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Metal–Free Stereoselective Addition of Propiolic acids to Ynamides: A Concise Synthetic Route to Highly Substituted Ene-Diyne-(*E*)-N,O-Acetals

Rangu Prasad, Suresh Kanikarapu, Shubham Dutta, SrinivasVangara, and Akhila K. Sahoo*

School of Chemistry, University of Hyderabad, Hyderabad 500046, India

E-mail: akhilchemistry12@gmail.com; akssc@uohyd.ac.in

SUPPORTING INFORMATION

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General Experimental Information

All the reactions were performed in oven-dried round bottom (RB) 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.

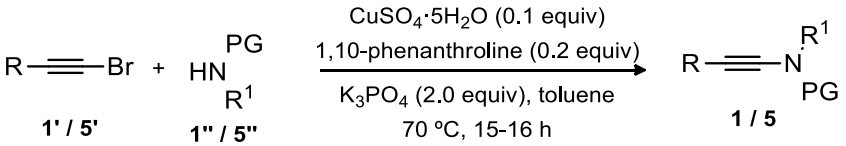
Proton, carbon, and fluorine nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR, and ^{19}F NMR) were recorded based on the resonating frequencies as follows: (^{1}H NMR, 400 MHz; ^{13}C NMR, 101 MHz; ^{19}F NMR, 376 MHz) and (^{1}H NMR, 500 MHz; ^{13}C NMR, 126 MHz; ^{19}F NMR, 470 MHz) having 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 reference standard. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet; bs= broad singlet; d = doublet; dd= doublet of doublet; bd= broad doublet; t = triplet; bt= 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, ^{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 electro-thermal heating and are uncorrected. X-ray data was collected at 293 K using graphite monochromated Mo-Kαradiation (0.71073 Å).

Materials: Unless otherwise noted, all the reagents and intermediates were obtained commercially and used without purification. 1,4–Dioxane, dichloromethane (CH_2Cl_2; DCM), toluene, acetonitrile (CH_3CN), 1,2-dichloroethane (DCE), and acetone were distilled over CaH_2. THF was freshly distilled over sodium/benzophenone ketyl under dry nitrogen. Propiolic acid was purchased from Sigma–Aldrich and used as received. Phenylpropiolic acid and 2-thiophenepropiolic acid were synthesized in our laboratory.

Experimental Procedures

Following the reported procedures, the ynamides (**1a–1z, 1za–1ze** and **5a–5l**)[1] were prepared (Table S1). Analytical and spectral data of these compounds are exactly matching with the reported values.

General Procedure (GP-1):[1]



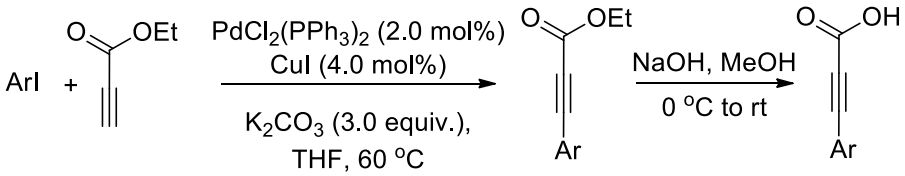
R = alkyl, aryl, hetero aryl groups;

R^1 = alkyl, aryl, allyl, propargyl, homo-propargyl groups

General Procedure for the Synthesis of Ynamide 1 & 5 (GP 1):[1]

To a mixture of **1″ / 5″**(2.0 mmol), $CuSO_4 \cdot 5H_2O$ (0.1 equiv), 1,10-phenanthroline (0.2 equiv) in dry toluene (8.0 mL), was added K_3PO_4 (2.0 equiv) portion wise. Subsequently, 1-bromo-2-arylacetylene **1′ / 5′** (2.4 mmol) was added. The reaction mixture was heated at 70 °C under 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 the reduced pressure. The crude residue was purified through column chromatography using ethyl acetate and hexane mixture on silica gel to provide **1 / 5**.

General procedure for the preparation of propiolic acid derivates 2b, 2c (GP 2):[2]

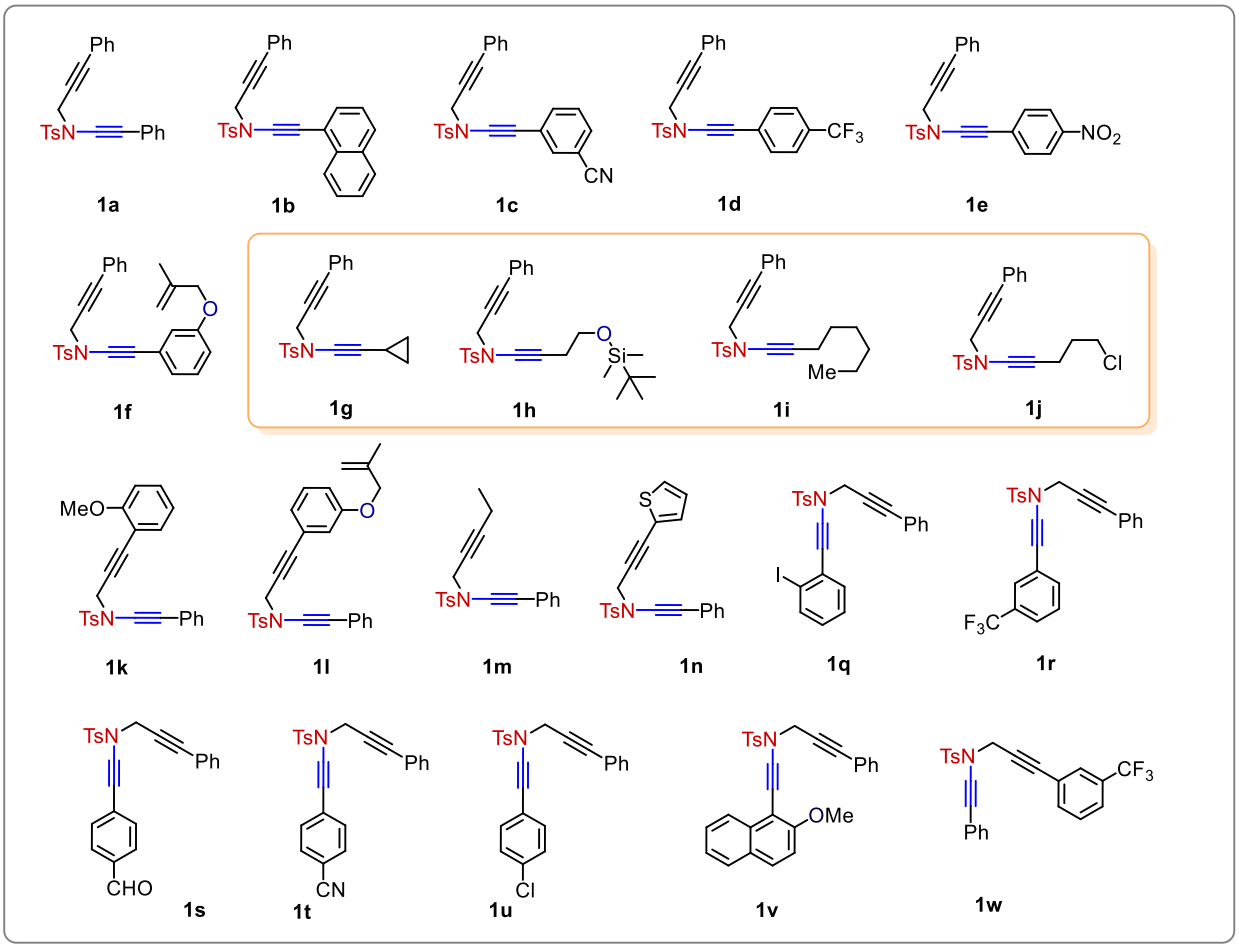


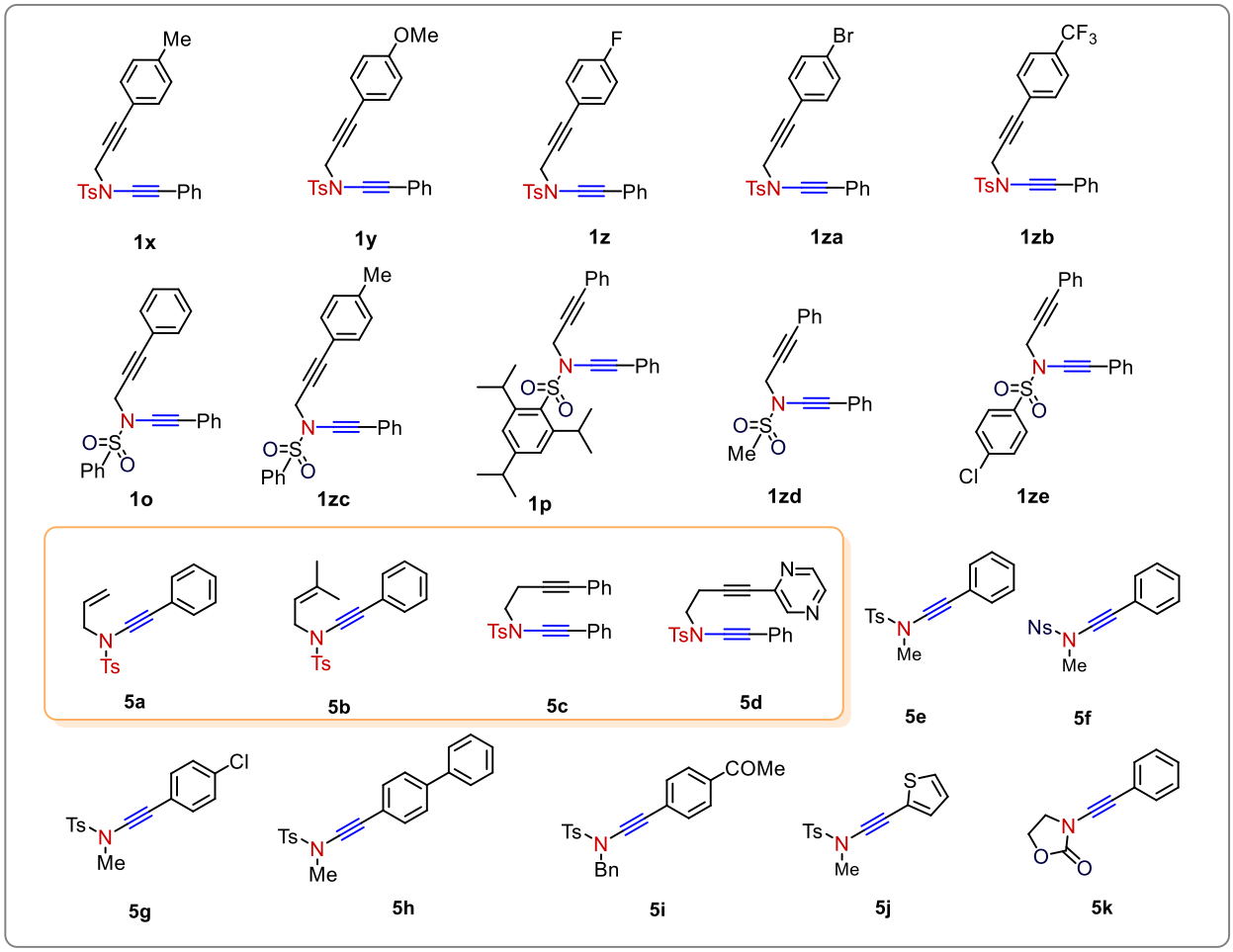
To a solution of aryl iodide (7.5 mmol), ethyl propiolate (5.0 mmol), and K_2CO_3 (15 mmol) in THF (30 mL) was added $PdCl_2(PPh_3)_2$ (0.02 mmol) and CuI (0.04 mmol). The resulting mixture was then heated under a nitrogen atmosphere at 60 °C for12 h. The reaction was monitored by TLC to establish the consumption of starting material. The mixture was then cooled to room

temperature, the solid was removed by filtration. The filtrate was diluted with EtOAc and washed with water.

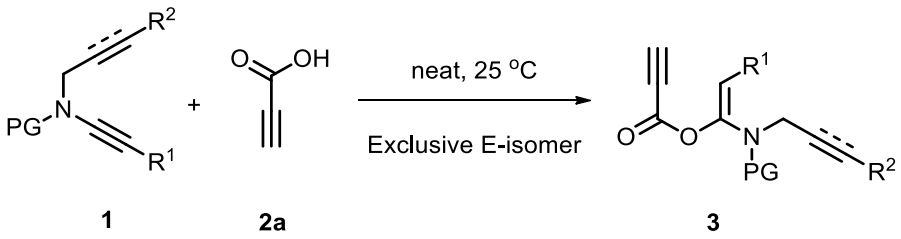
The combined organic layer was washed with brine and dried over Na_2SO_4. The resultant crude material was directly subjected to hydrolysis by subjecting to aqueous NaOH (1M, 3.0 equiv) in MeOH (5 mL) at 0 °C and then allowed to warm to rt and stirred overnight. The reaction mixture was acidified to pH = 1 by adding HCl (2M) and then extracted with DCM (1 × 10 mL). The organic layer was separated and the aqueous layer extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were dried over $MgSO_4$ and evaporated to yield the respective arylpropiolic acids.

Table S1: List of Ynamides





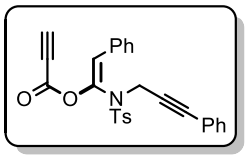
General procedure for the chemo-, regio-, and stereoselective hydropropioloxylation of ynamide 1 with terminal propiolic acid 2a (GP-3):



The ynamide **1** (0.3 mmol) was taken in an RB flask and then propiolic acid **2a** (0.36 mmol) was introduced drop wise. The reaction mixture was stirred at RT. The progress of the reaction was periodically monitored by TLC. After complete consumption of ynamide **1**, the reaction mixture was diluted with EtOAc and neutralized with saturated $NaHCO_3$ solution. The organic layer was

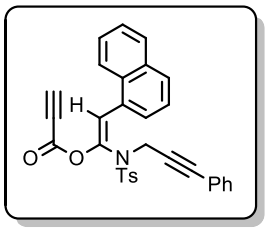
further extracted with EtOAc (10 mL) and dried over anhydrous Na_2SO_4. After evaporation of solvent under reduced pressure, the residue was purified by flash chromatography on silica gel (hexane/EtOAc) to afford the expected product **3**.

(*E*)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl propiolate (3a):



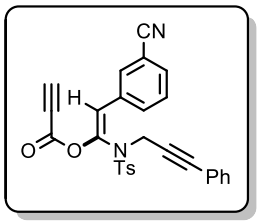
Following the general procedure GP−3, compound **3a** (134 mg) was obtained in 98% yield as colorless solid; mp= 124–126 °C; R_f = 0.49 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (d, J = 8.5 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.39–7.27 (m, 3H), 7.26–7.15 (m, 5H), 7.08 (d, J = 7.0 Hz, 2H), 6.51 (s, 1H), 4.43 (s, 2H), 2.93 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.9, 144.3, 137.0, 136.0, 131.6, 131.4, 129.4, 128.84, 128.81, 128.6, 128.52, 128.3, 127.9, 123.5, 122.1, 86.0, 81.9, 77.3, 73.8, 39.8, 21.4.; IR (Neat)ν_{max} 1724, 1351, 1264, 1100, 1052, 732,701 cm^{-1}; HRMS (ESI) for $C_{27}H_{21}NNaO_4S$ $(M+Na)^+$: calcd 478.1089, found 478.1084.

(*E*)-1-(4-Methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-(naphthalen-1-yl)vinyl propiolate (3b):



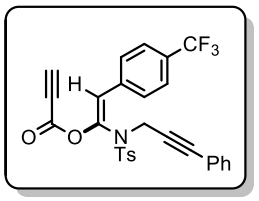
Following the general procedure GP−3, compound **3b** (146 mg) was obtained in 96% yield as colorless solid; mp = 126–128 °C; R_f = 0.51 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.99–7.89 (m, 2H), 7.87–7.76 (m, 2H), 7.72 (d, J = 8.4 Hz, 2H), 7.54–7.41 (m, 3H), 7.31–7.20 (m, 3H), 7.17–7.07 (m, 3H), 7.03 (d, J = 8.4 Hz, 2H), 4.33 (s, 2H), 3.07 (s, 1H), 2.25 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.0, 143.9, 138.8, 135.7, 133.3, 131.6, 131.4, 129.2, 128.8, 128.5, 128.4, 128.3, 128.0, 126.6, 126.4, 126.0, 125.5, 124.2, 122.1, 121.1, 85.9, 82.1, 77.5, 73.8, 40.0, 21.4; IR (Neat)ν_{max} 2128, 1748, 1351, 1157, 111.4, 1046, 685 cm^{-1}; HRMS (ESI) for $C_{31}H_{24}NO_4S$ $(M+H)^+$: calcd 506.1426, found 506.1423.

(*E*)-2-(3-Cyanophenyl)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl propiolate (3c):



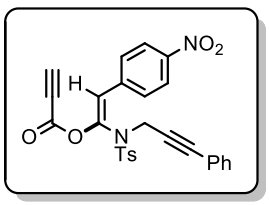
Following the general procedure GP–3, compound **3c** (137 mg) was obtained in 93% yield as colorless solid; mp = 129–131°C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88 (d, J = 7.8 Hz, 1H), 7.77 (d, J = 8.4 Hz, 2H), 7.73 (s, 1H), 7.50 (d, J = 7.8 Hz, 1H), 7.40 (t, J = 7.8 Hz, 1H), 7.27–7.17 (m, 5H), 7.10 (d, J = 7.2 Hz, 2H), 6.51 (s, 1H), 4.41 (s, 2H), 2.97 (s, 1H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.5, 144.8, 138.5, 135.2, 133.1, 132.8, 132.3, 132.2, 131.9, 131.6, 131.5, 129.7, 129.6, 129.5, 129.4, 128.6, 128.3, 128.04, 127.99, 121.80, 121.76, 118.3,112.7, 86.5, 81.2, 77.9, 77.7, 73.4, 39.6, 21.5; IR (Neat)ν_{max} 2227, 1745, 1509, 1349, 1272, 1159, 1099, 747, 625 cm^{-1}; HRMS (ESI) for $C_{28}H_{21}N_2O_4S$ $(M+H)^+$: calcd 481.1222, found 481.1222.

(*E*)-1-(4-Methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-(4-(trifluoromethyl)phenyl)vinyl propiolate (3d):



Following the general procedure GP–3, compound **3d** (151 mg) was obtained in 96% yield as colorless solid; mp = 121–123 °C; R_f = 0.46 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.79 (d, J = 7.8 Hz, 2H), 7.70 (d, J = 7.8 Hz, 2H), 7.55 (d, J = 7.8 Hz, 2H), 7.28–7.24 (m, 1H), 7.20 (t, J = 7.8 Hz, 4H), 7.08 (d, J = 6.6 Hz, 2H), 6.58 (s, 1H), 4.43 (s, 2H), 2.97 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 144.6, 138.4, 135.5, 135.2, 131.5, 130.3 (q, J = 32 Hz, 1C), 129.5, 129.1, 128.6, 128.4, 128.0, 125.4, 123.9 (q, J = 272 Hz, 1C), 122.5, 121.9, 121.2, 86.3, 81.4, 77.6, 73.5, 39.7, 21.4; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.7; IR (Neat)ν_{max} 2228, 1722, 1488, 1350, 1288, 1162, 1054, 737, 692 cm^{-1}; HRMS (ESI) for $C_{28}H_{21}F_3NO_4S$ $(M+H)^+$: calcd 524.1143, found 524.1144.

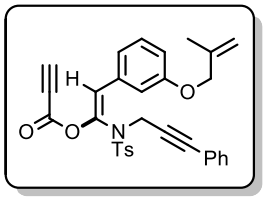
(*E*)-1-(4-Methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-(4-nitrophenyl)vinyl propiolate (3e):



Following the general procedure GP–3, compound **3e** (140 mg) was obtained in 93% yield as colorless solid; mp = 135–137 °C; R_f = 0.39 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.14 (d, J = 9.0 Hz, 2H), 7.80 (d, J = 7.8 Hz, 2H), 7.76 (d, J = 9.0 Hz, 2H),

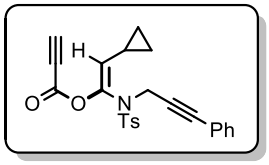
7.29–7.17 (m, 5H), 7.09 (d, J = 9.0 Hz, 2H), 6.63 (s, 1H), 4.42 (s, 2H), 2.98 (s, 1H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.4, 147.3, 144.8, 139.4, 138.4, 135.3, 131.6, 131.5, 129.8, 129.6, 128.7, 128.4, 128.2, 128.0, 127.97, 123.8, 123.6, 121.7, 86.5, 81.2, 78.0, 73.3, 39.7, 21.5; IR (Neat)ν_{max} 2125, 1722, 1524, 1347, 1163, 1026, 805, 668 cm^{-1}; HRMS (ESI) for $C_{27}H_{21}N_2O_6S$ $(M+H)^+$: calcd 501.1120, found 501.1121.

(*E*)-1-(4-Methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-(3-((2-methylallyl)oxy)phenyl)vinyl propiolate (3f):



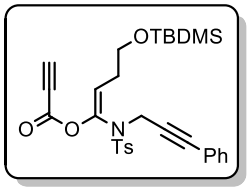
Following the general procedure GP–3, compound **3f** (144 mg) was obtained in 91% yield as colorless solid; mp = 127–129 °C; R_f = 0.5 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.86 (d, J = 8.4 Hz, 2H), 7.29–7.16 (m, 7H), 7.11 (d, J = 7.2 Hz, 1H), 7.08 (d, J = 7.2 Hz, 2H), 6.87 (dd, J = 8.4, 2.4 Hz, 1H), 6.48 (s, 1H), 5.07 (s, 1H), 4.97 (s, 1H), 4.43 (s, 2H), 4.40 (s, 2H), 2.93 (s, 1H), 2.32 (s, 3H), 1.81 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.8, 149.9, 144.3, 140.7, 137.1, 135.9, 132.5, 131.7, 131.5, 129.6, 129.4, 128.5, 128.3, 127.9, 123.5, 123.4, 122.1, 121.7, 116.32, 116.25, 113.9, 113.8, 112.6, 85.9, 81.9, 77.4, 73.7, 71.6, 39.8, 21.5, 19.4; IR (Neat)ν_{max} 2221, 1728, 1365, 1260, 1119, 1017, 729, 595 cm^{-1}; HRMS (ESI) for $C_{31}H_{28}NO_5$ $(M+H)^+$: calcd 526.1688, found 526.1687.

(*E*)-2-Cyclopropyl-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl propiolate (3g):



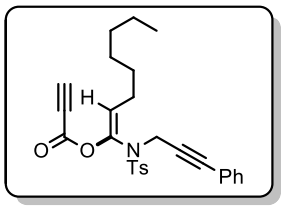
Following the general procedure GP–3, compound **3g** (122 mg) was obtained in 97% yield as colorless solid; mp = 118–120 °C; R_f = 0.53 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.87 (d, J = 7.8 Hz, 2H), 7.29–7.21 (m, 5H), 7.20–7.16 (m, 2H), 5.05 (d, J = 15.0 Hz, 1H), 4.52 (s, 2H), 2.87 (s, 1H), 2.35 (s, 3H), 1.70–1.60 (m, 1H), 0.77–0.68 (m, 2H), 0.48–0.41 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.5, 144.0, 136.5, 136.0, 131.6, 130.8, 130.6, 129.5, 129.4, 128.3, 128.0, 122.4, 85.5, 82.8, 76.7, 73.9, 40.3, 21.5, 9.64, 9.61, 7.3; IR (Neat)ν_{max} 2120, 1732, 1355, 1160, 1130, 690, 543 cm^{-1}; HRMS (ESI) for $C_{24}H_{21}NNaO_4S$ $(M+Na)^+$: calcd 442.1089, found 442.1088.

(*E*)-4-((*tert*-Butyldimethylsilyl)oxy)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)but-1-en-1-yl propiolate (3h):



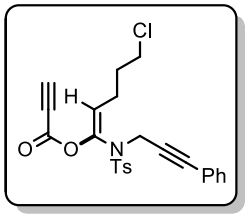
Following the general procedure GP–3, compound **3h** (145 mg) was obtained in 90% yield as colorless solid; mp = 126–128 °C; R_f = 0.55 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$):δ 7.86 (d, J = 8.5 Hz, 2H), 7.32–7.20 (m, 7H), 5.79 (t, J = 7.5 Hz, 1H), 4.47 (s, 2H), 3.69 (t, J = 6.5 Hz, 2H), 2.89 (s, 1H), 2.48 (q, J = 6.5 Hz, 2H), 2.37 (s, 3H), 0.89 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (126MHz, $CDCl_3$) δ 150.1, 144.1, 137.7, 136.2, 131.6, 129.5, 128.4, 128.3, 128.0, 123.3, 122.3, 85.5, 73.8, 61.7, 40.3, 31.0, 25.9, 21.5, 18.2, –5.5; IR (Neat)ν_{max} 2119, 1732, 1353, 1160, 1130, 1051, 757, 659 cm^{-1}; HRMS (ESI) for $C_{29}H_{36}NO_5SSi$ $(M+H)^+$: calcd 538.2083, found 538.1304.

(*E*)-1-(4-Methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)oct-1-en-1-yl propiolate (3i):



Following the general procedure GP–3, compound **3i** (135 mg) was obtained in 97% yield as colorless solid; mp = 121–123 °C; R_f = 0.52 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (d, J = 8.0 Hz, 2H), 7.35–7.20 (m, 7H), 5.66 (t, J = 7.5 Hz, 1H), 4.45 (s, 2H), 2.90 (s, 1H), 2.38 (s, 3H), 2.23 (q, J = 7.5 Hz, 2H), 1.44–1.33 (m, 2H), 1.32–1.15 (m, 6H), 0.85 (t, J = 6.5 Hz, 3H); ^{13}C NMR (126MHz, $CDCl_3$) δ 150.4, 144.1, 136.7, 136.2, 131.6, 129.4, 128.4, 128.2, 128.0, 126.6, 122.3, 85.4, 82.5, 77.3, 73.8, 40.2, 31.5, 29.0, 28.7, 27.2, 22.5, 21.5, 14.0; IR (Neat)ν_{max} 1733, 1356,1162, 1141, 1089, 661 cm^{-1}; HRMS (ESI) for $C_{27}H_{30}NO_4S$ $(M+H)^+$: calcd 464.1896, found 464.1886.

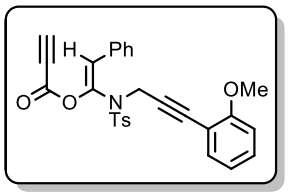
(*E*)-5-Chloro-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)pent-1-en-1-yl propiolate (3j):



Following the general procedure GP–3, compound **3j** (130 mg) was obtained in 95% yield as colorless solid; mp = 124–126 °C; R_f = 0.5 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, J = 8.0 Hz, 2H), 7.34–7.21 (m, 7H), 5.66 (t, J = 7.6 Hz, 1H), 4.46 (s, 2H), 3.53 (t, J = 6.4 Hz, 2H), 2.92 (s, 1H), 2.45 (q, J = 7.2 Hz, 2H), 2.39 (s, 3H), 1.99–1.85 (m, 2H);

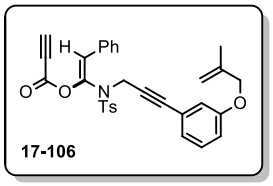
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.1, 144.3, 137.5, 135.9, 131.6, 129.5, 128.5, 128.2, 128.0, 124.7, 122.1, 85.6, 82.2, 77.0, 73.6, 44.1, 40.0, 31.4, 24.6, 21.4; IR (Neat)ν_{max} 2121,1733, 1353, 1157, 1126,1052, 657; HRMS (ESI) for $C_{24}H_{23}ClNO_4S(M+H)^+$: calcd 456.1036, found 456.1094.

(*E*)-1-(N-(3-(2-Methoxyphenyl)prop-2-yn-1-yl)-4-methylphenylsulfonamido)-2-phenylvinyl propiolate (3k):



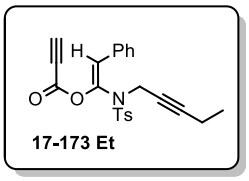
Following the general procedure GP–3, compound **3k** (137 mg) was obtained in 94% yield as colorless solid; mp = 128–130 °C; R_f = 0.48 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (d, J = 8.5 Hz, 2H),7.60 (t, J = 1.0 Hz, 2H),7.35–7.27 (m, 3H), 7.25–7.17 (m, 3H), 6.94 (dd, J = 7.5, 2.0 Hz, 1H), 6.81–6.75 (m, 2H), 6.54 (s, 1H), 4.49 (s, 2H), 3.77 (s, 3H), 2.93 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.9. 149.7, 144.1, 137.1, 135.9, 133.7, 131.4, 129.8, 129.3, 128.8, 128.7, 128.50, 128.45, 123.3, 119.9, 111.3, 110.3, 85.6, 82.5, 77.2, 73.8, 55.5, 40.0, 21.5; IR (Neat)ν_{max} 2927, 2120, 1733, 1491, 1352, 1292, 1160, 1019, 692, 660 cm^{-1}; HRMS (ESI) for $C_{28}H_{23}NNaO_5S$ $(M+Na)^+$: calcd 508.1195, found508.1192.

(*E*)-1-(4-Methyl-N-(3-(3-((2-methylallyl)oxy)phenyl)prop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl propiolate (3l):



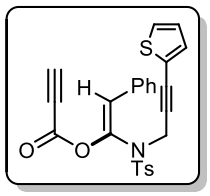
Following the general procedure GP–3, compound **3l** (147 mg) was obtained in 96% yield as colorless solid; mp = 128–130 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 7.6 Hz, 2H), 7.65 (d, J = 7.2 Hz, 2H), 7.48–7.25 (m, 5H), 7.14 (t, J = 8.0 Hz, 1H), 6.86 (d, J = 7.2 Hz, 1H), 6.80–6.69 (m, 2H), 6.55 (s, 1H), 5.10 (s, 1H), 5.02 (s, 1H), 4.47 (s, 2H), 4.37 (s, 2H), 2.99 (s, 1H), 2.38 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2, 150.0, 144.5, 140.6, 137.1, 136.0, 131.4, 129.5, 129.1, 129.0, 128.7, 128.6, 124.2, 123.6, 123.1, 117.8, 115.5, 112.9, 86.0, 81.8, 73.8, 71.7, 39.9, 21.6, 19.5; IR (Neat)ν_{max} 2226, 17321, 1698, 1358, 1163, 1108, 758 cm^{-1}; HRMS (ESI) for $C_{31}H_{28}NO_5S$ $(M+H)^+$: calcd 526.1688, found 526.1687.

(*E*)-1-(4-Methyl-N-(pent-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl propiolate (3m):



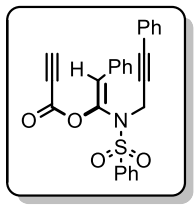
Following the general procedure GP–3, compound **3m** (120 mg) was obtained in 98% yield as colorless solid; mp= 118–120 °C; R_f = 0.51 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, J = 8.0 Hz, 2H), 7.59 (d, J = 7.5 Hz, 2H), 7.38–7.24 (m, 5H), 6.50 (s, 1H), 4.19 (s, 2H), 3.04 (s, 1H), 2.42 (s, 3H), 1.92 (q, J = 7.5 Hz, 2H), 0.88 (t, J = 7.5 Hz, 3H); ^{13}C NMR (121 MHz, $CDCl_3$) δ 149.8, 144.1, 136.9, 136.0, 131.4, 129.3, 128.8, 128.7, 128.5, 123.4, 88.1, 77.2, 73.8, 71.8, 39.3, 21.5, 13.1, 12.1; IR (Neat)ν_{max} 2119, 1735, 1348, 1160, 1114, 1015, 658, 533 cm^{-1}; HRMS (ESI) for $C_{23}H_{22}NO_4S$ $(M+H)^+$: calcd 408.1270, found 408.1267.

(*E*)-1-(4-Methyl-N-(3-(thiophen-2-yl)prop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl propiolate (3n):



Following the general procedure GP–3, compound **3n** (133 mg) was obtained in 96% yield as colorless solid; mp = 132–134 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.87 (d, J = 10.2 Hz, 2H), 7.59 (d, J = 9.0 Hz, 2H), 7.34 (t, J = 7.2 Hz, 2H), 7.33–7.27 (m, 1H), 7.24 (d, J = 7.8 Hz, 2H), 7.18 (dd, J = 5.4, 1.2 Hz, 1H), 6.93 (d, J = 2.4 Hz, 1H), 6.89–6.86 (m, 1H), 6.50 (s, 1H), 4.44 (s, 2H), 2.96 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.9, 144.4, 137.0, 135.9, 132.5, 131.3, 129.5, 128.9, 128.8, 128.6, 128.5, 127.3, 126.6, 123.5, 122.0, 85.8, 79.3, 77.3, 73.7. 40.0, 21.6; IR (Neat)ν_{max}2119, 1726, 1345, 1119, 1162, 1018, 691, 661, 534 cm^{-1}; HRMS (ESI) for $C_{25}H_{19}NNaO_4S_2$ $(M+Na)^+$: calcd 484.0653, found 484.0652.

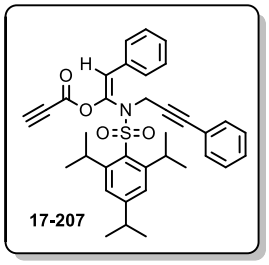
(*E*)-2-Phenyl-1-(N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl propiolate (3o):



Following the general procedure GP–3, compound **3o** (131 mg) was obtained in 99% yield as colorless solid; mp= 120–122 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.00 (d, J = 7.2 Hz, 2H), 7.61 (d, J = 7.2 Hz, 2H), 7.53 (t, J = 7.2 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.34 (t, J = 7.2 Hz, 2H), 7.29 (t, J = 7.8 Hz, 1H), 7.25 (t, J = 7.8 Hz, 1H), 7.19 (t, J = 7.8 Hz, 2H), 7.11–7.06 (m, 2H), 6.52 (s, 1H), 4.46 (s, 2H), 2.90 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.9, 139.0, 136.8, 133.3, 131.61, 131.56, 131.3, 128.9, 128.7, 128.5, 128.0, 123.6, 122.0, 86.1, 81.7, 77.3,

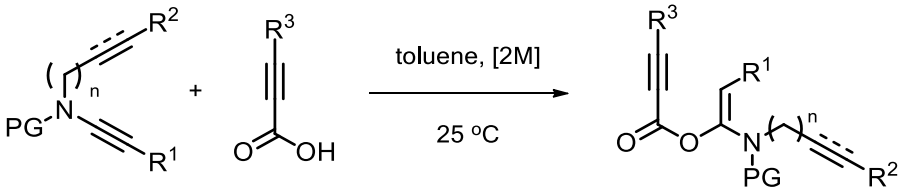
73.7, 40.0; IR (Neat)ν_{max} 1724, 1351, 1264, 1100, 1052, 732,701 cm^{-1}; HRMS (ESI) for $C_{26}H_{20}NO_4S$ $(M+H)^+$: calcd 442.1113, found 442.1110.

(*E*)-2-Phenyl-1-(2,4,6-triisopropyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl propiolate (3p):



Following the general procedure GP–3, compound **3p** (159 mg) was obtained in 97% yield as colorless solid; mp = 116–118 °C; R_f = 0.33 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70–7.59 (m, 2H), 7.35–7.22 (m, 5H), 7.21–7.15 (m, 3H), 7.13–7.03 (m, 2H), 6.58–6.50 (m, 1H), 4.70–4.60 (m, 2H), 4.19–3.95 (m, 2H), 2.95–2.81 (m, 2H), 1.45–1.20 (m, 18H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.5, 151.7, 150.5, 136.6, 133.3, 131.6, 131.5, 129.0, 128.8, 128.4, 128.3, 128.0, 124.2, 123.8, 122.4, 85.7, 82.7, 73.9, 39.0, 34.2, 30.5, 25.1, 23.5; IR (Neat)ν_{max} 2226, 1738, 1488, 1154, 1084, 1110, 750, 687 cm^{-1}; HRMS (ESI) for $C_{35}H_{37}NO_4S$ $(M+Na)^+$: calcd 568.2522, found 568.2521.

General procedure for the chemo-, regio-, and stereoselective hydropropioloxylation of ynamide 1 / 5 with arylpropiolic acids 2b / 2c (GP-4):

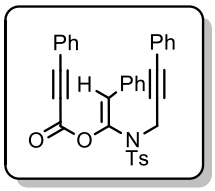


1 / 5 **2** **4 / 6**

To the solution of ynamide (0.3 mmol) in 2M toluene was introduced arylpropiolic acid **2** (0.36 mmol). The reaction mixture was stirred at RT. The progress of the reaction was periodically monitored by TLC. After complete consumption of ynamide, the reaction mixture was diluted with EtOAc and neutralized with saturated $NaHCO_3$ solution. The organic layer was further extracted with EtOAc (10 mL) and dried under anhydrous Na_2SO_4. After evaporation of solvent under reduced pressure, the residue was purified

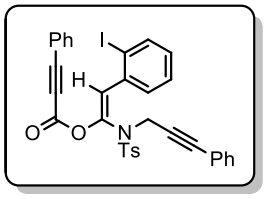
by flash chromatography on silica gel (Hexane/EtOAc) to afford the expected product **4 / 6**.

(*E*)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4a):



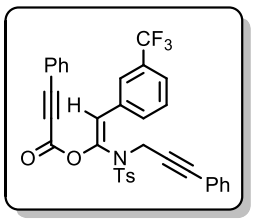
Following the general procedure GP–4, compound **4a** (157 mg) was obtained in 98% yield as colorless solid; mp = 131–133 °C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (d, J = 8.5 Hz, 2H), 7.66 (d, J = 7.5 Hz, 2H), 7.52–7.29 (m, 8H), 7.19 (d, J = 7.5 Hz, 3H), 7.16–7.06 (m, 4H), 6.57 (s, 1H), 4.49 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1, 144.1, 137.3, 136.2, 132.9, 131.6, 131.0, 129.3, 128.9, 128.71, 128.67, 128.6,128.2, 127.9, 123.3, 122.2, 119.1, 89.0, 85.9, 82.1, 79.8, 40.0, 21.4; IR (Neat)ν_{max} 1730, 1173, 1156, 1046, 1012, 682, 537cm^{-1}; HRMS (ESI) for $C_{33}H_{25}NNaO_4S$ $(M+Na)^+$: calcd 554.1403, found 554.1403.

(*E*)-2-(2-iodophenyl)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl 3-phenylpropiolate (4b):



Following the general procedure GP–4, compound **4b** (183 mg) was obtained in 92% yield as colorless solid; mp = 123–125 °C; R_f = 0.49 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93–7.83 (m, 4H), 7.55–7.49 (m, 3H), 7.47–7.34 (m, 4H), 7.25–7.17 (m, 6H), 7.02–6.94 (m, 1H), 6.68 (s, 1H), 4.39 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.8, 144.0, 139.2, 139.0, 135.9, 133.0, 131.7, 131.1, 129.7, 129.4, 128.3, 127.9, 125.8, 122.2, 119.0, 100.2, 89.3, 85.9, 82.1,80.0, 40.2, 21.4; IR (Neat)ν_{max} 1724, 1348, 1285, 1151, 1076, 1053, 761, 580 cm^{-1}; HRMS (ESI) for $C_{33}H_{24}INNaO_4S$ $(M+Na)^+$: calcd 680.0368, found 680.0366.

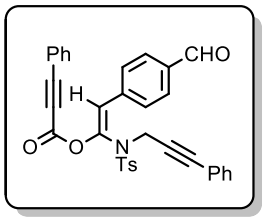
(*E*)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-(3-(trifluoromethyl) phenyl) vinyl 3-phenylpropiolate (4c):



Following the general procedure GP–4, compound **4c** (169 mg) was obtained in 94% yield as colorless solid; mp = 130–132 °C; R_f = 0.41 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 7.2 Hz, 2H), 7.50 (t, J = 7.2 Hz, 1H), 7.46–7.27 (m, 7H), 7.20 (d, J = 7.8 Hz, 2H), 7.06 (t, J = 7.2 Hz, 2H), 6.79 (t, J = 8.4 Hz, 2H), 6.55 (s, 1H),

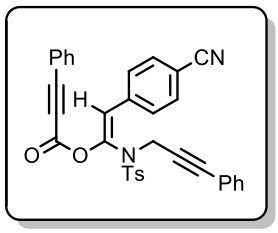
4.46 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9, 140.4, 138.5, 135.8, 133.0, 132.7, 131.7, 130.6, 131.3, 131.2, 131.0, 130.8, 136.5, 129.4, 129.1, 128.64, 128.62, 128.4, 128.0, 125.93, 125.90, 125.87, 125.84, 125.2, 125.1, 125.0, 122.8, 122.2, 122.0, 119.0, 89.4, 86.3, 81.6, 79.7, 39.8, 21.4; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.8 ppm; IR (Neat)ν_{max} 1737, 1350, 1156, 1108, 1013, 756, 687 cm^{-1}; HRMS (ESI) for $C_{34}H_{24}F_3NNaO_4S$ $(M+Na)^+$: calcd 622.1276, found 622.1309.

(*E*)-2-(4-formylphenyl)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl 3-phenylpropiolate (4d):



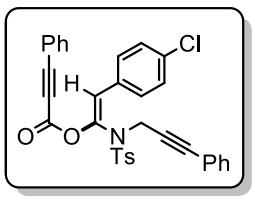
Following the general procedure GP–4, compound **4d** (166 mg) was obtained in 99% yield as colorless solid; mp = 138–140 °C; R_f = 0.46 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.97 (s, 1H), 7.89 (d, J = 8.0 Hz, 2H), 7.82 (q, J = 8.5 Hz, 4H), 7.49 (t, J = 7.5 Hz, 1H), 7.44 (d, J = 7.5 Hz, 2H), 7.38 (t, J = 8.0 Hz, 2H), 7.24–7.18 (m, 3H), 7.16–7.07 (m, 4H), 6.65 (s, 1H), 4.48 (s, 2H), 2.24 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.6, 150.7, 144.4, 139.2, 138.0, 135.9, 135.8, 133.0, 131.5, 131.2, 129.8, 129.44, 129.38, 128.62, 128.57, 128.4, 128.0, 122.2, 121.9, 118.8, 89.5, 86.3, 81.6, 79.6, 40.0, 21.4; IR (Neat)ν_{max} 2126, 1748, 1351, 1157, 1114, 1046, 754, 684 cm^{-1}; HRMS (ESI) for $C_{34}H_{25}NNaO_5S$ $(M+Na)^+$: calcd 582.1351, found 582.1350.

(*E*)-2-(4-cyanophenyl)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl 3-phenylpropiolate (4e):



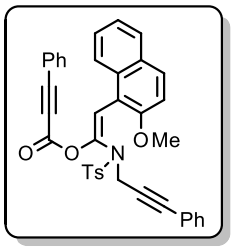
Following the general procedure GP–4, compound **4e** (159 mg) was obtained in 95% yield as colorless solid; mp = 133–135 °C; R_f = 0.38 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (d, J = 8.0 Hz, 2H), 7.76 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 8.5 Hz, 2H), 7.53–7.48 (m, 1H), 7.47–7.43 (m, 2H), 7.42–7.36 (m, 2H), 7.25–7.19 (m, 3H), 7.18–7.13 (m, 2H), 7.12–7.08 (m, 2H), 6.62 (s, 1H), 4.47 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.6, 144.6, 139.4, 136.7, 135.6, 133.0, 132.2, 131.5, 131.3, 129.5, 129.4, 128.7, 128.6, 128.0, 121.8, 118.8, 118.6, 111.8, 89.6, 86.4, 81.4, 79.5, 39.9, 21.4; IR (Neat)ν_{max} 2121, 1724, 1343, 1160, 1114, 997, 752, 690 cm^{-1}; HRMS (ESI) for $C_{34}H_{24}N_2NaO_4S$ $(M+Na)^+$: calcd 579.1354, found 579.1360.

(*E*)-1-(N-(3-(4-chlorophenyl)prop-2-yn-1-yl)-4-methylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4f):



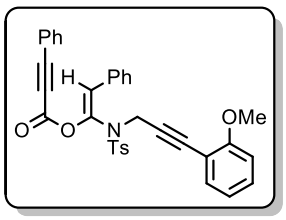
Following the general procedure GP–4, compound **4f** (165 mg) was obtained in 97% yield as colorless solid; mp = 128–130 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, J = 8.5 Hz, 2H), 7.64 (d, J = 7.5 Hz, 2H), 7.53–7.47 (m, 1H), 7.44–7.34 (m, 6H), 7.33–7.29 (m, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.09–7.05 (m, 2H), 7.03–6.96 (m, 2H), 6.56 (s, 1H), 4.47 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.2, 144.1, 137.2, 136.3, 134.3, 132.9, 132.8, 131.5, 131.1, 129.3, 128.9, 128.8, 128.71, 128.65, 128.6, 128.2, 123.5, 120.7, 119.0, 89.1, 84.8, 83.3, 79.8, 39.9, 21.4; IR (Neat)ν_{max} 2923, 1738, 1366, 1324, 1216, 1155, 812, 760cm^{-1}; HRMS (ESI) for $C_{33}H_{24}ClNNaO_4S$ $(M+Na)^+$: calcd 588.1012, found 588.1012.

(*E*)-1-(N-(3-(2-methoxynaphthalen-1-yl)prop-2-yn-1-yl)-4-methylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4g):



Following the general procedure GP–4, compound **4g** (172 mg) was obtained in 94% yield as pale yellow solid; mp = 140–142 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.04 (d, J = 8.5 Hz, 1H), 7.79 (dd, J = 21, 9.0 Hz, 2H), 7.71 (d, J = 8.5 Hz, 2H), 7.54–7.46 (m, 4H), 7.42–7.34 (m, 3H),7.26 (d, J = 9.0 Hz, 1H), 7.23–7.19 (m, 1H), 7.17–7.11 (m, 4H), 6.97 (d, J = 8.4, 2H), 6.71 (s, 1H), 4.34 (s, 2H), 4.00 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.2, 151.6, 143.4, 140.3, 136.8, 133.0, 132.6, 131.6, 130.9, 130.1, 129.0, 128.6, 128.1, 128.03, 127.96, 127.85, 126.9, 124.6, 123.8, 122.6, 119.2, 114.9, 114.2, 112.9, 89.2, 84.8, 83.4, 80.1, 56.3, 39.6, 21.3; IR (Neat)ν_{max} 1745, 1350, 1273, 1159, 1100, 1017, 813, 688cm^{-1}; HRMS (ESI) for $C_{38}H_{29}NNaO_5S$ $(M+Na)^+$: calcd 634.1664, found 634.1654.

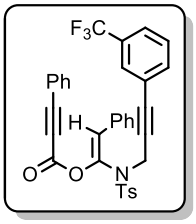
(*E*)-1-(N-(3-(2-Methoxyphenyl)prop-2-yn-1-yl)-4-methylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4h):



Following the general procedure GP–4, compound **4h** (161 mg) was obtained in 96% yield as colorless solid; mp = 124–126 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.91 (d, J = 9.0 Hz, 2H), 7.65 (d, J = 7.2 Hz, 2H), 7.49 (t, J = 7.8 Hz, 1H), 7.45

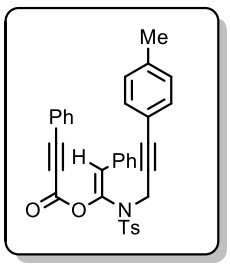
(d, J = 7.2 Hz, 2H), 7.38 (t, J = 7.8 Hz, 2H), 7.34 (t, J = 7.2 Hz, 2H), 7.29 (t, J = 7.2 Hz, 1H), 7.20–7.15 (m, 3H), 6.95 (dd, J = 7.8, 1.8 Hz, 1H), 6.75 (d, J = 8.4 Hz, 1H), 6.67 (t, J = 7.8 Hz, 1H), 6.59 (s, 1H), 4.54 (s, 2H), 3.77 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.9, 151.0, 143.9, 137.4, 136.2, 133.9, 133.6, 132.98, 132.96, 131.7, 131.0, 129.9, 129.6, 129.4, 129.1, 128.9, 128.7, 128.5, 123.0, 122.97, 120.0, 119.8, 119.2, 111.4, 110.3, 88.8, 85.9, 82.5, 79.9, 55.5, 40.2, 21.4; IR (Neat)ν_{max} 2235, 1738, 1488, 1349, 1154, 1110, 1017, 687, 660 cm^{-1}; HRMS (ESI) for $C_{34}H_{28}NO_5S$ $(M+H)^+$: calcd 562.1688, found 562.1691.

(*E*)-1-(4-Methyl-N-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4i):



Following the general procedure GP–4, compound **4i** (173 mg) was obtained in 96% yield as colorless solid; mp = 120–122 °C; R_f = 0.46 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 7.8 Hz, 2H), 7.50 (t, J = 7.2 Hz, 1H), 7.46 (d, J = 7.2 Hz, 2H), 7.42–7.35 (m, 4H), 7.34–7.26 (m, 1H), 7.22 (d, J = 8.4 Hz, 2H), 7.11–7.07 (m, 1H), 7.00–6.87 (d, J = 5.4 Hz, 2H), 6.69 (d, J = 9.6 Hz, 1H), 6.56 (s, 1H), 4.48 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.7, 161.1, 151.2, 144.2, 137.2, 136.2, 132.9, 131.5, 131.1, 129.7, 129.51, 129.46, 129.3, 129.2, 128.85, 128.81, 128.7, 128.64, 128.61, 128.2, 127.4, 124.0, 123.9, 123.4, 118.9, 118.4, 118.3, 115.6, 115.5, 89.2, 84.6, 83.2, 79.7, 39.9, 21.3; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.96 ppm;IR (Neat)ν_{max} 172, 1698, 1351, 1156, 1109, 1085, 813, 741 cm^{-1}; HRMS (ESI) for $C_{34}H_{24}F_3NNaO_4S$ $(M+Na)^+$: calcd 622.1276, found 622.1279.

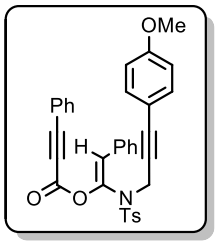
(*E*)-1-(4-methyl-N-(3-(p-tolyl)prop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4j):



Following the general procedure GP–4, compound **4j** (160 mg) was obtained in 98% yield as colorless solid; mp = 124–126 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (d, J = 8.5 Hz, 2H), 7.68 (d, J = 7.5 Hz, 2H), 7.51 (d, J = 7.0 Hz, 1H), 7.45–7.33 (m, 7H), 7.22 (d, J = 8.0 Hz, 2H), 7.01 (d, J =8.0 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H), 6.59 (s, 1H), 4.50 (s, 2H), 2.27 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.1, 144.0, 138.3,

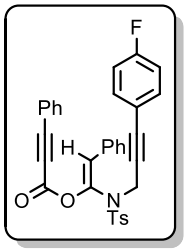
137.4, 136.3, 132.9, 131.6, 131.5, 130.9, 129.3, 128.9, 128.7, 128.62, 128.58, 128.5, 123.3, 119.2, 119.1, 88.9, 86.1, 81.4, 79.9, 40.0, 21.4, 21.3; IR (Neat)ν_{max} 1735, 1602, 1508, 1348, 1254, 1162, 1051, 754 cm^{-1}; HRMS (ESI) for $C_{34}H_{27}NNaO_5S$ $(M+Na)^+$: calcd 568.1558, found 568.1551.

(*E*)-1-(N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4k):



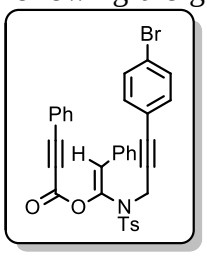
Following the general procedure GP–4, compound **4k** (167 mg) was obtained in 99% yield as colorless solid; mp = 136–138 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.92 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 8.5 Hz, 2H), 7.49–7.45 (m, 1H), 7.43–7.28 (m, 7H), 7.19 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 9.0 Hz, 2H), 6.62 (d, J = 9.0 Hz, 2H), 6.55 (s, 1H), 4.46 (s, 2H), 3.70 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 151.1, 144.0, 137.3, 136.2, 133.0, 132.9, 131.6, 131.0, 129.3, 128.9, 128.7, 128.6, 123.3, 119.1, 114.3, 113.5, 88.9, 85.9, 80.6, 79.8, 55.1, 40.1, 21.4; IR (Neat)ν_{max} 2228, 1724, 1504, 1350, 1287, 1152, 1052, 832, 693 cm^{-1}; HRMS (ESI) for $C_{34}H_{28}NO_5S$ $(M+H)^+$: calcd 562.1688, found 562.1678.

(*E*)-1-(N-(3-(4-fluorophenyl)prop-2-yn-1-yl)-4-methylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4l):



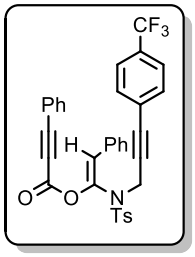
Following the general procedure GP–4, compound **4l** (106 mg) was obtained in 95% yield as colorless solid; mp = 127–129 °C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.93 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 7.2 Hz, 2H), 7.50 (t, J = 6.6 Hz, 1H), 7.47–7.27 (m, 7H), 7.20 (d, J = 7.8 Hz, 2H), 7.06 (bt, J = 7.2 Hz, 2H), 6.79 (t, J = 8.4 Hz, 2H), 6.55 (s, 1H), 4.46 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.3 (d, J = 250 Hz, 1C), 151.2, 144.1, 137.2, 136.2, 133.5 (d, J = 8.6 Hz, 1C), 132.9, 131.5, 131.1, 129.3, 128.9, 128.8, 128.71, 128.66, 128.6, 123.5, 115.2 (d, J = 23.1 Hz, 1C), 89.1, 84.9, 81.9, 79.8, 40.0, 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ –110.18; IR (Neat)ν_{max} 2128, 1732, 1353, 1160, 1116, 1087, 1018, 752, 660 cm^{-1}; HRMS (ESI) for $C_{33}H_{24}FNNaO_4S$ $(M+Na)^+$: calcd 572.1308, found 572.1302.

(*E*)–1–(N–(3–(4–bromophenyl)prop–2–yn–1–yl)–4-methylphenylsulfonamido) – 2–phenylvinyl 3-phenylpropiolate (4m):



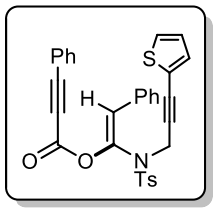
Following the general procedure GP–4, compound **4m** (181 mg) was obtained in 99% yield as colorless solid; mp = 133–135 °C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.92 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 7.5 Hz, 2H), 7.53–7.48 (m, 1H), 7.43–7.39 (m, 4H), 7.38–7.34 (m, 2H), 7.33–7.28 (m, 1H), 7.25–7.18 (m, 4H), 6.96–6.90 (m, 2H), 6.55 (s, 1H), 4.46 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 144.1, 137.1, 136.2, 133.0, 132.9, 131.5, 131.2, 129.3, 128.9, 128.8, 128.72, 128.67, 123.6, 122.6, 121.1, 119.0, 89.1, 84.8, 83.4, 79.8, 39.9, 21.4;IR (Neat)ν_{max} 1724, 1406, 1154, 1088, 820, 661, 549 cm^{-1}; HRMS (ESI) for $C_{33}H_{24}BrNNaO_4S$ $(M+Na)^+$: calcd 632.0507, found 632.0508.

(*E*)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-(4-(trifluoromethyl)phenyl)vinyl 3-phenylpropiolate (4n):



Following the general procedure GP–4, compound **4n** (171 mg) was obtained in 94% yield as colorless solid; mp = 128–130 °C; R_f = 0.39 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 7.0 Hz, 2H), 7.49 (bt, J = 7.0 Hz, 1H), 7.44–7.29 (m, 9H), 7.22 (d, J = 7.5 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 6.57 (s, 1H), 4.50 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.2, 144.2, 137.2, 136.3, 132.9, 131.8, 131.5, 130.0 (q, J = 32 Hz, 1C), 129.4, 128.9, 128.8, 128.72, 128.66, 127.0, 124.7 (q, J = 3.8 Hz, 1C), 124.3 (q, J = 212 Hz, 1C), 123.6, 118.9, 89.2, 84.9, 84.5, 79.8, 39.9, 21.3; ^{19}F NMR (471 MHz, $CDCl_3$) δ –62.94; IR (Neat)ν_{max} 2228, 1724, 1504, 1350, 1287,1102, 1052, 760, 542 cm^{-1}; HRMS (ESI) for $C_{34}H_{24}F_3NNaO_4S$ $(M+Na)^+$: calcd 622.1276, found 622.1270.

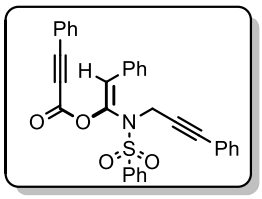
(*E*)-1-(4-methyl-N-(3-(thiophen-2-yl)prop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4o):



Following the general procedure GP–4, compound **4o** (156 mg) was obtained in 97% yield as colorless solid; mp = 139–141 °C; R_f = 0.37 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.92 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 7.0 Hz, 2H), 7.52–7.43 (m, 3H), 7.41–7.28 (m, 5H),

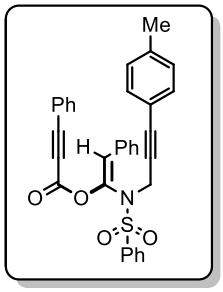
7.21 (d, J = 8.0 Hz, 2H), 7.12 (bd, J = 5.0 Hz, 1H), 6.94 (bd, J = 2.5 Hz, 1H), 6.84–6.78 (m, 1H), 6.55 (s, 1H), 4.49 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.1, 144.2, 137.4, 136.2, 133.0, 132.5, 131.5, 131.0, 129.4, 128.9, 128.7, 128.6, 127.2, 126.6, 123.2, 122.1, 119.2, 89.1, 86.1, 79.8, 79.3, 40.2, 21.4; IR (Neat)ν_{max} 2209, 1721, 1340, 1150, 1081, 790, 754, 730 cm^{-1}; HRMS (ESI) for $C_{31}H_{23}NNaO_4S_2$ $(M+Na)^+$: calcd 560.0966, found 560.0966.

(*E*)-2-phenyl-1-(N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)vinyl 3-phenylpropiolate (4p):



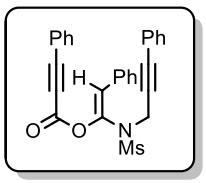
Following the general procedure GP–4, compound **4p** (154 mg) was obtained in 99% yield as colorless solid; mp = 123–125 °C; R_f = 0.41 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, J =7.0 Hz, 2H), 7.57 (d, J = 7.0 Hz, 2H), 7.43–7.20 (m, 12H), 7.06–7.00 (m, 4H), 6.49 (s, 1H), 4.42 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.1, 139.3, 137.2, 133.1, 133.0, 131.6, 131.5, 131.0, 128.9, 128.8, 128.7, 128.64, 128.60, 128.58, 128.3, 127.9, 123.3, 122.1, 119.1, 89.1, 86.0, 82.0, 79.7, 40.1; IR (Neat)ν_{max}2205, 1713, 1352, 1162, 1052, 890, 751, 667 cm^{-1}; HRMS (ESI) for $C_{32}H_{23}NNaO_4S$ $(M+Na)^+$: calcd 540.1245, found 540.1240.

(*E*)-2-Phenyl-1-(N-(3-(p-tolyl)prop-2-yn-1-yl)phenylsulfonamido)vinyl 3-phenylpropiolate (4q):



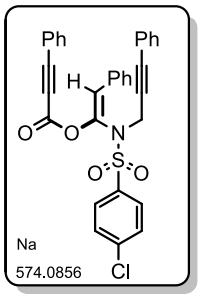
Following the general procedure GP–4, compound **4q** (152 mg) was obtained in 95% yield as colorless solid; mp = 126–128 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (d, 7.5 Hz, 2H), 7.65 (d, J =7.5 Hz, 2H), 7.52–7.46 (m, 2H), 7.45–7.40 (m, 4H), 7.40–7.34 (m, 4H), 7.33–7.28 (m, 1H), 7.00 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 8.0 Hz, 2H), 6.57 (s, 1H), 4.50 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1, 139.3, 138.4, 137.2, 133.1, 133.0, 131.5, 131.0, 128.9, 128.8, 128.7, 128.6, 123.4, 119.09,119.05, 89.0, 86.2, 81.2, 79.8, 40.2, 21.4; IR (Neat)ν_{max} 2121, 1724, 1344, 1160, 1088, 887, 752, 690 cm^{-1}; HRMS (ESI) for $C_{33}H_{25}NNaO_4S$ $(M+Na)^+$: calcd 554.1402, found 554.1404.

(*E*)-2-phenyl-1-(N-(3-phenylprop-2-yn-1-yl)methylsulfonamido)vinyl 3-phenylpropiolate (4r):



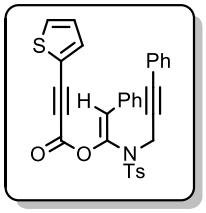
Following the general procedure GP–4, compound **4r** (135 mg) was obtained in 99% yield as colorless solid; mp = 127–129 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.61 (d, J = 7.5 Hz, 2H), 7.46 (bt, J = 7.5 Hz, 3H), 7.41 (d, J = 7.5 Hz, 2H), 7.39–7.28 (m, 5H), 7.27–7.23 (m, 1H), 7.19 (t, J = 7.5 Hz, 2H), 6.53 (s, 1H), 4.51 (s, 2H), 3.28 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.4, 137.4, 133.1, 131.7, 131.4, 131.2, 128.9, 128.8, 128.7, 128.6, 128.2, 122.7, 121.8, 118.8, 89.8, 86.5, 82.4, 79.7, 42.0, 40.1; IR (Neat)ν_{max} 1721, 1340, 1282, 1149, 1112, 1282, 1149, 1057, 961, 753 cm^{-1}; HRMS (ESI) for $C_{27}H_{21}NNaO_4S$ $(M+Na)^+$: calcd 478.1089, found 478.1113.

(*E*)-1-(4-Chloro-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (4s):



Following the general procedure GP–4, compound **4s** (157 mg) was obtained in 95% yield as colorless solid; mp = 132–134 °C; R_f = 0.39 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, J = 8.5 Hz, 2H), 7.65–7.60 (m, 2H), 7.52–7.47 (m, 1H), 7.46–7.42 (m, 2H), 7.41–7.37 (m, 2H), 7.38–7.31 (m, 5H), 7.23–7.18 (m, 1H), 7.16–7.09 (m, 4H), 6.57 (s,1H), 4.52 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.0, 139.8, 137.8, 137.0, 133.0, 131.6, 131.4, 131.1, 130.2, 128.90, 128.85, 128.71, 128.66, 128.5, 128.1, 123.6, 121.9, 118.9, 89.4, 86.4, 81.8, 79.7, 40.3; IR (Neat)ν_{max} 2225, 1731, 1358, 1164, 1107, 1050, 757 cm^{-1}; HRMS (ESI) for $C_{32}H_{22}ClNNaO_4S$ $(M+Na)^+$: calcd 574.0856, found 574.0857.

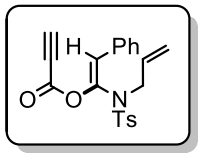
(*E*)-1-(4-methyl-N-(3-phenylprop-2-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-(thiophen-2-yl)propiolate (4t):



Following the general procedure GP–4, compound **4t** (150 mg) was obtained in 91% yield as colorless solid; mp = 138–140 °C; R_f = 0.38 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, J = 5.0 Hz, 2H), 7.65 (bs, 2H),7.53 (s, 1H), 7.47–6.98 (m, 12H), 6.56 (s, 1H), 4.48 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.0, 144.1, 137.3, 137.0, 136.2, 131.8, 131.5, 129.3,

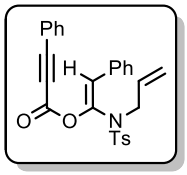
128.9, 128.63, 128.59, 128.2, 127.8, 127.7, 123.2, 122.1, 118.8, 86.0, 84.2, 83.1, 82.0, 40.0, 21.4; IR (Neat)ν_{max} 1678, 1414, 1299, 1260, 849, 747, 547 cm^{-1}; HRMS (ESI) for $C_{31}H_{23}NNaO_4S_2$ $(M+Na)^+$: calcd 560.0966, found 560.0966.

(*E*)-1-(N-Allyl-4-methylphenylsulfonamido)-2-phenylvinyl propiolate (6a):



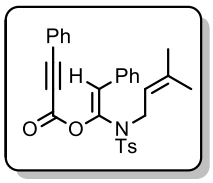
Following the general procedure GP–3, compound **6a** (101 mg) was obtained in 89%yield as colorless solid; mp = 121–123 °C; R_f = 0.39 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.80 (d, J = 10.2 Hz, 2H), 7.53 (d, J = 9.0 Hz, 2H), 7.30 (bs, 5H), 6.47 (s, 1H), 5.59 (s, 1H), 5.08–4.90 (m, 2H), 3.90 (s, 2H), 3.04 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.9, 144.2, 137.0, 136.1, 131.5, 131.3, 129.6, 128.9, 128.7, 128.5, 128.2, 122.8, 120.0, 77.3, 73.8, 52.2, 21.6; IR (Neat)ν_{max} 2118, 1729, 1347, 1189, 1157, 1015, 935, 758, 687 cm^{-1}; HRMS (ESI) for $C_{21}H_{20}NO_4S$ $(M+H)^+$: calcd 382.1113, found 382.1110.

(*E*)-1-(N-Allyl-4-methylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (6b):



Following the general procedure GP–4, compound **6b** (125 mg) was obtained in 91% yield as pale yellow solid; mp = 141–143 °C; R_f = 0.40 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.85 (d, J = 6.6 Hz, 2H), 7.62–7.56 (m, 4H), 7.54–7.50 (m, 1H), 7.45–7.41 (m, 2H), 7.38–7.34 (m, 2H), 7.32–7.26 (m, 3H), 6.52 (s, 1H), 5.70–5.60 (m, 1H), 5.10 (dd, J = 16.8, 0.6 Hz, 1H), 5.03 (d, J = 9.6 Hz, 1H), 3.95 (d, J = 7.2 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.2, 144.0, 137.3, 136.3, 133.1, 131.7, 131.5, 131.2, 129.63, 129.56, 129.47, 129.40, 128.9, 128.8, 128.7, 128.5, 128.2, 122.3, 119.1, 89.0, 79.7, 52.4, 21.5; IR (Neat)ν_{max} 1704, 1337, 1159, 1121, 1055, 811, 752, 589 cm^{-1}; HRMS (ESI) for $C_{27}H_{23}NNaO_4S$ $(M+Na)^+$: calcd 480.1245, found 480.1246.

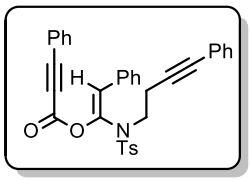
(*E*)-1-(4-methyl-N-(3-methylbut-2-en-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (6c):



Following the general procedure GP–4, compound **6c** (127 mg) was obtained in 87% yield as colorless solid; mp = 140–142 °C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, J = 8.5 Hz, 2H), 7.62–7.54 (m, 4H), 7.53–7.48 (m, 1H), 7.45–7.40 (m, 2H),

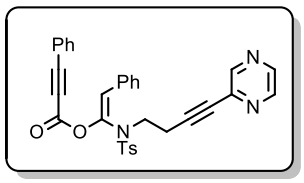
7.37–7.32 (m, 2H), 7.31–7.24 (m, 3H), 6.51 (s, 1H), 5.10–4.90 (m, 1H), 3.96 (d, J = 7.5 Hz, 2H), 2.32 (s, 3H), 1.50 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 143.8, 138.4, 137.6, 136.5, 133.1, 132.1, 131.1, 129.4, 128.9, 128.7, 128.4, 128.2, 122.5, 119.2, 117.5, 88.9, 79.8, 47.2, 25.6, 21.5, 17.7; IR (Neat)ν_{max} 1753, 1490, 1397, 1221, 1198, 1030, 756, 691 cm^{-1}; HRMS (ESI) for $C_{29}H_{28}NO_4S$ $(M+H)^+$: calcd 486.1739, found 486.1738.

(*E*)-1-(4-methyl-N-(4-phenylbut-3-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (6d):



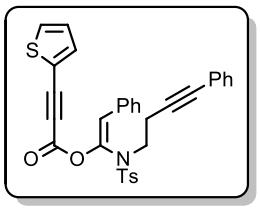
Following the general procedure GP–4, compound **6d** (153 mg) was obtained in 93% yield as colorless solid; mp = 136–138 °C; R_f = 0.49 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, J = 7.0 Hz, 2H), 7.68 (bd, J = 3.0 Hz, 2H), 7.59 (d, J = 7.5 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H), 7.45 (t, J = 7.5 Hz, 2H), 7.40–7.22 (m, 10H), 6.62 (s, 1H), 3.59 (s, 2H), 2.65 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.4, 144.2, 136.6, 136.0, 133.1, 131.6, 131.5, 131.2, 129.6, 129.0, 128.8, 128.7, 128.6, 128.2, 128.1,127.8, 123.6, 123.2, 119.0, 89.3, 85.9, 82.3, 79.6, 48.0, 21.4, 19.3; IR (Neat)ν_{max} 1721, 1358, 1144, 1103, 1012, 755, 684 cm^{-1}; HRMS (ESI) for $C_{34}H_{28}NO_4S$ $(M+H)^+$: calcd 546.1739, found 546.1739.

(*E*)-1-(4-Methyl-N-(4-(pyrazin-2-yl)but-3-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (6e):



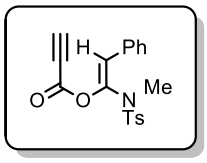
Following the general procedure GP–4, compound **6e** (153 mg) was obtained in 93% yield as colorless solid; mp = 149–151 °C; R_f = 0.32 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54–8.39 (m, 3H), 7.88 (d, J = 8.0 Hz, 2H), 7.68–7.27 (m, 12H), 6.58 (s, 1H), 3.57 (t, J = 6.8 Hz, 2H), 2.67 (t, J = 7.2 Hz, 2H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 147.6, 144.3, 144.1, 142.7, 140.0, 136.5, 135.7, 133.1, 131.28, 131.25, 129.7, 129.0, 128.9, 128.7, 128.6, 128.2, 123.8, 118.9, 90.9, 89.4, 79.5, 79.1, 47.5, 21.5, 19.4; IR (Neat)ν_{max} 2220, 1731, 1353, 1142, 1086, 1013, 687, 544 cm^{-1}; HRMS (ESI) for $C_{32}H_{26}N_3O_4S$ $(M+H)^+$: calcd 548.1644, found 548.1648.

(*E*)-1-(4-methyl-N-(4-phenylbut-3-yn-1-yl)phenylsulfonamido)-2-phenylvinyl 3-(thiophen-2-yl)propiolate(6f):



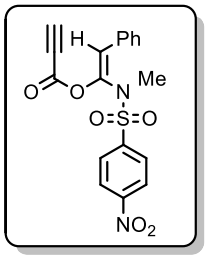
Following the general procedure GP–4, compound **6f** (141 mg) was obtained in 85% yield as colorless solid; mp = 138–140 °C; R_f = 0.38 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.92 (d, J = 8.5 Hz, 2H), 7.69 (d, J = 7.5 Hz, 2H), 7.55 (dd, J = 16.0, 5.0 Hz, 2H), 7.40–7.25 (m, 10H), 7.12 (t, J = 4.5 Hz, 1H), 6.62 (s, 1H), 3.59 (t, J = 7.5 Hz, 2H), 2.64 (t, J = 7.5 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 144.2, 137.2, 136.4, 135.8, 132.1, 131.5, 131.3, 129.6, 128.9, 128.7, 128.5, 128.1, 128.0, 127.8, 123.6, 123.1, 118.6, 85.8, 83.9, 83.4, 82.2, 47.9, 21.4, 19.2; IR (Neat)ν_{max} 1739, 1491, 1324, 1154, 1089, 1047, 814, 717, 663 cm^{-1}; HRMS (ESI) for $C_{32}H_{25}NNaO_4S_2$ $(M+Na)^+$: calcd 574.1123, found574.1113.

(*E*)-1-(N,4-Dimethylphenylsulfonamido)-2-phenylvinyl 3-phenylpropiolate (6g):



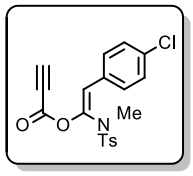
Following the general procedure GP–3, compound **6g** (109 mg) was obtained in 96% yield as colorless solid; mp = 120–122 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.79 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 7.8 Hz, 2H), 7.36 (t, J = 7.8 Hz, 2H), 7.33–7.28 (m, 3H), 6.31 (s, 1H), 3.03 (s, 1H), 2.99 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.5, 144.2, 139.0, 135.4, 131.2, 129.8, 128.7, 128.6, 127.8, 120.3, 77.4, 73.6, 36.3, 21.6; IR (Neat)ν_{max} 1730, 1349, 1320, 1158, 1105, 1012, 849, 682 cm^{-1}; HRMS (ESI) for $C_{19}H_{17}NNaO_4S$ $(M+Na)^+$: calcd 378.0776, found378.0779.

(*E*)-1-(N-Methyl-4-nitrophenylsulfonamido)-2-phenylvinyl propiolate (6h):



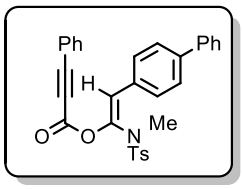
Following the general procedure GP–3, compound **6h** (112 mg) was obtained in 96% yield as colorless solid; mp = 132–134 °C; R_f = 0.38 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.33 (d, J = 8.4 Hz, 2H), 8.07 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 7.2 Hz, 2H), 7.37 (t, J = 6.6 Hz, 2H), 7.33 (d, J = 7.2 Hz, 1H), 6.38 (s, 1H), 3.08 (s, 3H), 3.07 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.3, 150.1, 144.0, 137.9, 130.7, 129.1, 128.8, 128.5, 124.3, 121.3 , 78.1, 73.1, 36.6; IR (Neat)ν_{max} 1742, 1693, 1527, 1347, 1308, 1104, 1080, 1014, 854, 683, 605 cm^{-1}; HRMS (ESI) for $C_{18}H_{15}N_2O_6S$ $(M+H)^+$: calcd 387.0651, found 387.0647.

(*E*)-2-(4-Chlorophenyl)-1-(N,4-dimethylphenylsulfonamido)vinyl propiolate (6i):



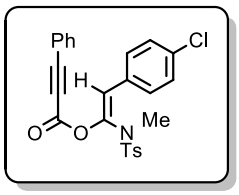
Following the general procedure GP–3, compound **6i** (108 mg) was obtained in 93% yield as colorless solid; mp = 122–124 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.78 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.35–7.29 (m, 4H), 6.27 (s, 1H), 3.02 (s, 1H), 2.98 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.4, 144.3, 139.4, 135.2, 134.5, 129.84, 129.80, 128.94, 127.86, 119.4, 77.5, 73.5, 36.2, 21.6; IR (Neat)ν_{max} 2912, 1713, 1570, 1445, 1337, 1235, 1162, 888, 694 cm^{-1}; HRMS (ESI) for $C_{19}H_{16}ClNNaO_4S$ $(M+Na)^+$: calcd 412.0386, found 412.0381.

(*E*)-2-([1,1'-Biphenyl]-4-yl)-1-(N,4-dimethylphenylsulfonamido)vinyl 3-phenylpropiolate (6j):



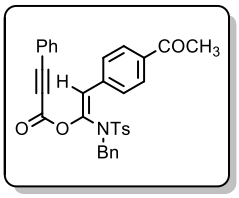
Following the general procedure GP–4, compound **6j** (143 mg) was obtained in 94% yield as colorless solid; mp = 124–126 °C; R_f = 0.48 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.85 (d, J = 7.2 Hz, 2H),7.67–7.58 (m, 8H), 7.53 (bt, J = 7.2 Hz, 1H), 7.49–7.42 (m, 4H), 7.37 (bt, J = 7.2 Hz, 1H), 7.29–7.24 (m, 1H), 6.38 (s, 1H), 3.10 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.8, 144.0, 141.2, 140.3, 139.3, 135.6, 133.1, 131.3, 130.4, 129.7, 129.1, 128.83, 128.77, 127.9, 127.6, 127.3, 127.0, 119.7, 119.0, 89.2, 79.6, 36.6, 21.5; IR (Neat)ν_{max} 1709, 1594, 1349, 1159, 1085, 1017, 813, 692, 582 cm^{-1}; HRMS (ESI) for $C_{31}H_{25}NNaO_4S$ $(M+Na)^+$: calcd 530.1402, found 530.1407.

(*E*)-2-(4-Chlorophenyl)-1-(N,4-dimethylphenylsulfonamido)vinyl 3-phenylpropiolate (6k):



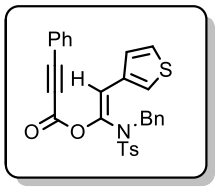
Following the general procedure GP–4, compound **6k** (130 mg) was obtained in 93% yield as colorless solid; mp = 128–130 °C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.82 (d, J = 8.4 Hz, 2H), 7.58 (d, J = 7.2 Hz, 2H), 7.55–7.48 (m, 3H), 7.44 (t, J = 7.8 Hz, 2H), 7.36–7.33 (m, 2H), 7.27 (d, J = 8.4 Hz, 2H), 6.30 (s, 1H), 3.03 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.7, 144.2, 139.7, 135.4, 134.4, 133.2, 131.3, 130.0, 129.9, 129.7, 128.9, 128.8, 127.9, 118.9, 89.4, 79.4, 36.4, 21.5; IR (Neat)ν_{max} 1727, 1355, 1157, 1111, 1086, 812, 750, 653 588 cm^{-1}; HRMS (ESI) for $C_{25}H_{20}ClNNaO_4S$ $(M+Na)^+$: calcd 488.0699, found 488.0694.

(*E*)-2-(4-Acetylphenyl)-1-(N-benzyl-4-methylphenylsulfonamido)vinyl 3-phenylpropiolate (6l):



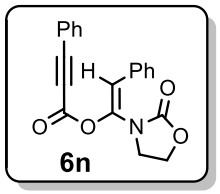
Following the general procedure GP–4, compound **6l** (155 mg) was obtained in 92% yield as colorless solid; mp = 130–132 °C; R_f = 0.4 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.83 (d, J = 7.8 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.61–7.50 (m, 3H), 7.46–7.37 (m, 4H), 7.29 (d, J = 7.8 Hz, 2H), 7.17–7.06 (m, 5H), 6.51 (s, 1H), 4.40 (s, 2H), 2.59 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.6, 150.9, 144.2, 138.3,136.6, 136.3, 135.9, 133.6, 133.1, 131.3, 129.7, 129.6, 128.80, 128.75, 128.3, 128.2, 128.1, 122.4, 119.0, 89.5, 79.5, 52.6, 26.6, 21.5; IR (Neat)ν_{max} 2219, 1728, 1701, 1348, 1161, 1103, 1044, 810, 709, 683cm^{-1}; HRMS (ESI) for $C_{33}H_{27}NNaO_5S$ $(M+Na)^+$: calcd 572.1508, found 572.1506.

(*E*)-1-(N-Benzyl-4-methylphenylsulfonamido)-2-(thiophen-3-yl)vinyl 3-phenylpropiolate (6m):



Following the general procedure GP–4, compound **6m** (134 mg) was obtained in 87% yield as colorless solid; mp = 131–133 °C; R_f = 0.36 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.87 (d, J = 8.4 Hz, 2H), 7.58–7.48 (m, 3H), 7.43 (t, J = 7.8 Hz, 2H), 7.36–7.28 (m, 3H), 7.23–7.09 (m, 7H), 6.54 (s, 1H), 4.44 (s, 2H), 2.36 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.0, 144.0, 136.0, 133.9, 133.1, 132.5, 131.2, 129.6, 128.7, 128.3, 128.1, 127.7, 126.0, 125.1, 119.1, 118.8, 89.0, 79.6, 52.4, 21.5; IR (Neat)ν_{max} 2226, 1717, 1350, 1277, 1165, 1150, 1106, 1077, 785, 685, 661 cm^{-1}; HRMS (ESI) for $C_{29}H_{23}NNaO_4S_2$ $(M+Na)^+$: calcd 536.0966, found 536.0960.

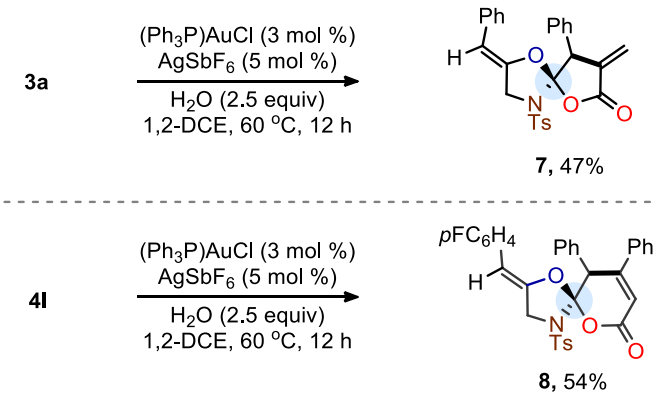
(*E*)-1-(2-Oxooxazolidin-3-yl)-2-phenylvinyl 3-phenylpropiolate (6n):



Following the general procedure GP–4, compound **6n** (106 mg) was obtained in 94% yield as pale yellow solid; mp = 126–128 °C; R_f = 0.42 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.63 (dd, J = 8.4, 2.4 Hz, 2H), 7.53–7.46 (m, 1H), 7.44–7.29 (m, 7H), 6.42 (s, 1H), 4.43–4.35 (m, 2H), 3.80–3.70 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.4, 152.0, 136.6, 133.3, 131.6, 131.2, 128.8, 128.7, 128.5, 128.2, 118.9, 117.4, 89.8, 79.5, 63.2, 44.3; IR (Neat)ν_{max} 2228,

1724, 1667, 1605, 1349, 1285, 1090, 1052, 653, 543 cm^{-1}; HRMS (ESI) for $C_{20}H_{15}NNaO_4S$ $(M+Na)^+$: calcd 356.0899, found 356.0896.

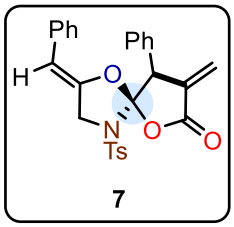
Au(I)-Catalyzed Spiro-Heterobicyclization; synthesis of 7 /8: General Procedure 5



General Procedure 5A: A solution of $[Au(PPh_3)]SbF_6$ in 1,2-DCE was prepared as following: $AuCl(PPh_3)$ (3 mol%) was dissolved in 1,2-DCE (3 mL). The solution was treated with $AgSbF_6$ (5 mol%) and stirred for 10 min. AgCl precipitation formed gradually and the supernatant was used for the following reactions.

General Procedure 5B: To a solution of **3a/4l** (1 equiv.) in 1,2-DCE was added water (2.5 equiv.) followed by $[Au(PPh_3)]SbF_6$ (3 mol%) (obtained from general procedure 5A). The resulting mixture was left to stir at 60 °C. The reaction mixture was monitored until TLC analysis indicated consumption of the starting material. The solution was filtered through a silica gel plug (1:1 hexanes:EtOAc), and the filtrate concentrated. The resulting residue was purified by flash column chromatography to afford the desired cyclized product **7**/**8**.

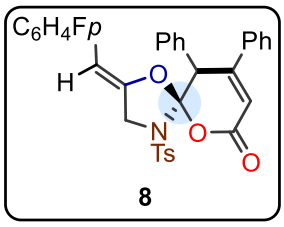
(5S,Z)-2-benzylidene-8-methylene-9-phenyl-4-tosyl-1,6-dioxa-4-azaspiro[4.4]nonan-7-one (7):



7

Compound **7** (94 mg, 47%) was obtained as colorless crystalline solid. Mp = 158–162 °C; R_f = 0.43 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): 7.84 (d, J = 8.4 Hz, 2H), 7.43–7.39 (m, 3H), 7.33–7.26 (m, 4H), 7.21–7.16 (m, 2H), 7.14–7.09 (m, 1H), 7.08–7.03 (m, 2H), 6.62 (d, J = 3.6 Hz, 1H), 5.70 (d, J = 3.2 Hz, 1H), 5.57 (t, J = 3.4 Hz, 1H), 5.14 (s, 1H), 4.27 (dd, J = 12.4, 1.2 Hz, 1H), 4.10 (dd, J = 12.4, 2 Hz, 1H), 2.47 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 165.8, 145.3, 143.6, 136.5, 133.4, 133.3, 133.1, 130.2, 129.9, 128.8, 128.6, 128.4, 128.0, 127.8, 126.4, 125.3, 117.6, 101.0, 54.0, 49.4, 29.7, 21.6; IR (Neat)ν_{max} 1723, 1597, 1503, 1151, 1052, 832, 613 cm^{-1}; HRMS (ESI) for $C_{27}H_{24}NO_5S$ $(M+H)^+$: calcd 474.1370, found 474.1334.

(5S,Z)-2-(4-fluorobenzylidene)-9,10-diphenyl-4-tosyl-1,6-dioxa-4-azaspiro[4.5]dec-8-en-7-one (8):



8

Compound **8** (113 mg, 54%) was obtained as colorless crystalline solid. Mp = 146-150 °C; R_f = 0.48 (3:2 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): 7.91 (d, J = 8.5, 2H), 7.41 (d, J = 8.0, 2H), 7.31–7.28 (m, 2H), 7.27–7.23 (m, 5H), 7.22–7.18 (m, 2H), 7.15–7.05 (m, 3H), 6.95 (br t, J = 8.8, 2H), 6.51 (d, J = 2.0, 1H), 5.79 (d, J = 2.5, 1H), 5.04 (s, 1H), 4.11 (dd, J = 12.5, 1.5 Hz, 1H), 3.96 (dd, J = 12.5, 1.0 Hz, 1H), 2.48 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 160.1 (d, J = 291 Hz, 1C), 145.1, 143.9 (d, J = 9.05 Hz, 1C), 136.2, 134.1, 133.4, 131.5, 129.8, 129.7, 129.23, 129.17, 128.9, 128.5, 128.0, 127.6, 127.4, 127.1, 116.5, 116.4, 115.1 (d, J = 85.1 Hz, 1C), 99.4, 51.0, 49.3, 21.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ –110.48; IR (Neat)ν_{max} 1731, 1504, 1360, 1107, 743, 724, 633 cm^{-1}; HRMS (ESI) for $C_{33}H_{27}FNO_5S$ $(M+H)^+$: calcd 568.1594, found 568.1594.

X-ray crystallography:

1. Single crystal X-ray data for the compound **3g** were collected using the 'Bruker D8 VENTURE Photon III detector' system [Mo-Kα fine focus sealed tube λ= 0.71073 Å] at 296K, 298K, and

294K graphite monochromator with a ω scan. Data reduction was performed using Bruker SAINT software. Intensities for absorption were corrected using SADABS 2014/5.Structure solution and refinement were carried out using Bruker SHELX-TL.

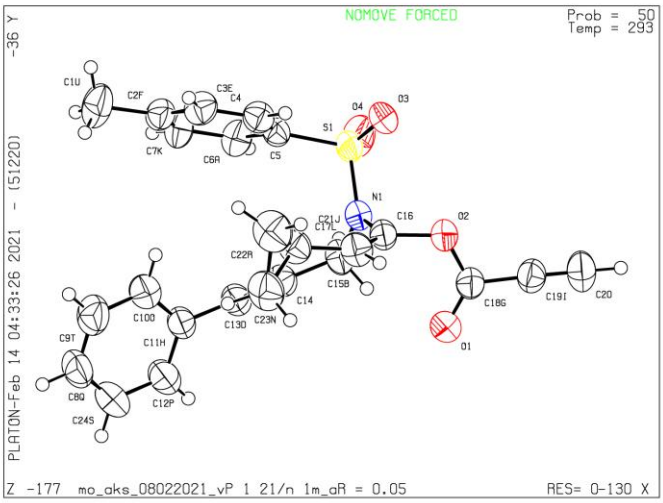


Figure S1. Molecular structure of compound **3g** (Oxygen (red), nitrogen (blue), and sulphur (yellow)

Compound	**3g**
formula	$C_{24}H_{21}NO_4S$
Formula weight	419.50
crystal system	Monoclinic
space group	P 1 21/n 1
T [K]	293 K
a [Å]	8.2335(3)
b [Å]	18.3922(8)
c [Å]	14.6378(6)
α [°]	90
β [°]	104.229(1)
γ [°]	90
V [Å^3]	2148.63(15)
Z	4

ρ_{calcd} [g cm^{-3}]	1.297
μ [mm^{-1}]	0.181
total reflns	5329
unique reflns	5318
observed	3710
R_1[I>2σ(I)]	0.0476
wR2 [all]	0.1404
GOF	1.056
Diffractometer	Bruker D8 VENTURE Photon IIIdetector
CCDC Number	2120261

Table S2. Crystallographic data for compound **3g**

2. Single crystal X-ray data for the compound **6b** were collected using the 'Bruker D8 VENTURE Photon III detector' system [Mo-Kα fine focus sealed tube λ= 0.71073 Å] at 296K, 298K, and 294K graphite monochromator with a ω scan. Data reduction was performed using Bruker SAINT software. Intensities for absorption were corrected using SADABS 2014/5.Structure solution and refinement were carried out using Bruker SHELX-TL.

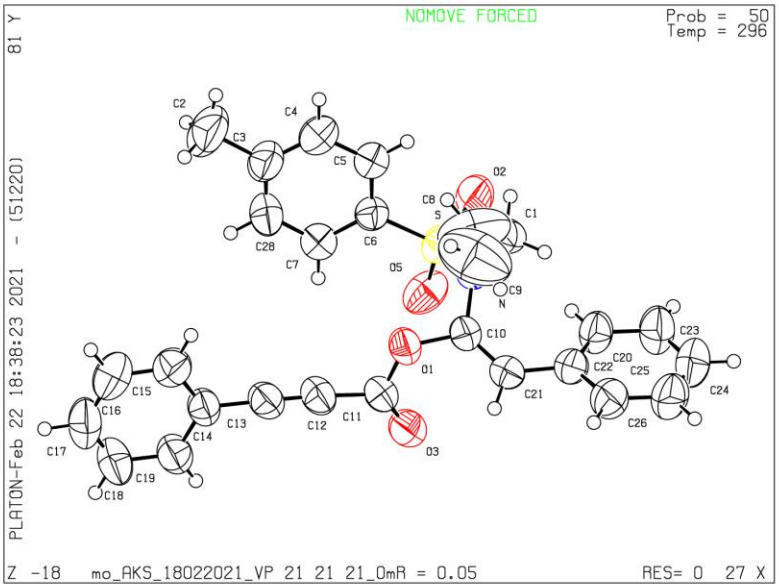


Figure S2. Molecular structure of compound **6b** (Oxygen (red), nitrogen (blue), and sulphur (yellow)

Compound	**6b**
formula	$C_{27}H_{23}NO_4S$
Formula weight	457.52
crystal system	Orthorhombic
space group	P 21 21 21
T [K]	296 K
a [Å]	8.793(3)
b [Å]	15.899(5)
c [Å]	17.594(6)
α [º]	90
β [º]	90
γ [º]	90
V [Å^3]	2459.6(14)
Z	4
ρ_{calcd} [g cm^{-3}]	1.236

μ [mm^{-1}]	0.164
total reflns	6130
unique reflns	6113
observed	3288
$R_1[I>2\sigma(I)]$	0.0462
wR2 [all]	0.1349
GOF	1.007
Diffractometer	Bruker D8 VENTURE Photon IIIdetector
CCDC Number	2120262

Table S3. Crystallographic data for compound **6b**

Hirshfeld Surface Analysis[3]

The Hirshfeld surface images (Fig. 1a & Fig. 1b) in which, the red spots signify the high contact populations, while blue and white spots are for low contact populations. This suggests that the negative (red) or positive value (blue and white) of d_{norm} depends on the intermolecular contacts being shorter (red) or longer (blue and white) than the van der Waals separations. For each point on the Hirshfeld surface, the normalized contact distance (d_{norm}) was determined by the equation as shown below.

$$[d_{norm}= (d_i – d_i^{vdW})/r_i^{vdW} + (d_e – d_e^{vdW}/r_e^{vdW}]$$

In which d_i is measured from the surface to the nearest atom interior to the surface interior, while d_e is measured from the surface to the nearest atom exterior to the surface interior, where r_i^{vdW} and r_e^{vdW} are the van der Waals radii of the atoms. Hirshfeld surface graphs and two-dimensional

fingerprint plots of **3g** and **6b** (Fig. S3 & Fig. S4) were analyzed using Crystalexplorer 17.5 software.

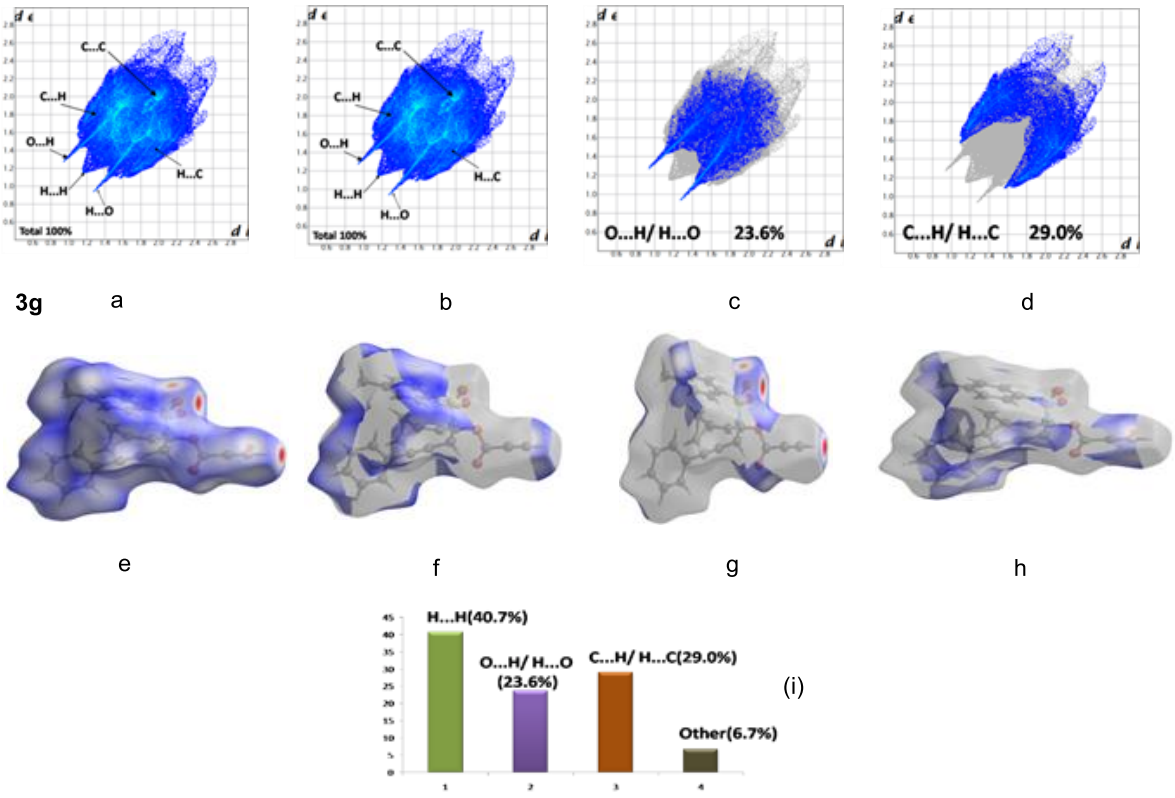


Figure S3: Hirshfeld surface calculations and 2D-fingerprint plots of compounds **3g**

Hirshfeld surface analysis indicated that H···H, H···C and H···O bond interactions are the primary contributors to the intermolecular stabilization in the crystal. The Hirshfeld surface and subsequent fingerprint plots were calculated for **3g** and **6b** individually, to quantify the intermolecular contacts present within the crystal structures of these compounds (Fig. S3 & Fig. S4). The X-ray single-crystal crystallographic information file of **3g** and **6b** were used as input files.

Significant intermolecular interactions are mapped in Fig. S3 & Fig. S4. On the Hirshfeld surfaces the H…H interactions appear as the largest region 40.7% for **3g** (Fig. S3) and 46.1% for **6b** (Fig. S4) of the fingerprint plot. Two sharp spikes on the fingerprint plot were observed for the O···H/H···O contacts, corresponding to the C···H···O interactions. These spikes are indicative of a strong hydrogen-bond interaction. The C···H/H···C contacts contribute to 29.0% for **3a** (Fig. S3) and 31.13% for **6b** (Fig. S4) of the Hirshfeld surface area.

All other contacts observed were found to contribute less than 6.7% (**3g)** and 1.2% (**6b**). It is therefore clear that the C···H/H···C, O···H/H···O and especially H···H contacts, were the most significant contributors among the interacting atoms. This finding therefore indicates the significance of these contacts in the packing arrangement of the crystal structure. Based on these findings a detailed model was constructed showing the most prominent short range intermolecular contacts that are responsible for the packing arrangement and formation of the three-dimensional network structure of **3g** and **6b** respectively (Fig. S3 & Fig. S4). 2-D column graphs (i) and (r) for **3g** and **6b** show the percentage contributions of the individual atomic contacts to the Hirshfeld surface.

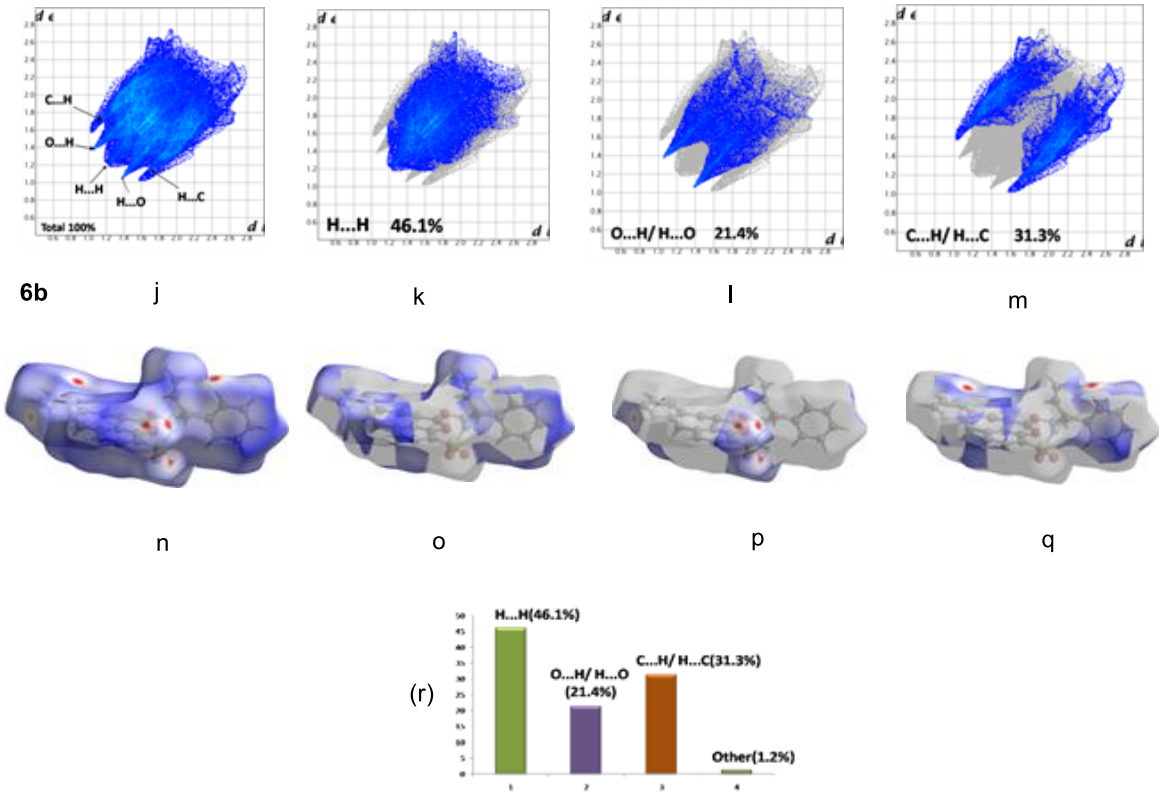


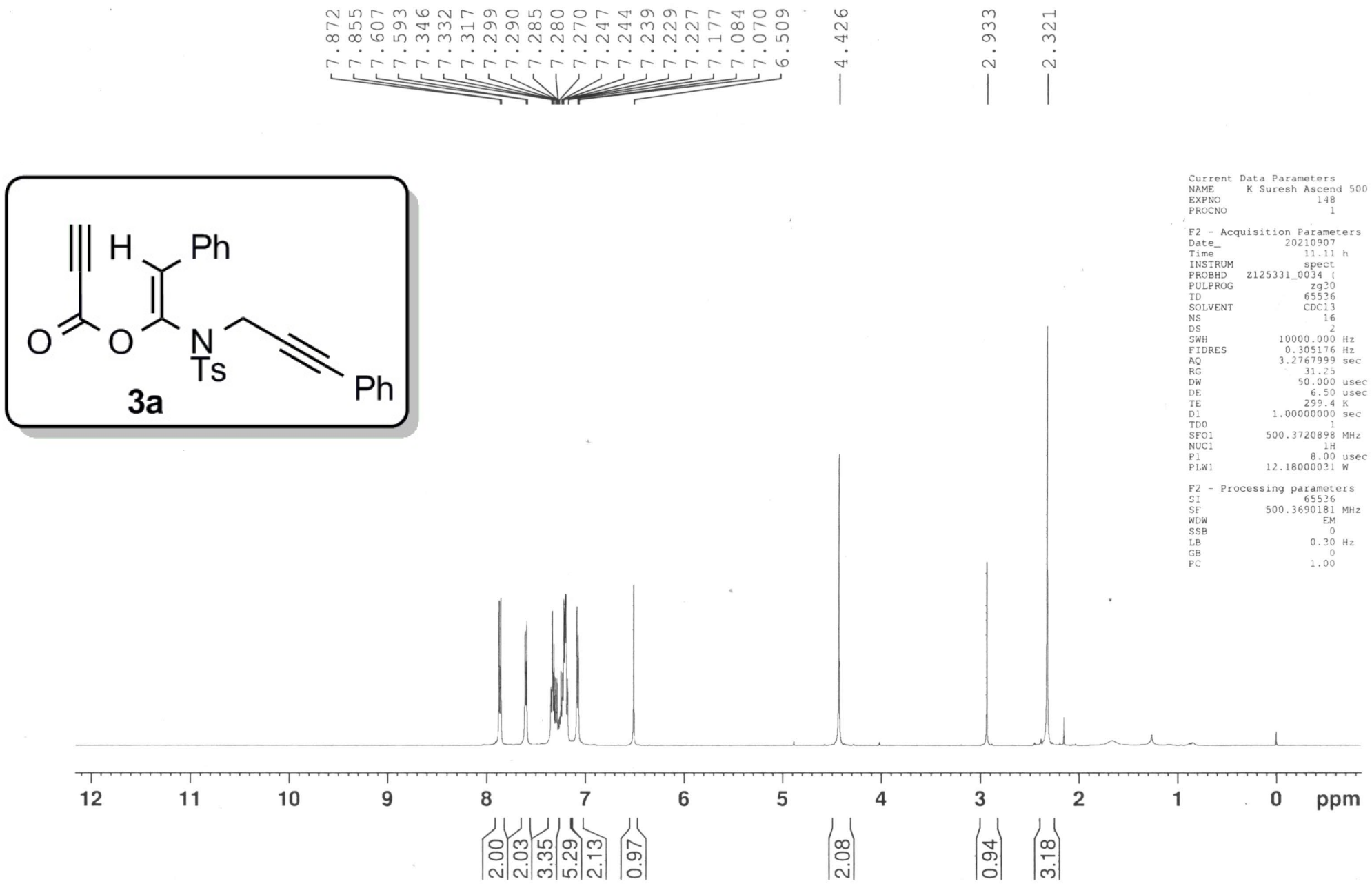
Figure S4: Hirshfeld surface calculations and 2D-fingerprint plots of compounds **6b.**

References

(1) (a) S. Dutta, R. K. Mallick, R. Prasad, V. Gandon, and A. K. Sahoo, *Angew. Chem. Int. Ed.*, 2019, **58,** 2289 –2294; (b) B. Prabagar, S. Nayak, R. K. Mallick, R. Prasad and A. K. Sahoo, *Org. Chem. Front.*, 2016, **3**, 110-115.

(2) (a) Hyun-Suk Yeom, Jaeyoung Koo, Hyun-Sub Park, Yi Wang, Yong Liang, Zhi-Xiang Yu, and Seunghoon Shin, *J. Am. Chem. Soc.*, 2012, **134,** 208–211; (b) Xia, Xiao-Feng; Zhao, Mingming; He, Wei; Zou, Lianghua; San, Xinxin; Wang, Dawei, *Advanced Synthesis & Catalysis*, 2020 **362,** 3621-3626.

(3) (a) M. A. Spackman, J. J. McKinnon, *CrystEngComm.*, 2002, **4,** 378–392; (b) M. A. Spackman, D. Jayatilake, Hirshfeld surface analysis, *CrystEngComm.* 2009, **11,** 19–32; (c) C. Zhang, X. Xue, Y. Cao, Y. Zhou, H. Li, J. Zhou, T. Gao, Intermolecular friction symbol derived from crystal information, *CrystEngComm.* 2013, **15,** 6837−6844; (d) M.J. Turner, J.J. McKinnon, S.K. Wolff, D.J. Grimwood, P.R. Spackman, D. Jayatilaka, M.A. Spackman, Crystal Explorer 17; University of Western Australia: Pert, Australia, 2017.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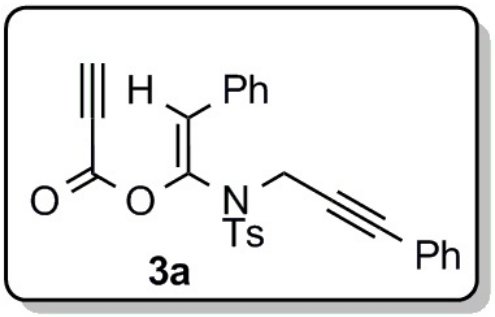

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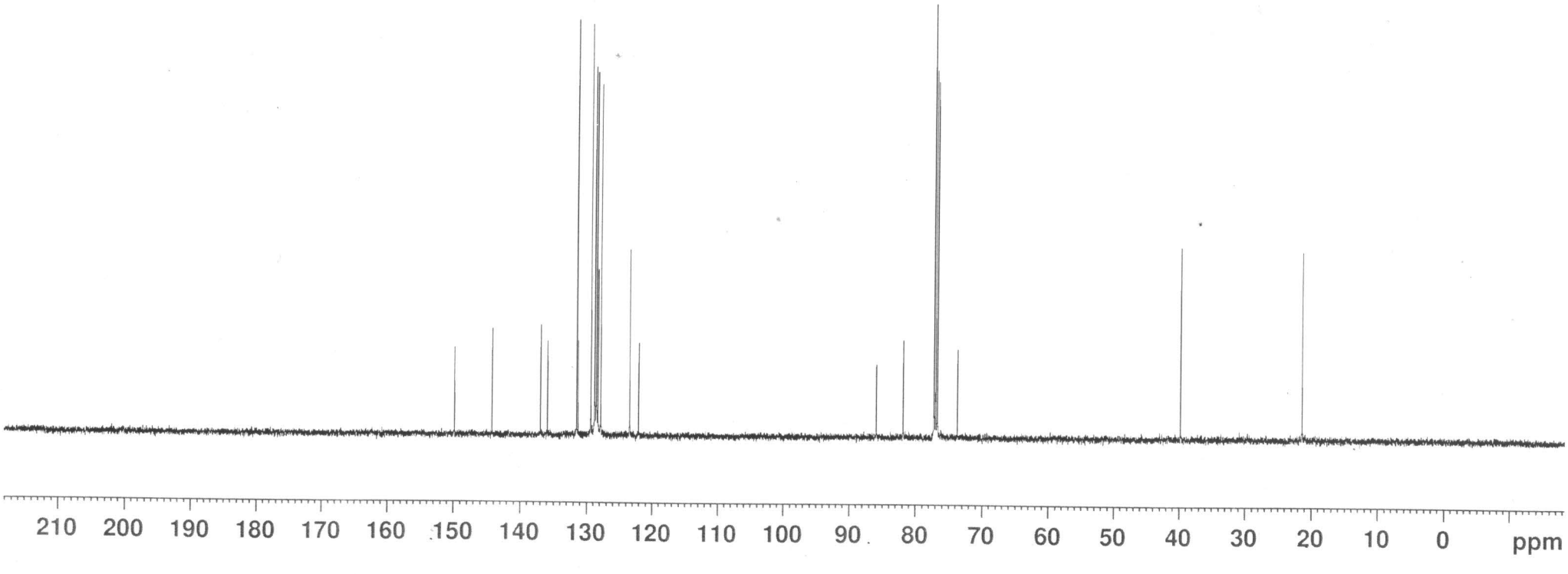

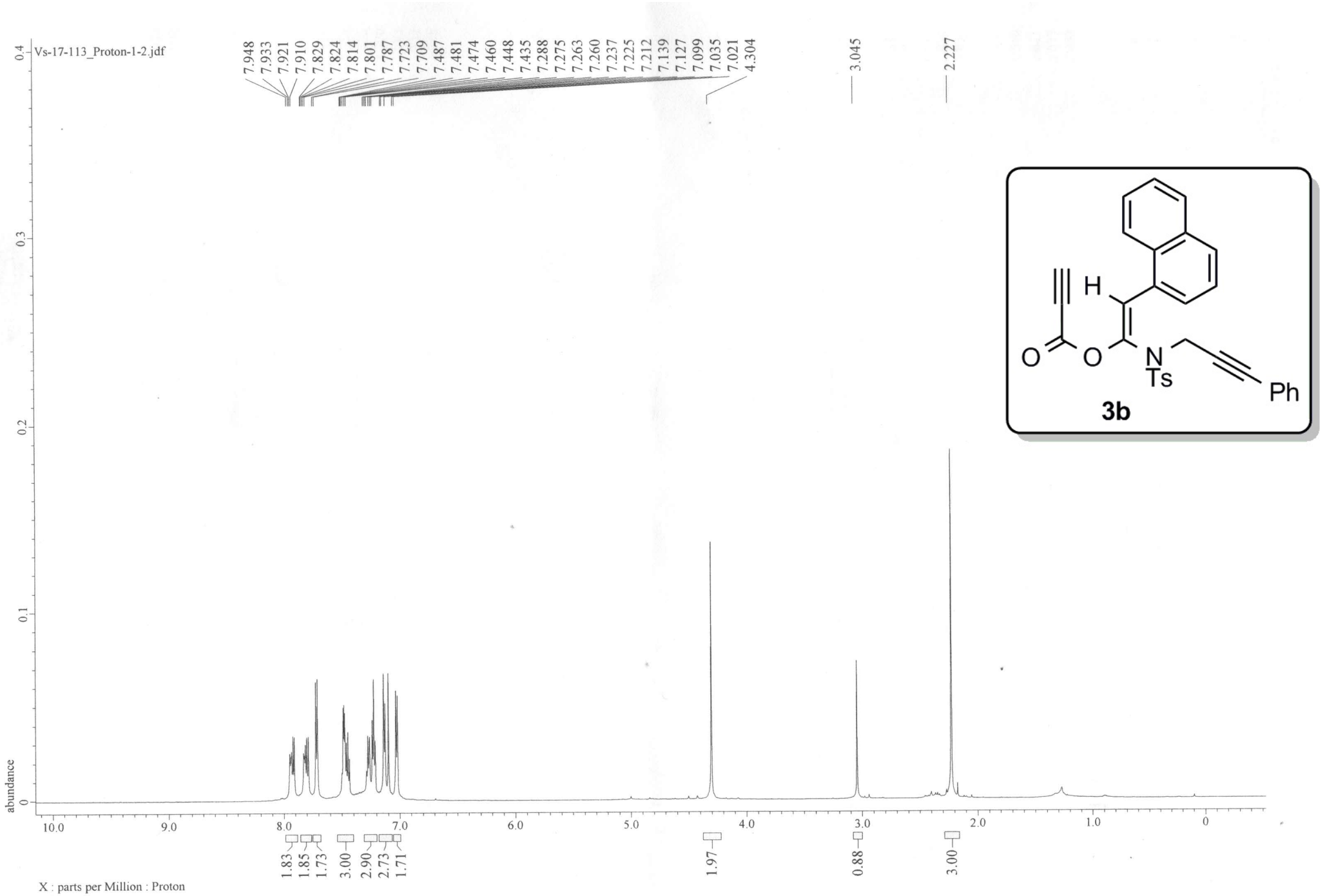
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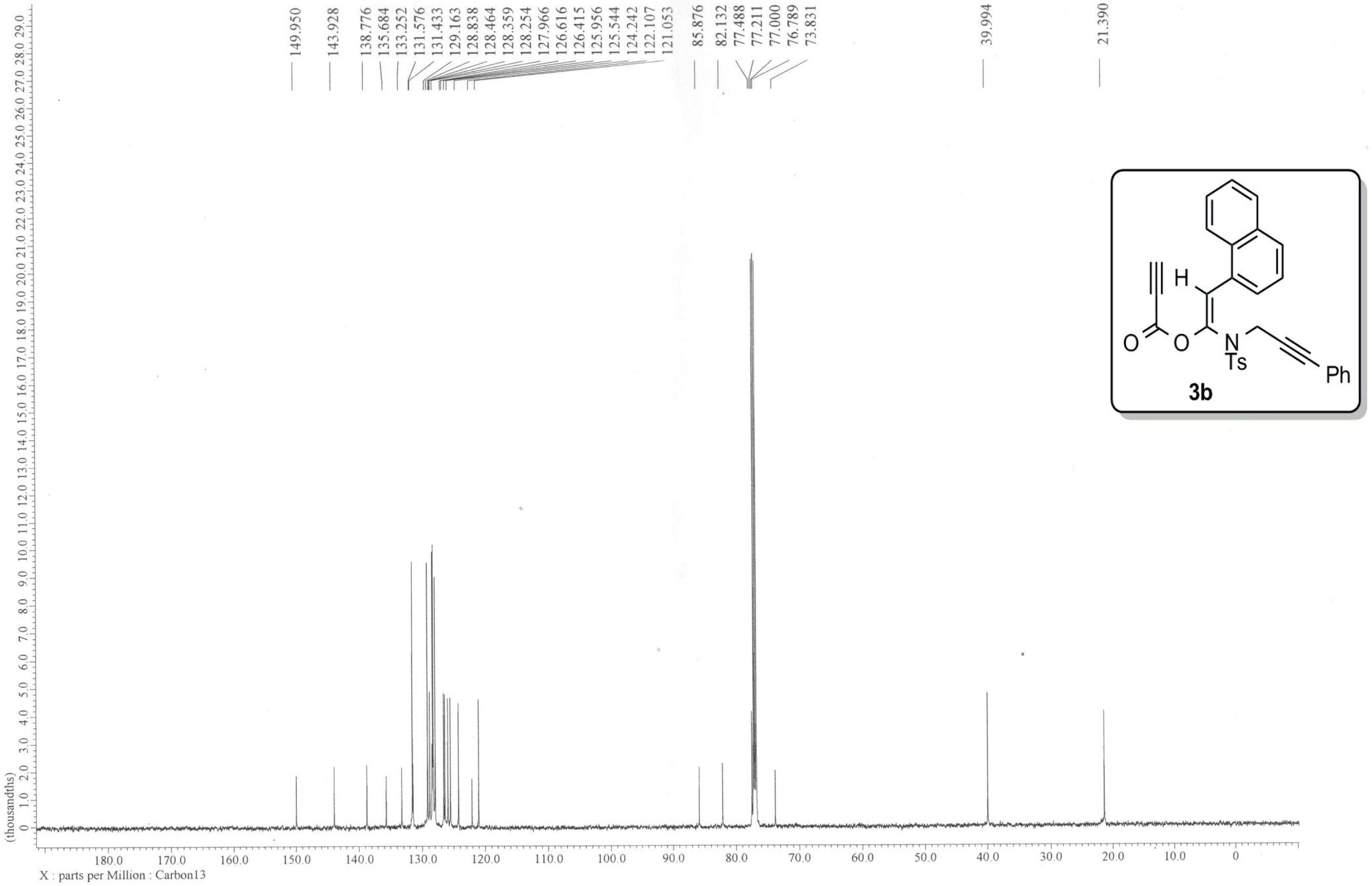
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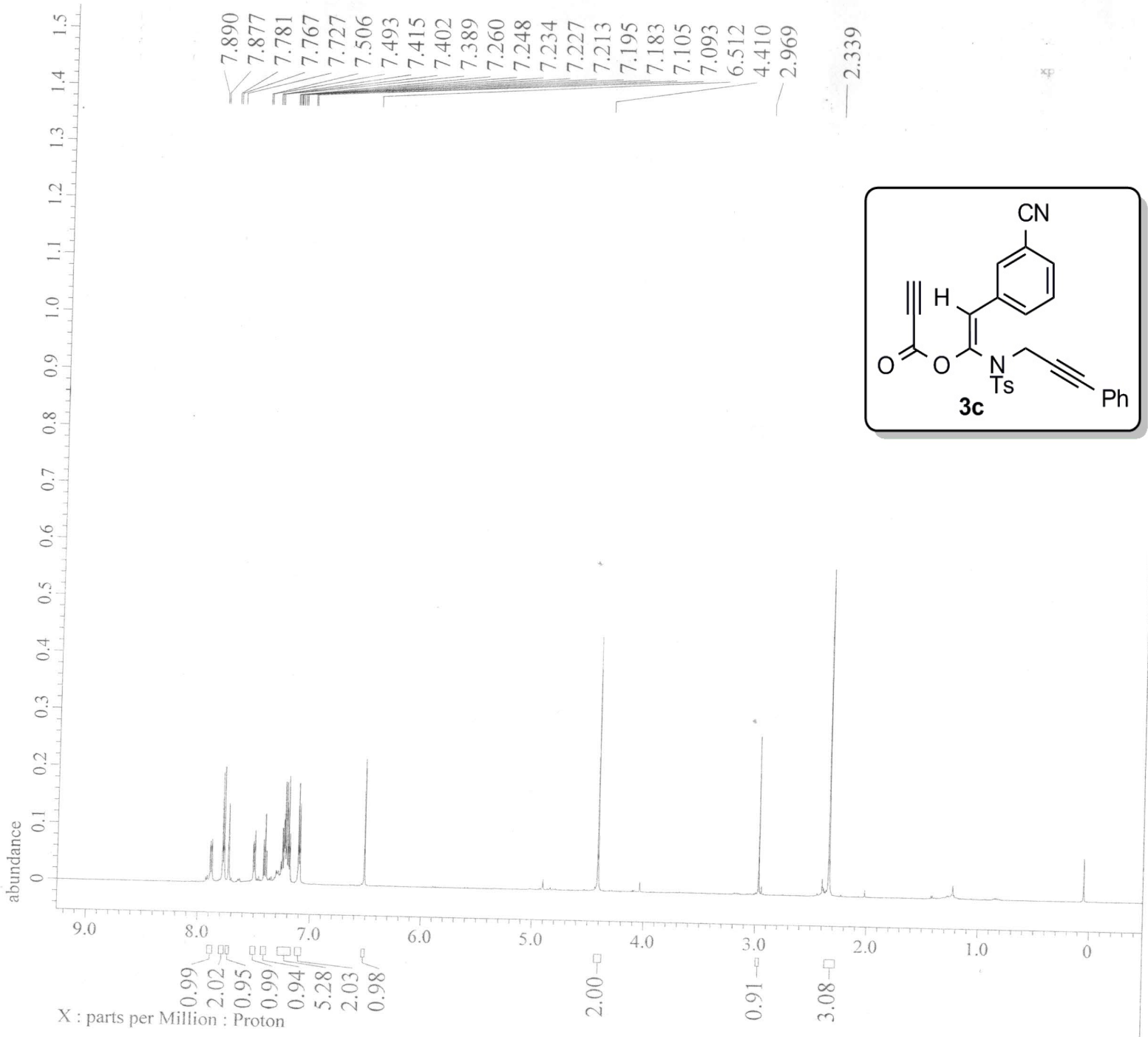

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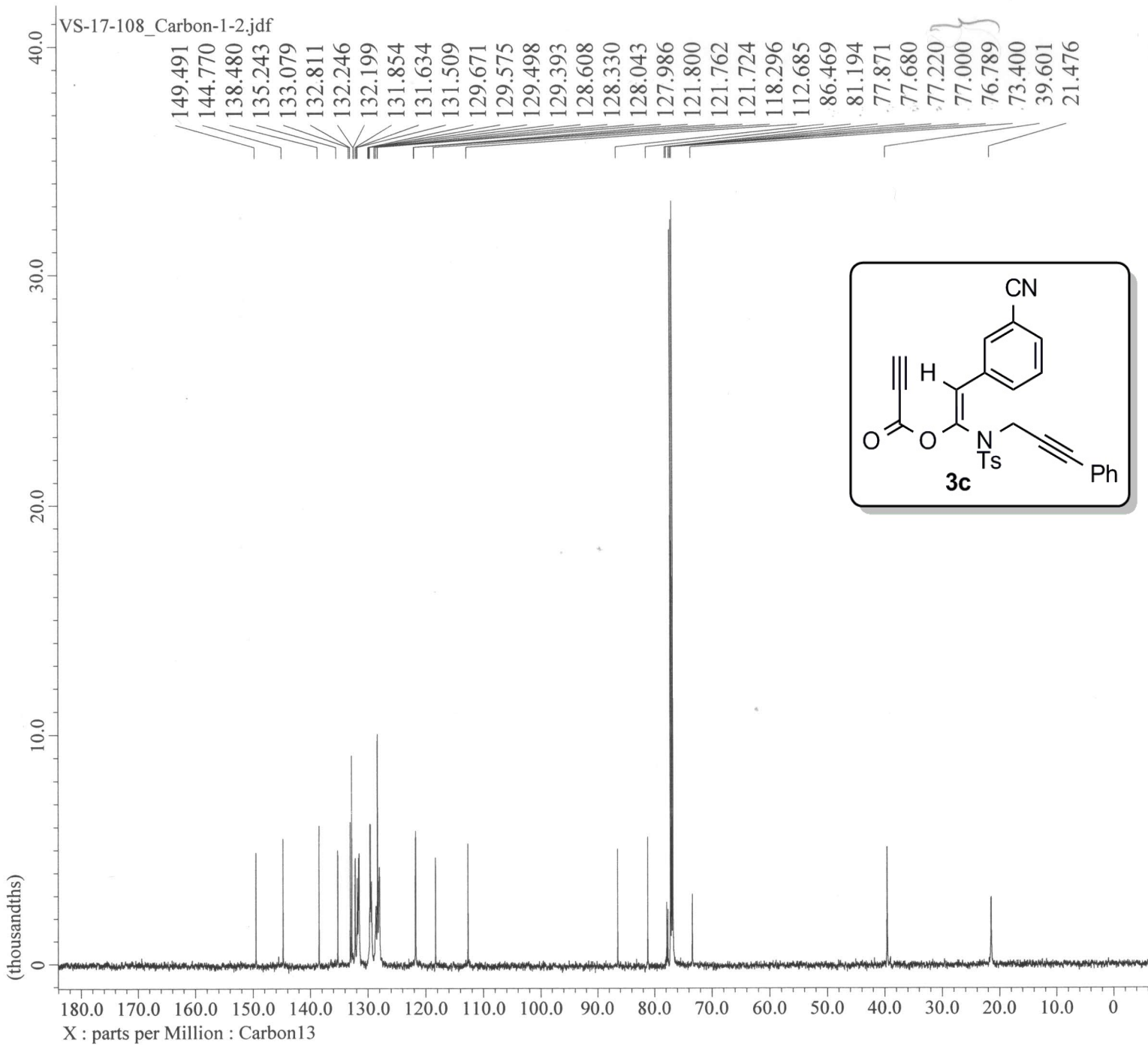

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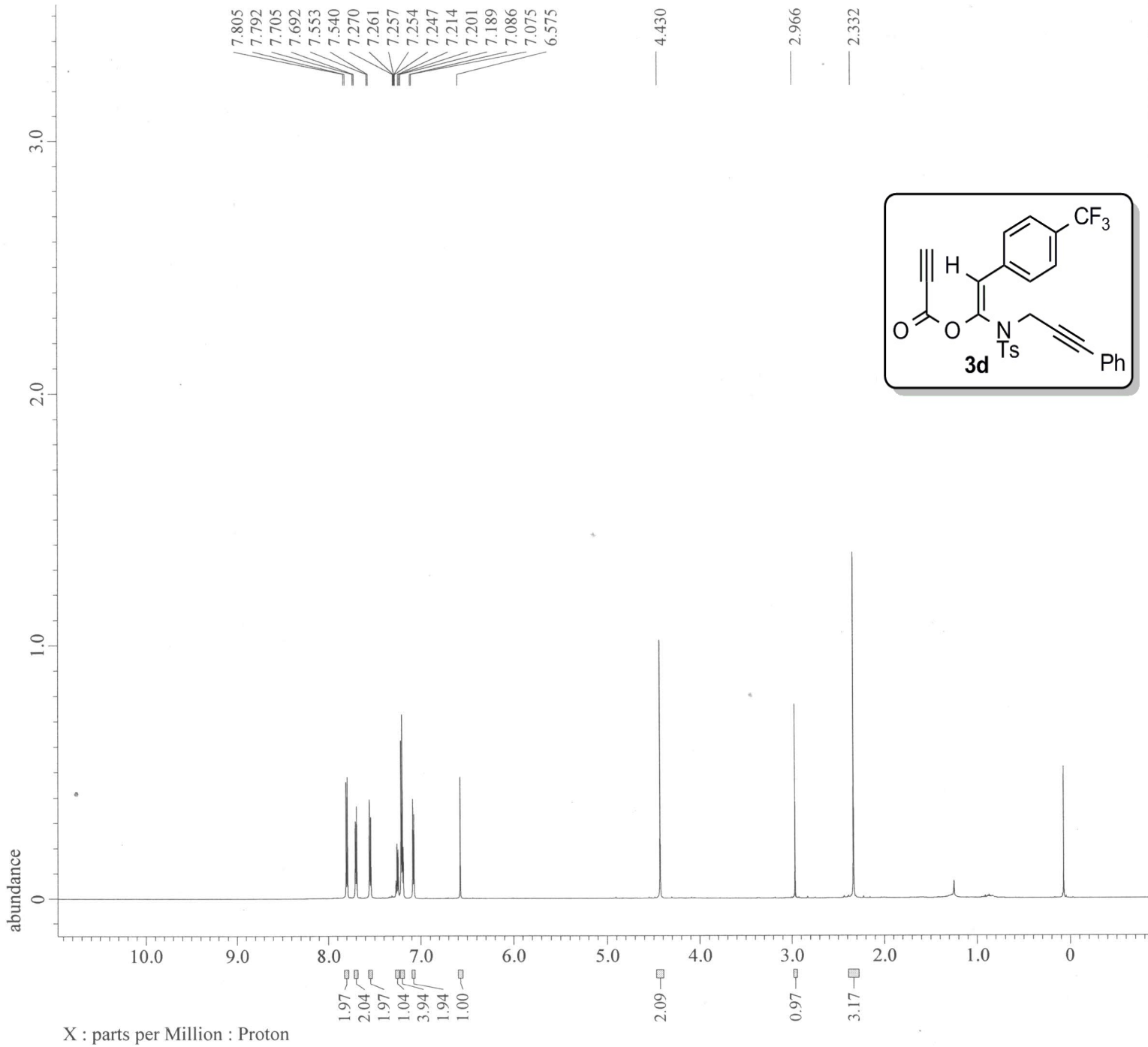
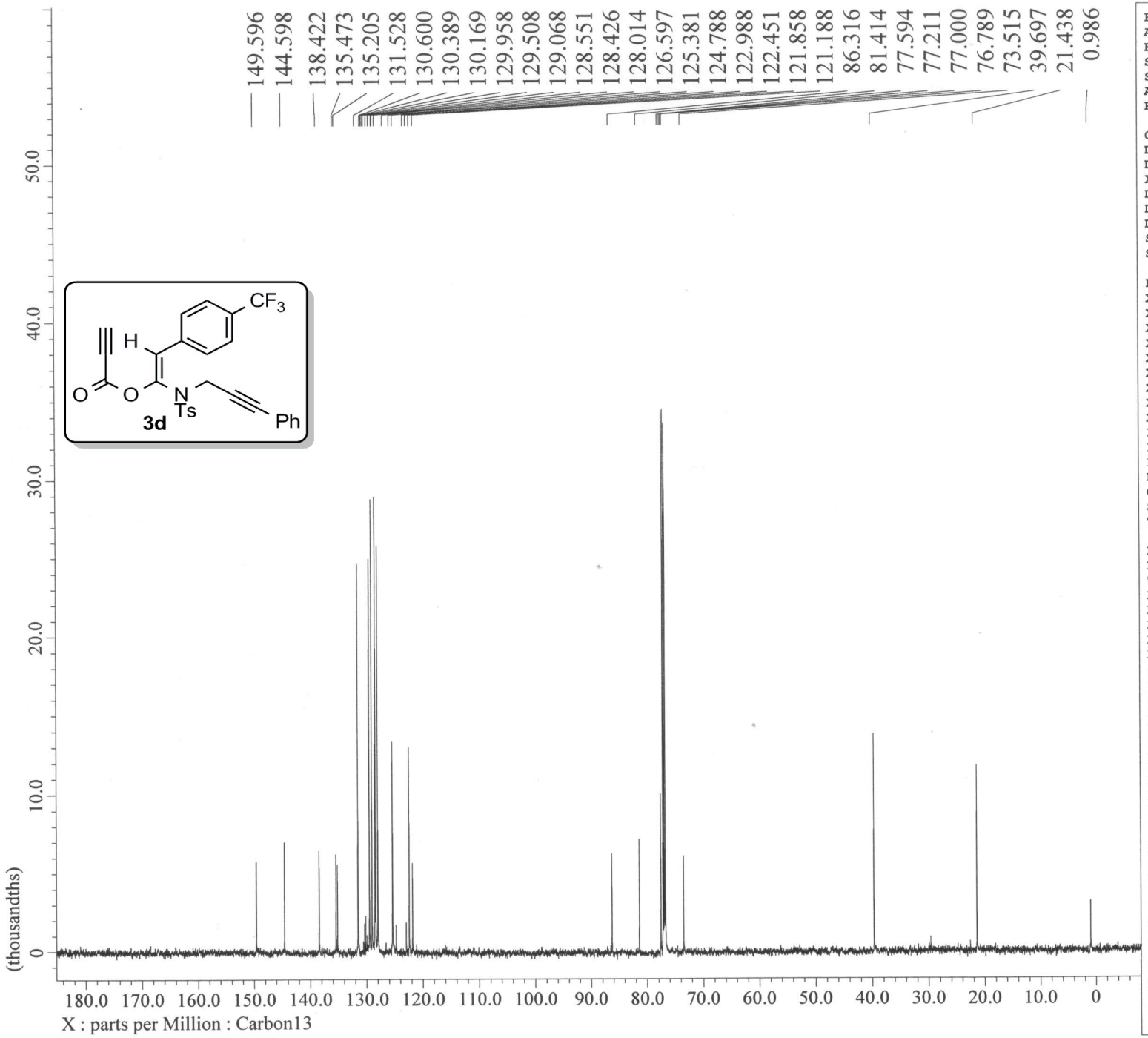
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]



JEOL

Filename	= vs-19-125_Proton-1-2.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= vs-19-125
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2021 11:44:53
Revision_Time	= 23-JAN-2021 21:19:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.9[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]

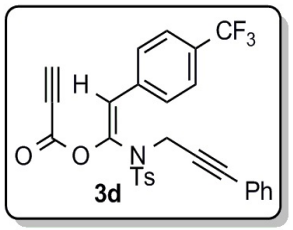



```
Filename                    = vs-19-125_Carbon-1
Author                      = delta
Experiment                  = carbon_auto.jxp
Sample_Id                   = vs-19-125
Solvent                     = CHLOROFORM-D
Actual_Start_Time           = 22-JAN-2021 11:47:
Revision_Time               = 16-JUL-2021 00:00:

Comment                     = single pulse decou
Data_Format                 = 1D COMPLEX
Dim_Size                    = 26214
X_Domain                    = Carbon13
Dim_Title                   = Carbon13
Dim_Units                   = [ppm]
Dimensions                  = X
Site                        = ACRHEM_UOH
Spectrometer                = JNM-ECZ600R/M1

Field_Strength              = 14.09636928[T] (60
X_Acq_Duration              = 0.34603008[s]
X_Domain                    = Carbon13
X_Freq                      = 150.91343039[MHz]
X_Offset                    = 100[ppm]
X_Points                    = 16384
X_Prescans                  = 4
X_Resolution                = 2.88992217[Hz]
X_Sweep                     = 47.34848485[kHz]
X_Sweep_Clipped             = 37.87878788[kHz]
Irr_Domain                  = Proton
Irr_Freq                    = 600.1723046[MHz]
Irr_Offset                  = 5[ppm]
Blanking                    = 2[us]
Clipped                     = FALSE
Scans                       = 256
Total_Scans                 = 256

Relaxation_Delay            = 2[s]
Recvr_Gain                  = 56
Temp_Get                    = 18.9[dC]
X_90_Width                  = 11[us]
X_Acq_Time                  = 0.34603008[s]
X_Angle                     = 30[deg]
X_Atn                       = 10.3[dB]
X_Pulse                     = 3.66666667[us]
Irr_Atn_Dec                 = 33.452[dB]
Irr_Atn_Dec_Calc            = 33.452[dB]
Irr_Atn_Dec_Default_Calc    = 33.452[dB]
Irr_Atn_Noe                 = 33.452[dB]
Irr_Dec_Bandwidth_Hz        = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm       = 12.05794078[ppm]
Irr_Dec_Freq                = 600.1723046[MHz]
Irr_Dec_Merit_Factor        = 2.2
Irr_Decoupling              = TRUE
Irr_Noe                     = TRUE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Temp1            = 76[us]
Irr_Wurst                   = FALSE
Decimation_Rate             = 0
Experiment_Path             = c:\Program Files\J
Initial_Wait                = 1[s]
Noe_Time                    = 2[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 2[s]
```

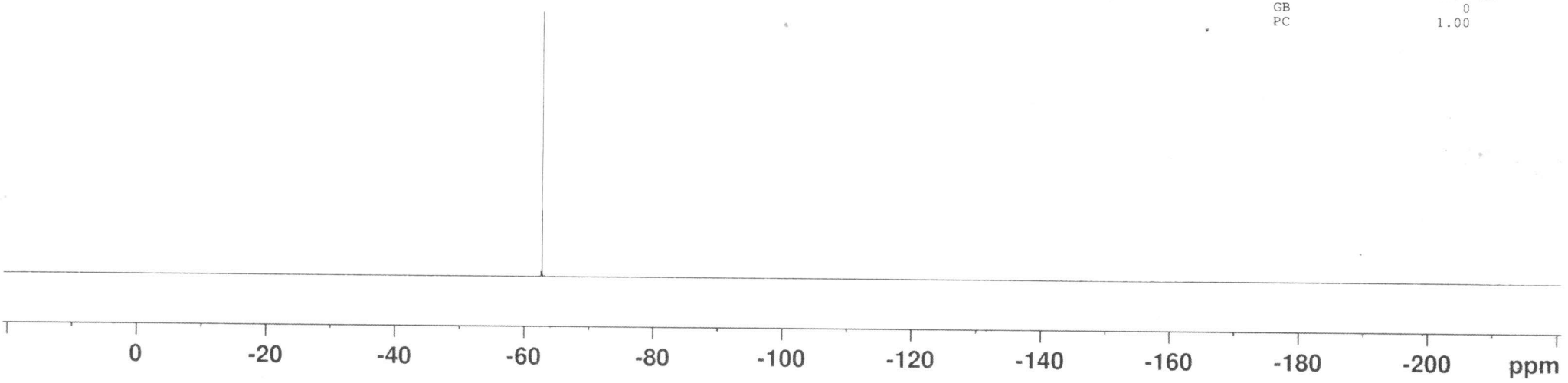


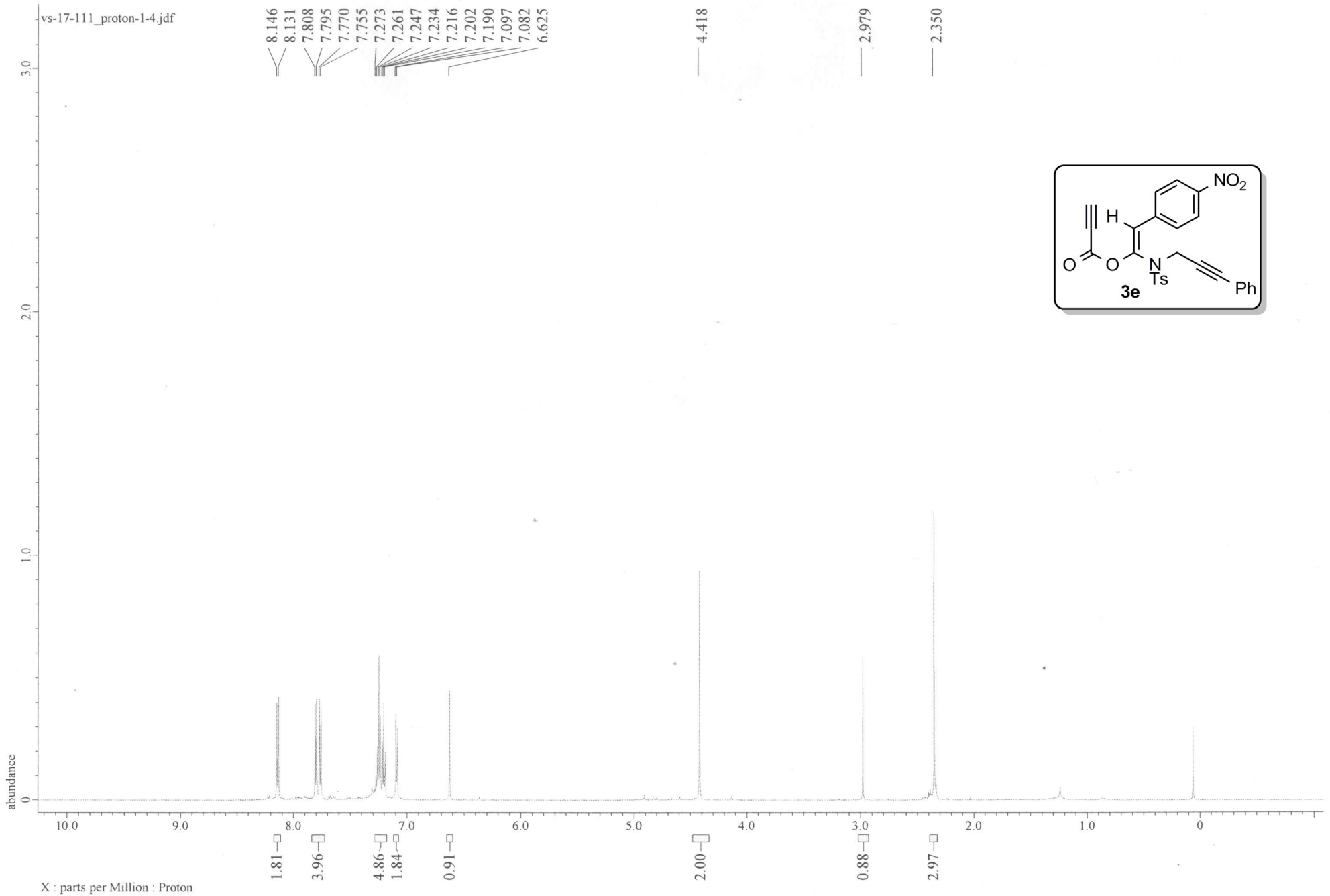
-62.69

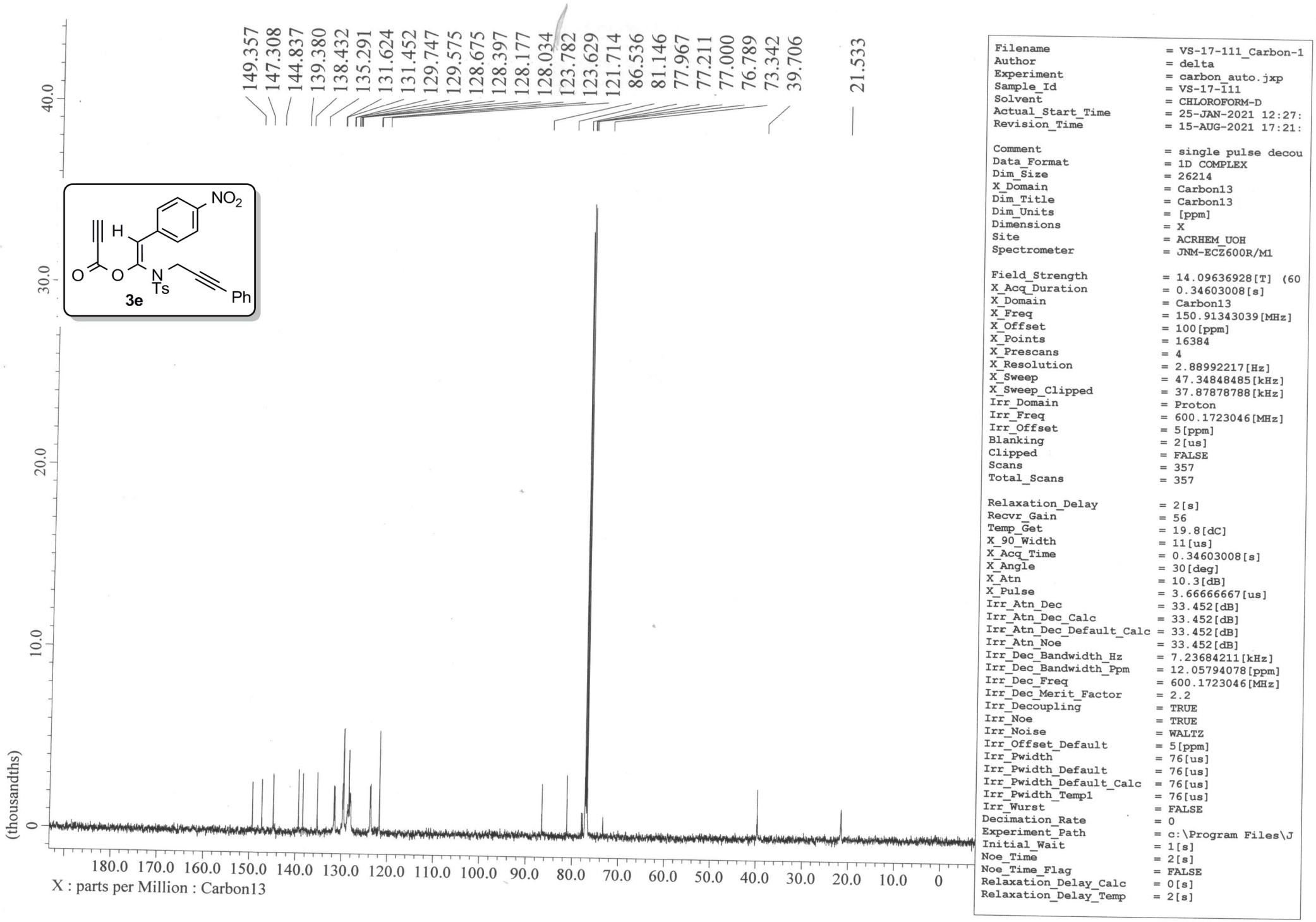
```
Current Data Parameters
NAME      K SURESH UPDATED 500
EXPNO                  142
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210915
Time              10.03 h
INSTRUM             spect
PROBHD    Z109128_0042 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
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                298.1 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

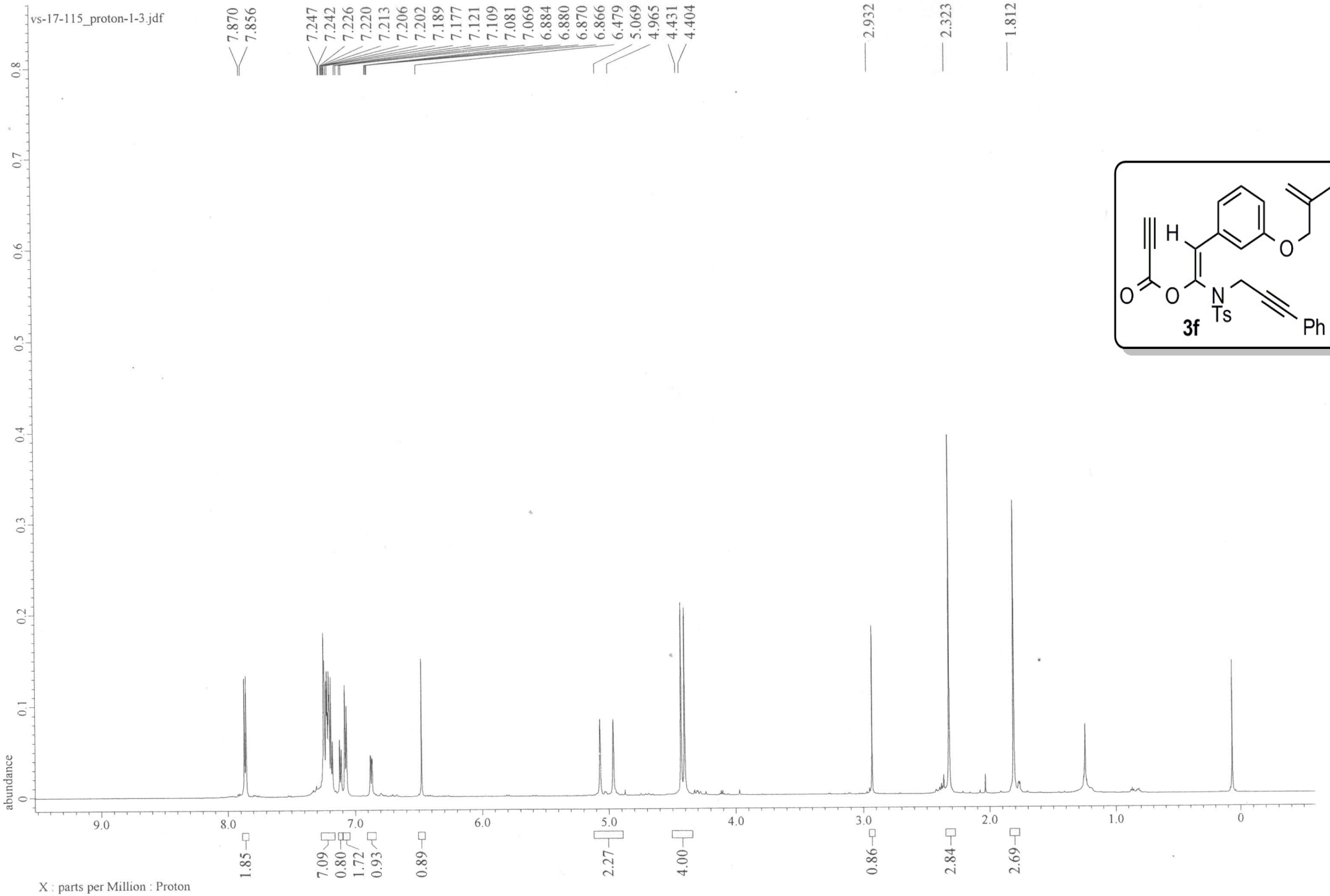
F2 - Processing parameters
SI                  65536
SF           470.6394242 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

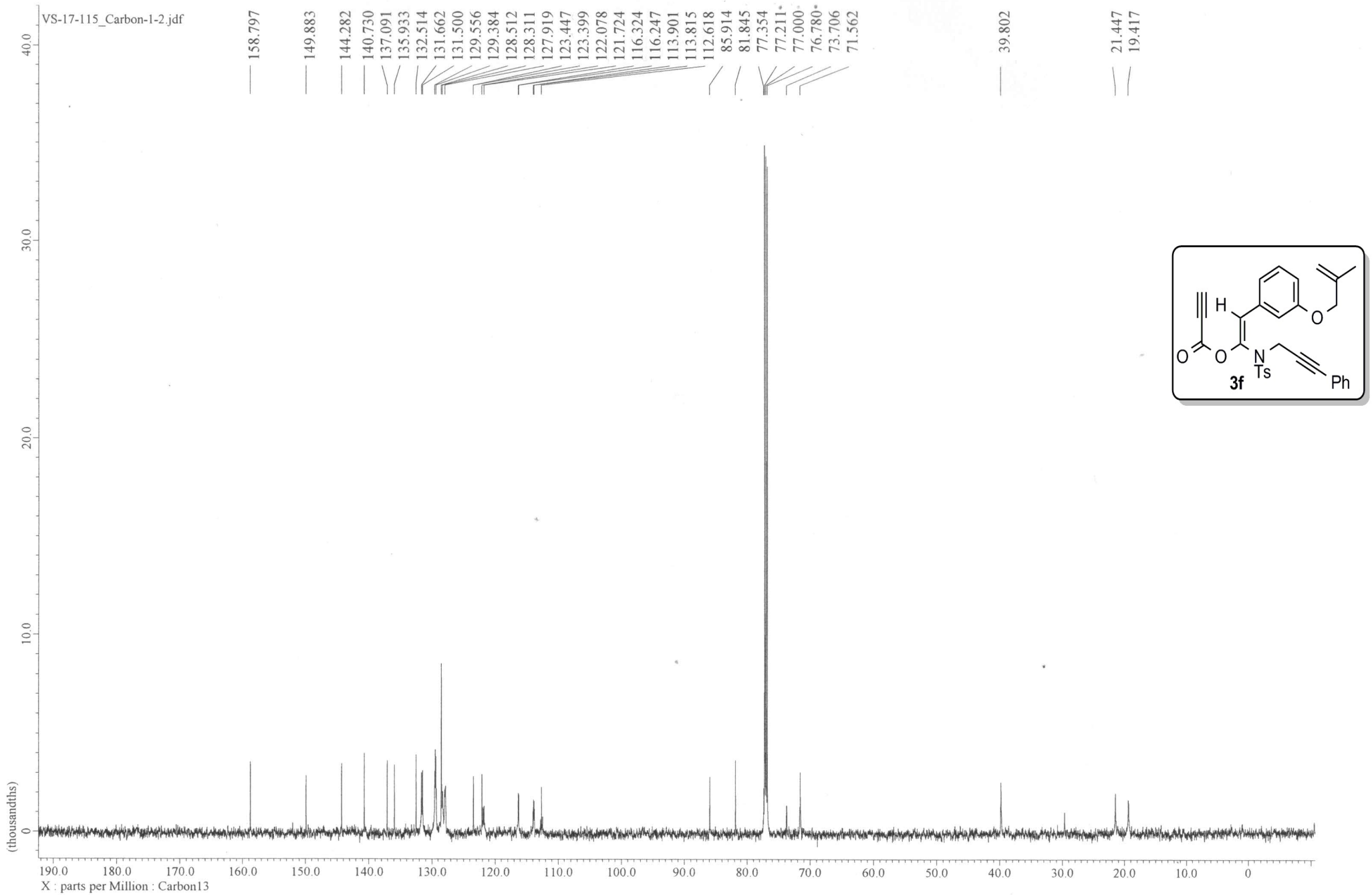


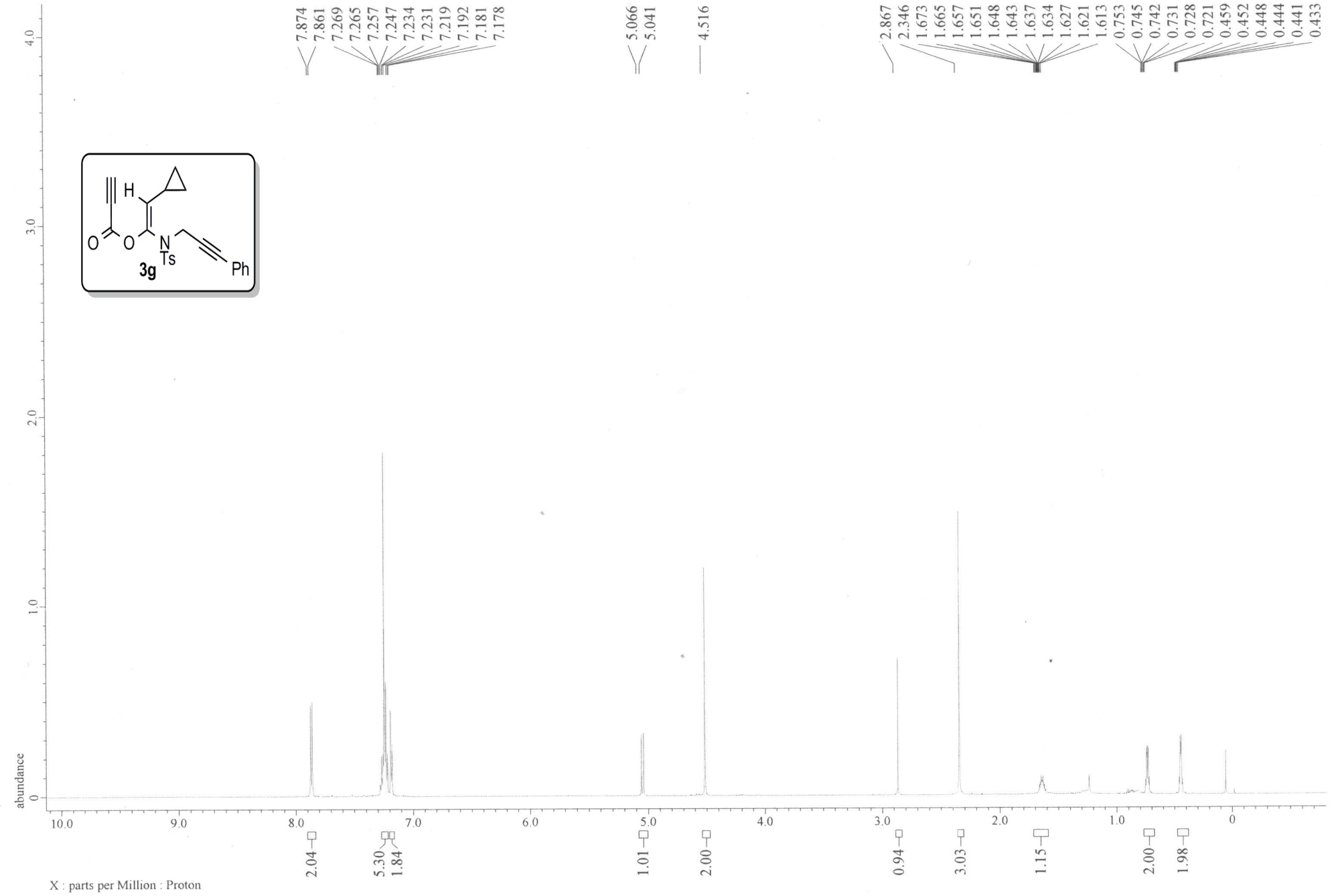

vs-17-111_proton-1-4.jdf
8.146
8.131
7.808
7.795
7.770
7.755
7.273
7.261
7.247
7.234
7.216
7.202
7.190
7.097
7.082
6.625
4.418
2.979
2.350
abundance
X : parts per Million : Proton
1.81
3.96
4.86
1.84
0.91
2.00
0.88
2.97
NO2
H
O
O
N
Ts
Ph
3e



Filename	= VS-17-111_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= VS-17-111
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JAN-2021 12:27:
Revision_Time	= 15-AUG-2021 17:21:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 357
Total_Scans	= 357
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.8[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]

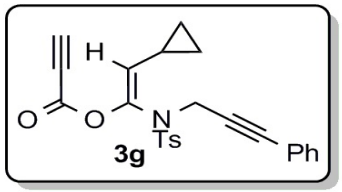

vs-17-115_proton-1-3.jdf
7.870
7.856
7.247
7.242
7.226
7.220
7.213
7.206
7.202
7.189
7.177
7.121
7.109
7.081
7.069
6.884
6.880
6.870
6.866
6.479
5.069
4.965
4.431
4.404
2.932
2.323
1.812
abundance
X : parts per Million : Proton
1.85
7.09
0.80
1.72
0.93
0.89
2.27
4.00
0.86
2.84
2.69
3f
Ph
Ts


VS-17-115_Carbon-1-2.jdf
158.797
149.883
144.282
140.730
137.091
135.933
132.514
131.662
131.500
129.556
129.384
128.512
128.311
127.919
123.447
123.399
122.078
121.724
116.324
116.247
113.901
113.815
112.618
85.914
81.845
77.354
77.211
77.000
76.780
73.706
71.562
39.802
21.447
19.417
40.0
30.0
20.0
10.0
0
(thousandths)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13
H
O
O
O
N
Ts
Ph
3f

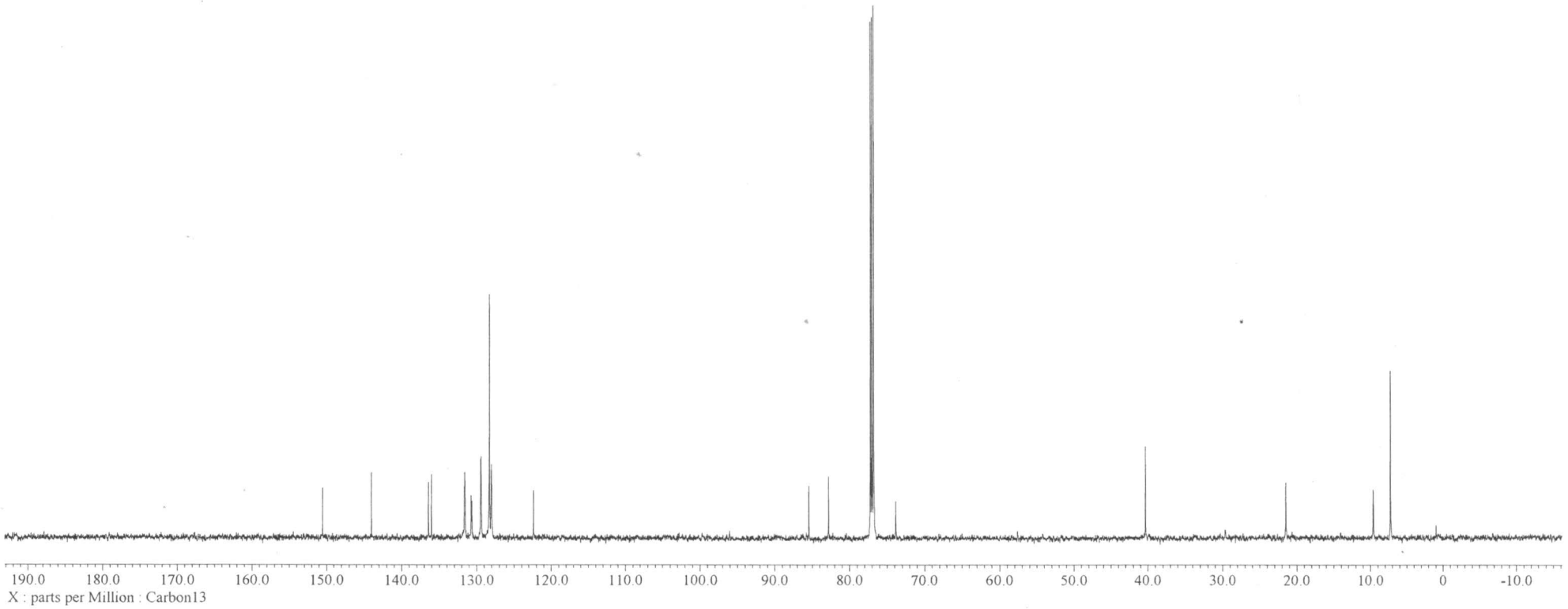

7.874
7.861
7.269
7.265
7.257
7.247
7.234
7.231
7.219
7.192
7.181
7.178
5.066
5.041
4.516
2.867
2.346
1.673
1.665
1.657
1.651
1.648
1.643
1.637
1.634
1.627
1.621
1.613
0.753
0.745
0.742
0.731
0.728
0.721
0.459
0.452
0.448
0.444
0.441
0.433
3g
Ts
Ph
abundance
X : parts per Million : Proton
2.04
5.30
1.84
1.01
2.00
0.94
3.03
1.15
2.00
1.98

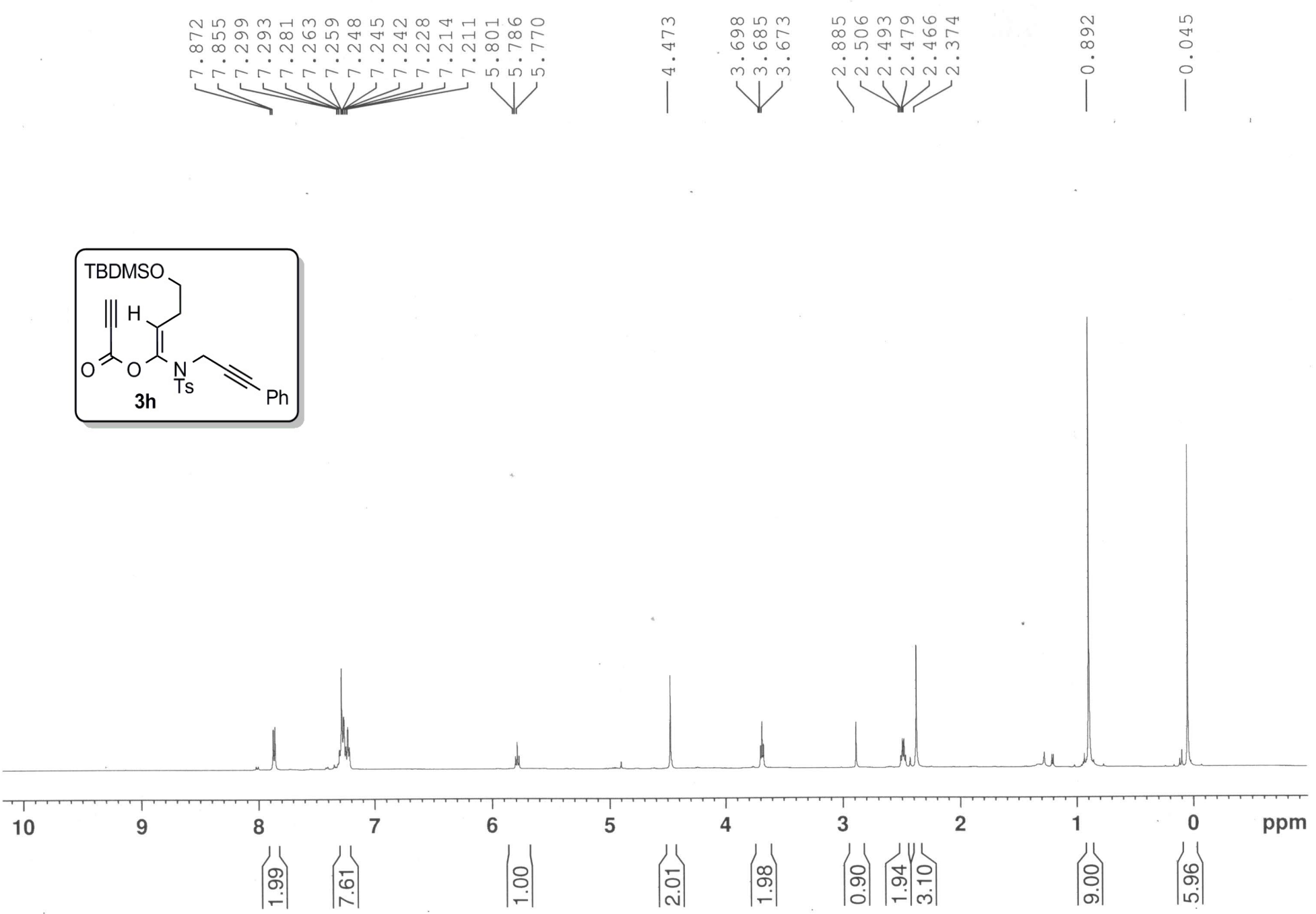
vs-16-82_Carbon-1-2.jdf

150.525
144.014
136.450
136.028
131.605
130.753
130.638
129.451
129.393
128.321
128.043
122.375
85.445
82.793
77.211
77.000
76.789
76.703
73.859
40.329
21.486
9.642
9.613
7.248



3g




7.872
7.855
7.299
7.293
7.281
7.263
7.259
7.248
7.245
7.242
7.228
7.214
7.211
5.801
5.786
5.770
4.473
3.698
3.685
3.673
2.885
2.506
2.493
2.479
2.466
2.374
0.892
0.045
TBDMSO
H
O
O
N
Ts
Ph
3h
10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
7.61
1.00
2.01
1.98
0.90
1.94
3.10
9.00
5.96

150.10
144.10
137.72
136.21
131.63
129.46
128.38
128.26
128.01
123.25
122.27

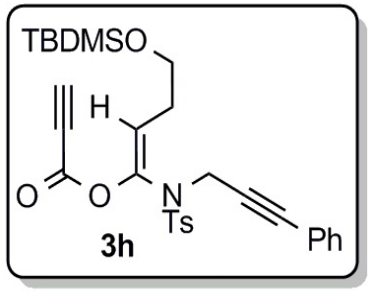
85.50
82.46
77.26
77.00
76.75
73.79

61.67

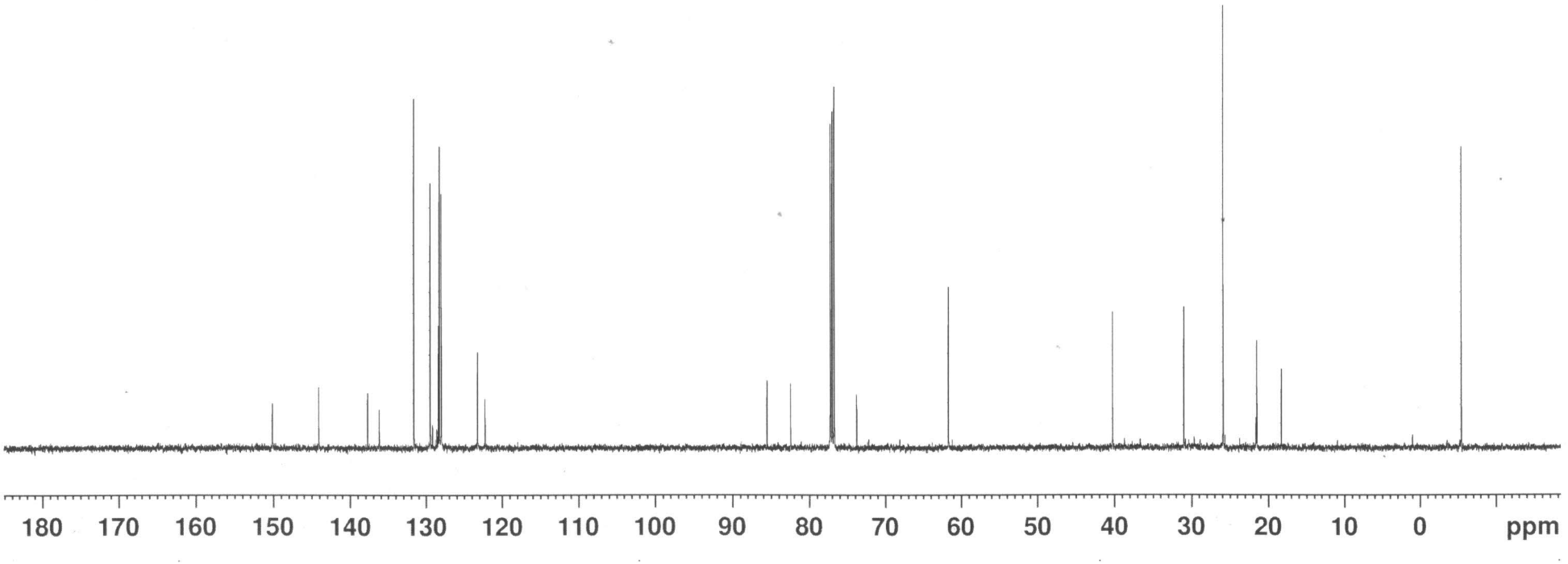
40.26

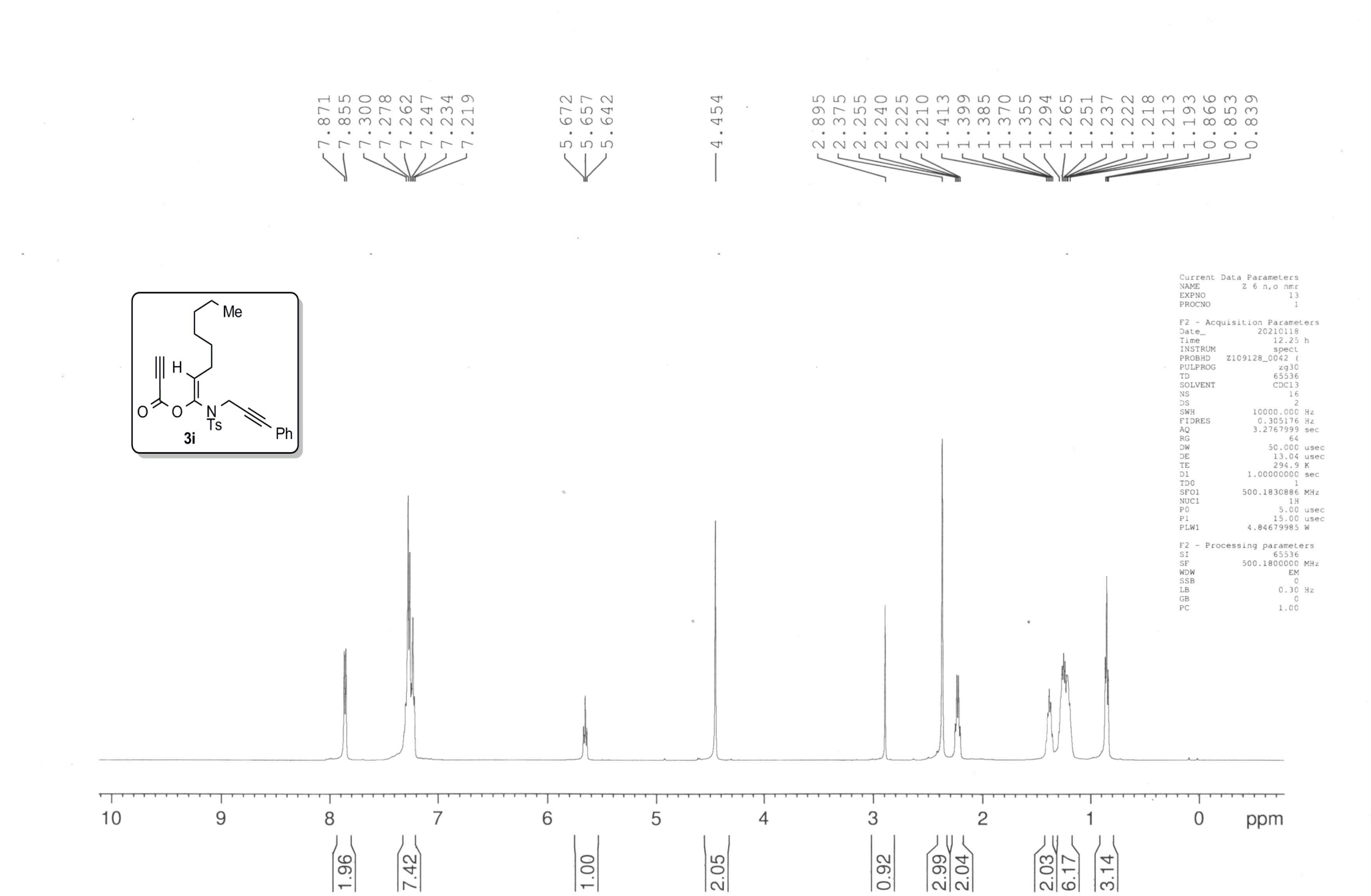
30.95
25.86
21.46
18.24

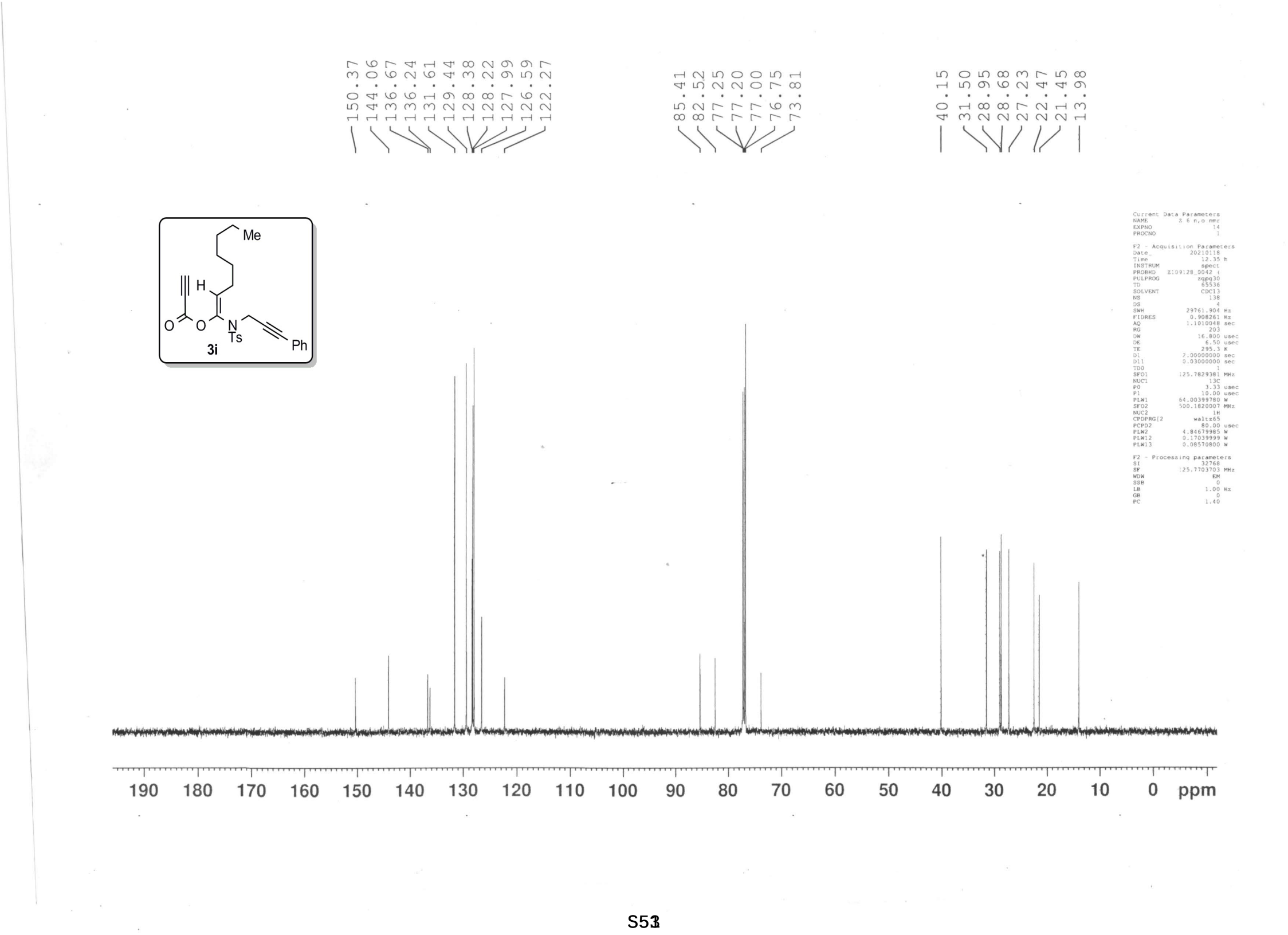
-5.47

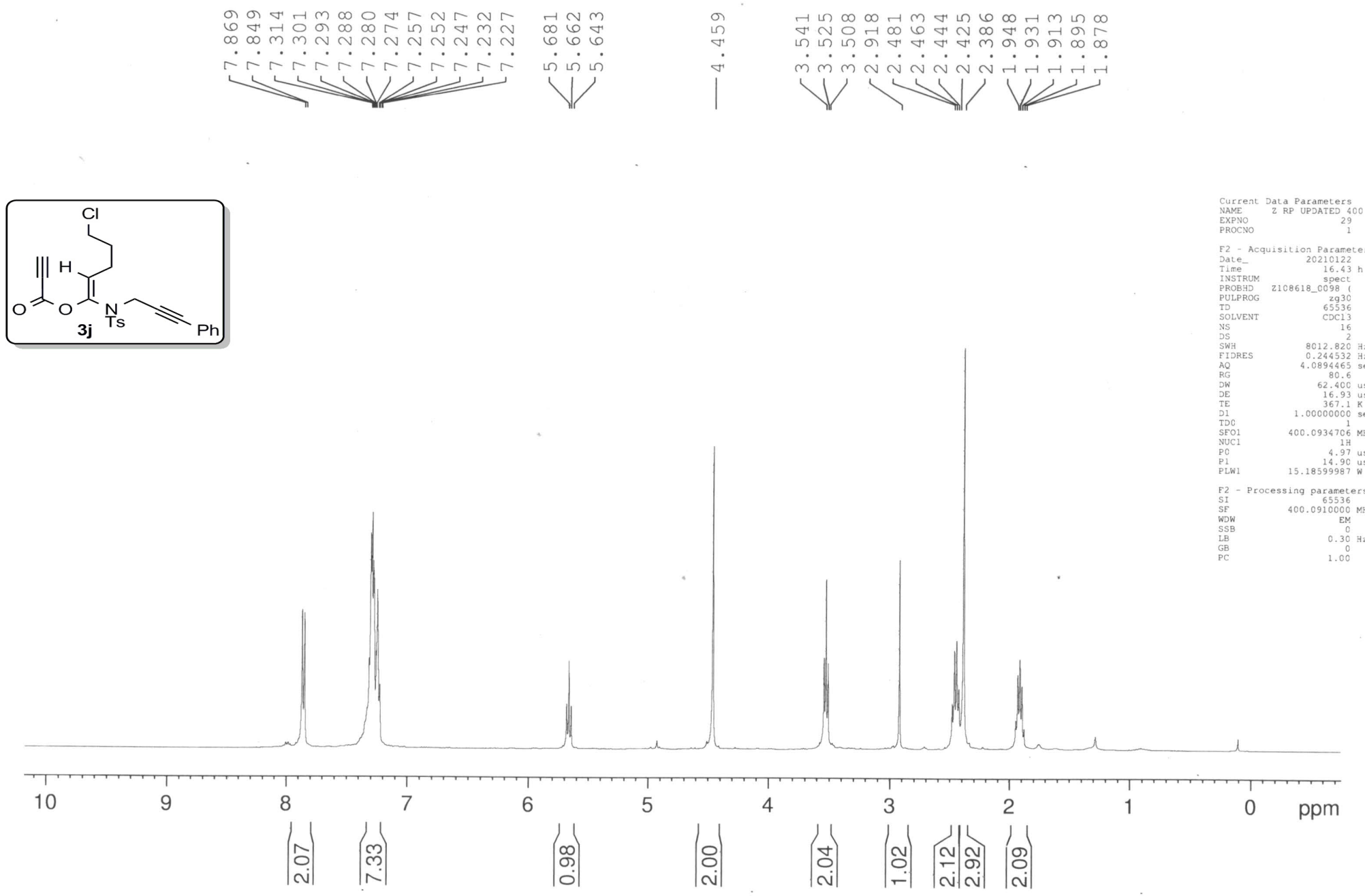


3h

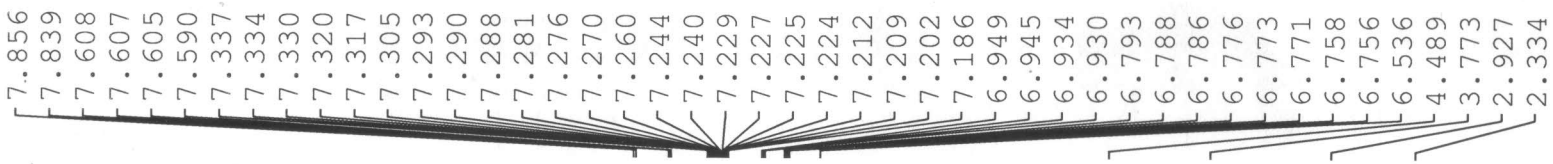



7.871
7.855
7.300
7.278
7.262
7.247
7.234
7.219
5.672
5.657
5.642
4.454
2.895
2.375
2.255
2.240
2.225
2.210
1.413
1.399
1.385
1.370
1.355
1.294
1.265
1.251
1.237
1.222
1.218
1.213
1.193
0.866
0.853
0.839
Me
H
O
O
N
Ts
Ph
3i
Current Data Parameters
NAME Z 6 n,o nmr
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210118
Time 12.25 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 294.9 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
1.96
7.42
1.00
2.05
0.92
2.99
2.04
2.03
6.17
3.14


150.37
144.06
136.67
136.24
131.61
129.44
128.38
128.22
127.99
126.59
122.27
85.41
82.52
77.25
77.20
77.00
76.75
73.81
40.15
31.50
28.95
28.68
27.23
22.47
21.45
13.98
Me
H
O
O
N
Ts
Ph
3i
Current Data Parameters
NAME Z 6 n,o nmr
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210118
Time 12.35 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 138
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 125.7703703 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 0 ppm


7.869
7.849
7.314
7.301
7.293
7.288
7.280
7.274
7.257
7.252
7.247
7.232
7.227
5.681
5.662
5.643
4.459
3.541
3.525
3.508
2.918
2.481
2.463
2.444
2.425
2.386
1.948
1.931
1.913
1.895
1.878
Cl
H
O
O
N
Ts
Ph
3j
Current Data Parameters
NAME Z RP UPDATED 400
EXPNO 29
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210122
Time 16.43 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 80.6
DW 62.400 usec
DE 16.93 usec
TE 367.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.0934706 MHz
NUC1 1H
P0 4.97 usec
P1 14.90 usec
PLW1 15.18599987 W
F2 - Processing parameters
SI 65536
SF 400.0910000 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
7.33
0.98
2.00
2.04
1.02
2.12
2.92
2.09

150.14
144.27
137.47
135.91
131.57
129.49
128.46
128.18
128.03
124.66
122.07
85.56
82.22
77.32
77.04
77.00
76.68
73.60
44.07
39.95
31.39
24.61
21.43
Cl
H
O
O
N
Ts
Ph
3j
Current Data Parameters
NAME Z RP UPDATED 400
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210122
Time 16.55 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 213
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 368.2 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 100.6029743 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 0 ppm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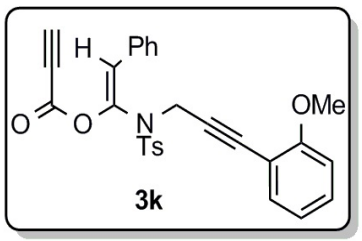
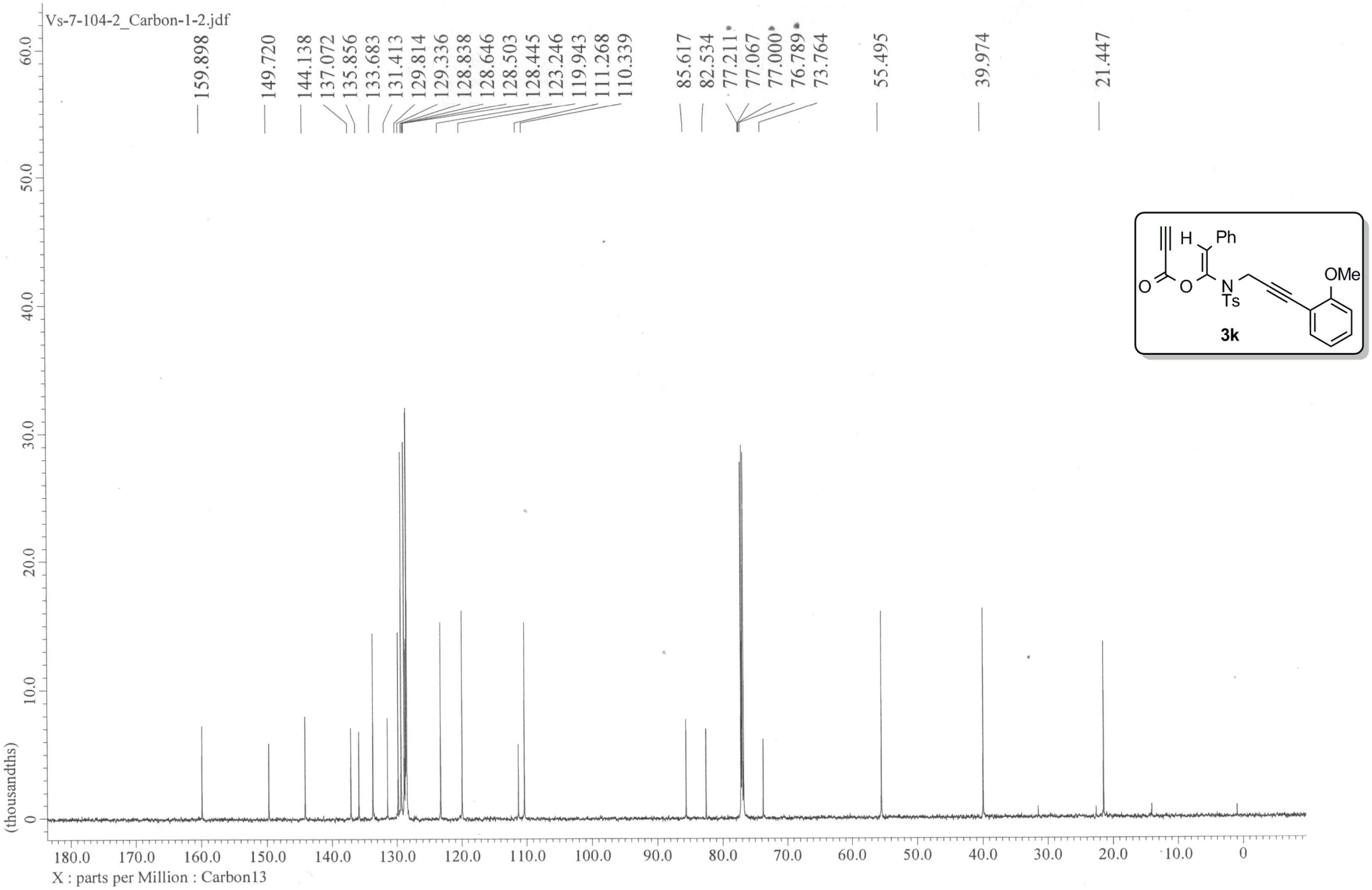
7.839
7.608
7.607
7.605
7.590
7.337
7.334
7.330
7.320
7.317
7.305
7.293
7.290
7.288
7.281
7.276
7.270
7.260
7.244
7.240
7.229
7.227
7.225
7.224
7.212
7.209
7.202
7.186
6.949
6.945
6.934
6.930
6.793
6.788
6.786
6.776
6.773
6.771
6.758
6.756
6.536
4.489
3.773
2.927
2.334


H
Ph
O
O
N
Ts
OMe
3k

12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.05
3.10
3.33
0.98
2.00
0.96
2.00
3.06
0.90
3.06


Vs-7-104-2_Carbon-1-2.jdf
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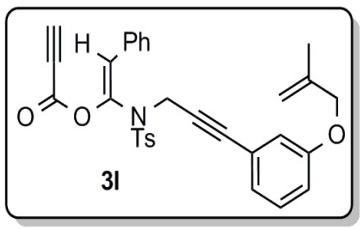
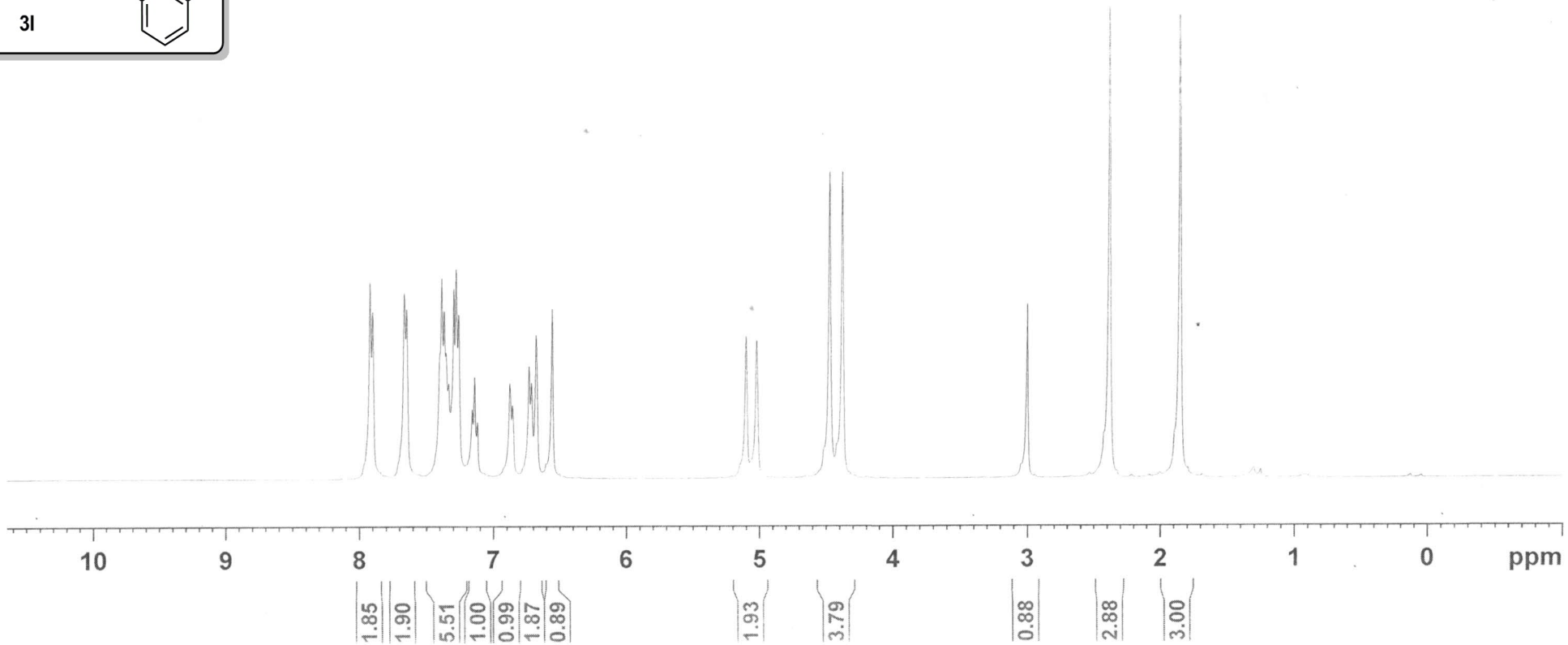
149.720
144.138
137.072
135.856
133.683
131.413
129.814
129.336
128.838
128.646
128.503
128.445
123.246
119.943
111.268
110.339
85.617
82.534
77.211
77.067
77.000
76.789
73.764
55.495
39.974
21.447
H
Ph
O
O
N
Ts
OMe
3k
(thousandths)
X : parts per Million : Carbon13

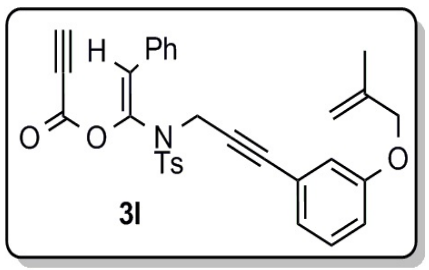


3l

7.915
7.896
7.660
7.642
7.379
7.361
7.349
7.329
7.289
7.272
7.253
7.156
7.136
7.117
6.874
6.853
6.727
6.709
6.674
6.552
5.098
5.018
4.465
4.373
2.994
2.375
1.845

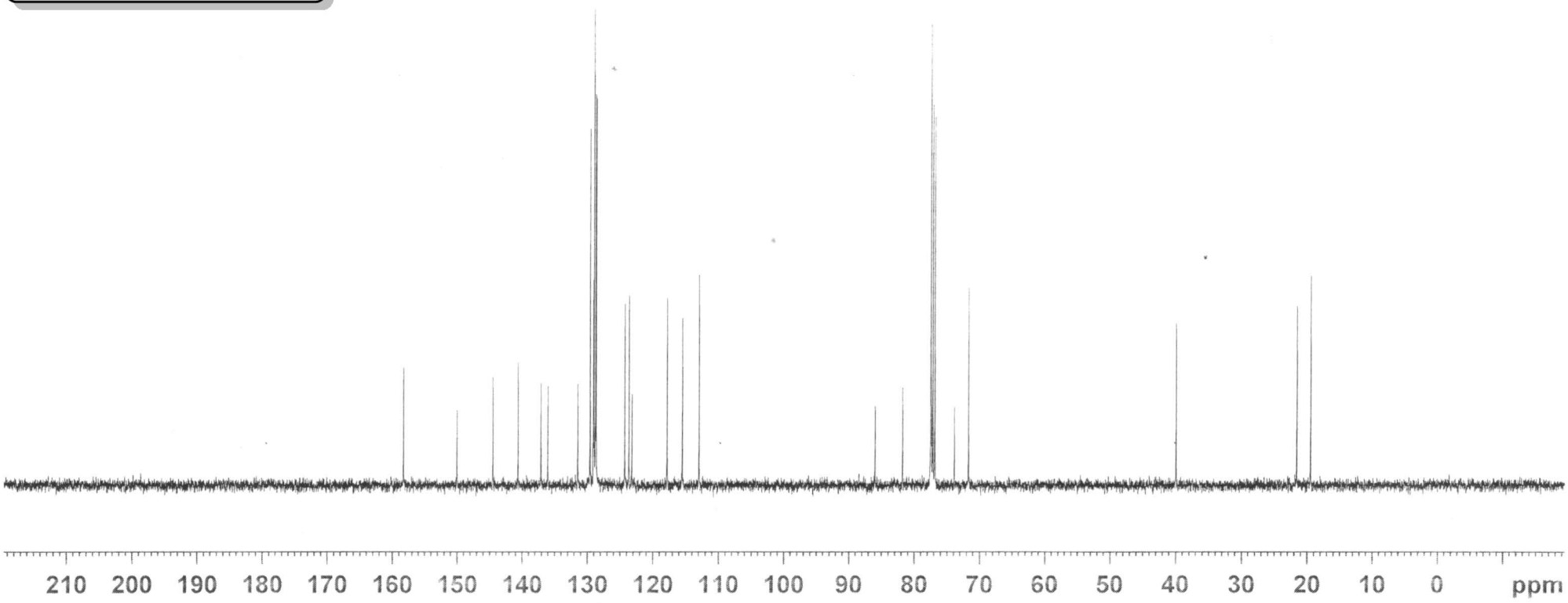


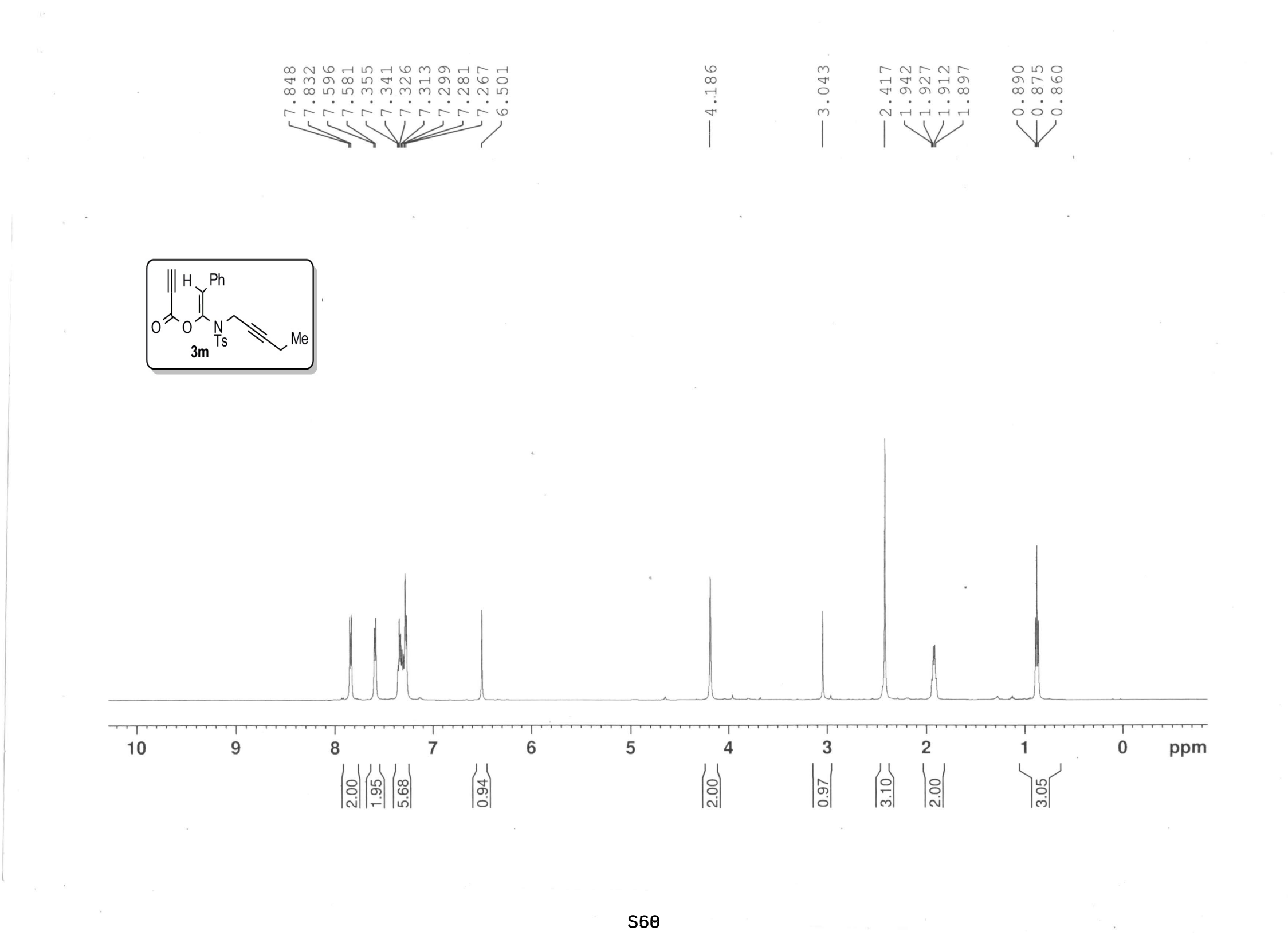
1.85
1.90
5.51
1.00
0.99
1.87
0.89
1.93
3.79
0.88
2.88
3.00



3l

158.23
149.98
144.46
140.57
137.05
135.98
131.41
129.54
129.05
128.95
128.71
128.60
124.24
123.59
123.13
117.77
115.45
112.90
85.95
81.76
77.45
77.33
77.13
76.81
73.84
71.65
39.88
21.57
19.45

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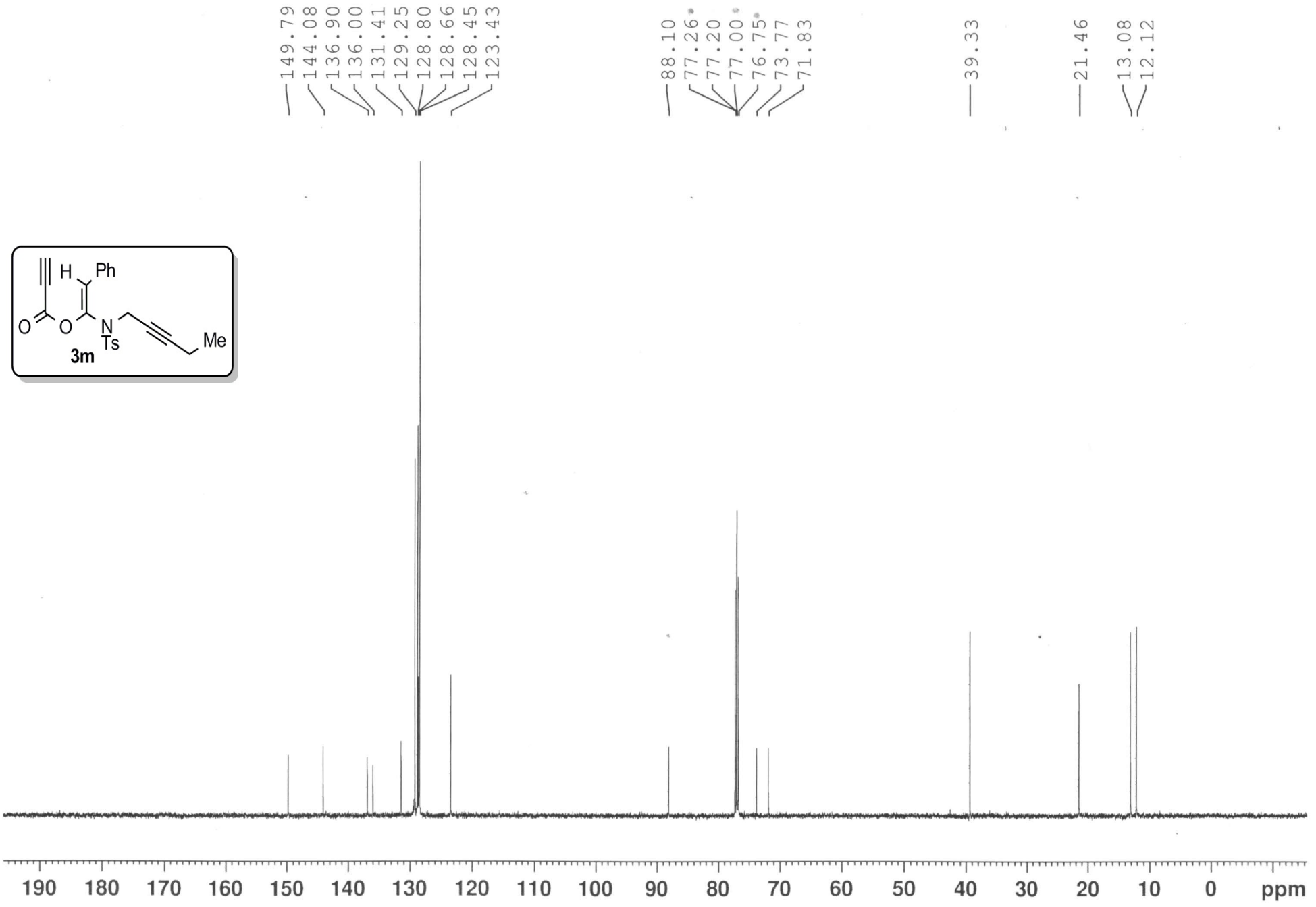
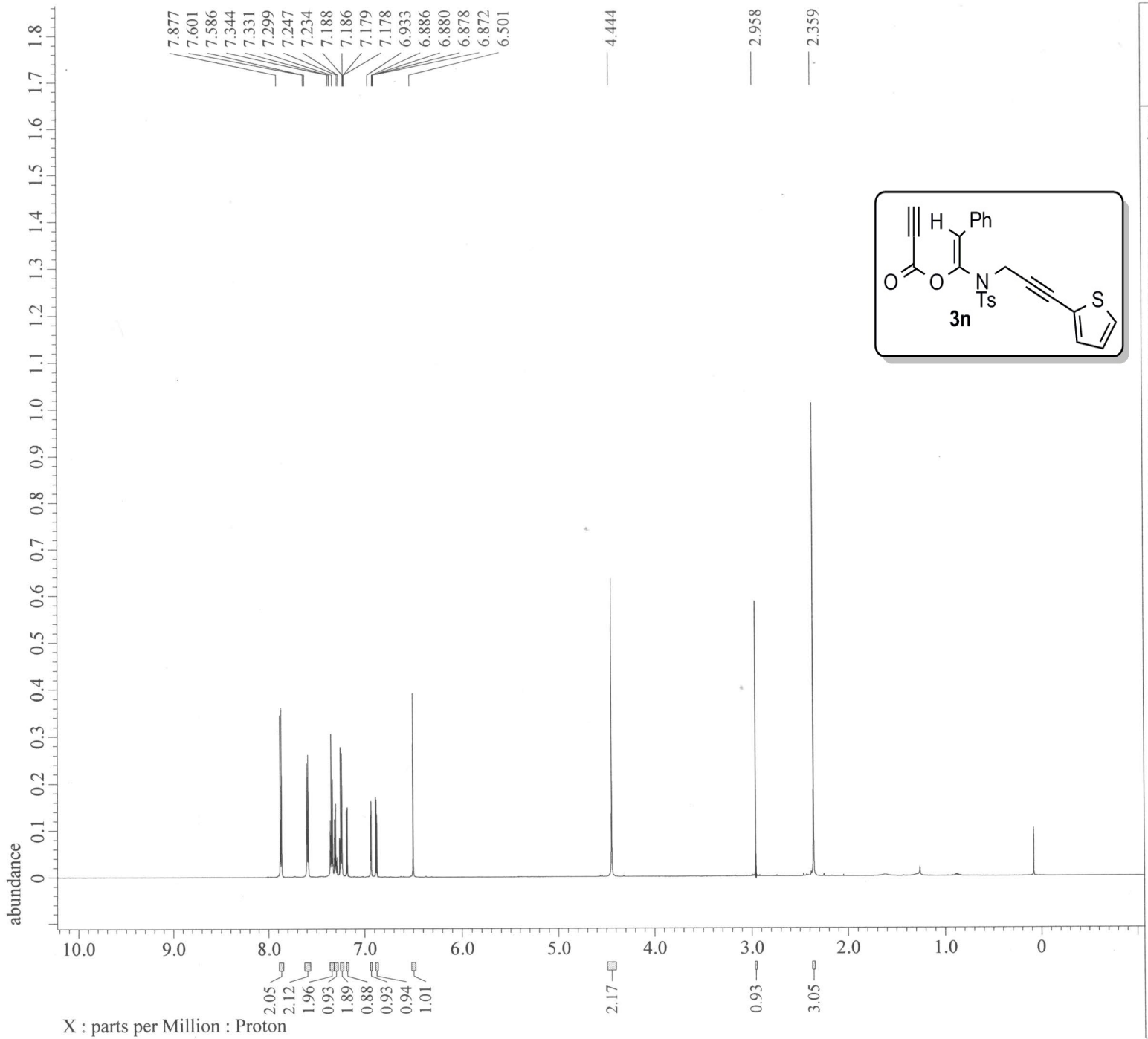
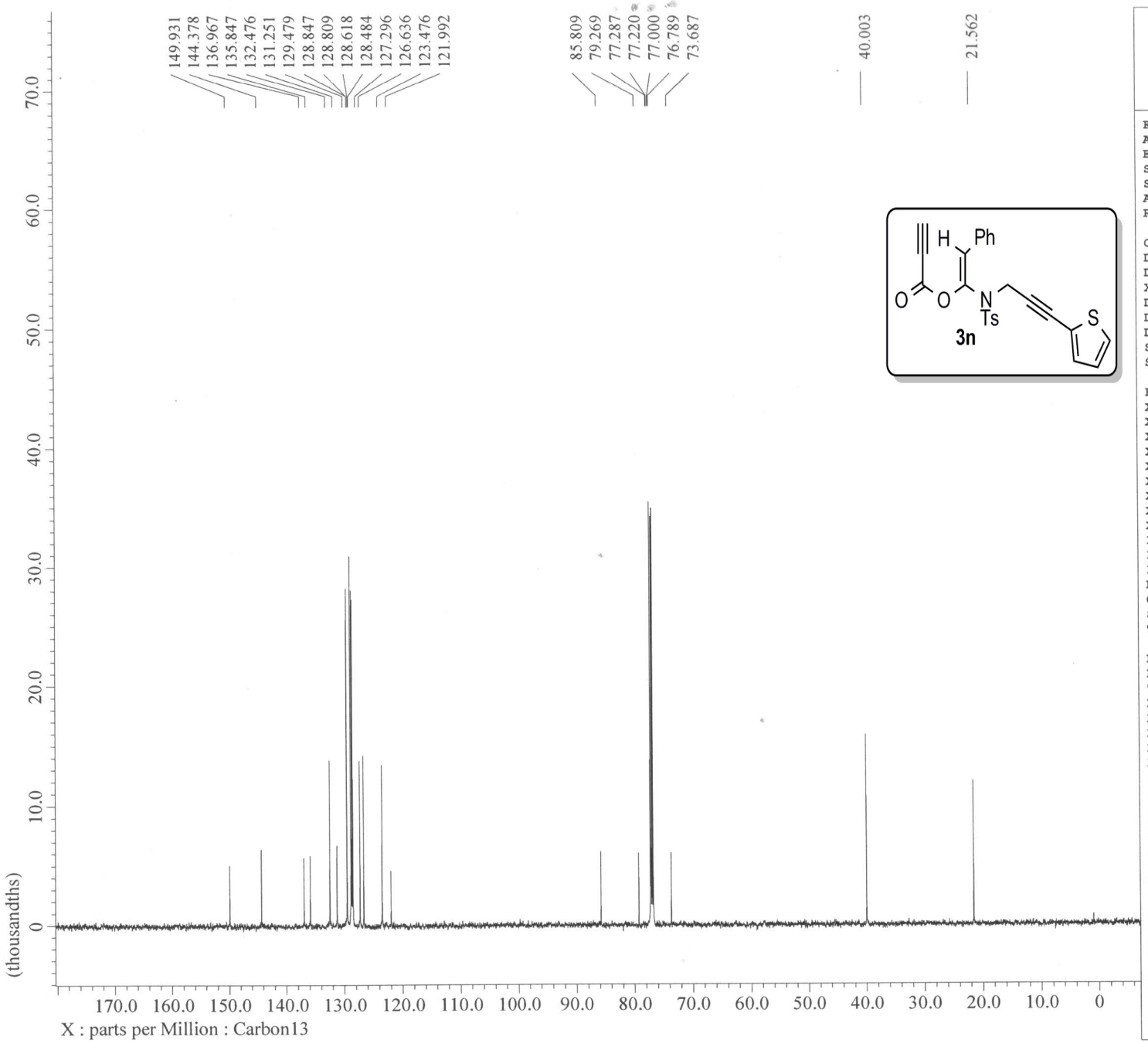
7.596
7.581
7.355
7.341
7.326
7.313
7.299
7.281
7.267
6.501
4.186
3.043
2.417
1.942
1.927
1.912
1.897
0.890
0.875
0.860
H
Ph
O
O
N
Ts
Me
3m
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.95
5.68
0.94
2.00
0.97
3.10
2.00
3.05


149.79
144.08
136.90
136.00
131.41
129.25
128.80
128.66
128.45
123.43
88.10
77.26
77.20
77.00
76.75
73.77
71.83
39.33
21.46
13.08
12.12
H
Ph
O
O
N
Ts
Me
3m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



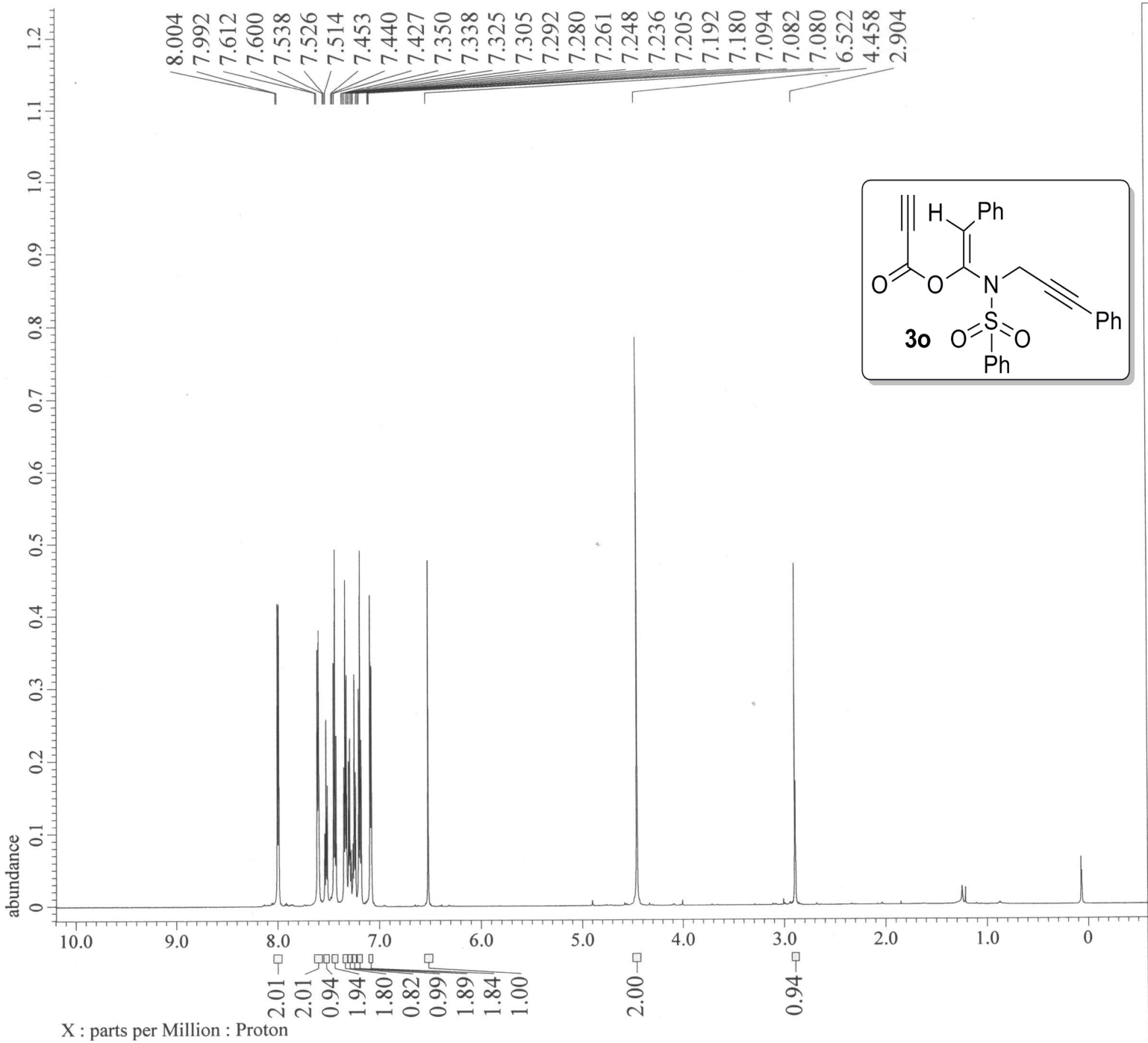
JEOL

Filename	= vs-17-120_Proton-1-3.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= vs-17-120
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2021 10:14:28
Revision_Time	= 23-JAN-2021 20:33:58
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 19.2[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]

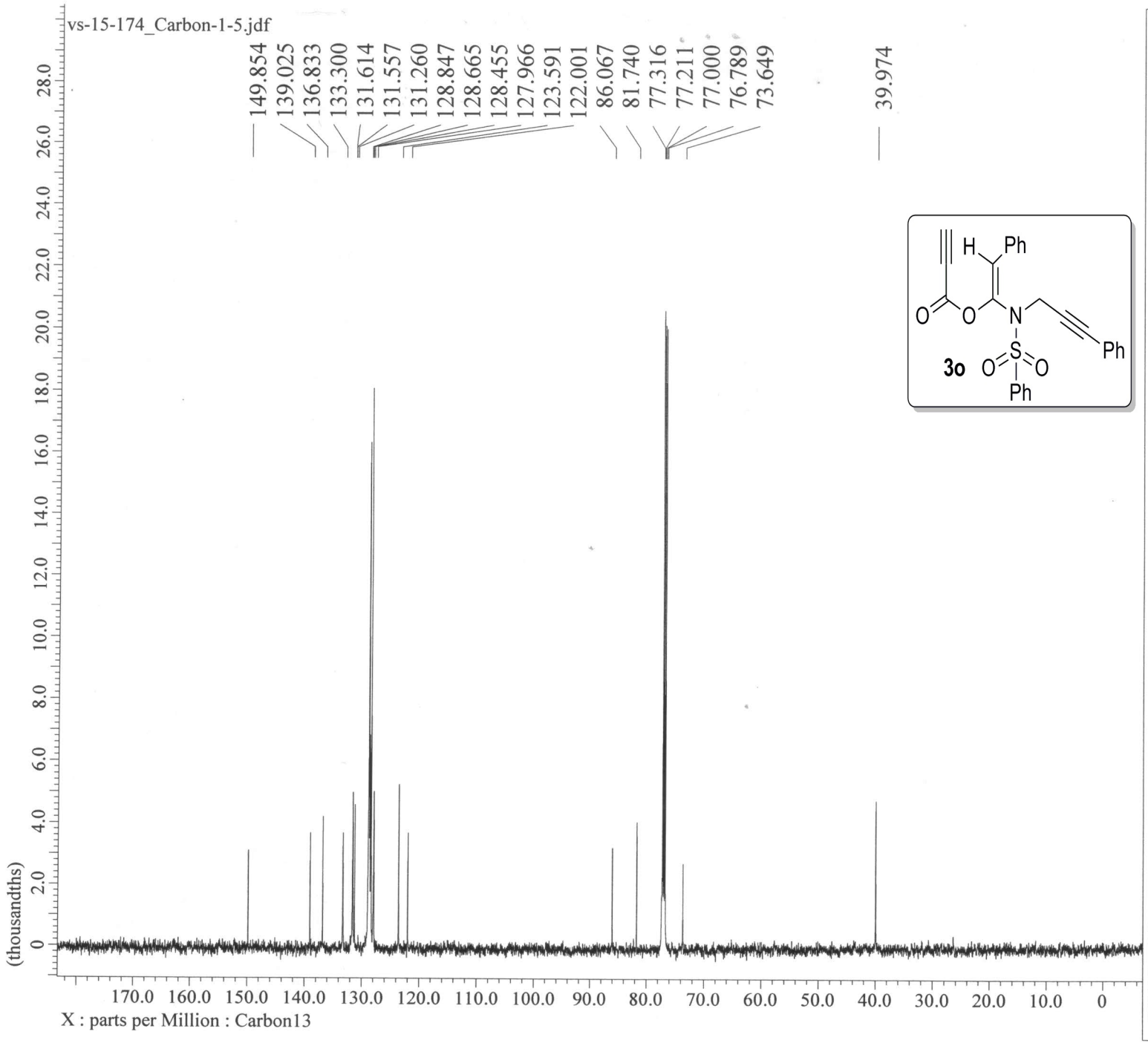


JEOL

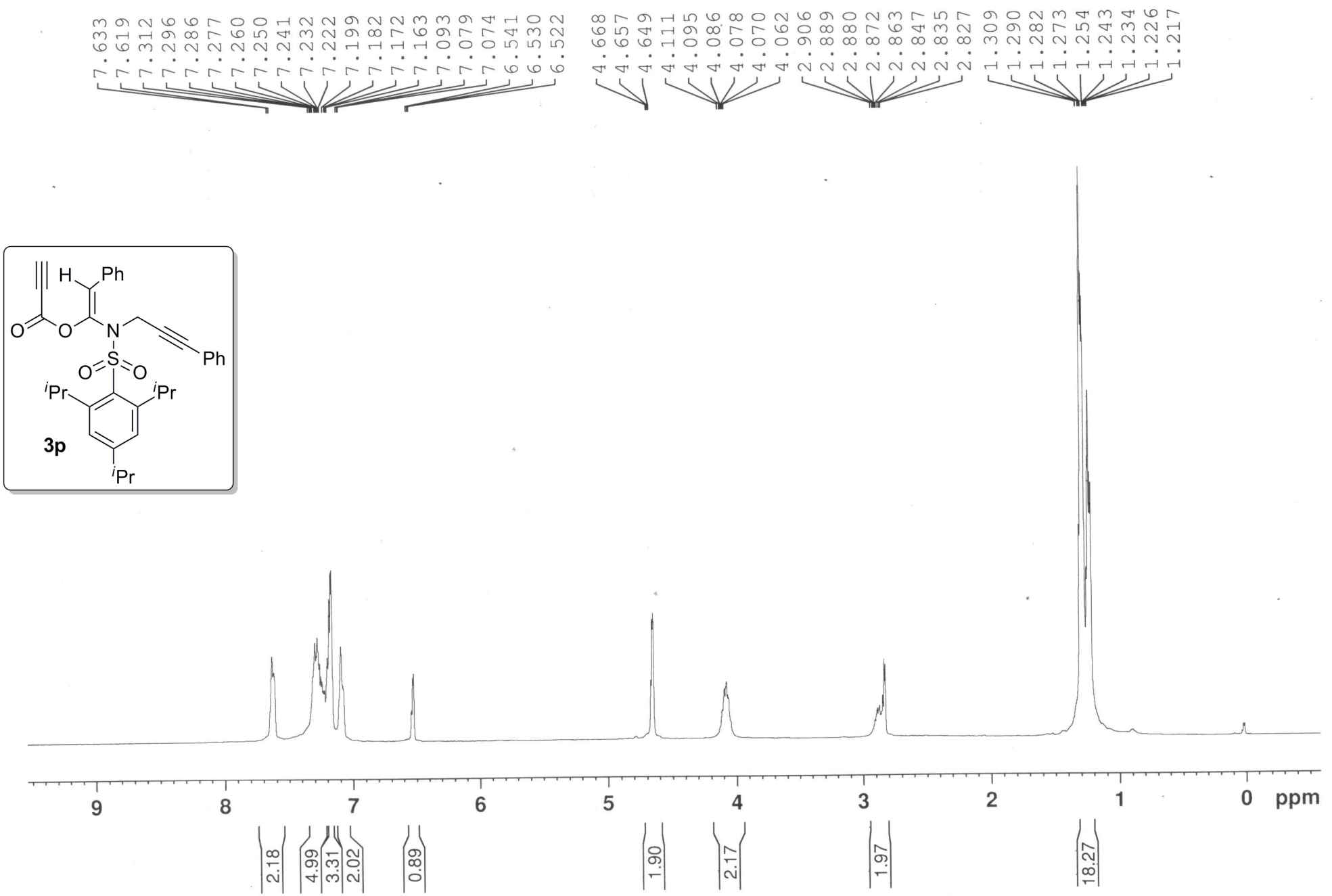
Filename	= vs-17-120_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= vs-17-120
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2021 10:16:
Revision_Time	= 23-JAN-2021 20:20:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.4[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0



Filename	= vs-15-174_Proton-1-8.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= vs-15-174
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2021 16:22:42
Revision_Time	= 10-FEB-2021 23:34:04
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.6[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]



Filename	= vs-15-174_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= vs-15-174
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2021 16:24:
Revision_Time	= 10-FEB-2021 23:30:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.5[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]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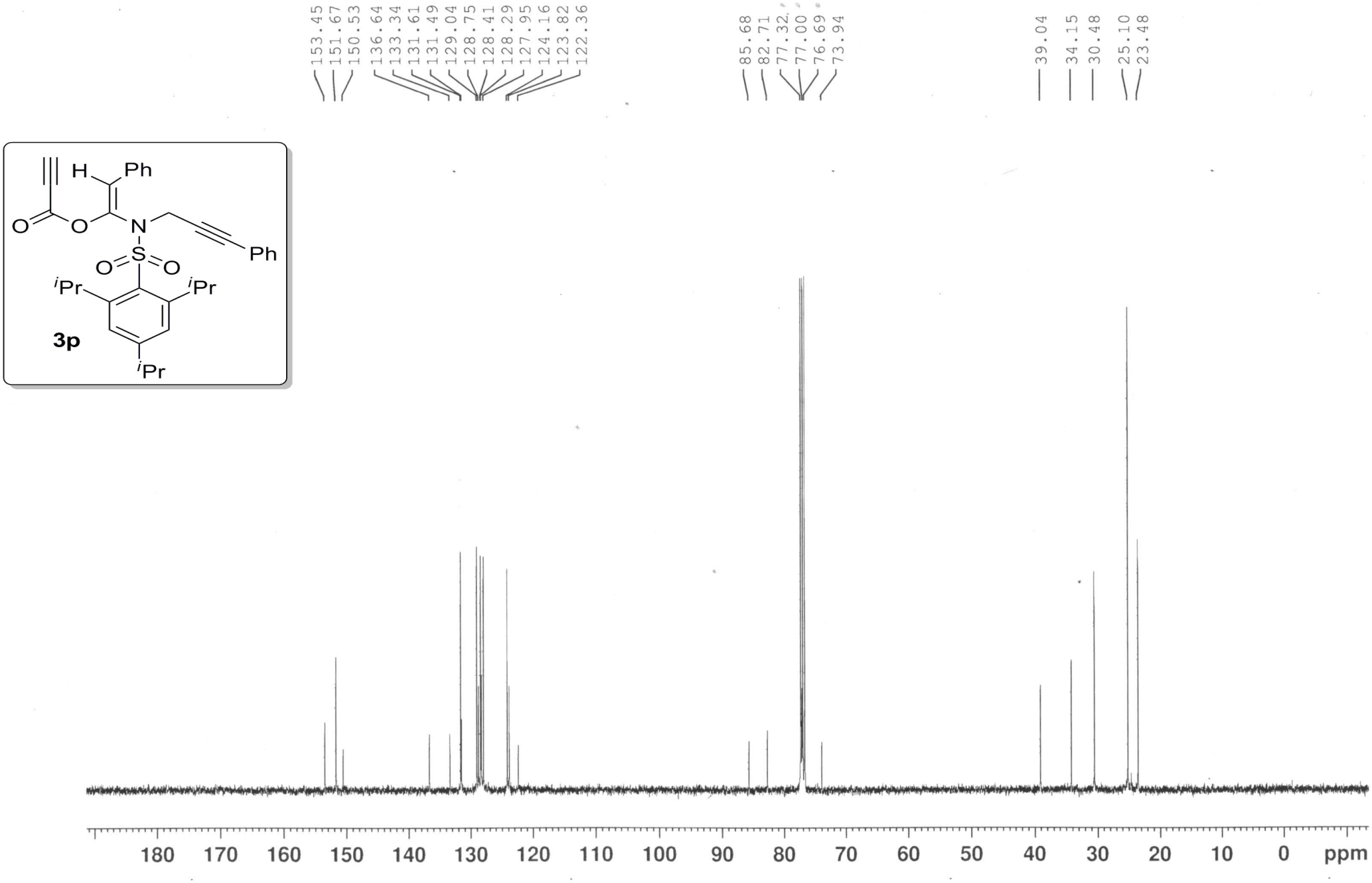
7.250
7.241
7.232
7.222
7.199
7.182
7.172
7.163
7.093
7.079
7.074
6.541
6.530
6.522
4.668
4.657
4.649
4.111
4.095
4.086
4.078
4.070
4.062
2.906
2.889
2.880
2.872
2.863
2.847
2.835
2.827
1.309
1.290
1.282
1.273
1.254
1.243
1.234
1.226
1.217
H
Ph
O
O
N
Ph
S
O
O
iPr
iPr
iPr
3p
9
8
7
6
5
4
3
2
1
0
ppm
2.18
4.99
3.31
2.02
0.89
1.90
2.17
1.97
18.27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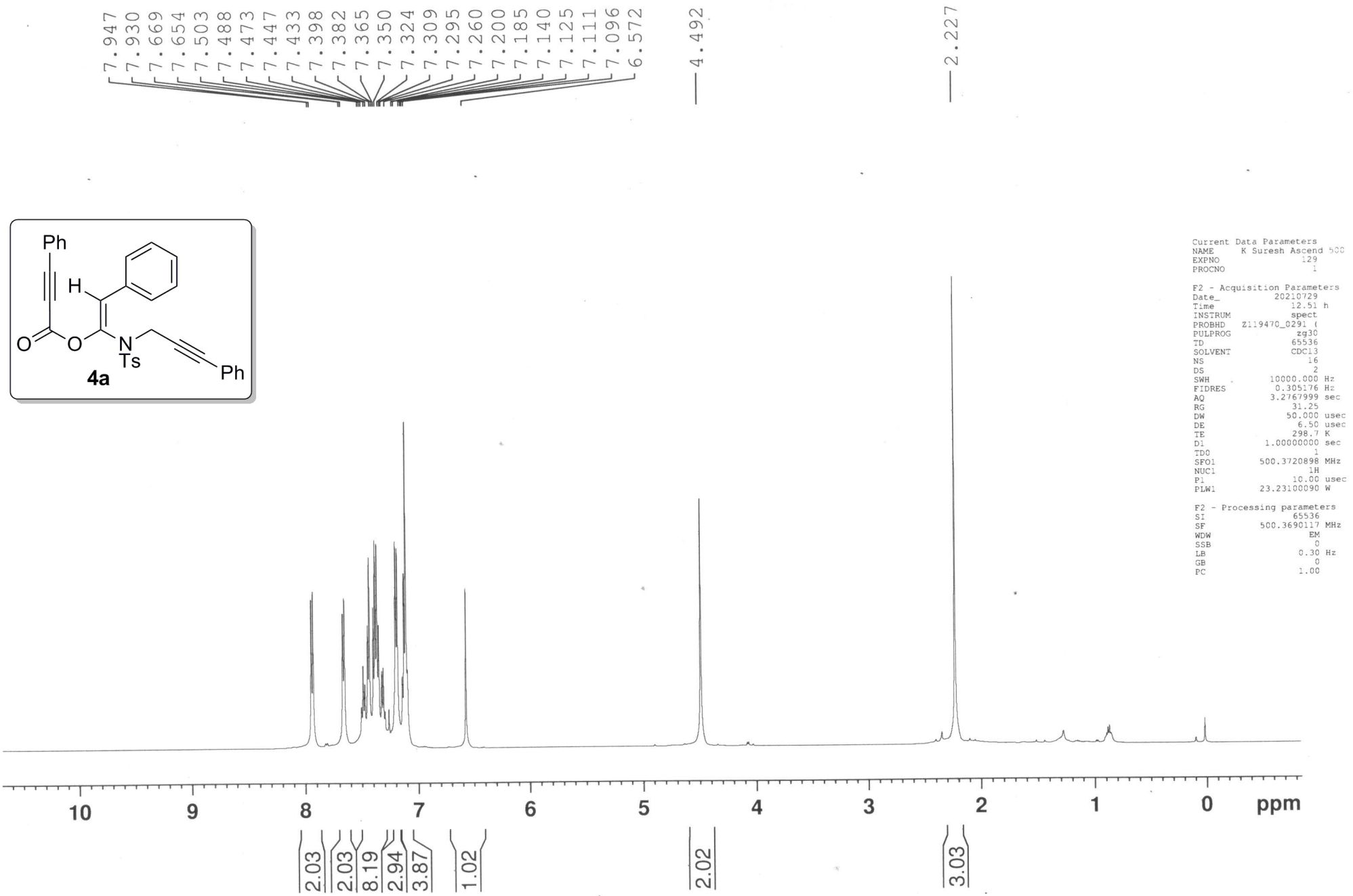
151.67
150.53
136.64
133.34
131.61
131.49
129.04
128.75
128.41
128.29
127.95
124.16
123.82
122.36
85.68
82.71
77.32
77.00
76.69
73.94
39.04
34.15
30.48
25.10
23.48
H
Ph
O
O
N
Ph
S
O
O
iPr
iPr
iPr
3p
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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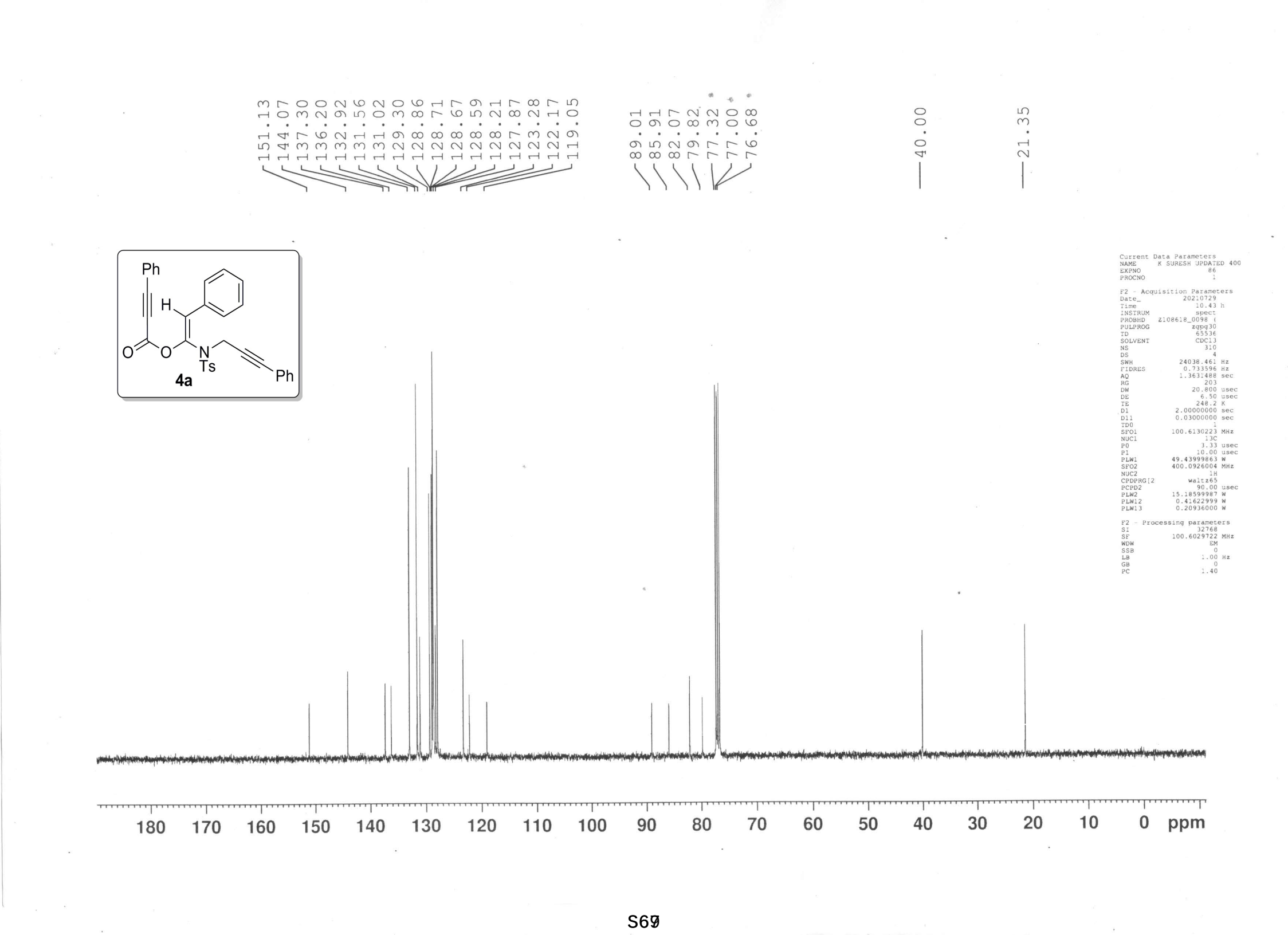
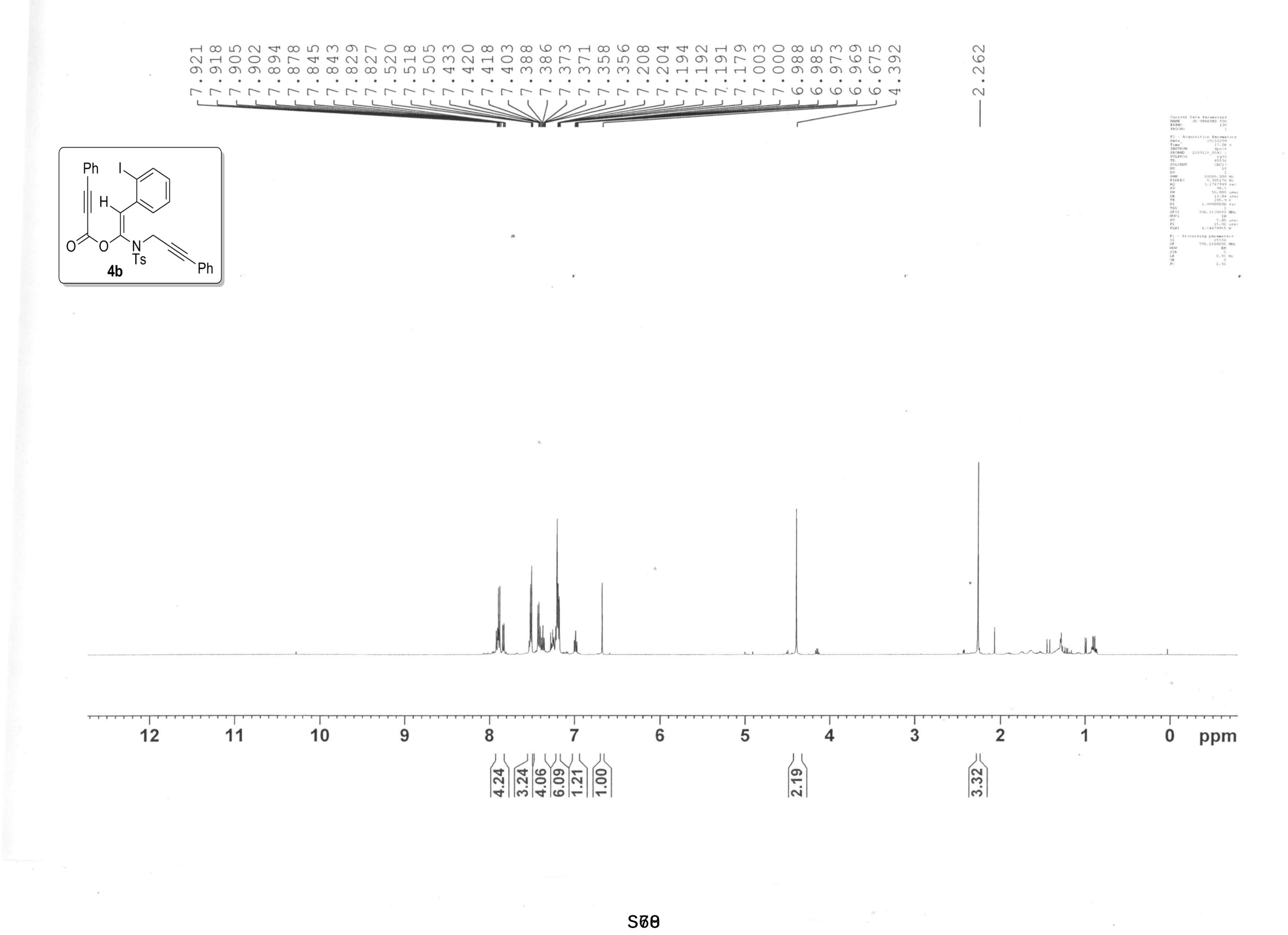
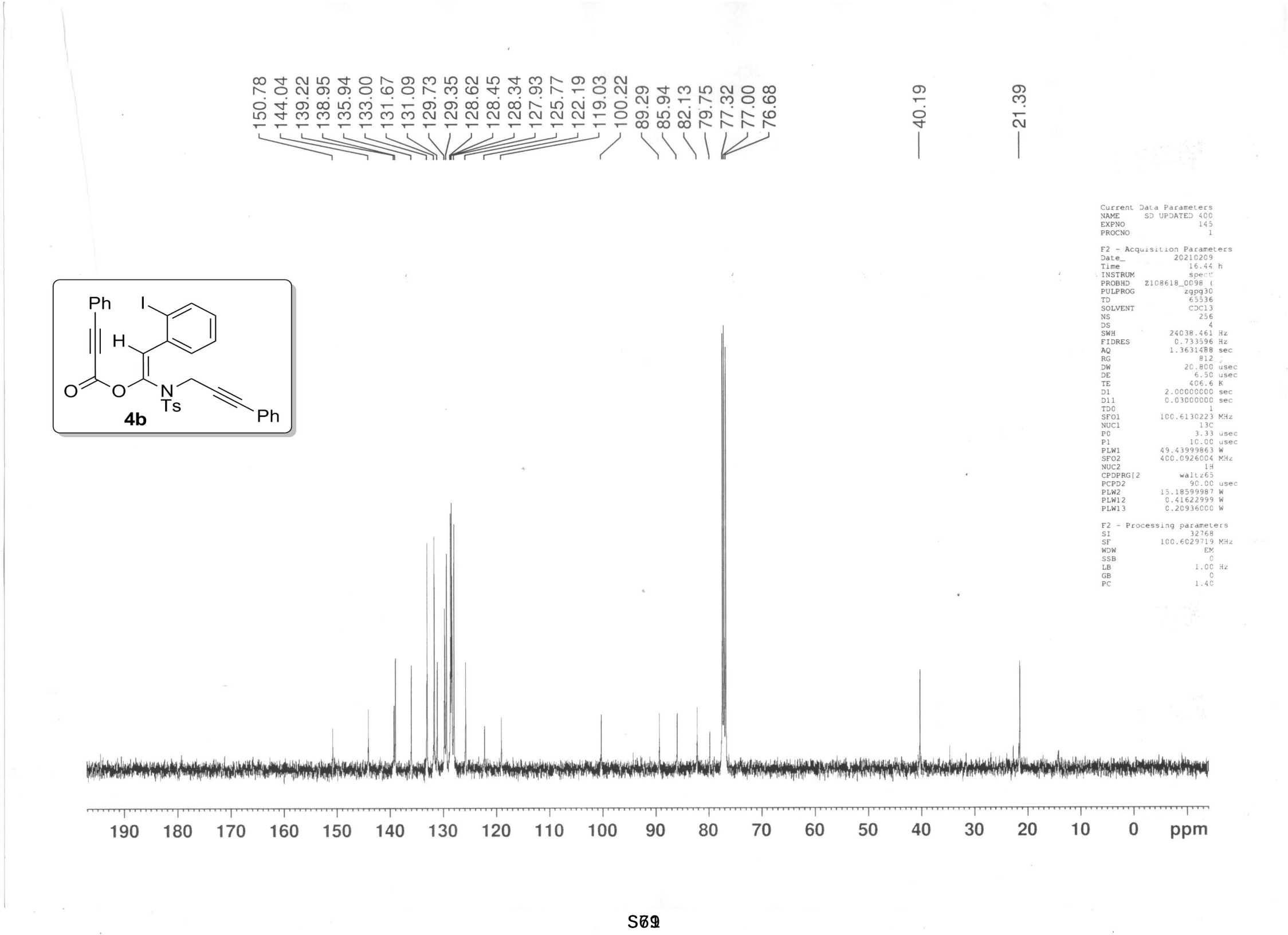
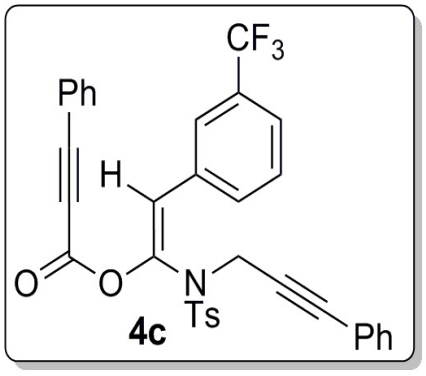
7.350
7.324
7.309
7.295
7.260
7.200
7.185
7.140
7.125
7.111
7.096
6.572
4.492
2.227
Ph
H
O
O
N
Ts
Ph
4a
Current Data Parameters
NAME K Suresh Ascend 500
EXPNO 129
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210729
Time 12.51 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 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 298.7 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 500.3690117 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
8.19
2.94
3.87
1.02
2.02
3.03


151.13
144.07
137.30
136.20
132.92
131.56
131.02
129.30
128.86
128.71
128.67
128.59
128.21
127.87
123.28
122.17
119.05
89.01
85.91
82.07
79.82
77.32
77.00
76.68
40.00
21.35
Ph
H
O
O
N
Ts
Ph
4a
Current Data Parameters
NAME K SURESH UPDATED 400
EXPNO 86
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210729
Time 10.43 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 310
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 248.2 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 100.6029722 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


7.921
7.918
7.905
7.902
7.894
7.878
7.845
7.843
7.829
7.827
7.520
7.518
7.505
7.433
7.420
7.418
7.403
7.388
7.386
7.373
7.371
7.358
7.356
7.208
7.204
7.194
7.192
7.191
7.179
7.003
7.000
6.988
6.985
6.973
6.969
6.675
4.392
2.262
Ph
I
H
O
O
N
Ts
Ph
4b
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.24
3.24
4.06
6.09
1.21
1.00
2.19
3.32

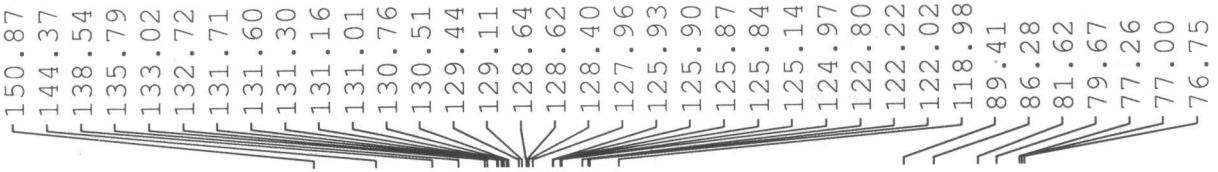

150.78
144.04
139.22
138.95
135.94
133.00
131.67
131.09
129.73
129.35
128.62
128.45
128.34
127.93
125.77
122.19
119.03
100.22
89.29
85.94
82.13
79.75
77.32
77.00
76.68
40.19
21.39
Ph
I
H
O
O
N
Ts
Ph
4b
Current Data Parameters
NAME SD UPDATED 400
EXPNO 145
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210209
Time 16.44 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
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 406.6 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 100.6029719 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 0 ppm

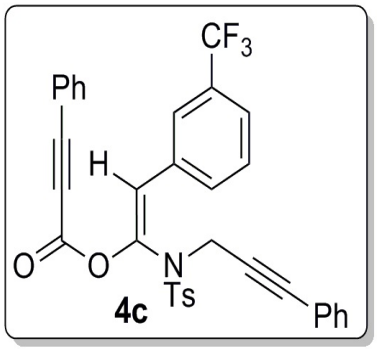


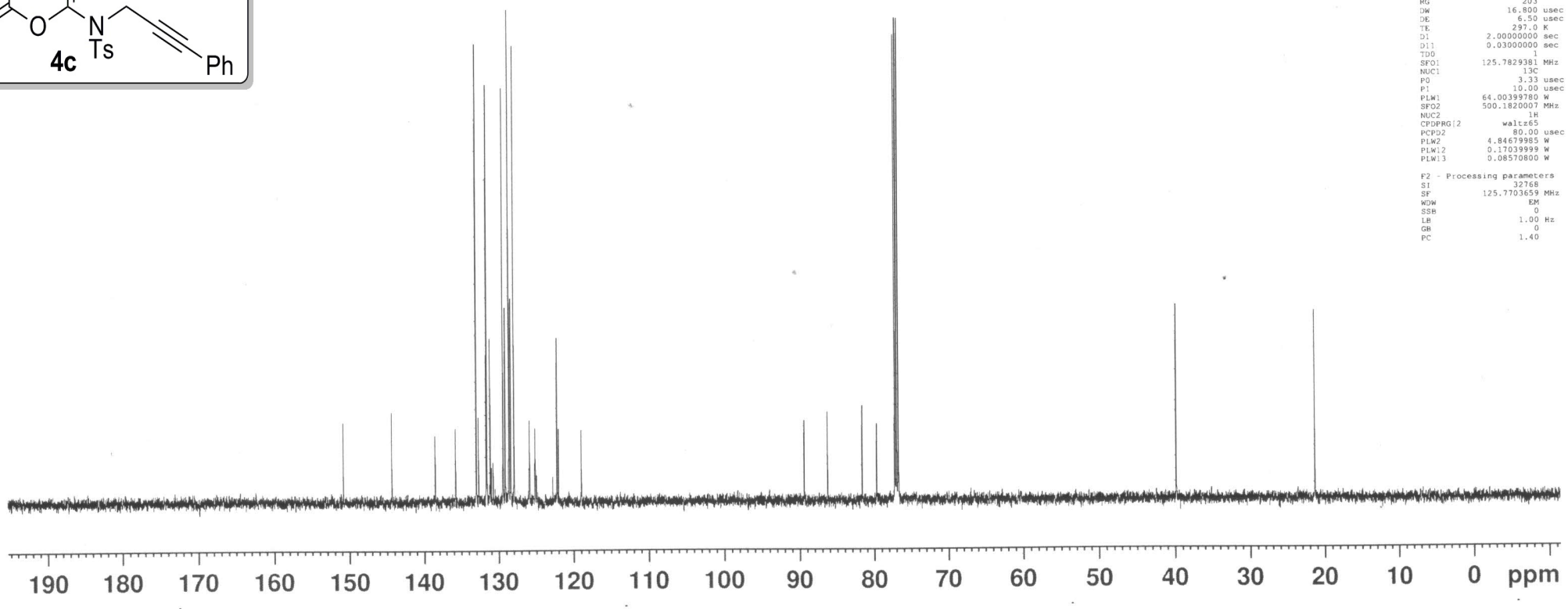

```
Current Data Parameters
NAME      K SURESH UPDATED 500
EXPNO                  121
PROCNO                   1

F2 - Acquisition Parameters
Date_               20210728
Time                    9.49 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                      114
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             500.1800096 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



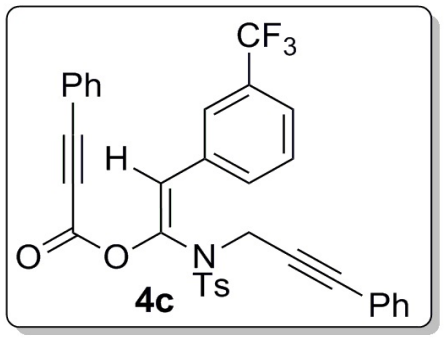





```
Current Data Parameters
NAME        K SURESH UPDATED 500
EXPNO                       122
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210728
Time                      10.02 h
INSTRUM                   spect
PROBHD    Z109128_0042 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         235
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                  125.7703659 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                       1.40
```

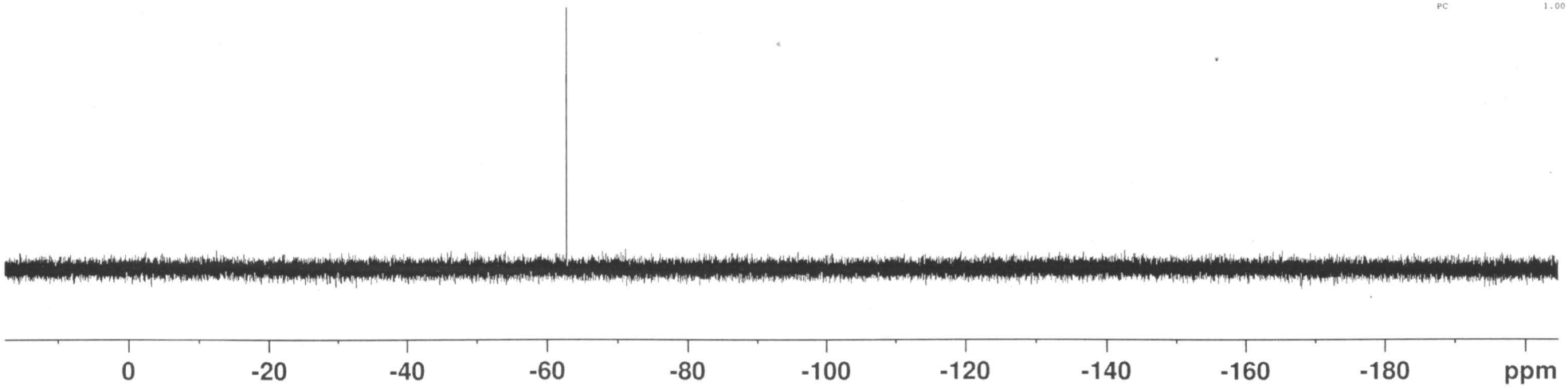


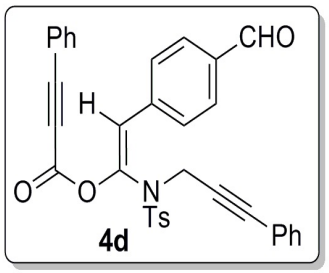
—62.79

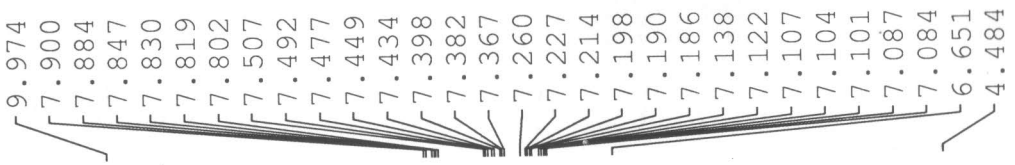
```
Current Data Parameters
NAME      K Suresh Ascend 500
EXPNO                  126
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210728
Time              15.21 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                    32
DS                     4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ             0.5767168 sec
RG                  7.96
DW                 4.400 usec
DE                 6.50 usec
TE                298.6 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

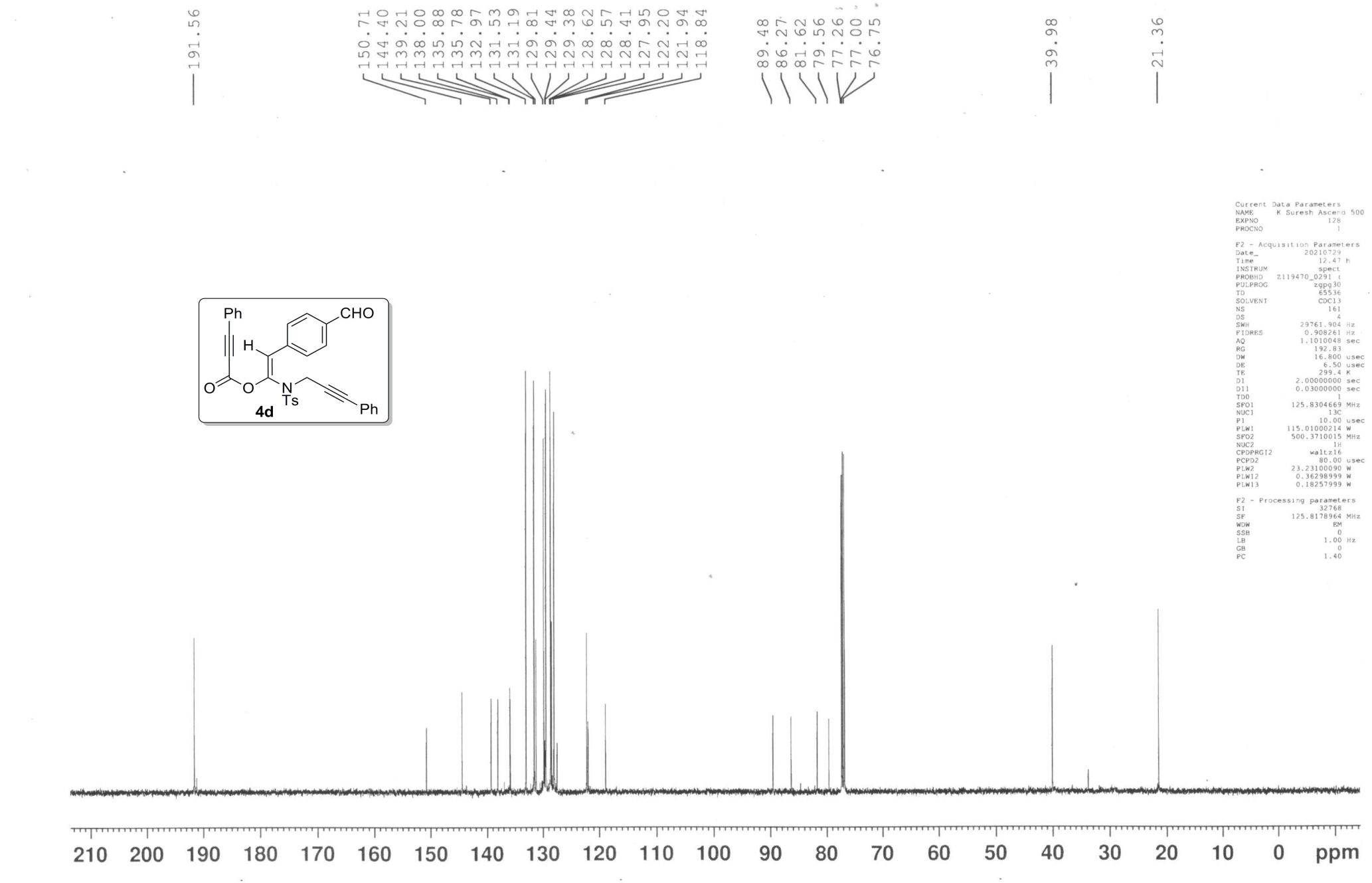
F2 - Processing parameters
SI                 65536
SF           470.8172619 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

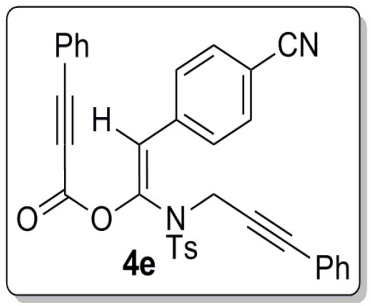


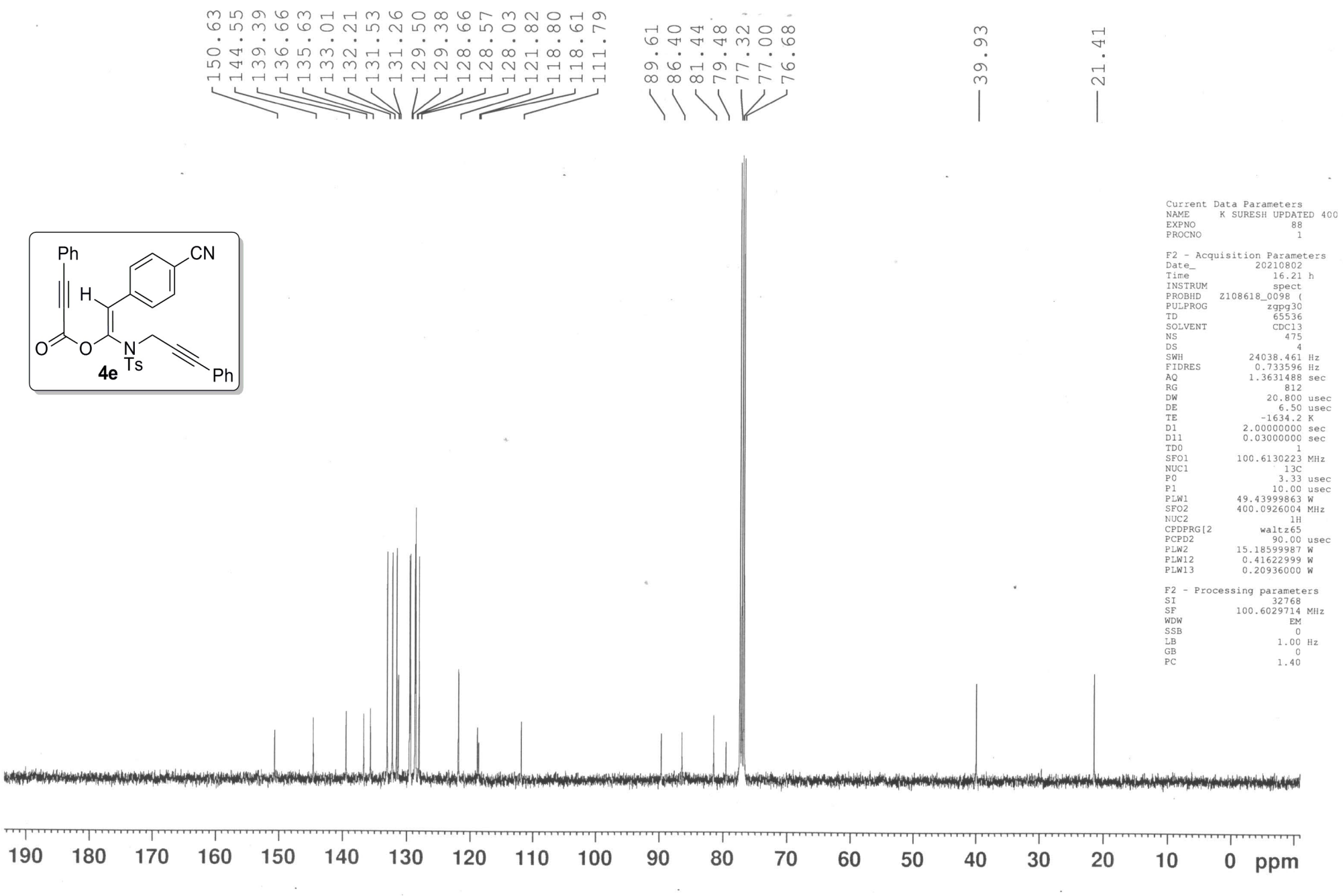

Ph
CHO
H
O
O
N
Ts
Ph
4d

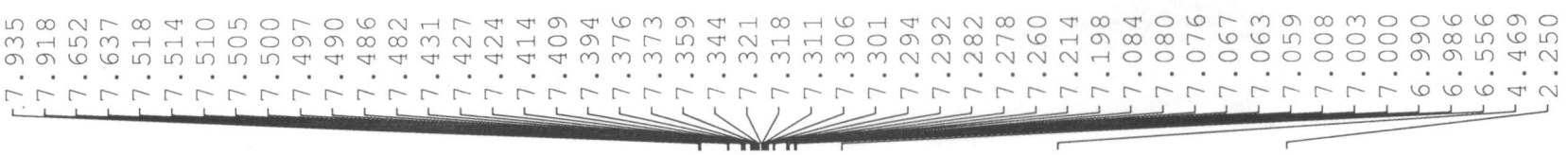

9.974
7.900
7.884
7.847
7.830
7.819
7.802
7.507
7.492
7.477
7.449
7.434
7.398
7.382
7.367
7.260
7.227
7.214
7.198
7.190
7.186
7.138
7.122
7.107
7.104
7.101
7.087
7.084
6.651
4.484
2.236

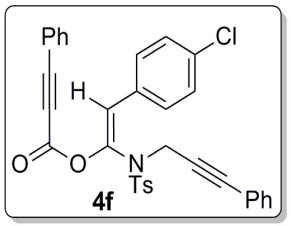
Current Data Parameters
NAME K Suresh Ascend 500
EXPNO 127
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210729
Time 12.37 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 298.6 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 500.3690117 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
0.97
2.00
4.00
1.01
1.99
2.06
3.02
4.06
1.01
2.00
3.03


191.56
150.71
144.40
139.21
138.00
135.88
135.78
132.97
131.53
131.19
129.81
129.44
129.38
128.62
128.57
128.41
127.95
122.20
121.94
118.84
89.48
86.27
81.62
79.56
77.26
77.00
76.75
39.98
21.36
Ph
CHO
H
O
O
N
Ts
Ph
4d
Current Data Parameters
NAME K Suresh Ascend 500
EXPNO 128
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210729
Time 12.47 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 161
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 299.4 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 125.8178964 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


Ph
CN
H
O
O
N
Ts
Ph
4e


150.63
144.55
139.39
136.66
135.63
133.01
132.21
131.53
131.26
129.50
129.38
128.66
128.57
128.03
121.82
118.80
118.61
111.79
89.61
86.40
81.44
79.48
77.32
77.00
76.68
39.93
21.41
Ph
CN
H
O
O
N
Ts
Ph
4e
Current Data Parameters
NAME K SURESH UPDATED 400
EXPNO 88
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210802
Time 16.21 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 475
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 -1634.2 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 100.6029714 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 0 ppm

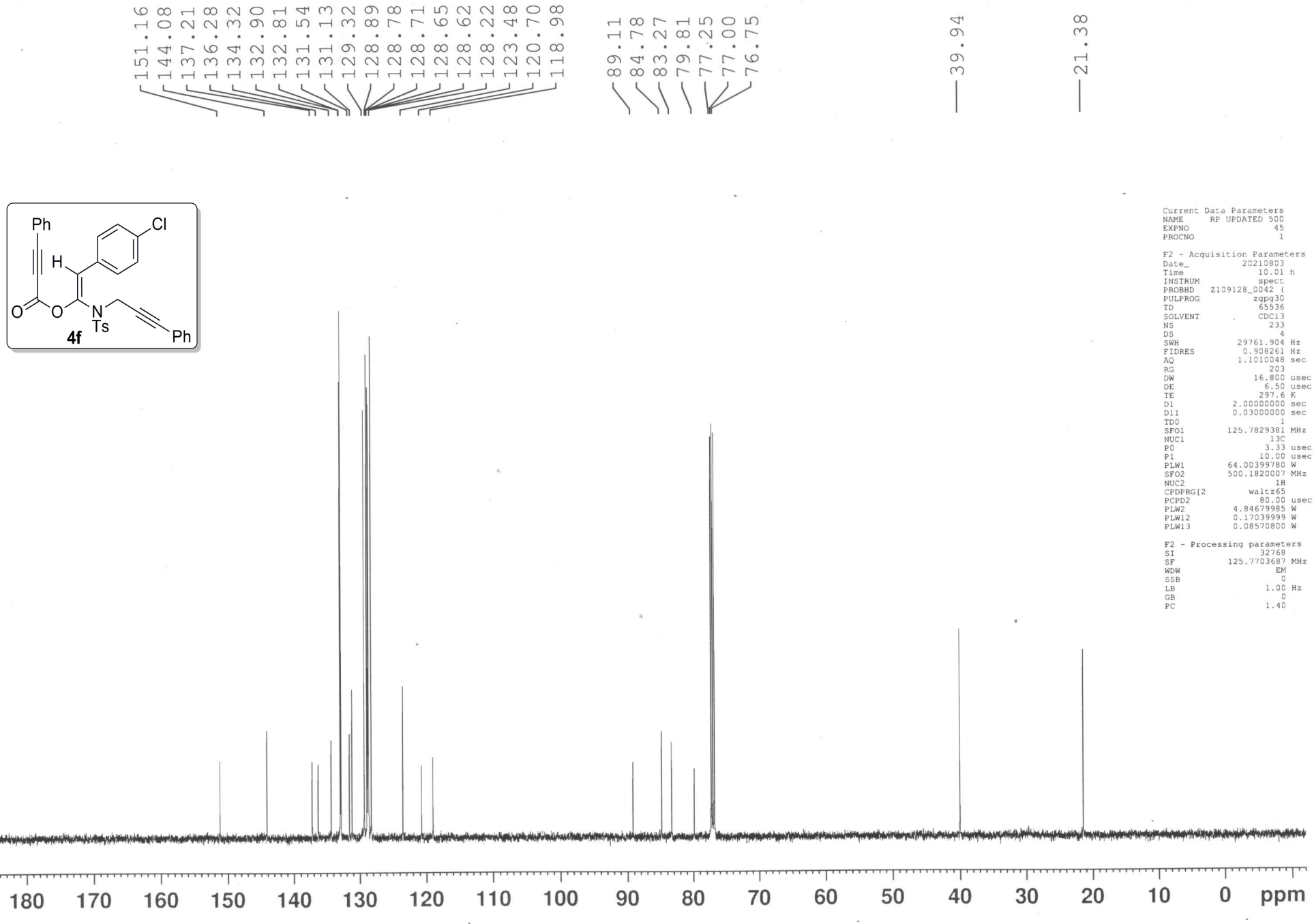


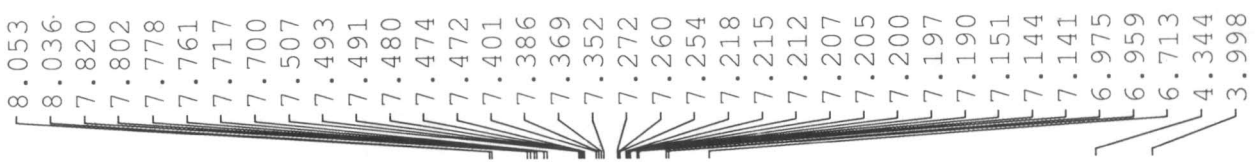


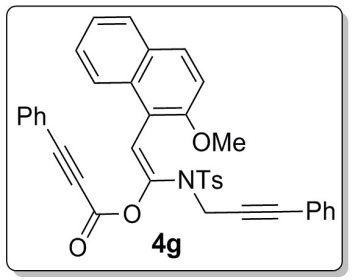
Current Data Parameters
NAME RP UPDATED 500
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210803
Time 9.48 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 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 500.1800109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


151.16
144.08
137.21
136.28
134.32
132.90
132.81
131.54
131.13
129.32
128.89
128.78
128.71
128.65
128.62
128.22
123.48
120.70
118.98
89.11
84.78
83.27
79.81
77.25
77.00
76.75
39.94
21.38
Ph
Cl
H
O
O
N
Ts
Ph
4f
Current Data Parameters
NAME RP UPDATED 500
EXPNO 45
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210803
Time 10.01 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 233
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 297.6 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 125.7703687 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

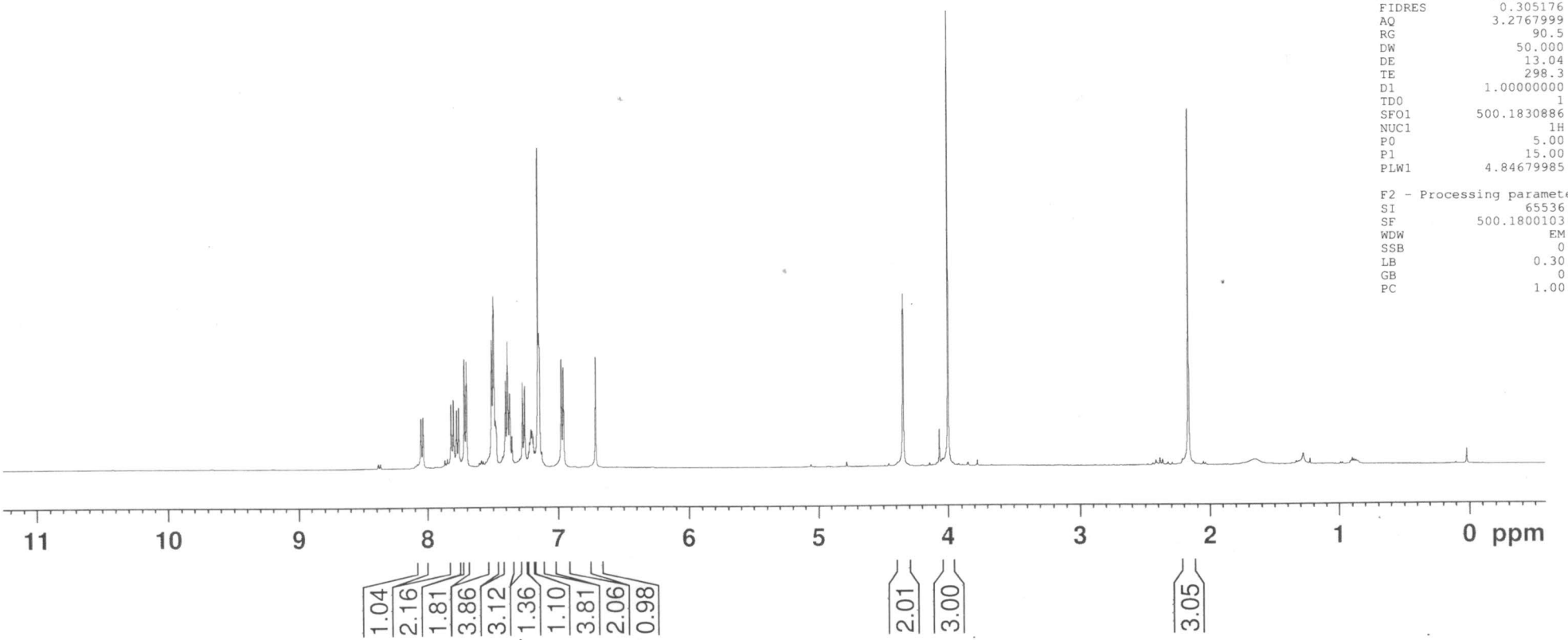


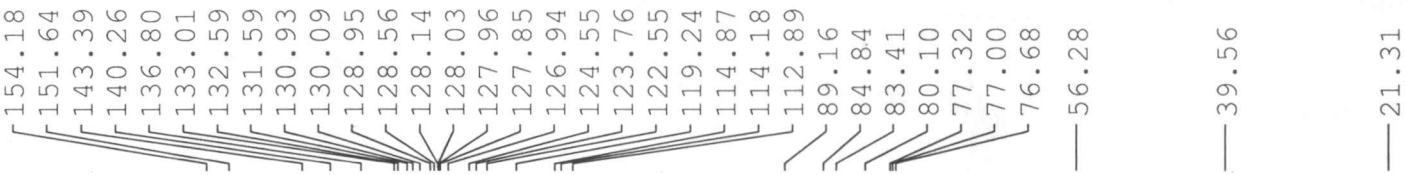


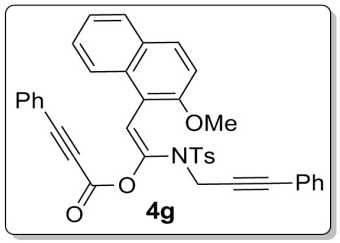
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 135
PROCNO 1

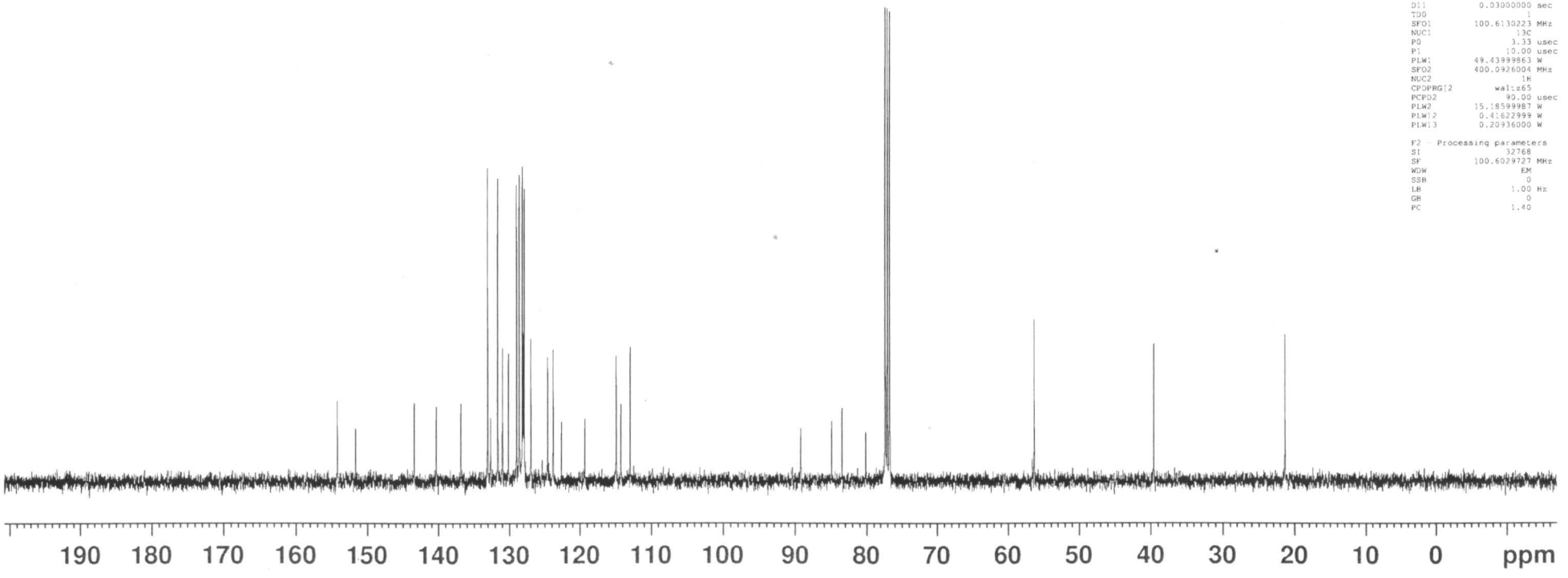
F2 - Acquisition Parameters
Date_ 20210812
Time 16.13 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 13.04 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W

F2 - Processing parameters
SI 65536
SF 500.1800103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





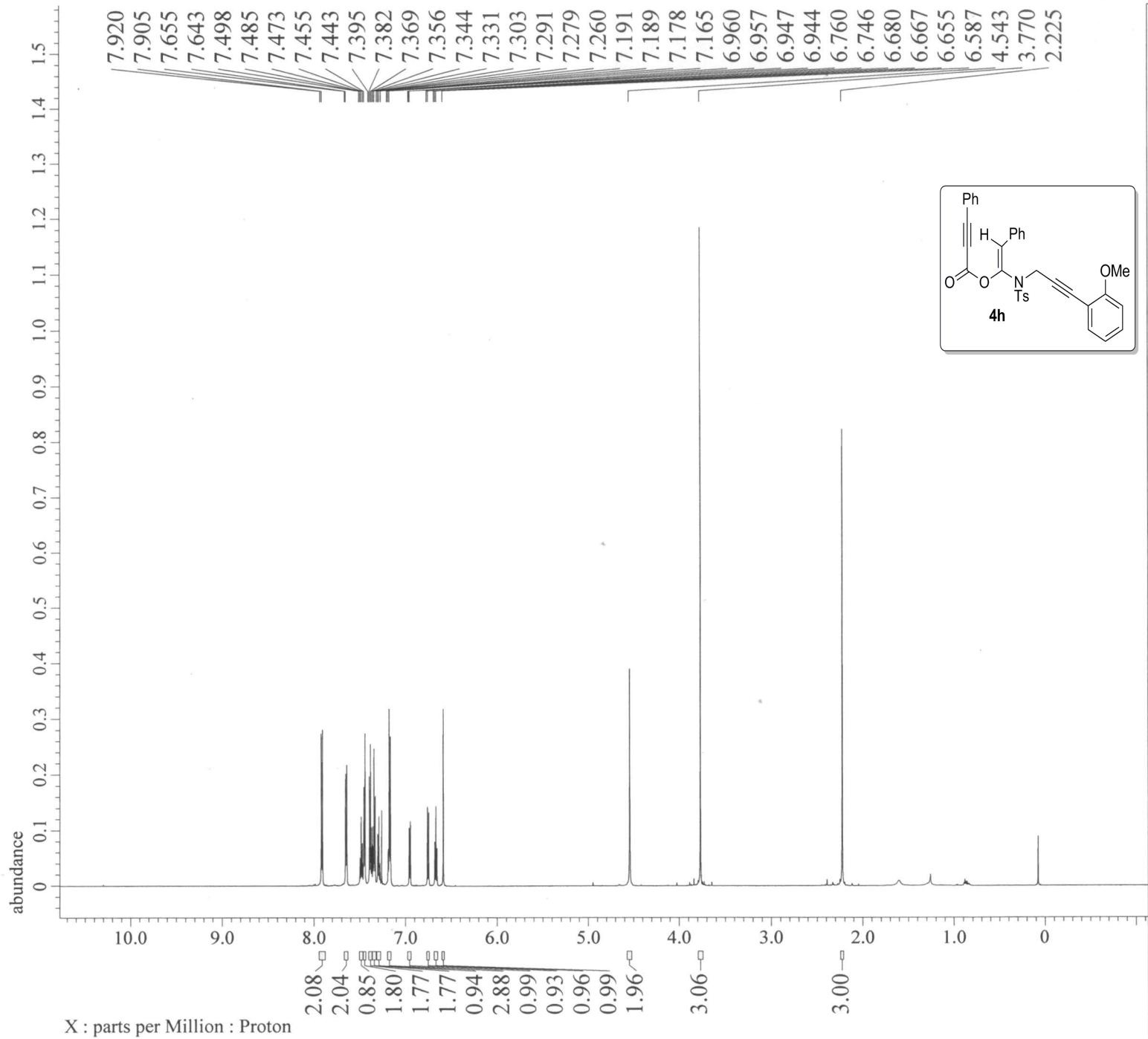




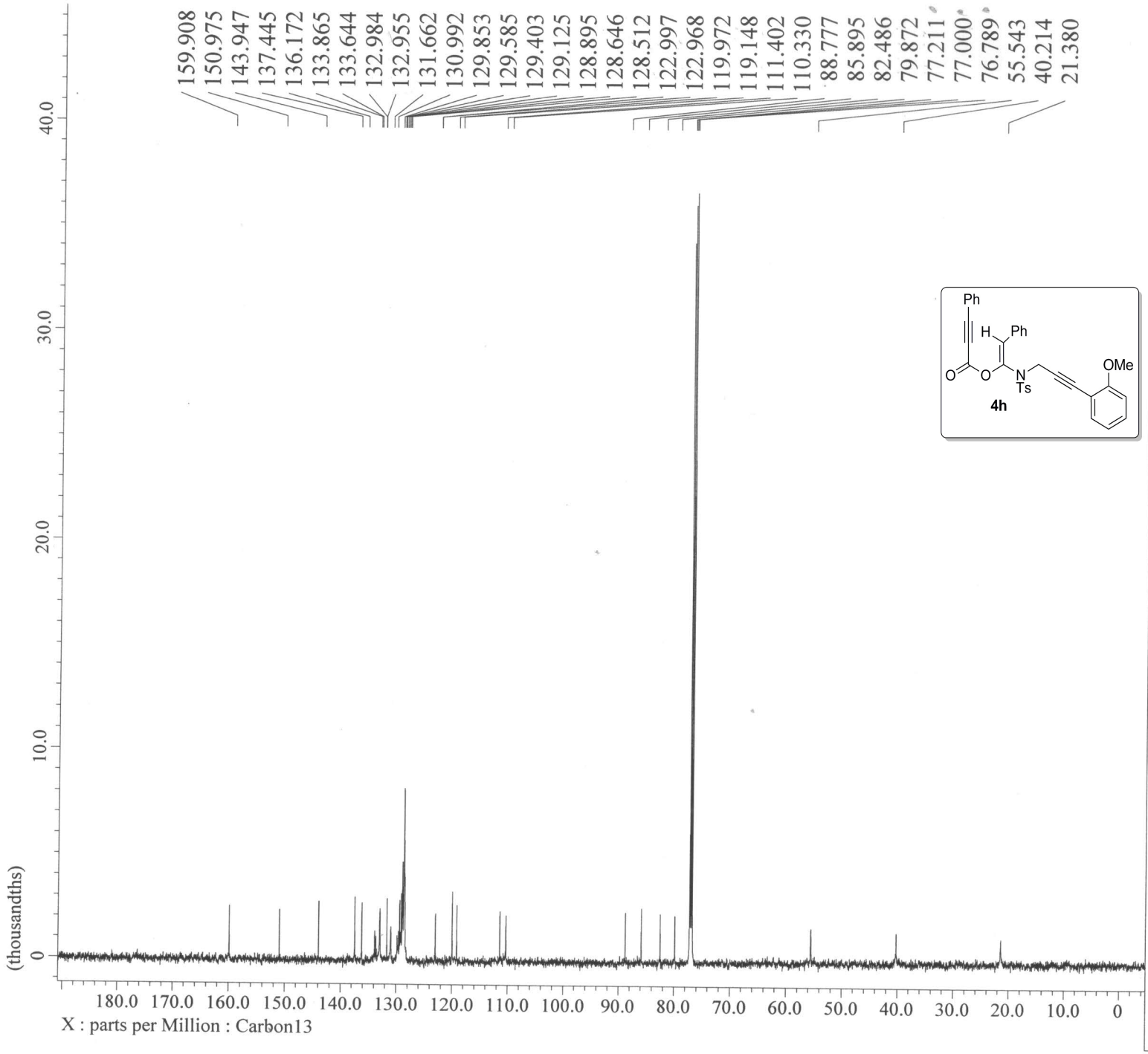

```
Current Data Parameters
NAME      K SURESH UPDATED 409
EXPNO                      92
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210812
Time                   16.05 h
INSTRUM                spect
PROBHD     Z108618_0098 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      268
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                   303.3 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

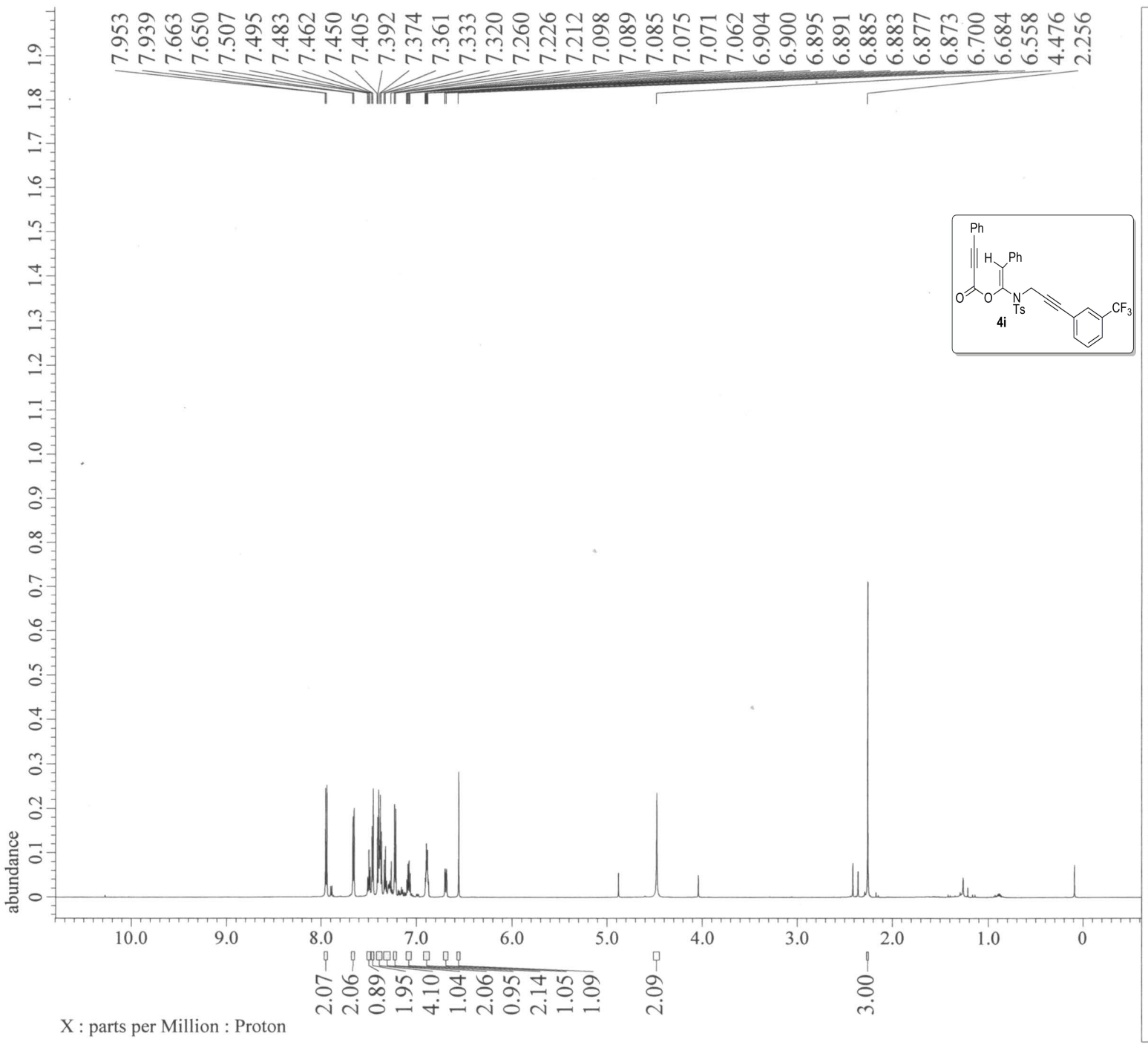
F2 - Processing parameters
SI                    32768
SF            100.6029727 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



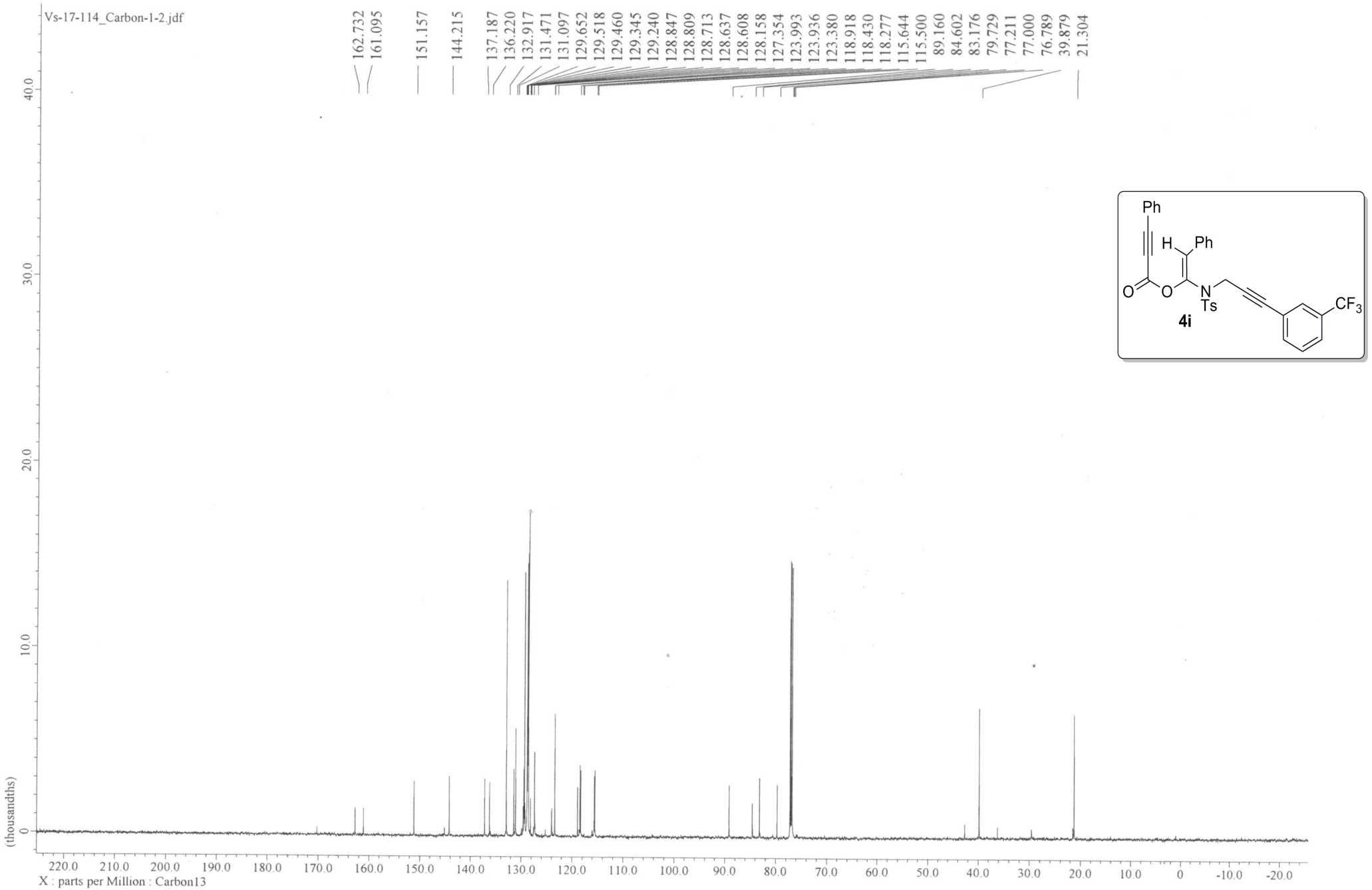
Filename	= Vs-19-105_Proton-1-3.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= Vs-19-105
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-FEB-2021 10:19:48
Revision_Time	= 15-AUG-2021 16:37:24
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.1[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]

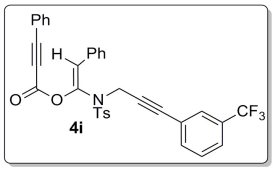


Filename	= Vs-19-105_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= Vs-19-105
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-FEB-2021 10:21:
Revision_Time	= 15-AUG-2021 16:41:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 402
Total_Scans	= 402
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.2[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]



Filename	= vs-19-114_Proton-1-4.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= vs-19-114
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2021 17:19:09
Revision_Time	= 15-AUG-2021 16:24:29
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 19.5[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]


Vs-17-114_Carbon-1-2.jdf
162.732
161.095
151.157
144.215
137.187
136.220
132.917
131.471
131.097
129.652
129.518
129.460
129.345
129.240
128.847
128.809
128.713
128.637
128.608
128.158
127.354
123.993
123.936
123.380
118.918
118.430
118.277
115.644
115.500
89.160
84.602
83.176
79.729
77.211
77.000
76.789
39.879
21.304
40.0
30.0
20.0
10.0
0
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13
Ph
H
Ph
O
O
N
Ts
CF3
4i



4i

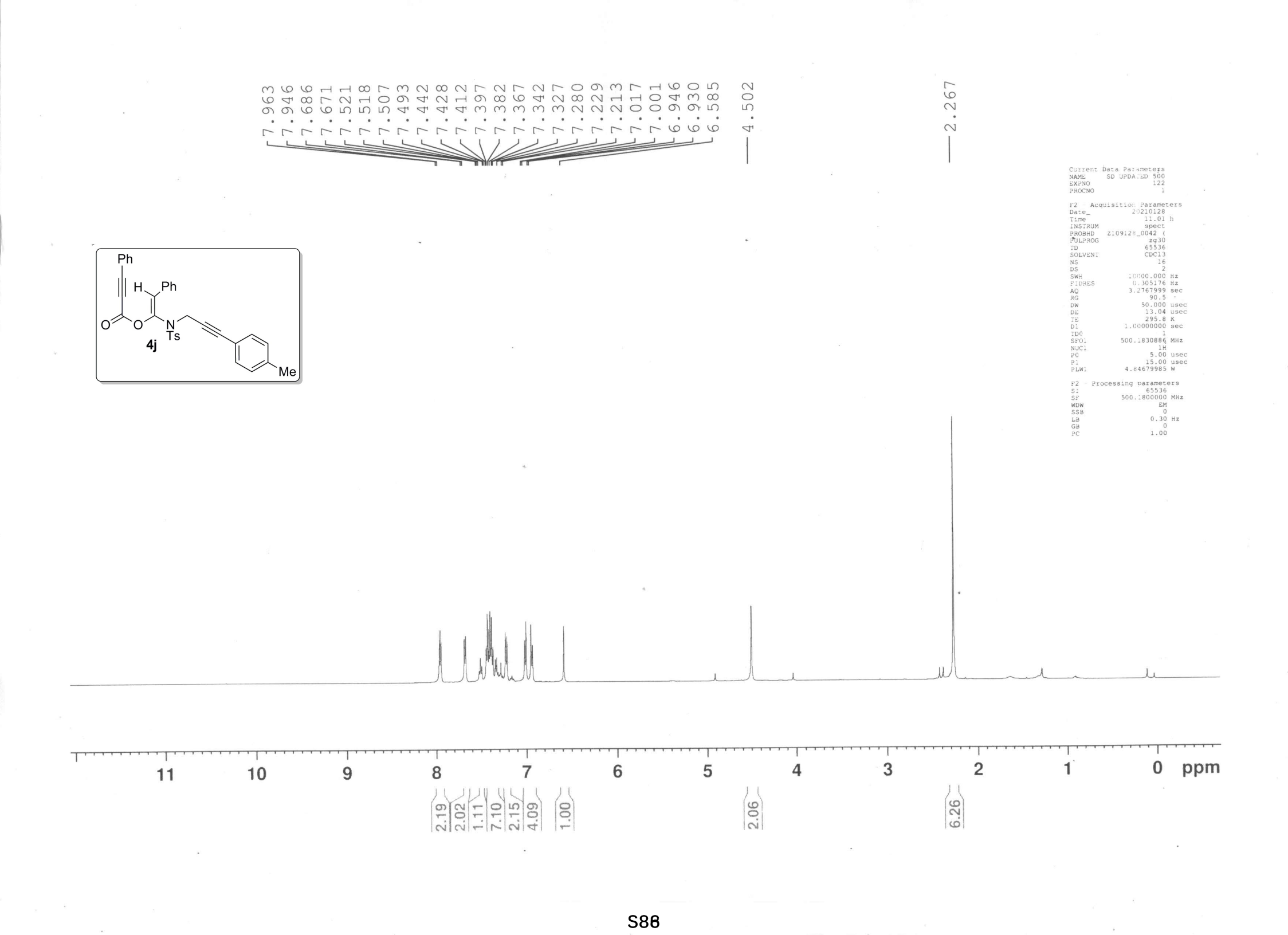
-62.96

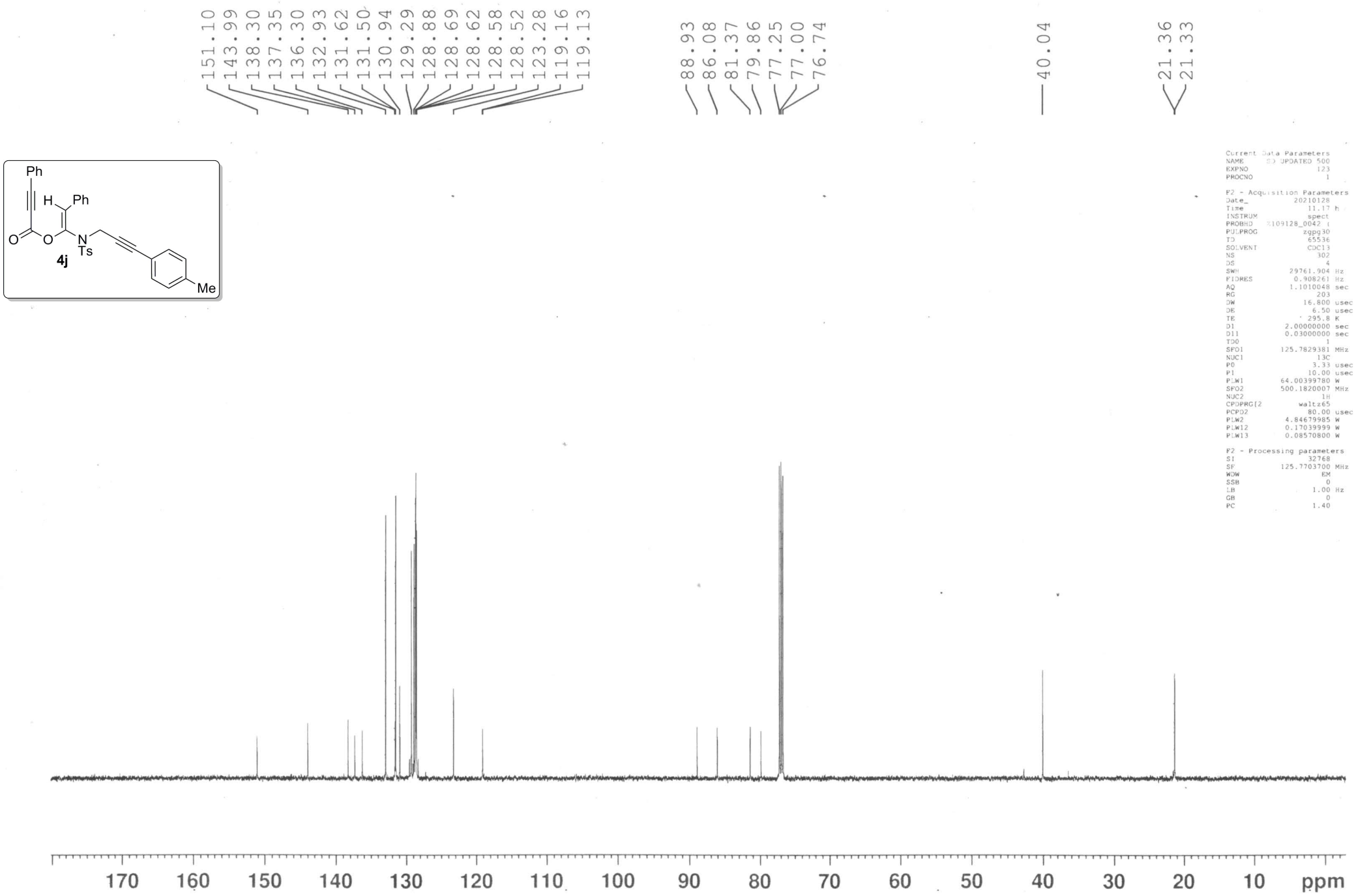
```
Current Data Parameters
NAME      K SURESH UPDATED 500
EXPNO                  143
PROCNO                   1

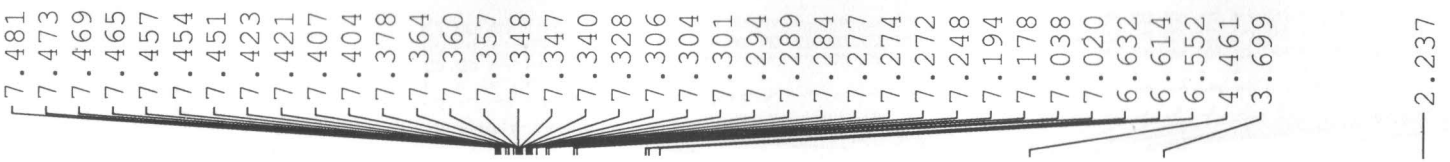
F2 - Acquisition Parameters
Date_           20210915
Time              10.07 h
INSTRUM             spect
PROBHD   Z109128_0042 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDC13
NS                     16
DS                      4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ              0.5767168 sec
RG                    456
DW                4.400 usec
DE                6.50 usec
TE                298.1 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

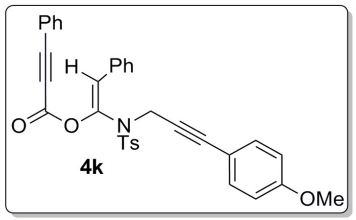
F2 - Processing parameters
SI                 65536
SF          470.6394242 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 ppm


7.963
7.946
7.686
7.671
7.521
7.518
7.507
7.493
7.442
7.428
7.412
7.397
7.382
7.367
7.342
7.327
7.280
7.229
7.213
7.017
7.001
6.946
6.930
6.585
4.502
2.267
Ph
H
Ph
O
O
N
Ts
4j
Me
Current Data Parameters
NAME SD_UPDA.ED_500
EXPNO 122
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210128
Time 11.01 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 295.8 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
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.19
2.02
1.11
7.10
2.15
4.09
1.00
2.06
6.26


151.10
143.99
138.30
137.35
136.30
132.93
131.62
131.50
130.94
129.29
128.88
128.69
128.62
128.58
128.52
123.28
119.16
119.13
88.93
86.08
81.37
79.86
77.25
77.00
76.74
40.04
21.36
21.33
Ph
H
Ph
O
O
N
Ts
4j
Me
Current Data Parameters
NAME SJ UPDATED 500
EXPNO 123
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210128
Time 11.17 h
INSTRUM spect
PROBHD %109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 302
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 295.8 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 125.7703700 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

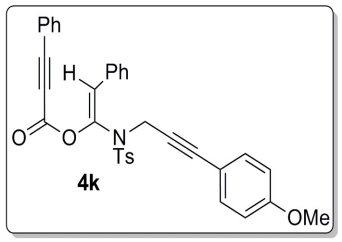





```
Current Data Parameters
NAME        SD ascend 500
EXPNO                357
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210122
Time              15.26 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                300.9 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            500.3690176 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

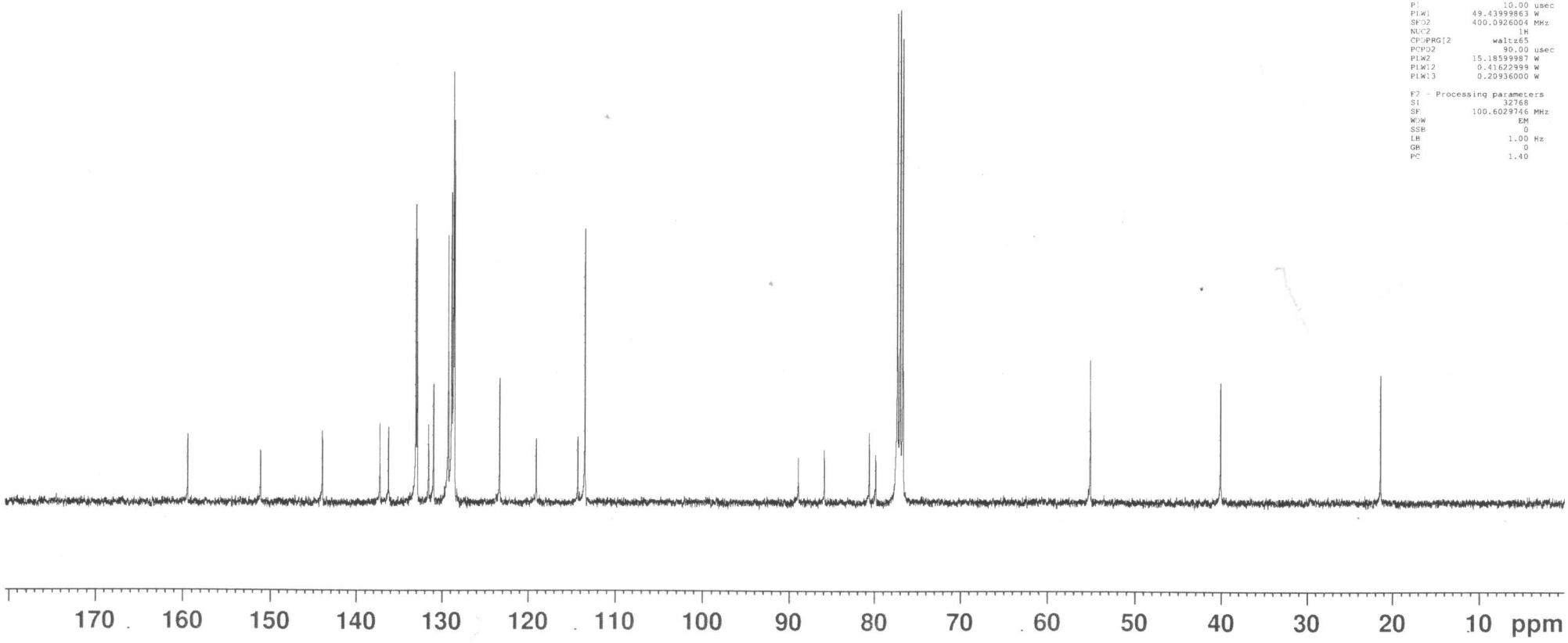


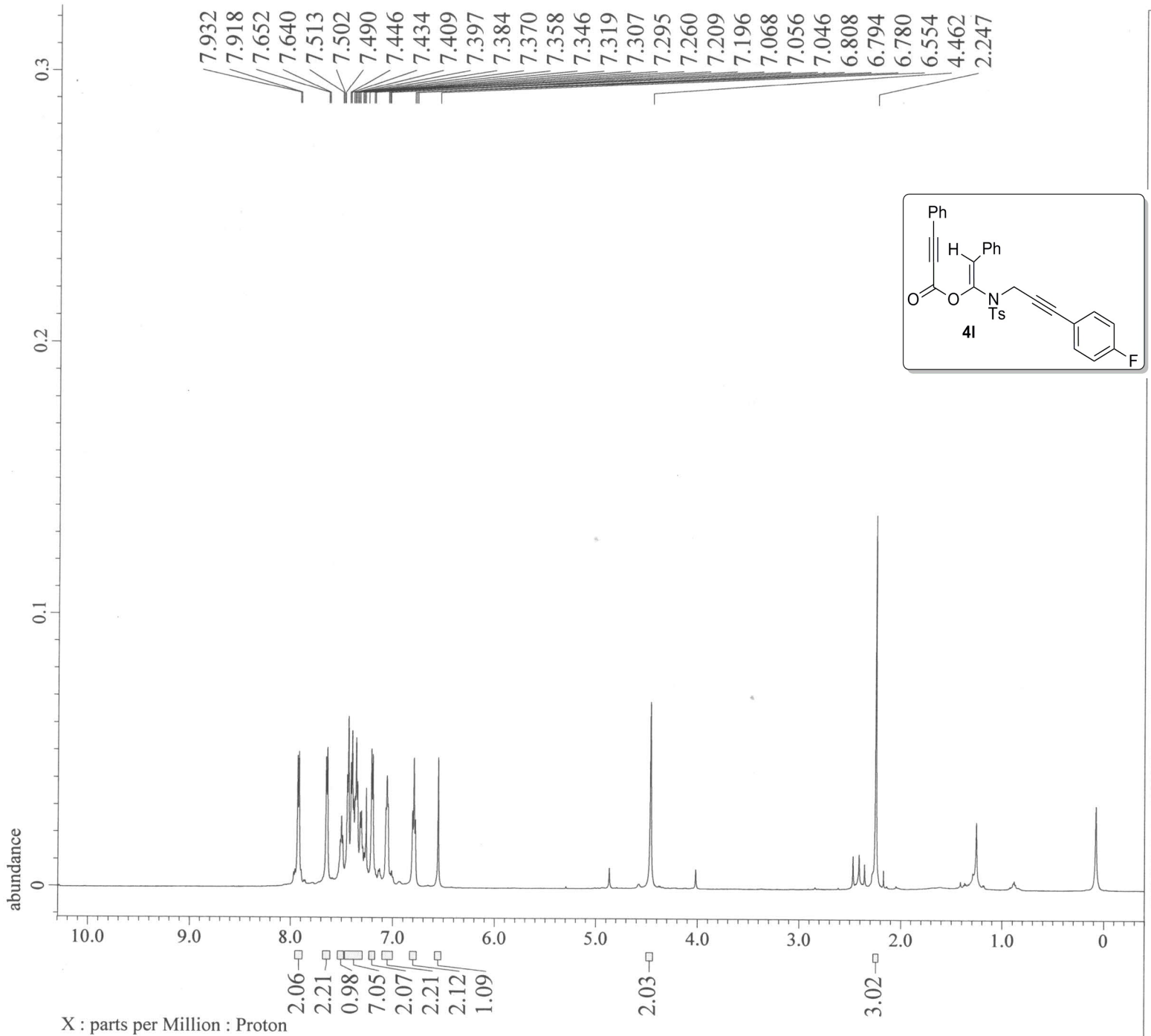
159.44
151.10
143.97
137.26
136.23
133.04
132.91
131.57
130.97
129.26
128.86
128.67
128.56
123.32
119.06
114.27
113.45
88.91
85.87
80.60
79.84
77.32
77.00
76.68
55.09
40.06
21.38

Current Data Parameters
NAME SD_UPDATED_400
EXPNO 142
PROCNO 1

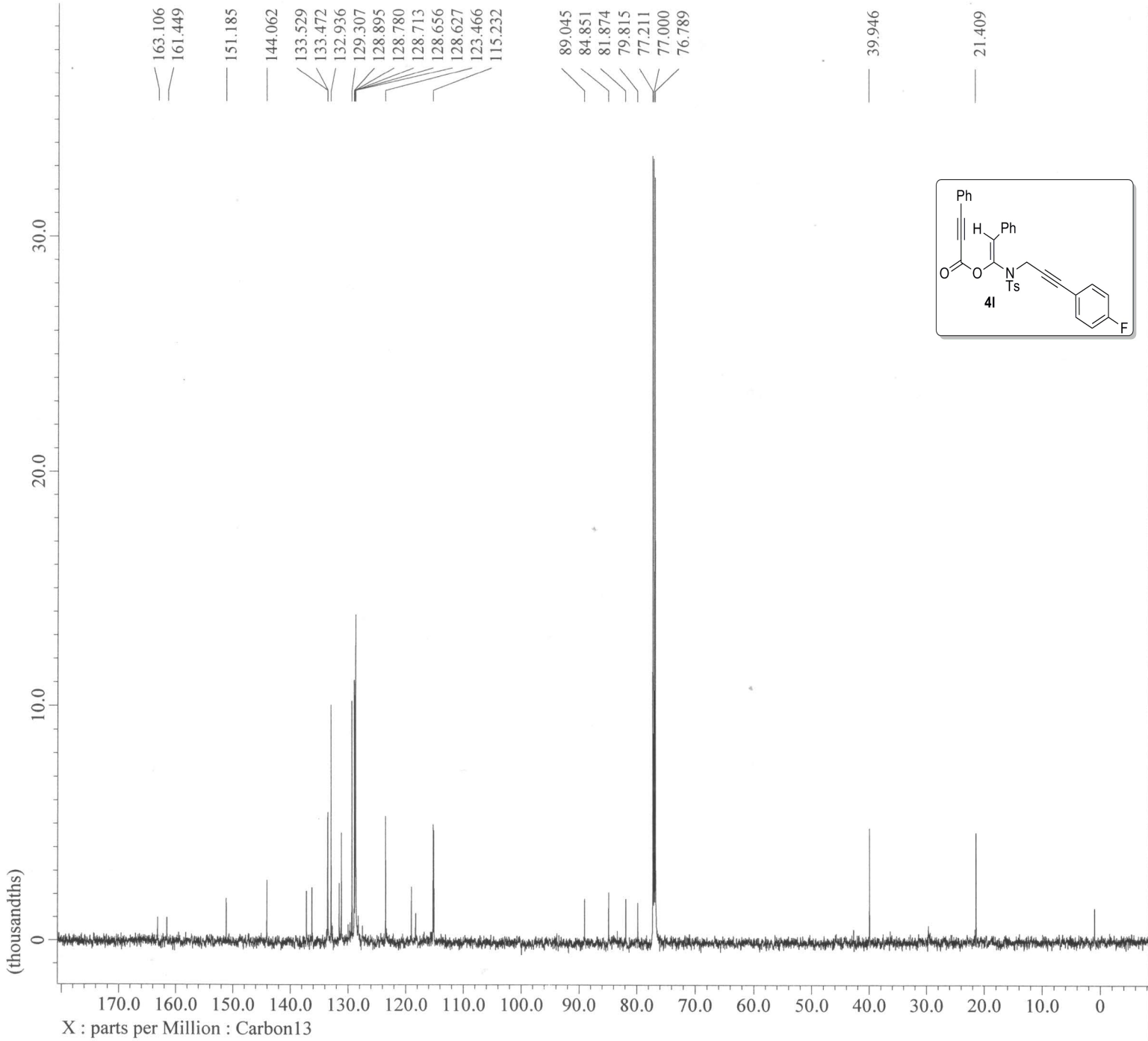
F2 - Acquisition Parameters
Date_ 20210127
Time 11.51 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 812
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6130223 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 100.6029746 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



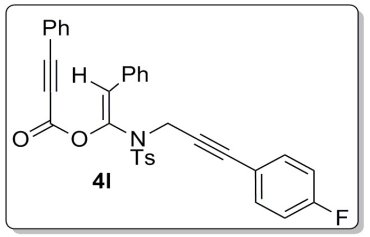


Filename	= vs-19-107_Proton-1-4.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= vs-19-107
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2021 16:56:02
Revision_Time	= 15-AUG-2021 16:10:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 19.4[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]



JEOL

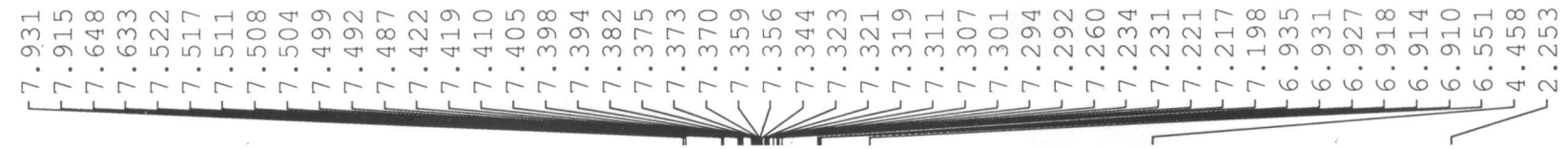
Filename	= vs-19-107_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= vs-19-107
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2021 16:58:
Revision_Time	= 23-JAN-2021 19:20:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.4[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0

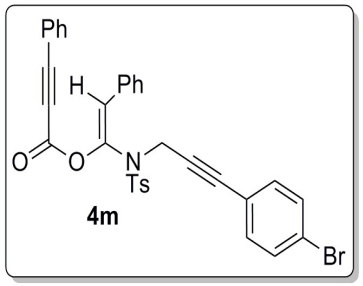



```
Current Data Parameters
NAME      K SURESH UPDATED 400
EXPNO                  108
PROCNO                   1

F2 - Acquisition Parameters
Date_               20211103
Time                   16.17 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                      724
DW                    5.600 usec
DE                    6.50 usec
TE                    580.1 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
```





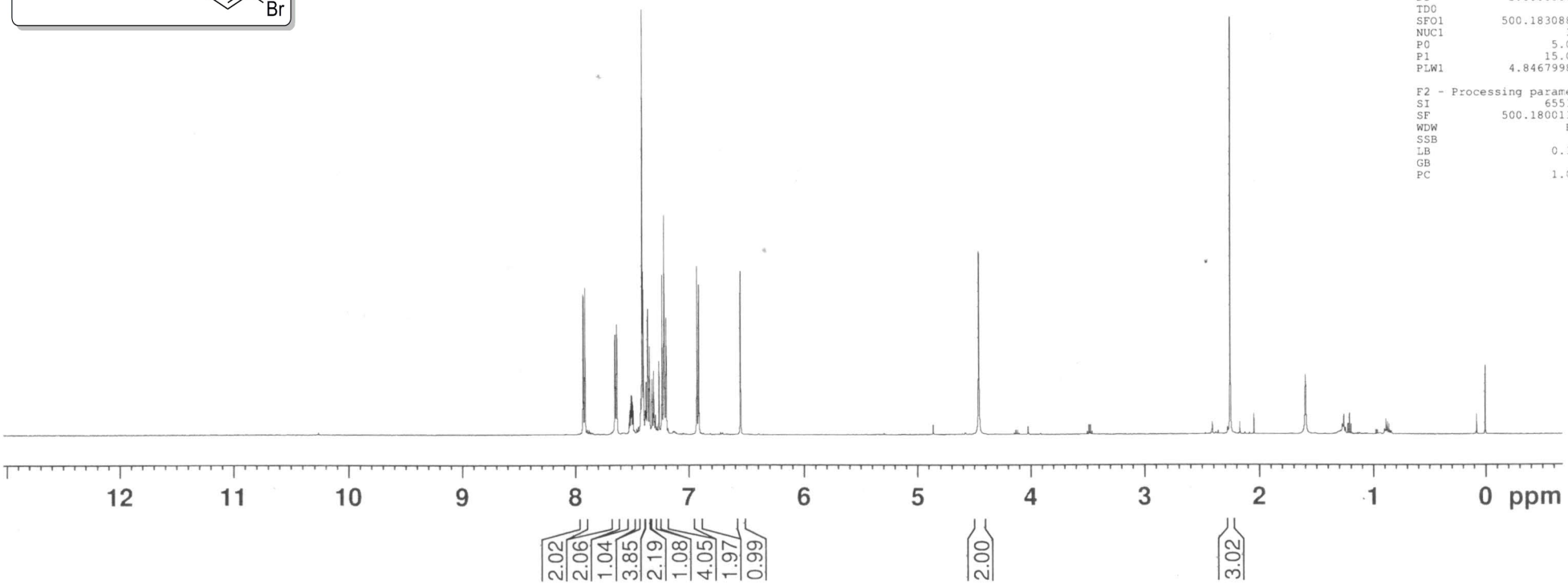
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 116
PROCNO 1

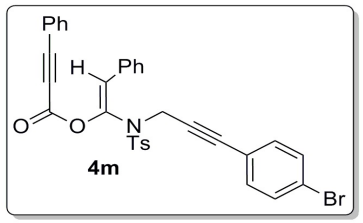
F2 - Acquisition Parameters

Date_	20210722
Time	13.22 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	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	500.1800110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





151.19
144.11
137.13
136.22
133.02
132.92
131.50
131.16
129.33
128.89
128.81
128.72
128.67
123.55
122.57
121.14
118.95

89.12
84.82
83.43
79.79
77.32
77.00
76.68

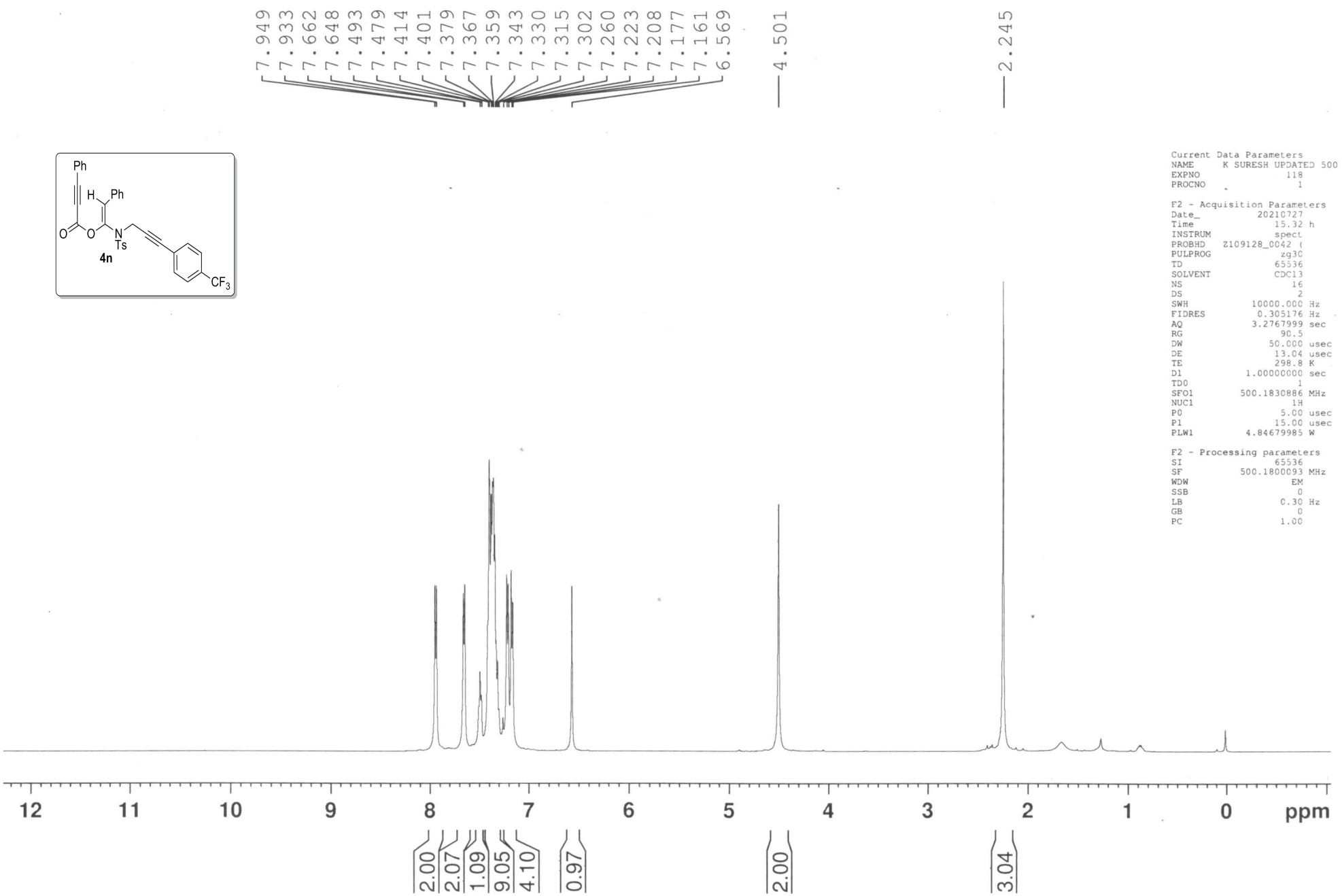
39.94

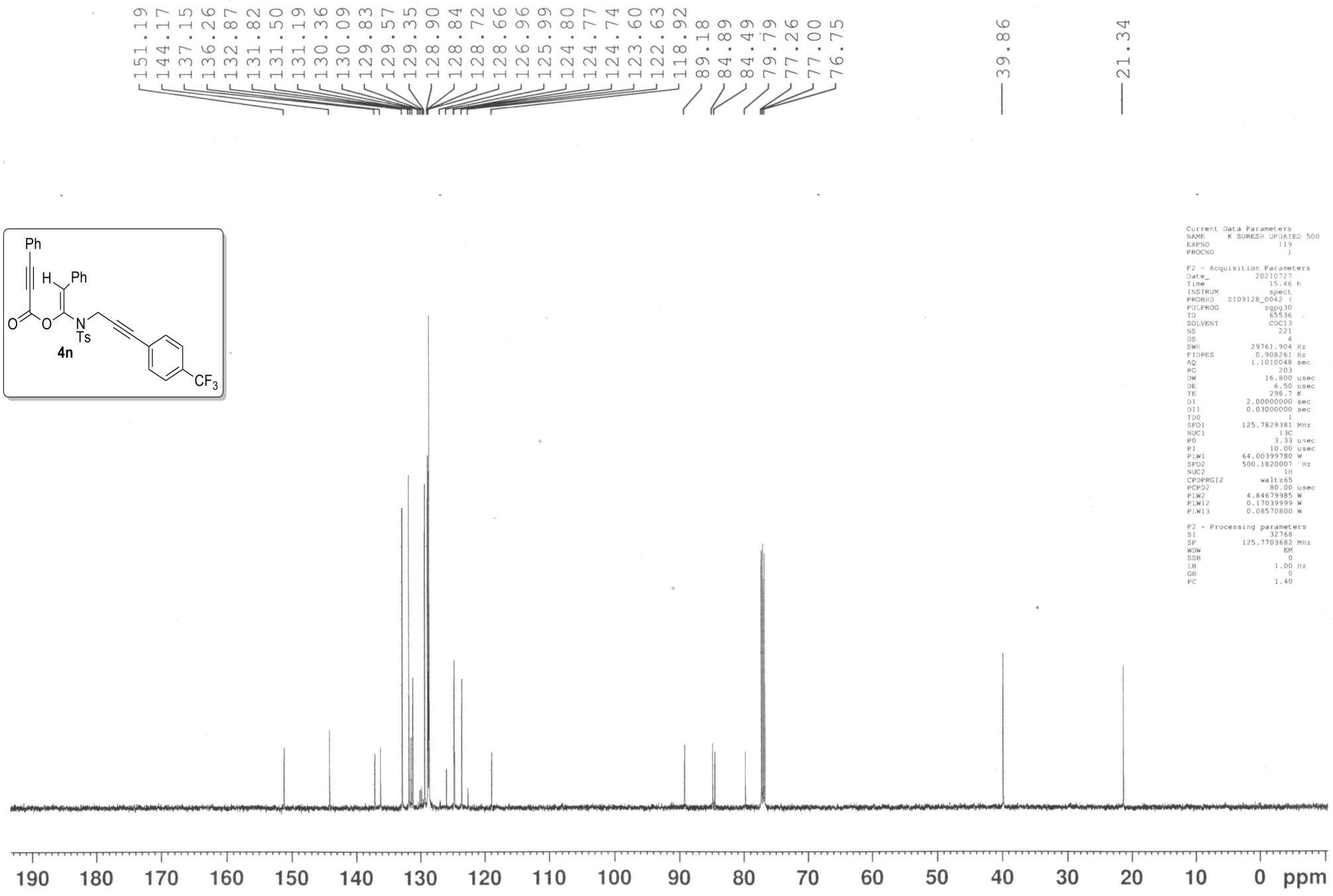
21.43

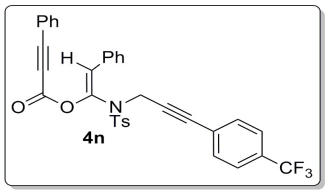
```
Current Data Parameters
NAME       K SURESH UPDATED 400
EXPNO              82
PROCNO              1

F2 - Acquisition Parameters
Date_          20210723
Time             17.29 h
INSTRUM            spect
PROBHD   Z108618_0098 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
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               878.1 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           100.6029703 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


7.949
7.933
7.662
7.648
7.493
7.479
7.414
7.401
7.379
7.367
7.359
7.343
7.330
7.315
7.302
7.260
7.223
7.208
7.177
7.161
6.569
4.501
2.245
Ph
H
Ph
O
O
N
Ts
4n
CF3
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 118
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210727
Time 15.32 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 298.8 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 500.1800093 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
2.00
2.07
1.09
9.05
4.10
0.97
2.00
3.04


151.19
144.17
137.15
136.26
132.87
131.82
131.50
131.19
130.36
130.09
129.83
129.57
129.35
128.90
128.84
128.72
128.66
126.96
125.99
124.80
124.77
124.74
123.60
122.63
118.92
89.18
84.89
84.49
79.79
77.26
77.00
76.75
39.86
21.34
Ph
H
Ph
O
O
N
Ts
4n
CF3
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 119
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210727
Time 15.46 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 221
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 298.7 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 125.7703682 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 0 ppm

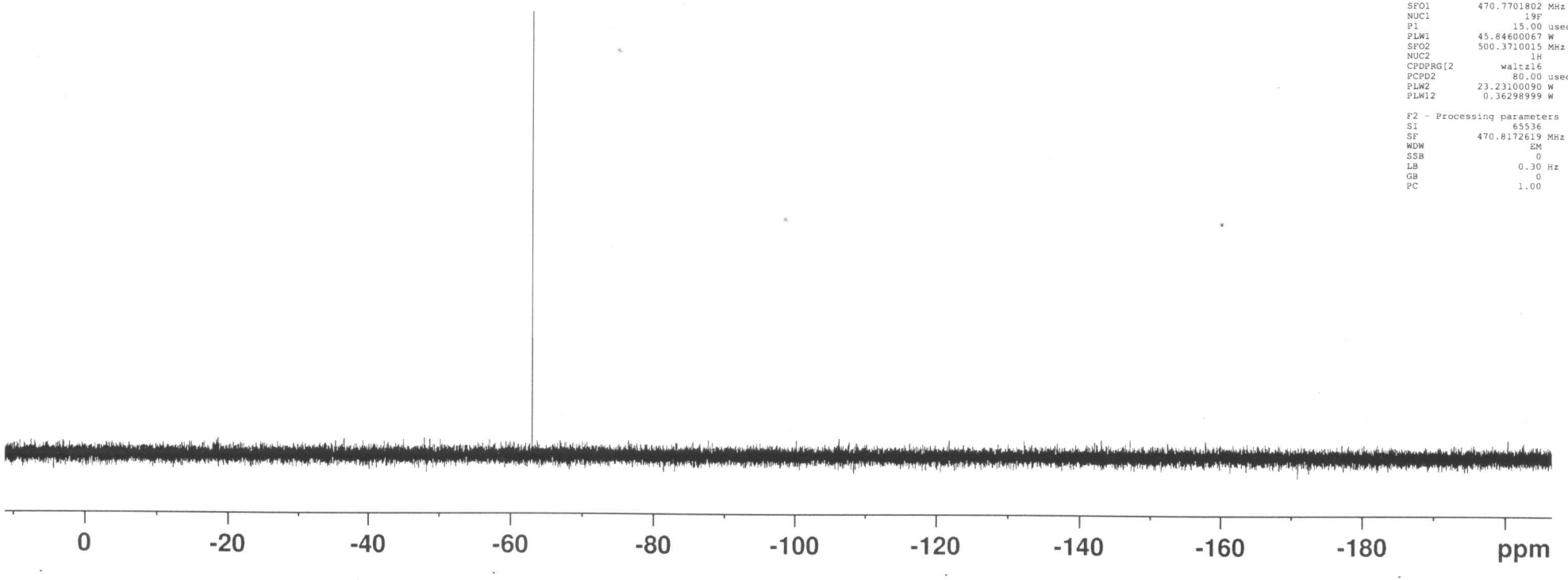


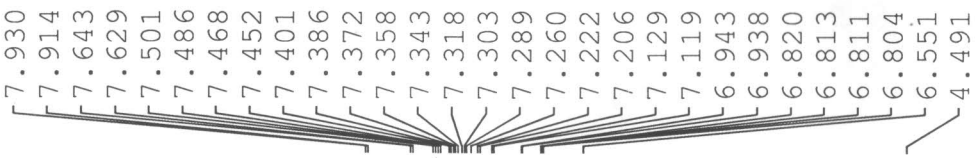
-62.94

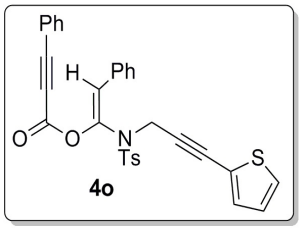
```
Current Data Parameters
NAME      K Suresh Ascend 500
EXPNO                  125
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210728
Time              15.15 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     32
DS                      4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ              0.5767168 sec
RG                   7.96
DW                4.400 usec
DE                6.50 usec
TE                298.6 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
```



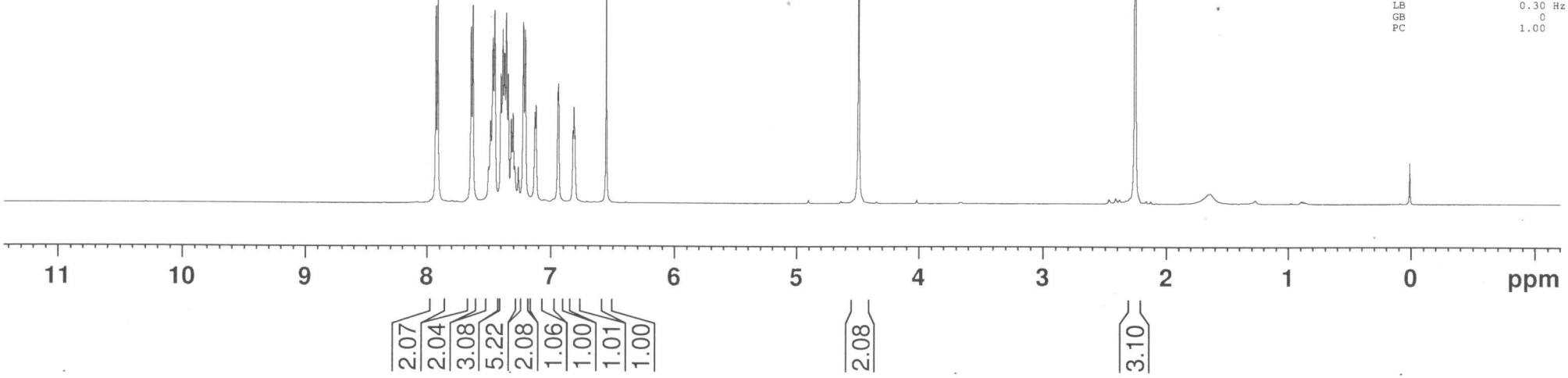


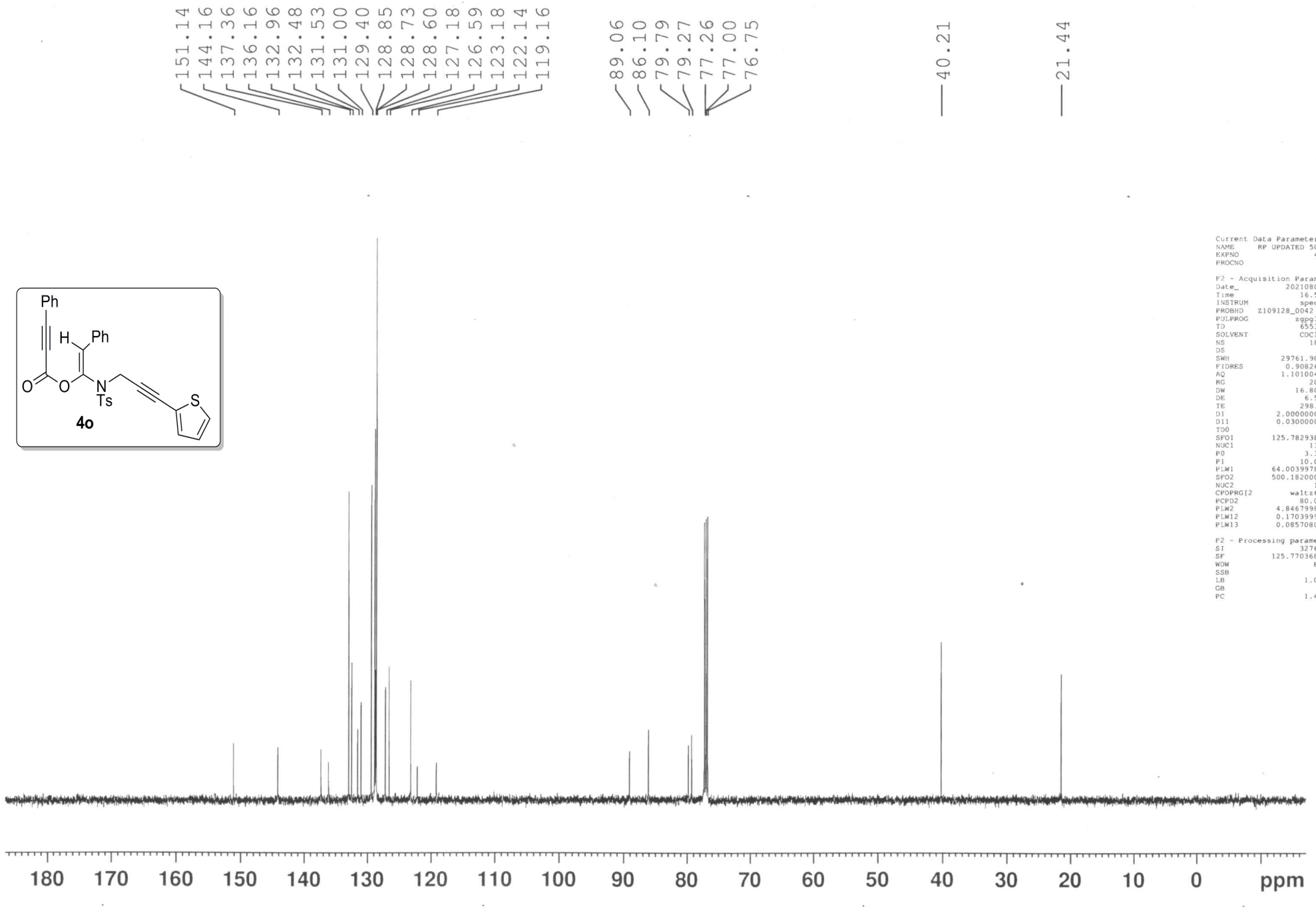


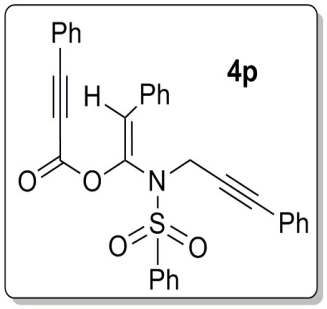

```
Current Data Parameters
NAME        RP UPDATED 500
EXPNO                  42
PROCNO                  1

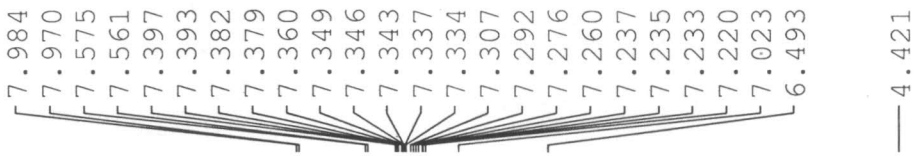
F2 - Acquisition Parameters
Date_            20210802
Time                16.40 h
INSTRUM              spect
PROBHD    Z109128_0042 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES              0.305176 Hz
AQ                3.2767999 sec
RG                    114
DW                 50.000 usec
DE                 13.04 usec
TE                 297.5 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

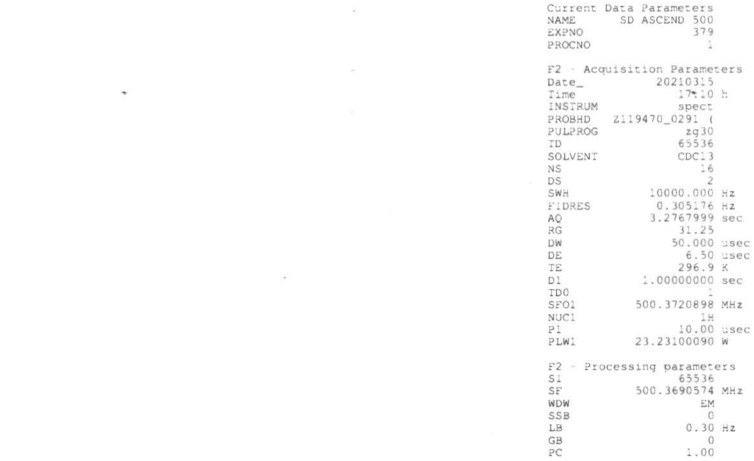
F2 - Processing parameters
SI                  65536
SF              500.1800095 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




151.14
144.16
137.36
136.16
132.96
132.48
131.53
131.00
129.40
128.85
128.73
128.60
127.18
126.59
123.18
122.14
119.16
89.06
86.10
79.79
79.27
77.26
77.00
76.75
40.21
21.44
Ph
H
Ph
O
O
N
Ts
S
4o
Current Data Parameters
NAME RP UPDATED 500
EXPNO 43
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210802
Time 16.50 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 182
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 125.7703681 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



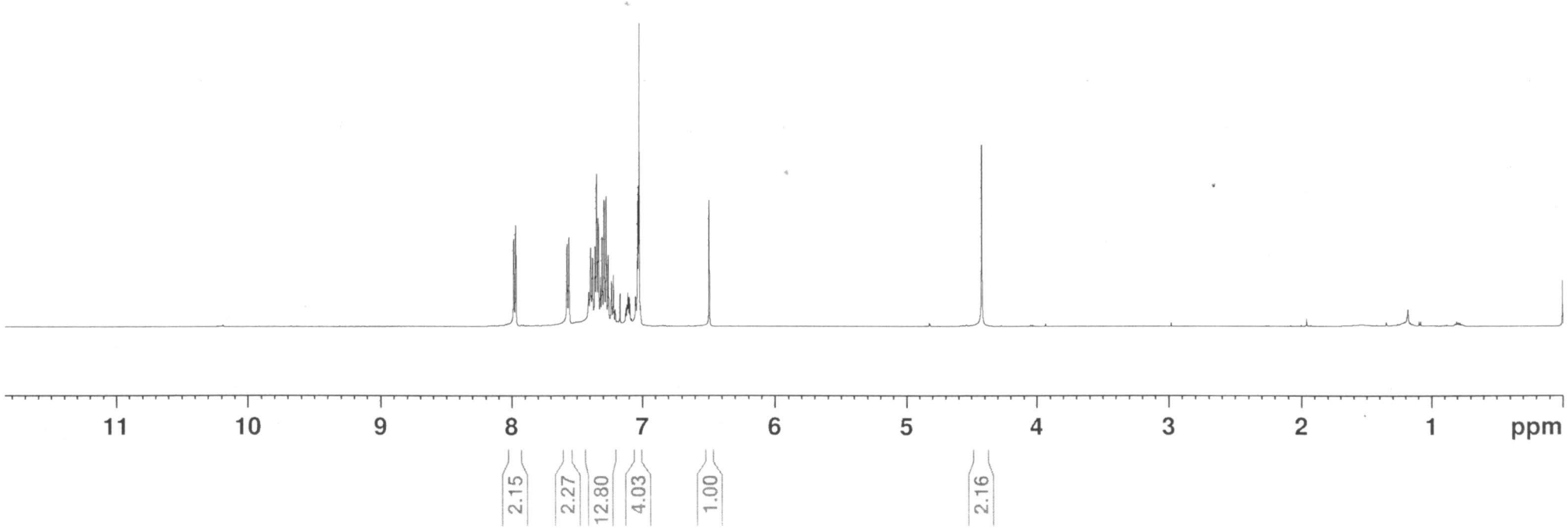


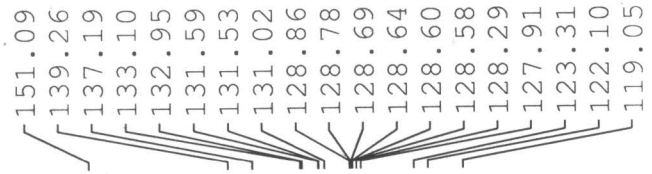


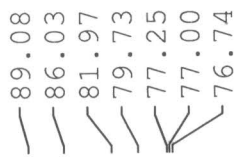
```
Current Data Parameters
NAME        SD ASCEND 500
EXPNO                379
PROCNO                 1

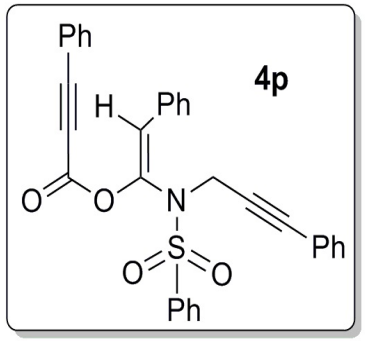
F2 - Acquisition Parameters
Date_           20210315
Time                17.10 h
INSTRUM              spect
PROBHD    Z119470_0291 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                  31.25
DW                 50.000 usec
DE                  6.50 usec
TE                 296.9 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            500.3690574 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```





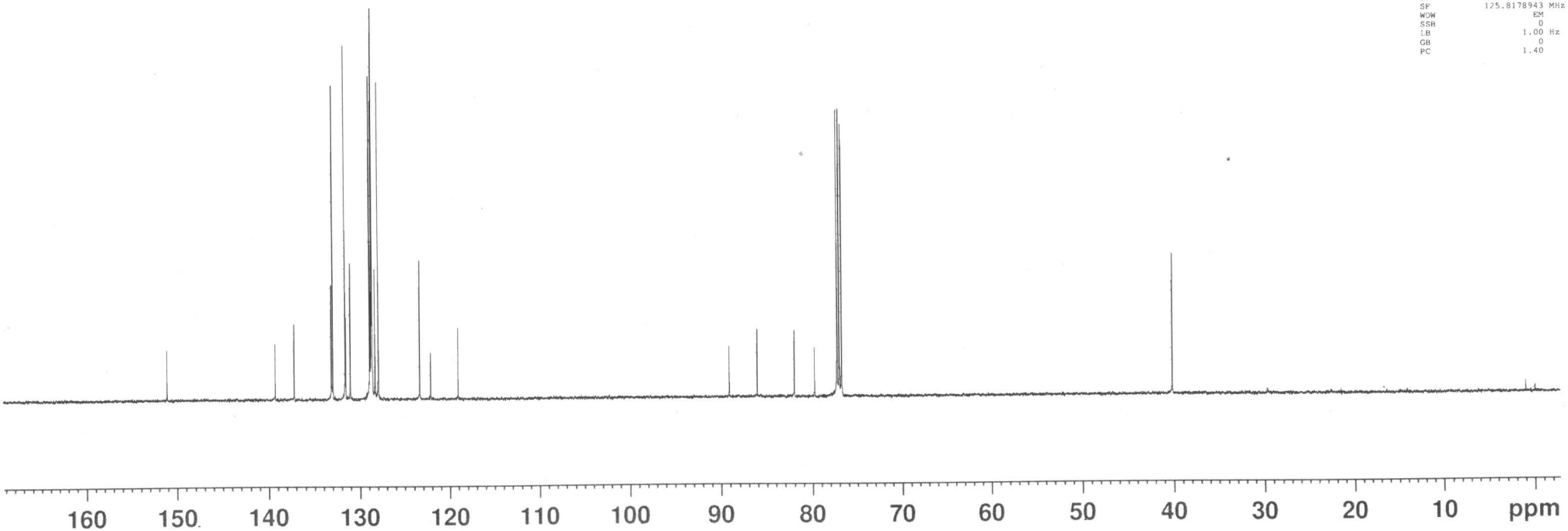


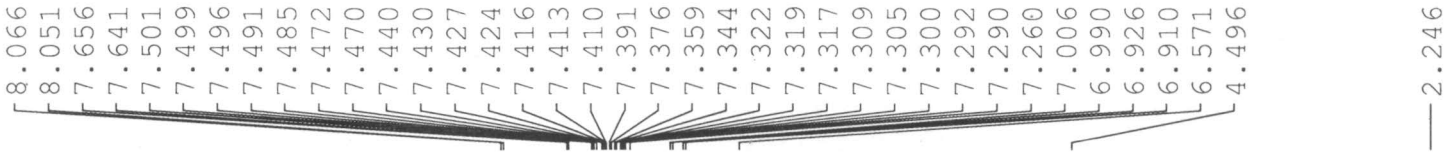


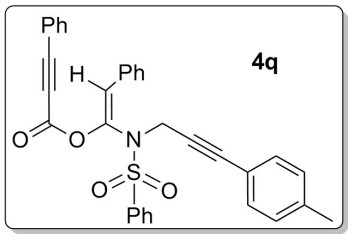

```
Current Data Parameters
NAME          SD ASCEND 500
EXPNO                  380
PROCNO                   1

F2 - Acquisition Parameters
Date_             20210316
Time                10.58 h
INSTRUM               spect
PROBHD     Z119470_0291 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     455
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                   299.3 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             125.8178943 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



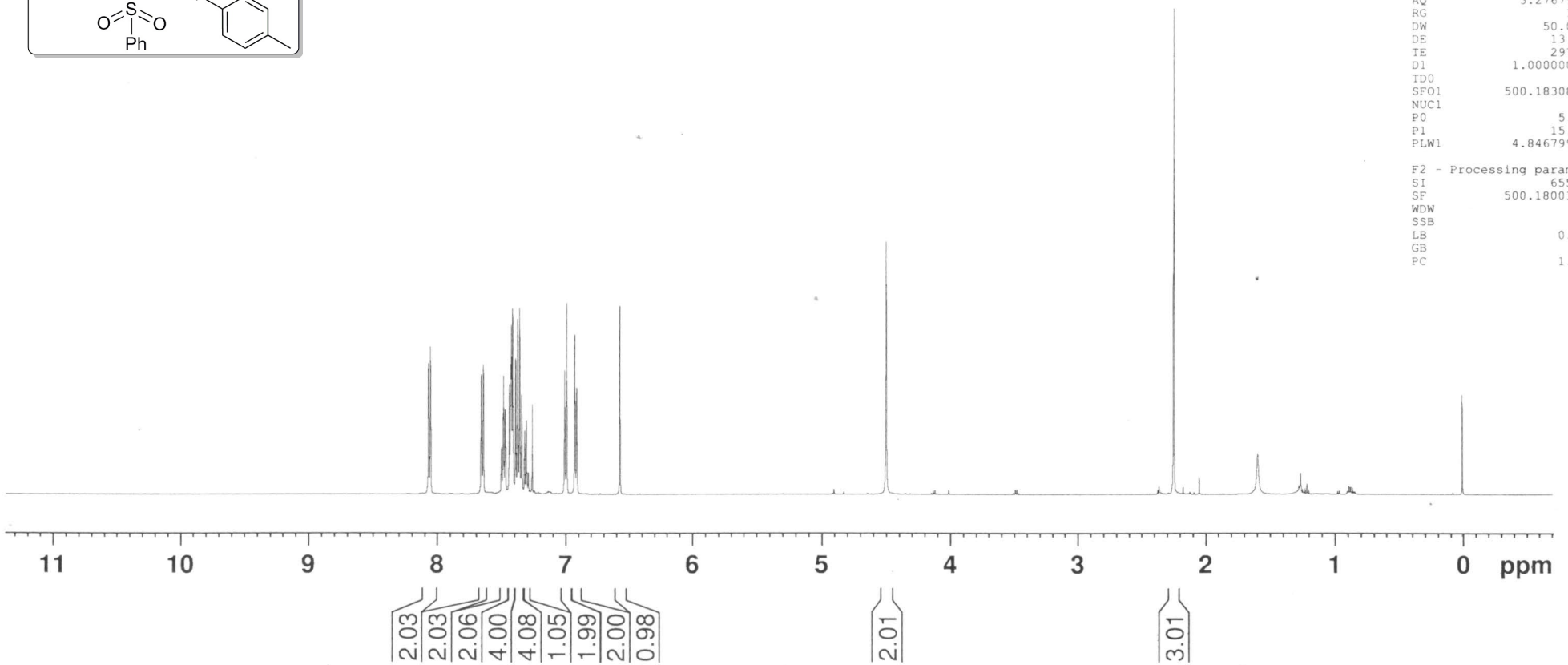


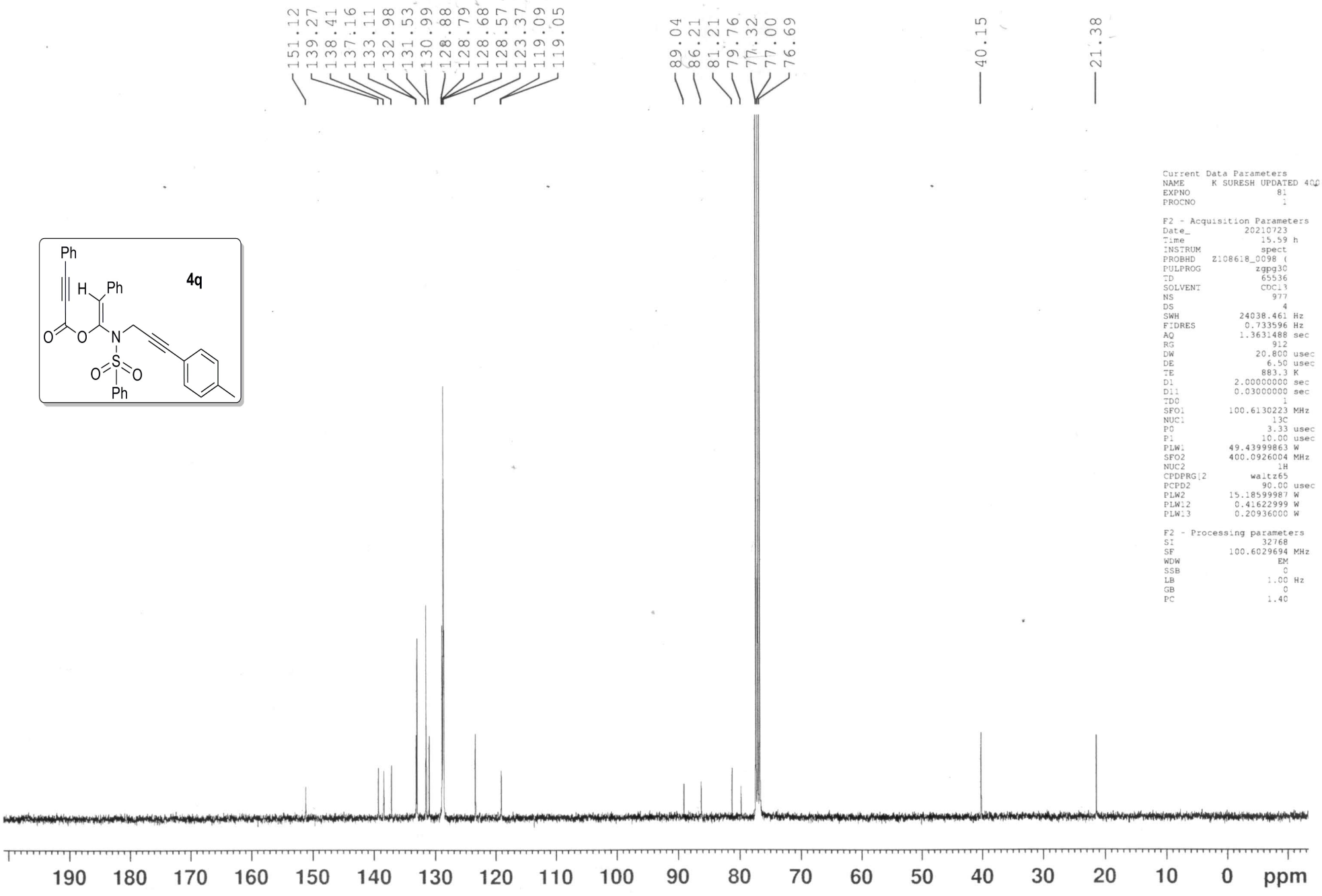


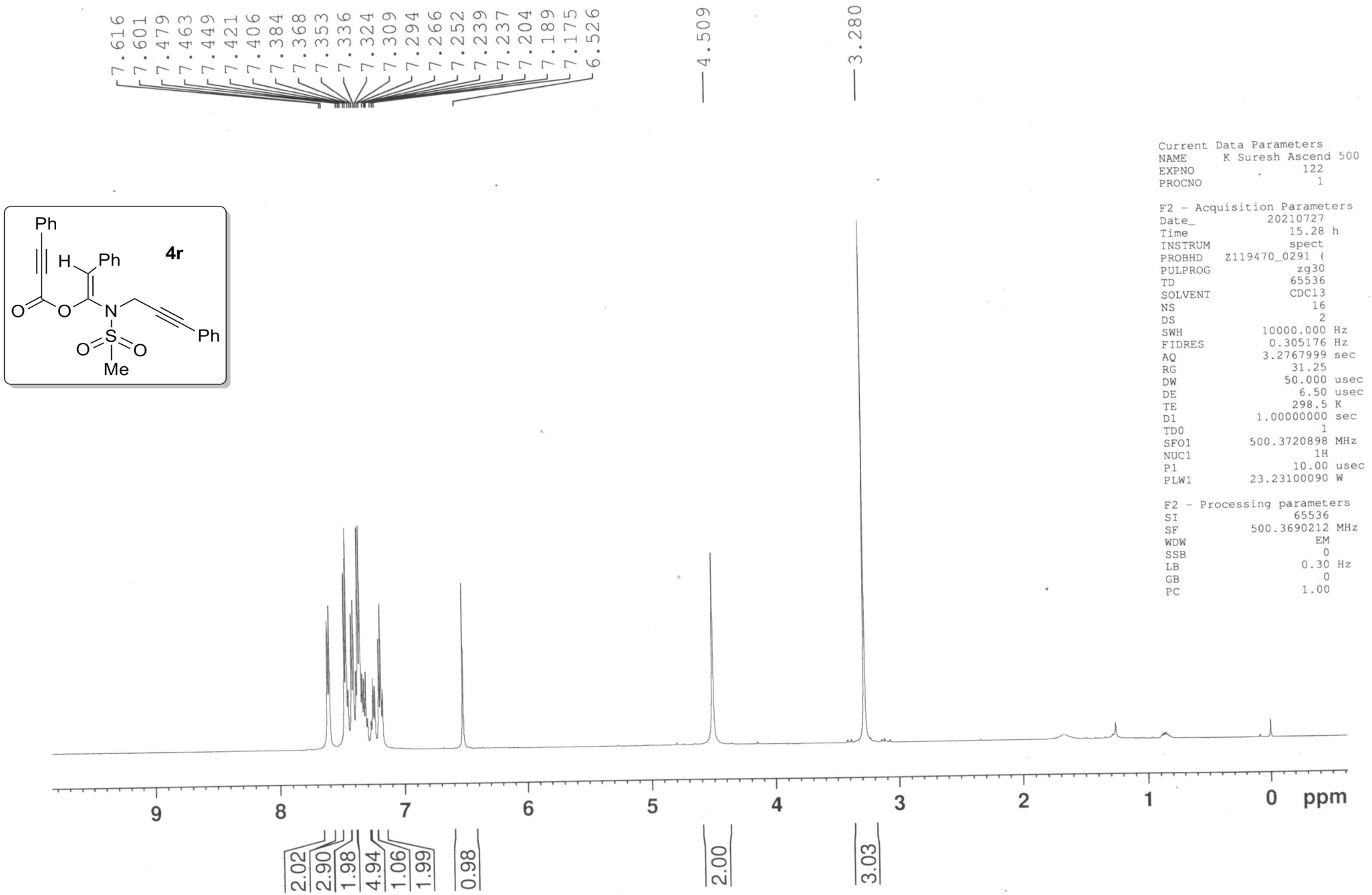
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 115
PROCNO 1

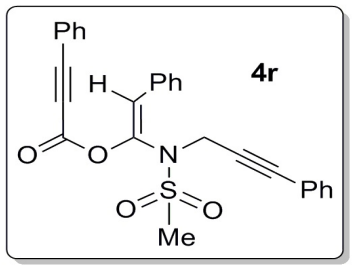
F2 - Acquisition Parameters
Date_ 20210722
Time 13.07 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 161
DW 50.000 usec
DE 13.04 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1830886 MHz
NUC1 1H
P0 5.00 usec
P1 15.00 usec
PLW1 4.84679985 W

F2 - Processing parameters
SI 65536
SF 500.1800112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




151.12
139.27
138.41
137.16
133.11
132.98
131.53
130.99
128.88
128.79
128.68
128.57
123.37
119.09
119.05
89.04
86.21
81.21
79.76
77.32
77.00
76.69
40.15
21.38
4q
Current Data Parameters
NAME K SURESH UPDATED 400
EXPNO 81
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210723
Time 15.59 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 977
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 883.3 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 100.6029694 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 0 ppm

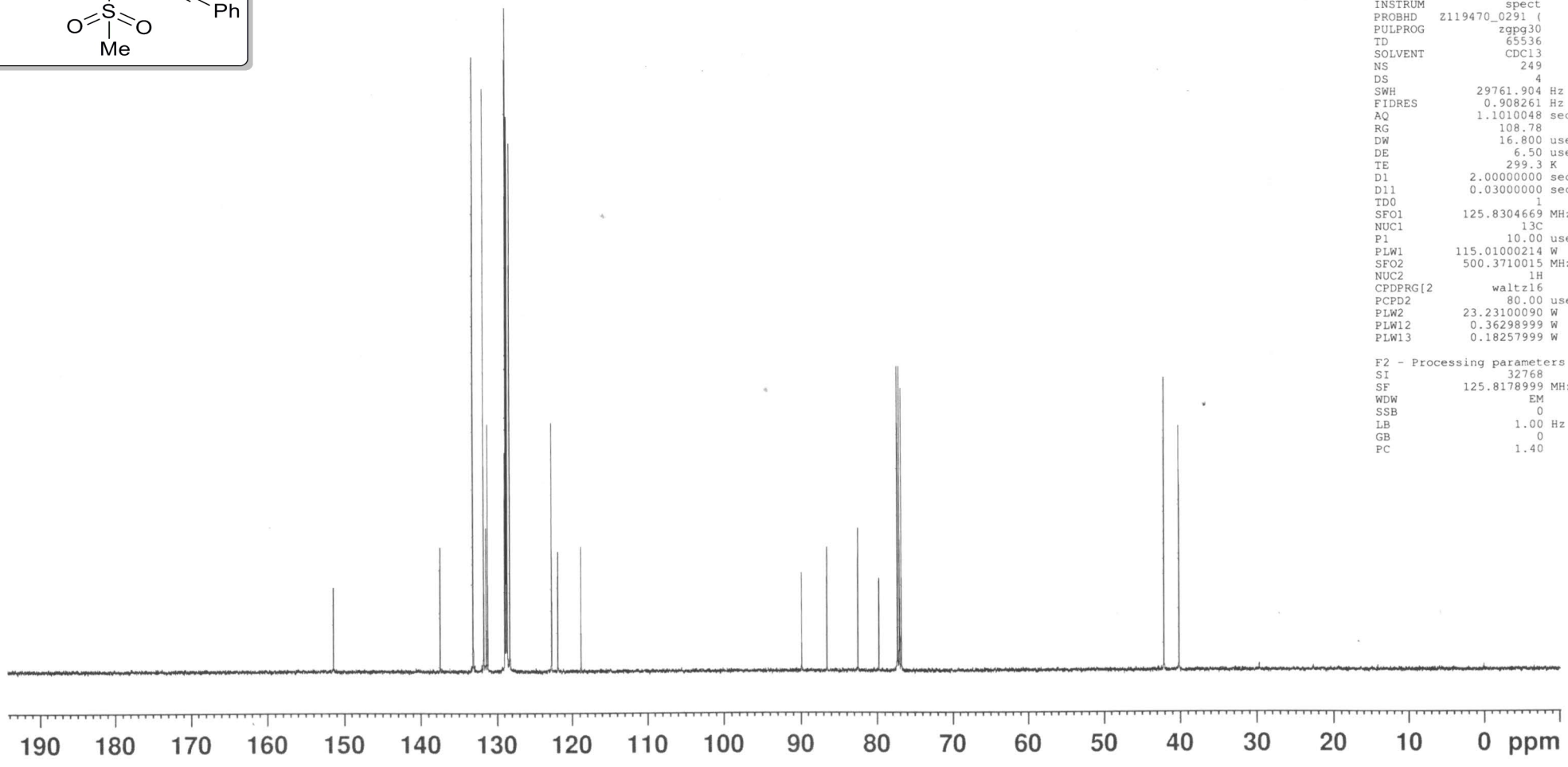

7.616
7.601
7.479
7.463
7.449
7.421
7.406
7.384
7.368
7.353
7.336
7.324
7.309
7.294
7.266
7.252
7.239
7.237
7.204
7.189
7.175
6.526
4.509
3.280
Ph
H
Ph
4r
O
O
N
S
O
O
Me
Ph
Current Data Parameters
NAME K Suresh Ascend 500
EXPNO 122
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210727
Time 15.28 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zg30
TD 65536
SOLVENT CDC13
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 298.5 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 500.3690212 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
2.90
1.98
4.94
1.06
1.99
0.98
2.00
3.03



151.35
137.40
133.06
131.69
131.37
131.16
128.89
128.77
128.71
128.58
128.22
122.67
121.84
118.77

89.81
86.45
82.43
79.68
77.26
77.00
76.75

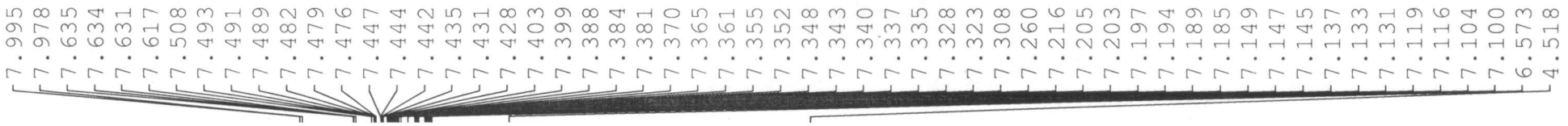
42.01
40.07

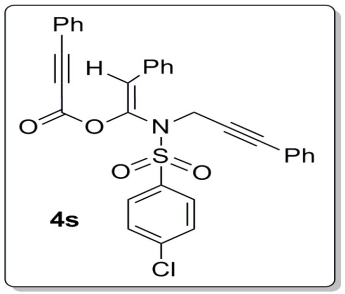


Current Data Parameters
NAME K Suresh Ascend 500
EXPNO 123
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210727
Time 15.43 h
INSTRUM spect
PROBHD Z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 249
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 299.3 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 125.8178999 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

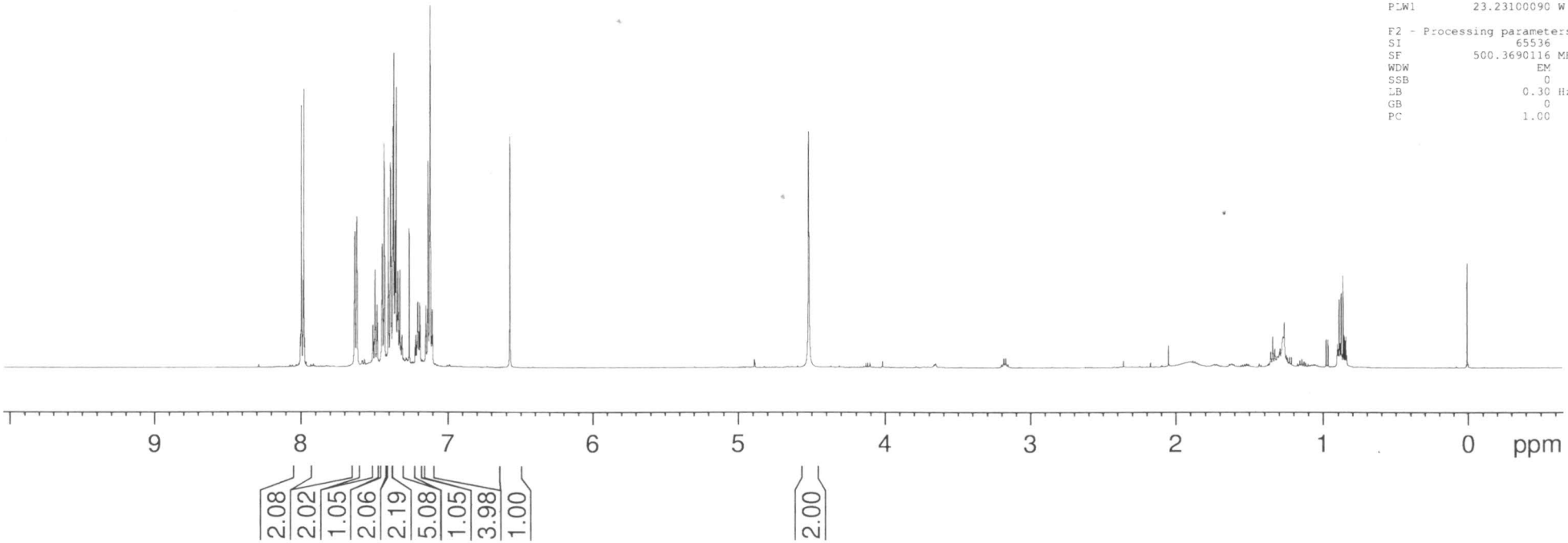


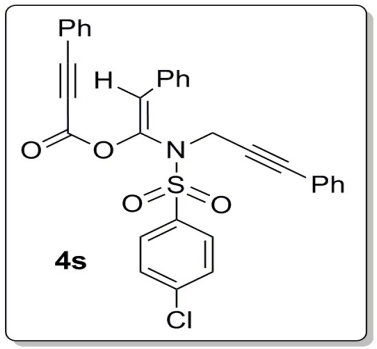



```
Current Data Parameters
NAME      K Suresh Ascend 500
EXPNO                  137
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210803
Time              11.20 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                 69.79
DW                50.000 usec
DE                 6.50 usec
TE                297.7 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            500.3690116 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



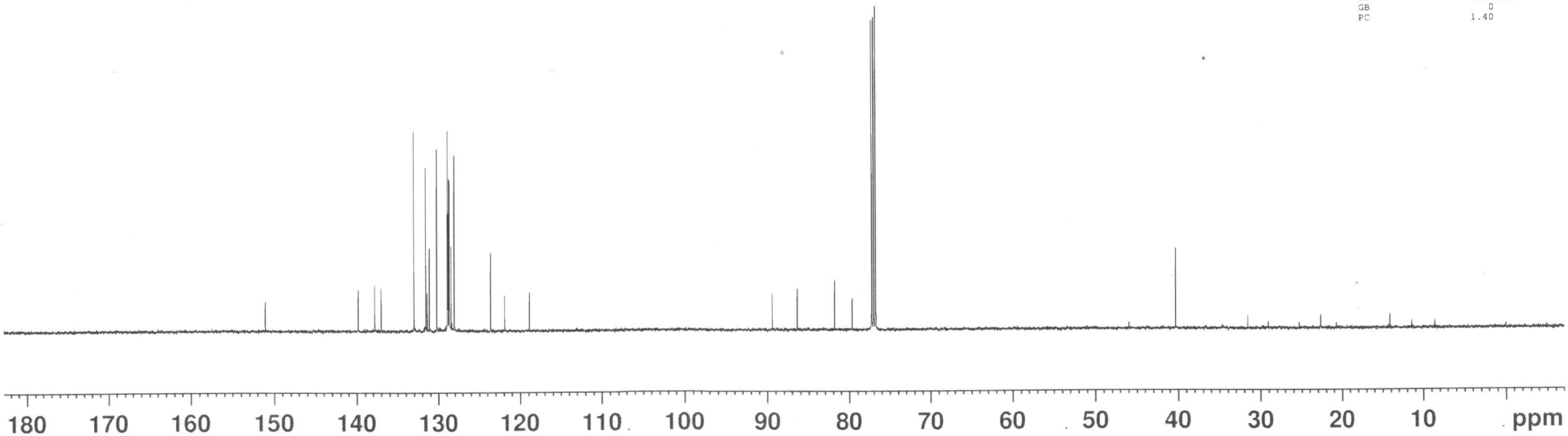


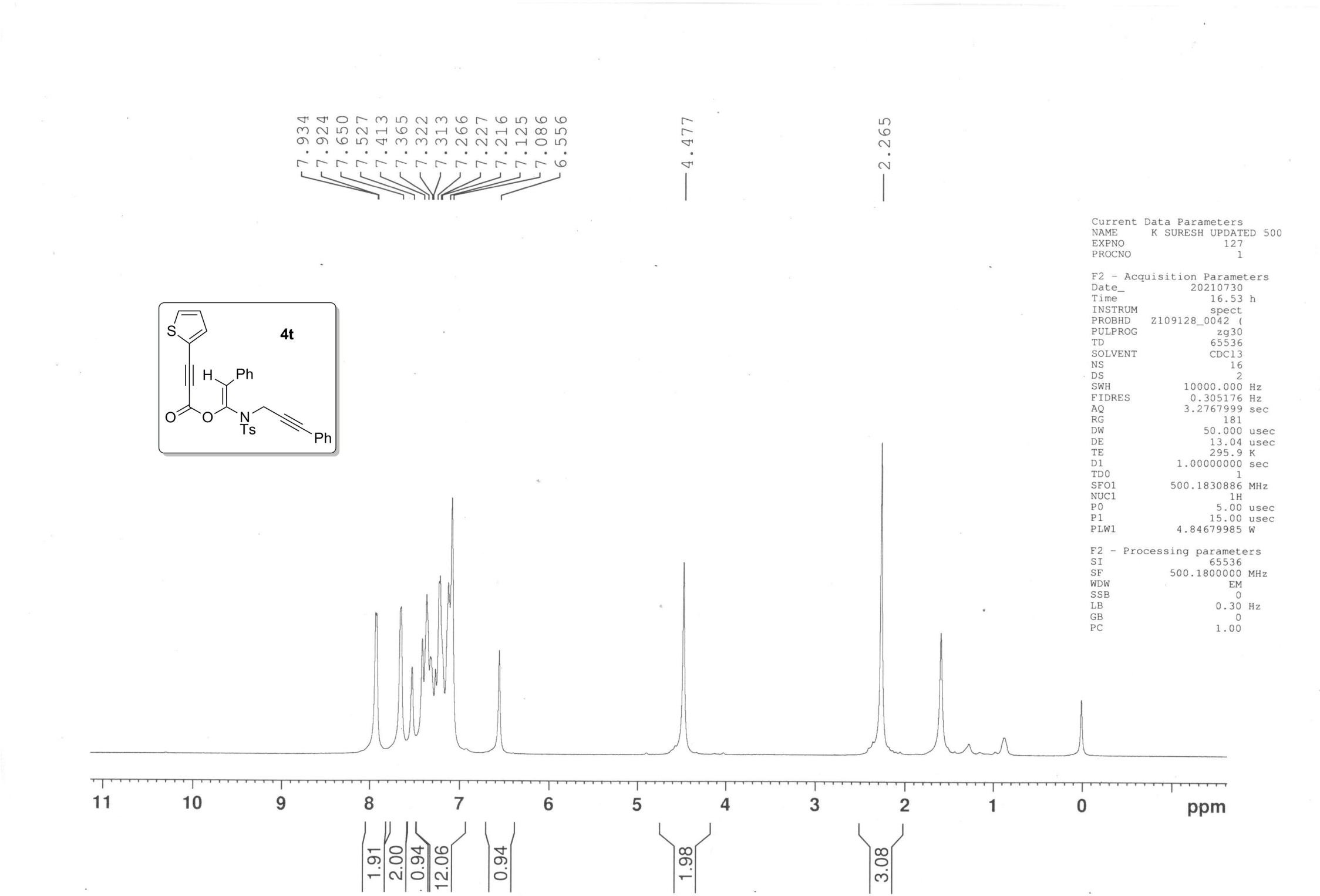
151.04
139.84
137.81
137.02
133.01
131.56
131.38
131.12
130.22
128.90
128.85
128.71
128.66
128.45
128.06
123.59
121.89
118.86
89.40
86.37
81.78
79.65
77.25
77.00
76.75
40.28

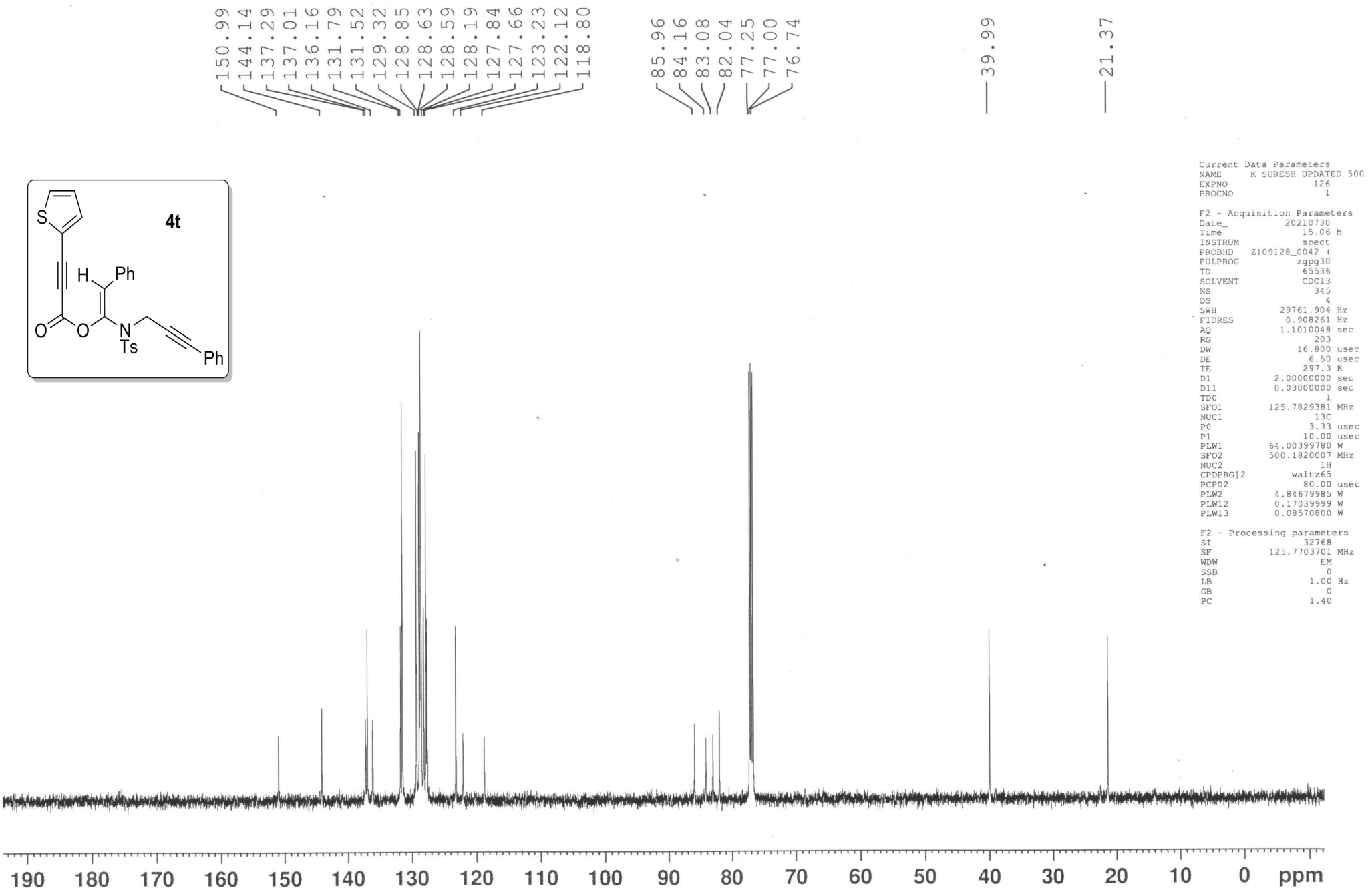
```
Current Data Parameters
NAME      K Suresh Ascend 500
EXPNO                  138
PROCNO                   1

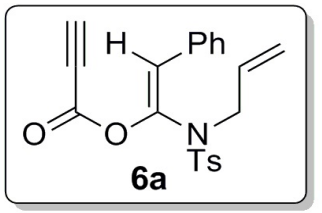
F2 - Acquisition Parameters
Date_           20210803
Time              11.41 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  368
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                87.13
DW                16.800 usec
DE                 6.50 usec
TE                298.6 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           125.8178905 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

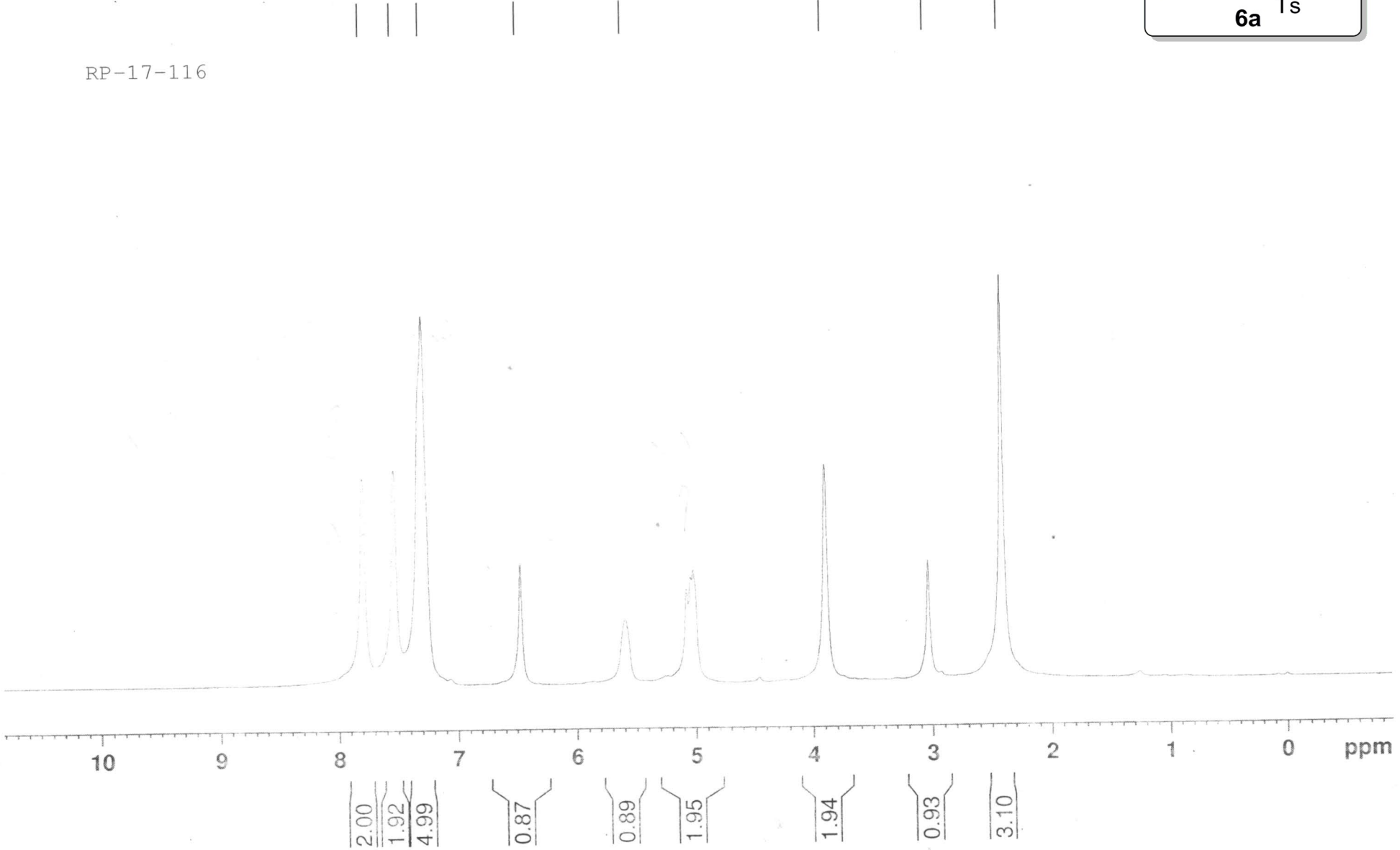


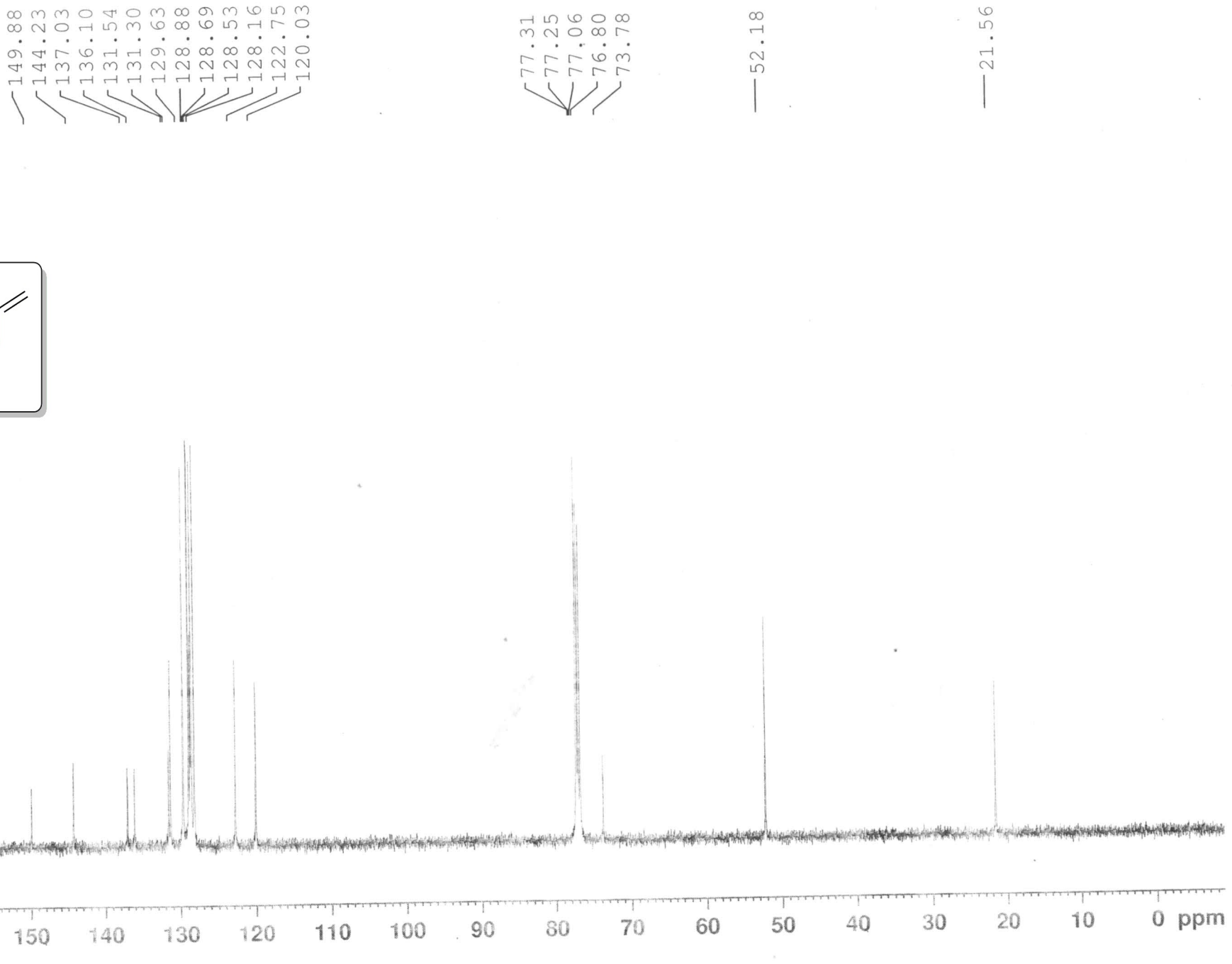

7.934
7.924
7.650
7.527
7.413
7.365
7.322
7.313
7.266
7.227
7.216
7.125
7.086
6.556
4.477
2.265
4t
S
H
Ph
O
O
N
Ts
Ph
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 127
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210730
Time 16.53 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 13.04 usec
TE 295.9 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
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.91
2.00
0.94
12.06
0.94
1.98
3.08

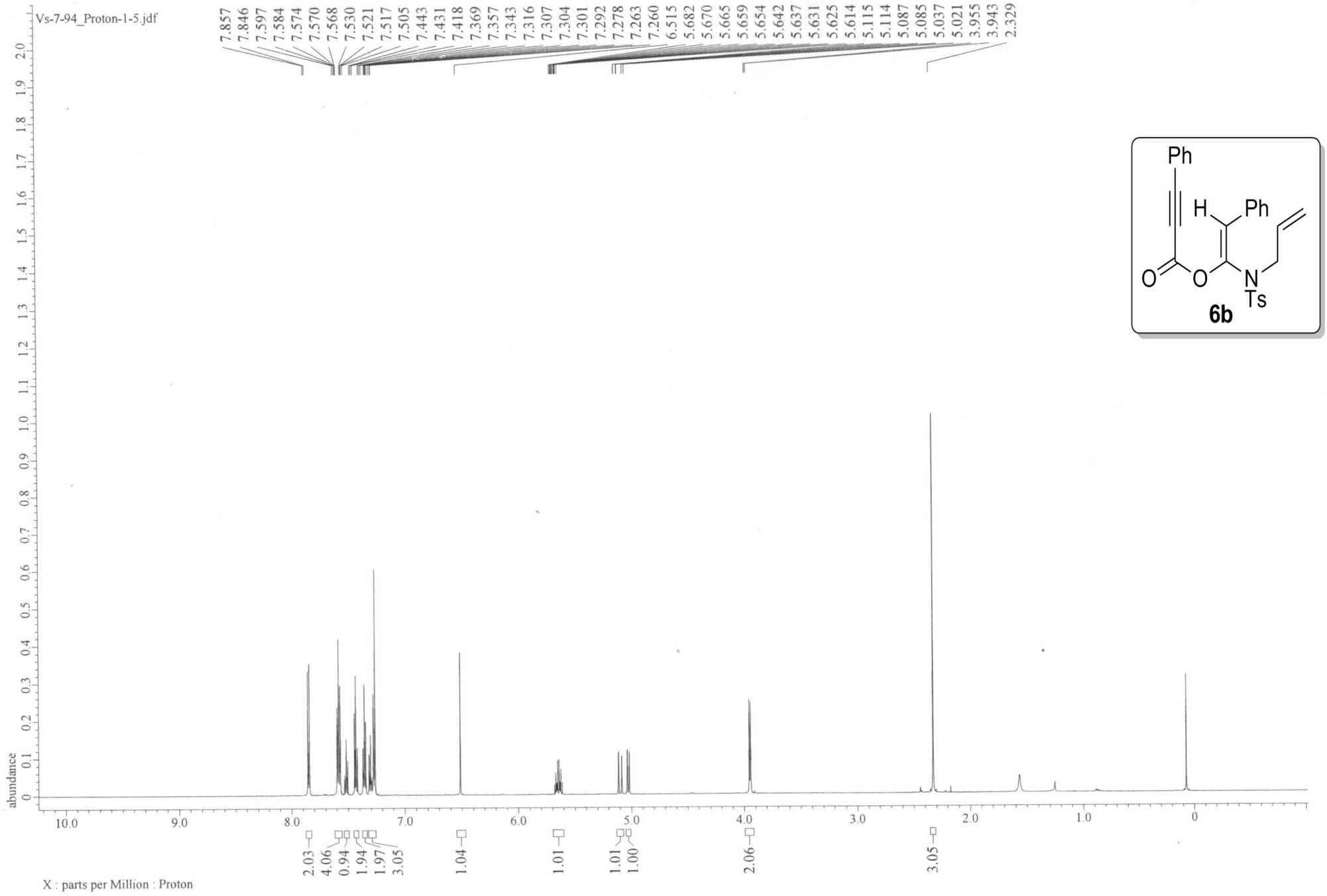

150.99
144.14
137.29
137.01
136.16
131.79
131.52
129.32
128.85
128.63
128.59
128.19
127.84
127.66
123.23
122.12
118.80
85.96
84.16
83.08
82.04
77.25
77.00
76.74
39.99
21.37
4t
S
H
Ph
O
O
N
Ts
Ph
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 126
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210730
Time 15.06 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 345
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 297.3 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 125.7703701 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 0 ppm

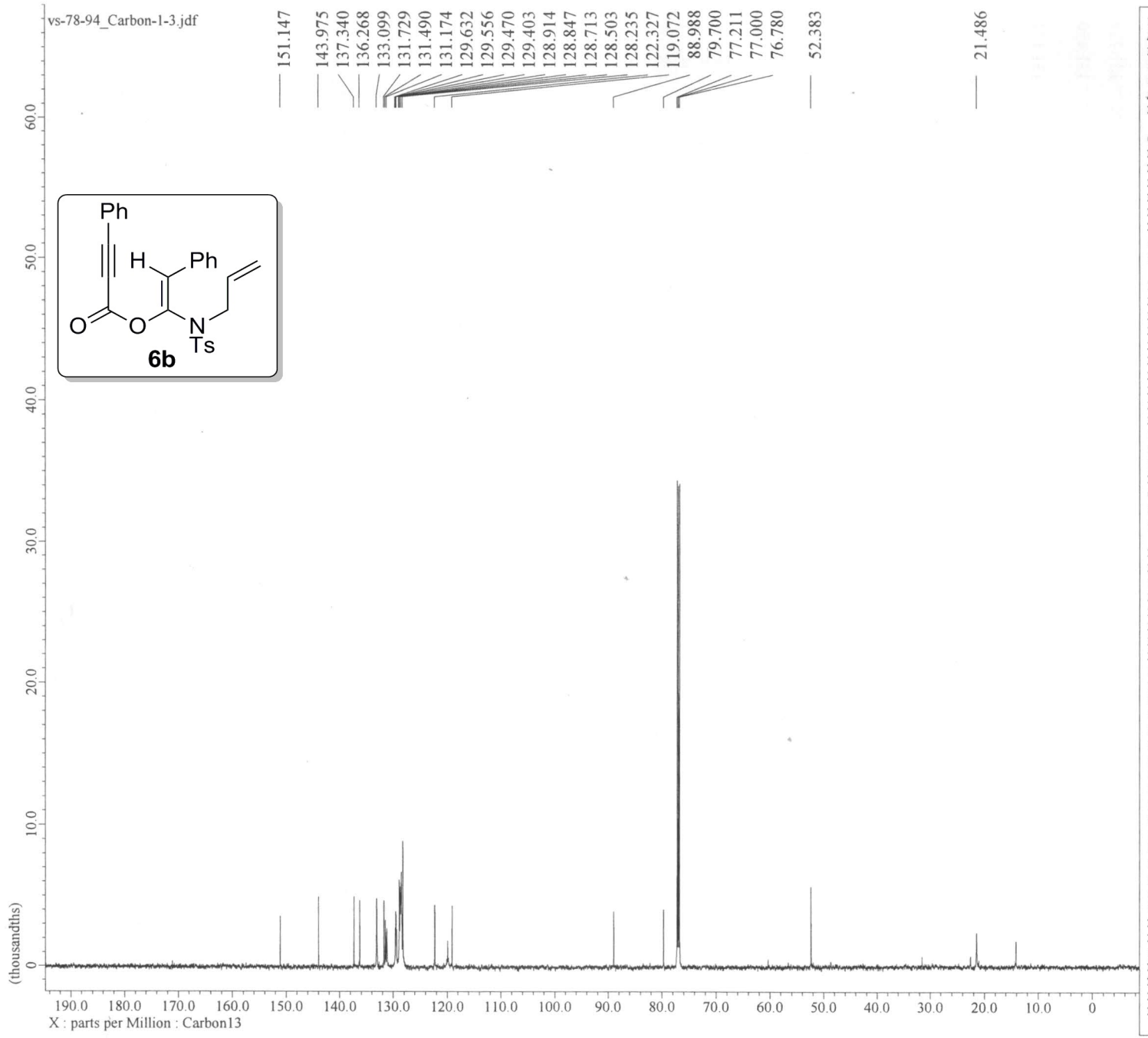

H
Ph
O
O
N
Ts
6a

RP-17-116

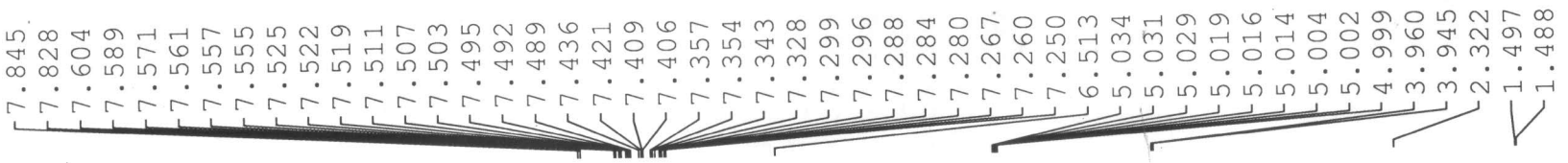

7.797
7.533
7.295
6.473
5.590
3.895
3.035
2.414
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.92
4.99
0.87
0.89
1.95
1.94
0.93
3.10

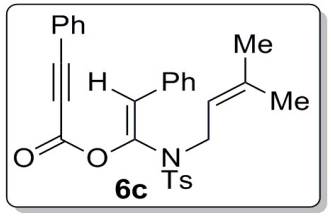

149.88
144.23
137.03
136.10
131.54
131.30
129.63
128.88
128.69
128.53
128.16
122.75
120.03
77.31
77.25
77.06
76.80
73.78
52.18
21.56
H
Ph
O
O
N
Ts
6a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


Vs-7-94_Proton-1-5.jdf
7.857
7.846
7.597
7.584
7.574
7.570
7.568
7.530
7.521
7.517
7.505
7.443
7.431
7.418
7.369
7.357
7.343
7.316
7.307
7.304
7.301
7.292
7.278
7.263
7.260
6.515
5.682
5.670
5.665
5.659
5.654
5.642
5.637
5.631
5.625
5.614
5.115
5.114
5.087
5.085
5.037
5.021
3.955
3.943
2.329
Ph
H
Ph
O
O
N
Ts
6b
abundance
X : parts per Million : Proton
2.03
4.06
0.94
1.94
1.97
3.05
1.04
1.01
1.01
1.00
2.06
3.05



Filename	= vs-78-94_Carbon-1-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= vs-78-94
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-FEB-2021 17:03:
Revision_Time	= 17-FEB-2021 01:17:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 562
Total_Scans	= 562
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.5[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]



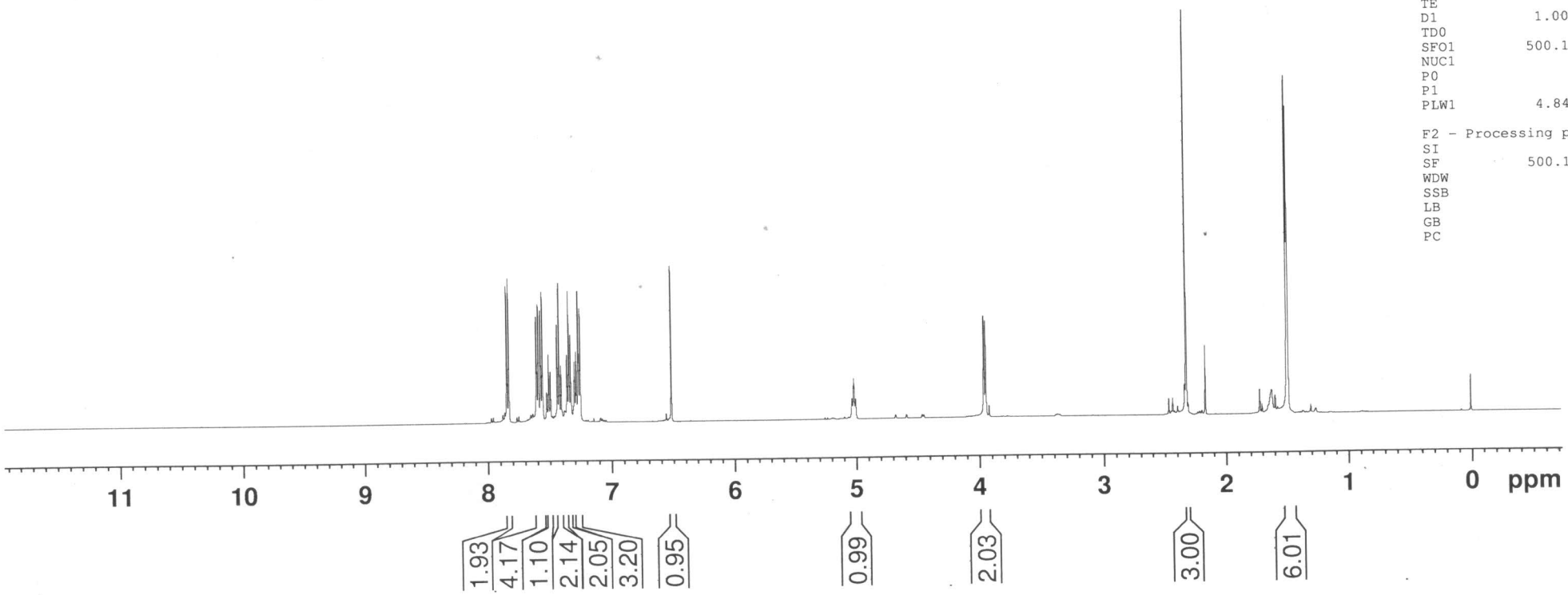


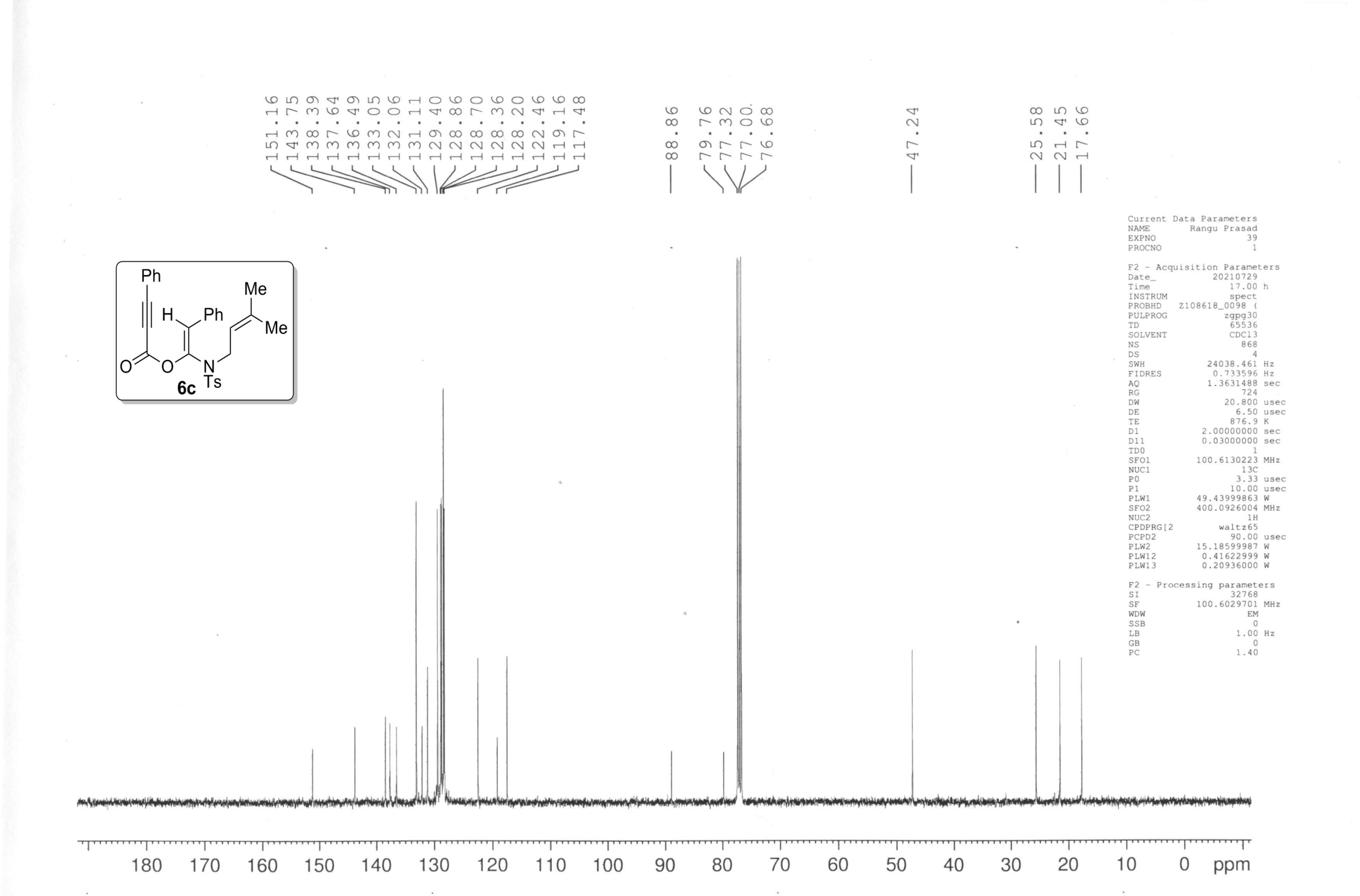
6c

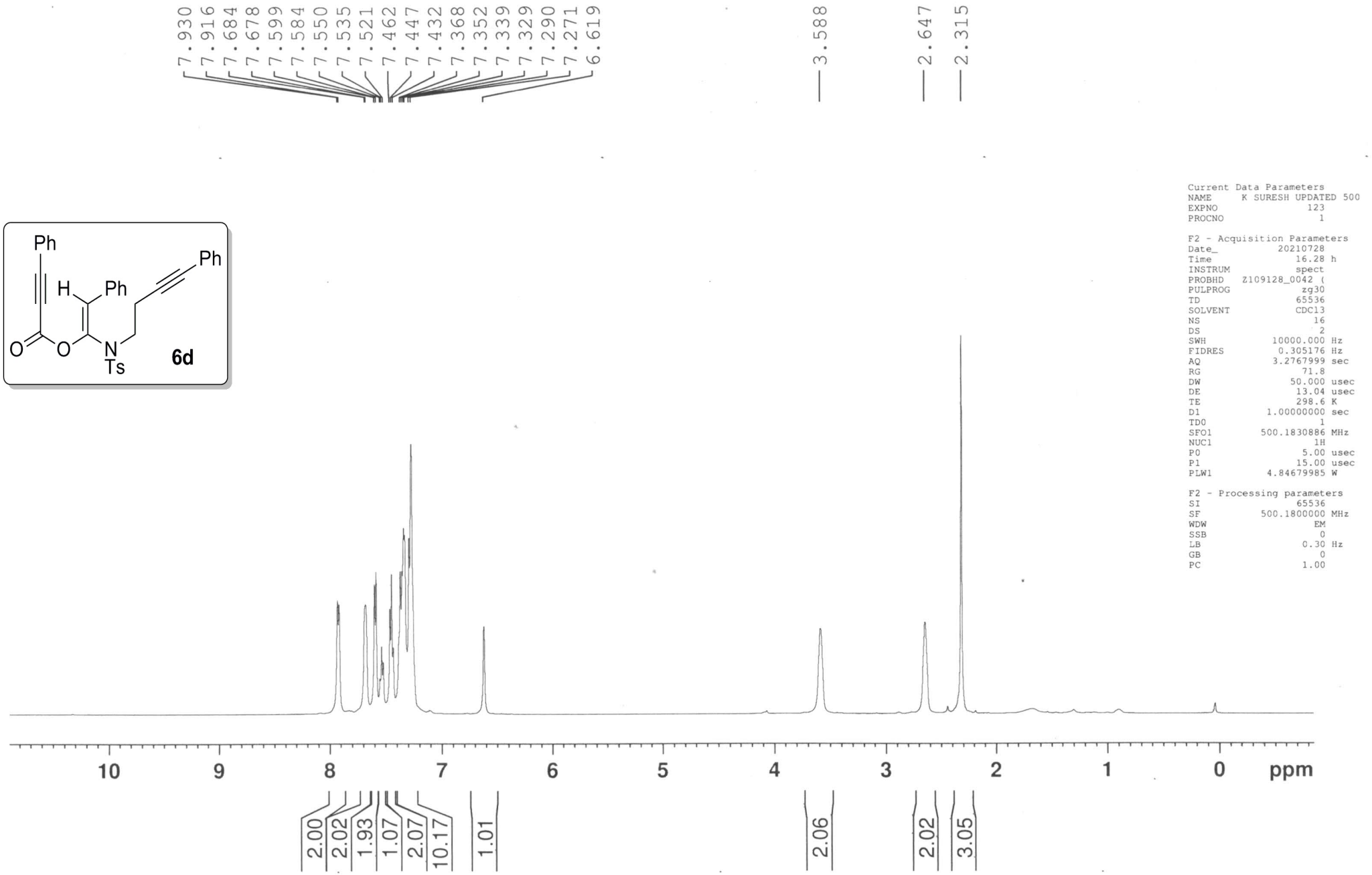
```
Current Data Parameters
NAME            Rangu Prasad
EXPNO                     38
PROCNO                     1

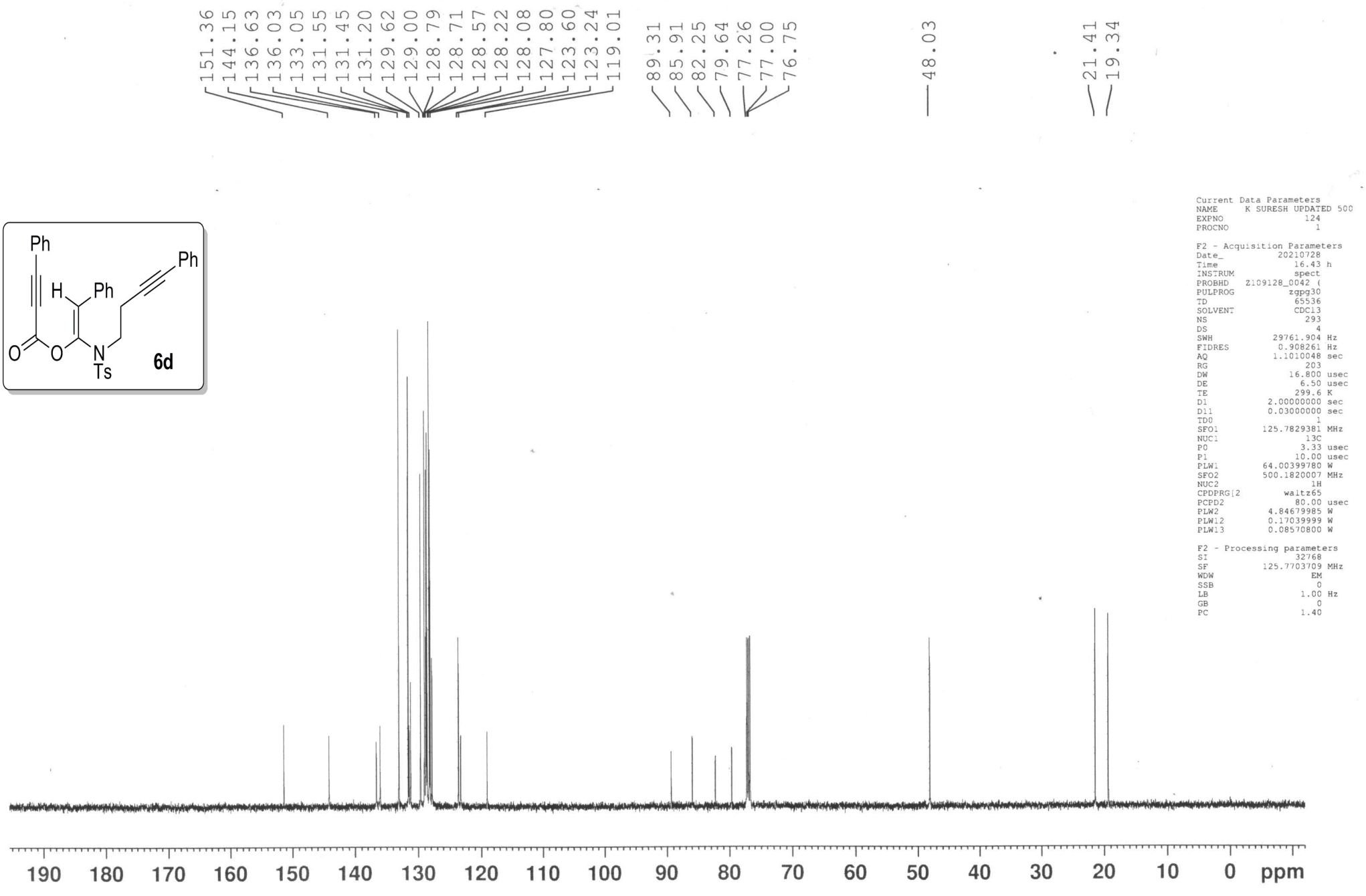
F2 - Acquisition Parameters
Date_               20210729
Time                  17.08 h
INSTRUM                spect
PROBHD    Z109128_0042 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ                3.2767999 sec
RG                      101
DW                 50.000 use
DE                 13.04 use
TE                 297.7 K
D1            1.00000000 sec
TD0                       1
SFO1          500.1830886 MHz
NUC1                    1H
P0                 5.00 use
P1                15.00 use
PLW1           4.84679985 W

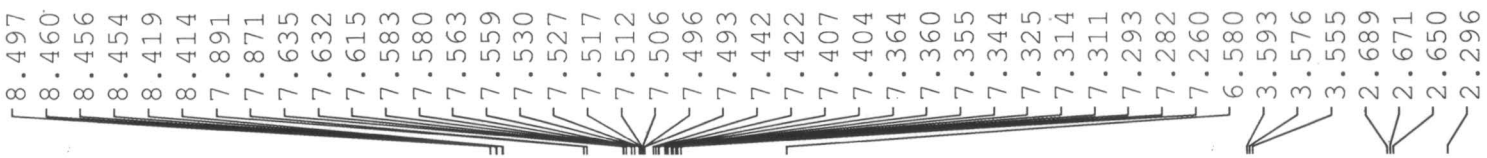
F2 - Processing parameters
SI                    65536
SF          500.1800108 MHz
WDW                     EM
SSB                      0
LB                0.30 Hz
GB                       0
PC                    1.00
```

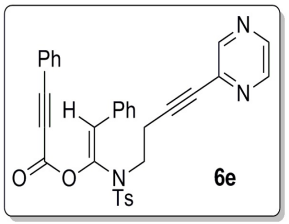


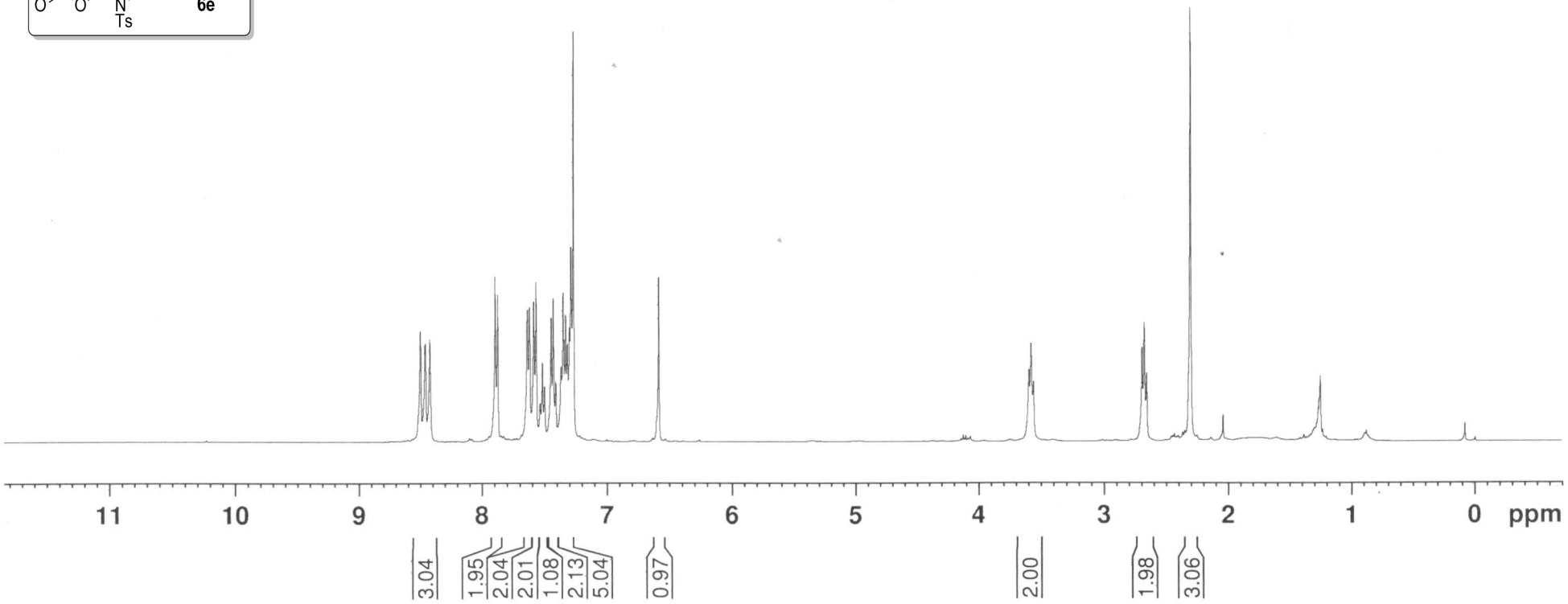

151.16
143.75
138.39
137.64
136.49
133.05
132.06
131.11
129.40
128.86
128.70
128.36
128.20
122.46
119.16
117.48
88.86
79.76
77.32
77.00
76.68
47.24
25.58
21.45
17.66
Ph
H
Ph
Me
Me
O
O
N
Ts
6c
Current Data Parameters
NAME Rangu Prasad
EXPNO 39
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210729
Time 17.00 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 868
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 876.9 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 100.6029701 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

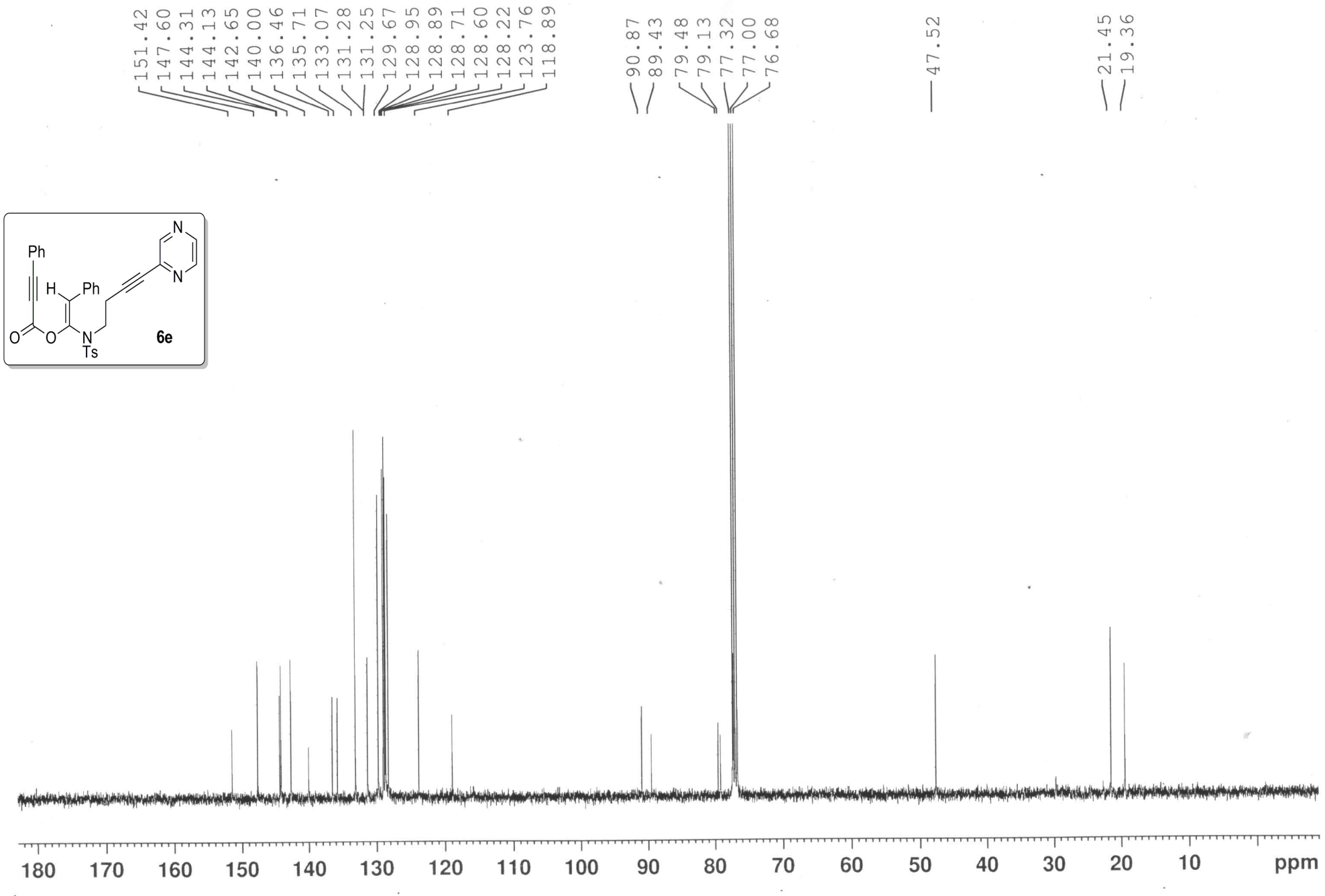

7.930
7.916
7.684
7.678
7.599
7.584
7.550
7.535
7.521
7.462
7.447
7.432
7.368
7.352
7.339
7.329
7.290
7.271
6.619
3.588
2.647
2.315
Ph
H
Ph
Ph
O
O
N
Ts
6d
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 123
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210728
Time 16.28 h
INSTRUM spect
PROBHD 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 298.6 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
2.00
2.02
1.93
1.07
2.07
10.17
1.01
2.06
2.02
3.05

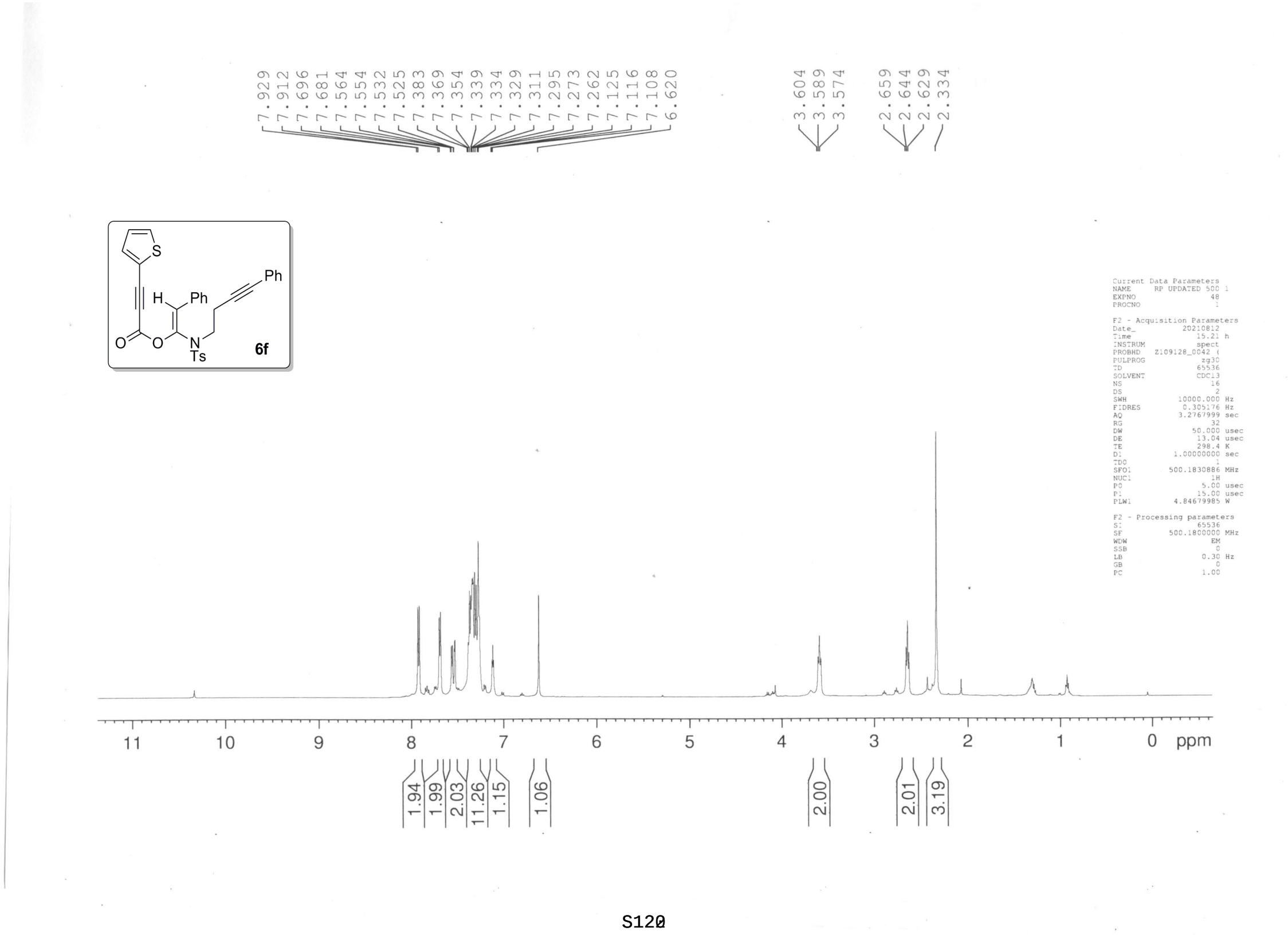

151.36
144.15
136.63
136.03
133.05
131.55
131.45
131.20
129.62
129.00
128.79
128.71
128.57
128.22
128.08
127.80
123.60
123.24
119.01
89.31
85.91
82.25
79.64
77.26
77.00
76.75
48.03
21.41
19.34
Ph
H
Ph
Ph
O
O
N
Ts
6d
Current Data Parameters
NAME K SURESH UPDATED 500
EXPNO 124
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210728
Time 16.43 h
INSTRUM spect
PROBHD Z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 293
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 299.6 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 125.7703709 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 0 ppm

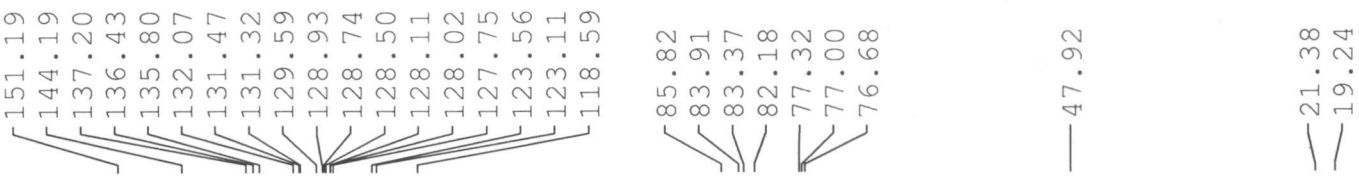

8.497
8.460
8.456
8.454
8.419
8.414
7.891
7.871
7.635
7.632
7.615
7.583
7.580
7.563
7.559
7.530
7.527
7.517
7.512
7.506
7.496
7.493
7.442
7.422
7.407
7.404
7.364
7.360
7.355
7.344
7.325
7.314
7.311
7.293
7.282
7.260
6.580
3.593
3.576
3.555
2.689
2.671
2.650
2.296

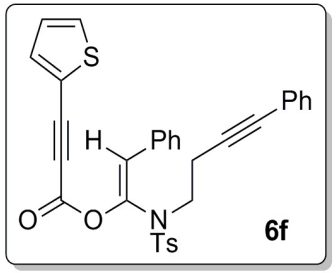

Ph
H
Ph
N
N
O
O
N
Ts
6e

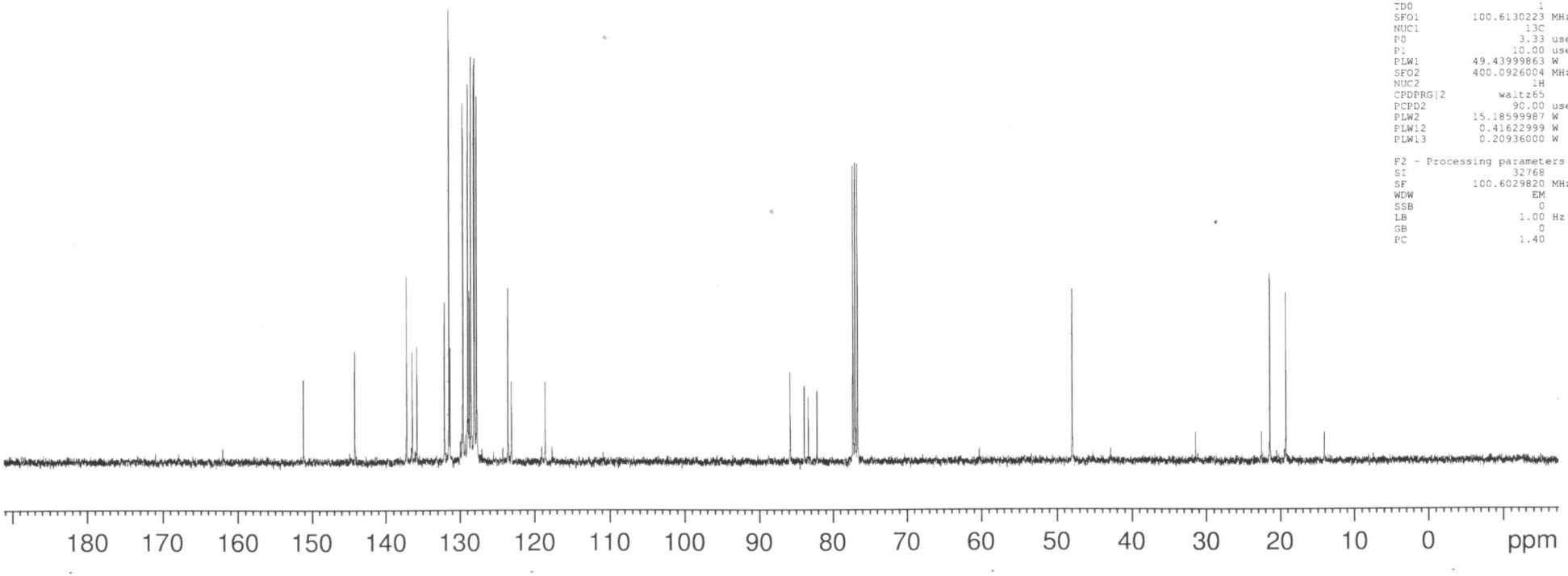

11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.04
1.95
2.04
2.01
1.08
2.13
5.04
0.97
2.00
1.98
3.06


151.42
147.60
144.31
144.13
142.65
140.00
136.46
135.71
133.07
131.28
131.25
129.67
128.95
128.89
128.71
128.60
128.22
123.76
118.89
90.87
89.43
79.48
79.13
77.32
77.00
76.68
47.52
21.45
19.36
Ph
H
Ph
N
N
O
O
N
Ts
6e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.929
7.912
7.696
7.681
7.564
7.554
7.532
7.525
7.383
7.369
7.354
7.339
7.334
7.329
7.311
7.295
7.273
7.262
7.125
7.116
7.108
6.620
3.604
3.589
3.574
2.659
2.644
2.629
2.334
S
Ph
H
Ph
O
O
N
Ts
6f
Current Data Parameters
NAME RP UPDATED 500 1
EXPNO 48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210812
Time 15.21 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 32
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
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.94
1.99
2.03
11.26
1.15
1.06
2.00
2.01
3.19



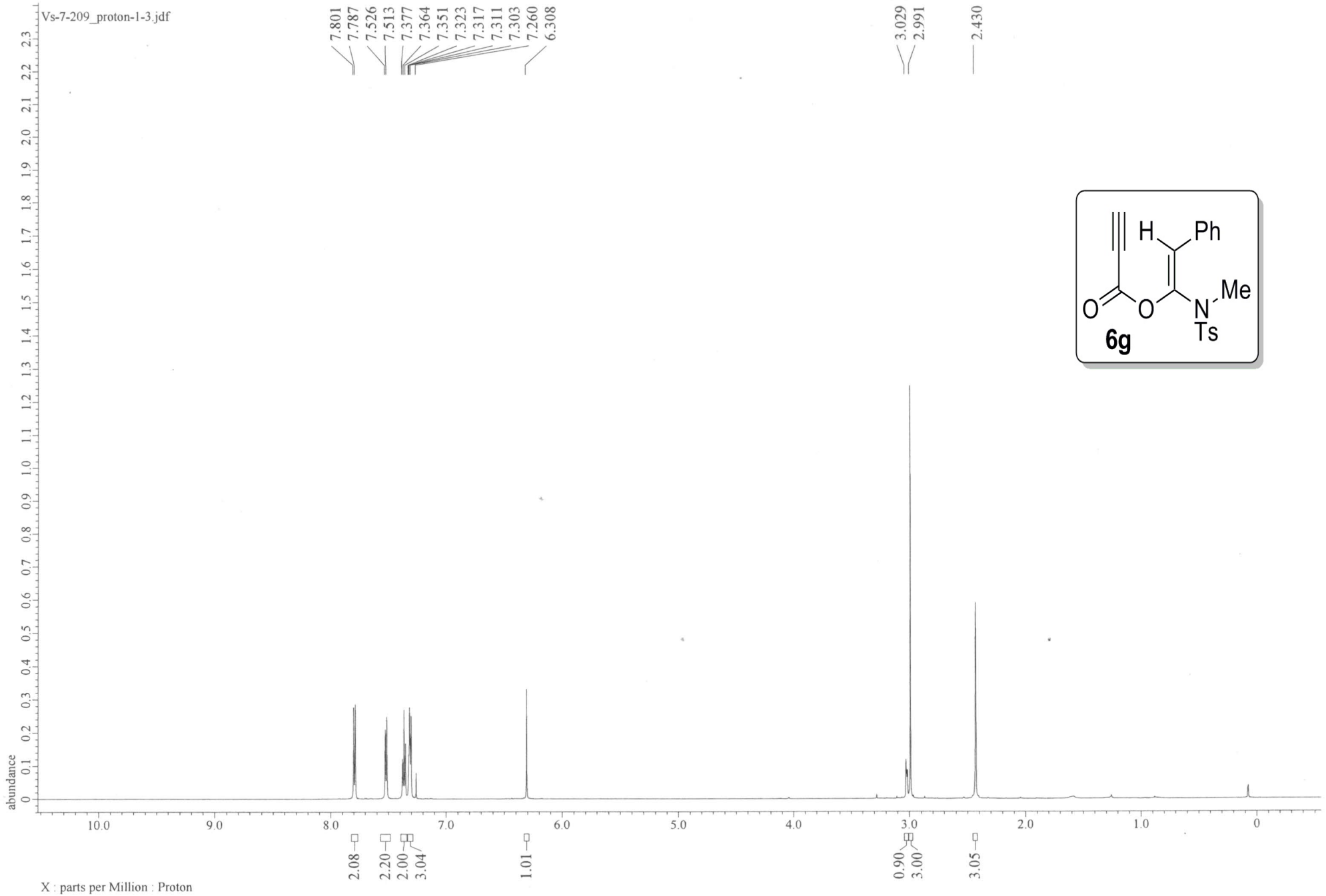


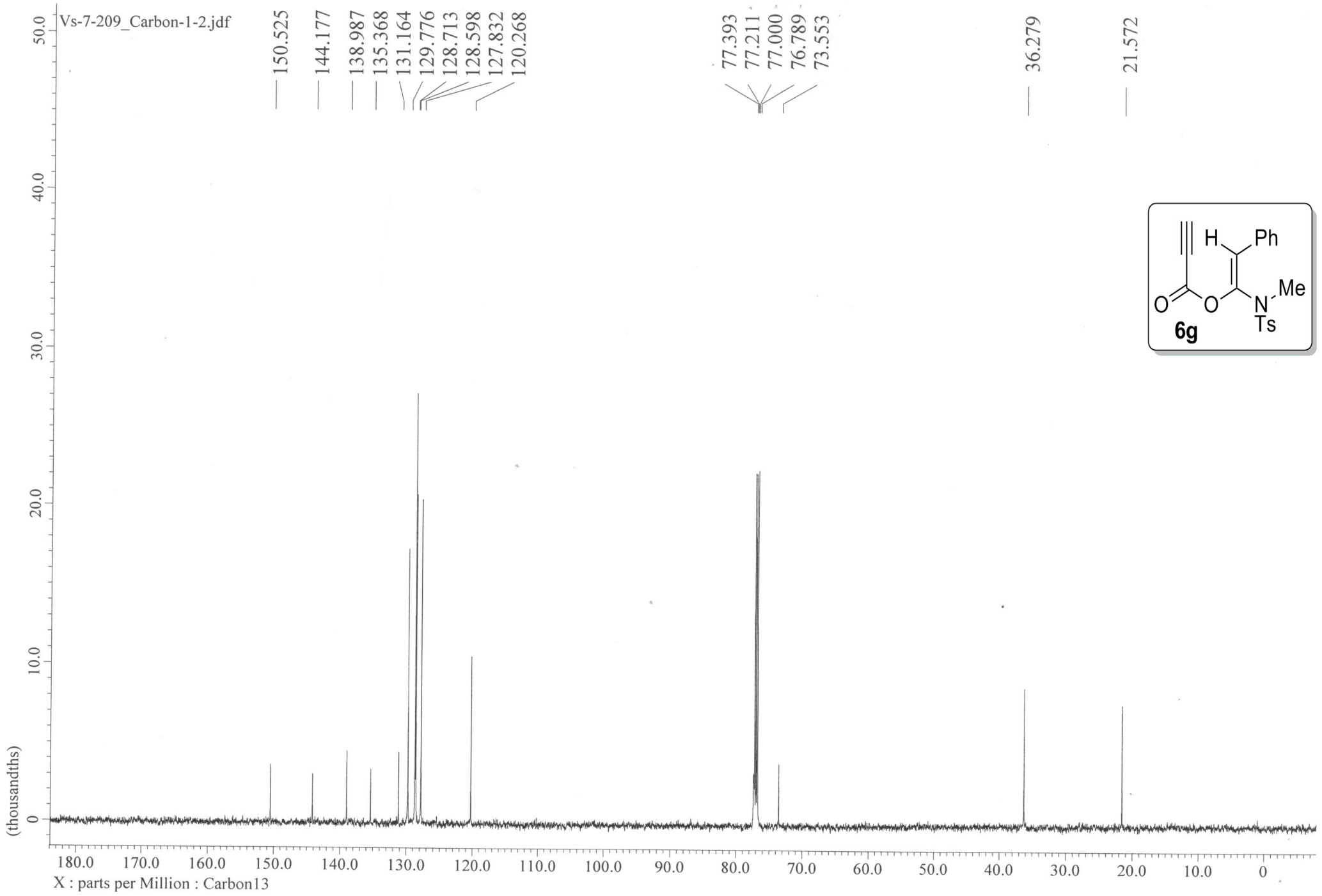


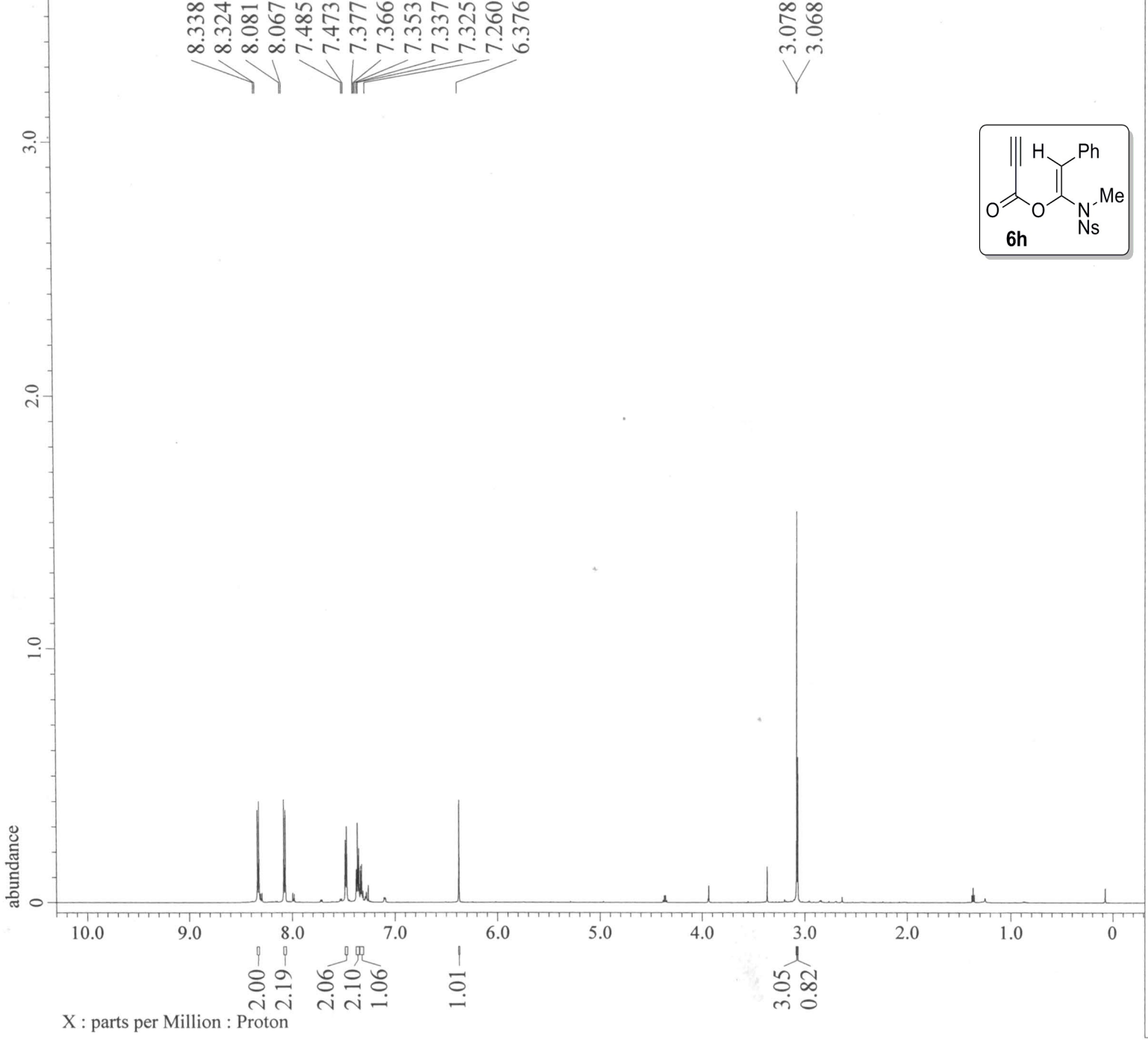

```
Current Data Parameters
NAME      RP Updated 400
EXPNO               42
PROCNO               1

F2 - Acquisition Parameters
Date_          20210812
Time              15.00 h
INSTRUM             spect
PROBHD    Z108618_0098 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  268
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                804.8 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           100.6029820 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

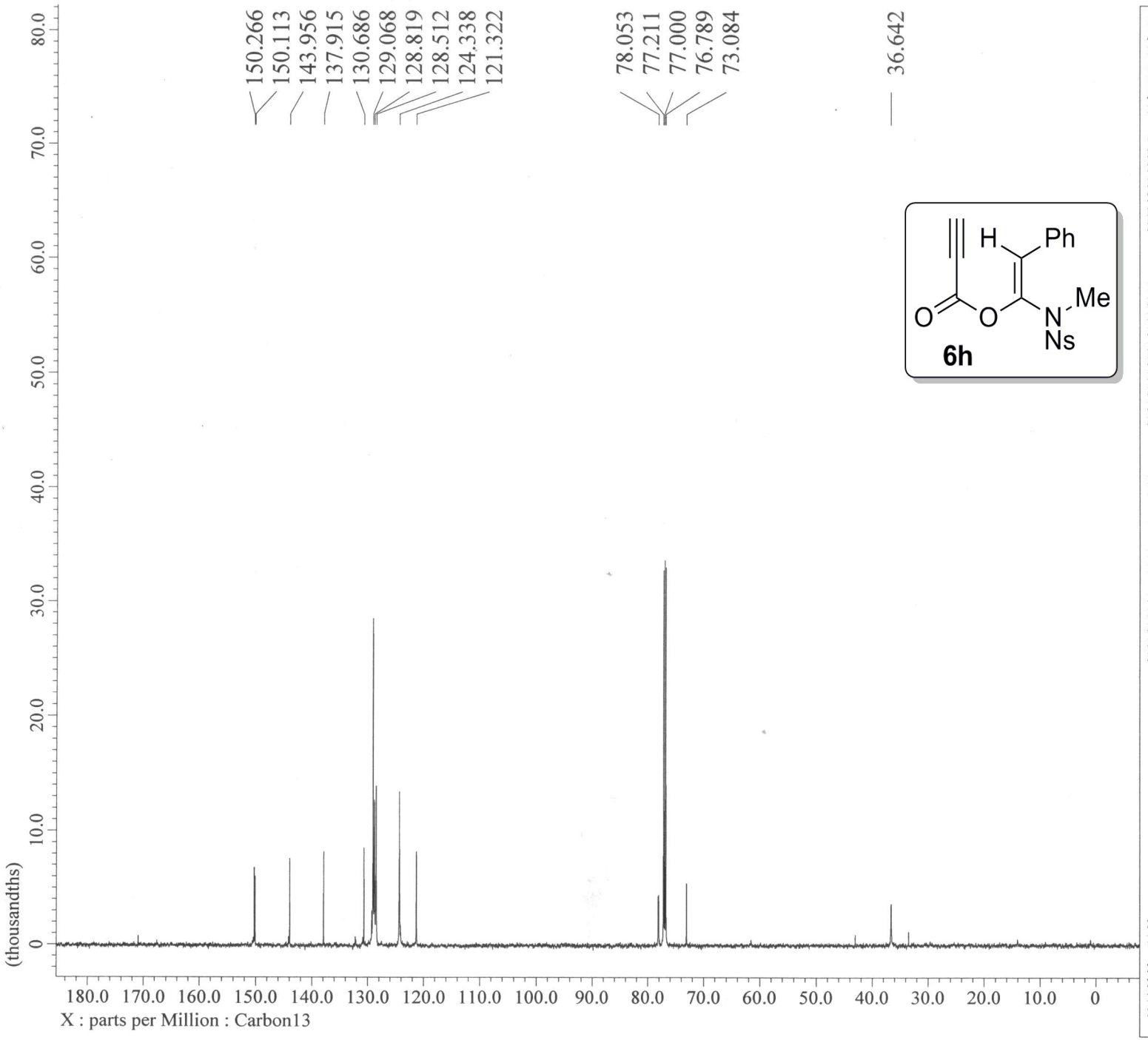

Vs-7-209_proton-1-3.jdf
7.801
7.787
7.526
7.513
7.377
7.364
7.351
7.323
7.317
7.311
7.303
7.260
6.308
3.029
2.991
2.430
H
Ph
O
O
N
Me
Ts
6g
abundance
X : parts per Million : Proton
2.08
2.20
2.00
3.04
1.01
0.90
3.00
3.05


Vs-7-209_Carbon-1-2.jdf
150.525
144.177
138.987
135.368
131.164
129.776
128.713
128.598
127.832
120.268
77.393
77.211
77.000
76.789
73.553
36.279
21.572
H
Ph
O
O
N
Me
Ts
6g
(thousandths)
X : parts per Million : Carbon13

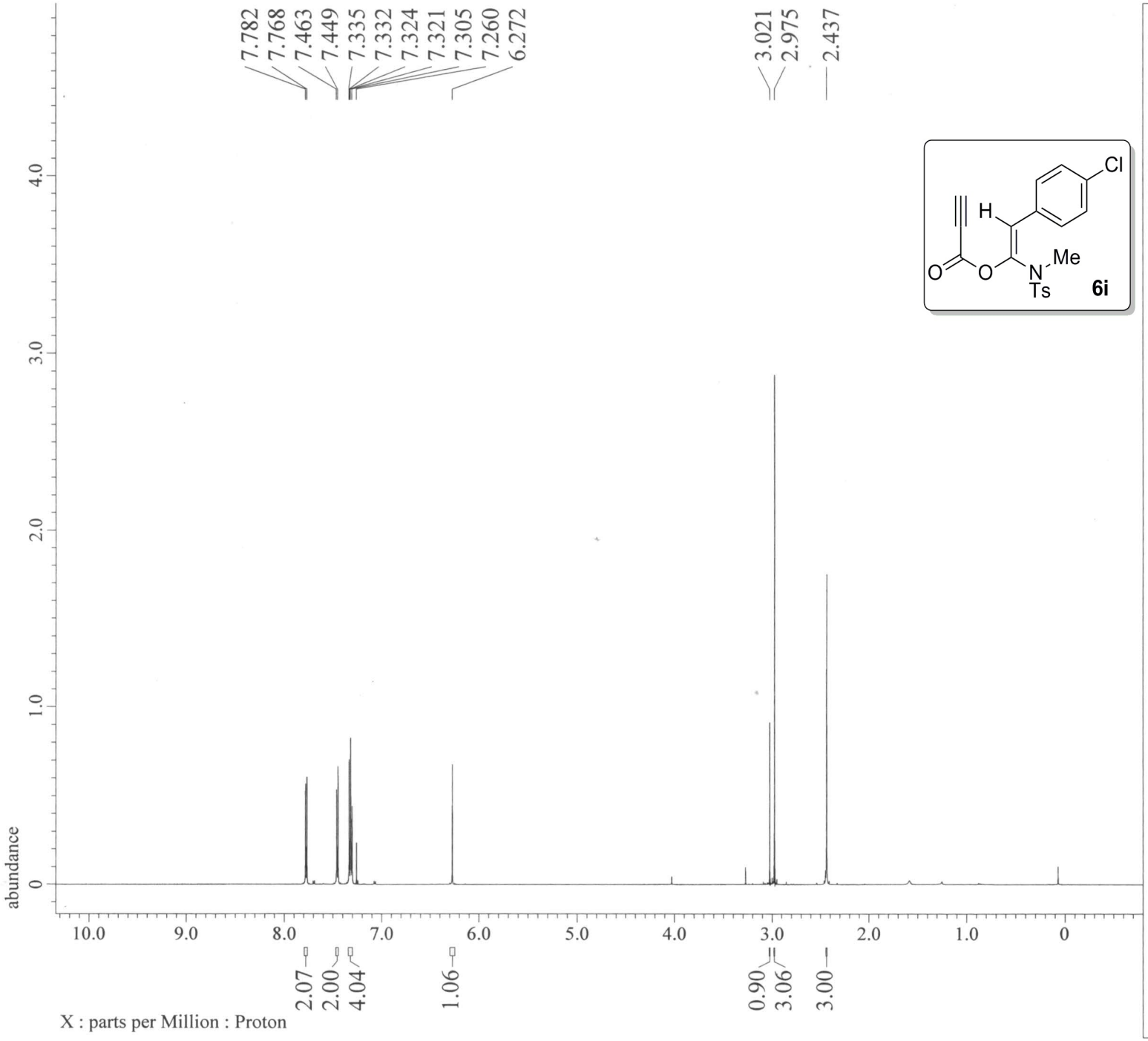


6h

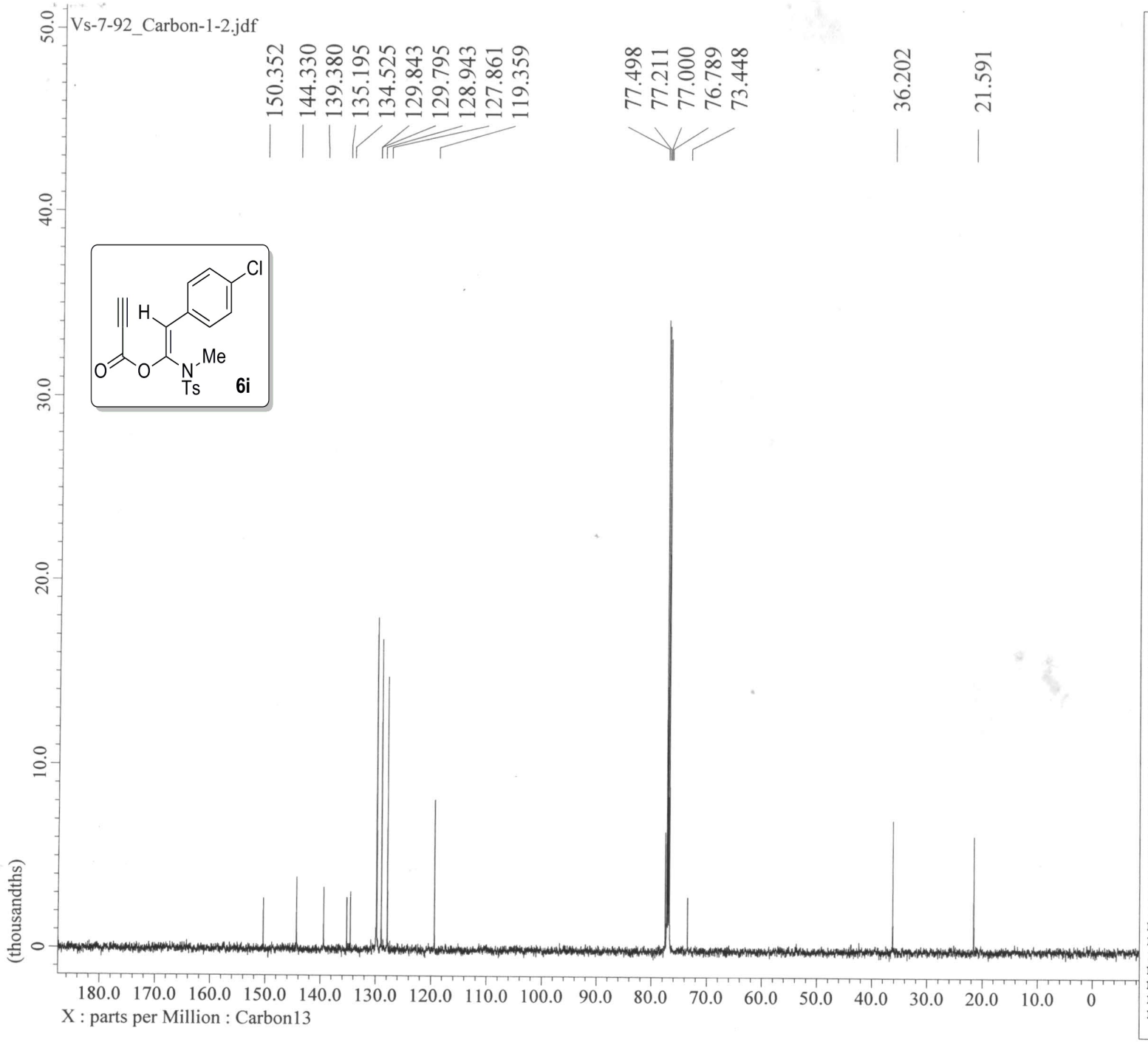
Filename	= vs-18-118_Proton-1-7.
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= vs-18-118
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2021 15:56:45
Revision_Time	= 15-AUG-2021 13:58:19
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.8[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]



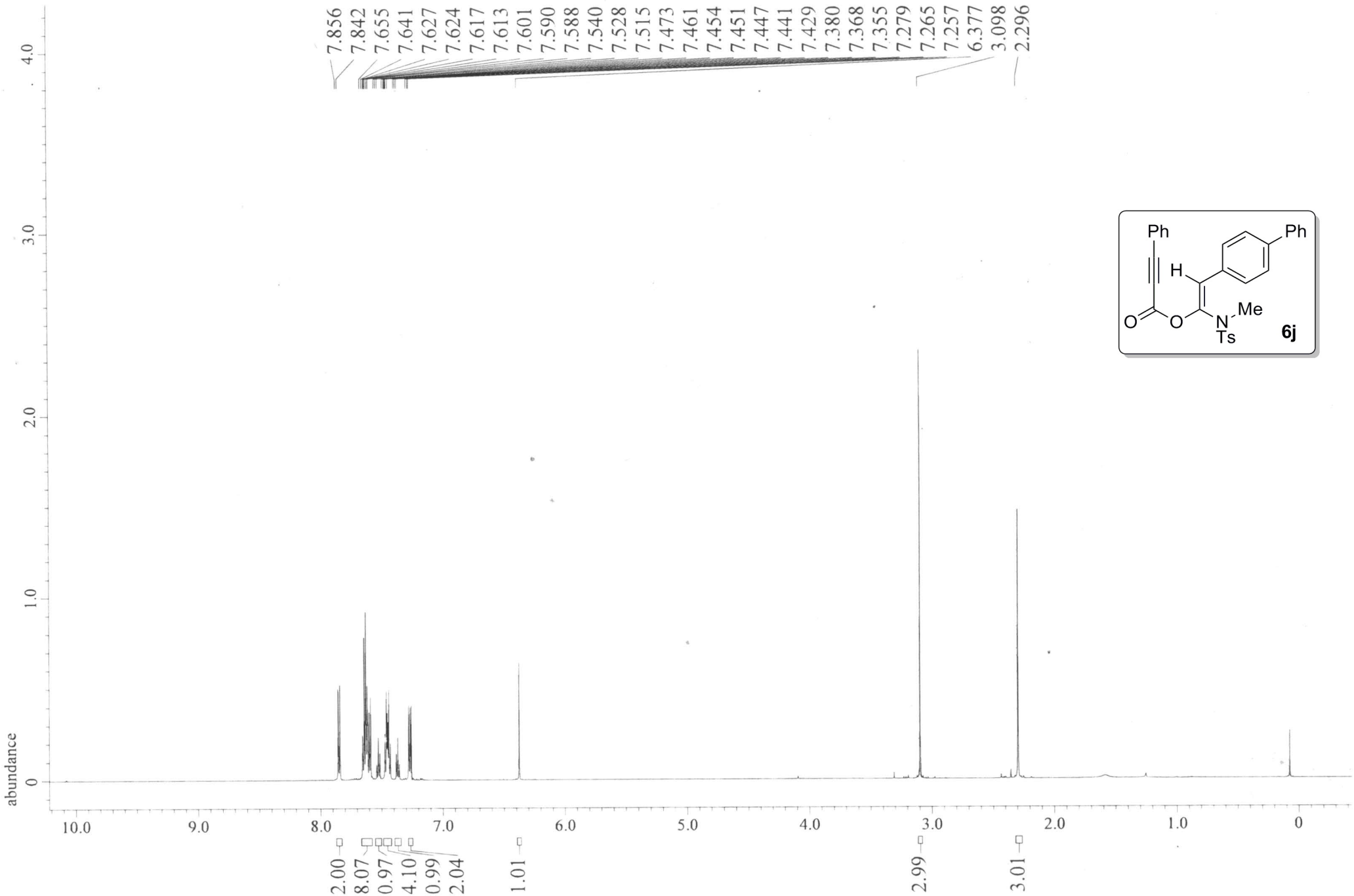
Filename	= vs-18-118_Carbon-1
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= vs-18-118
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2021 15:58:
Revision_Time	= 15-AUG-2021 14:25:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 401
Total_Scans	= 401
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.6[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]

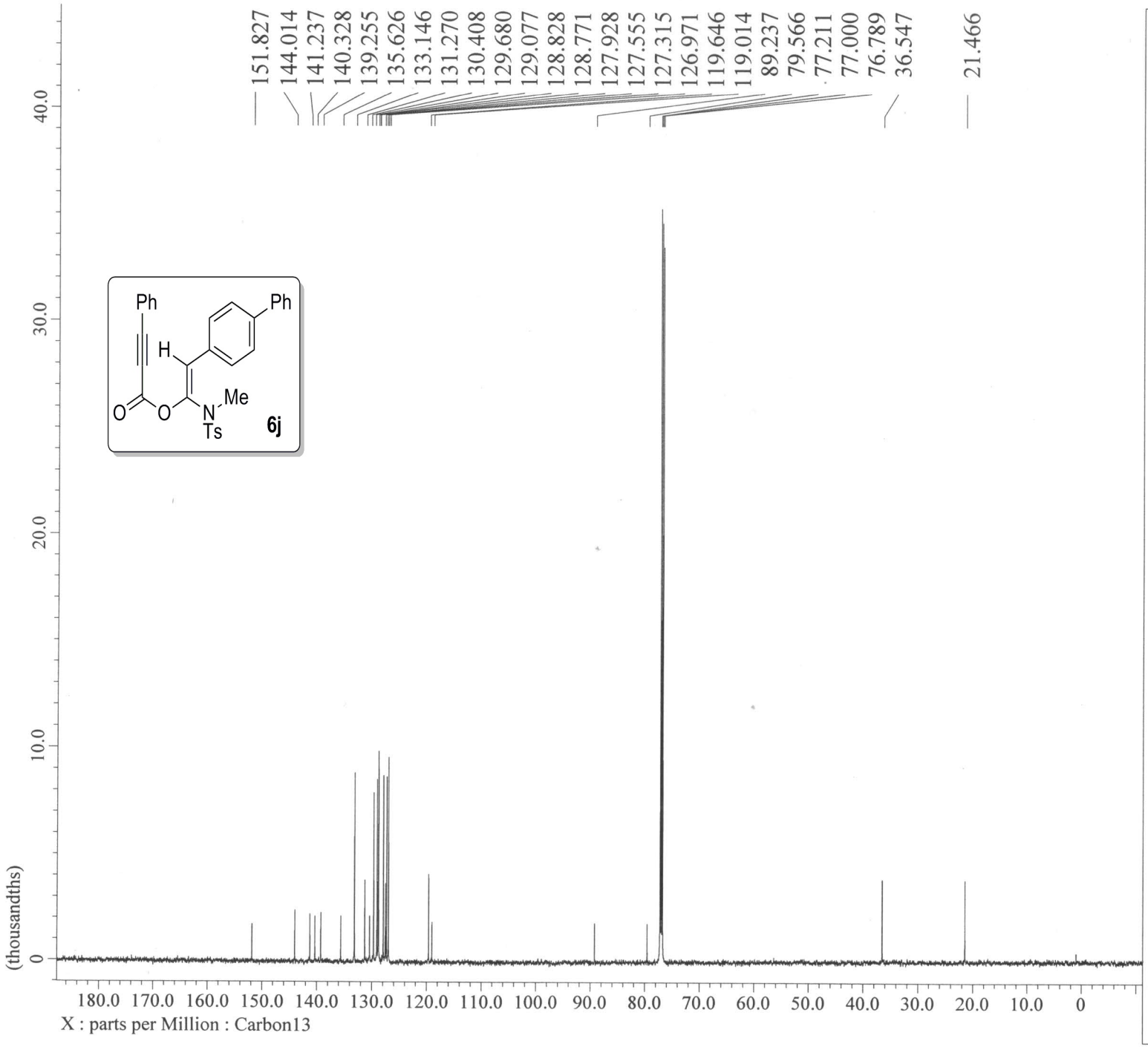


Filename	= Vs-7-92_proton-1-6.jd
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= Vs-7-92
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-FEB-2021 16:41:28
Revision_Time	= 15-AUG-2021 15:41:21
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.6[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Users\delta\Docume
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]

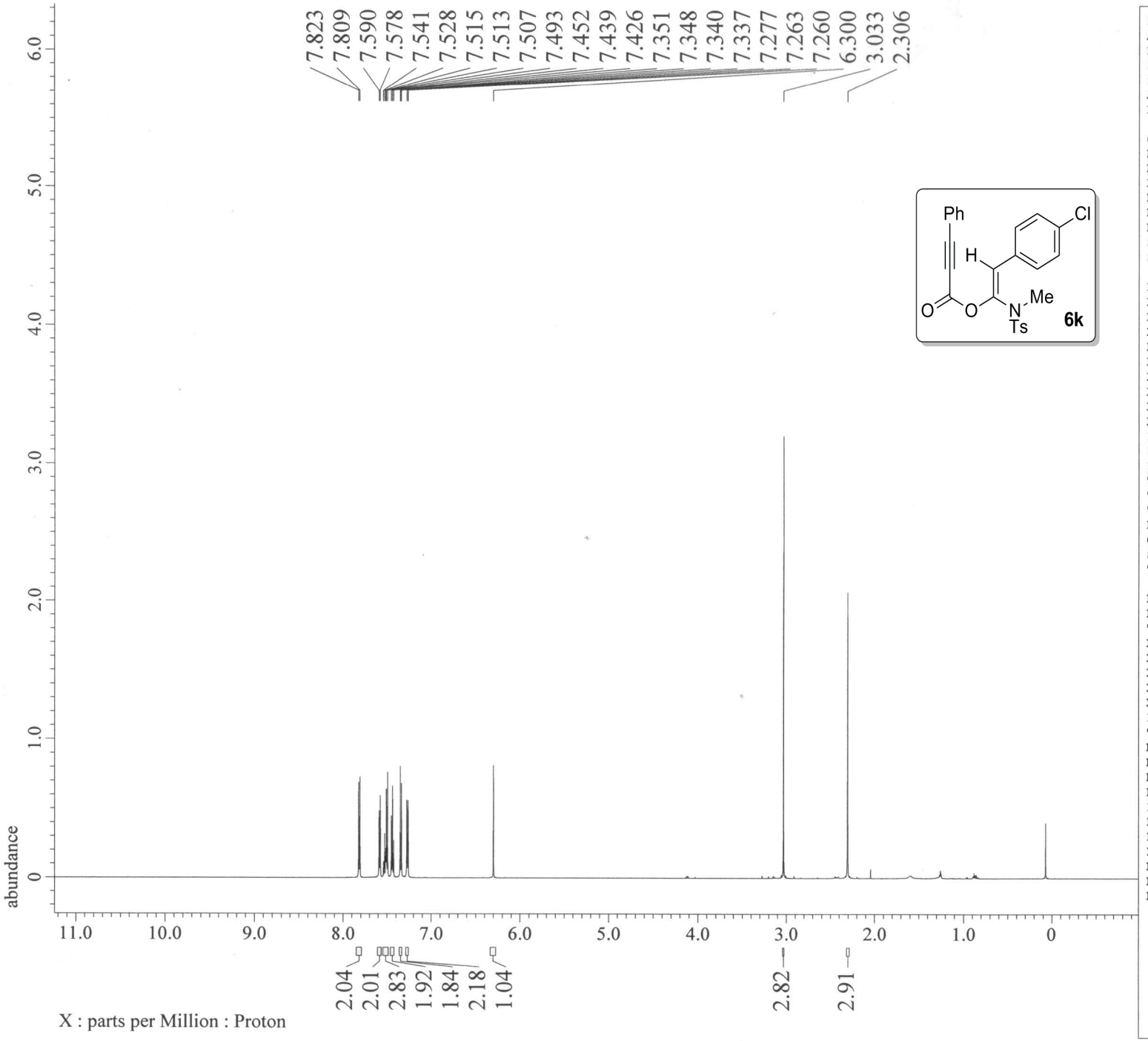


Filename	= Vs-7-92_Carbon-1-2
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= Vs-7-92
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-FEB-2021 16:43:
Revision_Time	= 2-MAR-2021 22:22:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 253
Total_Scans	= 253
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.7[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]

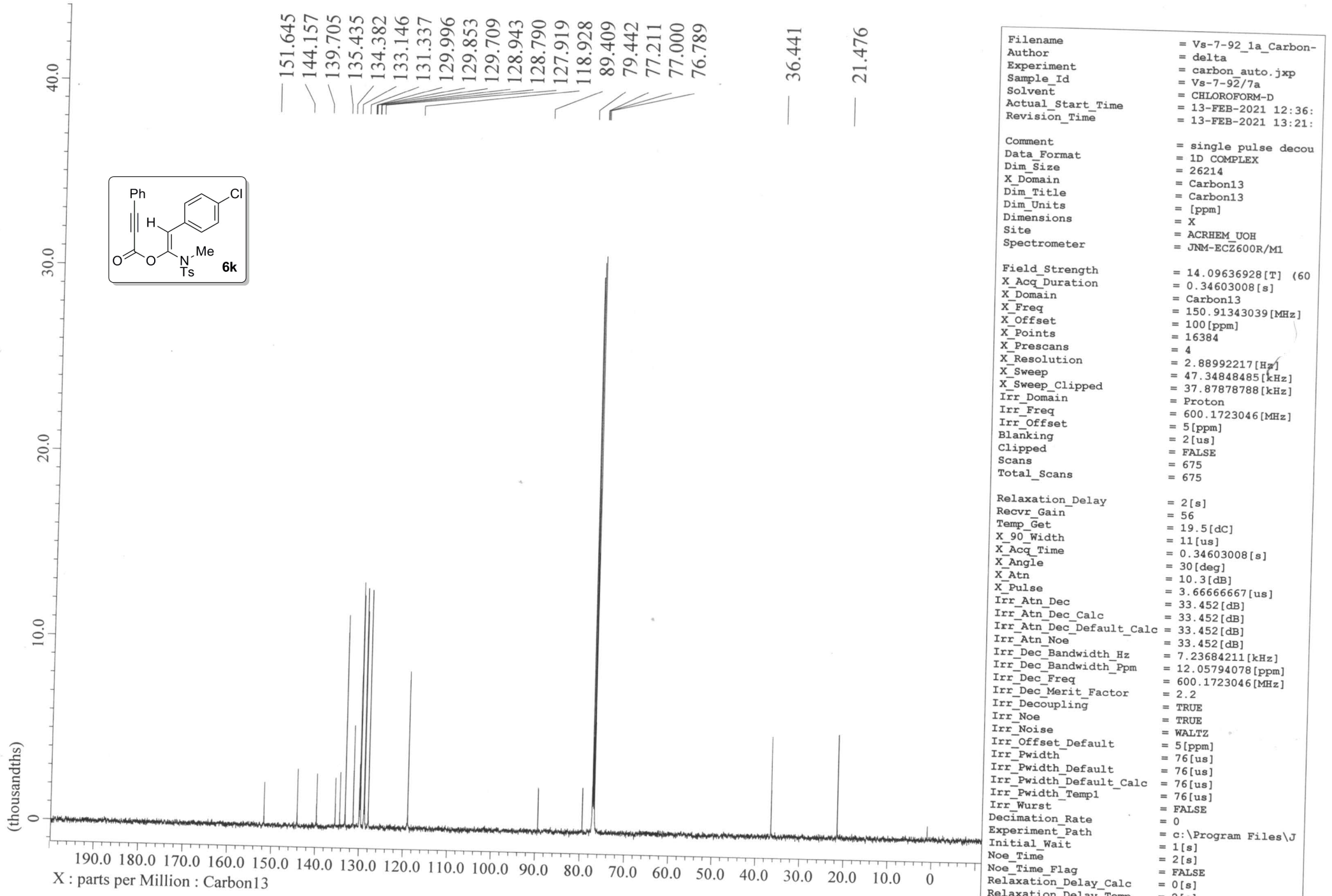

7.856
7.842
7.655
7.641
7.627
7.624
7.617
7.613
7.601
7.590
7.588
7.540
7.528
7.515
7.473
7.461
7.454
7.451
7.447
7.441
7.429
7.380
7.368
7.355
7.279
7.265
7.257
6.377
3.098
2.296
Ph
Ph
H
O
O
N
Me
Ts
6j
abundance
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
8.07
0.97
4.10
0.99
2.04
1.01
2.99
3.01
X : parts per Million : Proton



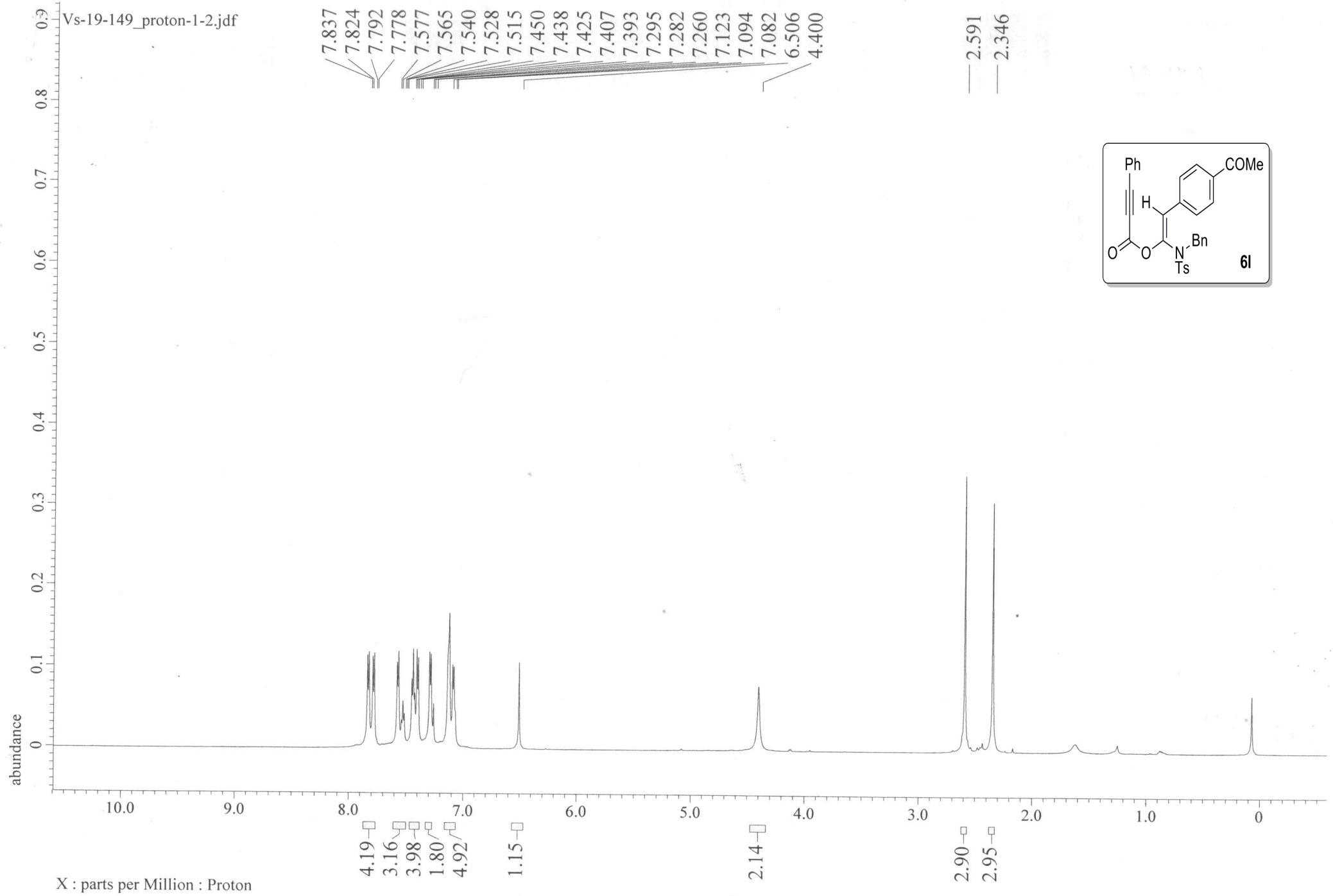
Filename	= Vs-7-93_Carbon-1-2
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= Vs-7-93
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-FEB-2021 15:56:
Revision_Time	= 13-FEB-2021 13:10:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.1[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]

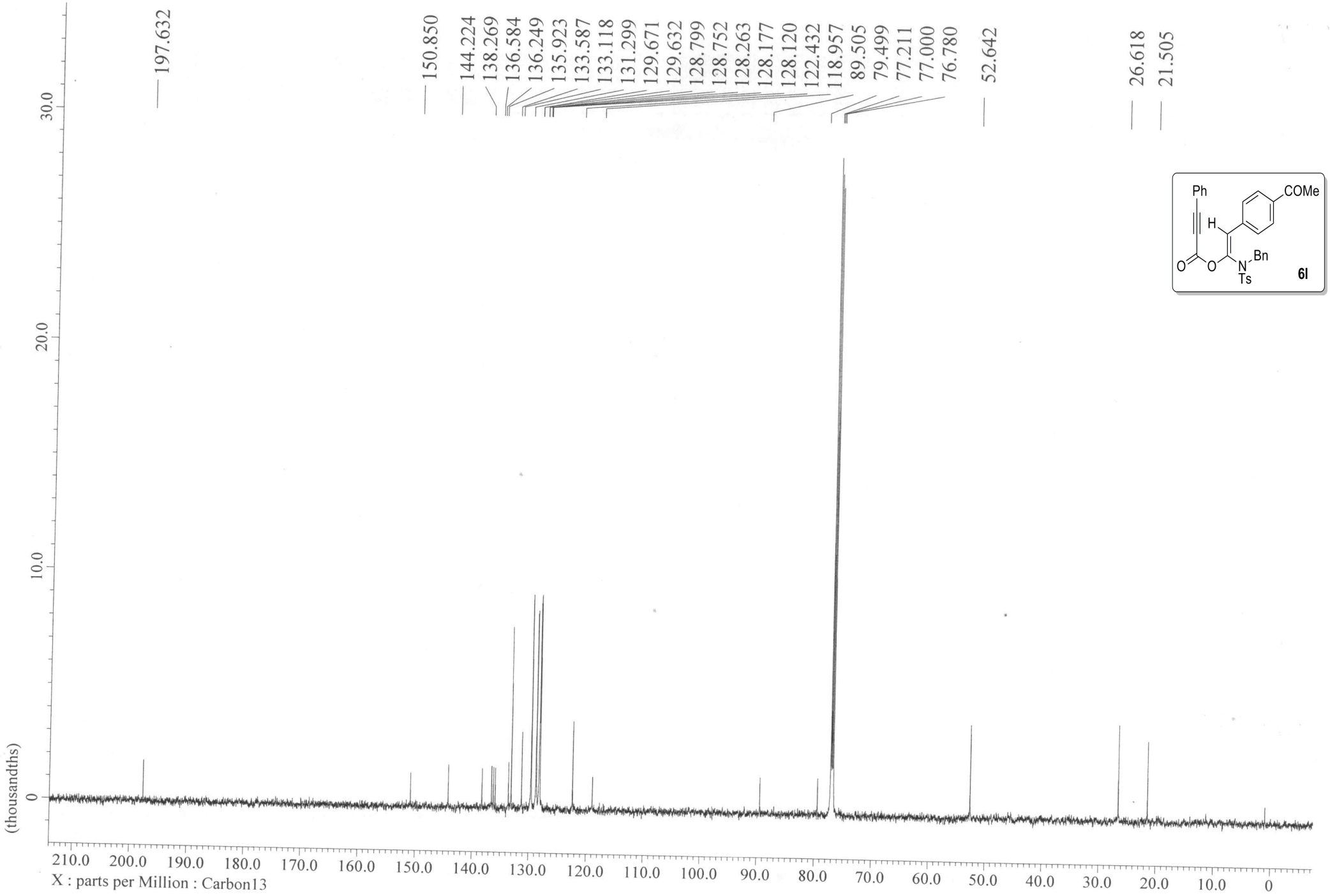


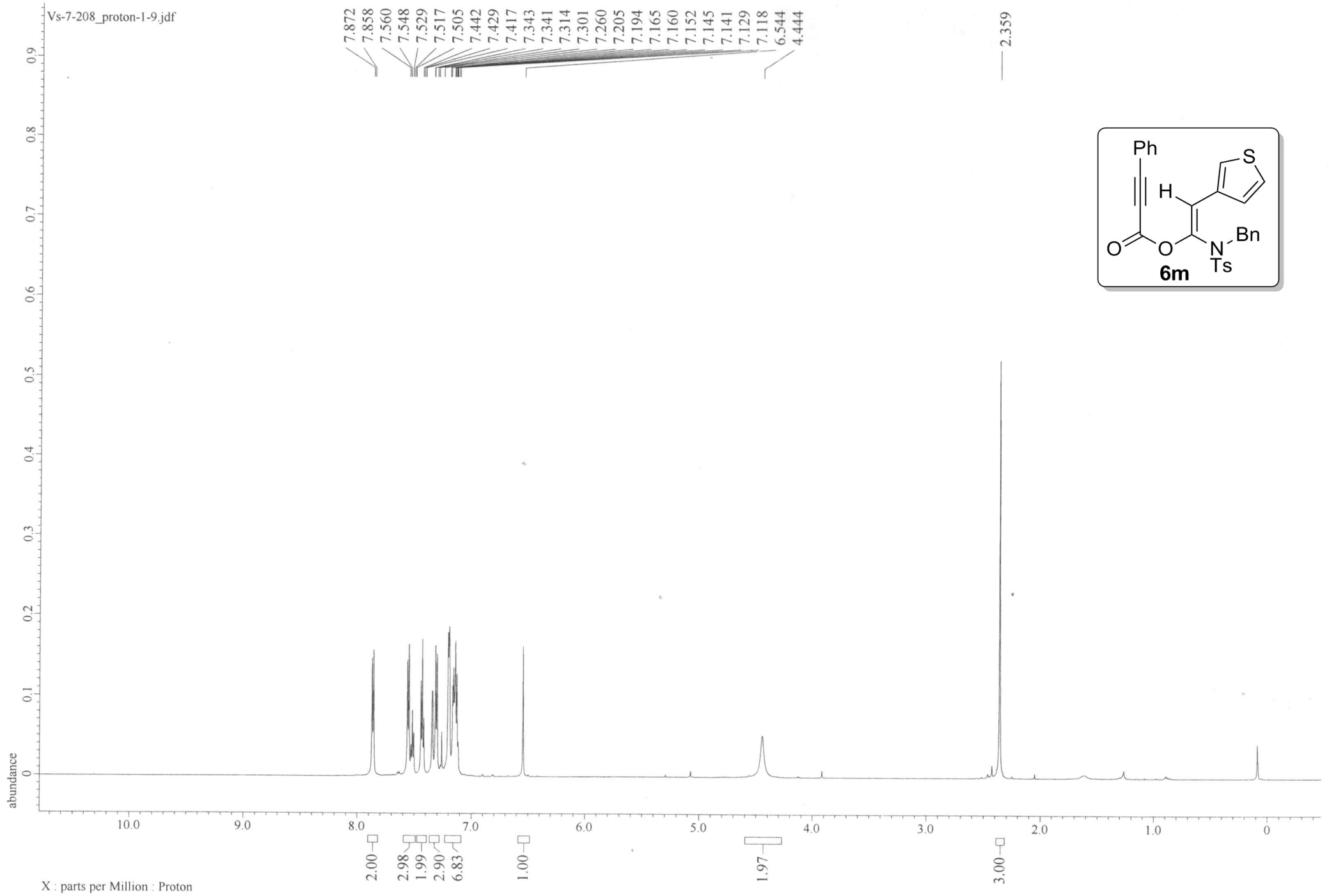
Filename	= Vs-7-92_1a_Proton-1-3
Author	= delta
Experiment	= proton_auto.jxp
Sample_Id	= Vs-7-92/7a
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-FEB-2021 12:34:10
Revision_Time	= 15-AUG-2021 15:03:08
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.72876032[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.37219326[Hz]
X_Sweep	= 22.48201439[kHz]
X_Sweep_Clipped	= 17.98561151[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.5[dC]
X_90_Width	= 6.89[us]
X_Acq_Time	= 0.72876032[s]
X_Angle	= 45[deg]
X_Atn	= 12.6[dB]
X_Pulse	= 3.445[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.72876032[s]

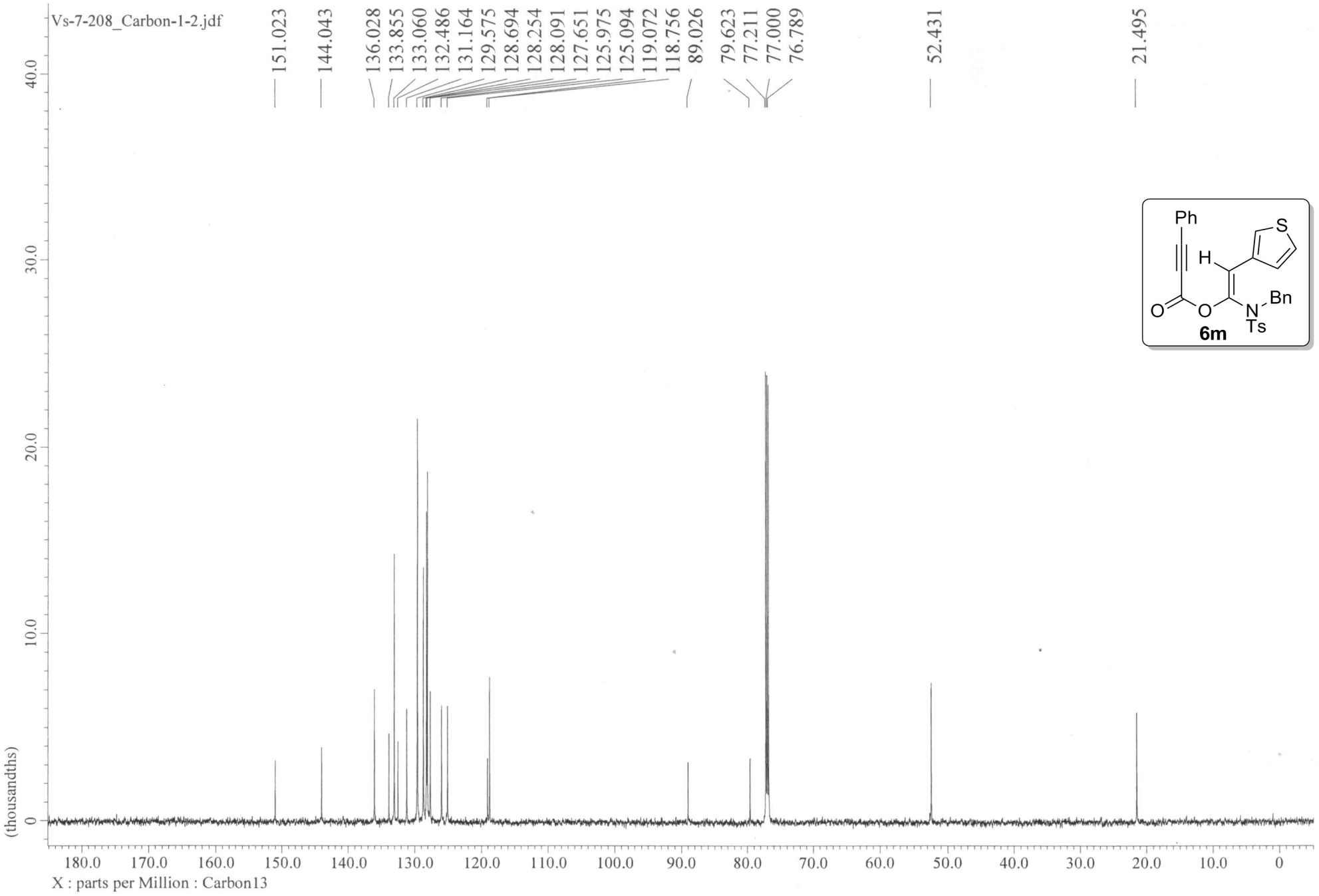


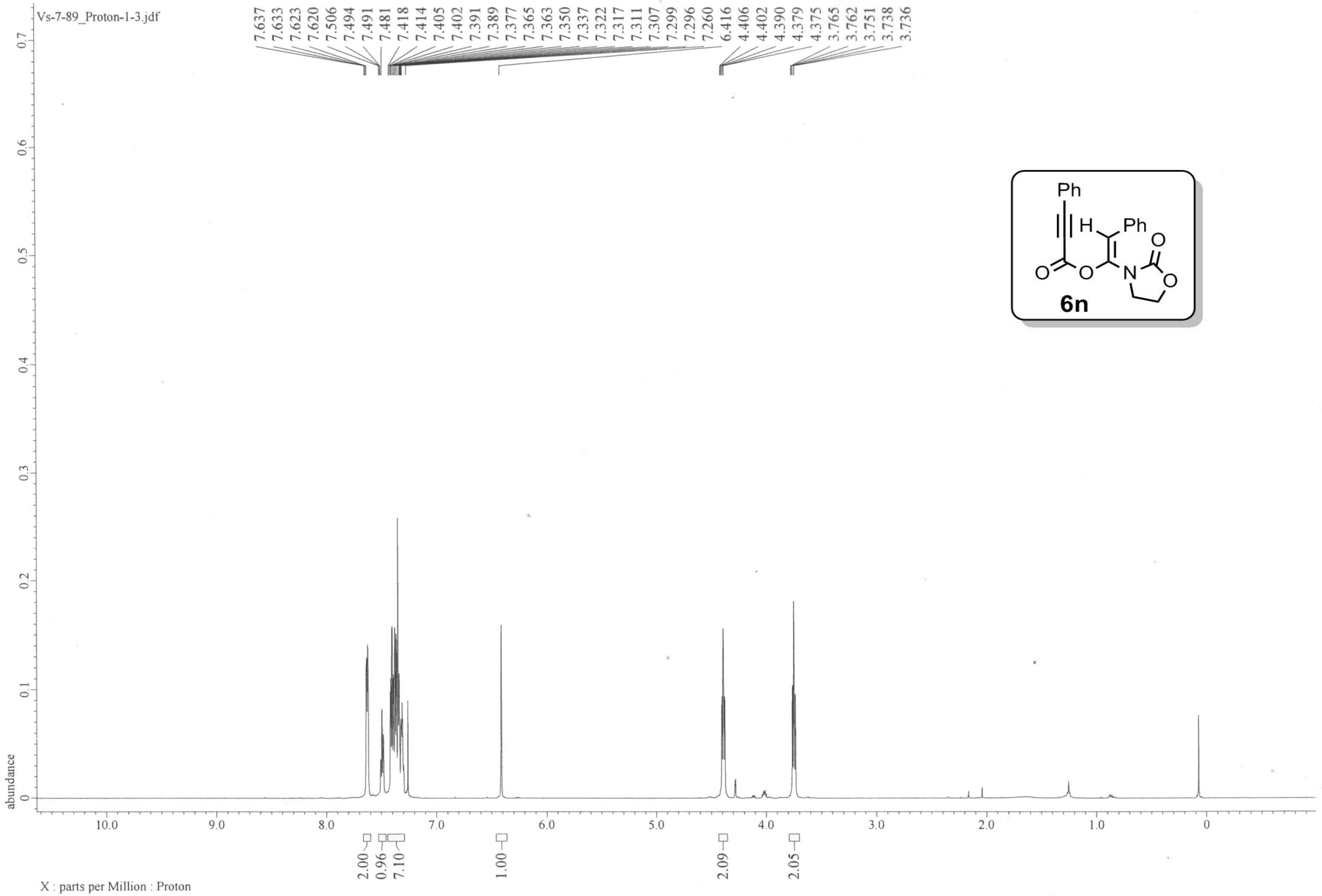
Filename	= Vs-7-92_1a_Carbon-
Author	= delta
Experiment	= carbon_auto.jxp
Sample_Id	= Vs-7-92/7a
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-FEB-2021 12:36:
Revision_Time	= 13-FEB-2021 13:21:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ACRHEM_UOH
Spectrometer	= JNM-ECZ600R/M1
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.34603008[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 2.88992217[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 675
Total_Scans	= 675
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 19.5[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 0.34603008[s]
X_Angle	= 30[deg]
X_Atn	= 10.3[dB]
X_Pulse	= 3.66666667[us]
Irr_Atn_Dec	= 33.452[dB]
Irr_Atn_Dec_Calc	= 33.452[dB]
Irr_Atn_Dec_Default_Calc	= 33.452[dB]
Irr_Atn_Noe	= 33.452[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\J
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]

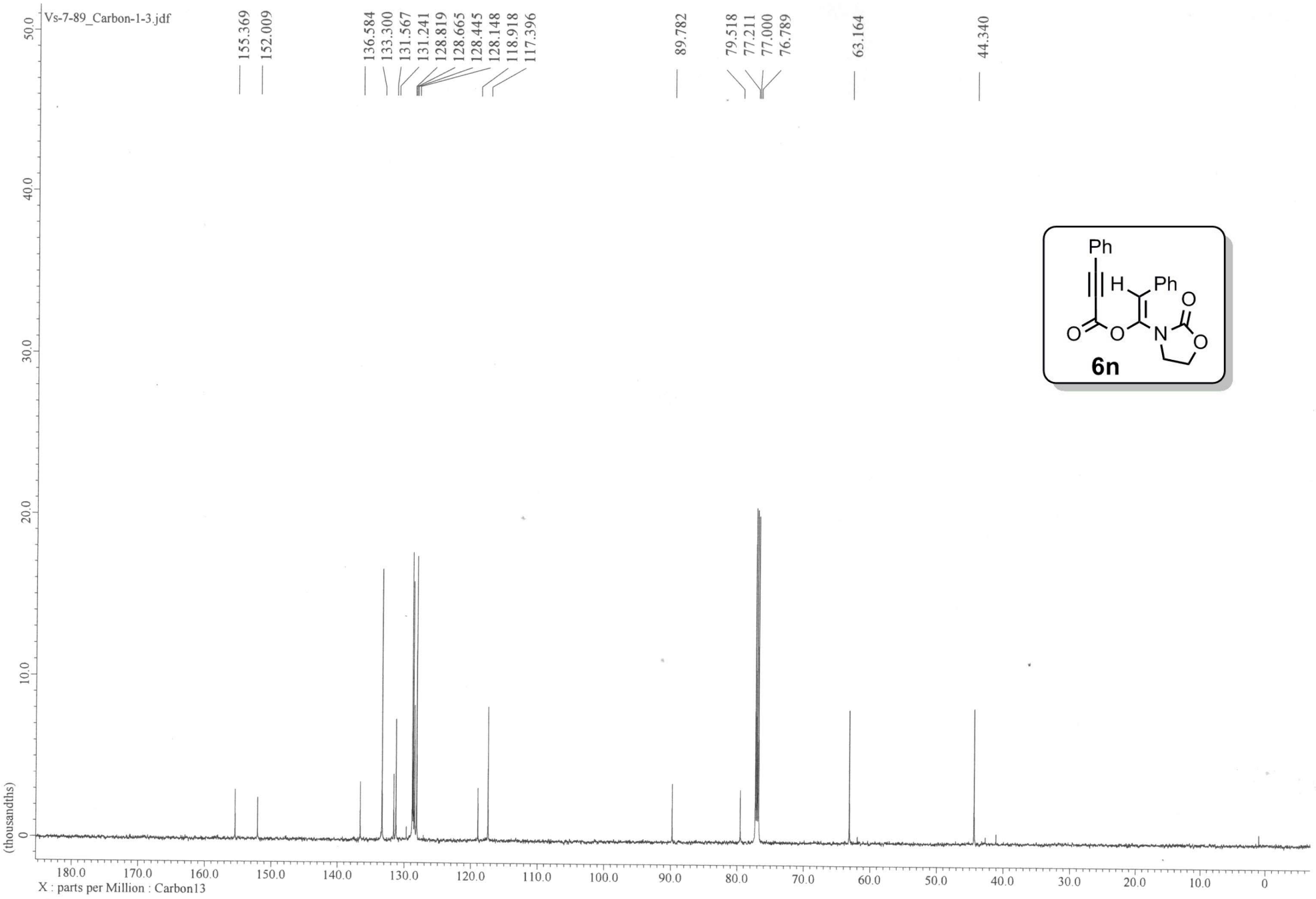

Vs-19-149_proton-1-2.jdf
7.837
7.824
7.792
7.778
7.577
7.565
7.540
7.528
7.515
7.450
7.438
7.425
7.407
7.393
7.295
7.282
7.260
7.123
7.094
7.082
6.506
4.400
2.591
2.346
Ph
COMe
H
O
O
N
Bn
Ts
6l
abundance
X : parts per Million : Proton
4.19
3.16
3.98
1.80
4.92
1.15
2.14
2.90
2.95

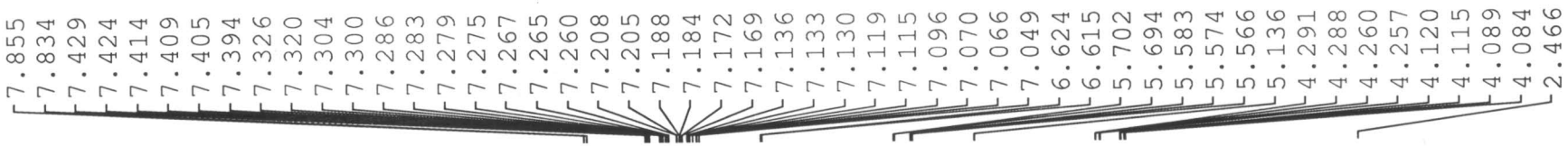

197.632
150.850
144.224
138.269
136.584
136.249
135.923
133.587
133.118
131.299
129.671
129.632
128.799
128.752
128.263
128.177
128.120
122.432
118.957
89.505
79.499
77.211
77.000
76.780
52.642
26.618
21.505
Ph
COMe
H
Bn
N
Ts
O
O
6l
30.0
20.0
10.0
0
(thousandths)
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : Carbon13

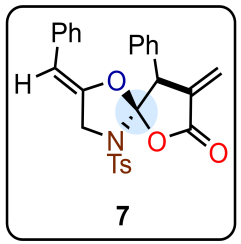

Vs-7-208_proton-1-9.jdf
7.872
7.858
7.560
7.548
7.529
7.517
7.505
7.442
7.429
7.417
7.343
7.341
7.314
7.301
7.260
7.205
7.194
7.165
7.160
7.152
7.145
7.141
7.129
7.118
6.544
4.444
2.359
Ph
S
H
Bn
O
O
N
Ts
6m
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
2.98
1.99
2.90
6.83
1.00
1.97
3.00
X : parts per Million : Proton


Vs-7-208_Carbon-1-2.jdf
151.023
144.043
136.028
133.855
133.060
132.486
131.164
129.575
128.694
128.254
128.091
127.651
125.975
125.094
119.072
118.756
89.026
79.623
77.211
77.000
76.789
52.431
21.495
Ph
S
H
O
O
N
Bn
Ts
6m
(thousandths)
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13

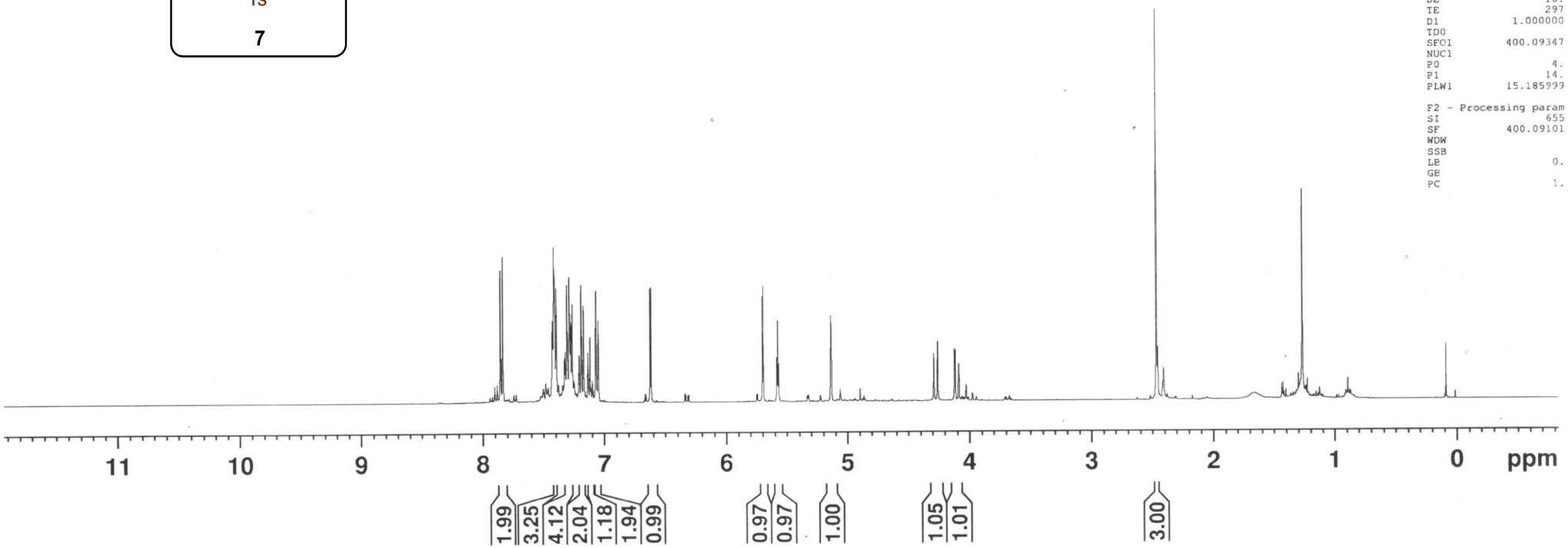

Vs-7-89_Proton-1-3.jdf
7.637
7.633
7.623
7.620
7.506
7.494
7.491
7.481
7.418
7.414
7.405
7.402
7.391
7.389
7.377
7.365
7.363
7.350
7.337
7.322
7.317
7.311
7.307
7.299
7.296
7.260
6.416
4.406
4.402
4.390
4.379
4.375
3.765
3.762
3.751
3.738
3.736
Ph
H
Ph
O
O
O
N
O
6n
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
0.96
7.10
1.00
2.09
2.05
X : parts per Million : Proton


Vs-7-89_Carbon-1-3.jdf
155.369
152.009
136.584
133.300
131.567
131.241
128.819
128.665
128.445
128.148
118.918
117.396
89.782
79.518
77.211
77.000
76.789
63.164
44.340
Ph
H
Ph
O
O
O
N
O
6n
(thousandths)
X : parts per Million : Carbon13





7




```
Current Data Paramete
NAME        Z Aryl Migra
EXPNO
PROCNO

F2 - Acquisition Para
Date_             201912
Time                15.
INSTRUM            spe
PROBHD    Z108618_0098
PULPROG              zg
TD                  655
SOLVENT             CDC
NS
DS
SWH              8012.8
FIDRES           0.2445
AQ              4.08944
RG                    1
DW                 62.4
DE                 16.
TE                  297
D1              1.000000
TD0
SFO1           400.09347
NUC1
P0                    4.
P1                   14.
PLW1           15.185999

F2 - Processing param
SI                  655
SF             400.09101
WDW
SSB
LB                    0.
GB
PC                    1.
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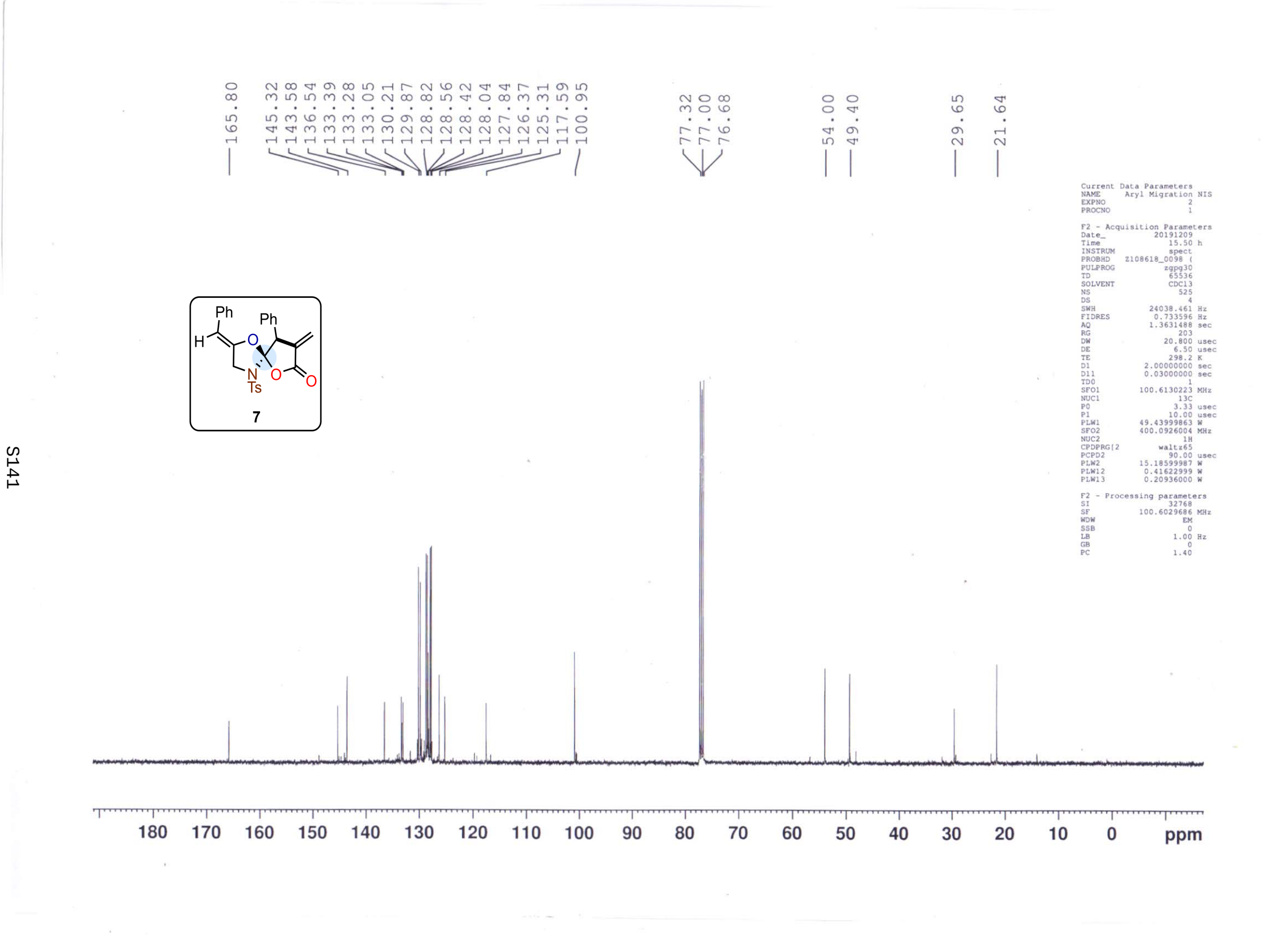
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145.32
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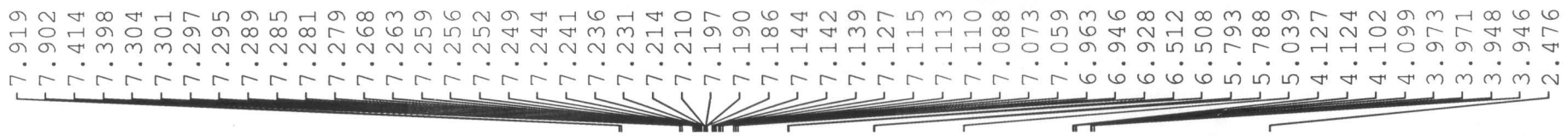
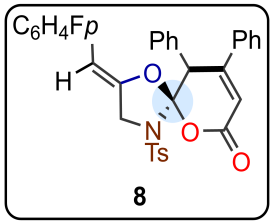
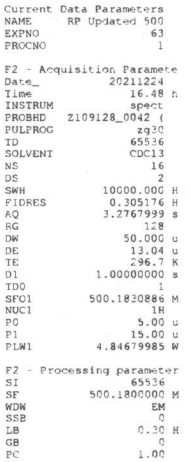
133.39
133.28
133.05
130.21
129.87
128.82
128.56
128.42
128.04
127.84
126.37
125.31
117.59
100.95
77.32
77.00
76.68
54.00
49.40
29.65
21.64
Ph
Ph
H
O
N
Ts
O
O
7
Current Data Parameters
NAME Aryl Migration NIS
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191209
Time 15.50 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 525
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 298.2 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 100.6029686 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


7.919
7.902
7.414
7.398
7.304
7.301
7.297
7.295
7.289
7.285
7.281
7.279
7.268
7.263
7.259
7.256
7.252
7.249
7.244
7.241
7.236
7.231
7.214
7.210
7.197
7.190
7.186
7.144
7.142
7.139
7.127
7.115
7.113
7.110
7.088
7.073
7.059
6.963
6.946
6.928
6.512
6.508
5.793
5.788
5.039
4.127
4.124
4.102
4.099
3.973
3.971
3.948
3.946
2.476


C6H4Fp
Ph
Ph
H
O
N
Ts
O
O

8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EXPNO 63
PROCNO 1
F2 - Acquisition Parameter
Date_ 20211224
Time 16.48 h
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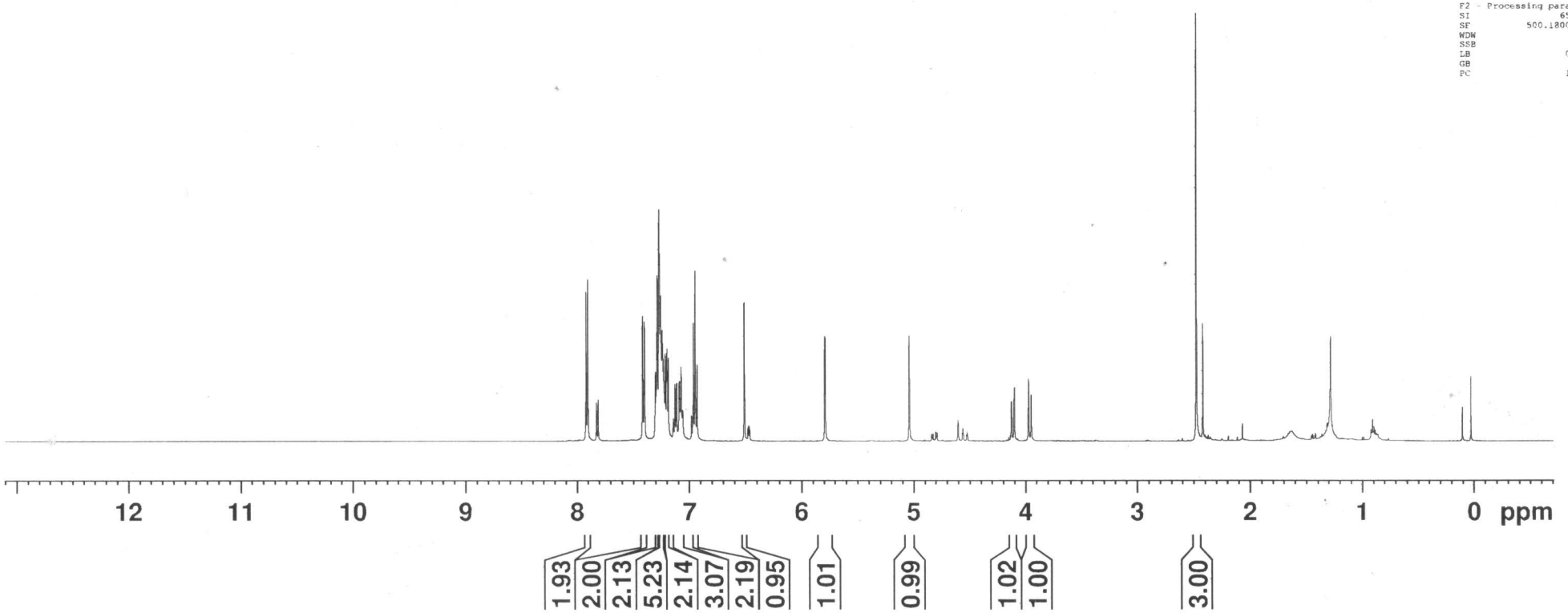
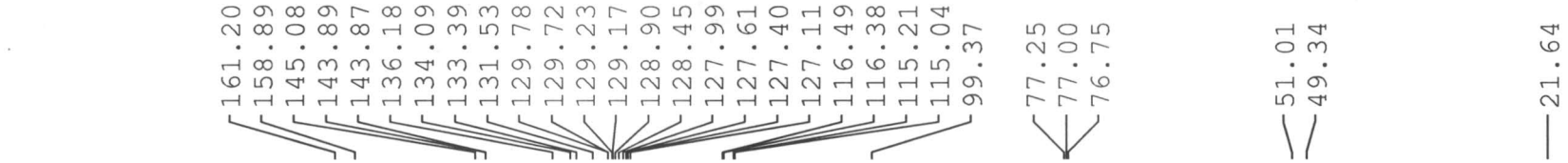
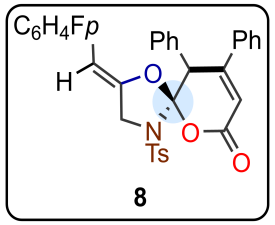
PROBHD Z109128_0042 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 H
FIDRES 0.305176 H
AQ 3.2767999 s
RG 128
DW 50.000 u
DE 13.04 u
TE 296.7 K
D1 1.00000000 s
TD0 1
SFO1 500.1830886 M
NUC1 1H
P0 5.00 u
P1 15.00 u
PLW1 4.84679985 W
F2 - Processing parameter
SI 65536
SF 500.1800000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00


12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.93
2.00
2.13
5.23
2.14
3.07
2.19
0.95
1.01
0.99
1.02
1.00
3.00

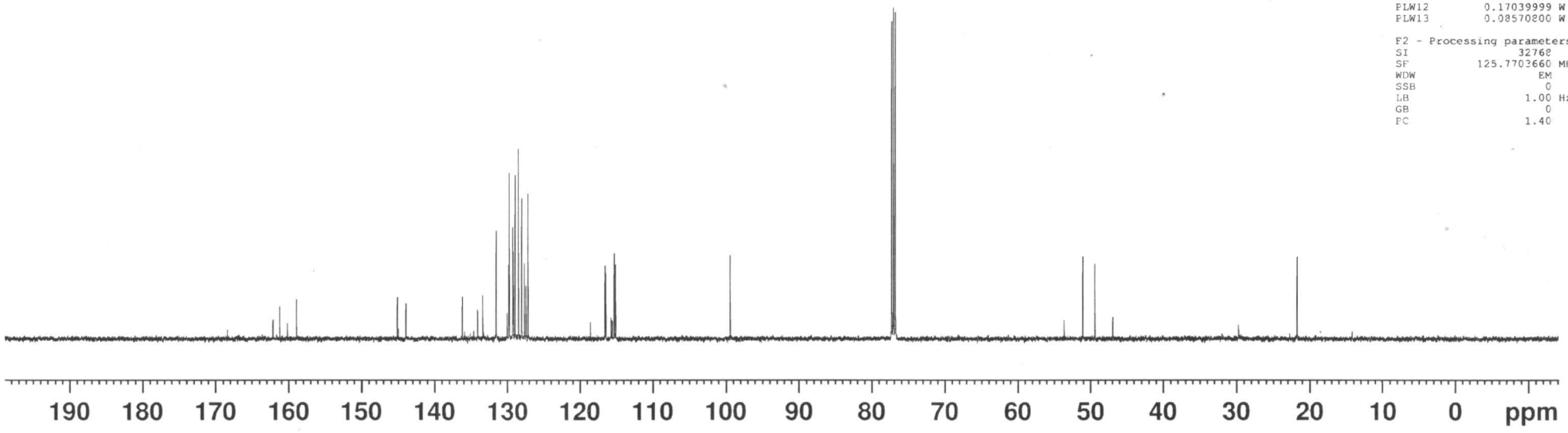


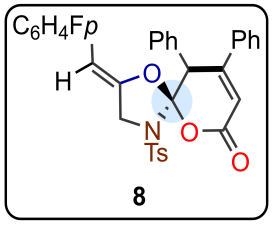



```
Current Data Parameters
NAME      RP Updated 500
EXPNO                 65
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211224
Time               17.14 h
INSTRUM             spect
PROBHD    Z109128_0042 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  365
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          64.00299780 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          125.7703660 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```





8

-110.48

Current Data Parameters
NAME RP Updated 400
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211129
Time 16.18 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
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 722.7 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