Regioselective *syn*-1,2-Hydroarylation of Internal Alkynes

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SUPPORTING INFORMATION

Table of Contents **Page**

General Experimental Information:

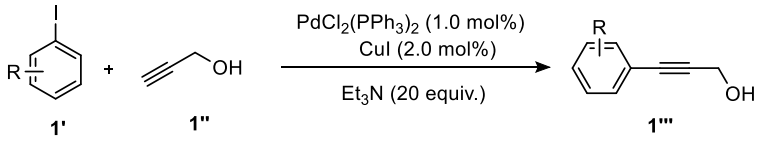
All the reactions were performed in oven-dried Schlenk flasks. Commercial grade solvents were distilled prior to use. Column chromatography was performed using either 100−200 Mesh or 230−400 Mesh silica gel or neutral alumina. Thin layer chromatography (TLC) was performed on silica gel GF254 plates and alumina plates.

Proton, carbon, and fluorine nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR, and ^{19}F NMR) were recorded based on the resonating frequencies as follows: (^{1}H NMR, 400 MHz; ^{13}C NMR, 101 MHz; ^{19}F NMR, 376 MHz) and (^{1}H NMR, 500 MHz; ^{13}C NMR, 126 MHz; ^{19}F NMR, 471 MHz) having the solvent resonance as internal standard (^{1}H NMR, $CDCl_3$ at 7.26 ppm, DMSO D_6 at 2.51 ppm; ^{13}C NMR, $CDCl_3$ at 77.0 ppm, DMSO D_6 at 39.8 ppm). In few cases, tetramethylsilane (TMS) was used as reference standard (at 0.00 ppm). Data for ^{1}H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet; bs= broad singlet; d = doublet; bd = broad doublet, t = triplet; bt = broad triplet; q = quartet; m = multiplet), coupling constants, J, in (Hz), and integration. Data for ^{13}C NMR, ^{19}F NMR are reported in terms of chemical shift (ppm). IR spectra are reported in cm^{-1}. High resolution mass spectra were obtained in ESI mode. Melting points were determined by electro-thermal heating and are uncorrected. X-ray data was collected at 293 K using graphite monochromatic Mo-Kα radiation (0.71073 Å).

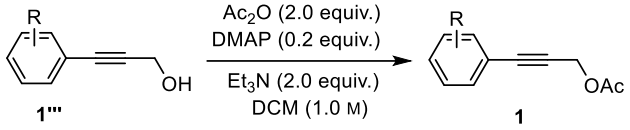
Materials: Unless otherwise noted, all the reagents and intermediates were obtained commercially and used without purification. Dichloromethane ($ClCH_2Cl$, DCM), acetone, toluene, and 1,4-dioxane were distilled over CaH_2 and DMF, and DMSO were used as received. $Pd_2(dba)_3$, $Pd_2(dba)_3 \cdot CHCl_3$ were purchased from commercially available source, and used as received. Commercially available propargyl alcohols and Ph_3SiH were purchased and directly used without purification. Following the known procedure, yne-acetates (**1a**–**1z**) and aryldiazonium salts (**2a**–**2x**) were prepared. Analytical and spectral data of all the known compounds are exactly matching with the reported values.

Experimental Procedures

Preparation of propargyl acetates: General Procedure (GP-1):[1-3]



Following the known synthetic procedure, $Pd(PPh_3)_2Cl_2$ (0.01 mmol) and CuI (0.02 mmol) were suspended in Et_3N (3.0 mL) under N_2 atmosphere in a screw capped reaction tube. Iodoarene (**1′**, 1.2 mmol) followed by propargyl alcohol (**1″**, 1.0 mmol) were added and the reaction was stirred at room temperature for 5.0 hours. Subsequent workup and column chromatography yielded the respective propargyl alcohols **1‴**.



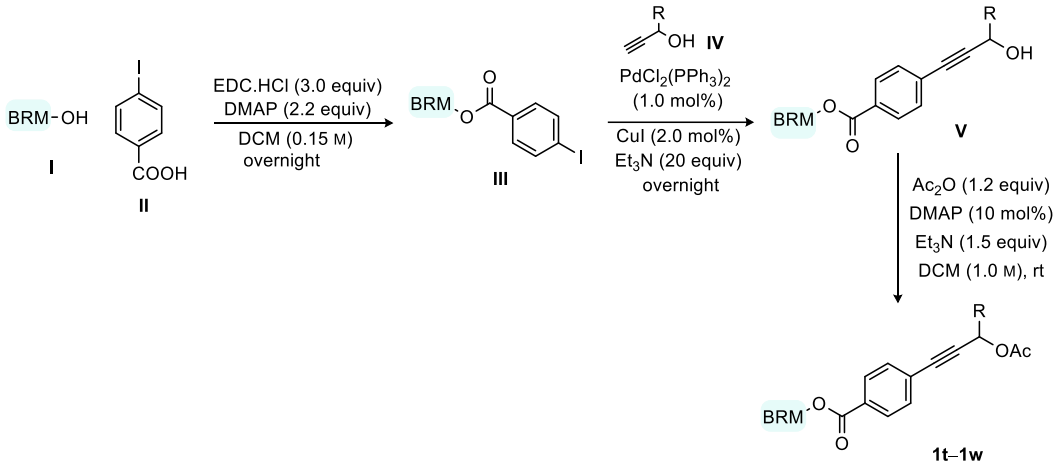
To a solution of acetic anhydride (2.0 mmol), triethylamine (30 mL), and N, N-dimethyl-4-aminopyridine (0.2 mmol) in dichloromethane (1.0 mL) was added propargyl alcohol (**1‴**, 1.0 mmol). The reaction mixture was stirred at room temperature for 16 h and then was quenched by aqueous 2N HCl (30 mL). The mixture was extracted with diethyl ether (20 mL x 3). The collected organic layer was dried over Na_2SO_4. The solvent was washed with saturated aqueous $NaHCO_3$ (80 mL x 2) and the solvent was evaporated under reduced pressure. The residue was purified by distillation under reduced pressure to give the product **1**.

General procedure for the preparation of biological relevant motif (BRM) bearing propargyl acetate 1t–1w (GP-2):[4-5]

A solution of N'-(3-dimethylaminopropyl)-N-ethylcarbodimide, hydrochloride salt (EDC·HCl) (1.15 g, 6.0 mmol, 3.0 equiv), 4-*N*,*N*-dimethylaminopyridine (DMAP; 538 mg, 4.4 mmol, 2.2 equiv) and 4-iodobenzoic acids **(II;** 546 mg, 2.2 mmol, 1.1 equiv) in CH_2Cl_2 (0.15 M, 13 mL) was stirred under argon atmosphere. Alcohol **I** (2.0 mmol, 1.0 equiv) was introduced dropwise (portion wise if the alcohol is solid) at 0 °C. The resulting reaction mixture was stirred for about 1 h at 0 °C and then 12 h at an ambient temperature. Upon complete consumption of alcohol, the solvent was filtered and evaporated under reduced pressure. The crude residue was purified using column chromatography on silica gel using hexane/ethyl acetate to afford **III**.

To a solution of $PdCl_2(PPh_3)_2$ (14 mg, 0.02 mmol, 0.01 equiv) and CuI (8.0 mg, 0.04 mmol, 0.02 equiv) in Et_3N (40.0 mmol, 20 equiv, 6.0 mL) were added aryl iodide **III** (2.6 mmol, 1.3 equiv) and substrate **IV** (2.0

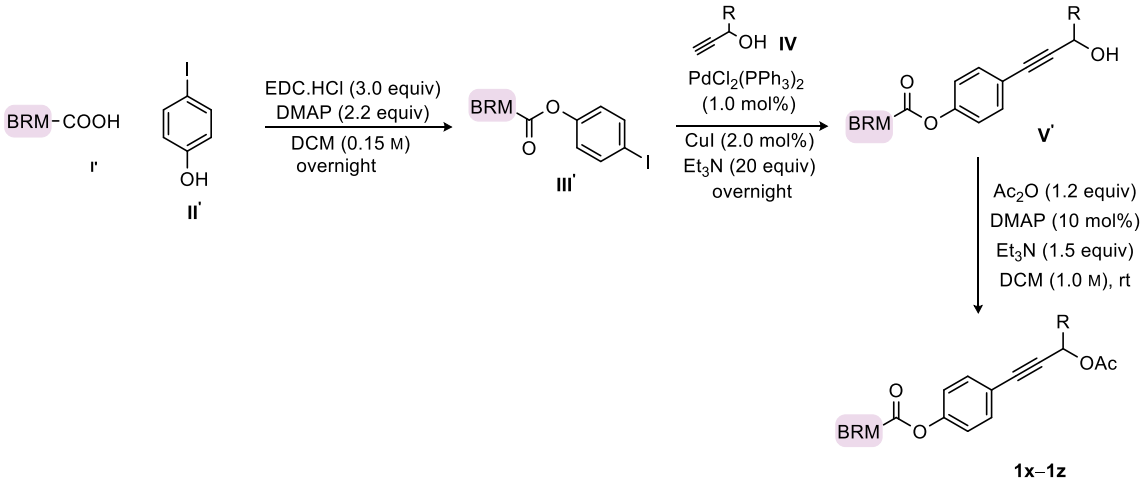
mmol, 1.0 equiv) successively under an argon atmosphere. The resulting mixture was stirred at room temperature overnight. The reaction progress was monitored by TLC on silica-gel. Upon reaction completion, the crude reaction mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified using column chromatography on silica gel to afford the respective propargyl alcohols **V**.



To a solution of an alcohol **V** (2.0 mmol, 1.0 equiv), Et_3N (3.0 mmol, 1.5 equiv, 0.4 mL), and DMAP (24 mg, 0.2 mmol, 0.1 equiv) in anhydrous CH_2Cl_2 (1.0 M, 2.0 mL) was added acetic anhydride dropwise (2.4 mmol, 1.2 equiv, 0.3 mL) at 0 °C. The mixture was stirred at room temperature for 2−3 h. The reaction progress was monitored by TLC on silica-gel. Upon reaction completion, the mixture was concentrated under reduced pressure and purified by column chromatography on silica gel eluting with hexane/EtOAc to give yne-acetates **1t–1w**.

General procedure for the preparation of biological relevant motif (BRM) bearing propargyl acetate 1x–1z (GP-2′):[4-5]

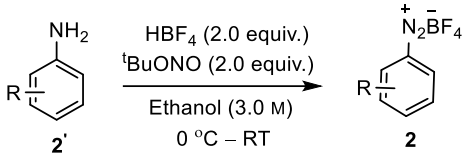
A solution of N'-(3-dimethylaminopropyl)-N-ethylcarbodimide. hydrochloride salt (EDC·HCl) (1.15 g, 6.0 mmol, 3.0 equiv), 4-N, N-dimethylaminopyridine (DMAP; 538 mg, 4.4 mmol, 2.2 equiv) and the respective carboxylic acid **(I′**; 2.2 mmol, 1.1 equiv, 0.35 mL) in CH_2Cl_2 (0.15 M, 13 mL) was stirred under an argon atmosphere. Next, 4-iodo phenol **(II′;** 440 mg, 2.0 mmol, 1.0 equiv) was introduced portion wise at 0 °C. The resulting reaction mixture was stirred for about 1 h at 0 °C and then 12 h at an ambient temperature. Upon complete consumption of carboxylic acid, the solvent was filtered and evaporated under reduced pressure. The crude residue was purified using column chromatography on silica gel using hexane/ethyl acetate to afford **III′**.



To a solution of $PdCl_2(PPh_3)_2$ (14 mg, 0.02 mmol, 0.01 equiv) and CuI (8.0 mg, 0.04 mmol, 0.02 equiv) in Et_3N (40.0 mmol, 20 equiv, 6.0 mL) were added aryl iodide **III′** (2.6 mmol, 1.3 equiv) and substrate **IV** (2.0 mmol, 1.0 equiv) successively under an argon atmosphere. The resulting mixture was stirred at room temperature overnight. The reaction progress was monitored by TLC. Upon reaction completion, the crude reaction mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified using column chromatography on silica gel to afford the respective propargyl alcohols **V′**.

To a solution of an alcohol **V′** (2.0 mmol, 1.0 equiv), Et_3N (3.0 mmol, 1.5 equiv, 0.4 mL) and DMAP (24 mg, 0.2 mmol, 0.1 equiv) in anhydrous CH_2Cl_2 (1.0 M, 2.0 mL) was added acetic anhydride (0.24 mmol, 1.2 equiv, 0.3 mL) at 0 °C. The mixture was stirred at room temperature for 2−3 h. Upon complete consumption of alcohol (monitored by TLC), the mixture was concentrated under reduced pressure and purified by column chromatography on silica gel eluting with hexane/EtOAc to give yne-acetates **1x–1z**.

General procedure for the preparation of aryldiazonium salts (GP-3):[6]



To the solution of HBF_4 (1.3 mL) and primary aryl amines (5.0 mmol) in EtOH (5.0 mL) was added ^tBuONO (1.4 mL) dropwise at 0 °C. The reaction mixture was stirred for 30 min at room temperature. Upon completion of the reaction, Et_2O (20 mL) was added to precipitate the diazonium salt. Next, the crude reaction mixture was filtered and the residue was washed Et_2O (3 × 10 mL).

Table S1: List of propargyl acetates

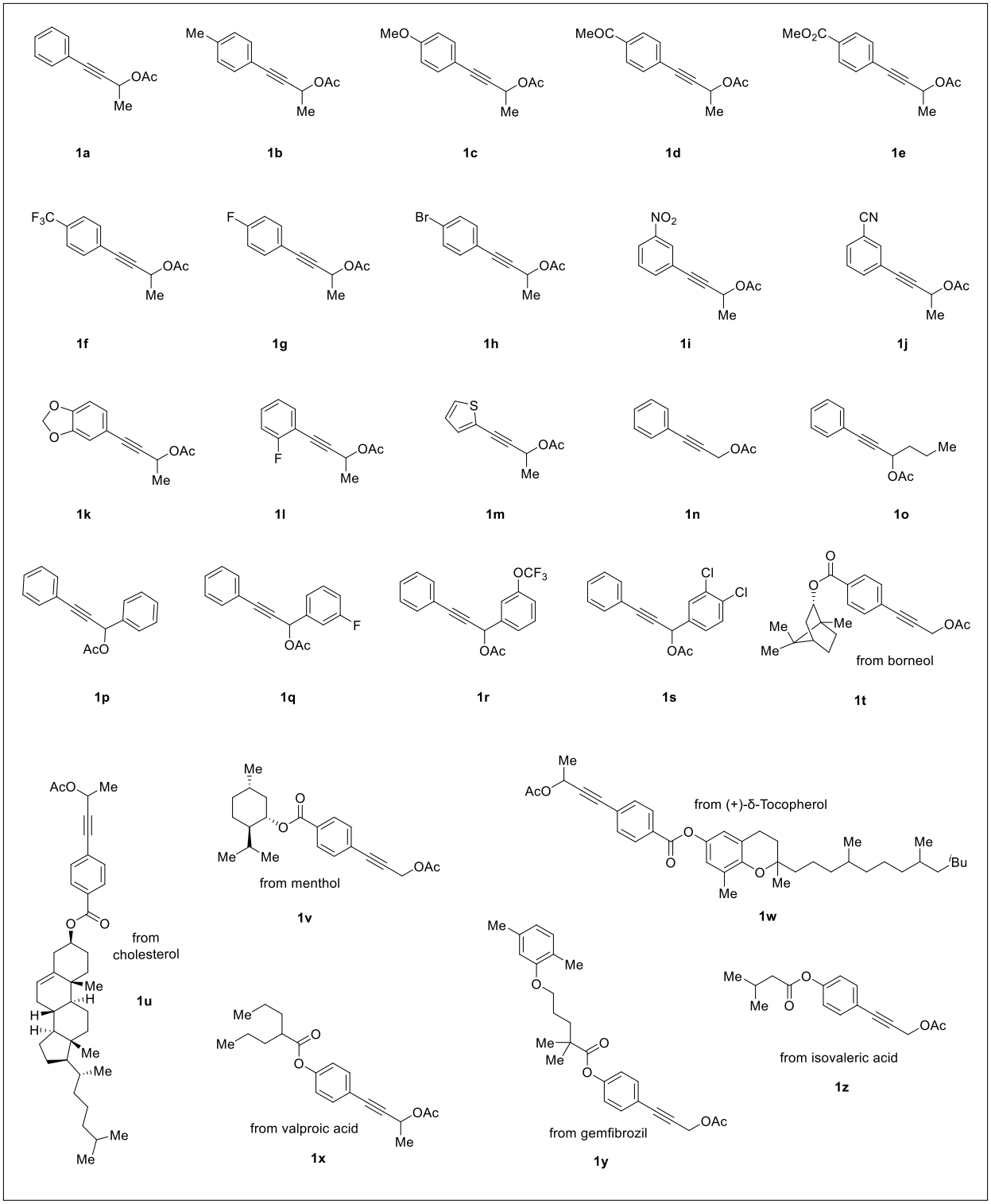
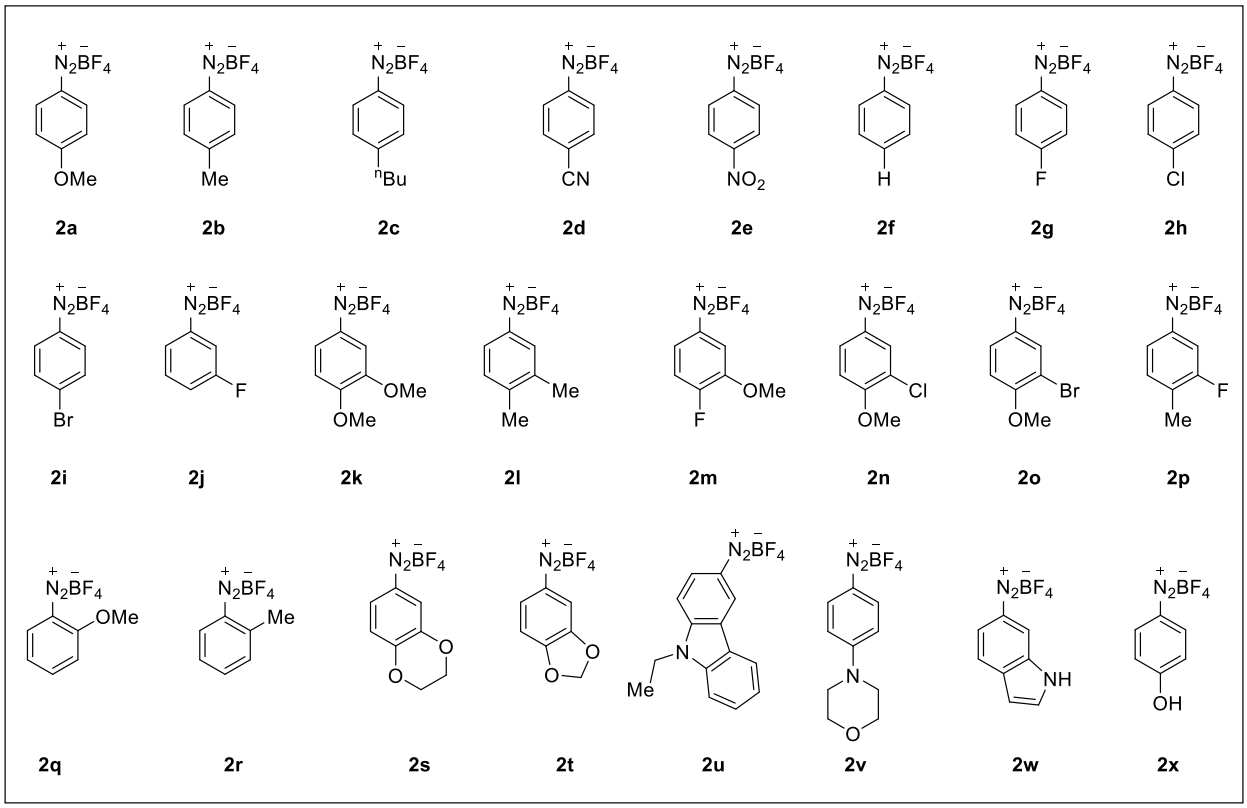
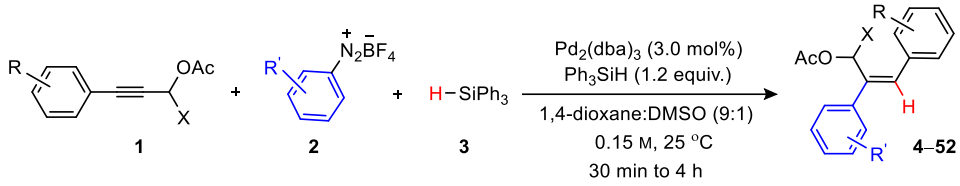


Table S2: List of diazonium salts

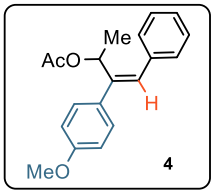


General procedure for regioselective *syn*-1,2-hydroarylation of propargyl acetates (1) with aryl diazonium salts (2) (GP-3):



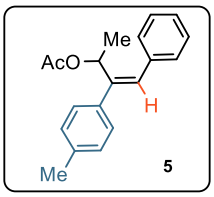
To a mixture of **1** (0.2 mmol), aryl diazonium-tetrafluoroborate **2** (0.6 mmol), Ph_3SiH **3** (0.24 mmol) and Pd_2dba_3 (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 30 min to 4.0 h. After completion of the reaction, DMSO was removed by water workup. The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was evaporated and purified by column chromatography using neutral alumina to afford **4–27**, **28–45**, and **46–52**.

(*Z*)-3-(4-Methoxyphenyl)-4-phenylbut-3-en-2-yl acetate (4):



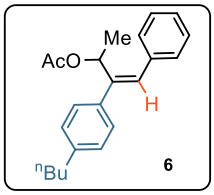
4 (56 mg, 94%) as pale-red liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.46 (dt, J = 9.5, 2.6 Hz, 2H), 7.40 (t, J = 7.5 Hz, 2H), 7.34–7.28 (m, 3H), 6.96 (dt, J = 9.2, 2.5 Hz, 2H), 6.69 (s, 1H), 5.99 (q, J = 6.7 Hz, 1H), 3.78 (s, 3H), 1.93 (s, 3H), 1.31 (d, J = 7.0 Hz, 3H) ; ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 159.1, 140.9, 136.9, 132.4, 131.0, 129.9, 129.2, 128.8, 127.6, 114.0, 69.0, 55.5, 21.4, 20.1; IR (Neat) ν_{max} 2924, 1733, 1604, 1508, 1369, 1234, 1030, 822 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{20}NaO_3^+$ $(M+Na)^+$: calcd. 319.1305 found 319.1308.

(*Z*)-4-Phenyl-3-(*p*-tolyl)but-3-en-2-yl acetate (5):



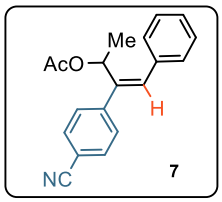
5 (49 mg, 87%) as pale-red liquid; R_f = 0.6 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.44–7.37(m, 4H), 7.34–7.29 (m, 3H), 7.21 (d, J = 8.0 Hz, 2H), 6.70 (s, 1H), 5.98 (q, J = 6.5 Hz, 1H), 2.33 (s, 3H), 1.92 (s, 3H), 1.31 (d, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 141.3, 137.3, 137.1, 136.8, 131.4, 129.22, 129.19, 128.8, 128.6, 127.7, 68.9, 21.4, 21.2, 20.0; IR (Neat) ν_{max} 2923, 1734, 1510, 1369, 1233, 1038, 811 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{20}NaO_2^+$ $(M+Na)^+$: calcd. 303.1356 found 303.1356.

(*Z*)-3-(4-Butylphenyl)-4-phenylbut-3-en-2-yl acetate (6):



6 (55 mg, 85%) as yellow liquid; R_f = 0.6 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.45–7.57 (m, 4H), 7.34–7.26 (m, 3H), 7.21 (d, J = 8.0 Hz, 2H), 6.71 (s, 1H), 5.98 (q, J = 6.7 Hz, 1H), 2.60 (t, J = 7.8 Hz, 2H), 1.92 (s, 3H), 1.62–1.52 (m, 2H), 1.37–1.28 (m, 5H), 0.91 (t, J = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 142.0, 141.3, 137.6, 136.8, 131.5, 129.2, 128.8, 128.6, 128.5, 127.7, 68.9, 35.0, 33.5, 22.3, 21.4, 20.0, 14.3; IR (Neat) ν_{max} 2927, 1736, 1619, 1369, 1236, 839 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{26}NaO_2^+$ $(M+Na)^+$: calcd. 345.1825 found 345.1828.

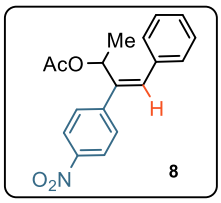
(*Z*)-3-(4-Cyanophenyl)-4-phenylbut-3-en-2-yl acetate (7):



7 (17 mg, 29%) as colorless liquid; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.88 (d, J = 8.5 Hz, 2H), 7.73 (d, J = 8.5 Hz, 2H), 7.43 (t, J = 7.5 Hz, 2H), 7.39–7.32 (m, 3H), 6.88 (s, 1H), 6.01 (q, J = 6.7 Hz, 1H), 1.95 (s, 3H), 1.33 (d, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.7, 145.1, 140.0, 136.1,

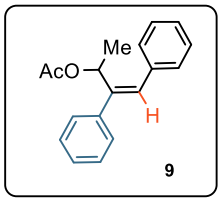
133.9, 132.6, 129.7, 129.3, 128.9, 128.2, 119.3, 110.6, 68.5, 21.3, 20.0; IR (Neat) ν_{max} 2927, 2227, 1735, 1602, 1370, 1232, 1039, 845cm^{-1}; **HRMS (ESI)** for $C_{19}H_{17}NNaO_2^+$ $(M+Na)^+$: calcd. 314.1151 found 314.1155.

(*Z*)-3-(4-Nitrophenyl)-4-phenylbut-3-en-2-yl acetate (8):



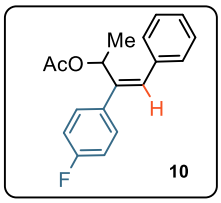
8 (20 mg, 32%) as red liquid; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 8.27 (dt, J = 9.3, 2.3 Hz, 2H), 7.82 (dt, J = 9.3, 2.3 Hz, 2H), 7.49–7.41 (m, 2H), 7.40–7.33 (m, 3H), 6.93 (s, 1H), 6.03 (q, J = 6.7 Hz, 1H), 1.96 (s, 3H), 1.36 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 147.1, 139.7, 136.1, 134.3, 130.1, 129.3, 129.0, 128.3, 123.8, 68.4, 21.4, 20.0; IR (Neat) ν_{max} 2929, 1735, 1594, 1515, 1341, 1231, 1039, 853 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{17}NNaO_4^+$ $(M+Na)^+$: calcd. 334.1050 found 334.1054.

(*Z*)-3,4-Diphenylbut-3-en-2-yl acetate (9):



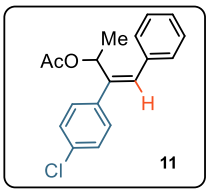
9 (41 mg, 77%) as red liquid; R_f = 0.7 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.54–7.48 (m, 2H), 7.44–7.38 (m, 4H), 7.37–7.29 (m, 4H), 6.73 (s, 1H), 6.00 (q, J = 6.5 Hz, 1H), 1.93 (s, 3H), 1.31 (d, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 141.5, 140.3, 136.7, 132.0, 129.2, 128.81, 128.76, 128.6, 127.9, 127.8, 68.8, 21.3, 20.0; IR (Neat) ν_{max} 2924, 1736, 1445, 1370, 1237, 1041, 936 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{18}NaO_2^+$ $(M+Na)^+$: calcd. 289.1199 found 289.1199.

(*Z*)-3-(4-Fluorophenyl)-4-phenylbut-3-en-2-yl acetate (10):



10 (39 mg, 69%) as pale-red liquid; R_f = 0.7 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.58–7.51(m, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.35–7.28 (m, 3H), 7.23 (tt, J = 8.8, 2.3 Hz, 2H), 6.73 (s, 1H), 5.96 (q, J = 6.7 Hz, 1H), 1.94 (s, 3H), 1.30 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 162.1 (d, J = 244.4 Hz, 1C), 140.4, 136.5, 132.2, 130.8 (d, J = 8.8 Hz, 1C), 129.0 (d, J = 50.4 Hz, 2C), 127.9, 115.4 (d, J = 21.4 Hz, 2C), 68.7, 21.3, 19.9; ^{19}F NMR (471 MHz, DMSO D_6) δ −115.1; IR (Neat) ν_{max} 2925, 1735, 1599, 1506, 1222, 1039, 837 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{17}FNaO_2^+$ $(M+Na)^+$: calcd. 307.1105 found 307.1101.

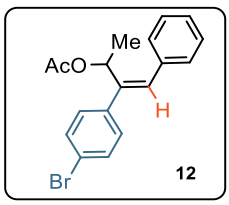
(*Z*)-3-(4-Chlorophenyl)-4-phenylbut-3-en-2-yl acetate (11):



11 (33 mg, 56%) as light yellow liquid; R_f = 0.7 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.54 (dt, J = 8.8, 2.3 Hz, 2H), 7.47 (dt, J = 8.8, 2.3 Hz, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.36–7.30 (m, 3H), 6.77 (s, 1H), 5.98 (q, J = 6.7 Hz, 1H), 1.94 (s,

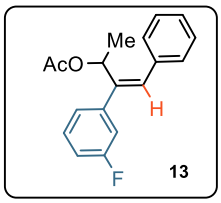
3H), 1.31 (d, J = 6.5 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO D_6) δ 169.8, 140.2, 139.0, 136.4, 132.7, 132.5, 130.6, 129.2, 128.9, 128.6, 127.9, 68.6, 21.4, 20.0; IR (Neat) ν_{max} 2923, 1736, 1600, 1507, 1225, 1040, 838 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{17}ClNaO_2^+$ $(M+Na)^+$: calcd. 323.0806 found 323.0809.

(*Z*)-3-(4-Bromophenyl)-4-phenylbut-3-en-2-yl acetate (12):



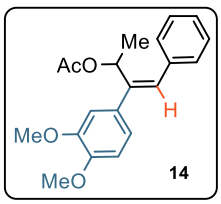
12 (39 mg, 55%) as red liquid; R_f = 0.7 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.60 (dt, J = 8.8, 2.3 Hz, 2H), 7.47 (dt, J = 8.8, 2.3 Hz, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.36–7.30 (m, 3H), 6.77 (s, 1H), 5.98 (q, J = 6.7 Hz, 1H), 1.94 (s, 3H), 1.31 (d, J = 6.5 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO D_6) δ 169.7, 140.3, 139.4, 136.4, 132.5, 131.5, 130.9, 129.2, 128.8, 127.9, 121.3, 68.6, 21.3, 20.0; IR (Neat) ν_{max} 2979, 1734, 1486, 1368, 1230, 1008, 934, 814 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{17}BrNaO_2^+$ $(M+Na)^+$: calcd. 367.0304 found 367.0304.

(*Z*)-3-(3-Fluorophenyl)-4-phenylbut-3-en-2-yl acetate (13):



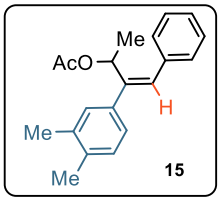
13 (29 mg, 51%) as red liquid; R_f = 0.7 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.49–7.44 (m, 1H), 7.42 (t, J = 7.5 Hz, 2H), 7.58 (dt, J = 8.0, 1.3 Hz, 1H), 7.35–7.29 (m, 4H), 7.23–7.15 (m, 1H), 6.83 (s, 1H), 5.99 (q, J = 6.7 Hz, 1H), 1.96 (s, 3H), 1.32 (d, J = 6.5 Hz, 3H) ; $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO D_6) δ 169.8, 162.3 (d, J = 244.4 Hz, 1C), 142.6 (d, J = 7.6 Hz, 1C), 140.1, 136.4, 132.9, 130.6 (d, J = 7.6 Hz, 1C), 129.3, 128.8, 128.0, 125.0 (d, J = 2.5 Hz, 1C), 115.5 (d, J = 21.4 Hz, 1C), 114.7 (d, J = 21.4 Hz, 1C), 68.6, 21.3, 19.9; ^{19}F NMR (471 MHz, DMSO D_6) δ −113.2; IR (Neat) ν_{max} 2923, 1735, 1600, 1507, 1370, 1224, 1158, 838 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{17}FNaO_2^+$ $(M+Na)^+$: calcd. 307.1105 found 307.1105.

(*Z*)-3-(3,4-Dimethoxyphenyl)-4-phenylbut-3-en-2-yl acetate (14):



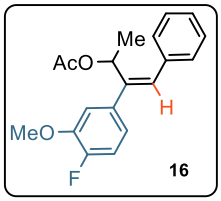
14 (56 mg, 86%) as colorless liquid; R_f = 0.2 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.40 (t, J = 7.8 Hz, 2H), 7.35–7.25 (m, 3H), 7.10 (d, J = 1.5 Hz, 1H), 7.07 (dd, J = 8.5, 2.0 Hz, 1H), 6.97 (d, J = 8.5 Hz, 1H), 6.74 (s, 1H), 6.00 (q, J = 6.5 Hz 1H), 3.80 (s, 3H), 3.78 (s, 3H), 1.95 (s, 3H), 1.32 (d, J = 6.5 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO D_6) δ 169.8, 148.9, 148.6, 141.0, 136.9, 132.8, 131.1, 129.2, 128.8, 127.6, 121.2, 112.6, 111.9, 69.0, 55.94, 55.92, 21.4, 20.1; IR (Neat) ν_{max} 2932, 1732, 1511, 1368, 1234, 1025, 855 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{22}NaO_4^+$ $(M+Na)^+$: calcd. 349.1410 found 349.1410.

(*Z*)-3-(3,4-Dimethylphenyl)-4-phenylbut-3-en-2-yl acetate (15):



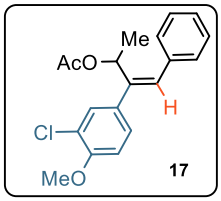
15 (53 mg, 90%) yellow liquid; R_f = 0.6 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.43–7.36 (m, 2H), 7.34–7.28 (m, 3H), 7.26 (s, 1H), 7.18 (dd, J = 8.0, 1.5 Hz, 1H), 7.15 (d, J = 8.0 Hz, 1H), 6.68 (s, 1H), 5.96 (q, J = 6.5 Hz 1H), 2.26 (s, 3H), 2.24 (s, 3H), 1.92 (s, 3H), 1.30 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 141.5, 137.8, 136.8, 136.3, 135.9, 131.3, 129.9, 129.6, 128.8, 127.6, 126.1, 69.0, 21.4, 20.1, 20.0, 19.5; IR (Neat) ν_{max} 2920, 1733, 1445, 1371, 1233, 1039, 826 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{22}NaO_2^+$ $(M+Na)^+$: calcd. 317.1512 found 317.1512.

(*Z*)-3-(3-Fluoro-4-methoxyphenyl)-4-phenylbut-3-en-2-yl acetate (16):



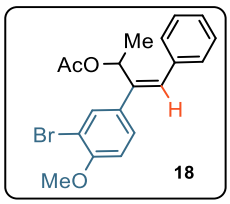
16 (40 mg, 64%) as yellow liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.44–7.35 (m, 3H), 7.34–7.27 (m, 4H), 7.19 (t, J = 8.8 Hz, 1H), 6.77 (s, 1H), 5.98 (q, J = 6.7 Hz, 1H), 3.87 (s, 3H), 1.95 (s, 3H), 1.32 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.7, 151.3 (d, J = 243.2 Hz, 1C), 147.0 (d, J = 11.3 Hz, 1C), 139.8, 136.6, 132.9 (d, J = 5.0 Hz, 1C), 131.9, 129.2, 128.8, 127.8, 125.1 (d, J = 2.5 Hz, 1C), 116.1 (d, J = 17.6 Hz, 1C), 114.0, 69.0, 56.4, 21.3, 20.0; ^{19}F NMR (471 MHz, DMSO D_6) δ −135.5; IR (Neat) ν_{max} 2922, 1734, 1513, 1445, 1233, 1025, 875 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}FNaO_3^+$ $(M+Na)^+$: calcd. 337.1210 found 337.1211.

(*Z*)-3-(3-Chloro-4-methoxyphenyl)-4-phenylbut-3-en-2-yl acetate (17):



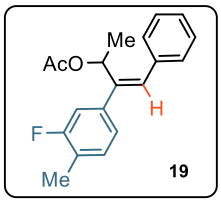
17 (40 mg, 60%) as yellow liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.56 (d, J = 7.0 Hz, 1H), 7.48 (dd, J = 8.5, 2.5 Hz, 1H), 7.46–7.37 (m, 2H), 7.35–7.29 (m, 3H), 7.18 (d, J = 9.0 Hz, 1H), 6.75 (s, 1H), 5.97 (q, J = 6.5 Hz, 1H), 3.89 (s, 3H), 1.95 (s, 3H), 1.31 (d, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.7, 154.4, 139.6, 136.6, 133.4, 132.0, 130.0, 129.2, 128.8, 127.8, 121.1, 112.9, 68.8, 56.6, 21.3, 20.0; IR (Neat) ν_{max} 2927, 1733, 1500, 1369, 1233, 1037, 1067, 809 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}ClNaO_3^+$ $(M+Na)^+$: calcd. 353.0915 found 353.0913.

(*Z*)-3-(3-Bromo-4-methoxyphenyl)-4-phenylbut-3-en-2-yl acetate (18):



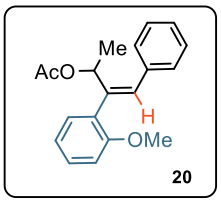
18 (40 mg, 53%) as pale-red liquid; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.59 (d, J = 8.5 Hz, 1H), 7.42 (t, J = 7.5 Hz, 2H), 7.38–7.30 (m, 3H), 7.19 (d, J = 2.0 Hz, 1H), 7.05 (dd, J = 8.0, 2.0 Hz, 1H), 6.83 (s, 1H), 6.00 (q, J = 6.5 Hz, 1H), 3.91 (s, 3H), 1.96 (s, 3H), 1.33 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 155.5, 141.3, 140.4, 132.9, 132.6, 129.3, 128.9, 128.0, 122.4, 113.1, 110.4, 68.7, 56.6, 21.4, 20.0; IR (Neat) ν_{max} 2932, 1731, 1586, 1447, 1236, 1042, 855 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}BrNaO_3^+$ $(M+Na)^+$: calcd. 397.0410 found 397.0412.

(*Z*)-3-(3-Fluoro-4-methylphenyl)-4-phenylbut-3-en-2-yl acetate (19):



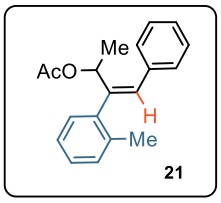
19 (43 mg, 72%) as pale-red liquid; R_f = 0.6 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.42 (t, J = 7.5 Hz, 2H), 7.35–7.30 (m, 4H), 7.29–7.24 (m, 2H), 6.79 (s, 1H), 5.97 (q, J = 6.7 Hz, 1H), 2.26 (s, 3H), 1.95 (s, 3H), 1.31 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 160.7 (d, J = 243.2 Hz, 1C), 140.0, 139.8 (d, J = 8.2 Hz, 1C), 136.5, 132.4, 131.8 (d, J = 5.0 Hz, 1C), 129.2, 128.8, 127.9, 124.6 (d, J = 2.5 Hz, 1C), 123.8 (d, J = 17.6 Hz, 1C), 115.1 (d, J = 22.7 Hz, 1C), 68.7, 21.4, 20.0, 14.4; ^{19}F NMR (471 MHz, DMSO D_6) δ −117.7; IR (Neat) ν_{max} 2926, 1736, 1505, 1369, 1232, 1040, 870 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}FNaO_2^+$ $(M+Na)^+$: calcd. 321.1261 found 321.1265.

(*Z*)-3-(2-Methoxyphenyl)-4-phenylbut-3-en-2-yl acetate (20):



20 (39 mg, 66%) as yellow liquid; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.41 (t, J = 7.5 Hz, 2H), 7.38–7.28 (m, 4H), 7.13 (dd, J = 7.5, 1.5 Hz, 1H), 7.04 (d, J = 7.5 Hz, 1H), 6.96 (td, J = 7.5, 1.0 Hz, 1H), 6.40 (s, 1H), 5.99 (q, J = 6.5 Hz, 1H), 3.76 (s, 3H), 1.83 (s, 3H), 1.28 (d, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.8, 157.6, 139.3, 136.6, 131.9, 131.6, 129.3, 128.8, 127.7, 120.3, 111.6, 68.6, 55.9, 21.3, 19.7; IR (Neat) ν_{max} 2933, 1734, 1489, 1368, 1241, 1025, 852 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{20}NaO_3^+$ $(M+Na)^+$: calcd. 319.1305 found 319.1307.

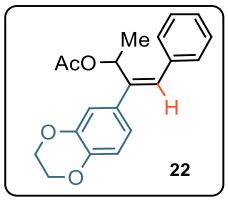
(*Z*)-4-Phenyl-3-(*o*-tolyl)but-3-en-2-yl acetate (21):



21 (34 mg, 61%) as yellow liquid; R_f = 0.7 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.42 (t, J = 7.5 Hz, 2H), 7.36–7.31 (m, 3H), 7.29 (d, J = 7.5 Hz, 1H), 7.26–7.19 (m, 3H), 6.45 (s, 1H), 5.98 (q, J = 6.7 Hz, 1H), 2.31 (s, 3H), 1.88 (s, 3H), 1.28 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 140.1, 139.7,

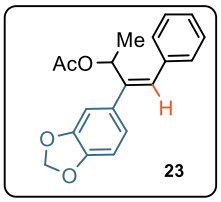
136.7, 136.4, 132.6, 130.6, 130.1, 129.1, 128.8, 127.8, 127.7, 125.4, 69.0, 21.4, 20.3, 19.7; IR (Neat) ν_{max} 2927, 1734, 1445, 1369, 1233, 1035, 802 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{20}NaO_2^+$ $(M+Na)^+$: calcd. 303.1356 found 303.1355.

(*Z*)-3-(2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)-4-phenylbut-3-en-2-yl acetate (22):



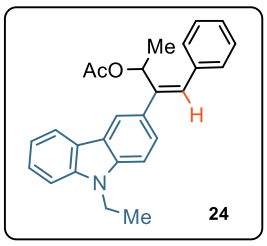
22 (46 mg, 71%) as light yellow liquid; R_f = 0.3 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.39 (t, J = 7.8 Hz, 2H), 7.33–7.27 (m, 3H), 7.02 (d, J = 2.0 Hz, 1H), 6.99 (dd, J = 8.5, 2.5 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H), 6.70 (s, 1H), 5.96 (q, J = 6.5 Hz, 1H), 4.26 (s, 4H), 1.94 (s, 3H), 1.30 (d, J = 6.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO D_6) δ 169.8, 143.5, 143.3, 140.6, 136.8, 133.4, 131.4, 129.3, 128.8, 127.7, 121.8, 117.4, 117.2, 68.9, 64.62, 64.56, 21.4, 20.0; IR (Neat) ν_{max} 2930, 1731, 1577, 1502, 1282, 1236, 1066, 808 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{20}NaO_4^+$ $(M+Na)^+$: calcd. 347.1254 found 347.1256.

(*Z*)-3-(Benzo[d][1,3]dioxol-5-yl)-4-phenylbut-3-en-2-yl acetate (23):



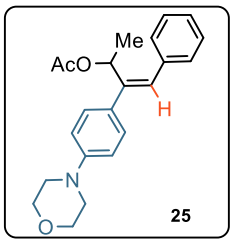
23 (28 mg, 45%) as yellow liquid; R_f = 0.4 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.40 (t, J = 7.5 Hz, 2H), 7.34–7.26 (m, 3H), 7.07 (d, J = 1.5 Hz, 1H), 7.00 (dd, J = 8.0, 1.5 Hz, 1H), 6.94 (d, J = 8.0 Hz, 1H), 6.71 (s, 1H), 6.05 (s, 2H), 5.95 (q, J = 6.5 Hz, 1H), 1.94 (s, 3H), 1.30 (d, J = 6.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO D_6) δ 169.8, 147.5, 147.2, 140.9, 136.7, 134.2, 131.7, 129.3, 128.8, 127.7, 122.4, 109.2, 108.5, 101.5, 68.9, 21.4, 20.0; IR (Neat) ν_{max} 2920, 1733, 1485, 1369, 1220, 1034, 934, 807 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{18}NaO_4^+$ $(M+Na)^+$: calcd. 333.1097 found 333.1098.

(*Z*)-3-(9-Ethyl-9H-carbazol-3-yl)-4-phenylbut-3-en-2-yl acetate (24):



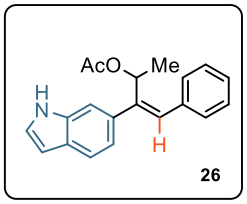
24 (58 mg, 76%) as fluorescent yellow liquid; R_f = 0.5 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 8.30 (d, J = 1.0 Hz 1H), 8.22 (d, J = 7.5 Hz 1H), 7.65 (dd, J = 8.5, 2.0 Hz 1H), 7.60 (d, J = 8.0 Hz 2H), 7.50–7.45 (m, 1H), 7.43 (t, J = 7.5 Hz, 2H), 7.38 (d, J = 7.0 Hz, 2H), 7.35–7.29 (m, 1H), 7.22 (t, J = 7.5 Hz, 1H), 6.82 (s, 1H), 6.11 (q, J = 6.5 Hz, 1H), 4.44 (q, J = 7.0 Hz, 2H), 1.97 (s, 3H), 1.39 (d, J = 7.0 Hz, 3H), 1.33 (t, J = 7.0 Hz, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, DMSO D_6) δ 169.9, 142.2, 140.4, 139.4, 137.1, 131.3, 131.1, 129.3, 128.8, 127.6, 126.7, 126.3, 122.7, 122.5, 120.9, 120.6, 119.3, 109.6, 109.0, 69.3, 37.5, 21.4, 20.3, 14.2; IR (Neat) ν_{max} 2924, 1731, 1596, 1472, 1331, 1230, 1037, 936, 805 cm^{-1}; **HRMS (ESI)** for $C_{26}H_{26}NO_2^+$ $(M+H)^+$: calcd. 384.1958 found 384.1956.

(*Z*)-3-(4-Morpholinophenyl)-4-phenylbut-3-en-2-yl acetate (25):



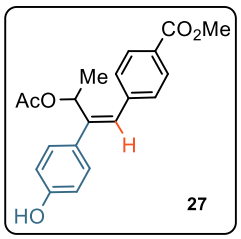
25 (40 mg, 57%) as colorless solid. mp = 206–208 °C; R_f = 0.2 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.49–7.36 (m, 4H), 7.35–7.25 (m, 3H), 6.96 (d, J = 8.5 Hz, 2H), 6.69 (s, 1H), 5.99 (q, J = 6.3 Hz 1H), 3.75 (bt, J = 4.5 Hz, 4H), 3.14 (bt, J = 4.0 Hz, 4H), 1.93 (s, 3H), 1.32 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 150.7, 141.0, 137.1, 130.6, 130.2, 129.3, 129.2, 128.8, 127.5, 69.1, 66.5, 48.6, 21.4, 20.1; IR (Neat) ν_{max} 2921, 2850, 1728, 1604, 1512, 1449, 1372, 1232, 1118, 1032, 925, 811 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{26}NO_3^+$ $(M+H)^+$: calcd. 352.1907 found 352.1906.

(*Z*)-3-(1H-indol-6-yl)-4-phenylbut-3-en-2-yl acetate (26):



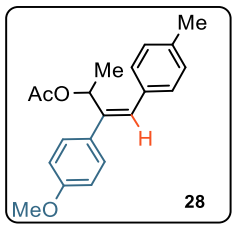
26 (23 mg, 38%) as colorless liquid; R_f = 0.1 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 11.13 (s, 1H), 7.55 (d, J = 8.0 Hz, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 7.36–7.28 (m, 3H), 7.18 (d, J = 8.5 Hz, 1H), 6.74 (s, 1H), 6.44 (bs, 1H), 6.03 (q, J = 6.5 Hz, 1H), 1.94 (s, 3H), 1.35 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 142.6, 137.2, 136.3, 133.2, 131.0, 129.3, 128.7, 127.5, 127.4, 126.4, 120.2, 120.0, 111.6, 69.4, 21.4, 20.2; IR (Neat) ν_{max} 3414, 2926, 1715, 1452, 1370, 1243, 1036, 809 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{19}NNaO_2^+$ $(M+Na)^+$: calcd. 328.1308 found 328.1306.

(*Z*)-Methyl-4-(3-acetoxy-2-(4-hydroxyphenyl)but-1-en-1-yl)benzoate (27):



27 (57 mg, 84%) as colorless solid. mp=185–187 °C; R_f = 0.2 (20% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 9.57 (s, 1H), 7.97 (d, J = 8.5 Hz, 2H), 7.44 (d, J = 8.0, 2H), 7.36 (d, J = 8.5 Hz, 2H), 6.81 (d, J = 9.0 Hz, 2H), 6.70 (s, 1H), 5.92 (q, J = 6.7 Hz, 1H), 3.86 (s, 3H), 1.89 (s, 3H), 1.33 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.7, 166.5, 157.6, 143.1, 142.1, 135.0, 130.4, 129.8, 129.6, 129.5, 129.1, 128.5, 115.5, 69.0, 52.6, 21.3, 20.1; IR (Neat) ν_{max} 3370, 2982, 1715, 1605, 1512, 1434, 1235, 1104, 1036, 834 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{20}NaO_5^+$ $(M+Na)^+$: calcd. 363.1203 found 363.1201.

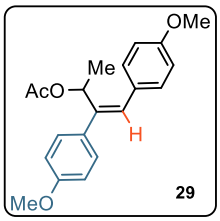
(*Z*)-3-(4-Methoxyphenyl)-4-(p-tolyl)but-3-en-2-yl acetate (28):



28 (48 mg, 77%) as red gummy liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.44 (d, J = 8.5 Hz, 2H), 7.24–7.16 (m, 4H), 6.95 (d, J = 8.5 Hz, 2H), 6.64 (s, 1H), 5.99 (q, J = 6.5 Hz, 1H), 3.78 (s, 3H), 2.32 (s, 3H), 1.94 (s, 3H), 1.29 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.8, 159.1, 140.4, 137.0, 134.0, 132.6, 131.1, 129.9, 129.4, 129.2, 114.0, 69.0, 55.5, 21.4, 21.3,

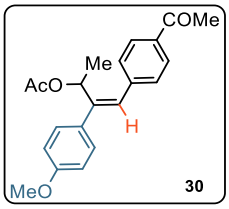
20.1; IR (Neat) ν_{max} 2929, 1733, 1605, 1510, 1285, 1235, 1178, 1032, 932, 829 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{22}NaO_3^+$ $(M+Na)^+$: calcd. 333.1461, found 333.1461.

(*Z*)-3,4-Bis(4-methoxyphenyl)but-3-en-2-yl acetate (29):



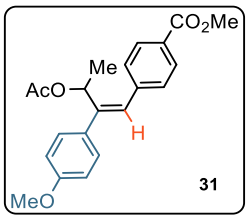
29 (26 mg, 40%) as red gummy liquid; R_f = 0.3 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.43 (dt, *J* = 8.5, 3.0 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 6.99–6.93 (m, 4H), 6.62 (s, 1H), 6.01 (q, *J* = 6.5 Hz, 1H), 3.78 (s, 6H), 1.95 (s, 3H), 1.31 (d, *J* = 6.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO D_6) δ 169.9, 159.0, 158.9, 139.5, 132.7, 130.8, 130.6, 129.9, 129.2, 114.3, 114.0, 69.0, 55.6, 55.5, 21.5, 20.0; IR (Neat) ν_{max} 2929, 2836, 1733, 1606, 1509, 1285, 1236, 1175, 1030, 828 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{22}NaO_4$ $(M+Na)^+$: calcd. 349.1410, found 349.1417.

(*Z*)-4-(4-Acetylphenyl)-3-(4-methoxyphenyl)but-3-en-2-yl acetate (30):



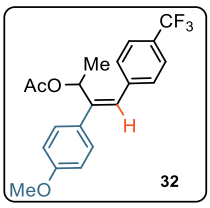
30 (62 mg, 74%) as pale-yellow liquid; R_f = 0.3 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.52–7.40 (m, 4H), 6.97 (dt, *J* = 7.0, 2.5 Hz, 2H), 6.75 (s, 1H), 5.95 (q, *J* = 6.5 Hz, 1H), 3.78 (s, 3H), 2.59 (s, 3H), 1.92 (s, 3H), 1.33 (d, *J* = 6.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO D_6) δ 197.9, 169.8, 159.4, 142.6, 141.8, 135.8, 132.0, 129.9, 129.6, 128.7, 114.1, 68.9, 55.6, 27.2, 21.3, 20.1; IR (Neat) ν_{max} 2930, 2040, 1733, 1679, 1600, 1506, 1360, 1234, 1179, 1031, 956 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{22}NaO_4^+$ $(M+Na)^+$: calcd. 361.1410, found 361.1409.

Methyl (*Z*)-4-(3-acetoxy-2-(4-methoxyphenyl)but-1-en-1-yl)benzoate (31):



31 (62 mg, 89%) as pale-red liquid; R_f = 0.3 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.97 (d, *J* = 8.5 Hz, 2H), 7.49–7.42 (m, 4H), 6.97 (dt, *J* = 9.0 Hz, 3.0 Hz, 2H), 6.73 (s, 1H), 5.93 (q, *J* = 6.5 Hz, 1H), 3.86 (s, 3H), 3.78 (s, 3H), 1.90 (s, 3H), 1.33 (d, *J* = 7.0 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO D_6) δ 169.8, 166.5, 159.4, 142.7, 142.0, 132.1, 129.9, 129.8, 129.61, 129.58, 128.6, 114.1, 68.9, 55.6, 52.6, 21.3, 20.1; IR (Neat) ν_{max} 2950, 2838, 1717, 1603, 1510, 1435, 1276, 1234, 1032, 829 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{22}NaO_5^+$ $(M+Na)^+$: calcd. 377.1359, found 377.1356.

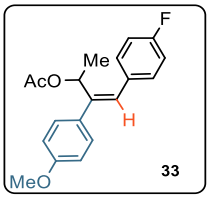
(*Z*)-3-(4-Methoxyphenyl)-4-(4-(trifluoromethyl)phenyl)but-3-en-2-yl acetate (32):



32 (53 mg, 76%) as pale-yellow liquid; R_f = 0.5 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.75 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.48 (dt, *J* = 9.0, 3.0 Hz, 2H), 6.98 (dt, *J* = 9.0, 3.0 Hz, 2H), 6.76 (s, 1H), 5.91 (q, *J* = 6.5 Hz, 1H), 3.79 (s, 3H), 1.90 (s, 3H), 1.33 (d, *J* = 6.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO

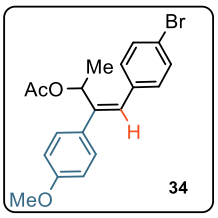
D_6) δ 169.8, 159.4, 142.8, 141.3, 131.9, 130.0, 129.9, 129.3, 127.9 (q, J = 31 Hz, 1C), 125.58, 125.55, 124.8 (q, J = 274 Hz, 1C), 114.1, 68.9, 55.6, 21.2, 20.0; ^{19}F NMR (471 MHz, DMSO D_6) δ –61.0; IR (Neat) ν_{max} 2935, 1736, 1606, 1509, 1370, 1321, 1287, 1235, 1162, 1065, 829 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{19}F_3NaO_3^+$ $(M+Na)^+$: calcd. 387.1179, found 387.1182.

(*Z*)-4-(4-Fluorophenyl)-3-(4-methoxyphenyl)but-3-en-2-yl acetate (33):



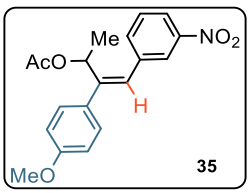
33 (47 mg, 75%) as colourless liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.44 (d, J = 9.0 Hz, 2H), 7.38–7.32 (m, 2H), 7.23 (t, J = 9.0 Hz, 2H), 6.96 (d, J = 8.5 Hz, 2H), 6.66 (s, 1H), 5.94 (q, J = 7 Hz, 1H), 3.78 (s, 3H), 1.92 (s, 3H), 1.31 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 161.7 (d, J = 246 Hz, 1C), 159.2, 141.1, 133.3 (d, J = 2.5 Hz, 1C), 132.3, 131.3 (d, J = 8.8 Hz, 2C), 129.9, 129.8, 115.6 (d, J = 21 Hz, 2C), 114.0, 68.9, 55.5, 21.3, 20.0; ^{19}F NMR (471 MHz, DMSO D_6) δ –114.9; IR (Neat) ν_{max} 2926, 2852, 1734, 1604, 1509, 1370, 1285, 1233, 1179, 1034, 831 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}FNaO_3^+$ $(M+Na)^+$: calcd. 337.1210, found 337.1211.

(*Z*)-4-(4-Bromophenyl)-3-(4-methoxyphenyl)but-3-en-2-yl acetate (34):



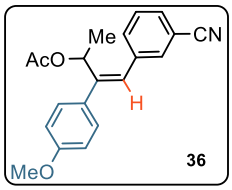
34 (53 mg, 70%) as pale yellow liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.58 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 9.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.5 Hz, 2H), 6.63 (s, 1H), 5.92 (q, J = 6.5Hz, 1H), 3.78 (s, 3H), 1.92 (s, 3H), 1.31 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.8, 159.3, 141.7, 136.2, 132.2, 131.7, 131.4, 129.9, 129.7, 120.9, 114.1, 68.9, 55.6, 21.3, 20.0; IR (Neat) ν_{max} 2918, 2850, 1725, 1603, 1509, 1485, 1287, 1238, 1072, 1028, 837 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}BrNaO_3^+$ $(M+Na)^+$: calcd. 397.0410, found 397.0407.

(*Z*)-3-(4-Methoxyphenyl)-4-(3-nitrophenyl)but-3-en-2-yl acetate (35):



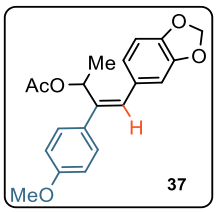
35 (55 mg, 83%) as pale-yellow liquid; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 8.21–8.15 (m, 2H), 7.79 (d, J = 7.5 Hz, 1H), 7.71 (t, J = 8.0 Hz, 1H), 7.49 (dt, J = 8.5, 3.0 Hz, 2H), 6.99 (dt, J = 8.5, 3.0 Hz, 2H), 6.80 (s, 1H), 5.87 (q, J = 6.5 Hz, 1H), 3.80 (s, 3H), 1.93 (s, 3H), 1.34 (d, J = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.8, 159.5, 148.2, 143.1, 138.7, 135.8, 131.8, 130.3, 129.9, 128.6, 123.8, 122.4, 114.1, 69.0, 55.6, 21.2, 20.0; IR (Neat) ν_{max} 2932, 1733, 1605, 1573, 1525, 1509, 1369, 1346, 1285, 1232, 1179, 1032, 832 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{19}NaO_5^+$ $(M+Na)^+$: calcd. 364.1155, found 364.1157.

(*Z*)-4-(3-Cyanophenyl)-3-(4-methoxyphenyl)but-3-en-2-yl acetate (36):



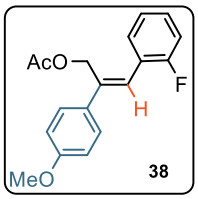
36 (41 mg, 63%) as pale yellow liquid; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.79–7.75 (m, 2H), 7.68–7.59 (m, 2H), 7.49–7.44 (m, 2H), 7.00–6.96 (m, 2H), 6.70 (s, 1H), 5.87 (q, *J* = 6.5 Hz, 1H), 3.79 (s, 3H), 1.91 (s, 3H), 1.32 (d, *J* = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.8, 159.4, 142.8, 138.3, 134.0, 132.8, 131.9, 131.2, 130.0, 129.9, 128.7, 119.2, 114.1, 111.9, 68.9, 55.6, 21.3, 20.0; IR (Neat) ν_{max} 3427, 1733, 1679, 1601, 1510, 1368, 1239, 1026, 825 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{19}NaO_3^+$ $(M+Na)^+$: calcd. 344.1257, found 344.1260.

(*Z*)-4-(Benzo[d][1,3]dioxol-5-yl)-3-(4-methoxyphenyl)but-3-en-2-yl acetate (37):



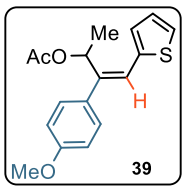
37 (38 mg, 67%) as pale-yellow liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.42 (dt, *J* = 9.0, 3.0 Hz, 2H), 6.98–6.91 (m, 3H), 6.89 (d, *J* = 1.5 Hz, 1H), 6.82–6.77 (m, 1H), 6.59 (s, 1H), 6.07–6.03 (m, 2H), 6.00 (q, *J* = 6.5 Hz, 1H), 3.78 (s, 3H), 1.96 (s, 3H), 1.29 (d, *J* = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.8, 159.1, 147.7, 146.9, 140.0, 132.5, 130.8, 130.7, 129.9, 123.1, 114.0, 109.4, 108.7, 101.6, 68.9, 55.5, 21.4, 20.0; IR (Neat) ν_{max} 2920, 1733, 1651, 1620, 1485, 1433, 1369, 1220, 1076, 1034, 934 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{20}NaO_5^+$ $(M+Na)^+$: calcd. 363.1203, found 363.1200.

(*Z*)-3-(2-Fluorophenyl)-2-(4-methoxyphenyl)allyl acetate (38):



38 (51 mg, 68%) as yellow gummy liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.53 (dt, *J* = 9.0, 3.0 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.29–7.22 (m, 2H), 7.00–6.95 (m, 3H), 5.00 (s, 2H), 3.78 (s, 3H), 1.93 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 170.7, 160.2 (d, *J* = 246 Hz, 1C), 159.7, 137.6, 131.7, 131.0 (d, *J* = 2.5 Hz, 1C), 130.2 (d, *J* = 8.8 Hz, 1C), 128.1, 124.9 (d, *J* = 3.8 Hz, 1C), 124.6 (d, *J* = 14.0 Hz, 1C), 123.5 (d, *J* = 2.5 Hz, 1C), 116.0 (d, *J* = 21.0 Hz, 1C), 114.4, 61.7, 55.6, 21.0; ^{19}F NMR (471 MHz, DMSO D_6) δ –114.6; IR (Neat) ν_{max} 2935, 1733, 1512, 1484, 1223, 1180, 1097, 1025, 956 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{17}FNaO_3^+$ $(M+Na)^+$: calcd. 323.1054, found 323.1053.

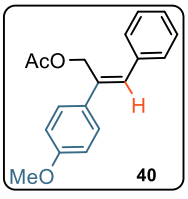
(*Z*)-3-(4-Methoxyphenyl)-4-(thiophen-2-yl)but-3-en-2-yl acetate (39):



39 (34 mg, 42%) as yellow liquid; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.63 (dd, *J* = 5.5, 4.5 Hz, 1H), 7.40 (dt, *J* = 9.0, 3.0 Hz, 2H), 7.20 (d, *J* = 3.0 Hz, 1H), 7.12 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.94 (dt, *J* = 8.5, 3.5 Hz, 2H), 6.77 (s, 1H), 6.23 (q, *J* = 6.5 Hz, 1H), 3.78 (s, 3H), 1.93 (s, 3H), 1.44 (d, *J* = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.9, 159.1, 139.3, 138.7, 132.2, 130.0,

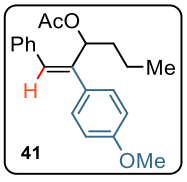
129.7, 127.9, 127.8, 122.9, 114.0, 69.2, 55.6, 21.3, 19.8; IR (Neat) ν_{max} 2918, 1733, 1604, 1508, 1455, 1369, 1383, 1286, 1237, 1177, 1030 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{18}NaO_3S^+$ $(M+Na)^+$: calcd. 325.0869, found 325.0867.

(*Z*)-2-(4-Methoxyphenyl)-3-phenylallyl acetate (40):



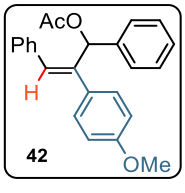
40 (45 mg, 79%) as colourless liquid; R_f = 0.5 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.52 (dt, J = 8.5, 3.5 Hz, 2H), 7.45–7.39 (m, 2H), 7.37 (d, J = 7.0 Hz, 2H), 7.34–7.30 (m, 1H), 7.12 (s, 1H), 6.97 (dt, J = 9.0, 3.0 Hz, 2H), 5.05 (s, 2H), 3.78 (s, 3H), 1.99 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, DMSO D_6) δ 170.8, 159.5, 137.0, 135.1, 132.5, 131.6, 129.2, 128.9, 127.88, 127.86, 114.4, 61.8, 55.6, 21.1; IR (Neat) ν_{max} 2923, 1735, 1606, 1512, 1462, 1244, 1181, 1027, 954, 826 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{18}NaO_3^+$ $(M+Na)^+$: calcd. 305.1148, found 305.1149.

(*Z*)-2-(4-Methoxyphenyl)-1-phenylhex-1-en-3-yl acetate (41):



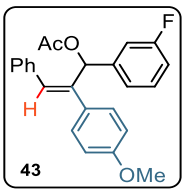
41 (46 mg, 71%) as yellow gummy liquid ; R_f = 0.6 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.47–7.43 (m, 2H), 7.41–7.37 (m, 2H), 7.34–7.27 (s, 3H), 6.98–6.93 (m, 2H), 6.72 (s, 1H), 5.92 (q, J = 1.5 Hz, 1H), 3.77 (s, 3H), 1.94 (s, 3H), 1.72–1.48 (m, 2H), 1.20–1.10 (m, 2H), 0.70 (t, J = 7.5 Hz, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, DMSO D_6) δ 169.4, 158.6, 139.6, 136.5, 132.2, 131.5, 129.4, 128.7, 128.2, 127.0, 113.5, 71.8, 55.0, 20.8, 18.3, 13.4; IR (Neat) ν_{max} 2957, 1734, 1509, 1286, 1232, 1028, 823, 697 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{24}NaO_3^+$ $(M+Na)^+$: calcd. 347.1618, found 347.1619.

(*Z*)-2-(4-Methoxyphenyl)-1,3-diphenylallyl acetate (42):



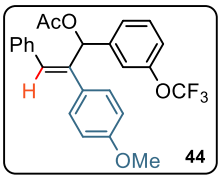
42 (35 mg, 55%) as red gummy liquid. R_f = 0.5 (10% EtOAc/Hex); ^1H NMR (500 MHz, DMSO D_6) δ 7.42–7.30 (m, 9H), 7.28–7.24 (m, 3H), 7.10 (s, 2H), 6.83 (dt, J = 8.0, 3.0 Hz, 2H), 3.71 (s, 3H), 2.02 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, DMSO D_6) δ 169.4, 158.6, 138.5, 137.6, 136.4, 131.6, 131.2, 129.1, 128.54, 128.48, 128.4, 127.5, 127.3, 125.8, 113.4, 72.6, 55.0, 20.7; IR (Neat) ν_{max} 2929, 1737, 1509, 1283, 1224, 1178, 1023, 748, 696 cm^{-1}; **HRMS (ESI)** for $C_{24}H_{22}NaO_3^+$ $(M+Na)^+$: calcd. 381.1461, found 381.1460.

(*Z*)-1-(3-Fluorophenyl)-2-(4-methoxyphenyl)-3-phenylallyl acetate (43):



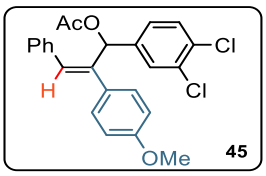
43 (45 mg, 60%) as yellow gummy liquid. R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.42–7.36 (m, 5H), 7.36–7.30 (m, 3H), 7.12–7.08 (m, 3H), 7.06–7.01 (m, 2H), 6.85 (dt, J = 8.0, 3.0 Hz, 2H), 3.72 (s, 3H), 2.01 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.5, 162.2 (d, J = 245 Hz, 1C), 141.55 (d, J = 7.1 Hz, 1C), 137.2, 136.3, 132.2, 130.7, 130.6 (d, J = 8.1 Hz, 1C), 129.1, 128.6, 128.5, 127.5, 114.4 (d, J = 21 Hz, 1C), 113.5, 112.7 (d, J = 22 Hz, 1C), 71.9, 55.0, 20.7; ^{19}F NMR (376 MHz, DMSO D_6) δ −112.6; IR (Neat) ν_{max} 2930, 2361, 1740, 1606, 1509, 1283, 1179, 1026, 825, 757, 722 cm^{-1}; **HRMS (ESI)** for $C_{24}H_{21}FNaO_3^+$ $(M+Na)^+$: calcd. 399.1367, found 399.1368.

(*Z*)-2-(4-Methoxyphenyl)-3-phenyl-1-(3-(trifluoromethoxy)phenyl)allyl acetate (44):



44 (45 mg, 51%) as yellow gummy liquid. R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.39 (d, J = 5.0 Hz, 4H), 7.38–7.34 (m, 3H), 7.34–7.29 (m, 4H), 7.11 (s, 1H), 7.07 (s, 1H), 6.85 (dt, J = 10.0, 3.0 Hz, 2H), 3.71 (s, 3H), 2.04 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 169.4, 158.7, 147.6, 137.8, 137.3, 136.3 132.1, 130.9, 129.1, 128.5, 128.4, 127.9, 127.4, 121.0, 120.0 (q, J = 257.0 Hz, 1C), 113.5, 72.0, 55.0, 20.6 ; ^{19}F NMR (376 MHz, DMSO D_6) δ −56.8; IR (Neat) ν_{max} 2934, 1741, 1508, 1508, 1217, 1158, 1018, 823 cm^{-1}; **HRMS (ESI)** for $C_{25}H_{21}F_3NaO_4^+$ $(M+Na)^+$: calcd.465.1284, found 465.1284.

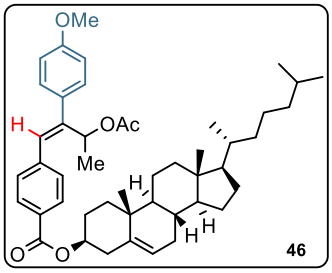
(*Z*)-1-(3,4-Dichlorophenyl)-2-(4-methoxyphenyl)-3-phenylallyl acetate (45):



45 (45 mg, 53%) as yellow gummy liquid. R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.59 (d, J = 8.5 Hz, 1H), 7.44–7.42 (m, 1H), 7.41–7.37 (m, 4H), 7.36 –7.29 (m, 3H), 7.26–7.22 (m, 1H), 7.13 (s, 1H), 7.00 (s, 1H), 6.86 (dt, J = 10.0, 3.0 Hz, 2H), 3.72 (s, 3H), 2.05 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 169.4, 158.8, 139.7, 136.7, 136.2, 132.5, 131.4, 130.8, 130.6, 130.3, 129.1, 128.6, 127.8, 127.6, 126.4, 113.6, 71.5, 55.0, 20.7; IR (Neat) ν_{max} 2931, 2360, 1598, 1740, 1509, 1221, 1179, 1025, 823, 729 cm^{-1}; **HRMS (ESI)** for $C_{24}H_{20}Cl_2NaO_3^+$ $(M+Na)^+$: calcd. 449.0682, found 449.0681.

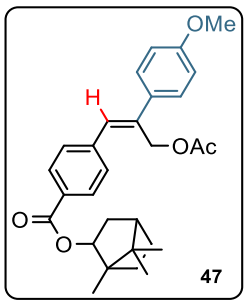
(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-((Z)-3-acetoxy-2-(4-methoxyphenyl)but-1-en-1-yl)benzoate (46):

46 (65 mg, 46%) as pale-yellow liquid ; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, J = 8.5 Hz, 2H), 7.47 (dt, J = 9.0, 3.0 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 6.94 (dt, J = 9.0, 2.5 Hz, 2H),



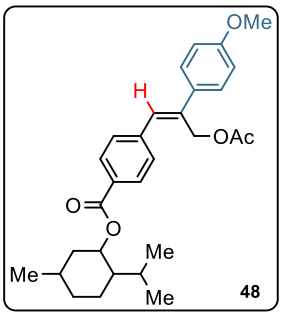
6.73 (s, 1H), 6.70 (s, 1H), 6.10 (q, *J* = 7.0 Hz, 1H), 5.45 (d, *J* = 4.0 Hz, 1H), 4.93–4.84 (m, 1H), 3.87 (s, 3H), 2.49 (d, *J* = 8.0 Hz, 2H), 2.07–1.94 (m, 10H), 1.63–1.48 (m, 9H), 1.42–1.36 (m, 4H), 1.29–1.26 (m, 4H), 1.14–1.00 (m, 4H), 0.95 (d, *J* = 6.5 Hz, 3H), 0.92–0.87 (m, 9H), 0.72 (s, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 170.0, 165.8, 159.2, 142.7, 141.5, 139.7, 132.4, 130.1, 129.60, 129.57, 128.8, 122.8, 116.2, 113.5, 74.6, 69.5, 56.7, 56.2, 55.3, 50.1, 42.4, 39.8, 39.5, 38.3, 37.1, 36.7, 36.2, 35.8, 32.0, 31.9, 28.3, 28.0, 24.3, 23.9, 22.8, 22.6, 21.2, 21.1, 19.8, 19.4, 18.7, 11.9; IR (Neat) ν_{max} 2922, 2851, 1740, 1714, 1606, 1511, 1463, 1369, 1272, 1244, 1178, 1035 cm^{-1}; **HRMS (ESI)** for $C_{47}H_{64}NaO_5^+$ $(M+Na)^+$: calcd. 731.4646, found 731.4647.

1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl (Z)-4-(3-acetoxy-2-(4-methoxyphenyl)prop-1-en-1-yl)benzoate (47):



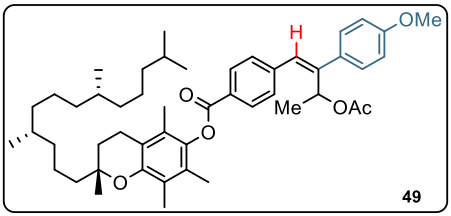
47 (72 mg, 78%) as pale-yellow liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 8.00 (d, *J* = 8.0 Hz, 2H), 7.57–7.48 (m, 4H), 7.16 (s, 1H), 6.97 (d, *J* = 8.5 Hz, 2H), 5.04 (s, 3H), 3.78 (s, 3H), 2.43–2.34 (m, 1H), 2.12–2.04 (m, 1H), 1.99 (s, 3H), 1.79–1.67 (m, 2H), 1.41–1.33 (m, 1H), 1.32–1.24 (m, 1H), 1.07 (dd, *J* = 14.0, 3.5 Hz, 1H), 0.92 (s, 3H), 0.87 (s, 3H), 0.86 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO D_6) δ 170.8, 166.0, 159.7, 141.8, 137.0, 132.1, 130.5, 129.7, 129.6, 129.2, 128.0, 114.4, 80.2, 61.5, 55.6, 49.2, 48.0, 44.8, 36.9, 28.1, 27.5, 21.1, 20.0, 19.1, 13.9; IR (Neat) ν_{max} 3384, 2924, 1737, 1710, 1653, 1604, 1512,1456, 1366, 1274, 1179, 1023, 992 cm^{-1}; **HRMS (ESI)** for $C_{29}H_{34}NaO_5^+$ $(M+Na)^+$: calcd. 485.2298, found 485.2299.

2-Isopropyl-5-methylcyclohexyl(*Z*)-4-(3-acetoxy-2-(4-methoxyphenyl)prop-1-en-1-yl)benzoate (48):



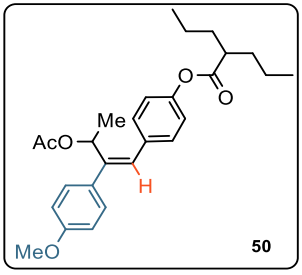
48 (60 mg, 65%) as pale yellow liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.98 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 9.0 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.17 (s, 1H), 6.97 (d, *J* = 9.0 Hz, 2H), 5.03 (s, 2H), 4.90–4.80 (m, 1H), 3.78 (s, 3H), 1.99 (s, 3H), 1.92–1.85 (m, 1H), 1.70–1.63 (m, 2H), 1.57–1.47 (m, 2H), 1.14–1.04 (m, 2H), 0.92–0.85 (m, 8H), 0.74 (d, *J* = 7.0 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO D_6) δ 170.7, 165.4, 159.7, 141.8, 137.0, 132.1, 130.4, 129.7, 129.5, 129.1, 128.0, 114.4, 74.6, 61.5, 55.6, 47.1, 34.2, 31.3, 26.7, 23.7, 22.3, 21.1, 20.9, 16.9; IR (Neat) ν_{max} 2953, 1738, 1708, 1603, 1513, 1271, 1246, 1178, 1102, 1019, 981 cm^{-1}; **HRMS (ESI)** for $C_{30}H_{36}NaO_5^+$ $(M+Na)^+$: calcd. 487.2455, found 487.2453.

(*R*)-2,5,7,8-Tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yl 4-((Z)-3-acetoxy-2-(4-methoxyphenyl)prop-1-en-1-yl)benzoate (49):



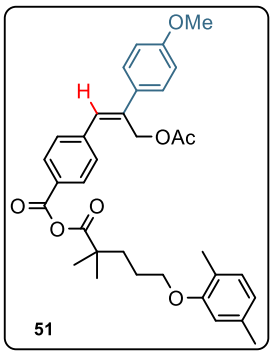
49 (102 mg, 69%) as pale yellow liquid; R_f = 0.2 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20–8.15 (m, 2H), 7.45 (dt, *J* = 9.0, 3.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 6.92 (dt, *J* = 9.0, 3.0 Hz, 2H), 6.81 (s, 1H), 6.75 (s, 1H), 6.70 (s, 1H), 6.05 (q, *J* = 6.5 Hz, 1H), 3.85 (s, 3H), 2.79–2.72 (m, 2H), 2.18 (s, 3H), 1.96 (s, 3H), 1.87–1.71 (m, 4H), 1.64–1.44 (m, 5H), 1.43–1.37 (m, 4H), 1.31–1.23 (m, 11H), 1.17–1.03 (m, 7H), 0.8–0.3 (m, 14H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 170.0, 165.7, 159.3, 149.9, 143.0, 142.7, 142.2, 132.3, 130.1, 129.9, 129.6, 129.0, 128.4, 127.4, 121.3, 121.1, 119.2, 113.6, 76.2, 69.5, 55.3, 40.2, 39.4, 37.5, 37.3, 32.8, 32.7, 31.1, 28.0, 24.8, 24.5, 24.3, 22.8, 22.7, 22.5, 21.2, 21.0, 19.9, 19.8, 19.7, 16.2; IR (Neat) ν_{max} 2924, 2865, 1734, 1605, 1510, 1468, 1374, 1222, 1176, 1138, 1073, 1033, 892 cm^{-1}; **HRMS (ESI)** for $C_{49}H_{69}O_6^+$ $(M+H)^+$: calcd. 753.5089, found 753.5088.

(*Z*)-4-(3-Acetoxy-2-(4-methoxyphenyl)but-1-en-1-yl)phenyl 2-propylpentanoate (50):



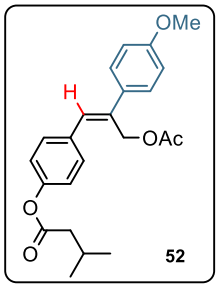
50 (56 mg, 64%) as pale-yellow liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.46 (dt, *J* = 8.5, 3.0 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.11 (dt, *J* = 8.5, 2.5 Hz, 2H), 6.96 (dt, *J* = 8.5, 3.0 Hz, 2H), 6.68 (s, 1H), 5.95 (q, *J* = 6.5 Hz, 1H), 3.78 (s, 3H), 2.65–2.58 (m, 1H), 1.93 (s, 3H), 1.71–1.62 (m, 2H), 1.59–1.50 (m, 2H), 1.44–1.35 (m, 4H), 1.32 (d, *J* = 6.5 Hz, 3H), 0.94 (t, *J* = 7.5 Hz, 6H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 174.8, 169.8, 159.2, 149.8, 141.2, 134.6, 132.4, 130.5, 130.0, 129.9, 122.1, 114.0, 69.0, 55.5, 45.0, 34.6, 21.4, 20.6, 20.1, 14.4; IR (Neat) ν_{max} 2957, 1736, 1605, 1509, 1370, 1285, 1236, 1197, 1105, 1034, 880 cm^{-1}; **HRMS (ESI)** for $C_{27}H_{34}NaO_5^+$ $(M+Na)^+$: calcd. 461.2298, found 461.2298.

(*Z*)-(*Z*)-4-(3-Acetoxy-2-(4-methoxyphenyl)prop-1-en-1-yl)benzoic 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoic anhydride (51):



51 (93 mg, 83%) as colorless liquid; R_f = 0.2 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.52 (d, J = 8.5 Hz, 2H), 7.39 (d, J = 8.5 Hz, 2H), 7.12–7.05 (m, 3H), 7.00–6.94 (m, 3H), 6.74 (s, 1H), 6.63 (d, J = 7.5 Hz, 1H), 5.03 (s, 2H), 4.00 (t, J = 6.0 Hz, 2H), 3.79 (s, 3H), 2.25 (s, 3H), 2.09 (s, 3H), 1.99 (s, 3H), 1.90–1.70 (m, 4H), 1.31 (s, 6H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 176.2, 170.8, 159.5, 156.9, 150.3, 136.6, 135.2, 134.6, 132.4, 130.8, 130.6, 130.4, 127.9, 123.0, 122.2, 121.0, 114.4, 112.5, 67.7, 61.8, 55.6, 42.4, 37.1, 25.2, 21.5, 21.2, 16.1; IR (Neat) ν_{max} 2923, 1737, 1606, 1509, 1462, 1244, 1201, 1164, 1107, 1027, 828 cm^{-1}; **HRMS (ESI)** for $C_{34}H_{39}O_7^+$ $(M+H)^+$: calcd. 531.2741, found 531.2741.

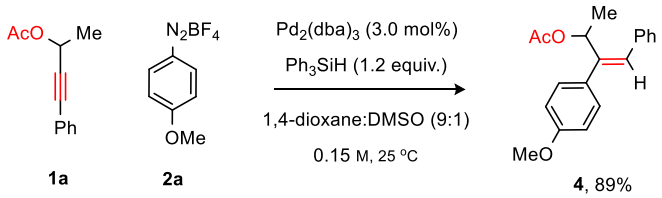
(*Z*)-4-(3-Acetoxy-2-(4-methoxyphenyl)prop-1-en-1-yl)phenyl 3-methylbutanoate (52):



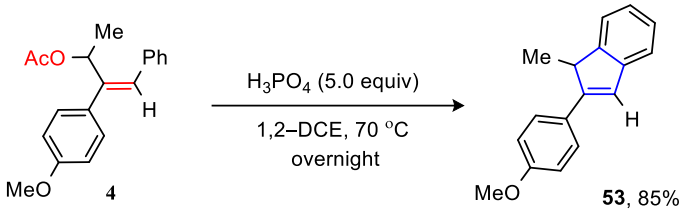
52 (56 mg, 73%) as colorless liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.51 (dt, J = 9.0, 3.0 Hz, 2H), 7.40 (d, J = 8.5 Hz, 2H), 7.18–7.14 (m, 2H), 7.10 (s, 1H), 6.96 (dt, J = 8.5, 3.0 Hz, 2H), 5.03 (s, 2H), 3.78 (s, 3H), 2.47 (d, J = 7.0 Hz, 2H), 2.17–2.07 (m, 1H), 1.98 (s, 3H), 1.00 (d, J = 6.5 Hz, 6H); ^{13}C{^{1}H} NMR (101 MHz, DMSO D_6) δ 171.5, 170.9, 159.5, 150.1, 135.2, 134.6, 132.4, 130.8, 130.4, 127.9, 122.4, 114.4, 61.7, 55.6, 42.9, 25.8, 22.6, 21.2; IR (Neat) ν_{max} 3408, 2958, 1755, 1730, 1606, 1361, 1239, 1199, 1100, 1022, 999, 888 cm^{-1}; **HRMS (ESI)** for $C_{23}H_{27}O_5^+$ $(M+H)^+$: calcd. 383.1853, found 383.1853.

Gram Scale Synthesis of 4:

To a mixture of **1a** (5.0 mmol, 0.9 g), *p*-methoxyphenyl diazonium tetrafluoroborate (**2a**) (15 mmol, 3.3 g), Ph_3SiH **3** (6.0 mmol, 1.5 g) and $Pd_2(dba)_3$ (0.15 mmol, 137.4 mg) was added 1,4-dioxane:dimethyl sulfoxide (9:1, 0.15 M, 33 mL). The reaction mixture was stirred at 25 °C for 4.0 h. After completion of the reaction, DMSO was removed by water workup. The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was evaporated and purified by column chromatography using neutral alumina to afford **4** (1.32 g, 89% yield).

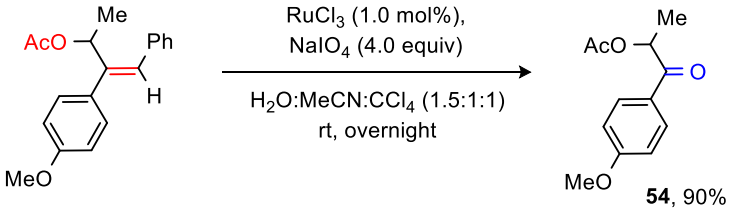


Synthesis of 2-(4-methoxyphenyl)-1-methyl-1H-indene (53):[7]



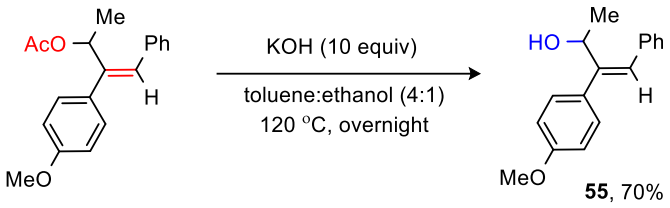
To a solution of **4** (0.2 mmol, 59 mg) in 1,2–dichloroethane (2.0 mL) was added H_3PO_4 (1.0 mmol, 98 mg, 52 µL). The resulting mixture was stirred at 70 °C overnight. The reaction progress was monitored by TLC. Upon completion, the crude mixture was concentrated under reduced pressure. The crude residue was purified using column chromatography on neutral alumina to afford **53** in 40 mg (85% yield) as colorless liquid; R_f = 0.8 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (dt, J = 8.5, 3.0 Hz, 2H), 7.50–7.45 (m, 1H), 7.42–7.38 (m, 1H), 7.33–7.29 (m, 1H), 7.25–7.20 (m, 1H), 7.01 (s, 1H), 7.00–6.96 (m, 2H), 3.92 (q, J = 7.5 Hz, 1H), 3.88 (s, 3H), 1.38 (d, J = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.1, 152.2, 149.3, 143.8, 129.4, 128.1, 126.7, 124.5, 124.2, 122.8, 120.7, 114.2, 55.4, 44.2, 17.5; IR (Neat) ν_{max} 2957, 2920, 2851, 1603, 1508, 1461, 1303, 1247, 1178, 1034, 828 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{17}O^+$ $(M+H)^+$: calcd. 237.1274, found 237.1270.

Synthesis of 1-(4-methoxyphenyl)-1-oxopropan-2-yl acetate (54):



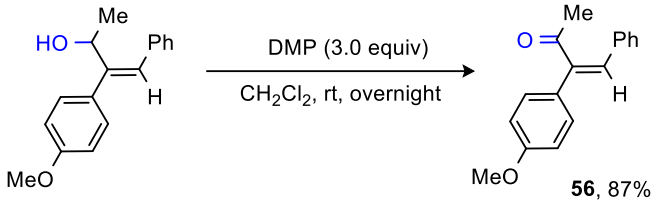
To a solution of **4** (0.2 mmol, 59 mg) in H_2O:MeCN:CCl_4 (1.5:1:1; 2.0 mL) was added $RuCl_3$ (0.002 mmol, 0.5 mg) and $NaIO_4$ (0.8 mmol, 171 mg). The resulting mixture was stirred at room temperature for overnight. The reaction progress was monitored by TLC. Upon completion, the crude mixture was concentrated under reduced pressure. The crude residue was purified using column chromatography on neutral alumina to afford **54** in 40 mg (90% yield) as colorless liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (dt, J = 9.0, 3.0 Hz, 2H), 6.97 (dt, J = 9.0, 3.0 Hz, 2H), 5.96 (q, J = 7.0 Hz, 1H), 3.89 (s, 3H), 2.16 (s, 3H), 1.54 (d, J = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 195.3, 170.5, 163.9, 130.8, 127.2, 114.0, 71.2, 55.5, 20.8, 17.4; IR (Neat) ν_{max} 2935, 1737, 1685, 1598, 1574, 1510, 1421, 1371, 1230, 1174, 1028, 841 cm^{-1}; **HRMS (ESI)** for $C_{12}H_{14}NaO_4^+$ $(M+Na)^+$: calcd. 245.0784, found 245.0788.

Synthesis of (*Z*)-3-(4-methoxyphenyl)-4-phenylbut-3-en-2-ol (55):[3]



To a solution of **4** (0.2 mmol, 59 mg) in toluene:ethanol (4:1; 2.0 mL) was added KOH (2.0 mmol, 112 mg). The resulting mixture was refluxed at 120 °C overnight. The reaction progress was monitored by TLC. Upon completion, the crude mixture was concentrated under reduced pressure. The crude residue was purified using column chromatography on neutral alumina to afford **55** in 36 mg (70% yield) as pale-yellow gummy liquid; R_f = 0.2 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6) δ 7.59 (dt, *J* = 9.0, 3.0 Hz, 2H), 7.43–7.36 (m, 4H), 7.30–7.25 (m, 1H), 6.92 (dt, *J* = 9.0, 3.0 Hz, 2H), 6.58 (s, 1H), 5.10 (d, *J* = 3.5 Hz, 1H), 5.00–4.90 (m, 1H), 3.77 (s, 3H), 1.13 (d, *J* = 6.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO D_6) δ 158.8, 145.4, 137.5, 133.6, 130.0, 129.4, 128.8, 128.6, 127.2, 113.6, 64.5, 55.5, 22.9; IR (Neat) ν_{max} 2929, 1605, 1507, 1442, 1283, 1241, 1177, 1105, 1029, 919 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{18}NaO_2^+$ $(M+Na)^+$: calcd. 277.1199, found 277.1199.

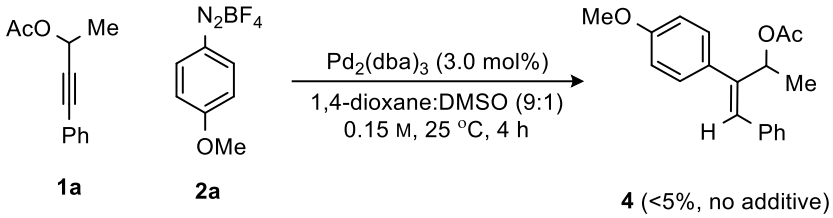
Synthesis of (*Z*)-3-(4-methoxyphenyl)-4-phenylbut-3-en-2-one (56):



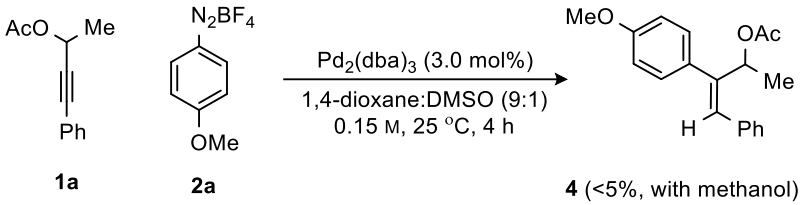
To a solution of **55** (0.2 mmol, 51 mg) in CH_2Cl_2 (2.0 mL) was added Dess-Martin periodinane (DMP; 0.6 mmol, 254 mg). The resulting mixture was stirred at room temperature overnight. The reaction progress was monitored by TLC. Upon completion, the crude mixture was concentrated under reduced pressure. The crude residue was purified using column chromatography on neutral alumina to afford **56** in 44 mg (87% yield) as colorless liquid; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.30 (m, 7H), 6.96–6.90 (m, 3H), 3.85 (s, 3H), 2.26 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 207.8, 159.8, 143.4, 135.9, 129.5, 128.7, 128.5, 128.1, 127.9, 127.6, 114.3, 55.4, 31.6; IR (Neat) ν_{max} 2932, 1954, 1695, 1572, 1509, 1417, 1282, 1246, 1205, 1181, 1030 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{16}NaO_2^+$ $(M+Na)^+$: calcd. 275.1043, found 275.1043.

Control Experiments

A. Hydride substitution vs protodemetalation



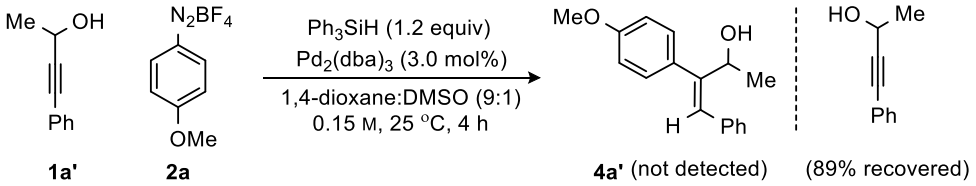
To a mixture of **1a** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), and $Pd_2(dba)_3$ (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 4.0 h. The reaction was monitored further for 24 h. Product **4** was not observed in detectable amount. **1a** was recovered in 88% yield.



To a mixture of **1a** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), and $Pd_2(dba)_3$ (0.006 mmol), and methanol (0.24 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 4.0 h. The reaction was monitored further for 24 h. Product **4** was not observed in detectable amount. **1a** was recovered in 90% yield.

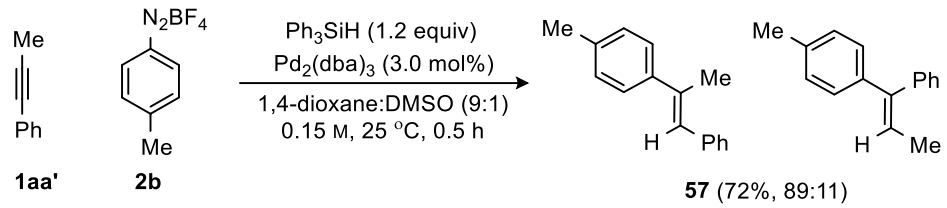
B. Role of acetate group

a)

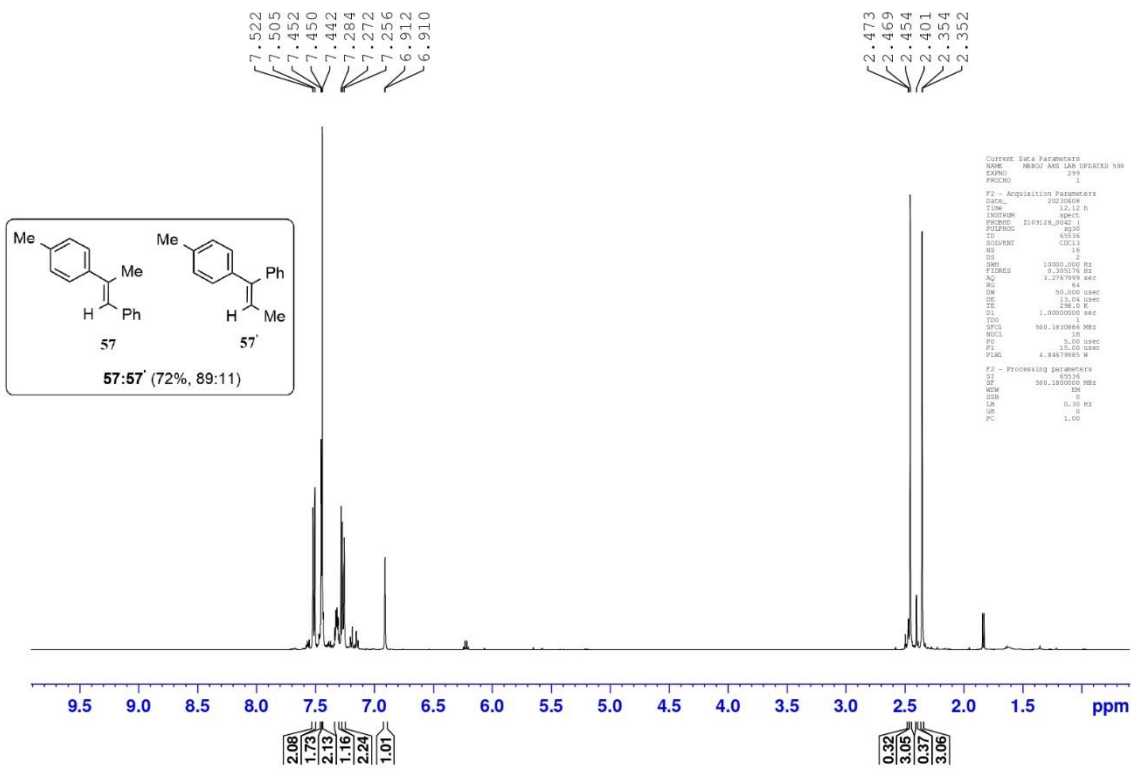


To a mixture of **1a'** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), and $Pd_2(dba)_3$ (0.006 mmol), and methanol (0.24 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 4.0 h. The reaction was monitored further for 24 h. Product **4a'** was not observed in detectable amount. **1a'** was recovered in 89% yield.

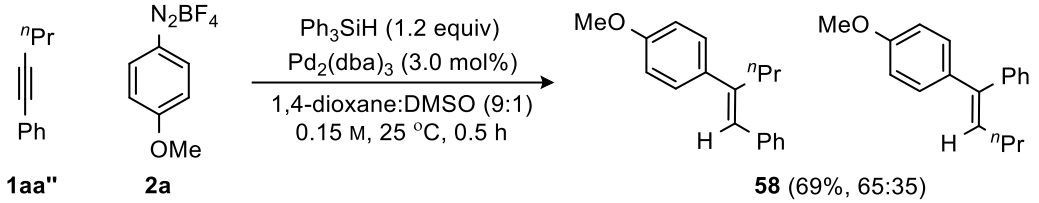
b)



To a mixture of **1aa'** (0.2 mmol), aryl diazonium-tetrafluoroborate **2b** (0.6 mmol), Ph_3SiH **3** (0.24 mmol) and $Pd_2(dba)_3$ (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 30 min. After completion of the reaction, DMSO was removed by water workup. The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was evaporated and purified by column chromatography using neutral alumina to afford **57** in 72% isolated yield of 89:11 regioisomeric mixture.

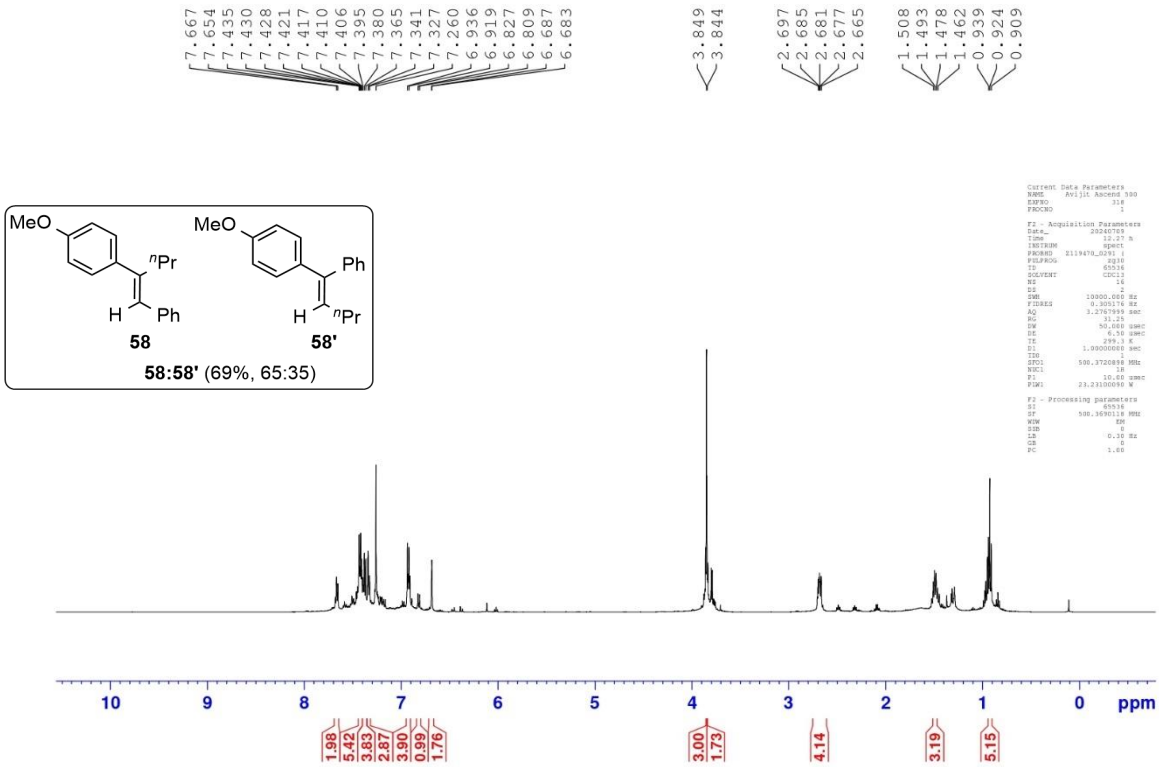


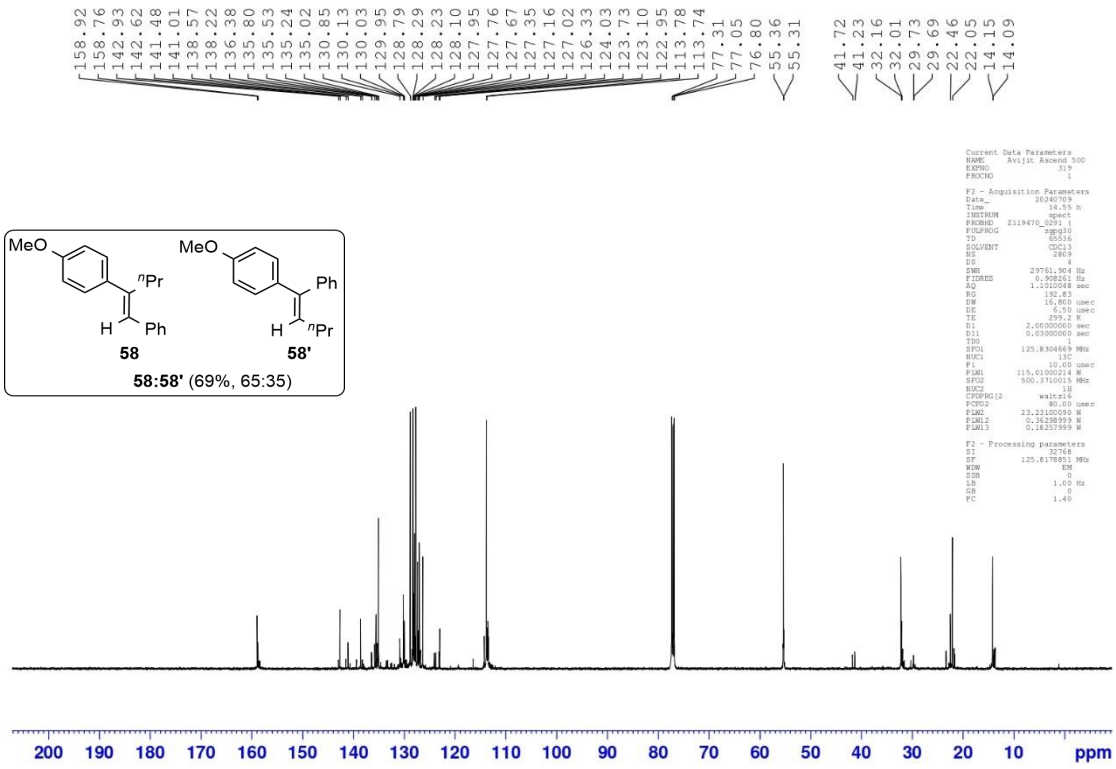
c)



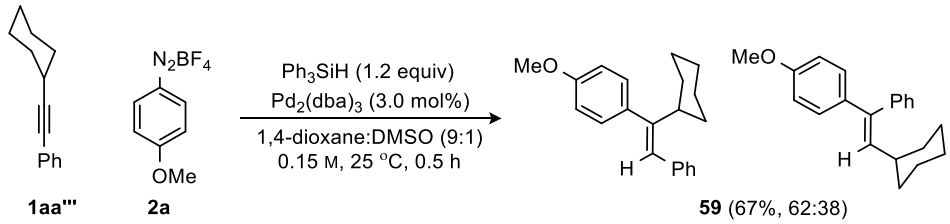
1aa" **2a** **58** (69%, 65:35)

To a mixture of **1aa''** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), Ph_3SiH **3** (0.24 mmol) and $Pd_2(dba)_3$ (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 30 min. After completion of the reaction, DMSO was removed by water workup. The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was evaporated and purified by column chromatography using neutral alumina to afford **58** in 69% isolated yield of 65:35 regioisomeric mixture.

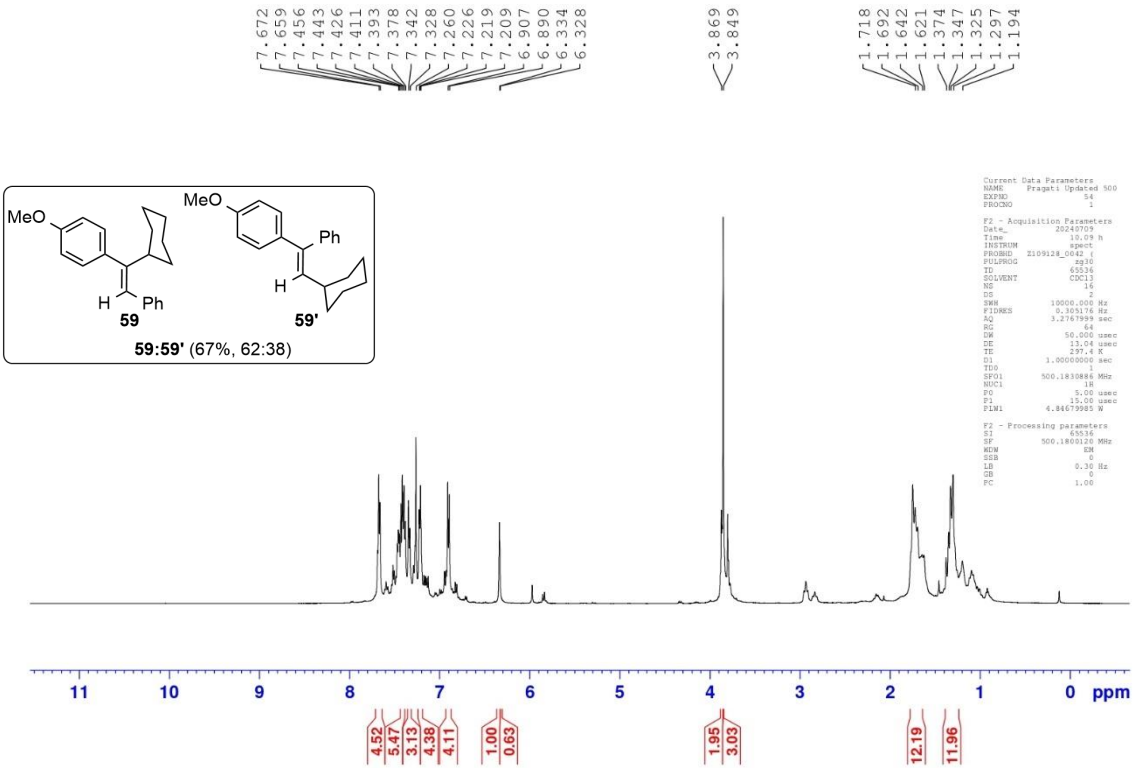


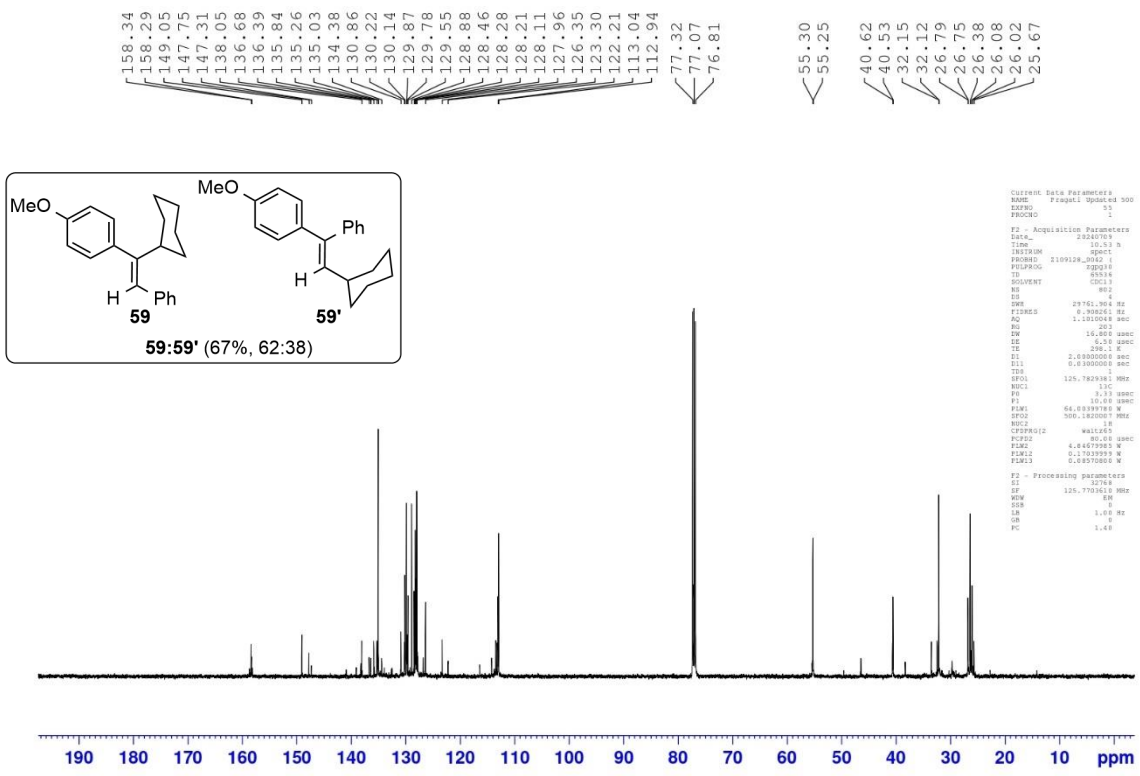


d)



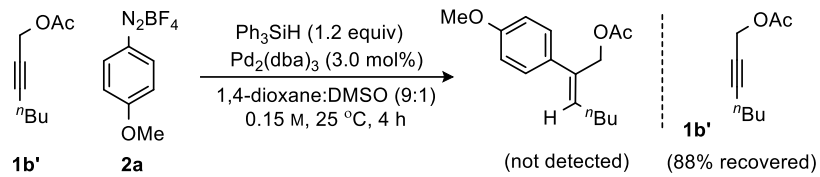
To a mixture of **1aa'''** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), Ph_3SiH **3** (0.24 mmol) and $Pd_2(dba)_3$ (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 30 min. After completion of the reaction, DMSO was removed by water workup. The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was evaporated and purified by column chromatography using neutral alumina to afford **59** in 67% isolated yield of 62:38 regioisomeric mixture.


7.672
7.659
7.456
7.443
7.426
7.411
7.393
7.378
7.342
7.328
7.260
7.226
7.219
7.209
6.907
6.890
6.334
6.328
3.869
3.849
1.718
1.692
1.642
1.621
1.374
1.347
1.325
1.297
1.194
MeO
H
Ph
59
MeO
Ph
H
59'
59:59' (67%, 62:38)
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.52
5.47
3.13
4.38
4.11
1.00
0.63
1.95
3.03
12.19
11.96


158.34
158.29
149.05
147.75
147.31
138.05
136.68
136.39
135.84
135.26
135.03
134.38
130.86
130.22
130.14
129.87
129.78
129.55
128.88
128.46
128.28
128.21
128.11
127.96
126.35
123.30
122.21
113.04
112.94
77.32
77.07
76.81
55.30
55.25
40.62
40.53
32.15
32.12
26.79
26.75
26.38
26.08
26.02
25.67
MeO
H
Ph
59
MeO
Ph
H
59'
59:59' (67%, 62:38)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

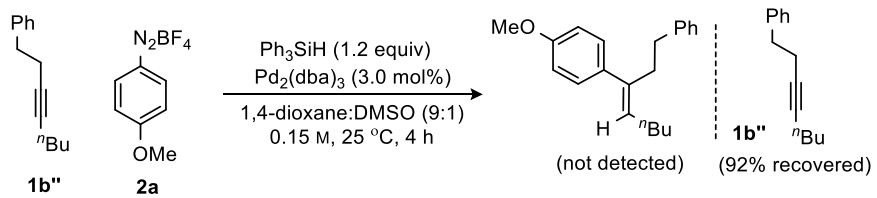
C. Other limiting alkynes

a)



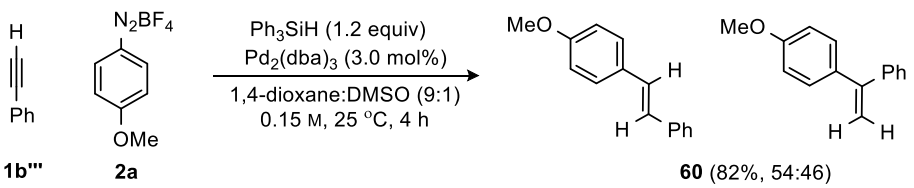
To a mixture of **1b′** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), and $Pd_2(dba)_3$ (0.006 mmol), and Ph_3SiH **3** (0.24 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 4.0 h. The reaction was monitored further for 24 h. The expected hydroarylation product was not observed in detectable amount. **1b′** was recovered in 88% yield.

b)



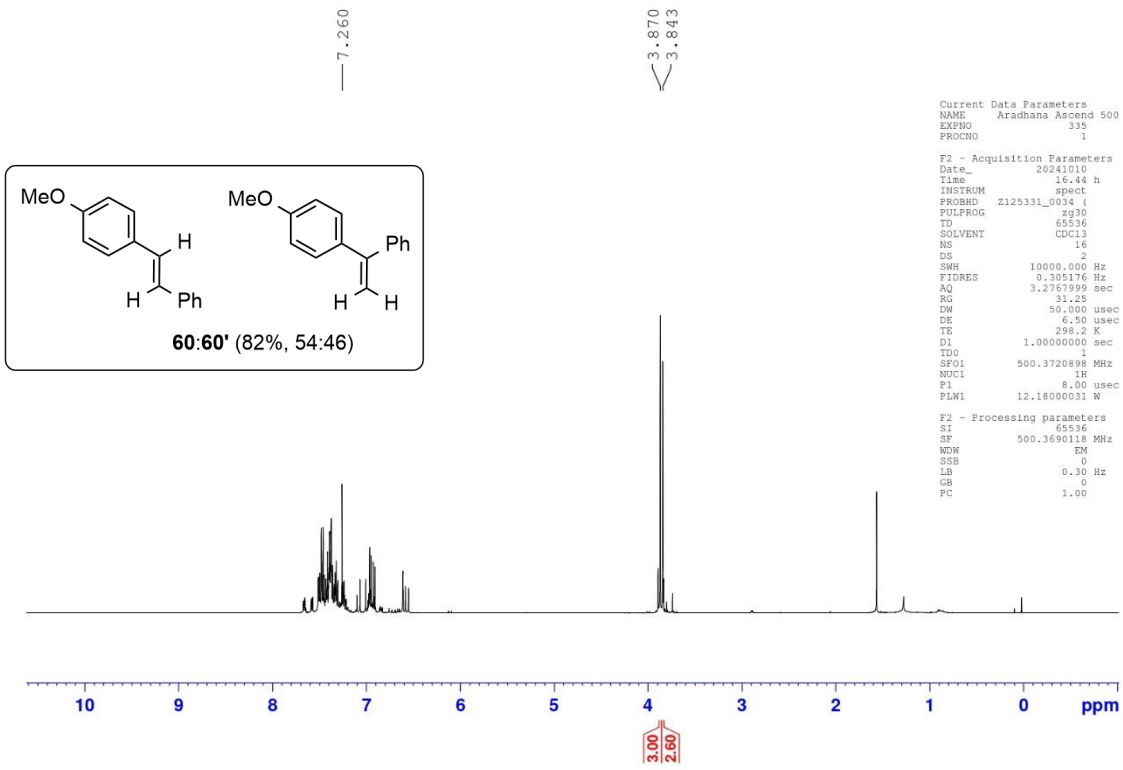
To a mixture of **1b″** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), and $Pd_2(dba)_3$ (0.006 mmol), and Ph_3SiH **3** (0.24 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 4.0 h. The reaction was monitored further for 24 h. The expected hydroarylation product was not observed in detectable amount. **1b″** was recovered in 92% yield.

c)

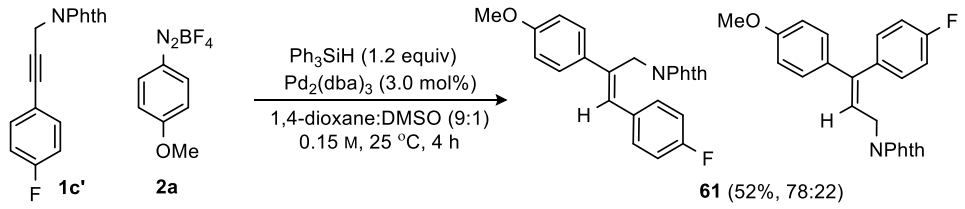


To a mixture of **1b‴** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), Ph_3SiH **3** (0.24 mmol) and $Pd_2(dba)_3$ (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 30 min. After completion of the reaction, DMSO was removed by water workup.

The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was evaporated and purified by column chromatography using neutral alumina to afford **60** in 82% isolated yield of 54:46 regioisomeric mixture.



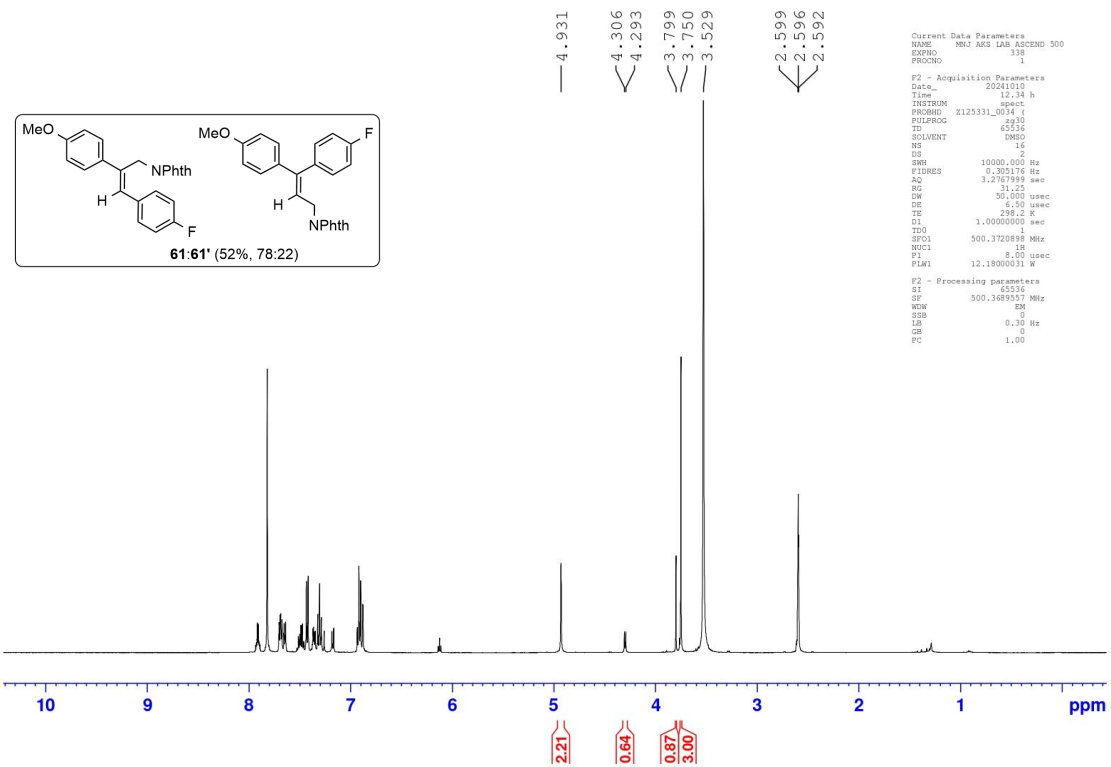
d)



(Phth = Phthalimide)

To a mixture of **1c'** (0.2 mmol), aryl diazonium-tetrafluoroborate **2a** (0.6 mmol), Ph_3SiH **3** (0.24 mmol) and $Pd_2(dba)_3$ (0.006 mmol) was added 1,4-dioxane: dimethyl sulfoxide (9:1, 0.15 M). The reaction mixture was stirred at 25 °C for 30 min. After completion of the reaction, DMSO was removed by water workup. The organic layer was extracted in ethyl acetate (3 × 10 mL) and dried over Na_2SO_4. The organic layer was

evaporated and purified by column chromatography using neutral alumina to afford **61** in 52% isolated yield of 78:22 regioisomeric mixture.



DFT Computations

Computational details: Following a recent DFT study on a related Pd-catalyzed reaction,[8] geometries (minima and transition states) were optimized at the BP86 level[9] of theory at 298 K and 1 atm using the Gaussian 16 software package.[10] The double-ζ basis set (LANL2DZ ECP) was used for Pd.[11] All other atoms were described by the 6-31G(d,p) basis set.[12] Frequency calculations were conducted at this level. Single point energy calculations were carried out at the M06L level of theory.[13] This method includes dispersion effects. The triple-ζ def2-TZVPP basis set was used for all atoms.[14] Solvent correction for 1,4-dioxane + DMSO (9:1) was obtained with the SMD[15] continuum solvation model as implemented in Gaussian. $Pd(DMSO)_2$ was used as starting point of the free energy profiles. The values discussed are Gibbs free energies (ΔG_{298}, kcal/mol). 3-Phenyl-2-propynylacetate **1a** was used as model substrate. Notably, we also tested the M06L functional and the SMD correction during optimization to evaluate the impact of dispersion and solvation on key steps. While this approach changed the energies, it did not alter the relative positioning of the computed species on the free energy profile. Therefore, the less computationally intensive method was preferred.

Results and discussion. In a previous study,[4] we have shown that $Pd(DMSO)_2$ is the most stable species in a DMSO/1,4-dioxane solution. We also reported that the oxidative addition of $Pd(DMSO)_2$ into the C–N bond of phenyl diazonium cation **A** to provide the cationic Pd-complex **B** is a barrierless and highly exergonic process releasing 64.0 kcal/mol of free energy (Figure S1). The different coordination modes of **1a** to **B** were also studied, revealing complex **C** as the best option (−6.7 kcal/mol). The *syn* insertion of the alkyne into the Pd–Ph bond leading to **D** (−19.1 kcal/mol) was achieved through $\mathbf{TS_{CD}}$, lying at 6.3 kcal/mol on the free energy surface. The exclusive α regioselectivity was already justified.[4]

From **D**, we studied the reaction with Ph_3SiH. At first, we envisaged the substitution of DMSO by the silane. It provided the σ-complex **E** (−11.1 kcal/mol) in which the Si–H bond serves as ligand (1.62 Å in **E** vs 1.50 Å in Ph_3SiH). The formation of **E** is endergonic by 8.0 kcal/mol. The breaking of the Si–H bond was modeled through $\mathbf{TS_{EF}}$, located at 9.0 kcal/mol (rate-determining step). The DMSO ligand plays a crucial role in this process as it captures the resulting silylium ion Ph_3Si^+ by its oxygen atom. Of note, in the absence of DMSO in the coordination sphere of Pd, we were unable to form a Pd–H bond. Thus, this assistance is a key point. The resulting hydride complex **F** (−2.9 kcal/mol) is coordinated to DMSO both by the S and the O atoms. Manifold efforts failed to obtain the reductive elimination of the latter. The $[Me_2SOSiPh_3]^+$ moiety can be used differently to coordinate the metal center and gain energy. In complex **G** (−13.7 kcal/mol), Pd is bound to one Ph group, allowing the S atom to establish a strong hydrogen bond with the hydride ligand (ρ_{max} = 0.028 eÅ^3). With the assistance of this noncovalent interaction, the reductive elimination becomes straightforward, the corresponding transition state $\mathbf{TS_{GH}}$ lying only 0.8 kcal/mol above **G** (−12.9 kcal/mol). This last step is strongly exergonic, leading to **H** at −50.8 kcal/mol. In this complex, the $[Me_2SOSiPh_3]^+$ moiety acts as a chelating ligand by the S atom and one Ph group. Finally, the recycling of the catalytically active species **B** from **H** is exergonic by 32.8 kcal/mol (see box).

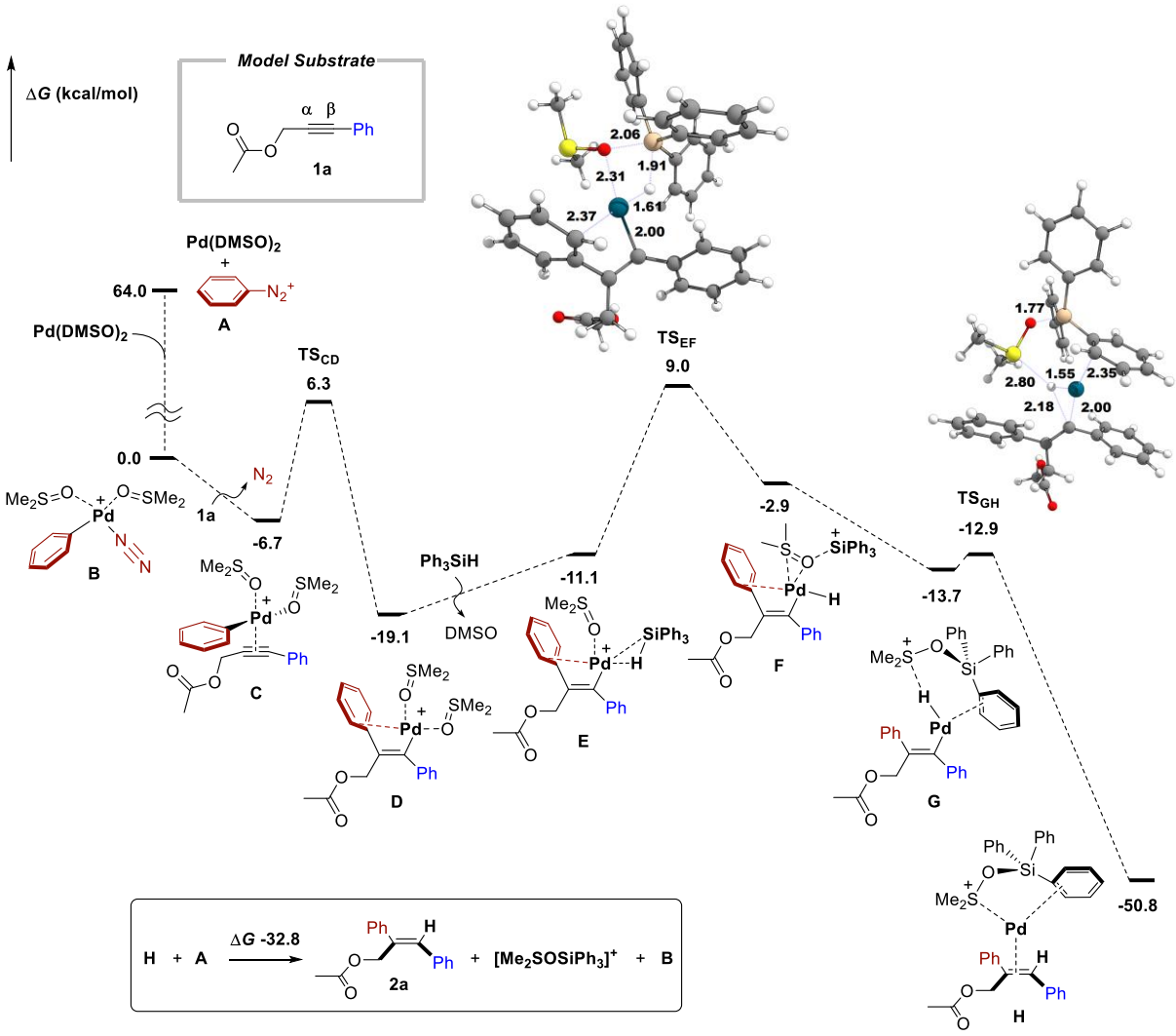


Figure S1. Computed free energy profile involving only tetravalent Pd species (M06L/def2-TZVPP; selected distances in Å).

We then studied the formation of a pentavalent addition complex between **D** and DMSO. Formation of the corresponding species **I** (-6.4 kcal/mol) is endergonic by 12.7 kcal/mol. However, the oxidative addition transition state $\mathbf{TS_{IJ}}$ (6.8 kcal/mol) lies 2.2 kcal/mol lower in energy than the tetravalent transition state $\mathbf{TS_{EF}}$ (9.0 kcal/mol; see Figure S2). Again here, the DMSO ligand assists the formation of the Pd–H bond by catching the ion Ph_3Si^+ ion. In the resulting Pd hydride **J**, the tetravalent neutral part is clearly separated from the $[Me_2SOSiPh_3]^+$ moiety. Its removal to give **K** (–17.4 kcal/mol) is exergonic by 5.8 kcal/mol. Reductive elimination takes place through $\mathbf{TS_{KL}}$ (–12.9 kcal/mol), with a low barrier of 4.5 kcal/mol. It yields the neutral species **L** (–25.3 kcal/mol), from which dissociation and regeneration of **B** is a highly favorable process (–58.3 kcal/mol, see box).

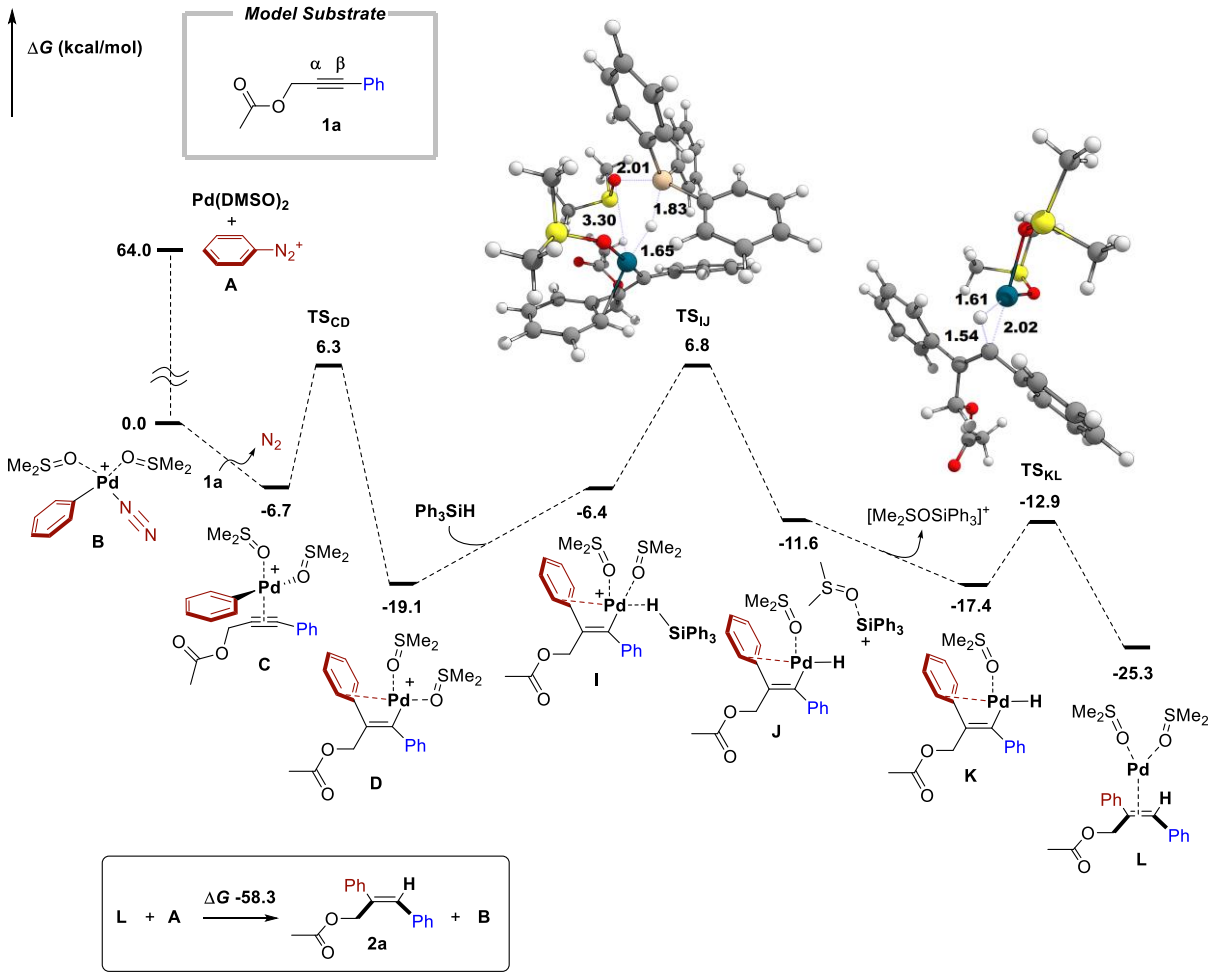


Figure S2. Computed free energy profile involving the pentavalent Pd species **I** (M06L/def2-TZVPP; selected distances in Å).

According to the above set of computations, DMSO is indispensable to promote the cleavage of the Si–H bond during the oxidative addition step. The proposed mechanism is consistent with the stereoselectivity of the title hydroarylation.

Table S3: Coordinates (x,y,z), energies (Hartree) and imaginary frequencies (cm^{-1}) of the computed species. Species **A** to **D** can be found in ref 4.

Ph_3SiH Thermal correction to Gibbs Free Energy= 0.224939 E(RM06L) = -985.237985717				**E** Thermal correction to Gibbs Free Energy= 0.532958 E(RM06L) = -2473.89086945			
Si	0.00104	-0.019119	0.921088	H	-0.52916	0.229176	-0.515258
C	-0.266108	1.767435	0.345273	Si	-2.090782	0.455473	-0.145375
C	-1.482729	2.182474	-0.243519	Pd	0.601961	-0.66039	0.452624
C	0.751206	2.737001	0.518827	C	1.864653	0.906249	0.645557
C	-1.679178	3.51495	-0.640884	C	3.100764	0.327409	0.618395
C	0.558696	4.069372	0.123754	C	3.022999	-1.154158	0.795848

C	-0.658818	4.460733	-0.457168
H	-2.285867	1.452407	-0.39489
H	1.711072	2.446169	0.962157
H	-2.62936	3.814155	-1.096473
H	1.359414	4.802992	0.26721
H	-0.810031	5.500207	-0.767509
C	1.688314	-0.647935	0.340905
C	2.258637	-0.227992	-0.884208
C	2.402213	-1.594431	1.113657
C	3.489238	-0.740596	-1.325244
C	3.633347	-2.107554	0.678095
C	4.177953	-1.682219	-0.544513
H	1.740622	0.520864	-1.494677
H	1.991893	-1.93216	2.07293
H	3.91339	-0.400865	-2.276342
H	4.170678	-2.836752	1.294011
H	5.139678	-2.080384	-0.885294
C	-1.402659	-1.132112	0.307169
C	-2.587395	-1.277035	1.067661
C	-1.315837	-1.825763	-0.922572
C	-3.649399	-2.074548	0.612918
C	-2.374291	-2.625447	-1.380487
C	-3.544028	-2.749549	-0.613665
H	-2.6805	-0.764249	2.032722
H	-0.403125	-1.748021	-1.524889
H	-4.556907	-2.173891	1.218257
H	-2.284916	-3.15644	-2.334378
H	-4.369732	-3.375522	-0.968575
H	-0.015836	-0.081548	2.424514

C	4.428766	1.054997	0.552246
C	3.786014	-2.103202	0.058348
C	2.145478	-1.635375	1.837782
C	1.466409	2.312716	0.674083
C	2.071925	3.275628	-0.176329
C	0.504041	2.747453	1.622268
H	2.815535	2.950978	-0.90873
C	1.736865	4.631457	-0.05709
H	0.030432	2.011095	2.279181
C	0.178036	4.103867	1.73378
H	2.219801	5.365907	-0.709837
C	0.792451	5.050135	0.895083
H	0.535802	6.110366	0.983957
H	-0.554773	4.425675	2.480176
O	4.716322	1.626363	-0.766796
H	5.254125	0.379144	0.827673
H	4.412127	1.931473	1.219312
C	5.492797	0.881037	-1.616978
C	5.790594	1.65683	-2.880995
O	5.89692	-0.245509	-1.360658
H	6.290741	0.998215	-3.60258
H	6.449811	2.509372	-2.646341
H	4.865745	2.06787	-3.315873
S	0.000228	-3.60753	-0.813722
O	-0.620763	-2.505027	0.116894
C	3.665482	-3.463222	0.339568
H	4.493748	-1.743969	-0.695242
C	2.020385	-3.032789	2.080157
H	1.809736	-0.932664	2.612551
C	2.772432	-3.937058	1.335909
H	4.279989	-4.180248	-0.215076
H	1.372503	-3.376983	2.892177
H	2.716156	-5.00955	1.548316
C	-0.898563	-5.119832	-0.318001
C	-0.760252	-3.391744	-2.466171
H	-1.978973	-4.912312	-0.345877
H	-0.6309	-5.938365	-1.004594
H	-0.578067	-5.365767	0.704161
H	-0.43922	-4.233592	-3.10112
H	-1.856477	-3.343826	-2.37993
H	-0.369464	-2.449855	-2.877037
C	-2.323673	2.165202	-0.895843
C	-2.439034	0.358788	1.702841
C	-3.063047	-0.794834	-1.170094

				C	-3.610743	2.759357	-0.839887
				C	-1.302339	2.840932	-1.601021
				C	-3.858677	3.994808	-1.457037
				H	-4.432587	2.253318	-0.31925
				C	-1.553077	4.074202	-2.223475
				H	-0.297464	2.409103	-1.656812
				C	-2.829672	4.6532	-2.150603
				H	-4.857509	4.439669	-1.402029
				H	-0.749026	4.583687	-2.764048
				H	-3.025046	5.614793	-2.636143
				C	-2.9106	1.504287	2.389705
				C	-2.269873	-0.842901	2.438674
				C	-3.210074	1.450392	3.760834
				H	-3.044554	2.446882	1.84833
				C	-2.567883	-0.893152	3.809401
				H	-1.896122	-1.741857	1.935331
				C	-3.039167	0.252561	4.472568
				H	-3.578423	2.34519	4.273074
				H	-2.435166	-1.829232	4.36219
				H	-3.273288	0.210872	5.54117
				C	-3.123707	-0.62851	-2.576065
				C	-3.803251	-1.851759	-0.588041
				C	-3.882818	-1.497539	-3.375091
				H	-2.587961	0.201903	-3.050651
				C	-4.570774	-2.717432	-1.384796
				H	-3.798432	-1.986728	0.498197
				C	-4.60696	-2.545583	-2.779902
				H	-3.923563	-1.348184	-4.459017
				H	-5.15569	-3.515909	-0.915762
				H	-5.212548	-3.214945	-3.399779
TS_{EF} Thermal correction to Gibbs Free Energy= 0.534401 E(RM06L) = -2473.86017991 Frequency -90.6929				**F** Thermal correction to Gibbs Free Energy= 0.533024 E(RM06L) = -2473.87788455			
H	0.251931	0.58952	-0.016491	H	0.750918	1.577099	-0.354505
Si	2.147597	0.377496	0.124801	Si	-2.957542	0.291166	-0.097109
Pd	-0.691947	-0.576631	-0.610256	Pd	0.919349	0.295393	0.510224
C	-2.361156	0.525817	-0.664893	C	2.895419	0.590265	0.477283
C	-3.360937	-0.404505	-0.634383	C	3.488908	-0.634191	0.657214
C	-2.841613	-1.796962	-0.848366	C	2.55903	-1.754016	1.000027
C	-4.84789	-0.128151	-0.526549	C	4.986182	-0.883573	0.635741
C	-3.18683	-2.9116	-0.030676	C	2.606369	-3.026886	0.373288
C	-1.974335	-2.022483	-1.973928	C	1.565704	-1.540575	2.009085

C	-2.372184	1.990775	-0.654711	C	3.509452	1.916262	0.296437
C	-3.298158	2.726745	0.130122	C	4.667724	2.115252	-0.49734
C	-1.462742	2.704597	-1.477522	C	2.952525	3.037563	0.963493
H	-3.994526	2.193375	0.782136	H	5.099246	1.273514	-1.043773
C	-3.322311	4.127779	0.06819	C	5.251206	3.38781	-0.598821
H	-0.732867	2.145163	-2.071669	H	2.043889	2.896787	1.5585
C	-1.498859	4.101794	-1.537443	C	3.547333	4.299952	0.869742
H	-4.044922	4.680918	0.677169	H	6.14088	3.522344	-1.222858
C	-2.429132	4.819868	-0.764911	C	4.700849	4.481644	0.085492
H	-2.453525	5.913296	-0.80968	H	5.160391	5.471718	0.00311
H	-0.798375	4.634448	-2.188361	H	3.107475	5.148003	1.404553
O	-5.273793	0.342781	0.796738	O	5.56855	-0.867061	-0.714774
H	-5.425286	-1.032454	-0.776011	H	5.22689	-1.852997	1.099148
H	-5.127259	0.701891	-1.195318	H	5.511962	-0.066814	1.15583
C	-5.721211	-0.597853	1.686249	C	5.829605	-2.069847	-1.313033
C	-6.233795	0.065184	2.946425	C	6.562442	-1.862209	-2.621427
O	-5.722643	-1.801866	1.465233	O	5.528768	-3.156192	-0.834
H	-6.408275	-0.69897	3.714923	H	6.527721	-2.788477	-3.209945
H	-7.183301	0.583216	2.72956	H	7.616781	-1.612939	-2.412149
H	-5.522922	0.822938	3.311393	H	6.132604	-1.023841	-3.19078
S	1.208146	-2.860793	0.699332	S	-0.4975	-1.536163	-1.150268
O	1.372633	-1.509241	-0.165901	O	-1.347656	-0.569478	-0.129863
C	-2.662527	-4.175817	-0.305197	C	1.665735	-4.01317	0.694207
H	-3.901014	-2.765805	0.785539	H	3.406535	-3.239845	-0.34233
C	-1.435392	-3.312915	-2.218163	C	0.612274	-2.540219	2.30953
H	-1.897057	-1.252427	-2.751277	H	1.650526	-0.662549	2.665096
C	-1.770226	-4.380636	-1.384603	C	0.648322	-3.770845	1.642663
H	-2.956851	-5.025101	0.32077	H	1.732039	-4.993224	0.208911
H	-0.800458	-3.469591	-3.096267	H	-0.117353	-2.363507	3.106657
H	-1.382007	-5.383369	-1.590308	H	-0.066803	-4.55982	1.898014
C	2.859375	-3.621893	0.886779	C	-1.649227	-2.92361	-1.493563
C	0.89469	-2.341406	2.419668	C	-0.498922	-0.713897	-2.775788
H	3.545114	-2.988839	1.466573	H	-2.609282	-2.584938	-1.907482
H	2.678234	-4.589248	1.385629	H	-1.117101	-3.588883	-2.19344
H	3.245163	-3.799226	-0.126995	H	-1.798172	-3.44307	-0.536374
H	0.775477	-3.259656	3.017765	H	-0.048112	-1.42972	-3.483452
H	1.731119	-1.732193	2.791843	H	-1.517736	-0.437759	-3.081865
H	-0.047143	-1.773126	2.410209	H	0.139751	0.17428	-2.672298
C	1.828869	1.78221	1.373519	C	-3.018096	1.560946	-1.473261
C	2.369734	0.890941	-1.671996	C	-2.777215	1.038736	1.606126
C	3.771791	-0.403909	0.764647	C	-4.315391	-1.000101	-0.237809
C	2.966403	2.545026	1.755591	C	-4.227735	1.814602	-2.17069
C	0.567712	2.174482	1.875691	C	-1.897292	2.384305	-1.756894
C	2.83454	3.665758	2.589957	C	-4.305689	2.836755	-3.130062

H	3.963522	2.267707	1.397142	H	-5.121576	1.220194	-1.954681
C	0.440293	3.280786	2.730195	C	-1.975547	3.400904	-2.719649
H	-0.328793	1.615991	1.584285	H	-0.955949	2.233663	-1.211988
C	1.572154	4.030992	3.085128	C	-3.179021	3.62594	-3.410189
H	3.721925	4.247754	2.859279	H	-5.248767	3.018592	-3.655125
H	-0.54718	3.561495	3.109842	H	-1.099392	4.024552	-2.924731
H	1.472346	4.89822	3.745816	H	-3.240589	4.422613	-4.158509
C	2.481352	2.269784	-1.975018	C	-3.092416	2.406171	1.797728
C	2.468015	-0.042325	-2.733005	C	-2.379084	0.272232	2.730958
C	2.69616	2.698391	-3.295072	C	-3.021826	2.985041	3.074395
H	2.402938	3.014418	-1.175449	H	-3.392408	3.023533	0.944194
C	2.679568	0.388628	-4.051603	C	-2.306958	0.85316	4.005406
H	2.367698	-1.113787	-2.528876	H	-2.115945	-0.784402	2.608074
C	2.794497	1.76014	-4.334813	C	-2.629545	2.210309	4.177651
H	2.78713	3.767983	-3.510557	H	-3.271042	4.042563	3.206774
H	2.754794	-0.346245	-4.859931	H	-1.999828	0.249776	4.865802
H	2.959953	2.09573	-5.363508	H	-2.573863	2.663121	5.172689
C	4.054533	-0.498315	2.151201	C	-4.812831	-1.438027	-1.493574
C	4.734509	-0.919252	-0.13827	C	-4.888841	-1.556129	0.932659
C	5.228661	-1.113529	2.618648	C	-5.828221	-2.402865	-1.57589
H	3.363555	-0.052939	2.878057	H	-4.419899	-1.004255	-2.421677
C	5.915536	-1.523737	0.322703	C	-5.904693	-2.522057	0.851933
H	4.567666	-0.830207	-1.217448	H	-4.55056	-1.21745	1.917811
C	6.159122	-1.635031	1.702309	C	-6.373021	-2.948927	-0.400767
H	5.426782	-1.169694	3.694296	H	-6.203383	-2.720217	-2.554221
H	6.65126	-1.901397	-0.395141	H	-6.337421	-2.934448	1.768915
H	7.079155	-2.106673	2.062346	H	-7.169273	-3.697412	-0.46313
G Thermal correction to Gibbs Free Energy= 0.534231 E(RM06L) = -2473.89626781				**TS_{GH}** Thermal correction to Gibbs Free Energy= 0.533709 E(RM06L) = -2473.89445172 Frequency -12.8667			
H	-0.239358	-0.675698	-1.420426	H	-0.576061	-0.44991	0.281295
C	-2.237529	0.566132	-0.769087	C	-2.383914	0.497283	-0.496323
Pd	-0.278469	0.825625	-1.06604	Pd	-0.404929	0.713654	-0.727384
C	-2.083723	-2.189069	-2.283787	C	-1.929941	-2.199777	-2.037803
S	1.055678	-2.526411	-0.953803	S	1.163033	-2.273829	-0.936622
C	-3.143019	-0.449429	-0.765286	C	-3.209617	-0.580362	-0.58397
C	-2.438072	1.976801	-0.384526	C	-2.786956	1.905567	-0.273696
C	-2.839845	-1.862175	-1.131536	C	-2.752764	-1.960277	-0.910504
C	-4.582783	-0.151319	-0.376686	C	-4.705194	-0.398963	-0.381894
C	-3.355895	-2.926912	-0.352487	C	-3.206152	-3.076764	-0.167919
O	-4.756419	-0.470818	1.047294	O	-5.023858	-0.795325	0.99328
H	-5.296927	-0.759071	-0.957342	H	-5.291421	-1.03035	-1.071842

H	-4.833205	0.910108	-0.528804	H	-5.015008	0.646835	-0.527493
C	-3.088183	-4.265298	-0.686113	C	-2.83331	-4.38332	-0.527409
H	-3.961049	-2.693436	0.528691	H	-3.859399	-2.90802	0.693255
C	-1.820321	-3.529175	-2.620998	C	-1.580599	-3.509385	-2.41468
H	-1.737393	-1.382559	-2.936297	H	-1.61036	-1.345602	-2.643553
C	-2.776473	2.353208	0.946684	C	-2.795018	2.480815	1.024247
C	-2.17352	3.00779	-1.334196	C	-3.154426	2.717528	-1.379633
H	-2.994109	1.565697	1.67455	H	-2.517362	1.859646	1.881541
C	-2.866606	3.702657	1.301007	C	-3.168767	3.817095	1.206162
H	-1.960288	2.731964	-2.373191	H	-3.16664	2.276693	-2.382226
C	-2.25404	4.359756	-0.961788	C	-3.527373	4.056014	-1.189067
H	-3.151639	3.978101	2.321611	H	-3.185844	4.243686	2.214352
C	-2.598452	4.709507	0.352426	C	-3.532494	4.610163	0.101478
H	-2.069492	5.139207	-1.70771	H	-3.824809	4.664365	-2.049325
H	-2.672514	5.763358	0.638368	H	-3.828366	5.653433	0.249689
C	-6.036172	-0.24224	1.511214	C	-6.340571	-0.580442	1.339502
C	-6.169931	-0.646927	2.964903	C	-6.612584	-1.055798	2.751734
O	-6.926788	0.207305	0.810166	O	-7.157553	-0.090551	0.577551
H	-6.631262	-1.648247	3.015201	H	-6.91721	-2.116404	2.723443
H	-6.84763	0.054662	3.472393	H	-7.445253	-0.47524	3.172325
H	-5.198091	-0.683923	3.477233	H	-5.720789	-0.972093	3.389772
O	2.398601	-1.714004	-0.48409	O	2.584921	-1.562242	-0.525424
Si	2.688731	-0.157042	0.322619	Si	2.945005	-0.017514	0.271854
C	2.00849	-0.204409	2.070782	C	2.622942	-0.168708	2.113065
C	2.028024	1.309256	-0.671628	C	1.962842	1.385762	-0.52336
C	4.56336	-0.201261	0.255886	C	4.764824	0.093791	-0.161914
C	1.847564	-4.162929	-1.147449	C	1.914817	-3.753191	-1.706982
C	0.09107	-2.850156	0.551438	C	0.559864	-3.04175	0.601667
C	-2.314143	-4.574949	-1.818984	C	-2.026194	-4.608724	-1.657162
H	-3.499903	-5.06925	-0.066905	H	-3.198155	-5.230936	0.0621
H	-1.270141	-3.755467	-3.541201	H	-1.003205	-3.671855	-3.332294
H	-2.133365	-5.618893	-2.095978	H	-1.778665	-5.630713	-1.963041
H	2.343675	-4.460295	-0.212199	H	2.66493	-4.179164	-1.024943
H	1.049191	-4.869365	-1.423771	H	1.098747	-4.462317	-1.910116
H	2.574638	-4.072389	-1.966981	H	2.382622	-3.426585	-2.646613
H	-0.691977	-3.574897	0.264552	H	-0.343469	-3.616374	0.329919
H	0.752615	-3.240623	1.33816	H	1.347258	-3.683665	1.022756
H	-0.373521	-1.900436	0.848371	H	0.29769	-2.229842	1.293659
C	2.833175	-0.665771	3.128054	C	3.675502	-0.580929	2.969338
C	0.696485	0.231044	2.386779	C	1.362309	0.12502	2.694324
C	1.966555	2.58724	-0.025549	C	1.852939	2.627487	0.17754
C	1.907081	1.285839	-2.098762	C	1.538191	1.354314	-1.892294
C	5.295164	-1.376646	0.55988	C	5.628349	-1.025841	-0.059103
C	5.285756	0.973855	-0.063647	C	5.316958	1.33238	-0.569269

C	2.357622	-0.707744	4.44784	C	3.471331	-0.711847	4.351488
H	3.86242	-0.978557	2.920359	H	4.668082	-0.786558	2.55378
C	0.223163	0.193632	3.706891	C	1.160413	-0.004202	4.077031
H	0.040387	0.602934	1.586373	H	0.534018	0.461089	2.057922
C	1.052224	-0.279275	4.738466	C	2.213584	-0.425544	4.906486
H	3.010201	-1.064461	5.25108	H	4.297135	-1.028513	4.996488
H	-0.790633	0.539472	3.933219	H	0.182319	0.230594	4.50961
H	0.684052	-0.305037	5.76922	H	2.05605	-0.522142	5.985577
C	1.829583	3.76775	-0.764688	C	1.348463	3.774285	-0.445966
H	2.043649	2.641902	1.066031	H	2.174478	2.682906	1.223468
C	1.759773	2.48741	-2.834428	C	0.993612	2.514154	-2.503685
H	2.044176	0.346544	-2.644276	H	1.736464	0.472628	-2.511976
C	1.732041	3.719431	-2.171966	C	0.901304	3.71435	-1.781926
H	1.799533	4.731233	-0.246768	H	1.287535	4.714914	0.109389
H	1.688785	2.44357	-3.925692	H	0.676954	2.472988	-3.550455
H	1.636385	4.646936	-2.744924	H	0.489899	4.607354	-2.261838
C	6.697638	-1.373926	0.552313	C	6.995841	-0.907603	-0.347511
H	4.76612	-2.307051	0.7943	H	5.229529	-2.001782	0.239358
C	6.689362	0.97714	-0.068276	C	6.686227	1.450876	-0.854094
H	4.750739	1.897109	-0.312523	H	4.674623	2.214942	-0.666659
C	7.396369	-0.195694	0.239882	C	7.526401	0.331783	-0.743327
H	7.246783	-2.291334	0.787702	H	7.6487	-1.78253	-0.264859
H	7.230754	1.895502	-0.316729	H	7.096086	2.416734	-1.166069
H	8.490992	-0.193597	0.233902	H	8.593909	0.423668	-0.967421
H Thermal correction to Gibbs Free Energy= 0.541870 E(RM06L) = -2473.96312110				**I** Thermal correction to Gibbs Free Energy= 0.601979 E(RM06L) = -3027.17342891			
H	2.790935	-0.686948	-1.993371	Si	2.492225	-0.530777	0.035415
C	2.561118	-0.04406	-1.131884	O	-1.15929	0.671652	-1.845647
Pd	0.435284	-0.457041	-0.650903	H	0.972711	-0.1868	0.167293
C	2.506033	-3.075051	-0.950894	Pd	-0.602204	0.755599	0.54013
S	-0.966393	0.69041	-2.070343	C	2.605147	-1.873161	-1.285458
C	2.565752	-0.751041	0.104083	C	3.000476	-1.123381	1.752338
C	2.715946	1.391373	-1.489981	C	3.472552	0.996201	-0.486861
C	2.932469	-2.207857	0.084301	C	-1.768698	-0.78796	1.103617
C	2.607681	-0.06371	1.457338	C	-1.482642	1.684281	2.486283
C	3.752424	-2.749154	1.102557	O	0.60996	2.532447	-0.00356
O	3.973852	0.362091	1.767379	C	-2.892589	-0.145144	1.505688
H	2.298829	-0.769524	2.24664	C	-1.409007	-2.199391	0.956525
H	1.951699	0.815393	1.519948	C	-2.606248	1.324843	1.649972
C	4.138148	-4.098663	1.077229	C	-4.224498	-0.722363	1.940109
H	4.133541	-2.100798	1.896875	C	-3.424335	2.363308	1.112444
C	2.894208	-4.420487	-0.977531	O	-4.891292	-1.586521	0.966827

H	1.835375	-2.692595	-1.730367	H	-4.906961	0.102069	2.208028
C	2.942044	1.665391	-2.866809	H	-4.101818	-1.388048	2.809495
C	2.664811	2.49924	-0.606278	C	-3.12914	3.695297	1.388521
H	3.016471	0.82542	-3.568496	H	-4.280943	2.080916	0.494788
C	3.096727	2.974842	-3.343358	C	-1.193785	3.056085	2.729003
H	2.51654	2.362045	0.46634	H	-1.027379	0.916744	3.122291
C	2.820488	3.808648	-1.085508	C	-2.104197	-3.065356	0.073823
H	3.285099	3.146182	-4.408346	C	-0.359366	-2.73651	1.747481
C	3.031641	4.059411	-2.45176	H	-2.910605	-2.661253	-0.541531
H	2.786601	4.641433	-0.375477	C	-1.770027	-4.42555	0.001624
H	3.160434	5.083796	-2.814413	H	0.194533	-2.076953	2.422223
C	4.089809	1.541227	2.462858	C	-0.034082	-4.095919	1.672368
C	5.534356	1.812246	2.81356	H	-2.324044	-5.084404	-0.675203
O	3.136135	2.253926	2.754718	C	-0.73732	-4.945405	0.799617
H	5.840177	1.15058	3.641968	H	0.773154	-4.49249	2.295446
H	5.642978	2.856863	3.133038	H	-0.481286	-6.008005	0.742757
H	6.193143	1.596352	1.958683	C	-5.384888	-0.986037	-0.14852
O	-2.530066	0.710083	-1.534735	C	-6.185284	-1.969627	-0.975889
Si	-2.761705	0.143095	0.15495	O	-5.224379	0.201358	-0.420161
C	-2.314581	1.535847	1.327302	H	-6.263008	-1.611005	-2.011126
C	-1.638562	-1.373539	0.330513	H	-7.204525	-2.037914	-0.557545
C	-4.580506	-0.283154	0.132993	H	-5.747749	-2.978348	-0.939938
C	-1.259033	0.196337	-3.802776	S	-0.050409	3.675994	-0.842207
C	-0.626029	2.4655	-2.28031	C	1.014106	5.118308	-0.477478
C	3.713684	-4.941061	0.038885	C	0.477843	3.391323	-2.571886
H	4.785117	-4.48764	1.870141	C	-2.008832	4.046788	2.187708
H	2.547405	-5.068397	-1.789286	H	-3.773599	4.485237	0.988645
H	4.016845	-5.992454	0.020098	H	-0.355148	3.319407	3.380901
H	-2.074806	0.805734	-4.219729	H	-1.812612	5.100901	2.410045
H	-0.316791	0.348942	-4.351423	H	2.065692	4.816725	-0.603165
H	-1.526071	-0.869461	-3.78892	H	0.748133	5.945275	-1.154819
H	0.367002	2.556333	-2.752906	H	0.820218	5.406823	0.565249
H	-1.423373	2.918622	-2.887891	H	0.126099	4.228019	-3.197064
H	-0.600336	2.895225	-1.268855	H	1.573557	3.287794	-2.606126
C	-3.325957	2.164998	2.094383	H	-0.01365	2.449447	-2.859558
C	-0.976032	1.970566	1.508155	C	3.808058	-2.069341	-2.008387
C	-0.724143	-1.523074	1.42396	C	1.518919	-2.742478	-1.551611
C	-1.914319	-2.538852	-0.458273	C	3.869461	-2.229071	1.90806
C	-5.531784	0.612012	-0.419182	C	2.557893	-0.45045	2.917564
C	-5.045215	-1.48967	0.711018	C	3.596698	1.348916	-1.853166
C	-3.00787	3.186652	3.003645	C	4.117028	1.813418	0.471486
H	-4.369189	1.849926	1.984392	C	3.922338	-3.096282	-2.960024
C	-0.652634	2.983742	2.422845	H	4.665353	-1.409504	-1.832736
H	-0.167965	1.494396	0.928819	C	1.6311	-3.766341	-2.506449

C	-1.674436	3.593114	3.171942
H	-3.803168	3.660366	3.58787
H	0.392558	3.277017	2.564683
H	-1.428498	4.380691	3.891424
C	-0.150643	-2.781008	1.72274
H	-0.560966	-0.683415	2.10813
C	-1.333078	-3.772967	-0.157298
H	-2.630516	-2.472483	-1.285929
C	-0.453352	-3.897804	0.939636
H	0.524945	-2.876883	2.577873
H	-1.576765	-4.651089	-0.763964
H	-0.013339	-4.870044	1.179341
C	-6.900407	0.30636	-0.396558
H	-5.203365	1.552719	-0.875236
C	-6.415657	-1.791089	0.737548
H	-4.333277	-2.201978	1.142565
C	-7.343121	-0.894689	0.183023
H	-7.622559	1.005148	-0.830752
H	-6.759046	-2.726648	1.190304
H	-8.411798	-1.131089	0.202385

H	0.58019	-2.630033	-0.997851
C	2.832893	-3.944852	-3.212479
H	4.862442	-3.232088	-3.504761
H	0.782506	-4.4343	-2.68918
H	2.921328	-4.745731	-3.953943
C	4.289766	-2.641453	3.183211
H	4.218658	-2.775837	1.02477
C	2.977435	-0.860607	4.193112
H	1.871516	0.401353	2.824982
C	3.845611	-1.957729	4.326391
H	4.963258	-3.498911	3.284216
H	2.627329	-0.327566	5.083545
H	4.172352	-2.280206	5.320332
C	4.331684	2.479244	-2.24636
H	3.127989	0.722884	-2.620996
C	4.847766	2.948061	0.083224
H	4.05847	1.553292	1.534167
C	4.955425	3.284537	-1.276546
H	4.434751	2.722537	-3.309699
H	5.347194	3.560796	0.841143
H	5.540158	4.158713	-1.58213
S	-2.072034	-0.407325	-2.497684
C	-1.182933	-0.947448	-4.008378
H	-0.268173	-1.457668	-3.670328
H	-1.819203	-1.650732	-4.569337
H	-0.929974	-0.070832	-4.624667
C	-3.442771	0.499296	-3.310148
H	-3.966835	-0.186975	-3.994956
H	-4.127117	0.820694	-2.510143
H	-3.032983	1.360793	-3.859881

TS_{IJ}
Thermal correction to Gibbs Free Energy= 0.608039
E(RM06L) = -3027.15844411
Frequency -55.7691

Si	2.009845	-0.629527	-0.237206
O	1.021924	0.174911	-1.793887
H	0.396356	-0.132085	0.474984
Pd	-0.748796	0.99275	0.866582
C	1.858444	-2.37904	-0.957757
C	2.383229	-0.886051	1.64154
C	3.521158	0.353779	-0.853588
C	-2.178657	-0.41203	1.042021
C	-2.511682	2.342376	1.742763

J
Thermal correction to Gibbs Free Energy= 0.601915
E(RM06L) = -3027.18176392

Si	3.504146	0.444696	0.080615
O	2.247328	0.473592	-1.182956
H	-1.863348	1.168824	1.151815
Pd	-2.897789	0.890584	0.029105
C	4.832485	-0.754345	-0.494629
C	2.686507	-0.124095	1.666367
C	4.032571	2.238767	0.059617
C	-2.882434	-1.039121	0.566674
C	-4.292952	-0.065523	-1.772992

O	0.817961	2.586293	0.734964	O	-2.944246	2.981562	-0.693973
C	-3.320013	0.236542	0.646637	C	-3.058123	-1.867387	-0.53042
C	-1.959742	-1.783228	1.519457	C	-2.783902	-1.449463	1.986952
C	-3.131356	1.723849	0.601703	C	-3.46974	-1.230965	-1.813579
C	-4.715245	-0.325798	0.471496	C	-3.07311	-3.37825	-0.4903
C	-3.600962	2.567841	-0.445642	C	-3.120498	-1.726499	-3.095755
O	-4.902983	-1.346285	-0.575186	O	-1.784684	-4.100802	-0.258426
H	-5.426491	0.493243	0.273537	H	-3.49147	-3.79554	-1.419576
H	-5.034852	-0.871421	1.374677	H	-3.663623	-3.742868	0.365443
C	-3.43613	3.951449	-0.366708	C	-3.53266	-1.065827	-4.262946
H	-4.092176	2.103584	-1.30478	H	-2.489948	-2.61604	-3.170954
C	-2.337435	3.749077	1.792453	C	-4.676492	0.61204	-2.944475
H	-2.374486	1.753177	2.658321	H	-4.787264	0.205639	-0.816815
C	-2.721658	-2.895777	1.073939	C	-2.193282	-2.65573	2.445692
C	-0.983612	-2.003746	2.527218	C	-3.364066	-0.599859	2.968641
H	-3.472398	-2.761005	0.292052	H	-1.699684	-3.325695	1.740147
C	-2.51857	-4.168271	1.628514	C	-2.200825	-2.997143	3.808096
H	-0.377613	-1.159525	2.869947	H	-3.807123	0.344316	2.634414
C	-0.790093	-3.275329	3.080585	C	-3.385479	-0.948537	4.323424
H	-3.119841	-5.01183	1.272898	H	-1.729717	-3.932621	4.128596
C	-1.556751	-4.365017	2.633084	C	-2.800617	-2.153376	4.753711
H	-0.032508	-3.414431	3.857686	H	-3.858125	-0.277324	5.048254
H	-1.404318	-5.36024	3.062658	H	-2.809532	-2.425867	5.814011
C	-4.669975	-1.013724	-1.868751	C	-0.658641	-3.795119	-0.918672
C	-4.981176	-2.182924	-2.780923	C	0.50588	-4.616568	-0.400608
O	-4.267379	0.085574	-2.243614	O	-0.559279	-2.942435	-1.809863
H	-4.810689	-1.891817	-3.825604	H	1.233766	-4.779337	-1.208084
H	-6.03052	-2.493269	-2.650239	H	0.169008	-5.578837	0.009754
H	-4.353981	-3.052195	-2.522781	H	1.002017	-4.055275	0.410925
S	0.704617	3.753245	-0.303675	S	-3.28746	3.999476	0.44569
C	1.054208	5.265171	0.668086	C	-1.685206	4.530468	1.164891
C	2.25998	3.71023	-1.264134	C	-3.670944	5.537954	-0.469953
C	-2.792696	4.549535	0.74378	C	-4.294711	0.115215	-4.198163
H	-3.81801	4.585967	-1.173846	H	-3.249533	-1.475715	-5.238712
H	-1.89445	4.198991	2.687178	H	-5.304912	1.50474	-2.868351
H	-2.697678	5.63902	0.796375	H	-4.608316	0.622568	-5.115503
H	1.980976	5.114808	1.242767	H	-1.005867	4.851679	0.360366
H	1.1465	6.121285	-0.019015	H	-1.869373	5.345574	1.882979
H	0.202167	5.41495	1.345251	H	-1.274531	3.653009	1.685291
H	2.290159	4.59461	-1.920922	H	-3.803228	6.361261	0.249681
H	3.120969	3.68722	-0.579048	H	-2.855222	5.752298	-1.177292
H	2.241273	2.786127	-1.859047	H	-4.610097	5.361638	-1.01372
C	2.755495	-2.838088	-1.955308	C	5.99979	-0.295007	-1.152335
C	0.827641	-3.256793	-0.538383	C	4.6717	-2.153211	-0.318197

C	3.016673	-2.088899	2.03213	C	3.4353	-0.813498	2.653063
C	2.153186	0.098248	2.629378	C	1.321753	0.152806	1.932627
C	3.805361	0.534762	-2.233559	C	4.300048	2.929128	-1.149047
C	4.453766	0.876671	0.076244	C	4.211984	2.92763	1.283534
C	2.623612	-4.119522	-2.515537	C	6.964974	-1.198194	-1.624481
H	3.576749	-2.194005	-2.288335	H	6.160177	0.780638	-1.285102
C	0.6868	-4.533677	-1.108645	C	5.63387	-3.057915	-0.794383
H	0.13211	-2.949895	0.249819	H	3.796596	-2.537879	0.220173
C	1.582456	-4.967469	-2.099268	C	6.78132	-2.57962	-1.44975
H	3.338361	-4.458804	-3.27287	H	7.86444	-0.823707	-2.123662
H	-0.118235	-5.191705	-0.765645	H	5.497543	-4.133752	-0.642458
H	1.479337	-5.966043	-2.536607	H	7.53644	-3.283379	-1.814503
C	3.407571	-2.297432	3.367538	C	2.840263	-1.209849	3.861303
H	3.205476	-2.876133	1.294834	H	4.491048	-1.047696	2.474669
C	2.549055	-0.105138	3.960819	C	0.720723	-0.26075	3.131181
H	1.66127	1.039422	2.353168	H	0.710491	0.69438	1.200081
C	3.174103	-1.308311	4.334364	C	1.482542	-0.939253	4.097466
H	3.891189	-3.239021	3.648926	H	3.435059	-1.737137	4.614272
H	2.368193	0.674208	4.709207	H	-0.341685	-0.062826	3.305578
H	3.475231	-1.472284	5.374214	H	1.013278	-1.260829	5.032612
C	4.963417	1.202205	-2.661523	C	4.737877	4.261723	-1.132169
H	3.105791	0.151258	-2.981639	H	4.157271	2.426394	-2.112253
C	5.607625	1.556732	-0.348286	C	4.655293	4.259325	1.29964
H	4.278856	0.745956	1.1483	H	4.002593	2.418969	2.23129
C	5.866721	1.720633	-1.718178	C	4.919033	4.926465	0.092644
H	5.16347	1.315861	-3.732458	H	4.93945	4.782402	-2.074018
H	6.310899	1.948702	0.394132	H	4.794085	4.776281	2.254666
H	6.770981	2.241349	-2.050284	H	5.265778	5.9649	0.105091
S	-0.423689	-0.399211	-2.179988	S	1.281549	-0.824579	-1.489476
C	-0.116214	-1.31426	-3.732003	C	2.001208	-1.467914	-3.032893
H	0.469381	-2.206806	-3.467684	H	2.989526	-1.878575	-2.778315
H	-1.092891	-1.606714	-4.149653	H	1.322979	-2.26348	-3.374808
H	0.437186	-0.676777	-4.43759	H	2.088298	-0.651534	-3.764581
C	-1.255229	1.058177	-2.876783	C	-0.155279	0.06838	-2.123342
H	-2.254783	0.740261	-3.217182	H	-0.798292	-0.658983	-2.640723
H	-1.374932	1.773289	-2.049897	H	-0.711372	0.476016	-1.255309
H	-0.646125	1.480583	-3.689915	H	0.207322	0.86576	-2.789108
$Me_2SOSiPh_3^+$ Thermal correction to Gibbs Free Energy= 0.290935 E(RM06L) = -1537.78623991				**K** Thermal correction to Gibbs Free Energy= 0.357694 E(RM06L) = -2042.67253380			
Si	-0.277843	-0.022634	0.015854	O	0.755746	-0.445804	1.812691
S	1.47712	0.048868	2.655259	H	1.348575	0.460656	-1.859273
O	0.137605	-0.118433	1.78412	Pd	1.192305	0.065104	-0.361102

C	2.513666	-1.405363	2.283629
C	2.489998	1.368136	1.9063
H	2.730975	-1.464355	1.207412
H	3.435098	-1.29541	2.879163
H	1.957866	-2.289485	2.627937
H	3.341586	1.525377	2.588799
H	2.833206	1.078406	0.903133
H	1.86763	2.274179	1.865634
C	-0.301443	1.805401	-0.381167
C	-1.957967	-0.826651	0.08505
C	1.027924	-0.982409	-0.932833
C	0.024677	2.279264	-1.676406
C	-0.734163	2.745638	0.589366
C	-0.065128	3.645801	-1.985574
H	0.34494	1.577204	-2.454129
C	-0.815453	4.111429	0.281423
H	-1.025737	2.406034	1.590277
C	-0.478709	4.562366	-1.006404
H	0.186976	3.993858	-2.992035
H	-1.15239	4.823623	1.041231
H	-0.547105	5.627614	-1.247842
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C	-2.198061	-2.032119	0.790866
C	-4.293741	-0.840075	-0.651454
H	-2.873847	0.705119	-1.170338
C	-3.464957	-2.631125	0.772729
H	-1.396773	-2.499711	1.373837
C	-4.512238	-2.036904	0.048512
H	-5.110807	-0.373073	-1.209787
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C	0.850659	-2.367576	-1.178127
C	3.197991	-1.112549	-2.079613
H	2.361404	0.71235	-1.283854
C	1.831874	-3.112775	-1.849506
H	-0.072085	-2.862906	-0.856677
C	3.008155	-2.488146	-2.295336
H	4.102792	-0.618847	-2.448056
H	1.673617	-4.179659	-2.035093
H	3.770297	-3.068855	-2.824182

C	-0.674431	0.669636	-0.634132
C	-0.611659	-2.136538	-1.992226
O	3.398303	-0.442481	-0.053043
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C	-0.802431	2.126122	-0.369024
C	-1.598832	-1.628773	-1.112435
C	-3.153851	0.369883	-0.853102
C	-2.499083	-2.555017	-0.528966
O	-3.770293	0.167742	0.479649
H	-3.787154	-0.154444	-1.58859
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H	0.077819	-1.432653	-2.467122
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C	-0.190872	3.083623	-1.218416
H	-1.990775	1.874872	1.425044
C	-1.621905	3.97779	1.019074
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H	-1.106631	5.985002	0.363743
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C	-5.631387	0.259845	1.951139
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H	-4.864791	0.398296	2.728089
H	-5.971919	-0.78929	1.996253
S	4.123906	0.696437	-0.839058
C	3.875698	2.255275	0.101907
C	5.893583	0.446755	-0.397123
C	-1.406382	-4.418069	-1.658924
H	-3.104982	-4.624765	-0.321181
H	0.249003	-3.872293	-2.955443
H	-1.333546	-5.490157	-1.871964
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H	6.494396	1.261732	-0.831404
H	5.999869	0.418941	0.698246
H	6.199021	-0.515595	-0.832978

				S	1.05744	-1.812918	2.478666
				C	2.872085	-1.864564	2.79111
				H	3.071688	-1.150614	3.604296
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				C	1.013759	-3.093127	1.168287
				H	1.338521	-4.054016	1.600671
				H	-0.026938	-3.163374	0.817511
				H	1.663549	-2.776613	0.336533
TS_{KL} Thermal correction to Gibbs Free Energy= 0.353643 E(RM06L) = -2042.66133434 Frequency -700.6390				**L** Thermal correction to Gibbs Free Energy= 0.363375 E(RM06L) = -2042.69080342			
H	0.490854	0.496184	-1.605176	H	-0.821596	-2.145327	-0.770672
C	-0.715391	0.671851	-0.667571	C	-1.000941	-1.137929	-1.172048
Pd	1.157509	0.081955	-0.202958	Pd	1.138585	0.284962	-0.207579
O	1.15333	-0.482108	2.058546	O	1.337492	2.245025	1.109444
S	1.456359	-1.912746	2.566013	S	0.874291	2.262377	2.590752
O	3.42864	-0.347454	-0.130342	O	2.105089	-0.970204	1.605867
C	-1.773892	-0.186883	-0.871727	C	-2.247505	-0.615434	-0.918598
C	-0.881019	2.121529	-0.369307	C	0.171626	-0.633747	-1.913788
S	3.918774	0.861304	-0.984412	S	2.740578	-2.047554	0.675868
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C	-0.608115	-2.125442	-2.053105	C	-3.273282	-2.80242	-0.125597
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C	-1.616671	2.555939	0.761748	C	0.460453	0.772798	-2.188594
C	-0.281956	3.110663	-1.189921	C	1.019999	-1.620252	-2.546891
C	-2.527092	-2.582185	-0.646771	C	-4.191681	-0.711654	0.683827
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H	-3.141021	-4.654413	-0.511964	H	-5.850032	-0.870097	2.063756
H	0.268056	-3.831293	-3.051386	H	-4.217346	-4.604673	0.605034
H	-2.073484	1.804614	1.412127	H	-0.277011	1.557438	-2.00298
C	-1.749461	3.922063	1.05316	C	1.546449	1.096467	-3.069423
H	0.298071	2.790973	-2.062932	H	0.804291	-2.678847	-2.357184
C	-0.430209	4.4744	-0.904832	C	2.038446	-1.263083	-3.420851

H	-2.318265	4.231628	1.93699	H	1.736595	2.152933	-3.287604
C	-1.160947	4.889049	0.222833	C	2.314584	0.108289	-3.676906
H	0.028377	5.218779	-1.565592	H	2.632111	-2.042023	-3.912152
H	-1.267689	5.954662	0.451605	H	3.12337	0.384585	-4.362041
C	-5.594259	0.133415	2.039892	C	-1.656287	3.969037	0.182648
O	-5.748175	0.943393	-0.255466	O	-2.335034	3.339974	-2.074049
H	-6.45703	0.775755	2.264549	H	-1.731007	5.007937	-0.165453
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C	3.718341	2.377357	0.037333	C	4.124312	-1.253404	-0.235879
C	5.760269	0.761933	-0.84519	C	3.801391	-3.037034	1.830223
H	4.146983	2.206583	1.037152	H	4.748365	-0.685792	0.472212
H	4.216047	3.218245	-0.473899	H	4.709188	-2.038671	-0.742988
H	2.633294	2.551492	0.110459	H	3.655302	-0.579676	-0.971631
H	6.212212	1.634175	-1.343957	H	4.366146	-3.789052	1.256058
H	6.046713	0.722253	0.217138	H	4.48235	-2.363847	2.373968
H	6.068373	-0.162051	-1.355887	H	3.121839	-3.53798	2.535082
H	-1.339376	-5.478658	-2.051415	H	-5.875458	-3.377965	2.031901
C	3.288176	-2.117337	2.541746	C	2.227688	1.506619	3.582379
C	1.085907	-3.064966	1.186636	C	-0.346008	0.901843	2.787413
H	3.684518	-1.508463	3.368254	H	3.073275	2.209917	3.550977
H	3.53892	-3.177829	2.706313	H	1.883572	1.381241	4.622154
H	3.666082	-1.740352	1.57738	H	2.495752	0.543634	3.116542
H	1.409104	-4.081624	1.465503	H	-0.685079	0.87288	3.836618
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H	1.595407	-2.703844	0.277425	H	0.123839	-0.04635	2.476939

X-ray crystallography

X-ray reflections for **25** were collected on Rigaku Oxford diffractometer using Mo-Kα, radiation. OLEX 2 program were used to solve and refine the data. All non-hydrogen atoms were refined anisotropically, and C−H hydrogens were fixed.[16] Crystal was grown in the mixture of 1,2-dichloromethane and hexane solvent medium.

Table S4: Crystallographic Data for Compound **25**

Compound	**25**	V [Å^3]	950.66 (15)
formula	$C_{22}H_{23}NO_3$	Z	2
Formula weight	349.41	ρ_{calcd} [g cm^{-3}]	1.221
crystal system	triclinic	μ [mm^{-1}]	0.081
space group	P -1	total reflns	36799
T [K]	297 K	unique reflns	4396
a [Å]	9.7695 (9)	observed	2694

b [Å]	10.1839 (8)
c [Å]	11.1377 (10)
α [°]	66.757 (3)
β [°]	79.058 (4)
γ [°]	69.275 (3)

R_1[I>2σ(I)]	0.0797 (2694)
wR2 [all]	0.1086 (4396)
GOF	1.013
Diffractometer	Rigaku Oxford
CCDC Number	CCDC 2170362

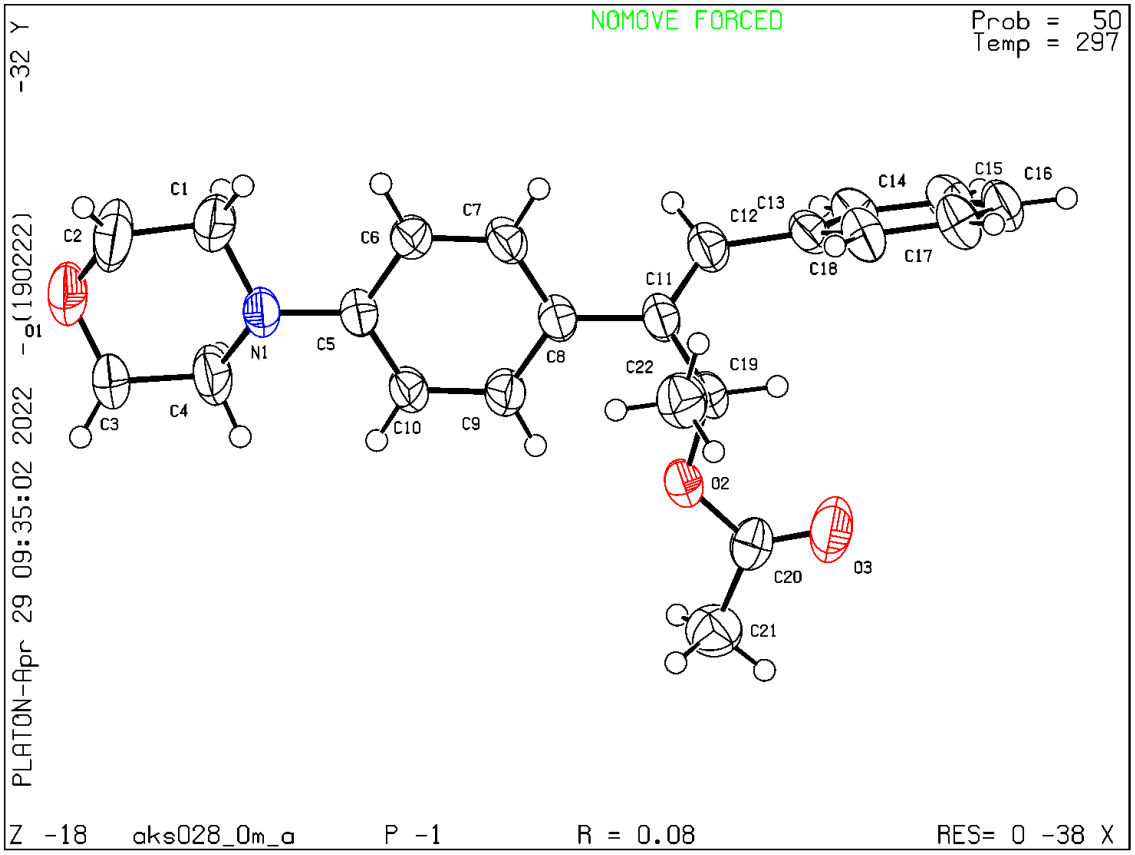

Figure S3: Molecular structure of compound **25**, (oxygen (red), nitrogen (blue), and sulphur (yellow)).

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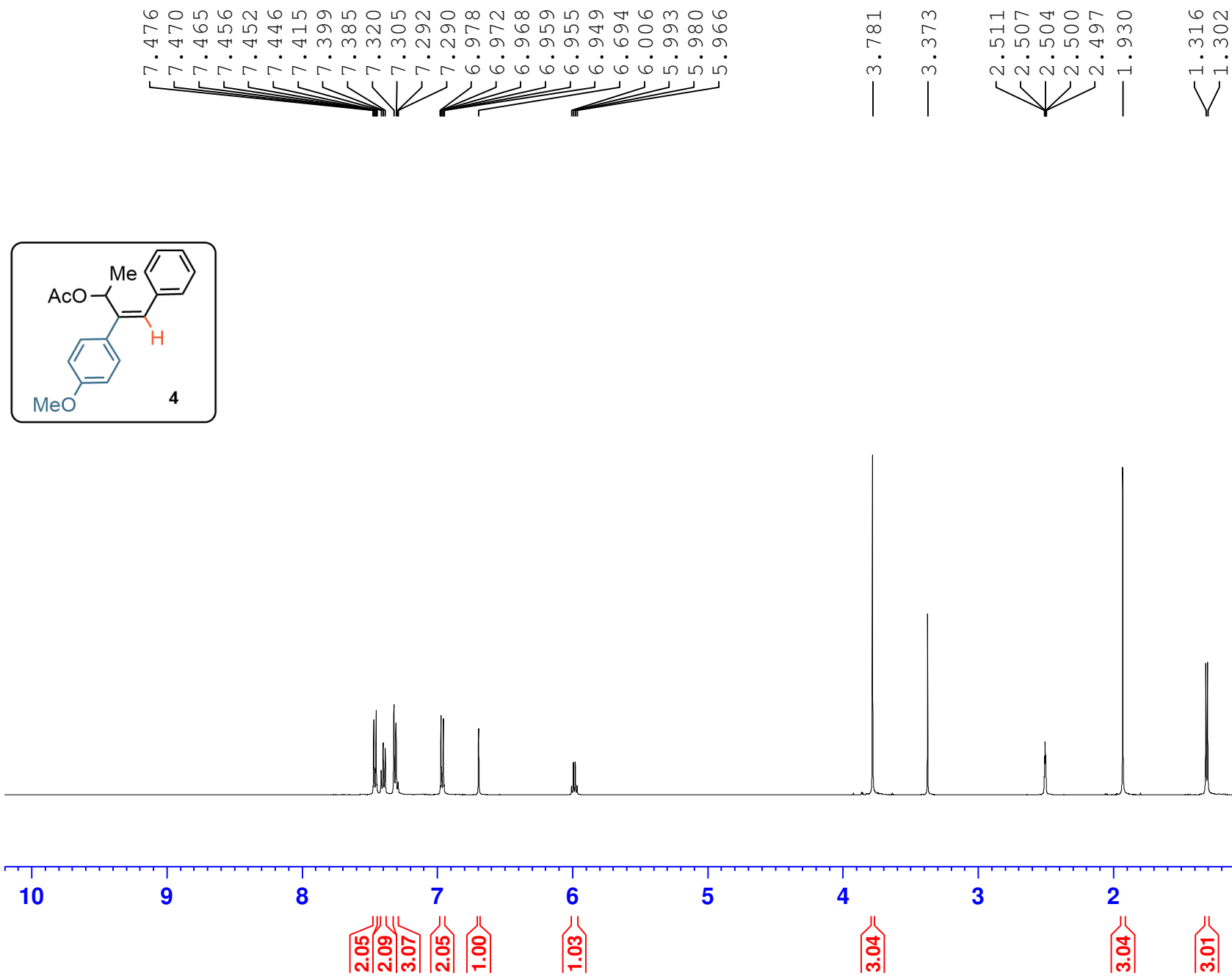
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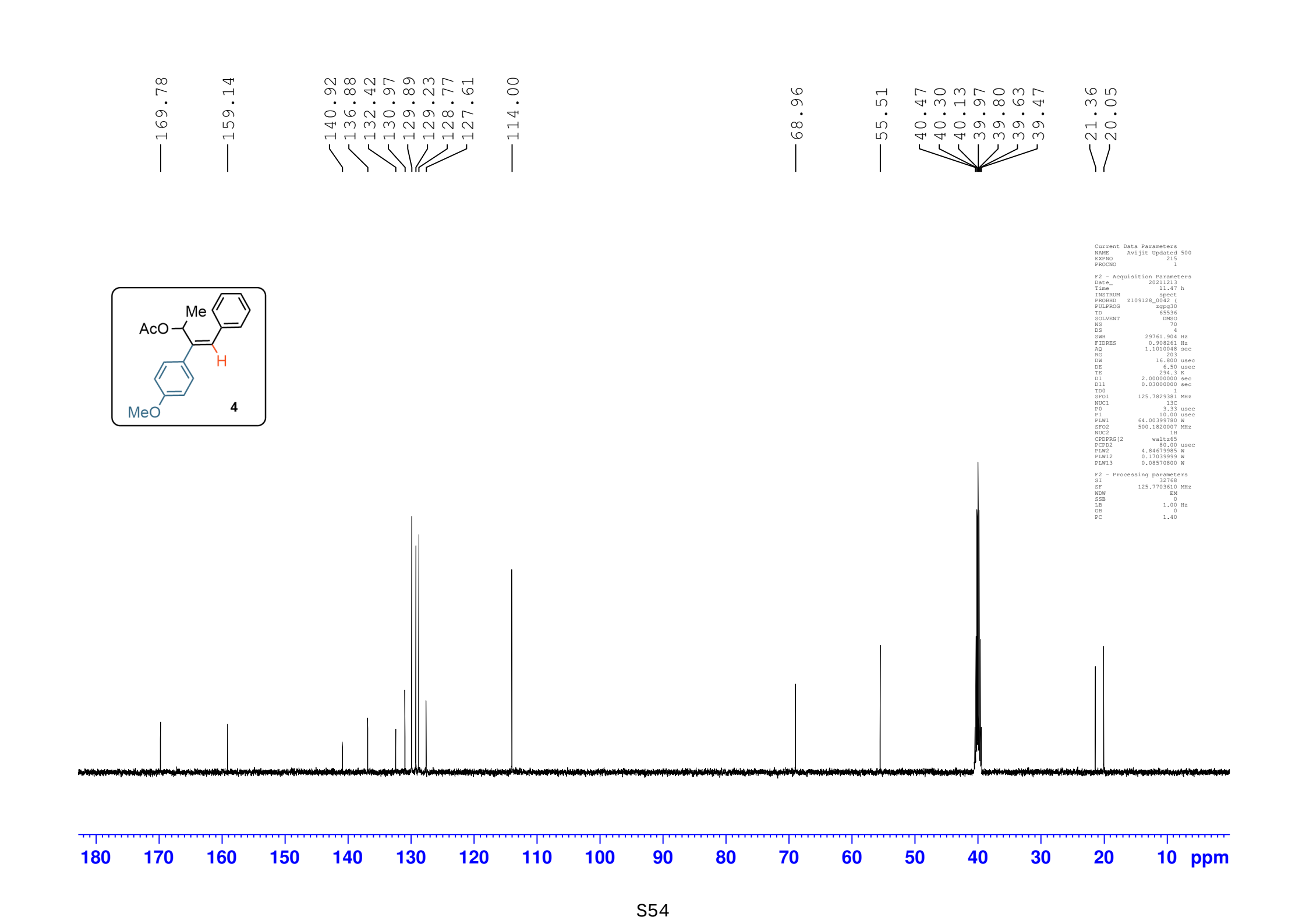
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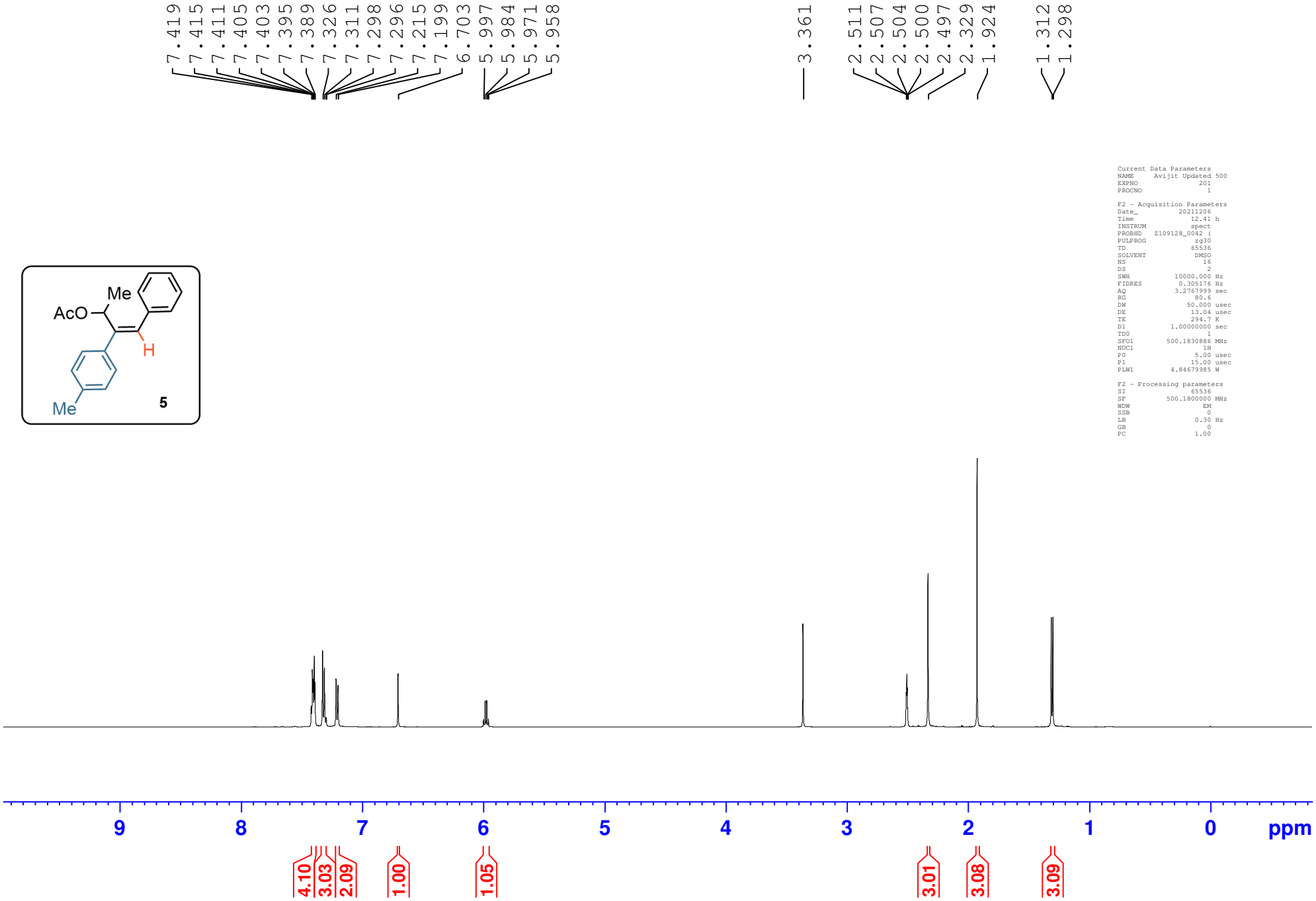
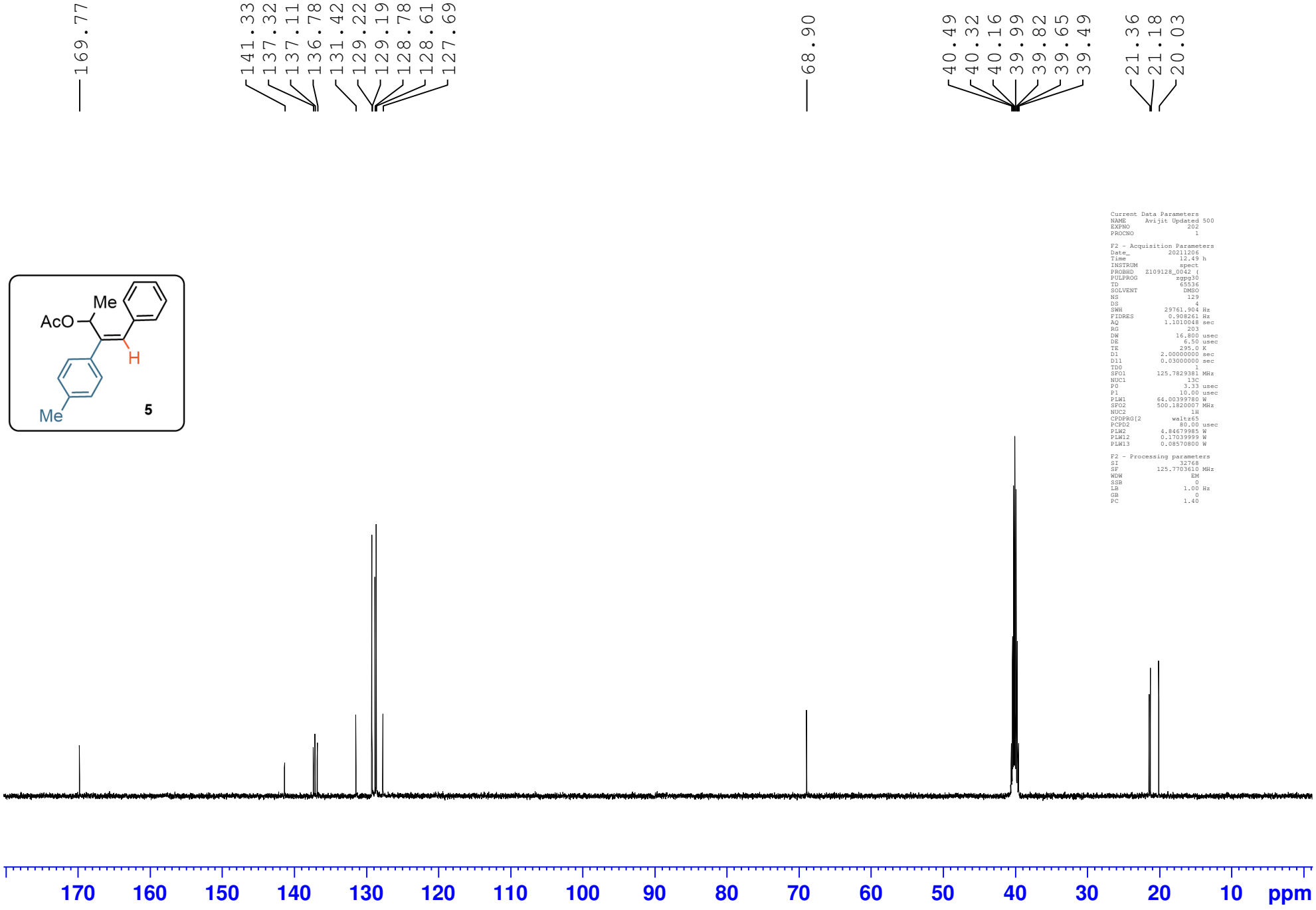
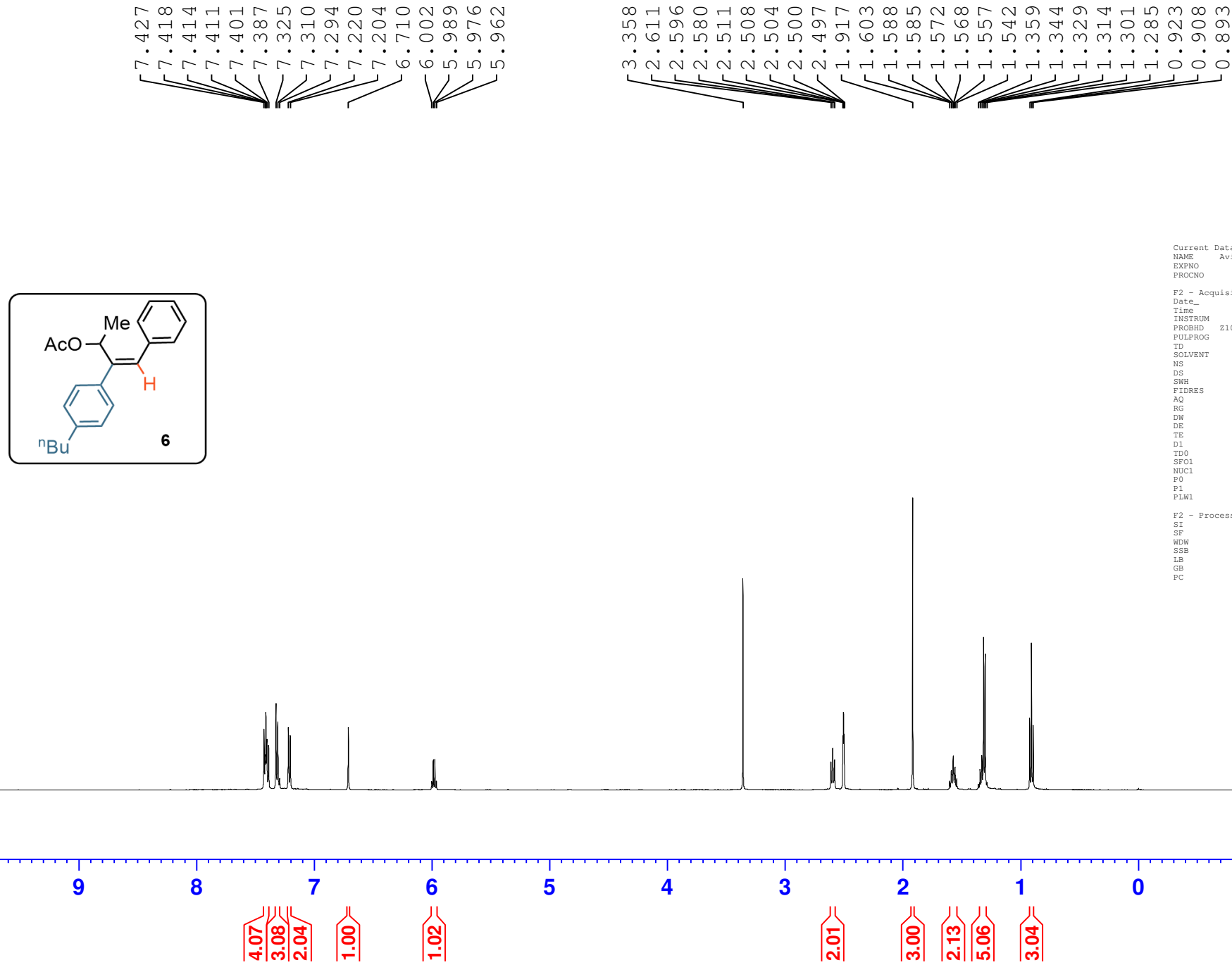
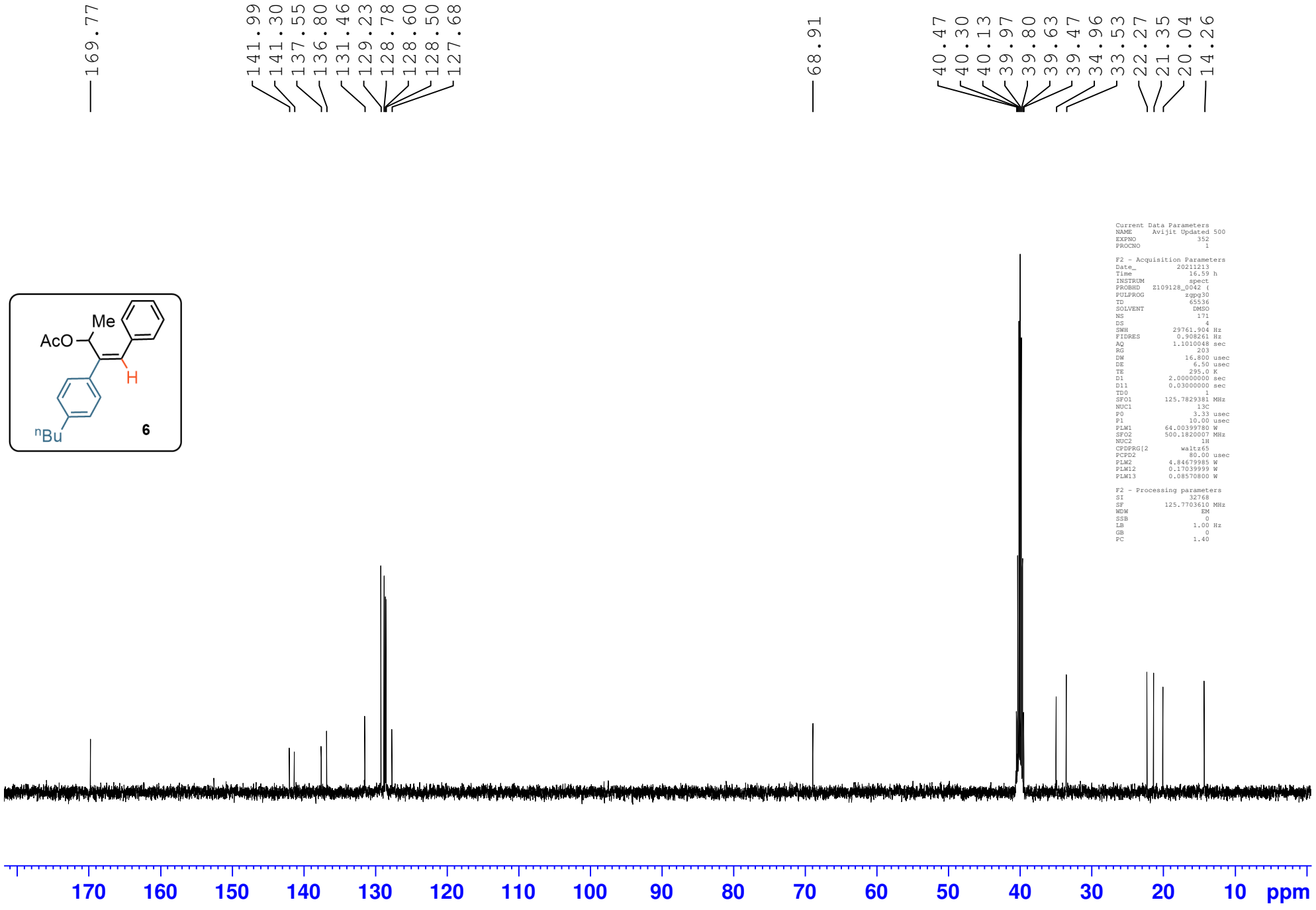
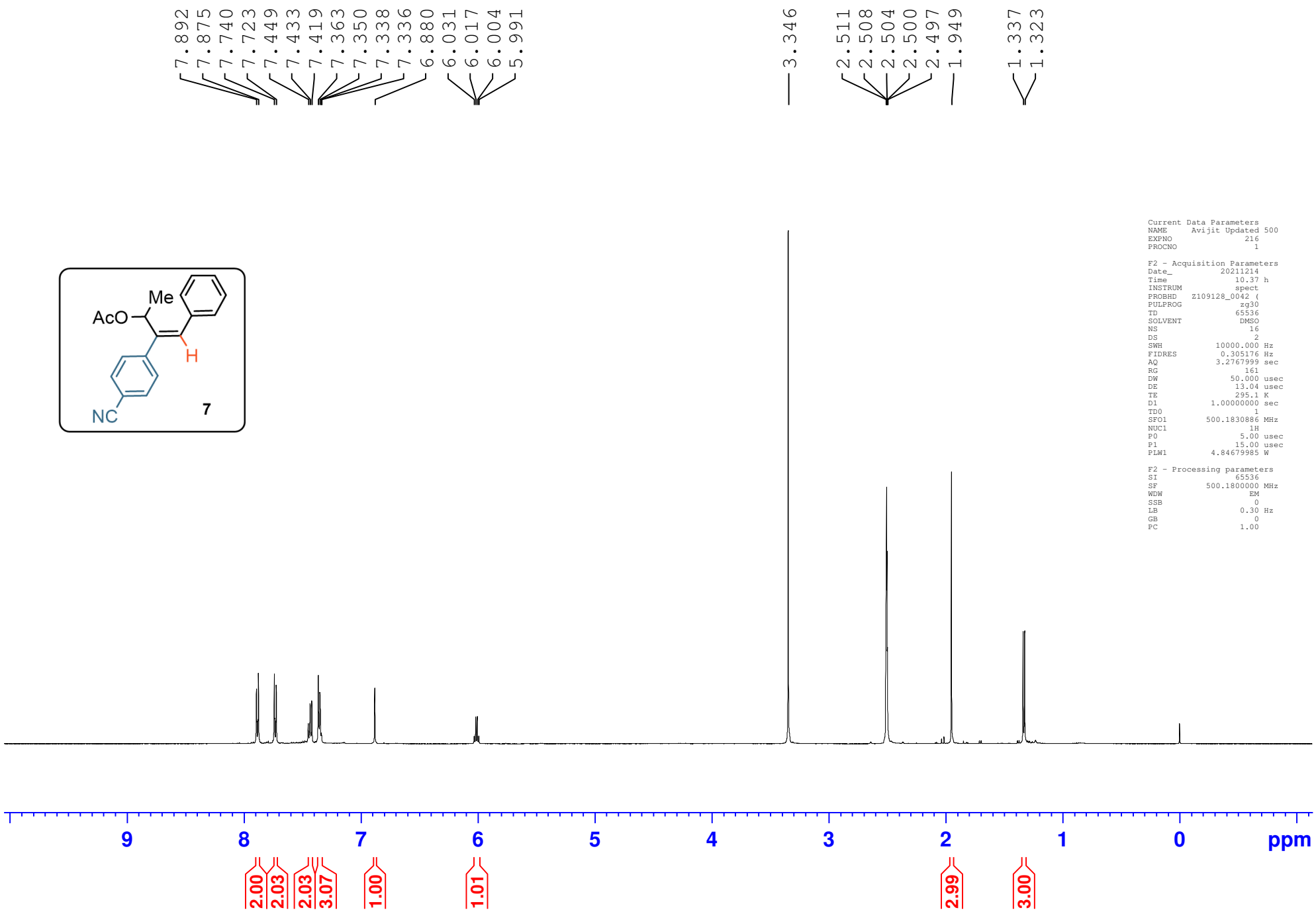
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

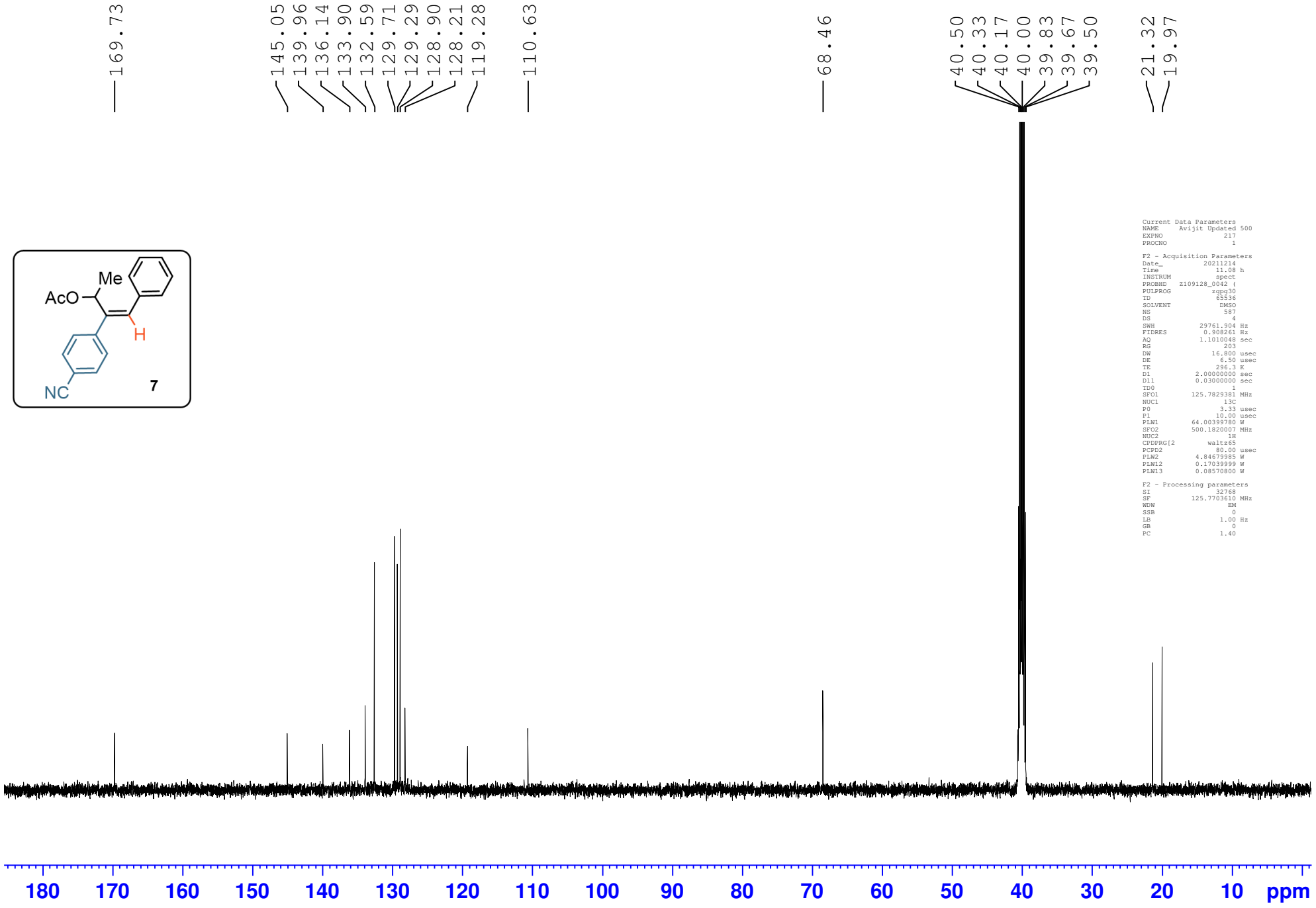

7.419
7.415
7.411
7.405
7.403
7.395
7.389
7.326
7.311
7.298
7.296
7.215
7.199
6.703
5.997
5.984
5.971
5.958
3.361
2.511
2.507
2.504
2.500
2.497
2.329
1.924
1.312
1.298
Me
AcO
H
Me
5
Current Data Parameters
NAME Avijit Updated 500
EXPNO 201
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 12.41 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 13.04 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
4.10
3.03
2.09
1.00
1.05
3.01
3.08
3.09

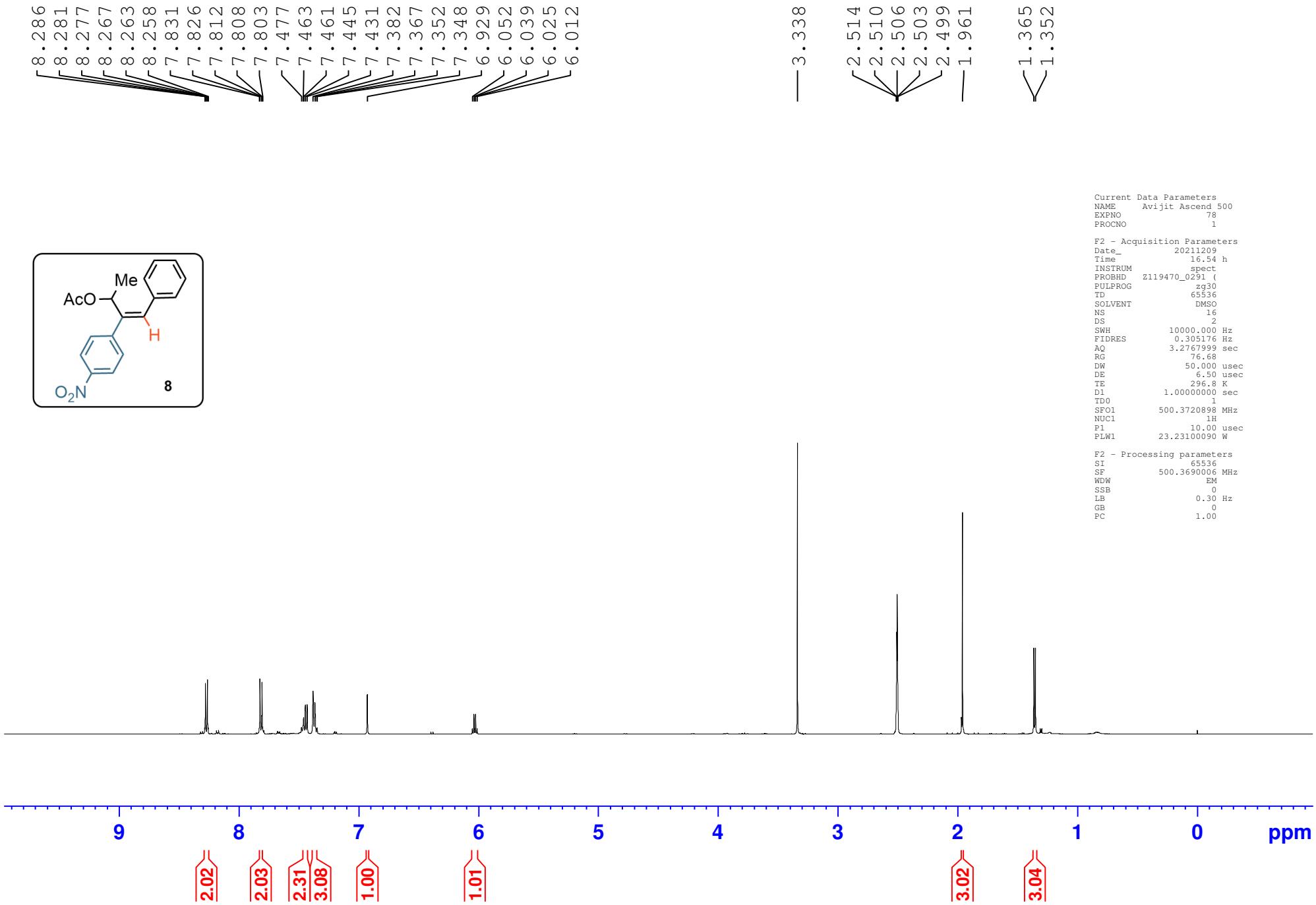

169.77
141.33
137.32
137.11
136.78
131.42
129.22
129.19
128.78
128.61
127.69
68.90
40.49
40.32
40.16
39.99
39.82
39.65
39.49
21.36
21.18
20.03
AcO
Me
H
Me
5
Current Data Parameters
NAME Avijit Updated 500
EXPNO 202
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 12.49 h
INSTRUM spect
PROBHD 2109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 129
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 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

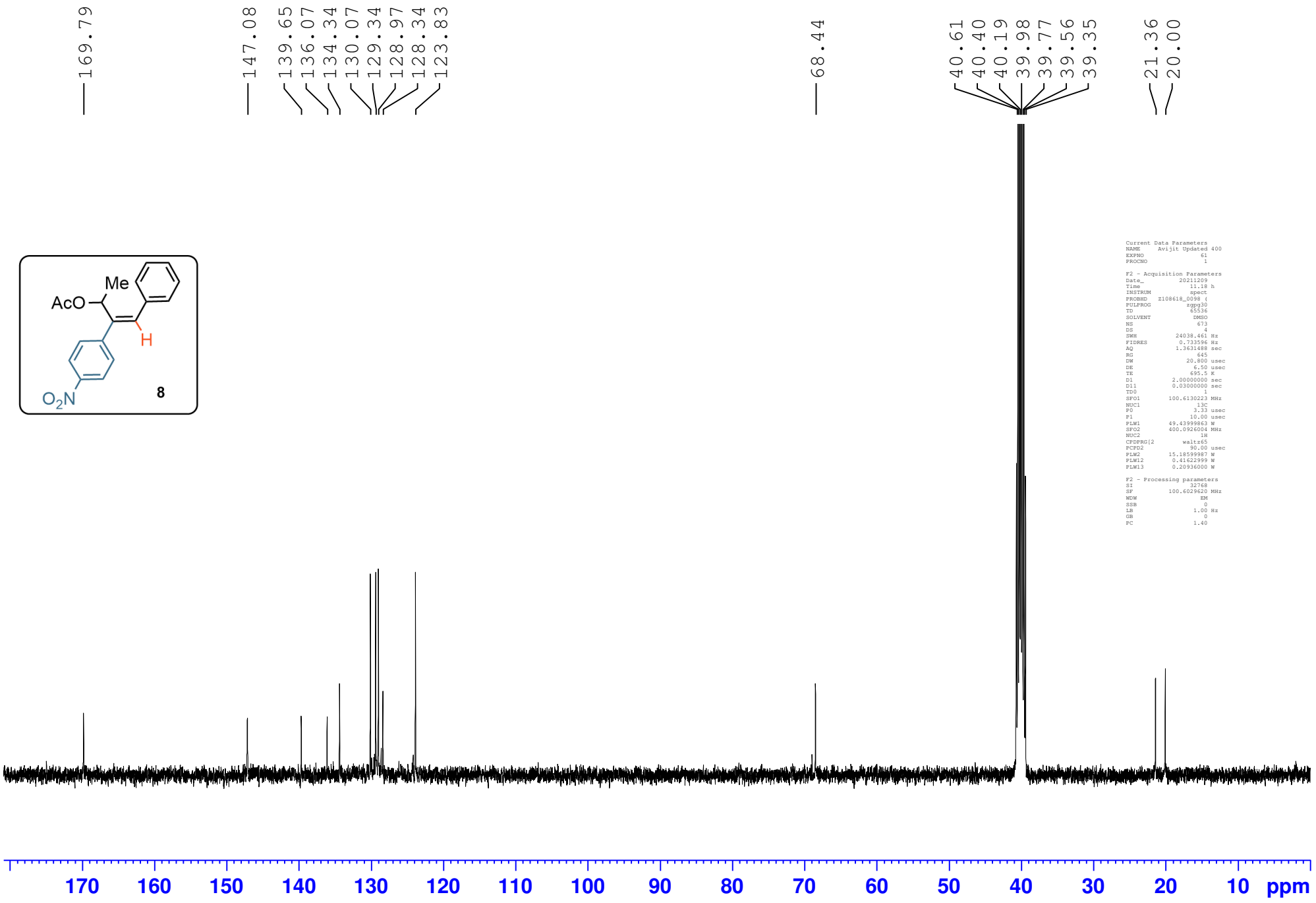

7.427
7.418
7.414
7.411
7.401
7.387
7.325
7.310
7.294
7.220
7.204
6.710
6.002
5.989
5.976
5.962
3.358
2.611
2.596
2.580
2.511
2.508
2.504
2.500
2.497
1.917
1.603
1.588
1.585
1.572
1.568
1.557
1.542
1.359
1.344
1.329
1.314
1.301
1.285
0.923
0.908
0.893
Me
AcO
H
nBu
6
Current Data Parameters
NAME Avijit Updated 500
EXPNO 351
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211213
Time 16.49 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 13.04 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
-1
ppm
4.07
3.08
2.04
1.00
1.02
2.01
3.00
2.13
5.06
3.04

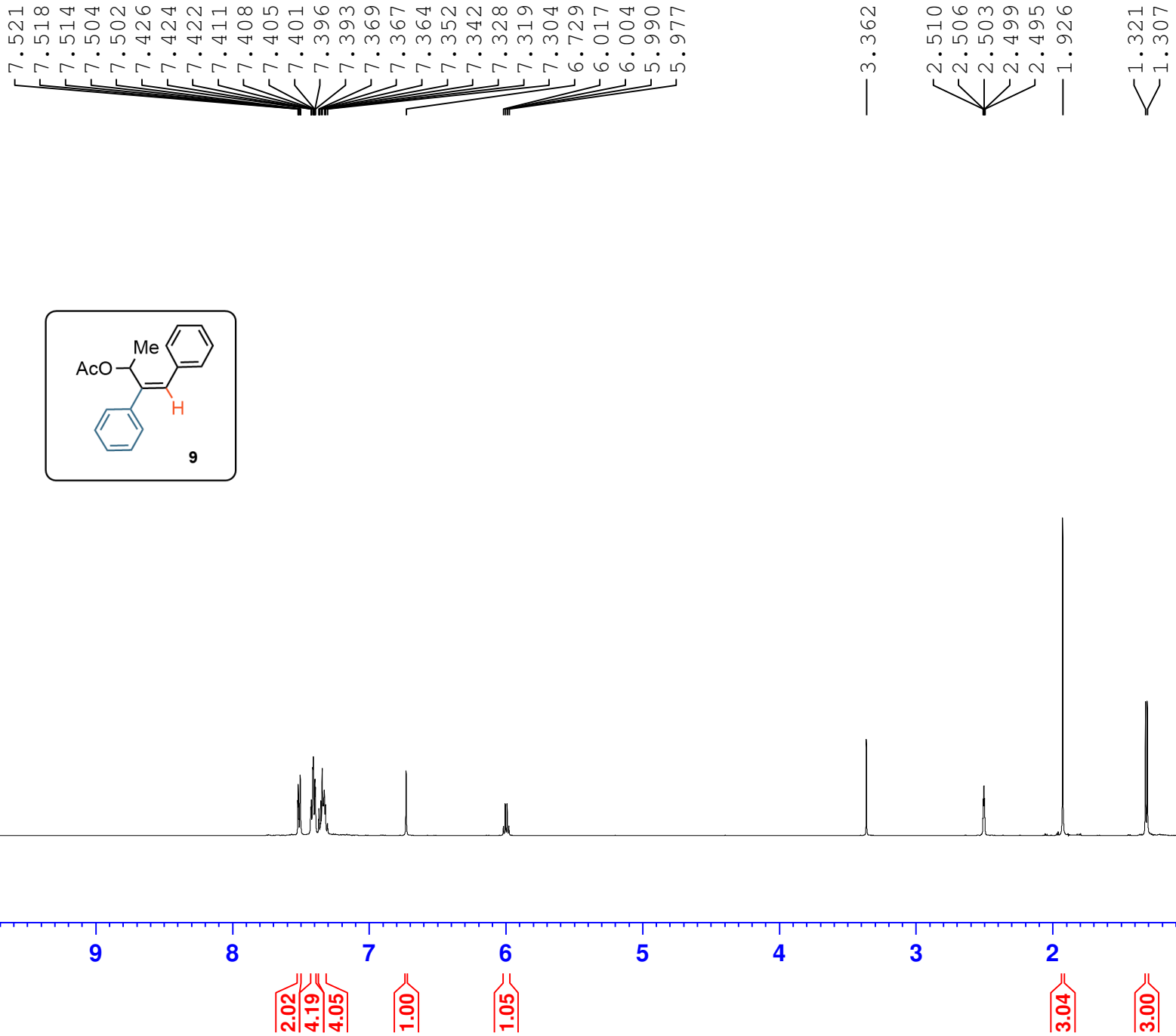

169.77
141.99
141.30
137.55
136.80
131.46
129.23
128.78
128.60
128.50
127.68
68.91
40.47
40.30
40.13
39.97
39.80
39.63
39.47
34.96
33.53
22.27
21.35
20.04
14.26
Me
AcO
H
nBu
6
Current Data Parameters
NAME Avijit Updated 500
EXPNO 352
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211213
Time 16.59 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 171
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 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

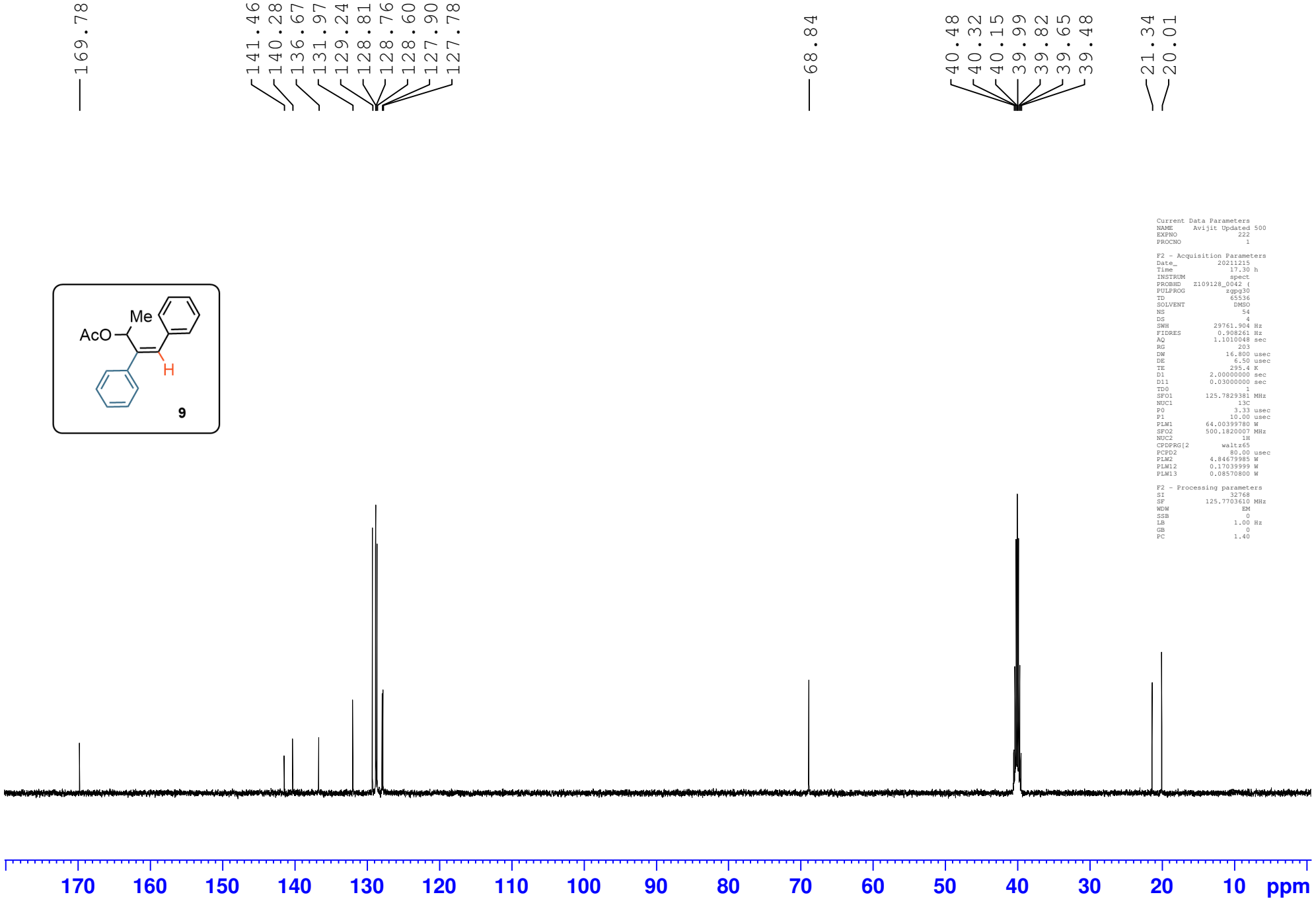

7.892
7.875
7.740
7.723
7.449
7.433
7.419
7.363
7.350
7.338
7.336
6.880
6.031
6.017
6.004
5.991
3.346
2.511
2.508
2.504
2.500
2.497
1.949
1.337
1.323
Me
AcO
H
NC
7
Current Data Parameters
NAME Avijit Updated 500
EXPNO 216
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211214
Time 10.37 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 161
DW 50.000 usec
DE 13.04 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.03
2.03
3.07
1.00
1.01
2.99
3.00

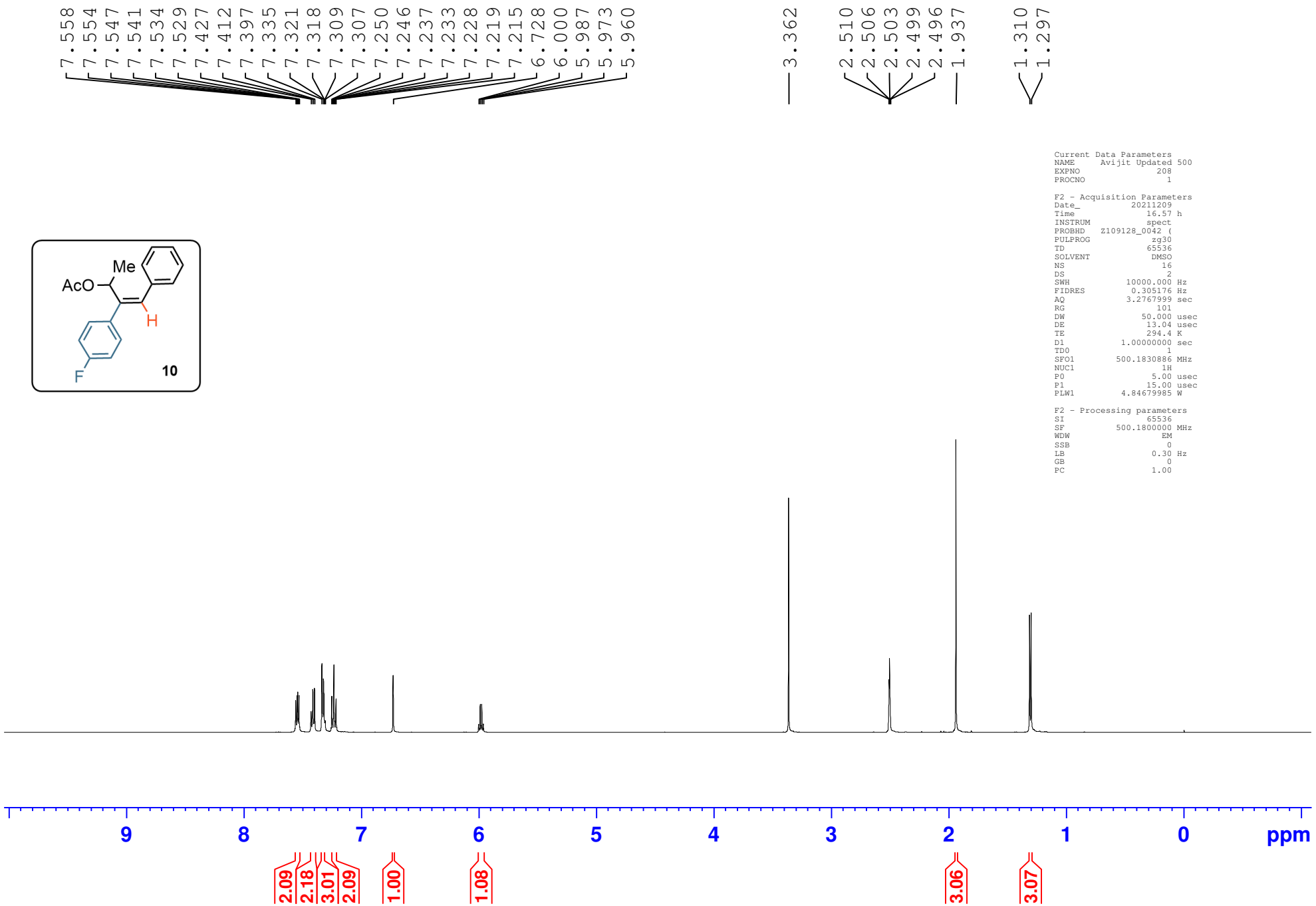

169.73
145.05
139.96
136.14
133.90
132.59
129.71
129.29
128.90
128.21
119.28
110.63
68.46
40.50
40.33
40.17
40.00
39.83
39.67
39.50
21.32
19.97
Me
AcO
H
NC
7
Current Data Parameters
NAME Avijit Updated 500
EXPNO 217
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211214
Time 11.08 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 587
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 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

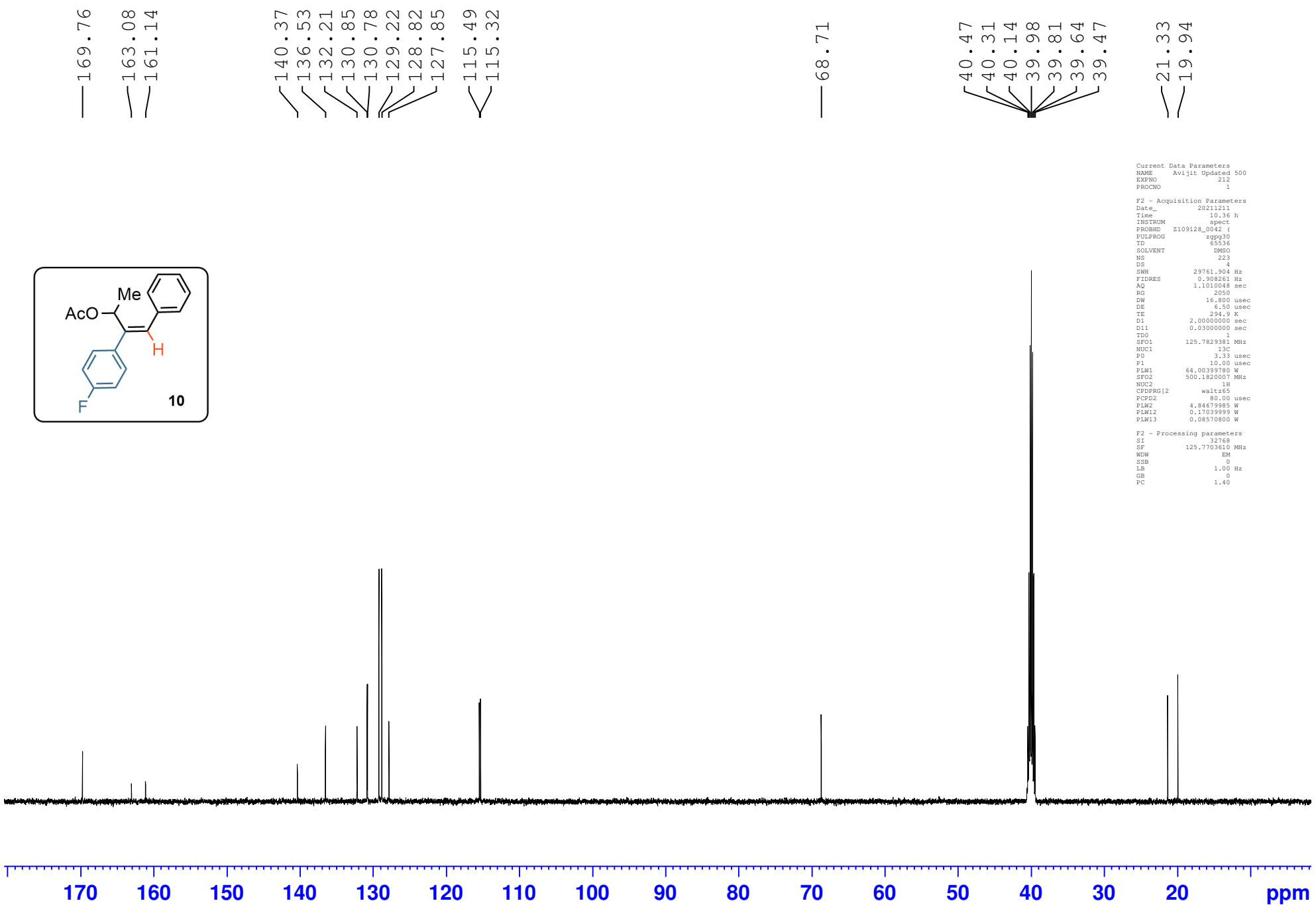

8.286
8.281
8.277
8.267
8.263
8.258
7.831
7.826
7.812
7.808
7.803
7.477
7.463
7.461
7.445
7.431
7.382
7.367
7.352
7.348
6.929
6.052
6.039
6.025
6.012
3.338
2.514
2.510
2.506
2.503
2.499
1.961
1.365
1.352
Me
AcO
H
O2N
8
Current Data Parameters
NAME Avijit Ascend 500
EXPNO 78
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211209
Time 16.54 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 76.68
DW 50.000 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690006 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.03
2.31
3.08
1.00
1.01
3.02
3.04

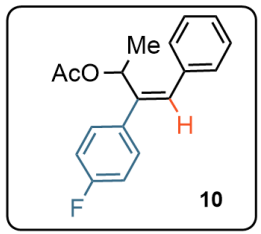

169.79
147.08
139.65
136.07
134.34
130.07
129.34
128.97
128.34
123.83
68.44
40.61
40.40
40.19
39.98
39.77
39.56
39.35
21.36
20.00
Me
AcO
H
O2N
8
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.521
7.518
7.514
7.504
7.502
7.426
7.424
7.422
7.411
7.408
7.405
7.401
7.396
7.393
7.369
7.367
7.364
7.352
7.342
7.328
7.319
7.304
6.729
6.017
6.004
5.990
5.977
3.362
2.510
2.506
2.503
2.499
2.495
1.926
1.321
1.307
AcO
Me
H
9
Current Data Parameters
NAME Avijit Updated 500
EXPNO 221
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211215
Time 17.23 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 71.8
DW 50.000 usec
DE 13.04 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.02
4.19
4.05
1.00
1.05
3.04
3.00


169.78
141.46
140.28
136.67
131.97
129.24
128.81
128.76
128.60
127.90
127.78
68.84
40.48
40.32
40.15
39.99
39.82
39.65
39.48
21.34
20.01
Me
AcO
H
9
Current Data Parameters
NAME Avijit Updated 500
EXPNO 222
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211215
Time 17.30 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 54
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 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.558
7.554
7.547
7.541
7.534
7.529
7.427
7.412
7.397
7.335
7.321
7.318
7.309
7.307
7.250
7.246
7.237
7.233
7.228
7.219
7.215
6.728
6.000
5.987
5.973
5.960
3.362
2.510
2.506
2.503
2.499
2.496
1.937
1.310
1.297
Me
AcO
H
F
10
Current Data Parameters
NAME Avijit Updated 500
EXPNO 208
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211209
Time 16.57 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 13.04 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.09
2.18
3.01
2.09
1.00
1.08
3.06
3.07


169.76
163.08
161.14
140.37
136.53
132.21
130.85
130.78
129.22
128.82
127.85
115.49
115.32
68.71
40.47
40.31
40.14
39.98
39.81
39.64
39.47
21.33
19.94
Me
AcO
H
F
10
Current Data Parameters
NAME Avijit Updated 500
EXPNO 212
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211211
Time 10.36 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 223
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

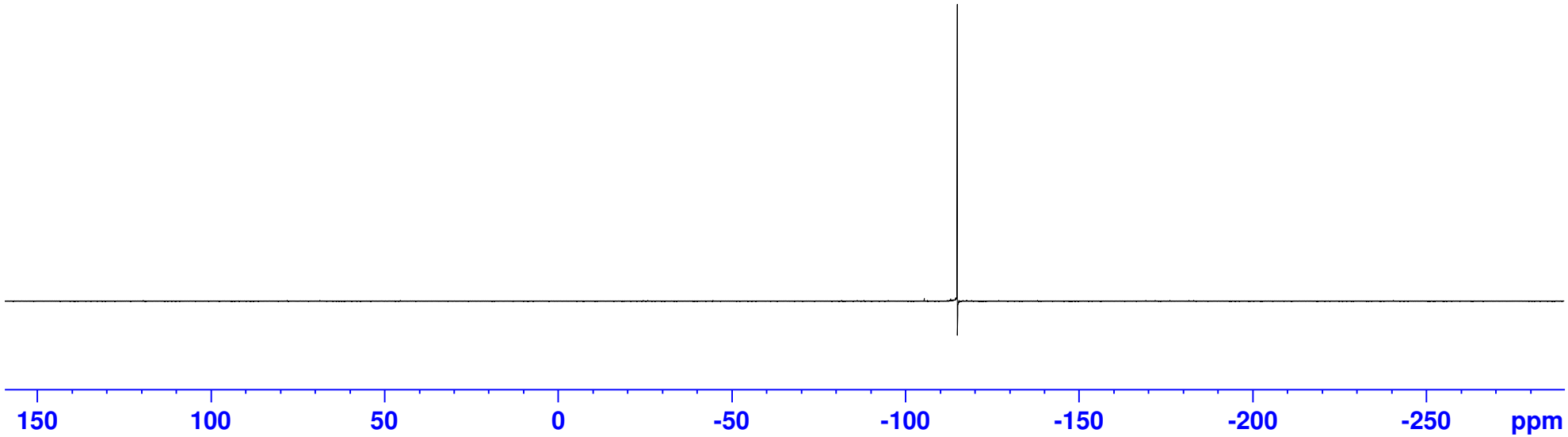


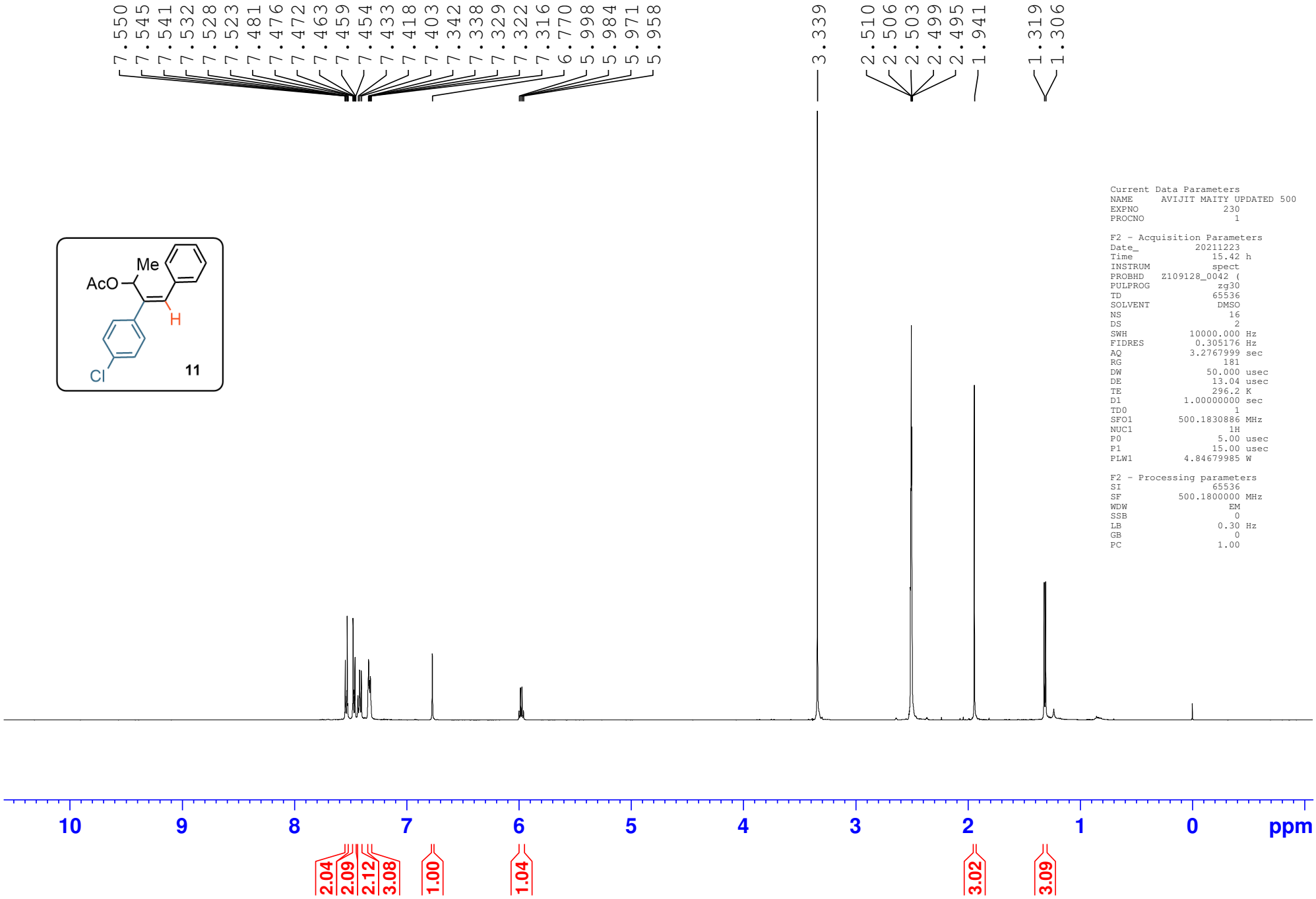
−115.06

```
Current Data Parameters
NAME      Avijit Updated 500
EXPNO                 209
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211209
Time              16.58 h
INSTRUM             spect
PROBHD    Z109128_0042 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT              DMSO
NS                     13
DS                      4
SWH           277777.781 Hz
FIDRES          4.238553 Hz
AQ             0.2359296 sec
RG                    203
DW                1.800 usec
DE                6.50 usec
TE                294.4 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1
SFO1         470.6394242 MHz
NUC1                  19F
P1                 12.00 usec
PLW1         36.12599945 W
SFO2         500.1820007 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          4.84679985 W
PLW12         0.17039999 W

F2 - Processing parameters
SI                 65536
SF           470.6394242 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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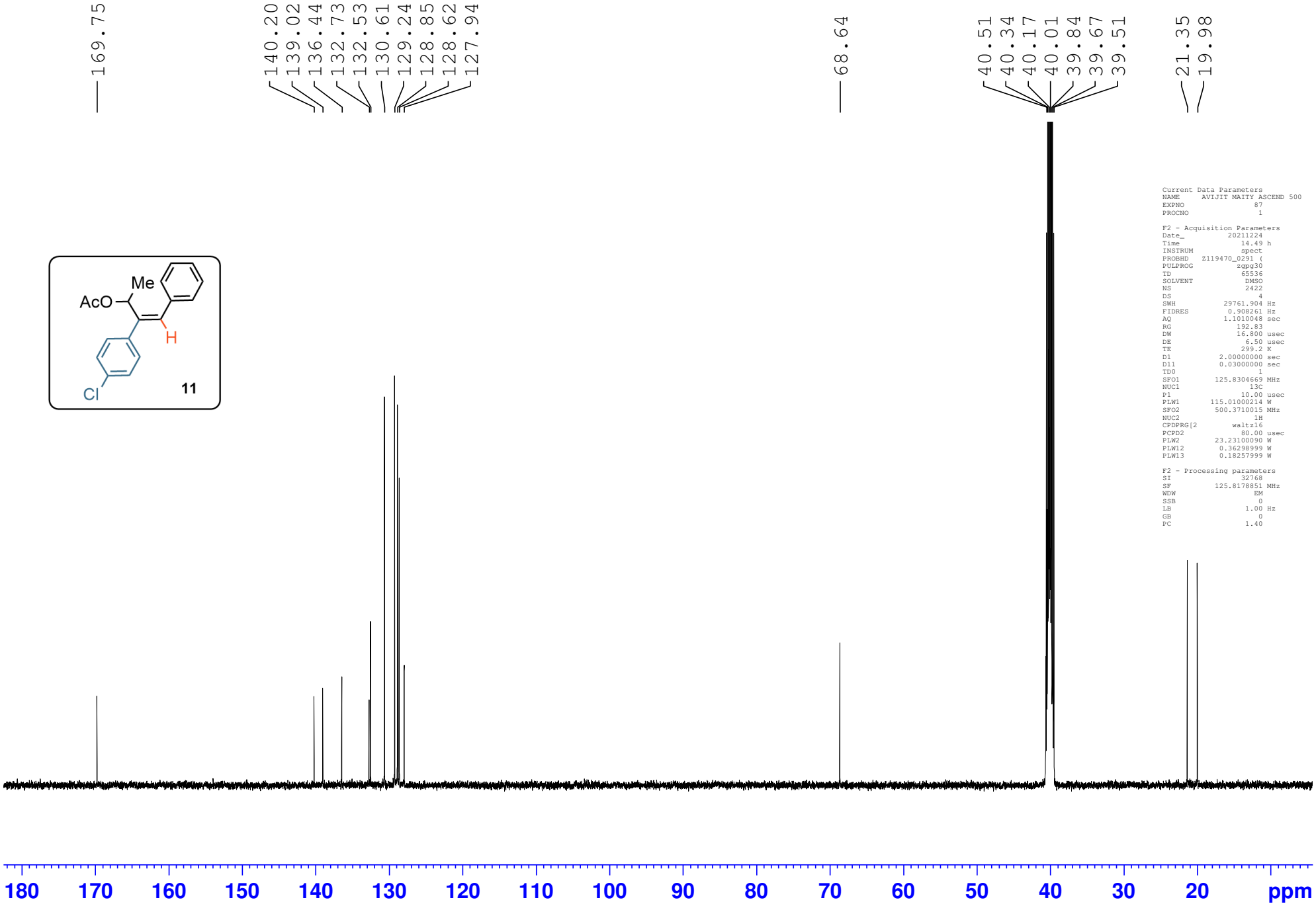
7.454
7.433
7.418
7.403
7.342
7.338
7.329
7.322
7.316
6.770
5.998
5.984
5.971
5.958
3.339
2.510
2.506
2.503
2.499
2.495
1.941
1.319
1.306
Me
AcO
H
Cl
11
Current Data Parameters
NAME AVIJIT MAITY UPDATED 500
EXPNO 230
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211223
Time 15.42 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 13.04 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
2.09
2.12
3.08
1.00
1.04
3.02
3.09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140.20
139.02
136.44
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129.24
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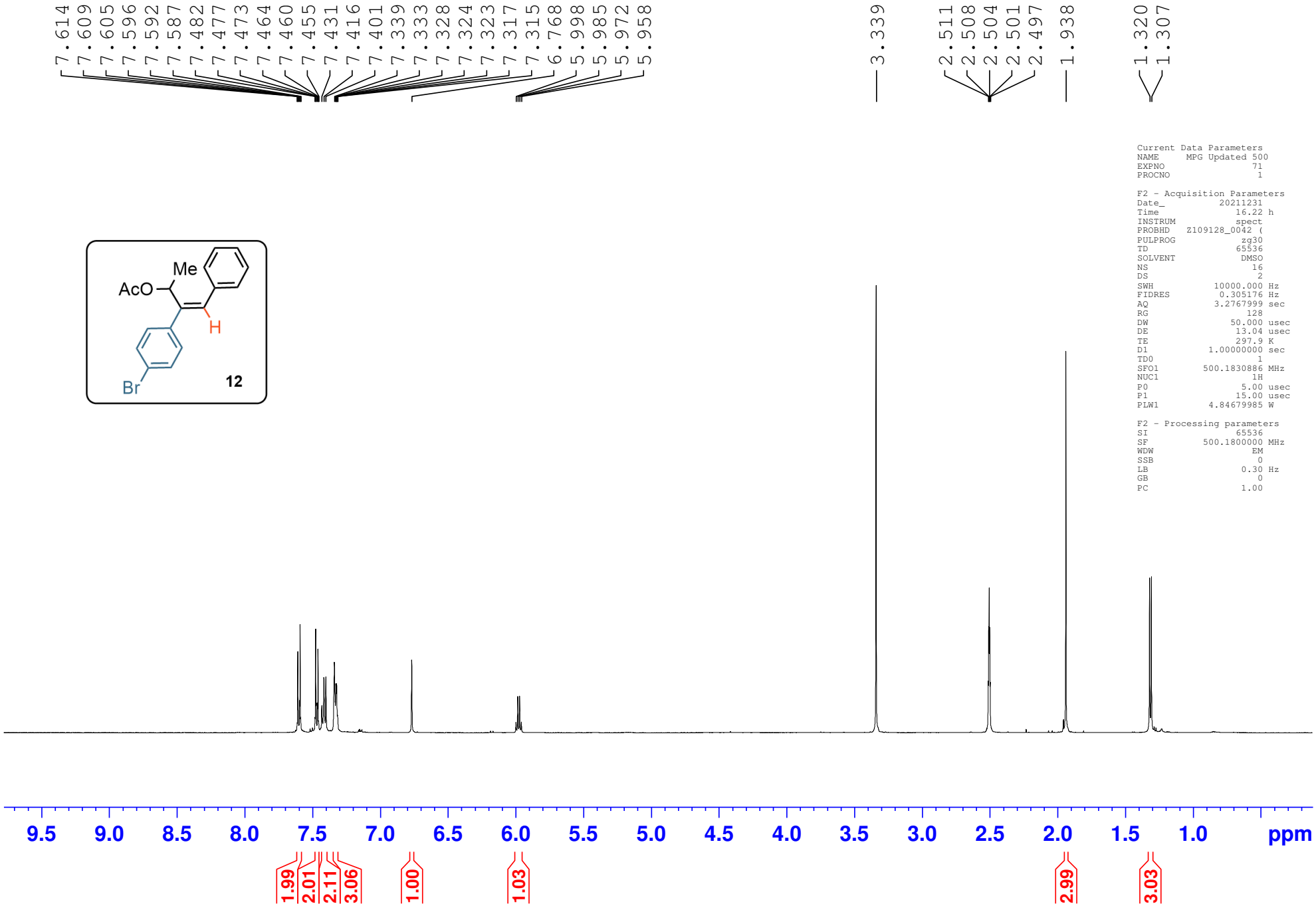
128.62
127.94
68.64
40.51
40.34
40.17
40.01
39.84
39.67
39.51
21.35
19.98
Me
AcO
H
Cl
11
Current Data Parameters
NAME AVIJIT MAITY ASCEND 500
EXPNO 87
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211224
Time 14.49 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2422
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.83
DW 16.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8304669 MHz
NUC1 13C
P1 10.00 usec
PLW1 115.01000214 W
SFO2 500.3710015 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.23100090 W
PLW12 0.36298999 W
PLW13 0.18257999 W
F2 - Processing parameters
SI 32768
SF 125.8178851 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.605
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7.460
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7.431
7.416
7.401
7.339
7.333
7.328
7.324
7.323
7.317
7.315
6.768
5.998
5.985
5.972
5.958
3.339
2.511
2.508
2.504
2.501
2.497
1.938
1.320
1.307
Me
AcO
H
Br
12
Current Data Parameters
NAME MPG Updated 500
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 16.22 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 13.04 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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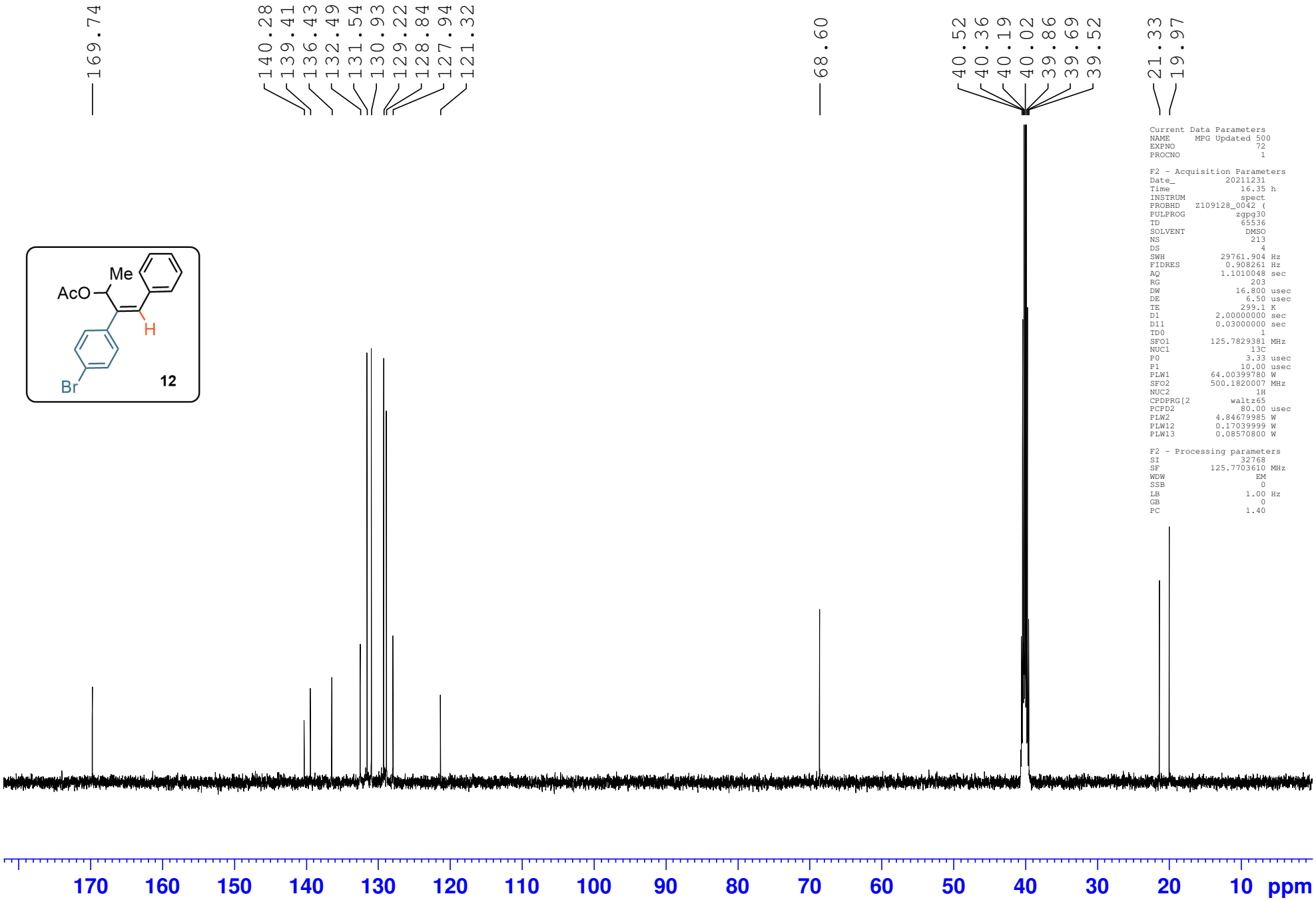
1.0
ppm
1.99
2.01
2.11
3.06
1.00
1.03
2.99
3.03


169.74
140.28
139.41
136.43
132.49
131.54
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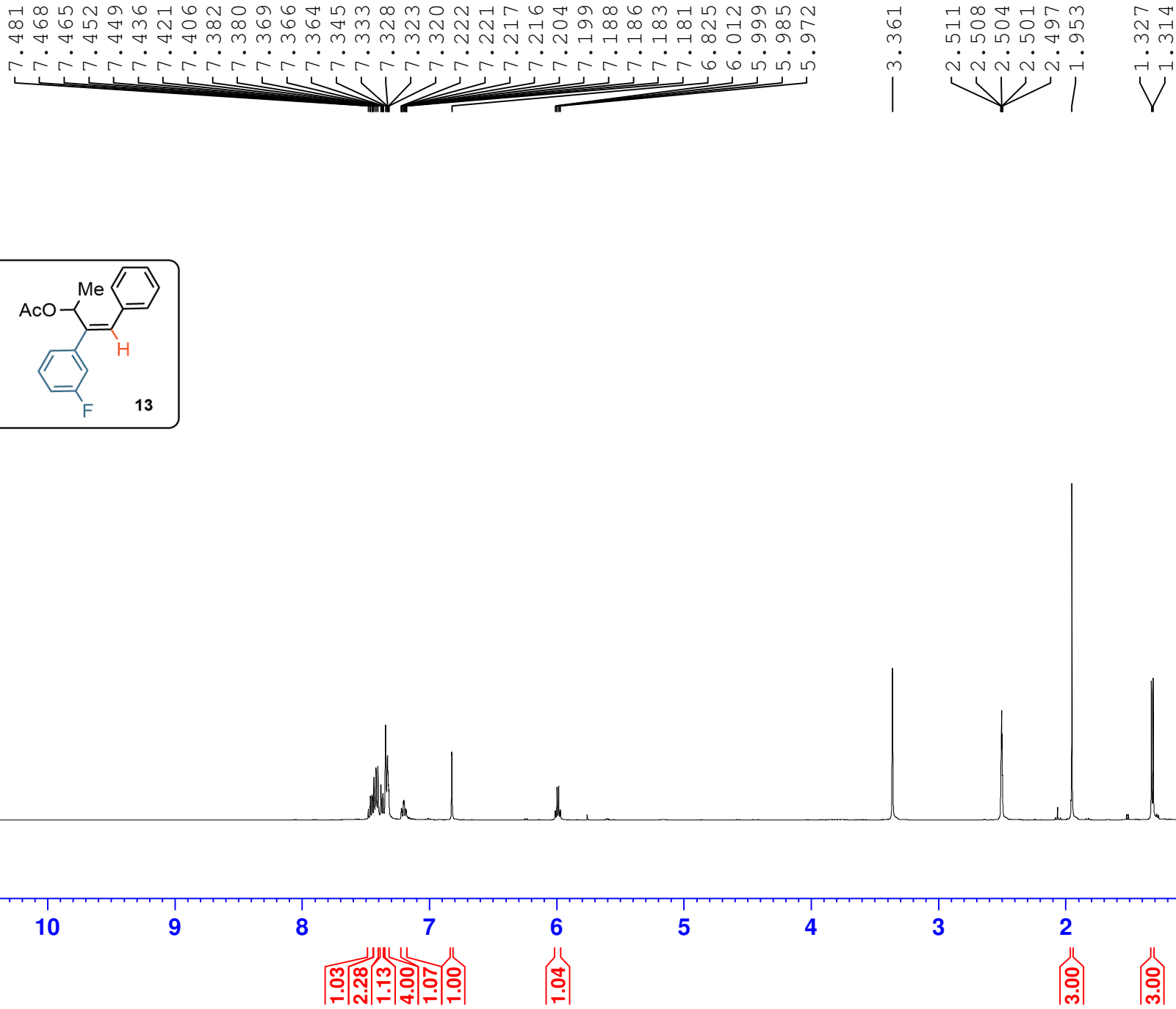
129.22
128.84
127.94
121.32
68.60
40.52
40.36
40.19
40.02
39.86
39.69
39.52
21.33
19.97
Me
AcO
H
Br
12
Current Data Parameters
NAME MPG Updated 500
EXPNO 72
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 16.35 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 213
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 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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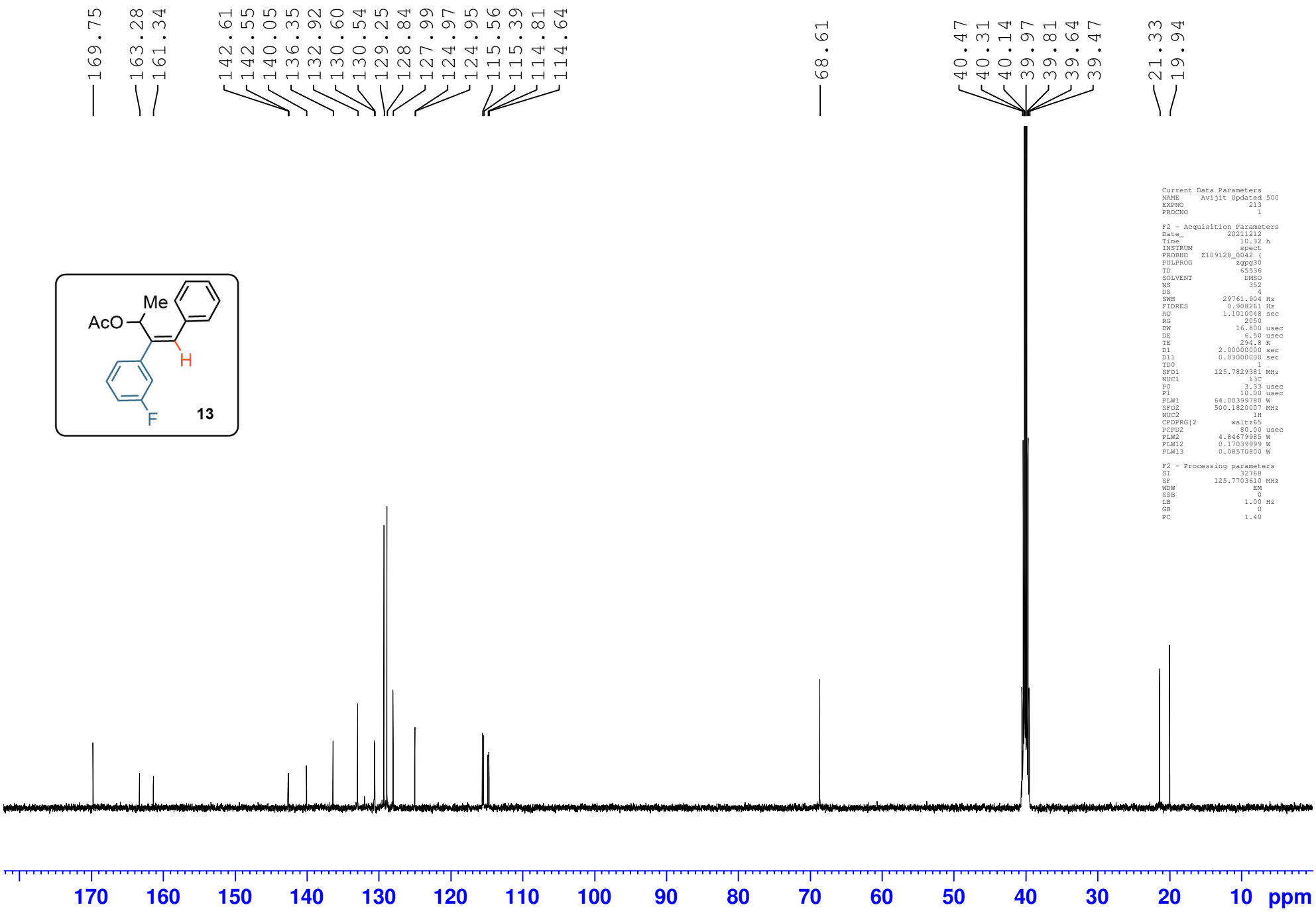
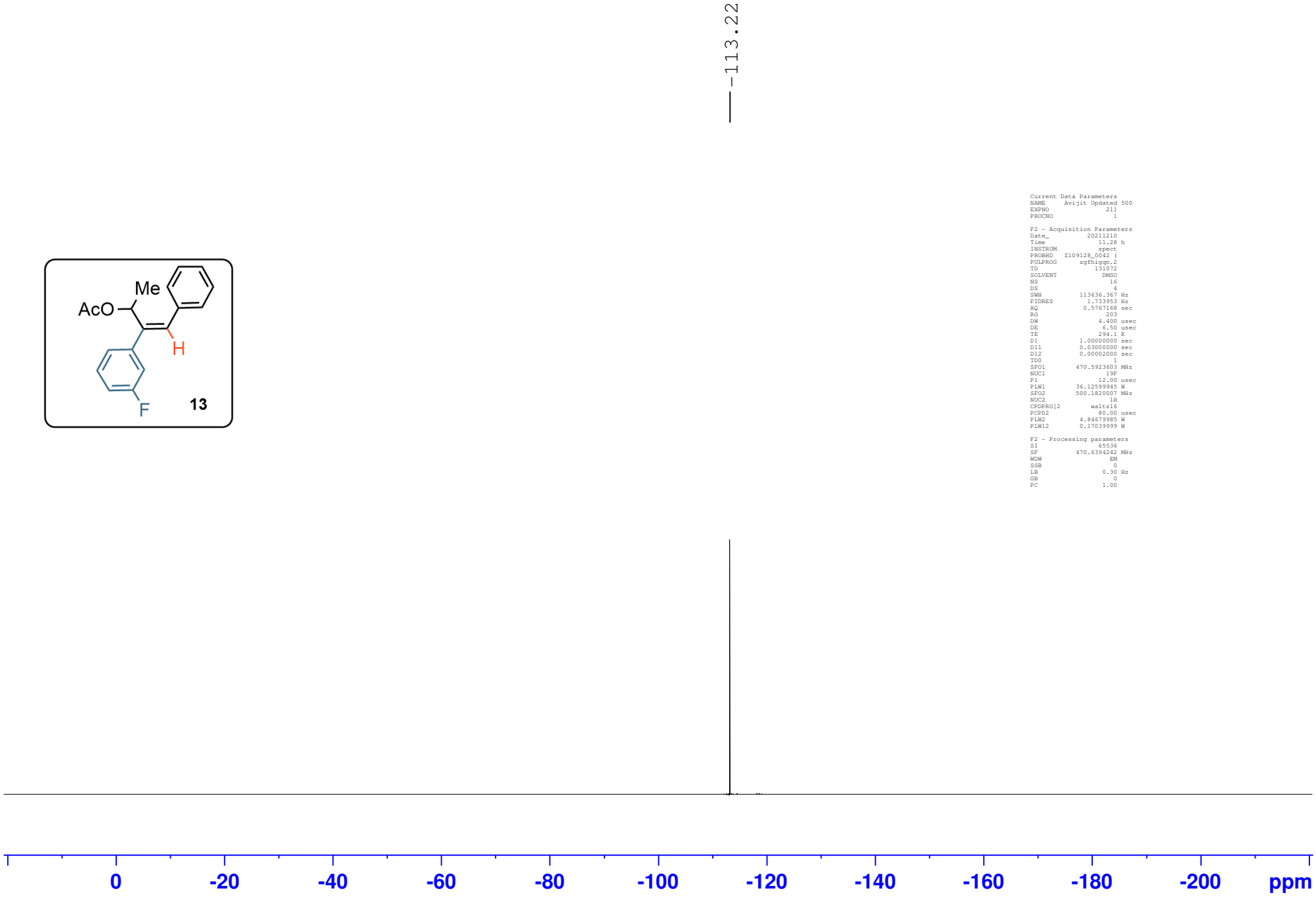
7.468
7.465
7.452
7.449
7.436
7.421
7.406
7.382
7.380
7.369
7.366
7.364
7.345
7.333
7.328
7.323
7.320
7.222
7.221
7.217
7.216
7.204
7.199
7.188
7.186
7.183
7.181
6.825
6.012
5.999
5.985
5.972
3.361
2.511
2.508
2.504
2.501
2.497
1.953
1.327
1.314
Me
AcO
H
F
13
Current Data Parameters
NAME Avijit Updated 500
EXPNO 210
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 11.26 h
INSTRUM spect
PROBHD 2109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 114
DW 50.000 usec
DE 13.04 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
2.28
1.13
4.00
1.07
1.00
1.04
3.00
3.00


169.75
163.28
161.34
142.61
142.55
140.05
136.35
132.92
130.60
130.54
129.25
128.84
127.99
124.97
124.95
115.56
115.39
114.81
114.64
68.61
40.47
40.31
40.14
39.97
39.81
39.64
39.47
21.33
19.94
Me
AcO
H
F
13
Current Data Parameters
NAME Avijit Updated 500
EXPNO 213
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211212
Time 10.32 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 352
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Me
AcO
H
F
13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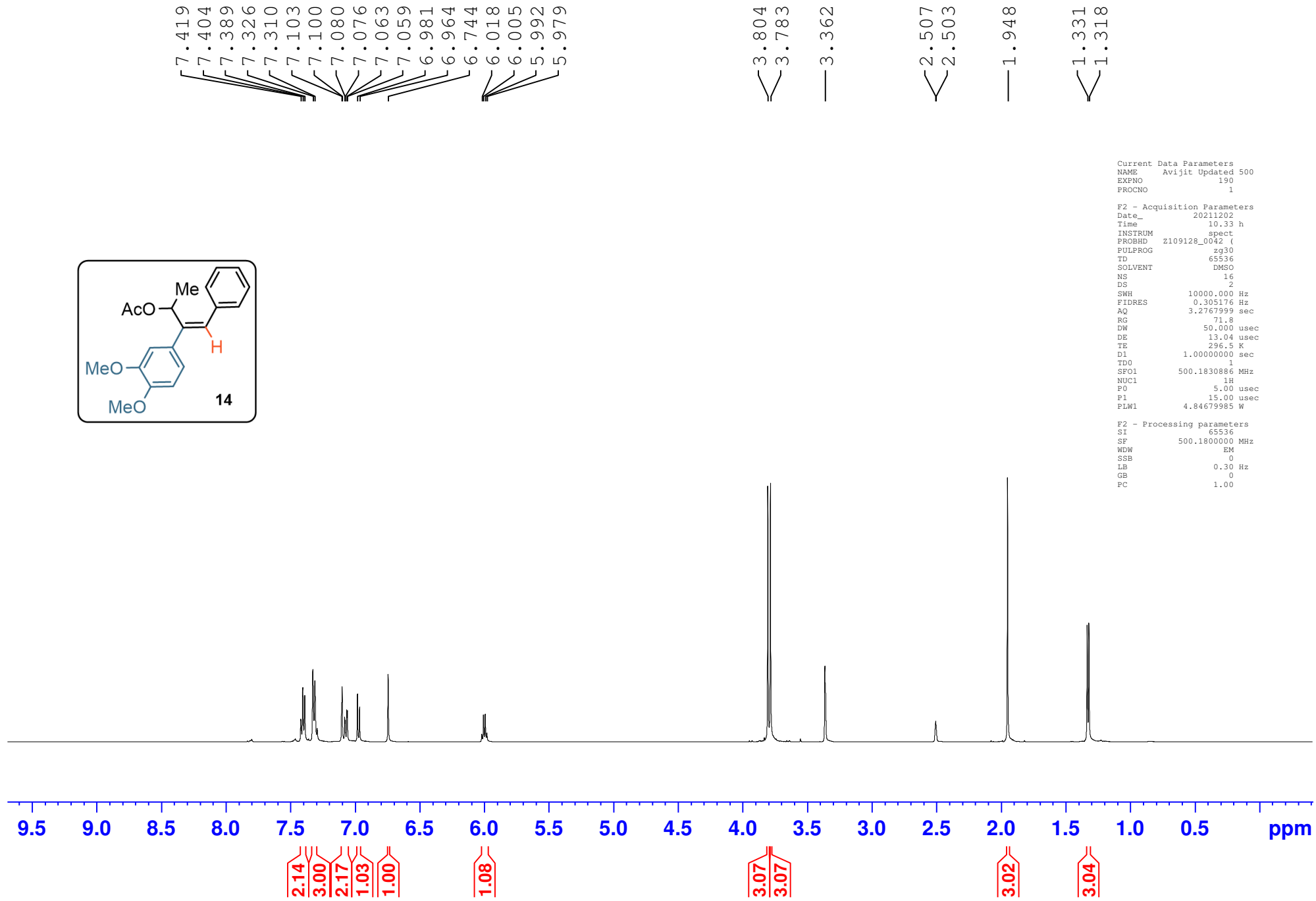
Current Data Parameters
NAME Avijit Updated 500
EXPNO 211
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 11.28 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 203
DW 4.400 usec
DE 6.50 usec
TE 294.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5923603 MHz
NUC1 19F
P1 12.00 usec
PLW1 36.12599945 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
F2 - Processing parameters
SI 65536
SF 470.6394242 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm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7.103
7.100
7.080
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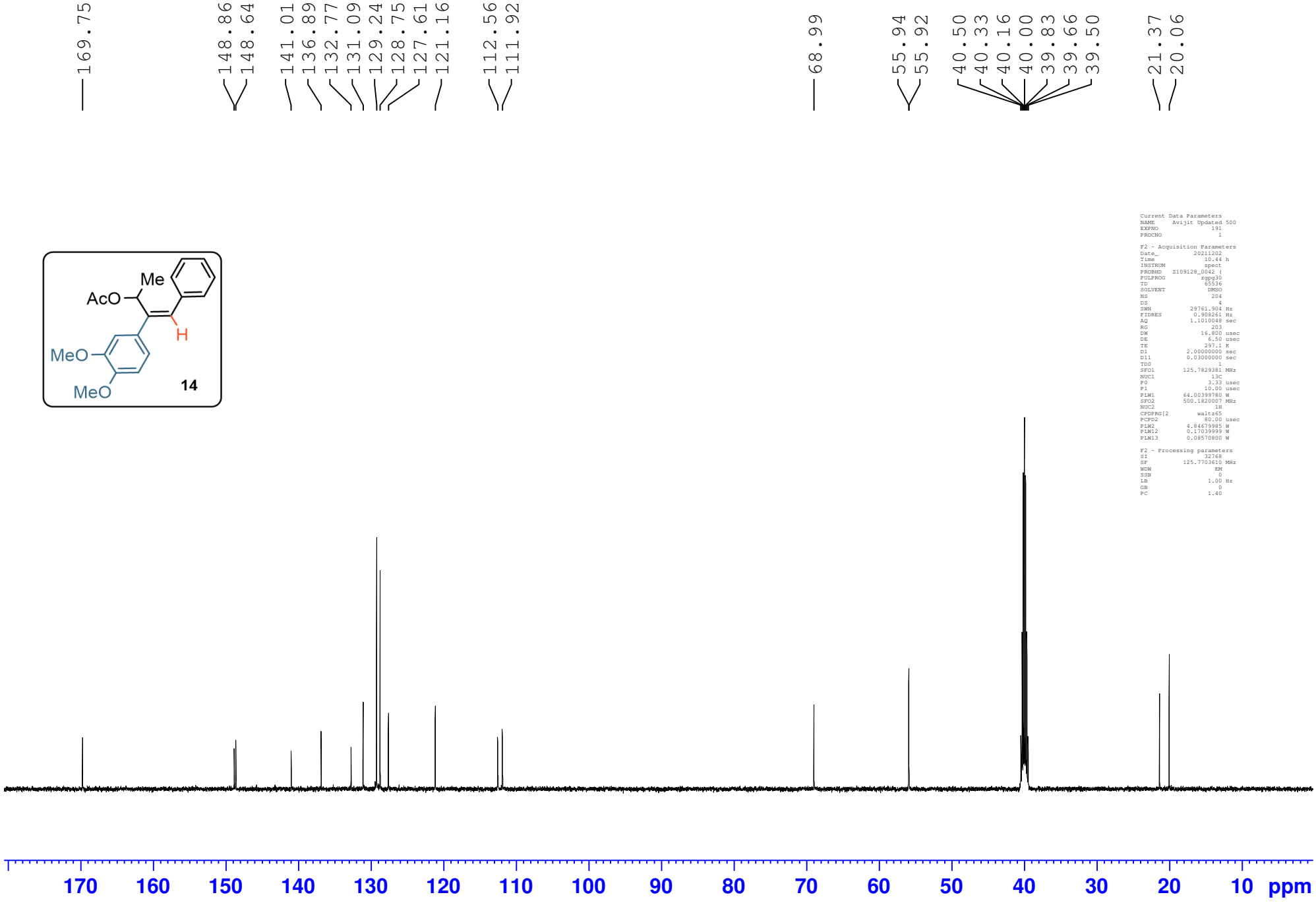
7.063
7.059
6.981
6.964
6.744
6.018
6.005
5.992
5.979
3.804
3.783
3.362
2.507
2.503
1.948
1.331
1.318
Me
AcO
H
MeO
MeO
14
Current Data Parameters
NAME Avijit Updated 500
EXPNO 190
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 10.33 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 71.8
DW 50.000 usec
DE 13.04 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.14
3.00
2.17
1.03
1.00
1.08
3.07
3.07
3.02
3.04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136.89
132.77
131.09
129.24
128.75
127.61
121.16
112.56
111.92
68.99
55.94
55.92
40.50
40.33
40.16
40.00
39.83
39.66
39.50
21.37
20.06
Me
AcO
H
MeO
MeO
14
Current Data Parameters
NAME Avijit Updated 500
EXPNO 191
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 10.44 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 204
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 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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150
140
130
120
110
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90
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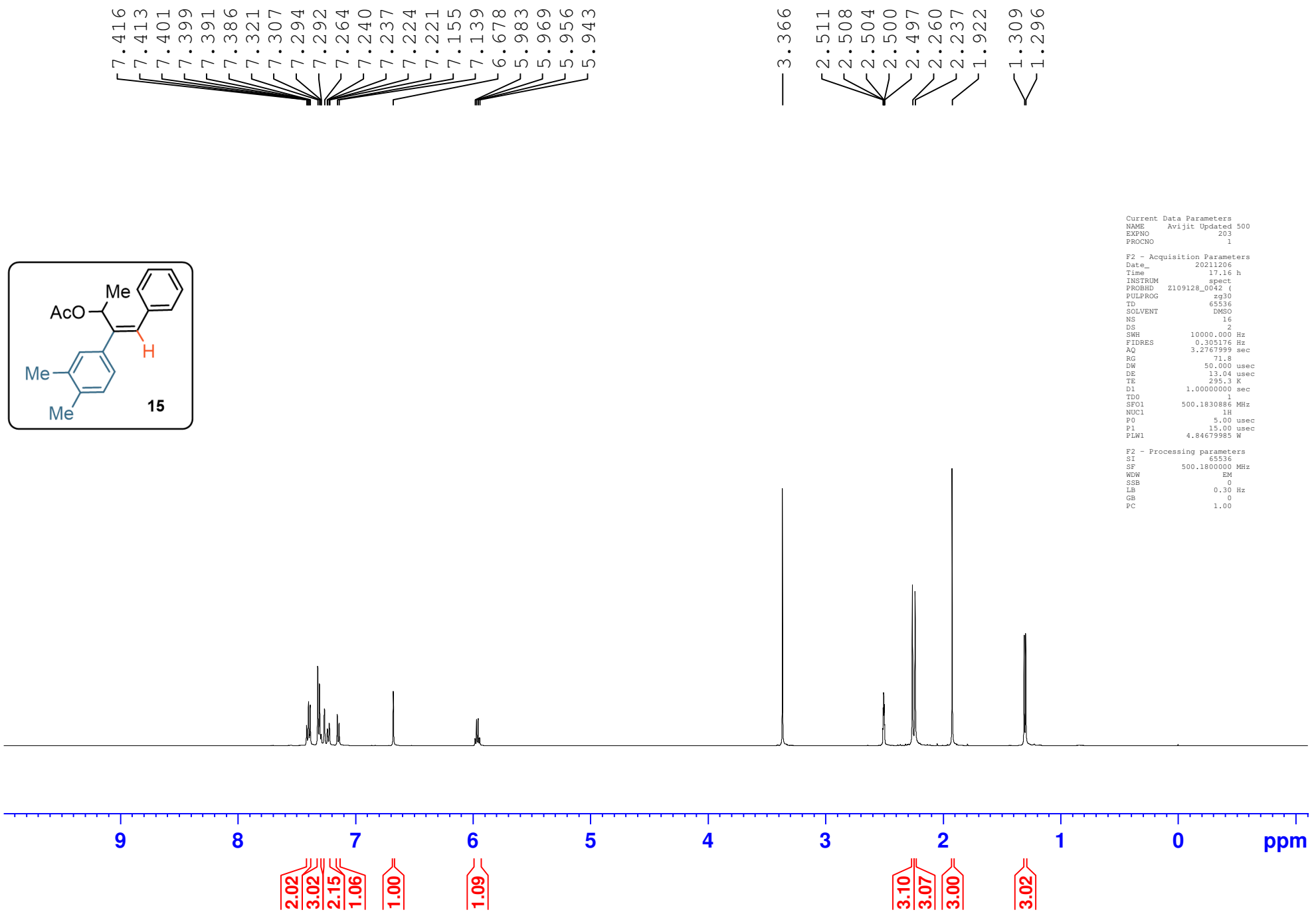
70
60
50
40
30
20
10
ppm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7.401
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7.321
7.307
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7.292
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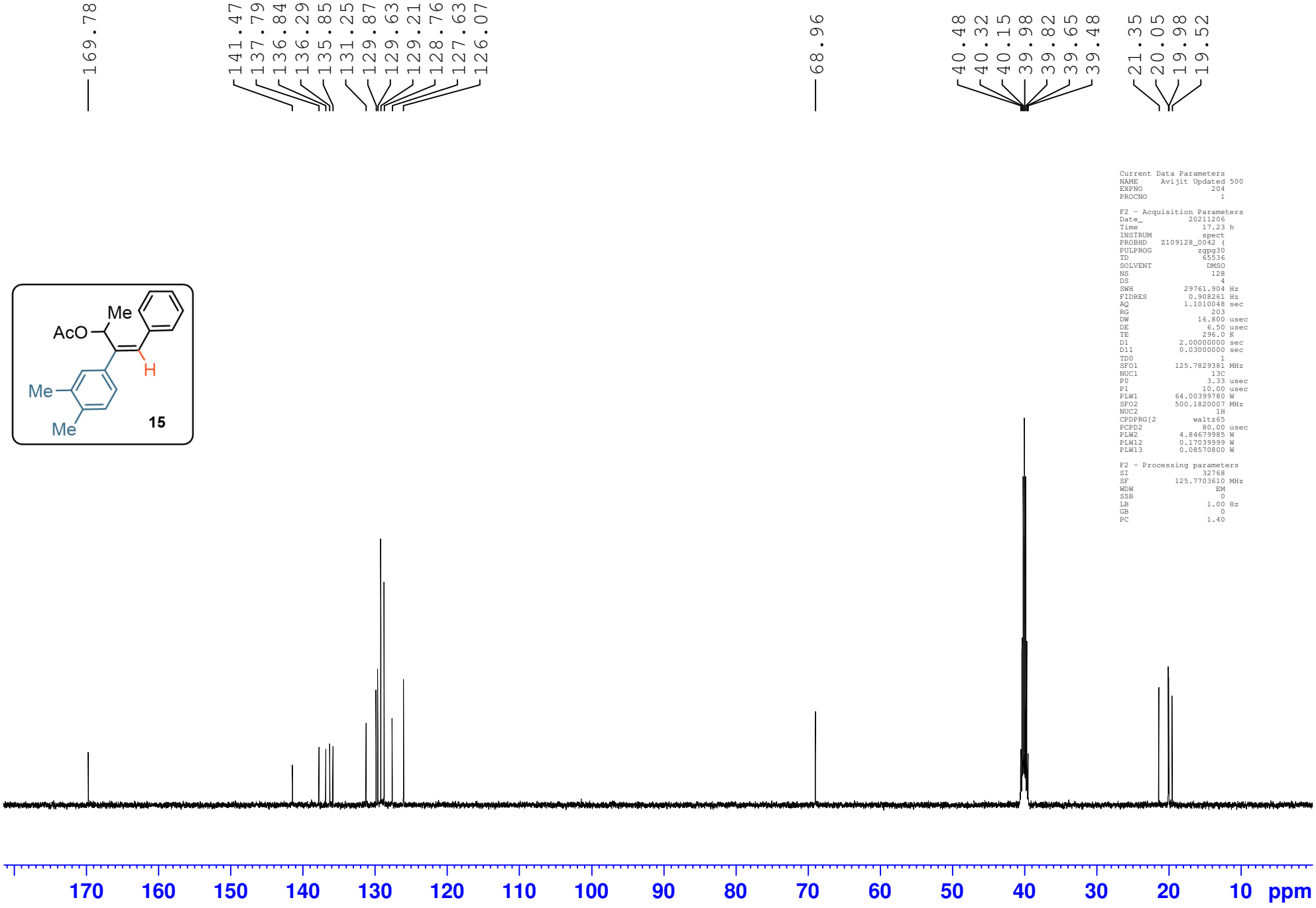
7.237
7.224
7.221
7.155
7.139
6.678
5.983
5.969
5.956
5.943
3.366
2.511
2.508
2.504
2.500
2.497
2.260
2.237
1.922
1.309
1.296
AcO
Me
H
Me
Me
15
Current Data Parameters
NAME Avijit Updated 500
EXPNO 203
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 17.16 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 71.8
DW 50.000 usec
DE 13.04 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.02
3.02
2.15
1.06
1.00
1.09
3.10
3.07
3.00
3.02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129.21
128.76
127.63
126.07
68.96
40.48
40.32
40.15
39.98
39.82
39.65
39.48
21.35
20.05
19.98
19.52
AcO
Me
H
Me
Me
15
Current Data Parameters
NAME Avijit Updated 500
EXPNO 204
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 17.23 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
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 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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140
130
120
110
100
90
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70
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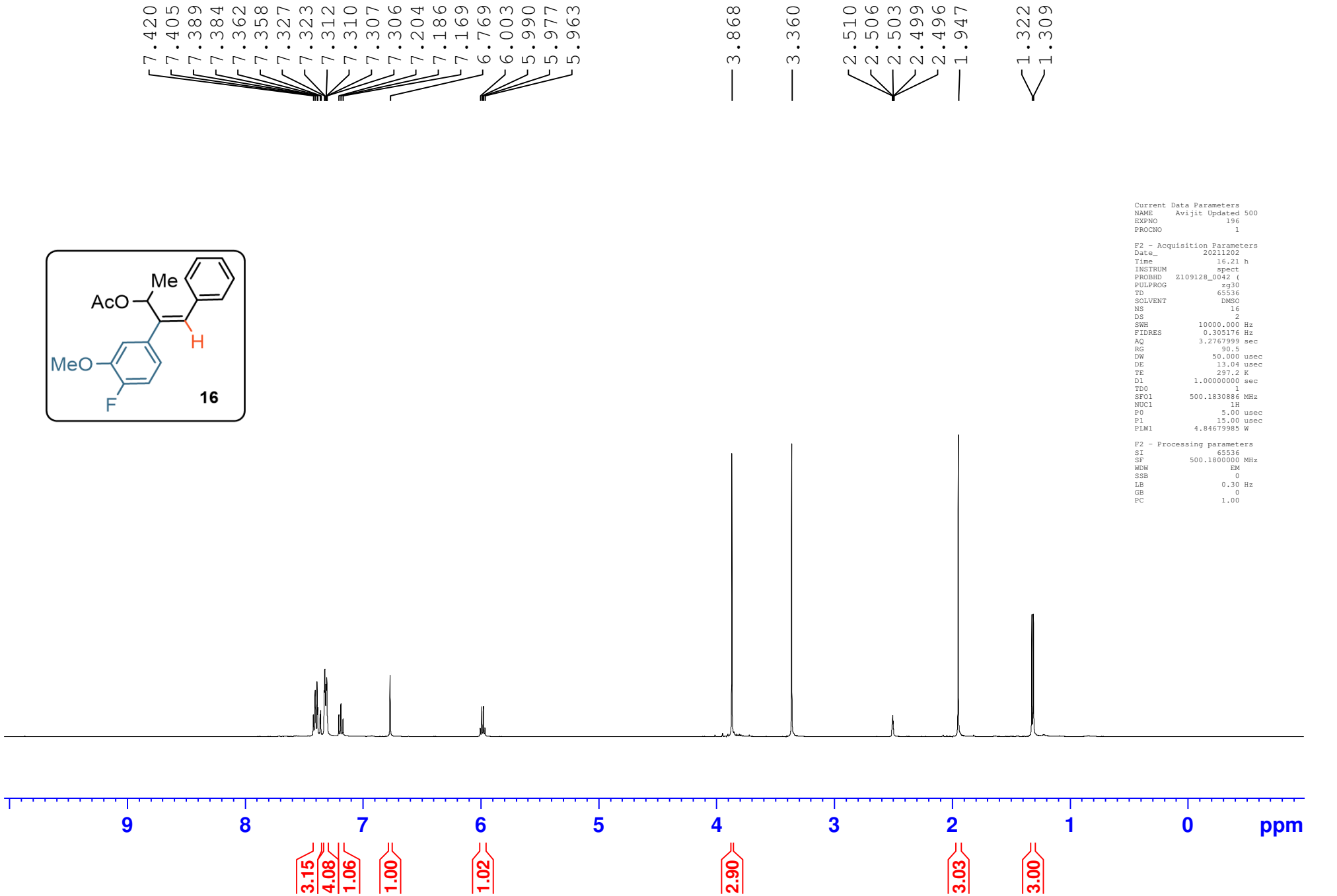
20
10
ppm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7.323
7.312
7.310
7.307
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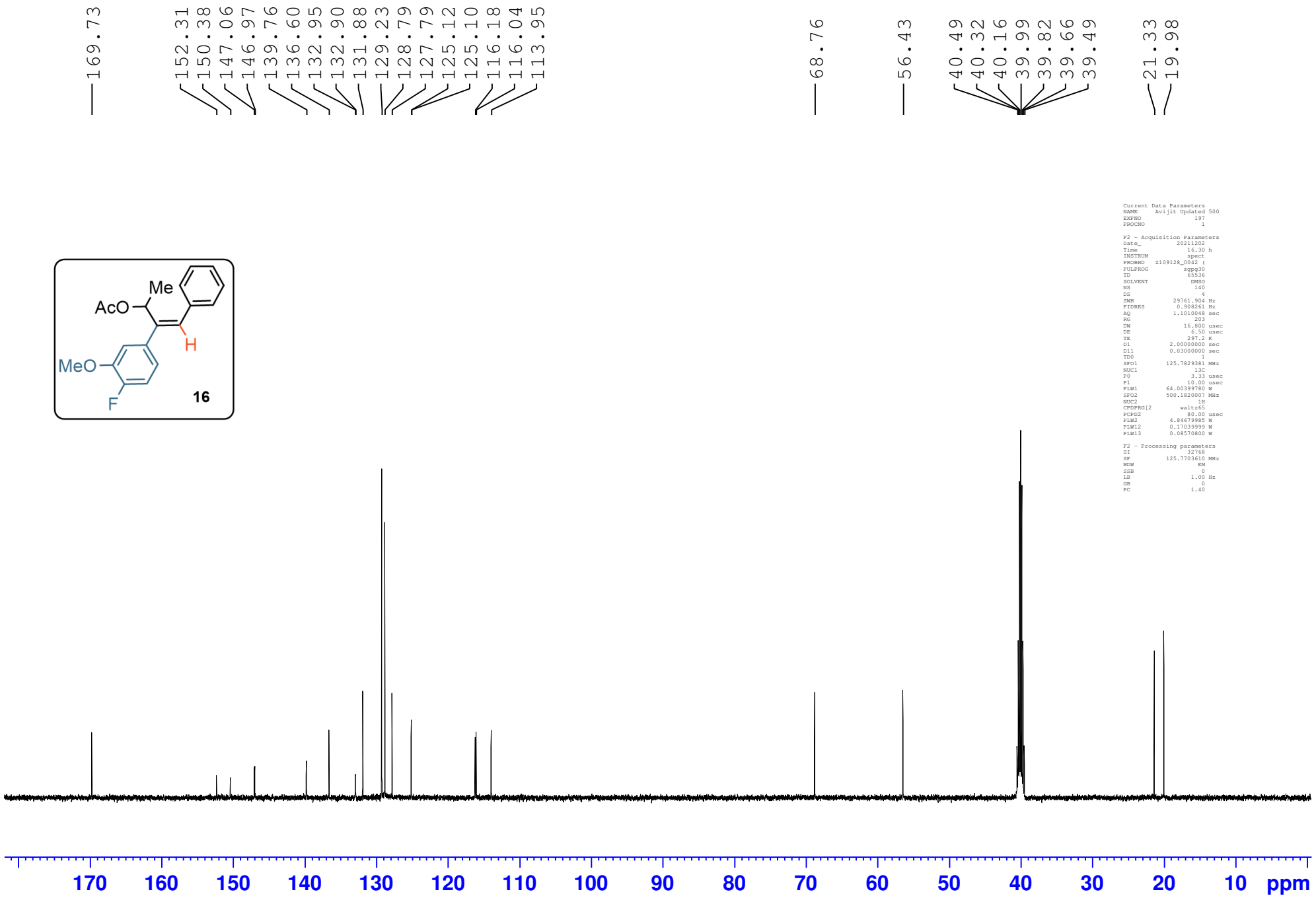
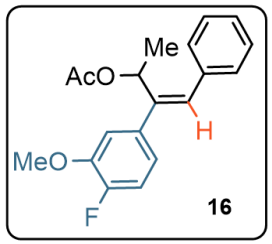
7.204
7.186
7.169
6.769
6.003
5.990
5.977
5.963
3.868
3.360
2.510
2.506
2.503
2.499
2.496
1.947
1.322
1.309
Me
AcO
H
MeO
F
16
Current Data Parameters
NAME Avijit Updated 500
EXPNO 196
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 16.21 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 13.04 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
3.15
4.08
1.06
1.00
1.02
2.90
3.03
3.00


169.73
152.31
150.38
147.06
146.97
139.76
136.60
132.95
132.90
131.88
129.23
128.79
127.79
125.12
125.10
116.18
116.04
113.95
68.76
56.43
40.49
40.32
40.16
39.99
39.82
39.66
39.49
21.33
19.98
Me
AcO
H
MeO
F
16
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

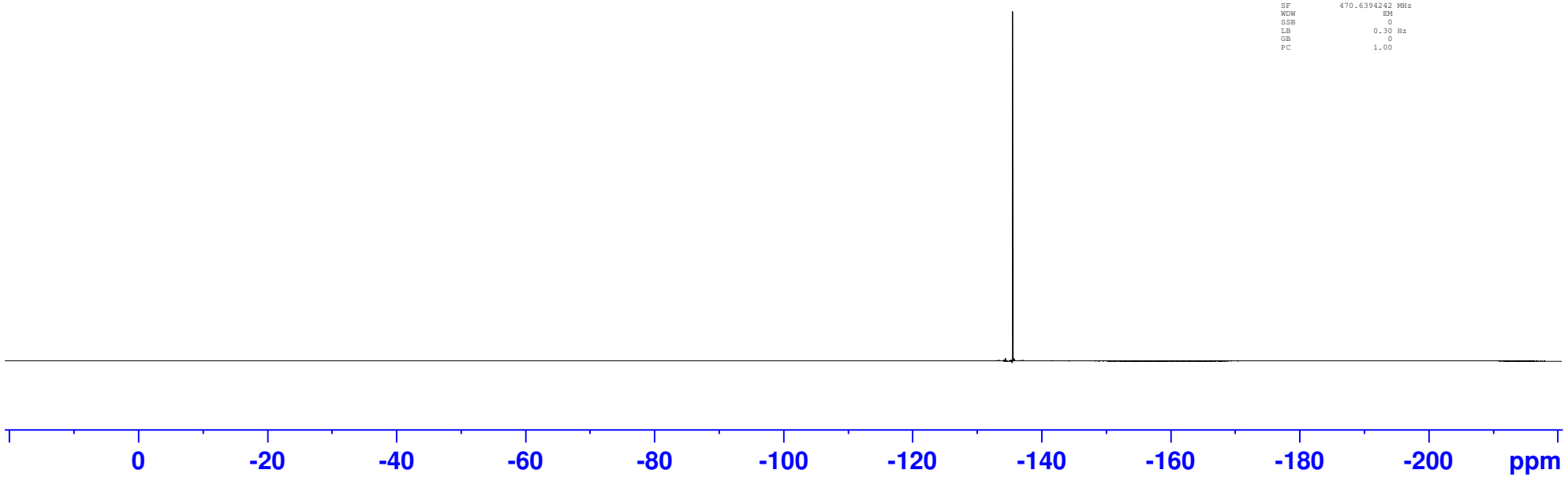


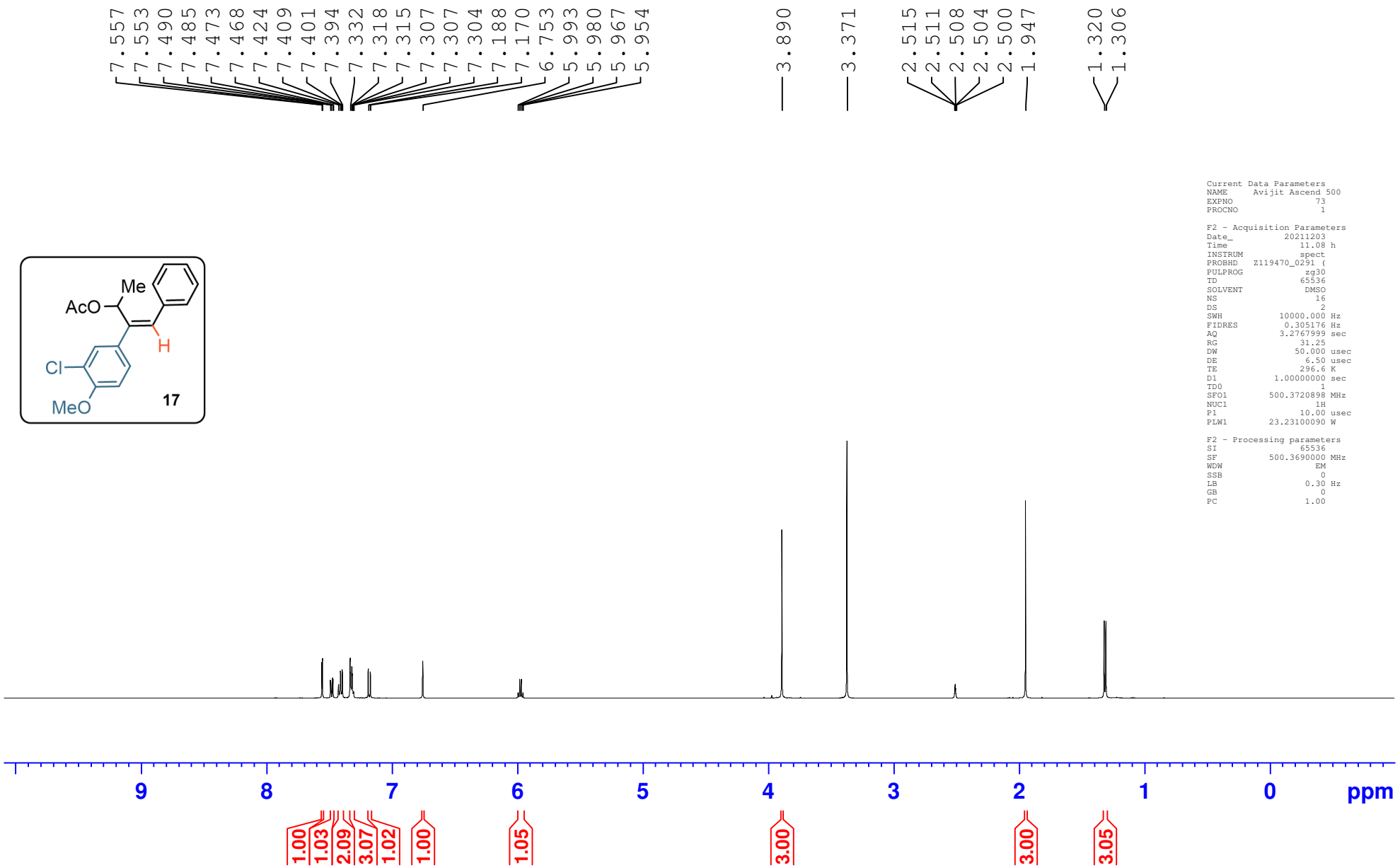
—135.51

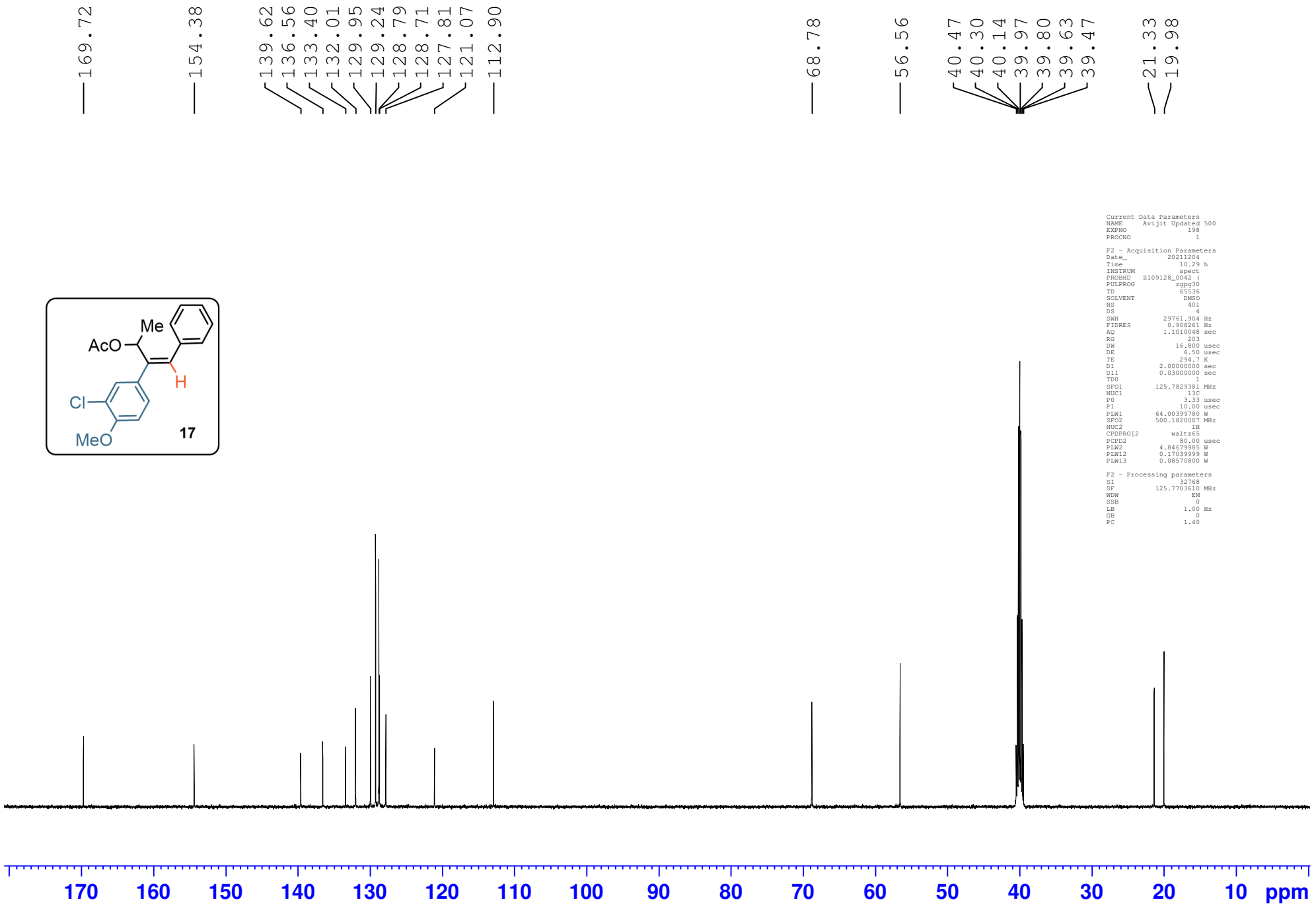
Current Data Parameters
NAME Avijit Updated 500
EXPNO 195
PROCNO 1

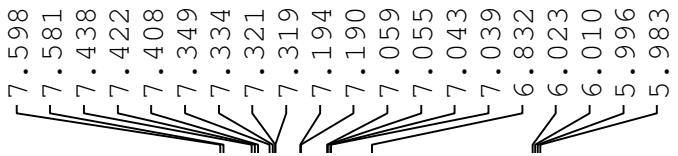
F2 - Acquisition Parameters
Date_ 20211202
Time 16.19 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 1.733953 Hz
AQ 0.5767168 sec
RG 406
DW 4.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5923603 MHz
NUC1 19F
P1 12.00 usec
PLW1 36.12599945 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W

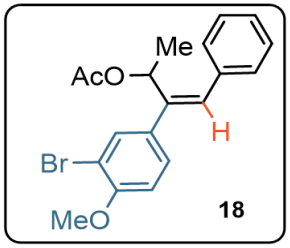
F2 - Processing parameters
SI 65536
SF 470.6394242 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



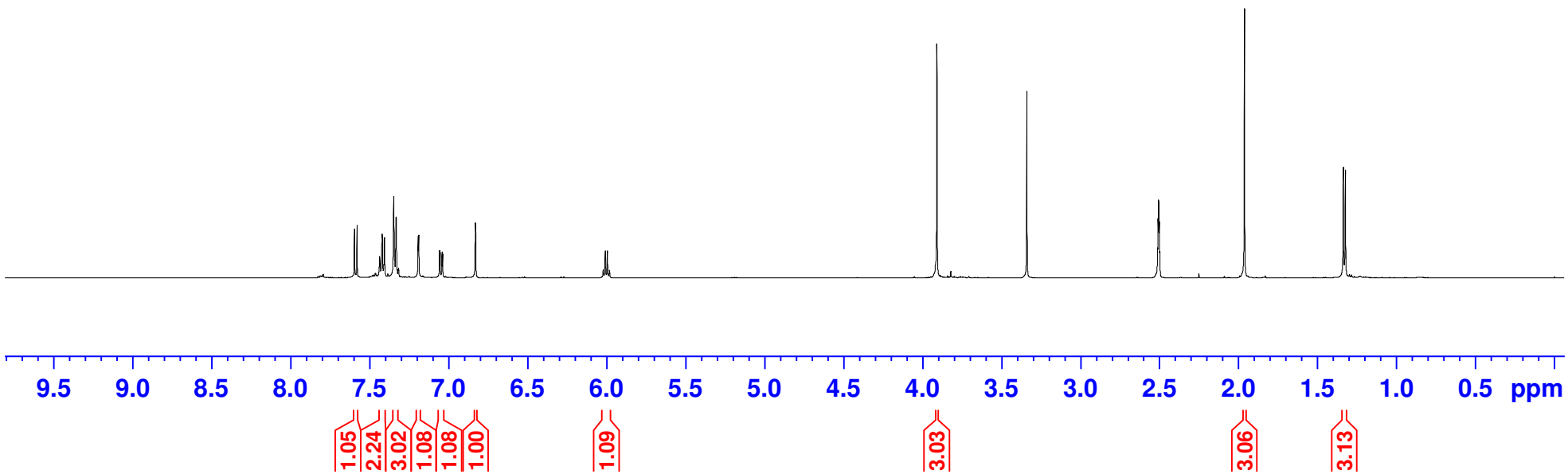

7.557
7.553
7.490
7.485
7.473
7.468
7.424
7.409
7.401
7.394
7.332
7.318
7.315
7.307
7.307
7.304
7.188
7.170
6.753
5.993
5.980
5.967
5.954
3.890
3.371
2.515
2.511
2.508
2.504
2.500
1.947
1.320
1.306
Me
AcO
H
Cl
MeO
17
Current Data Parameters
NAME Avijit Ascend 500
EXPNO 73
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211203
Time 11.08 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
2.09
3.07
1.02
1.00
1.05
3.00
3.00
3.05

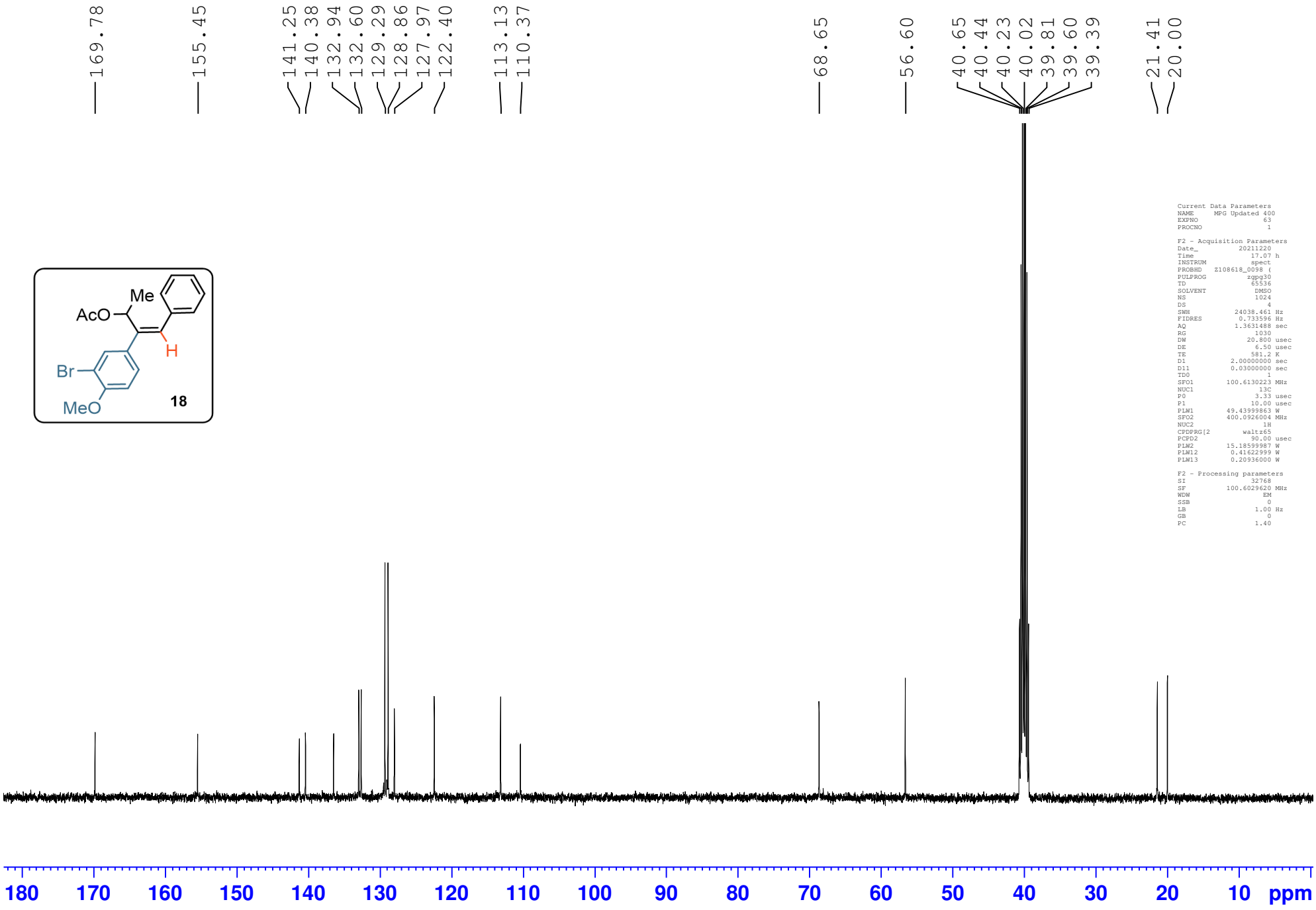

169.72
154.38
139.62
136.56
133.40
132.01
129.95
129.24
128.79
128.71
127.81
121.07
112.90
68.78
56.56
40.47
40.30
40.14
39.97
39.80
39.63
39.47
21.33
19.98
Me
AcO
H
Cl
MeO
17
Current Data Parameters
NAME Avijit Updated 500
EXPNO 198
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211204
Time 10.29 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 401
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 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

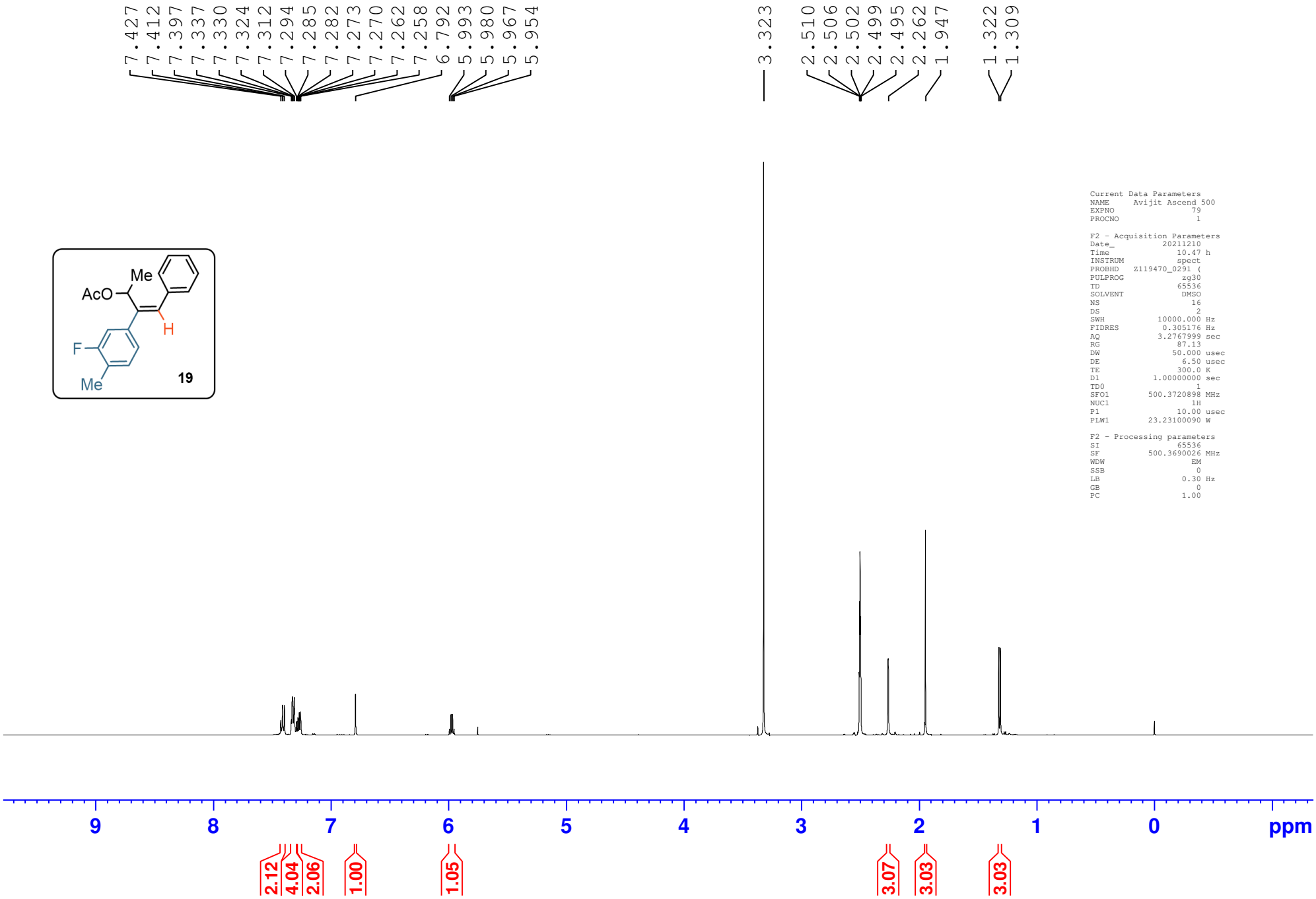


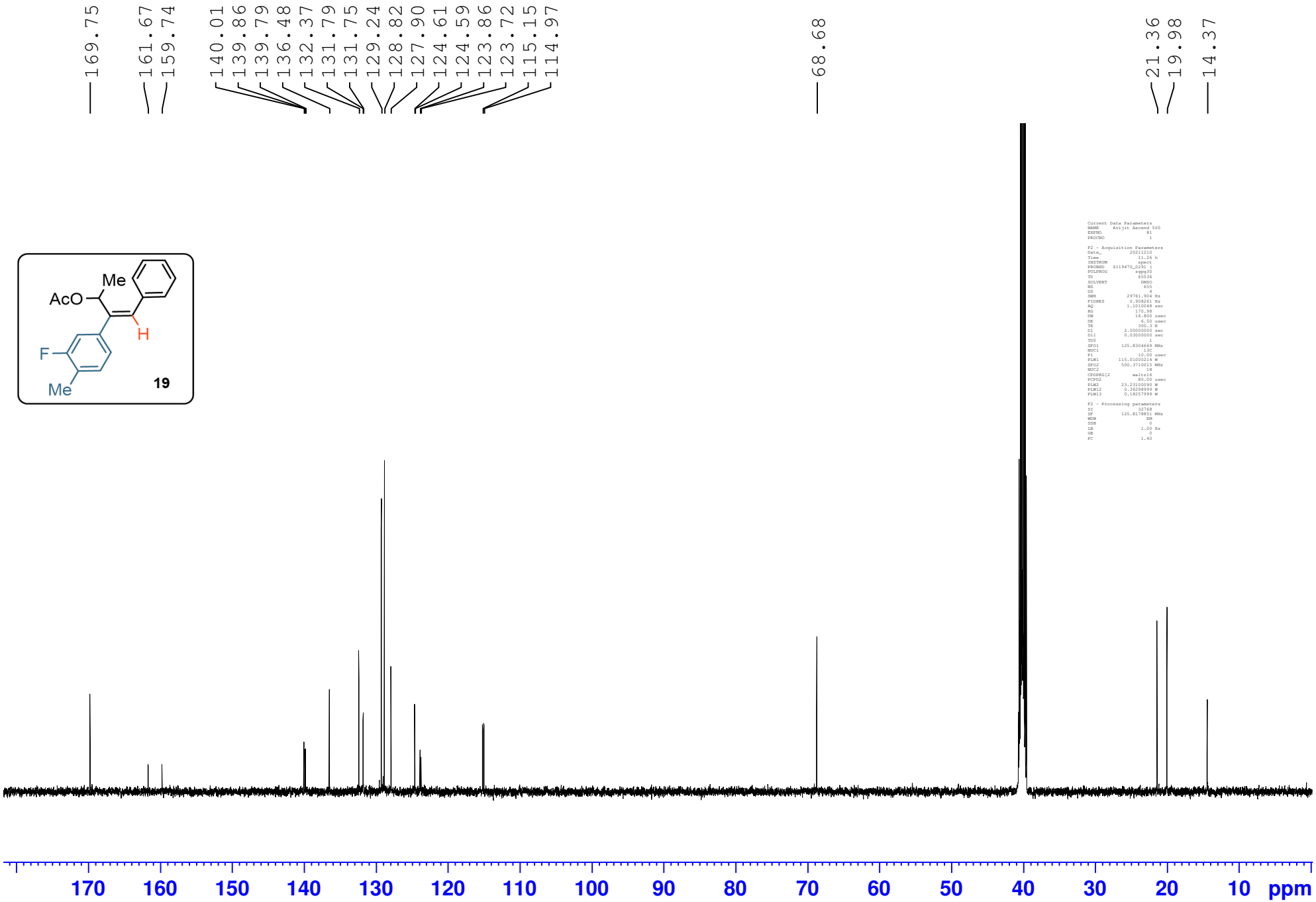


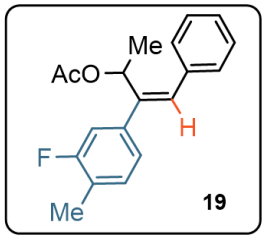

```
Current Data Parameters
NAME      MPG Ascend 500
EXPNO                73
PROCNO                1

F2 - Acquisition Parameters
Date_          20211220
Time              16.00 h
INSTRUM            spect
PROBHD   Z119470_0291 (
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                 48.7
DW               50.000 usec
DE                6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1
SFO1         500.3720898 MHz
NUC1                  1H
P1                10.00 usec
PLW1         23.23100090 W

F2 - Processing parameters
SI                 65536
SF           500.3690007 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




169.78
155.45
141.25
140.38
132.94
132.60
129.29
128.86
127.97
122.40
113.13
110.37
68.65
56.60
40.65
40.44
40.23
40.02
39.81
39.60
39.39
21.41
20.00
Me
AcO
H
Br
MeO
18
Current Data Parameters
NAME MPG Updated 400
EXPNO 63
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211220
Time 17.07 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 1030
DW 20.800 usec
DE 6.50 usec
TE 581.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

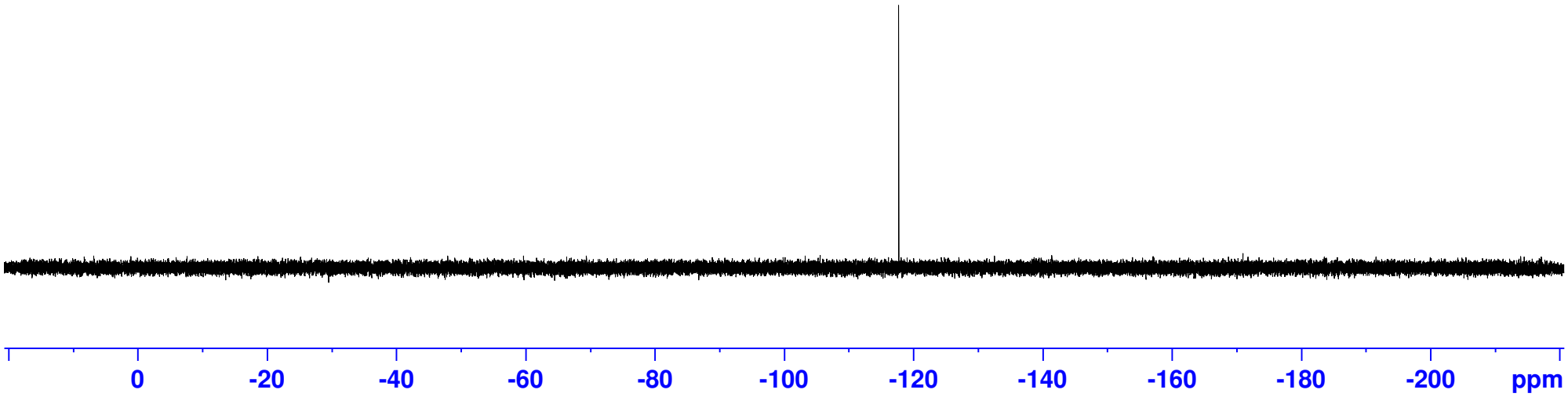

7.427
7.412
7.397
7.337
7.330
7.324
7.312
7.294
7.285
7.282
7.273
7.270
7.262
7.258
6.792
5.993
5.980
5.967
5.954
3.323
2.510
2.506
2.502
2.499
2.495
2.262
1.947
1.322
1.309
Me
AcO
H
F
Me
19
Current Data Parameters
NAME Avijit Ascend 500
EXPNO 79
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 10.47 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 87.13
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.12
4.04
2.06
1.00
1.05
3.07
3.03
3.03

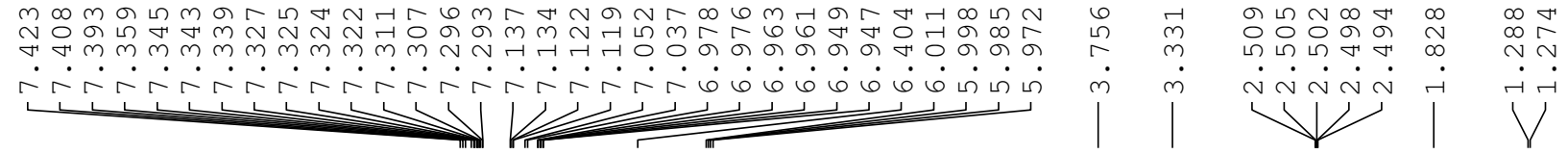

169.75
161.67
159.74
140.01
139.86
139.79
136.48
132.37
131.79
131.75
129.24
128.82
127.90
124.61
124.59
123.86
123.72
115.15
114.97
68.68
21.36
19.98
14.37
AcO
Me
H
F
Me
19
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

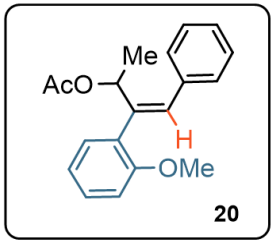


−117.72

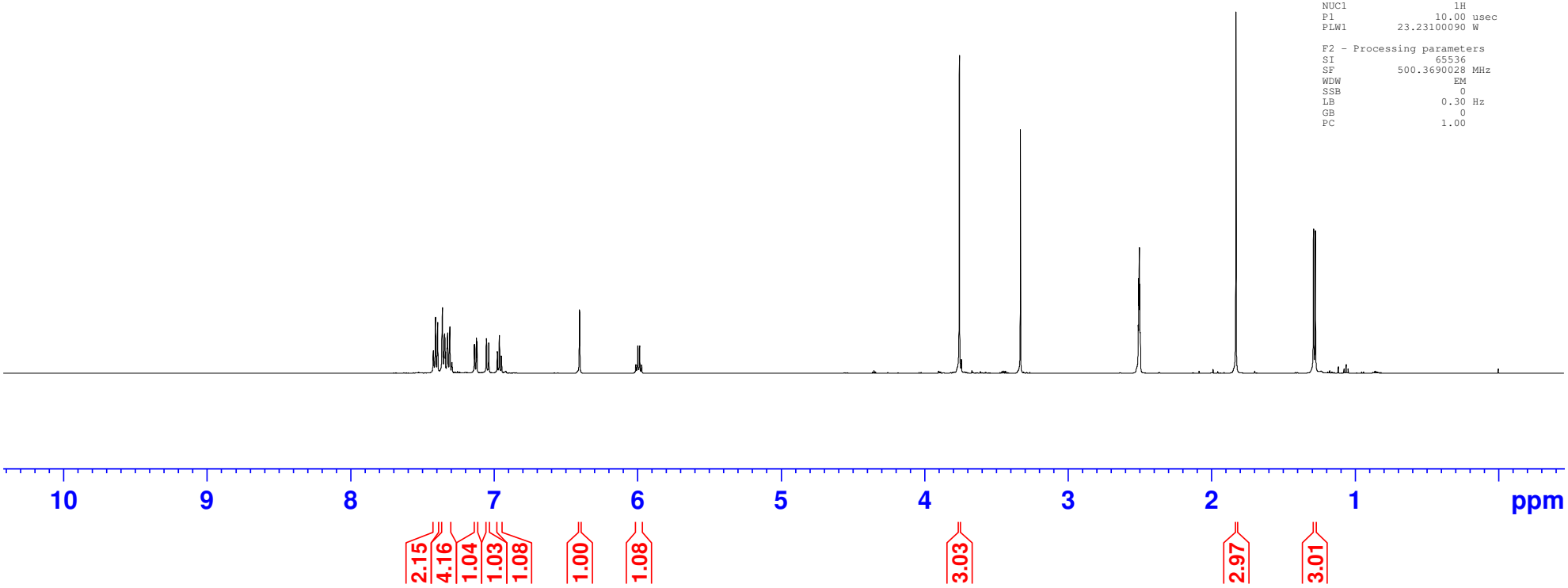
```
Current Data Parameters
NAME      Avijit Ascend 500
EXPNO                   80
PROCNO                   1

F2 - Acquisition Parameters
Date_            20211210
Time                10.49 h
INSTRUM              spect
PROBHD    Z119470_0291 (
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT               DMSO
NS                      16
DS                       4
SWH             113636.367 Hz
FIDRES            1.733953 Hz
AQ                0.5767168 sec
RG                     6.62
DW                 4.400 usec
DE                 6.50 usec
TE                   300.1 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                      1
SFO1           470.7701802 MHz
NUC1                   19F
P1                  15.00 usec
PLW1           45.84600067 W
SFO2           500.3710015 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           23.23100090 W
PLW12           0.36298999 W

F2 - Processing parameters
SI                   65536
SF             470.8172619 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

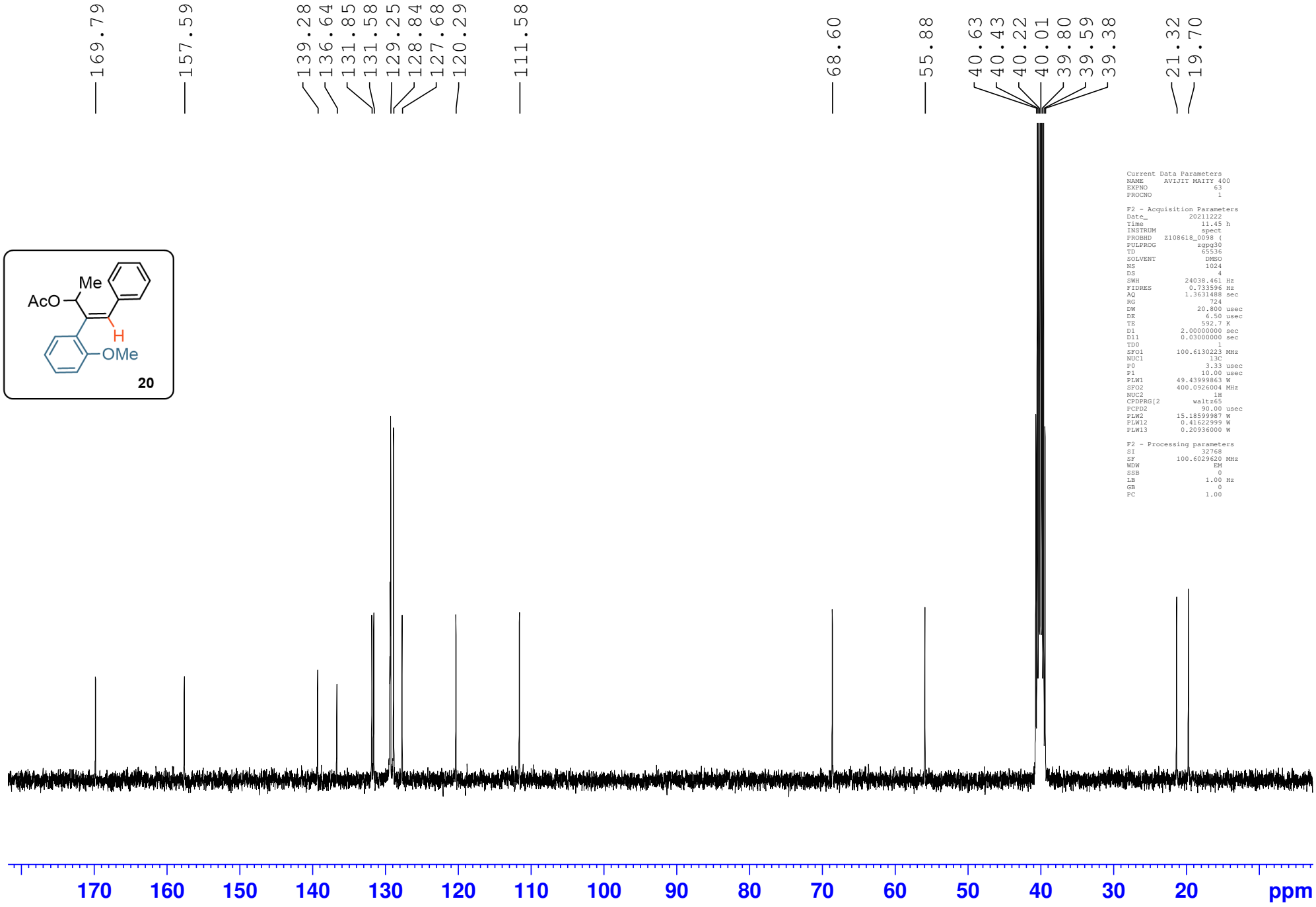


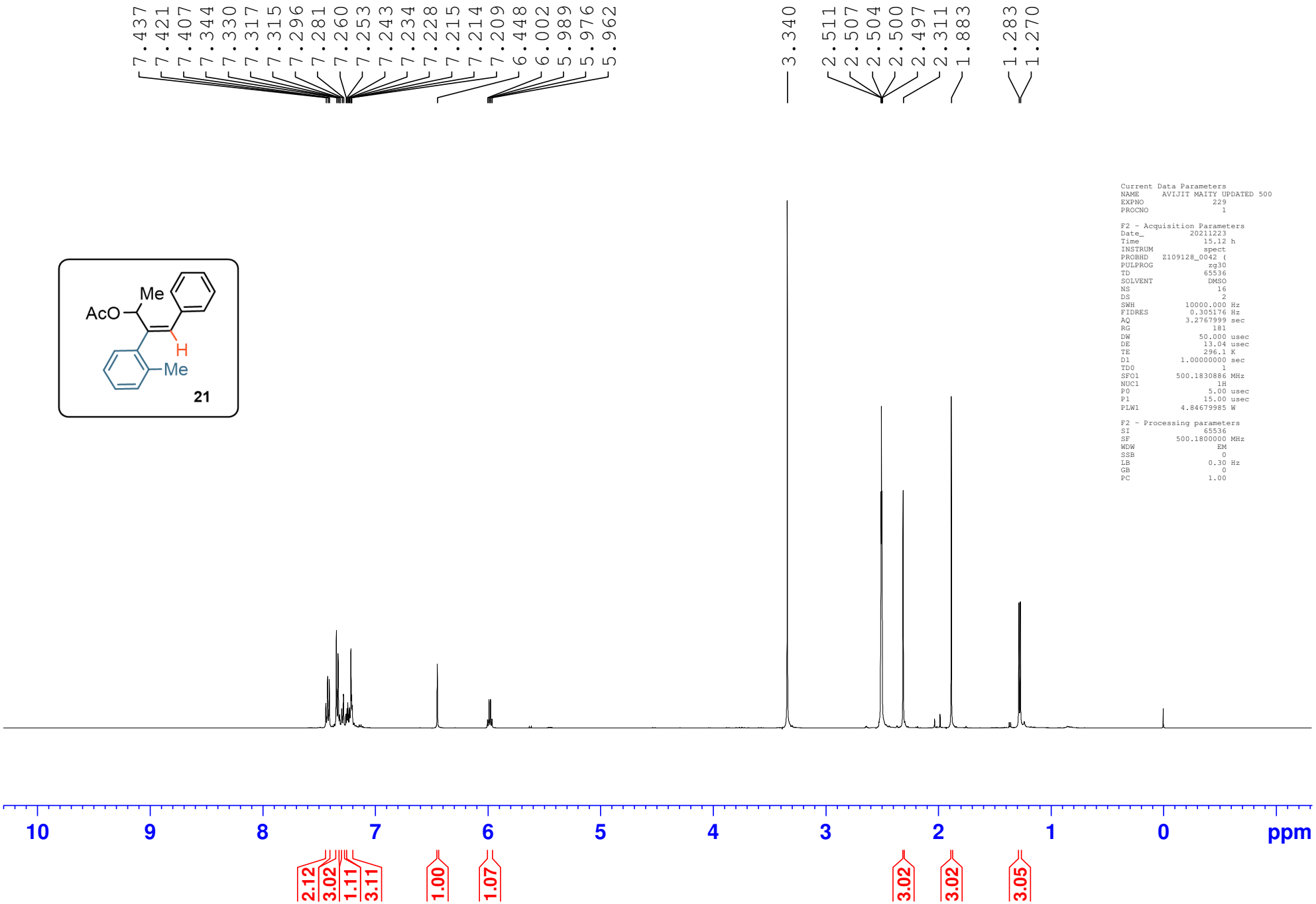


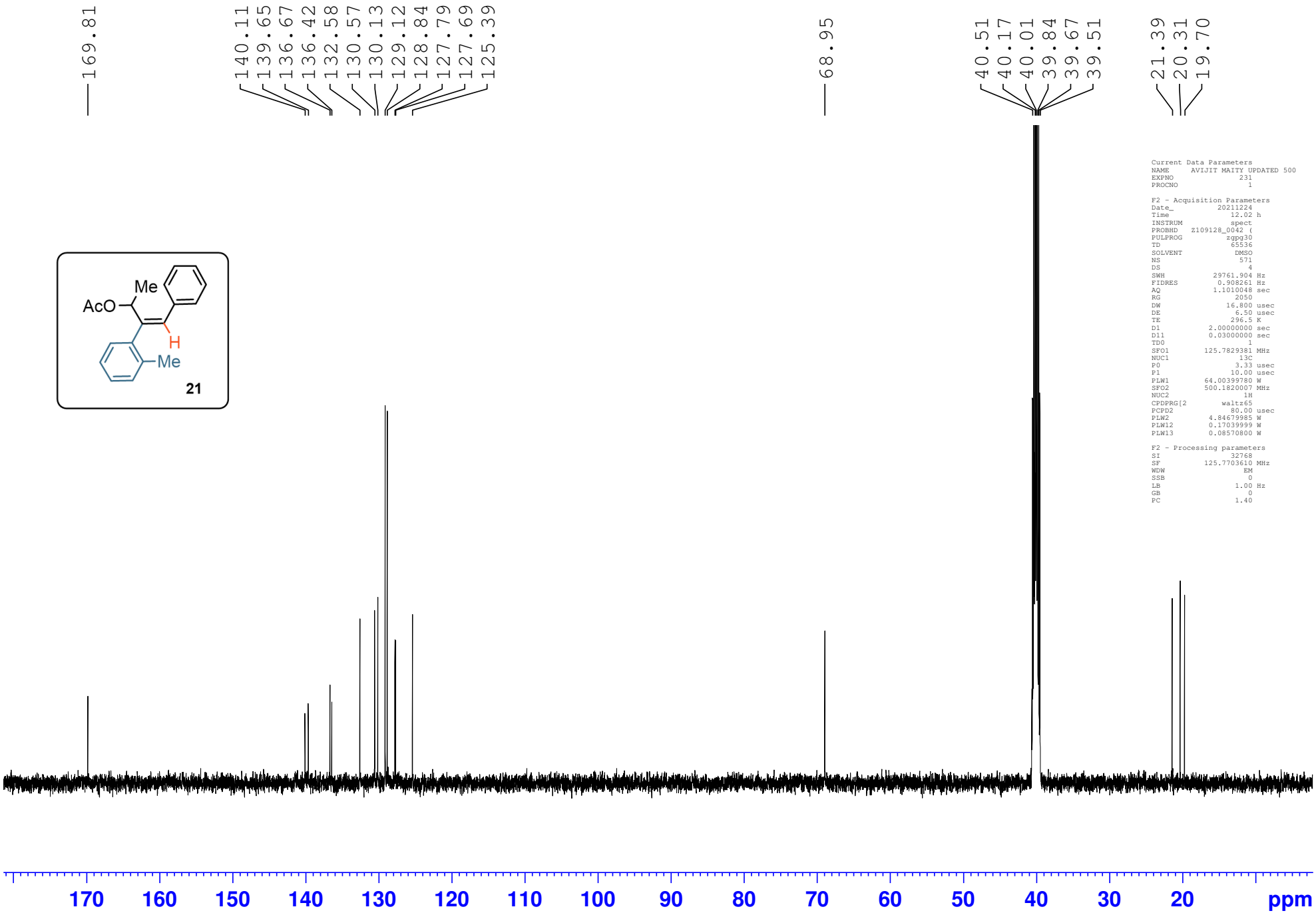


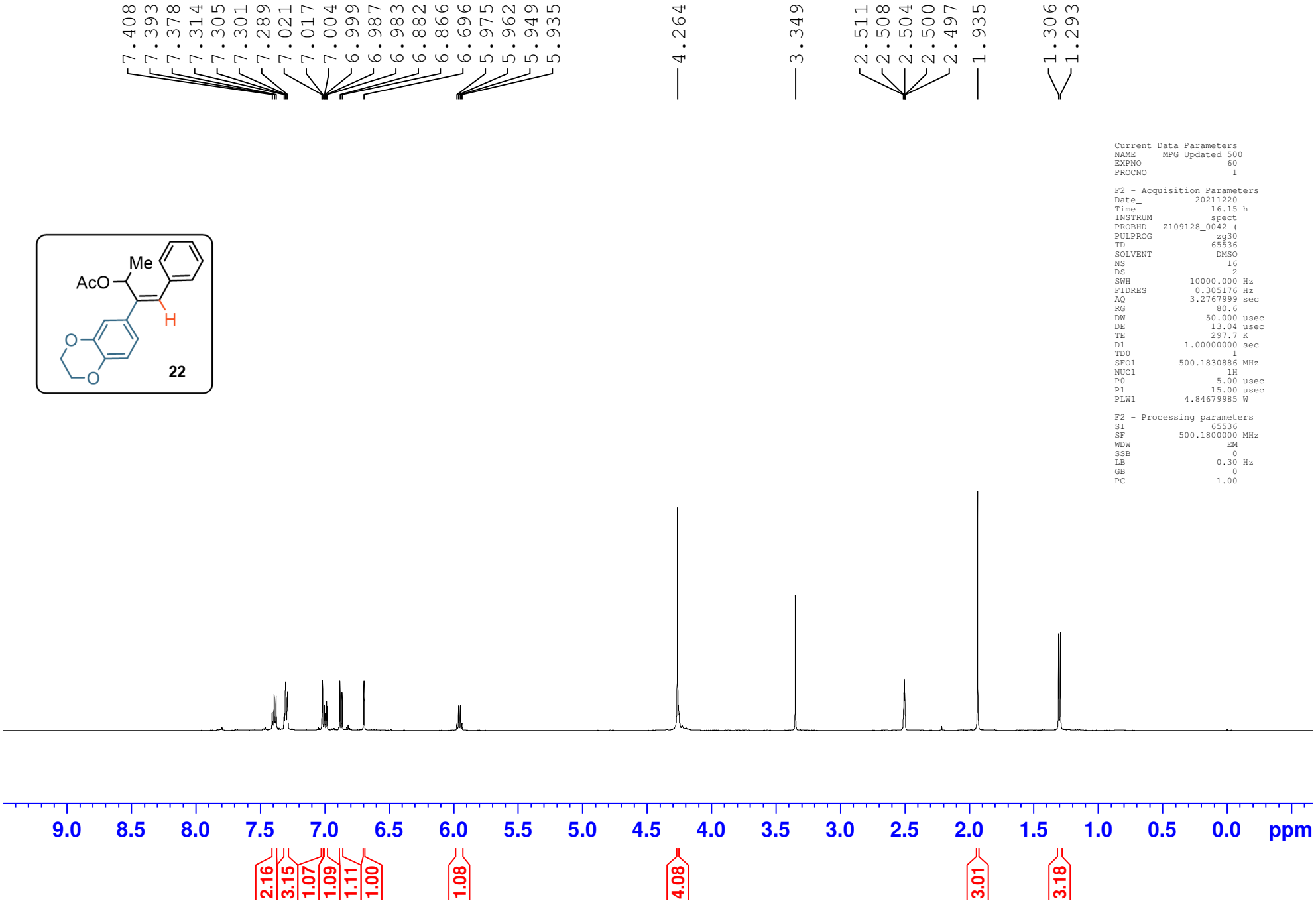

```
Current Data Parameters
NAME      AVIJIT MAITY ASCEND 500
EXPNO                 85
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211221
Time              15.04 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                 62.04
DW                50.000 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1
SFO1        500.3720898 MHz
NUC1                  1H
P1                10.00 usec
PLW1        23.23100090 W

F2 - Processing parameters
SI                 65536
SF          500.3690028 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

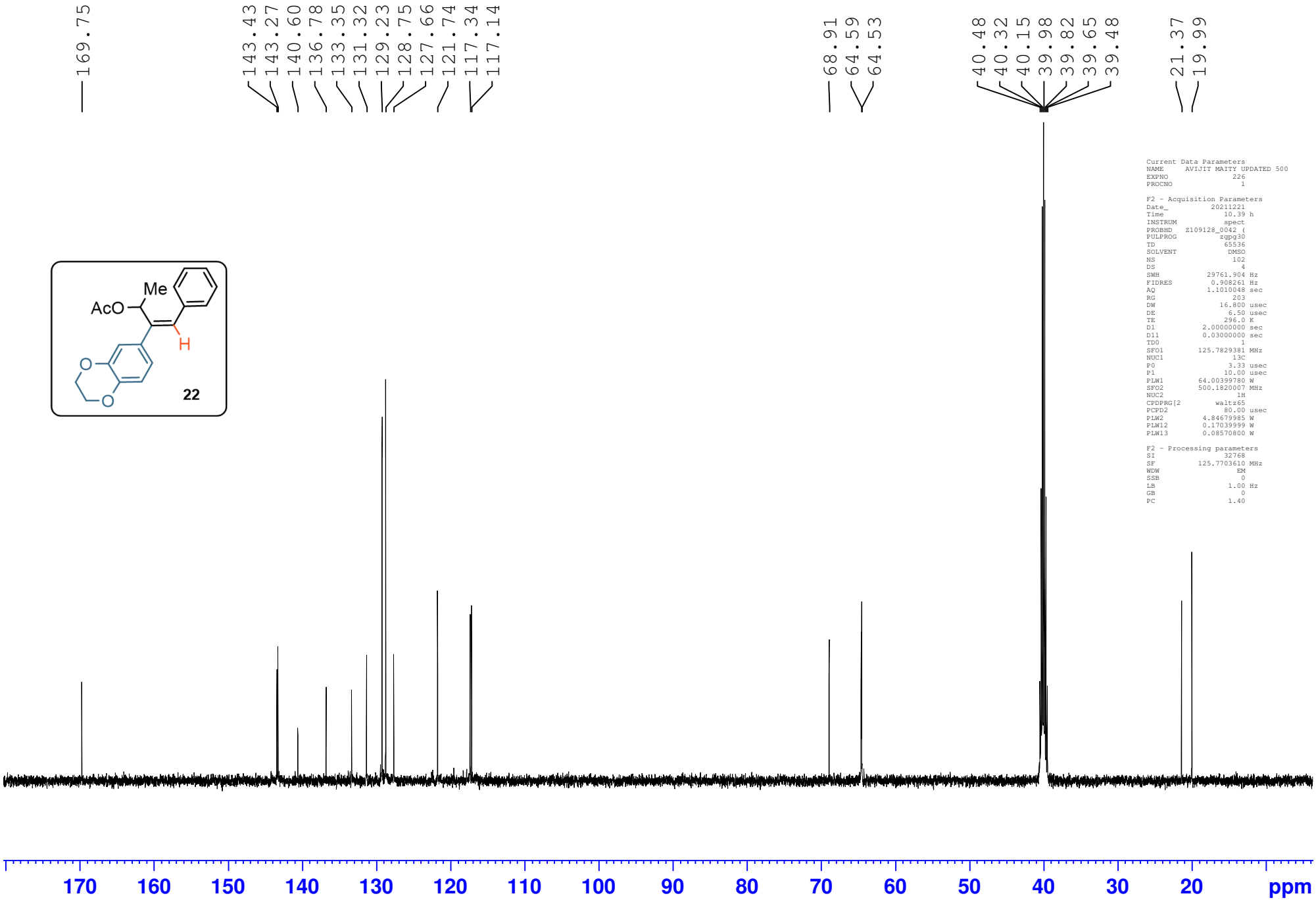


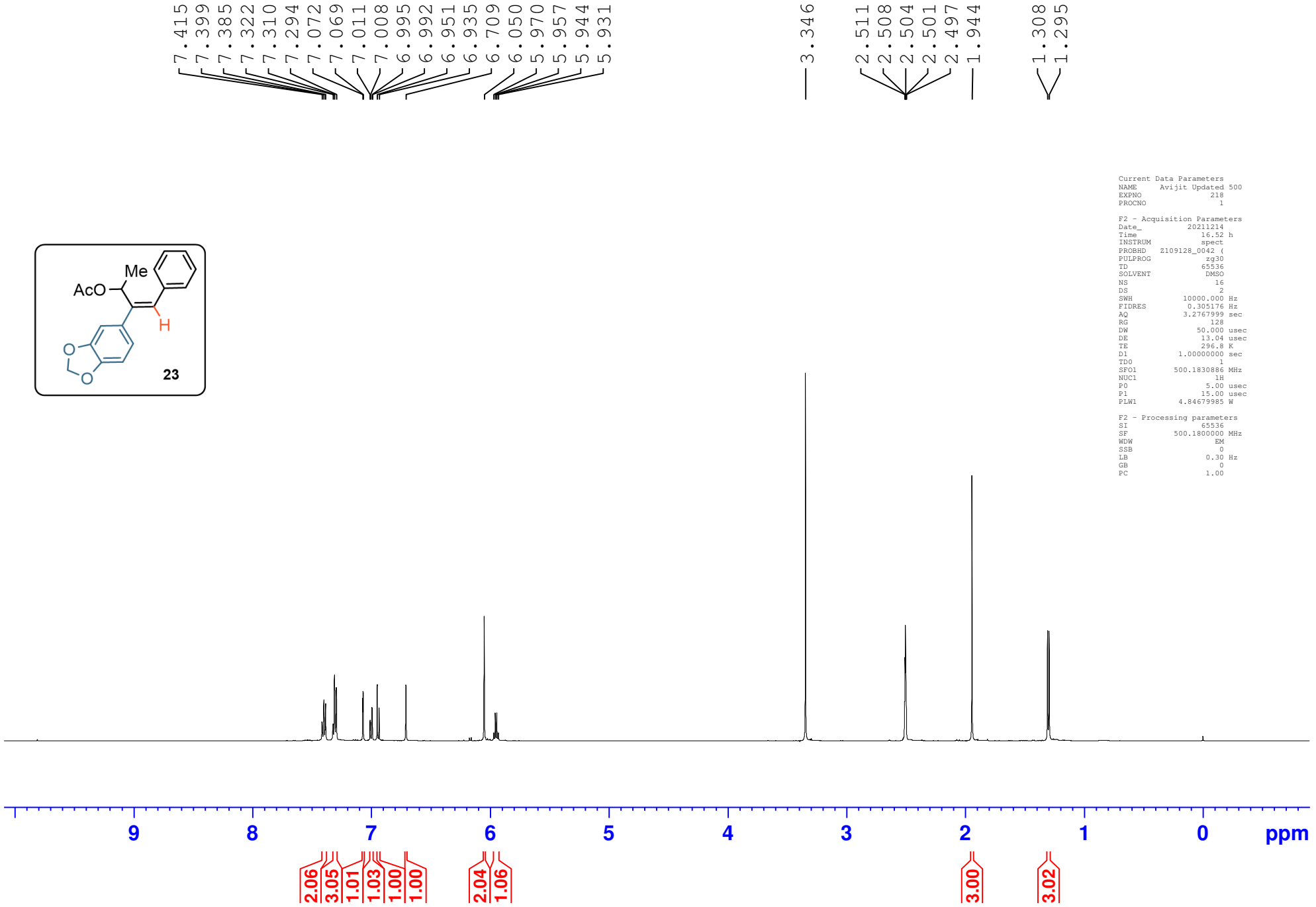

169.79
157.59
139.28
136.64
131.85
131.58
129.25
128.84
127.68
120.29
111.58
68.60
55.88
40.63
40.43
40.22
40.01
39.80
39.59
39.38
21.32
19.70
Me
AcO
H
OMe
20
Current Data Parameters
NAME AVIJIT MAITY 400
EXPNO 63
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 11.45 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 592.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

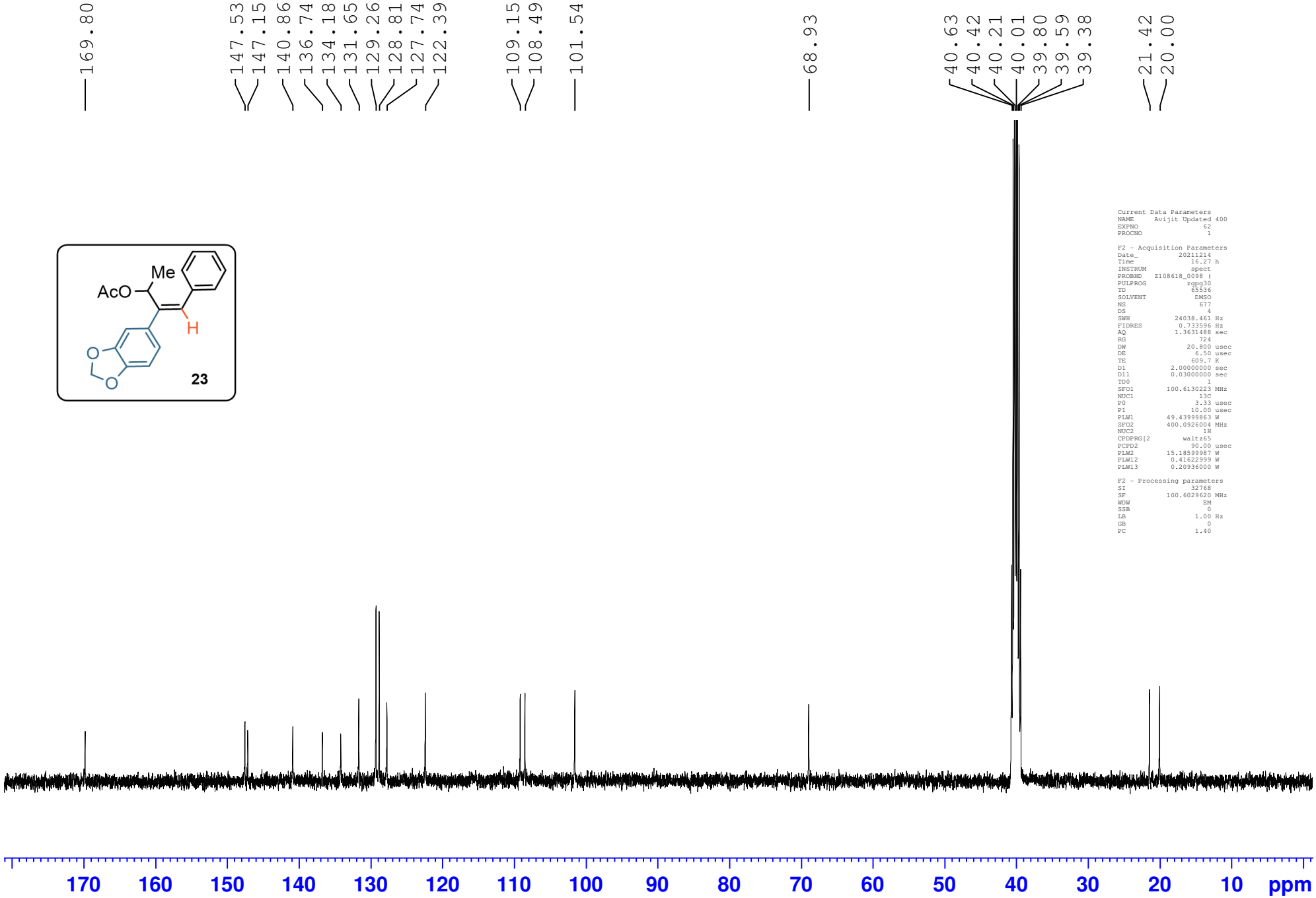

7.437
7.421
7.407
7.344
7.330
7.317
7.315
7.296
7.281
7.260
7.253
7.243
7.234
7.228
7.215
7.214
7.209
6.448
6.002
5.989
5.976
5.962
3.340
2.511
2.507
2.504
2.500
2.497
2.311
1.883
1.283
1.270
AcO
Me
H
Me
21
Current Data Parameters
NAME AVIJIT MAITY UPDATED 500
EXPNO 229
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211223
Time 15.12 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 13.04 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
3.02
1.11
3.11
1.00
1.07
3.02
3.02
3.05

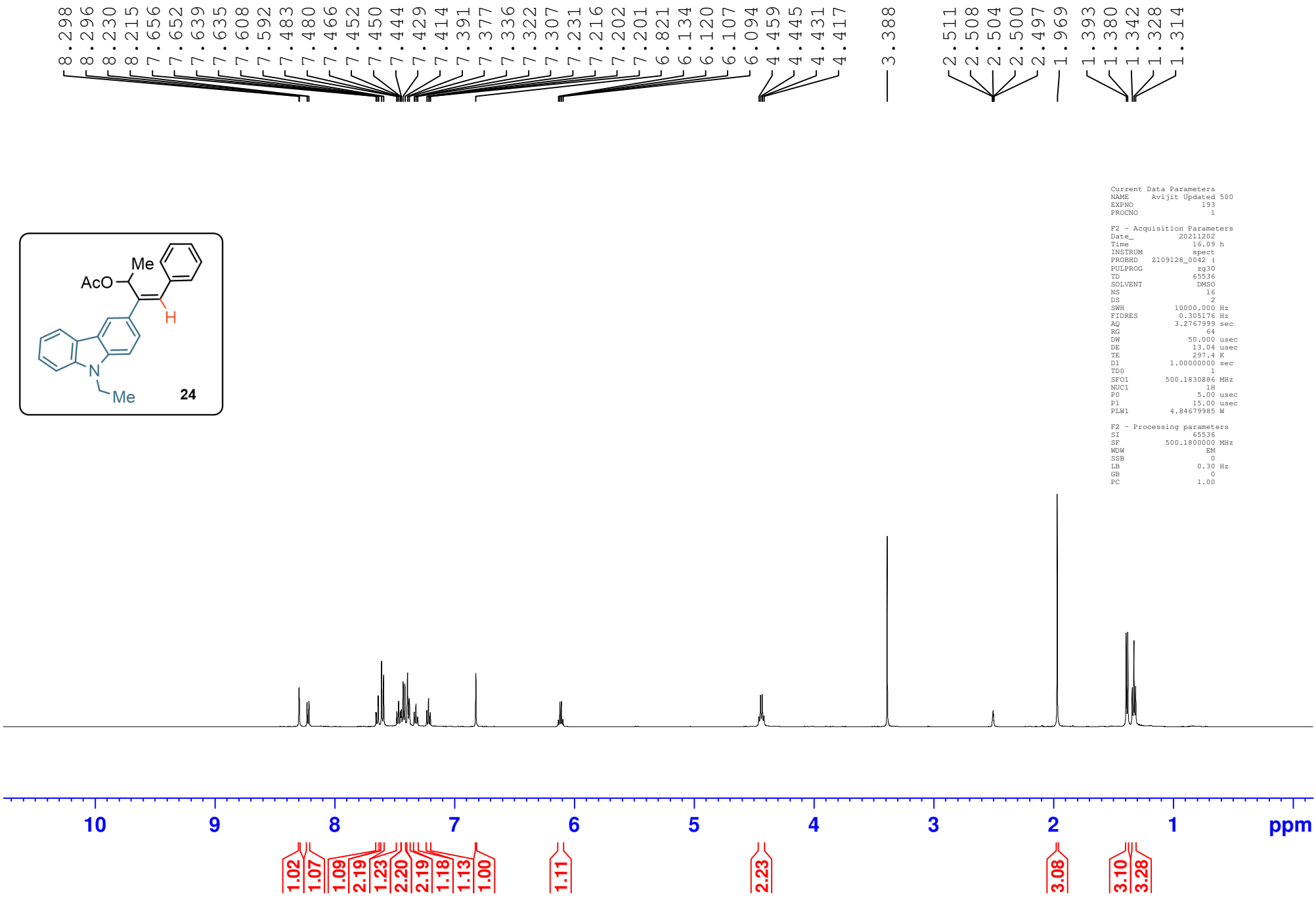

169.81
140.11
139.65
136.67
136.42
132.58
130.57
130.13
129.12
128.84
127.79
127.69
125.39
68.95
40.51
40.17
40.01
39.84
39.67
39.51
21.39
20.31
19.70
AcO
Me
H
Me
21
Current Data Parameters
NAME AVIJIT MAITY UPDATED 500
EXPNO 231
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211224
Time 12.02 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 571
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

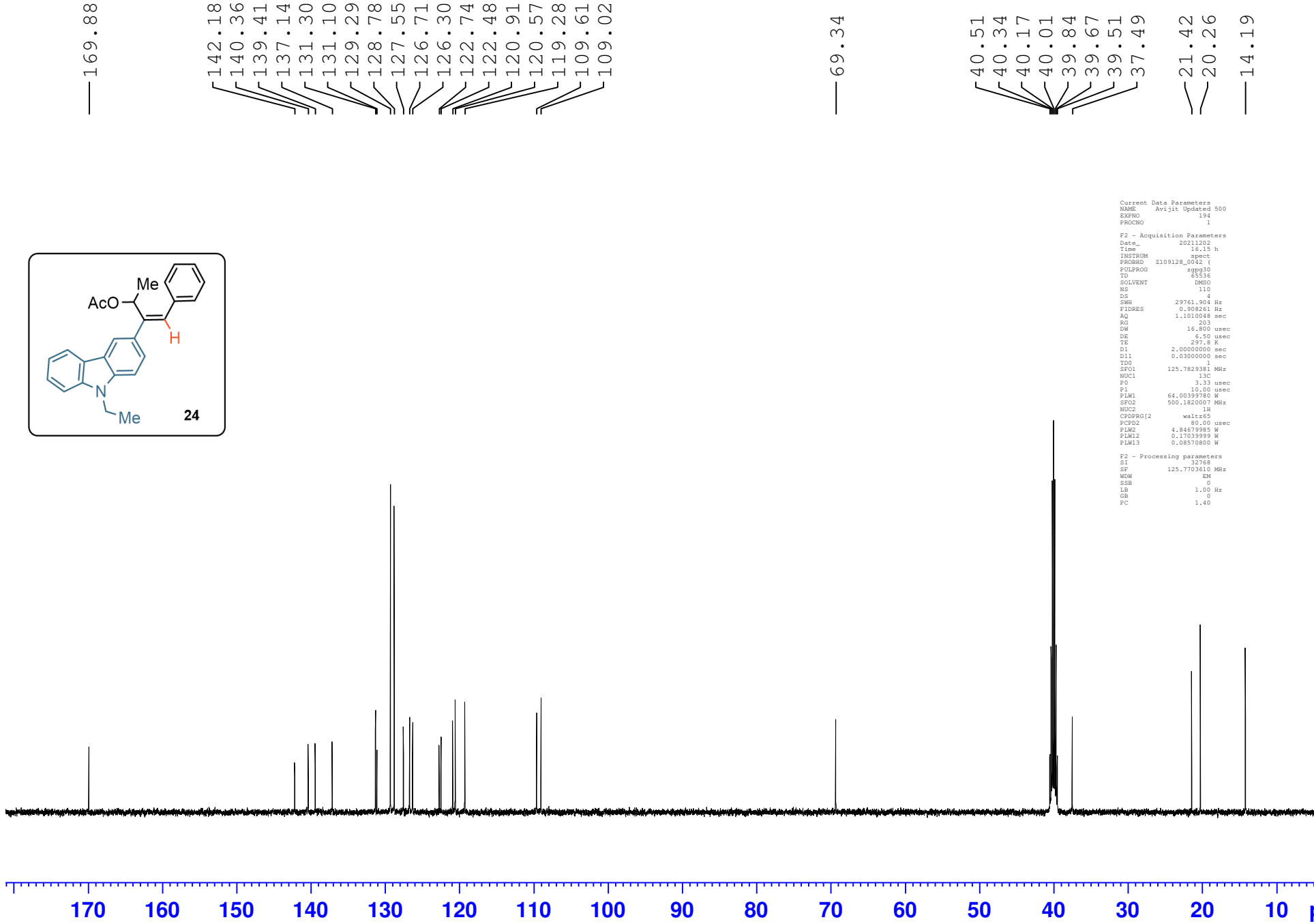

7.408
7.393
7.378
7.314
7.305
7.301
7.289
7.021
7.017
7.004
6.999
6.987
6.983
6.882
6.866
6.696
5.975
5.962
5.949
5.935
4.264
3.349
2.511
2.508
2.504
2.500
2.497
1.935
1.306
1.293
Me
AcO
H
O
O
O
22
Current Data Parameters
NAME MPG Updated 500
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211220
Time 16.15 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 13.04 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.16
3.15
1.07
1.09
1.11
1.00
1.08
4.08
3.01
3.18

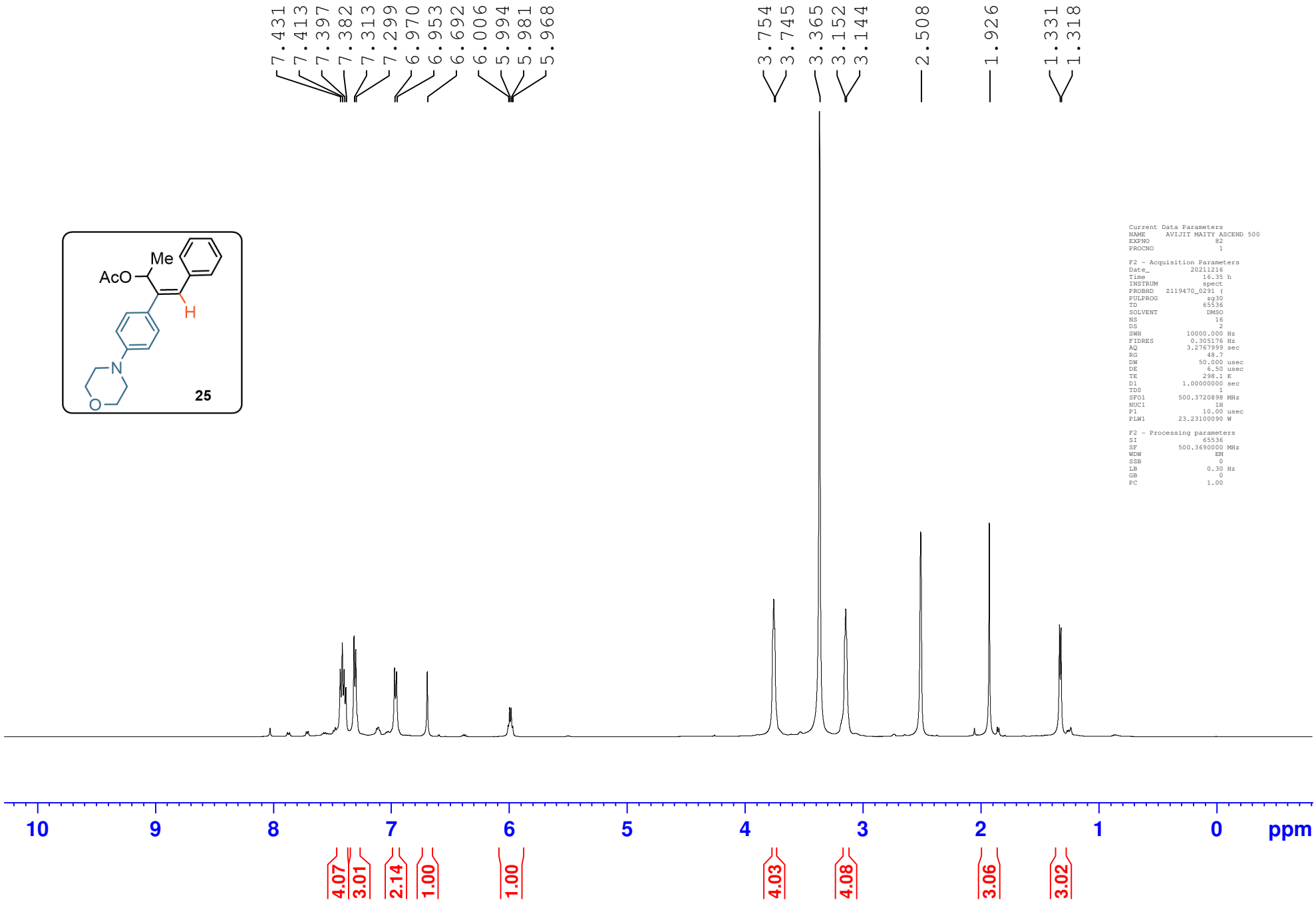

169.75
143.43
143.27
140.60
136.78
133.35
131.32
129.23
128.75
127.66
121.74
117.34
117.14
68.91
64.59
64.53
40.48
40.32
40.15
39.98
39.82
39.65
39.48
21.37
19.99
Me
AcO
H
O
O
O
22
Current Data Parameters
NAME AVIJIT MAITY UPDATED 500
EXPNO 226
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211221
Time 10.39 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 102
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 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

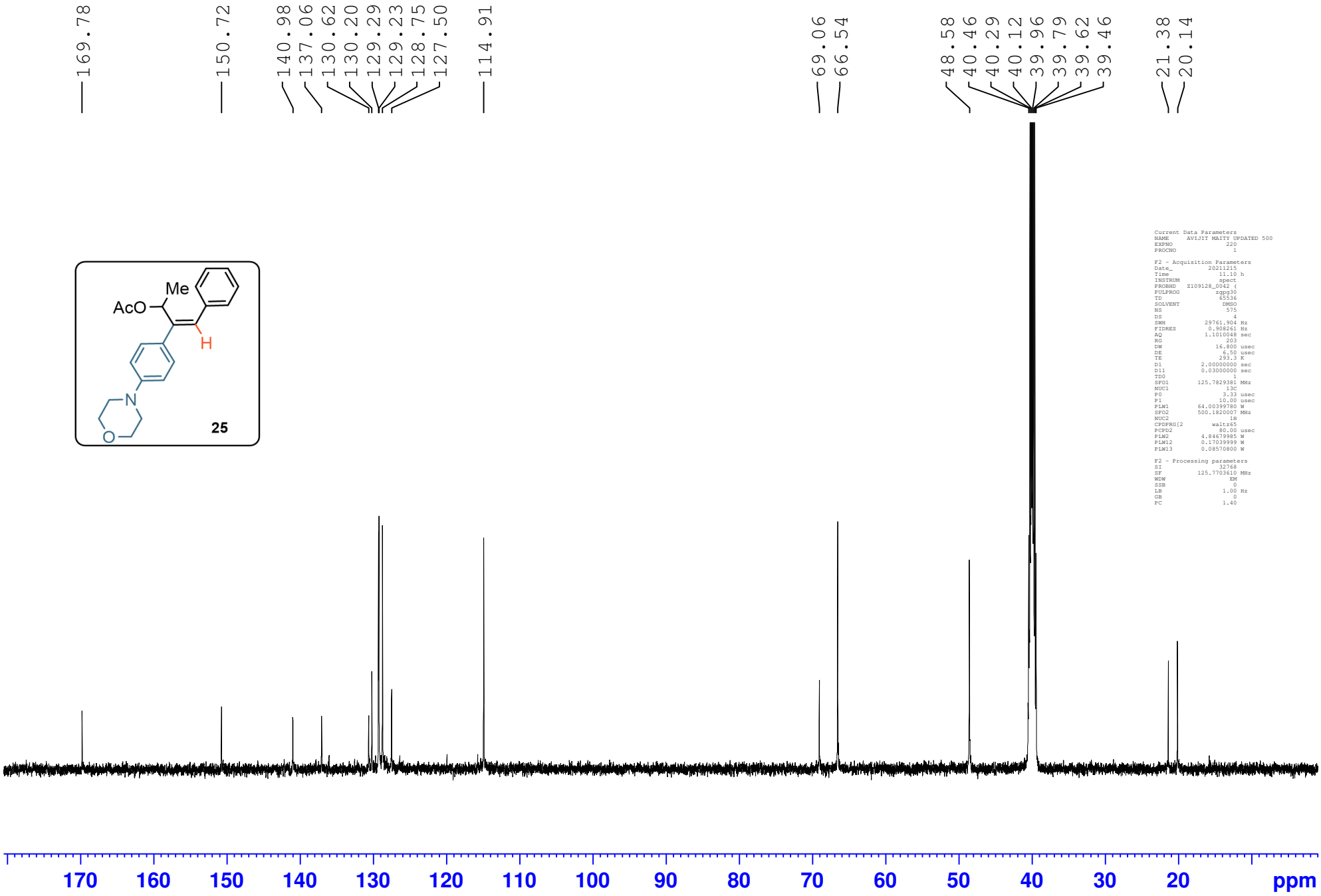

7.415
7.399
7.385
7.322
7.310
7.294
7.072
7.069
7.011
7.008
6.995
6.992
6.951
6.935
6.709
6.050
5.970
5.957
5.944
5.931
3.346
2.511
2.508
2.504
2.501
2.497
1.944
1.308
1.295
Me
AcO
H
O
O
O
23
Current Data Parameters
NAME Avijit Updated 500
EXPNO 218
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211214
Time 16.52 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 13.04 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.06
3.05
1.01
1.03
1.00
1.00
2.04
1.06
3.00
3.02

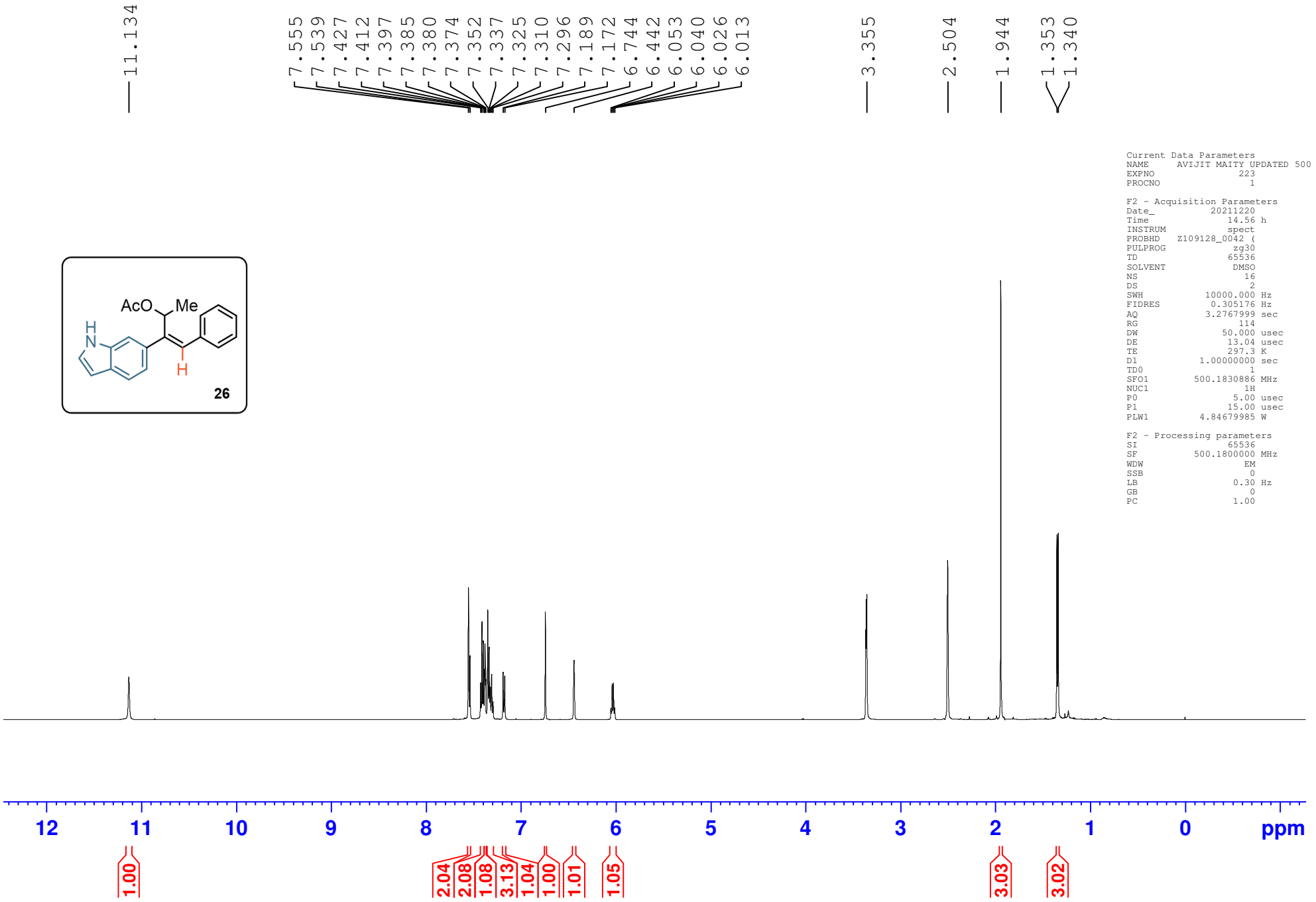

169.80
147.53
147.15
140.86
136.74
134.18
131.65
129.26
128.81
127.74
122.39
109.15
108.49
101.54
68.93
40.63
40.42
40.21
40.01
39.80
39.59
39.38
21.42
20.00
Me
AcO
H
23
Current Data Parameters
NAME Avijit Updated 400
EXPNO 62
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211214
Time 16.27 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 677
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 609.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

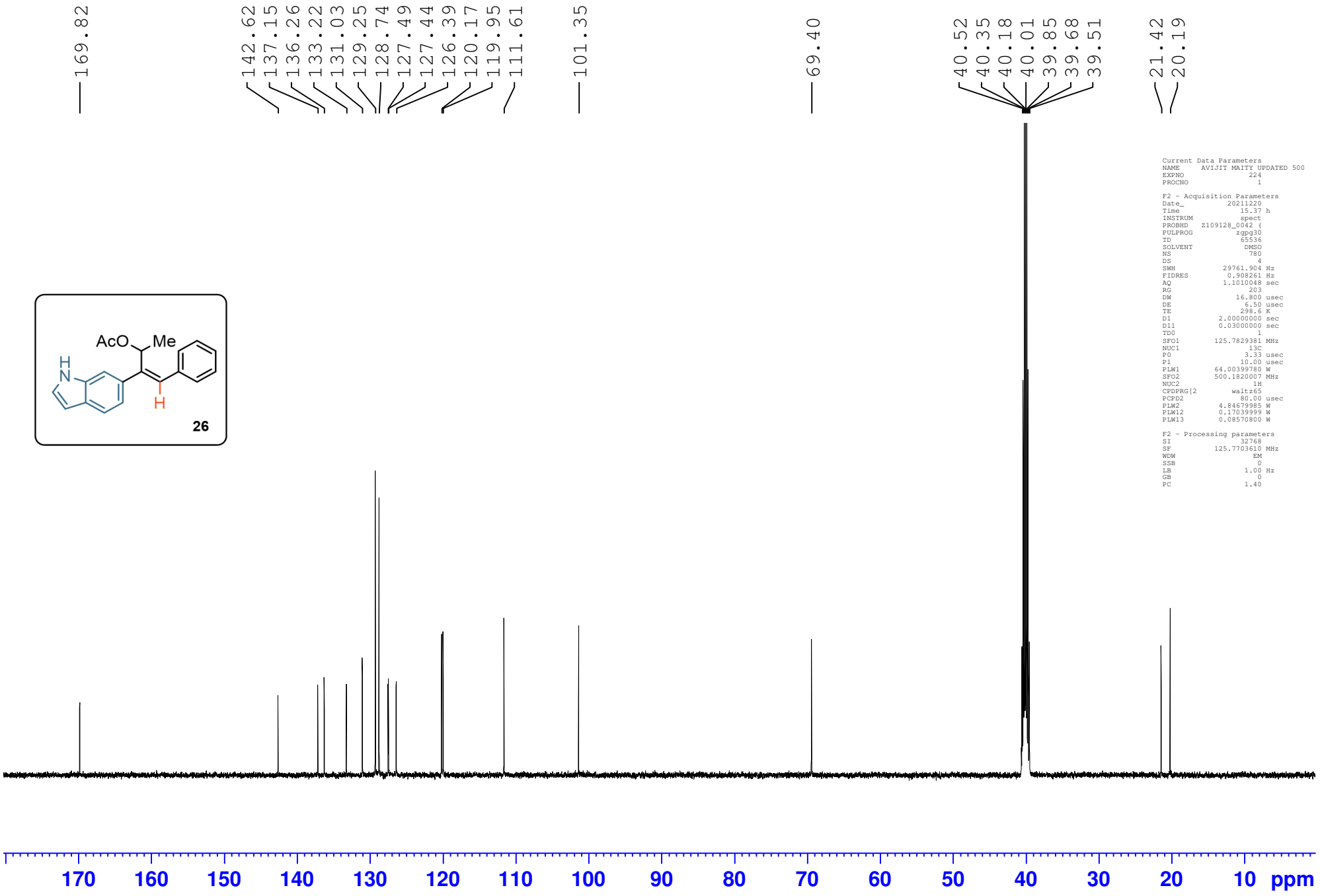

8.298
8.296
8.230
8.215
7.656
7.652
7.639
7.635
7.608
7.592
7.483
7.480
7.466
7.452
7.450
7.444
7.429
7.414
7.391
7.377
7.336
7.322
7.307
7.231
7.216
7.202
7.201
6.821
6.134
6.120
6.107
6.094
4.459
4.445
4.431
4.417
3.388
2.511
2.508
2.504
2.500
2.497
1.969
1.393
1.380
1.342
1.328
1.314
Me
AcO
H
N
Me
24
Current Data Parameters
NAME Avijit Updated 500
EXPNO 193
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 16.09 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 64
DW 50.000 usec
DE 13.04 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.07
1.09
2.19
1.23
2.20
2.19
1.18
1.13
1.00
1.11
2.23
3.08
3.10
3.28

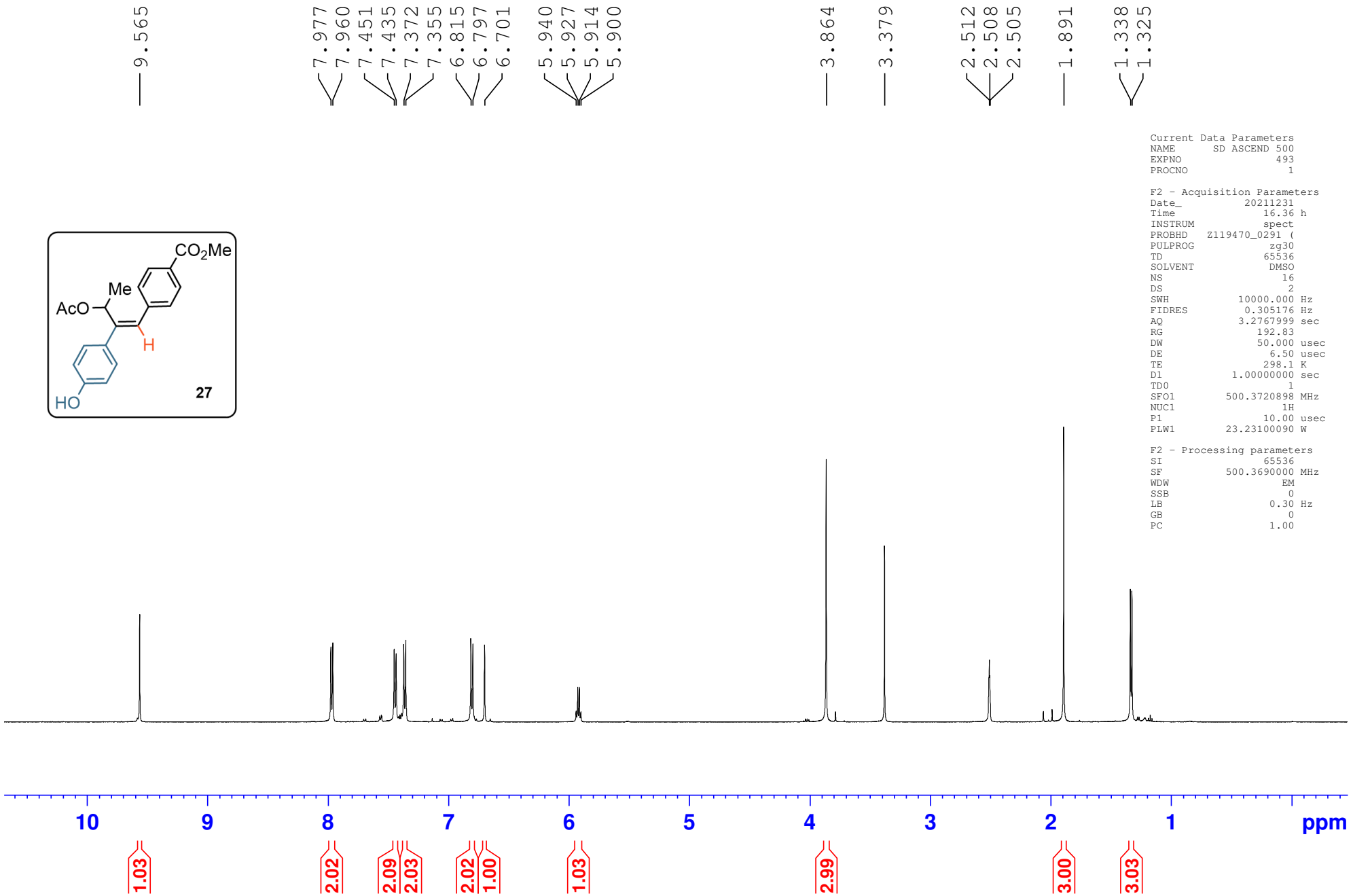

169.88
142.18
140.36
139.41
137.14
131.30
131.10
129.29
128.78
127.55
126.71
126.30
122.74
122.48
120.91
120.57
119.28
109.61
109.02
69.34
40.51
40.34
40.17
40.01
39.84
39.67
39.51
37.49
21.42
20.26
14.19
Me
AcO
H
N
Me
24
Current Data Parameters
NAME Avijit Updated 500
EXPNO 194
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 16.15 h
INSTRUM spect
PROBHD 2109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 110
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 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

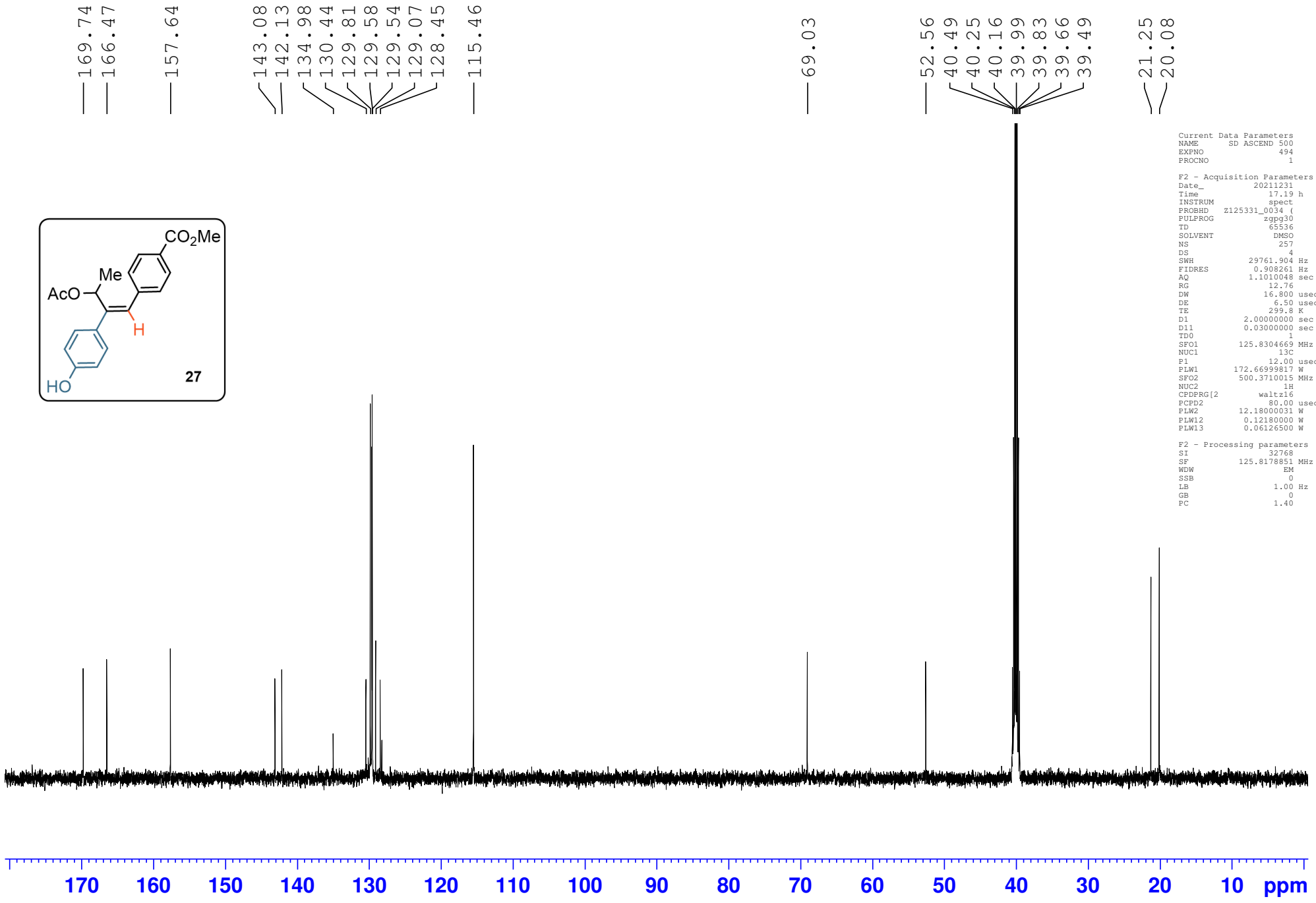

7.431
7.413
7.397
7.382
7.313
7.299
6.970
6.953
6.692
6.006
5.994
5.981
5.968
3.754
3.745
3.365
3.152
3.144
2.508
1.926
1.331
1.318
Me
AcO
H
N
O
25
Current Data Parameters
NAME AVIJIT MAITY ASCEND 500
EXPNO 82
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211216
Time 16.35 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 48.7
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
4.07
3.01
2.14
1.00
1.00
4.03
4.08
3.06
3.02

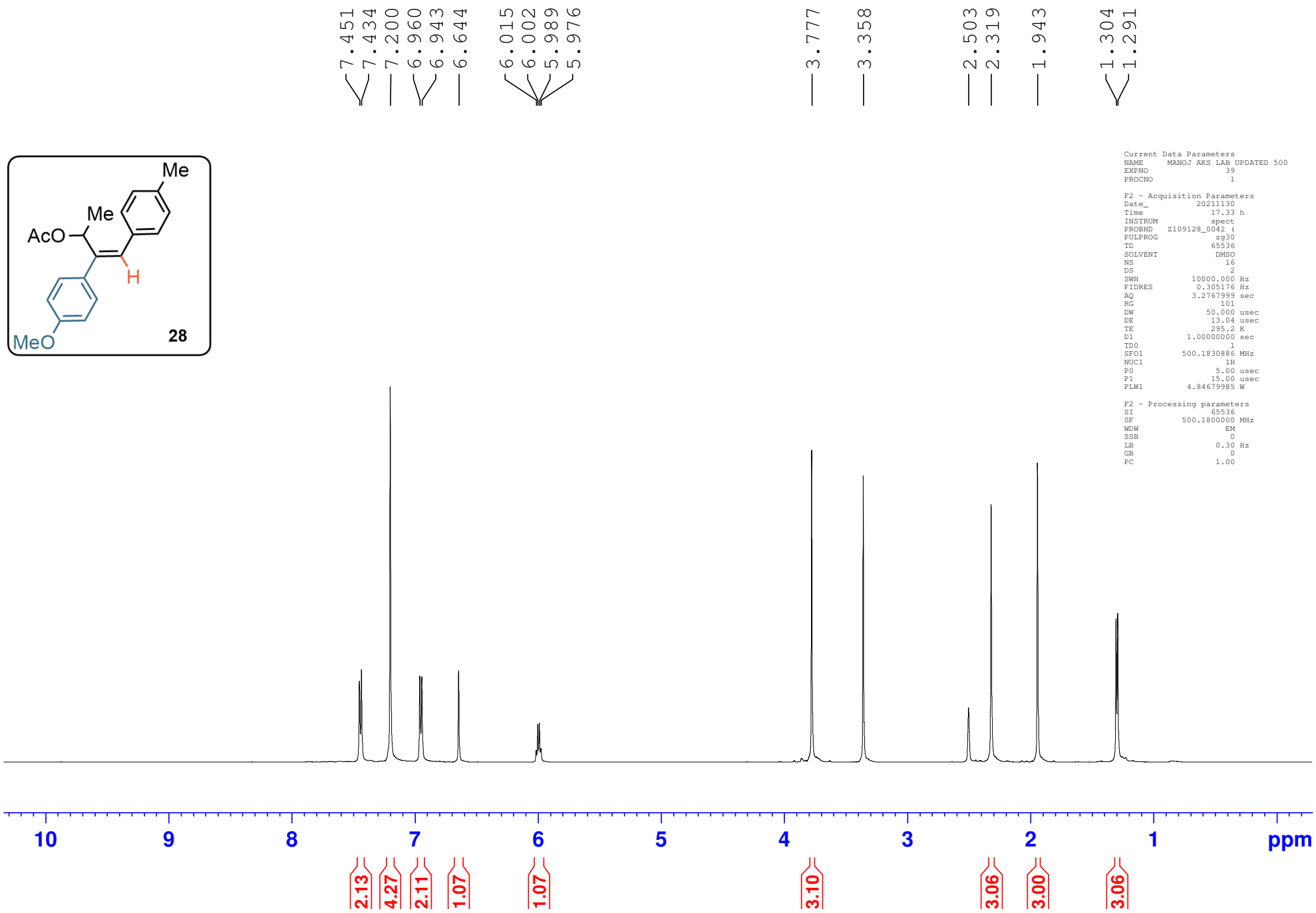

169.78
150.72
140.98
137.06
130.62
130.20
129.29
129.23
128.75
127.50
114.91
69.06
66.54
48.58
40.46
40.29
40.12
39.96
39.79
39.62
39.46
21.38
20.14
Me
AcO
H
N
O
25
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

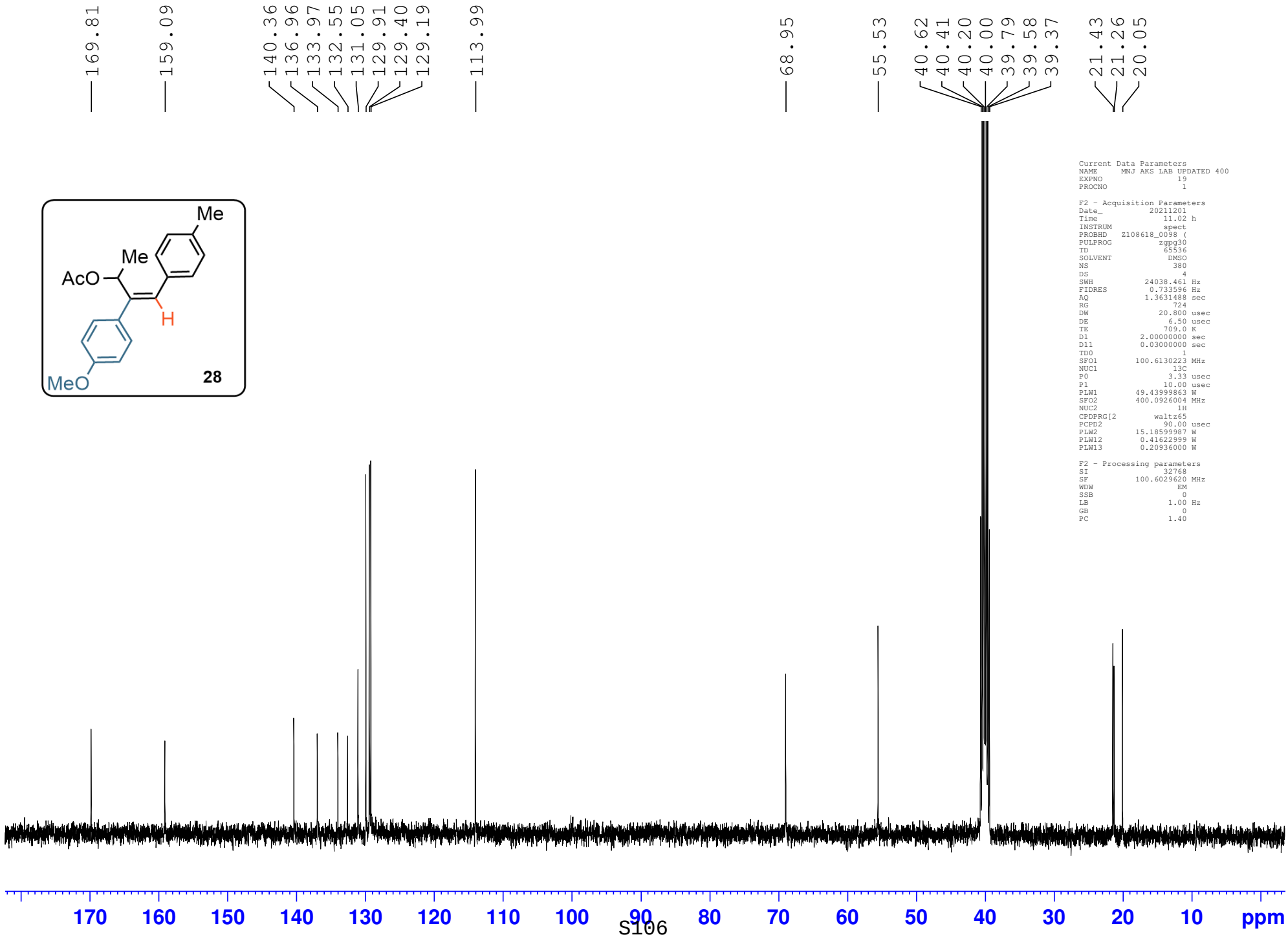

11.134
7.555
7.539
7.427
7.412
7.397
7.385
7.380
7.374
7.352
7.337
7.325
7.310
7.296
7.189
7.172
6.744
6.442
6.053
6.040
6.026
6.013
3.355
2.504
1.944
1.353
1.340
AcO
Me
H
N
H
26
Current Data Parameters
NAME AVIJIT MAITY UPDATED 500
EXPNO 223
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211220
Time 14.56 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 114
DW 50.000 usec
DE 13.04 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.04
2.08
1.08
3.13
1.04
1.00
1.01
1.05
3.03
3.02

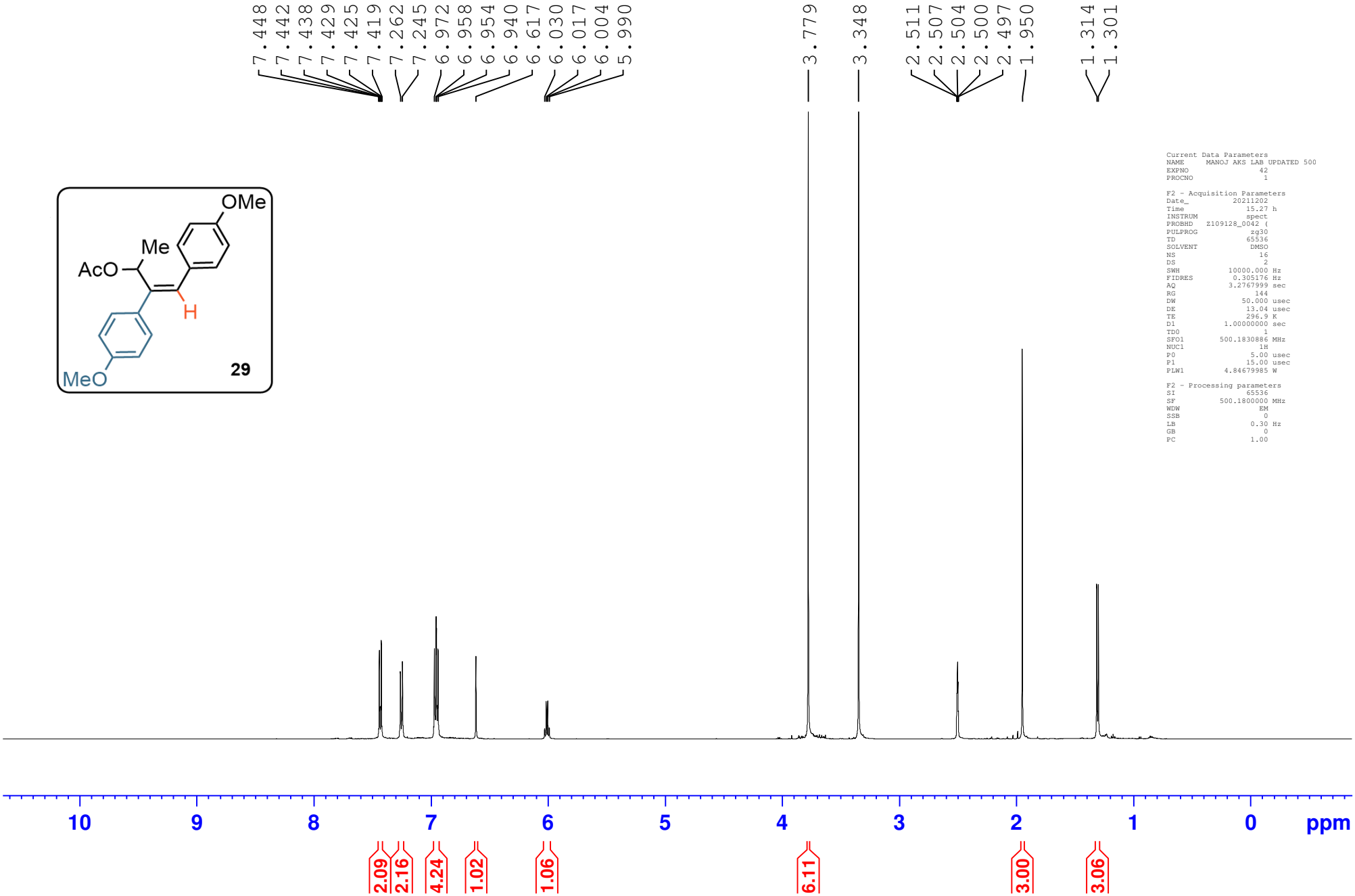

169.82
142.62
137.15
136.26
133.22
131.03
129.25
128.74
127.49
127.44
126.39
120.17
119.95
111.61
101.35
69.40
40.52
40.35
40.18
40.01
39.85
39.68
39.51
21.42
20.19
AcO
Me
H
N
H
26
Current Data Parameters
NAME AVIJIT MAITY UPDATED 500
EXPNO 224
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211220
Time 15.37 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 780
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 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

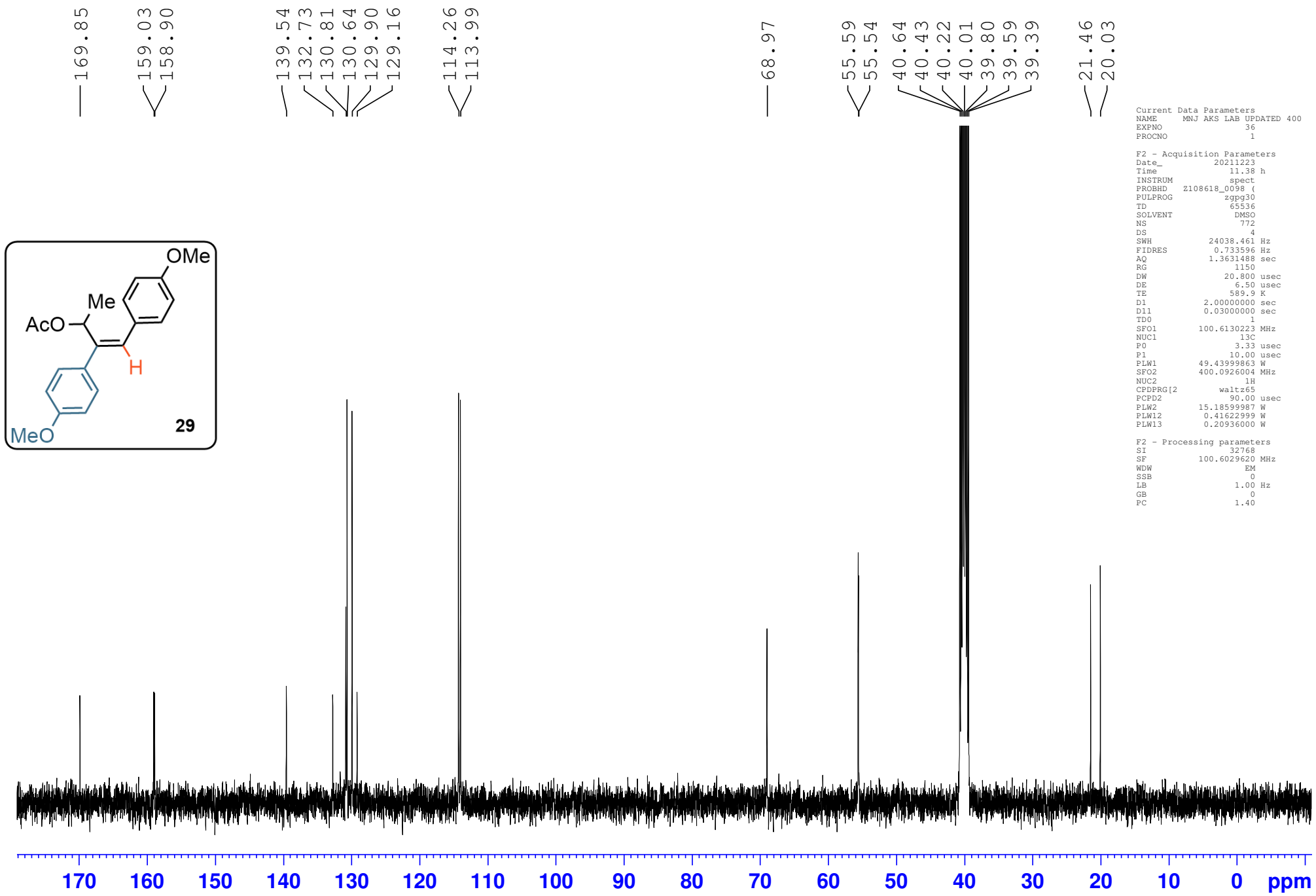

9.565
7.977
7.960
7.451
7.435
7.372
7.355
6.815
6.797
6.701
5.940
5.927
5.914
5.900
3.864
3.379
2.512
2.508
2.505
1.891
1.338
1.325
CO2Me
Me
AcO
H
HO
27
Current Data Parameters
NAME SD ASCEND 500
EXPNO 493
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 16.36 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 192.83
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.03
2.02
2.09
2.03
2.02
1.00
1.03
2.99
3.00
3.03

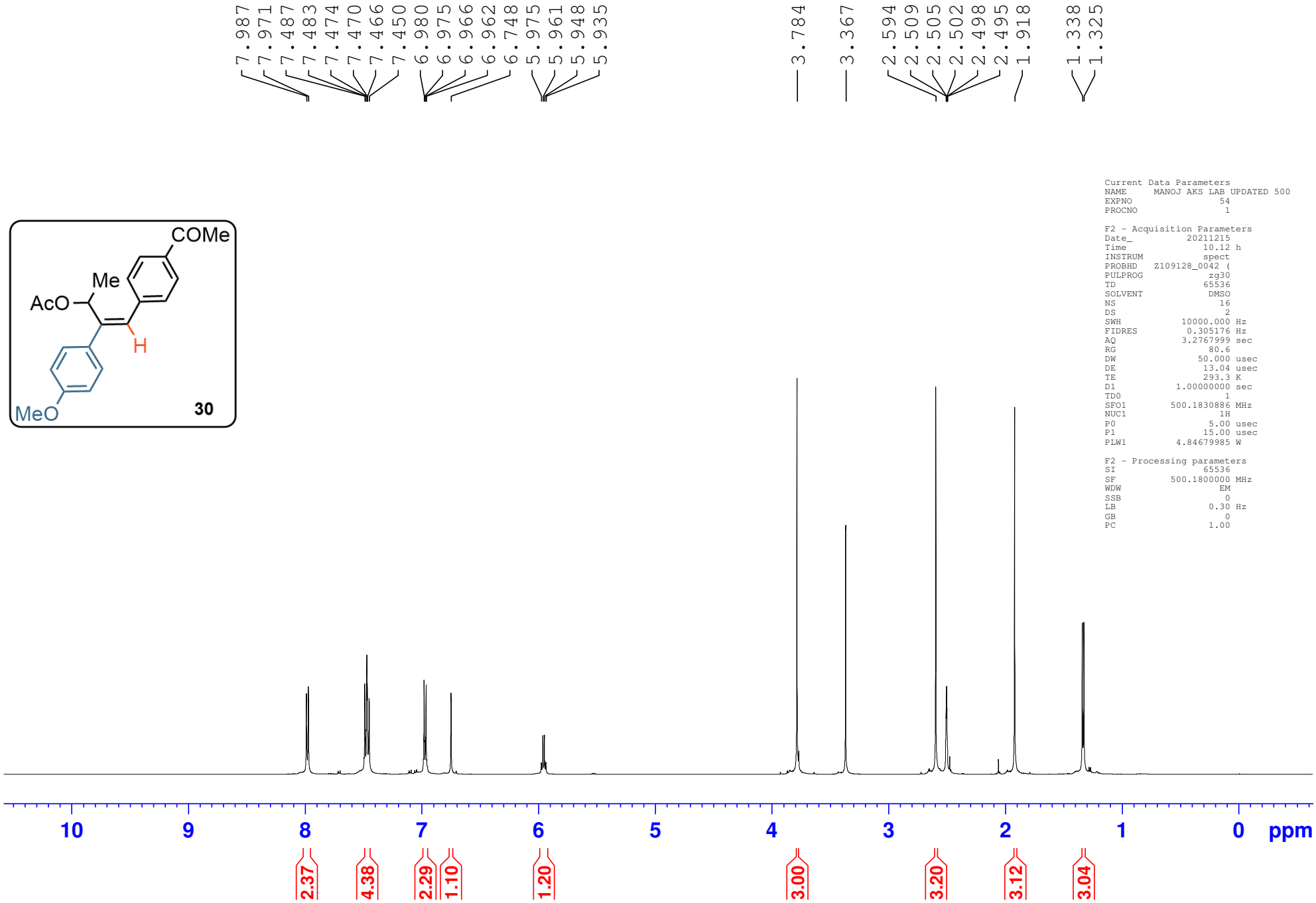

169.74
166.47
157.64
143.08
142.13
134.98
130.44
129.81
129.58
129.54
129.07
128.45
115.46
69.03
52.56
40.49
40.25
40.16
39.99
39.83
39.66
39.49
21.25
20.08
CO2Me
Me
AcO
H
HO
27
Current Data Parameters
NAME SD ASCEND 500
EXPNO 494
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 17.19 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 257
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 12.76
DW 16.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8304669 MHz
NUC1 13C
P1 12.00 usec
PLW1 172.66999817 W
SFO2 500.3710015 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.18000031 W
PLW12 0.12180000 W
PLW13 0.06126500 W
F2 - Processing parameters
SI 32768
SF 125.8178851 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

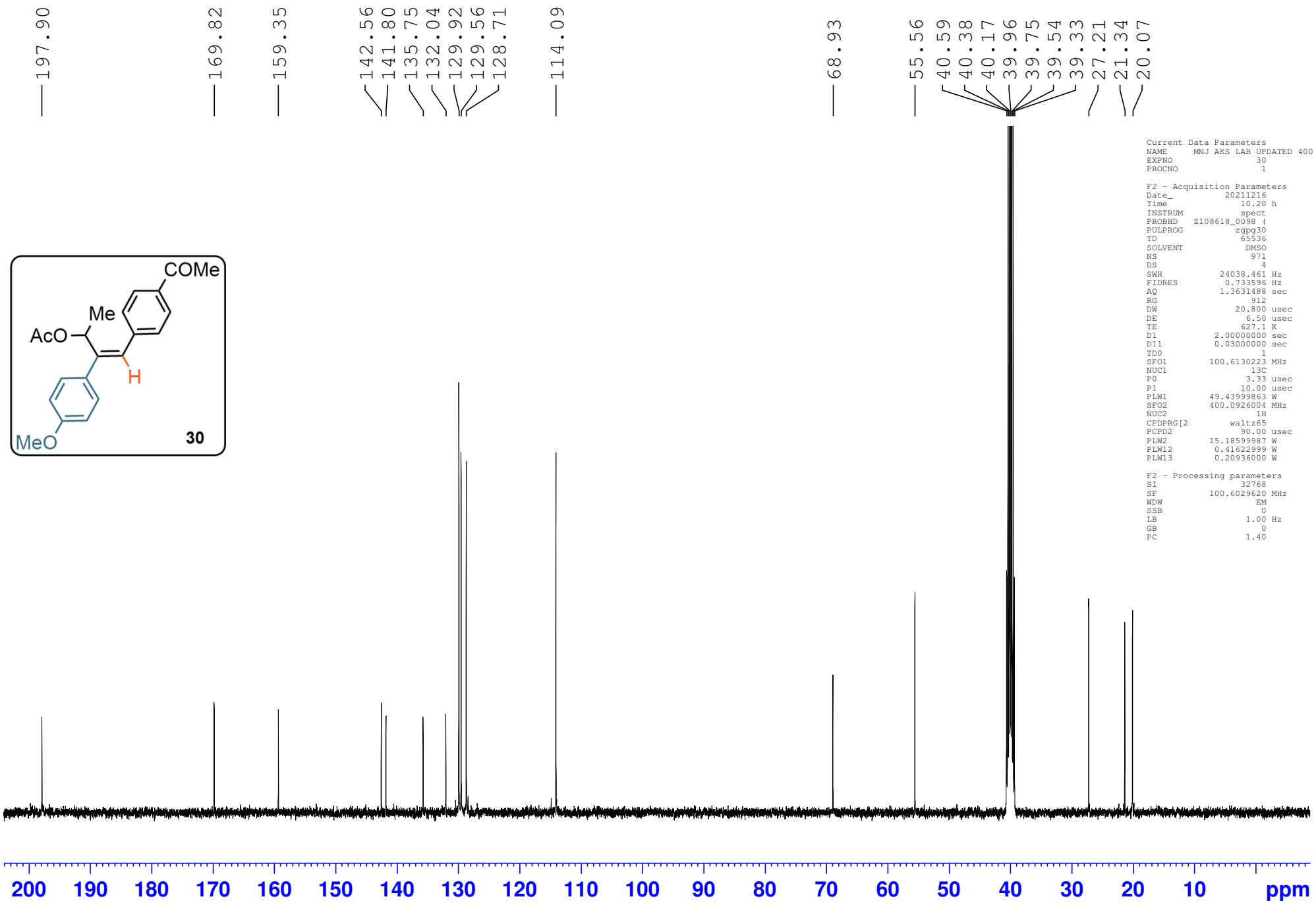

7.451
7.434
7.200
6.960
6.943
6.644
6.015
6.002
5.989
5.976
3.777
3.358
2.503
2.319
1.943
1.304
1.291
Me
Me
AcO
H
MeO
28
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 39
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211130
Time 17.33 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 13.04 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.13
4.27
2.11
1.07
1.07
3.10
3.06
3.00
3.06

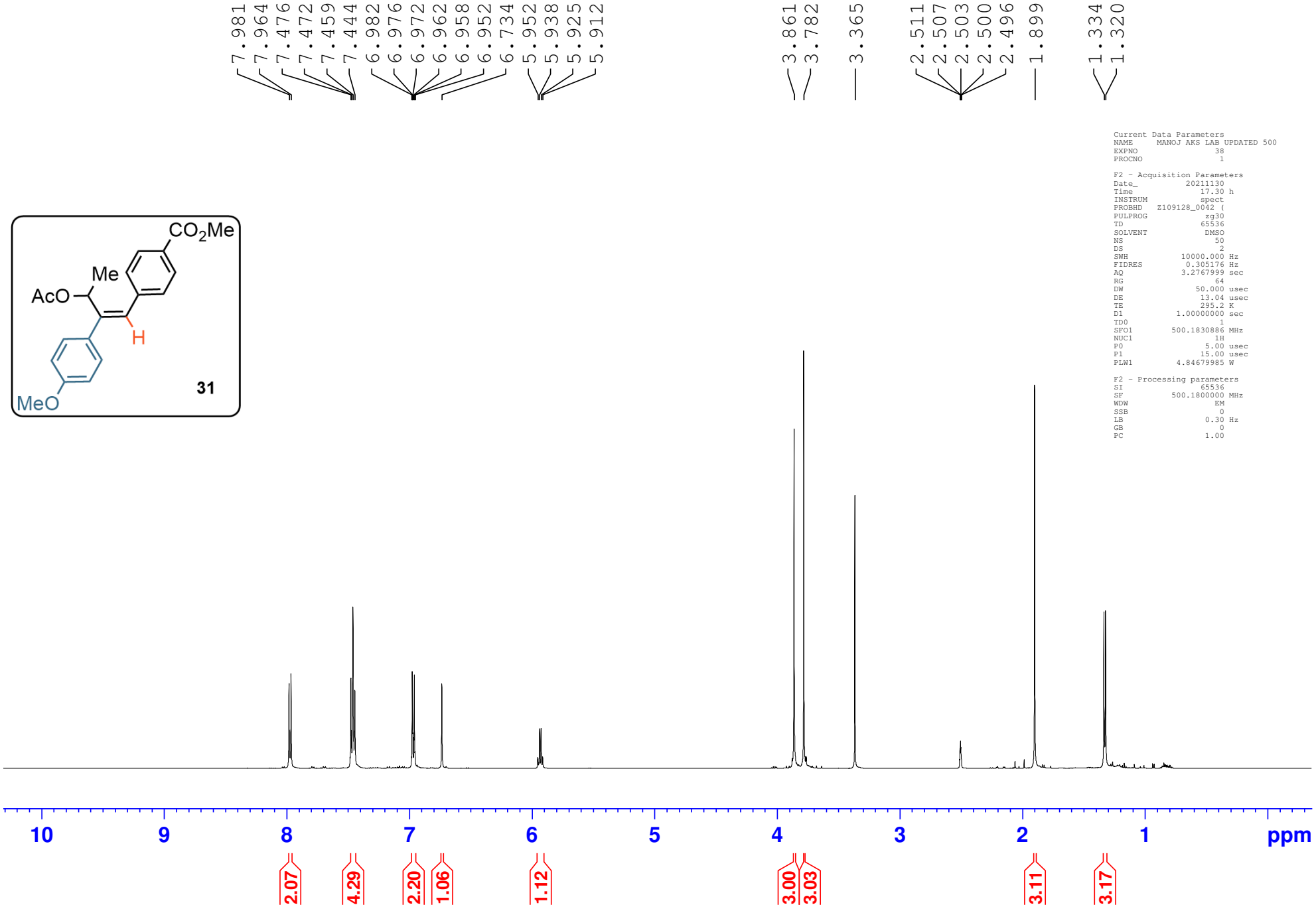

169.81
159.09
140.36
136.96
133.97
132.55
131.05
129.91
129.40
129.19
113.99
68.95
55.53
40.62
40.41
40.20
40.00
39.79
39.58
39.37
21.43
21.26
20.05
Me
Me
AcO
H
MeO
28
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 19
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 11.02 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 380
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 709.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.448
7.442
7.438
7.429
7.425
7.419
7.262
7.245
6.972
6.958
6.954
6.940
6.617
6.030
6.017
6.004
5.990
3.779
3.348
2.511
2.507
2.504
2.500
2.497
1.950
1.314
1.301
OMe
Me
AcO
H
MeO
29
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 15.27 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 144
DW 50.000 usec
DE 13.04 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.09
2.16
4.24
1.02
1.06
6.11
3.00
3.06


169.85
159.03
158.90
139.54
132.73
130.81
130.64
129.90
129.16
114.26
113.99
68.97
55.59
55.54
40.64
40.43
40.22
40.01
39.80
39.59
39.39
21.46
20.03
OMe
Me
AcO
H
MeO
29
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 36
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211223
Time 11.38 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 772
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 1150
DW 20.800 usec
DE 6.50 usec
TE 589.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.987
7.971
7.487
7.483
7.474
7.470
7.466
7.450
6.980
6.975
6.966
6.962
6.748
5.975
5.961
5.948
5.935
3.784
3.367
2.594
2.509
2.505
2.502
2.498
2.495
1.918
1.338
1.325
COMe
Me
AcO
H
MeO
30
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 54
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211215
Time 10.12 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 13.04 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.37
4.38
2.29
1.10
1.20
3.00
3.20
3.12
3.04


197.90
169.82
159.35
142.56
141.80
135.75
132.04
129.92
129.56
128.71
114.09
68.93
55.56
40.59
40.38
40.17
39.96
39.75
39.54
39.33
27.21
21.34
20.07
COMe
Me
AcO
H
MeO
30
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211216
Time 10.20 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 971
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 912
DW 20.800 usec
DE 6.50 usec
TE 627.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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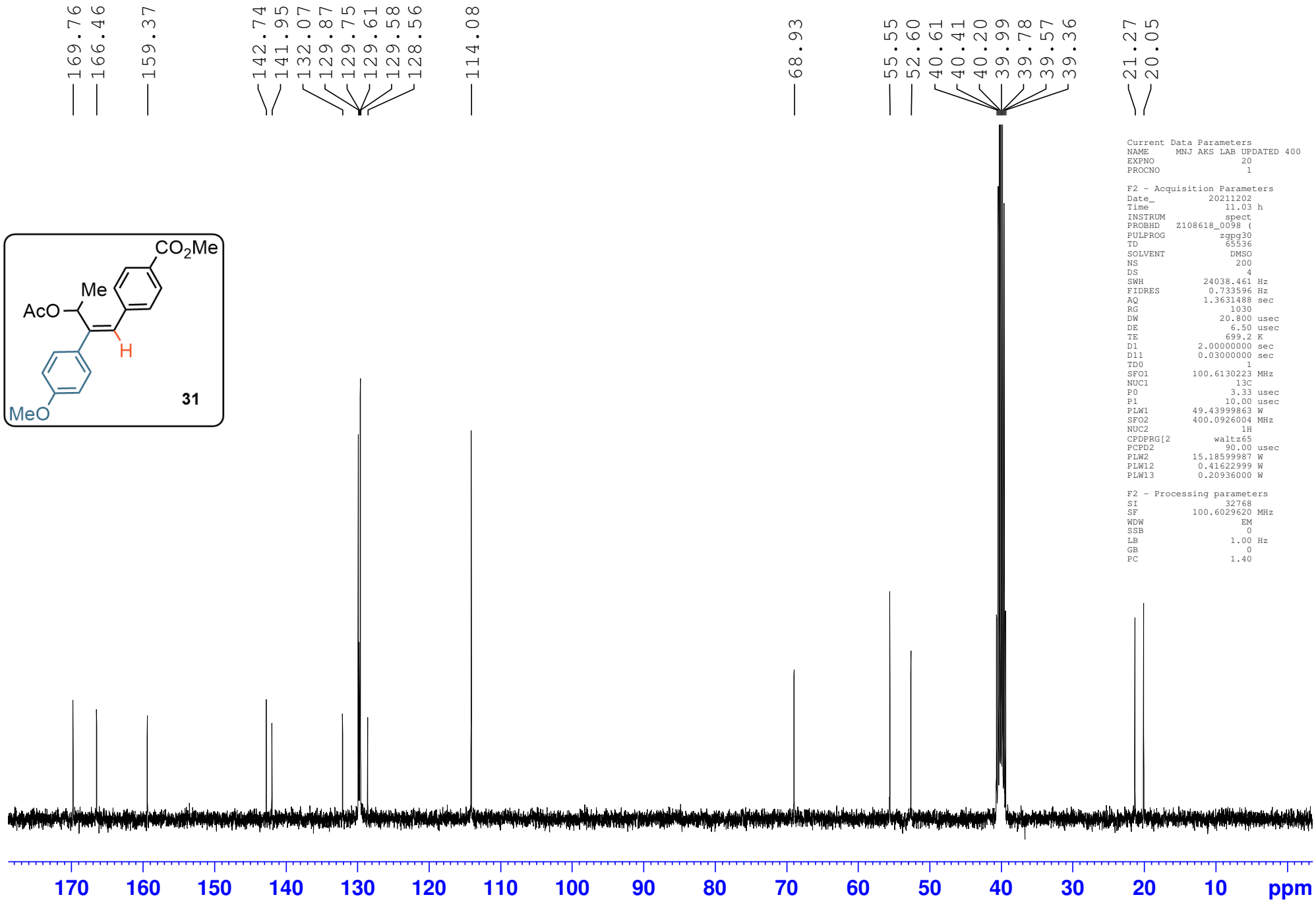
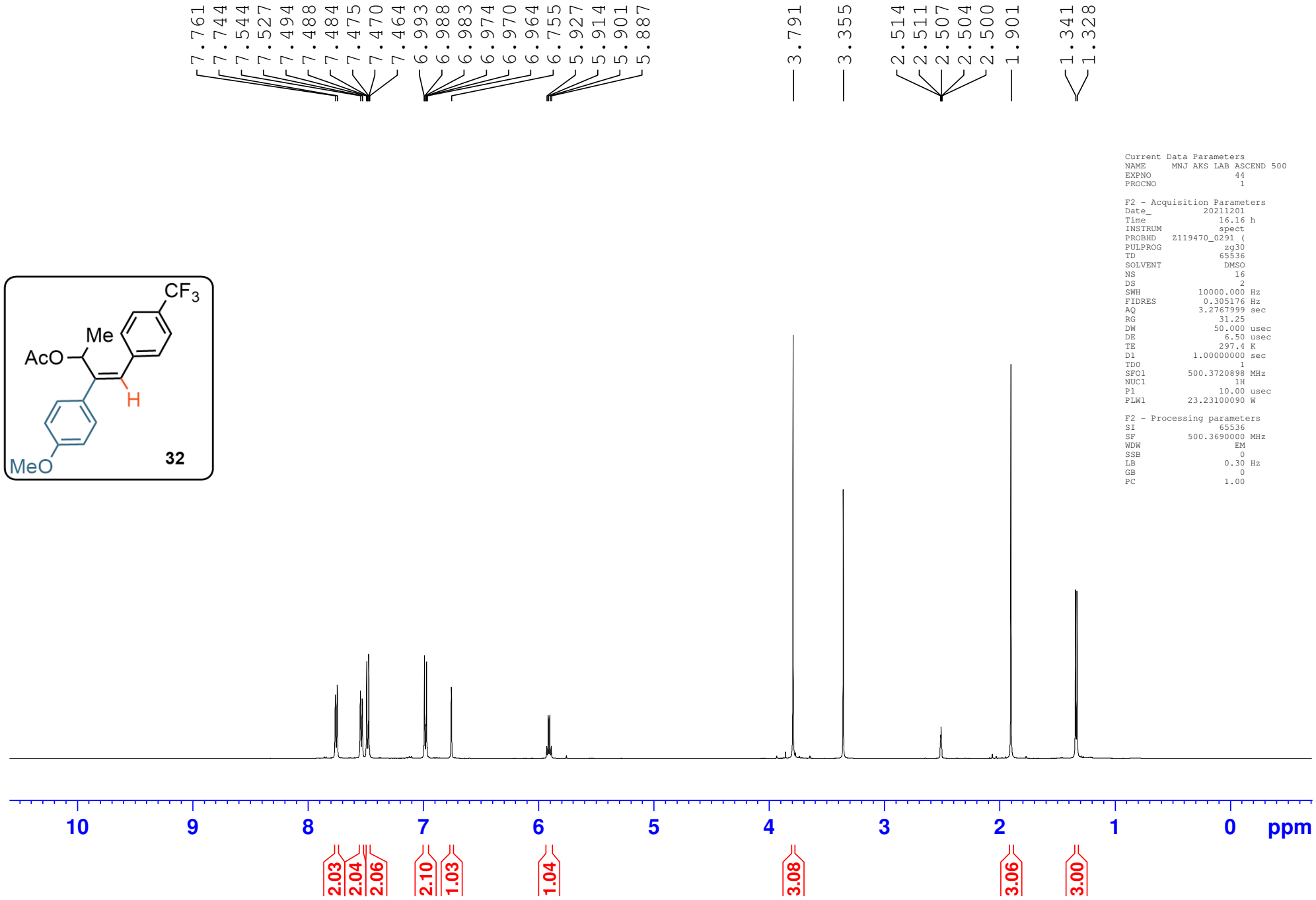
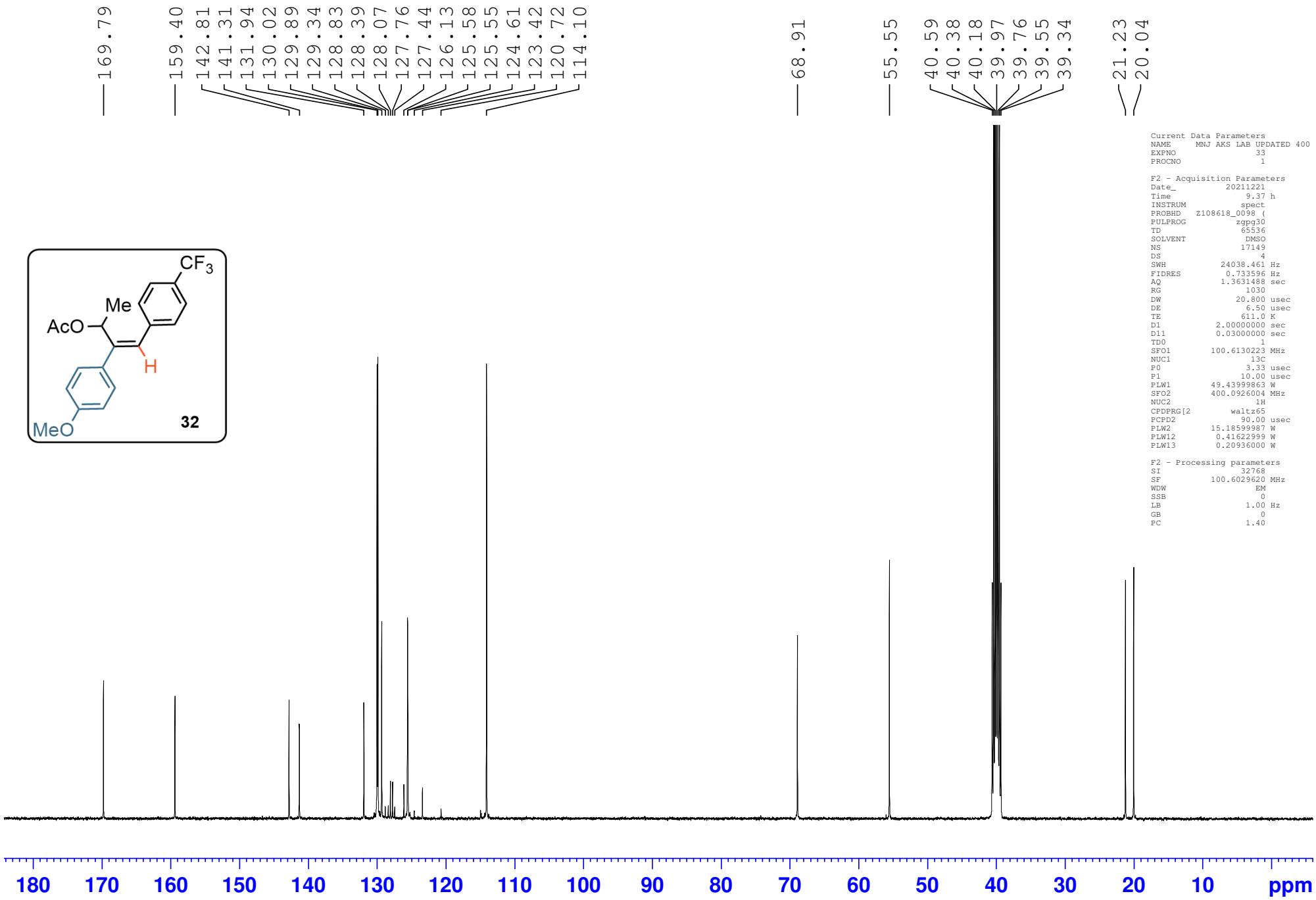
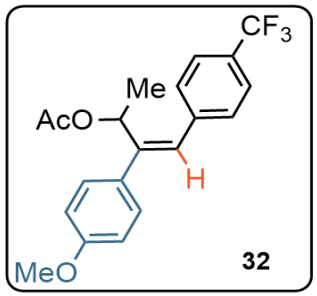
7.964
7.476
7.472
7.459
7.444
6.982
6.976
6.972
6.962
6.958
6.952
6.734
5.952
5.938
5.925
5.912
3.861
3.782
3.365
2.511
2.507
2.503
2.500
2.496
1.899
1.334
1.320
CO2Me
Me
AcO
H
MeO
31
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 38
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211130
Time 17.30 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 64
DW 50.000 usec
DE 13.04 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.07
4.29
2.20
1.06
1.12
3.00
3.03
3.11
3.17


169.76
166.46
159.37
142.74
141.95
132.07
129.87
129.75
129.61
129.58
128.56
114.08
68.93
55.55
52.60
40.61
40.41
40.20
39.99
39.78
39.57
39.36
21.27
20.05
CO2Me
Me
AcO
H
MeO
31
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 11.03 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 1030
DW 20.800 usec
DE 6.50 usec
TE 699.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

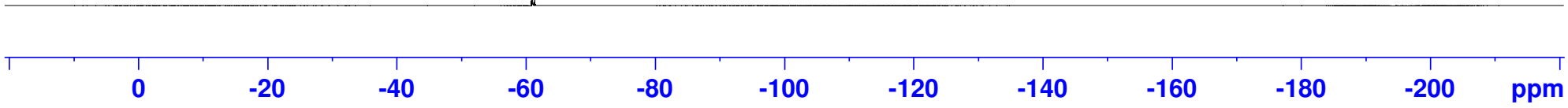

7.761
7.744
7.544
7.527
7.494
7.488
7.484
7.475
7.470
7.464
6.993
6.988
6.983
6.974
6.970
6.964
6.755
5.927
5.914
5.901
5.887
3.791
3.355
2.514
2.511
2.507
2.504
2.500
1.901
1.341
1.328
CF3
Me
AcO
H
MeO
32
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 44
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 16.16 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.04
2.06
2.10
1.03
1.04
3.08
3.06
3.00

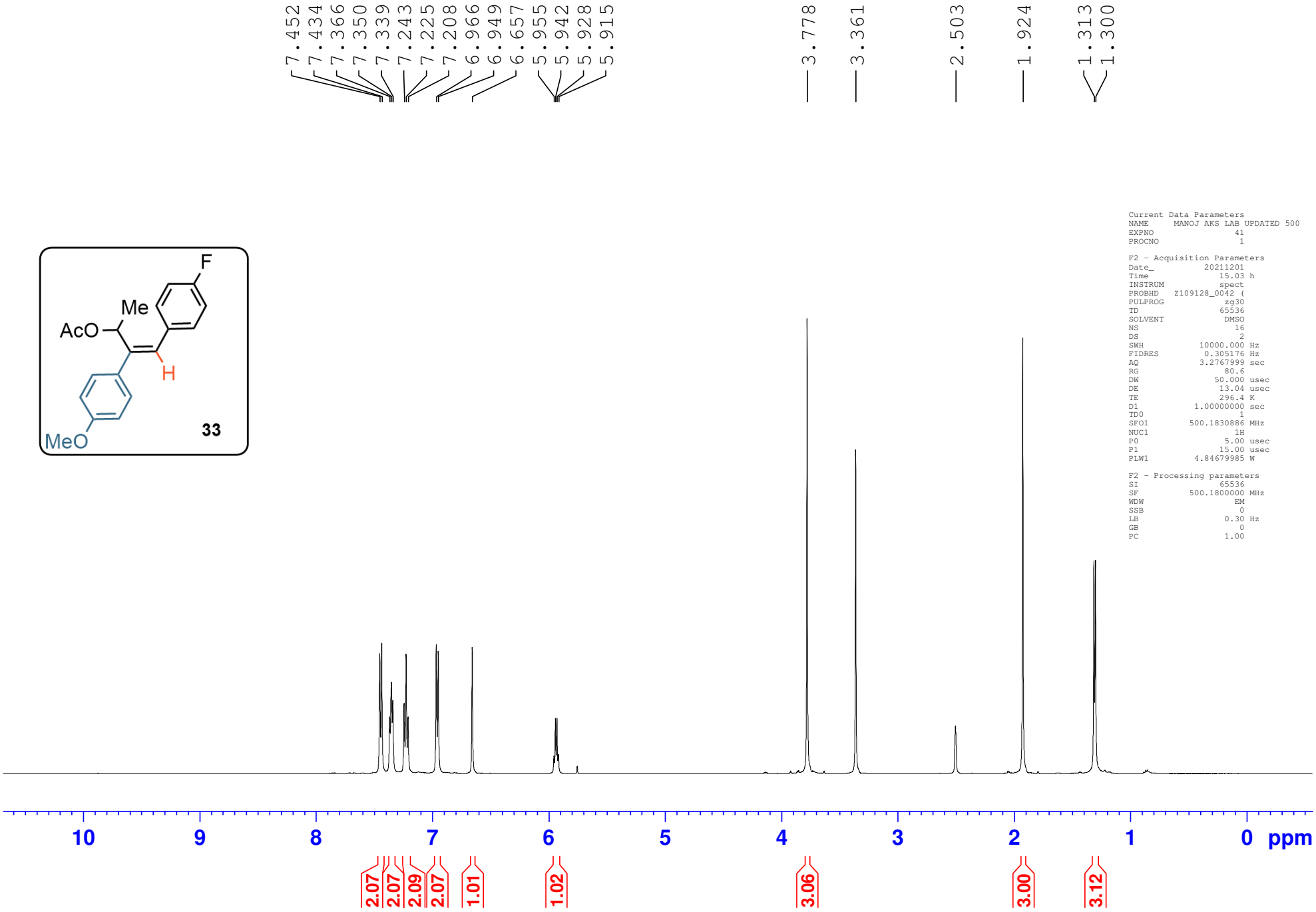

169.79
159.40
142.81
141.31
131.94
130.02
129.89
129.34
128.83
128.39
128.07
127.76
127.44
126.13
125.58
125.55
124.61
123.42
120.72
114.10
68.91
55.55
40.59
40.38
40.18
39.97
39.76
39.55
39.34
21.23
20.04
CF3
Me
AcO
H
MeO
32
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 33
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211221
Time 9.37 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 17149
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 1030
DW 20.800 usec
DE 6.50 usec
TE 611.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

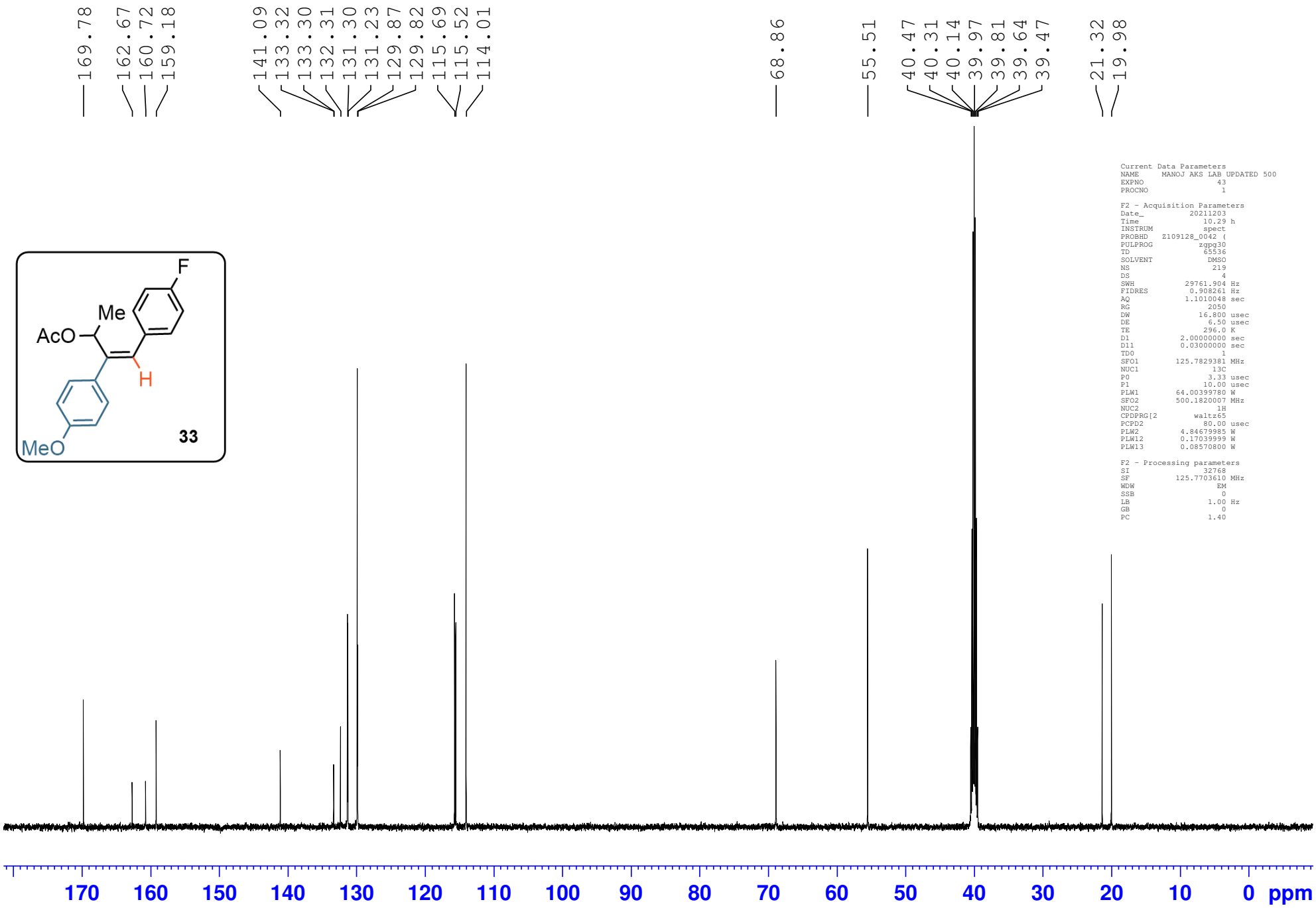


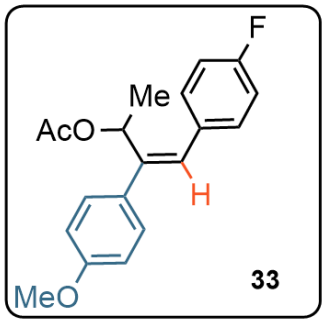
-60.98

```
Current Data Parameters
NAME      MANOJ AKS LAB UPDATED 500
EXPNO                44
PROCNO                1

F2 - Acquisition Parameters
Date_          20211206
Time              11.26 h
INSTRUM           spect
PROBHD   Z109128_0042 (
PULPROG       zgfhigqn.2
TD               131072
SOLVENT             DMSO
NS                    16
DS                     4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ             0.5767168 sec
RG                   362
DW                 4.400 usec
DE                 6.50 usec
TE                294.2 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1
SFO1         470.5923603 MHz
NUC1                 19F
P1                12.00 usec
PLW1         36.12599945 W
SFO2         500.1820007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          4.84679985 W
PLW12         0.17039999 W

F2 - Processing parameters
SI                65536
SF           470.6394242 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



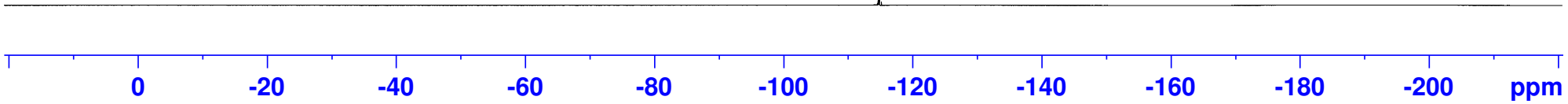

7.452
7.434
7.366
7.350
7.339
7.243
7.225
7.208
6.966
6.949
6.657
5.955
5.942
5.928
5.915
3.778
3.361
2.503
1.924
1.313
1.300
F
Me
AcO
H
MeO
33
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 15.03 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 13.04 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
2.07
2.09
2.07
1.01
1.02
3.06
3.00
3.12

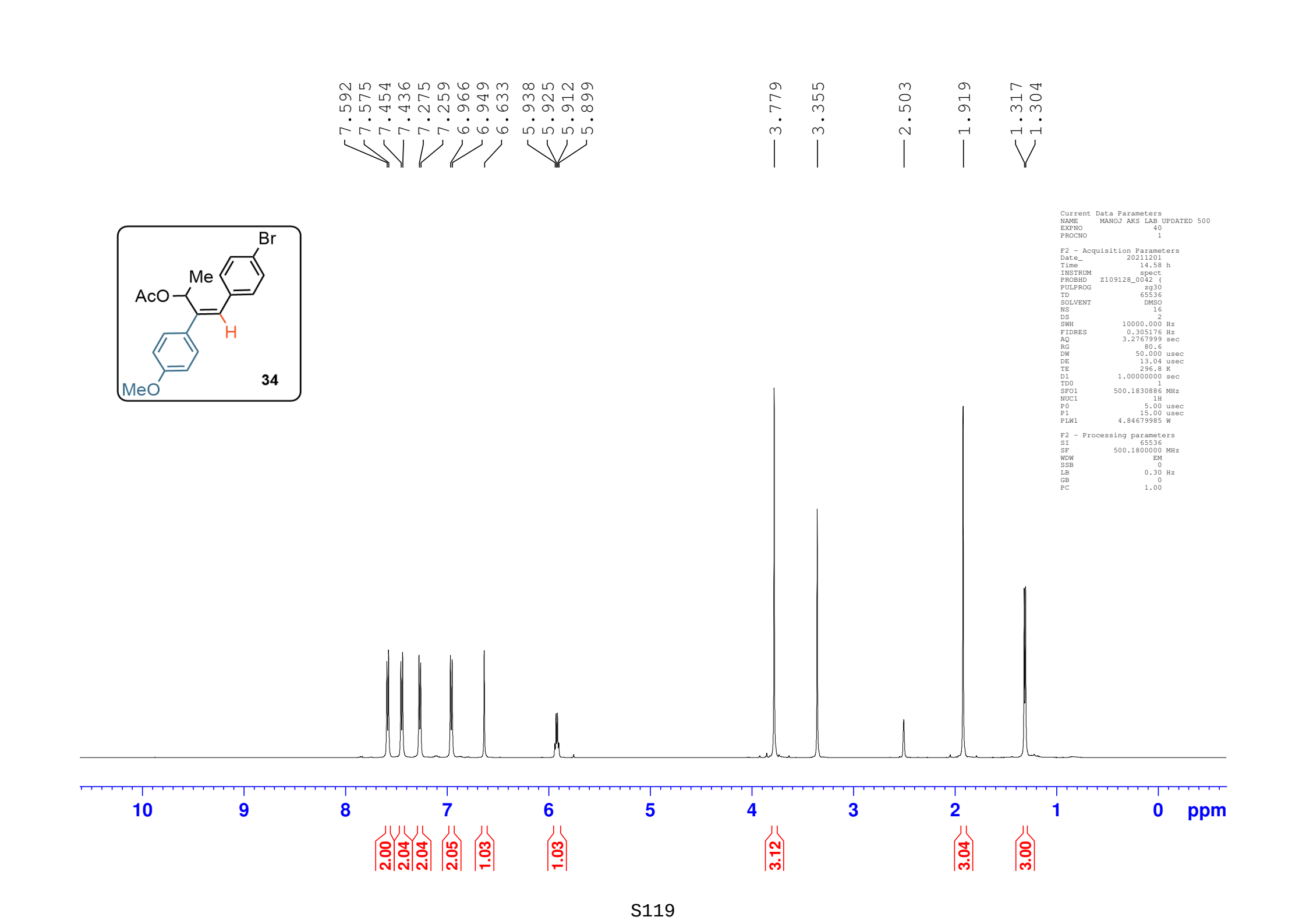

169.78
162.67
160.72
159.18
141.09
133.32
133.30
132.31
131.30
131.23
129.87
129.82
115.69
115.52
114.01
68.86
55.51
40.47
40.31
40.14
39.97
39.81
39.64
39.47
21.32
19.98
F
Me
AcO
H
MeO
33
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 43
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211203
Time 10.29 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 219
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

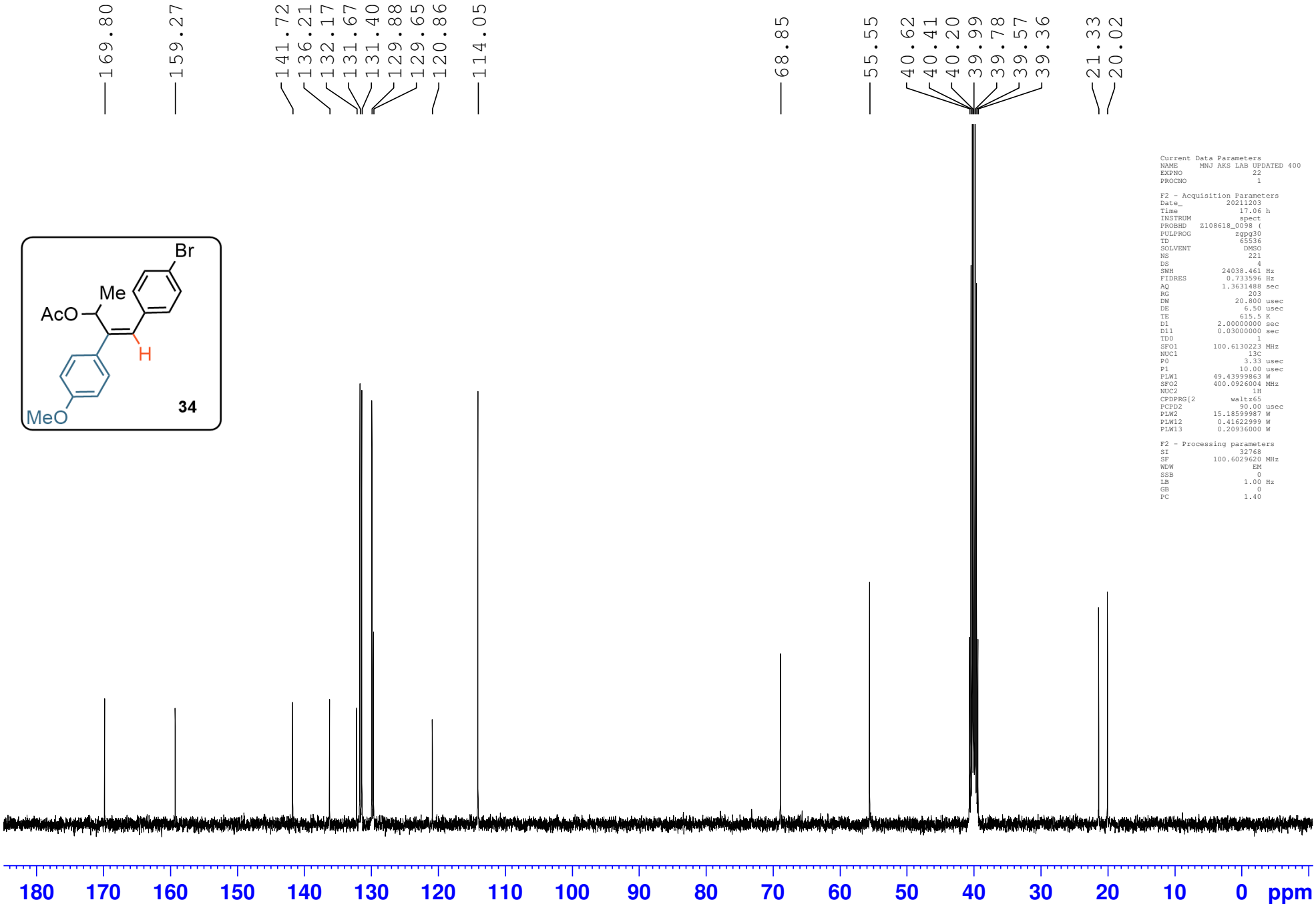


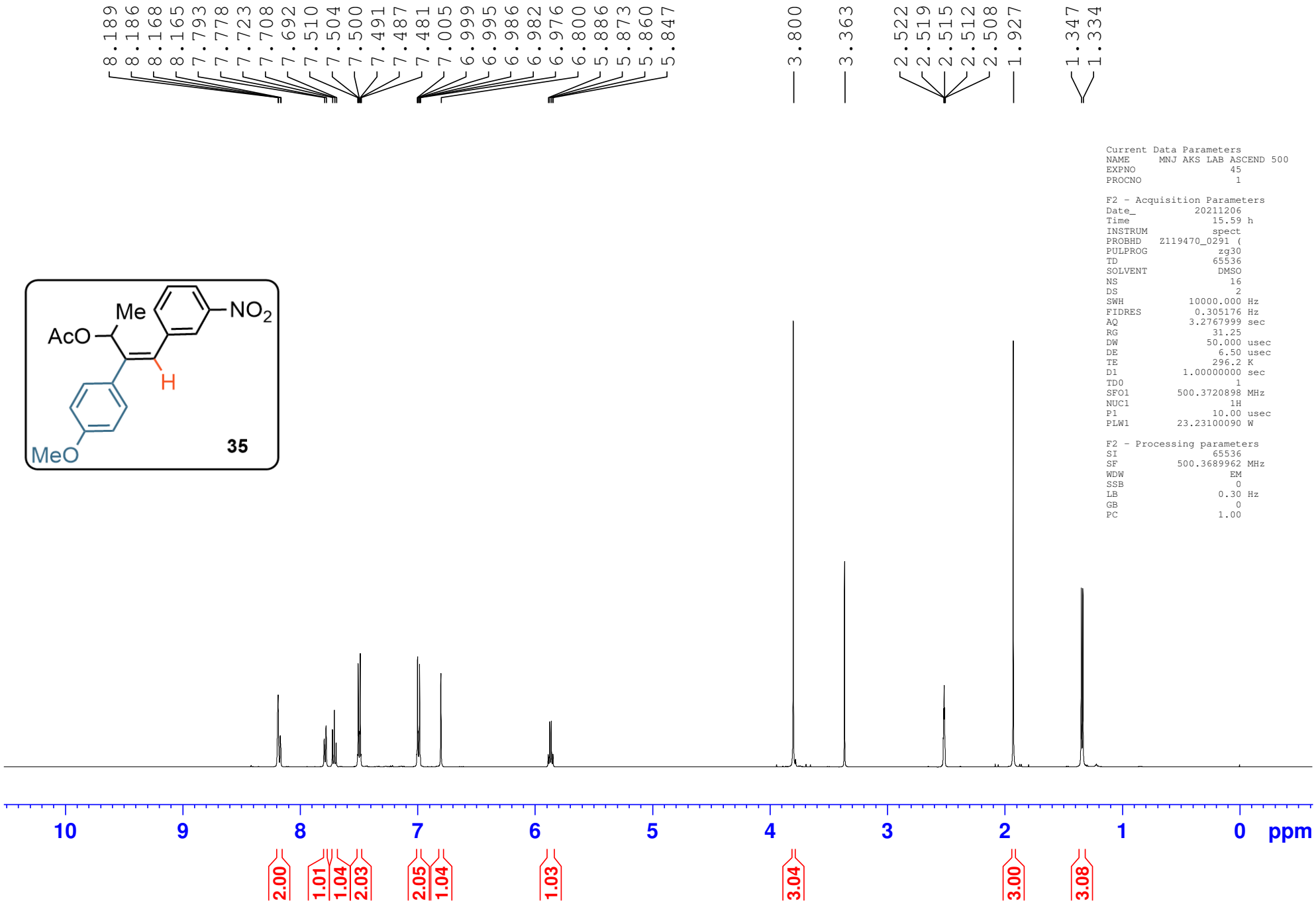
-114.86

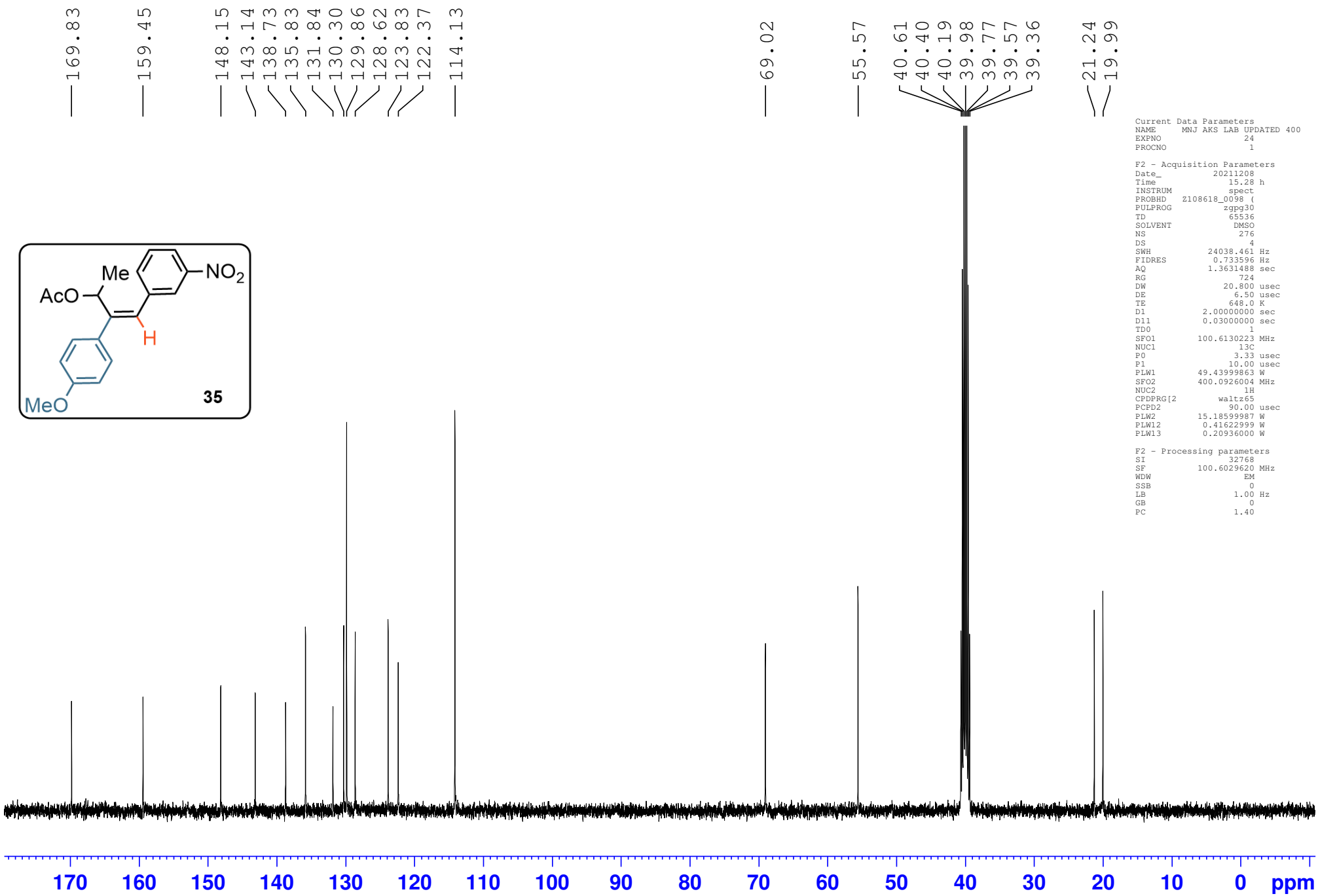
```
Current Data Parameters
NAME      MANOJ AKS LAB UPDATED 500
EXPNO                45
PROCNO                1

F2 - Acquisition Parameters
Date_          20211206
Time              11.36 h
INSTRUM             spect
PROBHD   Z109128_0042 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT              DMSO
NS                    16
DS                     4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ             0.5767168 sec
RG                   456
DW                 4.400 usec
DE                 6.50 usec
TE                293.9 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                    1
SFO1         470.5923603 MHz
NUC1                19F
P1                12.00 usec
PLW1         36.12599945 W
SFO2         500.1820007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          4.84679985 W
PLW12         0.17039999 W

F2 - Processing parameters
SI                 65536
SF           470.6394242 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

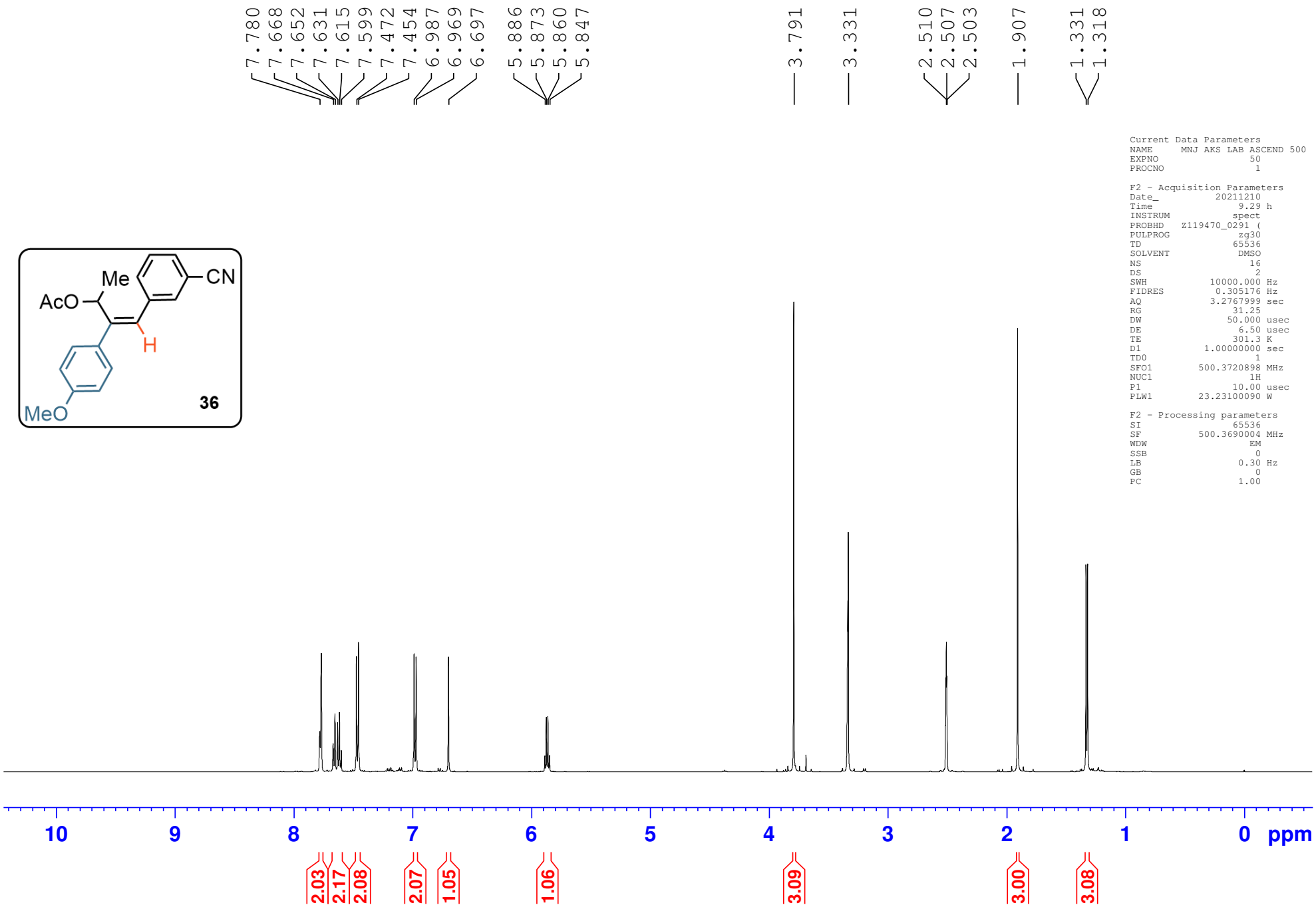



7.592
7.575
7.454
7.436
7.275
7.259
6.966
6.949
6.633
5.938
5.925
5.912
5.899
3.779
3.355
2.503
1.919
1.317
1.304
Br
Me
AcO
H
MeO
34
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 14.58 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 13.04 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.04
2.04
2.05
1.03
1.03
3.12
3.04
3.00


169.80
159.27
141.72
136.21
132.17
131.67
131.40
129.88
129.65
120.86
114.05
68.85
55.55
40.62
40.41
40.20
39.99
39.78
39.57
39.36
21.33
20.02
Br
Me
AcO
H
MeO
34
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211203
Time 17.06 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 221
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 615.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.189
8.186
8.168
8.165
7.793
7.778
7.723
7.708
7.692
7.510
7.504
7.500
7.491
7.487
7.481
7.005
6.999
6.995
6.986
6.982
6.976
6.800
5.886
5.873
5.860
5.847
3.800
3.363
2.522
2.519
2.515
2.512
2.508
1.927
1.347
1.334
Me
NO2
AcO
H
MeO
35
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 45
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 15.59 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3689962 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.01
1.04
2.03
2.05
1.04
1.03
3.04
3.00
3.08


169.83
159.45
148.15
143.14
138.73
135.83
131.84
130.30
129.86
128.62
123.83
122.37
114.13
69.02
55.57
40.61
40.40
40.19
39.98
39.77
39.57
39.36
21.24
19.99
Me
NO2
AcO
H
MeO
35
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 24
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211208
Time 15.28 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 276
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 648.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.780
7.668
7.652
7.631
7.615
7.599
7.472
7.454
6.987
6.969
6.697
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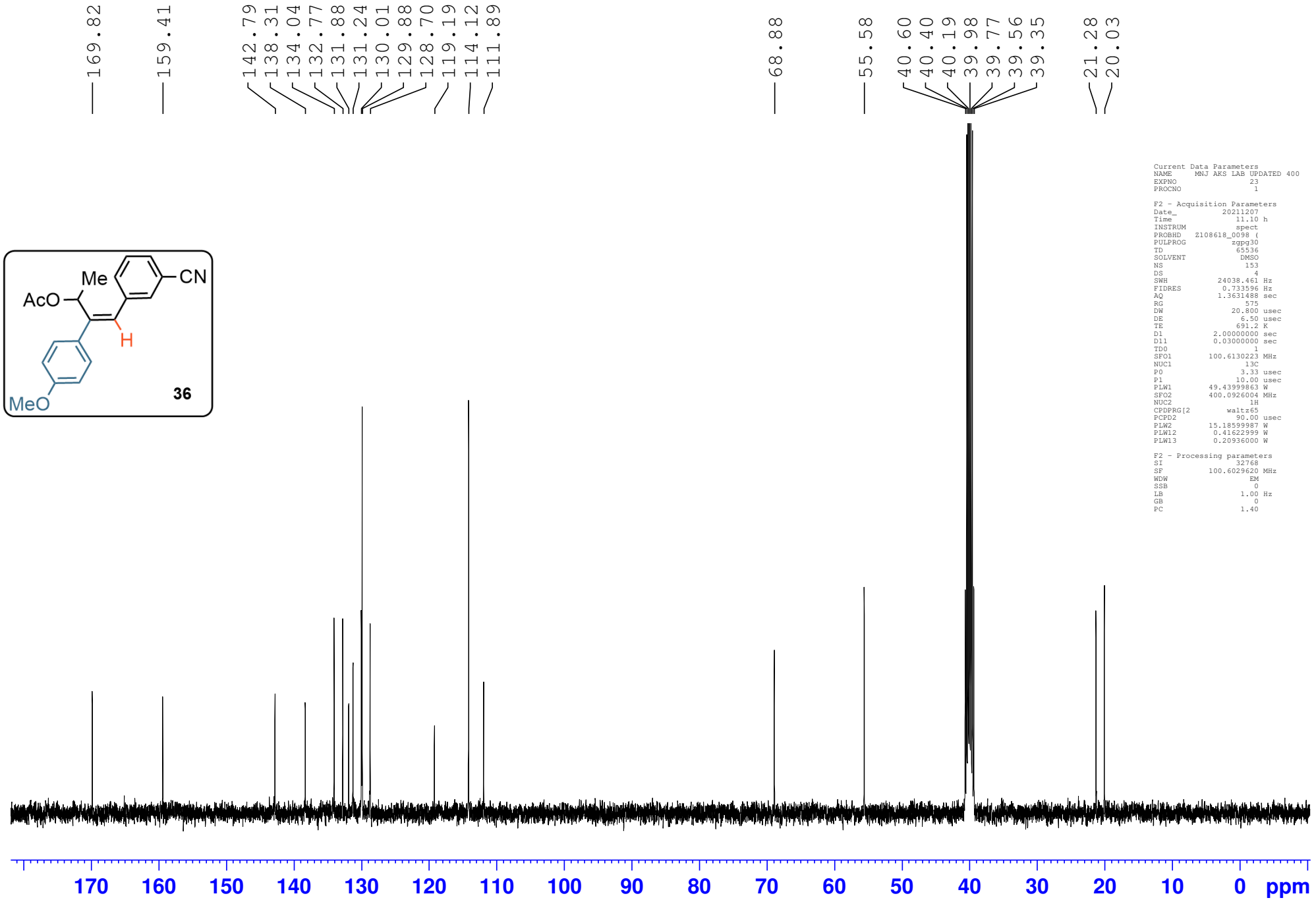
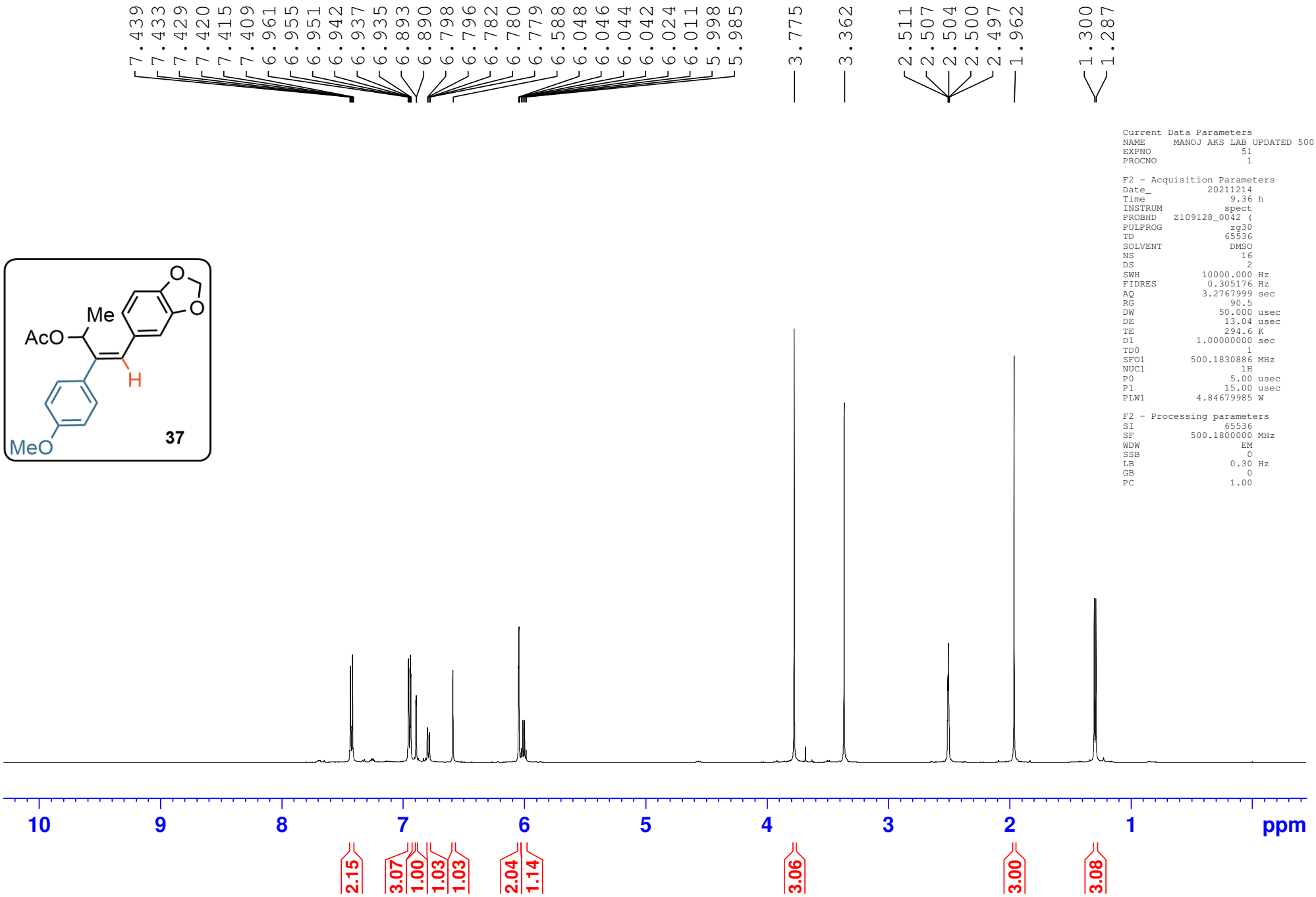
5.873
5.860
5.847
3.791
3.331
2.510
2.507
2.503
1.907
1.331
1.318
Me
CN
AcO
H
MeO
36
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 9.29 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 301.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690004 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.17
2.08
2.07
1.05
1.06
3.09
3.00
3.08


169.82
159.41
142.79
138.31
134.04
132.77
131.88
131.24
130.01
129.88
128.70
119.19
114.12
111.89
68.88
55.58
40.60
40.40
40.19
39.98
39.77
39.56
39.35
21.28
20.03
Me
CN
AcO
H
MeO
36
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 23
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211207
Time 11.10 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 153
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 575
DW 20.800 usec
DE 6.50 usec
TE 691.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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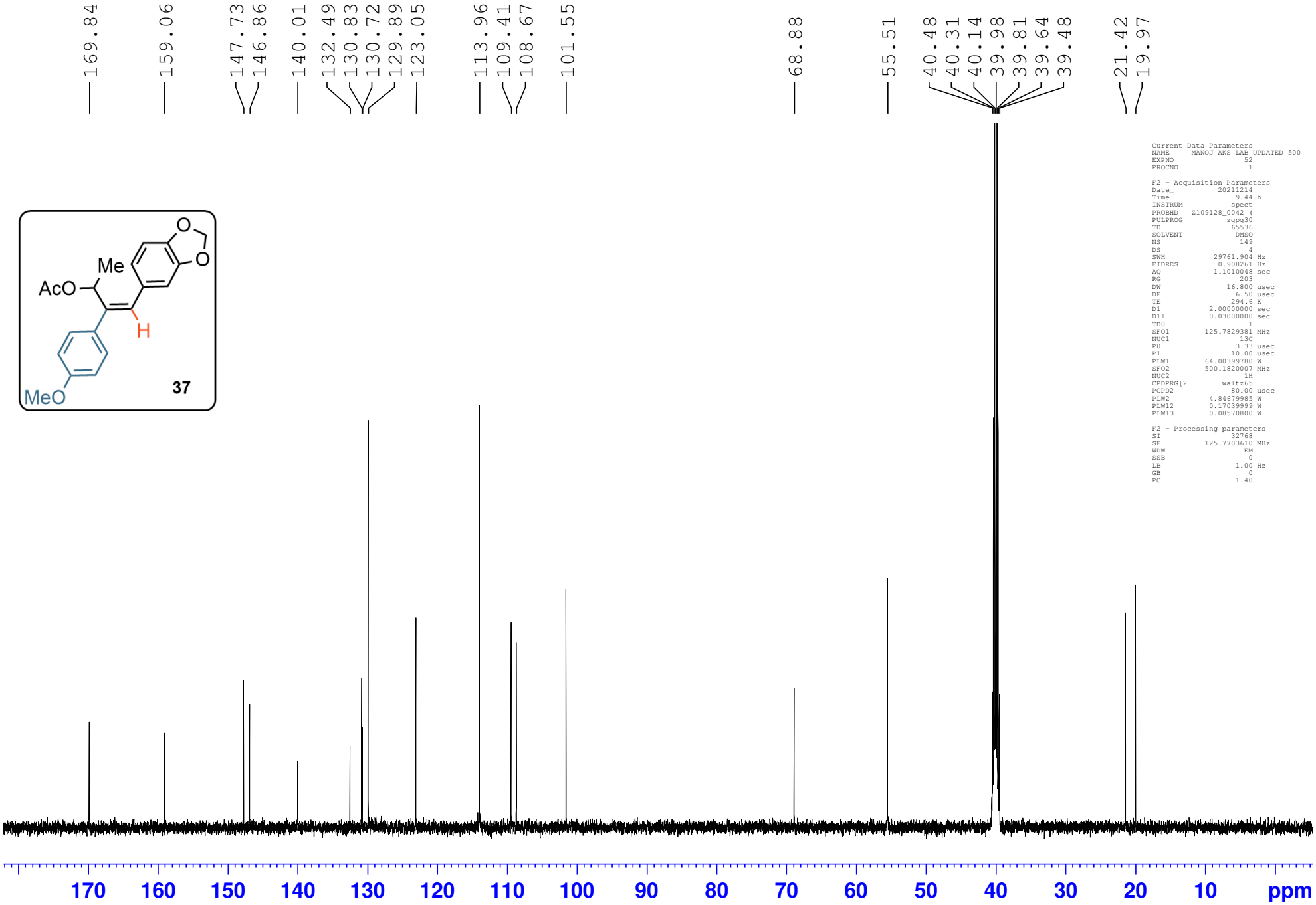
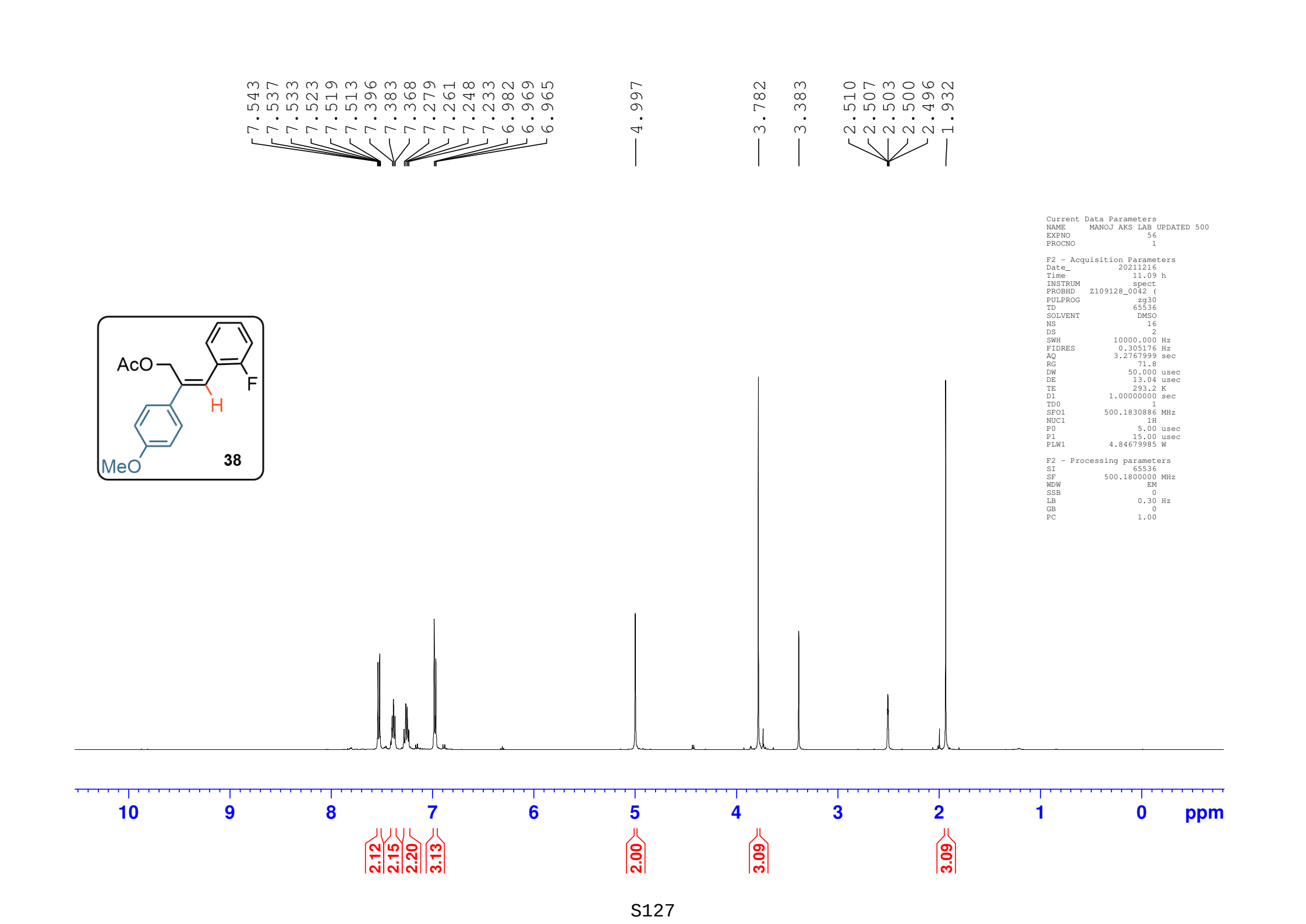
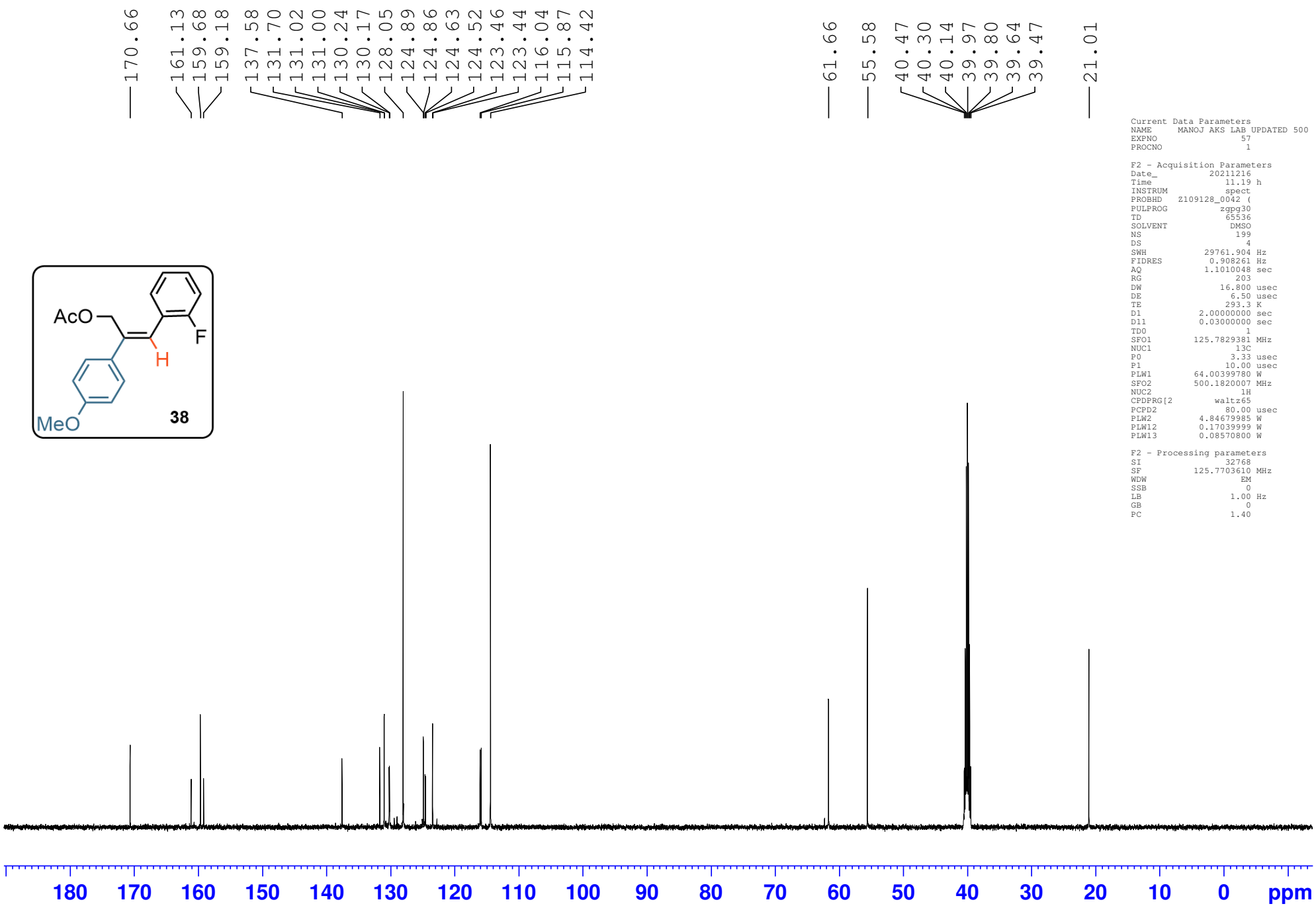
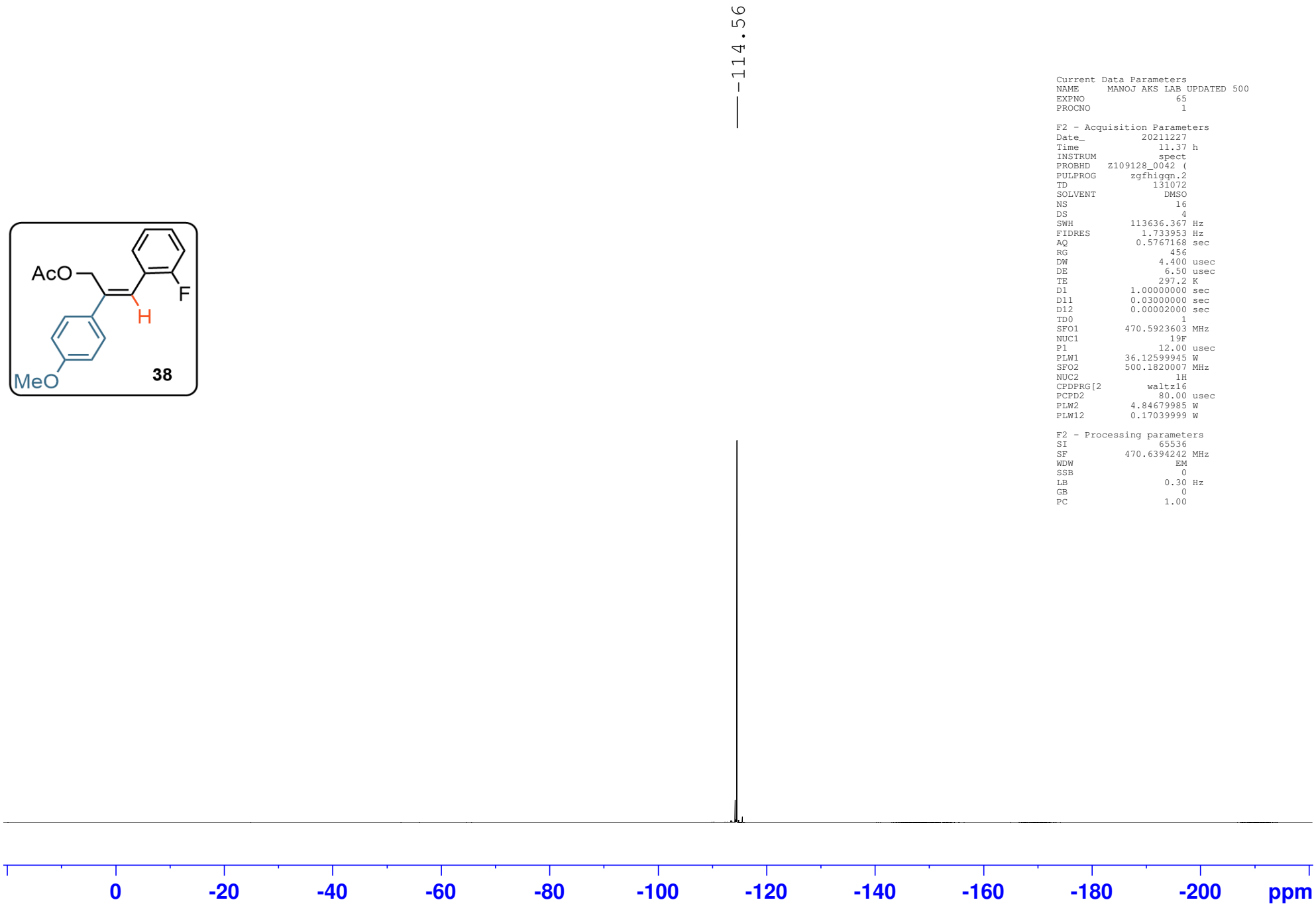
7.433
7.429
7.420
7.415
7.409
6.961
6.955
6.951
6.942
6.937
6.935
6.893
6.890
6.798
6.796
6.782
6.780
6.779
6.588
6.048
6.046
6.044
6.042
6.024
6.011
5.998
5.985
3.775
3.362
2.511
2.507
2.504
2.500
2.497
1.962
1.300
1.287
Me
AcO
O
O
H
MeO
37
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 51
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211214
Time 9.36 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 13.04 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.15
3.07
1.00
1.03
1.03
2.04
1.14
3.06
3.00
3.08


169.84
159.06
147.73
146.86
140.01
132.49
130.83
130.72
129.89
123.05
113.96
109.41
108.67
101.55
68.88
55.51
40.48
40.31
40.14
39.98
39.81
39.64
39.48
21.42
19.97
Me
AcO
H
MeO
O
O
37
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 52
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211214
Time 9.44 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 149
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 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.543
7.537
7.533
7.523
7.519
7.513
7.396
7.383
7.368
7.279
7.261
7.248
7.233
6.982
6.969
6.965
4.997
3.782
3.383
2.510
2.507
2.503
2.500
2.496
1.932
AcO
F
H
MeO
38
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 56
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211216
Time 11.09 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 71.8
DW 50.000 usec
DE 13.04 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
2.15
2.20
3.13
2.00
3.09
3.09

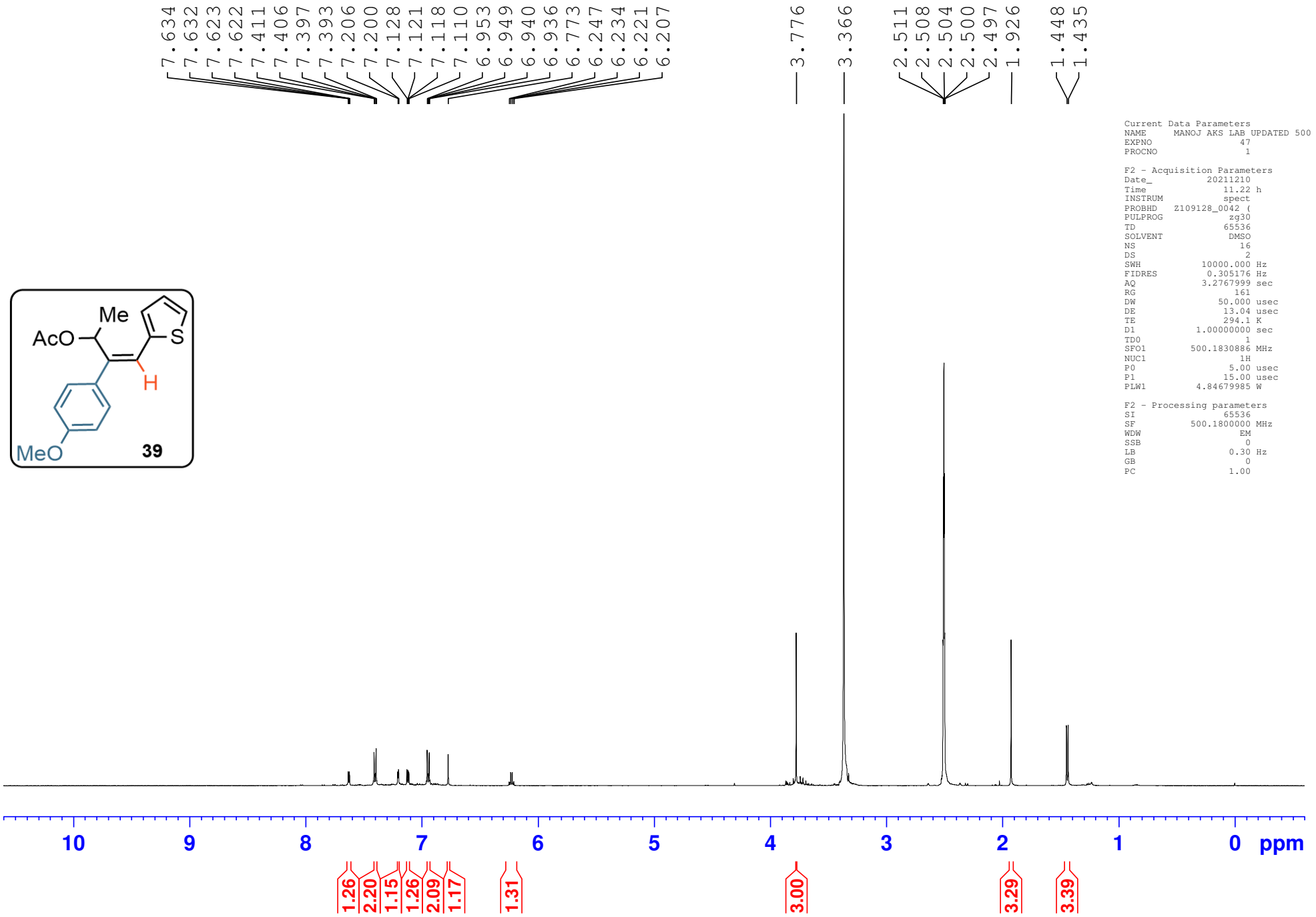

170.66
161.13
159.68
159.18
137.58
131.70
131.02
131.00
130.24
130.17
128.05
124.89
124.86
124.63
124.52
123.46
123.44
116.04
115.87
114.42
61.66
55.58
40.47
40.30
40.14
39.97
39.80
39.64
39.47
21.01
AcO
F
H
MeO
38
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 57
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211216
Time 11.19 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 199
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 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm




```
Current Data Parameters
NAME      MANOJ AKS LAB UPDATED 500
EXPNO                   65
PROCNO                   1

F2 - Acquisition Parameters
Date_           20211227
Time              11.37 h
INSTRUM             spect
PROBHD   Z109128_0042 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             DMSO
NS                    16
DS                     4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ             0.5767168 sec
RG                   456
DW                 4.400 usec
DE                 6.50 usec
TE                297.2 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                    1
SFO1         470.5923603 MHz
NUC1                 19F
P1                 12.00 usec
PLW1         36.12599945 W
SFO2         500.1820007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          4.84679985 W
PLW12         0.17039999 W

F2 - Processing parameters
SI                 65536
SF           470.6394242 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```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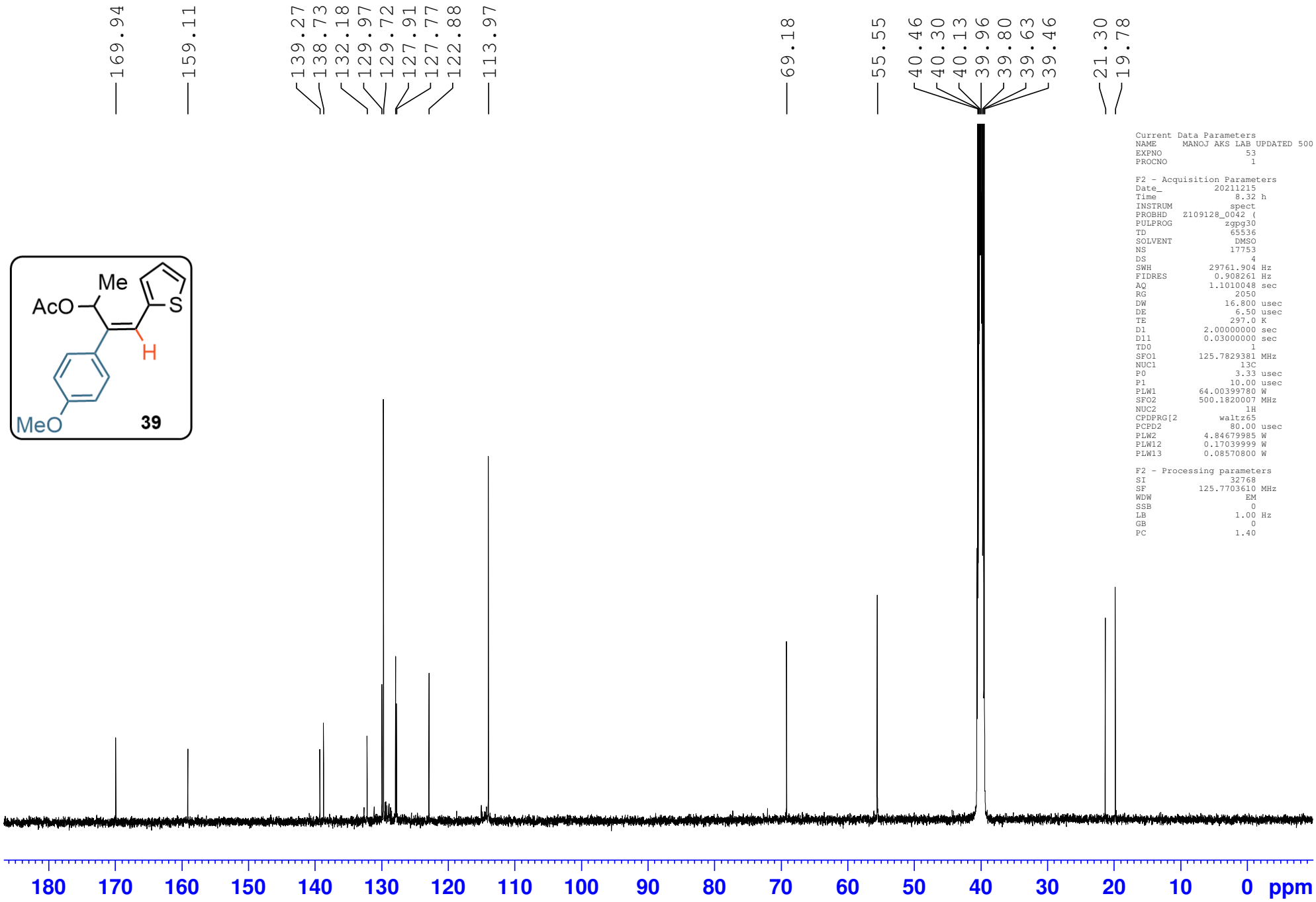
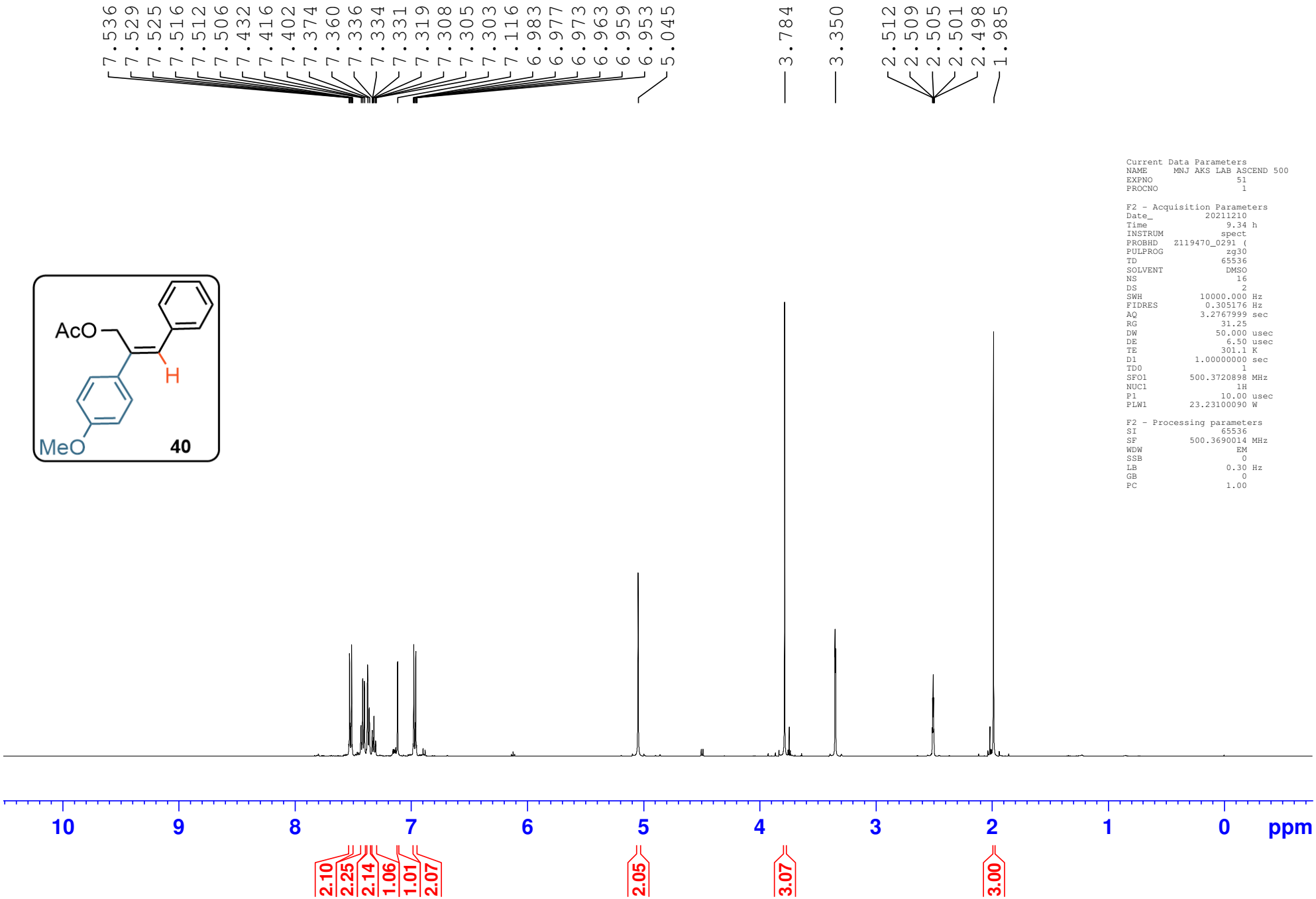
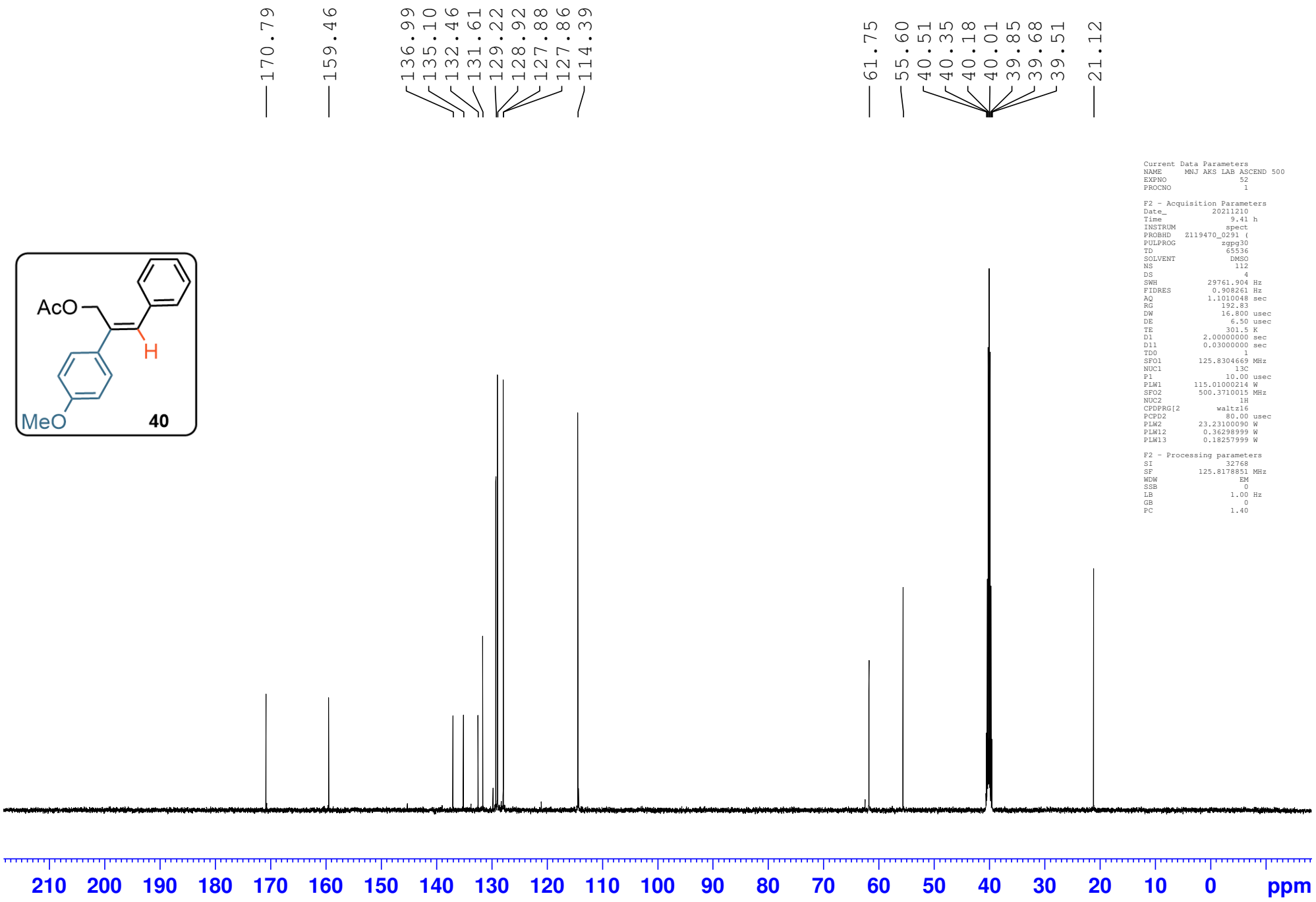
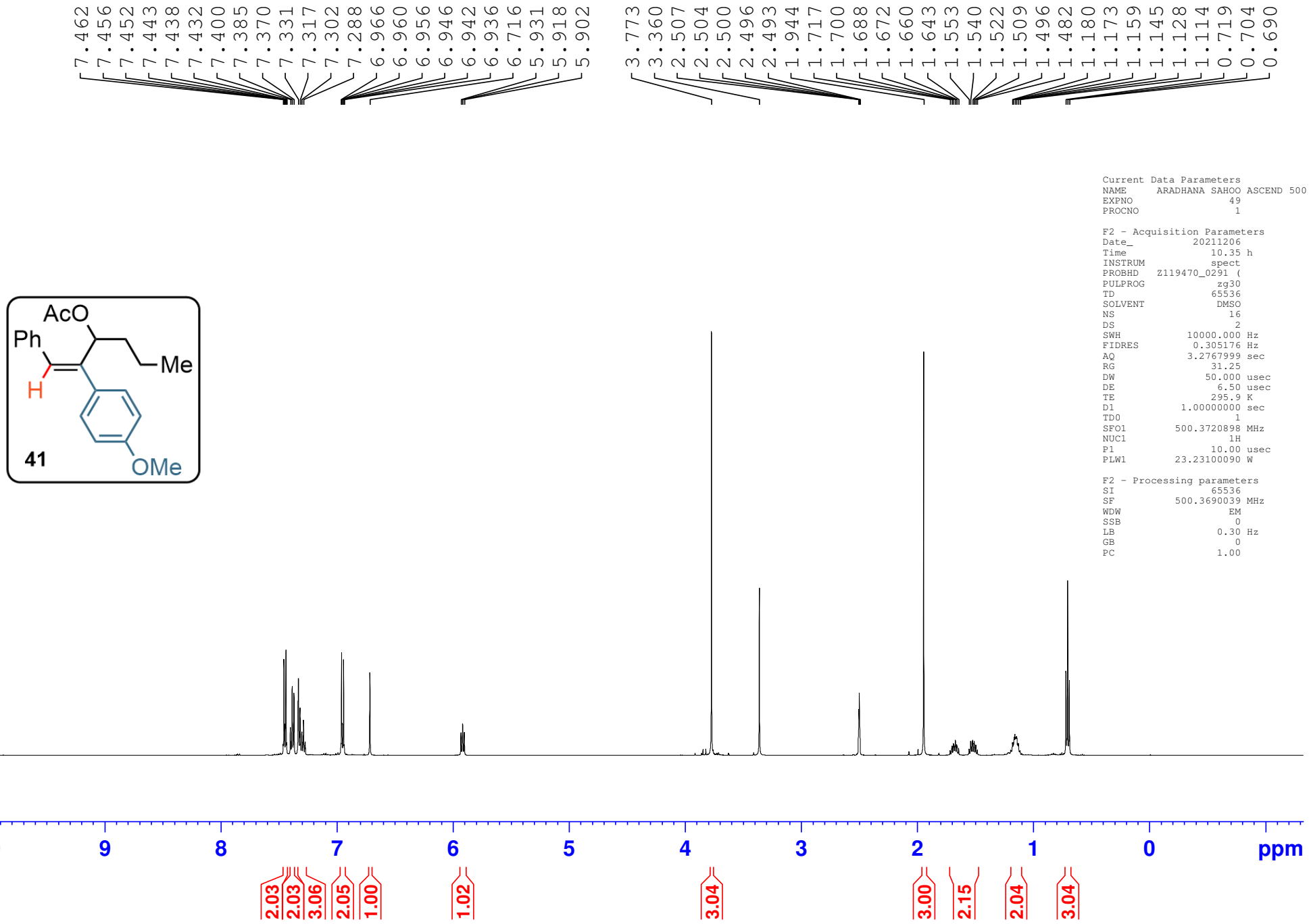
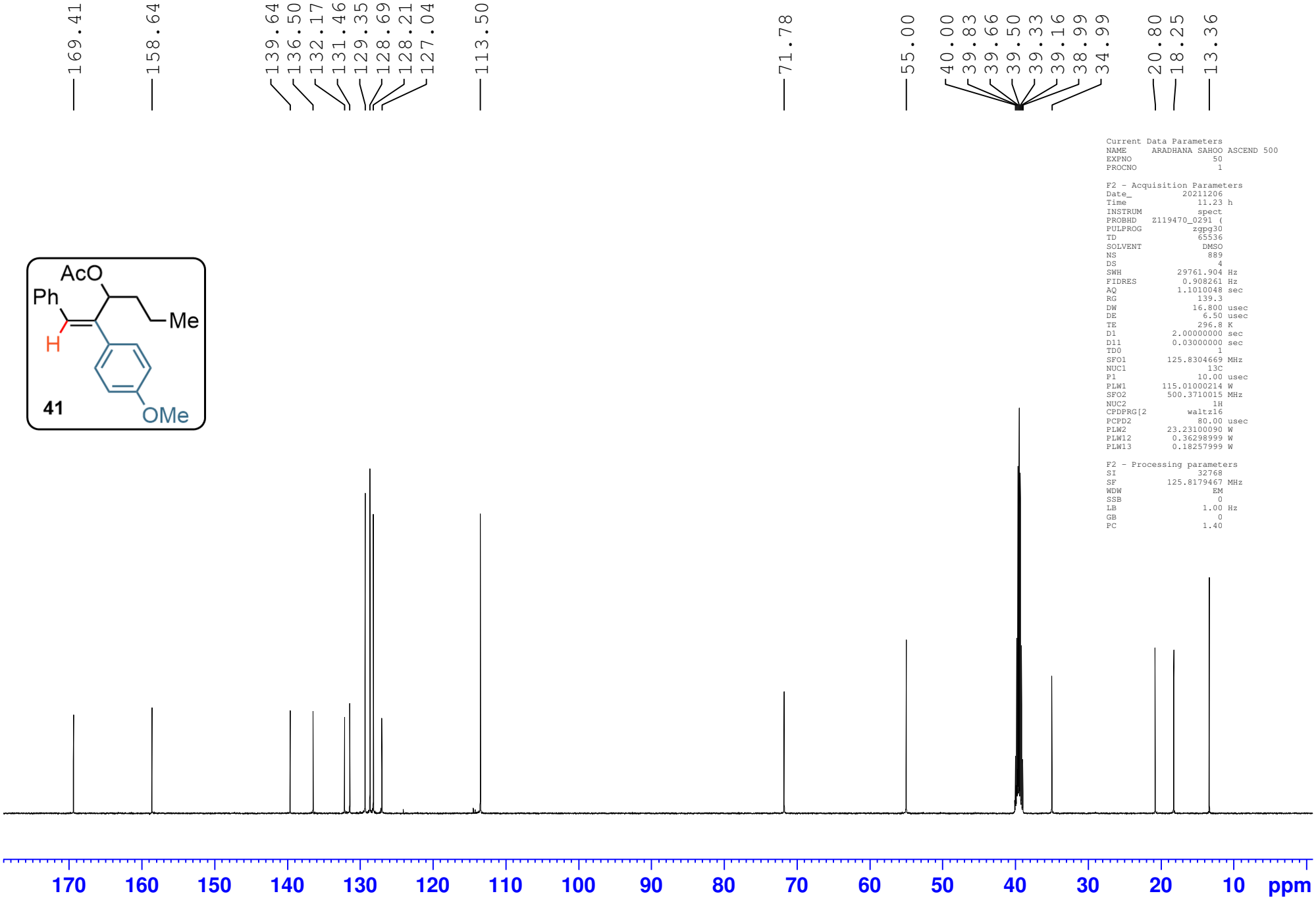
7.632
7.623
7.622
7.411
7.406
7.397
7.393
7.206
7.200
7.128
7.121
7.118
7.110
6.953
6.949
6.940
6.936
6.773
6.247
6.234
6.221
6.207
3.776
3.366
2.511
2.508
2.504
2.500
2.497
1.926
1.448
1.435
Me
AcO
S
H
MeO
39
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 47
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 11.22 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 161
DW 50.000 usec
DE 13.04 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.26
2.20
1.15
1.26
2.09
1.17
1.31
3.00
3.29
3.39

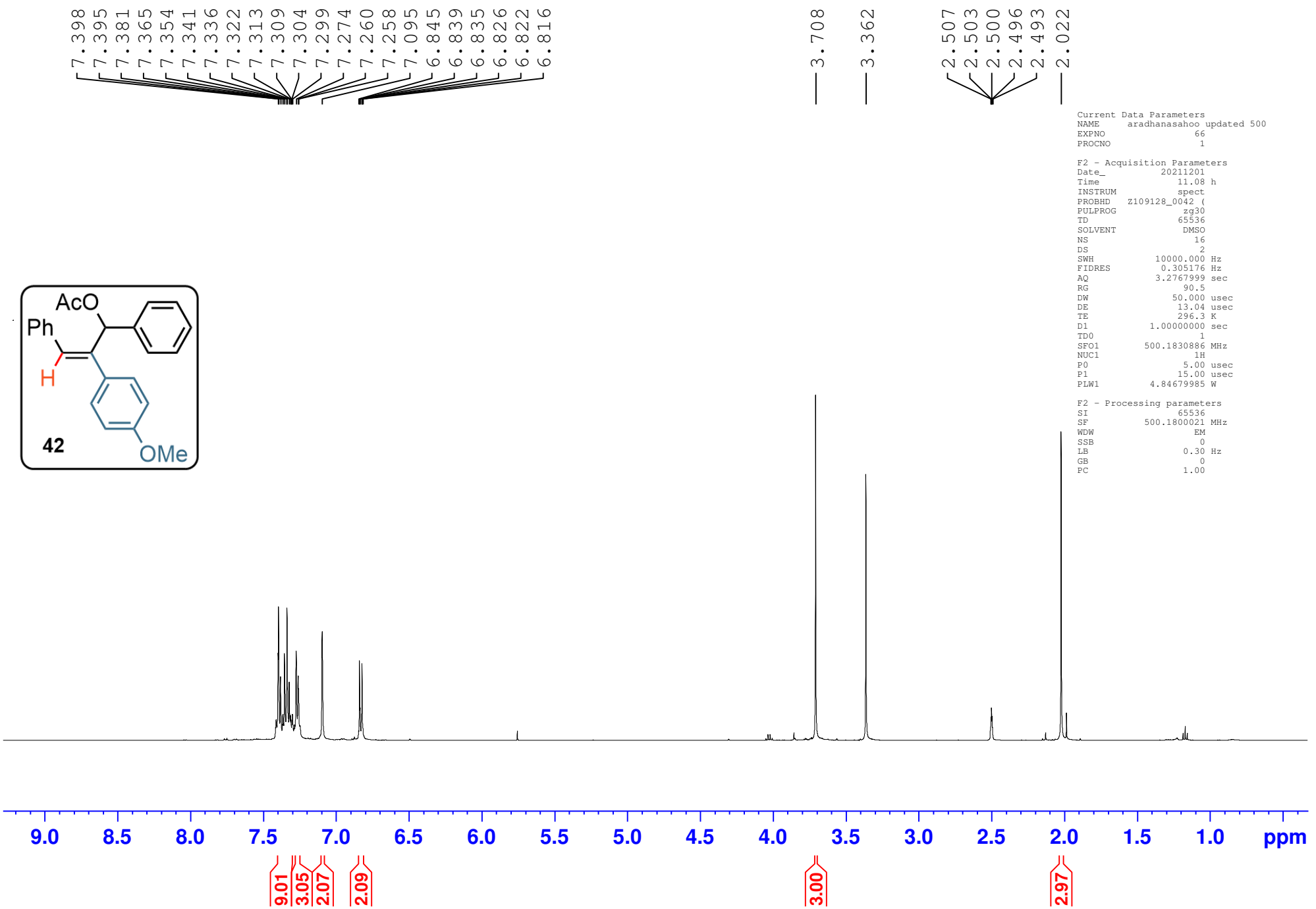

169.94
159.11
139.27
138.73
132.18
129.97
129.72
127.91
127.77
122.88
113.97
69.18
55.55
40.46
40.30
40.13
39.96
39.80
39.63
39.46
21.30
19.78
Me
AcO
S
H
MeO
39
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 53
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211215
Time 8.32 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 17753
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

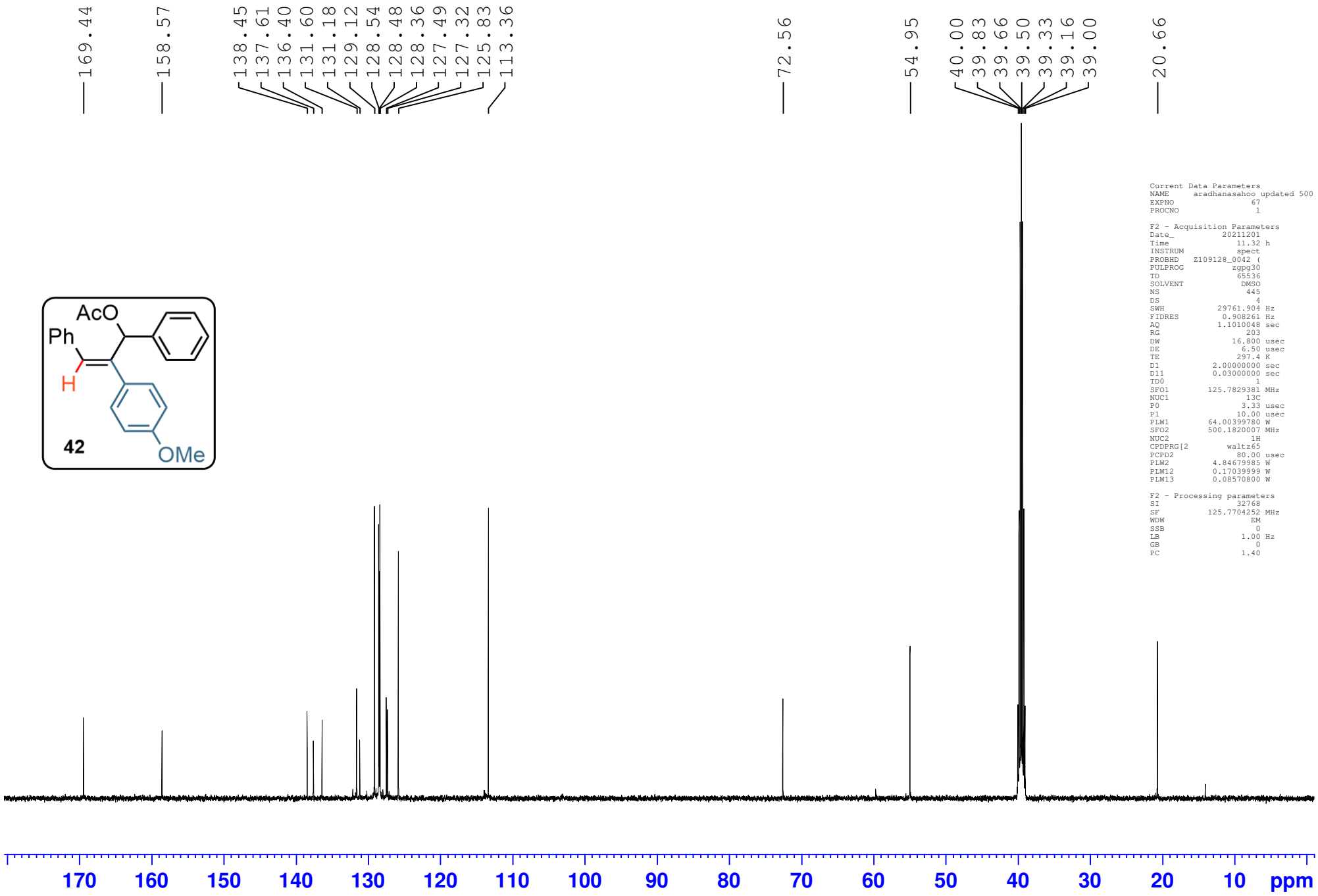

7.536
7.529
7.525
7.516
7.512
7.506
7.432
7.416
7.402
7.374
7.360
7.336
7.334
7.331
7.319
7.308
7.305
7.303
7.116
6.983
6.977
6.973
6.963
6.959
6.953
5.045
3.784
3.350
2.512
2.509
2.505
2.501
2.498
1.985
AcO
H
MeO
40
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 51
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 9.34 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 301.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.10
2.25
2.14
1.06
1.01
2.07
2.05
3.07
3.00

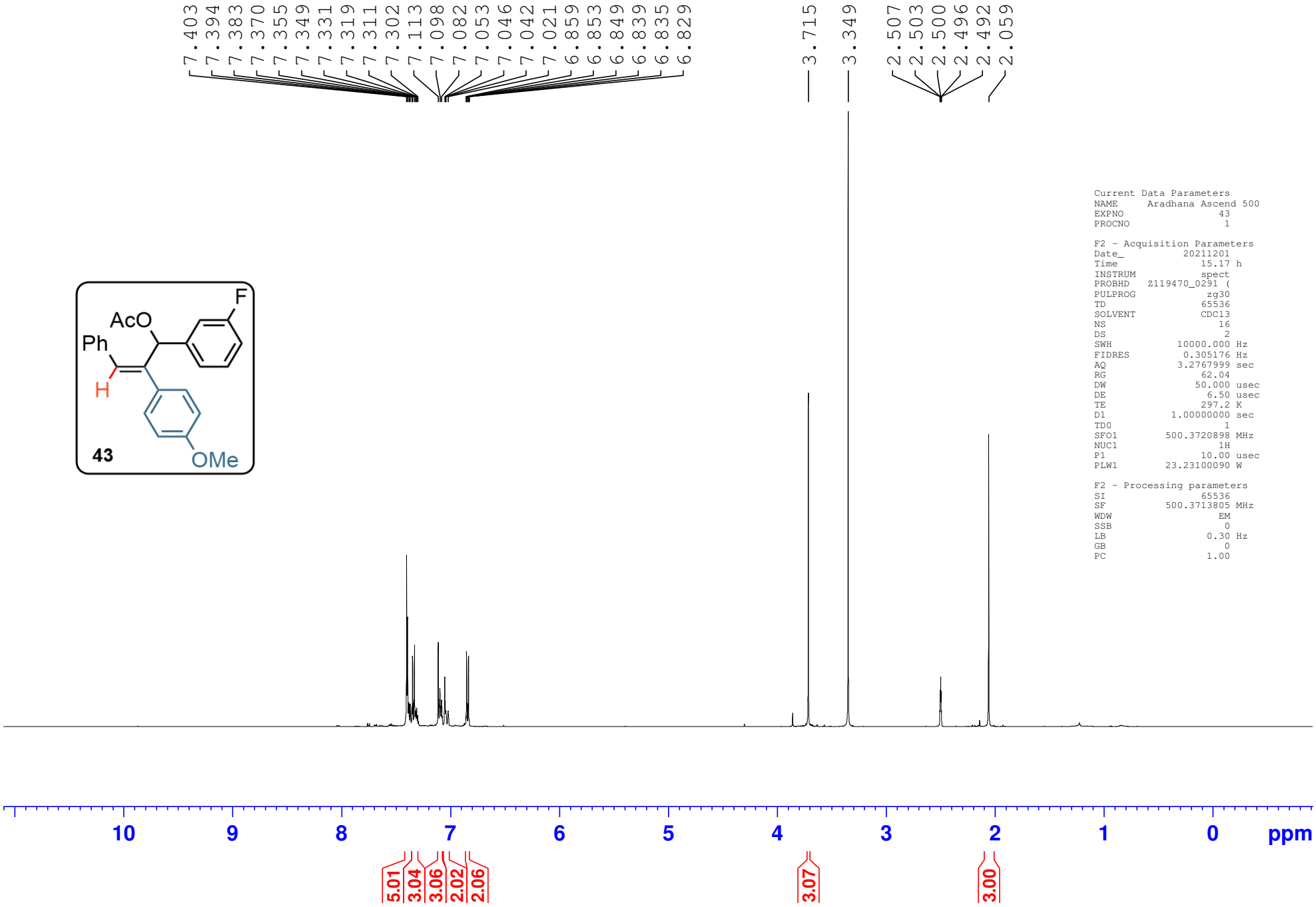

170.79
159.46
136.99
135.10
132.46
131.61
129.22
128.92
127.88
127.86
114.39
61.75
55.60
40.51
40.35
40.18
40.01
39.85
39.68
39.51
21.12
AcO
H
MeO
40
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 52
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 9.41 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 112
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.83
DW 16.800 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8304669 MHz
NUC1 13C
P1 10.00 usec
PLW1 115.01000214 W
SFO2 500.3710015 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.23100090 W
PLW12 0.36298999 W
PLW13 0.18257999 W
F2 - Processing parameters
SI 32768
SF 125.8178851 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

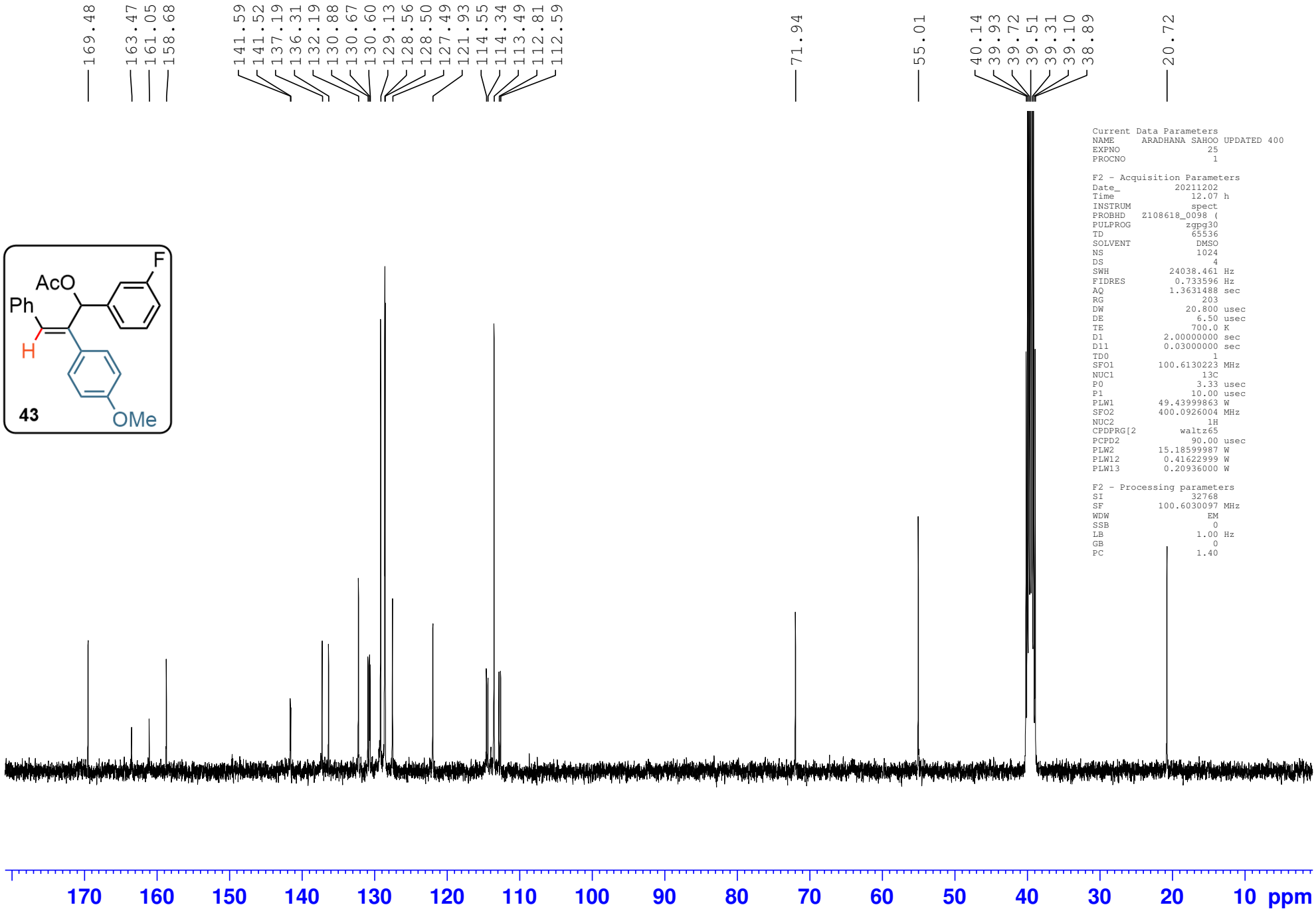

7.462
7.456
7.452
7.443
7.438
7.432
7.400
7.385
7.370
7.331
7.317
7.302
7.288
6.966
6.960
6.956
6.946
6.942
6.936
6.716
5.931
5.918
5.902
3.773
3.360
2.507
2.504
2.500
2.496
2.493
1.944
1.717
1.700
1.688
1.672
1.660
1.643
1.553
1.540
1.522
1.509
1.496
1.482
1.180
1.173
1.159
1.145
1.128
1.114
0.719
0.704
0.690
AcO
Ph
H
Me
OMe
41
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 49
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 10.35 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.03
3.06
2.05
1.00
1.02
3.04
3.00
2.15
2.04
3.04

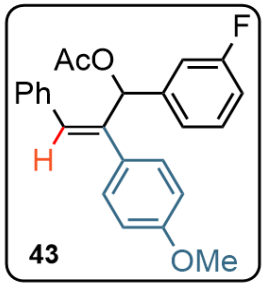

169.41
158.64
139.64
136.50
132.17
131.46
129.35
128.69
128.21
127.04
113.50
71.78
55.00
40.00
39.83
39.66
39.50
39.33
39.16
38.99
34.99
20.80
18.25
13.36
AcO
Ph
Me
H
41
OMe
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211206
Time 11.23 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 889
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 139.3
DW 16.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8304669 MHz
NUC1 13C
P1 10.00 usec
PLW1 115.01000214 W
SFO2 500.3710015 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.23100090 W
PLW12 0.36298999 W
PLW13 0.18257999 W
F2 - Processing parameters
SI 32768
SF 125.8179467 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.398
7.395
7.381
7.365
7.354
7.341
7.336
7.322
7.313
7.309
7.304
7.299
7.274
7.260
7.258
7.095
6.845
6.839
6.835
6.826
6.822
6.816
3.708
3.362
2.507
2.503
2.500
2.496
2.493
2.022
AcO
Ph
H
42
OMe
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 66
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 11.08 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 13.04 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
9.01
3.05
2.07
2.09
3.00
2.97


169.44
158.57
138.45
137.61
136.40
131.60
131.18
129.12
128.54
128.48
128.36
127.49
127.32
125.83
113.36
72.56
54.95
40.00
39.83
39.66
39.50
39.33
39.16
39.00
20.66
AcO
Ph
H
42
OMe
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 67
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 11.32 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 445
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 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7704252 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.403
7.394
7.383
7.370
7.355
7.349
7.331
7.319
7.311
7.302
7.113
7.098
7.082
7.053
7.046
7.042
7.021
6.859
6.853
6.849
6.839
6.835
6.829
3.715
3.349
2.507
2.503
2.500
2.496
2.492
2.059
AcO
Ph
H
F
OMe
43
Current Data Parameters
NAME Aradhana Ascend 500
EXPNO 43
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211201
Time 15.17 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 62.04
DW 50.000 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3713805 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
5.01
3.04
3.06
2.02
2.06
3.07
3.00

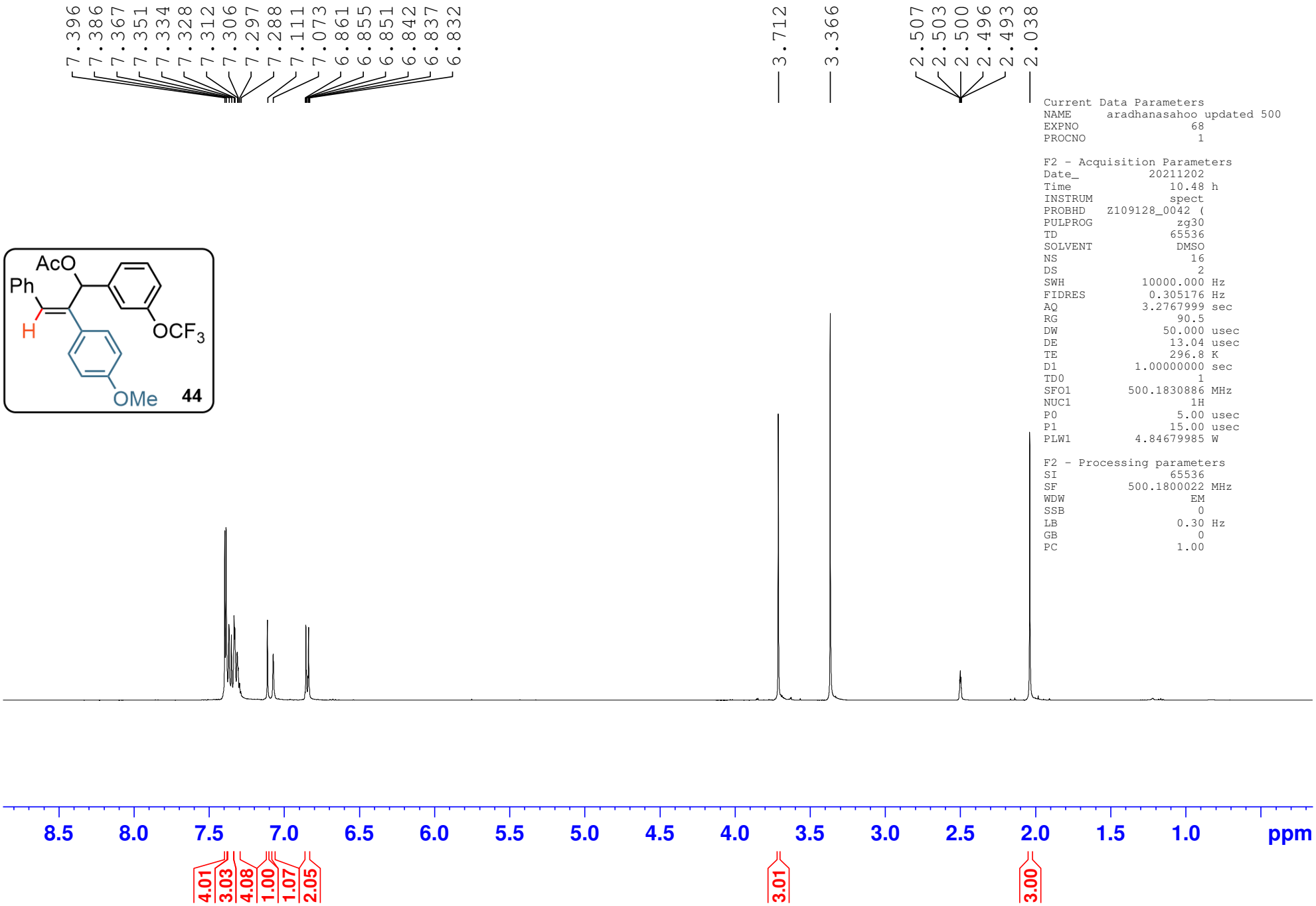

169.48
163.47
161.05
158.68
141.59
141.52
137.19
136.31
132.19
130.88
130.67
130.60
129.13
128.56
128.50
127.49
121.93
114.55
114.34
113.49
112.81
112.59
71.94
55.01
40.14
39.93
39.72
39.51
39.31
39.10
38.89
20.72
AcO
Ph
F
H
OMe
43
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 25
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 12.07 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 700.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6030097 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

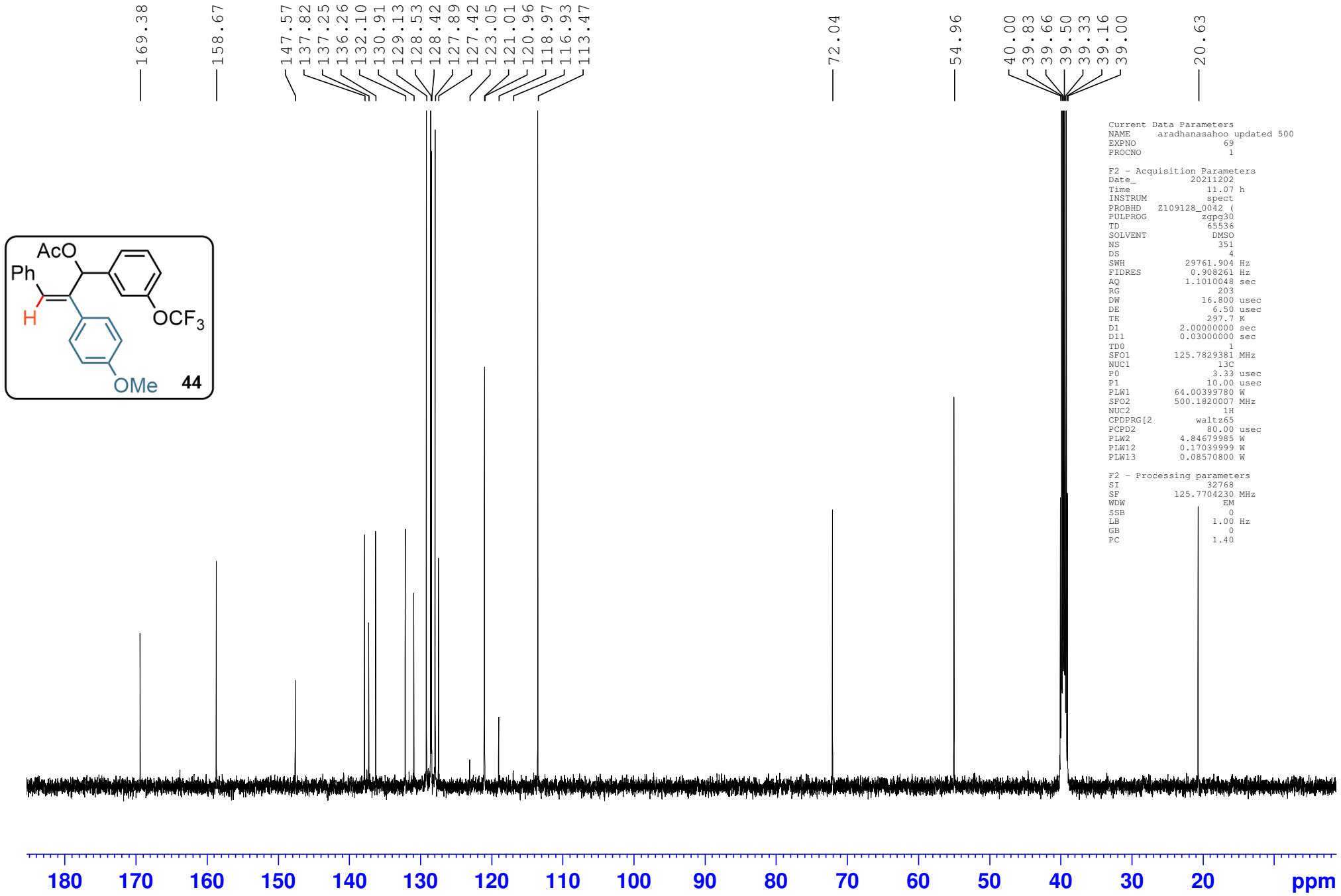


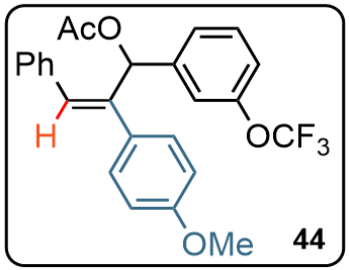
-112.56

```
Current Data Parameters
NAME      ARADHANA SAHOO UPDATED 400
EXPNO                 24
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211202
Time              11.07 h
INSTRUM             spect
PROBHD   Z108618_0098 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT              DMSO
NS                    16
DS                     4
SWH            89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                   645
DW                 5.600 usec
DE                 6.50 usec
TE                 702.5 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.4240234 MHz
NUC1                 19F
P1                14.80 usec
PLW1         18.11000061 W
SFO2         400.0926004 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         15.18599987 W
PLW12         0.41622999 W

F2 - Processing parameters
SI                 65536
SF           376.4616700 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

-40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 ppm


7.396
7.386
7.367
7.351
7.334
7.328
7.312
7.306
7.297
7.288
7.111
7.073
6.861
6.855
6.851
6.842
6.837
6.832
3.712
3.366
2.507
2.503
2.500
2.496
2.493
2.038
AcO
Ph
H
OCF3
OMe
44
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 68
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 10.48 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 13.04 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
4.01
3.03
4.08
1.00
1.07
2.05
3.01
3.00

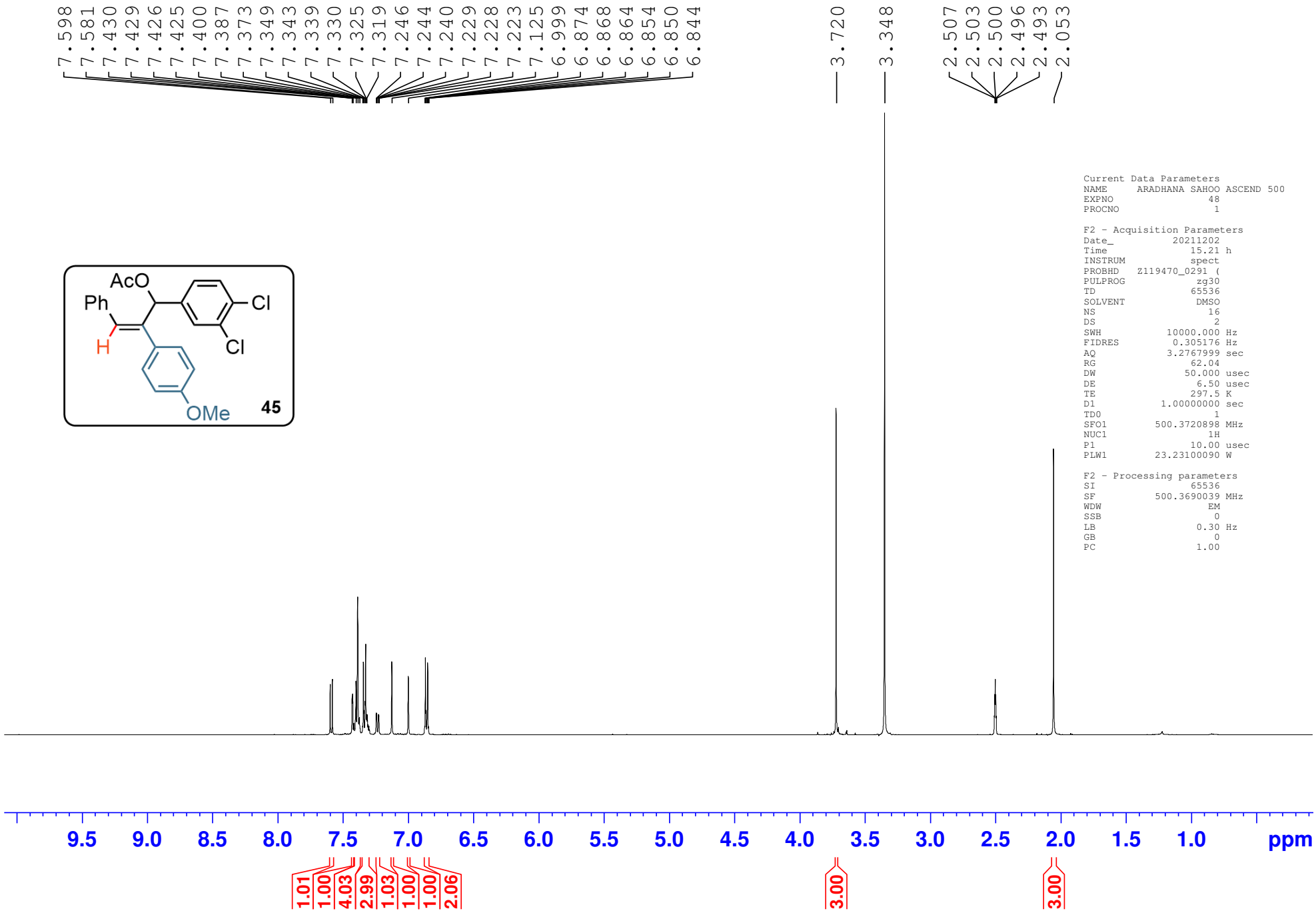

169.38
158.67
147.57
137.82
137.25
136.26
132.10
130.91
129.13
128.53
128.42
127.89
127.42
123.05
121.01
120.96
118.97
116.93
113.47
72.04
54.96
40.00
39.83
39.66
39.50
39.33
39.16
39.00
20.63
AcO
Ph
H
OCF3
OMe
44
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 69
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 11.07 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 351
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 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7704230 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

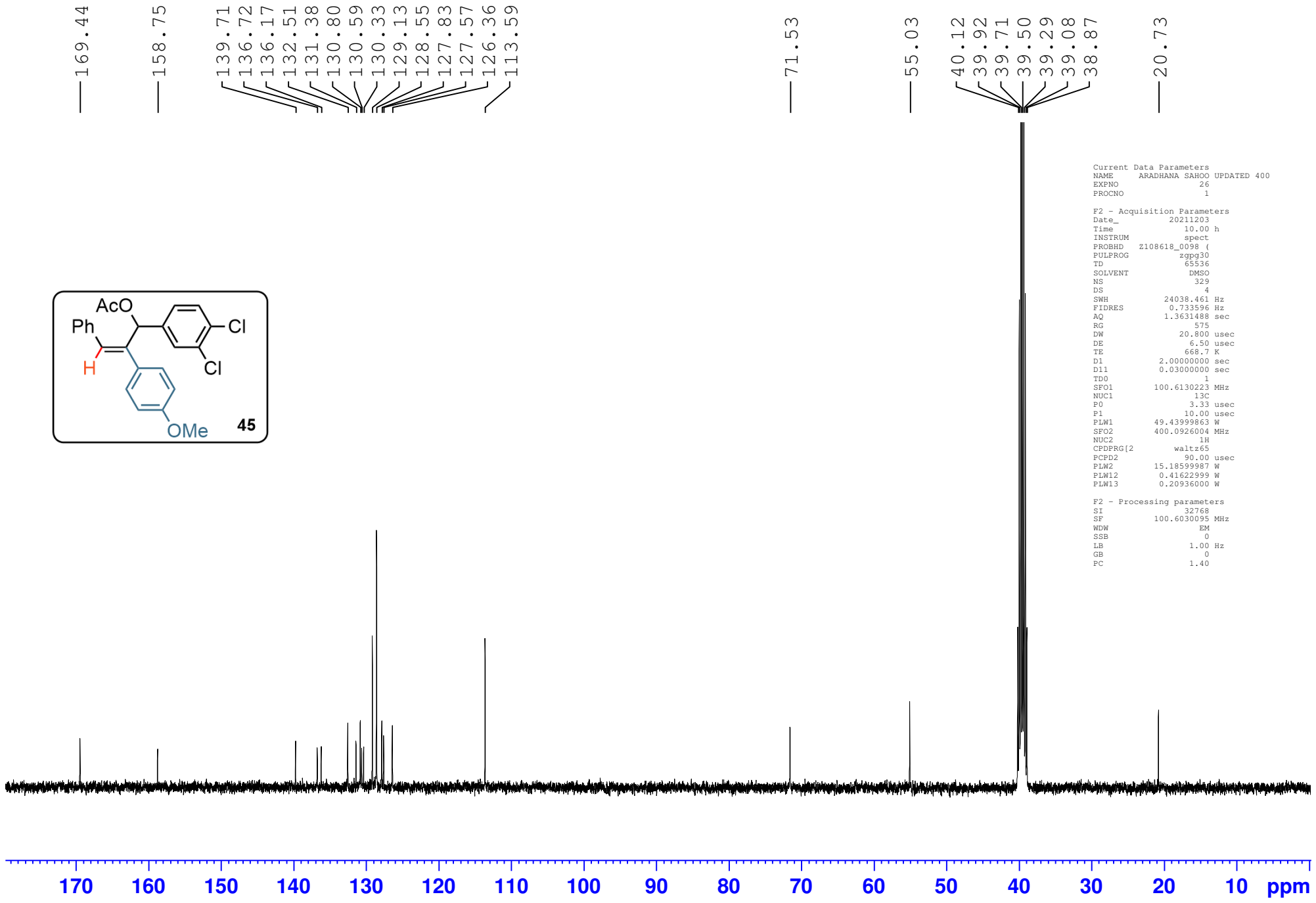


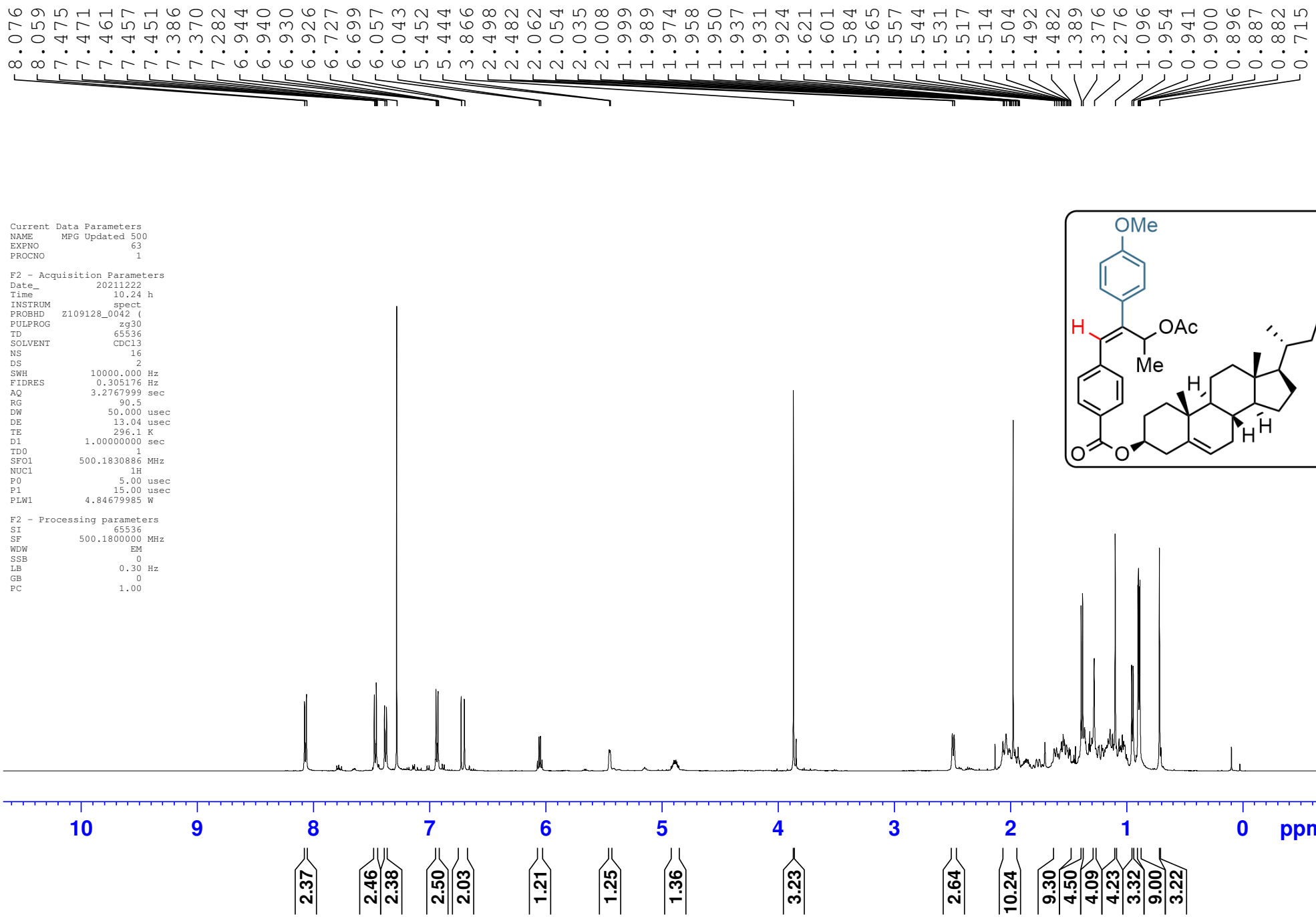
-56.84

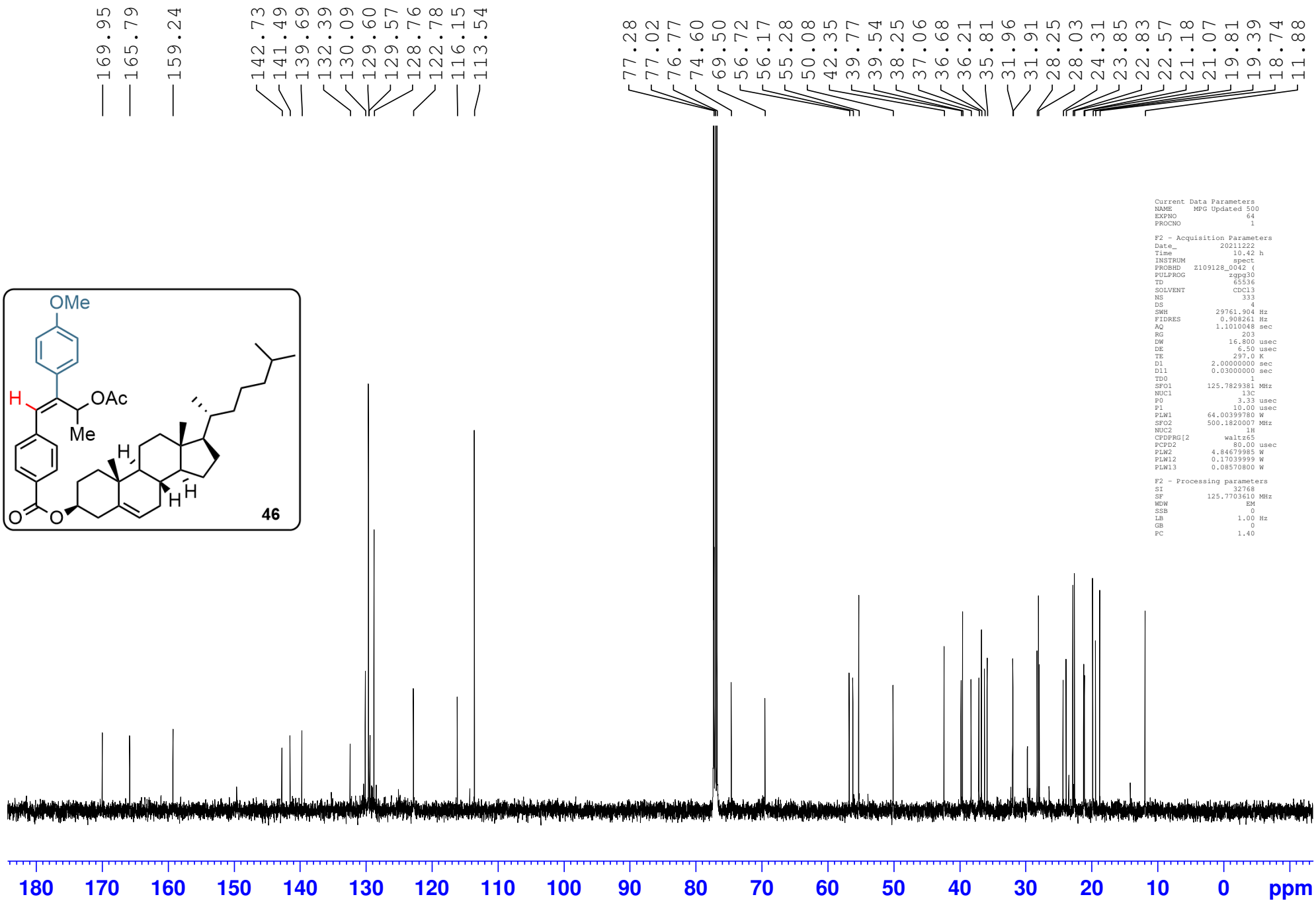
```
Current Data Parameters
NAME      ARADHANA SAHOO UPDATED 400
EXPNO                 27
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211203
Time              11.17 h
INSTRUM             spect
PROBHD   Z108618_0098 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT              DMSO
NS                      16
DS                       4
SWH             89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                     812
DW                 5.600 usec
DE                 6.50 usec
TE                 668.7 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                     1
SFO1         376.4240234 MHz
NUC1                  19F
P1                14.80 usec
PLW1         18.11000061 W
SFO2         400.0926004 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         15.18599987 W
PLW12         0.41622999 W

F2 - Processing parameters
SI                    65536
SF           376.4616700 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

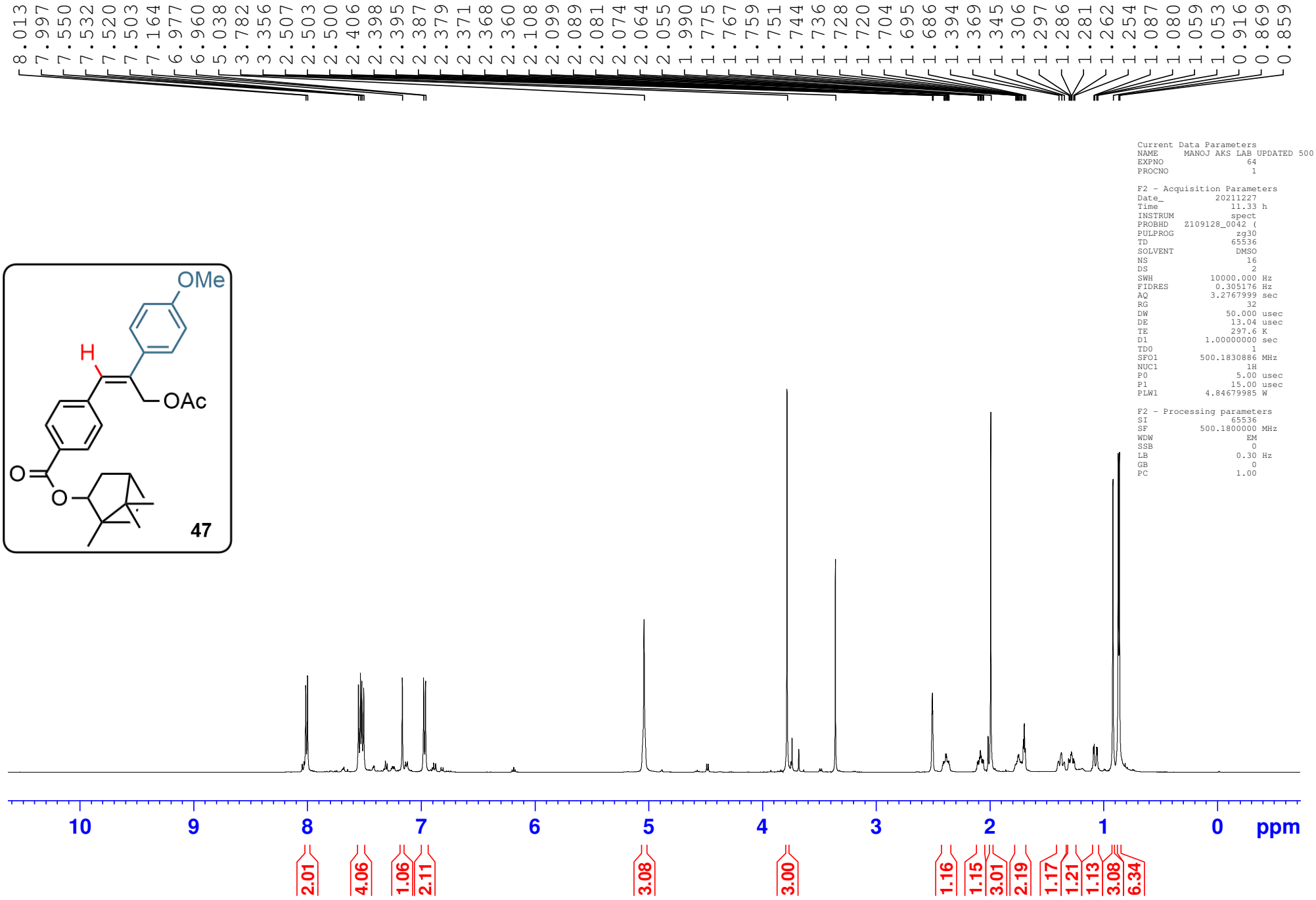
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 ppm

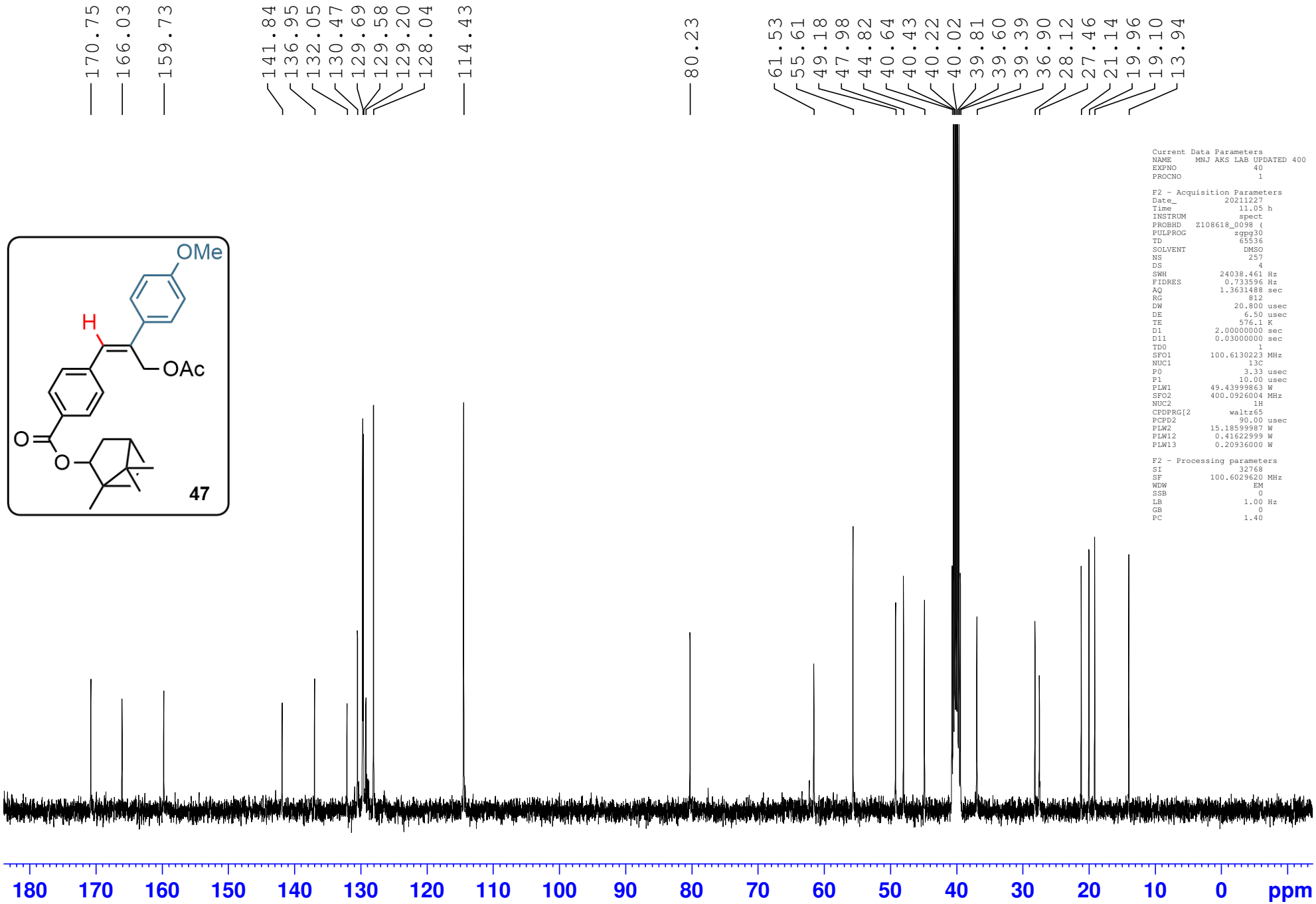

7.598
7.581
7.430
7.429
7.426
7.425
7.400
7.387
7.373
7.349
7.343
7.339
7.330
7.325
7.319
7.246
7.244
7.240
7.229
7.228
7.223
7.125
6.999
6.874
6.868
6.864
6.854
6.850
6.844
3.720
3.348
2.507
2.503
2.500
2.496
2.493
2.053
AcO
Ph
H
Cl
Cl
OMe
45
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211202
Time 15.21 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 62.04
DW 50.000 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.01 1.00 4.03 2.99 1.03 1.00 1.00 2.06
3.00
3.00

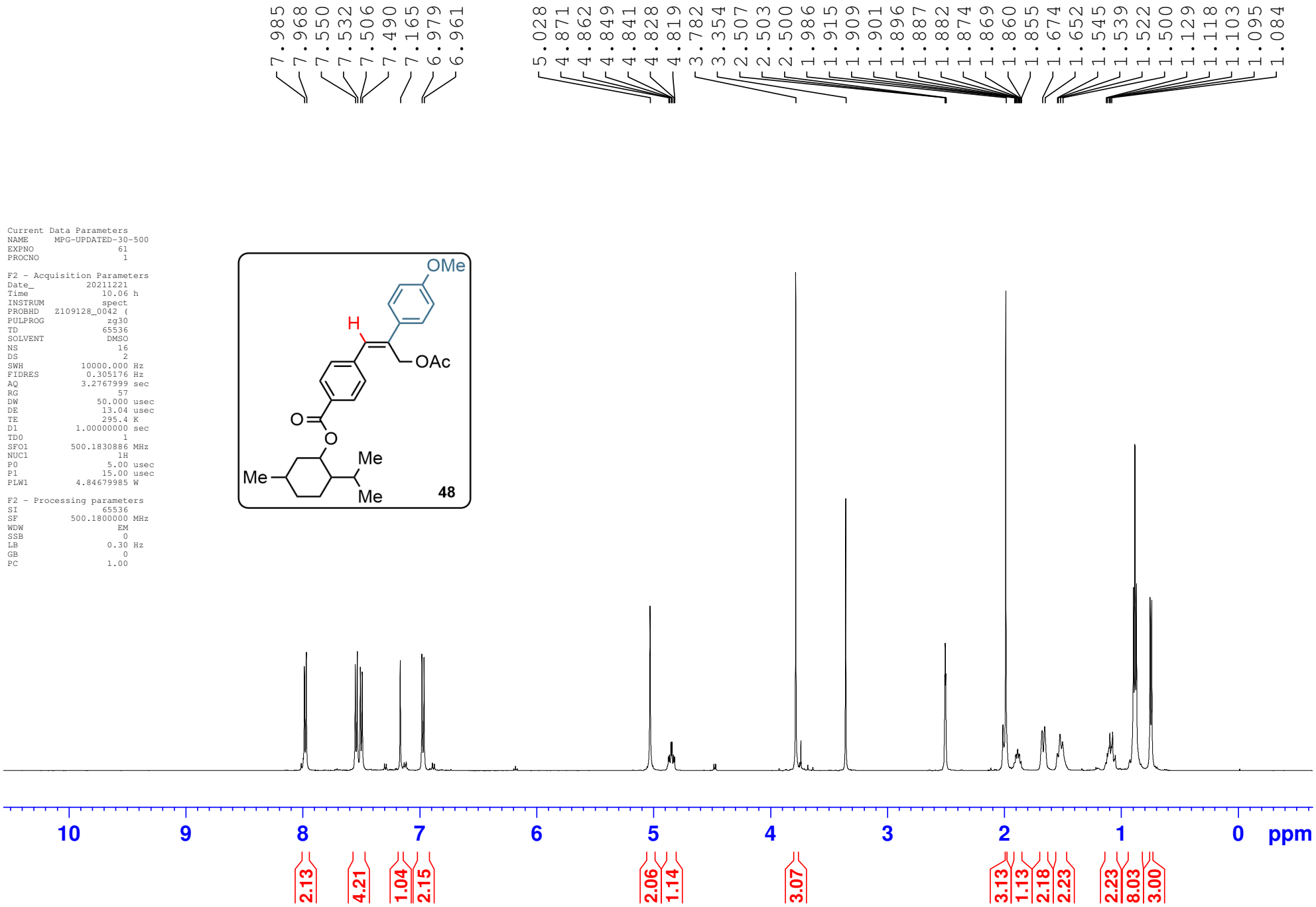

169.44
158.75
139.71
136.72
136.17
132.51
131.38
130.80
130.59
130.33
129.13
128.55
127.83
127.57
126.36
113.59
71.53
55.03
40.12
39.92
39.71
39.50
39.29
39.08
38.87
20.73
AcO
Ph
H
Cl
Cl
OMe
45
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 26
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211203
Time 10.00 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 329
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 575
DW 20.800 usec
DE 6.50 usec
TE 668.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6030095 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

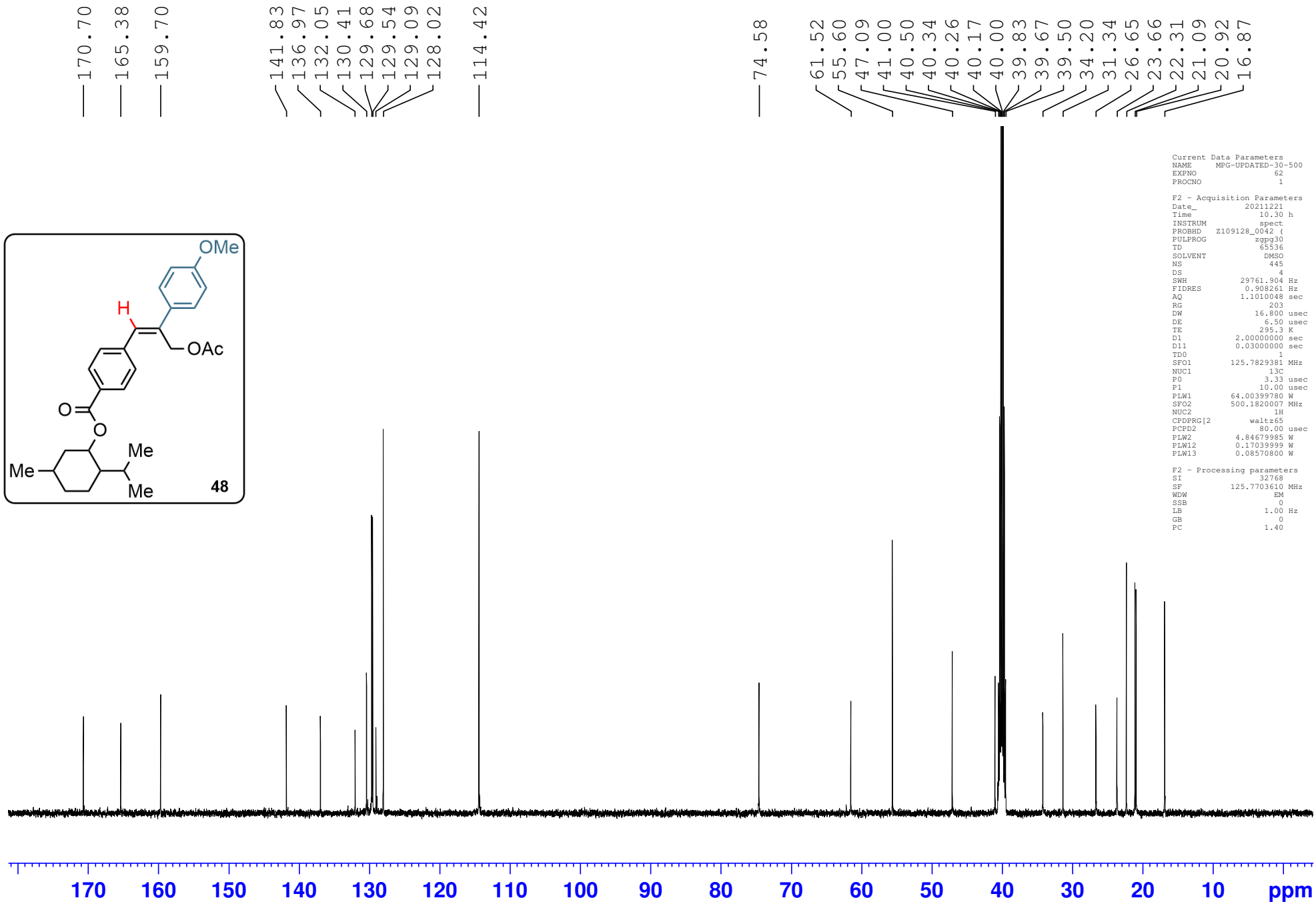

8.076 8.059 7.475 7.471 7.461 7.457 7.451 7.386 7.370 7.282 6.944 6.940 6.930 6.926 6.727 6.699 6.057 6.043 5.452 5.444 3.866 2.498 2.482 2.062 2.054 2.035 2.008 1.999 1.989 1.974 1.958 1.950 1.937 1.931 1.924 1.621 1.601 1.584 1.565 1.557 1.544 1.531 1.517 1.514 1.504 1.492 1.482 1.389 1.376 1.276 1.096 0.954 0.941 0.900 0.896 0.887 0.882 0.715
Current Data Parameters
NAME MPG Updated 500
EXPNO 63
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 10.24 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 13.04 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
H
OAc
Me
H
H
H
O
O
46
10 9 8 7 6 5 4 3 2 1 0 ppm
2.37 2.46 2.38 2.50 2.03 1.21 1.25 1.36 3.23 2.64 10.24 9.30 4.50 4.09 4.23 3.32 9.00 3.22

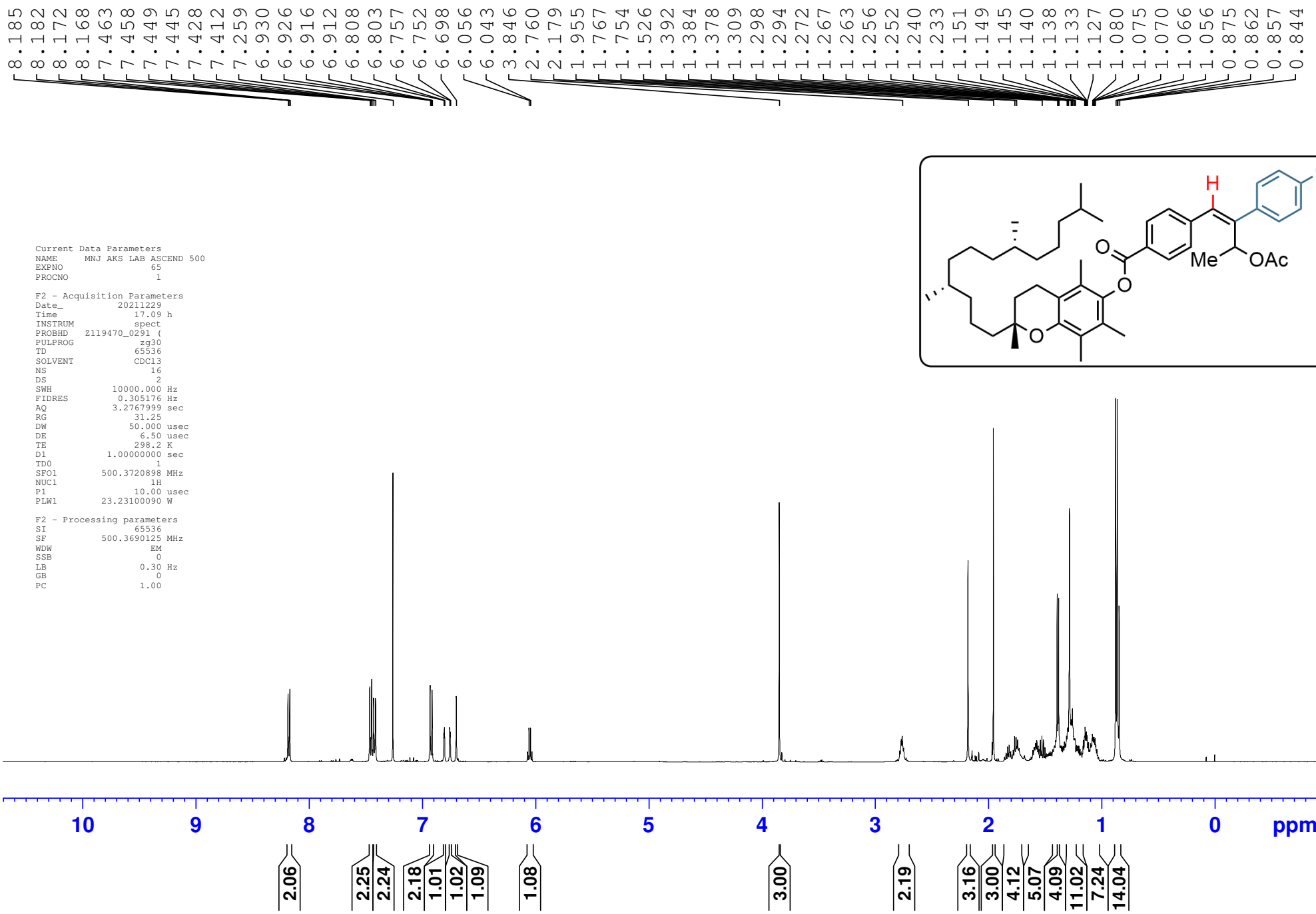

169.95
165.79
159.24
142.73
141.49
139.69
132.39
130.09
129.60
129.57
128.76
122.78
116.15
113.54
77.28
77.02
76.77
74.60
69.50
56.72
56.17
55.28
50.08
42.35
39.77
39.54
38.25
37.06
36.68
36.21
35.81
31.96
31.91
28.25
28.03
24.31
23.85
22.83
22.57
21.18
21.07
19.81
19.39
18.74
11.88
OMe
H
OAc
Me
H
H
H
O
O
46
Current Data Parameters
NAME MPG Updated 500
EXPNO 64
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 10.42 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 333
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 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

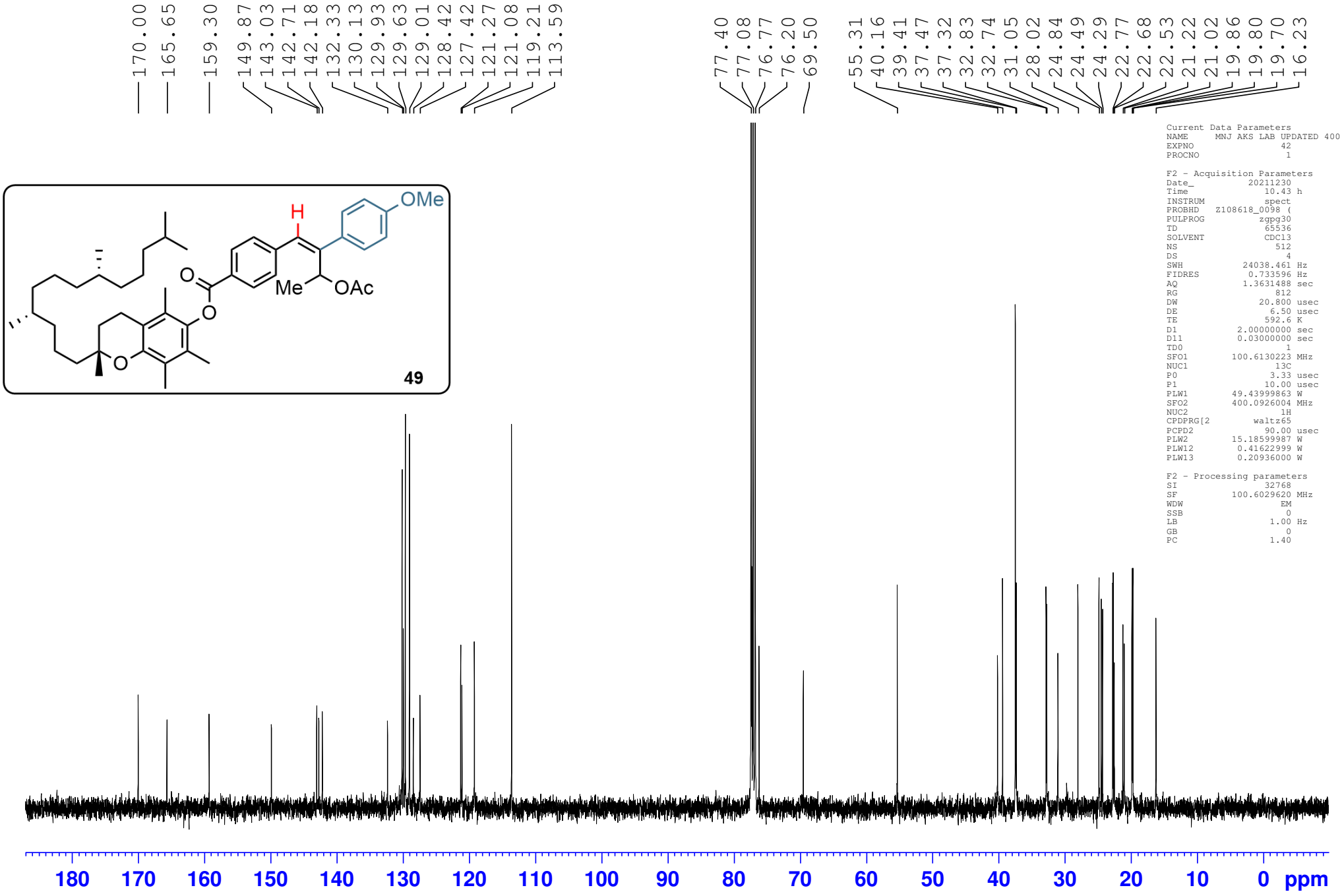

8.013
7.997
7.550
7.532
7.520
7.503
7.164
6.977
6.960
6.038
5.782
3.356
2.507
2.503
2.500
2.406
2.398
2.395
2.387
2.379
2.371
2.368
2.360
2.108
2.099
2.089
2.081
2.074
2.064
2.055
1.990
1.775
1.767
1.759
1.751
1.744
1.736
1.728
1.720
1.704
1.695
1.686
1.394
1.369
1.345
1.306
1.297
1.286
1.281
1.262
1.254
1.087
1.080
1.059
1.053
0.916
0.869
0.859
OMe
H
OAc
O
O
47
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 64
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211227
Time 11.33 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 32
DW 50.000 usec
DE 13.04 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
4.06
1.06
2.11
3.08
3.00
1.16
1.15
3.01
2.19
1.17
1.21
1.13
3.08
6.34

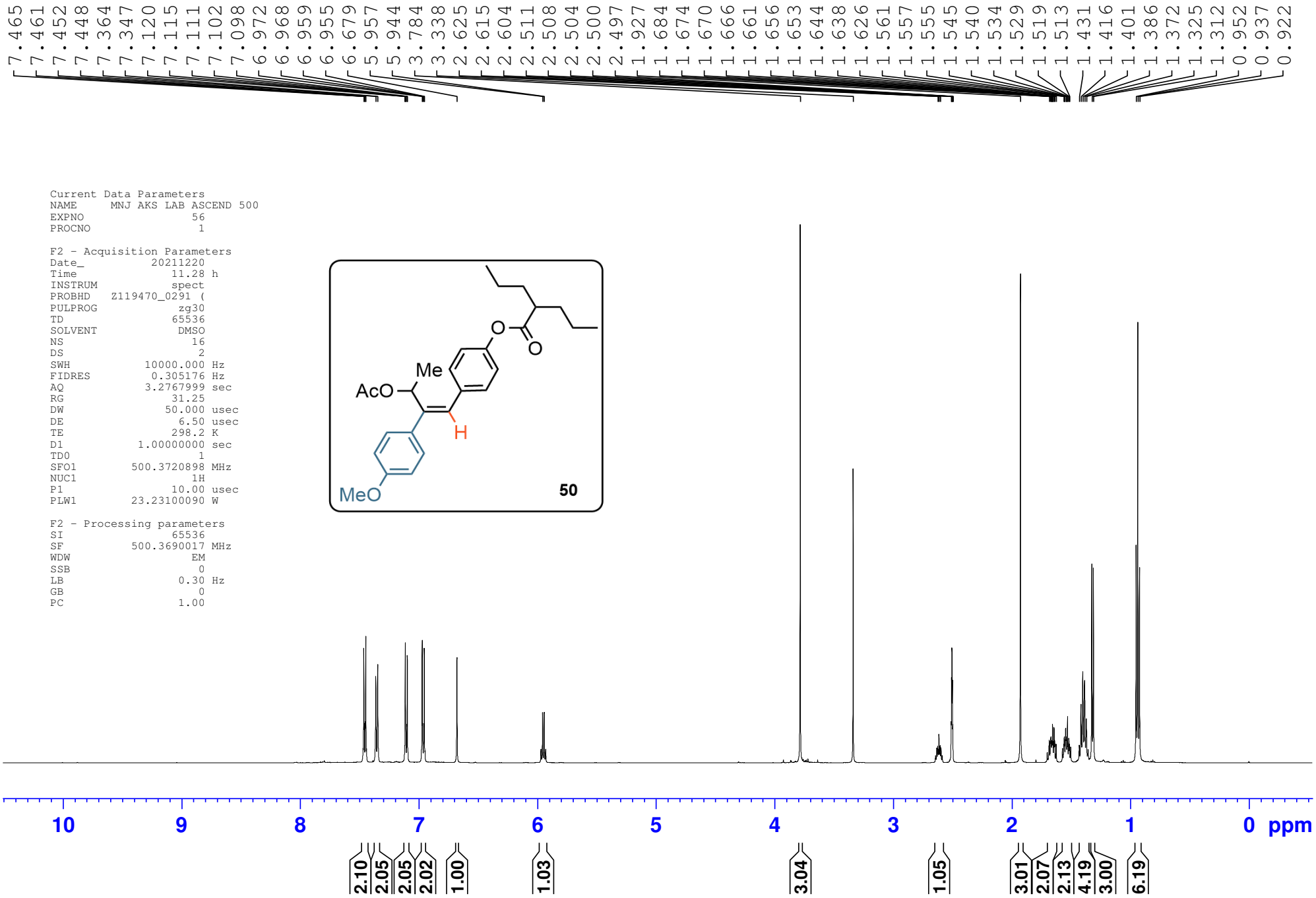

170.75
166.03
159.73
141.84
136.95
132.05
130.47
129.69
129.58
129.20
128.04
114.43
80.23
61.53
55.61
49.18
47.98
44.82
40.64
40.43
40.22
40.02
39.81
39.60
39.39
36.90
28.12
27.46
21.14
19.96
19.10
13.94
OMe
H
OAc
O
O
47
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211227
Time 11.05 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 257
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 812
DW 20.800 usec
DE 6.50 usec
TE 576.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

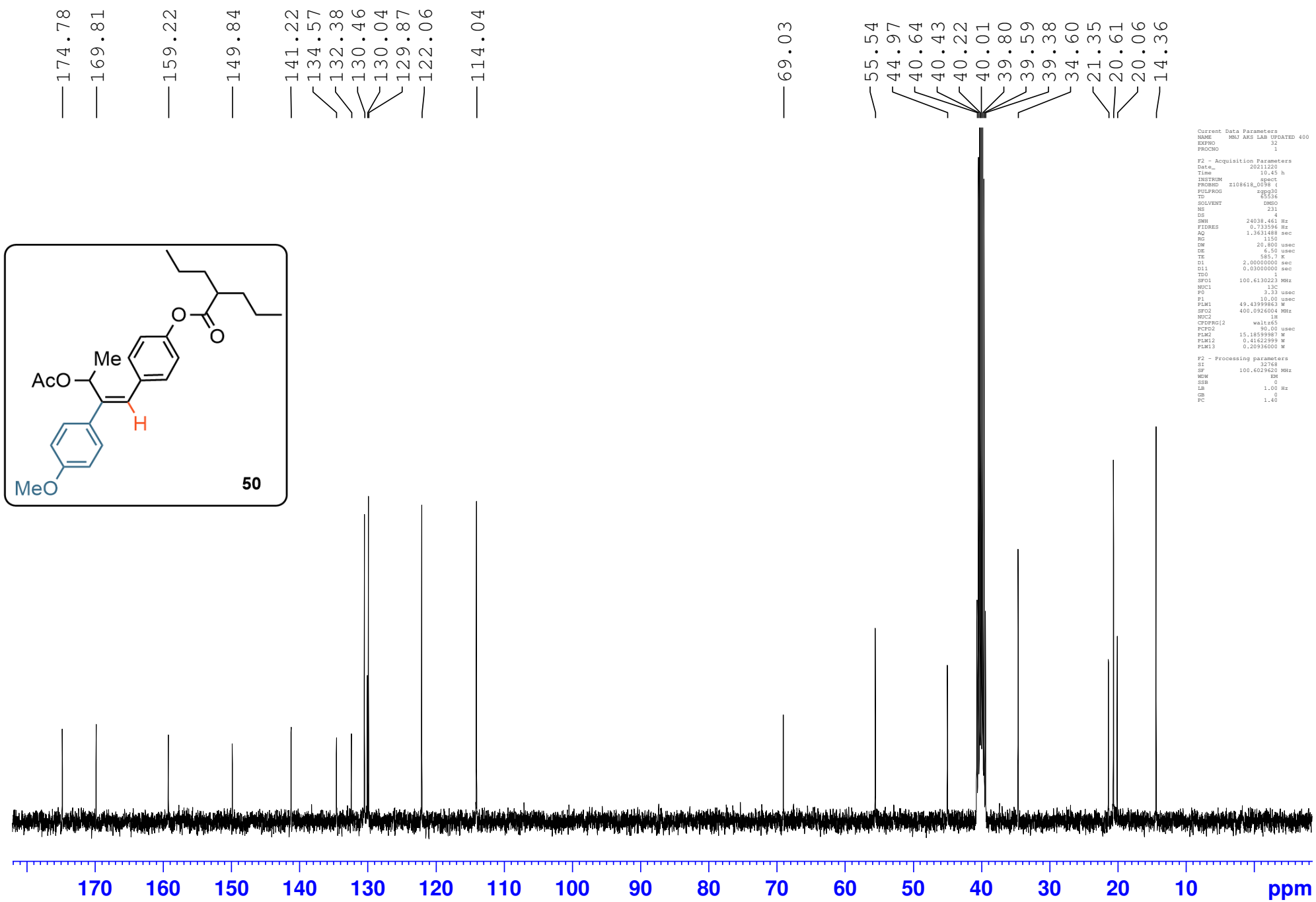

7.985
7.968
7.550
7.532
7.506
7.490
7.165
6.979
6.961
5.028
4.871
4.862
4.849
4.841
4.828
4.819
3.782
3.354
2.507
2.503
2.500
1.986
1.915
1.909
1.901
1.896
1.887
1.882
1.874
1.869
1.860
1.855
1.674
1.652
1.545
1.539
1.522
1.500
1.129
1.118
1.103
1.095
1.084
Current Data Parameters
NAME MPG-UPDATED-30-500
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211221
Time 10.06 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 57
DW 50.000 usec
DE 13.04 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
H
OAc
O
O
Me
Me
Me
48
10
9
8
7
6
5
4
3
2
1
0
ppm
2.13
4.21
1.04
2.15
2.06
1.14
3.07
3.13
1.13
2.18
2.23
2.23
8.03
3.00

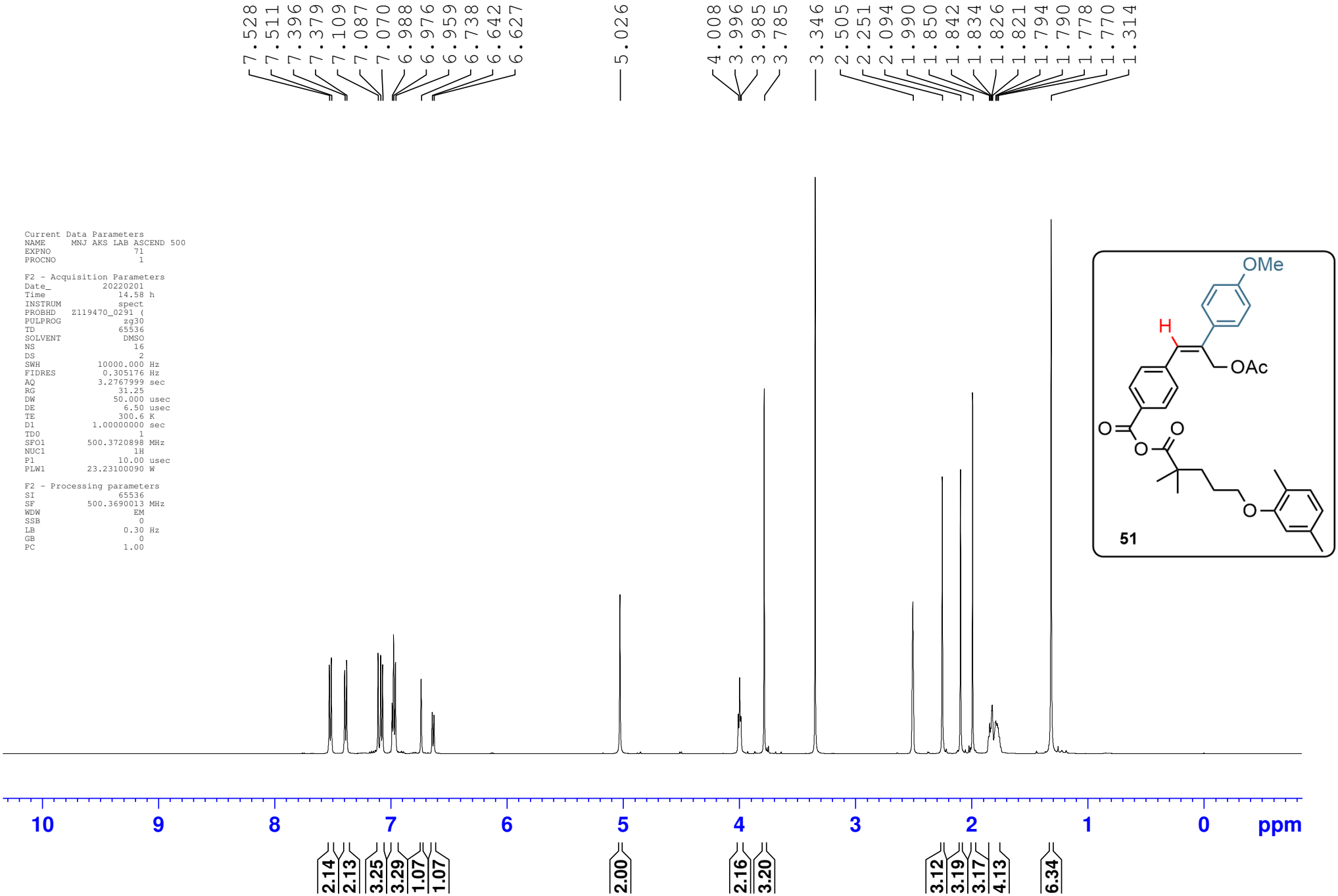

170.70
165.38
159.70
141.83
136.97
132.05
130.41
129.68
129.54
129.09
128.02
114.42
74.58
61.52
55.60
47.09
41.00
40.50
40.34
40.26
40.17
40.00
39.83
39.67
39.50
34.20
31.34
26.65
23.66
22.31
21.09
20.92
16.87
OMe
H
OAc
O
O
Me
Me
Me
48
Current Data Parameters
NAME MPG-UPDATED-30-500
EXPNO 62
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211221
Time 10.30 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 445
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 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

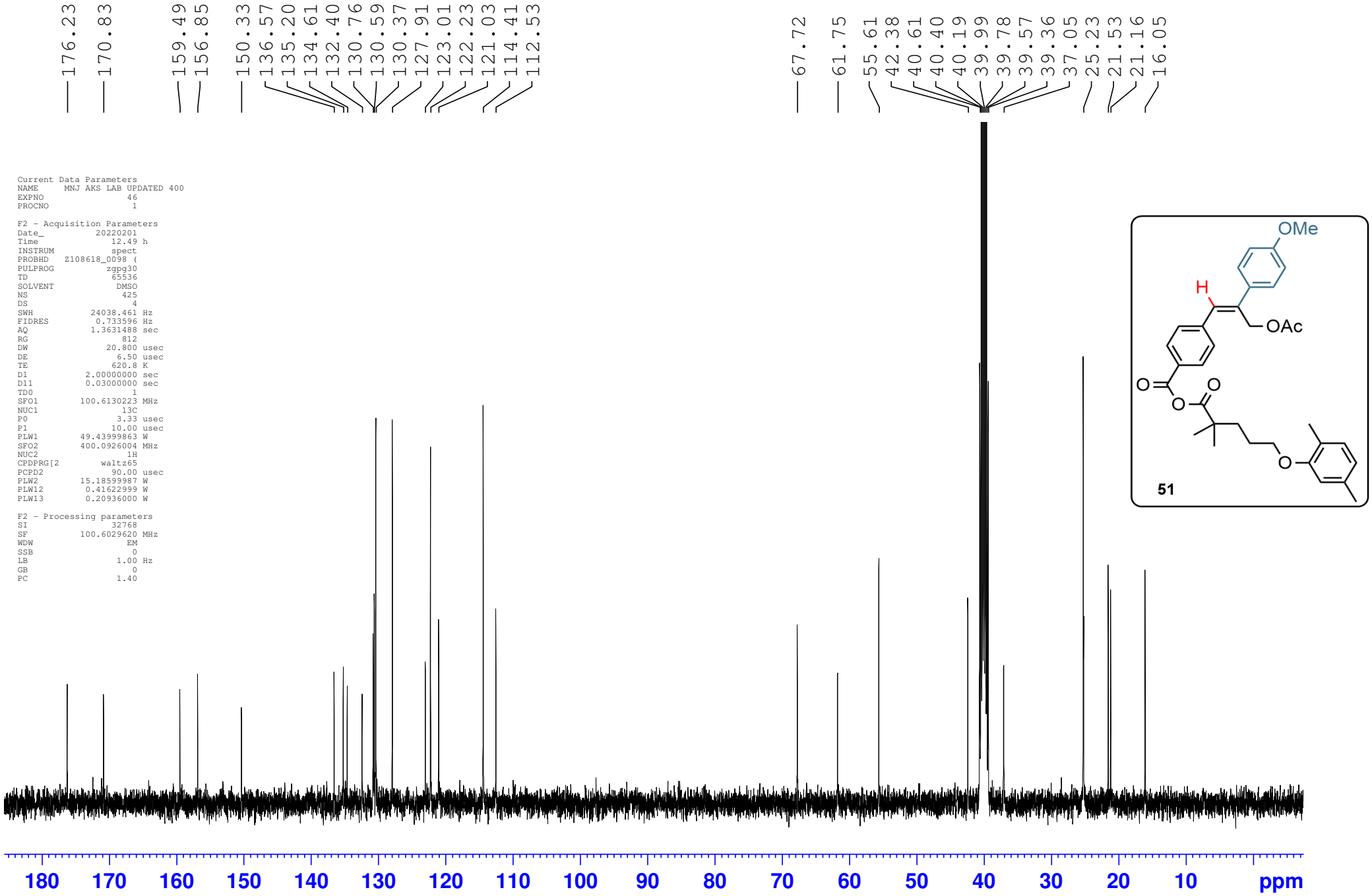

8.185
8.182
8.172
8.168
8.463
7.458
7.449
7.445
7.428
7.412
7.259
6.930
6.926
6.916
6.912
6.808
6.803
6.757
6.752
6.698
6.056
6.043
3.846
2.760
2.179
1.955
1.767
1.754
1.526
1.392
1.384
1.378
1.309
1.298
1.294
1.272
1.267
1.263
1.256
1.252
1.240
1.233
1.151
1.149
1.145
1.140
1.138
1.133
1.127
1.080
1.075
1.070
1.066
1.056
0.875
0.862
0.857
0.844
OMe
H
O
Me
OAc
O
O
49
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 65
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211229
Time 17.09 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
2.25
2.24
2.18
1.01
1.02
1.09
1.08
3.00
2.19
3.16
3.00
4.12
5.07
4.09
11.02
7.24
14.04

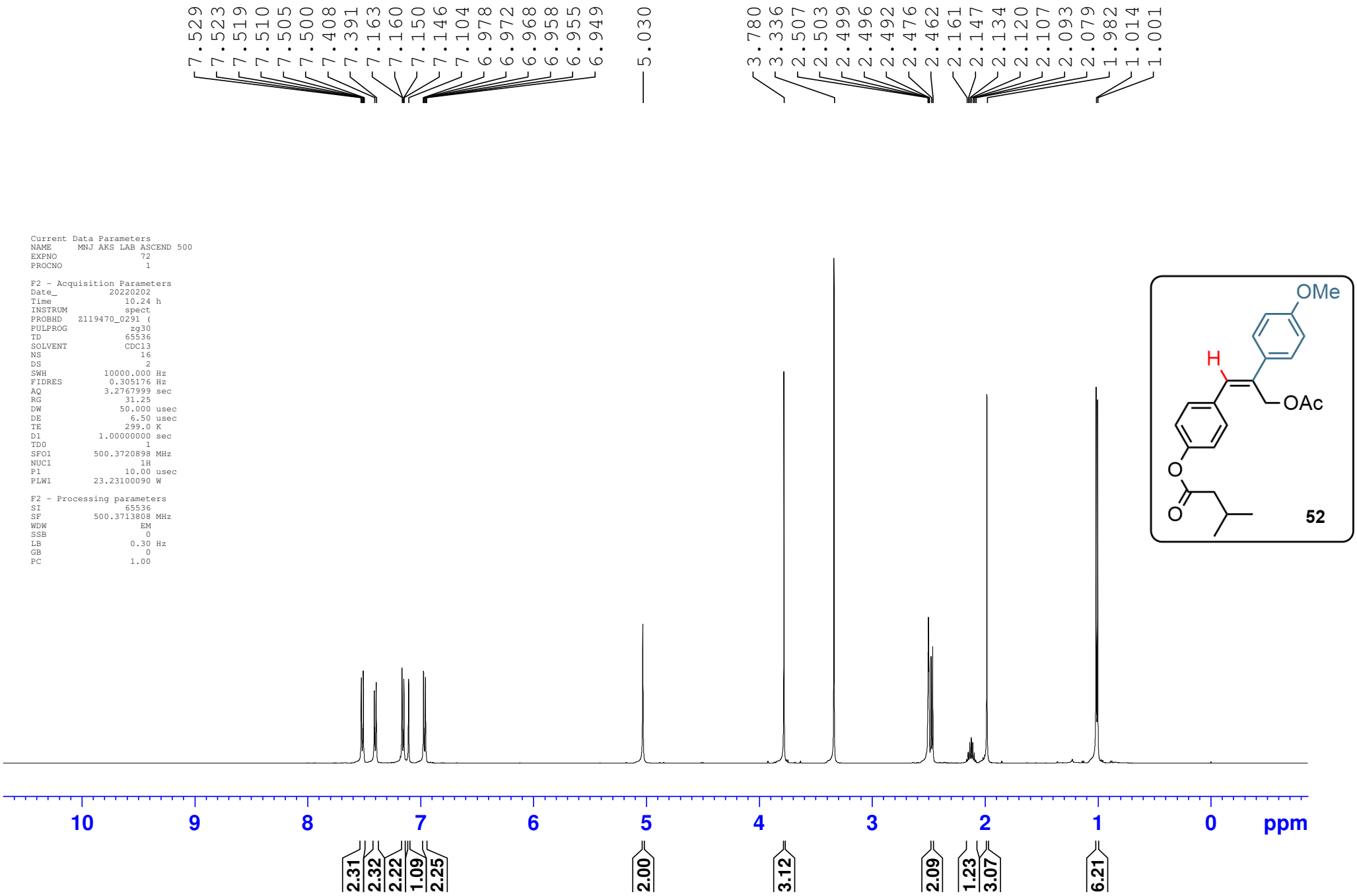

170.00
165.65
159.30
149.87
143.03
142.71
142.18
132.33
130.13
129.93
129.63
129.01
128.42
127.42
121.27
121.08
119.21
113.59
77.40
77.08
76.77
76.20
69.50
55.31
40.16
39.41
37.47
37.32
32.83
32.74
31.05
28.02
24.84
24.49
24.29
22.77
22.68
22.53
21.22
21.02
19.86
19.80
19.70
16.23
OMe
H
O
Me
OAc
O
O
49
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211230
Time 10.43 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 812
DW 20.800 usec
DE 6.50 usec
TE 592.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

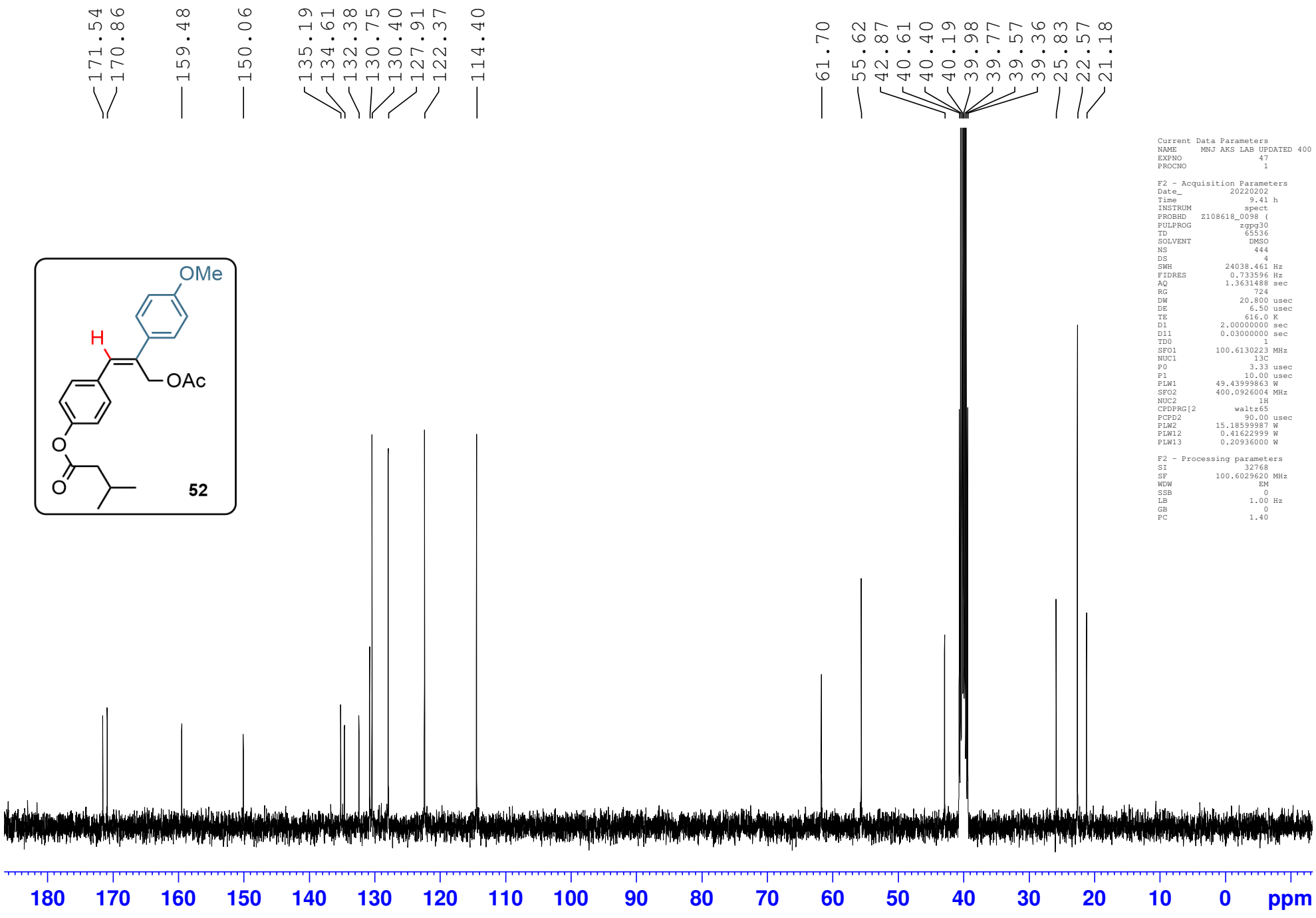

7.465
7.461
7.452
7.448
7.364
7.347
7.120
7.115
7.111
7.102
7.098
6.972
6.968
6.959
6.955
6.679
6.957
5.944
3.784
3.338
2.625
2.615
2.604
2.511
2.508
2.504
2.500
2.497
1.927
1.684
1.674
1.670
1.666
1.661
1.656
1.653
1.644
1.638
1.626
1.561
1.557
1.555
1.545
1.540
1.534
1.529
1.519
1.513
1.431
1.416
1.401
1.386
1.372
1.325
1.312
0.952
0.937
0.922
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 56
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211220
Time 11.28 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
AcO
Me
O
O
H
MeO
50
10
9
8
7
6
5
4
3
2
1
0 ppm
2.10
2.05
2.05
2.02
1.00
1.03
3.04
1.05
3.01
2.07
2.13
4.19
3.00
6.19

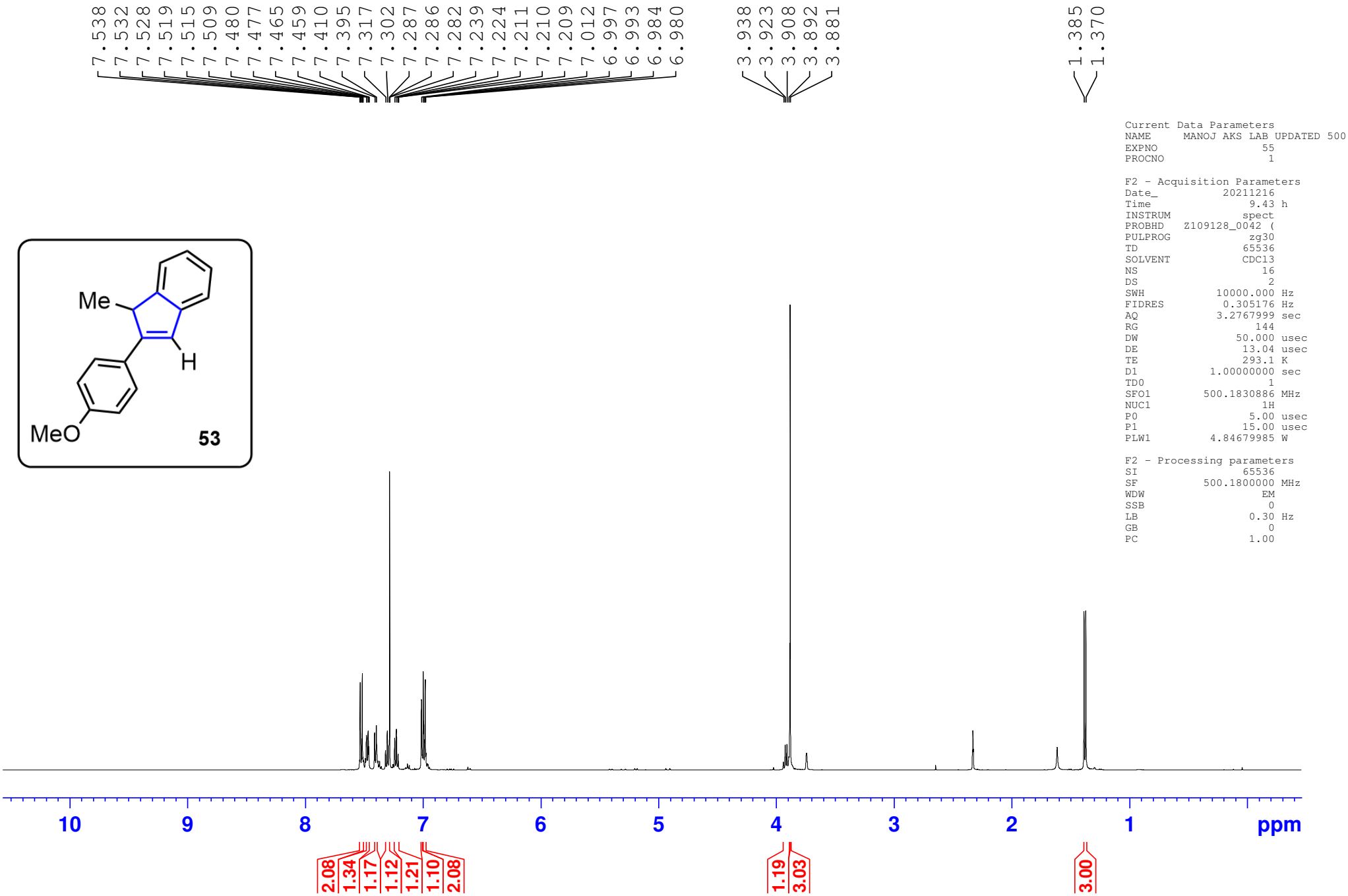

174.78
169.81
159.22
149.84
141.22
134.57
132.38
130.46
130.04
129.87
122.06
114.04
69.03
55.54
44.97
40.64
40.43
40.22
40.01
39.80
39.59
39.38
34.60
21.35
20.61
20.06
14.36
AcO
Me
O
O
H
MeO
50
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

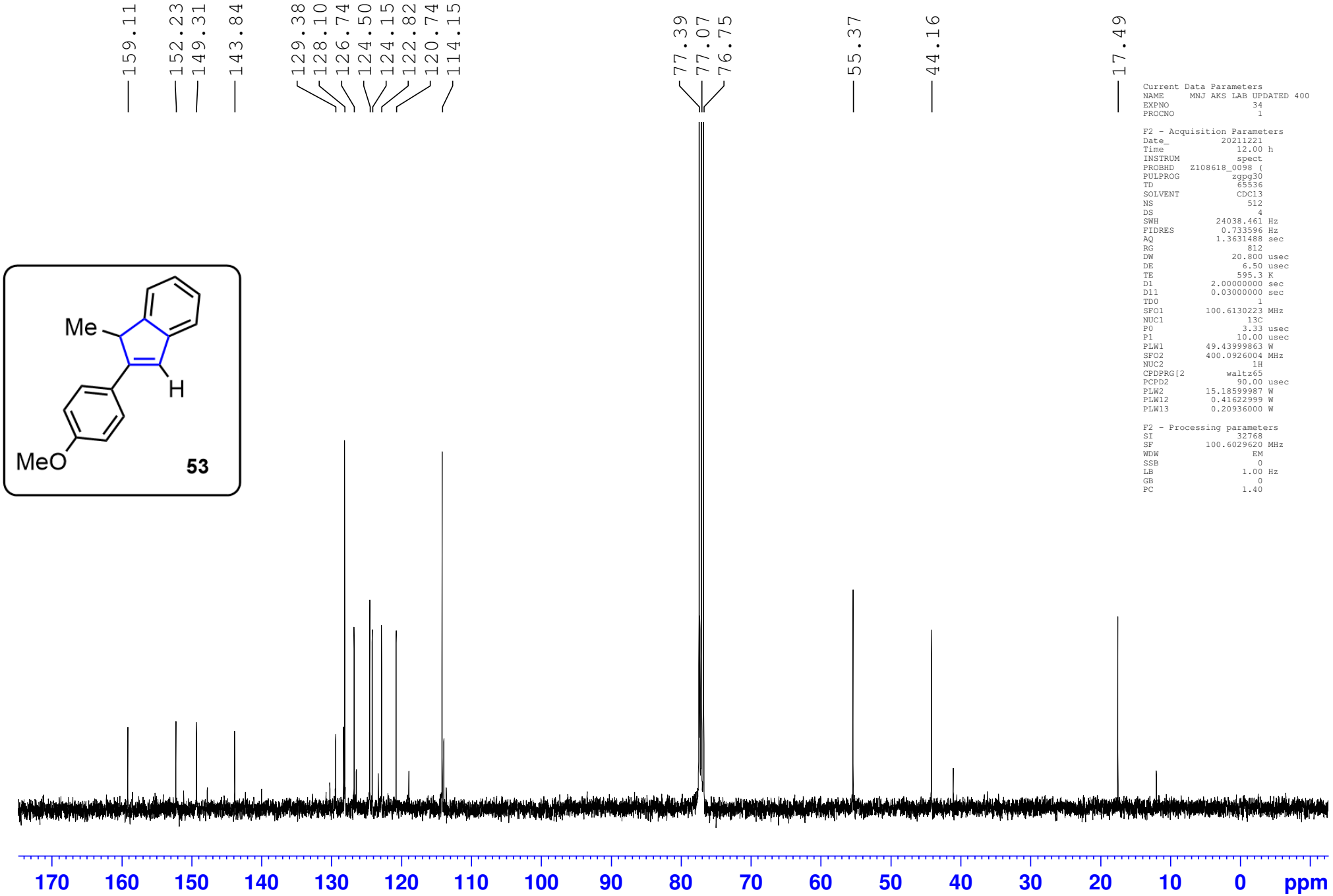

7.528
7.511
7.396
7.379
7.109
7.087
7.070
6.988
6.976
6.959
6.738
6.642
6.627
5.026
4.008
3.996
3.985
3.785
3.346
2.505
2.251
2.094
1.990
1.850
1.842
1.834
1.826
1.821
1.794
1.790
1.778
1.770
1.314
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220201
Time 14.58 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 300.6 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
H
OAc
O
O
O
O
51
10
9
8
7
6
5
4
3
2
1
0
ppm
2.14
2.13
3.25
3.29
1.07
1.07
2.00
2.16
3.20
3.12
3.19
3.17
4.13
6.34

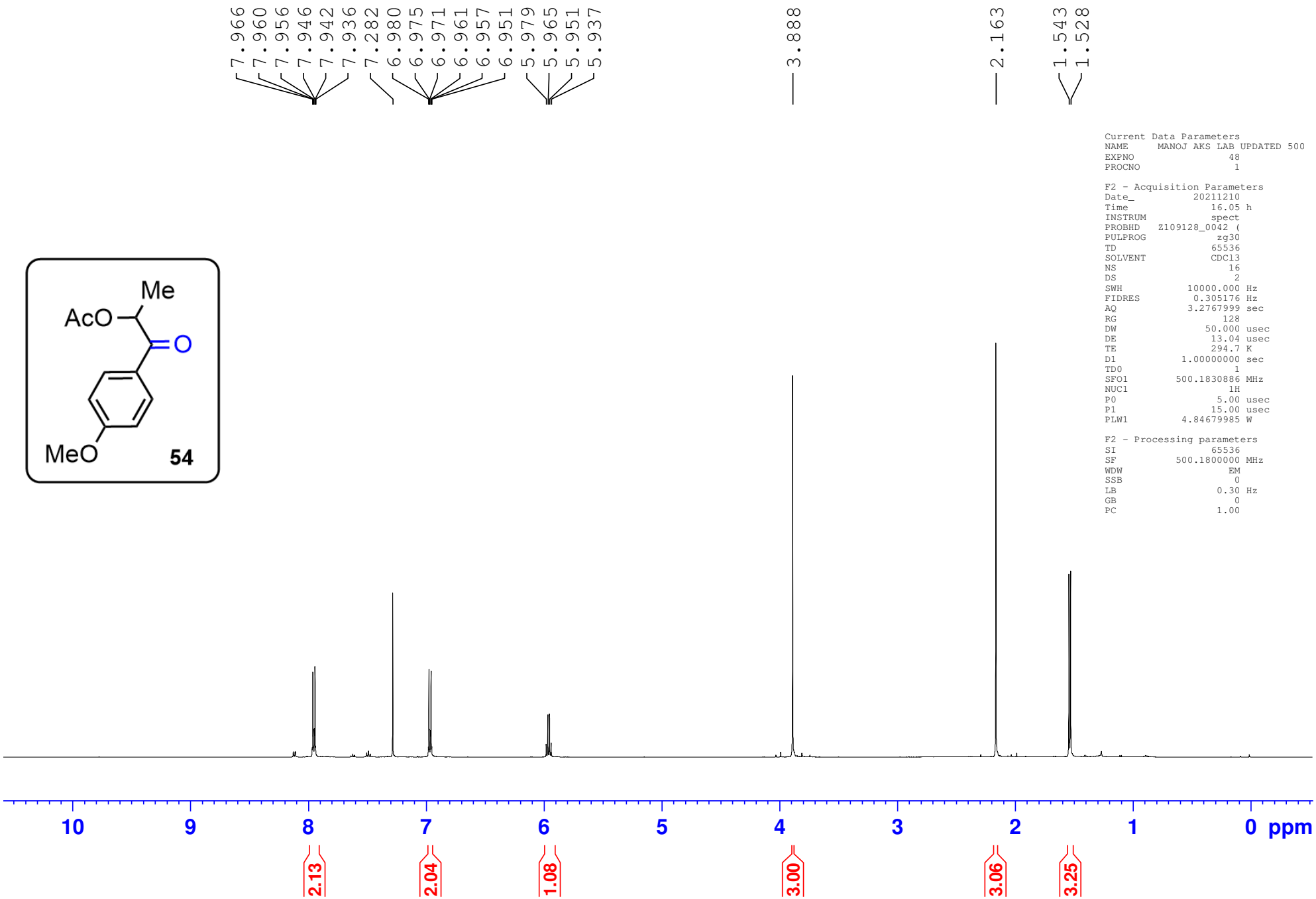

176.23
170.83
159.49
156.85
150.33
136.57
135.20
134.61
132.40
130.76
130.59
130.37
127.91
123.01
122.23
121.03
114.41
112.53
67.72
61.75
55.61
42.38
40.61
40.40
40.19
39.99
39.78
39.57
39.36
37.05
25.23
21.53
21.16
16.05
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 46
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220201
Time 12.49 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 425
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 812
DW 20.800 usec
DE 6.50 usec
TE 620.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OMe
H
OAc
O
O
O
O
51
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

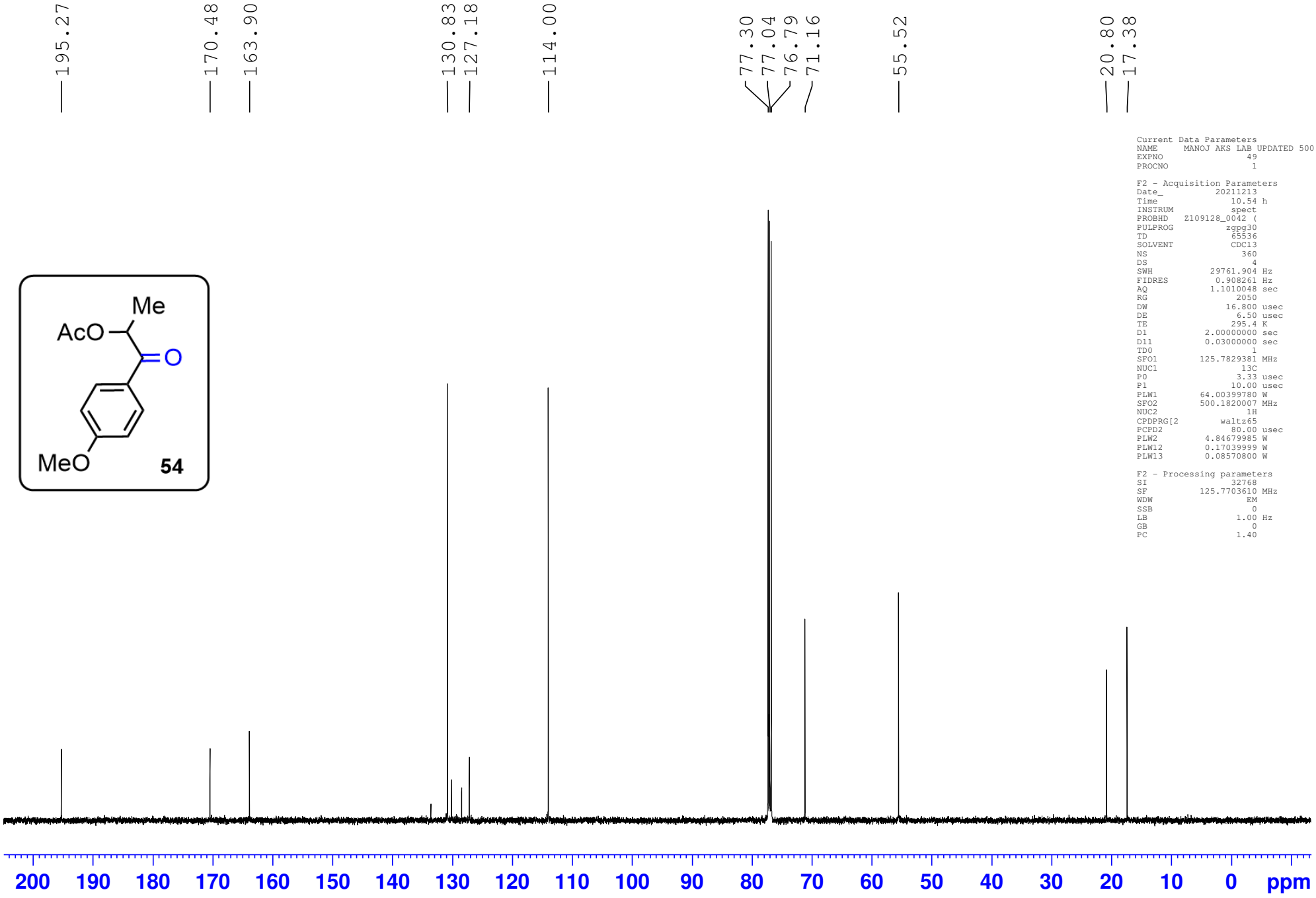

7.529
7.523
7.519
7.510
7.505
7.500
7.408
7.391
7.163
7.160
7.150
7.146
7.104
6.978
6.972
6.968
6.958
6.955
6.949
5.030
3.780
3.336
2.507
2.503
2.499
2.496
2.492
2.476
2.462
2.161
2.147
2.134
2.120
2.107
2.093
2.079
1.982
1.014
1.001
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 72
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220202
Time 10.24 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3713808 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
H
OAc
O
O
52
10
9
8
7
6
5
4
3
2
1
0
ppm
2.31
2.32
2.22
1.09
2.25
2.00
3.12
2.09
1.23
3.07
6.21

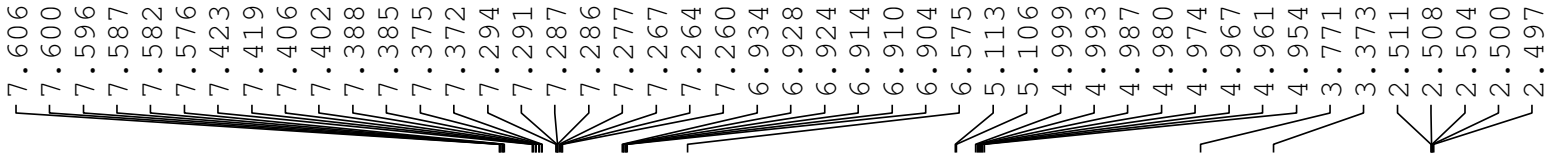

171.54
170.86
159.48
150.06
135.19
134.61
132.38
130.75
130.40
127.91
122.37
114.40
61.70
55.62
42.87
40.61
40.40
40.19
39.98
39.77
39.57
39.36
25.83
22.57
21.18
OMe
H
OAc
O
O
52
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 47
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220202
Time 9.41 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 444
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 616.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

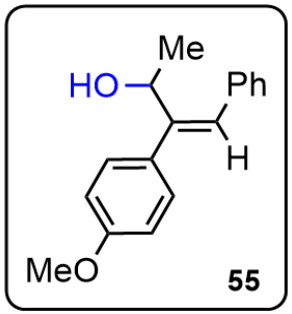

7.538
7.532
7.528
7.519
7.515
7.509
7.480
7.477
7.465
7.459
7.410
7.395
7.317
7.302
7.287
7.286
7.282
7.239
7.224
7.211
7.210
7.209
7.012
6.997
6.993
6.984
6.980
3.938
3.923
3.908
3.892
3.881
1.385
1.370
Me
H
MeO
53
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 55
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211216
Time 9.43 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 144
DW 50.000 usec
DE 13.04 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.08
1.34
1.17
1.12
1.21
1.10
2.08
1.19
3.03
3.00

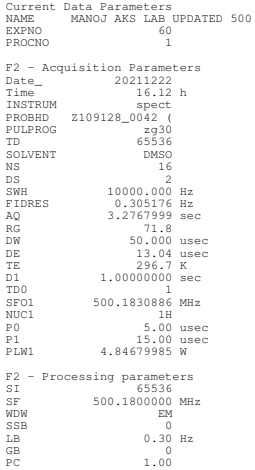

159.11
152.23
149.31
143.84
129.38
128.10
126.74
124.50
124.15
122.82
120.74
114.15
77.39
77.07
76.75
55.37
44.16
17.49
Me
H
MeO
53
Current Data Parameters
NAME MNJ AKS LAB UPDATED 400
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211221
Time 12.00 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 812
DW 20.800 usec
DE 6.50 usec
TE 595.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

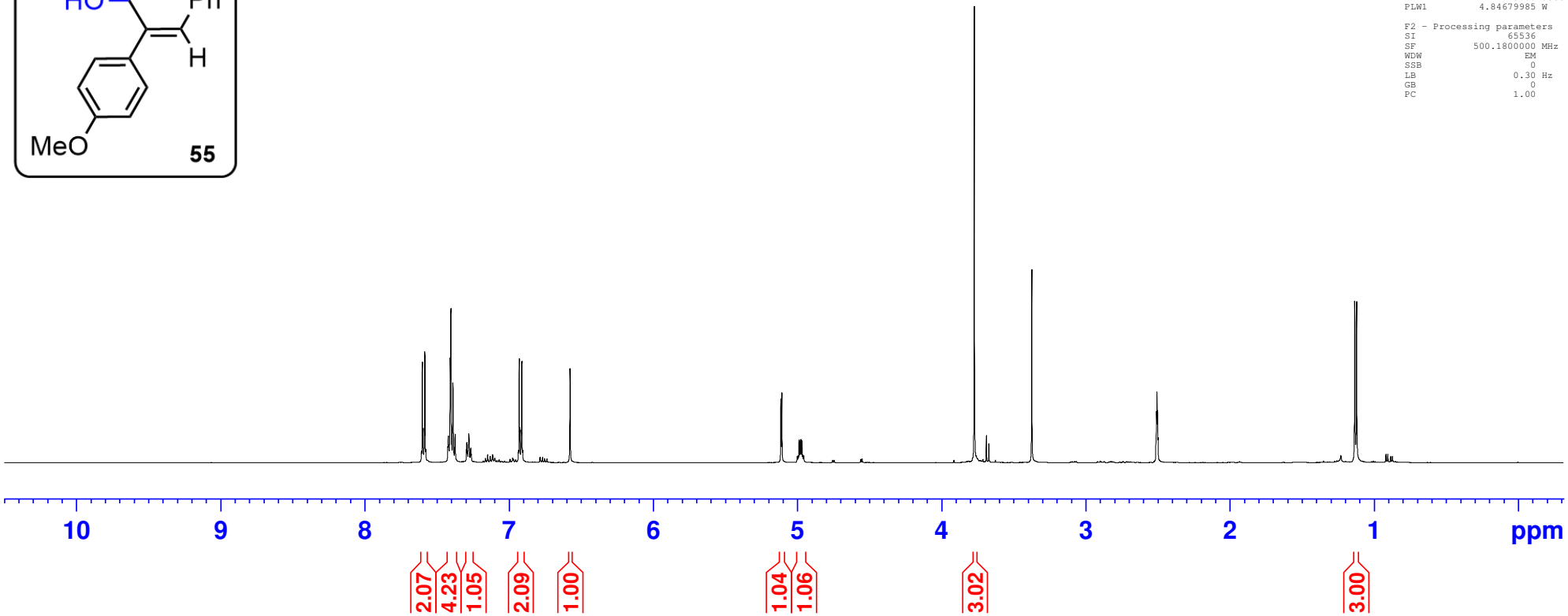

7.966
7.960
7.956
7.946
7.942
7.936
7.282
6.980
6.975
6.971
6.961
6.957
6.951
5.979
5.965
5.951
5.937
3.888
2.163
1.543
1.528
Me
AcO
O
MeO
54
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211210
Time 16.05 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 13.04 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0 ppm
2.13
2.04
1.08
3.00
3.06
3.25

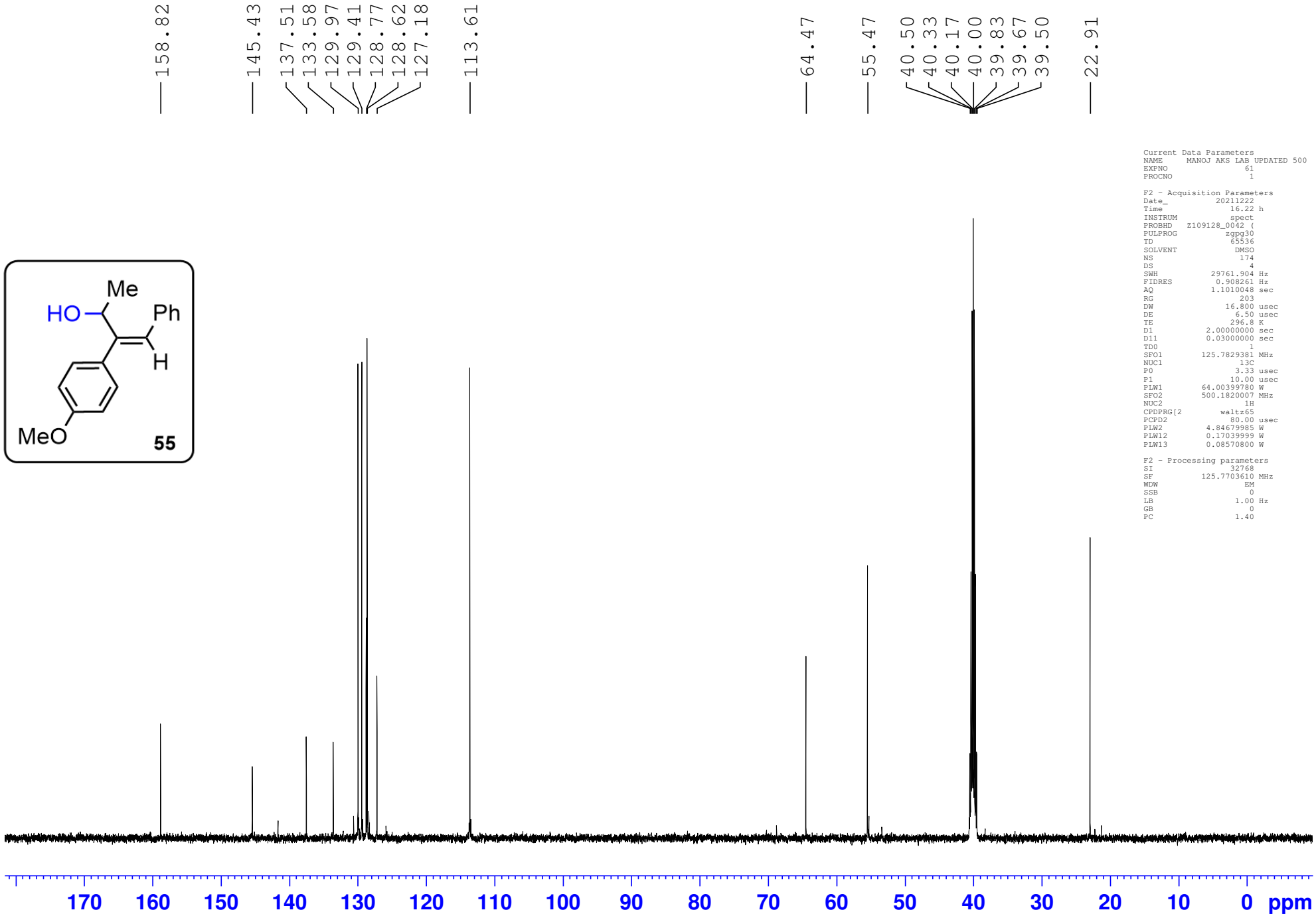

195.27
170.48
163.90
130.83
127.18
114.00
77.30
77.04
76.79
71.16
55.52
20.80
17.38
Me
AcO
O
MeO
54
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 49
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211213
Time 10.54 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 360
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

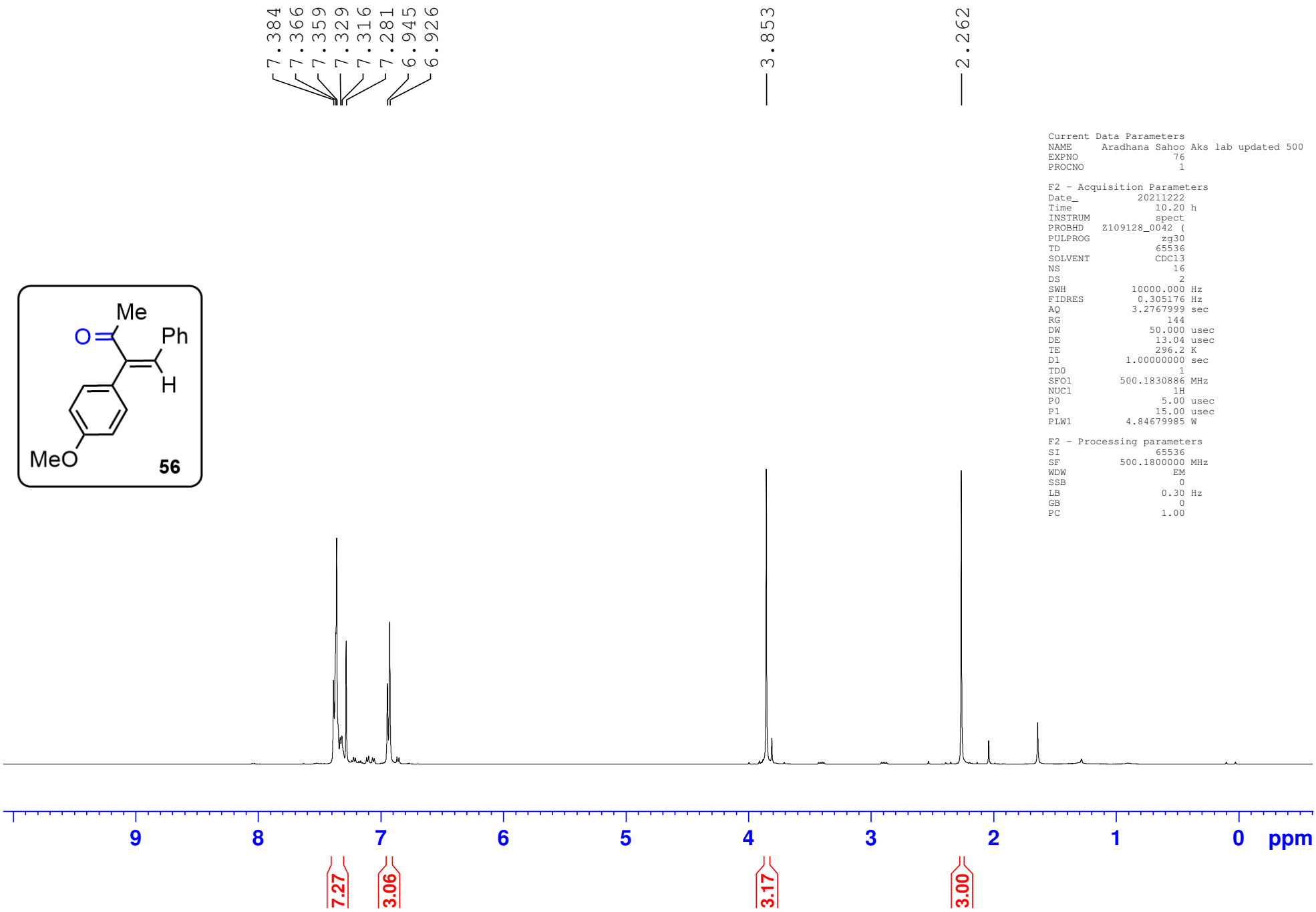

7.606
7.600
7.596
7.587
7.582
7.576
7.423
7.419
7.406
7.402
7.388
7.385
7.375
7.372
7.294
7.291
7.287
7.286
7.277
7.267
7.264
7.260
6.934
6.928
6.924
6.914
6.910
6.904
6.575
5.113
5.106
4.999
4.993
4.987
4.980
4.974
4.967
4.961
4.954
3.771
3.373
2.511
2.508
2.504
2.500
2.497
1.132
1.119

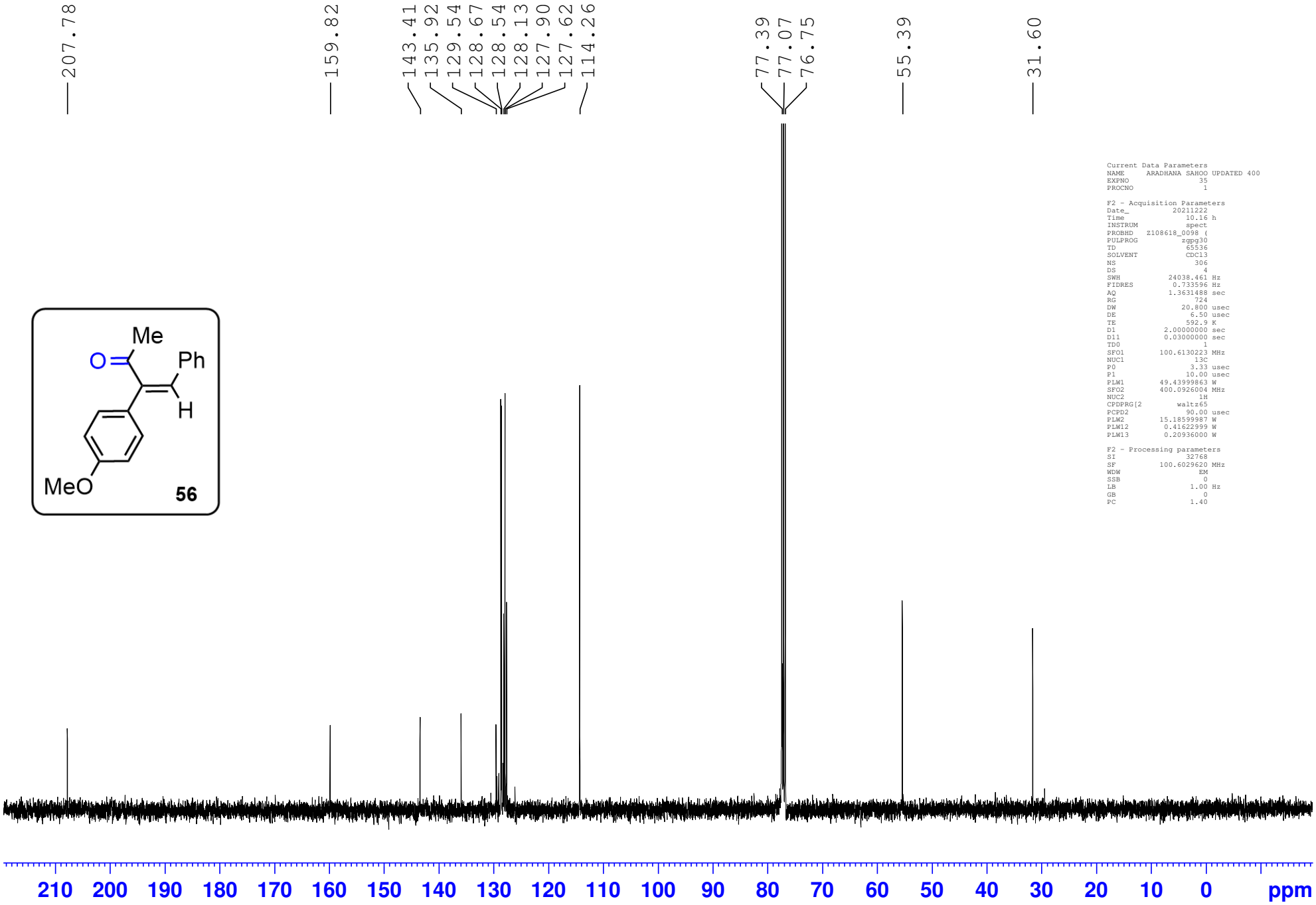

Me
HO
Ph
H
MeO
55

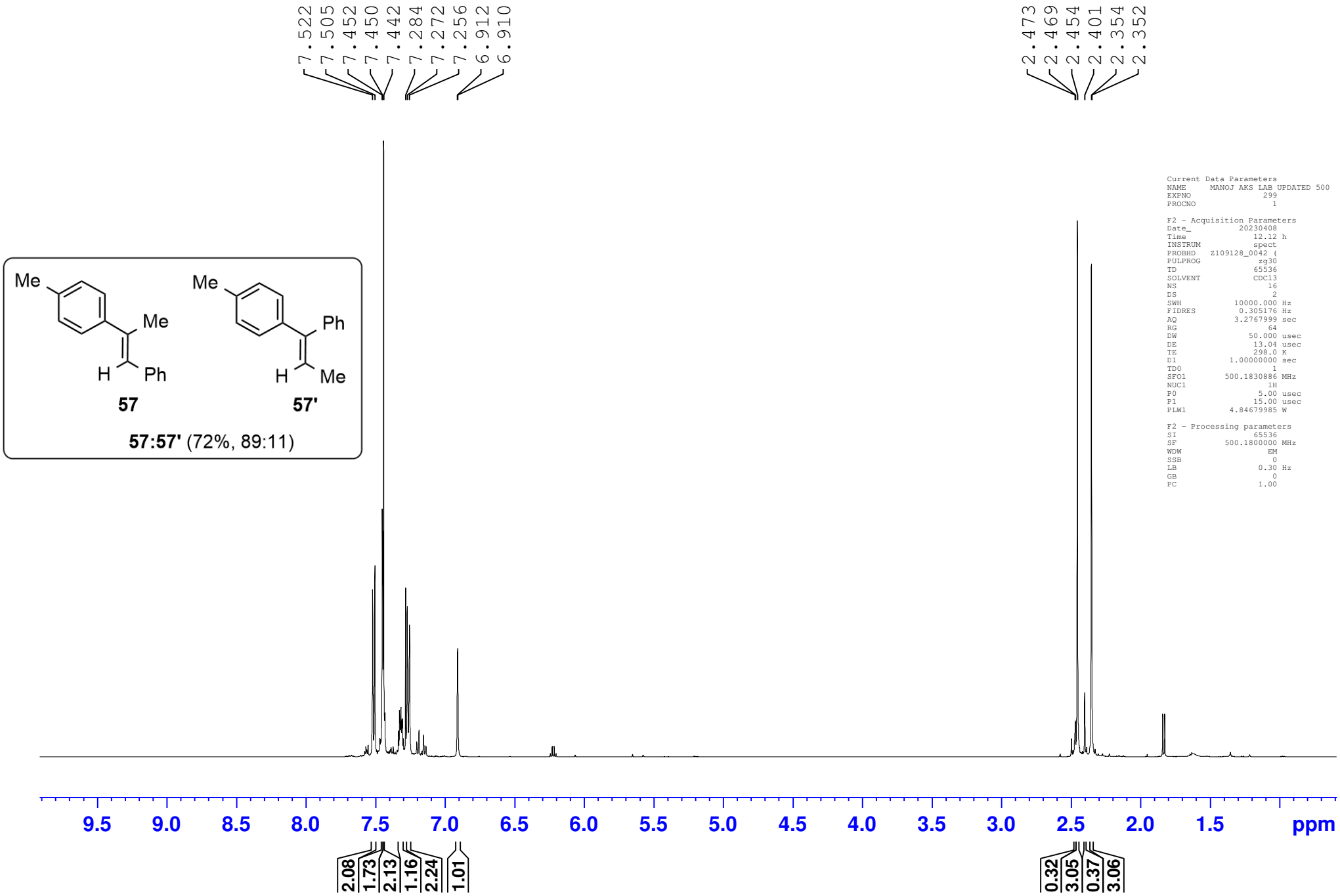

Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 16.12 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 71.8
DW 50.000 usec
DE 13.04 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

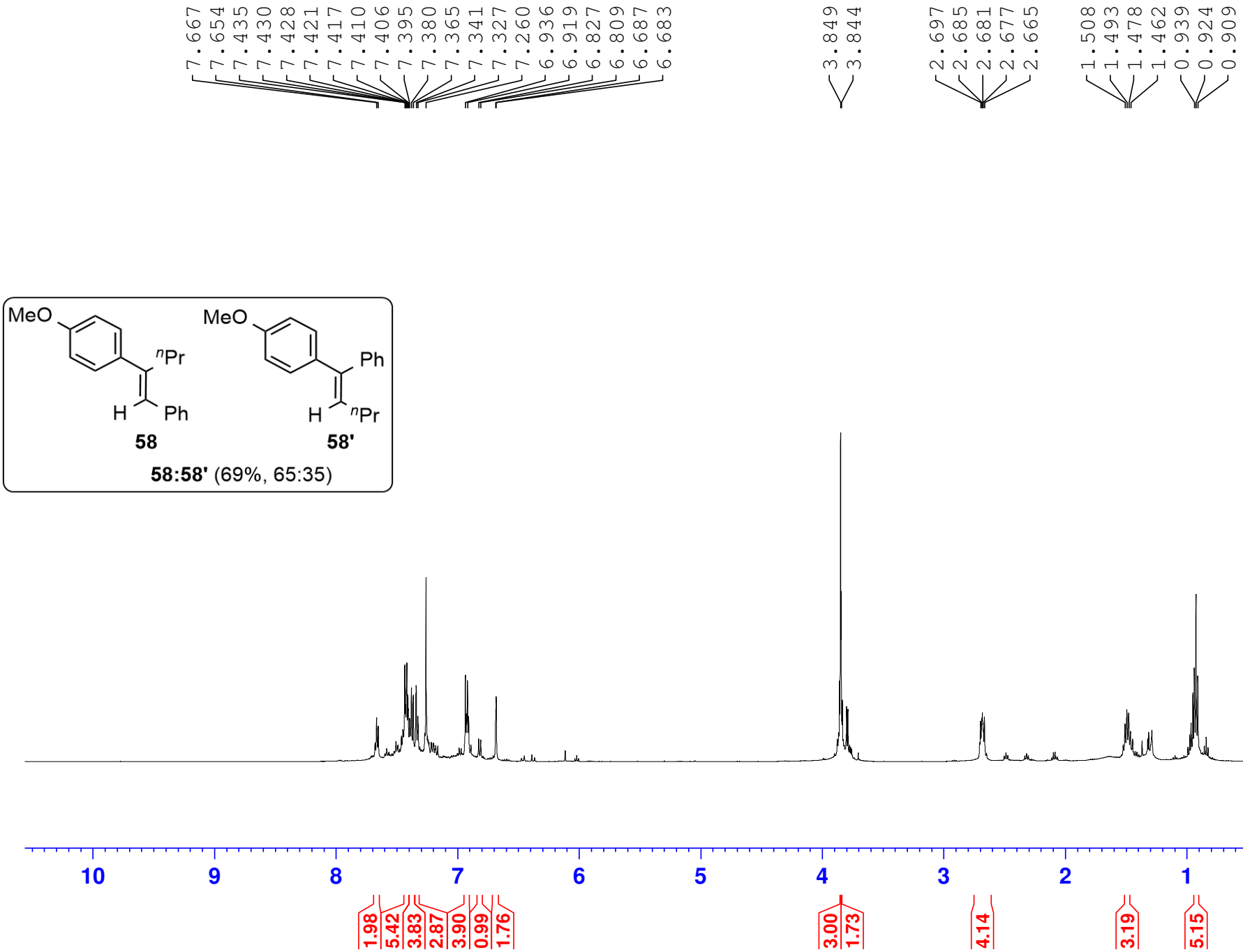

10
9
8
7
6
5
4
3
2
1
ppm
2.07
4.23
1.05
2.09
1.00
1.04
1.06
3.02
3.00

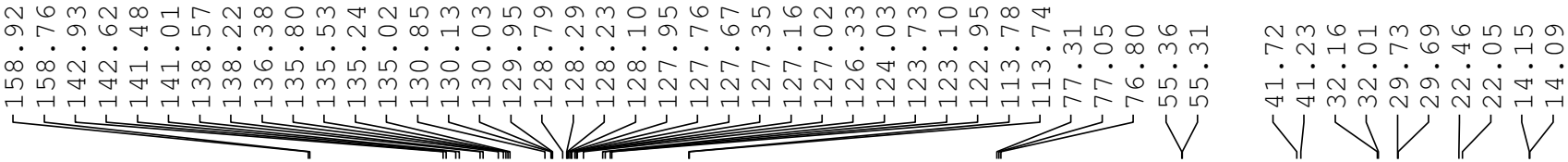

158.82
145.43
137.51
133.58
129.97
129.41
128.77
128.62
127.18
113.61
64.47
55.47
40.50
40.33
40.17
40.00
39.83
39.67
39.50
22.91
Me
HO
Ph
H
MeO
55
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 16.22 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 174
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 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

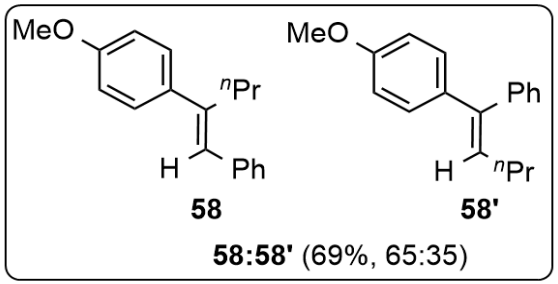

7.384
7.366
7.359
7.329
7.316
7.281
6.945
6.926
3.853
2.262
Me
O
Ph
H
MeO
56
Current Data Parameters
NAME Aradhana Sahoo Aks lab updated 500
EXPNO 76
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 10.20 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 144
DW 50.000 usec
DE 13.04 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
7.27
3.06
3.17
3.00


207.78
159.82
143.41
135.92
129.54
128.67
128.54
128.13
127.90
127.62
114.26
77.39
77.07
76.75
55.39
31.60
Me
O
Ph
H
MeO
56
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211222
Time 10.16 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 306
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.50 usec
TE 592.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 49.43999863 W
SFO2 400.0926004 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 15.18599987 W
PLW12 0.41622999 W
PLW13 0.20936000 W
F2 - Processing parameters
SI 32768
SF 100.6029620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

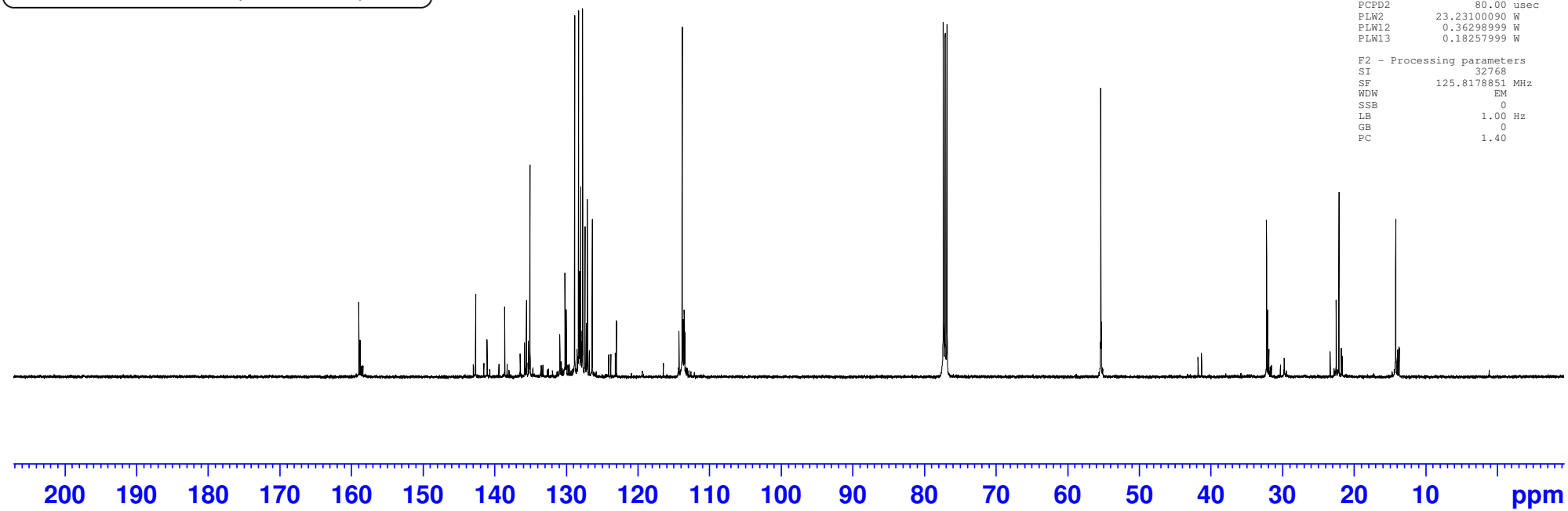

7.522
7.505
7.452
7.450
7.442
7.284
7.272
7.256
6.912
6.910
2.473
2.469
2.454
2.401
2.354
2.352
Me
Me
H
Ph
57
Me
Ph
H
Me
57'
57:57' (72%, 89:11)
Current Data Parameters
NAME MANOJ AKS LAB UPDATED 500
EXPNO 299
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230408
Time 12.12 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 64
DW 50.000 usec
DE 13.04 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
2.08
1.73
2.13
1.16
2.24
1.01
0.32
3.05
0.37
3.06

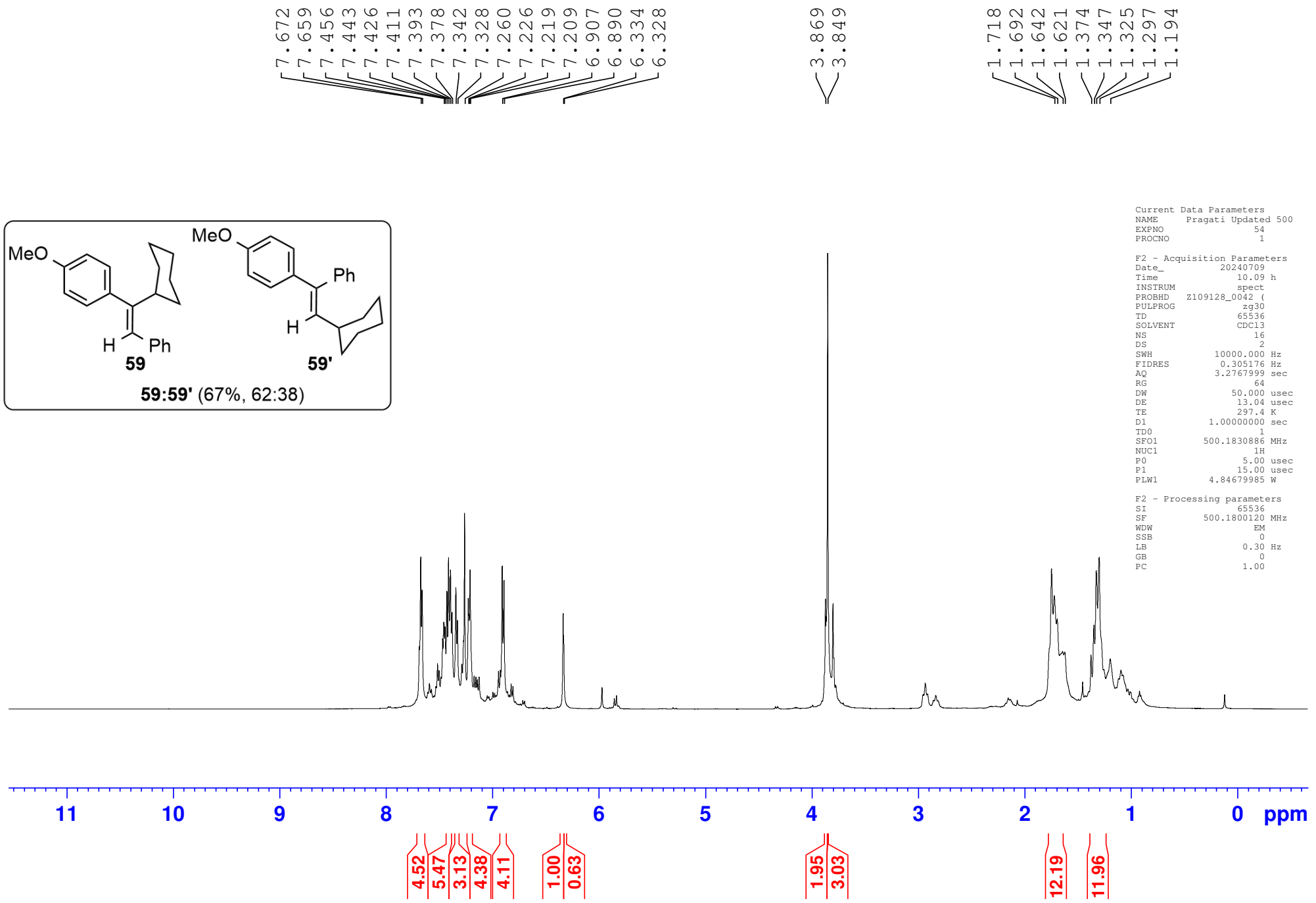

7.667
7.654
7.435
7.430
7.428
7.421
7.417
7.410
7.406
7.395
7.380
7.365
7.341
7.327
7.260
6.936
6.919
6.827
6.809
6.687
6.683
3.849
3.844
2.697
2.685
2.681
2.677
2.665
1.508
1.493
1.478
1.462
0.939
0.924
0.909
MeO
nPr
H
Ph
58
MeO
Ph
H
nPr
58'
58:58' (69%, 65:35)
Current Data Parameters
NAME Avijit Ascend 500
EXPNO 318
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240709
Time 12.27 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PLW1 23.23100090 W
F2 - Processing parameters
SI 65536
SF 500.3690118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.98
5.42
3.83
2.87
3.90
0.99
1.76
3.00
1.73
4.14
3.19
5.15

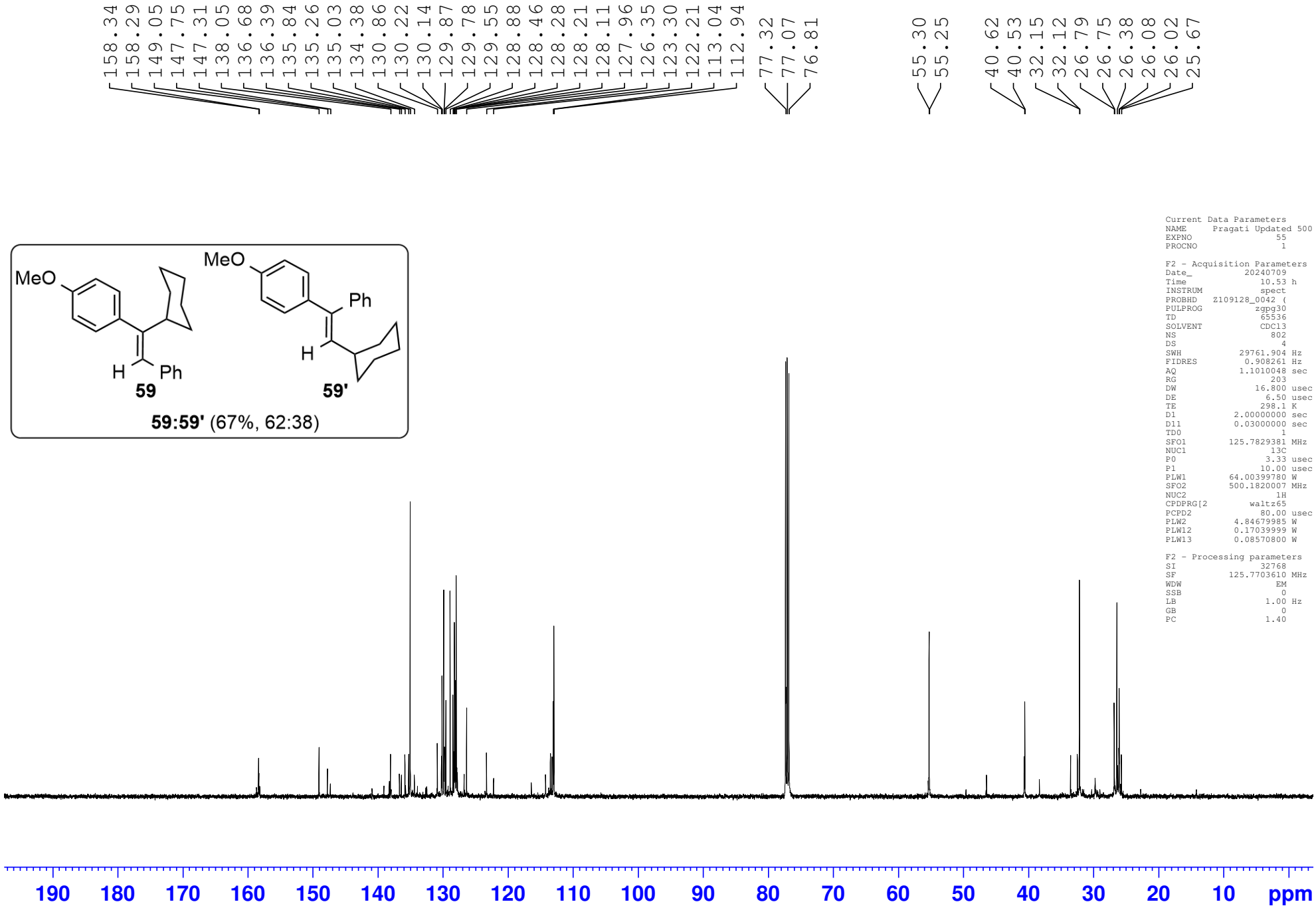


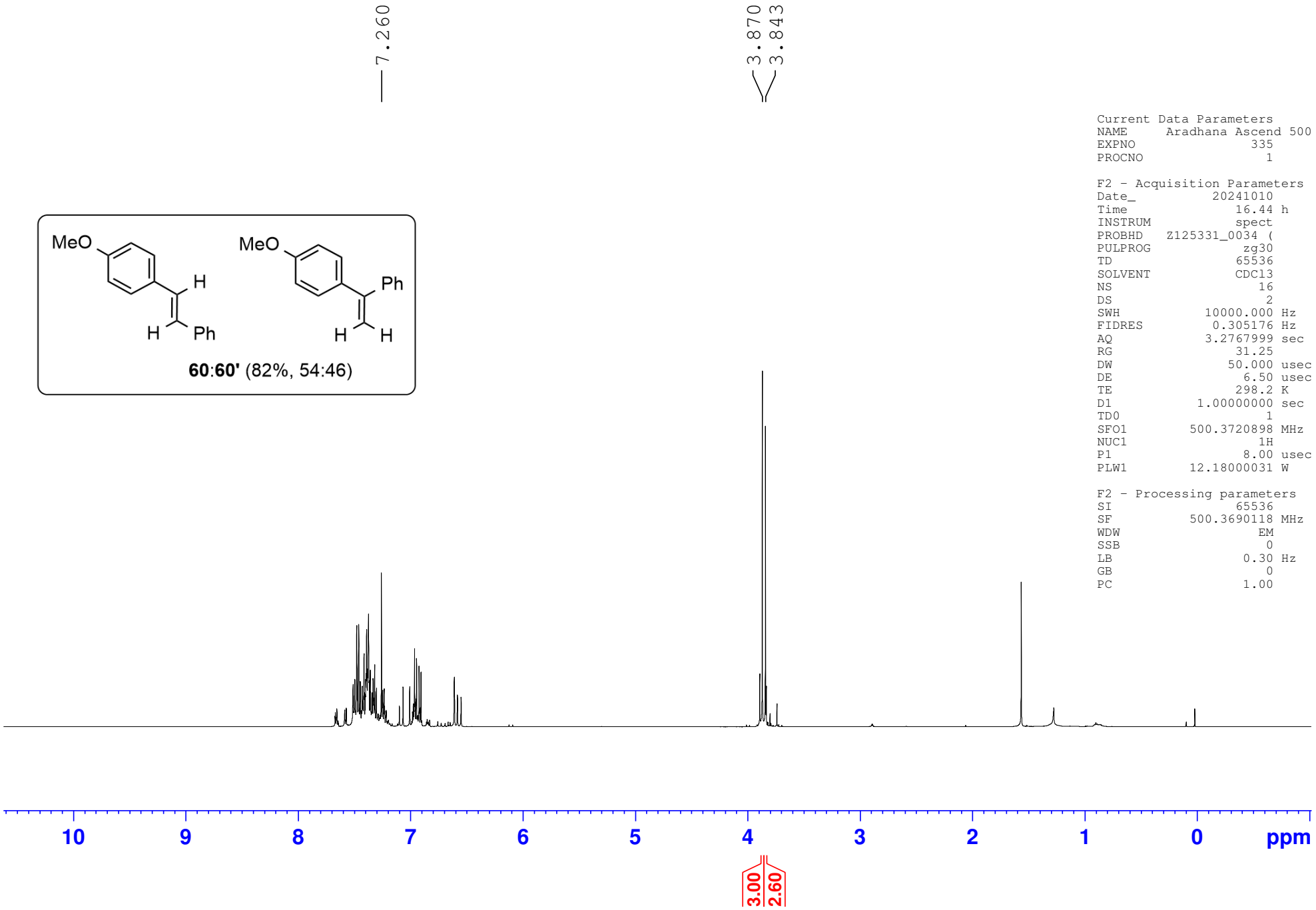


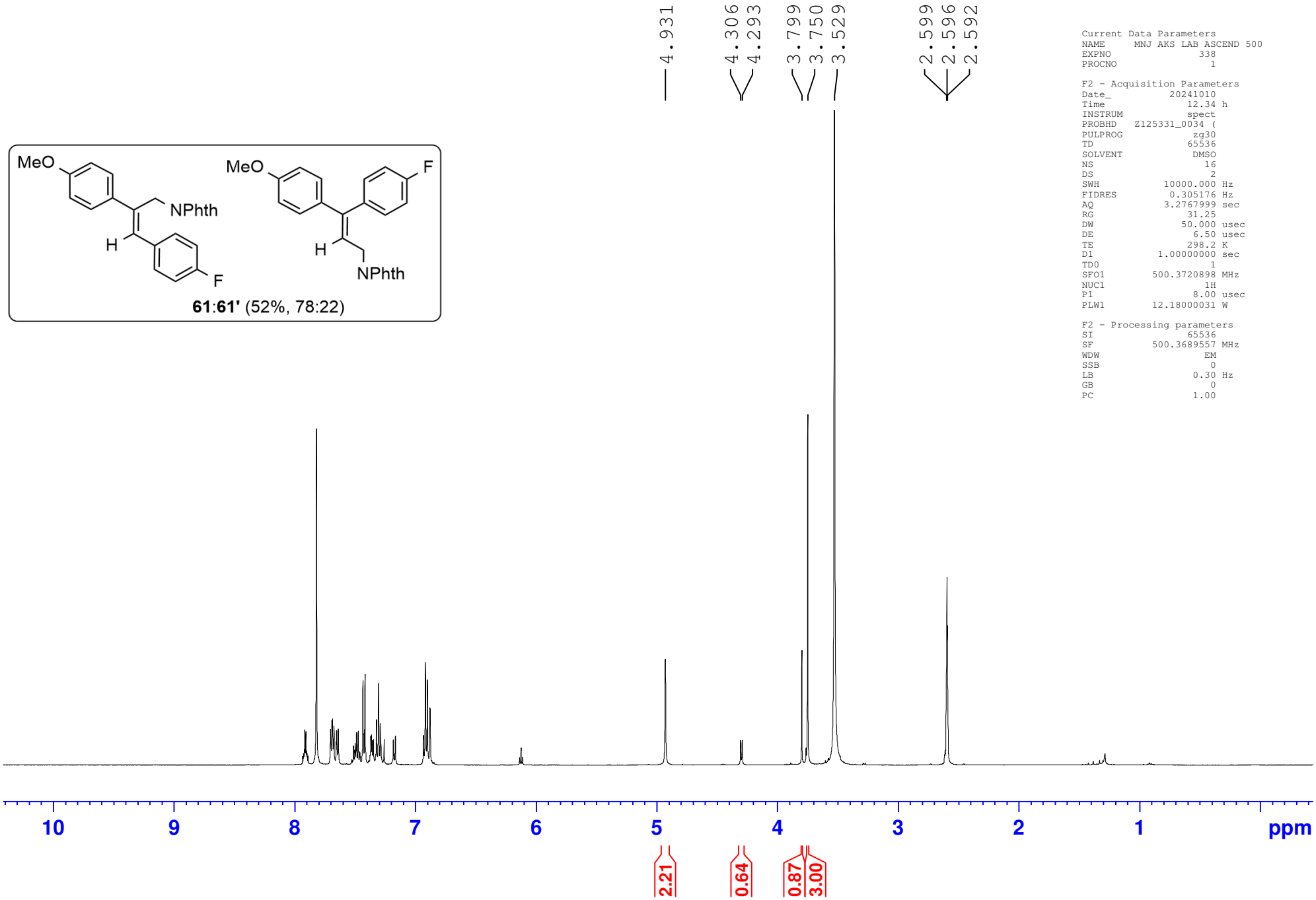

```
Current Data Parameters
NAME      Avijit Ascend 500
EXPNO                  319
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240709
Time              14.55 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2809
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                192.83
DW                16.800 usec
DE                 6.50 usec
TE                299.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.8304669 MHz
NUC1                13C
P1                 10.00 usec
PLW1        115.01000214 W
SFO2         500.3710015 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         23.23100090 W
PLW12         0.36298999 W
PLW13         0.18257999 W

F2 - Processing parameters
SI                 32768
SF           125.8178851 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




7.672
7.659
7.456
7.443
7.426
7.411
7.393
7.378
7.342
7.328
7.260
7.226
7.219
7.209
6.907
6.890
6.334
6.328
3.869
3.849
1.718
1.692
1.642
1.621
1.374
1.347
1.325
1.297
1.194
MeO
H
Ph
59
MeO
Ph
H
59'
59:59' (67%, 62:38)
Current Data Parameters
NAME Pragati Updated 500
EXPNO 54
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240709
Time 10.09 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 64
DW 50.000 usec
DE 13.04 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W
F2 - Processing parameters
SI 65536
SF 500.1800120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.52
5.47
3.13
4.38
4.11
1.00
0.63
1.95
3.03
12.19
11.96


158.34
158.29
149.05
147.75
147.31
138.05
136.68
136.39
135.84
135.26
135.03
134.38
130.86
130.22
130.14
129.87
129.78
129.55
128.88
128.46
128.28
128.21
128.11
127.96
126.35
123.30
122.21
113.04
112.94
77.32
77.07
76.81
55.30
55.25
40.62
40.53
32.15
32.12
26.79
26.75
26.38
26.08
26.02
25.67
MeO
H
Ph
59
MeO
Ph
H
59'
59:59' (67%, 62:38)
Current Data Parameters
NAME Pragati Updated 500
EXPNO 55
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240709
Time 10.53 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 802
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 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7829381 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 64.00399780 W
SFO2 500.1820007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 80.00 usec
PLW2 4.84679985 W
PLW12 0.17039999 W
PLW13 0.08570800 W
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.260
3.870
3.843
MeO
H
H
Ph
MeO
Ph
H
H
60:60' (82%, 54:46)
Current Data Parameters
NAME Aradhana Ascend 500
EXPNO 335
PROCNO 1
F2 - Acquisition Parameters
Date_ 20241010
Time 16.44 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.18000031 W
F2 - Processing parameters
SI 65536
SF 500.3690118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
3.00
2.60


4.931
4.306
4.293
3.799
3.750
3.529
2.599
2.596
2.592
MeO
NPhth
H
F
MeO
F
H
NPhth
61:61' (52%, 78:22)
Current Data Parameters
NAME MNJ AKS LAB ASCEND 500
EXPNO 338
PROCNO 1
F2 - Acquisition Parameters
Date_ 20241010
Time 12.34 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.18000031 W
F2 - Processing parameters
SI 65536
SF 500.3689557 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
2.21
0.64
0.87
3.00