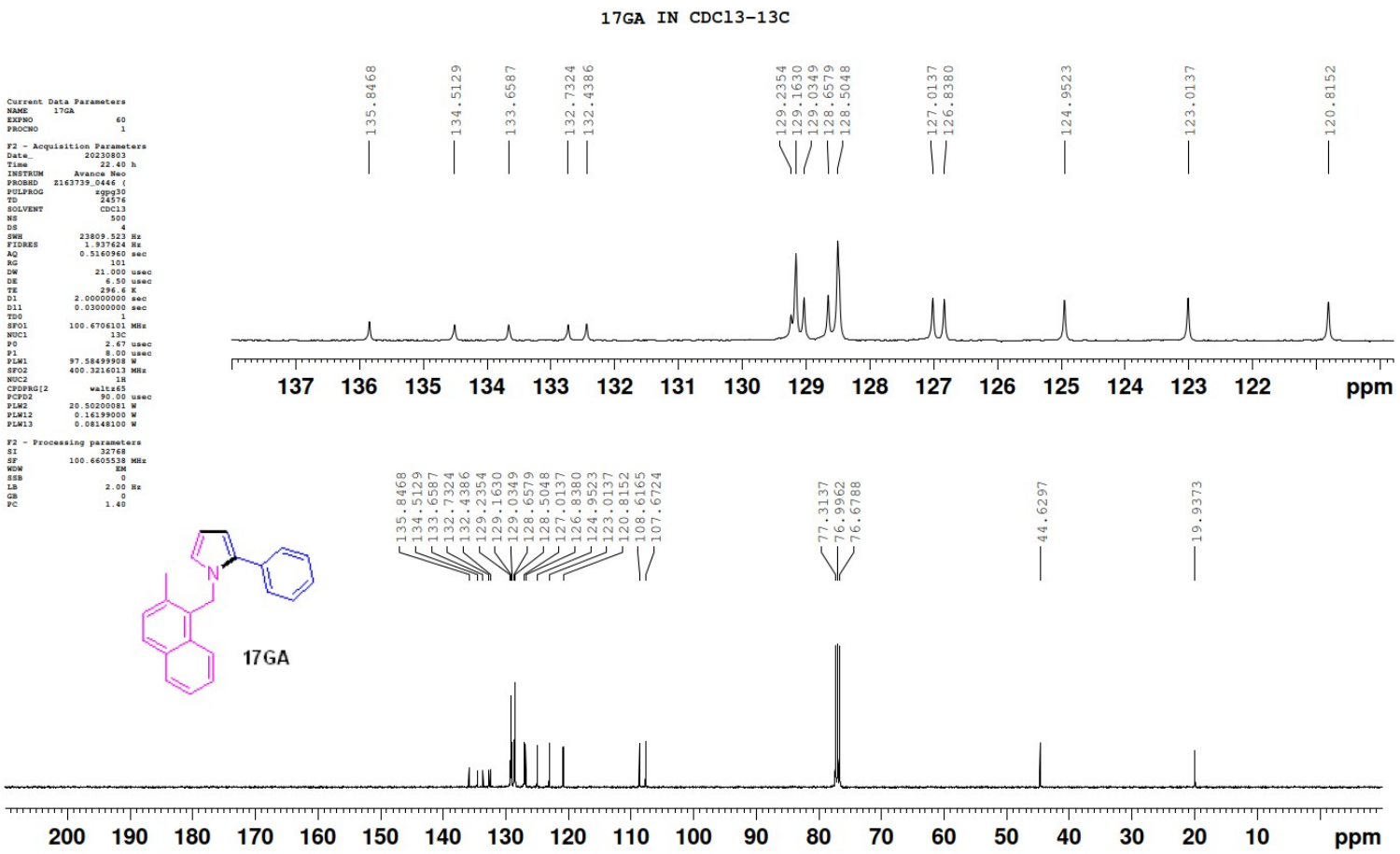



17GA IN CDCl3
Current Data Parameters
NAME 17GA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230803
Time 18.55 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.8344
7.8223
7.7869
7.7662
7.6494
7.6310
7.5271
7.5095
7.4906
7.4360
7.4245
7.4154
7.3959
7.3649
7.3439
7.2754
7.1725
6.2822
6.2215
6.0552
0.95
2.06
2.09
2.06
4.26
0.99
0.93
1.02
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
ppm
5.5336
2.4569
1.5675
1.2718
2.13
3.00
N
17GA
11
10
9
8
7
6
5
4
3
2
1
0
ppm

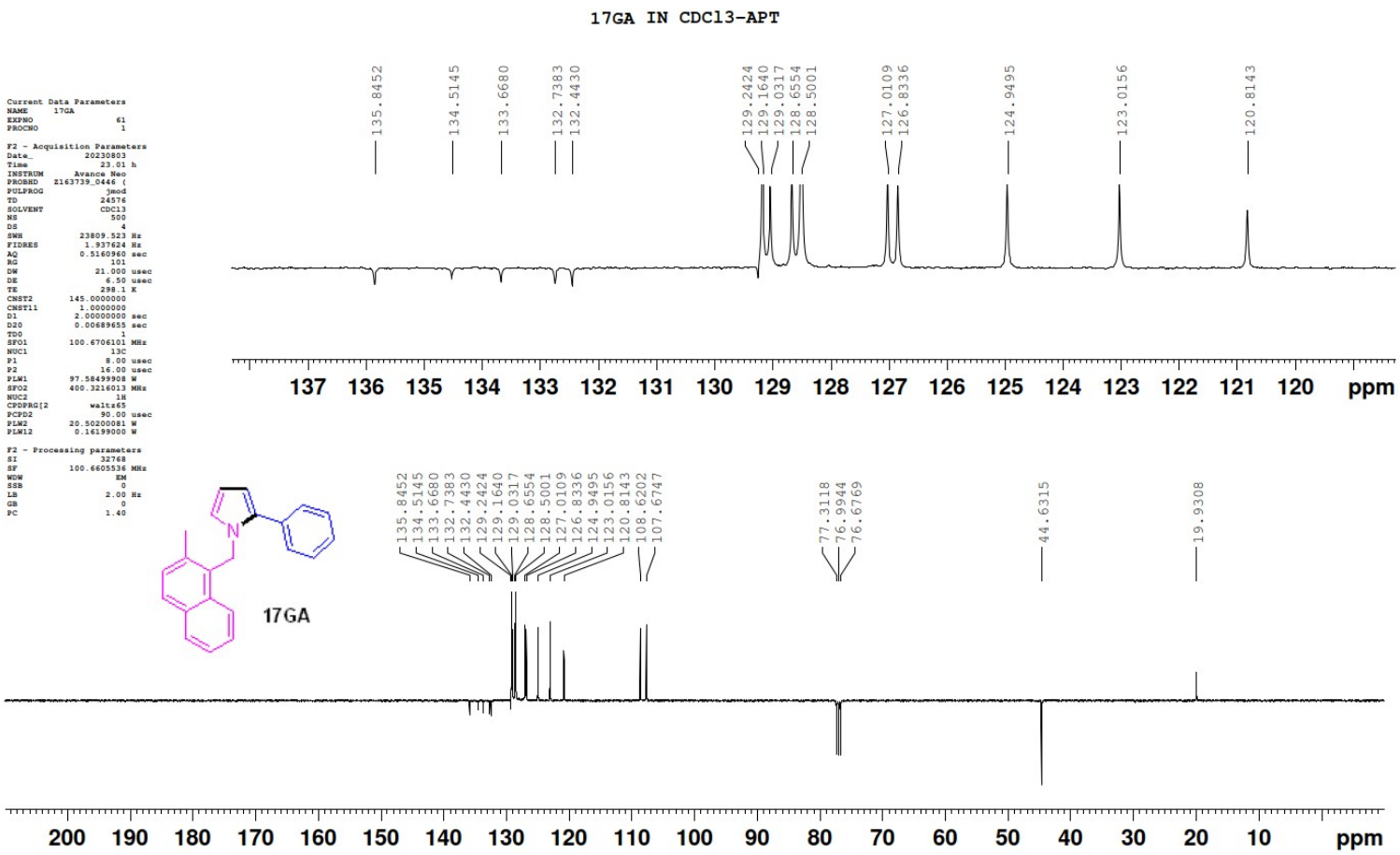
17GA IN MeOD


Current Data Parameters
NAME 17GA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221110
Time 0.48 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.813802 Hz
AQ 1.2288001 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 0 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 16384
SF 400.2300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.8279
7.8195
7.8089
7.8026
7.7819
7.7723
7.7614
7.7491
7.6109
7.5913
7.5017
7.4828
7.4655
7.3973
7.3901
7.3737
7.3577
7.3454
1.07
1.98
1.90
2.19
4.17
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
6.1471
6.1446
6.1406
6.1145
6.1083
6.1018
5.9487
5.9408
5.9331
5.5446
4.8611
3.2996
2.4054
1.2797
1.01
1.11
1.08
2.00
3.04
12
11
10
9
8
7
6
5
4
3
2
1
ppm
17GA

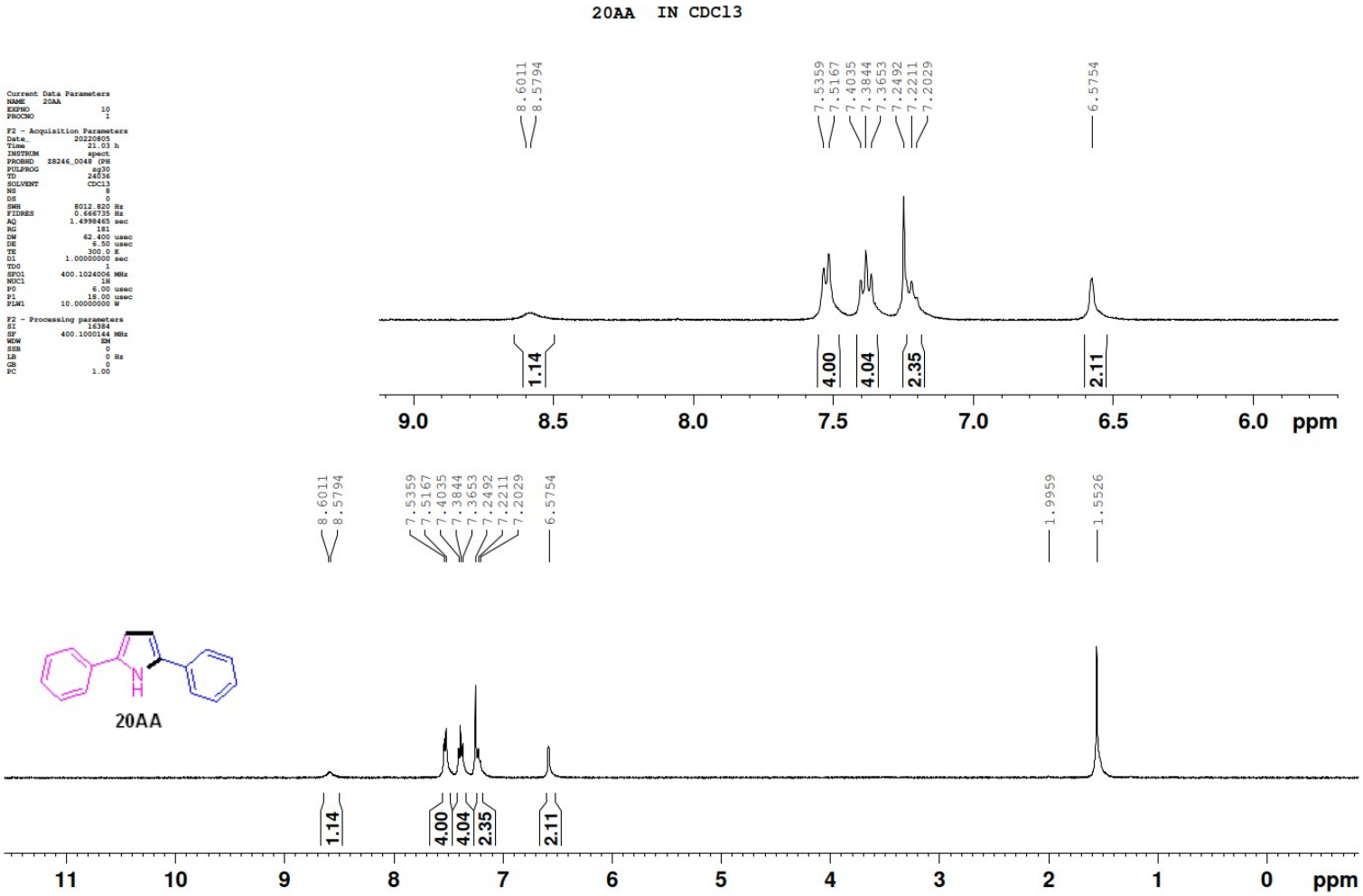
17GA IN CDCl3-13C

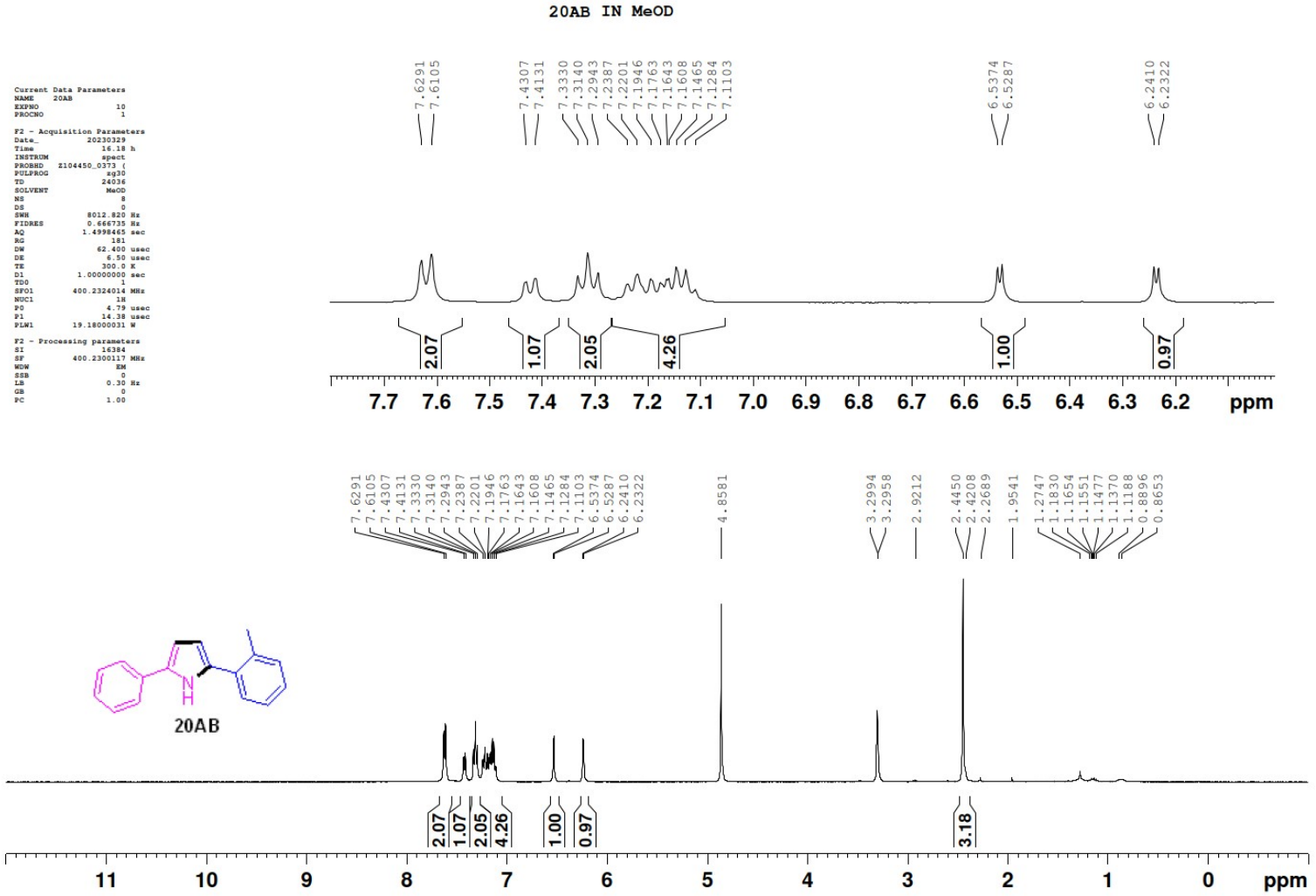


17GA IN CDCl3-APT

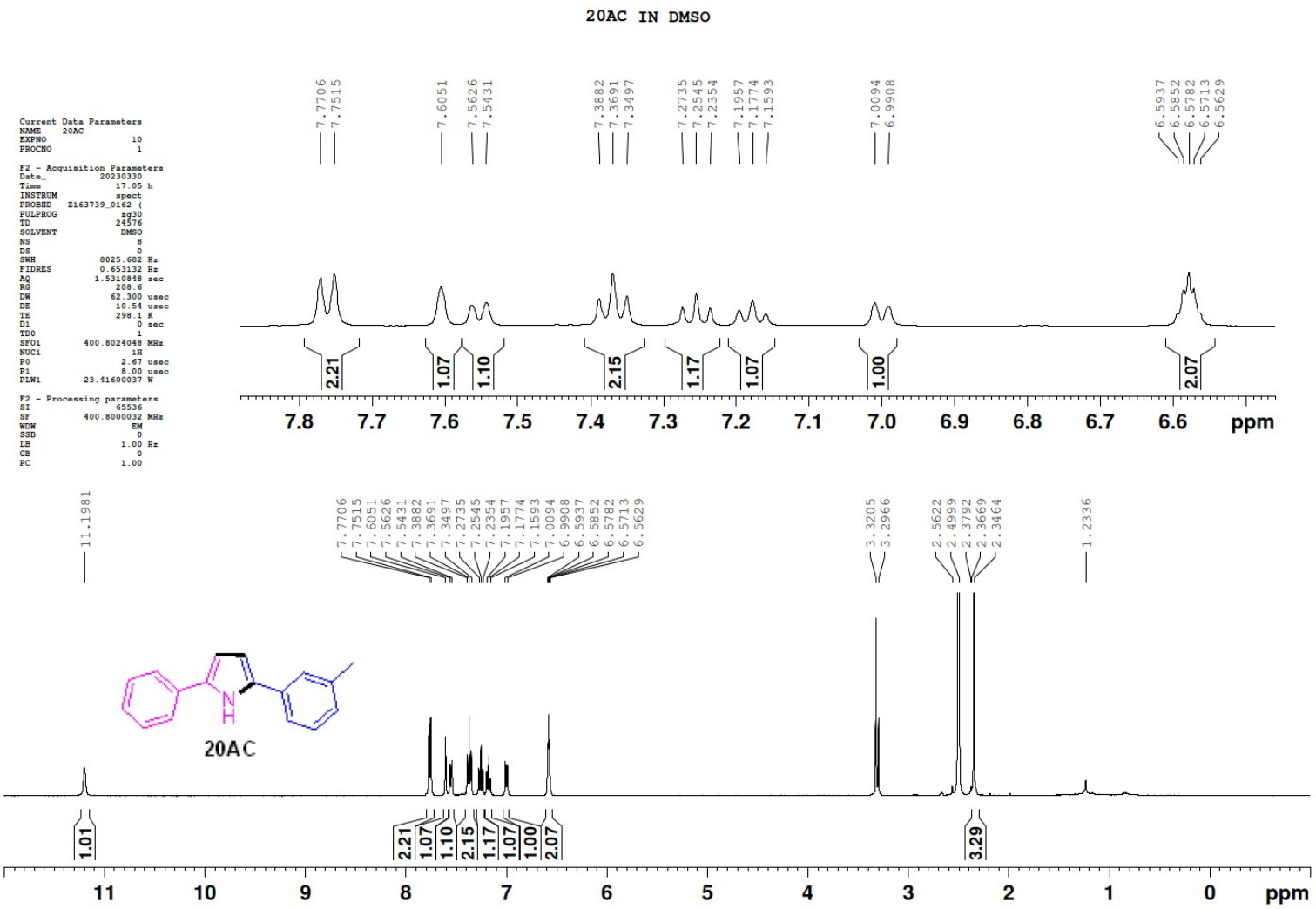


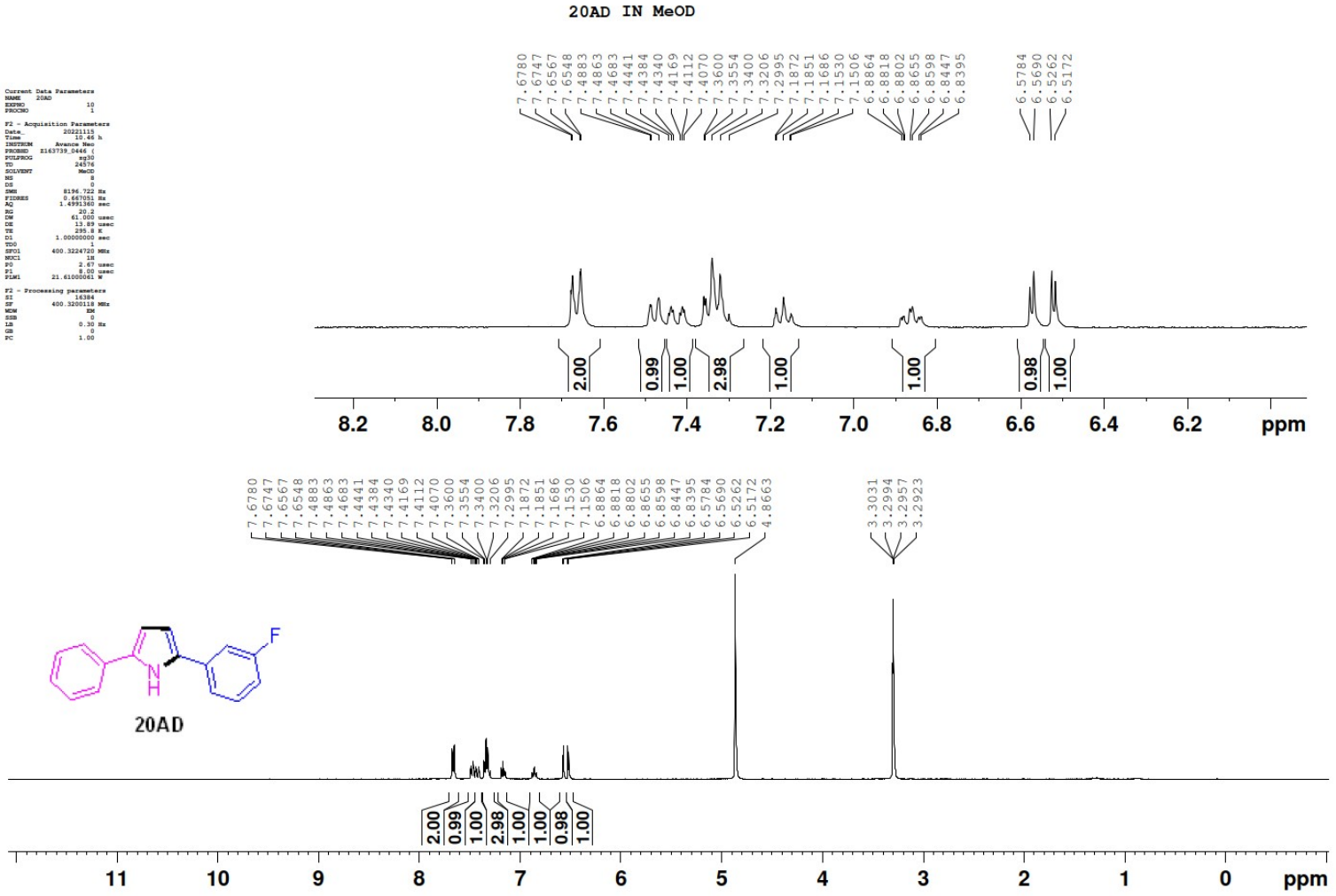
20AA IN CDCl3



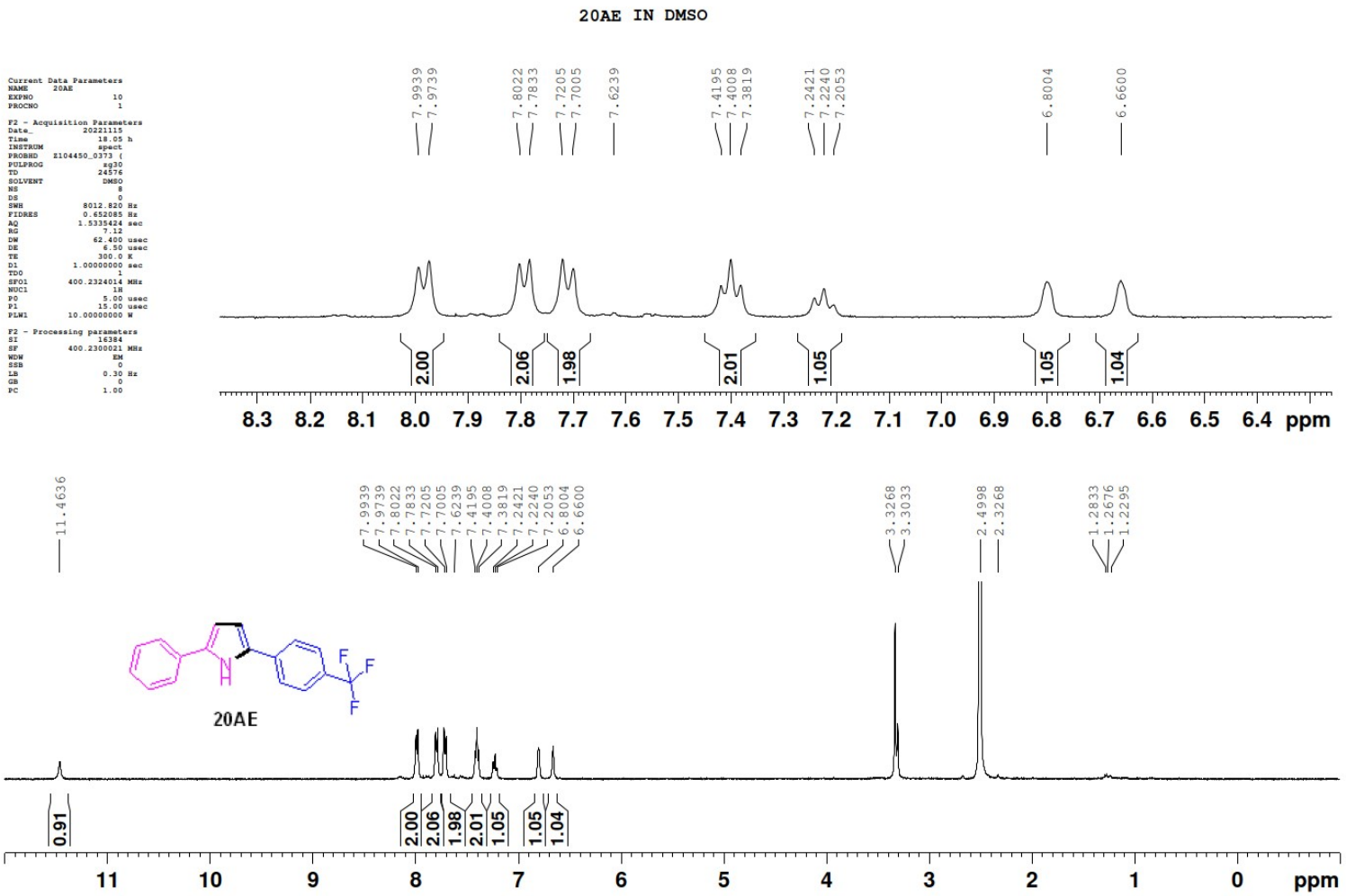

20AB IN MeOD
Current Data Parameters
NAME 20AB
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230329
Time 16.18 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.6291
7.6105
7.4307
7.4131
7.3330
7.3140
7.2943
7.2387
7.2201
7.1946
7.1763
7.1643
7.1608
7.1465
7.1284
7.1103
6.5374
6.5287
6.2410
6.2322
2.07
1.07
2.05
4.26
1.00
0.97
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 ppm
4.8581
3.2994
3.2958
2.9212
2.4450
2.4208
2.2689
1.9541
1.2747
1.1830
1.1654
1.1551
1.1477
1.1370
1.1188
0.8896
0.8653
3.18
20AB
11 10 9 8 7 6 5 4 3 2 1 0 ppm

20AC IN DMSO

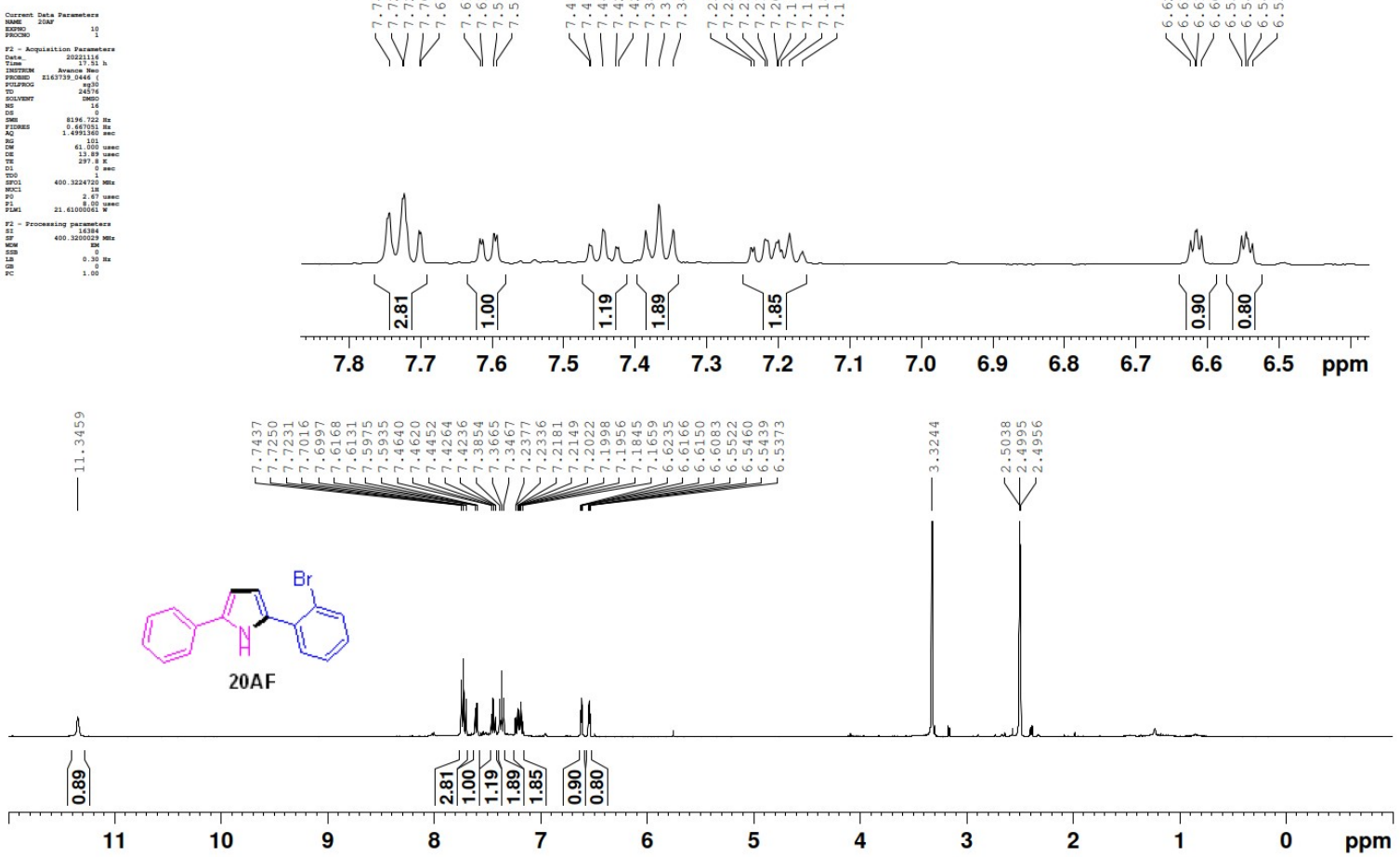

Current Data Parameters
NAME 20AC
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230330
Time 17.05 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8025.682 Hz
FIDRES 0.653132 Hz
AQ 1.5310848 sec
RG 208.6
DW 62.300 usec
DE 10.54 usec
TE 298.1 K
D1 0 sec
TD0 1
SFO1 400.8024048 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.41600037 W
F2 - Processing parameters
SI 65536
SF 400.8000032 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
7.7706
7.7515
7.6051
7.5626
7.5431
7.3882
7.3691
7.3497
7.2735
7.2545
7.2354
7.1957
7.1774
7.1593
7.0094
6.9908
6.5937
6.5852
6.5782
6.5713
6.5629
2.21
1.07
1.10
2.15
1.17
1.07
1.00
2.07
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
ppm
11.1981
3.3205
3.2966
2.5622
2.4999
2.3792
2.3669
2.3464
1.2336
1.01
3.29
11
10
9
8
7
6
5
4
3
2
1
0
20AC


20AD IN MeOD
Current Data Parameters
NAME 20AD
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221115
Time 10.46 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 20.2
DW 61.000 usec
DE 13.89 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.6780
7.6747
7.6567
7.6548
7.4883
7.4863
7.4683
7.4441
7.4384
7.4340
7.4169
7.4112
7.4070
7.3600
7.3554
7.3400
7.3206
7.2995
7.1872
7.1851
7.1686
7.1530
7.1506
6.8864
6.8818
6.8802
6.8655
6.8598
6.8447
6.8395
6.5784
6.5690
6.5262
6.5172
2.00
0.99
1.00
2.98
1.00
1.00
0.98
1.00
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
ppm
4.8663
3.3031
3.2994
3.2957
3.2923
F
N
H
20AD
11
10
9
8
7
6
5
4
3
2
1
0

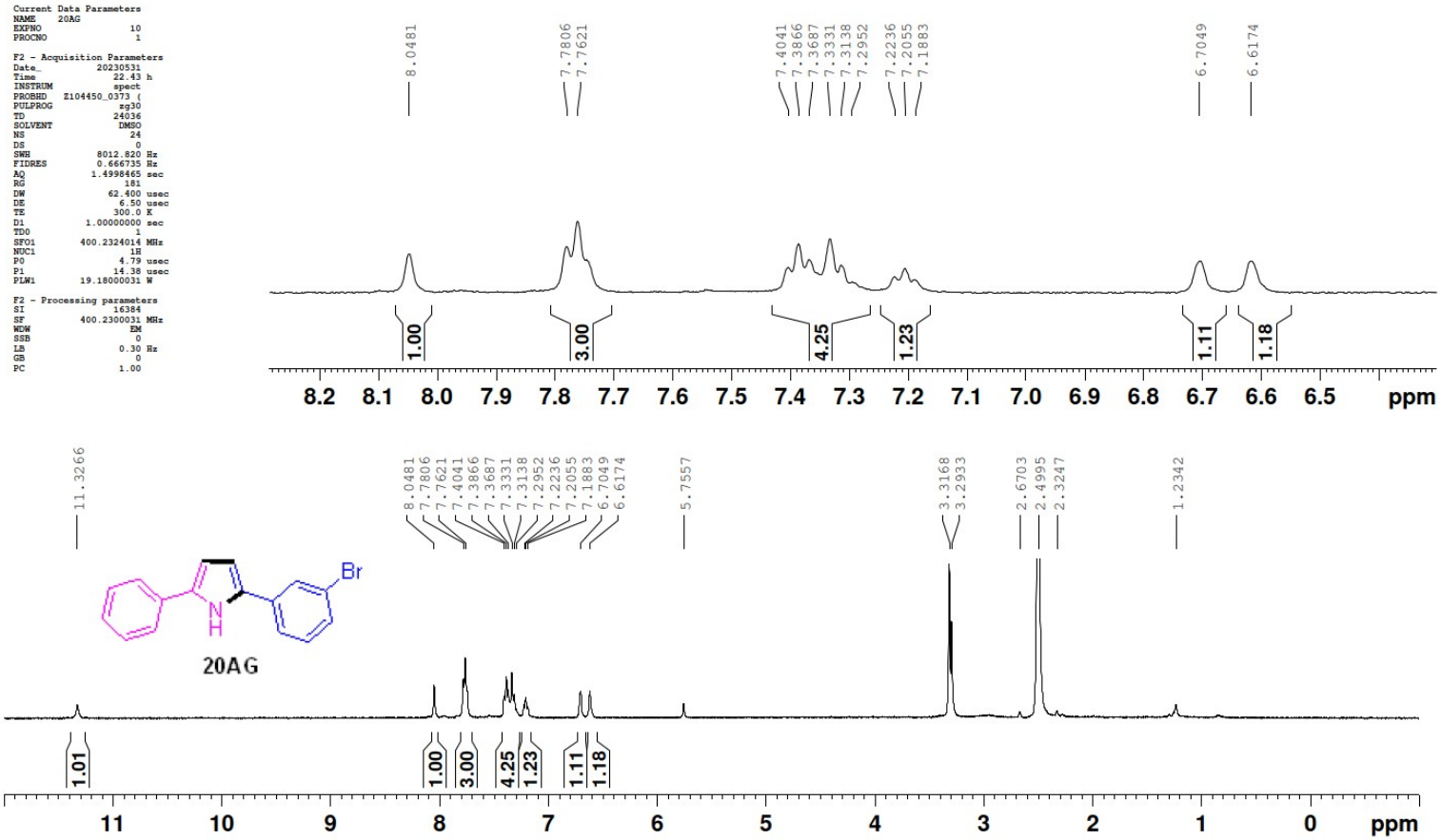
20AE IN DMSO

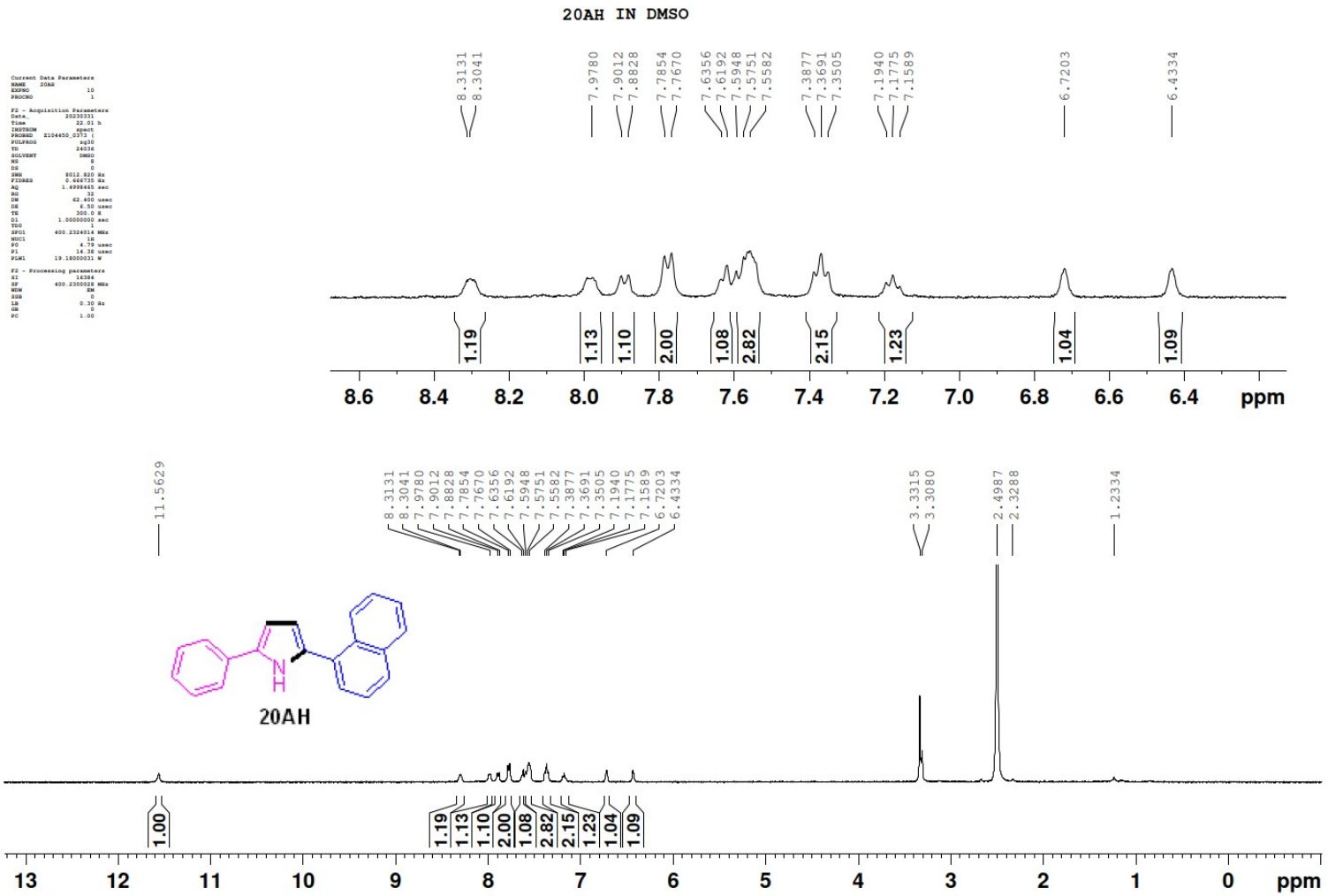

Current Data Parameters
NAME 20AE
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221115
Time 18.05 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.652085 Hz
AQ 1.5335424 sec
RG 7.12
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 16384
SF 400.2300021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.9939
7.9739
7.8022
7.7833
7.7205
7.7005
7.6239
7.4195
7.4008
7.3819
7.2421
7.2240
7.2053
6.8004
6.6600
2.00
2.06
1.98
2.01
1.05
1.05
1.04
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 ppm
11.4636
7.9939
7.9739
7.8022
7.7833
7.7205
7.7005
7.6239
7.4195
7.4008
7.3819
7.2421
7.2240
7.2053
6.8004
6.6600
3.3268
3.3033
2.4998
2.3268
1.2833
1.2676
1.2295
F
F
F
20AE
0.91
2.00
2.06
1.98
2.01
1.05
1.05
1.04
11 10 9 8 7 6 5 4 3 2 1 0 ppm

20AF IN DMSO

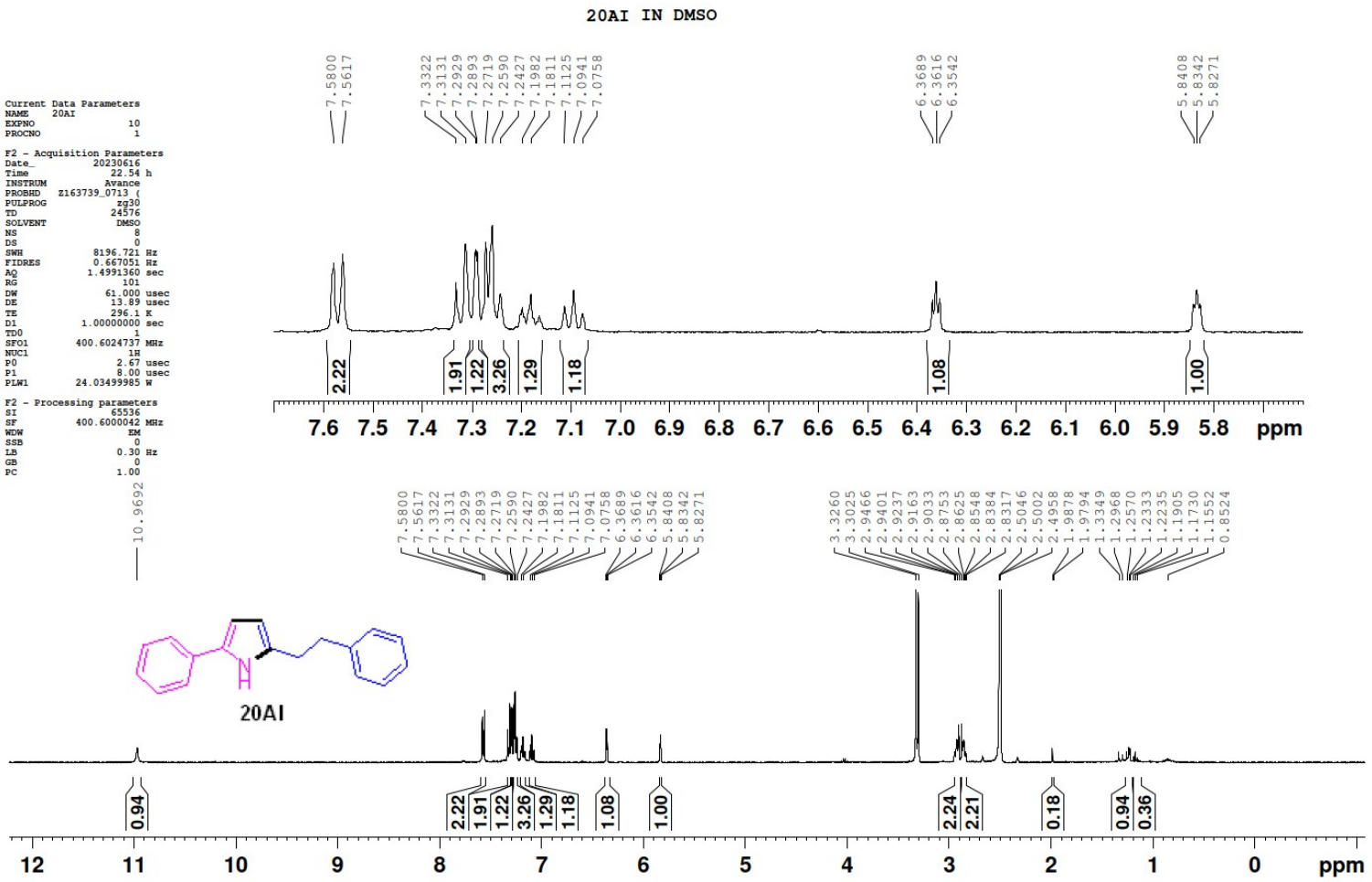

Current Data Parameters
NAME 20AF
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221116
Time 17.51 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 16
DS 0
SWH 8196.722 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.8 K
D1 0 sec
TD0 1
SFO1 400.3224720 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.61000061 W
F2 - Processing parameters
SI 16384
SF 400.3200029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.7437
7.7250
7.7231
7.7016
7.6997
7.6168
7.6131
7.5975
7.5935
7.4640
7.4620
7.4452
7.4264
7.4236
7.3854
7.3665
7.3467
7.2377
7.2336
7.2181
7.2149
7.2022
7.1998
7.1956
7.1845
7.1659
6.6235
6.6166
6.6150
6.6083
6.5522
6.5460
6.5439
6.5373
2.81
1.00
1.19
1.89
1.85
0.90
0.80
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
ppm
11.3459
3.3244
2.5038
2.4995
2.4956
Br
N
H
20AF
0.89
2.81
1.00
1.19
1.89
1.85
0.90
0.80
11
10
9
8
7
6
5
4
3
2
1
0
ppm

20AG IN DMSO

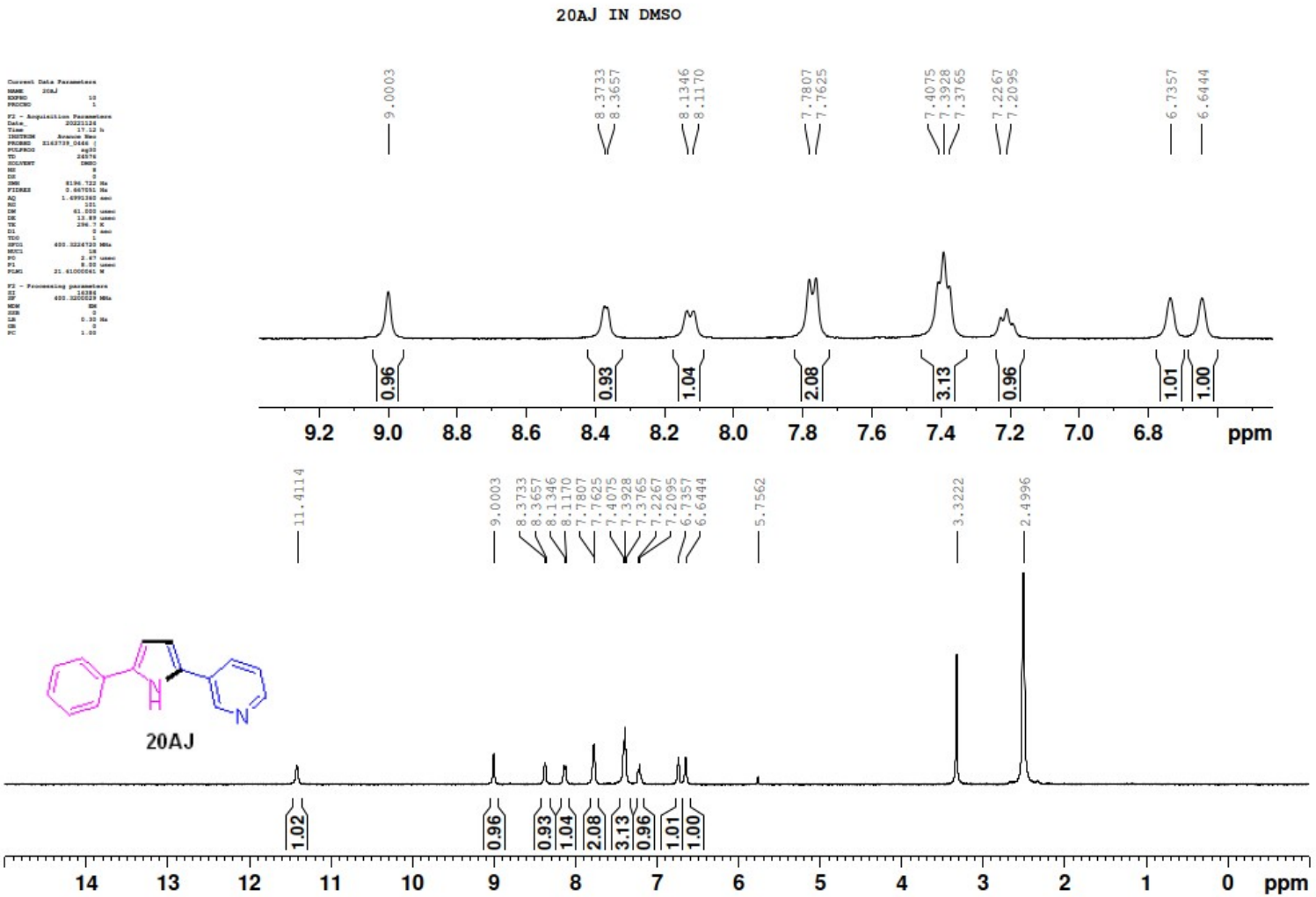

Current Data Parameters
NAME 20AG
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230531
Time 22.43 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0481
7.7806
7.7621
7.4041
7.3866
7.3687
7.3331
7.3138
7.2952
7.2236
7.2055
7.1883
6.7049
6.6174
1.00
3.00
4.25
1.23
1.11
1.18
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 ppm
11.3266
5.7557
3.3168
3.2933
2.6703
2.4995
2.3247
1.2342
Br
N
H
20AG
1.01
11 10 9 8 7 6 5 4 3 2 1 0 ppm


20AH IN DMSO
Current Data Parameters
NAME 20AH
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230331
Time 22.01 h
INSTRUM spect
PROBHD 2104450_5mm_C
PULPROG zg30
TD 24034
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998445 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3131
8.3041
7.9780
7.9012
7.8828
7.7854
7.7670
7.6356
7.6192
7.5948
7.5751
7.5582
7.3877
7.3691
7.3505
7.1940
7.1775
7.1589
6.7203
6.4334
1.19
1.13
1.10
2.00
1.08
2.82
2.15
1.23
1.04
1.09
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
ppm
11.5629
3.3315
3.3080
2.4987
2.3288
1.2334
1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
20AH

20AI IN DMSO

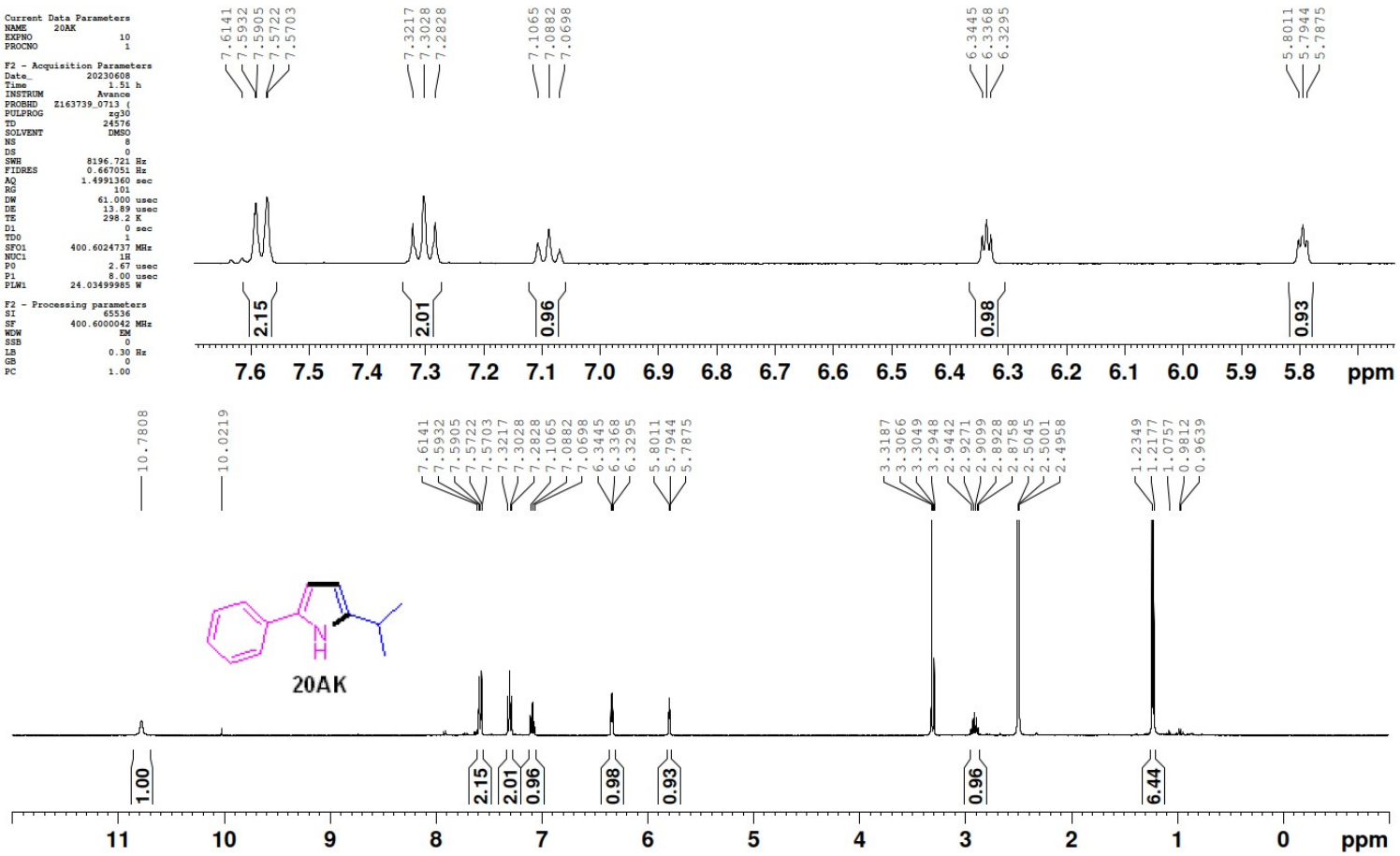

Current Data Parameters
NAME 20AI
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230616
Time 22.54 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5800
7.5617
7.3322
7.3131
7.2929
7.2893
7.2719
7.2590
7.2427
7.1982
7.1811
7.1125
7.0941
7.0758
6.3689
6.3616
6.3542
5.8408
5.8342
5.8271
2.22
1.91
1.22
3.26
1.29
1.18
1.08
1.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 ppm
10.9692
3.3260
3.3025
2.9466
2.9401
2.9237
2.9163
2.9033
2.8753
2.8625
2.8548
2.8384
2.8317
2.5046
2.5002
2.4958
1.9878
1.9794
1.3349
1.2968
1.2570
1.2333
1.2235
1.1905
1.1730
1.1552
0.8524
20AI
0.94
2.24
2.21
0.18
0.36
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

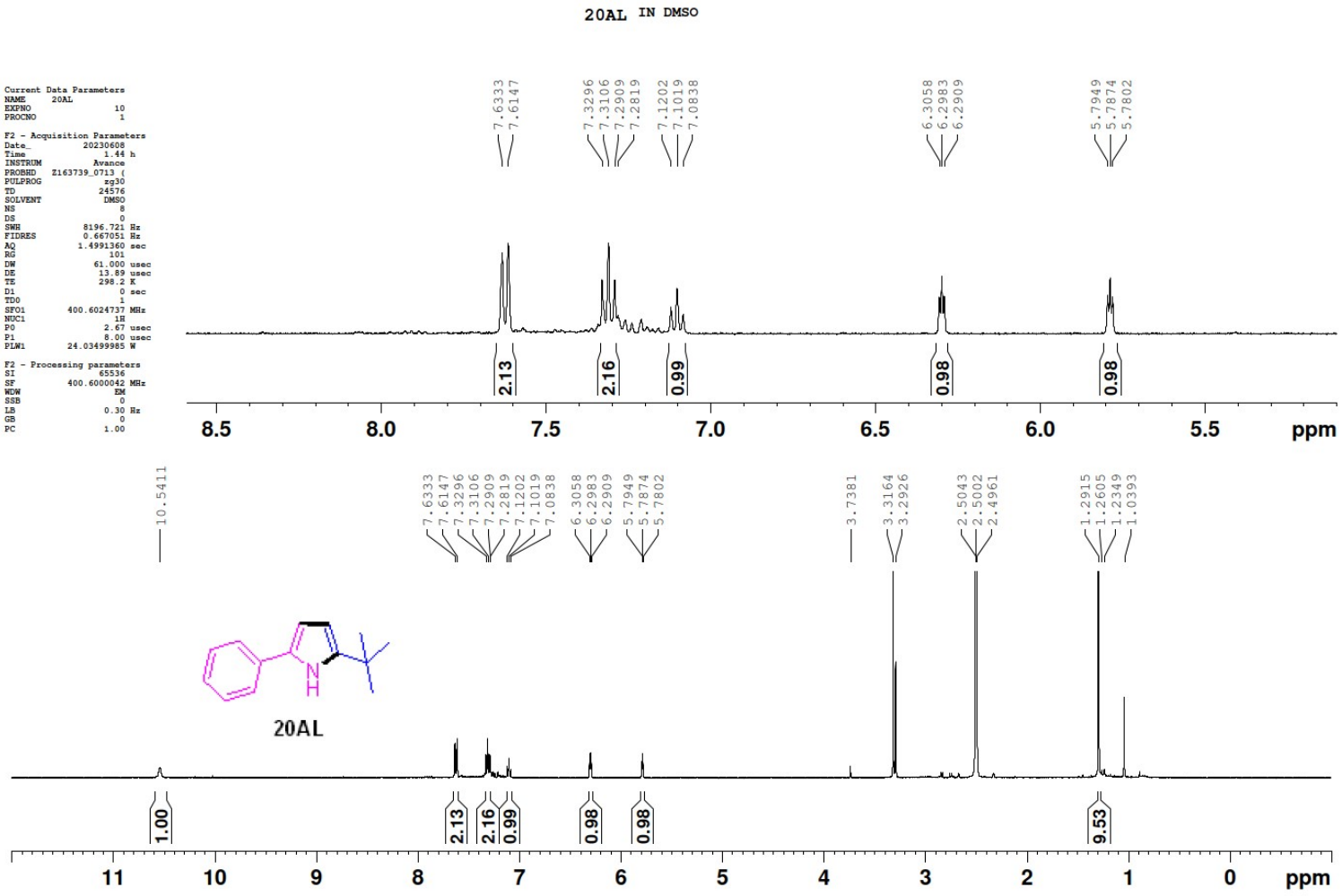
20AJ IN DMSO



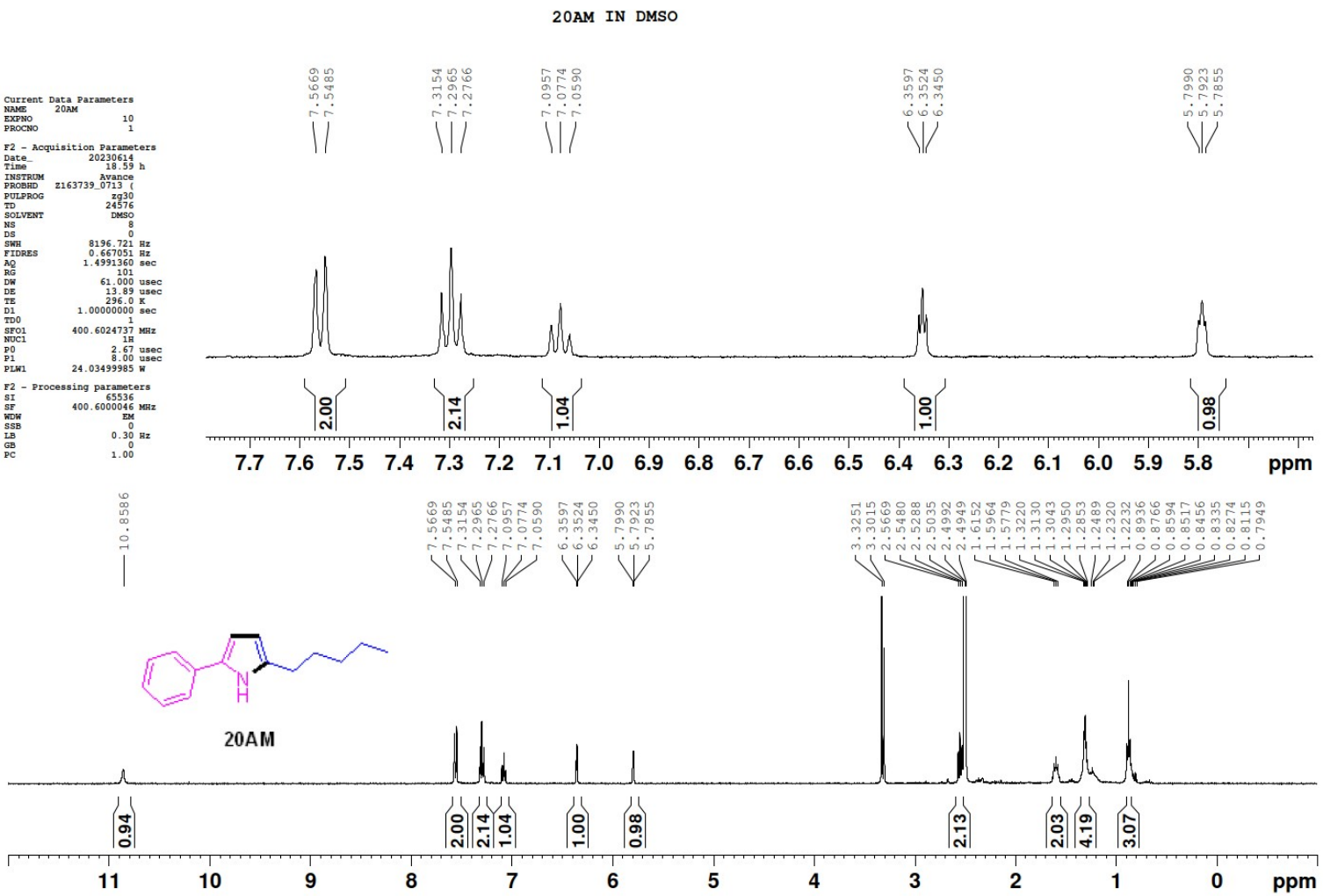
20AJ

20AK IN DMSO


Current Data Parameters
NAME 20AK
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230608
Time 1.51 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 0 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.6141
7.5932
7.5905
7.5722
7.5703
7.3217
7.3028
7.2828
7.1065
7.0882
7.0698
6.3445
6.3368
6.3295
5.8011
5.7944
5.7875
2.15
2.01
0.96
0.98
0.93
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 ppm
10.7808
10.0219
3.3187
3.3066
3.3049
3.2948
2.9442
2.9271
2.9099
2.8928
2.8758
2.5045
2.5001
2.4958
1.2349
1.2177
1.0757
0.9812
0.9639
20AK
1.00
2.15
2.01
0.96
0.98
0.93
0.96
6.44
11 10 9 8 7 6 5 4 3 2 1 0 ppm


20AL IN DMSO
Current Data Parameters
NAME 20AL
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230608
Time 1.44 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 0 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.6333
7.6147
7.3296
7.3106
7.2909
7.2819
7.1202
7.1019
7.0838
6.3058
6.2983
6.2909
5.7949
5.7874
5.7802
2.13
2.16
0.99
0.98
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
ppm
10.5411
3.7381
3.3164
3.2926
2.5043
2.5002
2.4961
1.2915
1.2605
1.2349
1.0393
1.00
2.13
2.16
0.99
0.98
0.98
9.53
20AL
11
10
9
8
7
6
5
4
3
2
1
0
ppm

20AM IN DMSO

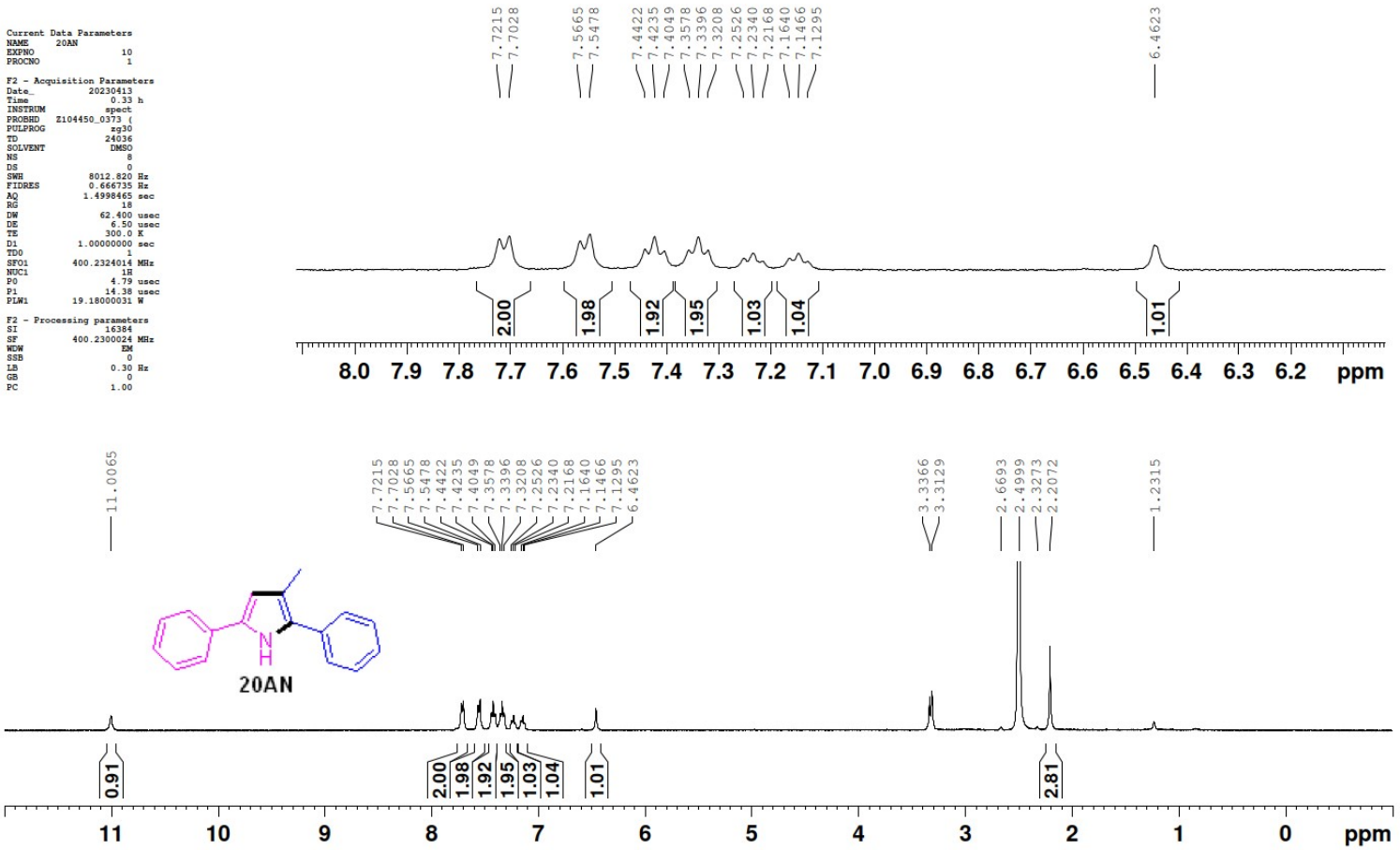

Current Data Parameters
NAME 20AM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230614
Time 18.59 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5669
7.5485
7.3154
7.2965
7.2766
7.0957
7.0774
7.0590
6.3597
6.3524
6.3450
5.7990
5.7923
5.7855
2.00
2.14
1.04
1.00
0.98
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 ppm
10.8586
3.3251
3.3015
2.5669
2.5480
2.5288
2.5035
2.4992
2.4949
1.6152
1.5964
1.5779
1.3220
1.3130
1.3043
1.2950
1.2853
1.2489
1.2320
1.2232
0.8936
0.8766
0.8594
0.8517
0.8456
0.8335
0.8274
0.8115
0.7949
20AM
0.94
2.00
2.14
1.04
1.00
0.98
2.13
2.03
4.19
3.07
11 10 9 8 7 6 5 4 3 2 1 0 ppm

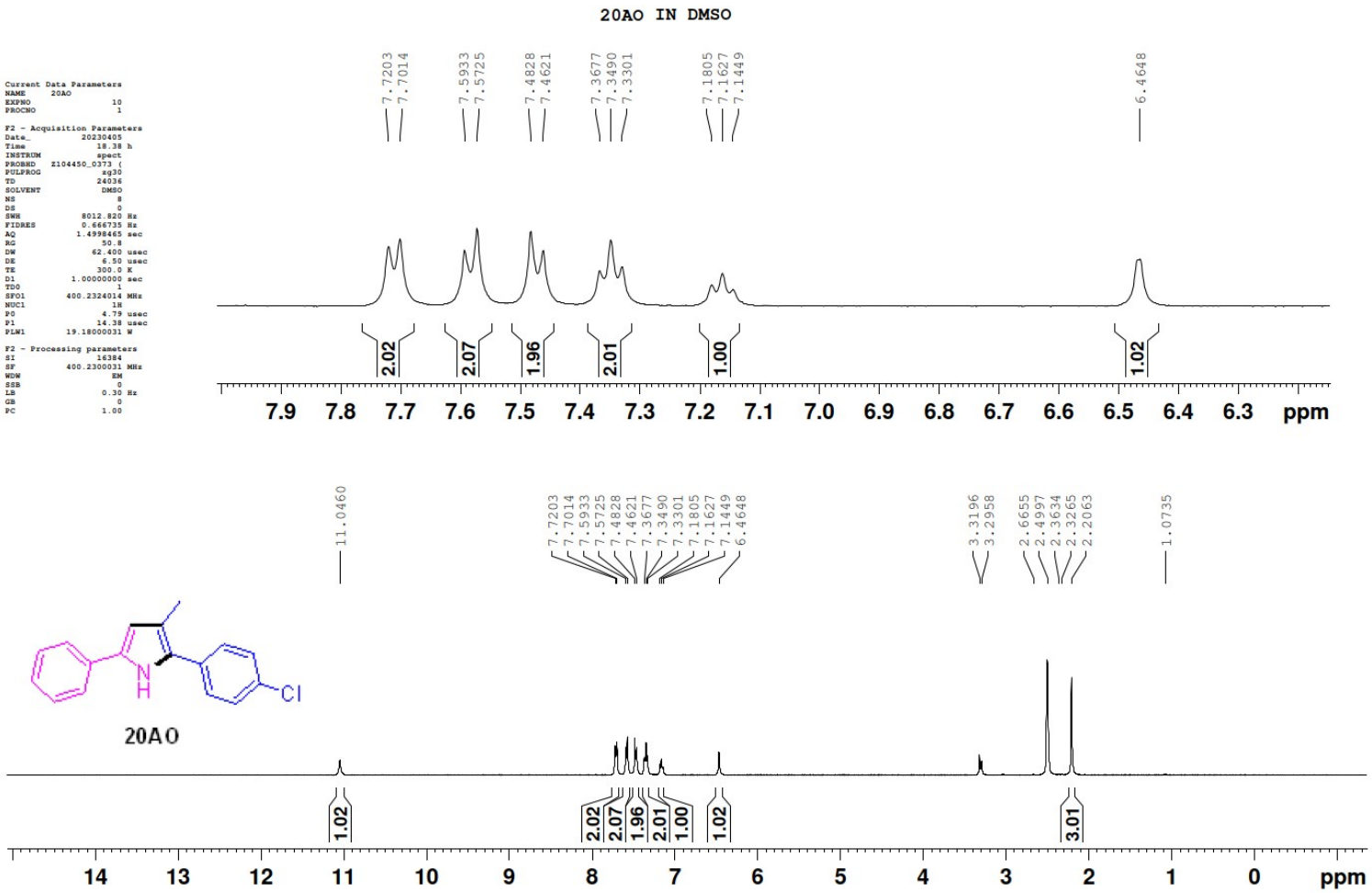
20AN IN DMSO

```
Current Data Parameters
NAME      20AN
EXPNO       10
PROCNO       1

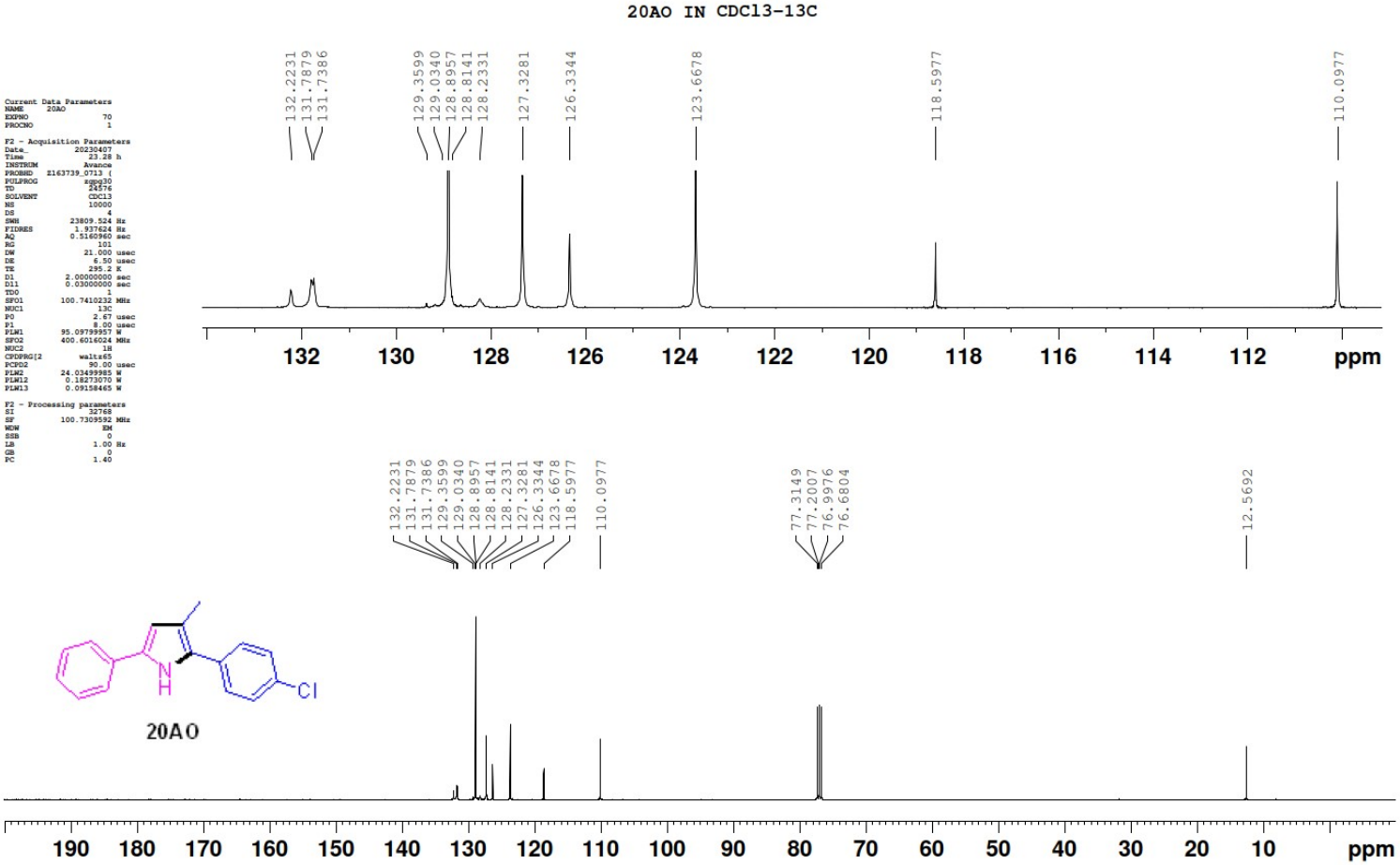
F2 - Acquisition Parameters
Date_     20230413
Time          0.33 h
INSTRUM       spect
PROBHD   Z104450_0373 (
PULPROG       zg30
TD           24036
SOLVENT       DMSO
NS               8
DS               0
SWH       8012.820 Hz
FIDRES    0.666735 Hz
AQ        1.4998465 sec
RG              18
DW           62.400 usec
DE            6.50 usec
TE           300.0 K
D1        1.00000000 sec
TD0              1
SFO1    400.2324014 MHz
NUC1           1H
P0            4.79 usec
P1           14.38 usec
PLW1     19.18000031 W

F2 - Processing parameters
SI           16384
SF      400.2300024 MHz
WDW            EM
SSB             0
LB           0.30 Hz
GB              0
PC           1.00
```



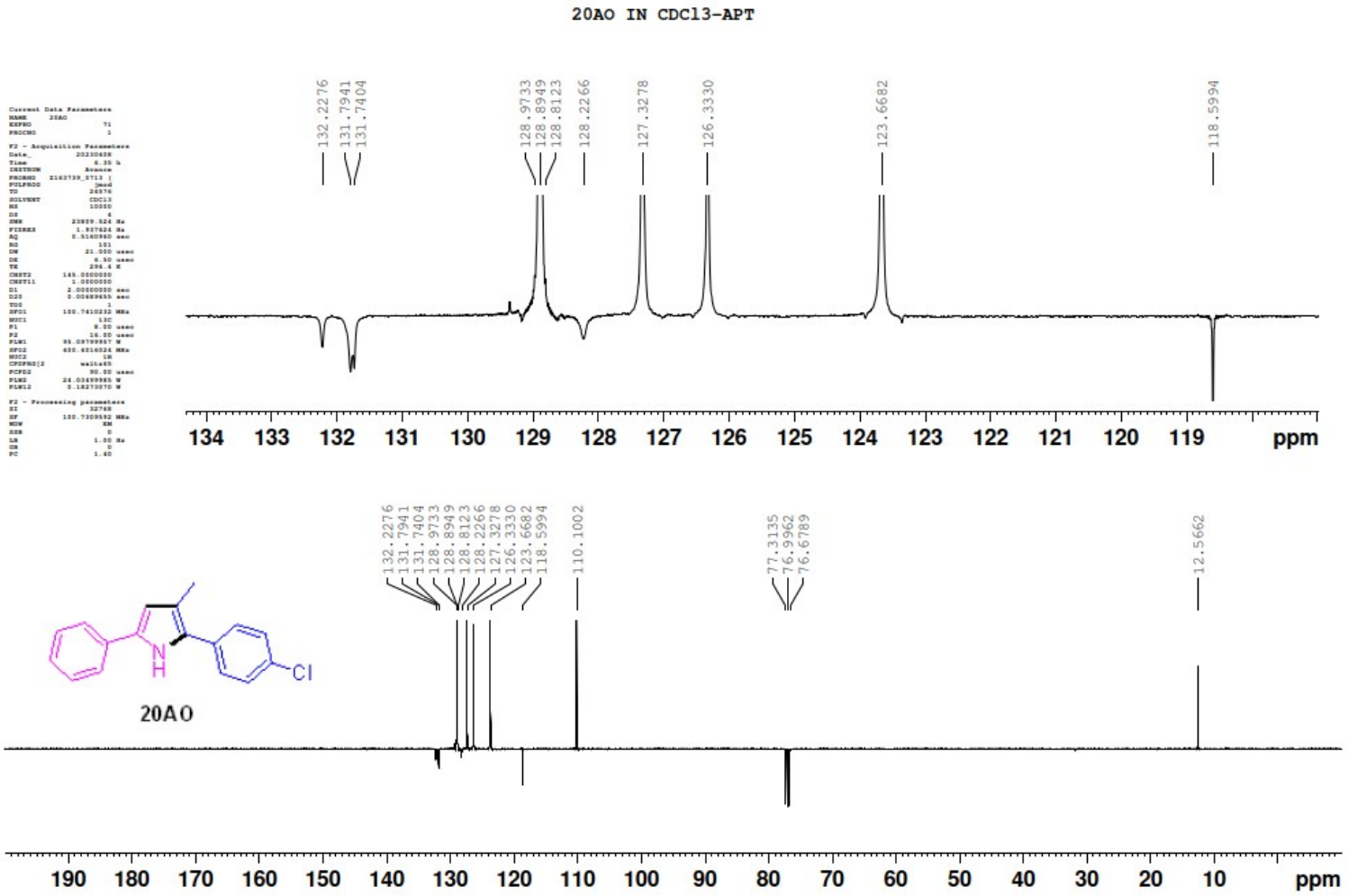

20AO IN DMSO
Current Data Parameters
NAME 20AO
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230405
Time 18.38 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.7203
7.7014
7.5933
7.5725
7.4828
7.4621
7.3677
7.3490
7.3301
7.1805
7.1627
7.1449
6.4648
2.02
2.07
1.96
2.01
1.00
1.02
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 ppm
11.0460
7.7203
7.7014
7.5933
7.5725
7.4828
7.4621
7.3677
7.3490
7.3301
7.1805
7.1627
7.1449
6.4648
3.3196
3.2958
2.6655
2.4997
2.3634
2.3265
2.2063
1.0735
N
H
Cl
20AO
1.02
2.02
2.07
1.96
2.01
1.00
1.02
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

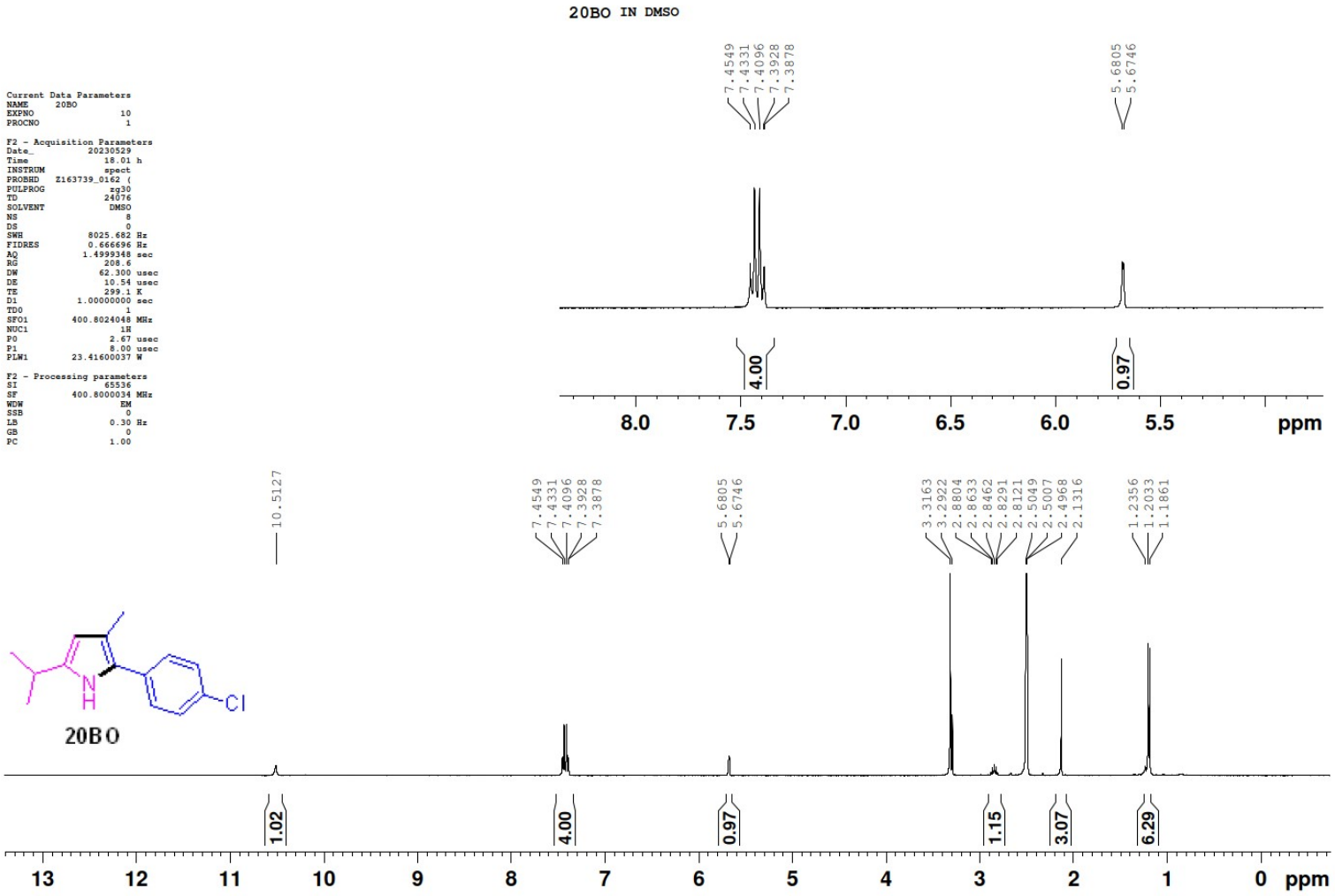
20AO IN CDCl3-13C



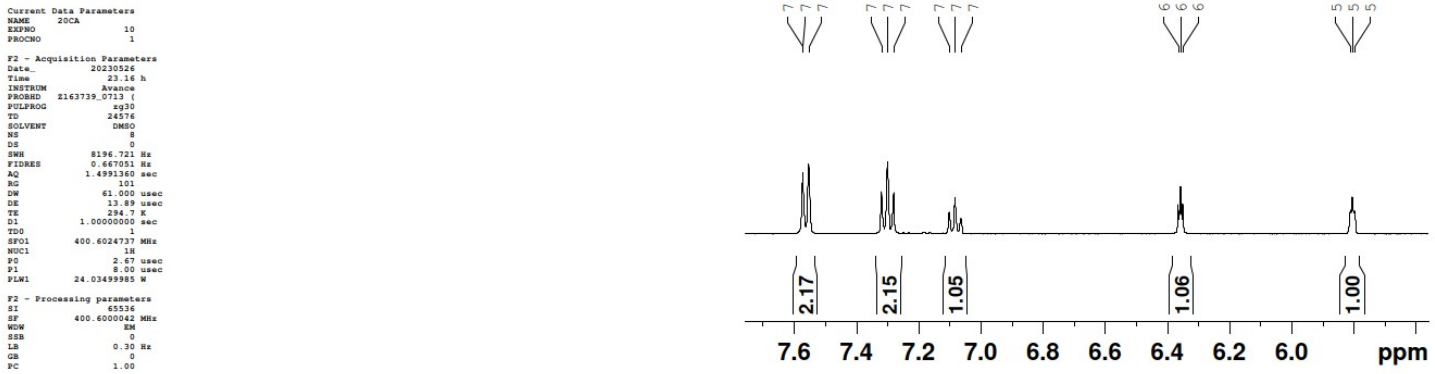
20AO

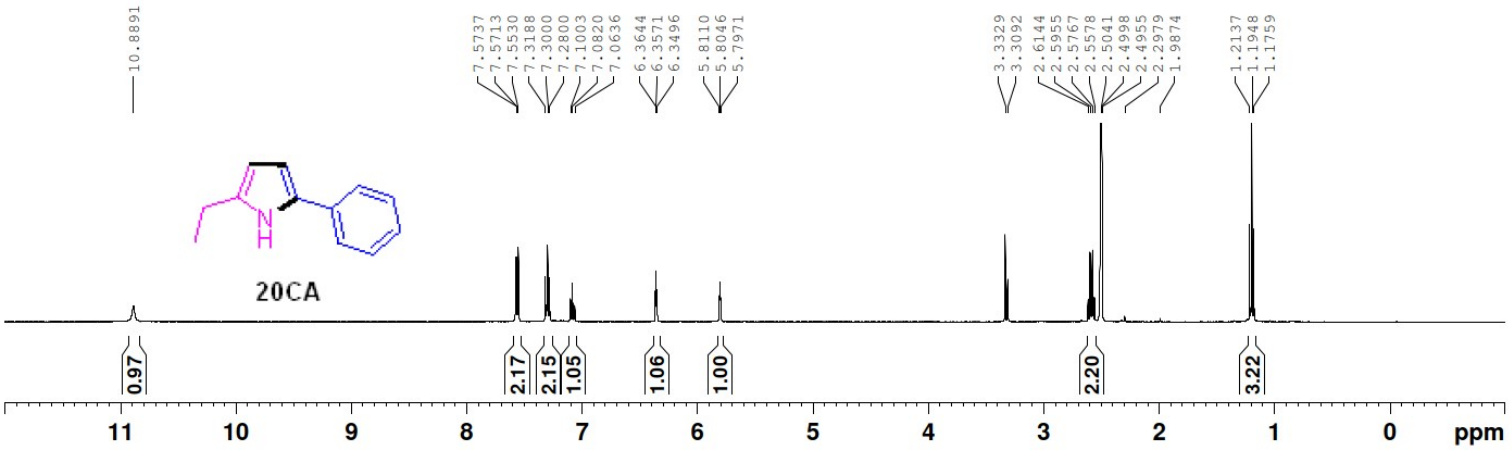
20AO IN CDCl3-APT

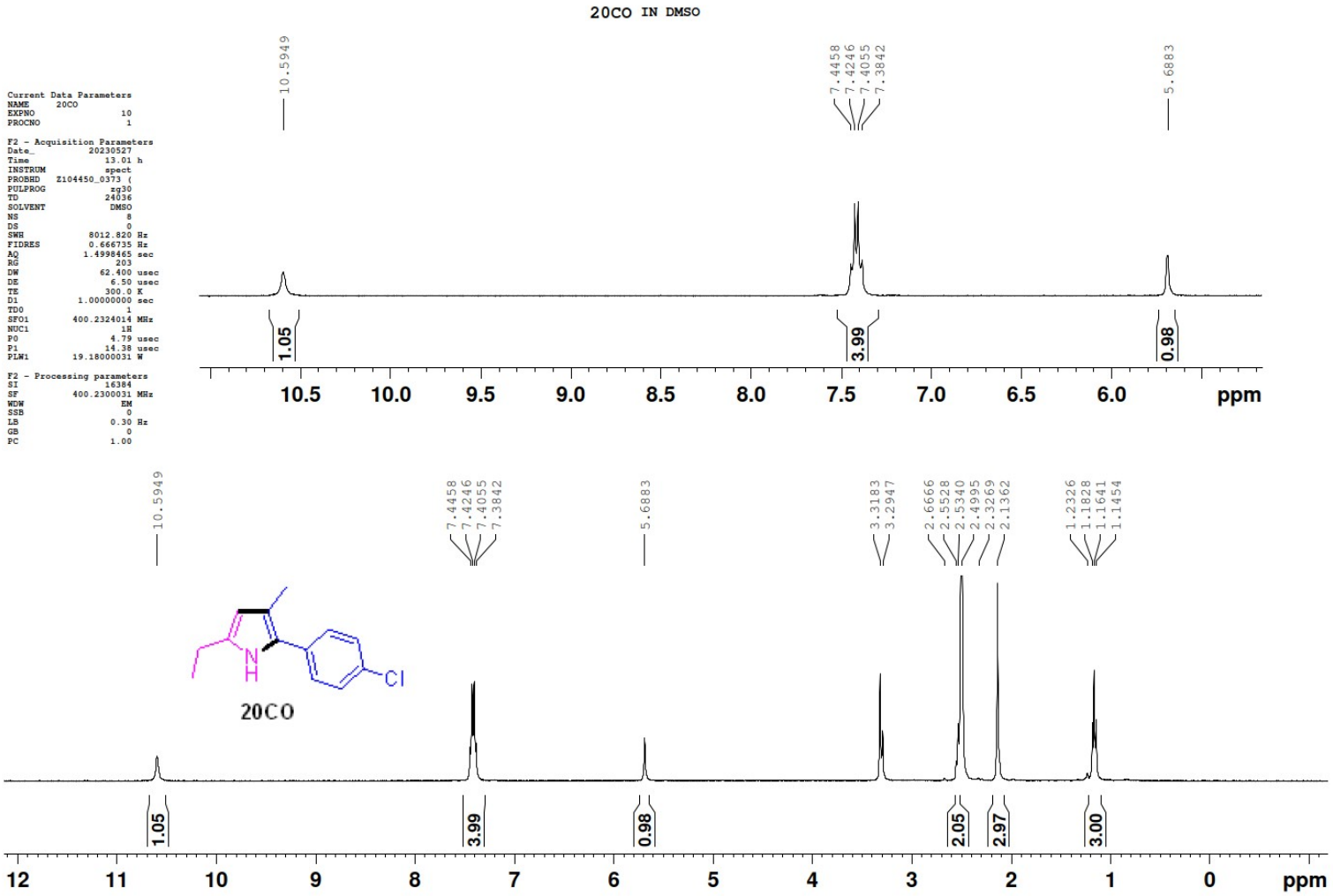



20BO IN DMSO
Current Data Parameters
NAME 20BO
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230529
Time 18.01 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24076
SOLVENT DMSO
NS 8
DS 0
SWH 8025.682 Hz
FIDRES 0.666696 Hz
AQ 1.4999348 sec
RG 208.6
DW 62.300 usec
DE 10.54 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.8024048 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.41600037 W
F2 - Processing parameters
SI 65536
SF 400.8000034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.4549
7.4331
7.4096
7.3928
7.3878
5.6805
5.6746
4.00
0.97
8.0
7.5
7.0
6.5
6.0
5.5
ppm
10.5127
3.3163
3.2922
2.8804
2.8633
2.8462
2.8291
2.8121
2.5049
2.5007
2.4968
2.1316
1.2356
1.2033
1.1861
1.02
1.15
3.07
6.29
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
N
H
Cl
20BO

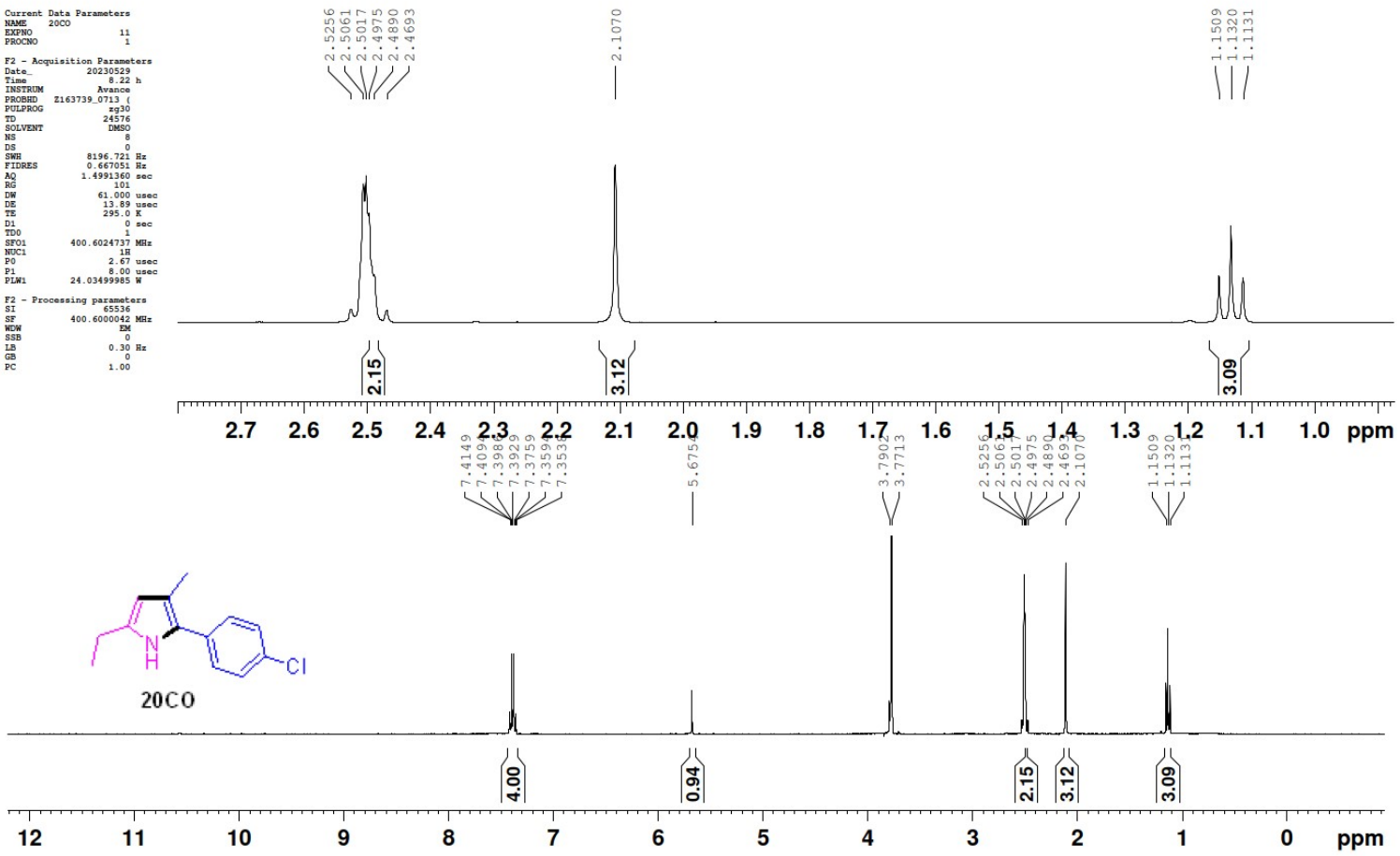
20CA IN DMSO


Current Data Parameters
NAME 20CA
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230526
Time 23.16 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5737
7.5713
7.5530
7.3188
7.3000
7.2800
7.1003
7.0820
7.0636
6.3644
6.3571
6.3496
5.8110
5.8046
5.7971
2.17
2.15
1.05
1.06
1.00
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
ppm


10.8891
7.5737
7.5713
7.5530
7.3188
7.3000
7.2800
7.1003
7.0820
7.0636
6.3644
6.3571
6.3496
5.8110
5.8046
5.7971
3.3329
3.3092
2.6144
2.5955
2.5767
2.5578
2.5041
2.4998
2.4955
2.2979
1.9874
1.2137
1.1948
1.1759
20CA
0.97
2.17
2.15
1.05
1.06
1.00
2.20
3.22
11
10
9
8
7
6
5
4
3
2
1
0
ppm


20CO IN DMSO
Current Data Parameters
NAME 20CO
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230527
Time 13.01 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10.5949
7.4458
7.4246
7.4055
7.3842
5.6883
1.05
3.99
0.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 ppm
10.5949
7.4458
7.4246
7.4055
7.3842
5.6883
3.3183
3.2947
2.6666
2.5528
2.5340
2.4995
2.3269
2.1362
1.2326
1.1828
1.1641
1.1454
N
H
Cl
20CO
1.05
3.99
0.98
2.05
2.97
3.00
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

20CO D2O EXCHANGE

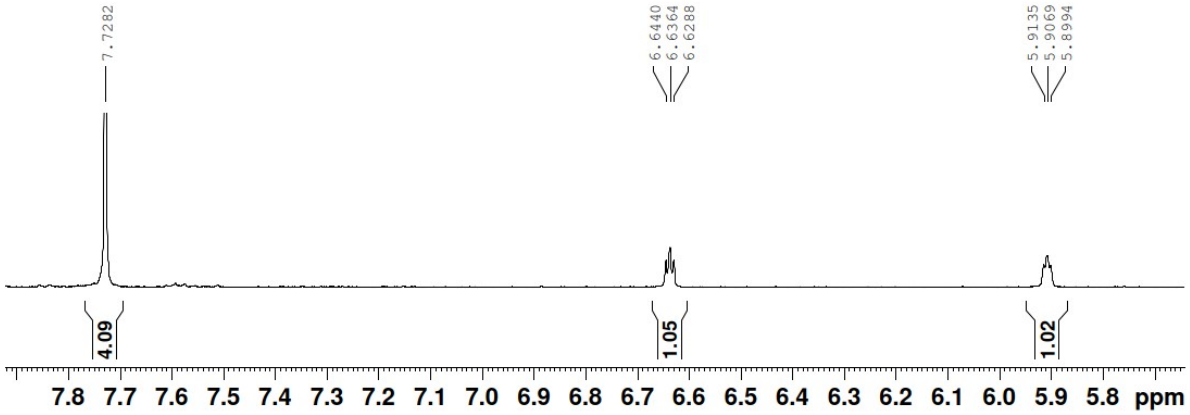


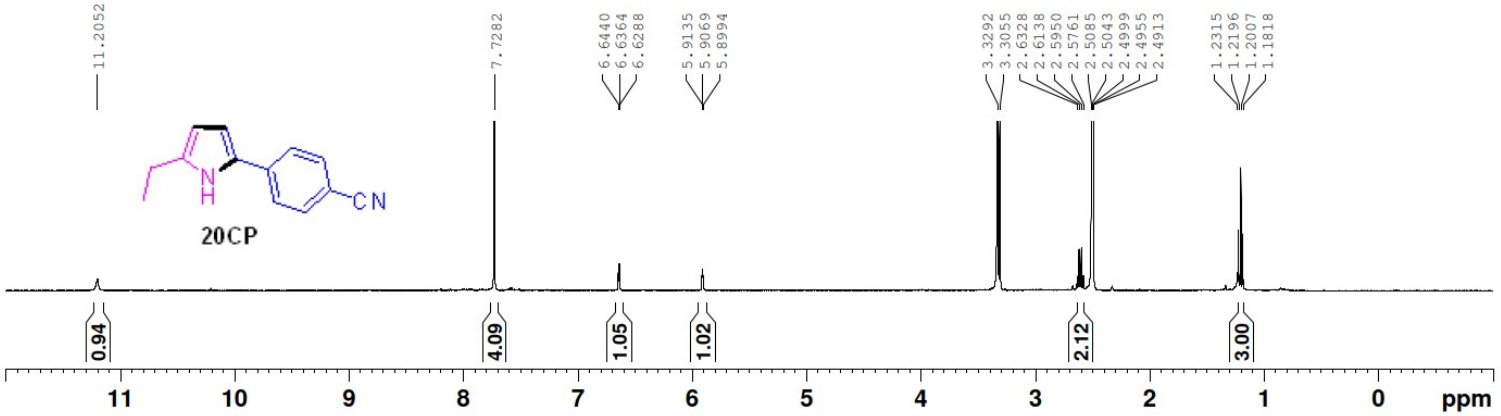
20CP IN DMSO

```
Current Data Parameters
NAME      20CP
EXPNO       10
PROCNO       1

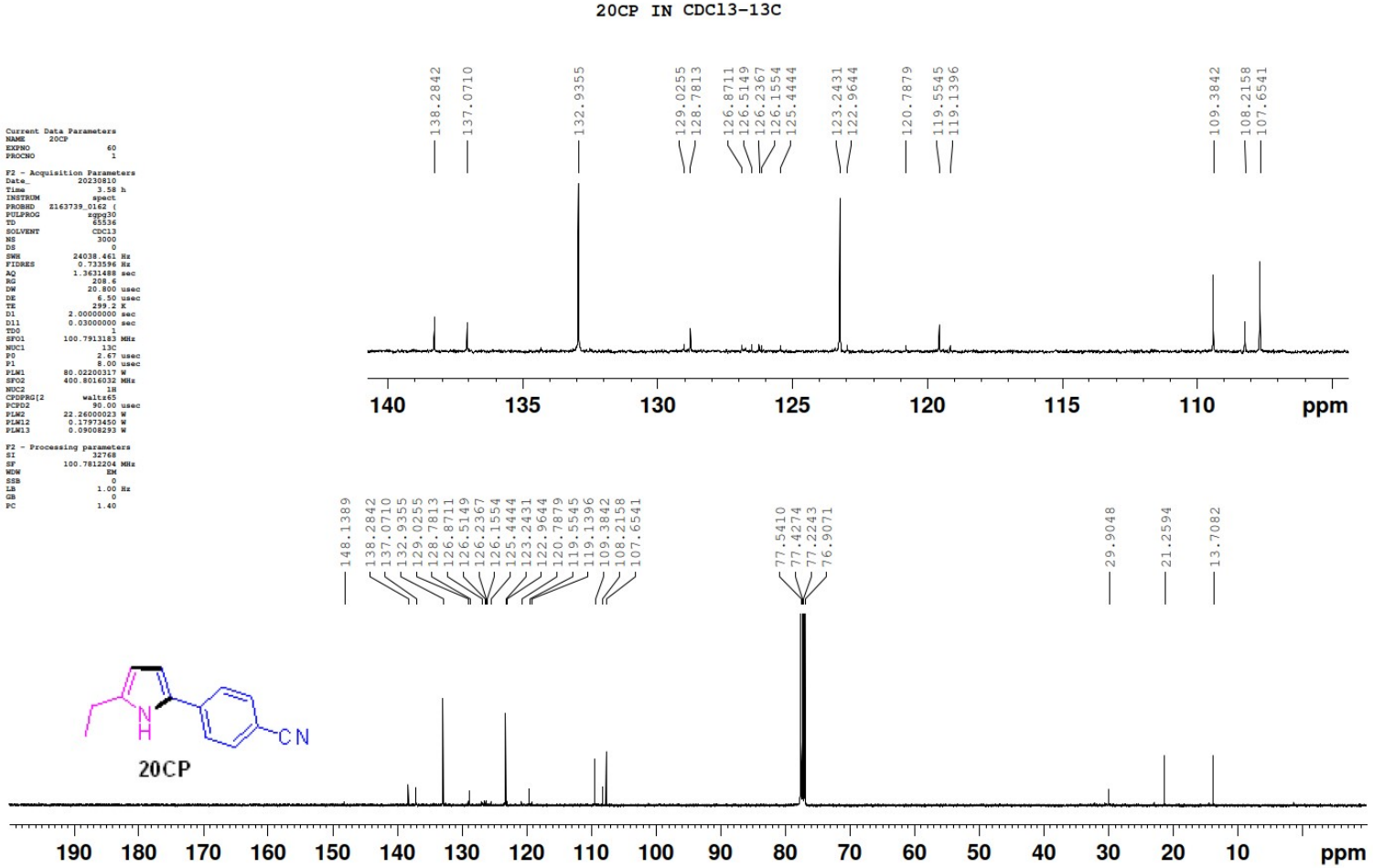
F2 - Acquisition Parameters
Date_     20230530
Time        21.51 h
INSTRUM      Avance
PROBHD   Z163739_0713 (
PULPROG       zg30
TD           24576
SOLVENT       DMSO
NS               8
DS               0
SWH       8196.721 Hz
FIDRES    0.667051 Hz
AQ        1.4991360 sec
RG             101
DW          61.000 usec
DE          13.89 usec
TE           295.7 K
D1        1.00000000 sec
TD0              1
SFO1    400.6024737 MHz
NUC1           1H
P0           2.67 usec
P1           8.00 usec
PLW1     24.03499985 W

F2 - Processing parameters
SI           65536
SF      400.6000042 MHz
WDW             EM
SSB              0
LB            0.30 Hz
GB               0
PC            1.00
```

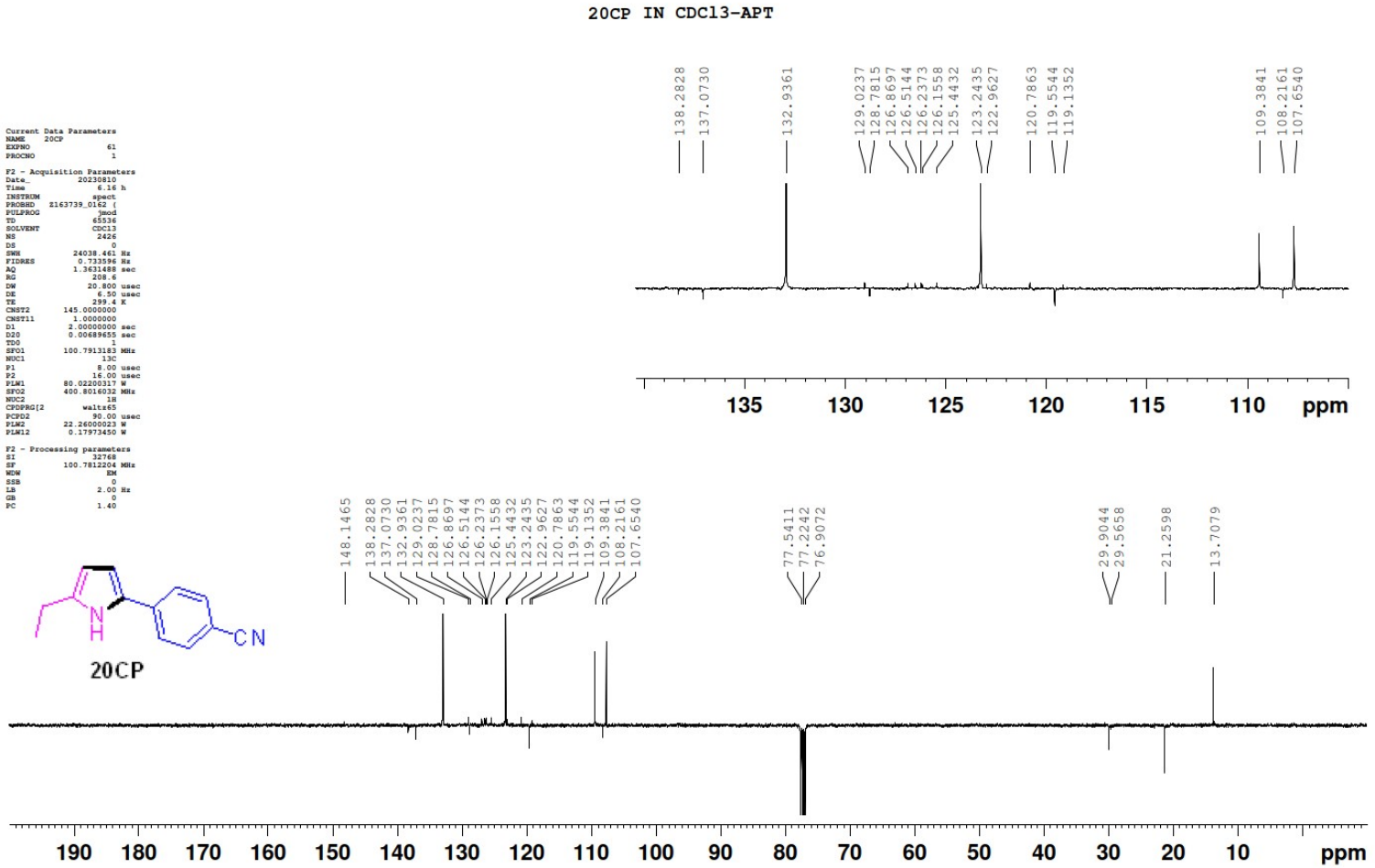


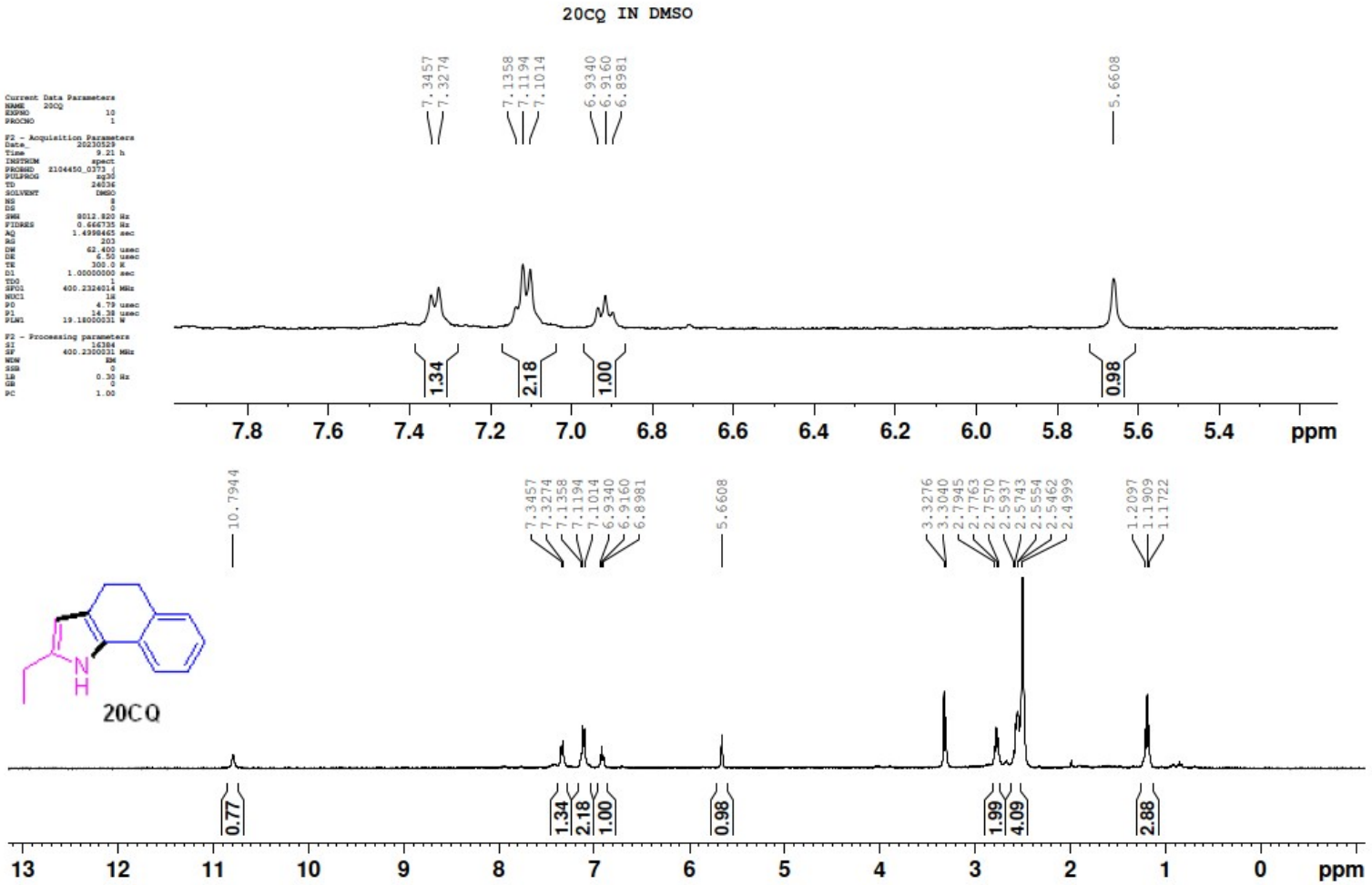


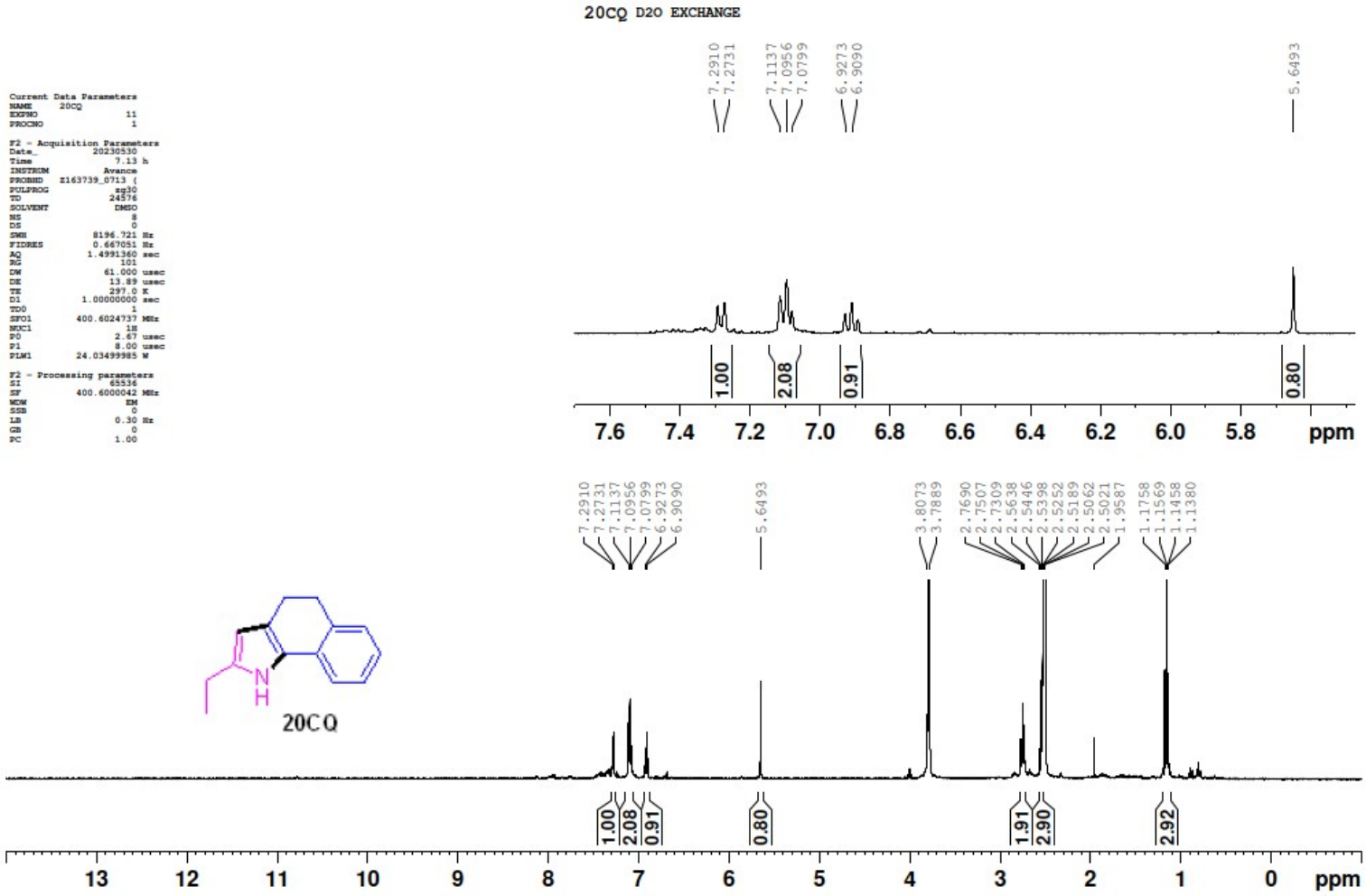
20CP IN CDCl3-13C

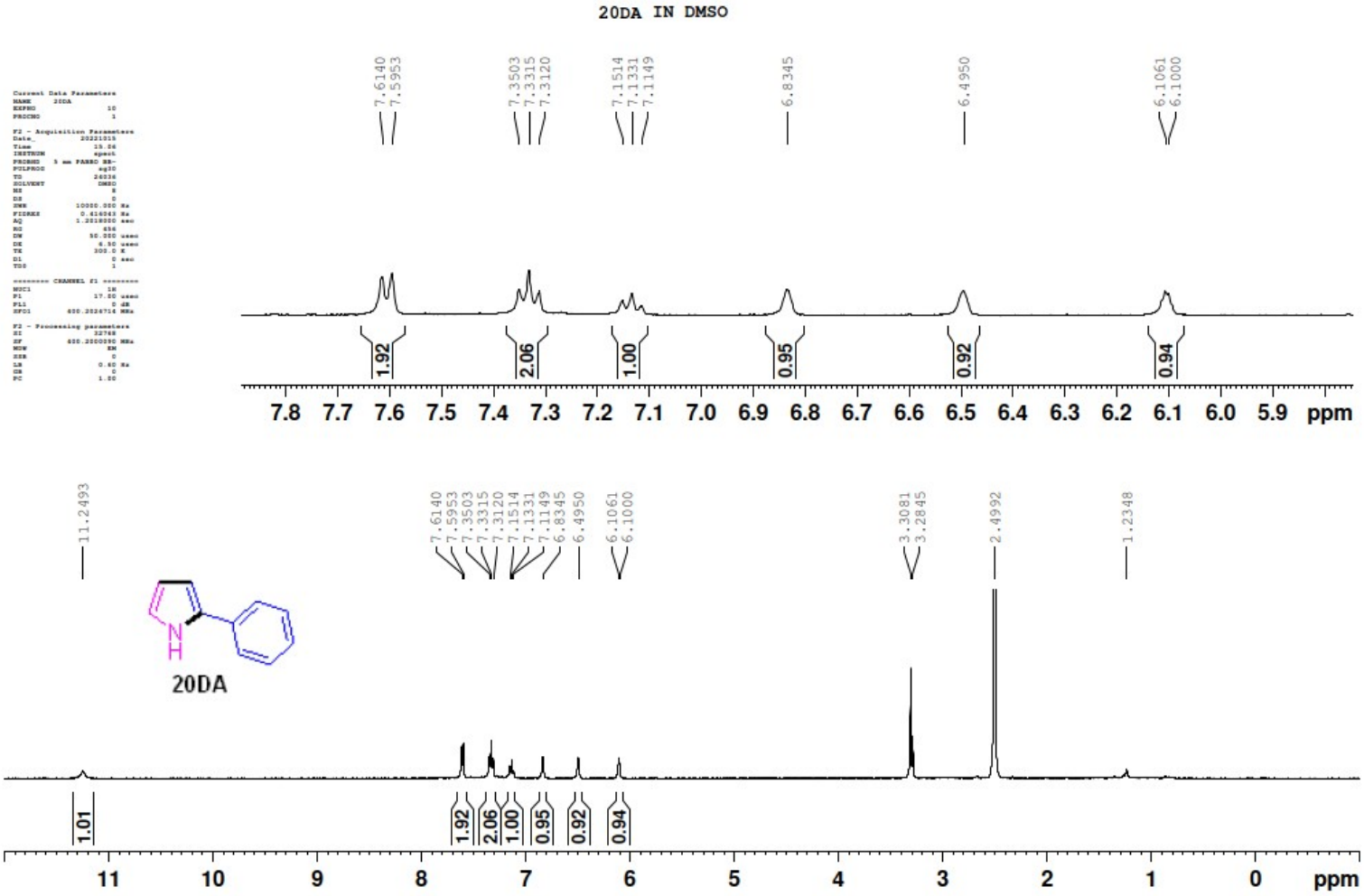


20CP IN CDCl3-APT

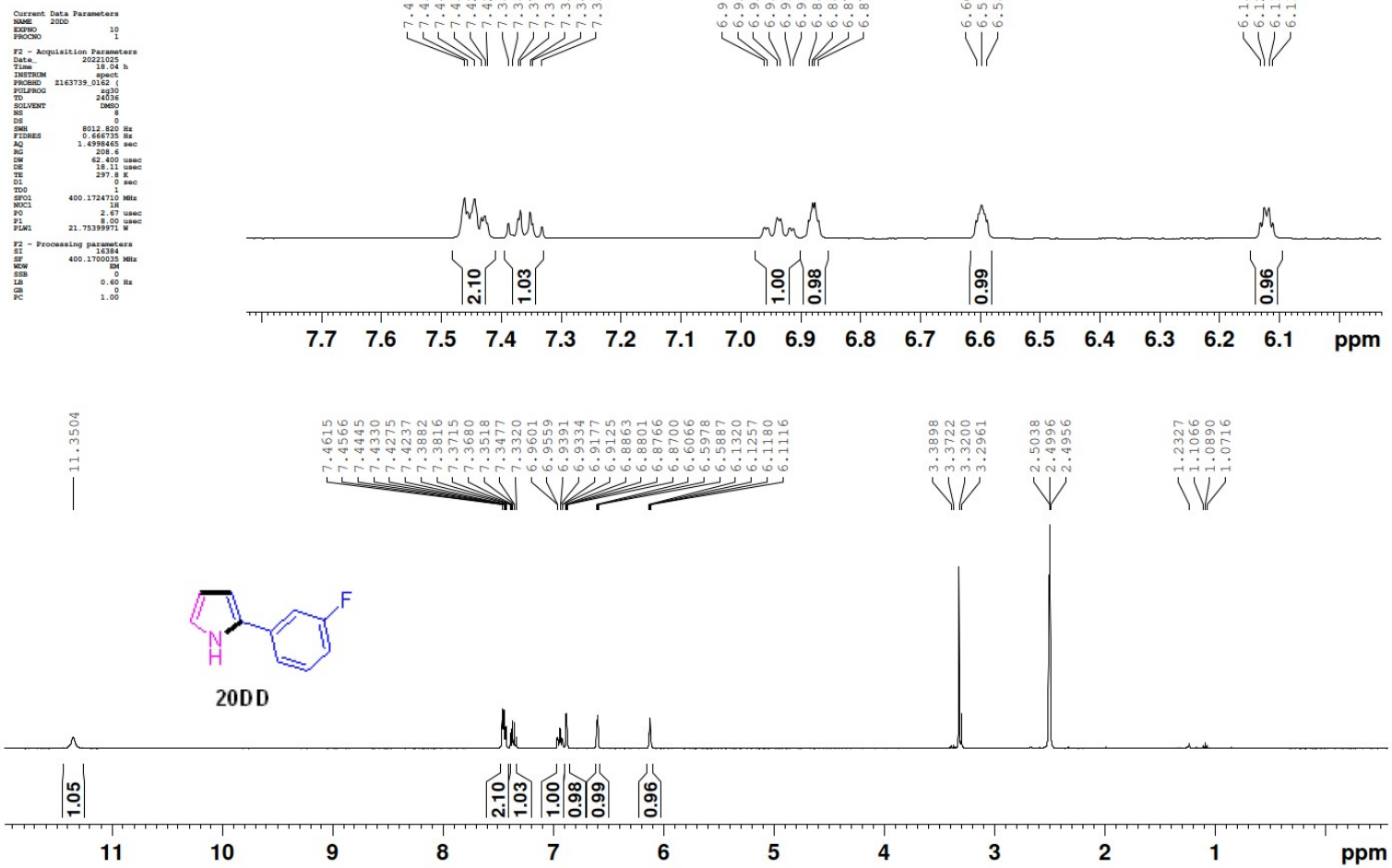



20CQ IN DMSO
Current Data Parameters
NAME 20CQ
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230529
Time 9.21 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4996465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3457
7.3274
7.1358
7.1194
7.1014
6.9340
6.9160
6.8981
5.6608
1.34
2.18
1.00
0.98
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
ppm
10.7944
7.3457
7.3274
7.1358
7.1194
7.1014
6.9340
6.9160
6.8981
5.6608
3.3276
3.3040
2.7945
2.7763
2.7570
2.5937
2.5743
2.5554
2.5462
2.4999
1.2097
1.1909
1.1722
N
H
20CQ
0.77
1.34
2.18
1.00
0.98
1.99
4.09
2.88
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

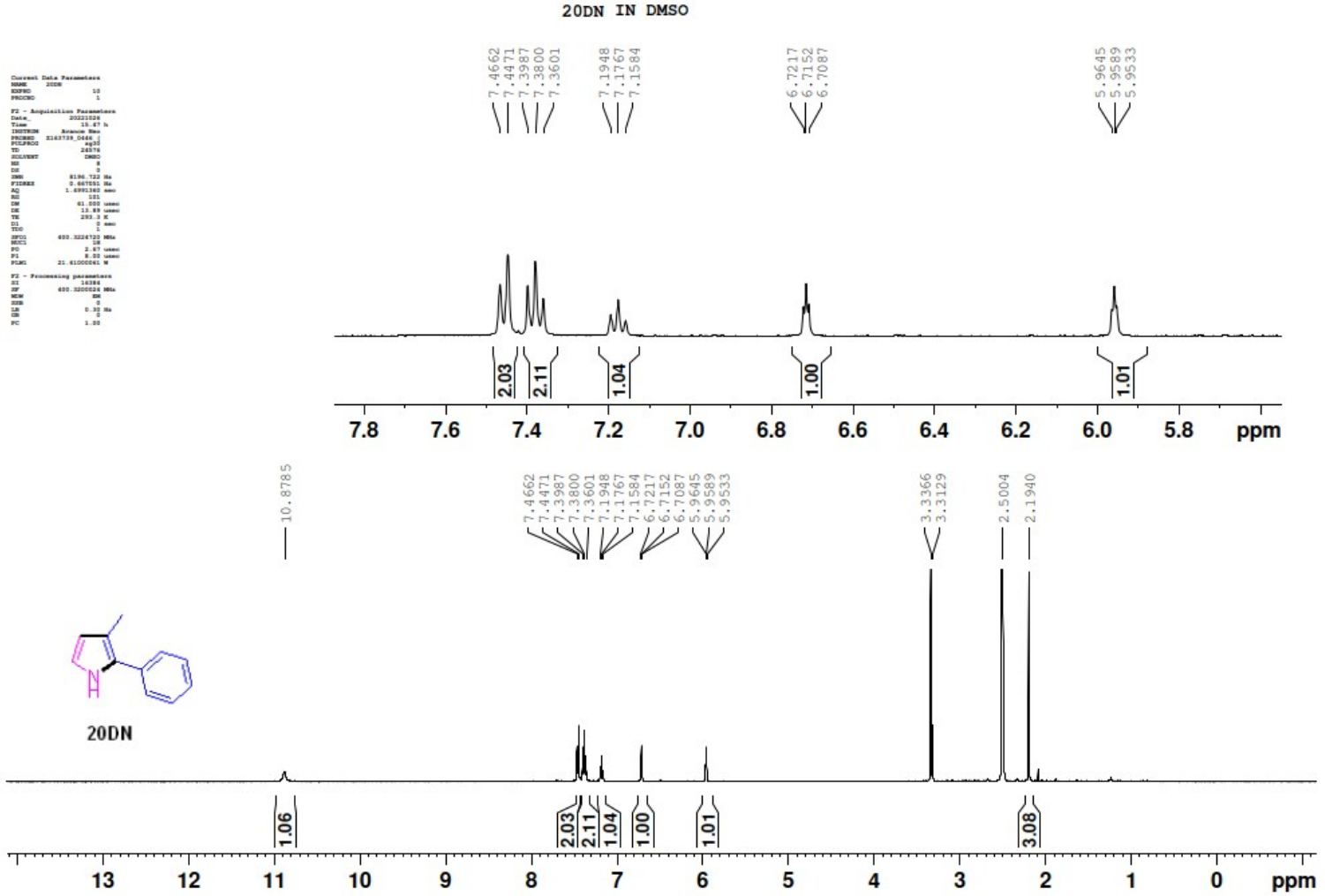

20CQ D2O EXCHANGE
Current Data Parameters
NAME 20CQ
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230530
Time 7.13 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.2910
7.2731
7.1137
7.0956
7.0799
6.9273
6.9090
5.6493
1.00
2.08
0.91
0.80
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
ppm
3.8073
3.7889
2.7690
2.7507
2.7309
2.5638
2.5446
2.5398
2.5252
2.5189
2.5062
2.5021
1.9587
1.1758
1.1569
1.1458
1.1380
1.91
2.90
2.92
20CQ
13
12
11
10
9
8
7
6
5
4
3
2
1
0


20DA IN DMSO
7.6140
7.5953
7.3503
7.3315
7.3120
7.1514
7.1331
7.1149
6.8345
6.4950
6.1061
6.1000
1.92
2.06
1.00
0.95
0.92
0.94
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 ppm
11.2493
3.3081
3.2845
2.4992
1.2348
1.01
11 10 9 8 7 6 5 4 3 2 1 0 ppm
20DA

20DD IN DMSO

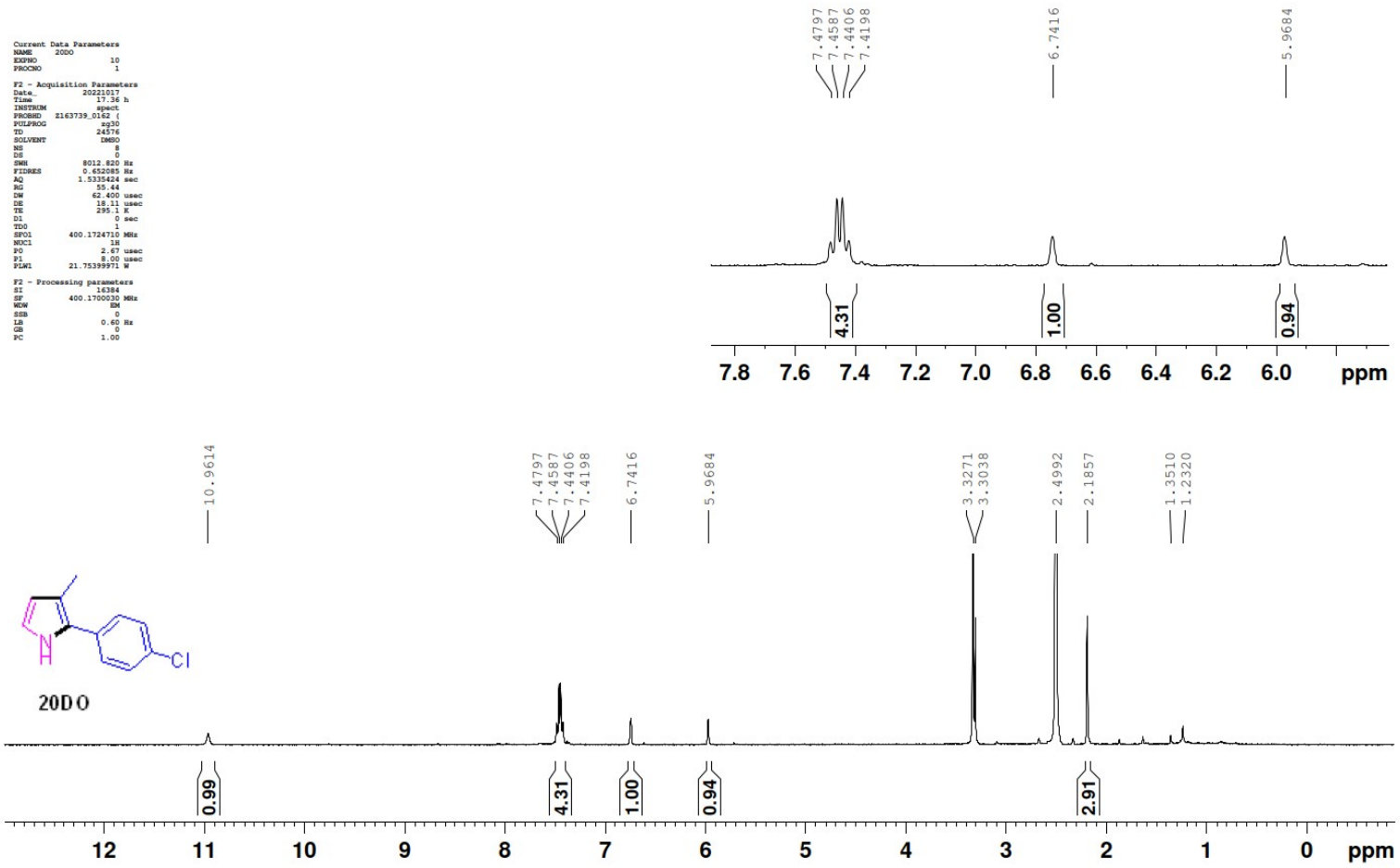

Current Data Parameters
NAME 20DD
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221025
Time 18.04 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 208.6
DW 62.400 usec
DE 18.11 usec
TE 297.8 K
D1 0 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.75399971 W
F2 - Processing parameters
SI 16384
SF 400.1700035 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
7.4615
7.4566
7.4445
7.4330
7.4275
7.4237
7.3882
7.3816
7.3715
7.3680
7.3518
7.3477
7.3320
6.9601
6.9559
6.9391
6.9334
6.9177
6.9125
6.8863
6.8801
6.8766
6.8700
6.6066
6.5978
6.5887
6.1320
6.1257
6.1180
6.1116
2.10
1.03
1.00
0.98
0.99
0.96
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 ppm
11.3504
7.4615
7.4566
7.4445
7.4330
7.4275
7.4237
7.3882
7.3816
7.3715
7.3680
7.3518
7.3477
7.3320
6.9601
6.9559
6.9391
6.9334
6.9177
6.9125
6.8863
6.8801
6.8766
6.8700
6.6066
6.5978
6.5887
6.1320
6.1257
6.1180
6.1116
3.3898
3.3722
3.3200
3.2961
2.5038
2.4996
2.4956
1.2327
1.1066
1.0890
1.0716
F
N
H
20DD
1.05
2.10
1.03
1.00
0.98
0.99
0.96
11 10 9 8 7 6 5 4 3 2 1 ppm

20DN IN DMSO

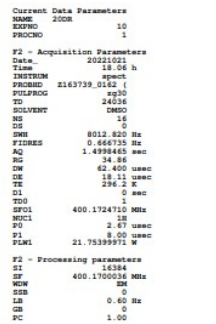


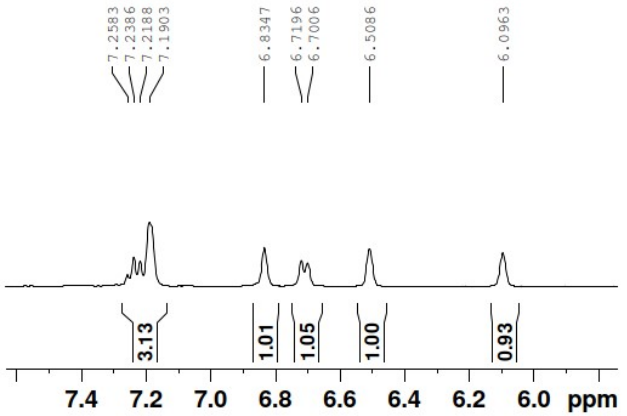
20DN

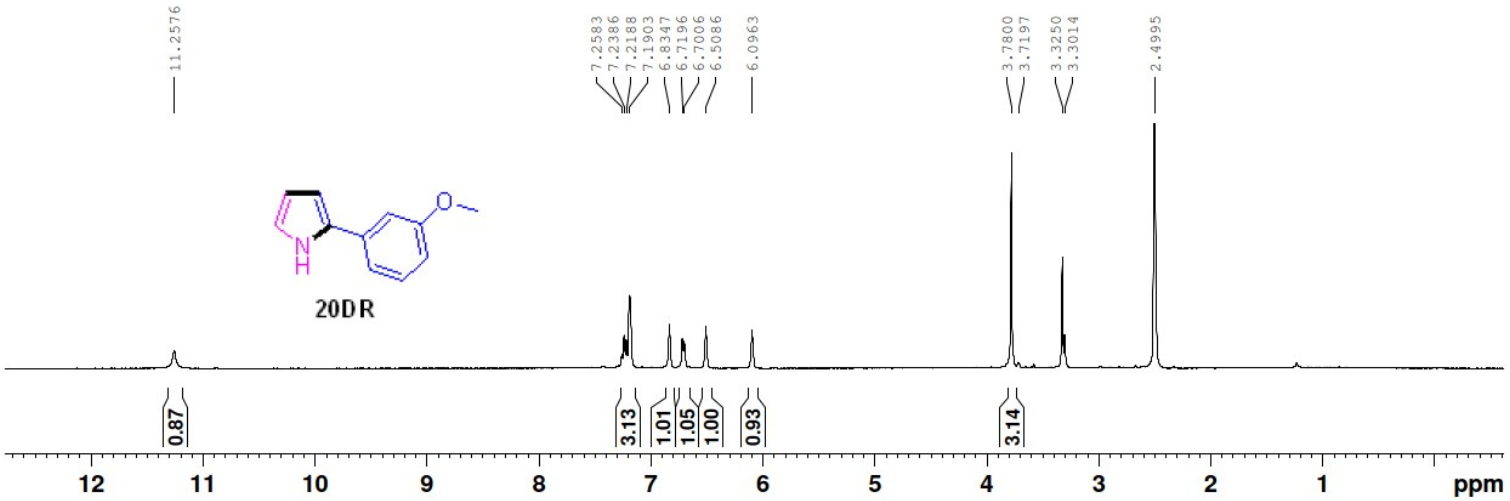
20DO IN DMSO


Current Data Parameters
NAME 20DO
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221017
Time 17.36 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24576
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.652085 Hz
AQ 1.5335424 sec
RG 55.44
DW 62.400 usec
DE 18.11 usec
TE 295.1 K
D1 0 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.75399971 W
F2 - Processing parameters
SI 16384
SF 400.1700030 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
7.4797
7.4587
7.4406
7.4198
6.7416
5.9684
4.31
1.00
0.94
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 ppm
10.9614
7.4797
7.4587
7.4406
7.4198
6.7416
5.9684
3.3271
3.3038
2.4992
2.1857
1.3510
1.2320
Cl
H
N
20DO
0.99
4.31
1.00
0.94
2.91
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

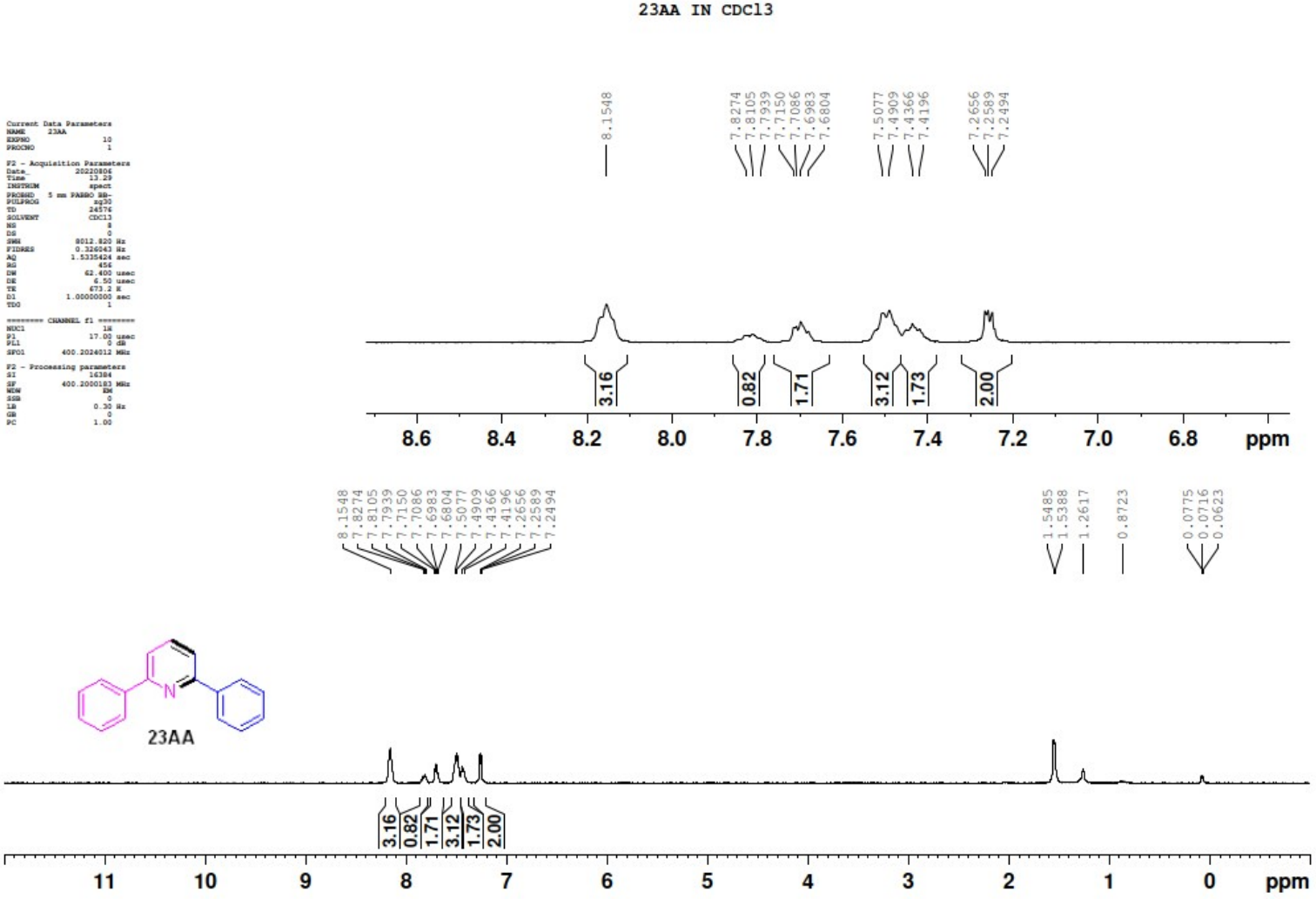
20DR IN DMSO


Current Data Parameters
NAME 20DR
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221021
Time 18.06 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 34.86
DW 62.400 usec
DE 18.11 usec
TE 296.2 K
D1 0 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 21.75399971 W
F2 - Processing parameters
SI 16384
SF 400.1700036 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

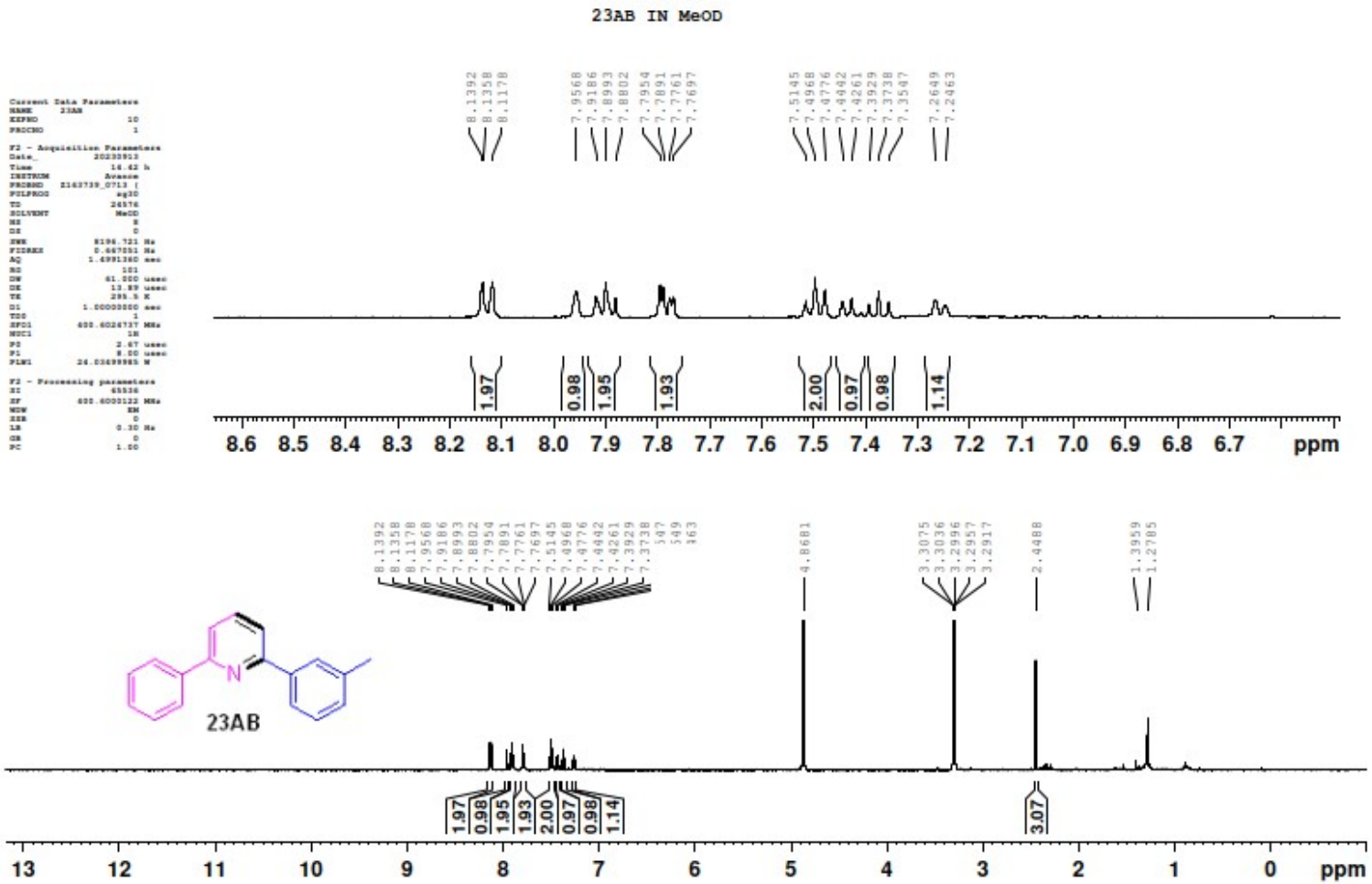

7.2583
7.2386
7.2188
7.1903
6.8347
6.7196
6.7006
6.5086
6.0963
3.13
1.01
1.05
1.00
0.93
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
ppm


11.2576
7.2583
7.2386
7.2188
7.1903
6.8347
6.7196
6.7006
6.5086
6.0963
3.7800
3.7197
3.3250
3.3014
2.4995
20DR
0.87
3.13
1.01
1.05
1.00
0.93
3.14
12
11
10
9
8
7
6
5
4
3
2
1
ppm

23AA IN CDCl3

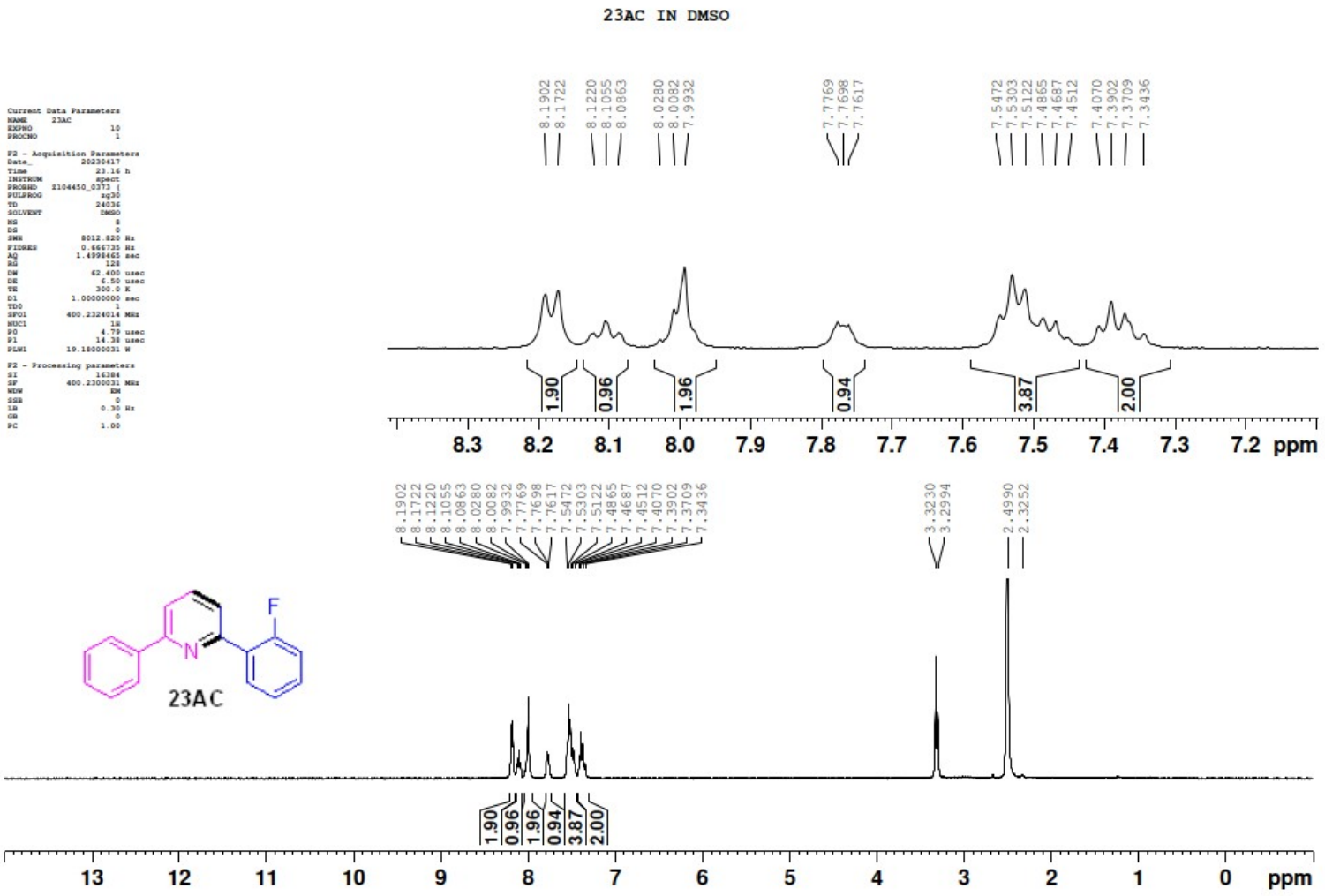


23AB IN MeOD



23AB

23AC IN DMSO

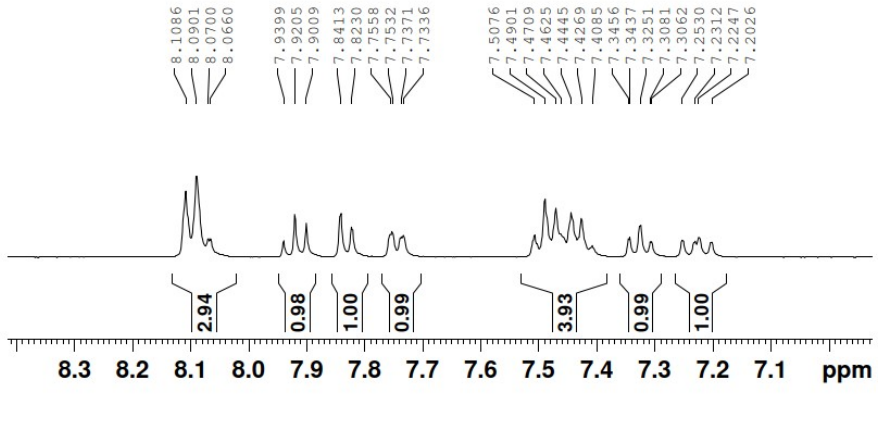

Current Data Parameters
NAME 23AC
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230417
Time 23.16 h
INSTRUM spect
PROBHD 2104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.1902
8.1722
8.1220
8.1055
8.0863
8.0280
8.0082
7.9932
7.7769
7.7698
7.7617
7.5472
7.5303
7.5122
7.4865
7.4687
7.4512
7.4070
7.3902
7.3709
7.3436
1.90
0.96
1.96
0.94
3.87
2.00
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
3.3230
3.2994
2.4990
2.3252
F
N
23AC
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

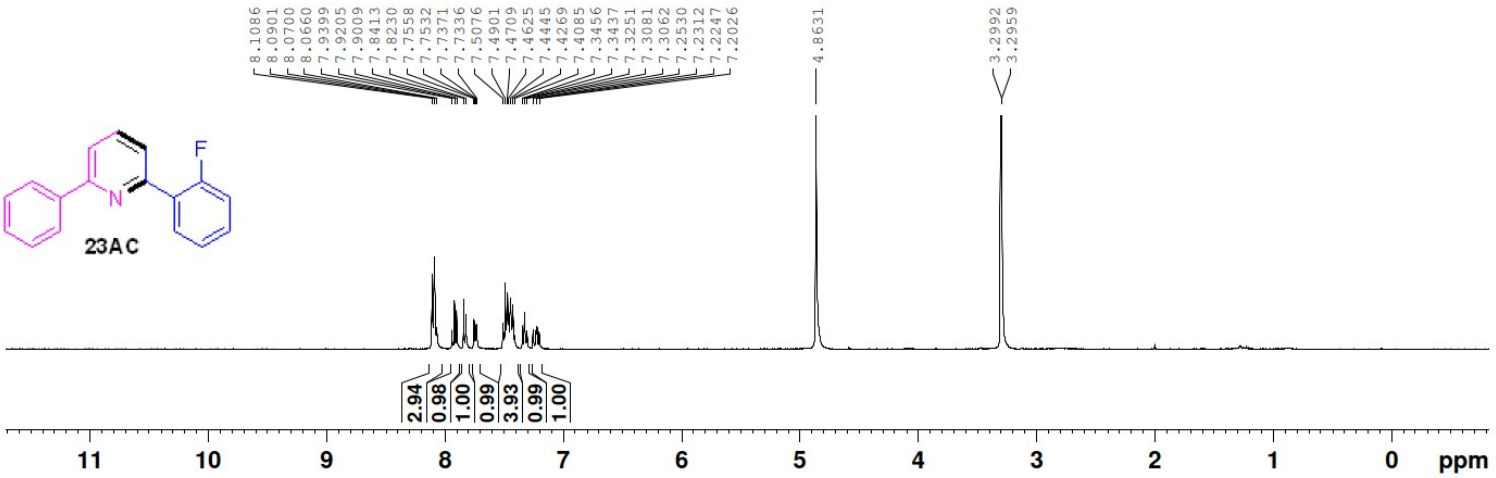
23AC IN MeOD

```
Current Data Parameters
NAME          23AC
EXPNO           10
PROCNO           1

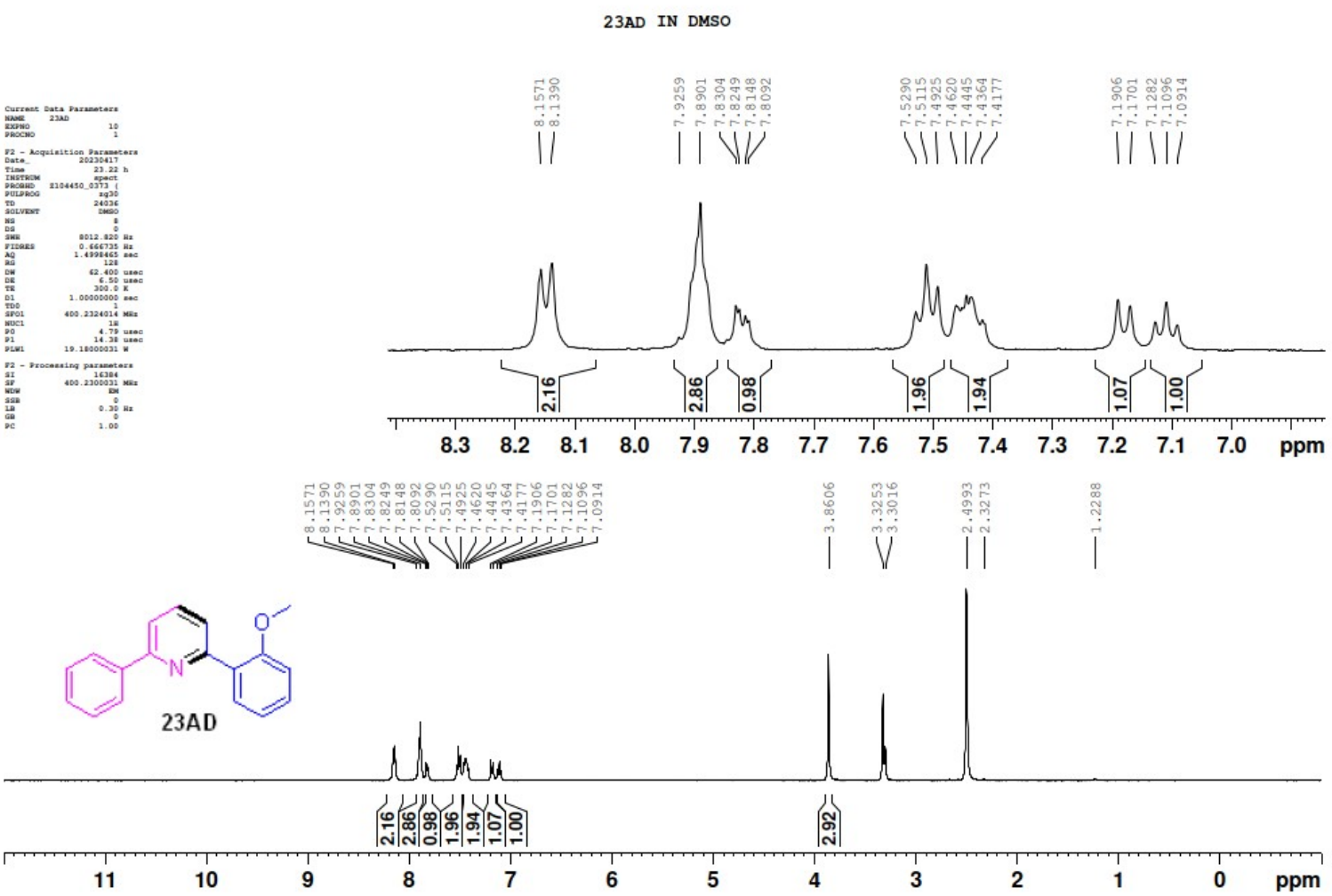
F2 - Acquisition Parameters
Date_        20230413
Time           16.21 h
INSTRUM      Avance Neo
PROBHD   Z163739_0446 (
PULPROG         zg30
TD             24576
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8196.722 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE            296.1 K
D1          1.00000000 sec
TD0                1
SFO1        400.3224019 MHz
NUC1               1H
P0             2.67 usec
P1             8.00 usec
PLW1       21.61000061 W

F2 - Processing parameters
SI             16384
SF          400.3200118 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```





23AD IN DMSO

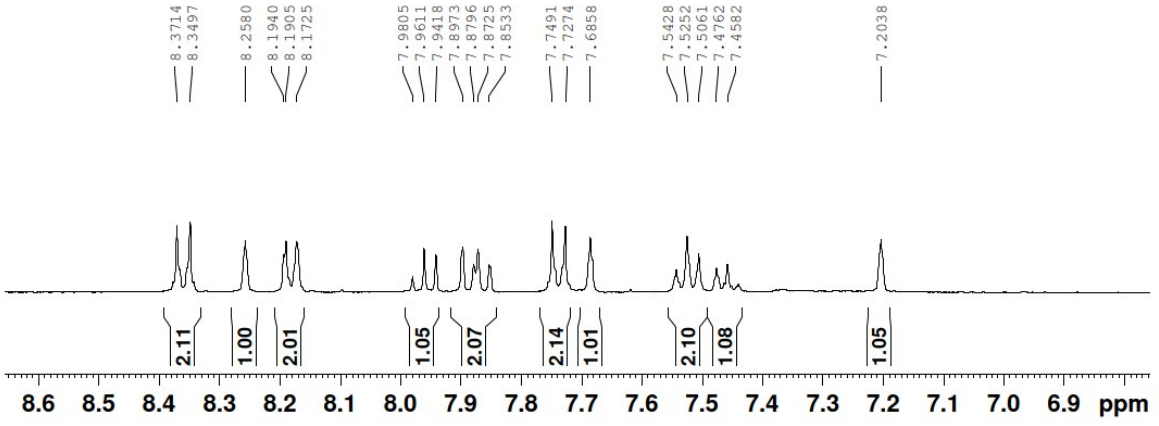

Current Data Parameters
NAME 23AD
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230417
Time 23.22 h
INSTRUM spect
PROBHD 2104450_0373 (
PULPROG zg30
TD 24036
SOLVENT DMSO
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.1571
8.1390
7.9259
7.8901
7.8304
7.8249
7.8148
7.8092
7.5290
7.5115
7.4925
7.4620
7.4445
7.4364
7.4177
7.1906
7.1701
7.1282
7.1096
7.0914
2.16
2.86
0.98
1.96
1.94
1.07
1.00
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
3.8606
3.3253
3.3016
2.4993
2.3273
1.2288
2.92
23AD
11 10 9 8 7 6 5 4 3 2 1 0 ppm

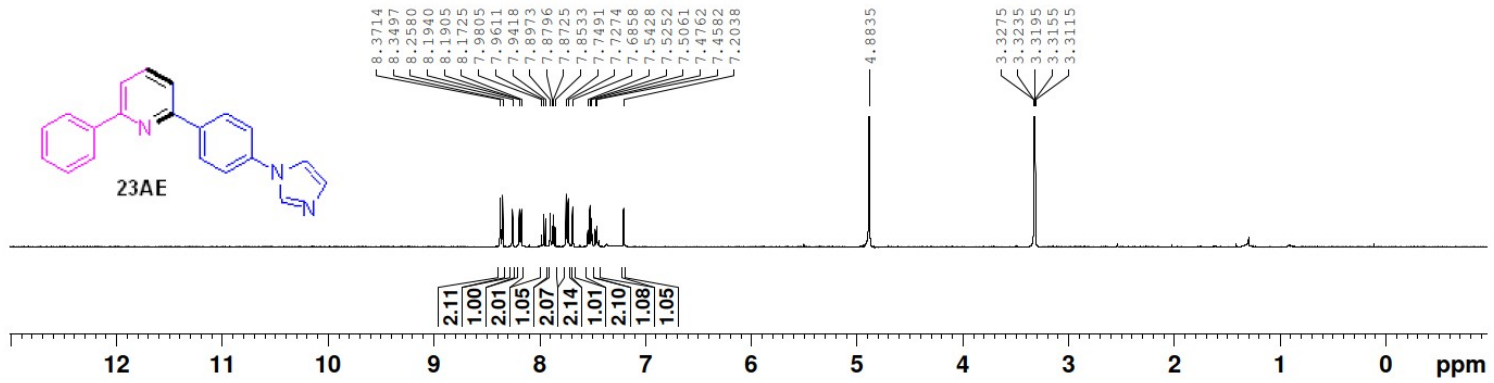
23AE IN MeOD

```
Current Data Parameters
NAME      23AE
EXPNO           10
PROCNO           1

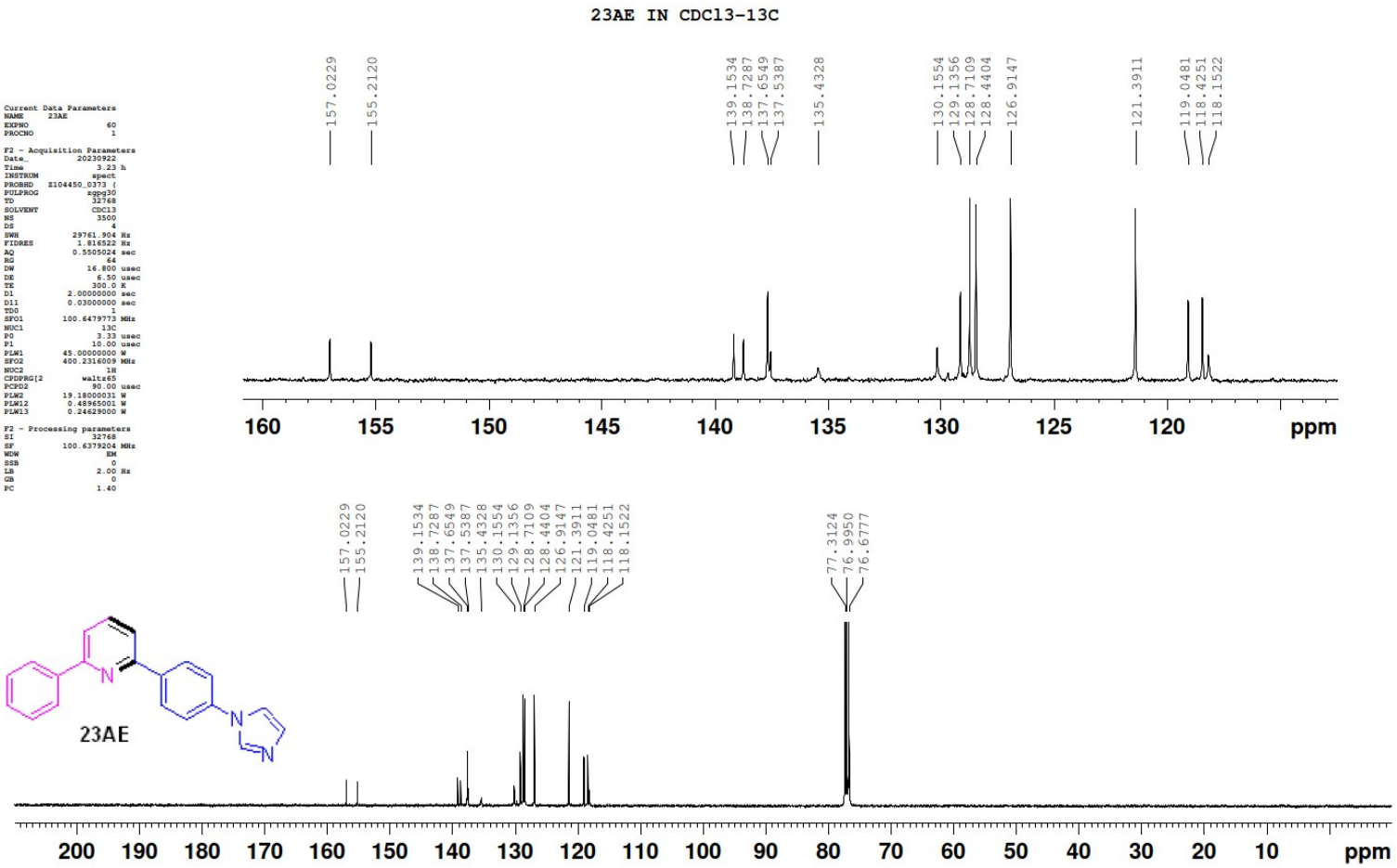
F2 - Acquisition Parameters
Date_      20230918
Time           6.51 h
INSTRUM      Avance
PROBHD   Z163739_0713 (
PULPROG         zg30
TD             24576
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8196.721 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE            296.2 K
D1          1.00000000 sec
TD0                1
SFO1        400.6024737 MHz
NUC1               1H
P0             2.67 usec
P1             8.00 usec
PLW1       24.03499985 W

F2 - Processing parameters
SI             65536
SF        400.6000042 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

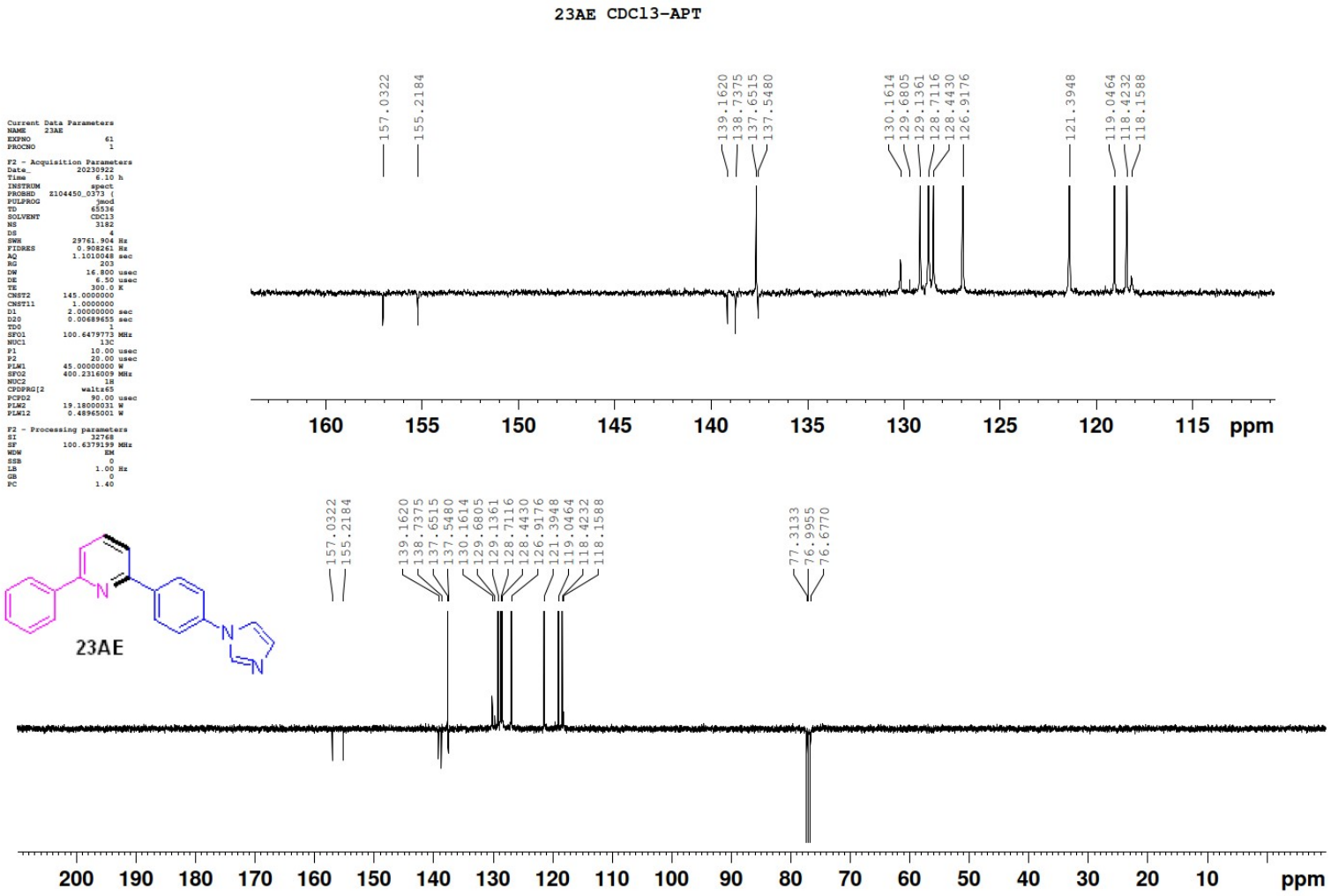




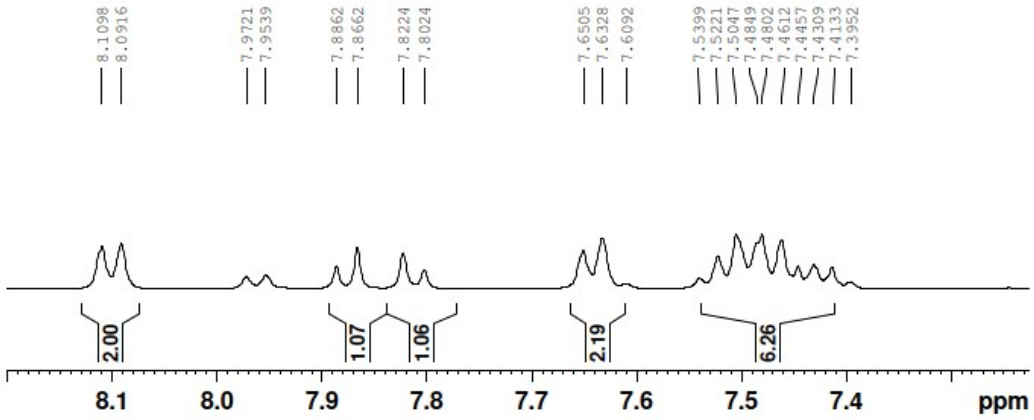
23AE IN CDCl3-13C

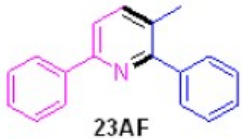


23AE CDCl3-APT



23AF IN DMSO





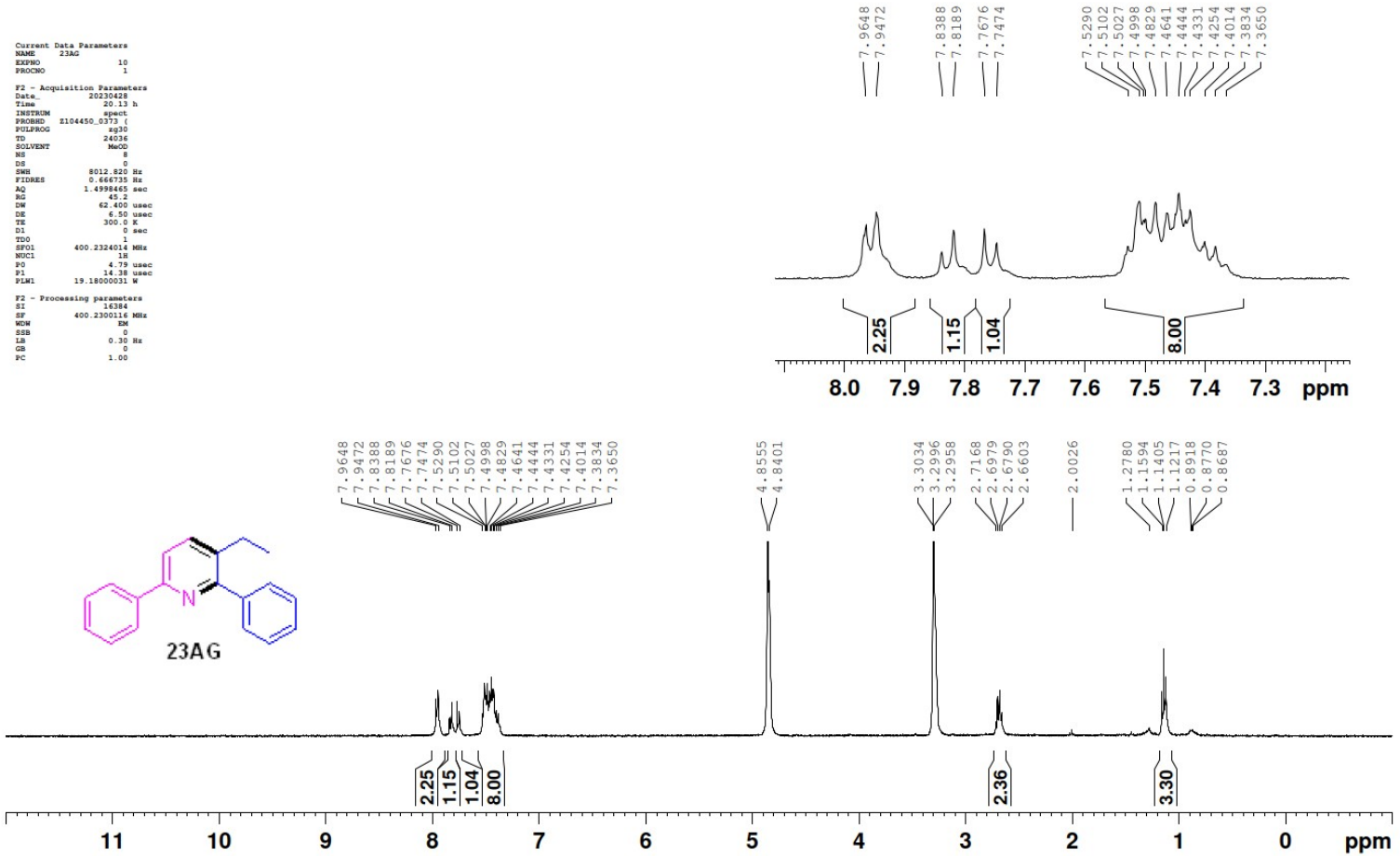
23AF

23AG IN MeOD

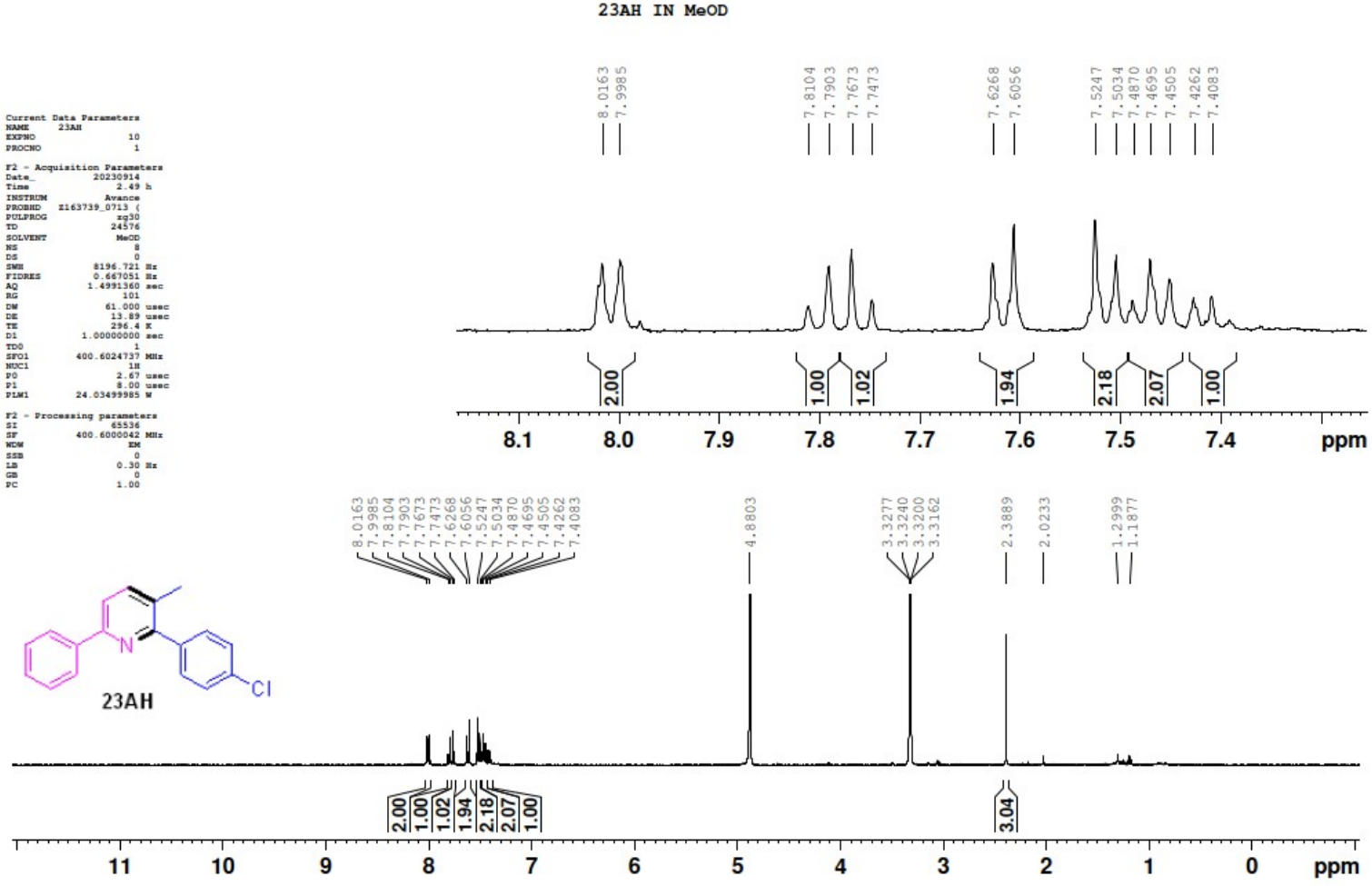
```
Current Data Parameters
NAME      23AG
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20230428
Time            20.13 h
INSTRUM          spect
PROBHD   Z104450_0373 (
PULPROG          zg30
TD              24036
SOLVENT          MeOD
NS                8
DS                0
SWH          8012.820 Hz
FIDRES       0.666735 Hz
AQ           1.4998465 sec
RG               45.2
DW              62.400 usec
DE               6.50 usec
TE              300.0 K
D1                0 sec
TD0               1
SFO1     400.2324014 MHz
NUC1             1H
P0               4.79 usec
P1              14.38 usec
PLW1    19.18000031 W

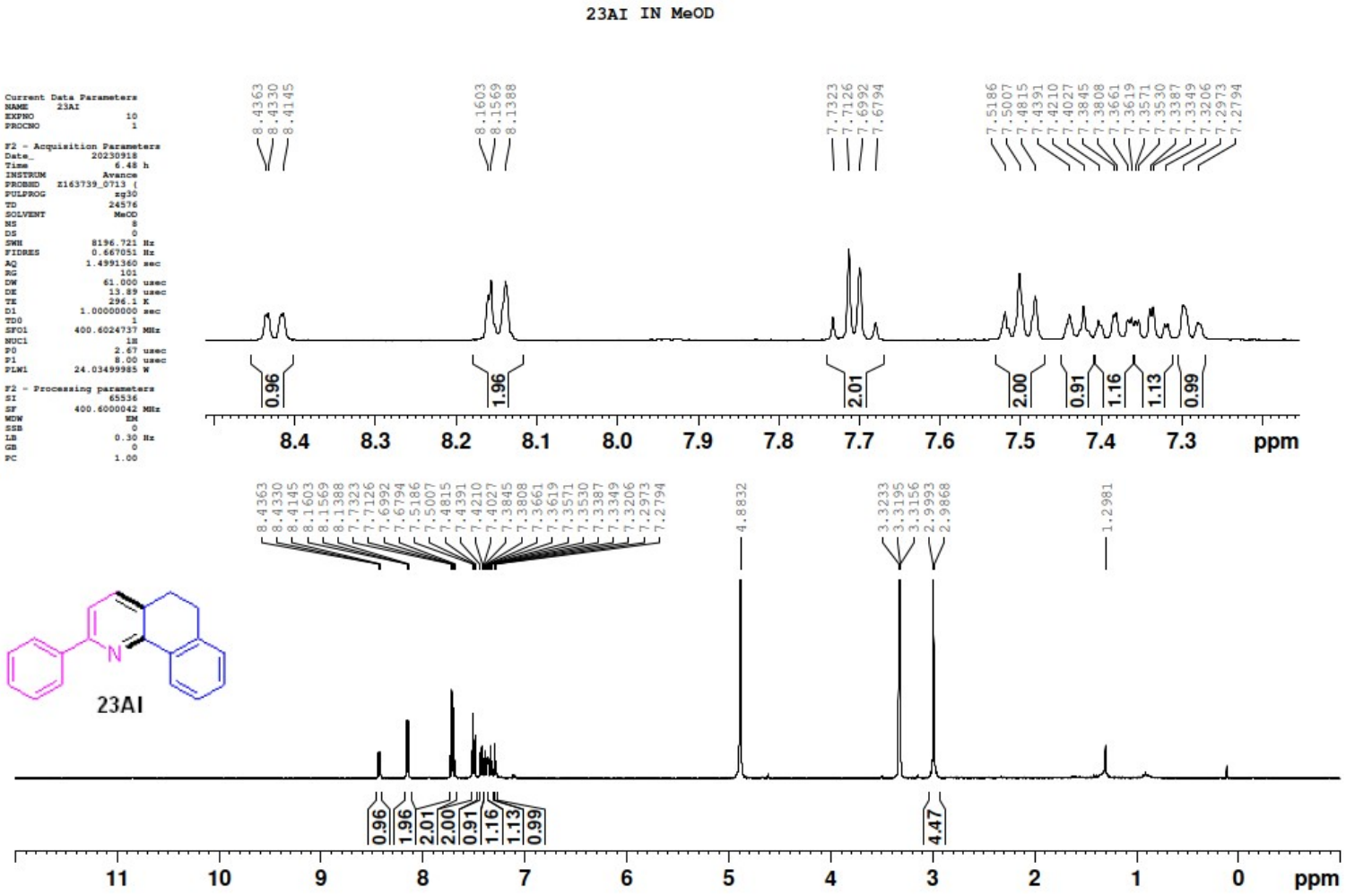
F2 - Processing parameters
SI               16384
SF       400.2300116 MHz
WDW              EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```

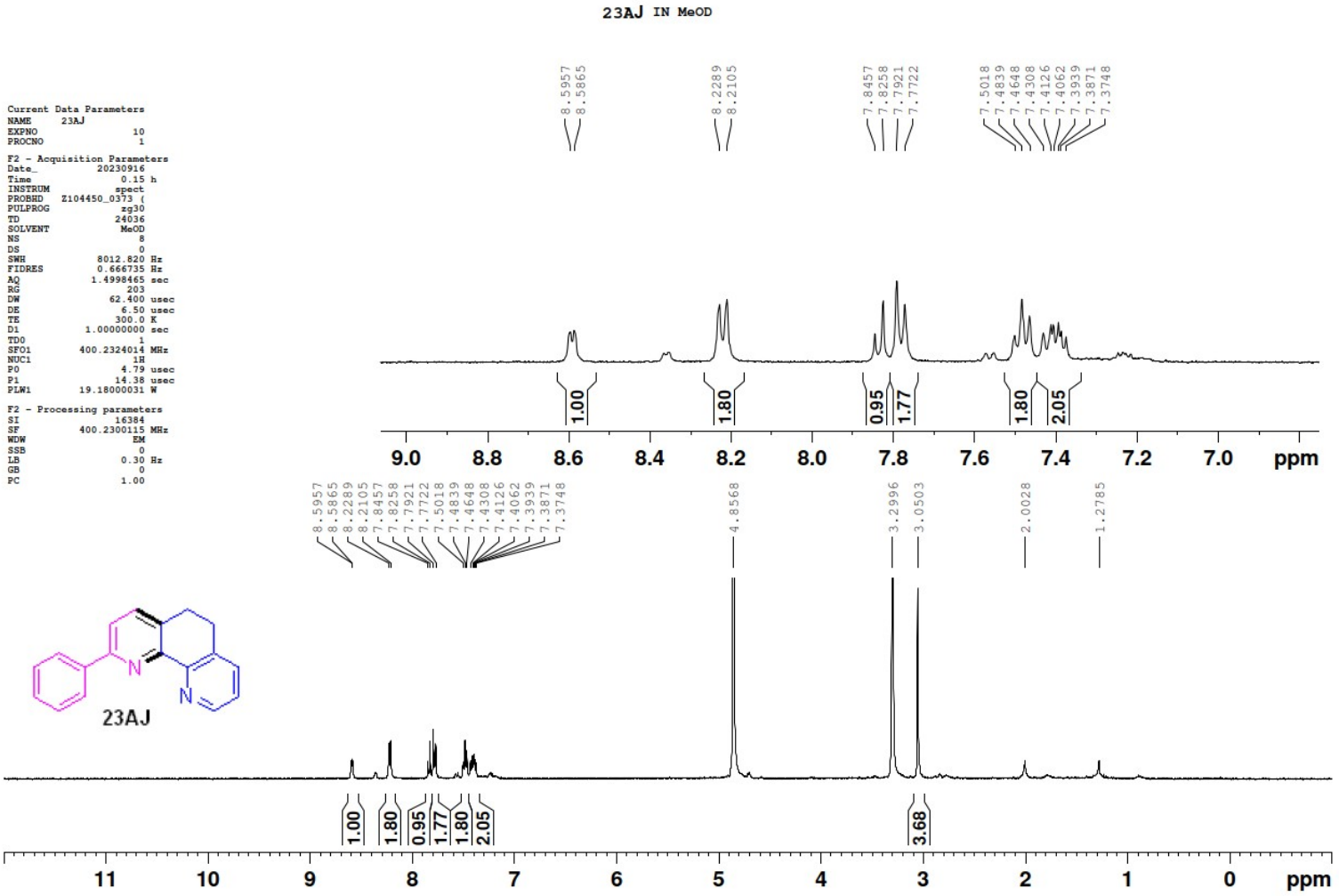


23AH IN MeOD


Current Data Parameters
NAME 23AH
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230914
Time 2.49 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0163
7.9985
7.8104
7.7903
7.7673
7.7473
7.6268
7.6056
7.5247
7.5034
7.4870
7.4695
7.4505
7.4262
7.4083
2.00
1.00
1.02
1.94
2.18
2.07
1.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
4.8803
3.3277
3.3240
3.3200
3.3162
2.3889
2.0233
1.2999
1.1877
3.04
N
Cl
23AH
11
10
9
8
7
6
5
4
3
2
1
0
ppm

23AI IN MeOD


Current Data Parameters
NAME 23AI
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230918
Time 6.48 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.4363
8.4330
8.4145
8.1603
8.1569
8.1388
7.7323
7.7126
7.6992
7.6794
7.5186
7.5007
7.4815
7.4391
7.4210
7.4027
7.3845
7.3808
7.3661
7.3619
7.3571
7.3530
7.3387
7.3349
7.3206
7.2973
7.2794
0.96
1.96
2.01
2.00
0.91
1.16
1.13
0.99
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 ppm
4.8832
3.3233
3.3195
3.3156
2.9993
2.9868
1.2981
4.47
11 10 9 8 7 6 5 4 3 2 1 0 ppm
N
23AI

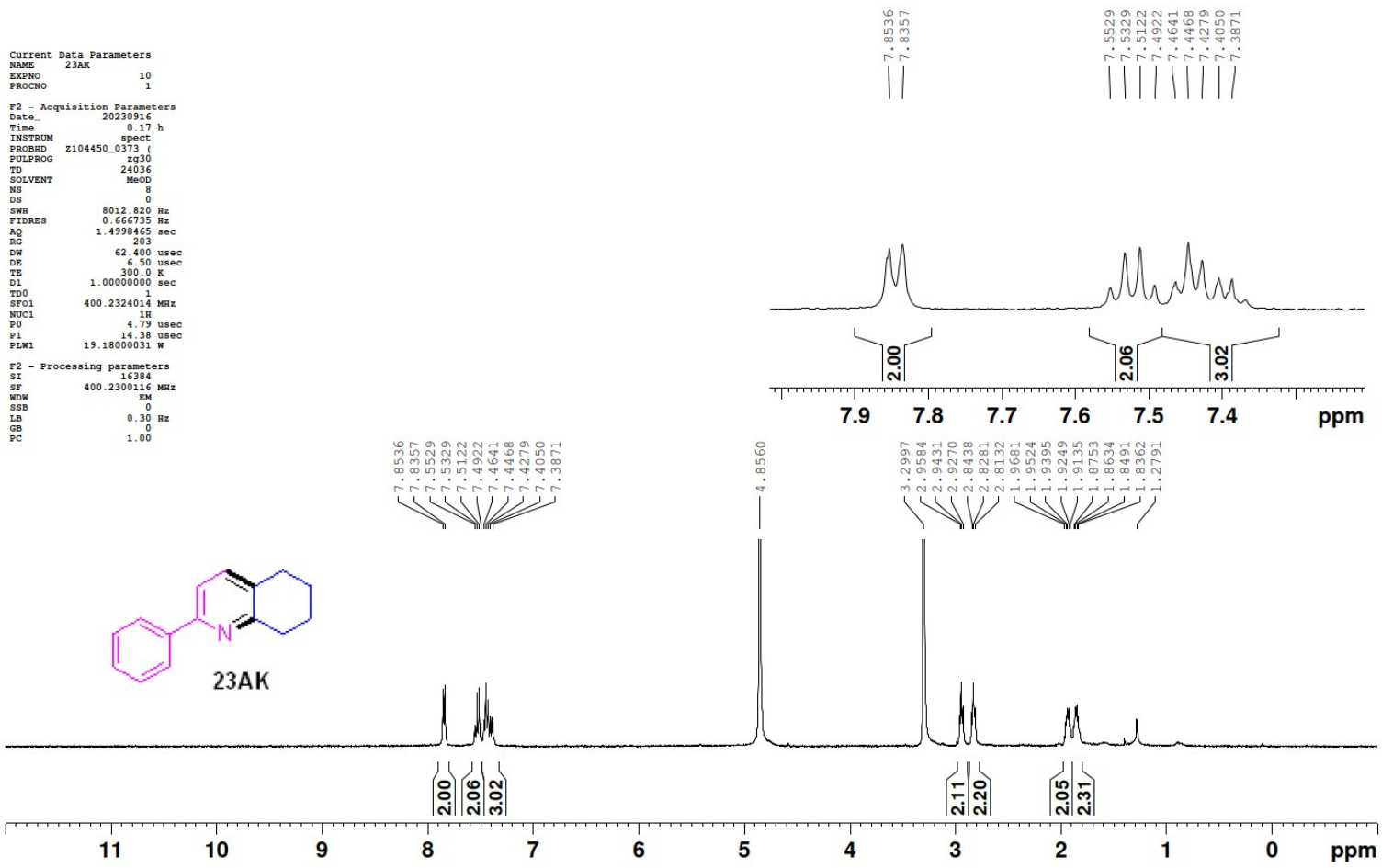

23AJ IN MeOD
Current Data Parameters
NAME 23AJ
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230916
Time 0.15 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5957
8.5865
8.2289
8.2105
7.8457
7.8258
7.7921
7.7722
7.5018
7.4839
7.4648
7.4308
7.4126
7.4062
7.3939
7.3871
7.3748
1.00
1.80
0.95
1.77
1.80
2.05
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm
4.8568
3.2996
3.0503
2.0028
1.2785
3.68
11
10
9
8
7
6
5
4
3
2
1
0
N
N
23AJ

23AK IN MeOD

```
Current Data Parameters
NAME      23AK
EXPNO               10
PROCNO               1

F2 - Acquisition Parameters
Date_         20230916
Time              0.17 h
INSTRUM          spect
PROBHD    Z104450_0373 (
PULPROG           zg30
TD               24036
SOLVENT           MeOD
NS                   8
DS                   0
SWH           8012.820 Hz
FIDRES        0.666735 Hz
AQ            1.4998465 sec
RG                 203
DW               62.400 usec
DE                6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                  1
SFO1         400.2324014 MHz
NUC1                1H
P0                4.79 usec
P1               14.38 usec
PLW1         19.18000031 W

F2 - Processing parameters
SI                16384
SF           400.2300116 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

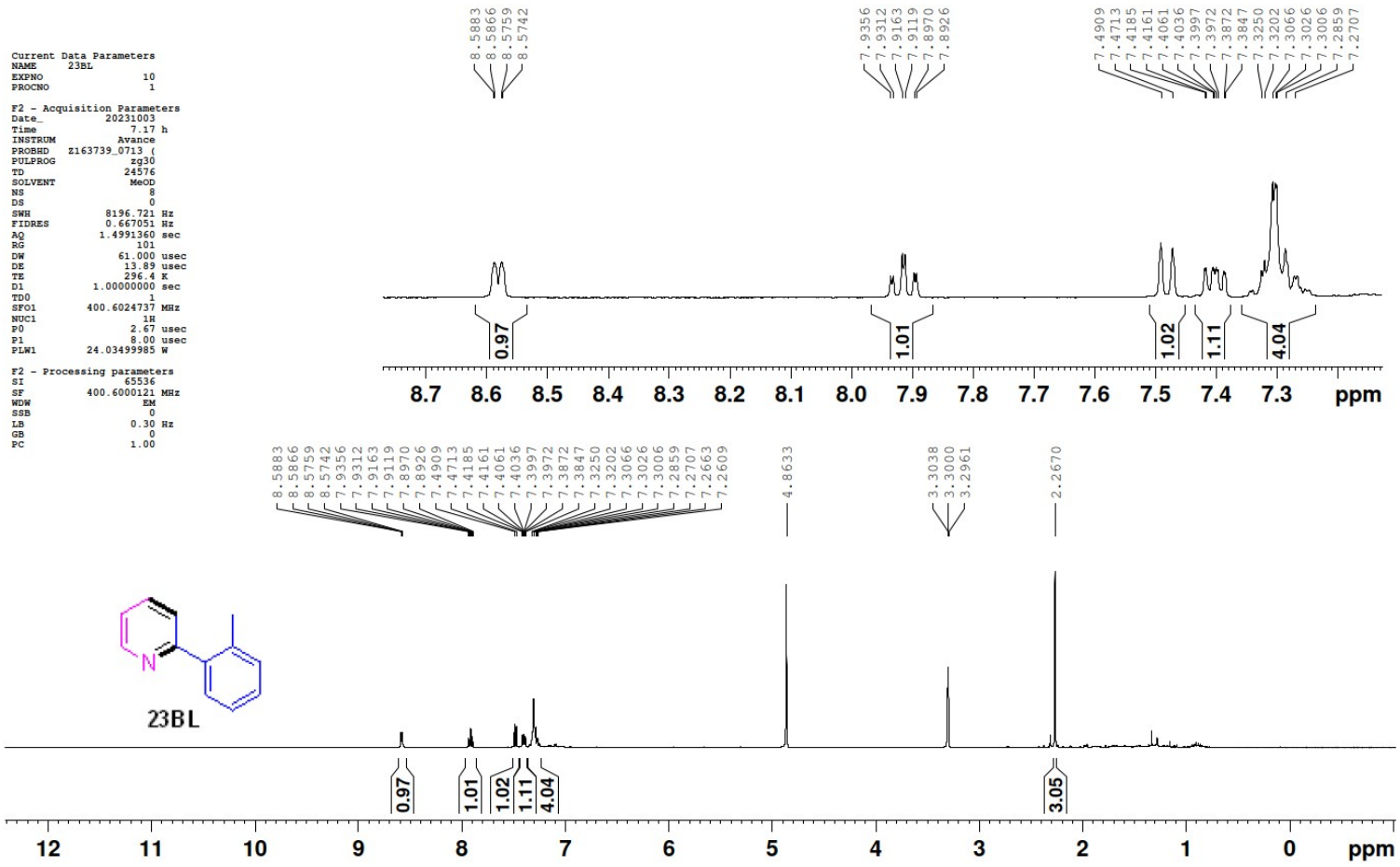


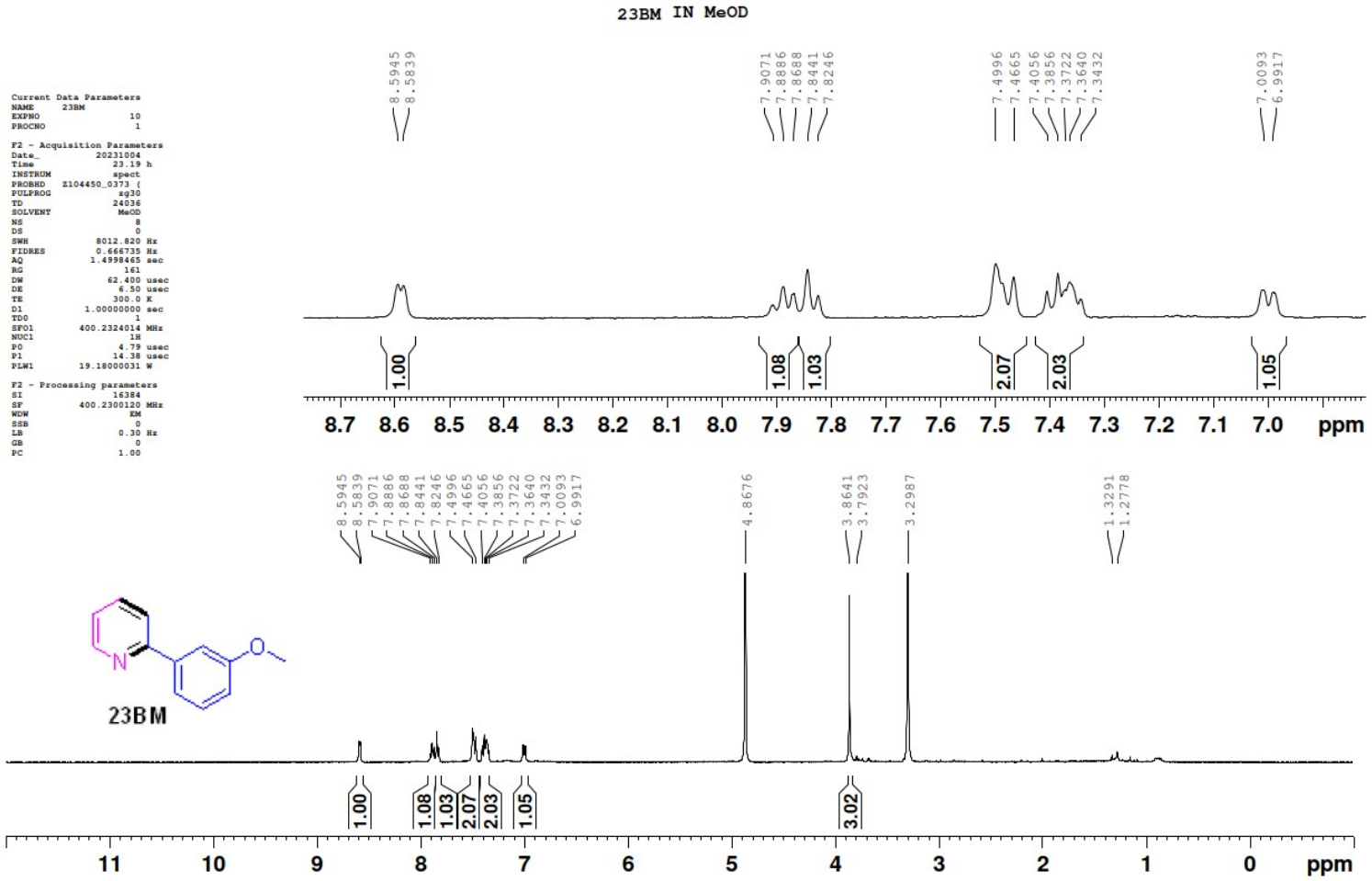
23BL IN MeOD

```
Current Data Parameters
NAME      23BL
EXPNO           10
PROCNO           1

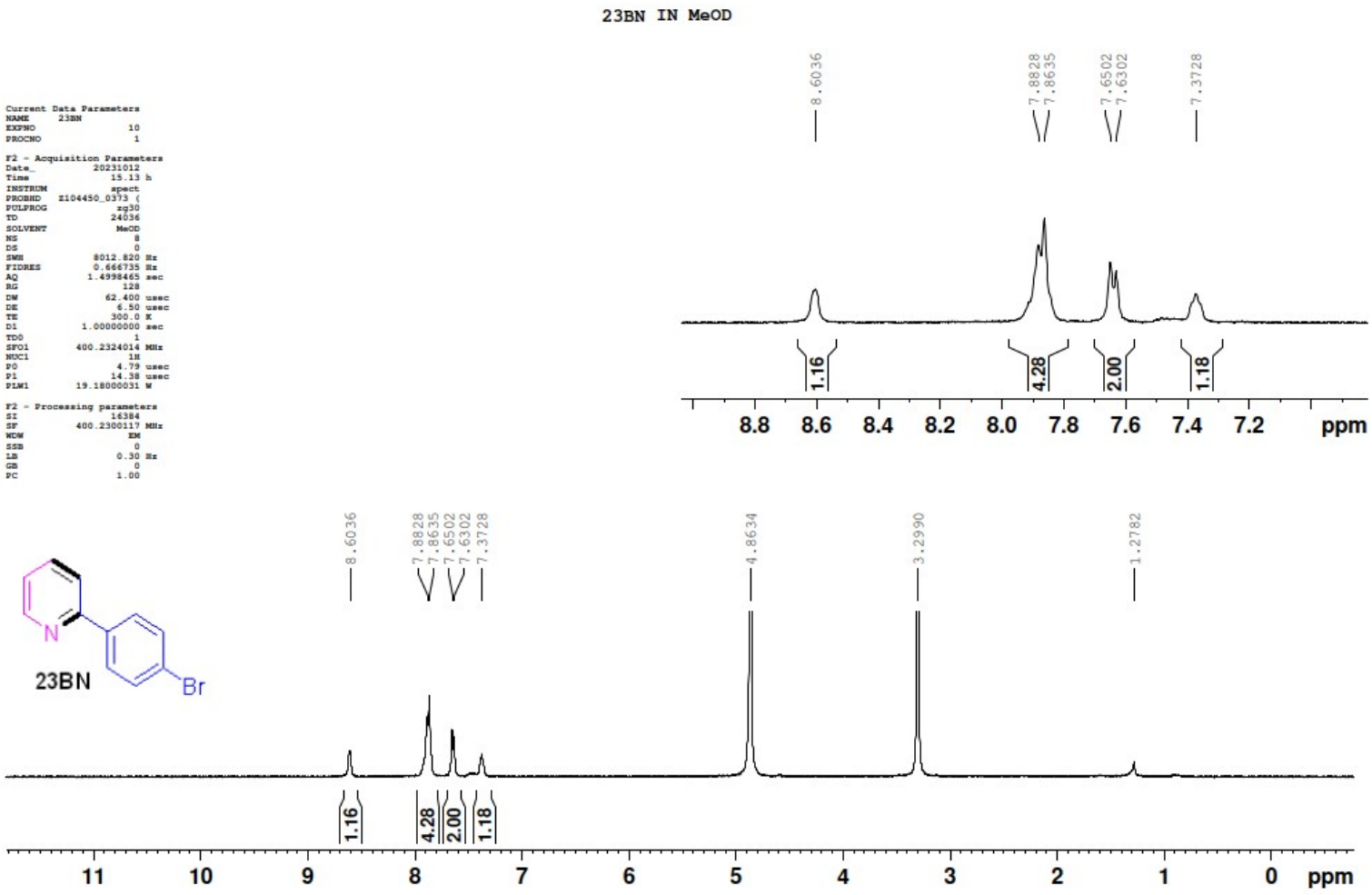
F2 - Acquisition Parameters
Date_      20231003
Time           7.17 h
INSTRUM       Avance
PROBHD   Z163739_0713 (
PULPROG         zg30
TD             24576
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8196.721 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE            296.4 K
D1          1.00000000 sec
TD0                1
SFO1        400.6024737 MHz
NUC1               1H
P0             2.67 usec
P1             8.00 usec
PLW1       24.03499985 W

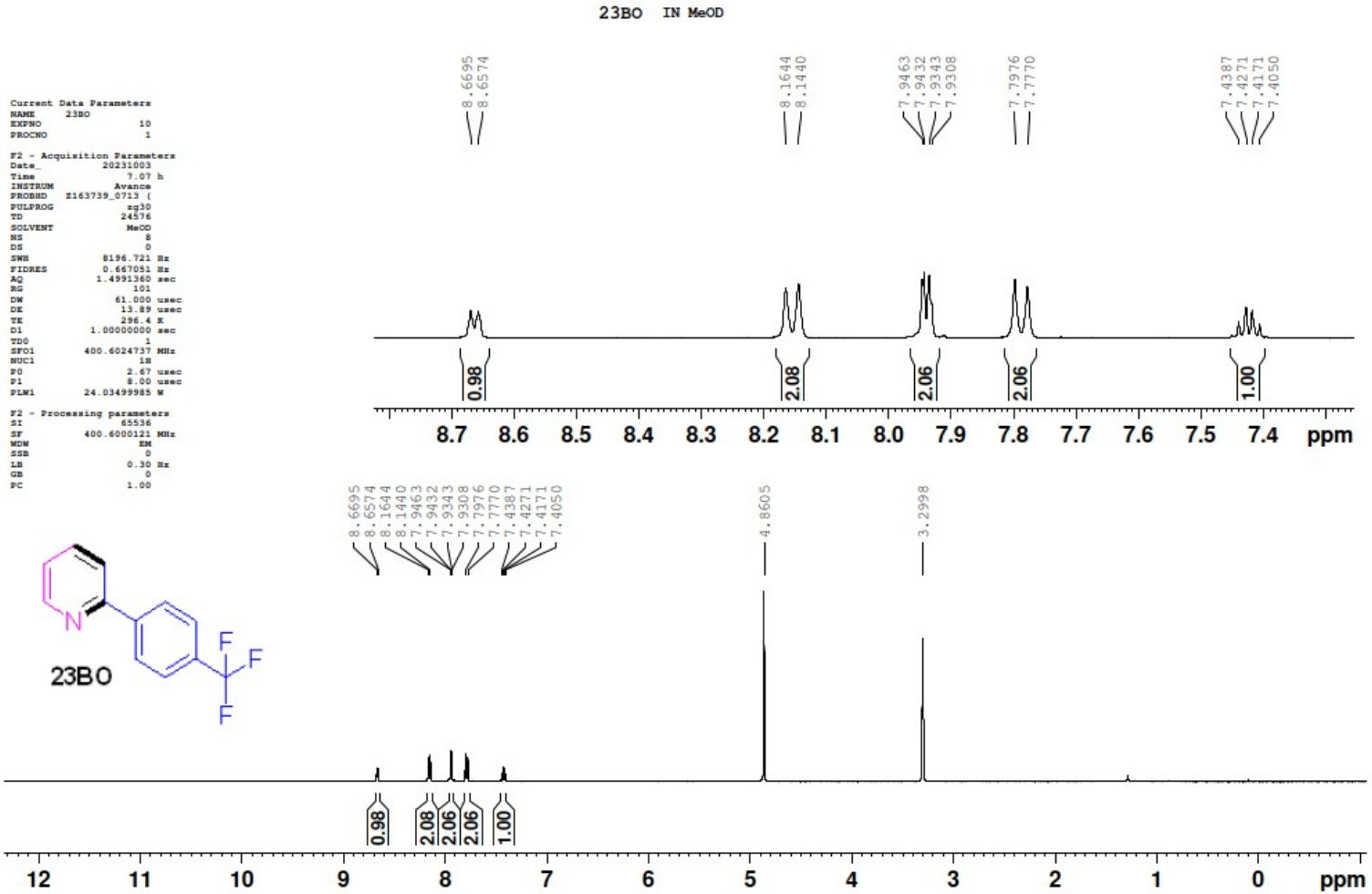
F2 - Processing parameters
SI             65536
SF        400.6000121 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```




23BM IN MeOD
Current Data Parameters
NAME 23BM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231004
Time 23.19 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5945
8.5839
7.9071
7.8886
7.8688
7.8441
7.8246
7.4996
7.4665
7.4056
7.3856
7.3722
7.3640
7.3432
7.0093
6.9917
1.00
1.08
1.03
2.07
2.03
1.05
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
4.8676
3.8641
3.7923
3.2987
1.3291
1.2778
3.02
11 10 9 8 7 6 5 4 3 2 1 0 ppm
23BM

23BN IN MeOD


Current Data Parameters
NAME 23BN
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231012
Time 15.13 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.6036
7.8828
7.8635
7.6502
7.6302
7.3728
1.16
4.28
2.00
1.18
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 ppm
N
Br
23BN
4.8634
3.2990
1.2782
11 10 9 8 7 6 5 4 3 2 1 0 ppm

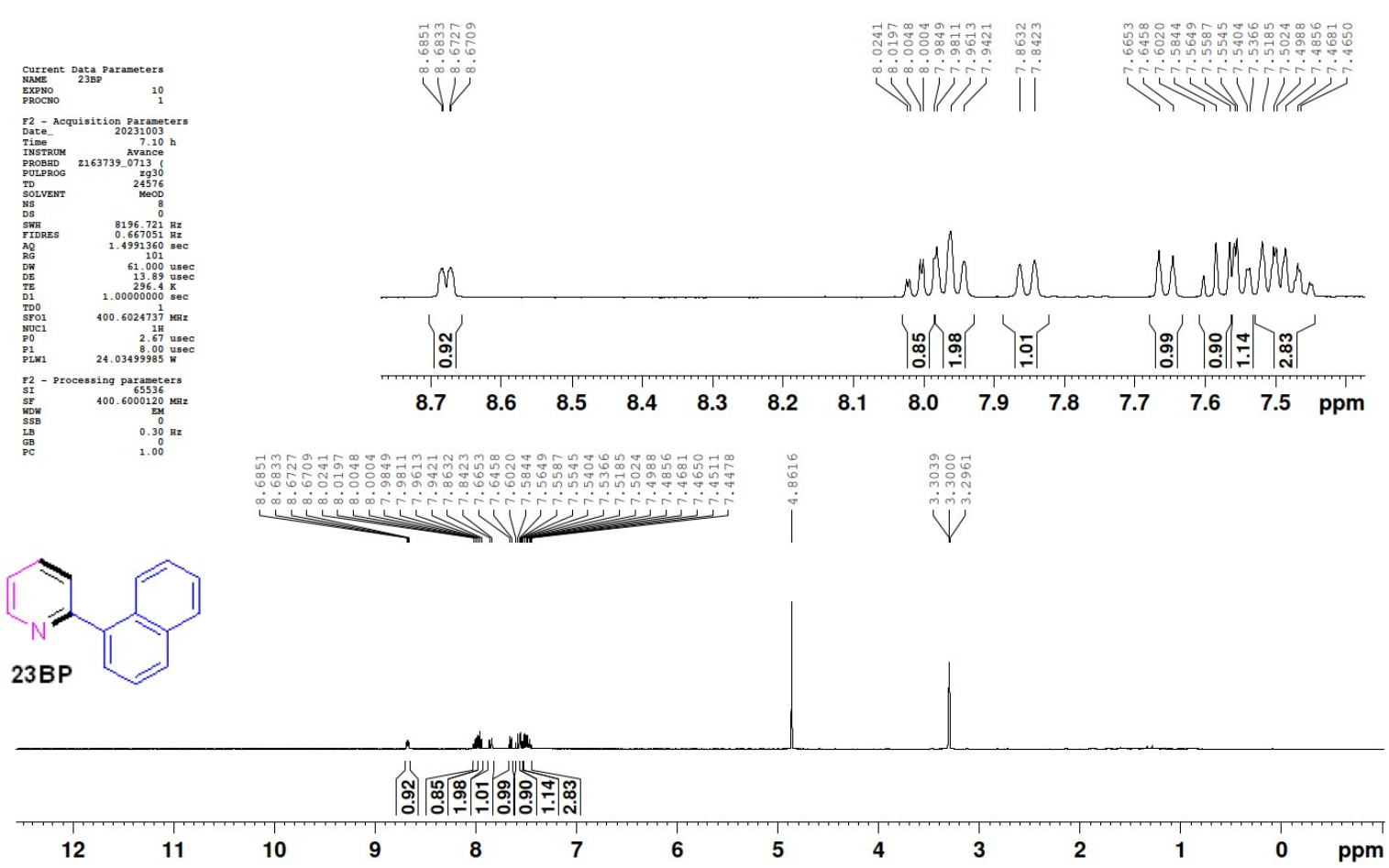

23BO IN MeOD
Current Data Parameters
NAME 23BO
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231003
Time 7.07 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT MeOD
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.6695
8.6574
8.1644
8.1440
7.9463
7.9432
7.9343
7.9308
7.7976
7.7770
7.4387
7.4271
7.4171
7.4050
0.98
2.08
2.06
2.06
1.00
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
4.8605
3.2998
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
N
F
F
F
23BO

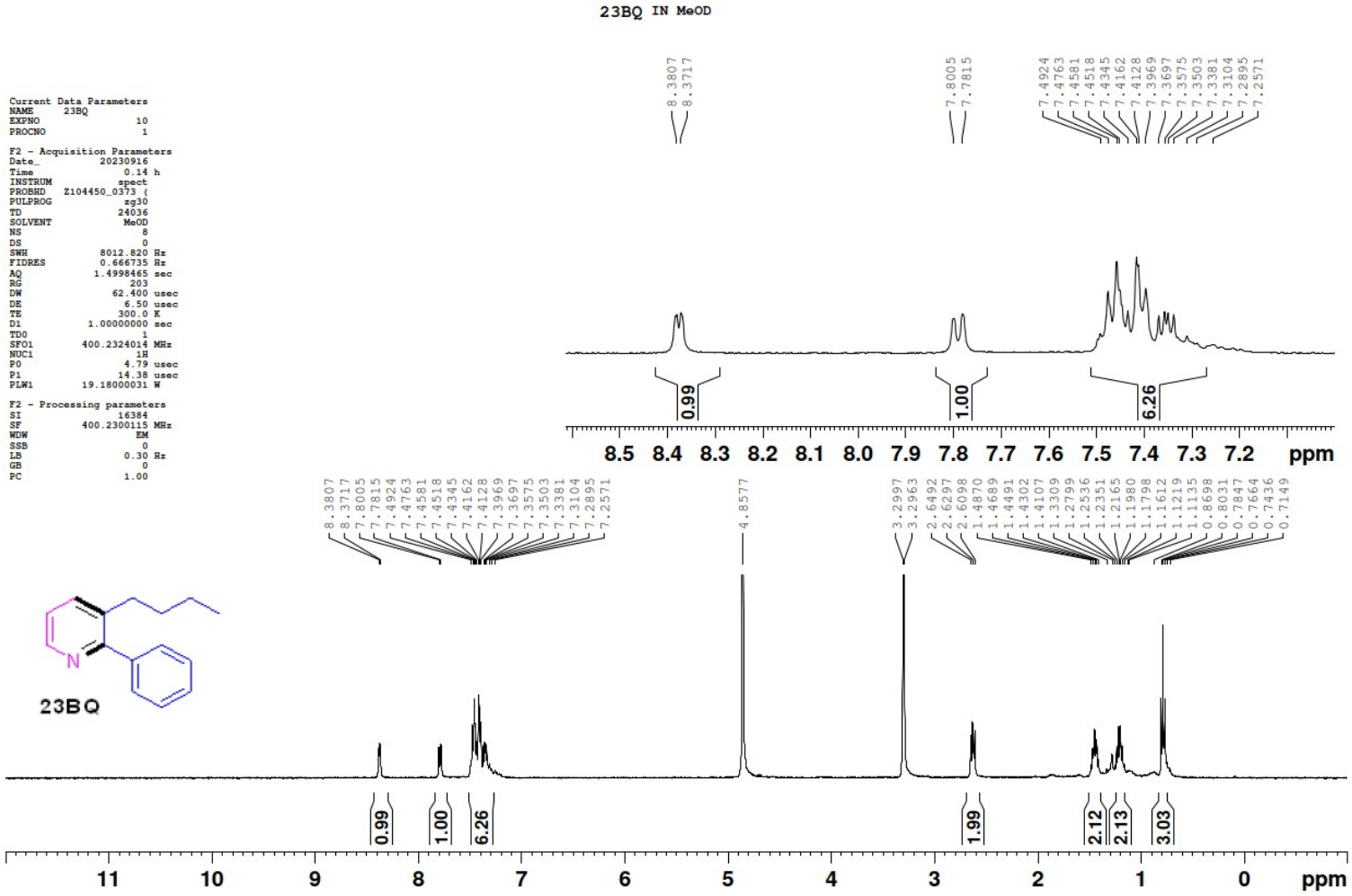
23BP IN MeOD

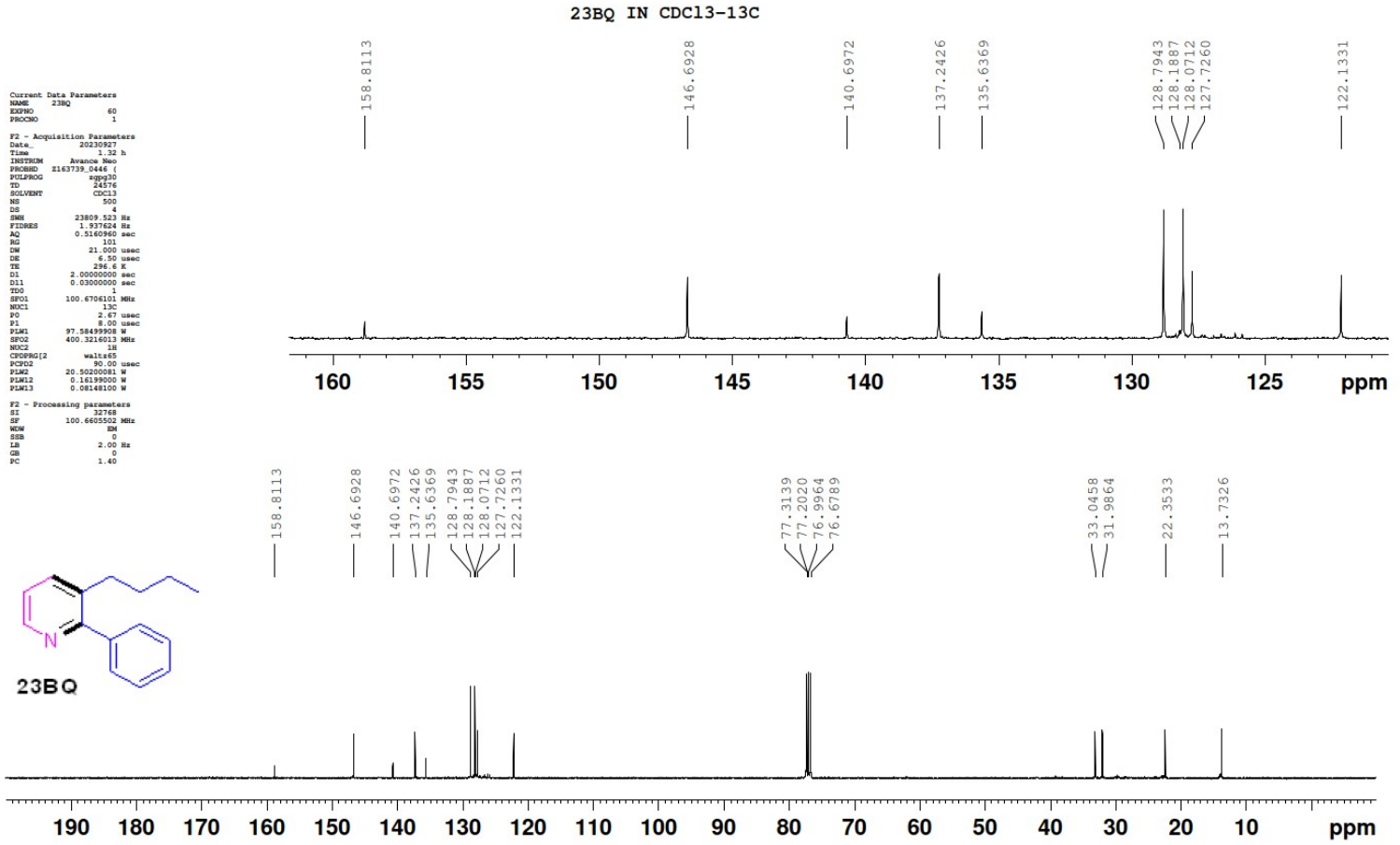
```
Current Data Parameters
NAME      23BP
EXPNO           10
PROCNO           1

F2 - Acquisition Parameters
Date_      20231003
Time           7.10 h
INSTRUM       Avance
PROBHD   Z163739_0713 (
PULPROG         zg30
TD             24576
SOLVENT         MeOD
NS                 8
DS                 0
SWH         8196.721 Hz
FIDRES      0.667051 Hz
AQ          1.4991360 sec
RG               101
DW            61.000 usec
DE            13.89 usec
TE             296.4 K
D1          1.00000000 sec
TD0                1
SFO1        400.6024737 MHz
NUC1               1H
P0             2.67 usec
P1             8.00 usec
PLW1       24.03499985 W

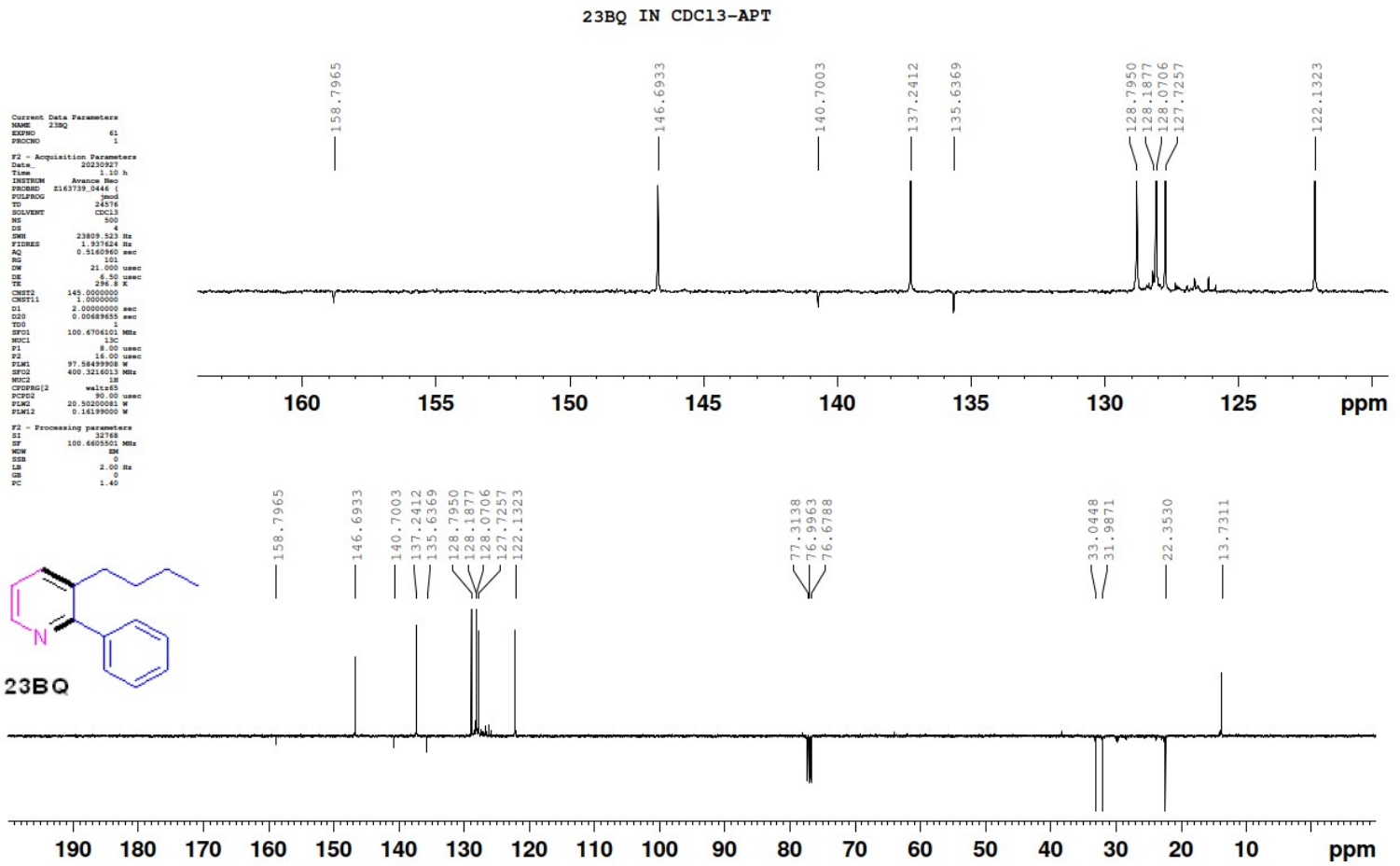
F2 - Processing parameters
SI             65536
SF        400.6000120 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```




23BQ IN MeOD
Current Data Parameters
NAME 23BQ
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230916
Time 0.14 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3807
8.3717
7.8005
7.7815
7.4924
7.4763
7.4581
7.4518
7.4345
7.4162
7.4128
7.3969
7.3697
7.3575
7.3503
7.3381
7.3104
7.2895
7.2571
0.99
1.00
6.26
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
4.8577
3.2997
3.2963
2.6492
2.6297
2.6098
1.4870
1.4689
1.4491
1.4302
1.4107
1.3309
1.2799
1.2536
1.2351
1.2165
1.1980
1.1798
1.1612
1.1219
1.1135
0.8698
0.8031
0.7847
0.7664
0.7436
0.7149
N
23BQ
0.99
1.00
6.26
1.99
2.12
2.13
3.03
11 10 9 8 7 6 5 4 3 2 1 0 ppm


23BQ IN CDCl3-13C
Current Data Parameters
NAME 23BQ
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230927
Time 1.32 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG zgpg30
TD 24576
SOLVENT CDCl3
NS 500
DS 4
SWH 23809.523 Hz
FIDRES 1.937624 Hz
AQ 0.5160960 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
PO 2.67 usec
P1 8.00 usec
PLW1 97.58499908 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 20.50200081 W
PLW12 0.16199000 W
PLW13 0.08148100 W
F2 - Processing parameters
SI 32768
SF 100.6605502 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
158.8113
146.6928
140.6972
137.2426
135.6369
128.7943
128.1887
128.0712
127.7260
122.1331
160
155
150
145
140
135
130
125
ppm
77.3139
77.2020
76.9964
76.6789
33.0458
31.9864
22.3533
13.7326
N
23BQ
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

23BQ IN CDCl3-APT

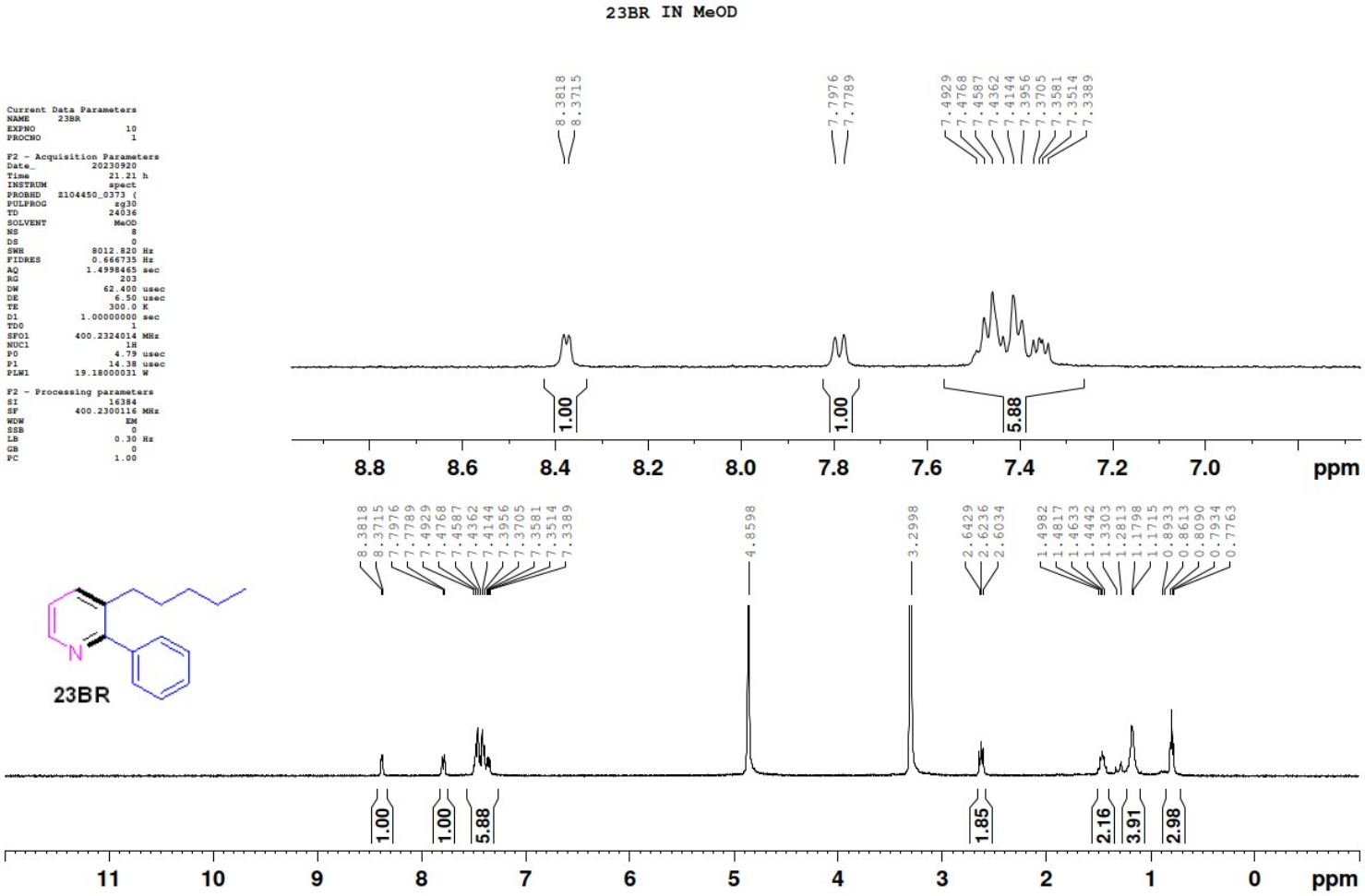


Current Data Parameters
NAME 23BQ
EXPNO 61
PROCNO 1

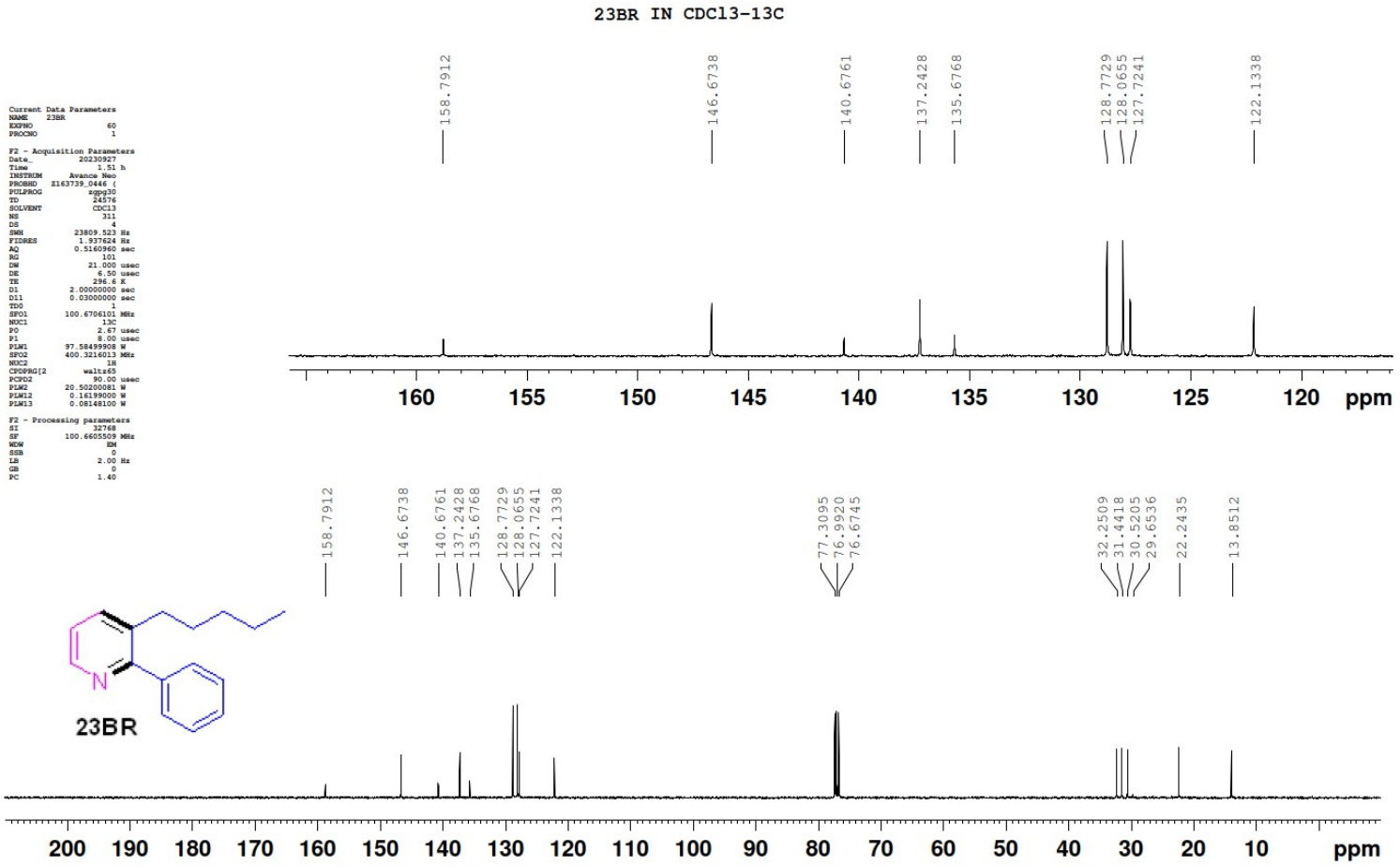
F2 - Acquisition Parameters
Date 20230927
Time 1.10 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG jmod
TD 24576
SOLVENT CDCl3
NS 500
DS 4
SWH 23809.523 Hz
FIDRES 1.937624 Hz
AQ 0.5160960 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 296.8 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 97.58499908 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 20.50200081 W
PLW12 0.16199000 W

F2 - Processing parameters
SI 32768
SF 100.6605501 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

23BR IN MeOD


Current Data Parameters
NAME 23BR
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230920
Time 21.21 h
INSTRUM spect
PROBHD Z104450_0373 (
PULPROG zg30
TD 24036
SOLVENT MeOD
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324014 MHz
NUC1 1H
P0 4.79 usec
P1 14.38 usec
PLW1 19.18000031 W
F2 - Processing parameters
SI 16384
SF 400.2300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.3818
8.3715
7.7976
7.7789
7.4929
7.4768
7.4587
7.4362
7.4144
7.3956
7.3705
7.3581
7.3514
7.3389
1.00
1.00
5.88
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm
4.8598
3.2998
2.6429
2.6236
2.6034
1.4982
1.4817
1.4633
1.4442
1.3303
1.2813
1.1798
1.1715
0.8933
0.8613
0.8090
0.7934
0.7763
N
23BR
1.00
1.00
5.88
1.85
2.16
3.91
2.98
11
10
9
8
7
6
5
4
3
2
1
0
ppm

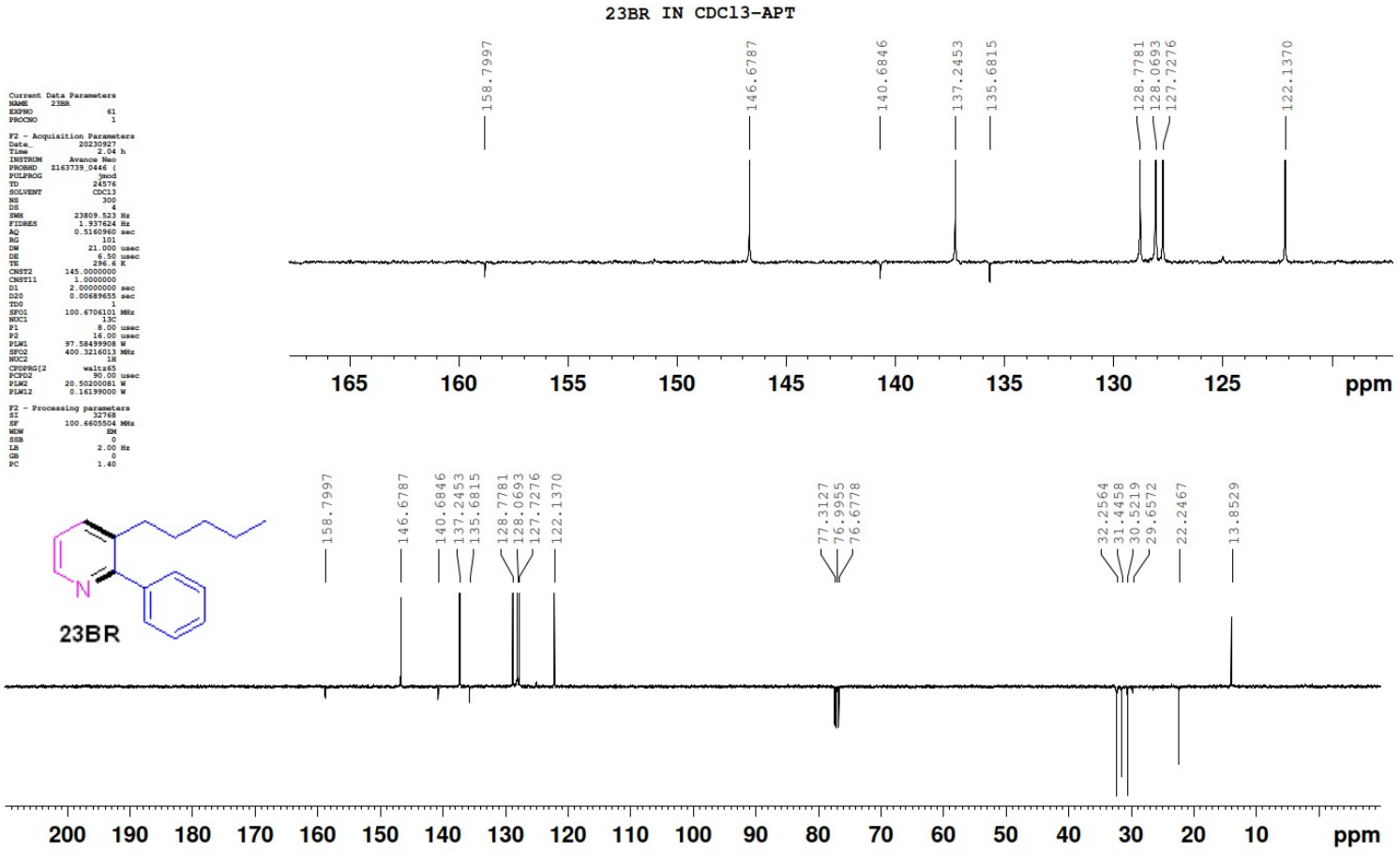
23BR IN CDCl3-13C



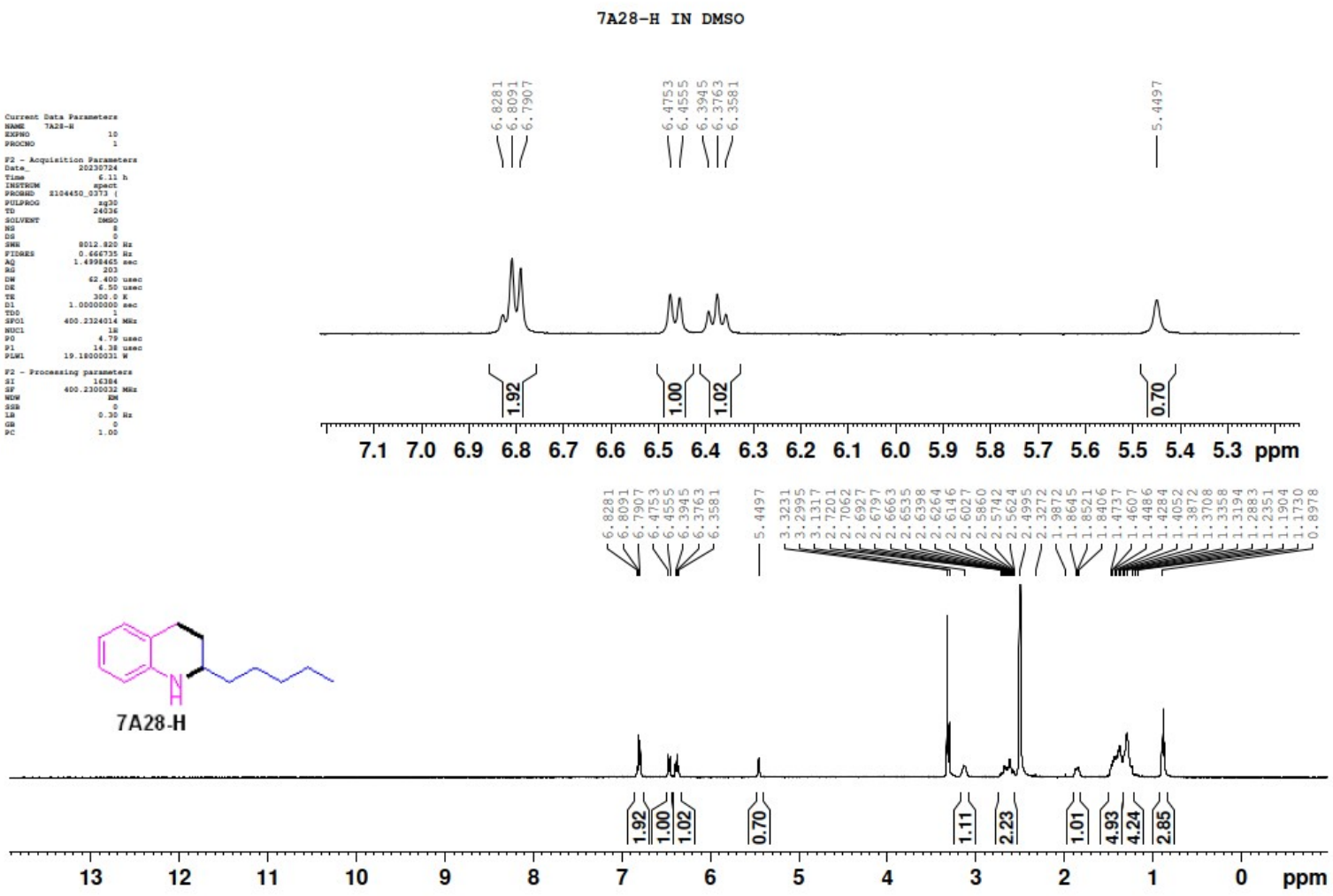

```
Current Data Parameters
NAME      23BR
EXPNO           60
PROCNO           1

F2 - Acquisition Parameters
Date_        20230927
Time            1.51 h
INSTRUM       Avance Neo
PROBHD   Z163739_0446 (
PULPROG        zgpg30
TD             24576
SOLVENT        CDCl3
NS               311
DS                 4
SWH        23809.523 Hz
FIDRES      1.937624 Hz
AQ          0.5160960 sec
RG               101
DW            21.000 usec
DE             6.50 usec
TE            296.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0              1
SFO1     100.6706101 MHz
NUC1            13C
P0             2.67 usec
P1             8.00 usec
PLW1      97.58499908 W
SFO2     400.3216013 MHz
NUC2            1H
CPDPRG[2     waltz65
PCPD2         90.00 usec
PLW2      20.50200081 W
PLW12      0.16199000 W
PLW13      0.08148100 W

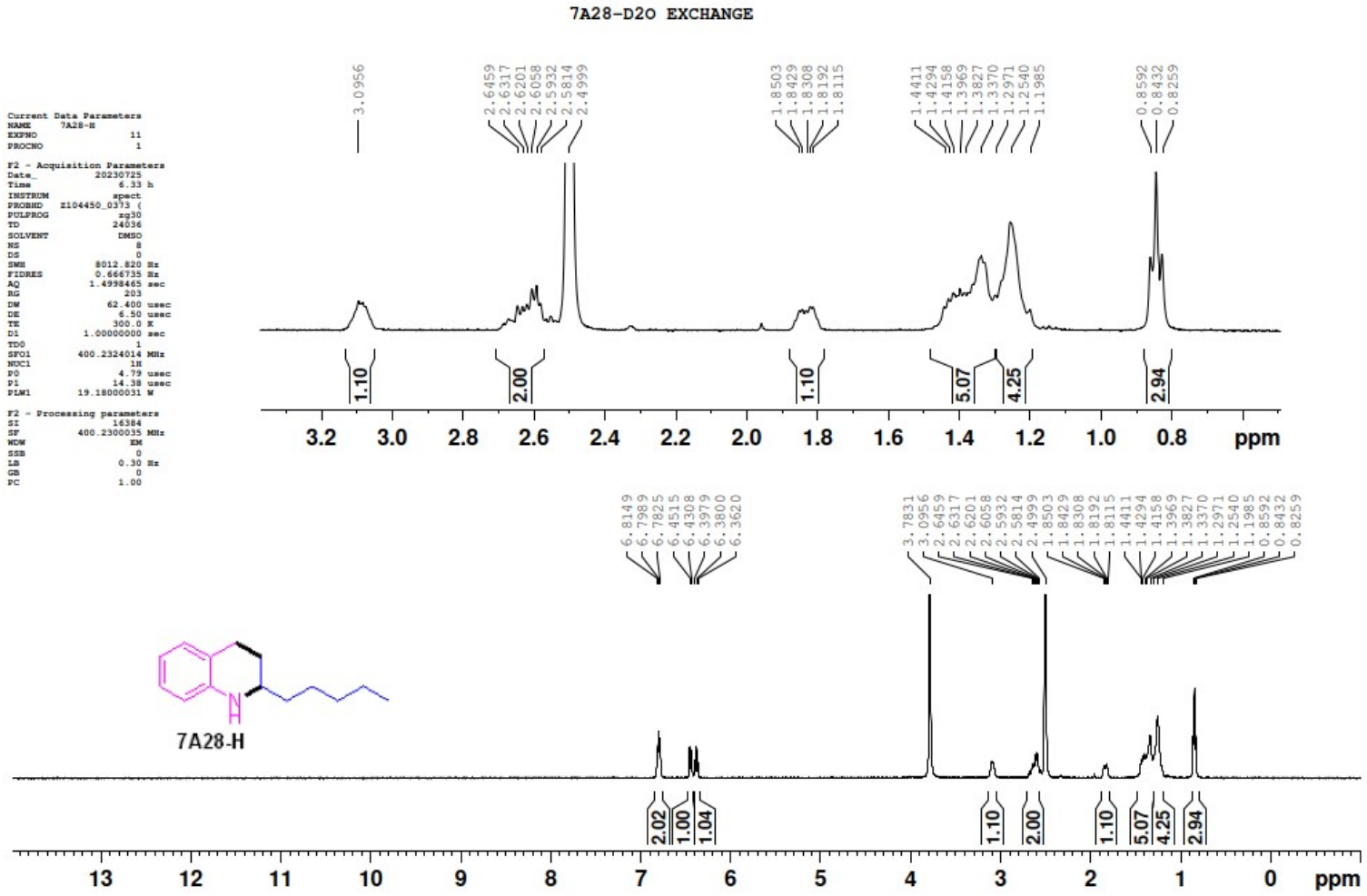
F2 - Processing parameters
SI             32768
SF        100.6605509 MHz
WDW              EM
SSB               0
LB             2.00 Hz
GB                0
PC             1.40
```


23BR IN CDCl3-APT
Current Data Parameters
NAME 23BR
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230927
Time 2.04 h
INSTRUM Avance Neo
PROBHD Z163739_0446 (
PULPROG jmod
TD 24576
SOLVENT CDCl3
NS 300
DS 4
SWH 23809.523 Hz
FIDRES 1.937624 Hz
AQ 0.5160960 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 296.6 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6706101 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 97.58499908 W
SFO2 400.3216013 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 20.50200081 W
PLW12 0.16199000 W
F2 - Processing parameters
SI 32768
SF 100.6605504 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
158.7997
146.6787
140.6846
137.2453
135.6815
128.7781
128.0693
127.7276
122.1370
165
160
155
150
145
140
135
130
125
ppm
N
23BR
158.7997
146.6787
140.6846
137.2453
135.6815
128.7781
128.0693
127.7276
122.1370
77.3127
76.9955
76.6778
32.2564
31.4458
30.5219
29.6572
22.2467
13.8529
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

7A28-H IN DMSO



7A28-D2O EXCHANGE

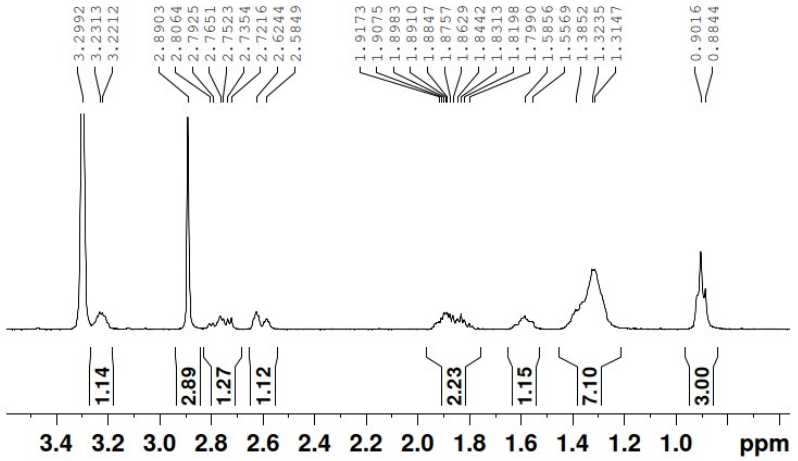


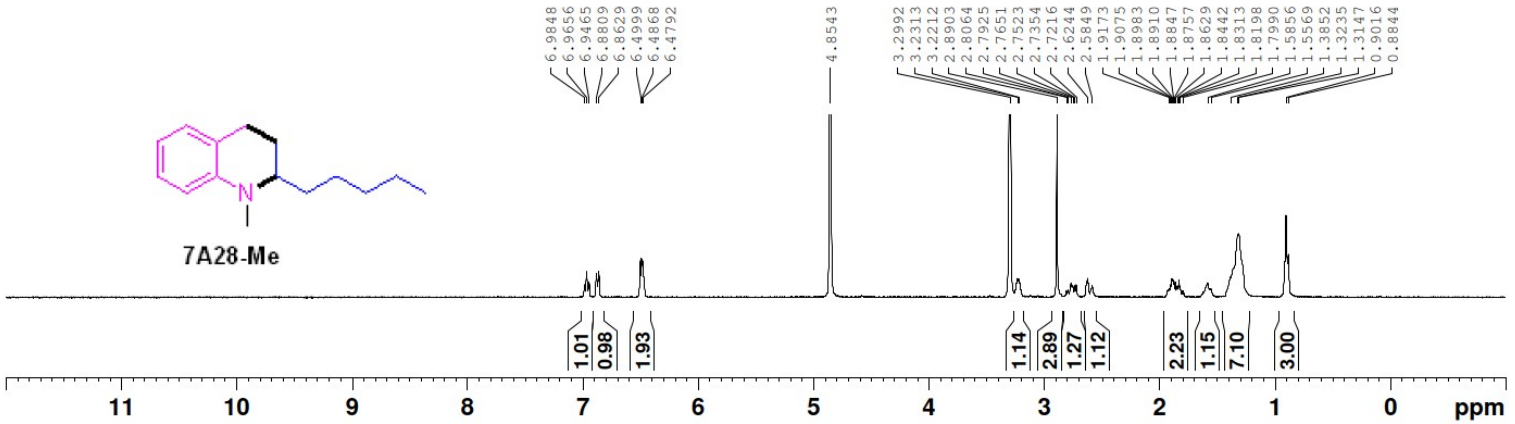
7A28-Me IN MeOD

```
Current Data Parameters
NAME        7A28-Me
EXPNO            10
PROCNO            1

F2 - Acquisition Parameters
Date_        20230727
Time            22.50 h
INSTRUM          spect
PROBHD   2104450_0373 (
PULPROG          zg30
TD              24036
SOLVENT          MeOD
NS                  8
DS                  0
SWH          8012.820 Hz
FIDRES       0.666735 Hz
AQ           1.4998465 sec
RG                 50.8
DW              62.400 usec
DE               6.50 usec
TE              300.0 K
D1          1.00000000 sec
TD0                 1
SFO1       400.2324014 MHz
NUC1               1H
P0              4.79 usec
P1             14.38 usec
PLW1       19.18000031 W

F2 - Processing parameters
SI              16384
SF         400.2300119 MHz
WDW               EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

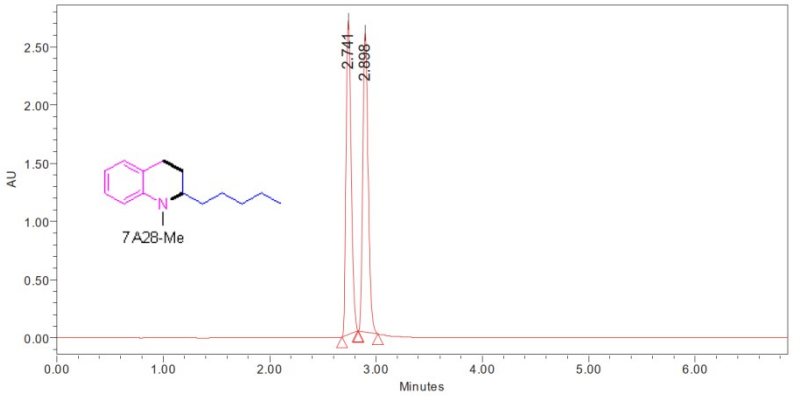




Empower 3 SOFTWARE

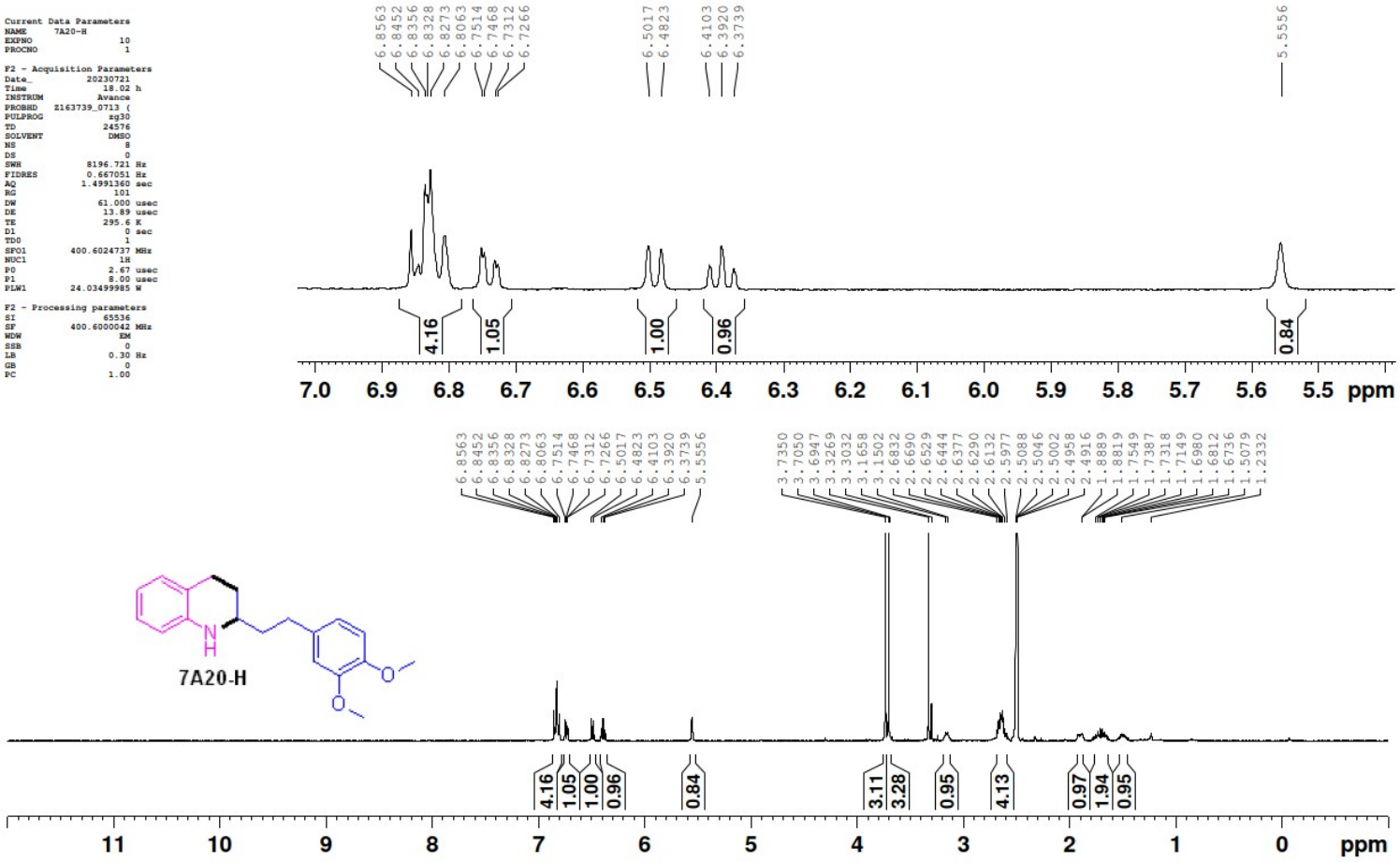
SAMPLE INFORMATION

Sample Name: 7A28-Me		Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	10082023
Vial:	1:B,2	Acq. Method Set:	B4_C5_3_80_CO2
Injection #:	1	Processing Method	002574
Injection Volume:	3.00 ul	Channel Name:	254.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	PDA Spectrum PDA 254.0 nm
		Column Name I	CELLULOSE J
Date Acquired:	10-08-2023 08:30:04 IST	CoSolvent 0.5% IPamine_MEOH	
Date Processed:	10-08-2023 08:37:59 IST		

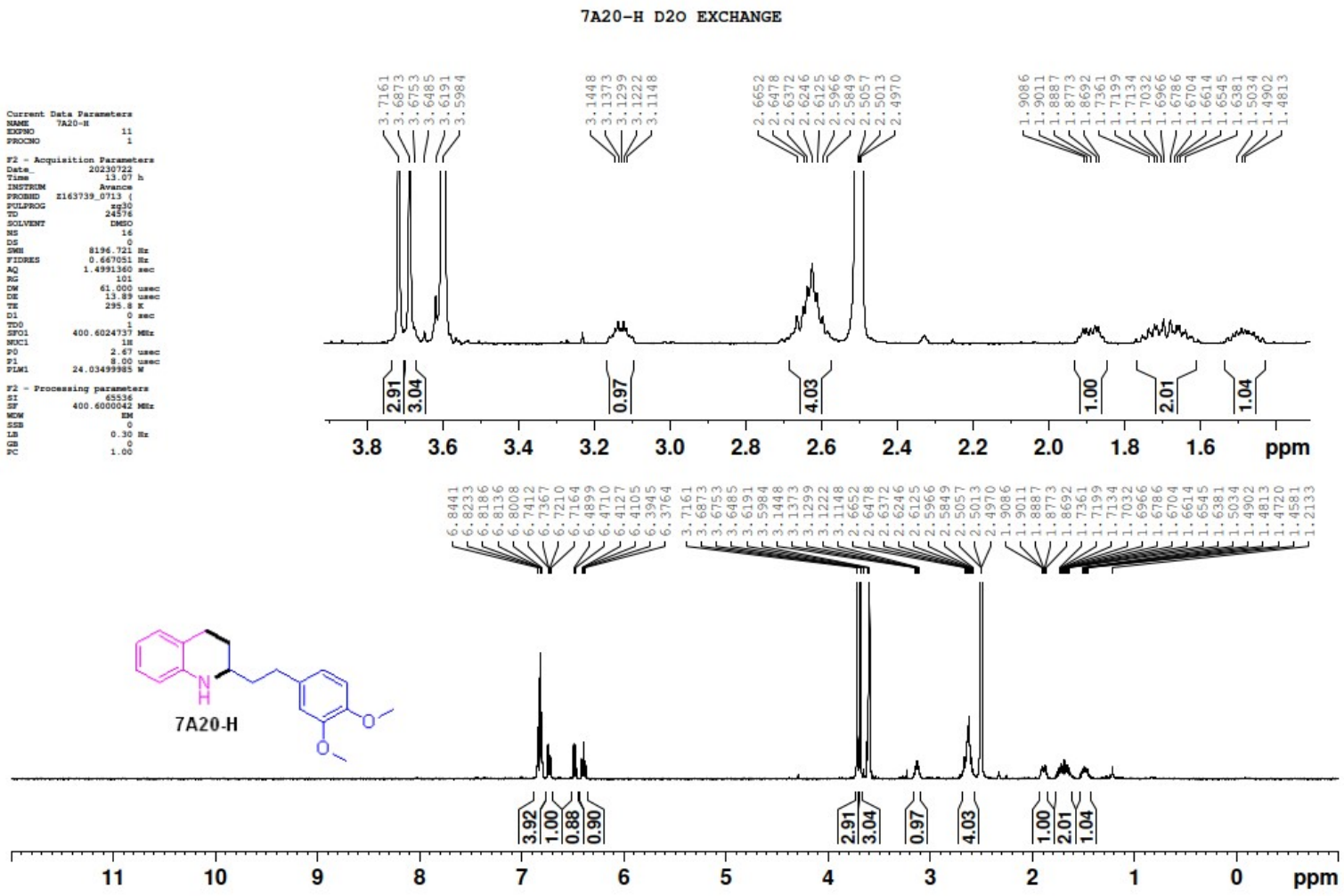


	RT	Height	Area	% Area
1	2.741	2697416	8805751	49.65
2	2.898	2576921	8928948	50.35

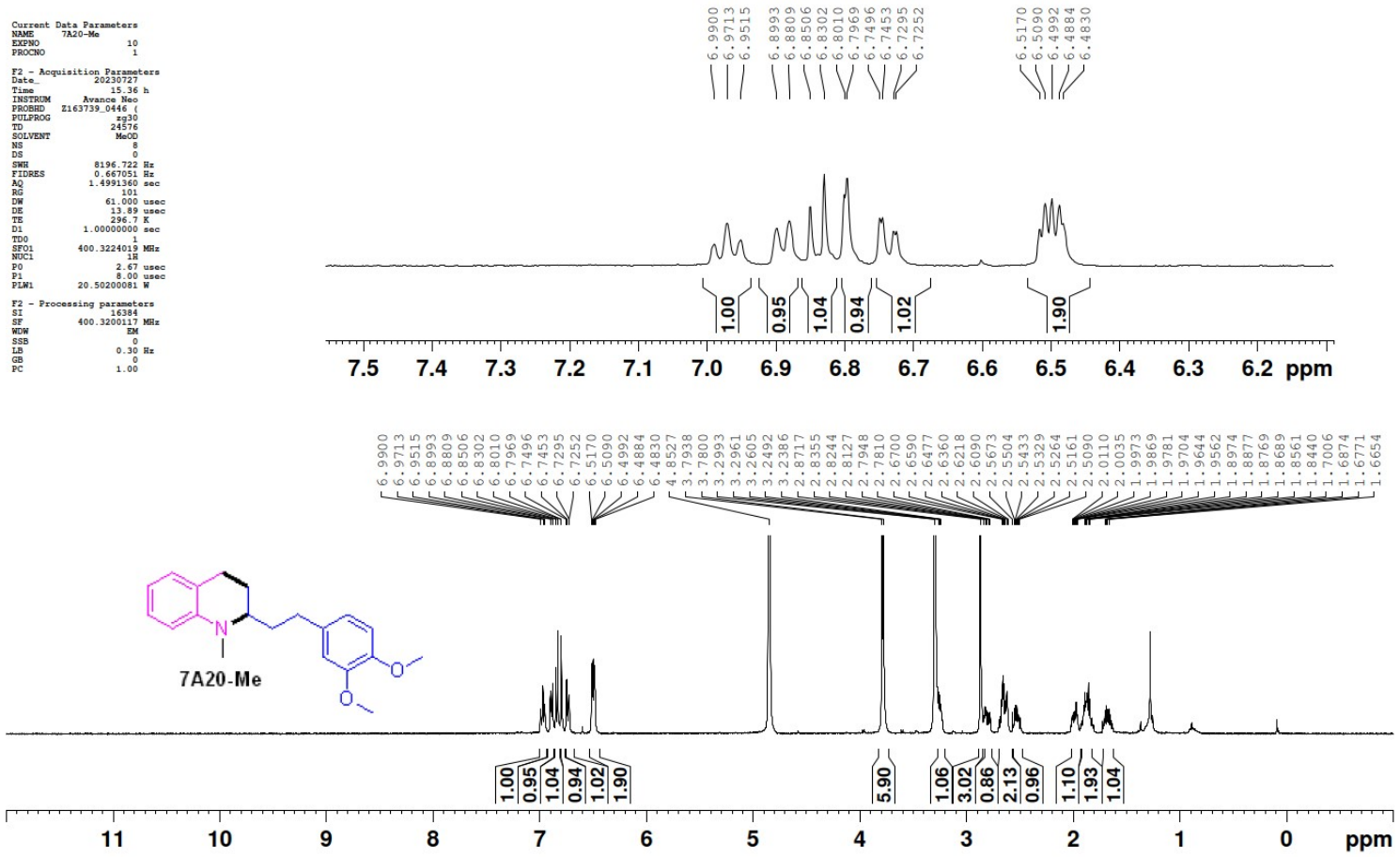
7A20-H IN DMSO



7A20-H D2O EXCHANGE



7A20-Me IN MeOD



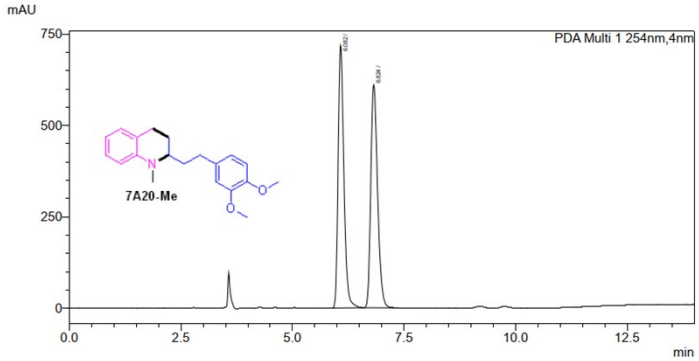
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample ID	: 7A20-Me		
Data Filename	: 02082023031.lcd		
Method Filename	: AB_METHOD-4.lcm		
Batch Filename	: 02082023.lcb		
Vial #	: 1-89	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 03-08-2023 12:12:16 AM	Acquired by	:------
Date Processed	: 03-08-2023 12:57:20 AM	Processed by	:------
Token Number	: 17		
COLUMN	:CHIRALCEL OD-H (250X4.6)mm,5µ M.P.- Hexane/EtOH/IPAmine : 80/20/0.1 Flow Rate - 1.0 ml/min		

<Chromatogram>

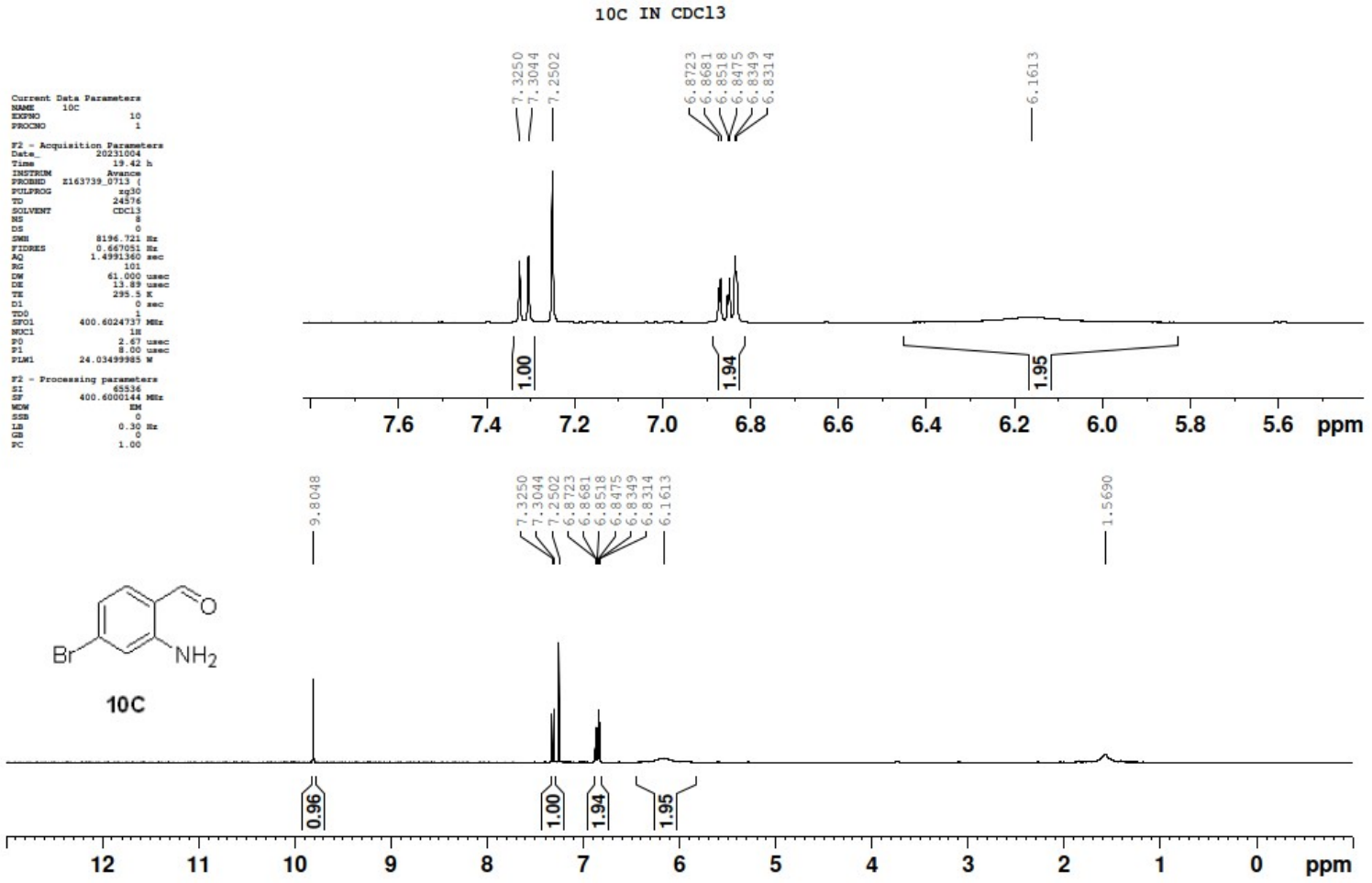


<Batch Table>

Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	6.082	6465561	50.112
2	6.824	6436655	49.888
Total		12902216	100.000

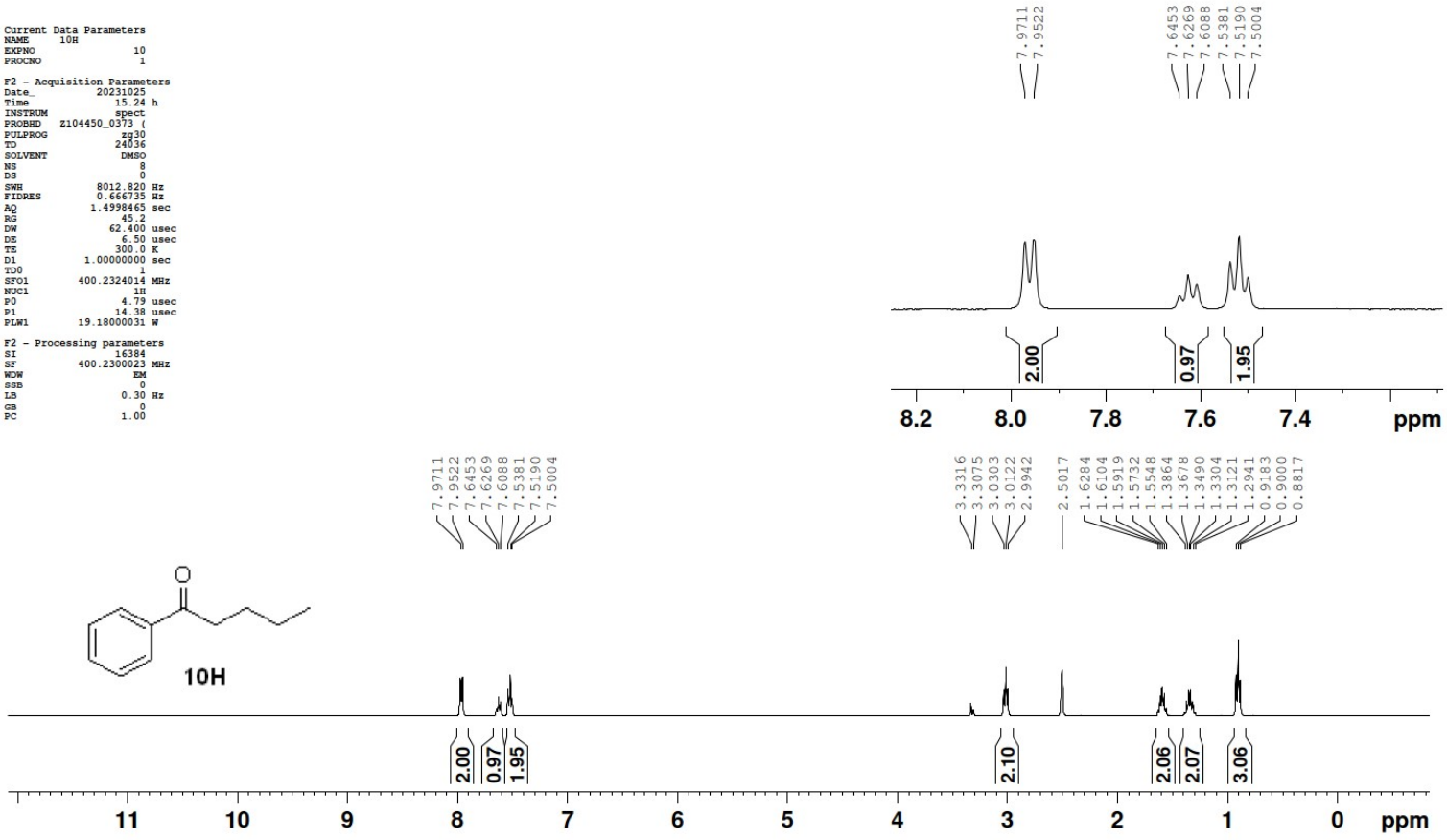

10C IN CDCl3
Current Data Parameters
NAME 10C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231004
Time 19.42 h
INSTRUM Avance
PROBHD Z163739_0713 (
PULPROG zg30
TD 24576
SOLVENT CDCl3
NS 8
DS 0
SWH 8196.721 Hz
FIDRES 0.667051 Hz
AQ 1.4991360 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 295.5 K
D1 0 sec
TD0 1
SFO1 400.6024737 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.03499985 W
F2 - Processing parameters
SI 65536
SF 400.6000144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.3250
7.3044
7.2502
6.8723
6.8681
6.8518
6.8475
6.8349
6.8314
6.1613
1.00
1.94
1.95
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
ppm
9.8048
1.5690
Br
NH2
O
10C
0.96
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

10H IN DMSO

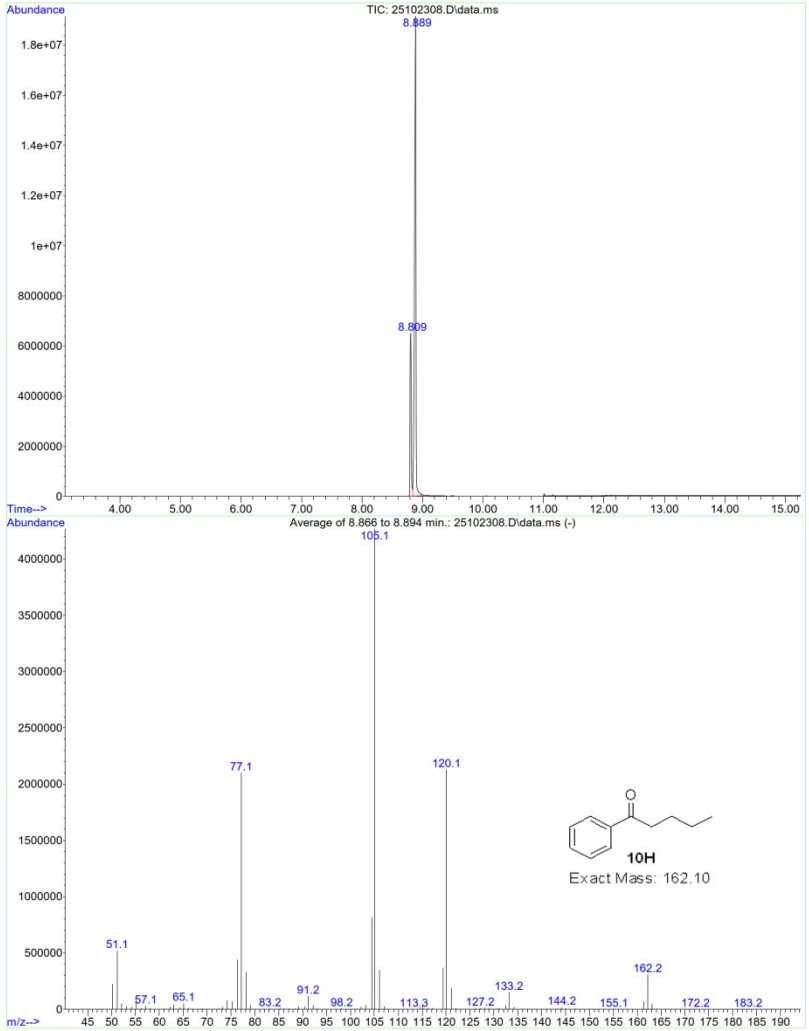
```
Current Data Parameters
NAME      10H
EXPNO          10
PROCNO          1

F2 - Acquisition Parameters
Date_      20231025
Time           15.24 h
INSTRUM         spect
PROBHD   Z104450_0373 (
PULPROG         zg30
TD             24036
SOLVENT         DMSO
NS                 8
DS                 0
SWH         8012.820 Hz
FIDRES      0.666735 Hz
AQ          1.4998465 sec
RG              45.2
DW             62.400 usec
DE              6.50 usec
TE             300.0 K
D1          1.00000000 sec
TD0                1
SFO1      400.2324014 MHz
NUC1               1H
P0              4.79 usec
P1             14.38 usec
PLW1      19.18000031 W

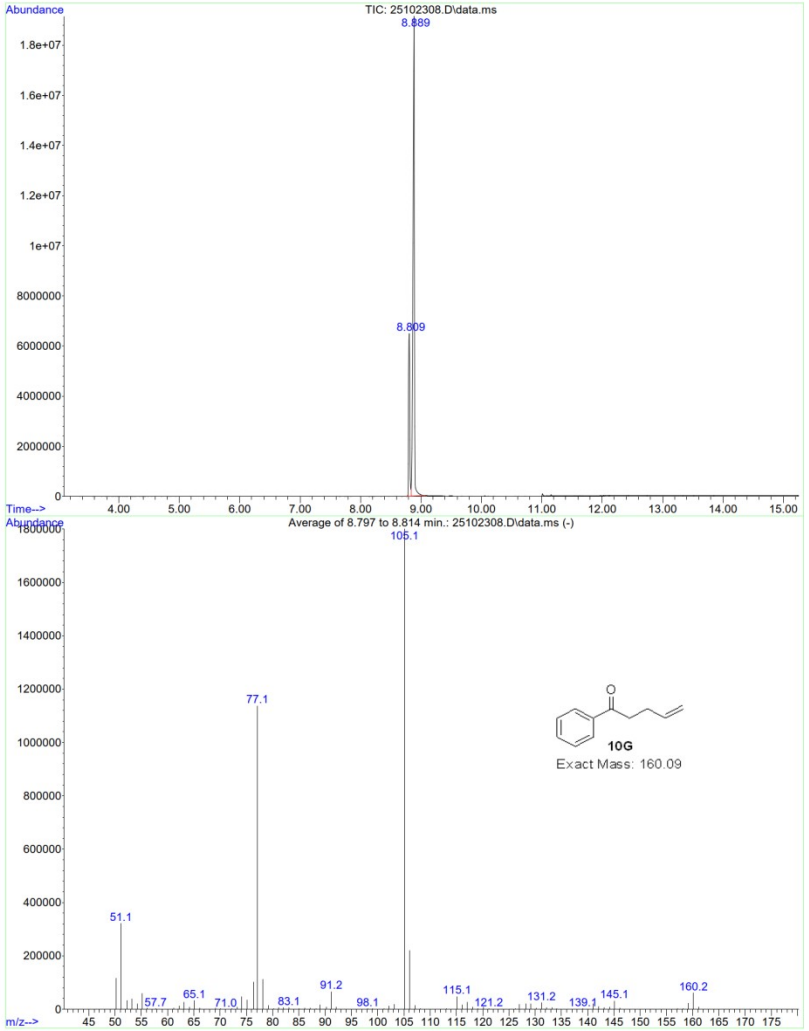
F2 - Processing parameters
SI             16384
SF        400.2300023 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

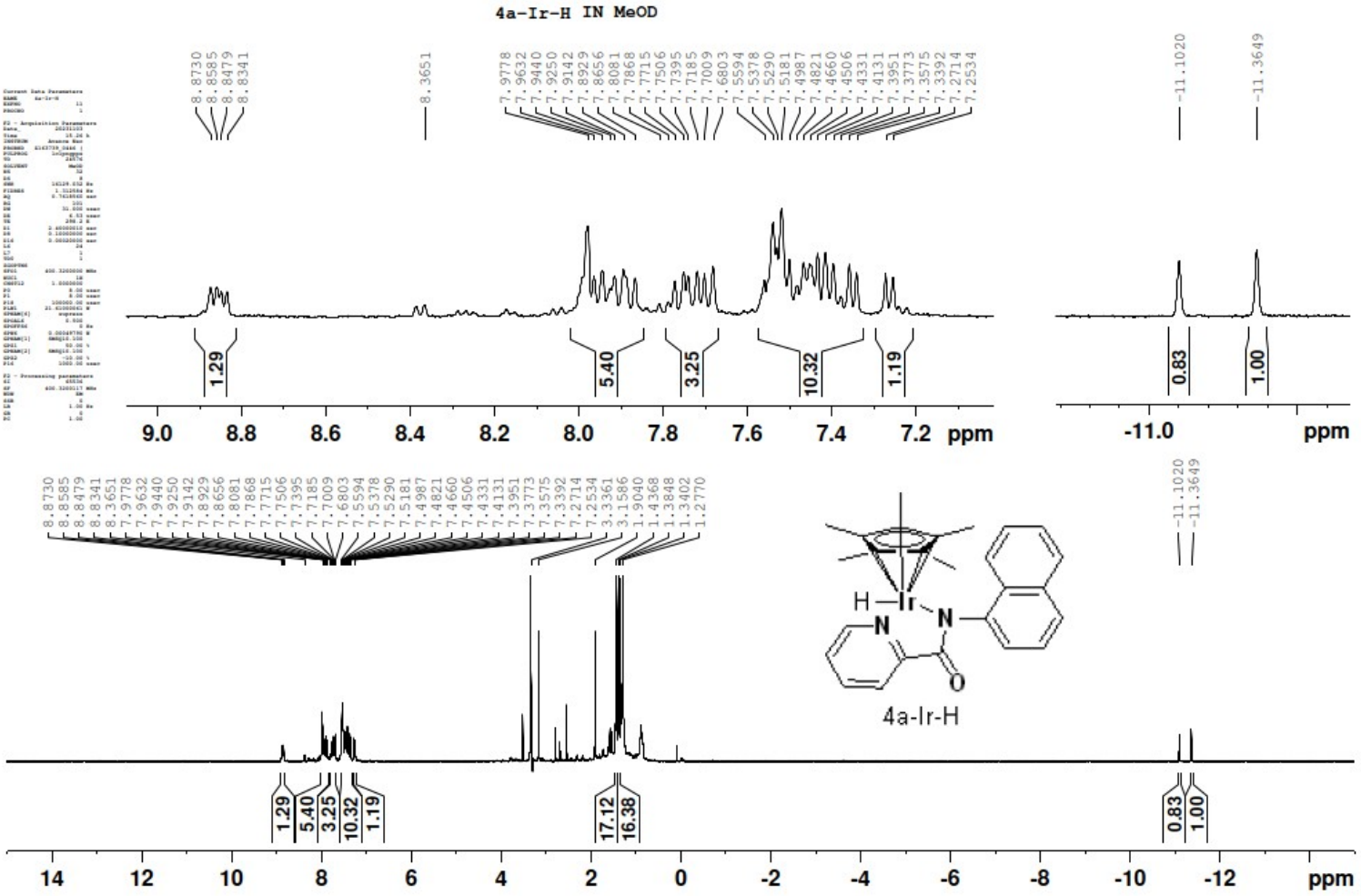


File :D:\DATA\OCT-23A\25102308.D
Operator :
Acquired : 25 Oct 2023 13:32 using AcqMethod TCG50.M
Instrument : GCMS
Sample Name: 10H
Misc Info :
Vial Number: 6



File :D:\DATA\OCT-23A\25102308.D
Operator :
Acquired : 25 Oct 2023 13:32 using AcqMethod TCG50.M
Instrument : GCMS
Sample Name: 10H
Misc Info :
Vial Number: 6



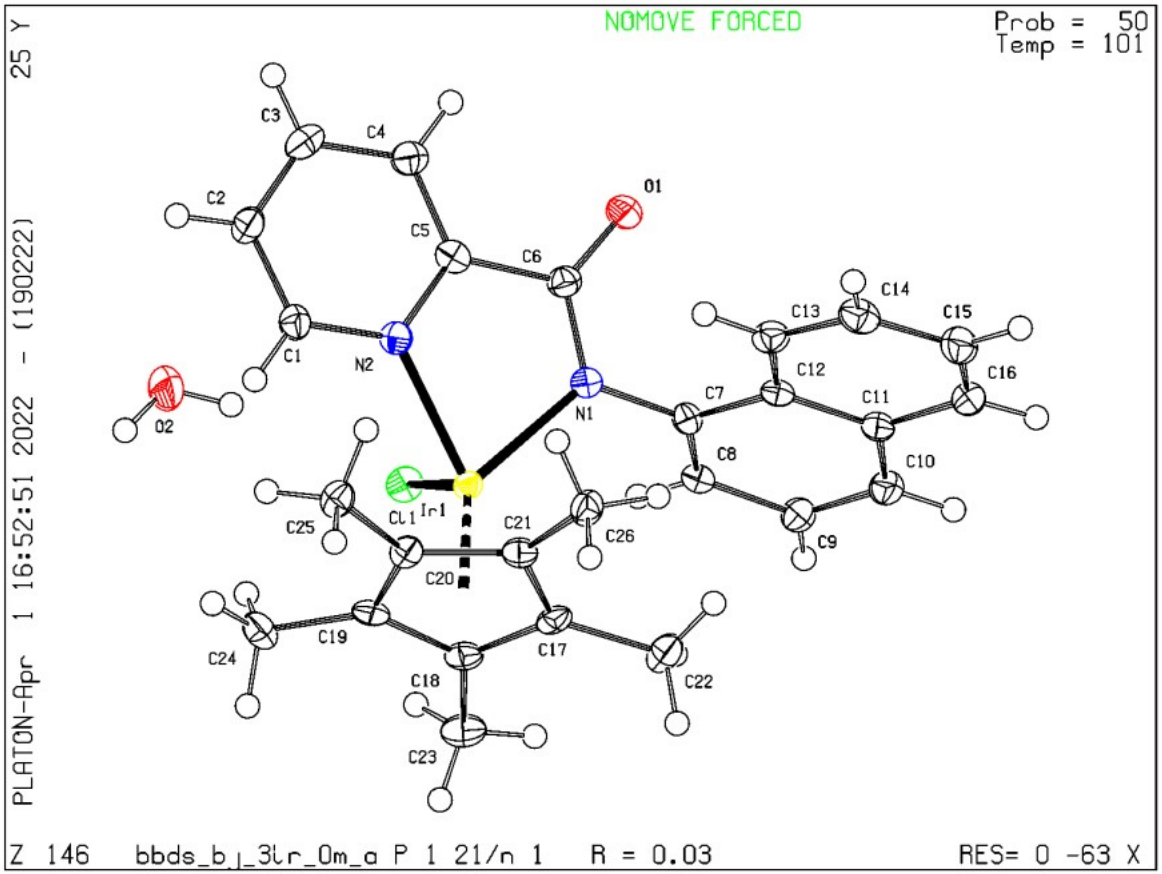

4a-Ir-H IN MeOD
8.8730
8.8585
8.8479
8.8341
8.3651
7.9778
7.9632
7.9440
7.9250
7.9142
7.8929
7.8656
7.8081
7.7868
7.7715
7.7506
7.7395
7.7185
7.7009
7.6803
7.5594
7.5378
7.5290
7.5181
7.4987
7.4821
7.4660
7.4506
7.4331
7.4131
7.3951
7.3773
7.3575
7.3392
7.2714
7.2534
-11.1020
-11.3649
1.29
5.40
3.25
10.32
1.19
0.83
1.00
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
-11.0
ppm
3.3361
3.1586
1.9040
1.4368
1.3848
1.3402
1.2770
17.12
16.38
H
Ir
N
N
O
4a-Ir-H
14
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
-12
ppm

7. Crystallographic data and refinement details of **4a-Ir**.

Crystal Structure Determination: The single-crystal data for 4a-Ir were collected on a Bruker-

APEX-II CCD X-ray diffractometer.

X-ray determined molecular structure of **4a-Ir (CCDC 2165585).**



Bond precision: C-C = 0.0050 A Wavelength=1.54178

Cell: a=9.4305(7) b=11.9858(9) c=20.8802(17)
alpha=90 beta=100.870(2) gamma=90
Temperature: 101 K

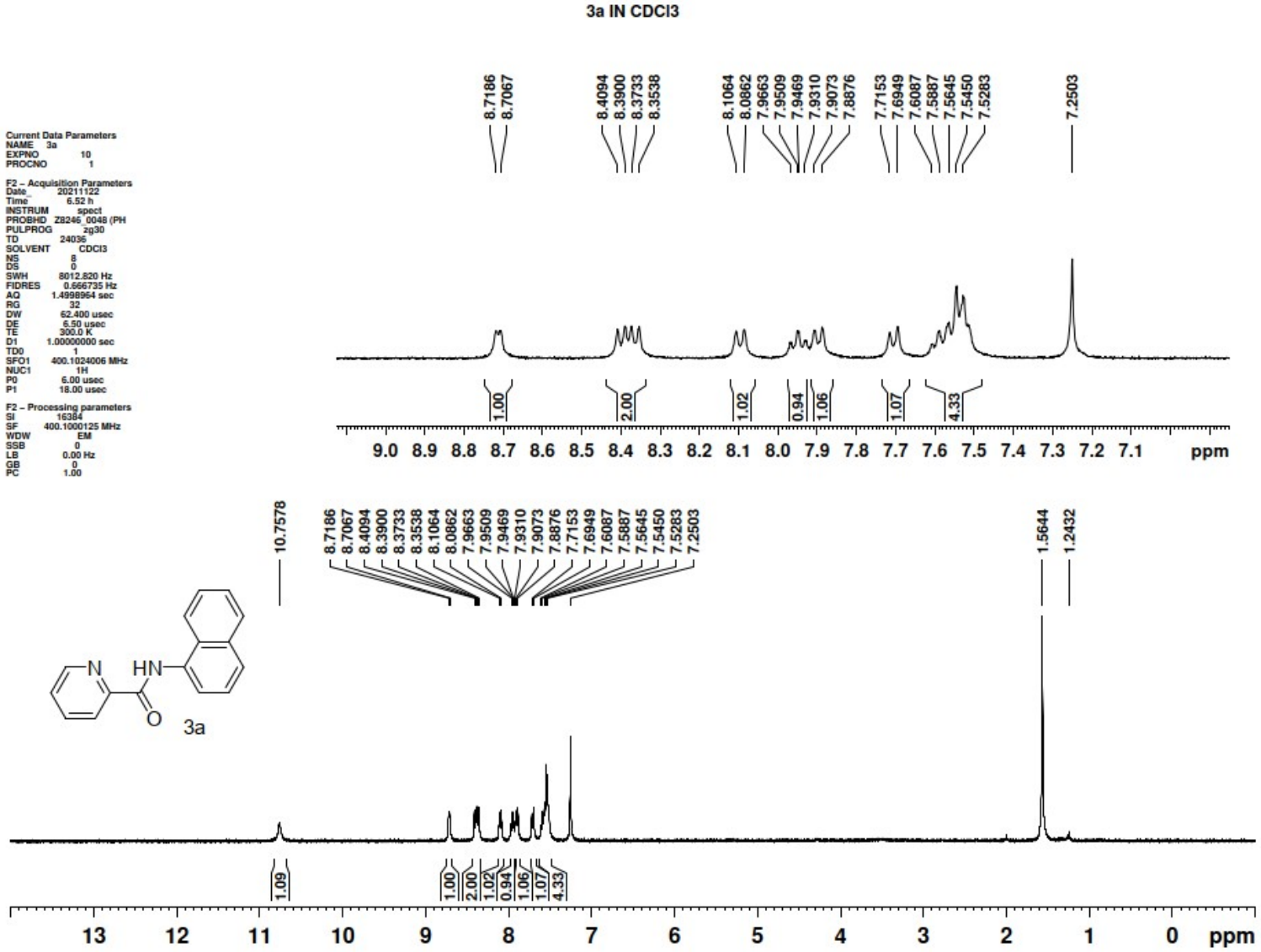
	Calculated	Reported
Volume	2317.8(3)	2317.8(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H26 Cl Ir N2 O, H2 O	C26 H26 Cl Ir N2 O, H2 O
Sum formula	C26 H28 Cl Ir N2 O2	C26 H22 Cl Ir N2 O2
Mr	628.17	622.10
Dx,g cm-3	1.800	1.783
Z	4	4
Mu (mm-1)	12.417	12.416
F000	1232.0	1208.0
F000'	1216.95	
h,k,lmax	11,14,25	11,14,25
Nref	4246	4146
Tmin,Tmax	0.209,0.289	0.355,0.753
Tmin'	0.067	

Correction method= # Reported T Limits: Tmin=0.355 Tmax=0.753
AbsCorr = MULTI-SCAN

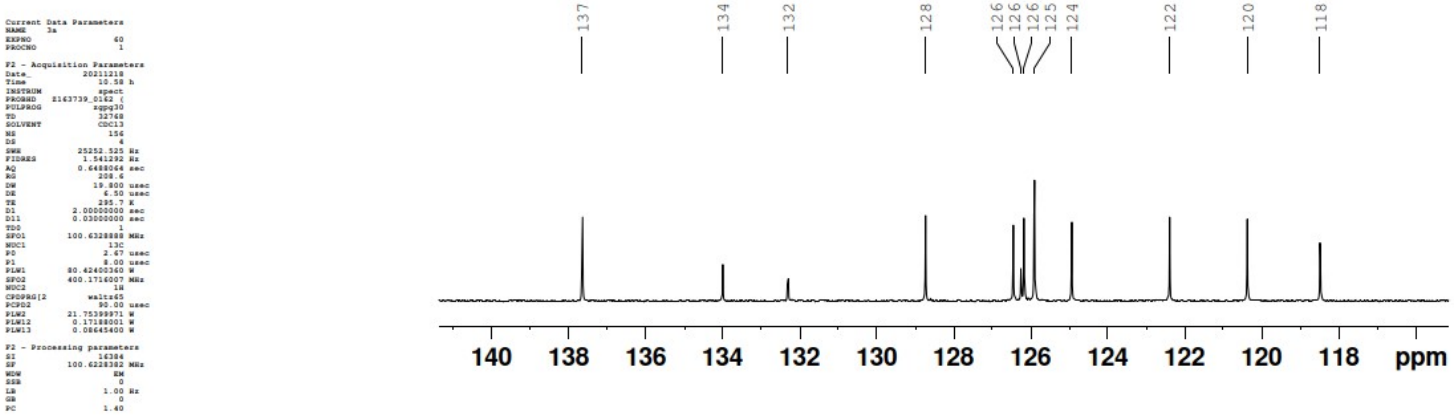
Data completeness= 0.976 Theta(max)= 68.246

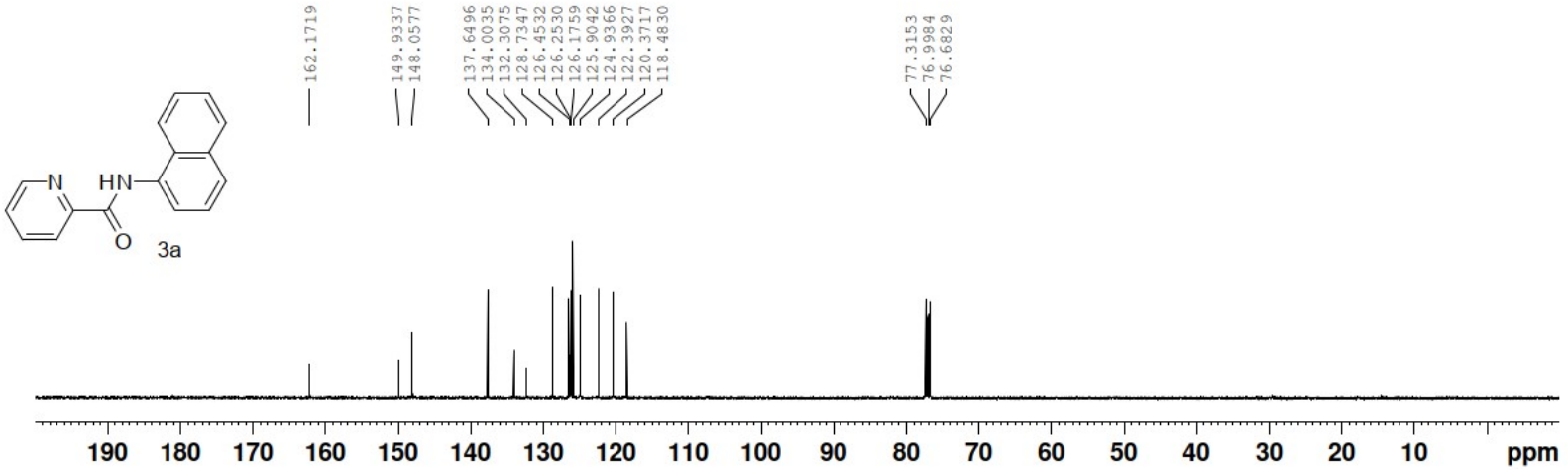
R(reflections)= 0.0303(4099) wR2(reflections)= 0.0839(4146)

S = 1.198 Npar= 298


3a IN CDCl3
Current Data Parameters
NAME 3a
EXPNO 10
PROCNO 1
F2 – Acquisition Parameters
Date_ 20211122
Time 6.52 h
INSTRUM spect
PROBHD Z8246_0048 (PH
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998964 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1024006 MHz
NUC1 1H
P0 6.00 usec
P1 18.00 usec
F2 – Processing parameters
SI 16384
SF 400.1000125 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.7186
8.7067
8.4094
8.3900
8.3733
8.3538
8.1064
8.0862
7.9663
7.9509
7.9469
7.9310
7.9073
7.8876
7.7153
7.6949
7.6087
7.5887
7.5645
7.5450
7.5283
7.2503
1.00
2.00
1.02
0.94
1.06
1.07
4.33
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
10.7578
1.5644
1.2432
N
HN
O
3a
1.09
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

3a IN CDC13-13C



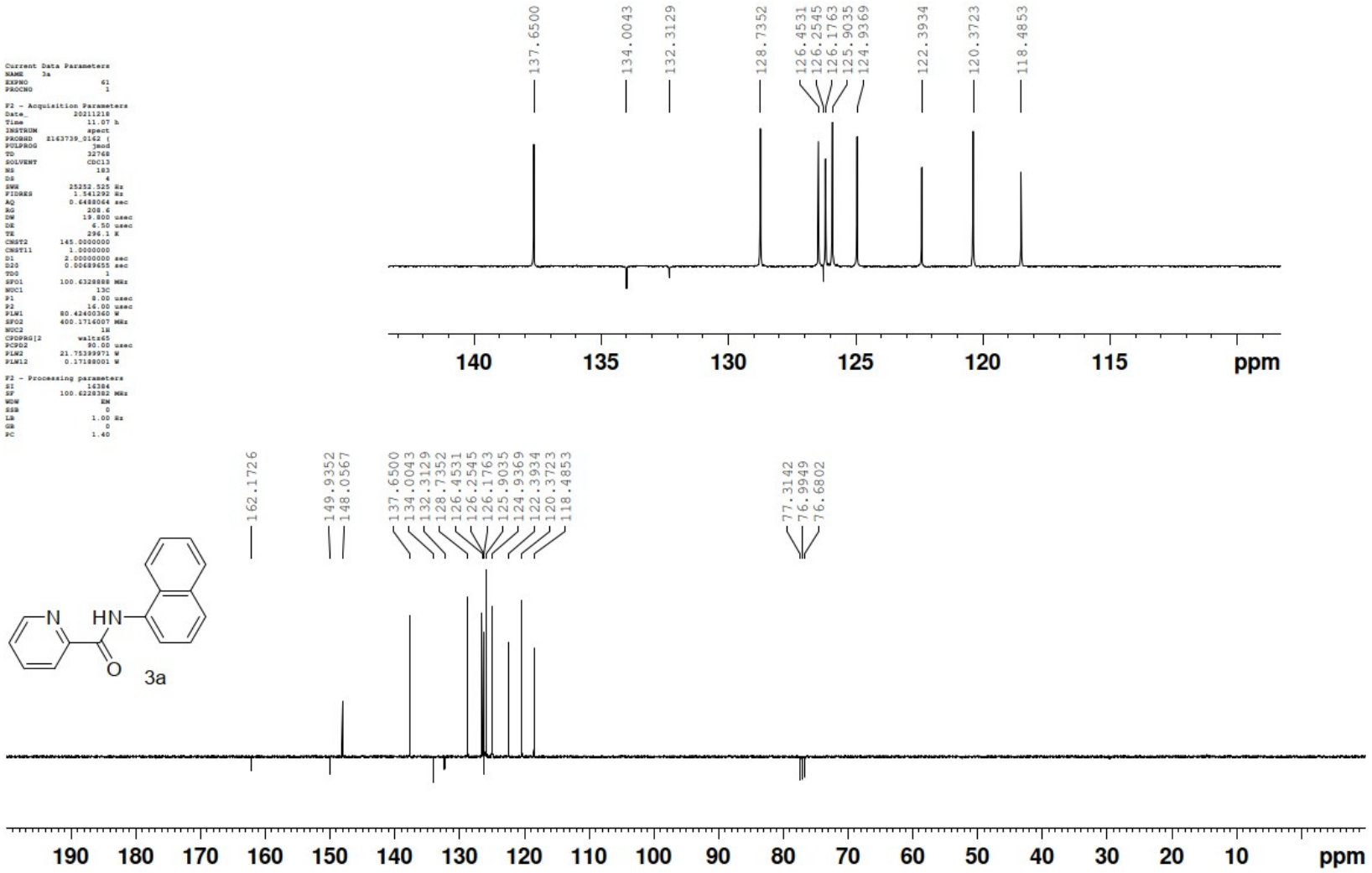


Current Data Parameters
NAME 3a
EXPNO 40
PROCNO 1

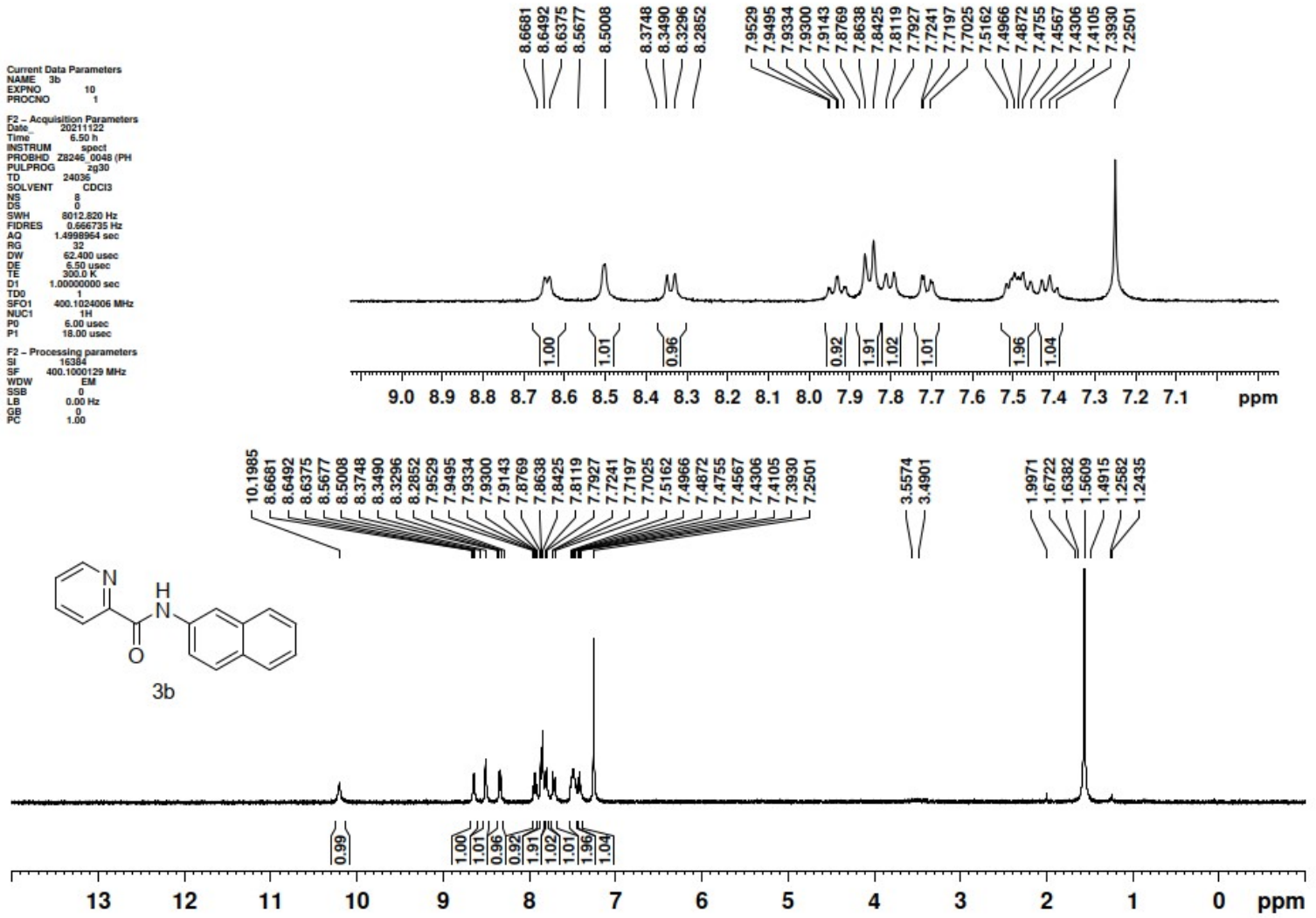
F2 - Acquisition Parameters
Date_ 20211218
Time 10.58 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 154
DS 4
SWH 25252.525 Hz
FIDRES 1.541292 Hz
AQ 0.64488064 sec
RG 208.6
DW 19.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 2.47 usec
P1 8.00 usec
PLW1 80.42400340 W
SFO2 400.1716007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 21.75399971 W
PLW12 0.17188001 W
PLW13 0.08645400 W

F2 - Processing parameters
SI 16384
SF 100.6228382 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

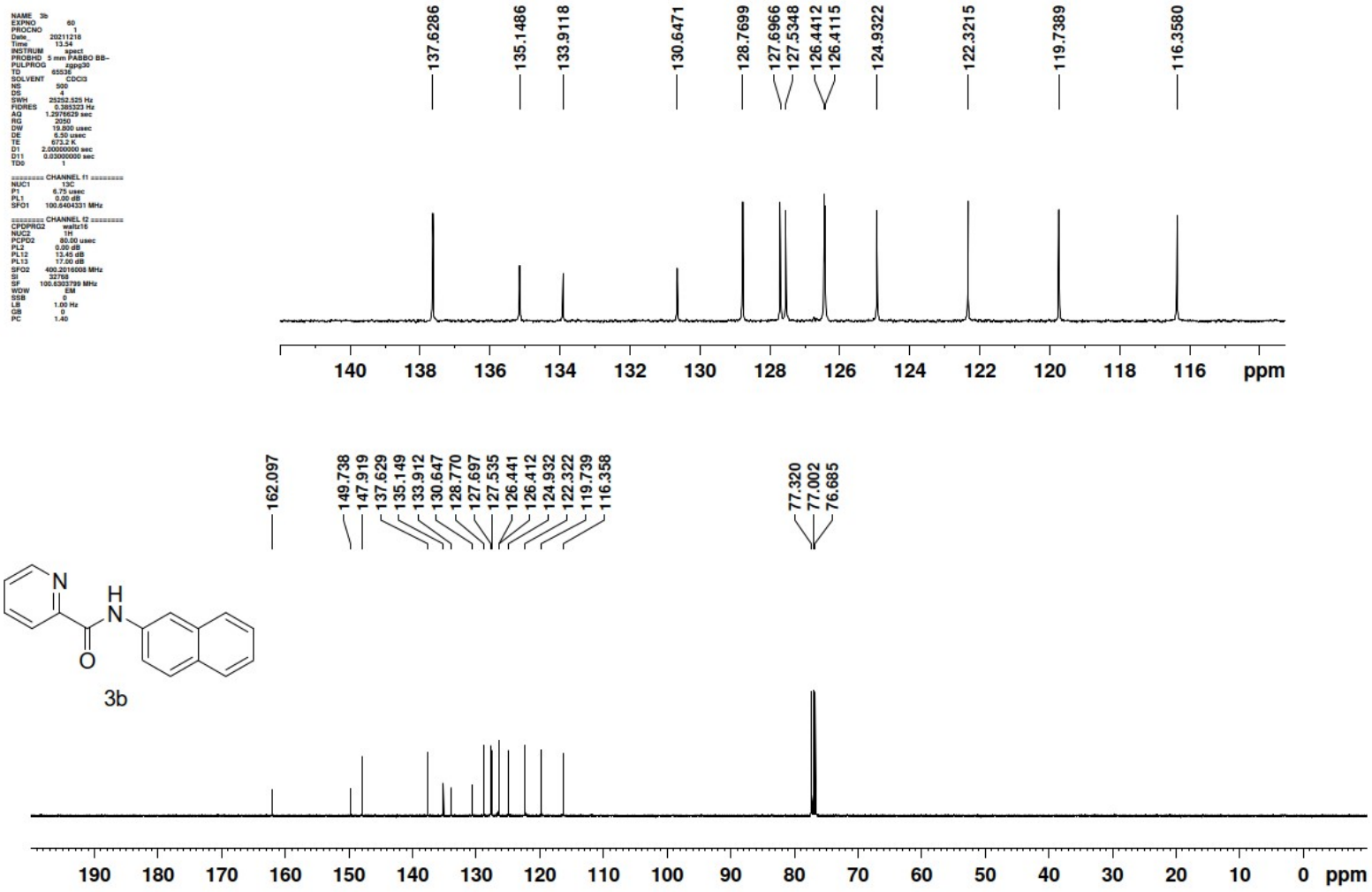
3a IN CDCl3-APT



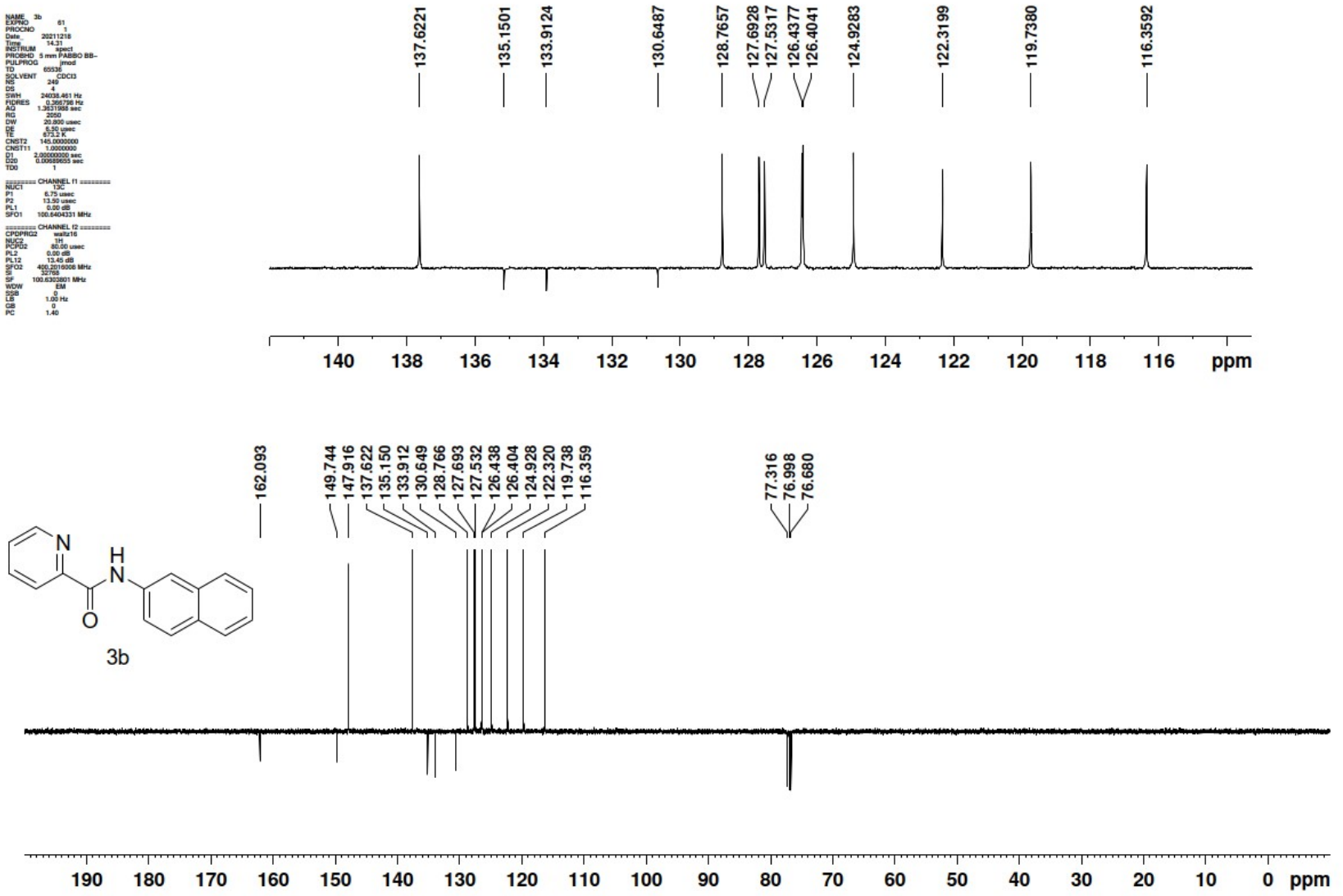
3b IN CDCl3


Current Data Parameters
NAME 3b
EXPNO 10
PROCNO 1
F2 – Acquisition Parameters
Date 20211122
Time 6.50 h
INSTRUM spect
PROBHD Z8246_0048 (PH
PULPROG zg30
TD 24036
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998964 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1024006 MHz
NUC1 1H
P0 6.00 usec
P1 18.00 usec
F2 – Processing parameters
SI 16384
SF 400.1000129 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.6681 8.6492 8.6375 8.5677 8.5008 8.3748 8.3490 8.3296 8.2852 7.9529 7.9495 7.9334 7.9300 7.9143 7.8769 7.8638 7.8425 7.8119 7.7927 7.7241 7.7197 7.7025 7.5162 7.4966 7.4872 7.4755 7.4567 7.4306 7.4105 7.3930 7.2501
1.00 1.01 0.96 0.92 1.91 1.02 1.01 1.96 1.04
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
10.1985 8.6681 8.6492 8.6375 8.5677 8.5008 8.3748 8.3490 8.3296 8.2852 7.9529 7.9495 7.9334 7.9300 7.9143 7.8769 7.8638 7.8425 7.8119 7.7927 7.7241 7.7197 7.7025 7.5162 7.4966 7.4872 7.4755 7.4567 7.4306 7.4105 7.3930 7.2501
3.5574 3.4901
1.9971 1.6722 1.6382 1.5609 1.4915 1.2582 1.2435
N
H
N
O
3b
0.99 1.00 1.01 0.96 0.92 1.91 1.02 1.01 1.96 1.04
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

3b IN CDCl3–13C



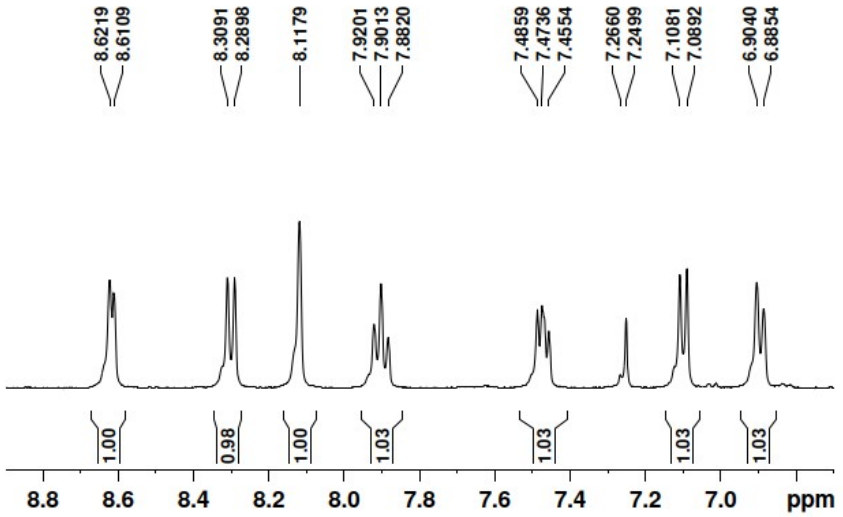
3b IN CDCl3–APT

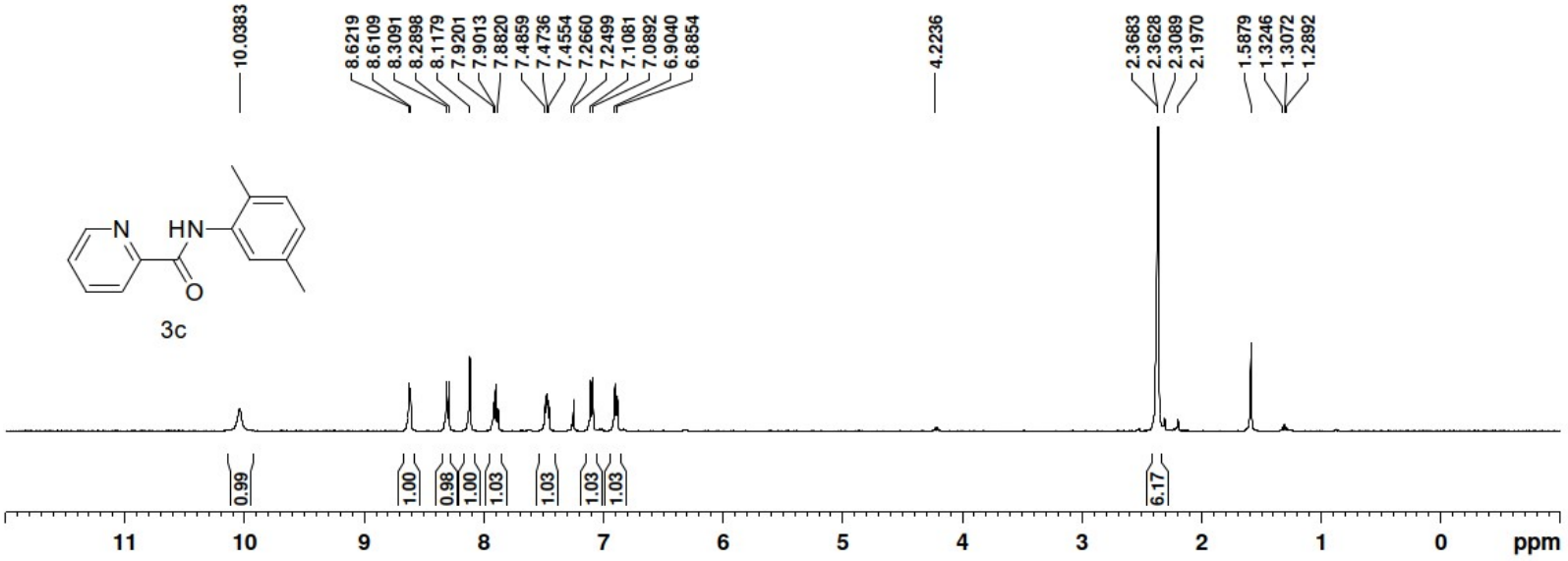


3c IN CDCl3

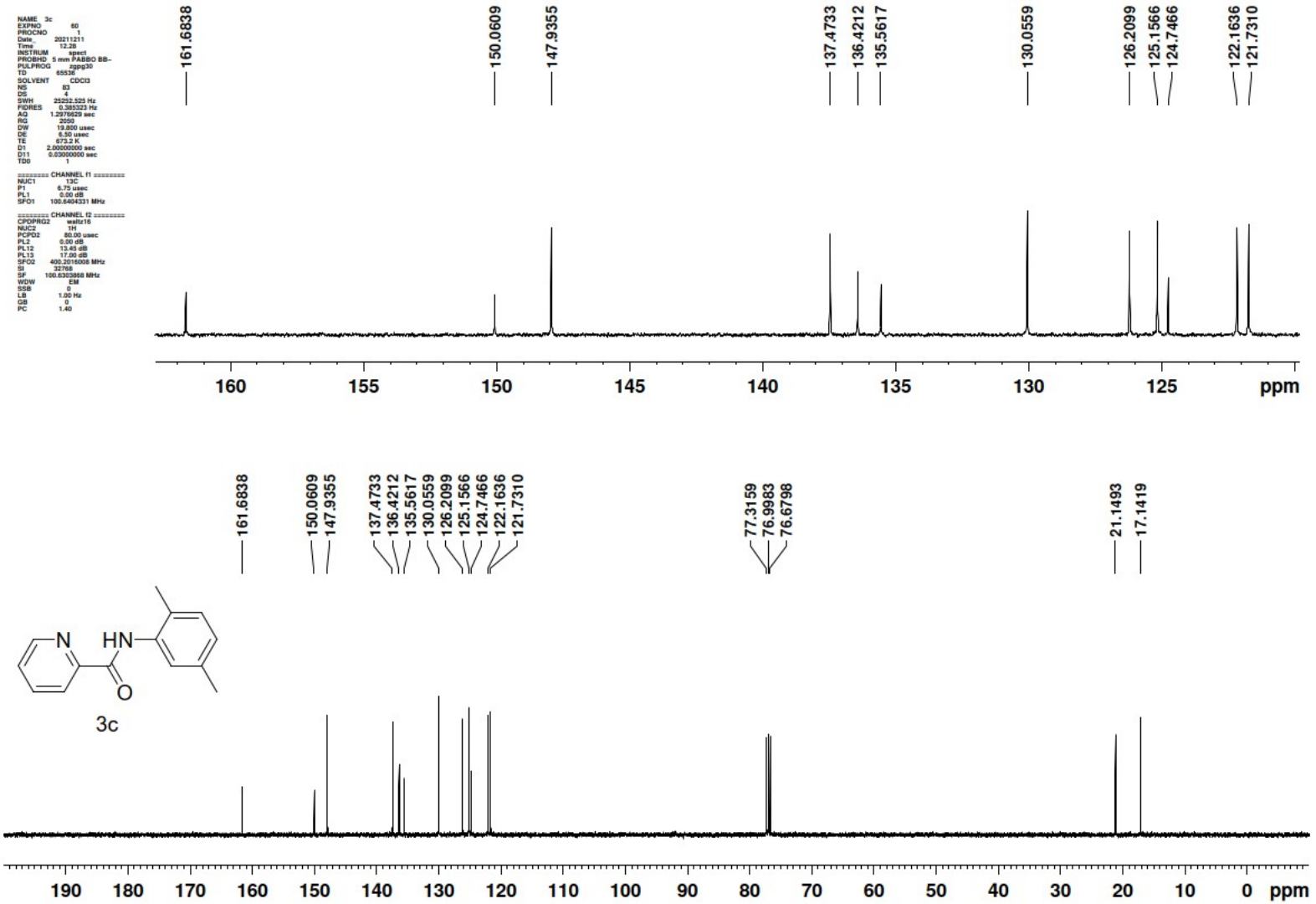
```
NAME   3c
EXPNO        10
PROCNO        1
Date_      20211211
Time_         12.21
INSTRUM       spect
PROBHD_ 5 mm PABBO BB-
PULPROG       zg30
TD           24576
SOLVENT       CDCl3
NS               8
DS               0
SWH        8012.820 Hz
FIDRES        0.326043 Hz
AQ         1.5335923 sec
RG             256
DW          62.400 usec
DE           6.50 usec
TE           673.2 K
D1         1.00000000 sec
TD0              1

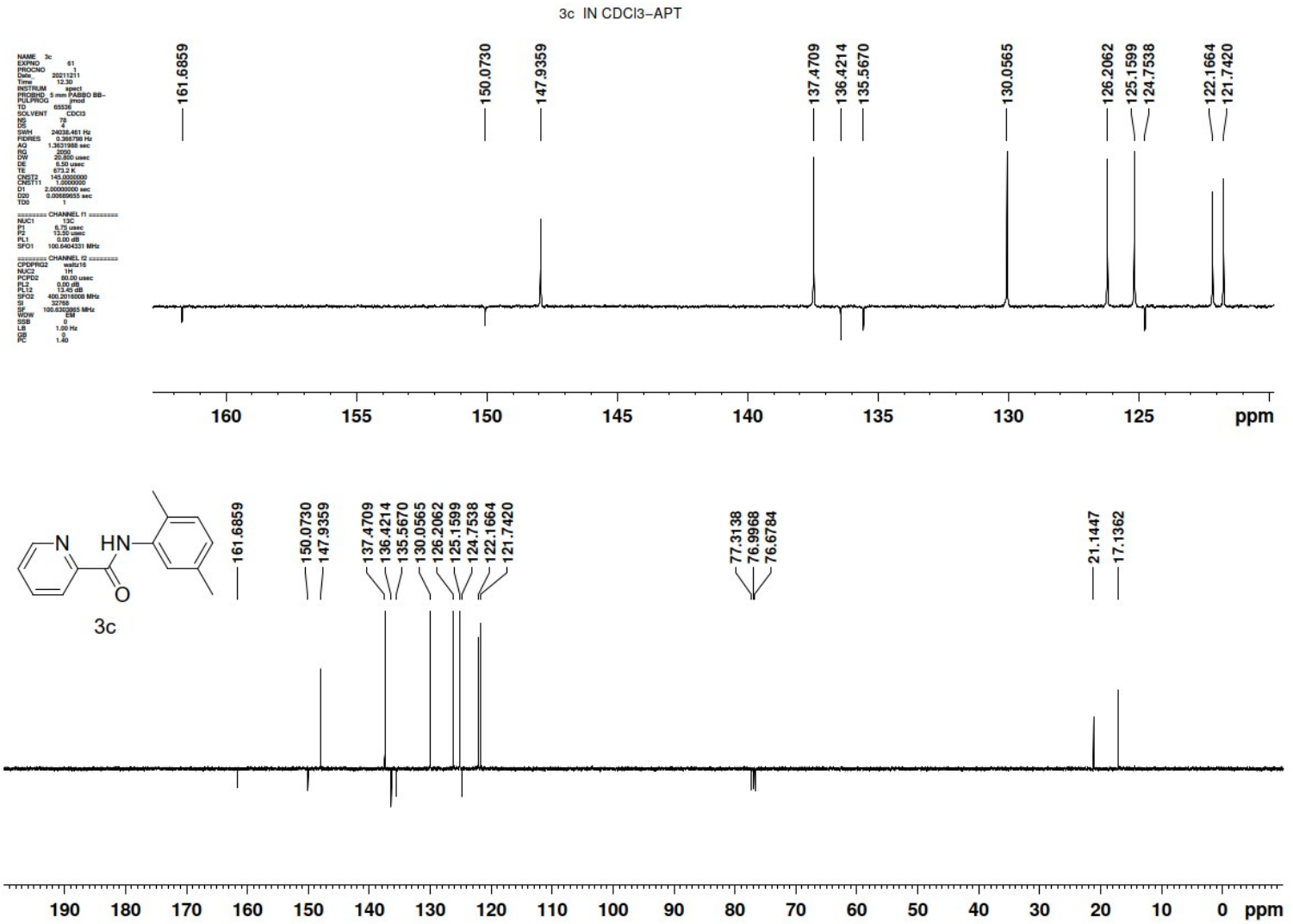
======== CHANNEL f1 ========
NUC1           1H
P1          17.00 usec
PL1          0.00 dB
SFO1    400.2024714 MHz
SI           16384
SF      400.2000182 MHz
WDW            EM
SSB              0
LB            0.30 Hz
GB               0
PC            1.00
```





3c IN CDCl3-13C



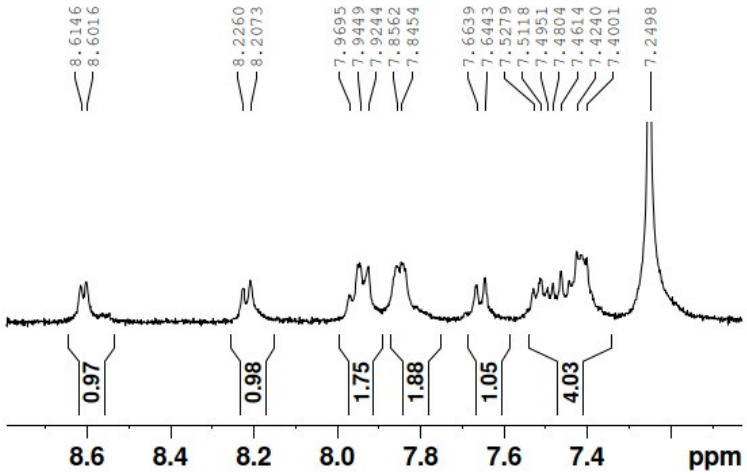

3c IN CDCl3–APT
NAME 3c
EXPNO 61
PROCNO 1
Date_ 20211211
Time 12.30
INSTRUM spect
PROBHD 5 mm PABBO BB–
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 72
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00680655 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.75 usec
P2 13.50 usec
PL1 0.00 dB
SFO1 100.6404331 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 13.45 dB
SFO2 400.2016008 MHz
SI 32768
SF 100.6303655 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
161.6859
150.0730
147.9359
137.4709
136.4214
135.5670
130.0565
126.2062
125.1599
124.7538
122.1664
121.7420
160
155
150
145
140
135
130
125
ppm
N
HN
O
3c
161.6859
150.0730
147.9359
137.4709
136.4214
135.5670
130.0565
126.2062
125.1599
124.7538
122.1664
121.7420
77.3138
76.9968
76.6784
21.1447
17.1362
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

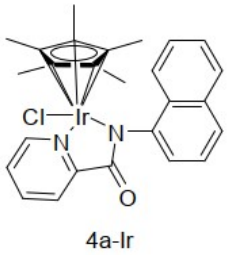
4a-Ir IN CDCl3

```
Current Data Parameters
NAME      4a-Ir
EXPNO             10
PROCNO             1

F2 - Acquisition Parameters
Date_        20220518
Time              0.09 h
INSTRUM          spect
PROBHD   Z8246_0048 (PH
PULPROG          zg30
TD              24036
SOLVENT          CDCl3
NS                 8
DS                 0
SWH           8012.820 Hz
FIDRES        0.666735 Hz
AQ            1.4998465 sec
RG                128
DW             62.400 usec
DE              6.50 usec
TE             300.0 K
D1          1.00000000 sec
TD0                1
SFO1        400.1024006 MHz
NUC1               1H
P0              6.00 usec
P1             18.00 usec
PLW1       10.00000000 W

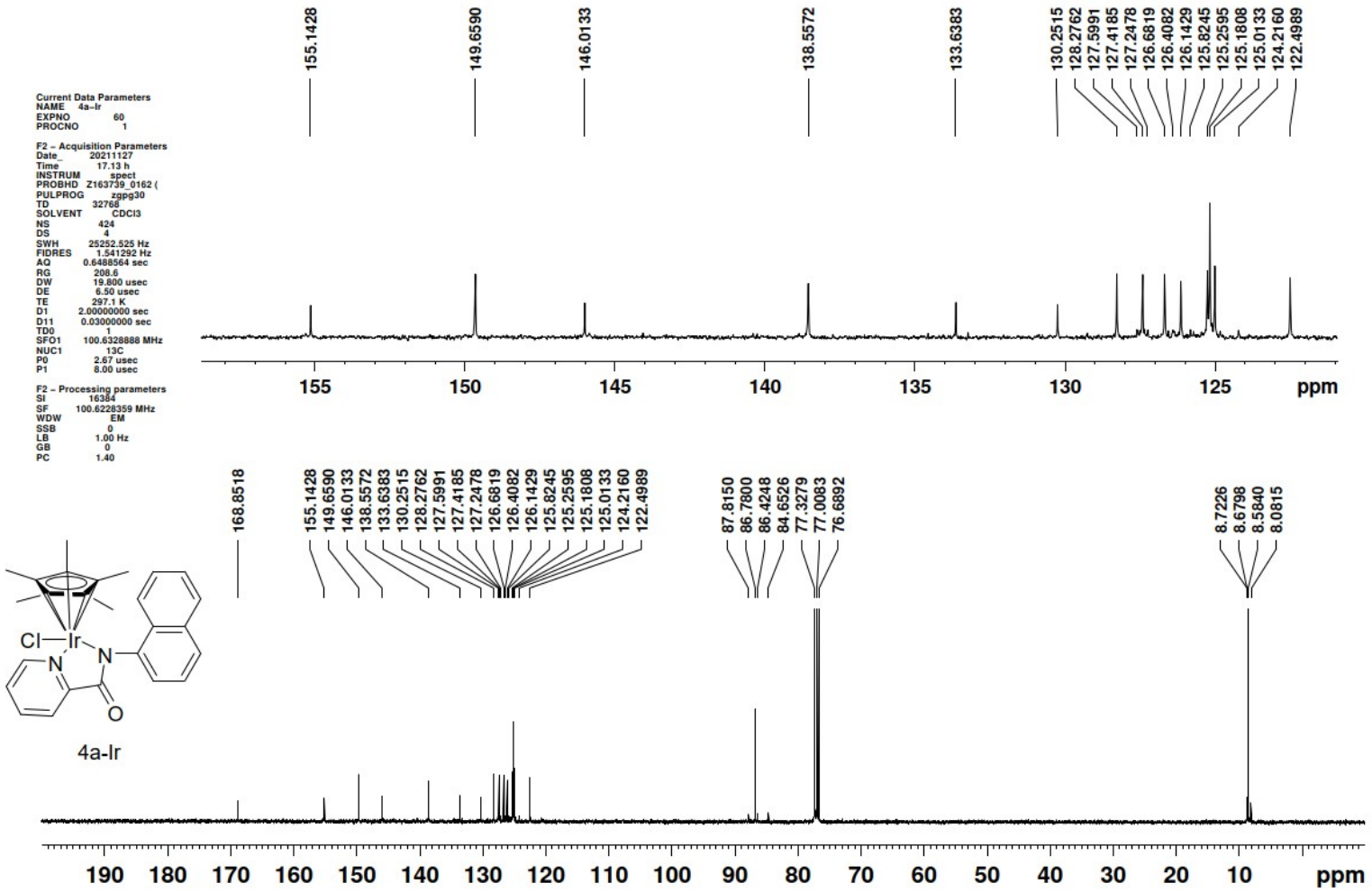
F2 - Processing parameters
SI             16384
SF          400.1000139 MHz
WDW               EM
SSB                0
LB                 0 Hz
GB                 0
PC              1.00
```





4a-Ir

4a–Ir IN CDCl3–13C

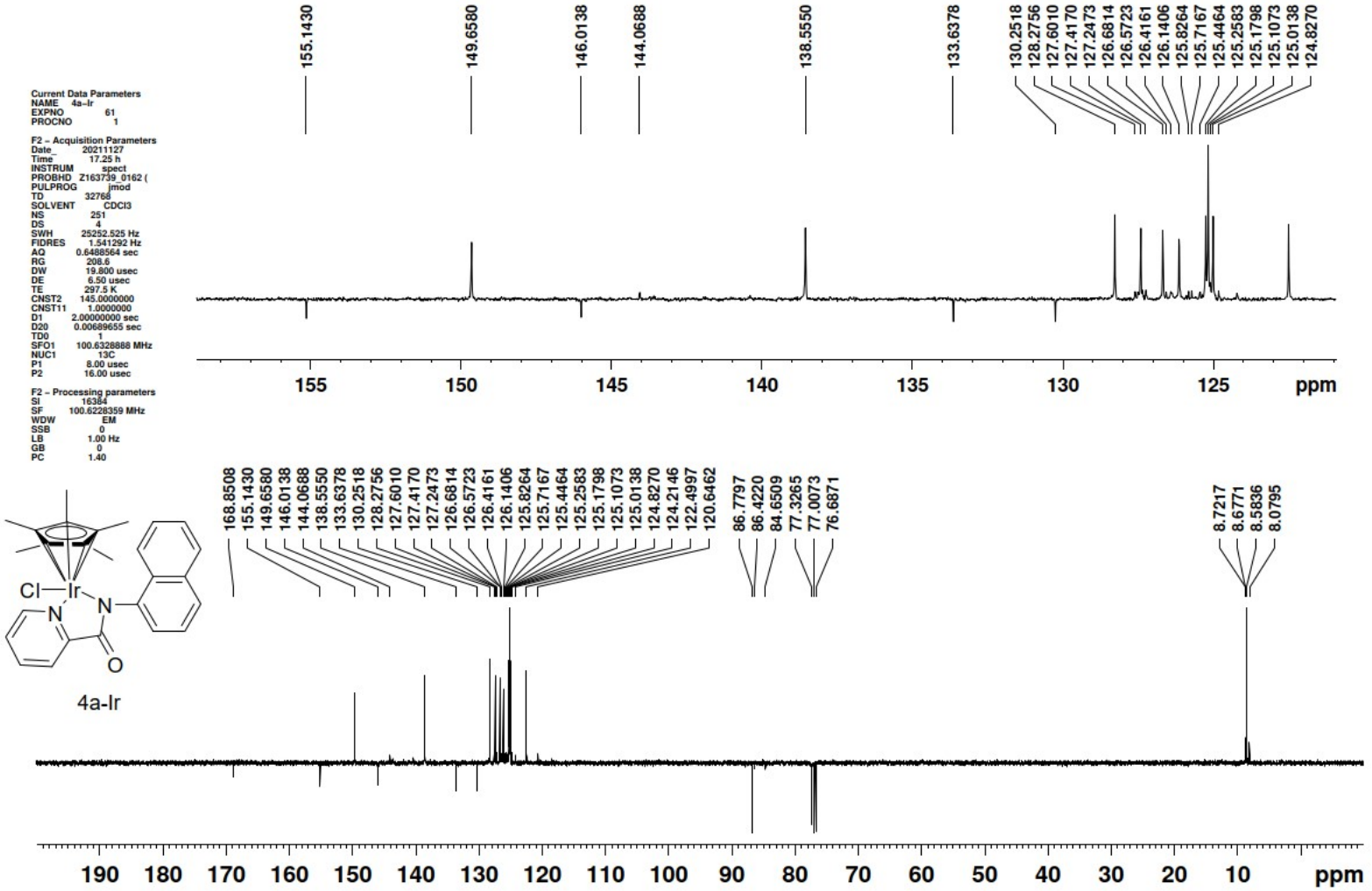


Current Data Parameters
NAME 4a–Ir
EXPNO 60
PROCNO 1

F2 – Acquisition Parameters
Date_ 20211127
Time 17.13 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 424
DS 4
SWH 25252.525 Hz
FIDRES 1.541292 Hz
AQ 0.6488564 sec
RG 208.6
DW 19.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec

F2 – Processing parameters
SI 16384
SF 100.6228359 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4a–Ir IN CDCl3–APT

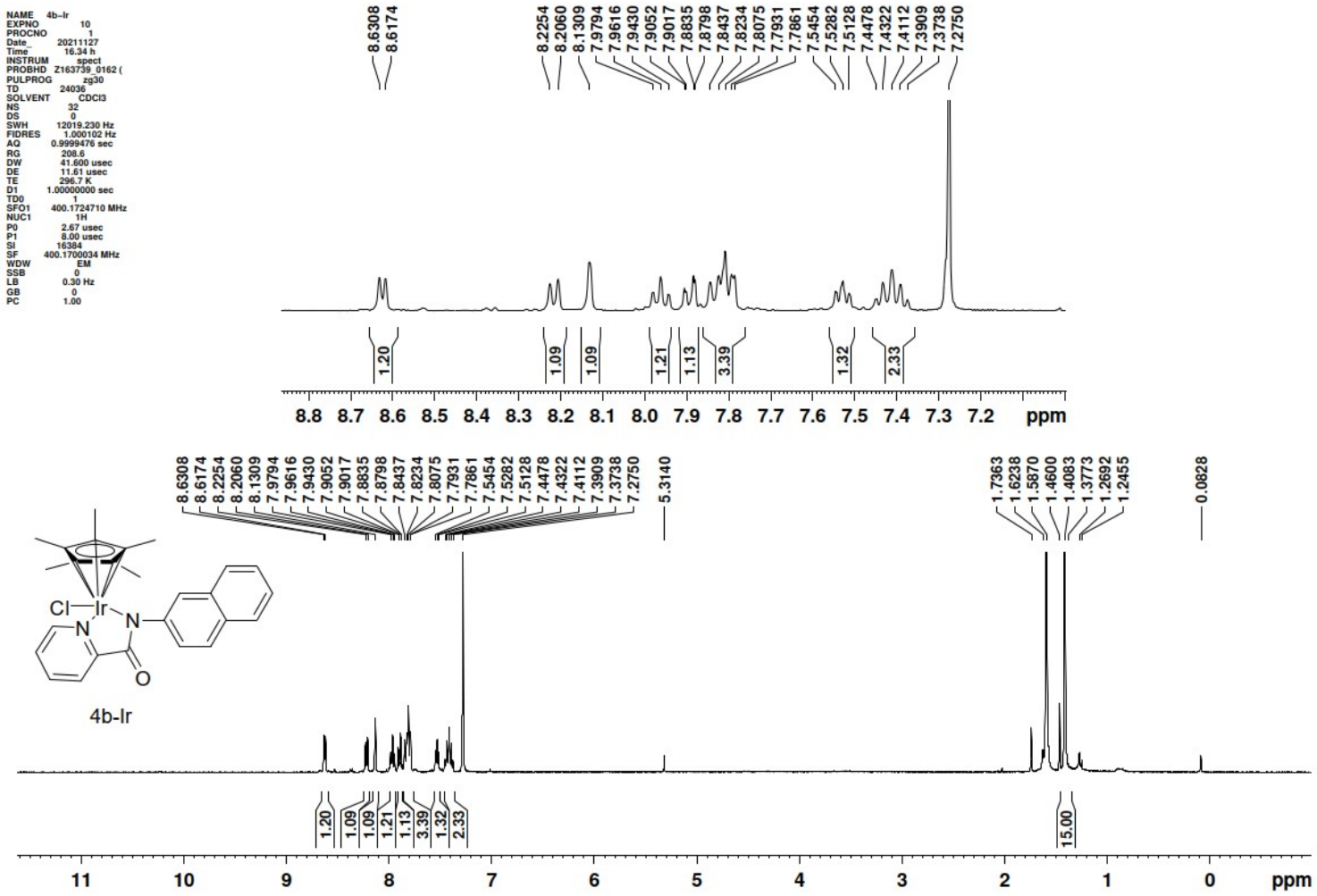


Current Data Parameters
NAME 4a–Ir
EXPNO 61
PROCNO 1

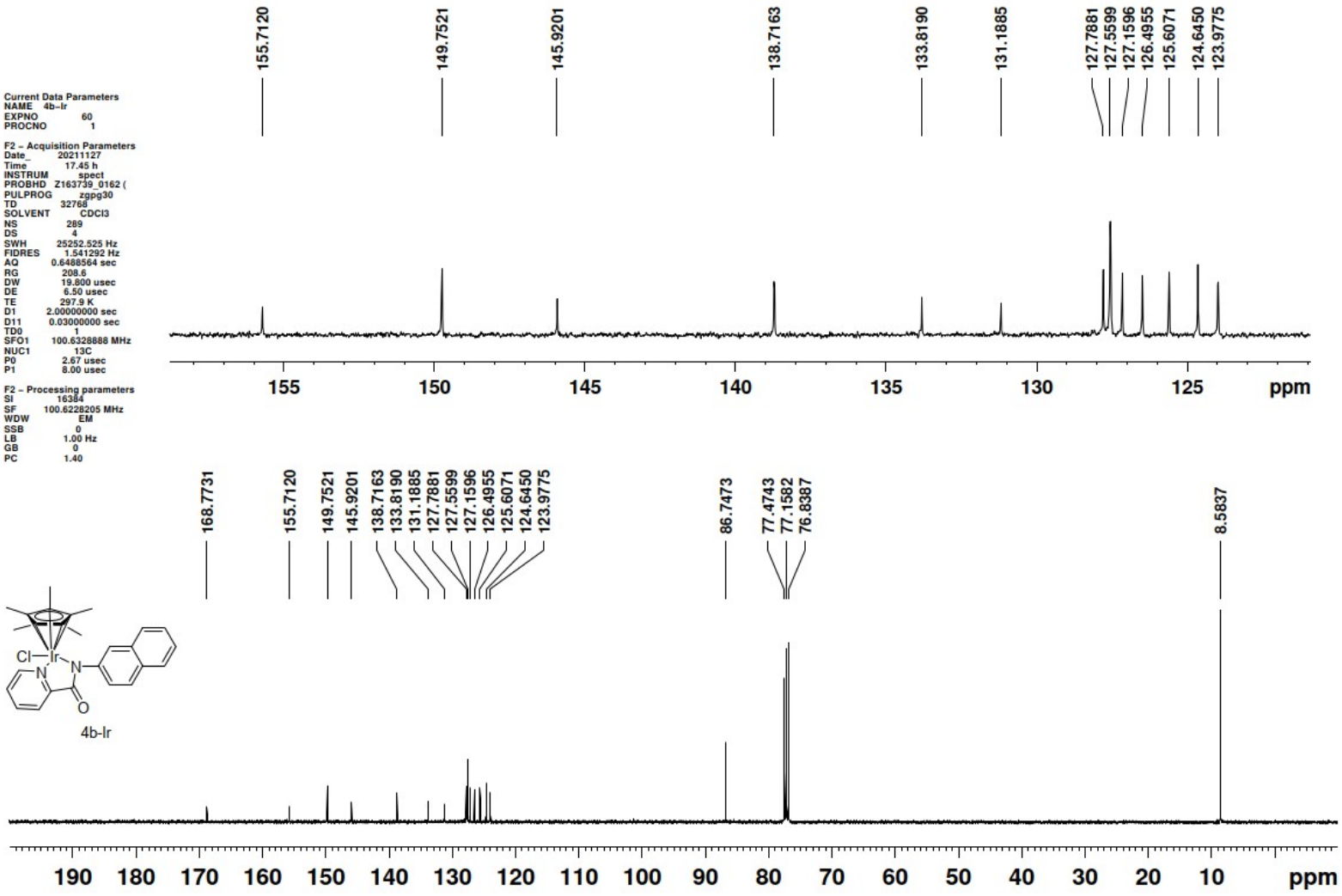
F2 – Acquisition Parameters
Date_ 20211127
Time 17.25 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG jmod
TD 32768
SOLVENT CDCl3
NS 251
DS 4
SWH 25252.525 Hz
FIDRES 1.541292 Hz
AQ 0.6488564 sec
RG 208.6
DW 19.800 usec
DE 6.50 usec
TE 297.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec

F2 – Processing parameters
SI 16384
SF 100.6228359 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4b–Ir IN CDCl3



4b–Ir IN CDCl3–13C

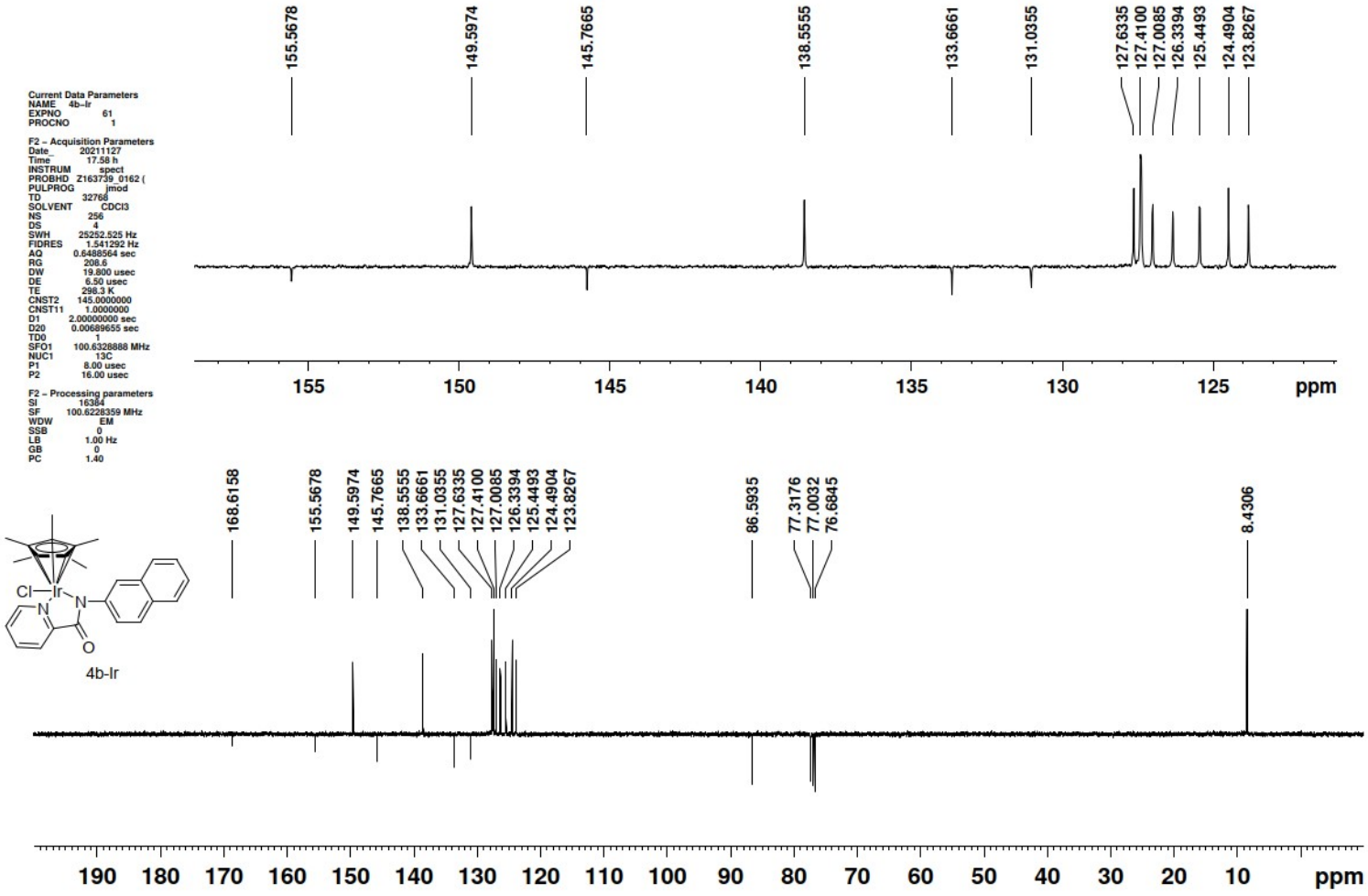


Current Data Parameters
NAME 4b–Ir
EXPNO 60
PROCNO 1

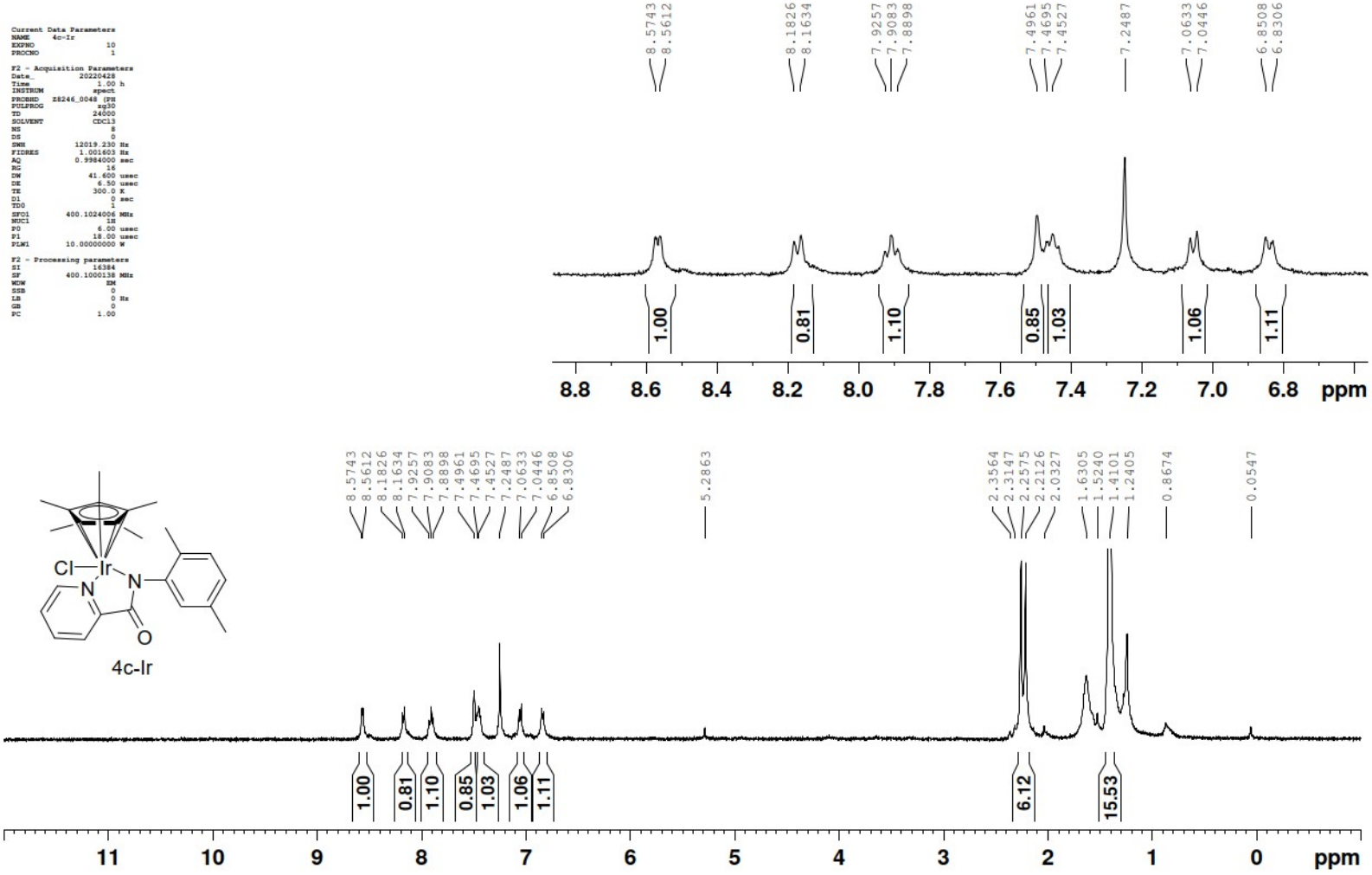
F2 – Acquisition Parameters
Date_ 20211127
Time 17.45 h
INSTRUM spect
PROBHD Z163739_0162 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 289
DS 4
SWH 25252.525 Hz
FIDRES 1.541292 Hz
AQ 0.6488564 sec
RG 208.6
DW 19.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec

F2 – Processing parameters
SI 16384
SF 100.6228205 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

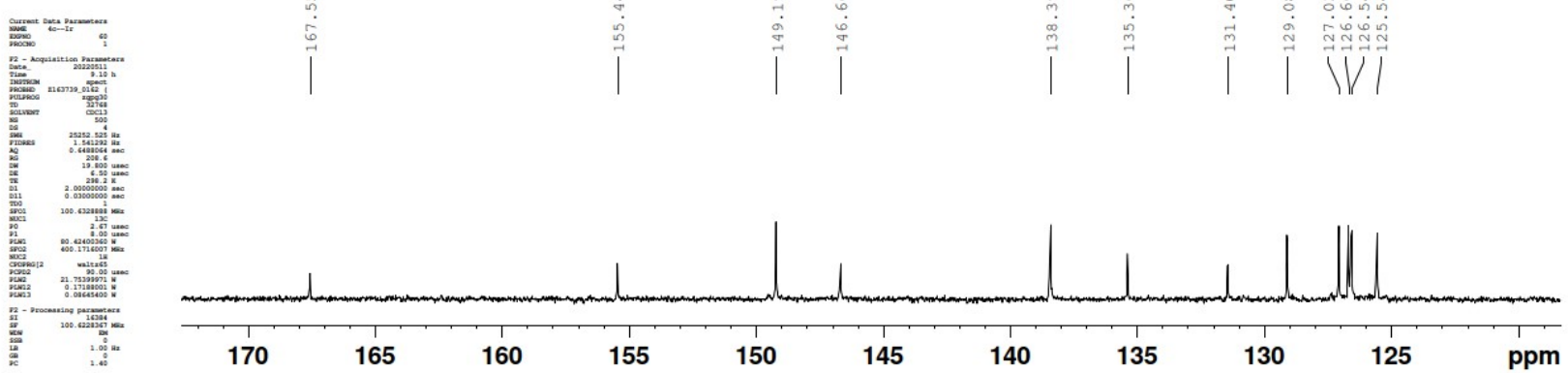
4b–Ir IN CDCl3–APT

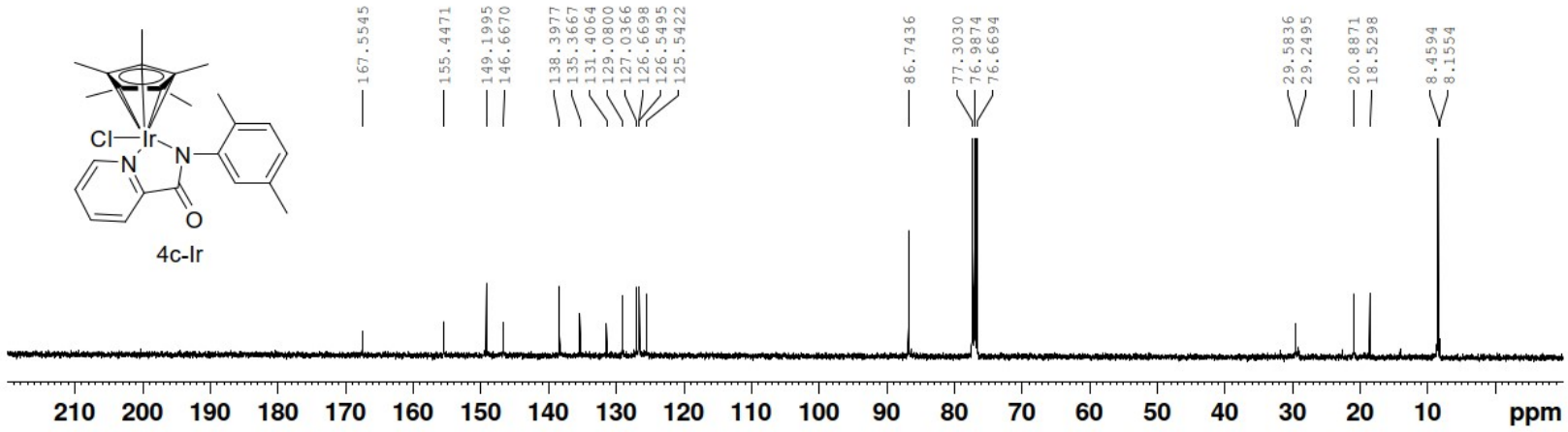


4c-Ir IN CDC13

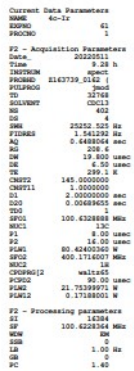


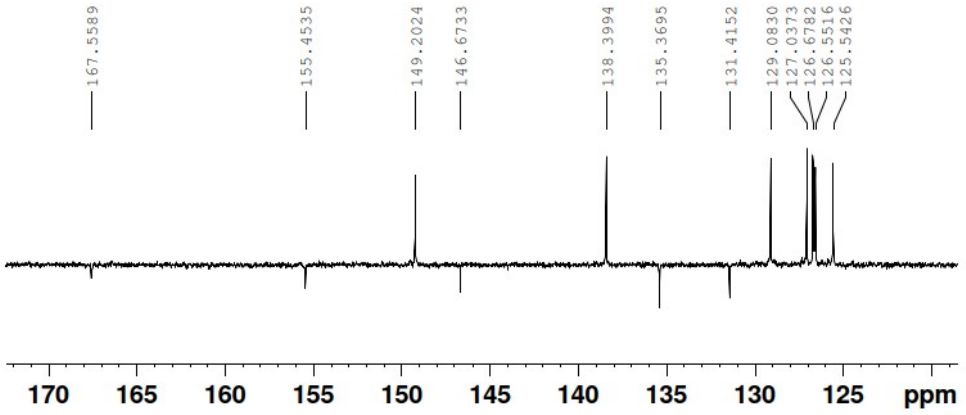
4c-Ir IN CDCl3-13C

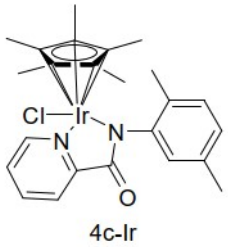




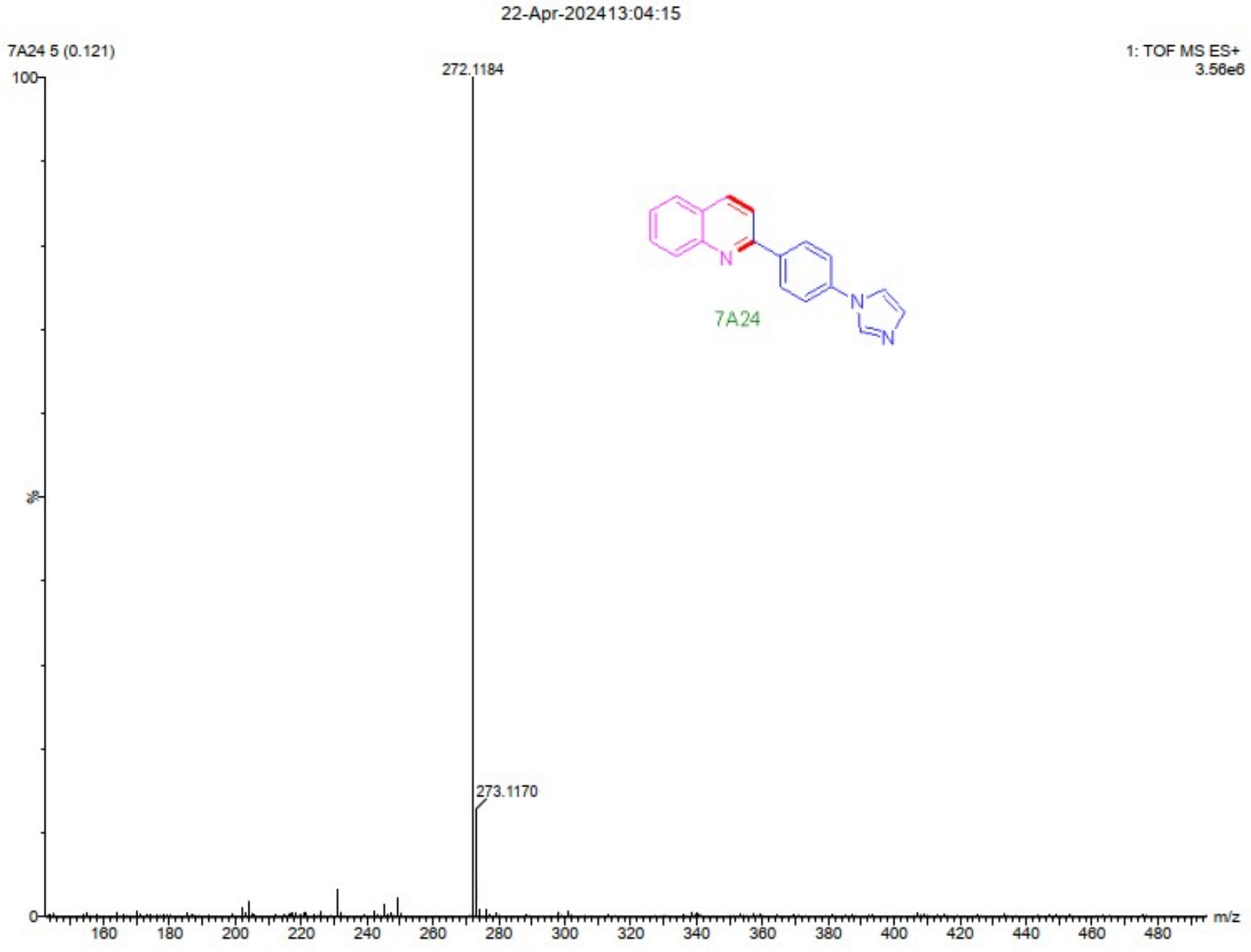
4c-Ir IN CDCl3-APT







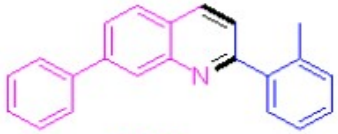
4c-Ir


22-Apr-202413:04:15
7A24 5 (0.121)
1: TOF MS ES+
3.56e6
100
272.1184
%
273.1170
0
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
m/z
N
N
N
7A24

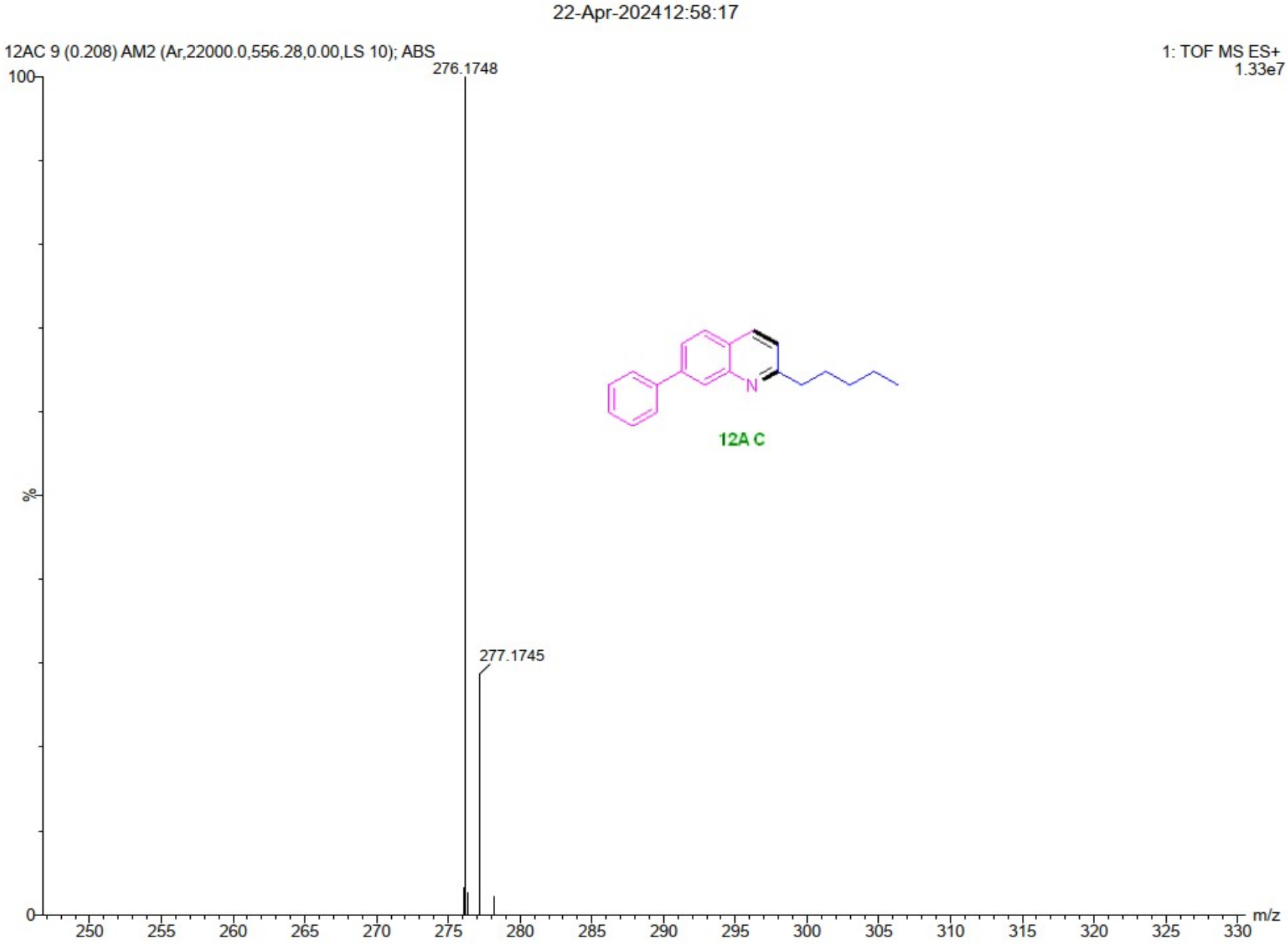
22-Apr-202416:20:08

12AB 9 (0.208) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
1.30e7



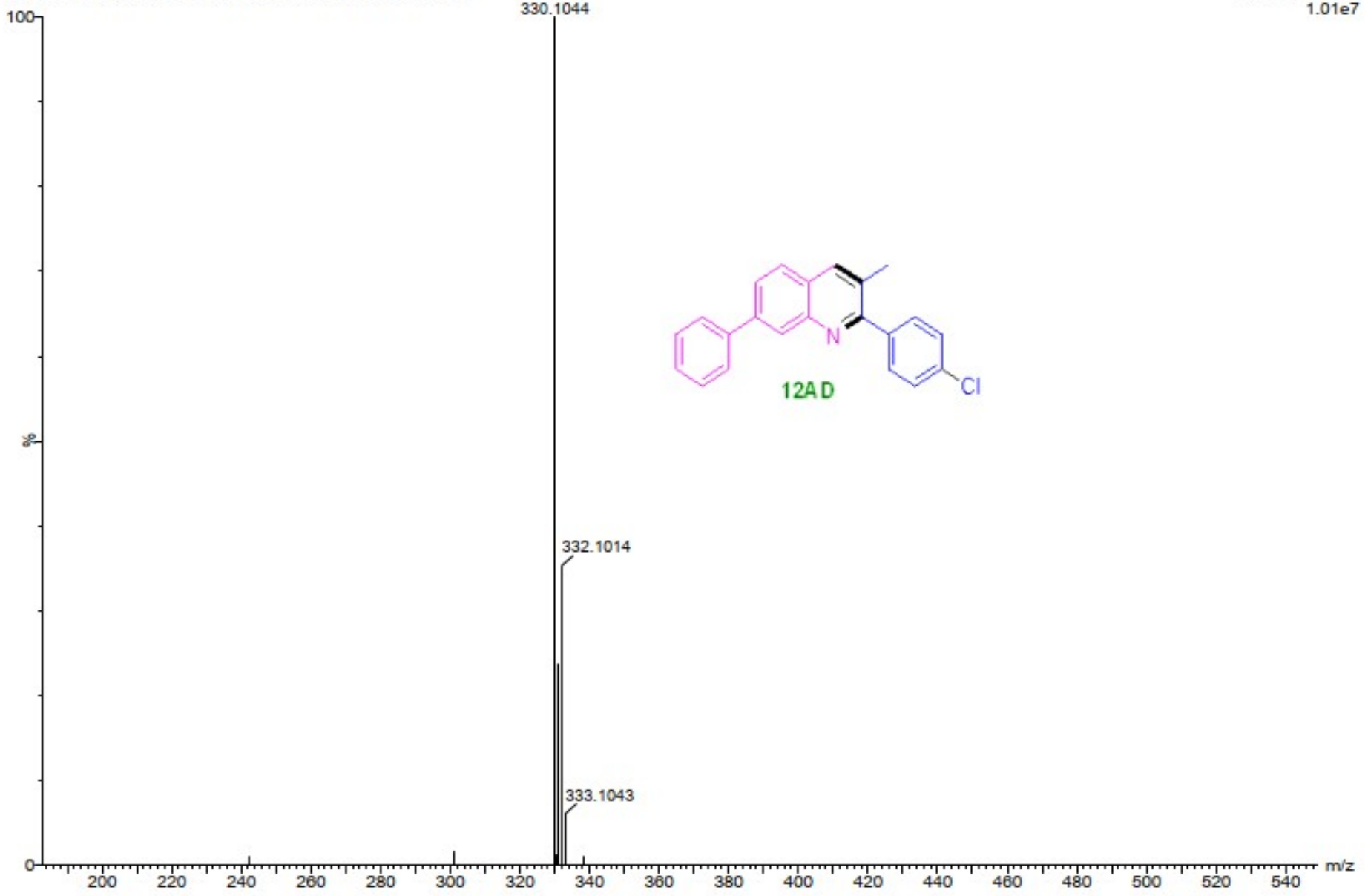
12AB


22-Apr-202412:58:17
12AC 9 (0.208) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
1.33e7
276.1748
277.1745
100
%
0
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
325
330
m/z
N
12A C

PKT22-Apr-202415:49:09

12AD 10 (0.225) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

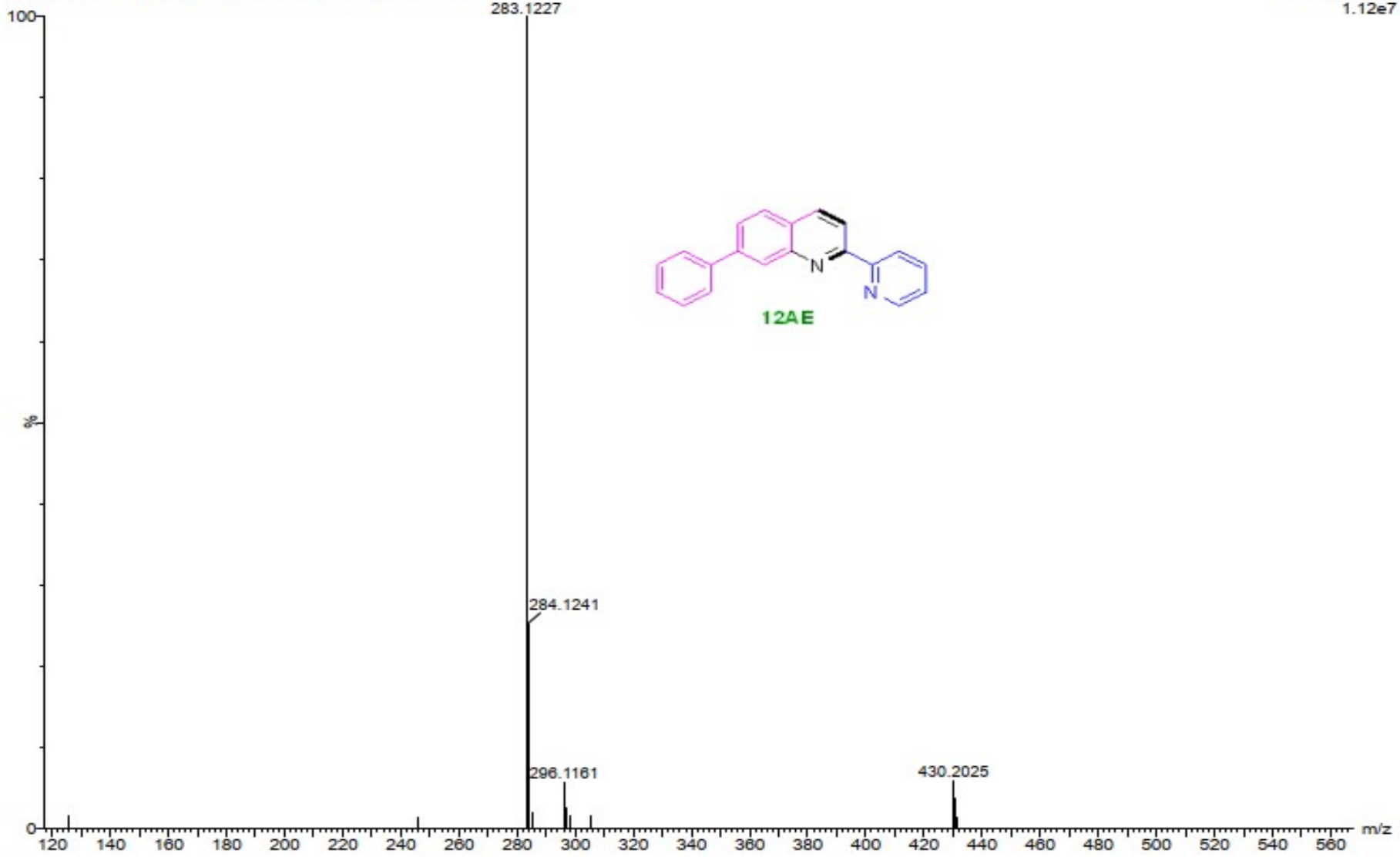
1: TOF MS ES+
1.01e7



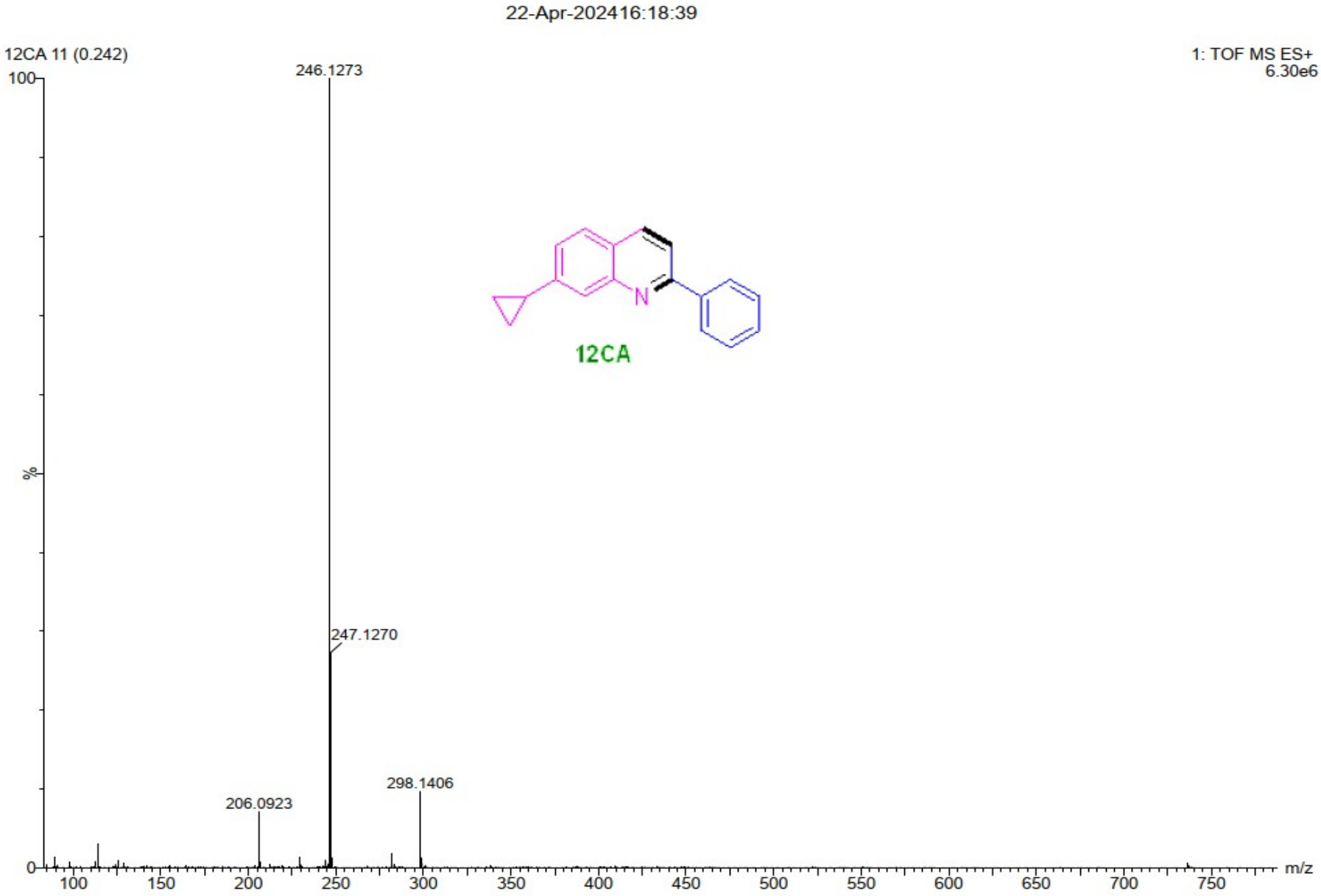
22-Apr-202416:48:59

12AE 6 (0.138) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
1.12e7



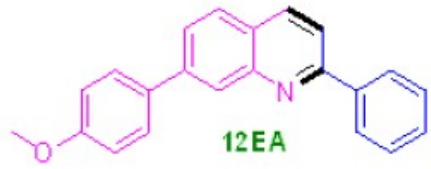
12AE

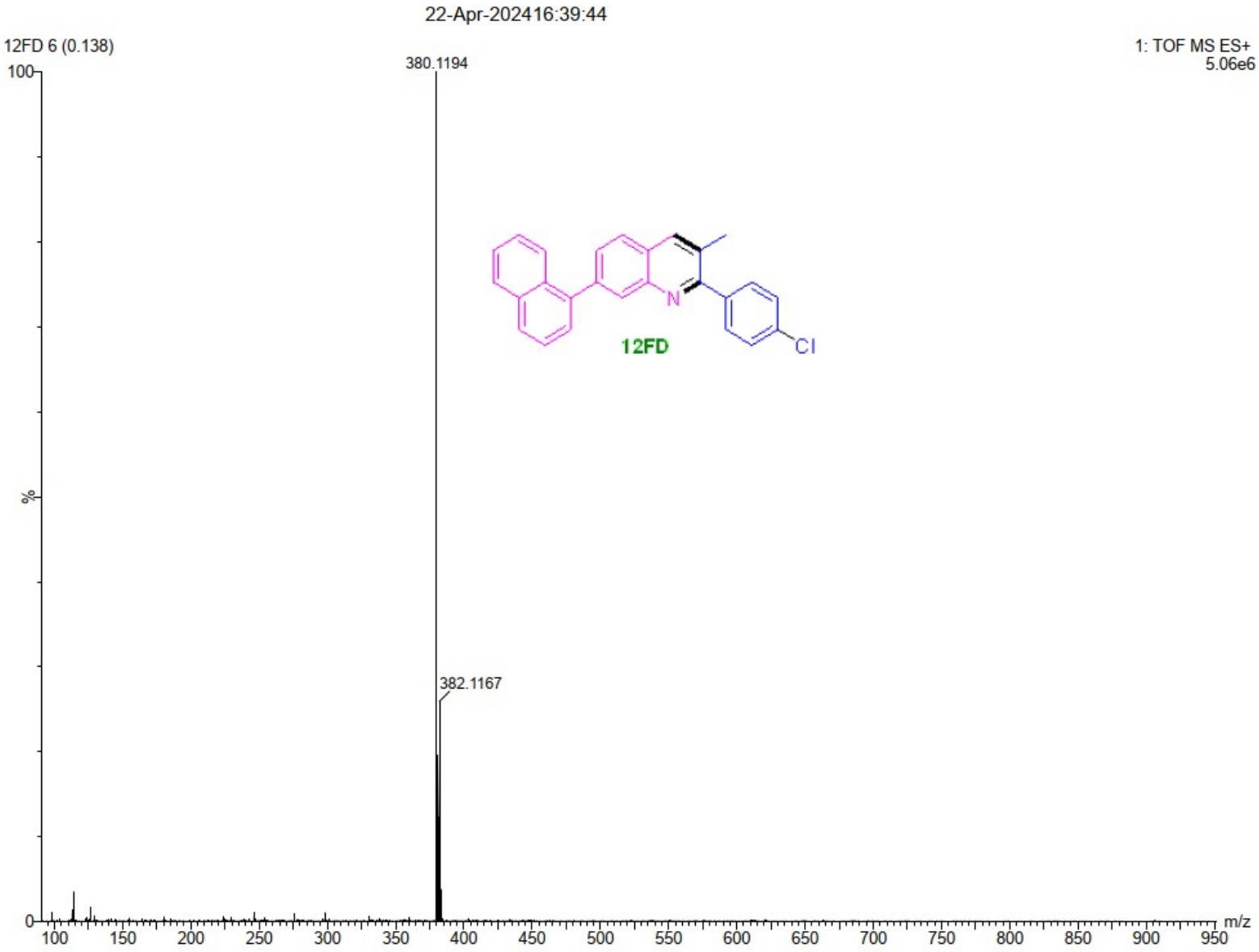

22-Apr-202416:18:39
12CA 11 (0.242)
1: TOF MS ES+
6.30e6
100
%
0
246.1273
247.1270
298.1406
206.0923
N
12CA
100
150
200
250
300
350
400
450
500
550
600
650
700
750
m/z

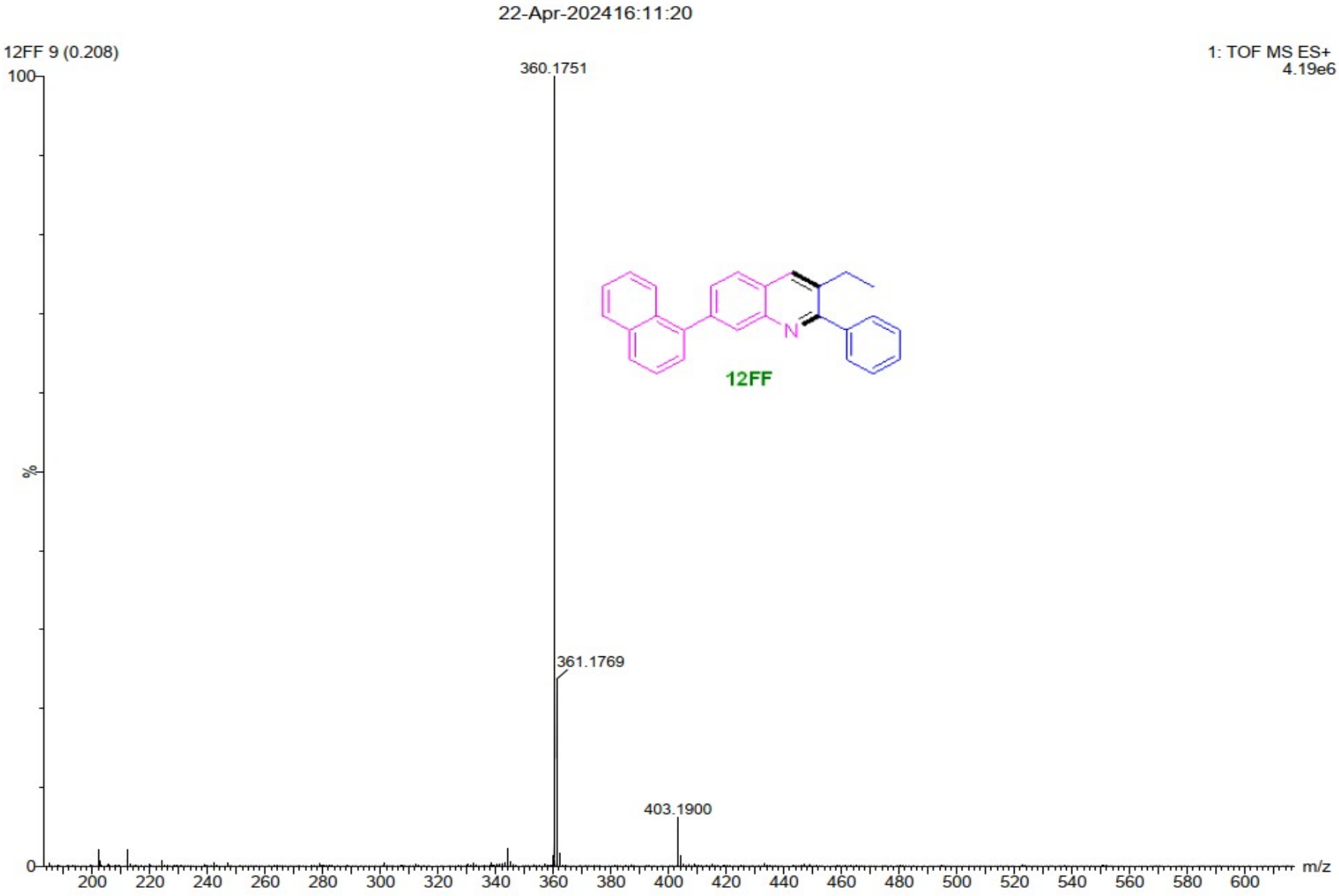
22-Apr-202412:53:22

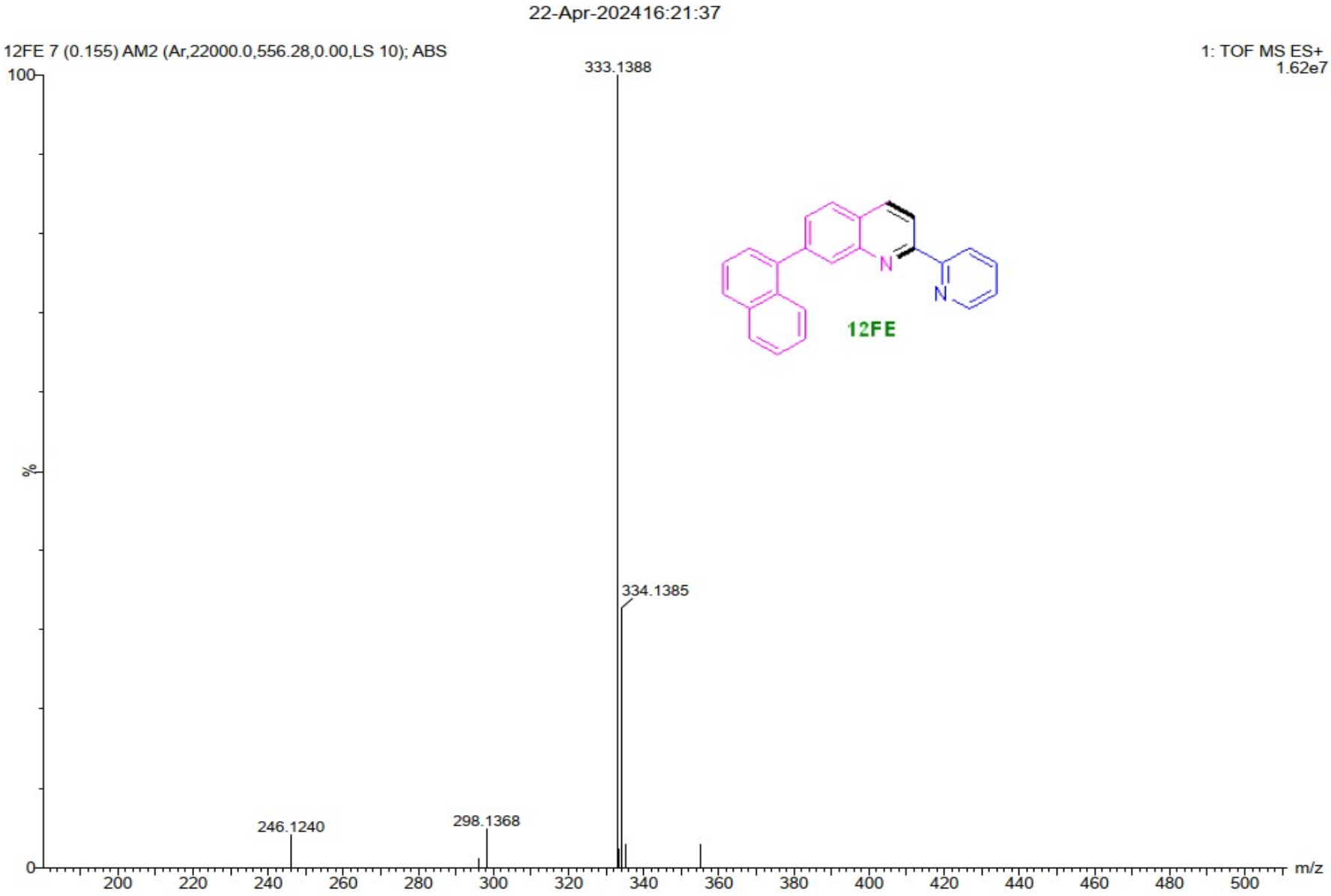
12EA 4 (0.104) AM2 (Ar,22000.0,556.27,0.00,LS 10); ABS

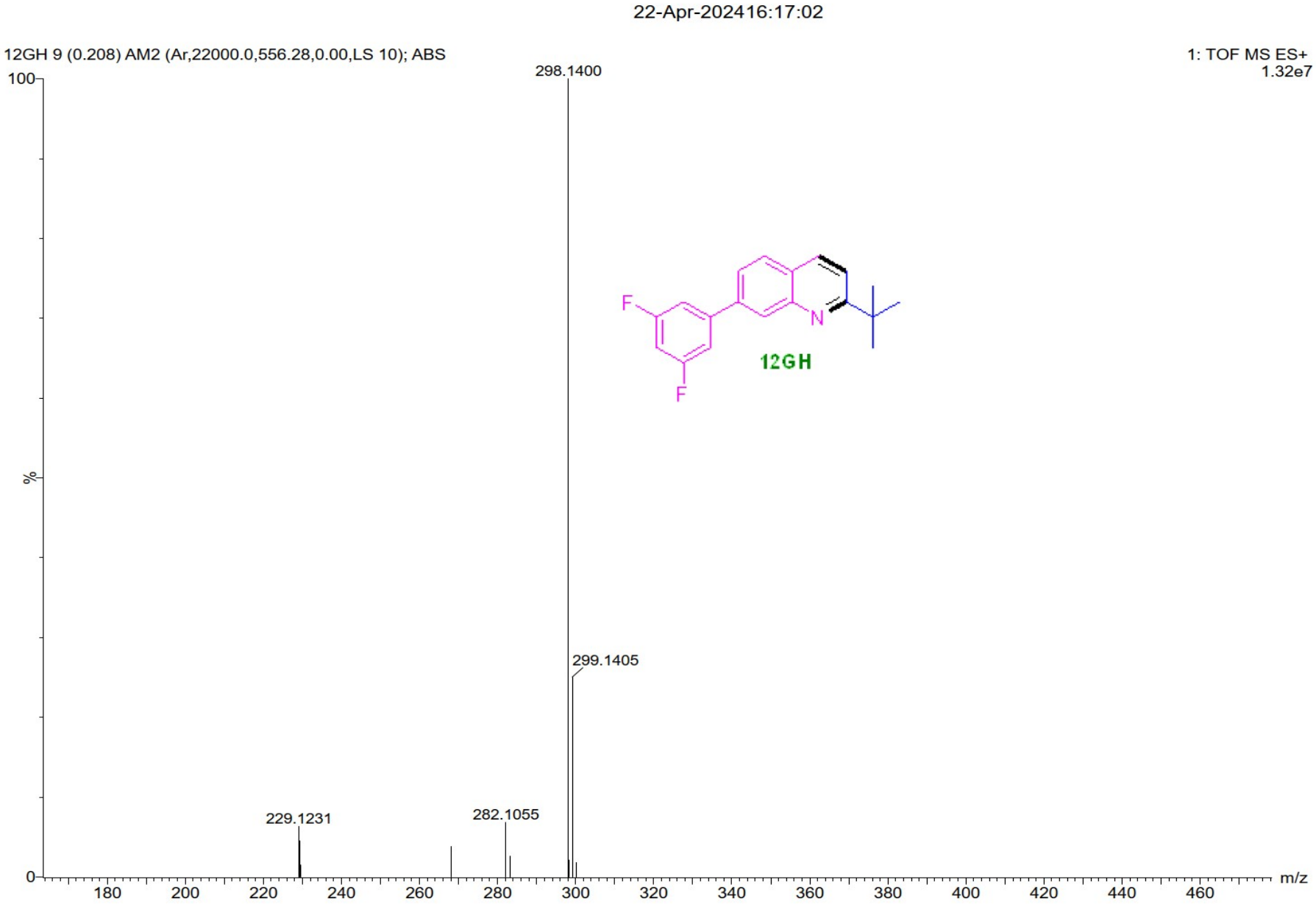
1: TOF MS ES+
3.29e7

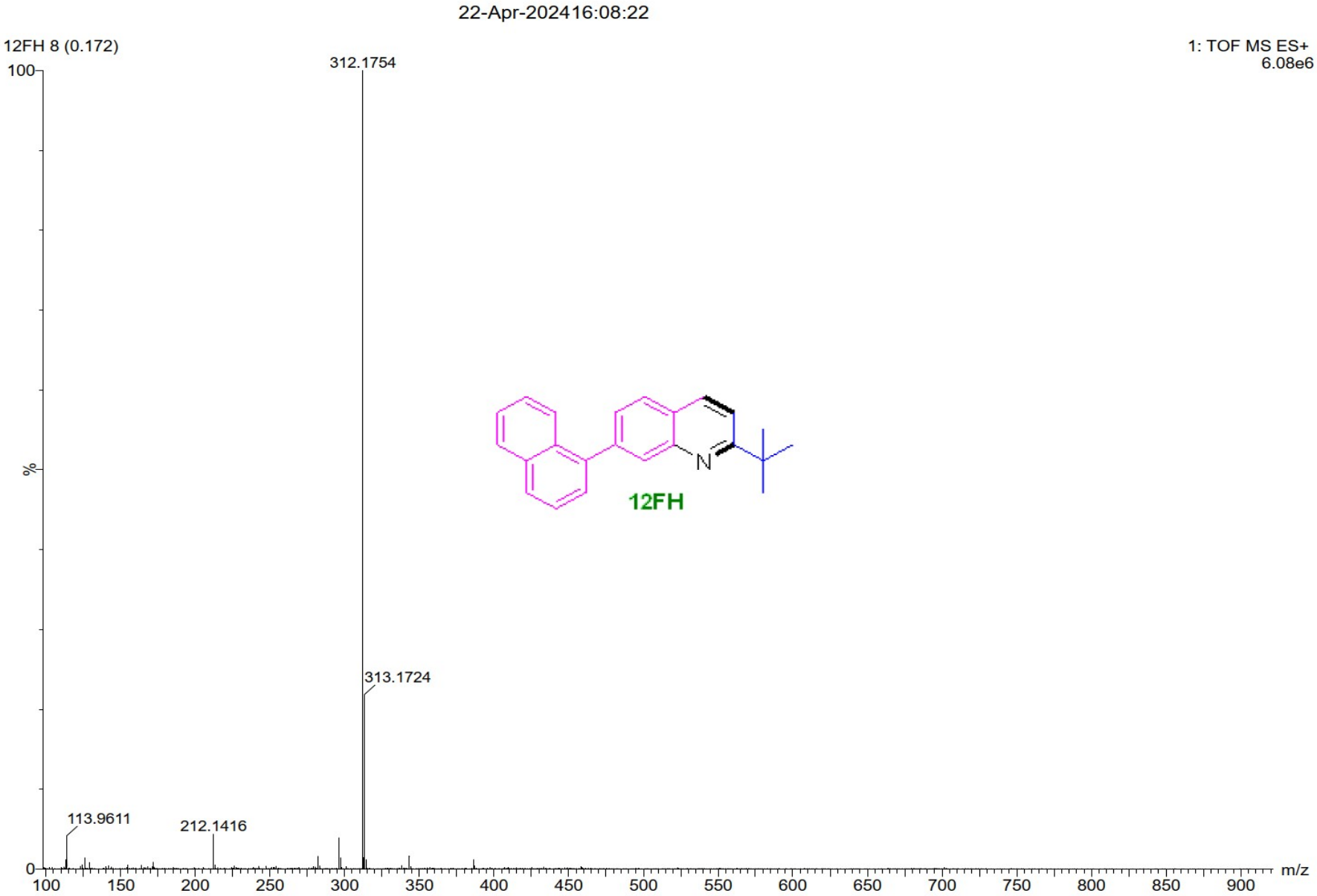



22-Apr-202416:39:44
12FD 6 (0.138)
1: TOF MS ES+
5.06e6
100
%
0
380.1194
382.1167
N
Cl
12FD
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
m/z


22-Apr-202416:11:20
12FF 9 (0.208)
1: TOF MS ES+
4.19e6
100
%
0
360.1751
361.1769
403.1900
N
12FF
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
m/z


22-Apr-202416:21:37
12FE 7 (0.155) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
1.62e7
100
%
0
333.1388
334.1385
246.1240
298.1368
N
N
12FE
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
m/z

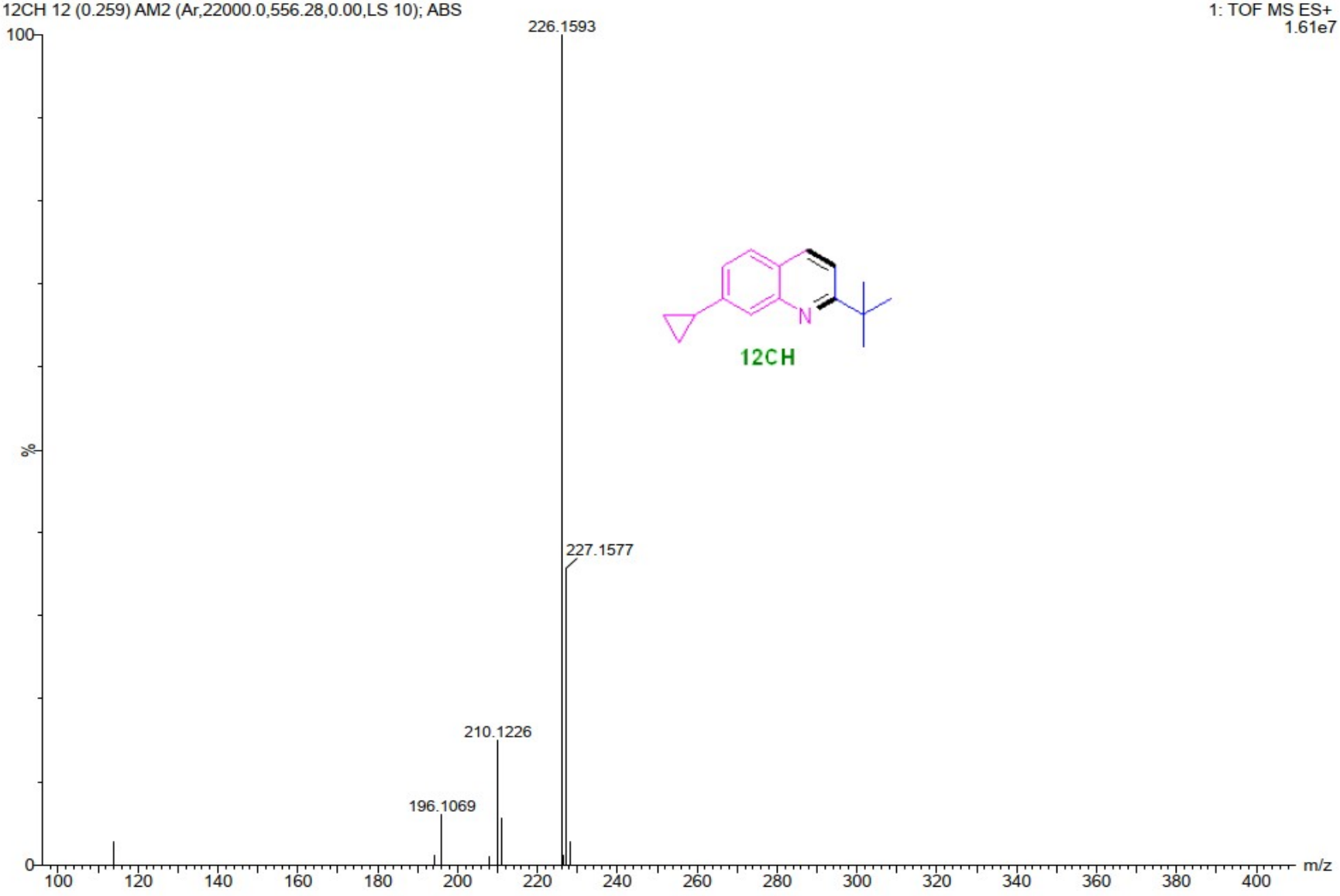

22-Apr-202416:17:02
12GH 9 (0.208) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
1.32e7
100
%
0
298.1400
299.1405
229.1231
282.1055
F
F
N
12GH
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
m/z

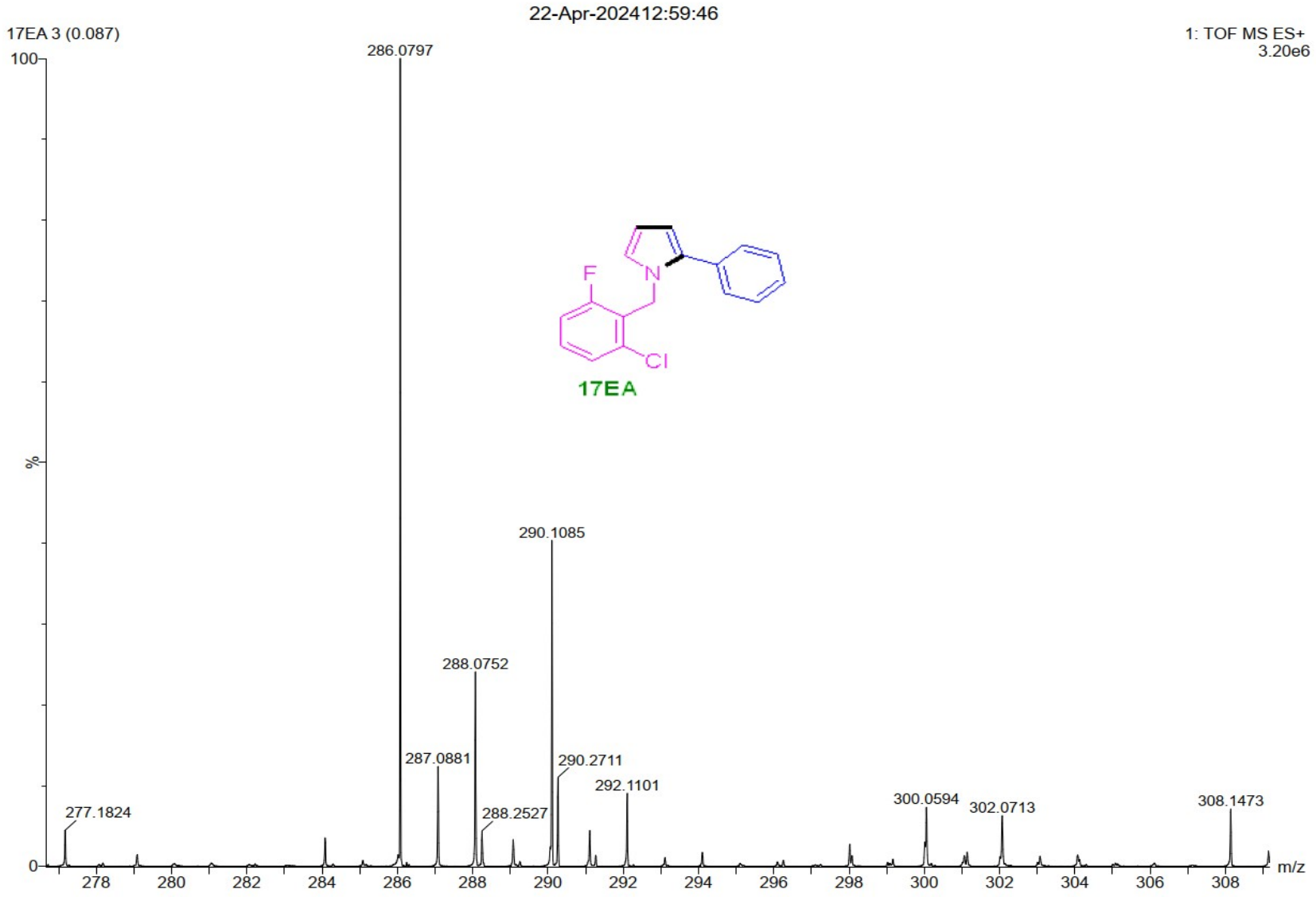

22-Apr-202416:08:22
12FH 8 (0.172)
1: TOF MS ES+
6.08e6
100
%
0
312.1754
313.1724
113.9611
212.1416
N
12FH
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z

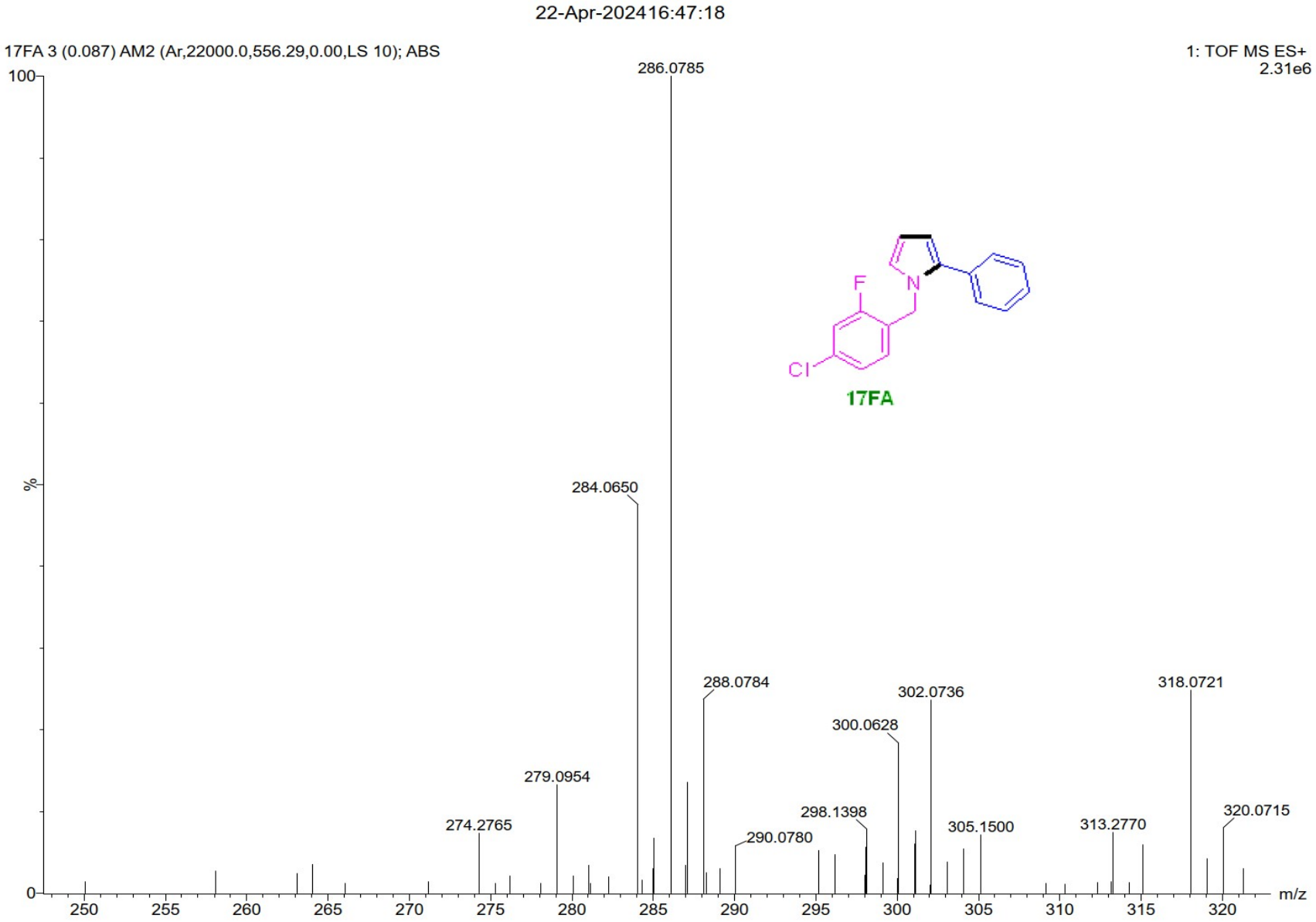
22-Apr-202416:50:37

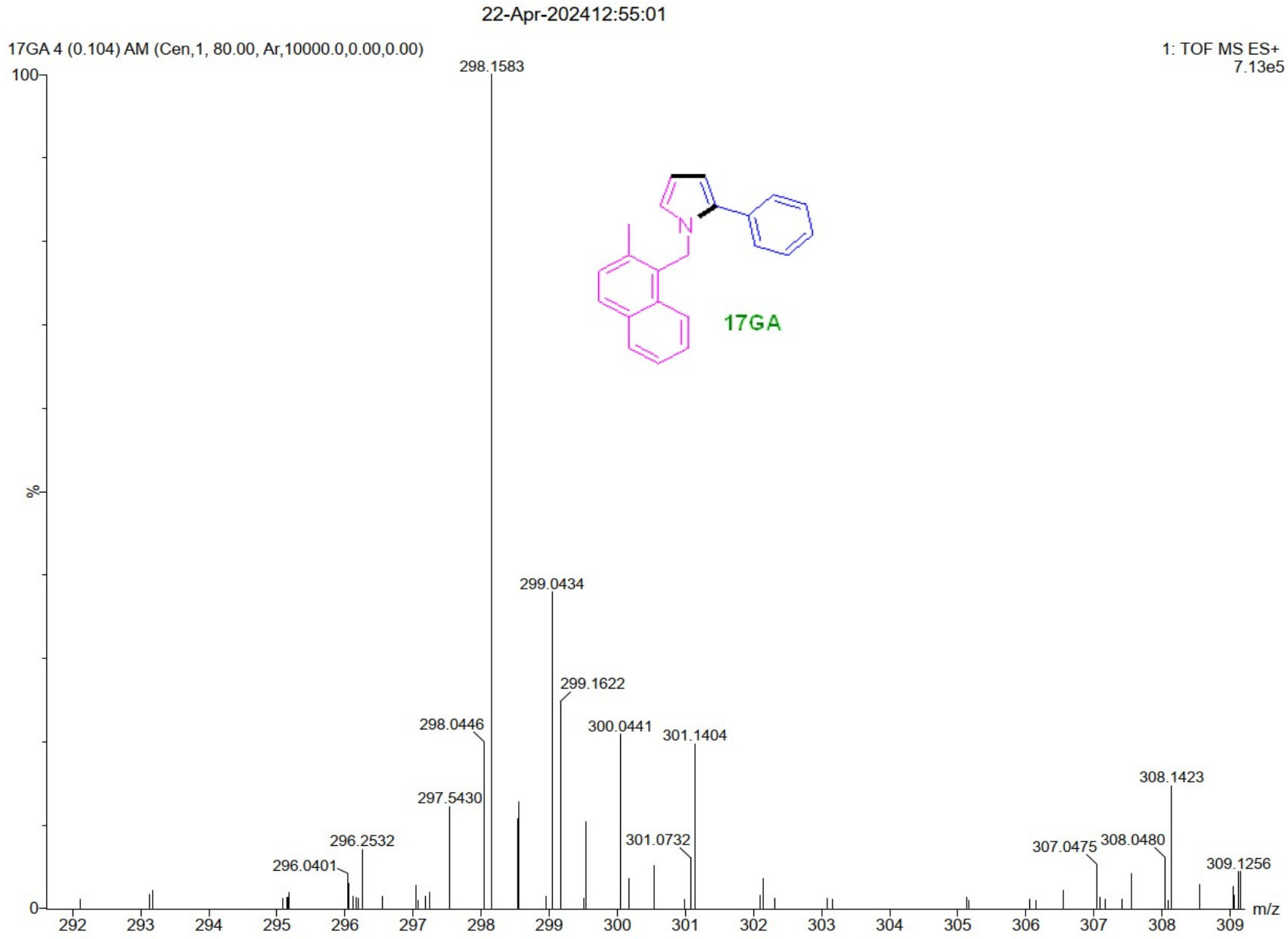
12CH 12 (0.259) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
1.61e7




22-Apr-202412:59:46
17EA 3 (0.087)
1: TOF MS ES+
3.20e6
100
%
0
286.0797
290.1085
288.0752
287.0881
290.2711
292.1101
277.1824
288.2527
300.0594
302.0713
308.1473
278
280
282
284
286
288
290
292
294
296
298
300
302
304
306
308
m/z
F
N
Cl
17EA

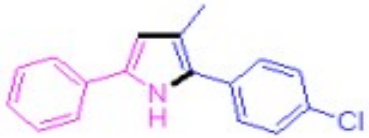

22-Apr-202416:47:18
17FA 3 (0.087) AM2 (Ar,22000.0,556.29,0.00,LS 10); ABS
1: TOF MS ES+
2.31e6
100
%
0
286.0785
284.0650
288.0784
302.0736
318.0721
300.0628
279.0954
298.1398
320.0715
274.2765
290.0780
305.1500
313.2770
F
N
Cl
17FA
250
255
260
265
270
275
280
285
290
295
300
305
310
315
320
m/z


22-Apr-202412:55:01
17GA 4 (0.104) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00)
1: TOF MS ES+
7.13e5
100
%
0
298.1583
299.0434
299.1622
298.0446
300.0441
301.1404
297.5430
308.1423
296.2532
301.0732
307.0475
308.0480
296.0401
309.1256
N
17GA
292
293
294
295
296
297
298
299
300
301
302
303
304
305
306
307
308
309
m/z

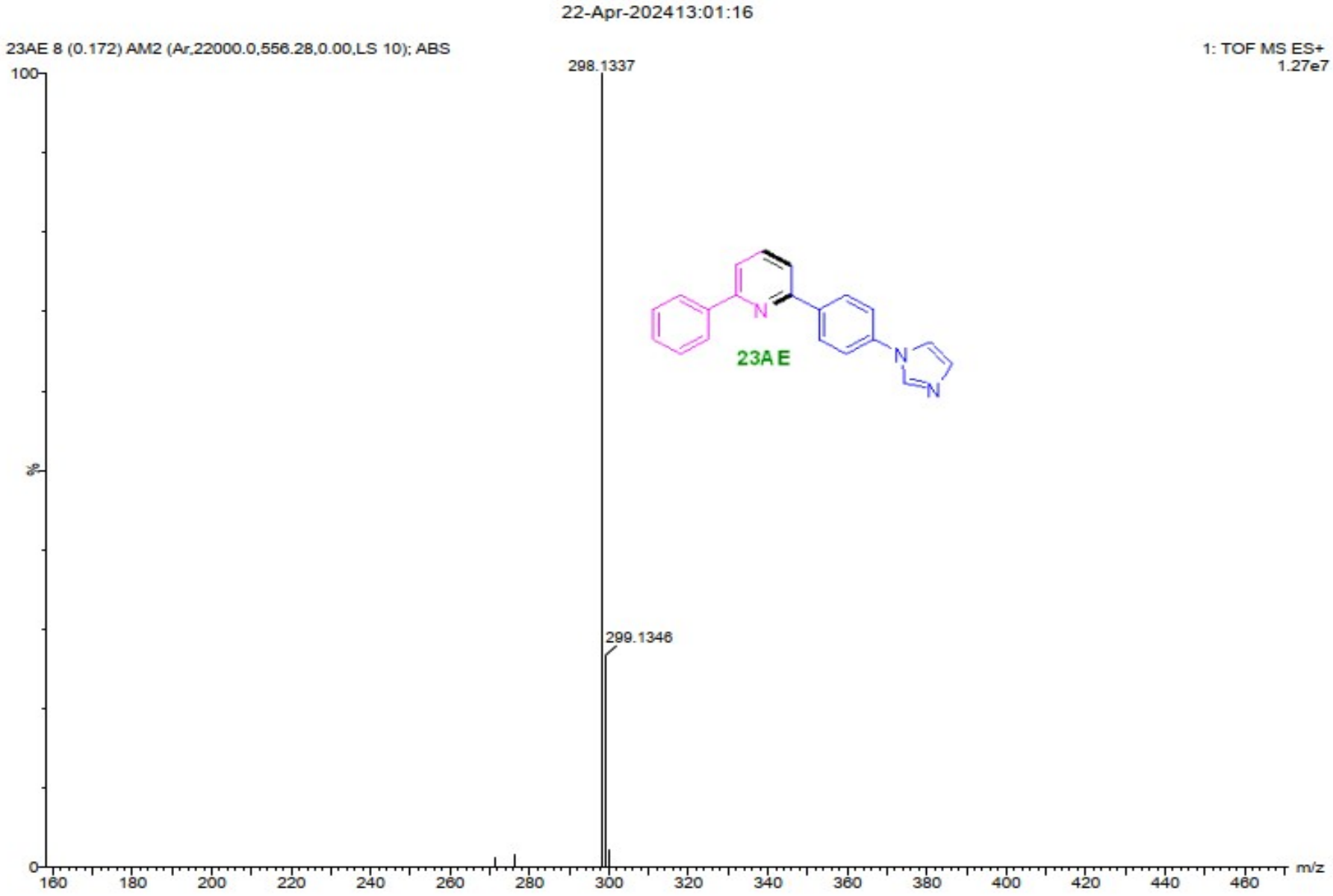
22-Apr-202416:12:50

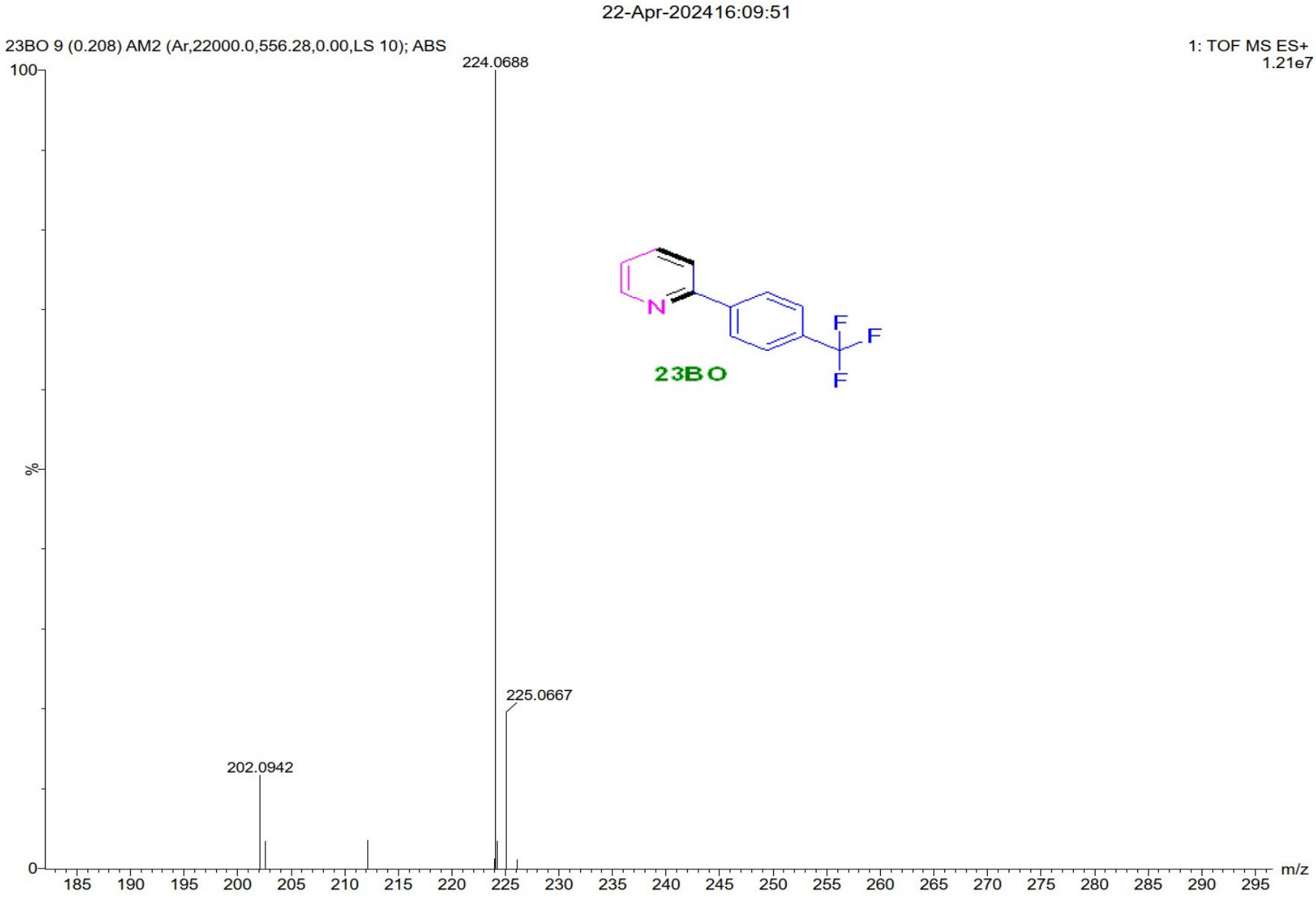
20AO 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

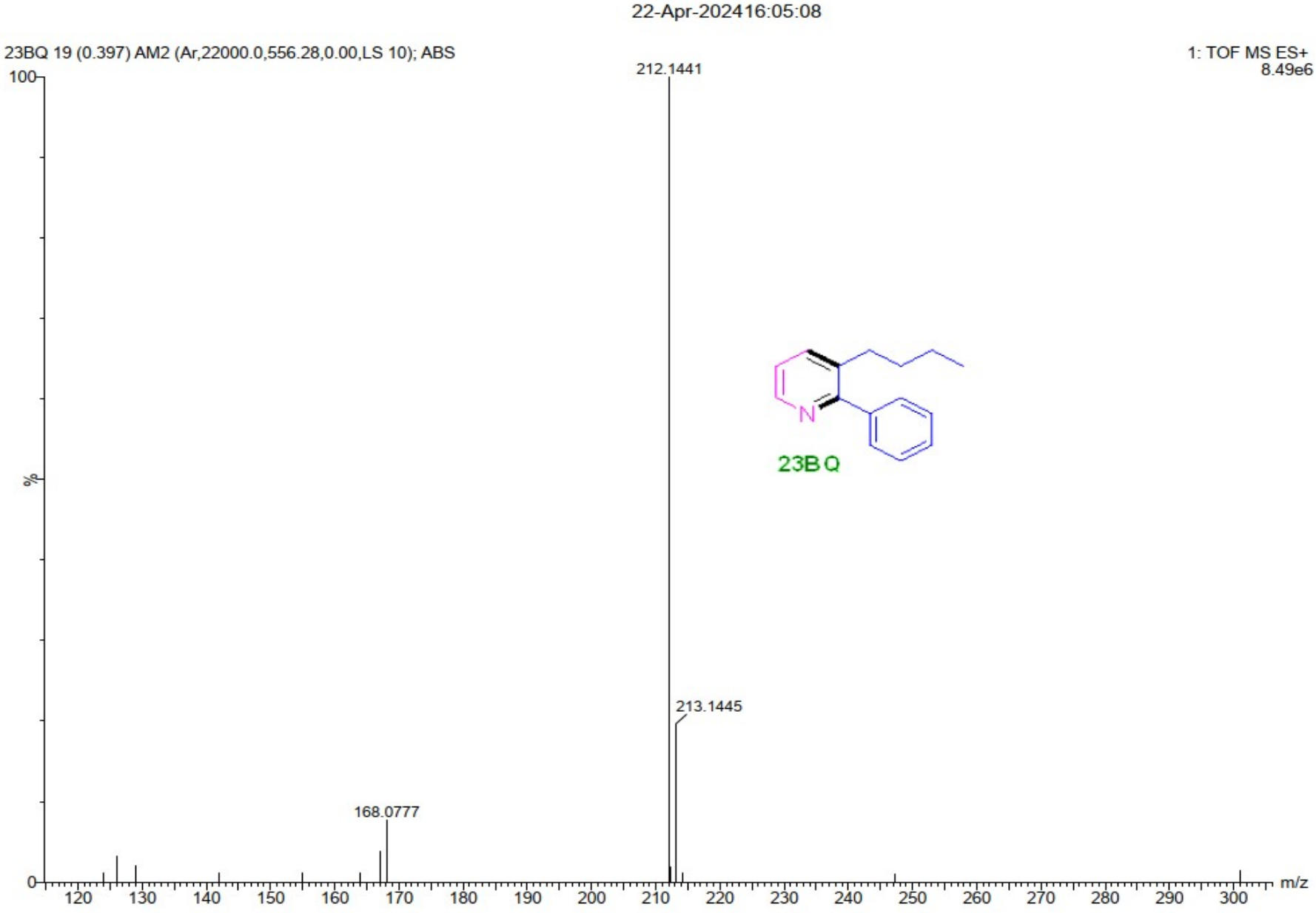
1: TOF MS ES+
4.44e6

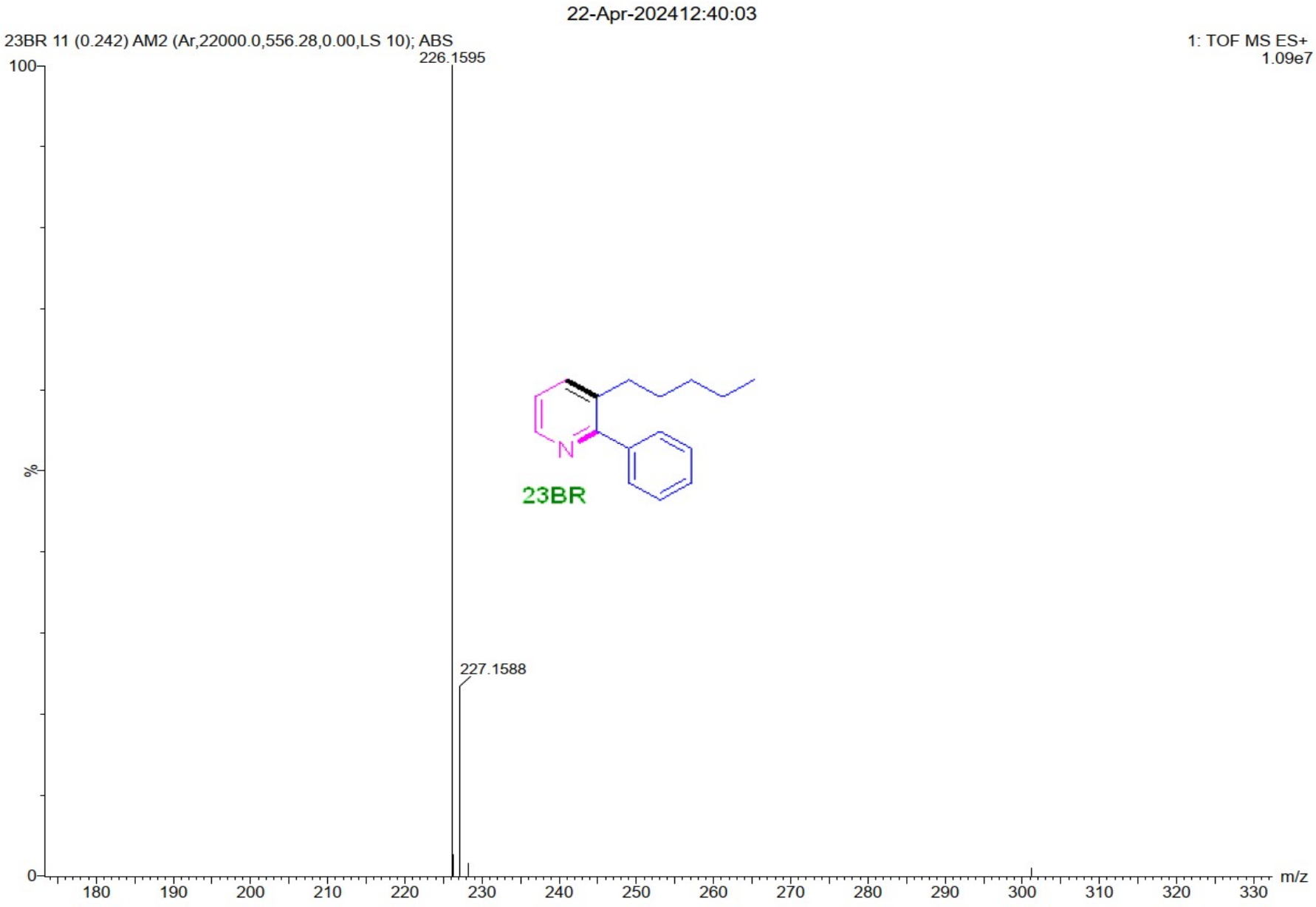


20A O


22-Apr-202413:01:16
23AE 8 (0.172) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
1.27e7
298.1337
299.1346
100
%
0
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
m/z
N
N
N
23A E


22-Apr-202416:09:51
23BO 9 (0.208) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
1.21e7
100
%
0
224.0688
225.0667
202.0942
N
F
F
F
23BO
185 190 195 200 205 210 215 220 225 230 235 240 245 250 255 260 265 270 275 280 285 290 295
m/z


22-Apr-202416:05:08
23BQ 19 (0.397) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
8.49e6
100
%
0
212.1441
213.1445
168.0777
N
23BQ
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
m/z


22-Apr-202412:40:03
23BR 11 (0.242) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS
1: TOF MS ES+
1.09e7
226.1595
227.1588
100
%
0
23BR
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
m/z

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