Two-Component Symmetrical Diarylation of Ynamides

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SUPPORTING INFORMATION

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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, 470 MHz) having the solvent resonance as internal standard (^{1}H NMR, $CDCl_3$ at 7.26 ppm; ^{13}C NMR, $CDCl_3$ at 77.0 ppm). Few cases tetramethylsilane (TMS) at 0.00 ppm was used as the reference standard. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet; br s = broad singlet; d = doublet; br d = broad doublet, t = triplet; br t = broad triplet; q = quartet; m = multiplet; tt = triplet of triplet; dq = doublet of quartet), coupling constant, *J*, in (Hz), and integration. Data for ^{13}C NMR, and ^{19}F NMR were reported in terms of chemical shift (ppm). IR spectra were reported in cm^{-1}. High resolution mass spectra were obtained in ESI mode. Melting points were determined by electrothermal heating and are uncorrected. X−ray data was collected at 293 K using graphite monochromatic Mo-Kα radiation (0.71073 Å).

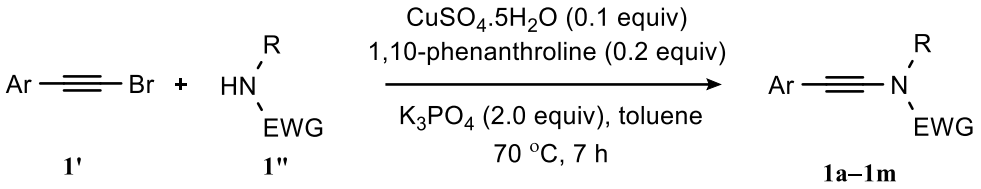
Materials:

Unless otherwise noted, all the reagents and intermediates were obtained commercially and used without purification. CH_3CN, toluene, and 1,4-dioxane were distilled over CaH_2. $Pd(OAc)_2$ and aryl boronic acids were purchased from commercially available source and used as received. Analytical and spectral data of all the known compounds are exactly matching with the reported values.

Following the known procedure, the ynamides (**1a**−**n**)[1,2] were prepared (Table S1). Analytical and spectral data of these compounds are exactly matching with the reported values.

Experimental Procedures

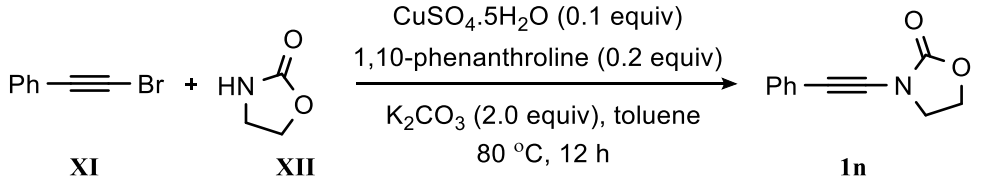
Preparation of Ynamides (1): General Procedure (GP-1):[1,2]



General Procedure for the Synthesis of 1a–1m (GP 1):[1]

To a mixture of **1″** (2.0 mmol), $CuSO_4 \cdot 5H_2O$ (0.2 mmol), 1,10–phenanthroline (0.4 mmol), and K_3PO_4 (4.0 mmol) in dry toluene (8.0 mL) was added 1-bromo-2-arylacetylene **(1′)**. The reaction mixture was heated at 70 °C under a nitrogen atmosphere. Progress of the reaction was monitored periodically by TLC. Upon completion, the reaction mixture was cooled to room temperature and diluted with dichloromethane (10 mL). The crude mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified through column chromatography using ethyl acetate and hexane mixture on silica gel to provide **1a–m**.

Preparation of 2-oxazolidinone ynamide (1n):[2]



To a mixture of **XII** (2.0 mmol), $CuSO_4 \cdot 5H_2O$ (0.2 mmol), 1,10–phenanthroline (0.4 mmol), and K_2CO_3 (4.0 mmol) in dry toluene (8.0 mL) was added **XI** (2.4 mmol). The reaction mixture was heated at 80 °C under a nitrogen atmosphere. Progress of the reaction was monitored periodically by TLC. Upon completion, the reaction mixture was cooled to room temperature and diluted with dichloromethane (10 mL). The crude 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 (eluting with EA/hexane : 1/4) to obtain **1n**.

Table S1: List of Ynamides

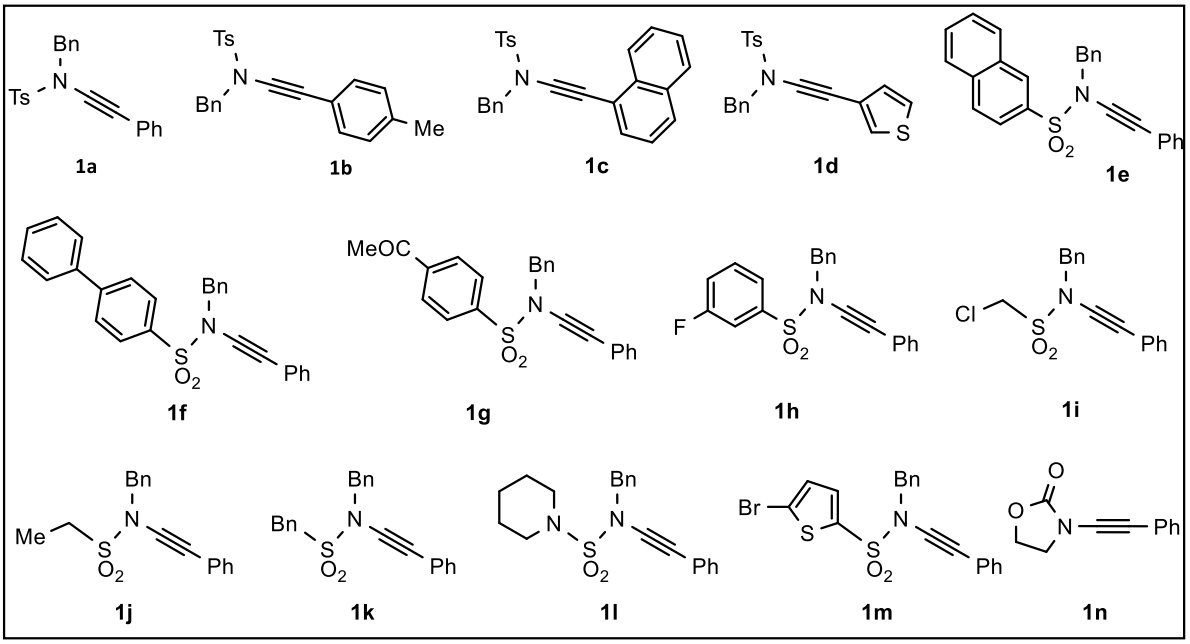
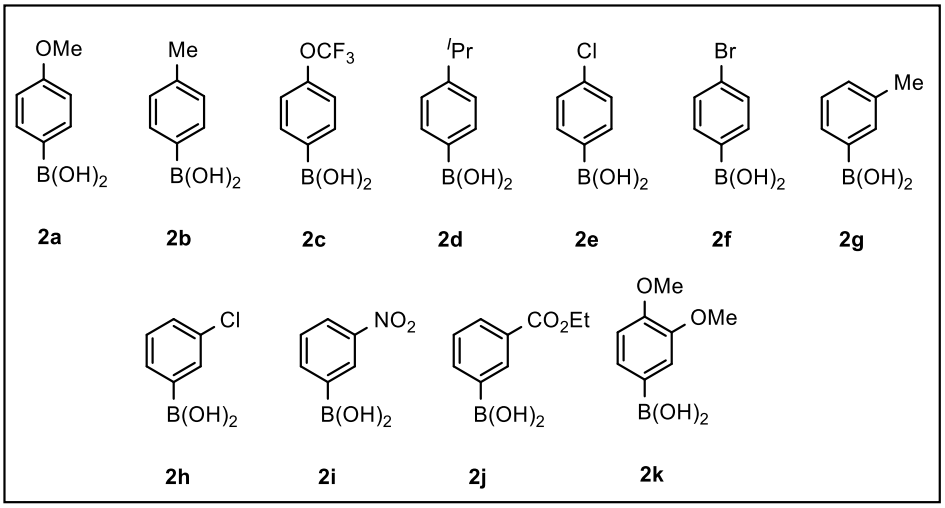
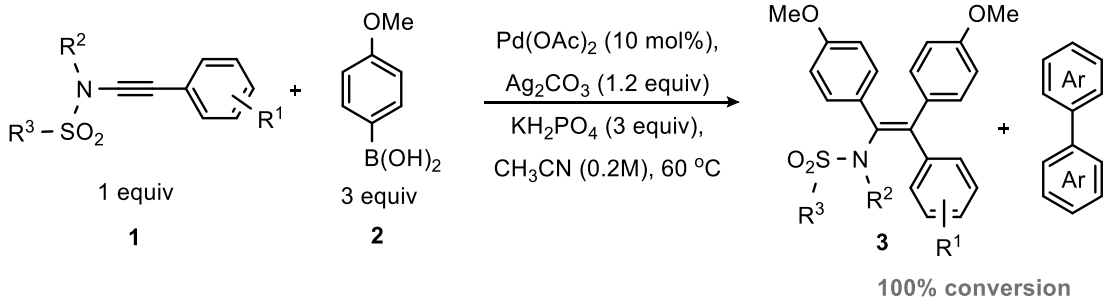


Table S2: List of Boronic Acids

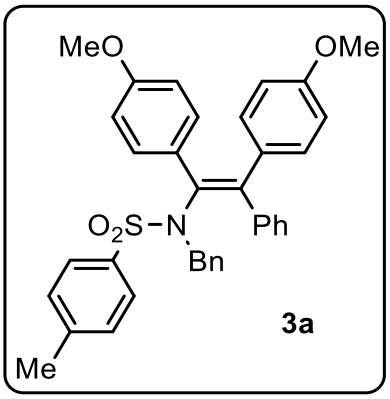


General Procedure for the symmetrical diarylation of N-sulfonyl Ynamides (1) with Aryl Boronic Acids (2) (GP-2):



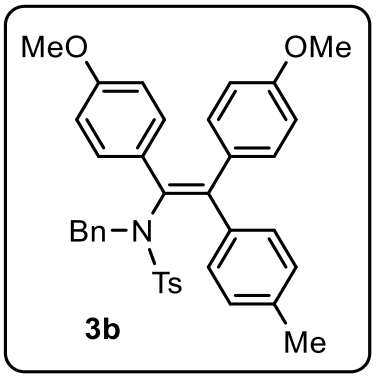
To a mixture of **1** (0.3 mmol) and 4-methoxyphenyl boronic acid **2** (136.8 mg, 0.9 mmol), $Pd(OAc)_2$ (6.7 mg, 0.03 mmol), KH_2PO_4 (122.5mg, 0.9 mmol), and Ag_2CO_3 (99.3 mg, 0.36 mmol) was added acetonitrile (CH_3CN; 1.5 mL). The reaction mixture was stirred at 60 °C for 5 h. Progress of the reaction was monitored periodically by TLC. Upon completion, the reaction mixture was diluted with ethyl acetate (10 mL). The crude mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified through column chromatography to afford **3a–m.**

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)-4-methylbenzenesulfonamide (3a):



3a (134 mg, 77%) as yellow solid; M.P = 210–212 °C; R_f = 0.6 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.31–7.29 (m, 2H), 7.29–7.27 (m, 1H), 7.23 (t, J = 8.0 Hz, 3H), 7.10 (br d, J = 6.5 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 8.0 Hz, 2H), 6.84 (d, J = 8.5 Hz, 2H), 6.78 (s, 1H), 6.76 (dt, J = 7.5, 2.5 Hz, 3H), 6.58–6.55 (m, 4H), 4.25 (br d, J = 14.5 Hz, 1H), 3.98 (br d, J = 14.5 Hz, 1H), 3.74 (s, 3H), 3.70 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ158.7, 158.2, 142.9, 142.2, 141.3, 137.8, 136.2, 135.0, 133.0, 132.9, 132.5, 130.2, 130.1, 129.7, 128.9, 128.3, 128.2, 128.1, 128.0, 127.2, 113.2, 113.1, 55.1, 55.0, 51.0, 21.4; IR (Neat) ν_{max} 1604, 1508, 1248, 1152, 1027, 659 cm^{-1}; HRMS (ESI) for $C_{36}H_{33}NO_4SNa^+$ $(M+Na)^+$: calcd. 598.2023, found 598.2019.

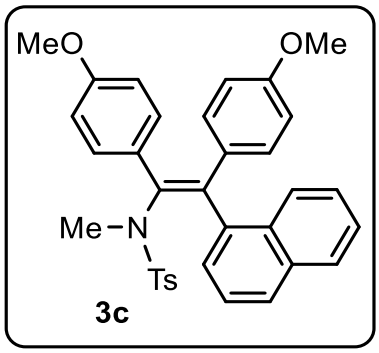
(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-(*p*-tolyl)vinyl)-4-methylbenzenesulfonamide (3b):



3b (93 mg, 53%) as yellow solid; M.P = 141–143 °C; R_f = 0.7 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.33 (d, J = 5.0 Hz, 1H), 7.30 (t, J = 6.5 Hz, 2H), 7.15 (d, J = 8.5 Hz, 2H), 7.12 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 8.5 Hz, 3H), 6.97 (s, 1H), 6.85 (d, J = 7.0 Hz, 2H), 6.66–6.63 (m, 4H), 6.57 (d, J = 9.0 Hz, 2H), 6.52 (d, J = 9.0 Hz, 2H), 4.30 (br d, J = 14.5 Hz, 1H), 3.86 (br d, J = 14.5 Hz, 1H), 3.67 (s, 3H), 3.64 (s, 3H), 2.37 (d, J = 2.5 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 158.5, 158.0, 142.8, 140.8, 139.1,138.0, 137.1, 136.3, 135.0, 132.7, 132.4, 130.2, 129.9, 128.9, 128.8, 128.3, 128.1, 127.9,

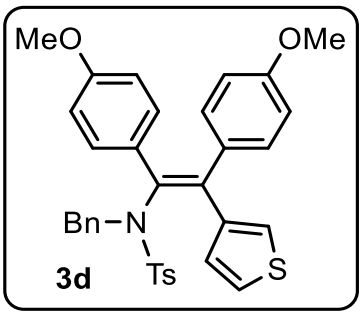
113.0, 55.1, 55.0, 51.0, 29.7, 21.5, 21.3; IR (Neat): ν_{max} 1703, 1352, 1155, 1087, 732, 699 cm^{-1}; HRMS (ESI) for $C_{37}H_{36}NO_4S^+$ $(M+H)^+$: calcd.590.2360, found 590.2357.

(*Z*)-*N*-(1,2-Bis(4-methoxyphenyl)-2-(naphthalen-1-yl)vinyl)-*N*,4-dimethylbenzenesulfonamide (3c):



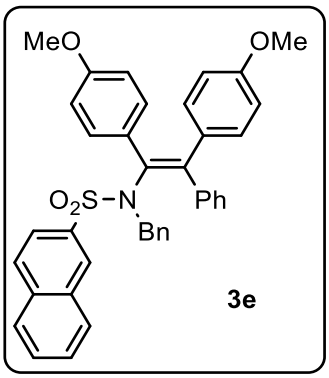
3c (101 mg, 61%) as yellow solid; M.P = 218–220 °C; R_f = 0.2 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.94–7.48 (m, 6H), 7.46–7.31 (m, 3H), 7.22–7.06 (m, 2H), 6.90–6.83 (m, 3H), 6.80–6.76 (m, 3H), 6.63–6.58 (m, 2H), 3.73 (s, 3H), 3.59 (s, 3H), 2.63 (br s, 3H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, DMSO–D_6): δ 159.1, 158.3, 142.9, 139.0, 136.9, 134.2, 133.6, 132.3, 131.5, 129.5, 129.3, 128.7, 128.3, 126.9, 126.5, 126.0, 113.9, 113.8, 55.5, 55.3, 37.5, 29.5, 21.3; IR (Neat): ν_{max} 1604, 1508, 1337, 1247, 1028, 790 cm^{-1}; HRMS (ESI) for $C_{34}H_{31}NO_4SNa^+$ $(M+Na)^+$: calcd.572.1866, found 572.1866.

(*Z*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-(thiophen-3-yl)vinyl)-4-methylbenzenesulfonamide (3d):



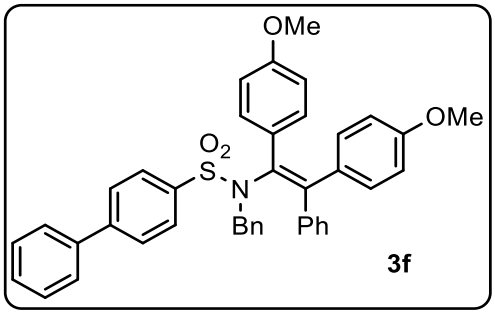
3d (84 mg, 48%) as yellow solid; M.P = 190-192 °C; R_f = 0.6 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO D_6): δ 7.64 (dd, J = 5.0, 3.0 Hz, 1H), 7.42–7.34 (m, 3H), 7.23 (d, J = 8.0 Hz, 2H), 7.21 (dd, J = 3.0, 1.5 Hz, 1H), 7.17 (d, J = 8.5 Hz, 2H), 7.12 (dd, J = 5.0, 1.0 Hz, 1H), 7.07–7.02 (m, 2H), 6.76–7.69 (m, 4H), 6.52–6.48 (m, 4H), 4.57 (br d, J = 14.5 Hz, 1H), 4.01 (br d, J = 14.5 Hz, 1H), 3.71 (s, 3H), 3.70 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, DMSO–D_6): δ 159.2, 158.4, 143.3, 134.4, 133.2, 132.6, 132.1, 131.6, 130.1, 130.0, 129.5, 129.2, 128.7, 128.4, 128.0, 127.6, 127.0, 125.9, 113.9, 55.7, 55.4, 46.7, 21.3; IR (Neat): ν_{max} 1601, 1507, 1244, 1152, 747 cm^{-1}; HRMS (ESI) for $C_{34}H_{35}N_2O_4S_2^+$ $(M+NH_4)^+$: calcd.599.2033, found 599.2033.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)naphthalene-2-sulfonamide (3e):



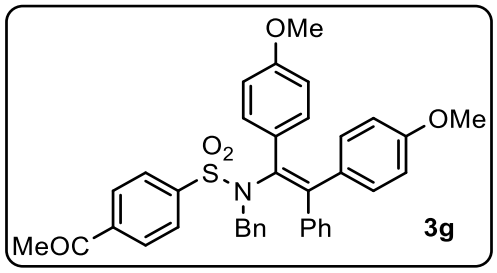
3e (112 mg, 62%) as yellow solid; M.P = 215–218 °C; R_f = 0.8 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.5 Hz, 1H), 7.71 (d, *J* = 8.5 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.62–7.57 (m, 1H), 7.56–7.50 (m, 2H), 7.38–7.30 (m, 5H), 7.20 (t, *J* = 7.5 Hz, 2H), 7.15 (dd, *J* = 9.0, 2.0 Hz, 2H), 6.90 (d, *J* = 7.0 Hz, 2H), 6.78 (dt, *J* = 8.5, 3.0 Hz, 2H), 6.71 (br d, *J* = 8.0 Hz, 2H), 6.58 (dt, *J* = 9.0, 2.5 Hz, 2H), 6.39 (d, *J* = 8.5 Hz, 2H), 4.45 (br d, *J* = 14.5 Hz, 1H), 4.02 (br d, *J* = 14.5 Hz, 1H), 3.70 (s, 3H), 3.59 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 158.5, 158.1, 141.0, 140.6, 137.8, 136.2, 134.7, 134.4, 133.3, 132.8, 132.5, 131.8, 130.2, 130.1, 129.41, 129.39, 129.2, 128.42, 128.36, 128.33, 128.28, 128.2, 127.6, 127.5, 126.9, 123.0, 113.1, 113.0, 55.0, 54.9, 51.6; IR (Neat): ν_{max} 1604, 1507, 1246, 1153, 1024, 698 cm^{-1}; HRMS (ESI) for $C_{39}H_{34}NO_4S^+$ $(M+H)^+$: calcd.612.2203, found 612.2200.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)-[1,1'-biphenyl]-4-sulfonamide (3f):



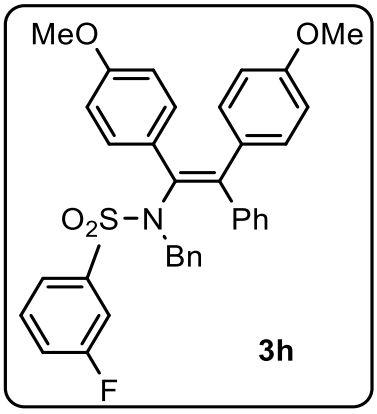
3f (118 mg, 65%) as yellow solid; M.P = 205–207 °C; R_f = 0.9 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60 (d, *J* =7.0 Hz, 2H), 7.52–7.44 (m, 5H), 7.42 (dt, *J* = 7.5, 2.0 Hz 1H), 7.34–7.29 (m, 4H), 7.25 (d, *J* =7.0 Hz, 1H), 7.17 (br d, *J* = 5.5 Hz, 2H), 7.14 (dt, *J* = 8.5, 2.0 Hz 2H), 6.87 (d, *J* =7.0 Hz, 2H), 6.85 (d, *J* = 6.5 Hz, 2H), 6.79 (dt, *J* = 9.0, 3.0 Hz, 2H), 6.59 (dt, *J* = 8.5, 3.0 Hz, 2H) 6.56 (d, *J* = 9.0 Hz, 2H), 4.35 (br d, *J* = 15.0 Hz, 1H), 4.05 (br d, *J* = 14.5 Hz, 1H), 3.73 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 158.6, 158.1, 144.9, 142.1, 141.2, 139.4, 139.3, 136.0, 134.8, 133.0, 132.8, 132.4, 130.2, 130.1, 129.6, 129.0, 128.37, 128.35, 128.32, 128.25, 128.2, 127.3, 127.2, 126.8, 113.12, 113.06, 55.1, 55.0, 51.3; IR (Neat): ν_{max} 1604, 1507, 1245, 1155, 1026, 698 cm^{-1}; HRMS (ESI) for $C_{41}H_{35}NO_4SNa^+$ $(M+Na)^+$: calcd.660.2179, found 660.2173.

(*E*)-4-Acetyl-*N*-benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)benzenesulfonamide (3g):



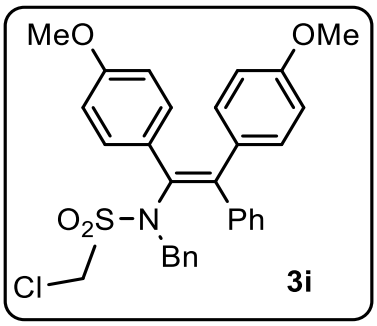
3g (88 mg, 49%) as yellow solid; M.P = 160–162 °C; R_f = 0.1 (10% EtOAc/Hex; ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.84 (d, J = 8.0 Hz, 2H), 7.38–7.33 (m, 5H), 7.32–7.22 (m, 4H), 7.21–7.18 (m, 2H), 6.98 (d, J = 8.0 Hz, 2H), 6.69–6.64 (m, 4H), 6.50–6.47 (m, 3H), 4.45 (br d, J = 14.5 Hz, 1H), 3.90 (br d, J = 14.5 Hz, 1H), 3.36 (s, 6H), 2.62 (s, 3H); ^{13}C NMR (126 MHz, DMSO–D_6): δ 197.8, 158.9, 158.4, 144.4, 141.9, 140.5, 139.8, 136.0, 134.6, 133.2, 132.6, 132.4, 130.5, 130.0, 129.8, 129.5, 129.0, 128.9, 128.8, 128.7, 128.2, 127.8, 113.9, 113.6, 55.5, 55.4, 51.5, 27.5; IR (Neat): ν_{max} 1604, 1508, 1337, 1247, 1028, 790 cm^{-1}; HRMS (ESI) for $C_{37}H_{33}NO_5SNa^+$ $(M+Na)^+$: calcd. 626.1972, found 626.1973.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)-3-fluorobenzenesulfonamide (3h):



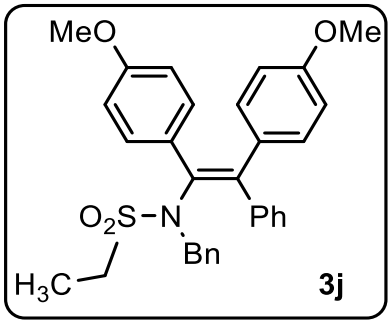
3h (106 mg, 60%) as yellow solid; M.P = 76–79 °C; R_f = 0.5 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.48-7.40 (m, 3H), 7.38–7.35 (m, 4H), 7.32 (t, J = 7.5 Hz, 2H), 7.22 (d, J = 7.0 Hz, 1H), 7.21–7.17 (m, 2H), 6.96 (d, J = 7.0 Hz, 2H), 6.67 (q, J = 9.5 Hz, 4H),), 6.54–6.52 (m, 3H), 6.49 (d, J = 8.5 Hz, 1H), 4.42 (br d, J = 14.5 Hz, 1H), 3.90 (br d, J = 14.0 Hz, 1H), 3.65 (d, J = 6.5 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 161.9 (d, J = 251 Hz, 1C), 158.8, 158.2, 141.8, 141.1, 135.9, 134.6, 132.9, 132.7, 132.4, 130.2, 129.9, 129.8, 129.7, 129.4, 129.1, 128.8, 128.7, 128.5, 128.3, 127.7, 123.4 (d, J = 2.5 Hz, 1C), 119.3 (d, J = 21 Hz, 1C), 115.1 (d, J = 24 Hz, 1C), 113.1 (d, J = 11 Hz, 1C), 55.0 (d, J = 10 Hz, 1C), 51.6; ^{19}F NMR (400 MHz, $CDCl_3$): δ –110.43; IR (Neat): ν_{max} 1603, 1508, 1348, 1247, 1149, 1024, 694 cm^{-1}; HRMS (ESI) for $C_{35}H_{31}FNO_4S^+$ $(M+H)^+$: calcd. 580.1952, found 580.1951.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)-1-chloromethanesulfonamide (3i):



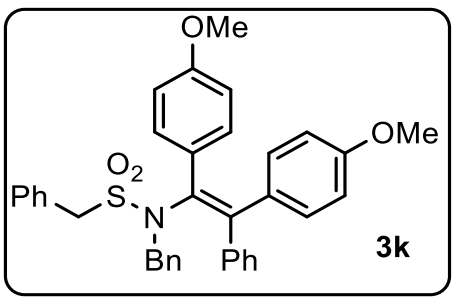
3i (105 mg, 65%) as yellow solid; M.P = 112–115 °C; R_f = 0.9 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 6.18–6.14 (m, 3H), 6.05–6.01 (m, 2H), 6.00–5.95 (m, 3H), 5.62–5.58 (m, 2H), 5.49 (d, J = 7.5 Hz, 4H), 5.38–5.35 (m, 4H), 3.01 (d, J = 11.5 Hz, 1H), 2.89 (t, J = 5.0 Hz, 2H), 2.41 (d, J = 3.0 Hz, 3H), 2.34 (d, J = 3.0 Hz, 3H), 1.94 (br d, J = 10.5 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 159.0, 158.4, 141.6, 140.7, 135.6, 134.1, 133.2, 132.2, 130.8, 129.6, 128.8, 128.7, 128.6, 128.4, 127.7, 113.6, 113.2, 57.2, 55.1, 55.0, 52.7; IR (Neat): ν_{max} 1604, 1508, 1348, 1245, 1027, 733 cm^{-1}; HRMS (ESI) for $C_{30}H_{29}ClNO_4S^+$ $(M+H)^+$: calcd. 534.1500, found 534.1500.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)ethanesulfonamide (3j):



3j (109 mg, 70%) as yellow solid; M.P = 170–172 °C; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 6.59–6.55 (m, 3H), 6.41–6.38 (m, 2H), 6.36–6.31 (m, 3H), 6.06 (d, J = 8.5 Hz, 2H), 6.98–6.95 (m, 2H), 5.87 (d, J = 9.0 Hz, 2H), 5.82 (d, J = 8.5 Hz, 2H), 5.76 (d, J = 9.0 Hz, 2H), 3.24 (q, J = 15.0 Hz, 2H), 2.80 (s, 3H), 2.74 (s, 3H), 1.75–1.66 (m, 1H), 1.93–0.94 (m, 1H), 0.08 (t, J = 7.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 158.8, 158.1, 142.2, 140.2, 136.5, 134.6, 134.2, 132.4, 132.3, 130.4, 129.8, 129.4, 128.6, 128.3, 128.0, 127.2, 113.5, 113.1, 55.1, 55.0, 51.9, 49.4, 7.8; IR (Neat): ν_{max} 1604, 1507, 1329, 1244, 1141, 1027, 699 cm^{-1}; HRMS (ESI) for $C_{31}H_{31}NO_4SNa^+$ $(M+Na)^+$: calcd.536.1866, found 536.1868.

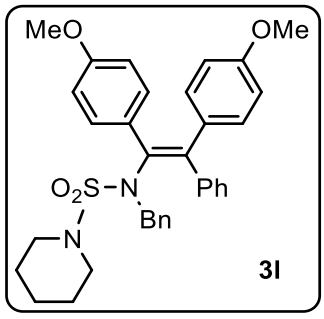
(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)-1-phenylmethanesulfonamide (3k):



3k (94 mg, 55%) as yellow solid; M.P = 188–190 °C; R_f = 0.3 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.43 (t, J = 3.5 Hz, 3H), 7.32–7.27 (m, 5H), 7.24 (dt, J = 7.0, 2.0 Hz, 1H), 7.21–7.18 (m, 2H), 7.16–7.12 (m, 2H), 7.11 (d, J = 8.5 Hz, 2H), 7.06 (br d, J = 7.0 Hz, 2H), 6.85 (d, J = 8.5 Hz, 2H), 6.75 (d, J =

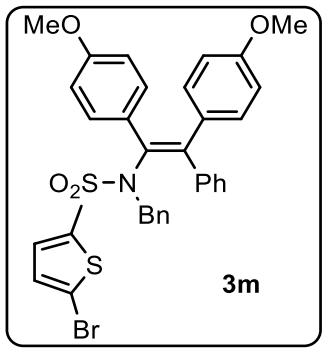
9.0 Hz, 2H), 6.61 (dt, J = 9.0, 3.0 Hz, 2H), 4.32 (br d, J = 14.5 Hz, 1H) 4.20 (br d, J = 14.5 Hz, 1H), 3.78 (s, 3H), 3.72 (s, 3H), 3.50 (br d, J = 13.5 Hz, 1H), 2.77 (br d, J = 13.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.9, 158.2, 142.4, 140.5, 136.2, 134.5, 132.5, 132.3, 130.8, 130.6, 130.0, 129.2, 128.7, 128.6, 128.4, 128.3, 128.1, 127.3, 113.6, 113.1, 60.5, 55.1, 55.0, 52.4; IR (Neat) ν_{max} 1604, 1508, 1245, 1144, 1027, 698 cm^{-1}; HRMS (ESI) for $C_{36}H_{37}N_2O_4S^+$ $(M+NH_4)^+$: calcd. 593.2469, found 593.2467.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)piperidine-1-sulfonamide (3l):



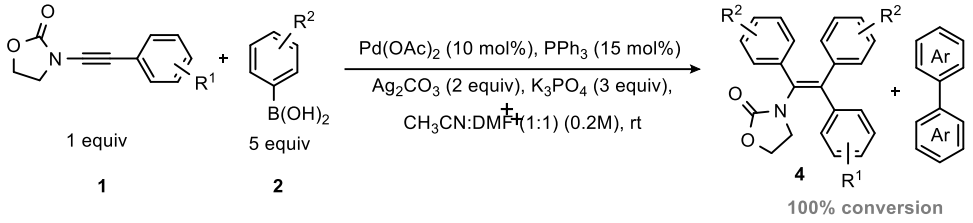
3l (99 mg, 58%) %) as yellow solid; M.P = 225–227 ^{o}C; R_f = 0.9 (15% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.49–7.45 (m, 3H), 7.20–7.16 (m, 3H), 7.15–7.12 (m, 2H), 7.08 (d, J = 8.0 Hz, 2H), 6.77 (d, J = 8.5 Hz, 2H), 6.69–6.61 (m, 6H), 4.01 (br d, J = 14.0 Hz, 1H) 3.88 (br d, J = 14.0 Hz, 1H), 3.71 (s, 3H), 3.63 (s, 3H), 2.58–2.51 (m, 3H), 1.39–1.34 (m, 2H), 1.31–1.20 (m, 5H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 158.7, 158.0, 142.6, 142.3, 136.4, 135.2, 133.9, 133.0, 132.3, 130.6, 130.3, 129.7, 128.3, 128.1, 127.9, 127.6, 126.8, 113.3, 113.0, 55.1, 55.0, 51.4, 46.9, 46.4, 25.5, 23.8; IR (Neat): ν_{max} 1604, 1508, 1246, 1141, 1030, 733, 699 cm^{-1}; HRMS (ESI) for $C_{34}H_{37}N_2O_4S^+$ $(M+H)^+$: calcd. 569.2469, found 569.2468.

(*E*)-*N*-Benzyl-*N*-(1,2-bis(4-methoxyphenyl)-2-phenylvinyl)-5-bromothiophene-2-sulfonamide (3m):



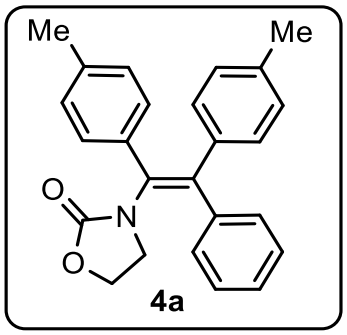
3m (90 mg, 46%) as yellow solid; M.P = 196–199 ^{o}C; R_f = 0.4 (10% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.39 (t, J = 8.0 Hz, 3H), 7.35–7.32 (m, 3H), 7.18 (d, J = 4.0 Hz, 1H), 7.16–7.14 (m, 2H), 7.08 (t, J = 6.5 Hz, 2H), 6.89 (d, J = 4.5 Hz, 1H), 6.67 (q, J = 9.5 Hz, 4H), 6.56 (q, J = 9.0 Hz, 4H), 4.41 (br d, J = 14.5 Hz, 1H), 3.96 (br d, J = 14.5 Hz, 1H) 3.67 (s, 3H), 3.64 (s, 3H); ^{13}C NMR (126 MHz, DMSO–D_6): δ 159.0, 158.4, 142.9, 141.9, 140.9, 135.8, 134.4, 133.4, 133.2, 132.6, 132.3, 131.2, 130.9, 130.6, 129.8, 129.4, 129.03, 129.00, 128.8, 128.1, 119.9, 114.3, 113.9, 113.6, 56.0, 55.5, 55.4, 52.1, 26.9; IR (Neat) ν_{max} 1604, 1507, 1244, 1149, 1023, 699 cm^{-1}; HRMS (ESI) for $C_{33}H_{28}BrNO_4S_2Na^+$ $(M+Na)^+$: calcd. 668.0535, found 668.0540.

General Procedure for the symmetrical diarylation of oxazolidone Ynamides (1) with Aryl Boronic Acids (2) (GP-3):



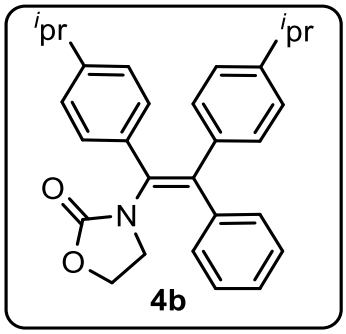
To a mixture of **1** (0.15 mmol) and aryl boronic acid **2** (0.75 mmol), $Pd(OAc)_2$ (3.4mg, 0.015 mmol), K_3PO_4 (95.5mg, 0.45 mmol), and Ag_2CO_3 (82.7mg, 0.3 mmol) was added acetonitrile and dimethylformamide in the ratio 1:1 (CH_3CN:DMF (1:1); 0.75 mL). The reaction mixture was stirred at 25 °C 4–5 hrs. Progress of the reaction was monitored periodically by TLC. Upon completion, the reaction mixture was diluted with ethyl acetate (10 mL). The crude mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified through column chromatography to afford **4a–j.**

(*E*)-3-(2-Phenyl-1,2-di-*p*-tolylvinyl)oxazolidin-2-one (4a):



4a (33 mg, 59%) as yellow solid; M.P = 224–226 °C; R_f = 0.6 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36–7.31 (m, 2H), 7.30–7.27 (m, 2H), 7.26–7.25 (m, 1H), 7.09 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 8.0 Hz, 2H), 6.94–6.90 (m, 4H), 4.18 (t, J = 8.0 Hz, 2H), 3.50 (t, J = 8.0 Hz, 2H), 2.89 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.9, 142.0, 140.0, 137.8, 136.9, 133.3, 131.6, 130.8, 129.4, 129.0, 128.6, 128.4, 127.6, 62.1, 46.1, 21.3, 21.2; IR (Neat): ν_{max} 1753, 1611, 1401, 1343, 1180, 681 cm^{-1}; HRMS (ESI) for $C_{25}H_{24}NO_2^+$ $(M+H)^+$: calcd. 370.1802, found 370.1804.

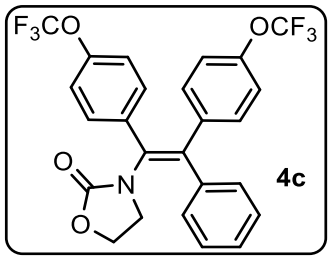
(*E*)-3-(1,2-Bis(4-isopropylphenyl)-2-phenylvinyl)oxazolidin-2-one (4b):



4b (50 mg, 40%) as yellow solid; M.P = 175–178 °C; R_f = 0.6 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36–7.31 (m, 2H), 7.30–7.26 (m, 3H), 7.11 (dt, J = 8.0, 2.0 Hz, 2H), 7.02 (d, J = 8.5 Hz, 2H), 6.97–6.91 (m, 4H), 4.18 (t, J = 8.5 Hz, 2H), 3.51 (t, J = 8.0 Hz, 2H), 2.87–2.77 (m, 2H), 1.20 (d, J = 7.0 Hz, 6H), 1.19 (d, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$):

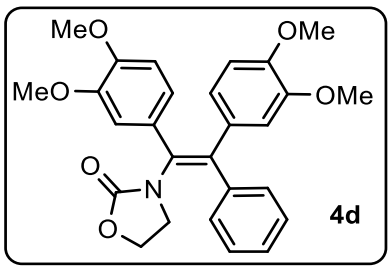
δ 155.9, 148.6, 147.8, 142.1, 140.3, 138.0, 133.5, 131.6, 130.8, 129.4, 129.0, 128.3, 127.5, 126.2, 125.8, 62.0, 46.2, 33.7, 33.6, 23.8, 23.7; IR (Neat): ν_{max} 1758, 1408, 1203, 1150, 1072, 758 cm^{-1}; HRMS (ESI) for $C_{29}H_{32}NO_2^+$ $(M+H)^+$: calcd. 426.2428, found 426.2431.

(*E*)-3-(2-Phenyl-1,2-bis(4-(trifluoromethoxy)phenyl)vinyl)oxazolidin-2-one (4c):



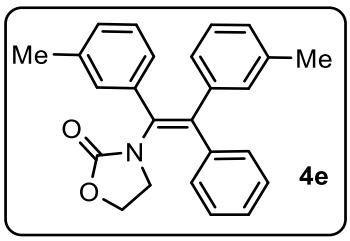
4c (47 mg, 30%) as yellow solid; M.P = 185–187 °C; R_f = 0.5 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 (tt, *J* = 7.5, 2.0 Hz, 2H), 7.33 (tt, *J* = 7.5, 3.0 Hz, 1H), 7.27–7.25 (m, 2H), 7.25 (t, *J* = 1.5 Hz, 1H), 7.21 (dt, *J* = 9.0, 2.5 Hz, 2H), 7.07–7.05 (m, 1H), 7.03 (dt, *J* = 9.0, 2.5 Hz, 3H), 6.98 (d, *J* = 8.0 Hz, 2H), 4.22 (t, *J* = 8.0 Hz, 2H), 3.50 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.7, 148.8, 148.5, 140.8, 140.0, 138.8, 134.6, 132.3, 131.7, 131.1, 128.9, 128.7, 128.3, 120.7, 120.4, 120.3 (q, *J* = 258.3 Hz, 1C), 62.2, 45.9; ^{19}F NMR (400 MHz, $CDCl_3$): δ –57.81, –57.86; IR (Neat): ν_{max} 1750, 1505, 1403, 1203, 1151, 762, 700 cm^{-1}; HRMS (ESI) for $C_{25}H_{19}F_6NO_4^+$ $(M+H)^+$: calcd. 510.1135, found 510.1137.

(*E*)-3-(1,2-Bis(3,4-dimethoxyphenyl)-2-phenylvinyl)oxazolidin-2-one (4d):



4d (24 mg, 35%) as yellow solid; M.P = 115–117 °C; R_f = 0.7 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38–7.33 (m, 2H), 7.31–7.27 (m, 3H), 6.82 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 2.0 Hz, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.59–6.54 (m, 2H), 4.20 (t, *J* = 8.0 Hz, 2H), 3.84 (s, 3H), 3.81 (s, 3H), 3.56 (s, 3H), 3.55–3.50 (m, 5H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.8, 148.8, 148.5, 148.31, 148.26, 141.7, 139.4, 133.5, 131.1, 129.0, 128.9, 128.4, 127.7, 123.6, 121.6, 114.3, 113.2, 110.8, 110.6, 62.1, 55.79, 55.75, 55.70, 55.66, 46.2; IR (Neat) ν_{max} 1748, 1510, 1404, 1260, 1137, 1024, 732 cm^{-1}; HRMS (ESI) for $C_{27}H_{28}NO_6^+$ $(M+H)^+$: calcd.462.1911, found 462.1916.

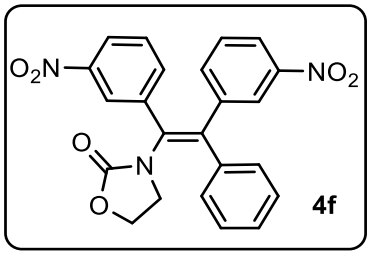
(*E*)-3-(1,2-Bis(3-nitrophenyl)-2-phenylvinyl)oxazolidin-2-one (4e):



4e (21 mg, 38%) as yellow solid; M.P = 183–185 °C; R_f = 0.5 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (tt, *J* = 7.5, 1.5 Hz, 2H), 7.31–7.29 (m, 1H), 7.29–7.26 (m, 2H), 7.05 (t, *J* = 7.5 Hz, 1H), 7.02–6.93 (m, 5H), 6.85–6.80 (m, 2H), 4.20 (t,

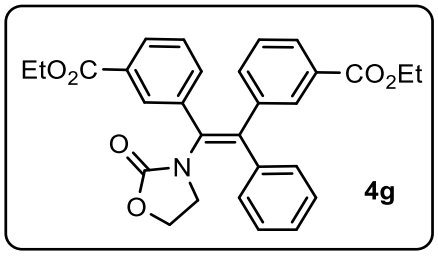
J = 8.0 Hz, 2H), 3.52 (t, J = 8.0 Hz, 2H), 2.21 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.9, 141.8, 140.8, 140.5, 137.7, 137.3, 136.0, 132.0, 131.5, 129.9, 128.9, 128.8, 128.4, 128.1, 127.9, 127.6, 126.9, 62.1, 46.1, 21.3, 21.2; IR (Neat): ν_{max} 1748, 1401, 1220, 1036, 699 cm^{-1}. HRMS (ESI) for $C_{25}H_{24}NO_2^+$ $(M+H)^+$: calcd.370.1802, found 370.1805.

(*E*)-3-(1,2-Bis(3-nitrophenyl)-2-phenylvinyl)oxazolidin-2-one (4f):



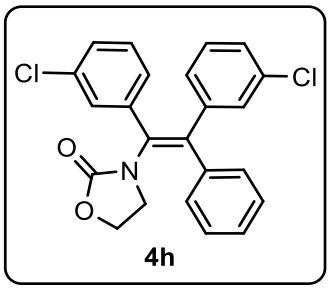
4f (17 mg, 26%) as yellow solid; M.P = 195–197 °C; R_f = 0.2 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10–8.05 (m, 2H), 8.04 (dt, J = 7.5, 3.0 Hz, 1H), 7.87–7.84 (m, 1H), 7.53–7.49 (m, 1H), 7.45–7.41 (m, 3H), 7.41–7.36 (m, 2H), 7.36–7.32 (m, 2H), 7.28 (d, J = 2.0 Hz, 1H), 4.29 (t, J = 8.0 Hz, 2H), 3.52 (t, J = 8.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.6, 148.3, 148.1, 141.6, 139.48, 139.45, 137.7, 136.9, 135.8, 132.6, 129.6, 129.4, 129.2, 129.1, 129.0, 125.6, 124.2, 123.5, 122.8, 62.6, 45.8; IR (Neat): ν_{max} 1752, 1526, 1348, 1265, 733 cm^{-1}. HRMS (ESI) for $C_{23}H_{18}N_3O_6^+$ $(M+H)^+$: calcd.432.1190, found 432.1183.

Diethyl 3,3'-(1-(2-oxooxazolidin-3-yl)-2-phenylethene-1,2-diyl)(*E*)-dibenzoate (4g):



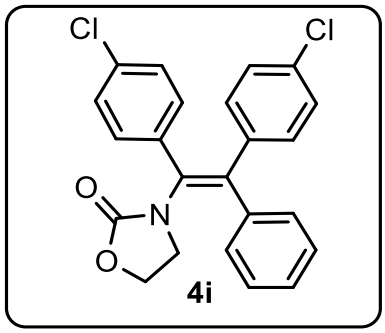
4g (31 mg, 43%) as yellow solid; M.P = 158–160 °C; R_f = 0.2 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (tt, J = 9.0, 1.5 Hz, 2H), 7.82 (dt, J = 6.5, 2.0 Hz, 1H), 7.70–7.68 (m, 1H), 7.37 (tt, J = 7.5, 1.5 Hz, 2H), 7.35–7.32 (m, 2H), 7.28 (d, J = 1.5 Hz, 1H),), 7.27–7.26 (m, 1H), 7.24–7.18 (m, 3H), 4.30 (q, J = 7.5 Hz, 2H), 4.27–4.22 (m, 4H), 3.52 (t, J = 8.0 Hz, 2H), 1.32 (t, J = 7.5 Hz, 3H), 1.29 (t, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 166.1, 166.0, 155.7, 140.7, 140.6, 140.2, 136.4, 135.3, 134.3, 132.4, 131.9, 130.7, 130.4, 130.3, 129.3, 129.0, 128.7, 128.5, 128.4, 128.3, 128.1, 62.3, 61.0, 60.9, 46.0, 14.19, 14.15; IR (Neat): ν_{max} 1752, 1713, 1400, 1247, 1105, 733 cm^{-1}; HRMS (ESI) for $C_{29}H_{27}NO_6$ $(M+Na)^+$: calcd. 508.1731, found 508.1735.

(*E*)-3-(1,2-Bis(3-chlorophenyl)-2-phenylvinyl)oxazolidin-2-one (4h):



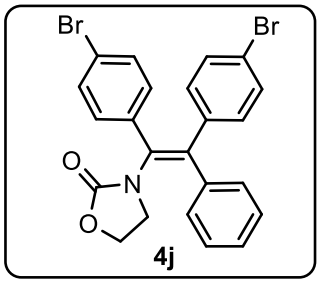
4h (17 mg, 28%) as yellow solid; M.P = 190–193 °C; R_f = 0.4 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, DMSO–D_6): δ 7.42 (t, *J* = 8.0 Hz, 2H), 7.36 (tt, *J* = 7.5, 2.5 Hz, 1H), 7.30 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.28 (d, *J* = 7.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 2.0 Hz, 1H), 7.21–7.19 (m, 2H), 7.16 (dt, *J* = 7.5, 1.5 Hz, 1H), 6.98 (t, *J* = 2.0 Hz, 1H), 6.94 (dt, *J* = 7.5, 1.5 Hz, 1H), 4.22 (t, *J* = 8.5 Hz, 2H), 3.47 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (126 MHz, DMSO–D_6): δ 155.7, 143.1, 140.9, 138.7, 133.3, 133.2, 132.9, 130.6, 130.54, 130.48, 129.8, 129.7¸129.22, 129.15, 128.9, 128.62, 128.58, 127.9, 63.0, 45.8; IR (Neat): ν_{max} 1751, 1401, 1264, 1079, 733 cm^{-1}. HRMS (ESI) for $C_{23}H_{18}Cl_2NO_2^+$ $(M+H)^+$: calcd.410.0709, found 410.0707.

(*E*)-3-(1,2-Bis(4-chlorophenyl)-2-phenylvinyl)oxazolidin-2-one (4i):



4i (21 mg, 35%) as yellow solid; M.P = 272–274 °C; R_f = 0.4 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.39–7.31 (m, 3H), 7.25–7.22 (m, 2H), 7.19 (dt, *J* = 8.5, 2.5 Hz, 2H), 7.14–7.09 (m, 4H), 6.94 (dt, *J* = 8.5, 2.5 Hz, 2H), 4.21 (t, *J* = 8.0 Hz, 2H), 3.48 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.7, 140.9, 139.8, 138.8, 134.5, 134.1, 133.5, 132.2, 131.6, 130.8, 128.9, 128.8, 128.7, 128.4, 128.2, 62.2, 45.9; IR (Neat): ν_{max} 1750, 1401, 1264, 1088, 736 cm^{-1}; HRMS (ESI) for $C_{23}H_{18}Cl_2NO_2$ $(M+H)^+$: calcd. 410.0709, found 410.0711.

(*E*)-3-(1,2-Bis(4-bromophenyl)-2-phenylvinyl)oxazolidin-2-one (4j):



4j (29 mg, 36%) as yellow solid; M.P = 270–272 °C; R_f = 0.4 (30% EtOAc/Hex); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44–7.40 (m, 1H), 7.38–7.34 (m, 3H), 7.34–7.31 (m, 2H), 7.29–7.27 (m, 1H), 7.25–7.21 (m, 2H), 7.06 (dt, *J* = 8.5, 2.5 Hz, 2H), 6.88 (dt, *J* = 8.5, 2.5 Hz, 2H), 4.21 (t, *J* = 8.5 Hz, 2H), 3.48 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, DMSO–D_6): δ 155.6, 141.3, 140.3, 138.8, 135.8, 133.2, 132.6, 132.2, 131.7, 129.2, 129.1, 128.5, 121.8, 121.2, 62.9, 45.8, 29.5; IR (Neat) ν_{max} 1750, 1401, 1222, 1070, 804, 706 cm^{-1}; HRMS (ESI) for $C_{23}H_{18}Br_2NO_2$ $(M+H)^+$: calcd. 497.9699, found 497.9697.

X-ray crystallography:[3]

X-ray reflections for **3c** were collected on Rigaku Oxford CCD diffractometer using Mo-Kα, radiation. Data reduction was performed using CrysAlisPro (version 1.171.33.55). Apex 2 and SHELXL 97 program were used to solve and refine the data. All non-hydrogen atoms were refined anisotropically, and C−H hydrogens were fixed. The crystal has been grown by slow evaporation of CH_2Cl_2 and hexane.

Table S3. Crystallographic Data for Compound **3c**

Compound	**3c**		
formula	$C_{34}H31NO_4S$	V [Å^3]	653.00 (8)
Formula weight	549.66	Z	4
crystal system	Monoclinic	ρ_{calcd} [g cm^{-3}]	1.252
space group	P 21/n	μ [mm^{-1}]	0.150
T [K]	258 K	total reflns	35706
a [Å]	13.3009(3)	unique reflns	6241
b [Å]	11.1099 (3)	observed	3511
c [Å]	19.7682 (5)	R_1[I>2σ(I)]	0.0568 (3511)
α [º]	90	wR2 [all]	0.1660 (6241)
β [º]	93.282 (2)	GOF	1.020
γ [º]	90	Diffractometer	Rigaku Oxford
		CCDC Number	CCDC 2262318

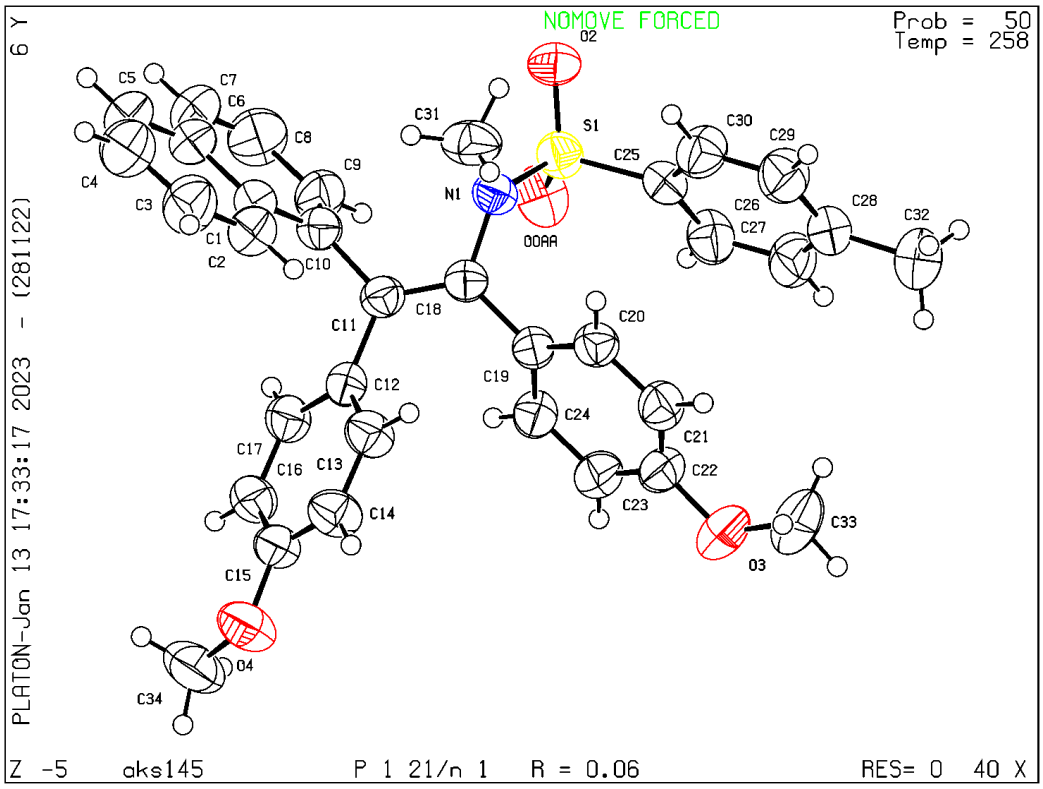


Figure S1. Molecular structure of compound **3c**, (Oxygen (red), nitrogen (blue), and sulphur (yellow)). The ellipsoid contour % probability level is 50%.

X-ray reflections for **4c** were collected on Rigaku Oxford CCD diffractometer using Mo-Kα, radiation. Data reduction was performed using CrysAlisPro (version 1.171.33.55). Apex 2 and SHELXL 97 program were used to solve and refine the data. All non-hydrogen atoms were refined anisotropically, and C−H hydrogens were fixed. The crystal has been grown by slow evaporation of CH_2Cl_2 and hexane.

Table S4. Crystallographic Data for Compound **4c**

Compound	**4c**
formula	$C_{25}H_{17}F_6NO_4$
Formula weight	509.40
crystal em	Monoclinic
space group	P 21/c
T [K]	298 K
a [Å]	15.0723 (4)
b [Å]	9.1985 (3)
c [Å]	16.7522 (4)
α [°]	90

V [Å^3]	2320.85 (11)
Z	4
ρ_{calcd} [g cm^{-3}]	1.458
μ [mm^{-1}]	0.130
total reflns	26409
unique reflns	4087
observed	2930
R_1[I>2σ(I)]	0.0876 (2930)
wR2 [all]	0.2919 (4087)
GOF	1

β [°]	92.202 (2)	Diffractometer	Rigaku Oxford
γ [°]	90	CCDC Number	CCDC 2262319

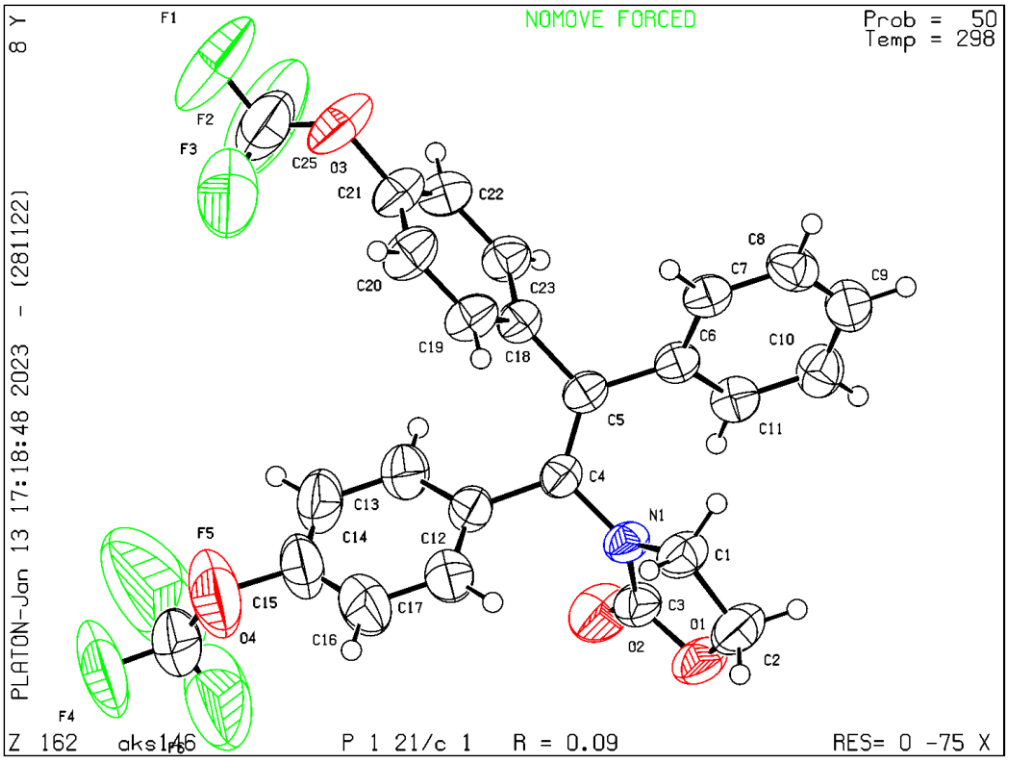
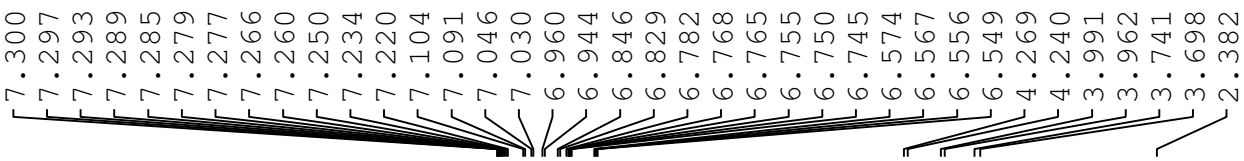
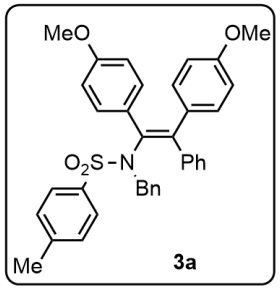


Figure S2. Molecular structure of compound **4c**, (Oxygen (red), nitrogen (blue), and fluorine (green). The ellipsoid contour % probability level is 50%.

Reference:

1. S. Dutta, S. Yang, R. Vanjari, R. K. Mallick, V. Gandon, A. K. Sahoo, Angew. *Chem.Int. Ed*, 2020, **59**, 10785.
2. M. Chen, N. Sun, H. Chen, Y. Liu, *Chem. Commun*, 2016, **52**, 6324.
3. (a) SAINT-Plus, version 6.45, Bruker AXS Inc. Madison, WI, 2003. (b) G. M. Sheldrick, SADABS, Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen, Germany, 1997. (c) SMART (version 5.625), SHELX-TL (version 6.12), Bruker AXS Inc. Madison, WI, 2000; (d) G. M. Sheldrick, SHELXS-97, SHELXL-97, University of Gottingen, Germmany, 1997. (e) O. V. Dolomanov, A. J. Blake, N. R. Champness, M. Schroder, *J. Appl. Cryst.* 2003, **36**, 1283.



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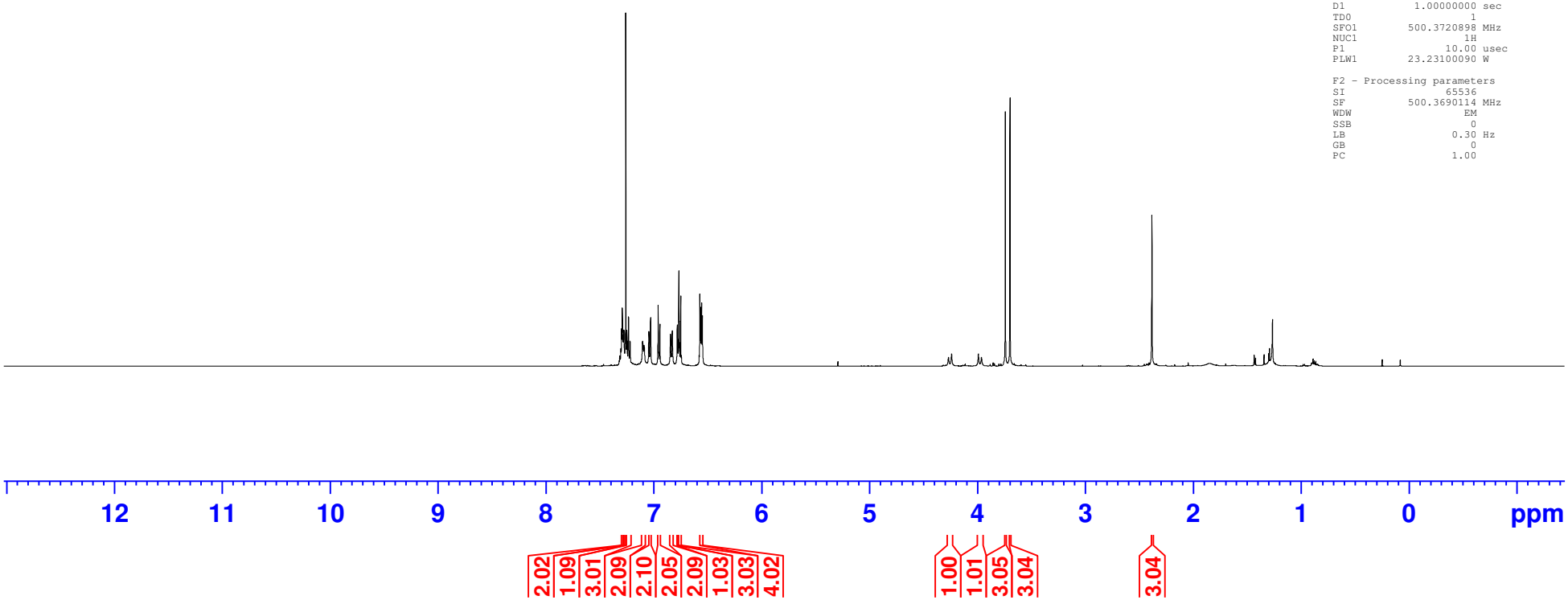

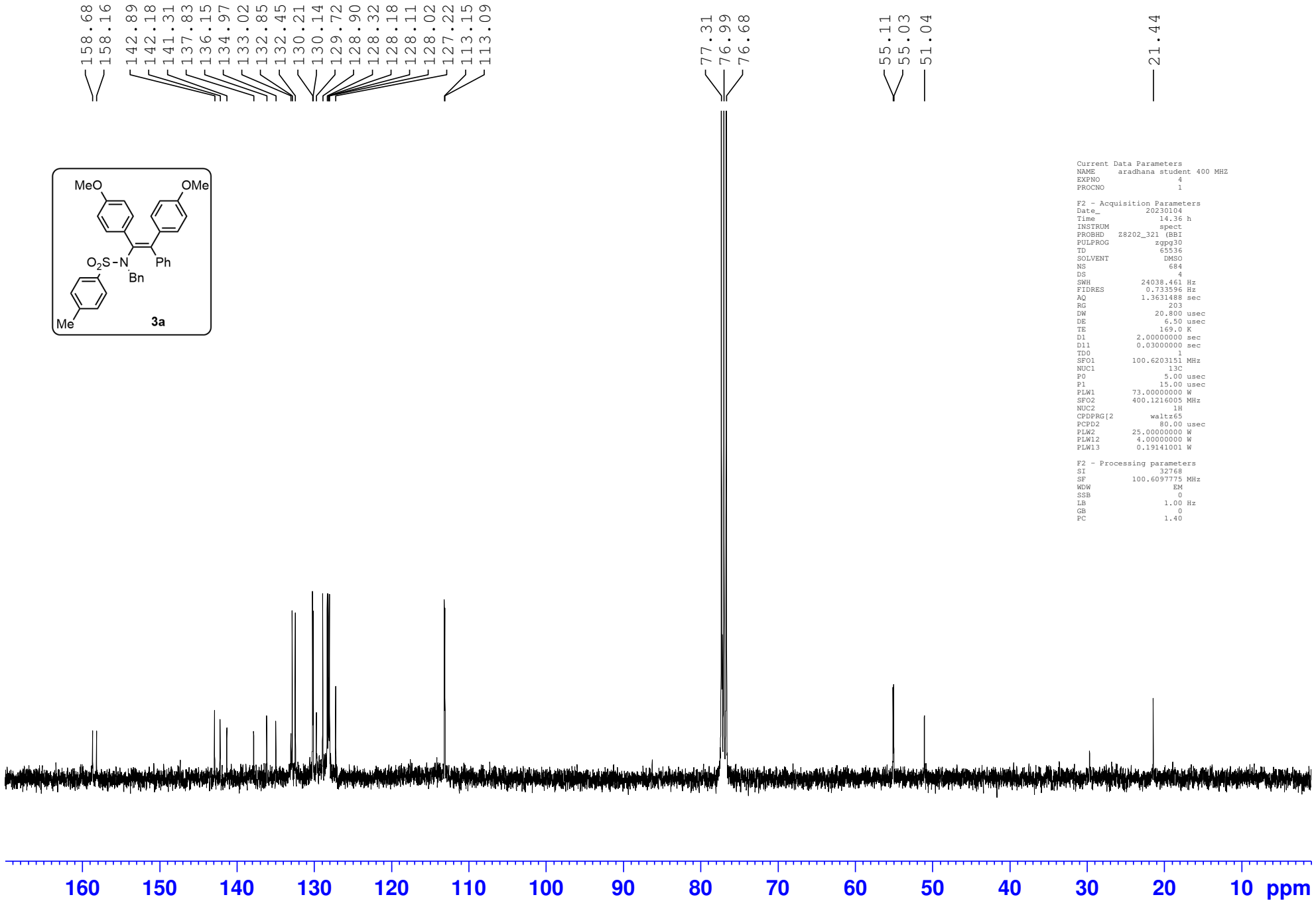
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128.11
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76.68
55.11
55.03
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Bn
Ph
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FIDRES 0.733596 Hz
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RG 203
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DE 6.50 usec
TE 169.0 K
D1 2.00000000 sec
D11 0.03000000 sec
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NUC1 13C
P0 5.00 usec
P1 15.00 usec
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SSB 0
LB 1.00 Hz
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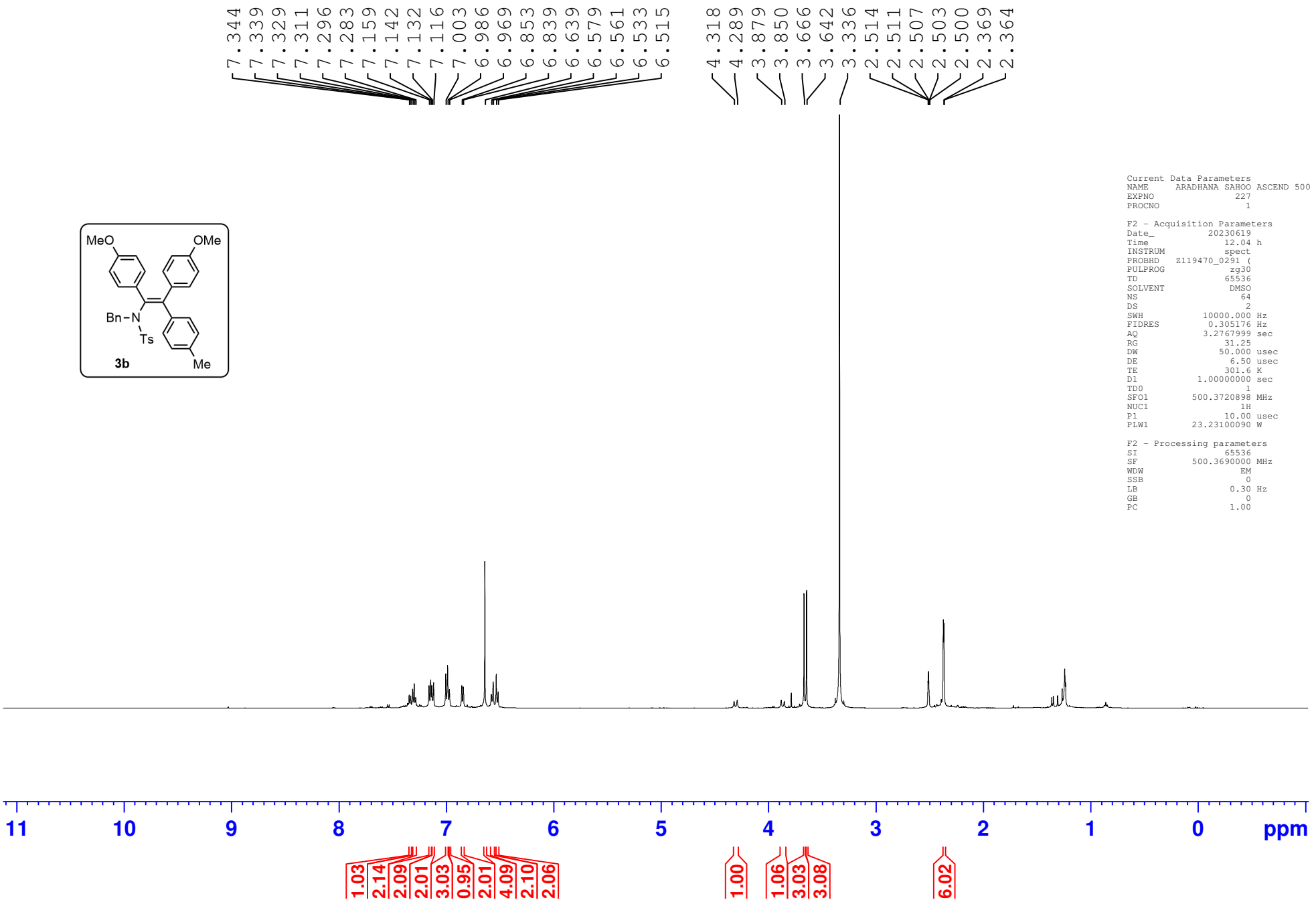
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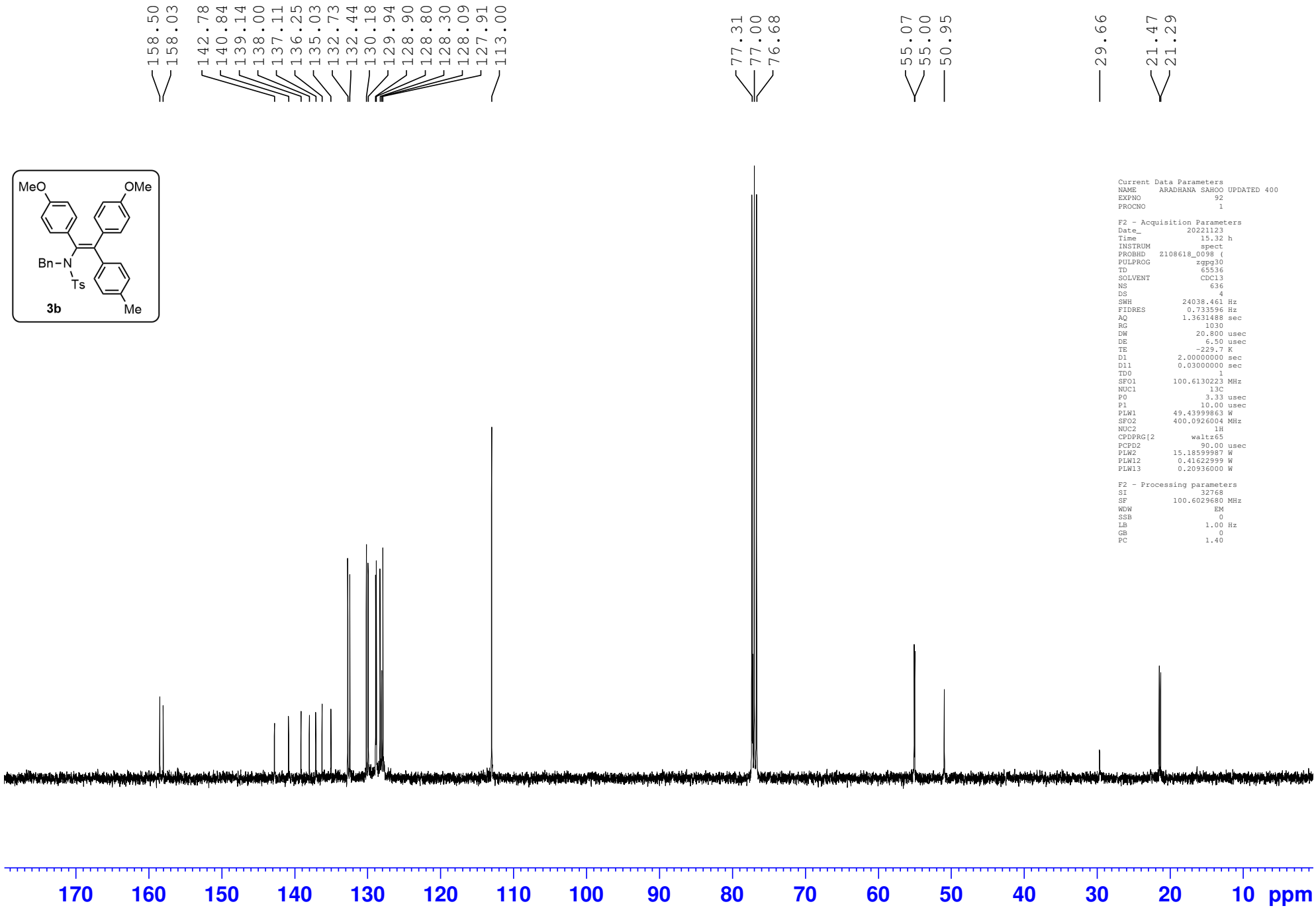
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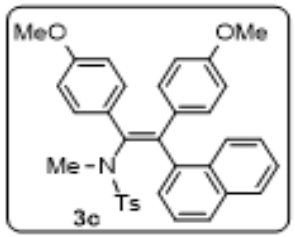
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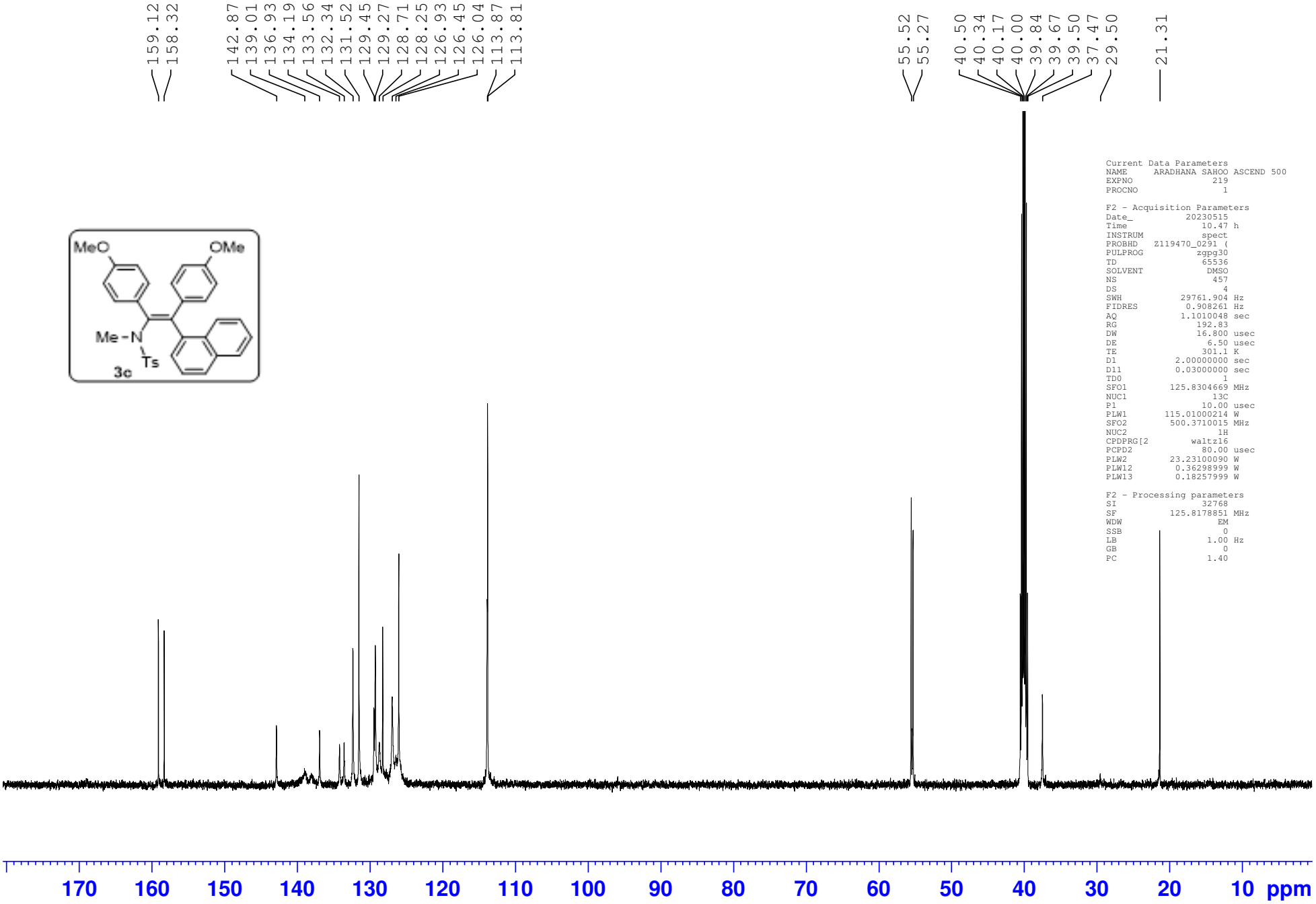
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Me-N
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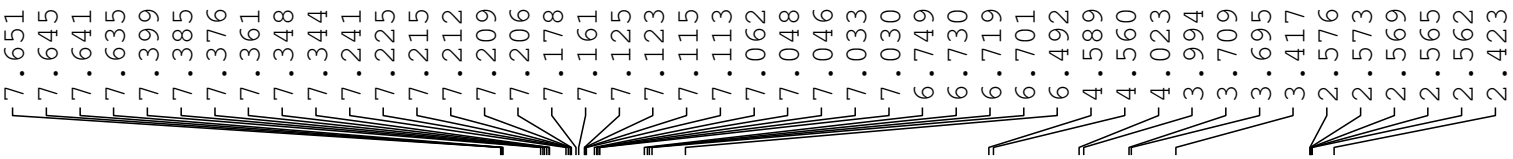

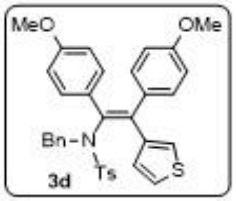


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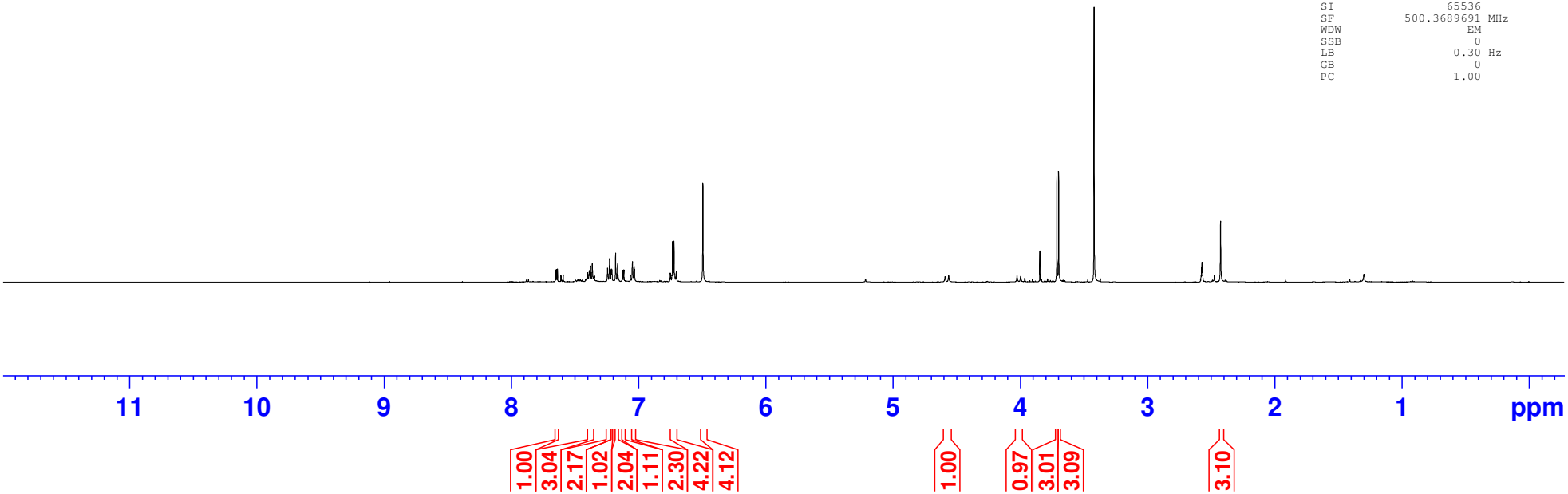

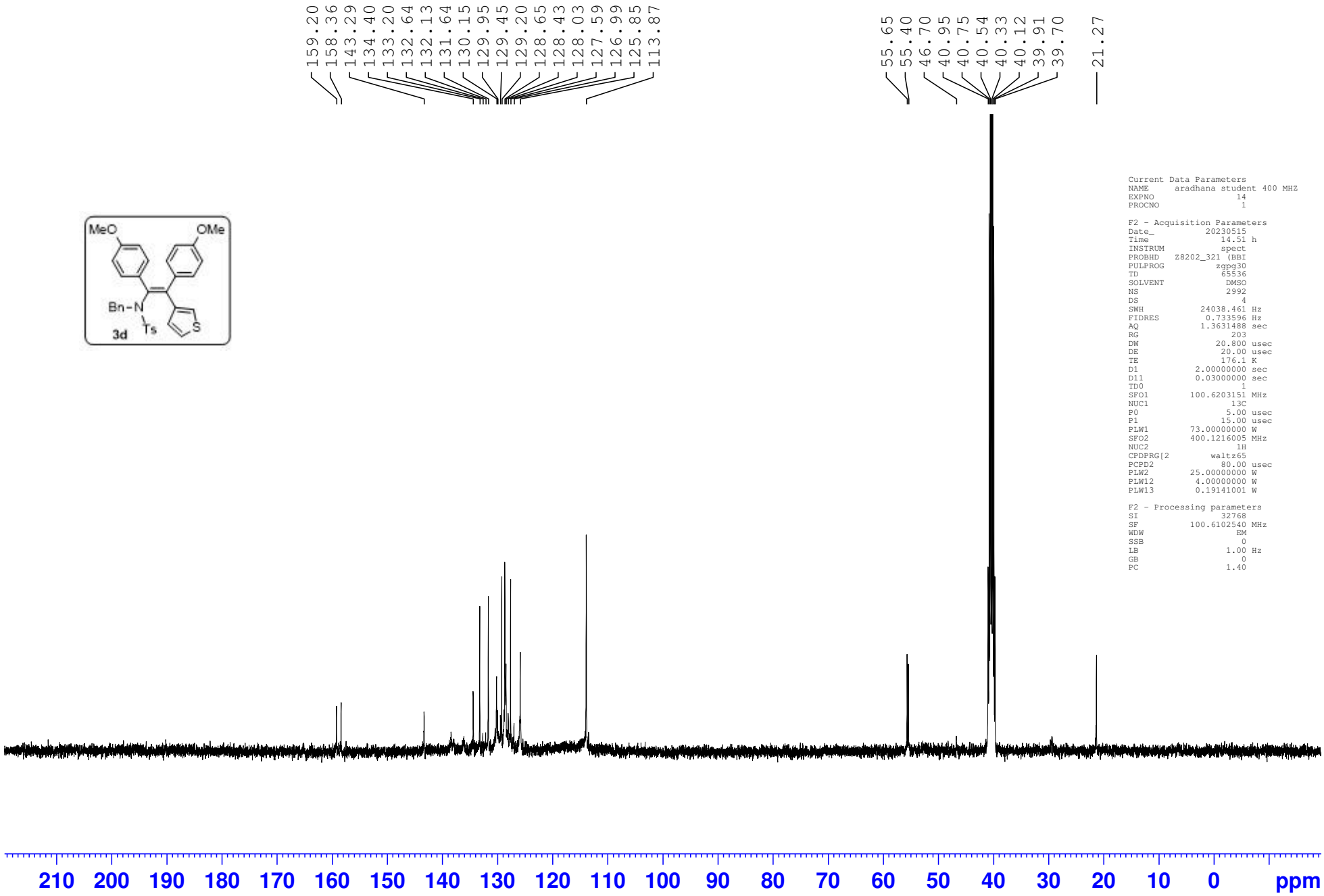
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RG 203
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TE 176.1 K
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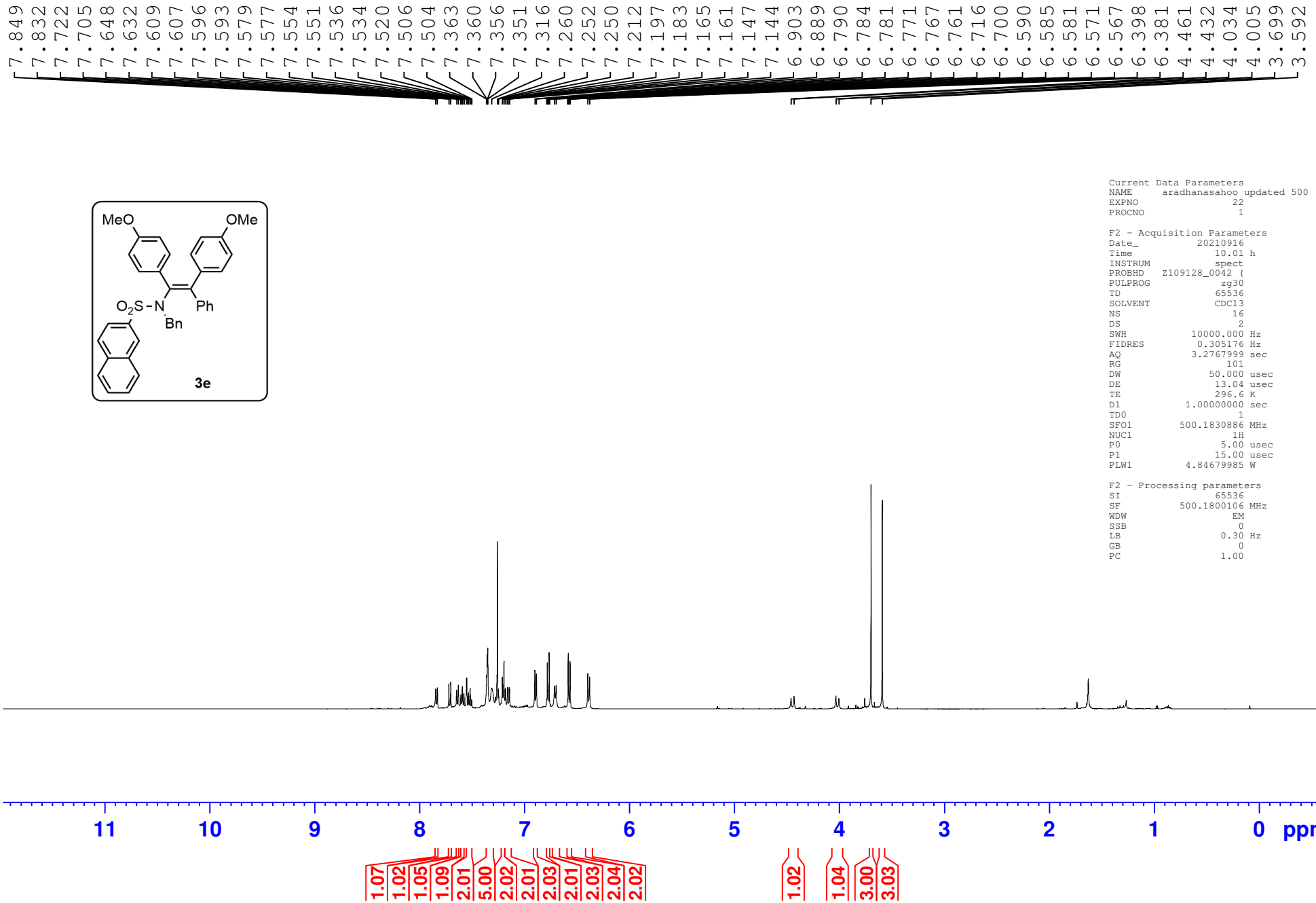
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LB 0.30 Hz
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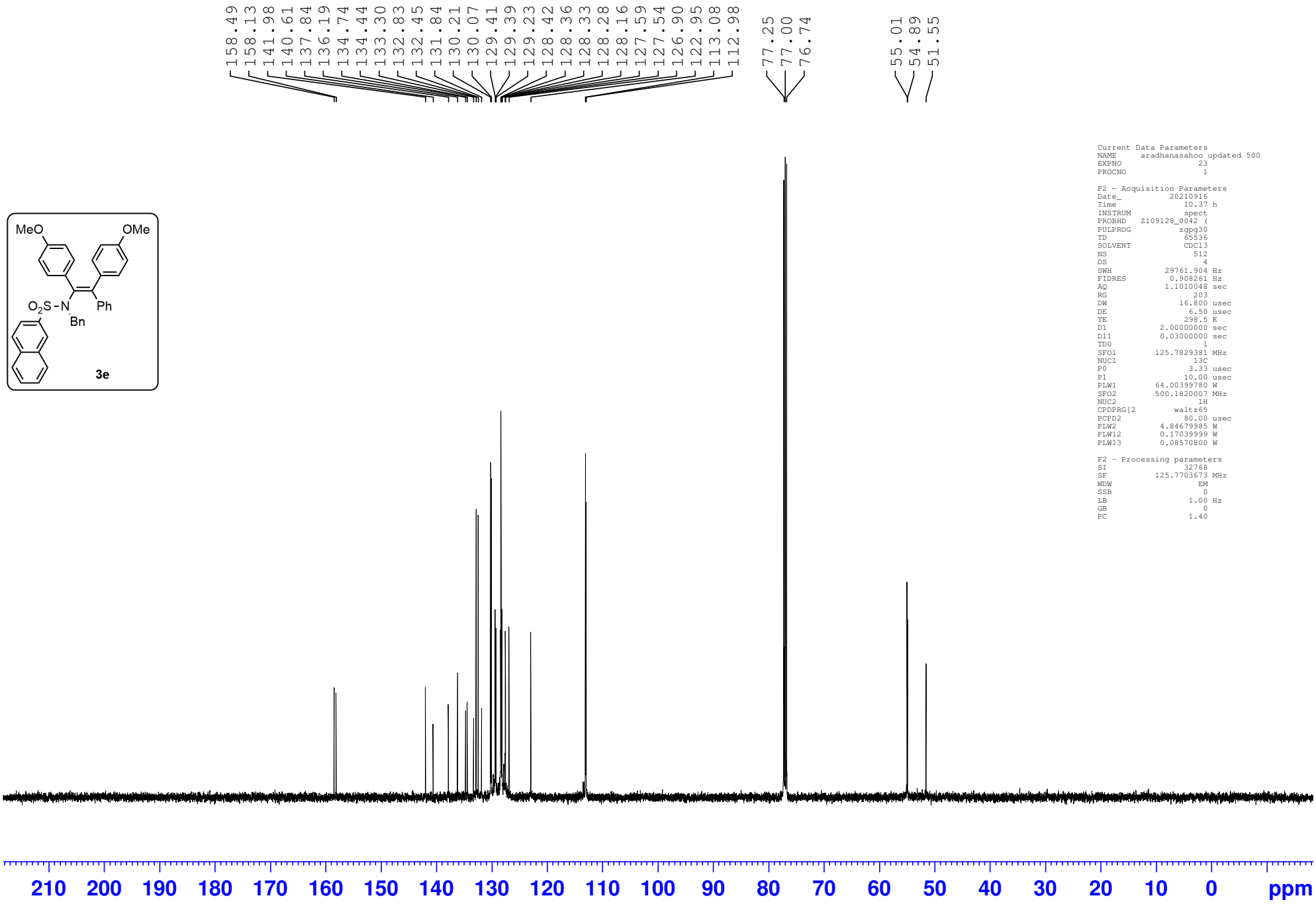
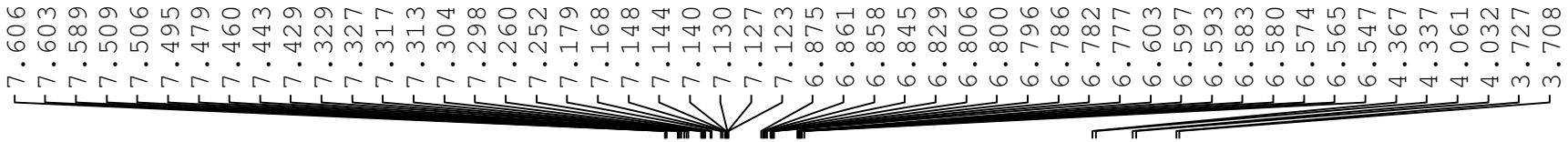
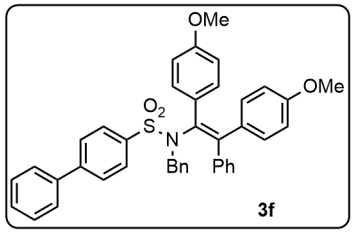
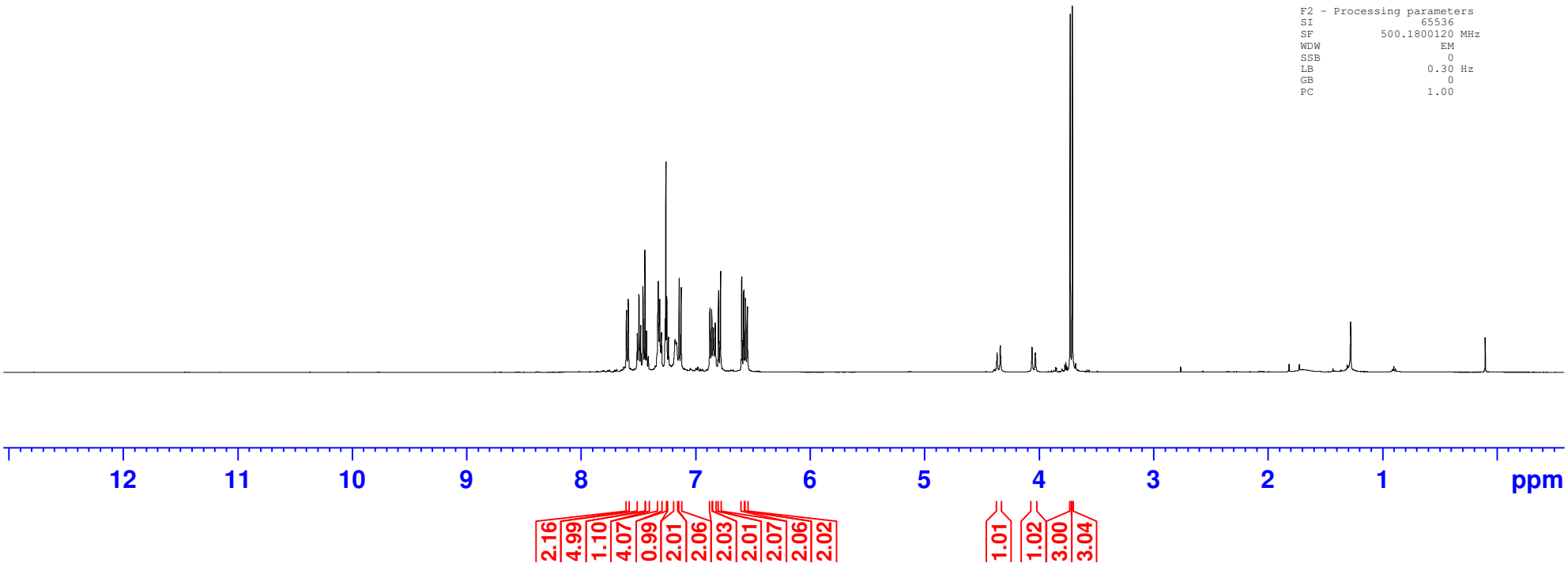
1.04
3.00
3.03

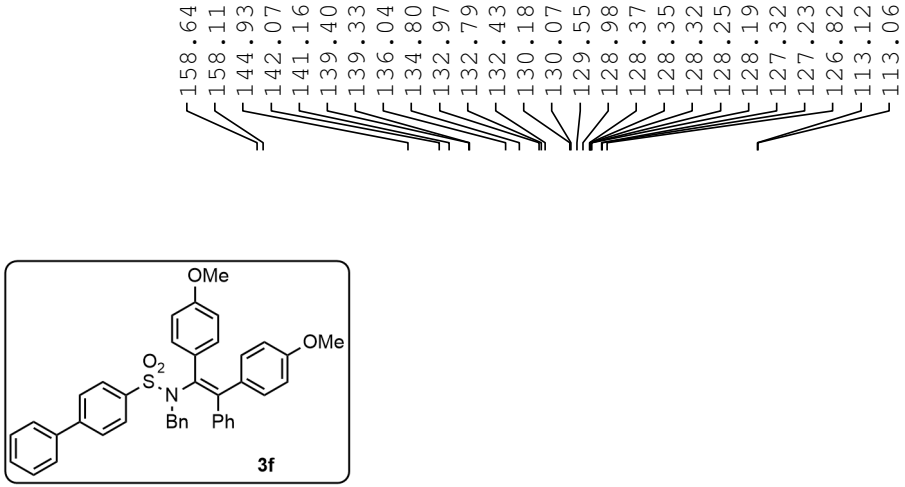

158.49
158.13
141.98
140.61
137.84
136.19
134.74
134.44
133.30
132.83
132.45
131.84
130.21
130.07
129.41
129.39
129.23
128.42
128.36
128.33
128.28
128.16
127.59
127.54
126.90
122.95
113.08
112.98
77.25
77.00
76.74
55.01
54.89
51.55
MeO
OMe
O2S-N
Bn
Ph
3e
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 23
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210916
Time 10.37 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
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 298.5 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 125.7703673 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

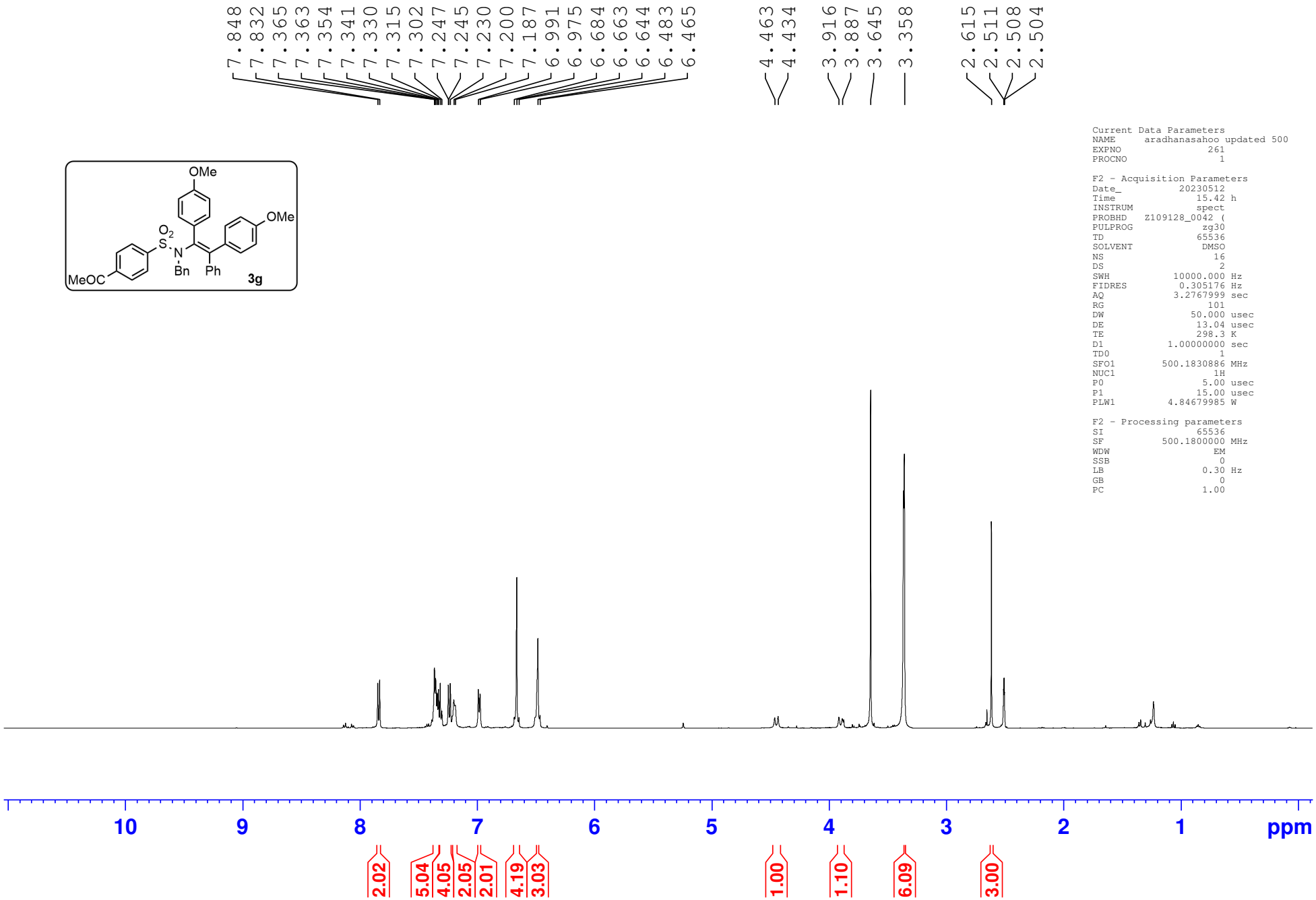


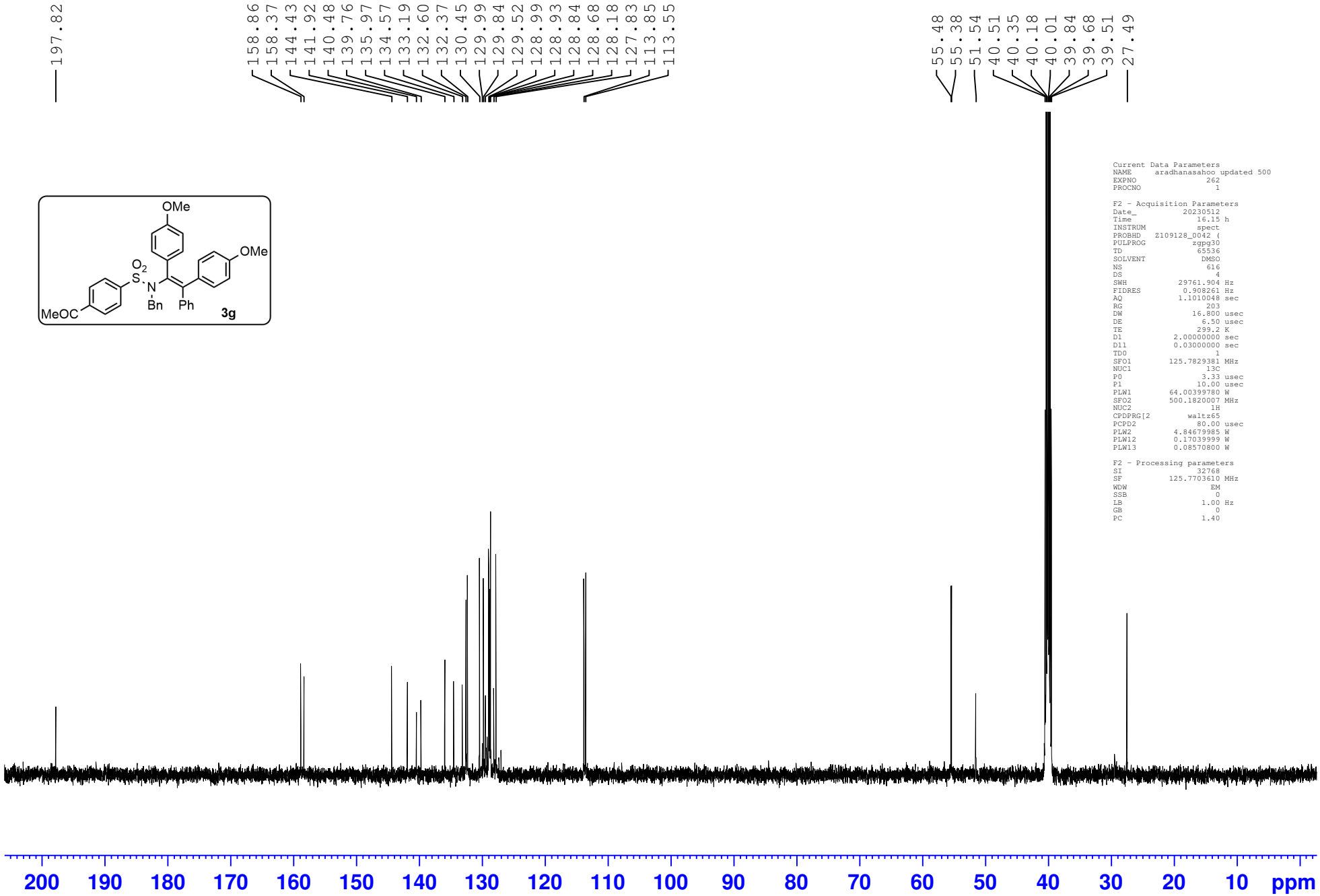


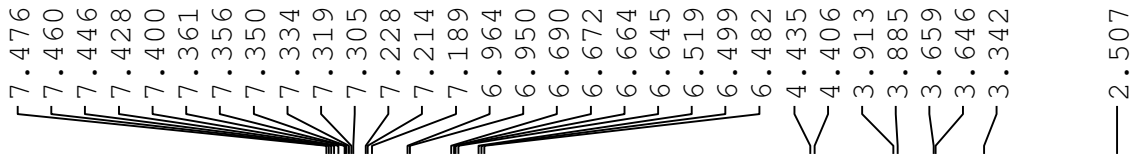

```
Current Data Parameters
NAME      aradhanasahoo updated 500
EXPNO                210
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221202
Time              11.00 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                 71.8
DW                50.000 usec
DE                13.04 usec
TE                297.1 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          500.1800120 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

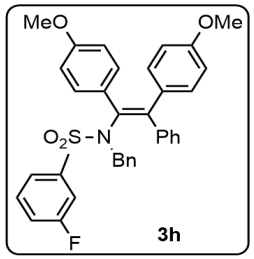



158.64
158.11
144.93
142.07
141.16
139.40
139.33
136.04
134.80
132.97
132.79
132.43
130.18
130.07
129.55
128.98
128.37
128.35
128.32
128.25
128.19
127.32
127.23
126.82
113.12
113.06
77.25
77.00
76.74
55.07
55.00
51.26
OMe
OMe
O2
S
N
Bn
Ph
3f
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 211
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221202
Time 11.11 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 202
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 125.7703709 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

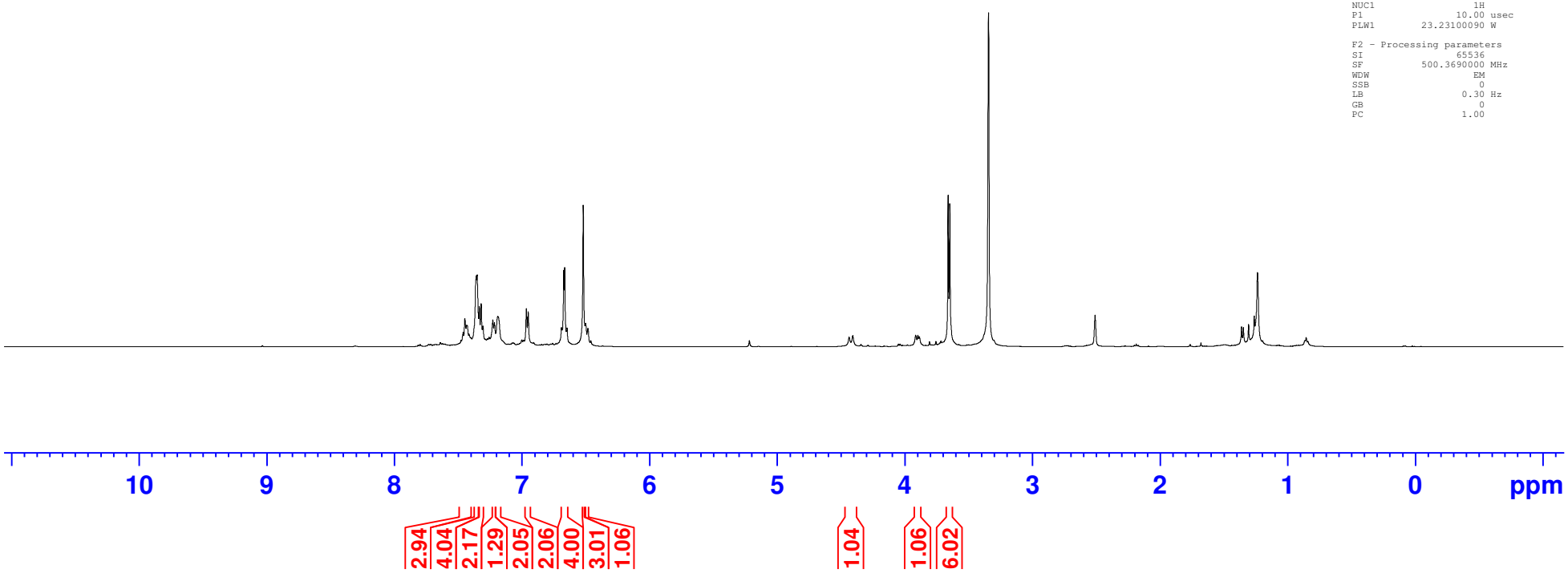

7.848
7.832
7.365
7.363
7.354
7.341
7.330
7.315
7.302
7.247
7.245
7.230
7.200
7.187
6.991
6.975
6.684
6.663
6.644
6.483
6.465
4.463
4.434
3.916
3.887
3.645
3.358
2.615
2.511
2.508
2.504
OMe
OMe
O2
S
N
Bn
Ph
MeOC
3g
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 261
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230512
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 101
DW 50.000 usec
DE 13.04 usec
TE 298.3 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
ppm
2.02
5.04
4.05
2.05
2.01
4.19
3.03
1.00
1.10
6.09
3.00

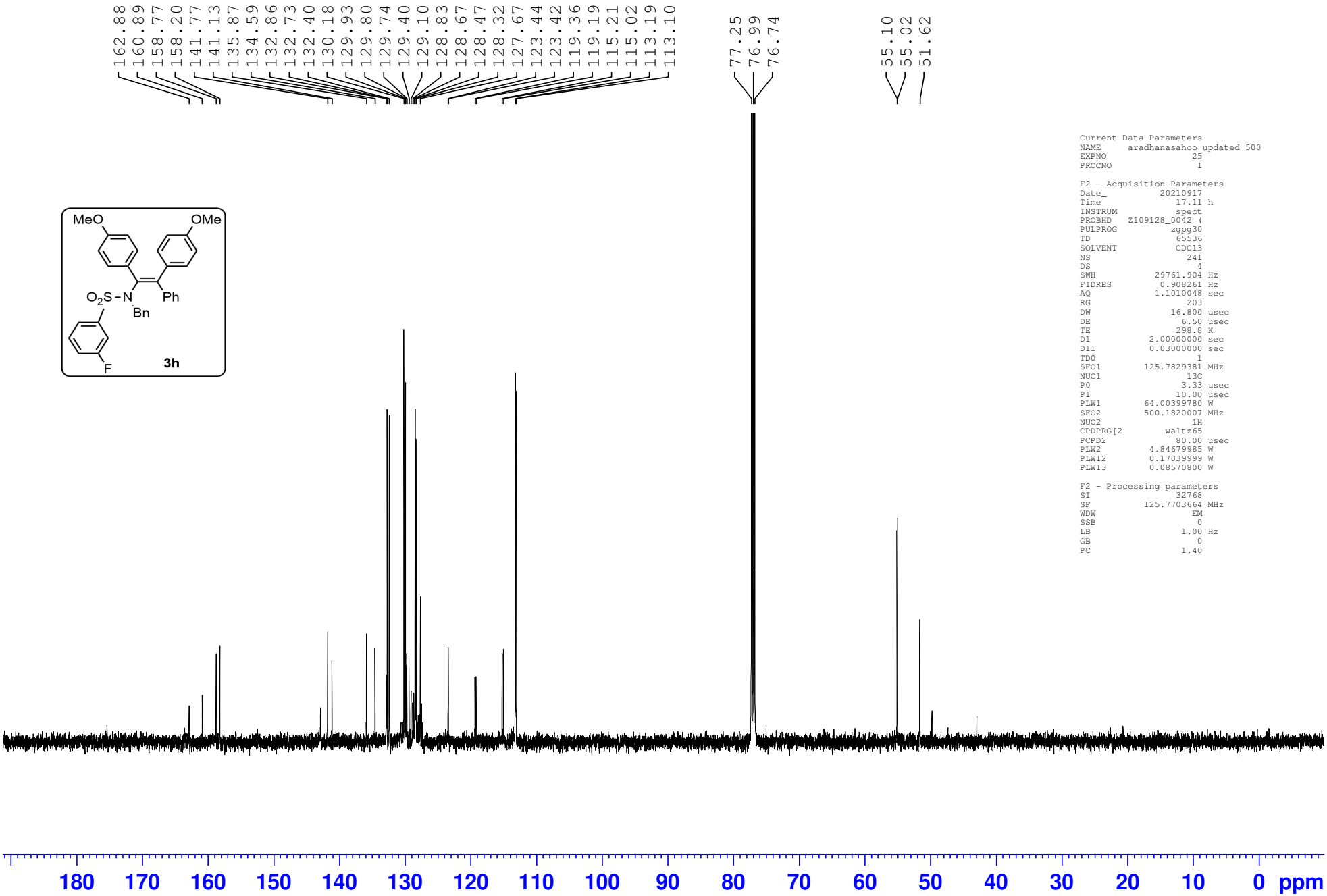

197.82
158.86
158.37
144.43
141.92
140.48
139.76
135.97
134.57
133.19
132.60
132.37
130.45
129.99
129.84
129.52
128.99
128.93
128.84
128.68
128.18
127.83
113.85
113.55
55.48
55.38
51.54
40.51
40.35
40.18
40.01
39.84
39.68
39.51
27.49
OMe
OMe
O2
S
N
Bn
Ph
MeOC
3g
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 262
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230512
Time 16.15 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 616
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 299.2 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
ppm

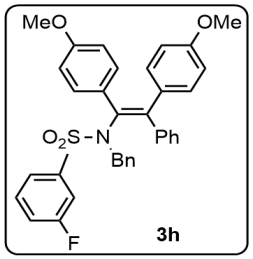





```
Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                228
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230619
Time              12.19 h
INSTRUM            spect
PROBHD   Z119470_0291 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    64
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                 54.81
DW                50.000 usec
DE                 6.50 usec
TE                301.6 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
```



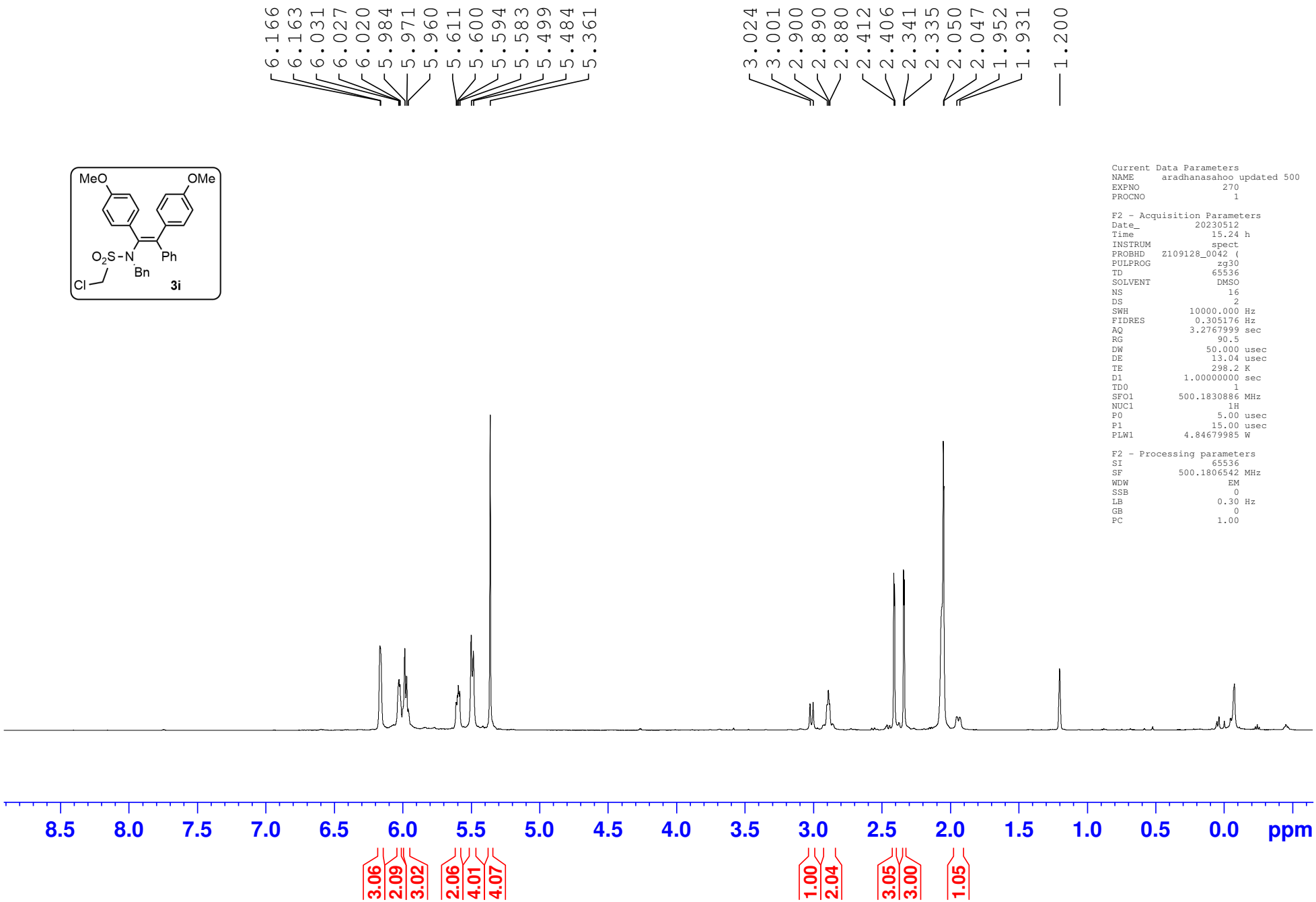

162.88
160.89
158.77
158.20
141.77
141.13
135.87
134.59
132.86
132.73
132.40
130.18
129.93
129.80
129.74
129.40
129.10
128.83
128.67
128.47
128.32
127.67
123.44
123.42
119.36
119.19
115.21
115.02
113.19
113.10
77.25
76.99
76.74
55.10
55.02
51.62
MeO
OMe
O2S-N
Bn
Ph
F
3h
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 25
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210917
Time 17.11 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 241
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 298.8 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 125.7703664 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

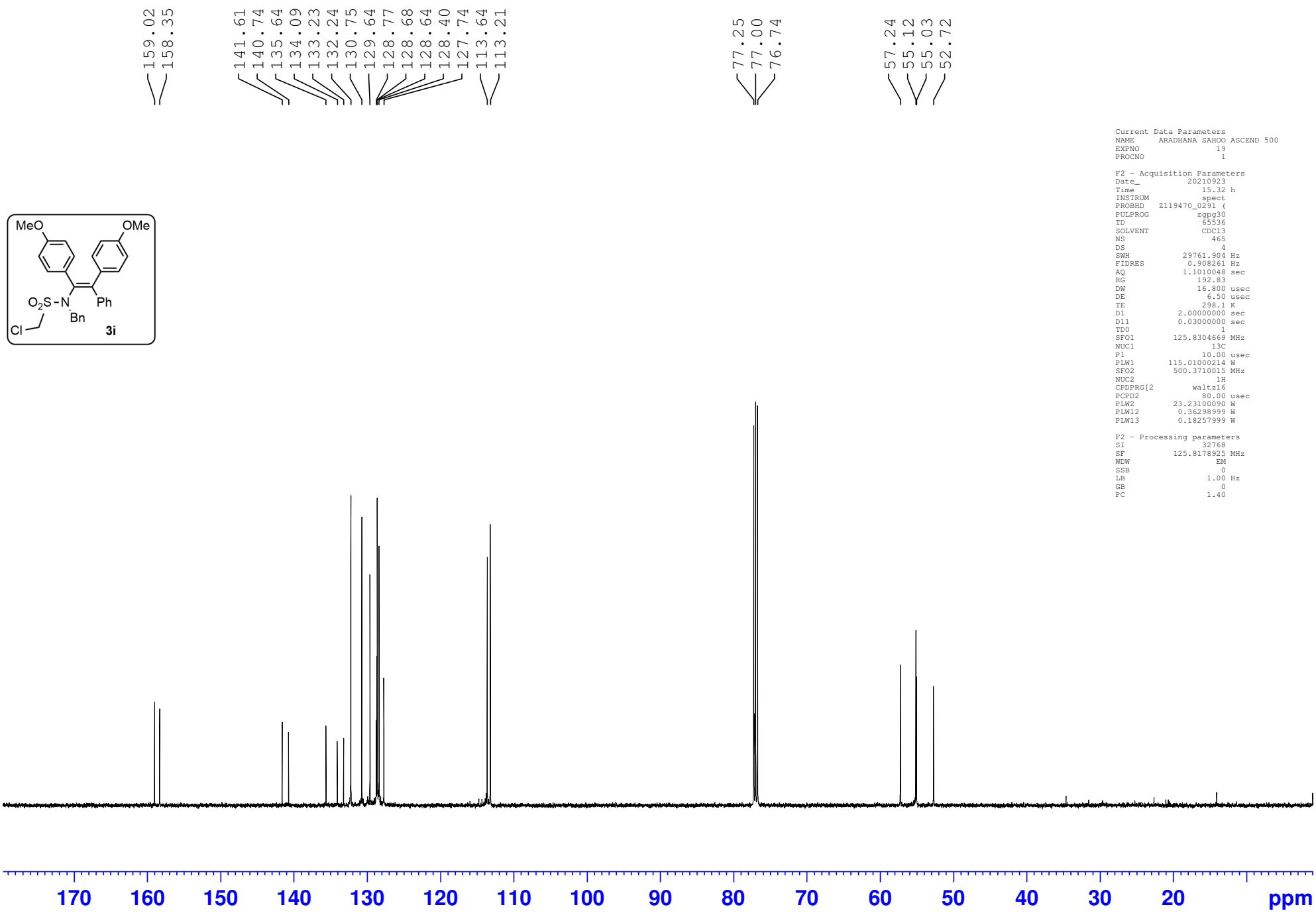


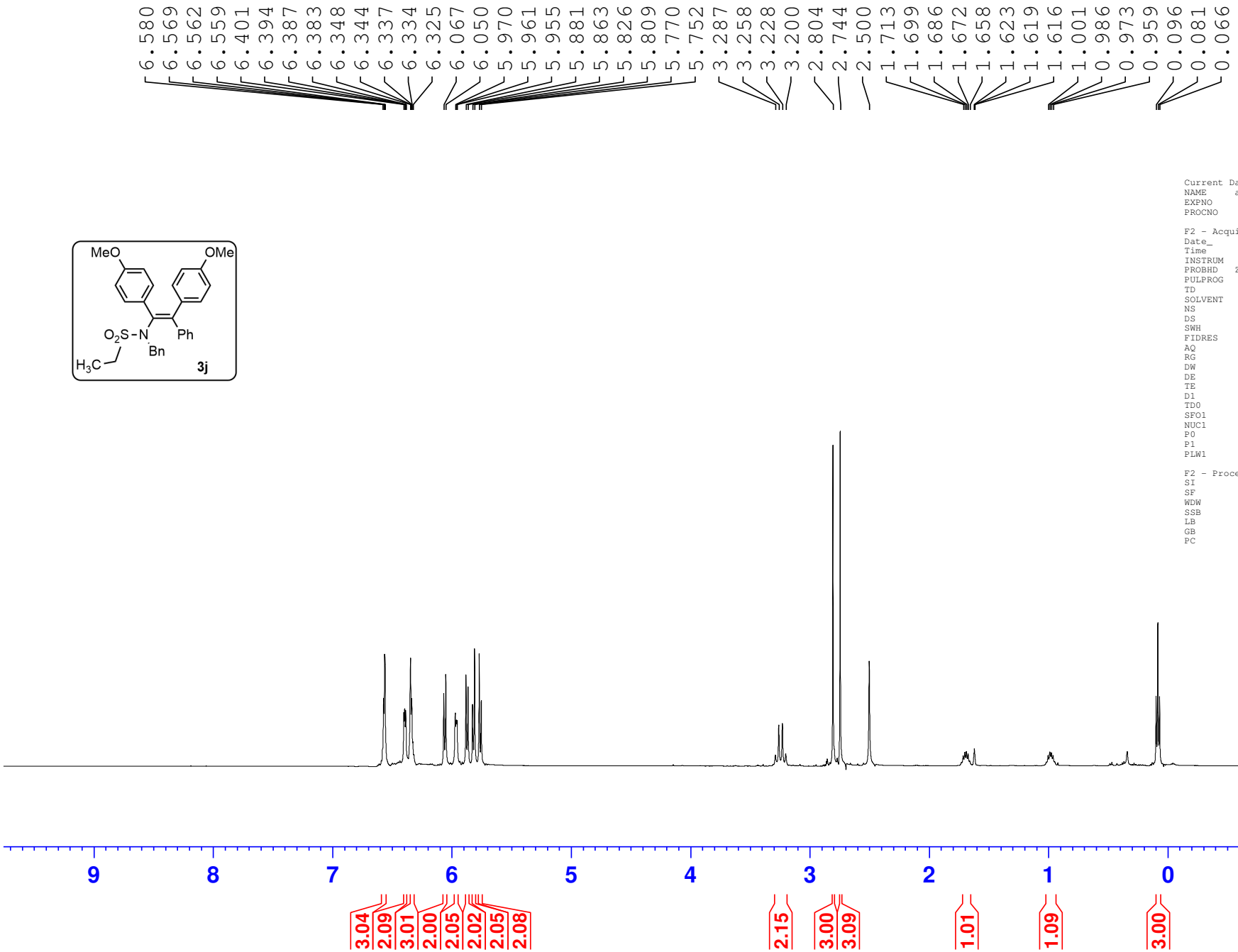
-110.43

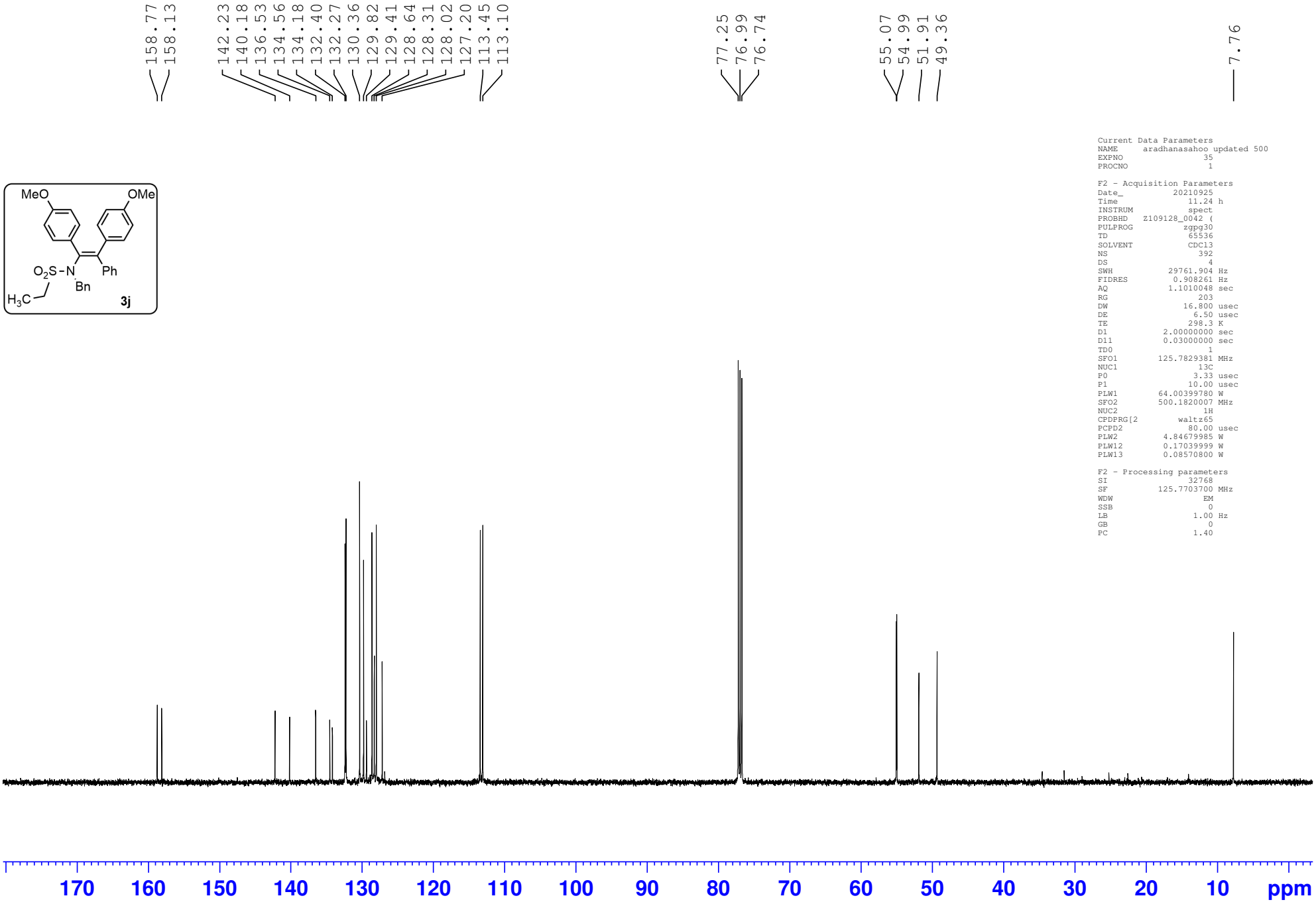
```
Current Data Parameters
NAME      ARADHANA SAHOO UPDATED 400
EXPNO                111
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230510
Time              11.27 h
INSTRUM             spect
PROBHD   Z108618_0098 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDC13
NS                     32
DS                      4
SWH             89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                    724
DW                  5.600 usec
DE                  6.50 usec
TE                428.2 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
```

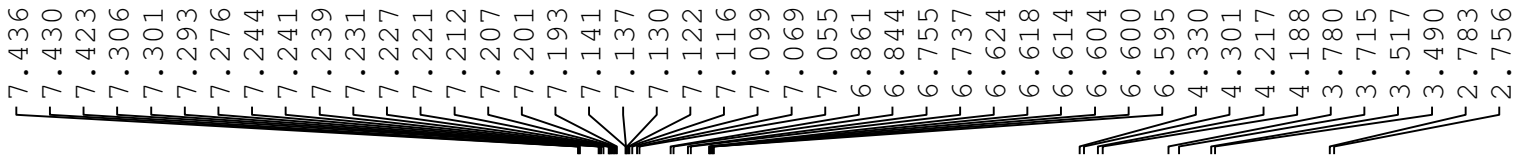
-110.1 -110.2 -110.3 -110.4 -110.5 -110.6 ppm

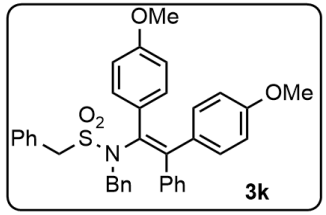

6.166
6.163
6.031
6.027
6.020
5.984
5.971
5.960
5.611
5.600
5.594
5.583
5.499
5.484
5.361
3.024
3.001
2.900
2.890
2.880
2.412
2.406
2.341
2.335
2.050
2.047
1.952
1.931
1.200
MeO
OMe
O2S-N
Ph
Bn
Cl
3i
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 270
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230512
Time 15.24 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 298.2 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 500.1806542 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
0.5
0.0
ppm
3.06
2.09
3.02
2.06
4.01
4.07
1.00
2.04
3.05
3.00
1.05


159.02
158.35
141.61
140.74
135.64
134.09
133.23
132.24
130.75
129.64
128.77
128.68
128.64
128.40
127.74
113.64
113.21
77.25
77.00
76.74
57.24
55.12
55.03
52.72
MeO
OMe
O2S-N
Bn
Ph
Cl
3i
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 19
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210923
Time 15.32 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 465
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 298.1 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 125.8178925 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

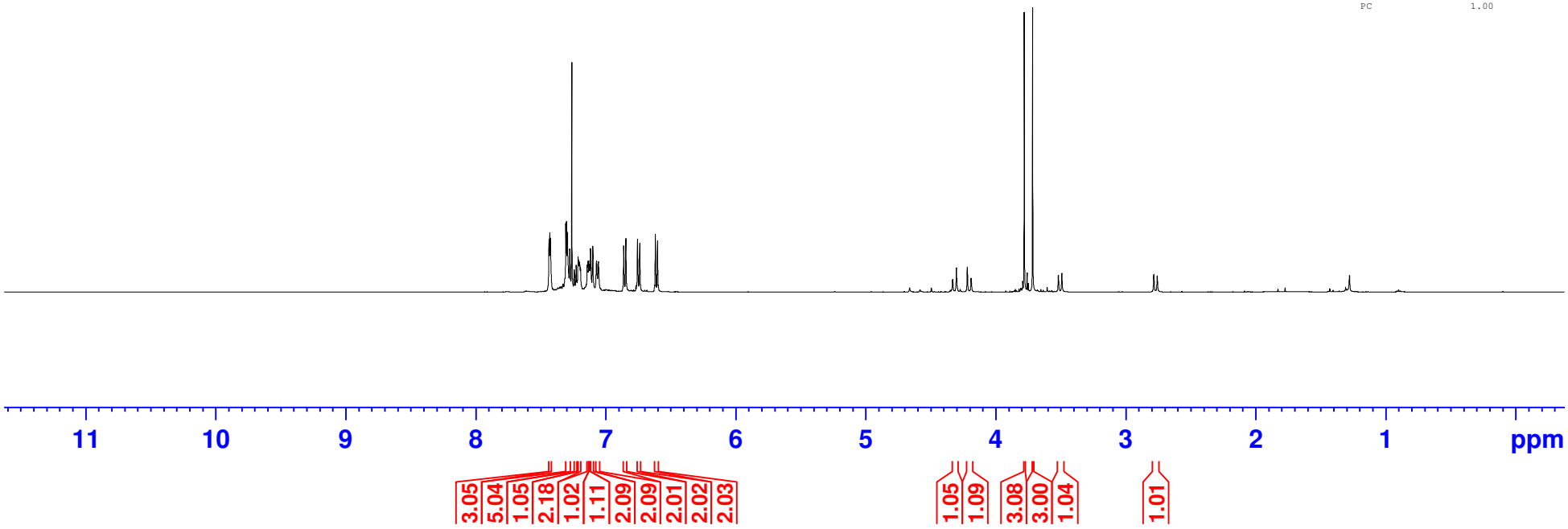

6.580
6.569
6.562
6.559
6.401
6.394
6.387
6.383
6.348
6.344
6.337
6.334
6.325
6.067
6.050
5.970
5.961
5.955
5.881
5.863
5.826
5.809
5.770
5.752
3.287
3.258
3.228
3.200
2.804
2.744
2.500
1.713
1.699
1.686
1.672
1.658
1.623
1.619
1.616
1.001
0.986
0.973
0.959
0.096
0.081
0.066
MeO
OMe
O2S-N
Ph
Bn
H3C
3j
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 260
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230512
Time 15.29 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 298.2 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 500.1804445 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
3.04
2.09
3.01
2.00
2.05
2.02
2.05
2.08
2.15
3.00
3.09
1.01
1.09
3.00

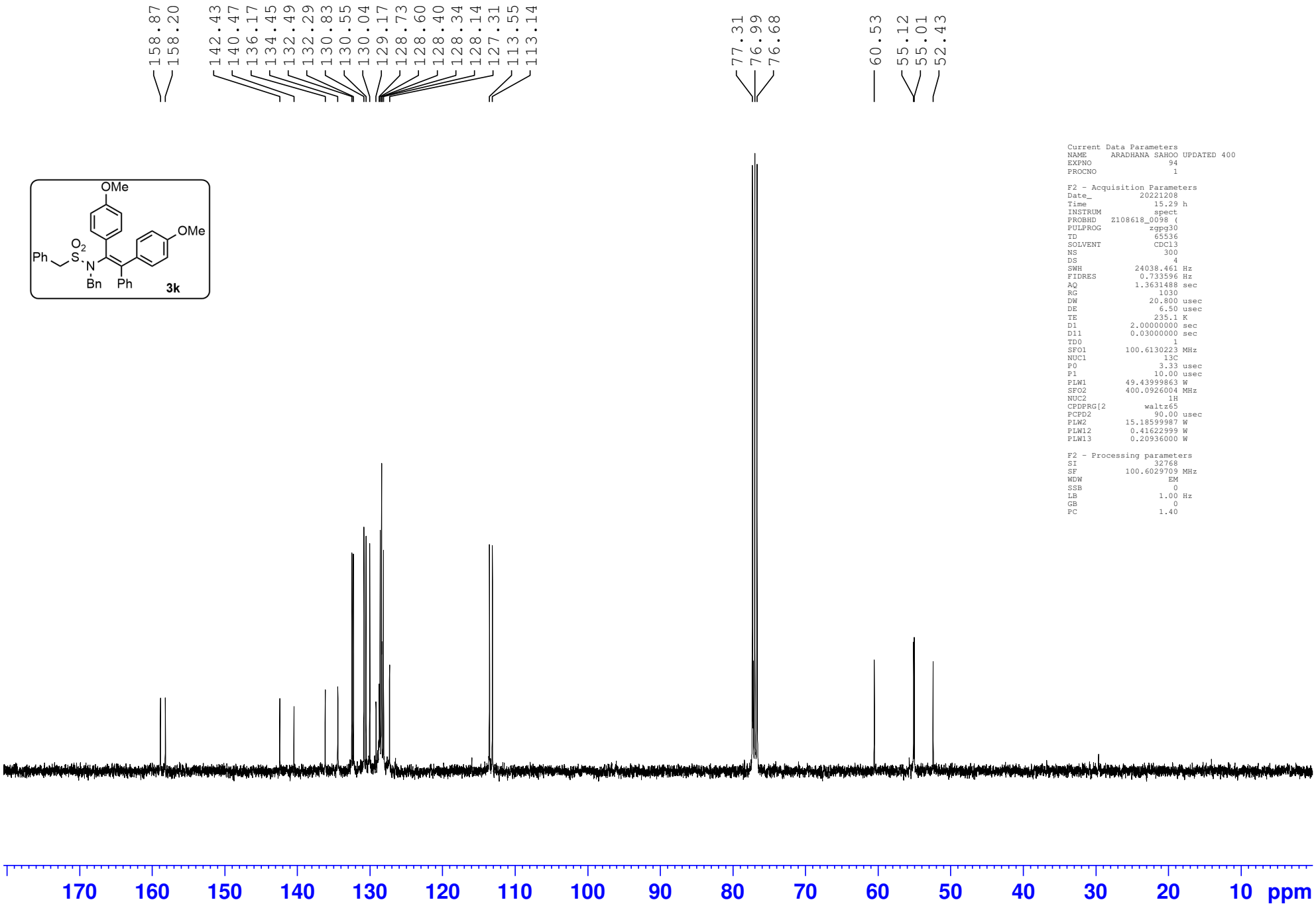

158.77
158.13
142.23
140.18
136.53
134.56
134.18
132.40
132.27
130.36
129.82
129.41
128.64
128.31
128.02
127.20
113.45
113.10
77.25
76.99
76.74
55.07
54.99
51.91
49.36
7.76
MeO
OMe
O2S-N
Bn
Ph
H3C
3j
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210925
Time 11.24 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 392
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 298.3 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 125.7703700 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

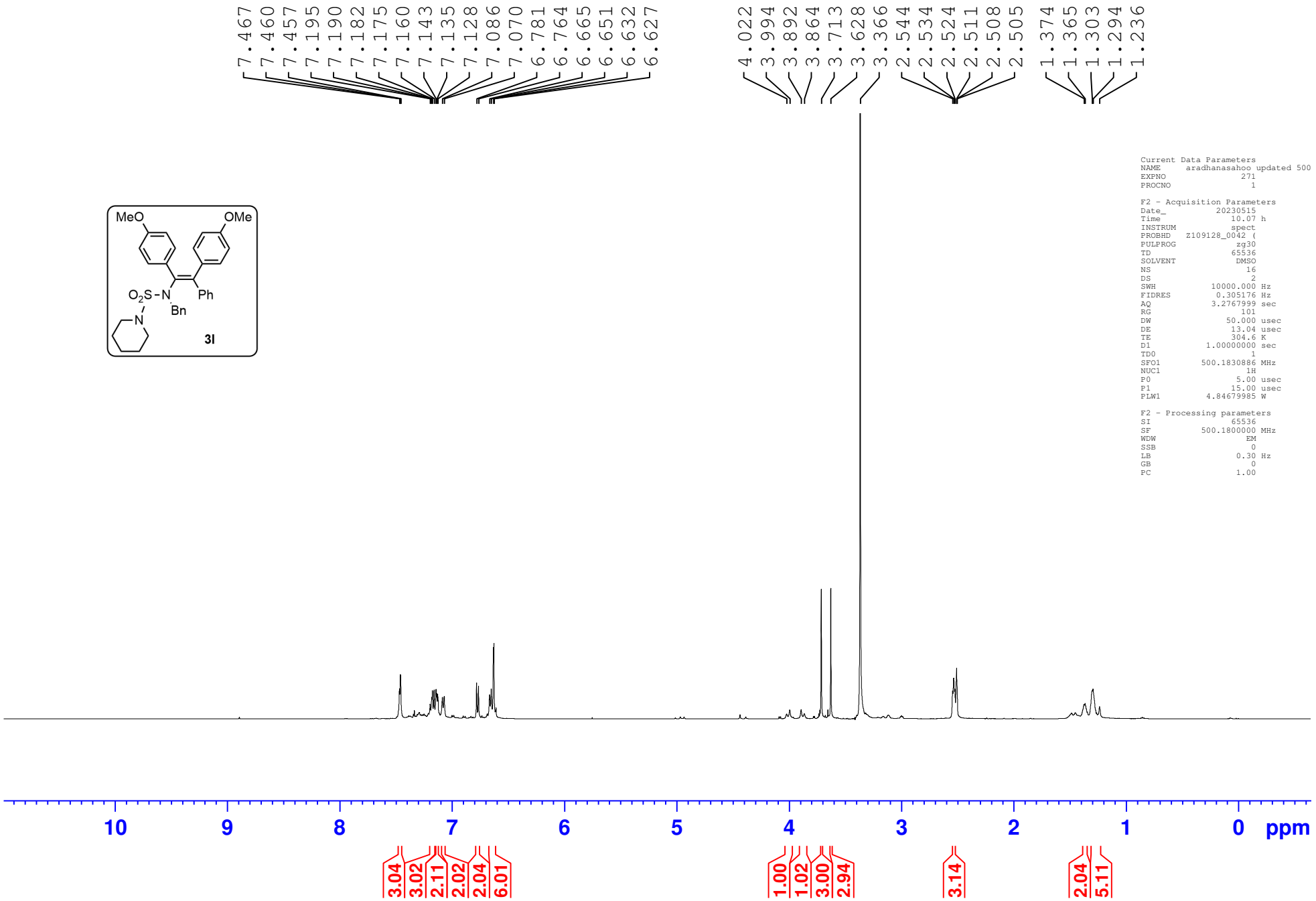





```
Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                183
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221208
Time              14.42 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                298.9 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            500.3690118 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

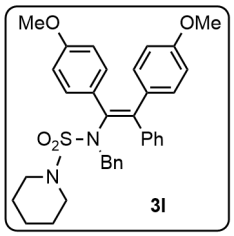



158.87
158.20
142.43
140.47
136.17
134.45
132.49
132.29
130.83
130.55
130.04
129.17
128.73
128.60
128.40
128.34
128.14
127.31
113.55
113.14
77.31
76.99
76.68
60.53
55.12
55.01
52.43
OMe
OMe
O2
S
N
Ph
Bn
Ph
3k
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 94
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221208
Time 15.29 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
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 235.1 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 100.6029709 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


7.467
7.460
7.457
7.195
7.190
7.182
7.175
7.160
7.143
7.135
7.128
7.086
7.070
6.781
6.764
6.665
6.651
6.632
6.627
4.022
3.994
3.892
3.864
3.713
3.628
3.366
2.544
2.534
2.524
2.511
2.508
2.505
1.374
1.365
1.303
1.294
1.236
MeO
OMe
O2S-N
Ph
Bn
N
3l
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 271
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230515
Time 10.07 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 304.6 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
3.04
3.02
2.11
2.02
2.04
6.01
1.00
1.02
3.00
2.94
3.14
2.04
5.11

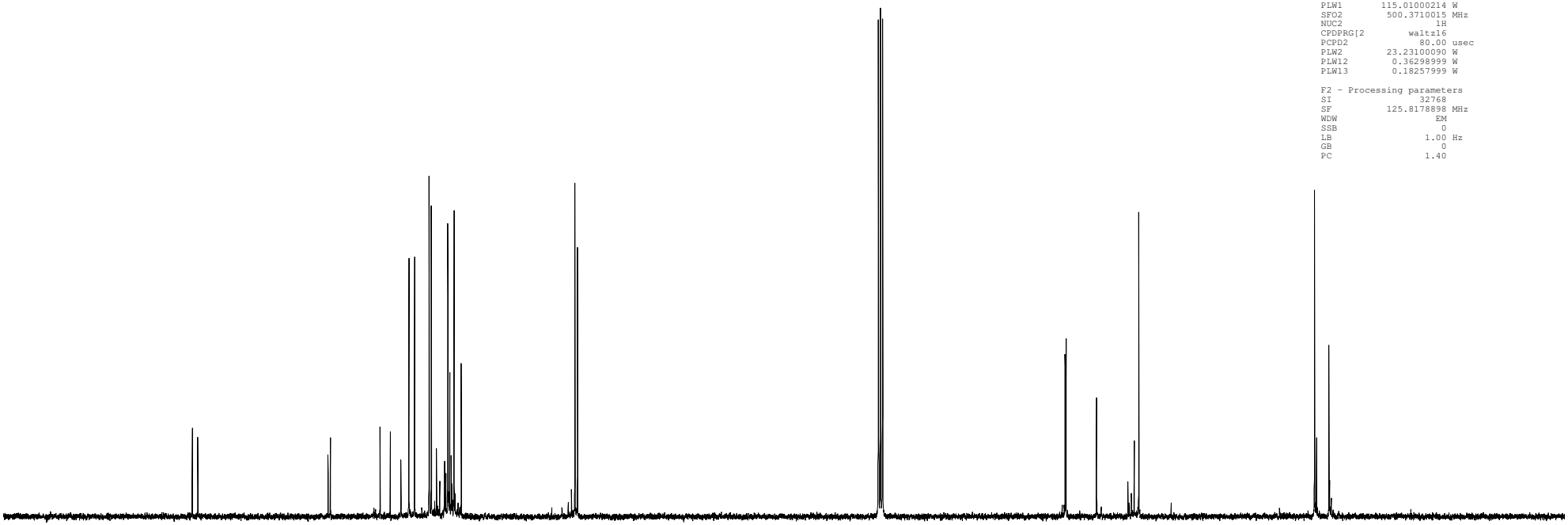
ARS-1-216

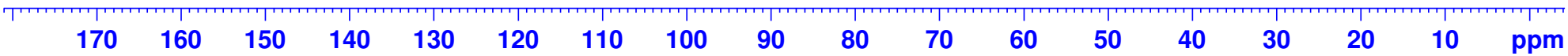
158.68
158.02
142.56
142.27
136.40
135.17
133.92
132.96
132.30
130.57
130.31
129.71
128.34
128.11
127.94
127.59
126.76
113.26
112.96
77.25
77.00
76.74
55.09
54.99
51.37
46.89
46.35
25.49
23.79

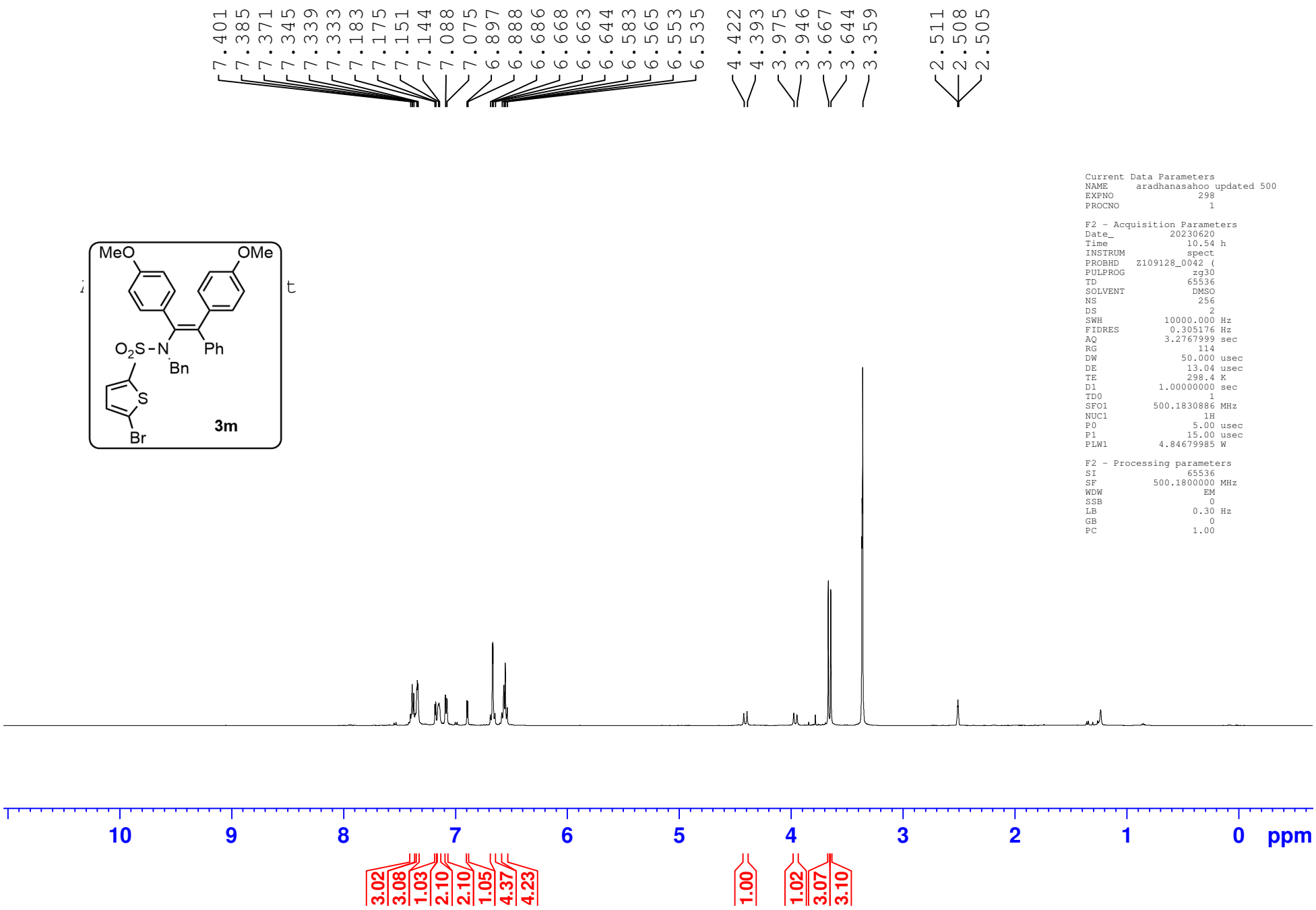


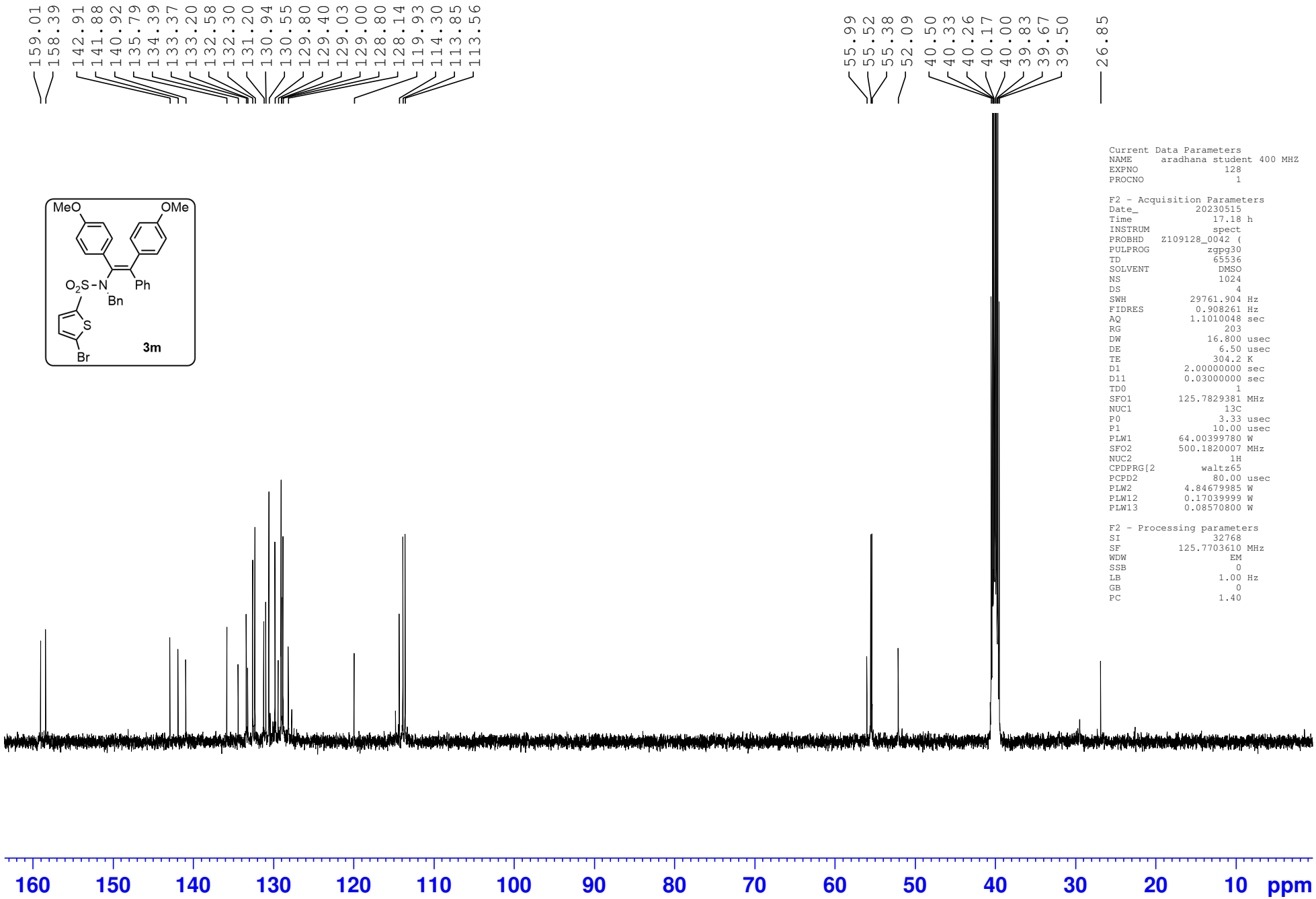
3l

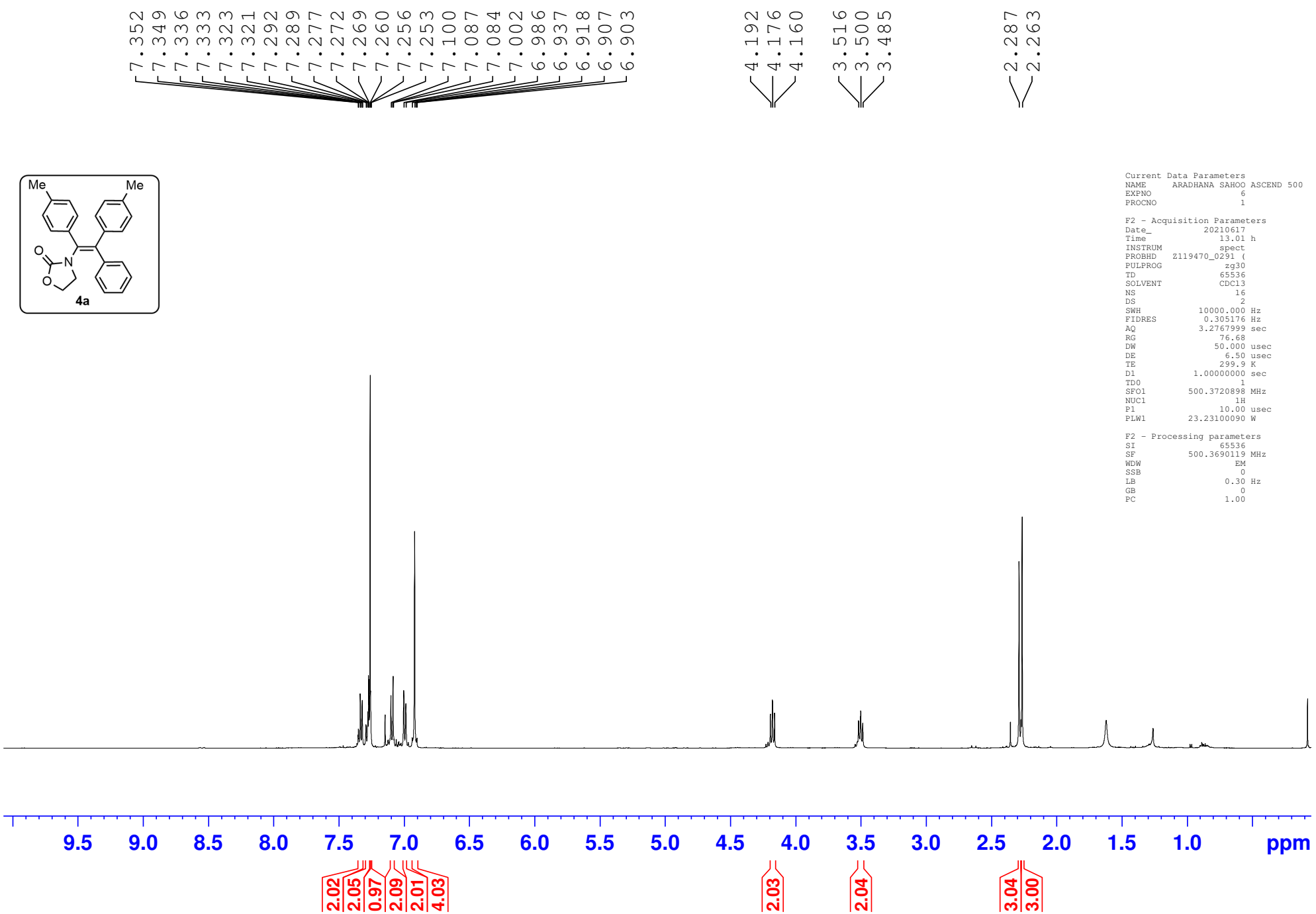
```
Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                 17
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210917
Time              10.35 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDC13
NS                  585
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG                108.78
DW                16.800 usec
DE                 6.50 usec
TE                300.8 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          125.8178898 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

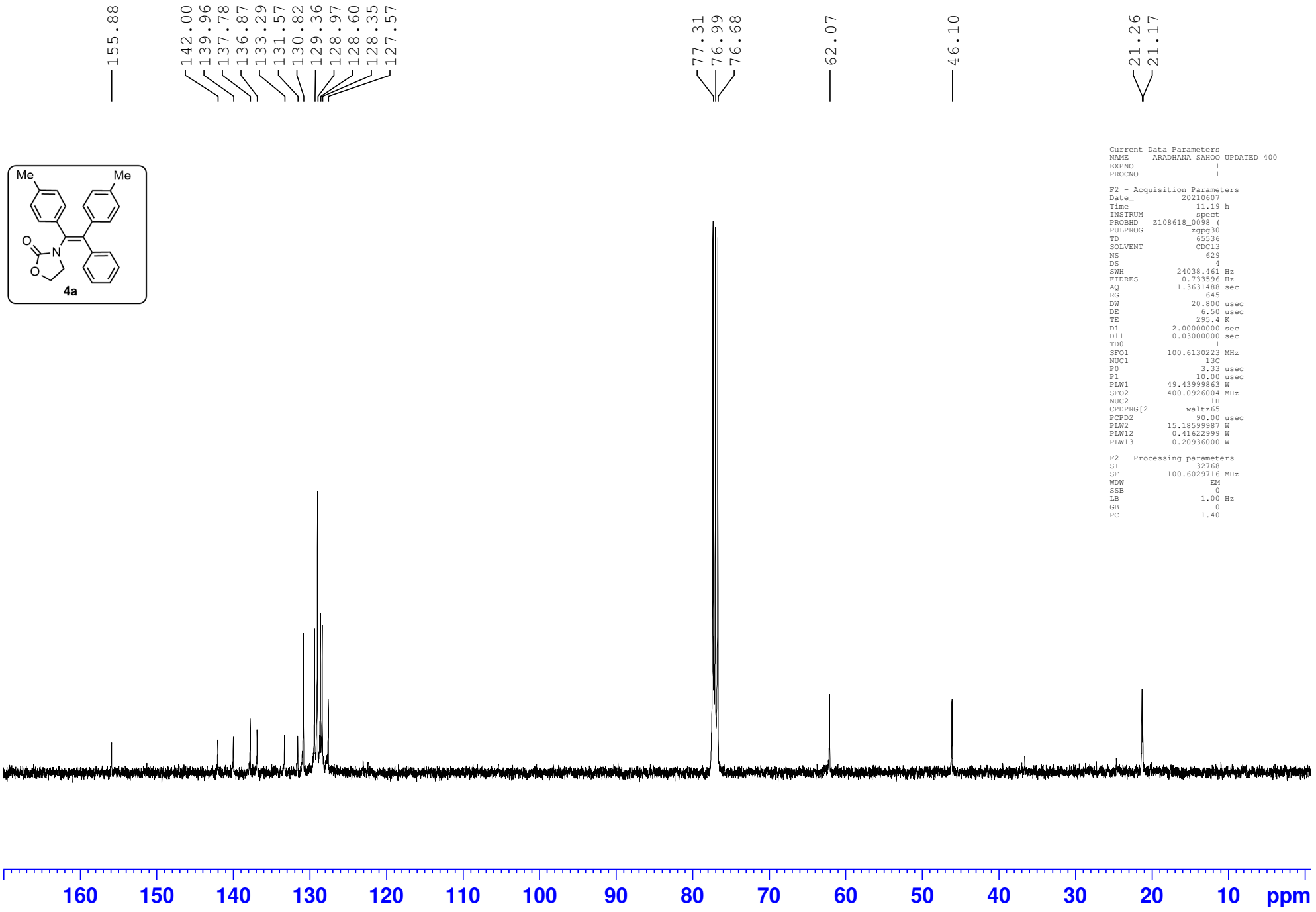


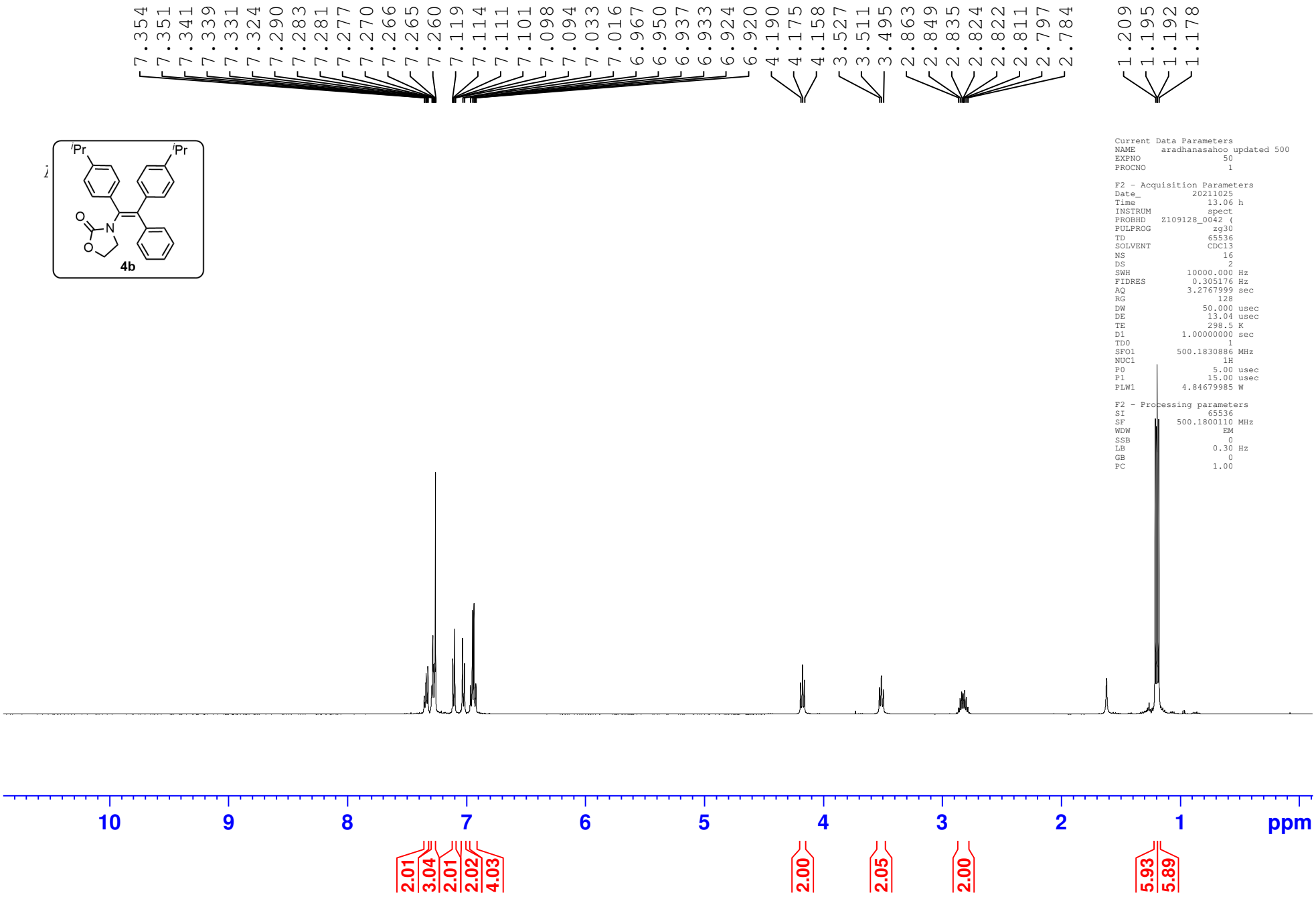


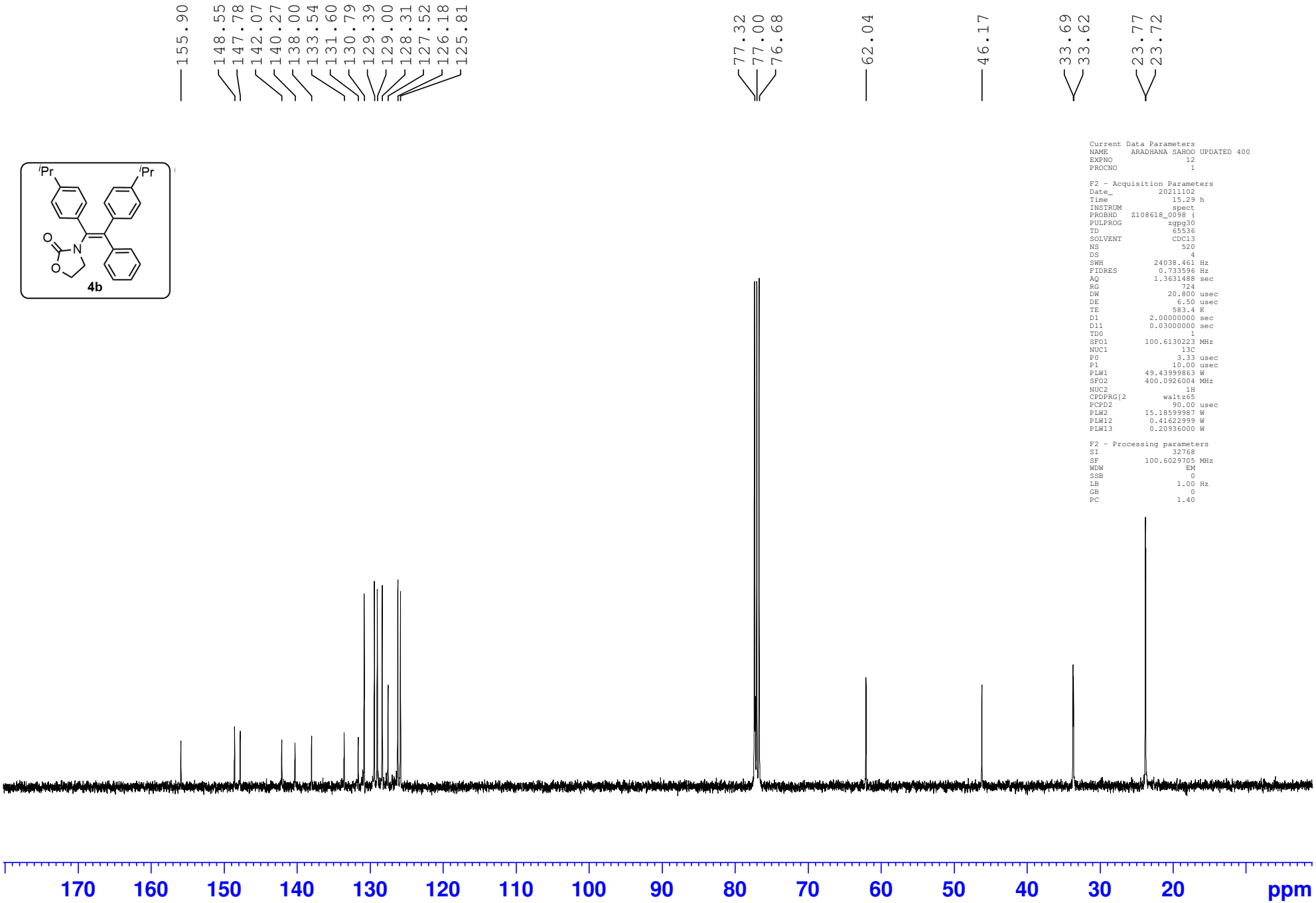

7.401
7.385
7.371
7.345
7.339
7.333
7.183
7.175
7.151
7.144
7.088
7.075
6.897
6.888
6.686
6.668
6.663
6.644
6.583
6.565
6.553
6.535
4.422
4.393
3.975
3.946
3.667
3.644
3.359
2.511
2.508
2.505
MeO
OMe
O2S-N
Ph
Bn
S
Br
3m
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 298
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230620
Time 10.54 h
INSTRUM spect
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 256
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 298.4 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
3.02
3.08
1.03
2.10
2.10
1.05
4.37
4.23
1.00
1.02
3.07
3.10

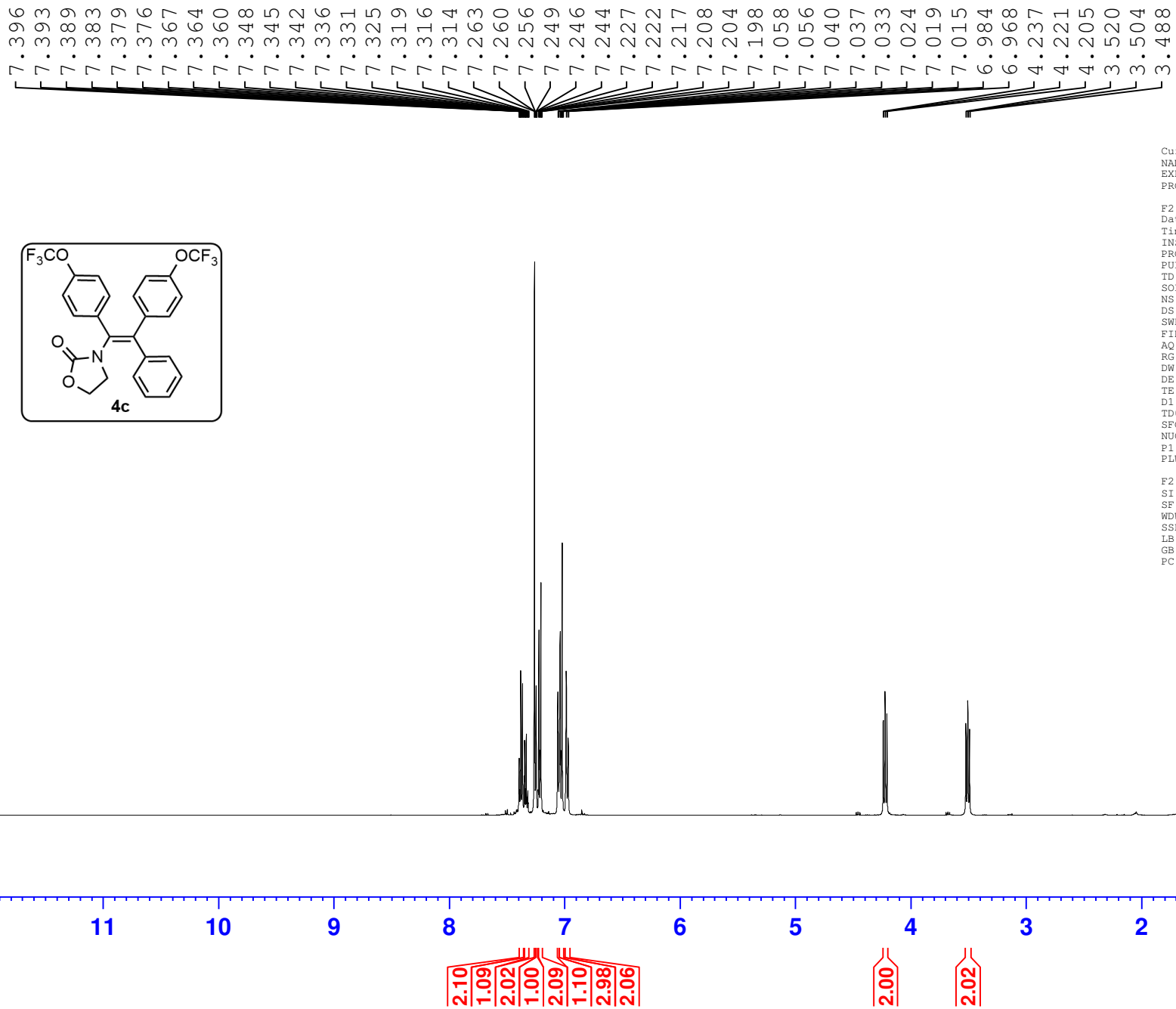

159.01
158.39
142.91
141.88
140.92
135.79
134.39
133.37
133.20
132.58
132.30
131.20
130.94
130.55
129.80
129.40
129.03
129.00
128.80
128.14
119.93
114.30
113.85
113.56
55.99
55.52
55.38
52.09
40.50
40.33
40.26
40.17
40.00
39.83
39.67
39.50
26.85
MeO
OMe
O2S-N
Bn
Ph
S
Br
3m
Current Data Parameters
NAME aradhana student 400 MHZ
EXPNO 128
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230515
Time 17.18 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
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 304.2 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
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

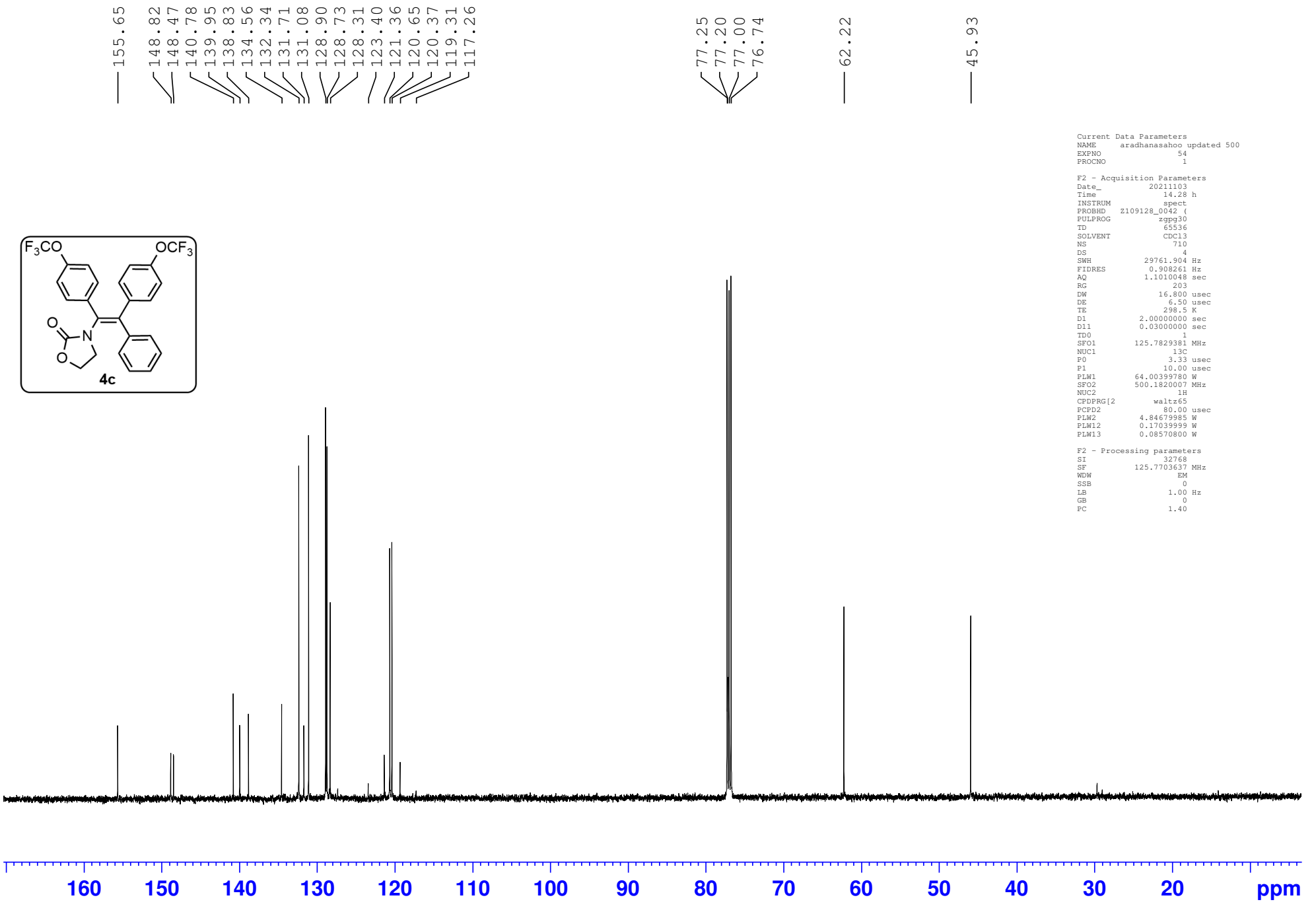

7.352
7.349
7.336
7.333
7.323
7.321
7.292
7.289
7.277
7.272
7.269
7.260
7.256
7.253
7.100
7.087
7.084
7.002
6.986
6.937
6.918
6.907
6.903
4.192
4.176
4.160
3.516
3.500
3.485
2.287
2.263
Me
Me
O
N
O
4a
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210617
Time 13.01 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 76.68
DW 50.000 usec
DE 6.50 usec
TE 299.9 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 500.3690119 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
2.02
2.05
0.97
2.09
2.01
4.03
2.03
2.04
3.04
3.00

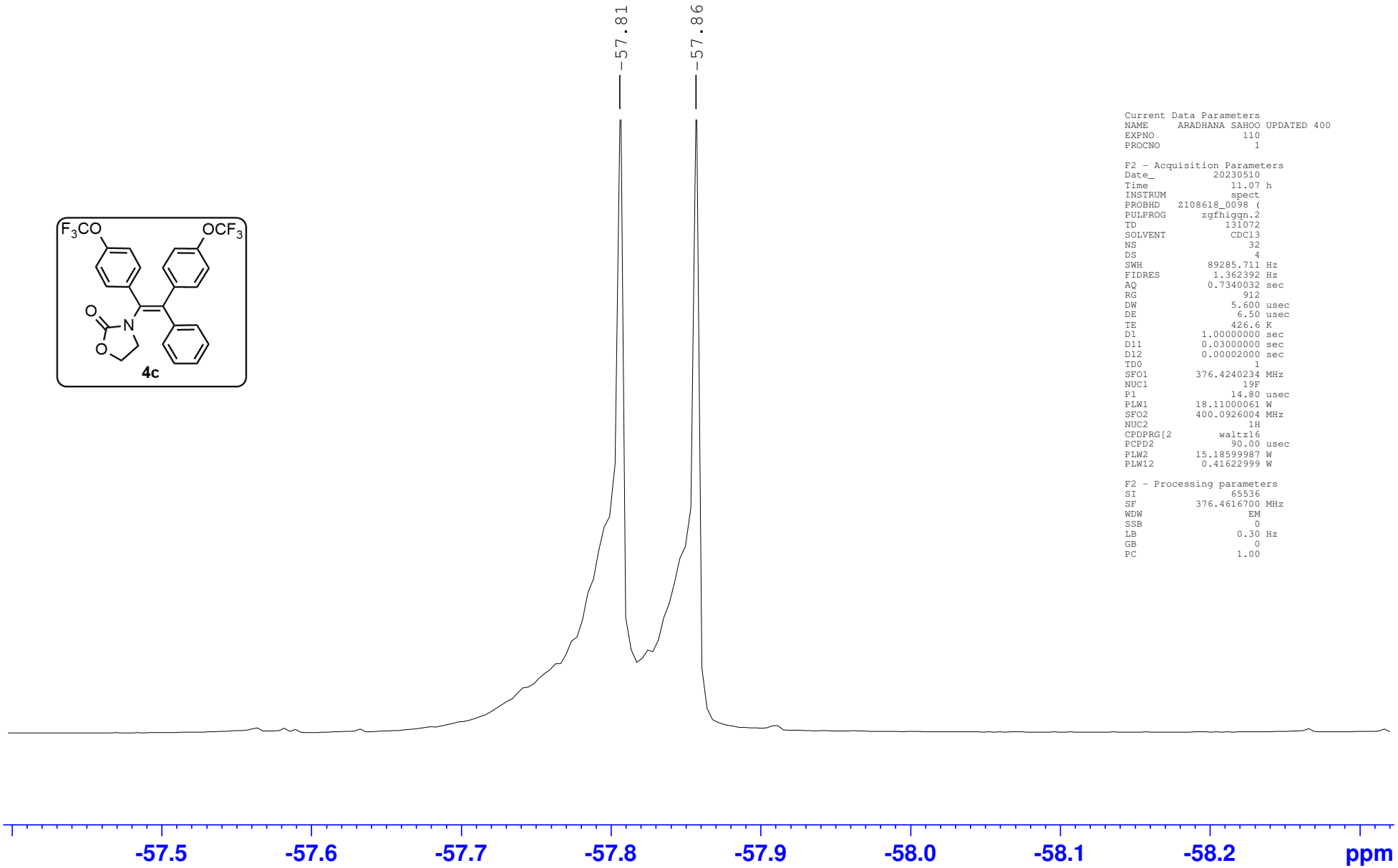

155.88
142.00
139.96
137.78
136.87
133.29
131.57
130.82
129.36
128.97
128.60
128.35
127.57
77.31
76.99
76.68
62.07
46.10
21.26
21.17
Me
Me
O
N
O
4a
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210607
Time 11.19 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 629
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 645
DW 20.800 usec
DE 6.50 usec
TE 295.4 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 100.6029716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.354
7.351
7.341
7.339
7.331
7.324
7.290
7.283
7.281
7.277
7.270
7.266
7.265
7.260
7.119
7.114
7.111
7.101
7.098
7.094
7.033
7.016
6.967
6.950
6.937
6.933
6.924
6.920
4.190
4.175
4.158
3.527
3.511
3.495
2.863
2.849
2.835
2.824
2.822
2.811
2.797
2.784
1.209
1.195
1.192
1.178
iPr
iPr
O
N
O
4b
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211025
Time 13.06 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 298.5 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 500.1800110 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
2.01
3.04
2.01
2.02
4.03
2.00
2.05
2.00
5.93
5.89

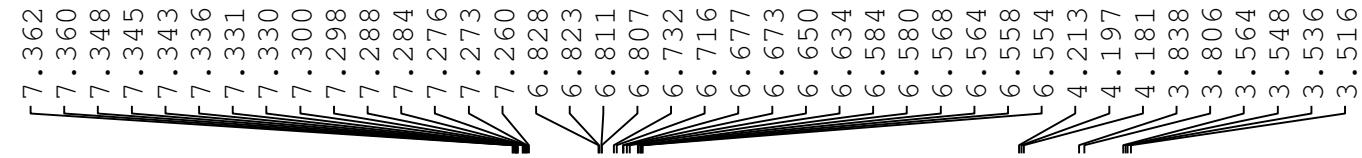

155.90
148.55
147.78
142.07
140.27
138.00
133.54
131.60
130.79
129.39
129.00
128.31
127.52
126.18
125.81
77.32
77.00
76.68
62.04
46.17
33.69
33.62
23.77
23.72
4b
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211102
Time 15.29 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 520
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 583.4 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 100.6029705 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

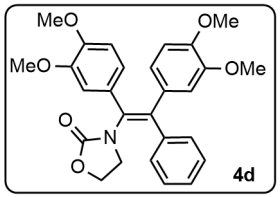

7.396
7.393
7.389
7.383
7.379
7.376
7.367
7.364
7.360
7.348
7.345
7.342
7.336
7.331
7.325
7.319
7.316
7.314
7.263
7.260
7.256
7.249
7.246
7.244
7.227
7.222
7.217
7.208
7.204
7.198
7.058
7.056
7.040
7.037
7.033
7.024
7.019
7.015
6.984
6.968
4.237
4.221
4.205
3.520
3.504
3.488
F3CO
OCF3
O
N
O
4c
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 33
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211111
Time 14.17 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 54.81
DW 50.000 usec
DE 6.50 usec
TE 295.6 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 500.3690121 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
ppm
2.10
1.09
2.02
1.00
2.09
1.10
2.98
2.06
2.00
2.02


155.65
148.82
148.47
140.78
139.95
138.83
134.56
132.34
131.71
131.08
128.90
128.73
128.31
123.40
121.36
120.65
120.37
119.31
117.26
77.25
77.20
77.00
76.74
62.22
45.93
F3CO
OCF3
O
N
O
4c
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 54
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211103
Time 14.28 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 710
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 298.5 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 125.7703637 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

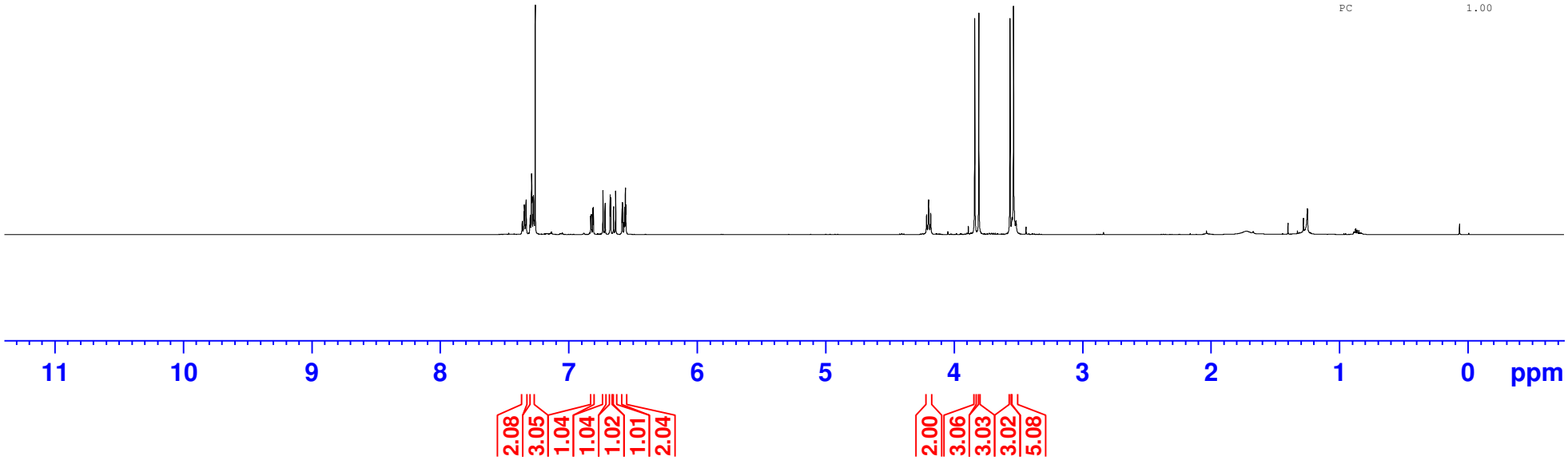


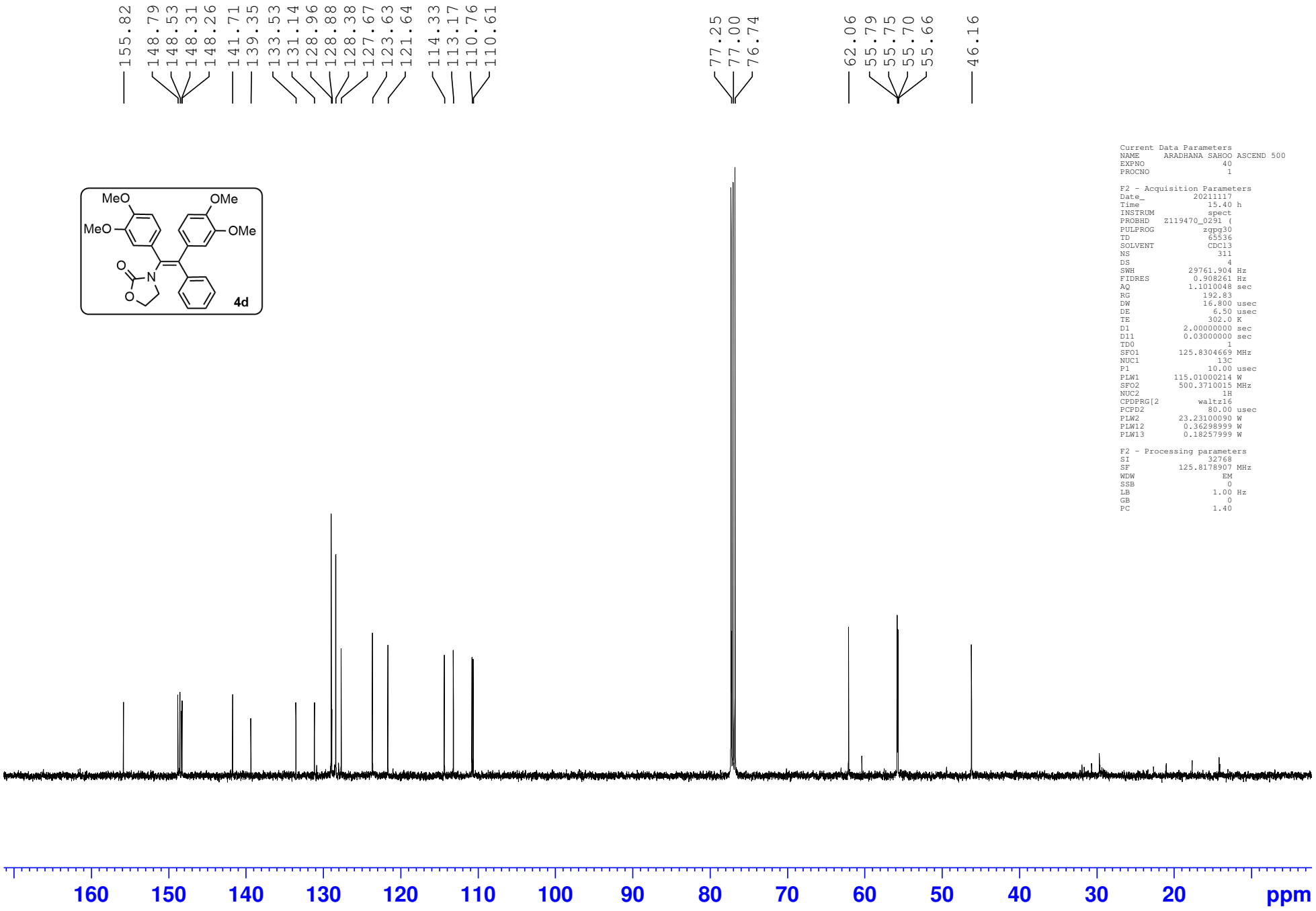

```
Current Data Parameters
NAME      ARADHANA SAHOO UPDATED 400
EXPNO                110
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230510
Time              11.07 h
INSTRUM             spect
PROBHD   Z108618_0098 (
PULPROG       zgfhigqn.2
TD               131072
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                   912
DW                 5.600 usec
DE                 6.50 usec
TE                426.6 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
```

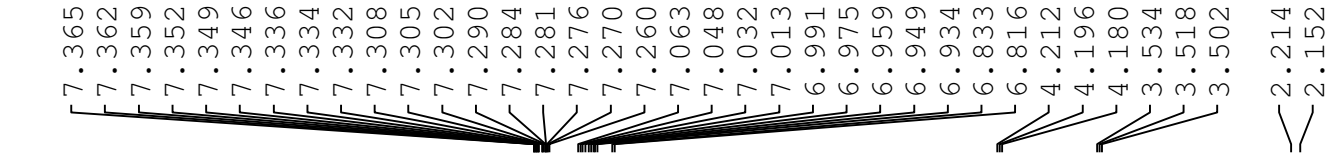


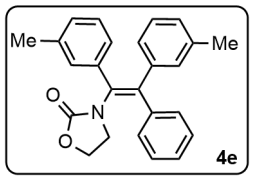



```
Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                 46
PROCNO                 1

F2 - Acquisition Parameters
Date_              20211123
Time                 12.05 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                    76.68
DW                 50.000 usec
DE                  6.50 usec
TE                  298.7 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             500.3690119 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

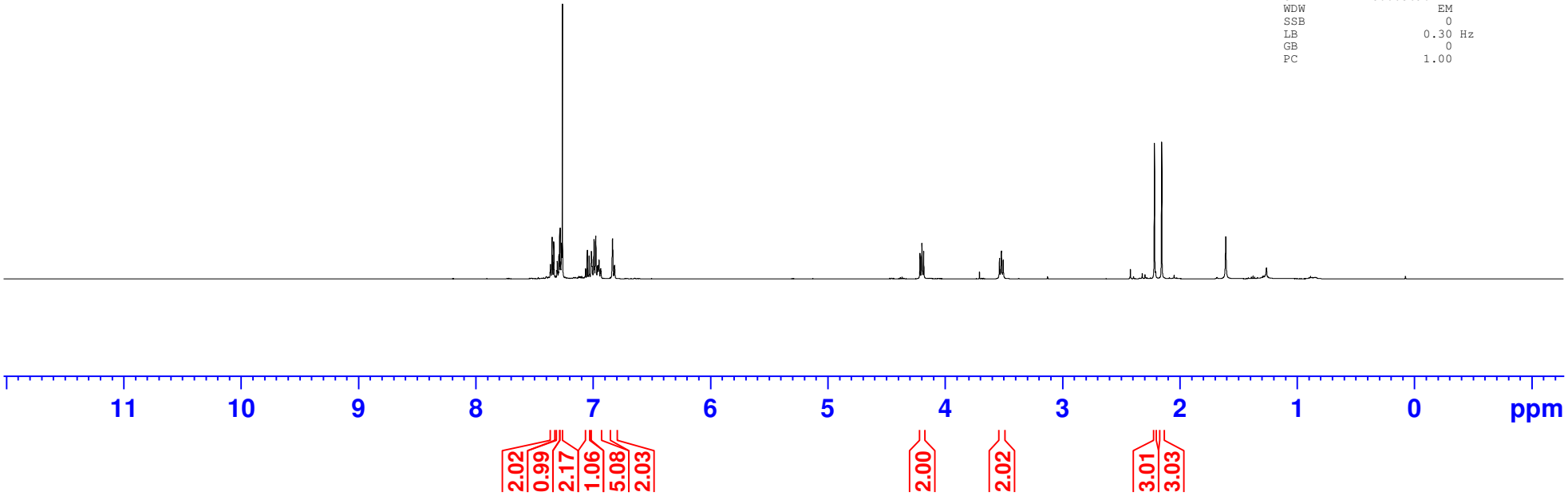


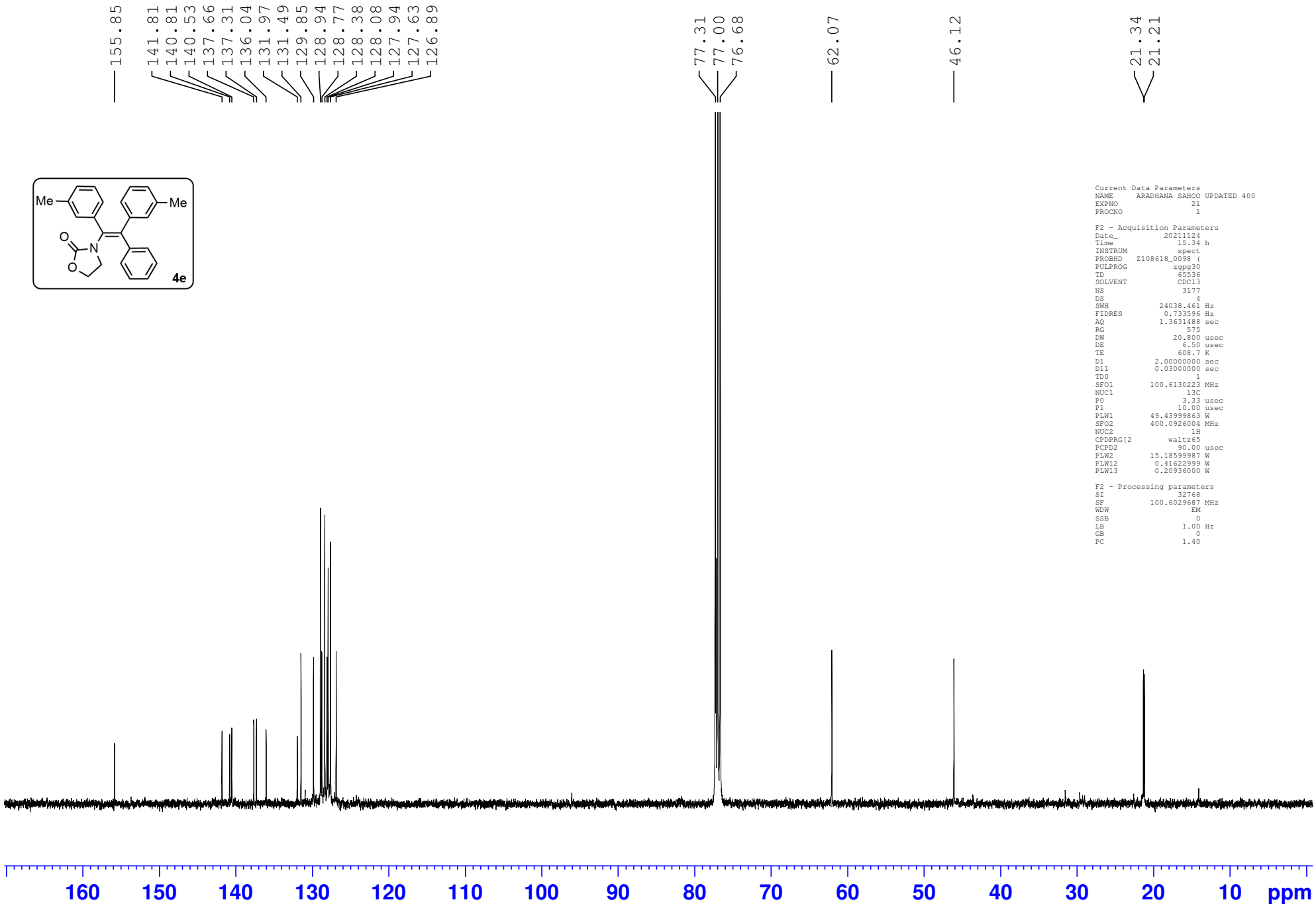

155.82
148.79
148.53
148.31
148.26
141.71
139.35
133.53
131.14
128.96
128.88
128.38
127.67
123.63
121.64
114.33
113.17
110.76
110.61
77.25
77.00
76.74
62.06
55.79
55.75
55.70
55.66
46.16
MeO
MeO
OMe
OMe
O
N
O
4d
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211117
Time 15.40 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 311
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 302.0 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 125.8178907 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

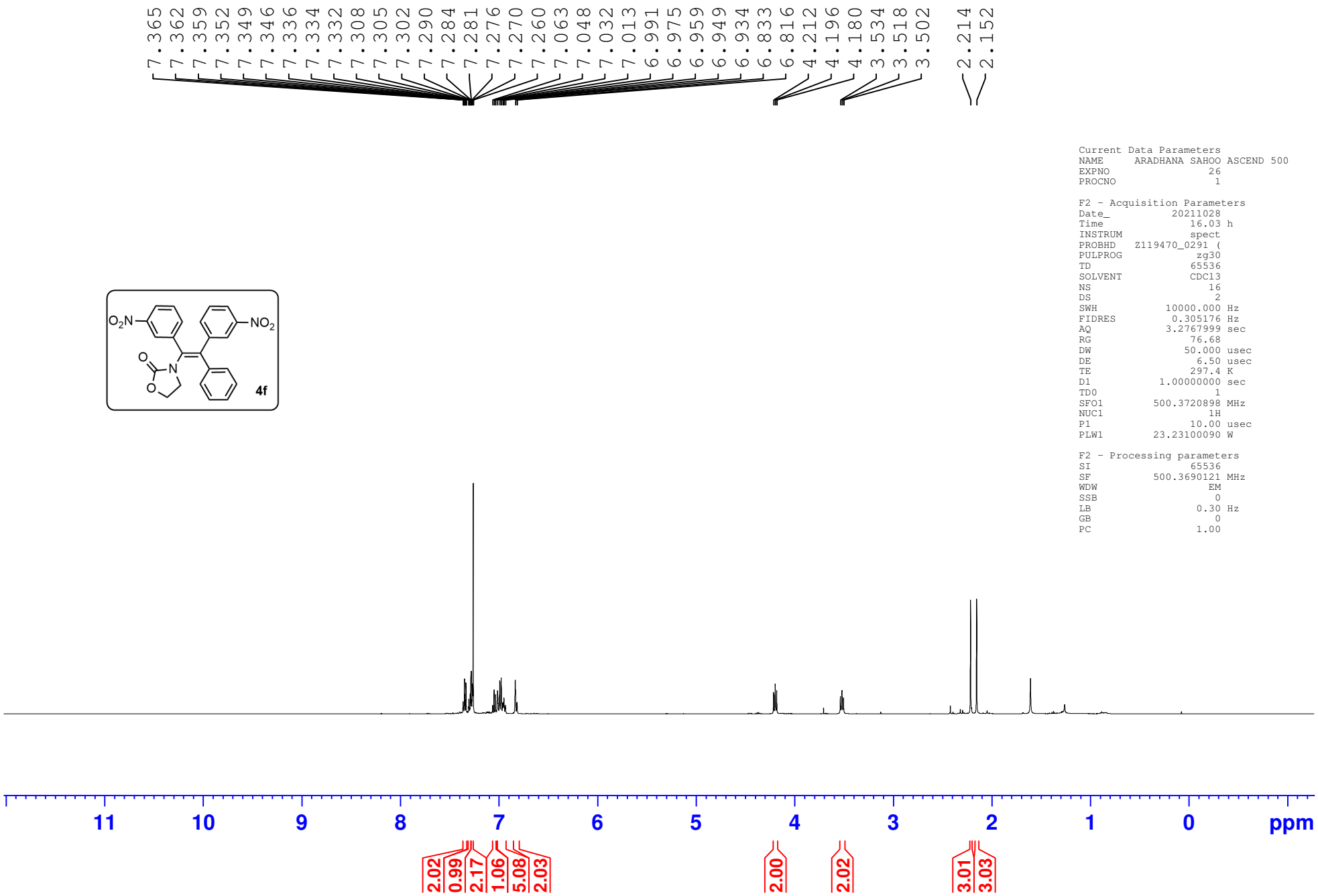


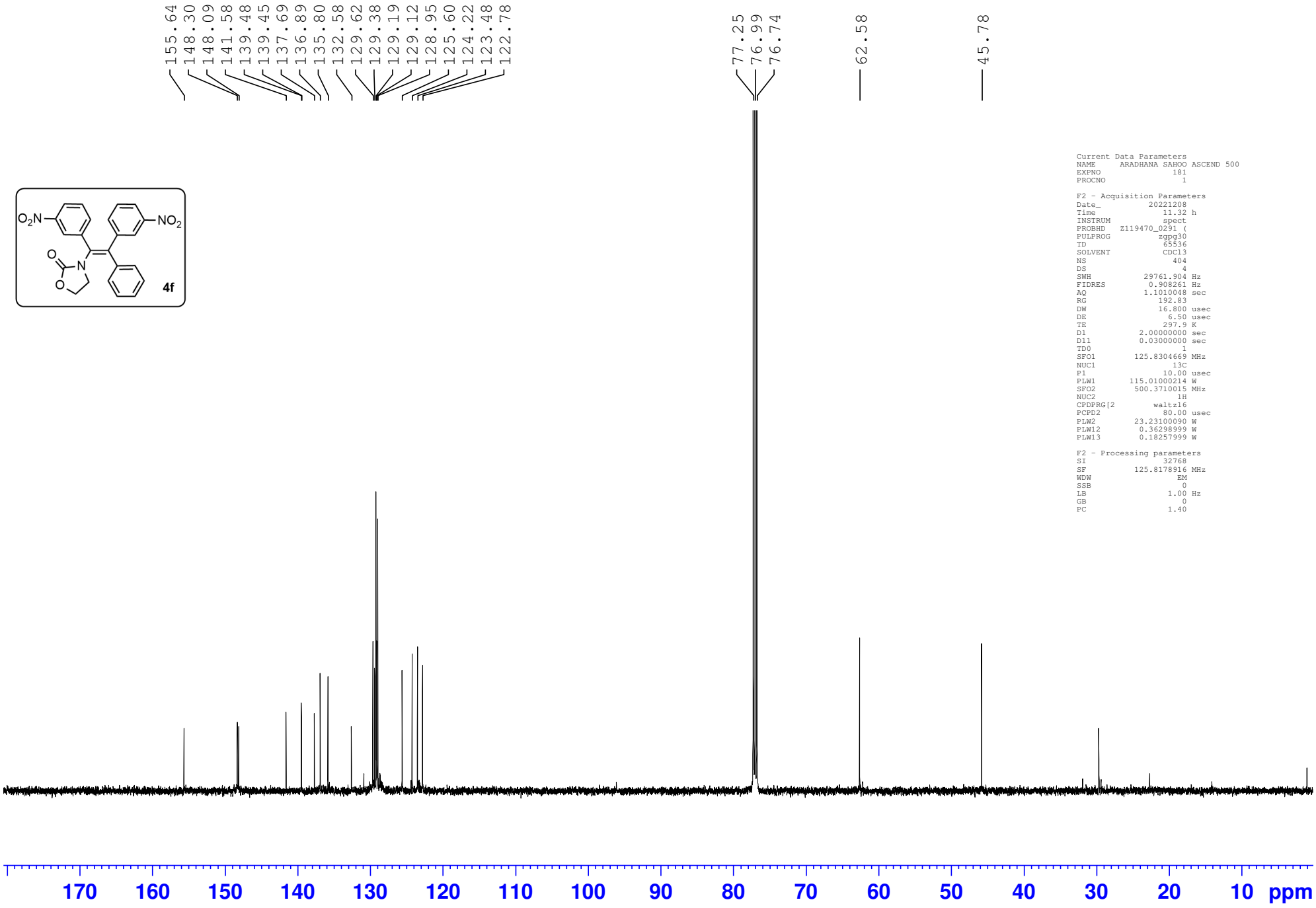


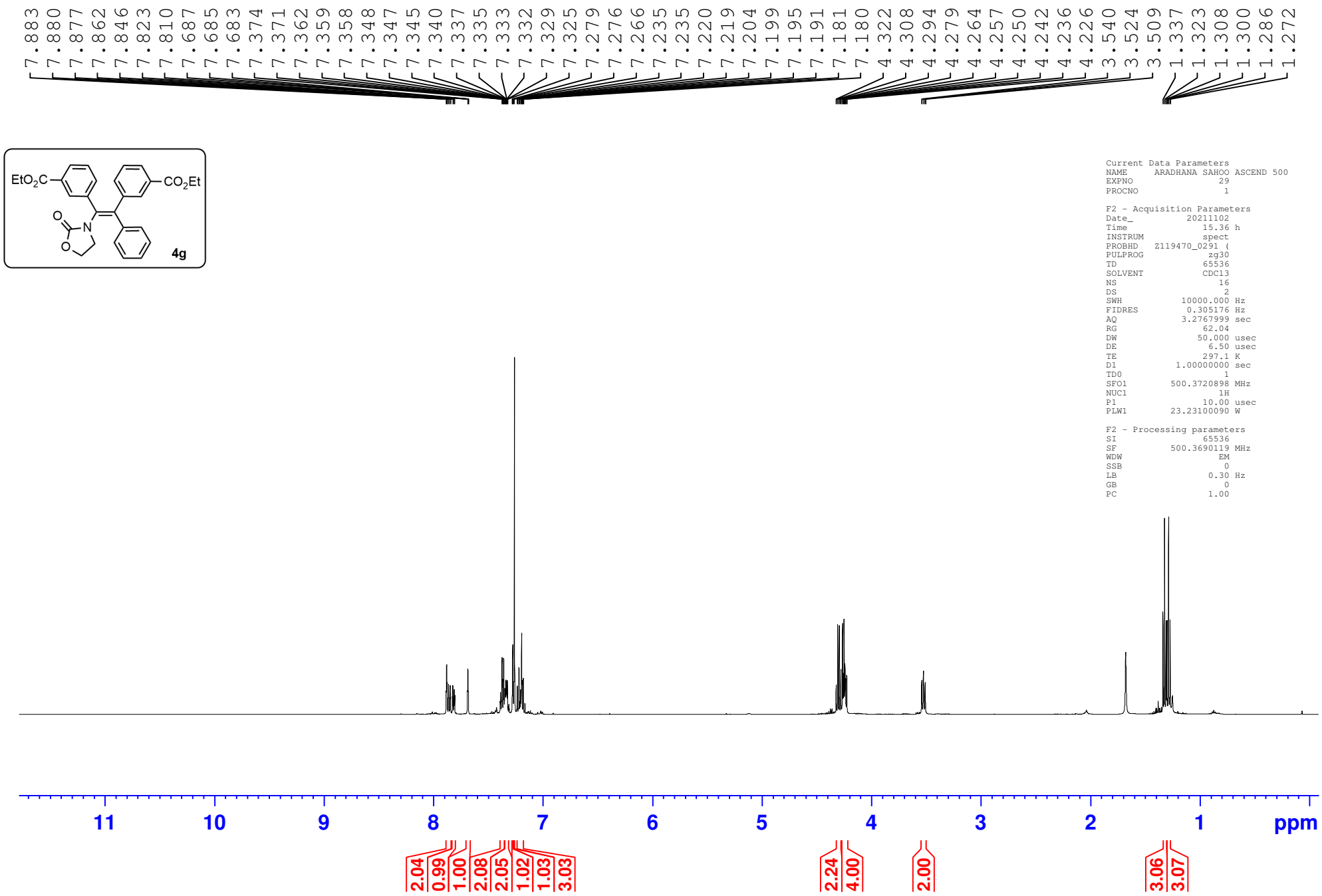

```
Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                 26
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211028
Time               16.03 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                 76.68
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           500.3690121 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

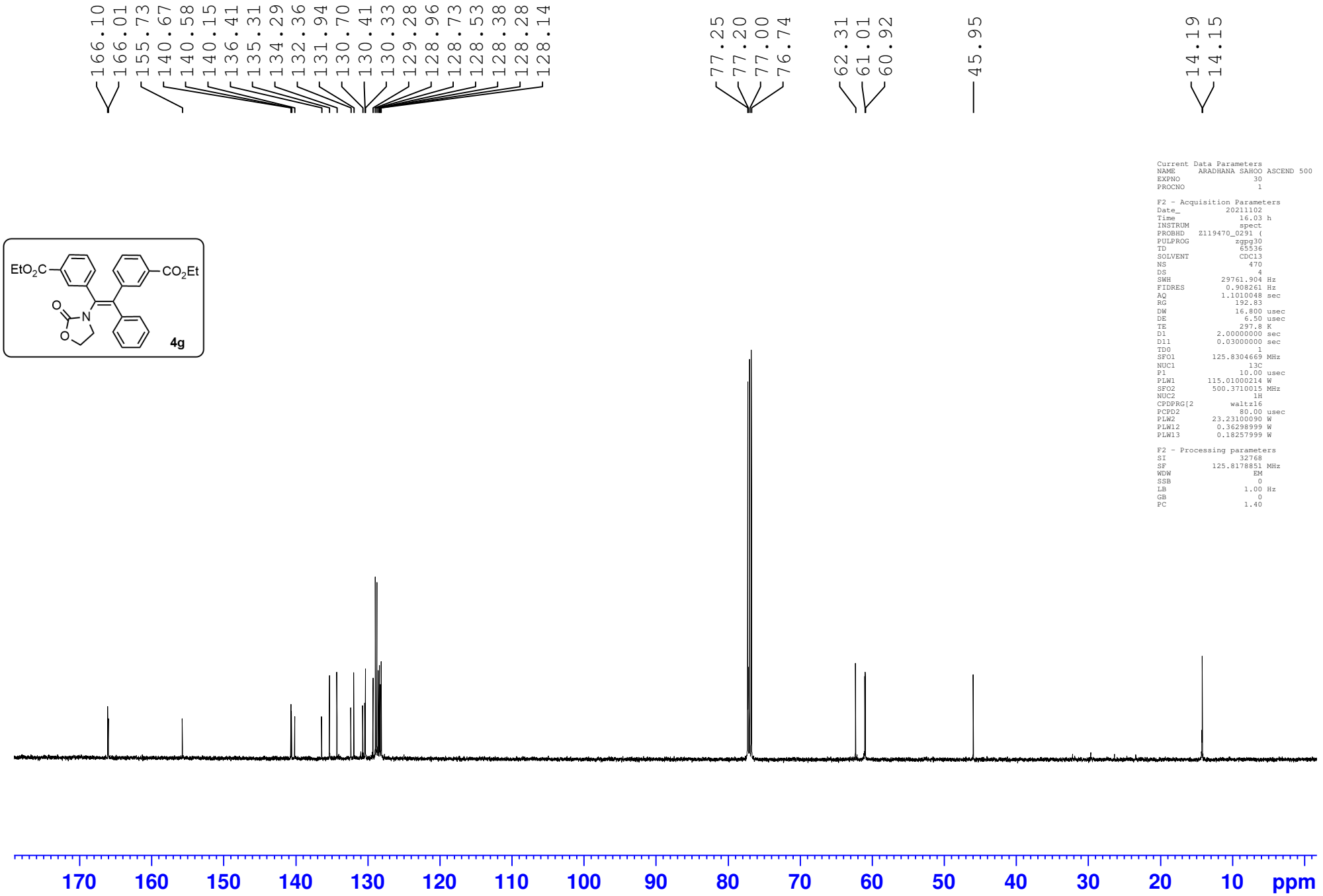


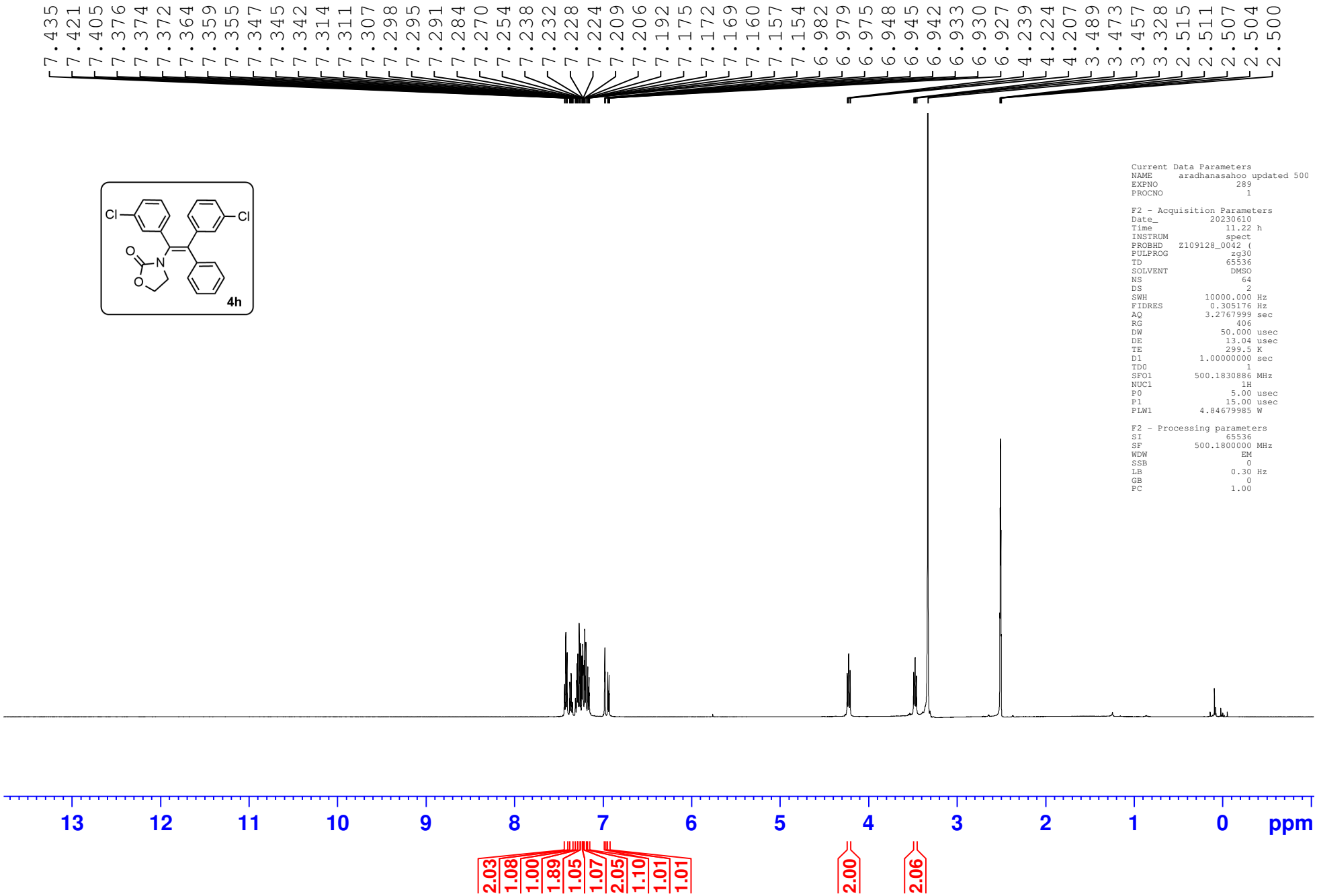

155.85
141.81
140.81
140.53
137.66
137.31
136.04
131.97
131.49
129.85
128.94
128.77
128.38
128.08
127.94
127.63
126.89
77.31
77.00
76.68
62.07
46.12
21.34
21.21
Me
Me
O
N
O
4e
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211124
Time 15.34 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3177
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 608.7 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 100.6029687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

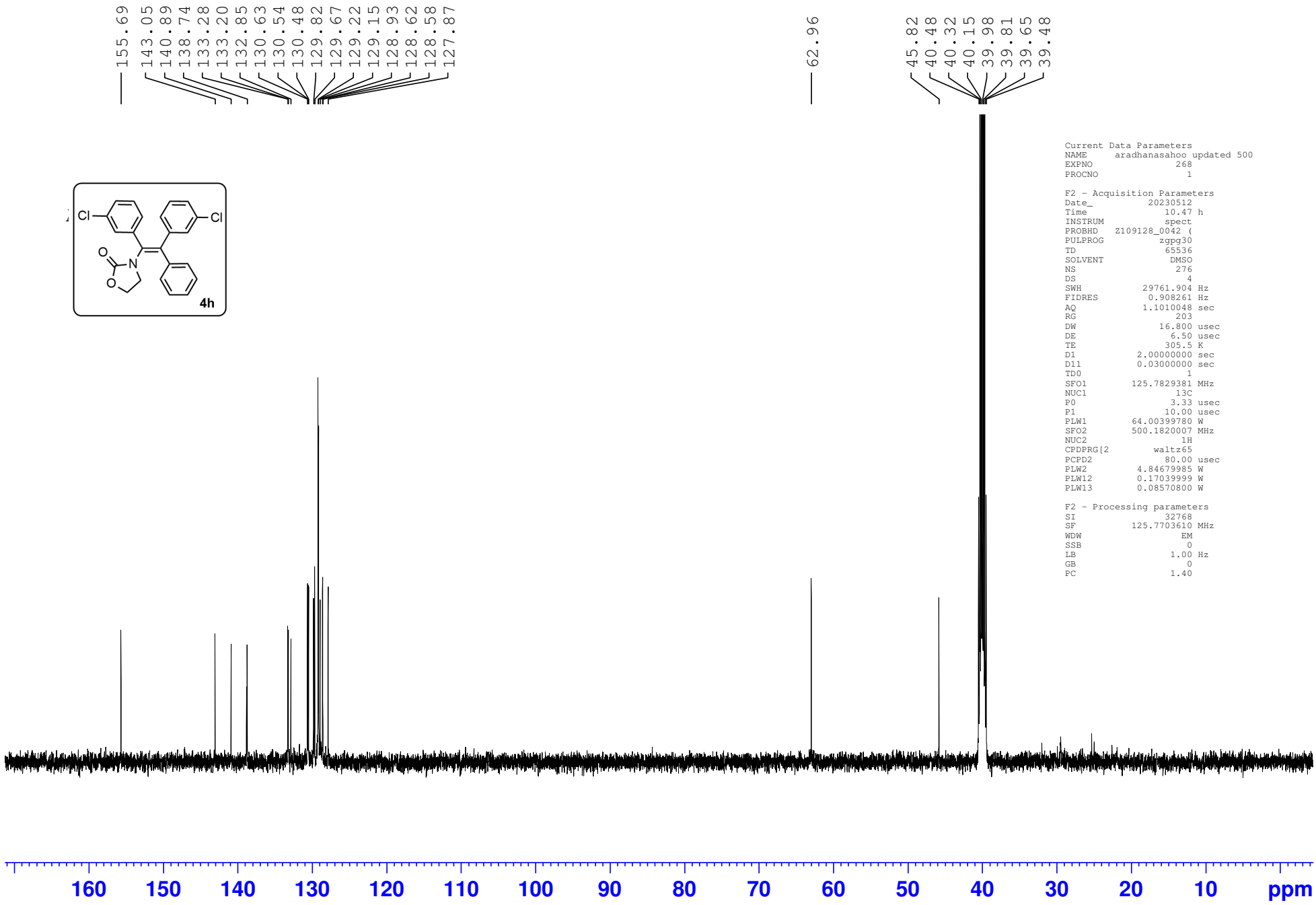

7.365
7.362
7.359
7.352
7.349
7.346
7.336
7.334
7.332
7.308
7.305
7.302
7.290
7.284
7.281
7.276
7.270
7.260
7.063
7.048
7.032
7.013
6.991
6.975
6.959
6.949
6.934
6.833
6.816
4.212
4.196
4.180
3.534
3.518
3.502
2.214
2.152
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 26
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211028
Time 16.03 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 76.68
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 500.3690121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O2N
NO2
O
N
O
4f
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
0.99
2.17
1.06
5.08
2.03
2.00
2.02
3.01
3.03

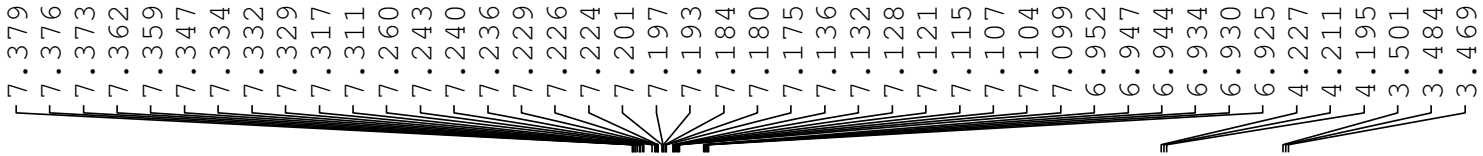

155.64
148.30
148.09
141.58
139.48
139.45
137.69
136.89
135.80
132.58
129.62
129.38
129.19
129.12
128.95
125.60
124.22
123.48
122.78
77.25
76.99
76.74
62.58
45.78
4f
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 181
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221208
Time 11.32 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 404
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 297.9 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 125.8178916 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

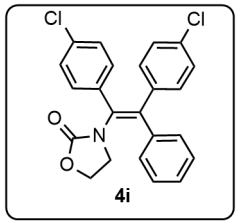

7.883
7.880
7.877
7.862
7.846
7.823
7.810
7.687
7.685
7.683
7.374
7.371
7.362
7.359
7.358
7.348
7.347
7.345
7.340
7.337
7.335
7.333
7.332
7.329
7.325
7.279
7.276
7.266
7.235
7.235
7.220
7.219
7.204
7.199
7.195
7.191
7.181
7.180
4.322
4.308
4.294
4.279
4.264
4.257
4.250
4.242
4.236
4.226
3.540
3.524
3.509
1.337
1.323
1.308
1.300
1.286
1.272
EtO2C
CO2Et
O
N
O
4g
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 29
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211102
Time 15.36 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 297.1 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 500.3690119 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
ppm
2.04
0.99
1.00
2.08
2.05
1.02
1.03
3.03
2.24
4.00
2.00
3.06
3.07


166.10
166.01
155.73
140.67
140.58
140.15
136.41
135.31
134.29
132.36
131.94
130.70
130.41
130.33
129.28
128.96
128.73
128.53
128.38
128.28
128.14
77.25
77.20
77.00
76.74
62.31
61.01
60.92
45.95
14.19
14.15
EtO2C
CO2Et
O
N
O
4g
Current Data Parameters
NAME ARADHANA SAHOO ASCEND 500
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211102
Time 16.03 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 470
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 297.8 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 125.8178851 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


7.435
7.421
7.405
7.376
7.374
7.372
7.364
7.359
7.355
7.347
7.345
7.342
7.314
7.311
7.307
7.298
7.295
7.291
7.284
7.270
7.254
7.238
7.232
7.228
7.224
7.209
7.206
7.192
7.175
7.172
7.169
7.160
7.157
7.154
6.982
6.979
6.975
6.948
6.945
6.942
6.933
6.930
6.927
4.239
4.224
4.207
3.489
3.473
3.457
3.328
2.515
2.511
2.507
2.504
2.500
Cl
Cl
O
N
O
4h
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 289
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230610
Time 11.22 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 406
DW 50.000 usec
DE 13.04 usec
TE 299.5 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
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
1.08
1.00
1.89
1.05
1.07
2.05
1.10
1.01
1.01
2.00
2.06


155.69
143.05
140.89
138.74
133.28
133.20
132.85
130.63
130.54
130.48
129.82
129.67
129.22
129.15
128.93
128.62
128.58
127.87
62.96
45.82
40.48
40.32
40.15
39.98
39.81
39.65
39.48
Cl
Cl
O
N
O
4h
Current Data Parameters
NAME aradhanasahoo updated 500
EXPNO 268
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230512
Time 10.47 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 276
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 305.5 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
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm





4i

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Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                34
PROCNO                1

F2 - Acquisition Parameters
Date_          20211111
Time              14.41 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                87.13
DW               50.000 usec
DE                6.50 usec
TE               295.5 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          500.3690122 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
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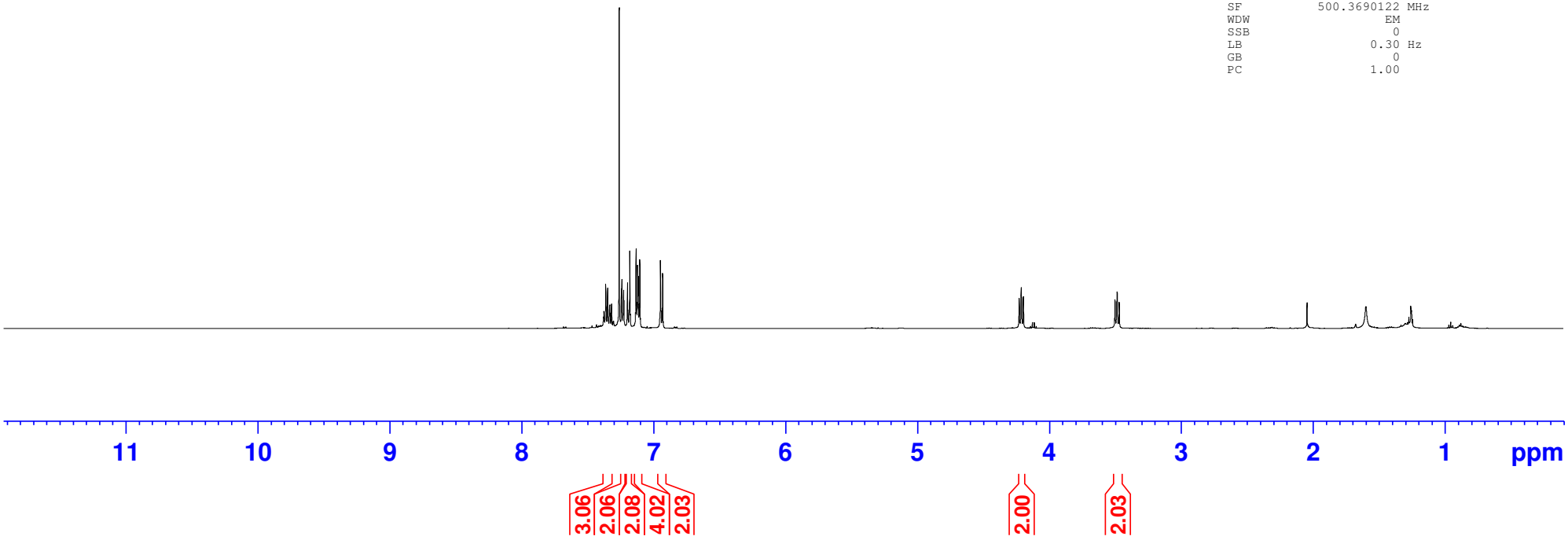
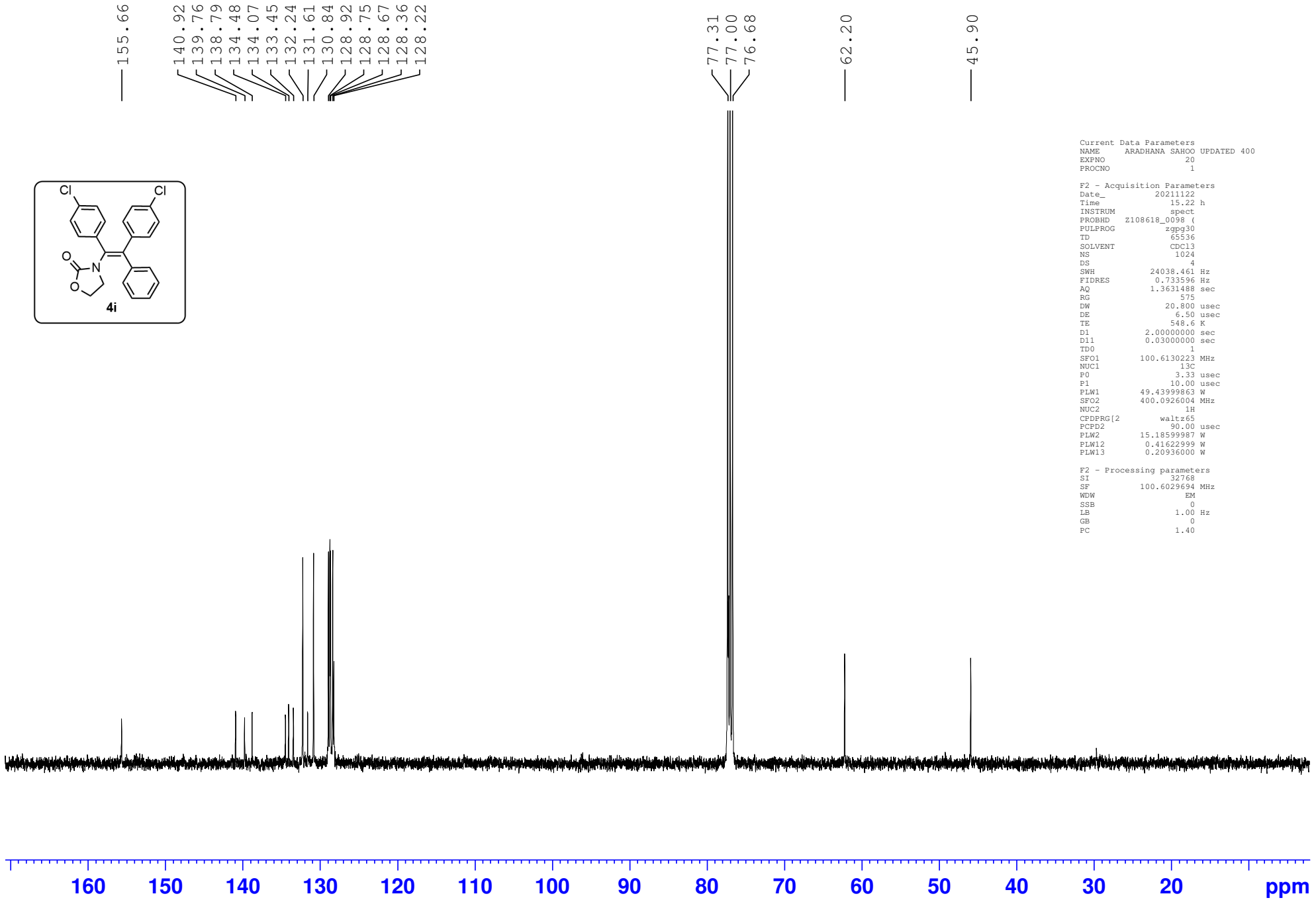
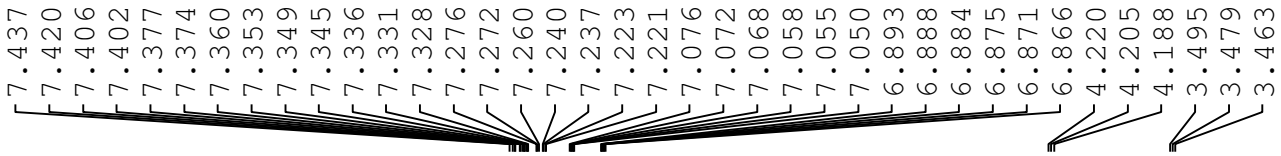
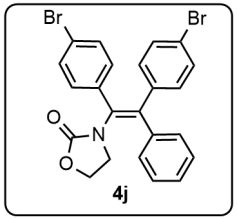



155.66
140.92
139.76
138.79
134.48
134.07
133.45
132.24
131.61
130.84
128.92
128.75
128.67
128.36
128.22
77.31
77.00
76.68
62.20
45.90
Cl
Cl
O
N
O
4i
Current Data Parameters
NAME ARADHANA SAHOO UPDATED 400
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211122
Time 15.22 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
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 548.6 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 100.6029694 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

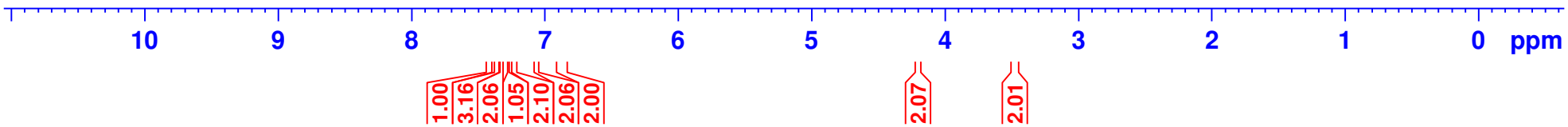


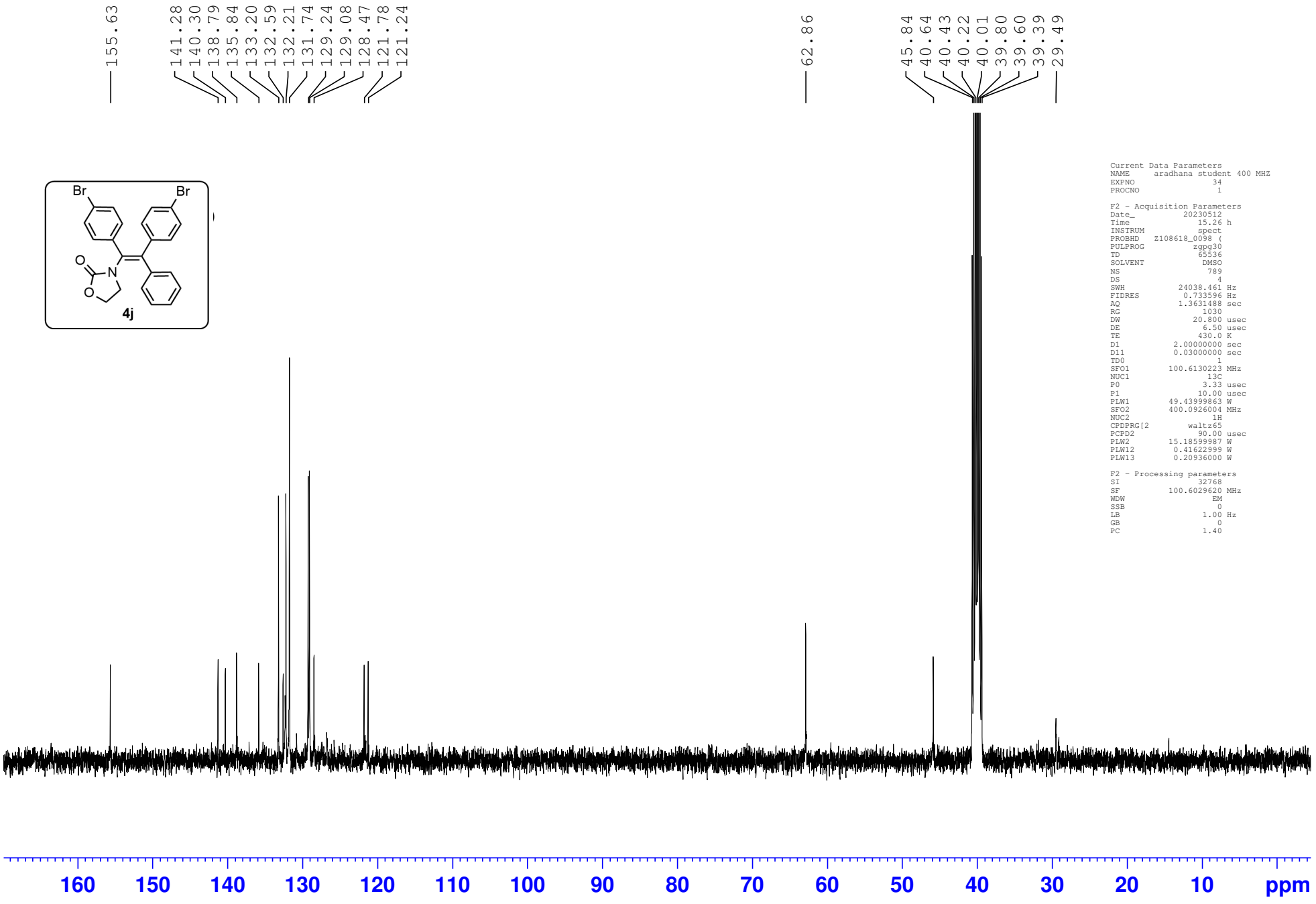



```
Current Data Parameters
NAME      ARADHANA SAHOO ASCEND 500
EXPNO                45
PROCNO                1

F2 - Acquisition Parameters
Date_          20211123
Time              12.00 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                87.13
DW              50.000 usec
DE               6.50 usec
TE              298.8 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           500.3690119 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```




155.63
141.28
140.30
138.79
135.84
133.20
132.59
132.21
131.74
129.24
129.08
128.47
121.78
121.24
62.86
45.84
40.64
40.43
40.22
40.01
39.80
39.60
39.39
29.49
Br
Br
O
N
O
4j
Current Data Parameters
NAME aradhana student 400 MHZ
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230512
Time 15.26 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 789
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 430.0 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
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm