Supporting Information

for

Gold-catalyzed bicyclic annulations between 4-hydroxy-1,5-diynamides and nitrones for the synthesis of cyclopentene-fused isoxazole carboxamides

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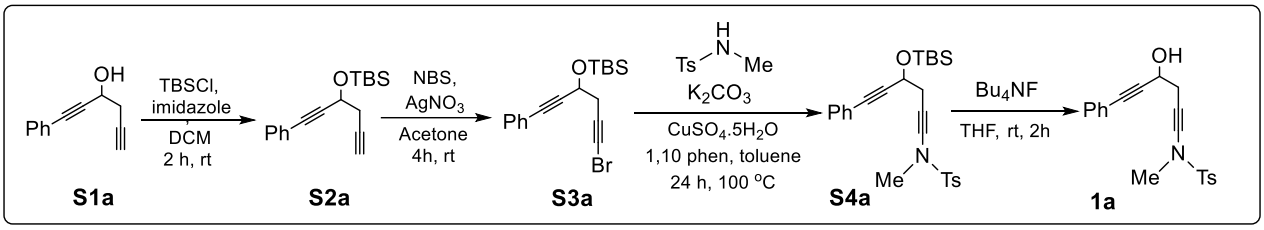
(1) General methods:

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under nitrogen atmosphere. Toluene and DCE were distilled from CaH_2 under nitrogen. THF was distilled from Na metal under nitrogen. All other commercial reagents were used without further purification unless otherwise indicated. ^1H NMR and ^{13}C NMR spectra were recorded on Varian 700 MHz, Bruker 400 MHz and Bruker 500 MHz Spectrometers using chloroform-d ($CDCl_3$: δ_H = 7.24 ppm, δ_C = 77.00) and dichloromethane-d (CD_2Cl_2: δ_H = 5.32 ppm, δ_C = 53.50) as solvents and Me_4Si as an internal standard. Chemical Shift (δ) and Spin-Spin coupling constant (J). The following abbreviations were used to show the multiplicities: s: singlet, bs: broad singlet, d: doublet, t: triplet, q: quadruplet, dd: doublet of doublet, tt: triplet of triplet, qt: quadruplet of triplet, tq: triplet of quadruplet, m: multiplet. Mass spectrometry was performed in the positive electrospray ionization (ESI+) mode, positive electron ionization (EI+) mode, positive field ionization (FI+) mode and field desorption (FD+) mode. All heating reactions were carried out with oil bath as heat source. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f - 254) using UV light as visualizing agents. Single-crystal X-ray diffraction intensity data were collected on a Bruker X8 APEX diffractometer equipped with a CCD area detector and Mo Kα radiation (λ = 0.71073 Å) at 100 K; all data calculations were performed by using the PC version of the APEX2 program package. All the substrate ynol-ynamides and nitrones were prepared according to the literature procedures described below.

(2) General procedure for synthesis of substrates:

2.1.a. General procedure for synthesis of 4-hydroxy-1,5-diyn-1-amides.



To a solution of compound **S1a** (5 g, 29.37 mmol) and imidazole (3.19 g, 47.00 mmol), in dry DCM (60 mL) was added TBSC1 (14.17 g, 94.00 mmol) under N_2 atmosphere at room temperature. The reaction mixture was stirred at room temperature for 2 h. The mixture was quenched with H_2O and extracted with DCM. The organic layers were separated and washed with H_2O, brine solution, and then dried over $MgSO_4$. The solvent was removed under reduced pressure. The residue was purified by column chromatography over silica gel with 2% EtOAc/Hexane to give a pale-yellow liquid of **S2a** (7.5 g, 90%).

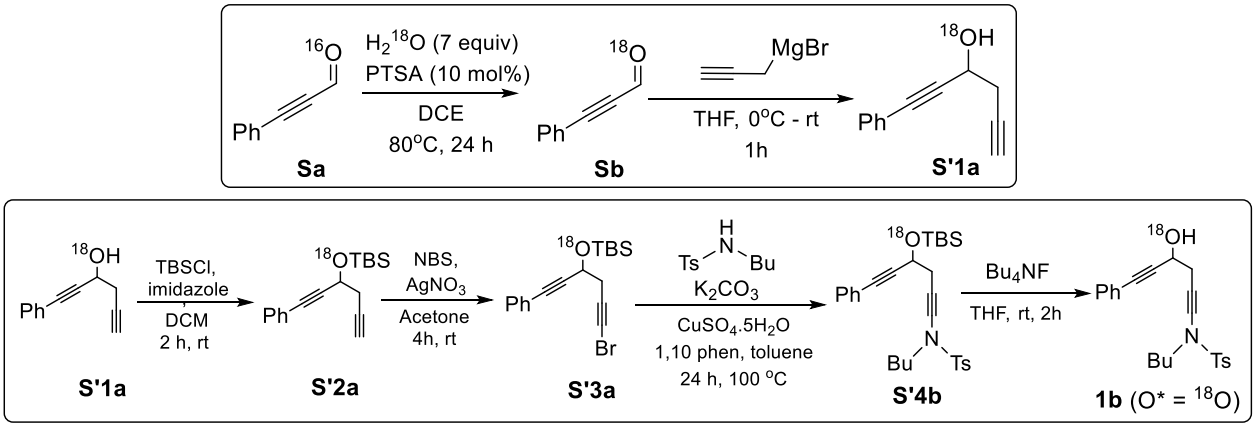
$AgNO_3$ (178 mg, 1.05 mmol) was added to a solution of **S2a** (3 g, 10.54 mmol) in acetone (50 mL). Then NBS (2 g, 11.6 mmol) was added in portions. The mixture was stirred for 4 h at room temperature and then concentrated in vacuo. The residue was dissolved in petroleum ether and filtered through a short column of silica gel with 2% EtOAc/Hexane. The solvent was removed in vacuo to afford a pale-yellow oil of **S3a** (3.2 g, 83%).

To a solution of the **S3a** (2 g, 5.50 mmol) in toluene (30 mL) were added $CuSO_4 \cdot 5H_2O$ (137.3 mg, 0.55 mmol), 1,10-phenanthroline (99 mg, 0.55 mmol), K_2CO_3 (1.9 g, 13.75 mmol) and amide (1.2 g, 6.60 mmol) at room temperature under Ar. After being stirred at 80 °C for 24 h, the reaction mixture was cooled to room temperature, filtered through a pad of Celite, and washed with CH_2Cl_2. The residue was concentrated in vacuo and purified by column chromatography on silica gel with 10% EtOAc/Hexane to give the corresponding product **S4a** (2.1 g, 82%).

To a stirred solution of **S4a** (1 g, 2.14 mmol) in THF (15 mL) was added tetra-n-butyl-ammonium fluoride (TBAF) (615 mg, 2.35 mmol) slowly. The reaction mixture was stirred at room temperature for 2 h. The reaction mixture was diluted with 1 N HCl. The aqueous layer was extracted with EtOAc. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography over silica gel with 25% EtOAc/Hexane to give **1a** (680 mg, 90%) as a colorless oil.

Other 4-hydroxy-1,5-diyn-1-amides **1a, 1b, 1c, 1d, 1e, 1f, 1g, 1h, 1i, 1j, 1k, 1l, 1m** and **1n** were prepared according to the above-mentioned procedure.
All the intermediates **S1** were prepared according to the procedure reported in the literature.[1]

2.1.b. Procedure for synthesis of ^{18}O substituted 4-hydroxy-1,5-diyn-1-amide {1b (O* = ^{18}O)}.



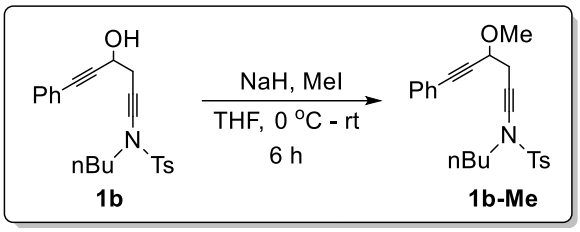
A Schlenk tube was charged with 3 ml DCE solution of **Sa** (600 mg, 4.6 mmol). $H_2{}^{18}O$ (7 equiv, 650 mg, 32.2 mmol) (98 atom% ^{18}O) and PTSA (0.46 mmol) were added to this solution, and the solution was stirred for 24 hours at 80 °C. The reaction was cooled down and filtered through a short celite pad, concentrated in vacuo to obtain **Sb** (98%), and was then used for further reaction.

The other steps were performed according to the above-mentioned procedure.

2.2. Synthetic procedure for 6-((*N*-butyl-4-methylphenyl)sulfonamido)-1-phenylhexa-1,5-diyn-3-yl acetate (1b-Ac).

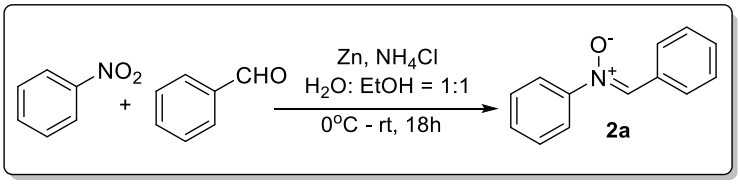
Compound **1b** (500 mg, 1.26 mmol) was added to 15 mL of dichloromethane, NEt_3 (3.78 mmol, 3 equiv.) was added, and the reaction was stirred for 10 minutes. The acetic anhydride (1.8 mmol, 1.2 equiv.) was added slowly and reacted for 12 hours at ambient temperature. The reaction mixture was quenched with aqueous NH_4Cl solution and extracted with dichloromethane. The organic layer was dried over sodium sulfate, filtered and the solvent was concentrated in vacuo and purified by column chromatography on silica gel with 5% EtOAc/Hexane to give the corresponding product **1b-Ac** (492 mg, 89%).

2.3. Synthetic procedure for *N*-butyl-*N*-(4-methoxy-6-phenylhexa-1,5-diyn-1-yl)-4-methyl benzene sulfonamide (1b-Me).



Compound **1b** (500 mg, 1.26 mmol) was added to 15 mL of tetrahydrofuran, the temperature was lowered to 0 °C, NaH (36 mg, 1.5 mmol) was added, and the temperature was raised to 25 ° C and stirred for 1.0 hours. The methyl iodide (6.3 mmol) was added and reacted for 5 hours at ambient temperature. The reaction mixture was diluted with water (30 mL) and extracted with ethyl acetate. The organic layer was dried over sodium sulfate, filtered and the solvent was concentrated in vacuo and purified by column chromatography on silica gel with 5% EtOAc/Hexane to give the corresponding product **1b-Me** (480 mg, 93%).

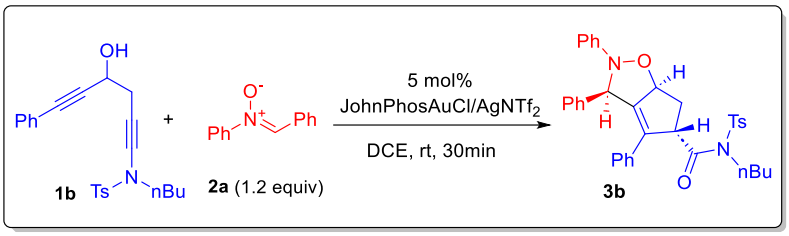
2.4. General procedure for synthesis of Nitrones.



Nitrobenzene (20 mmol, 1.0 equiv), aldehyde (22 mmol, 1.1 equiv) and NH_4Cl (26 mmol, 1.3 equiv) were dissolved in a mixture of EtOH and water (1:1) and cooled to 0 °C (ice bath). Then zinc powder (40 mmol, 2.0 equiv) was added to the resulting mixture over 1 hour, and the reaction was allowed to warm to room temperature and stirred for 18 hours. The reaction mixture was filtered and washed with CH_2Cl_2. The filtrate was extracted with CH_2Cl_2 (4 × 50 mL), and the combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure to give crude nitrones. Recrystallization of the crude product with DCM/pentane afforded (*Z*)-*N*,1-diphenylmethanimine oxide **2a** (3.35 g, 16.98 mmol, 85%) as a Colorless solid.

All the nitrones were prepared according to the procedure reported in the literature.[2]

(3) Standard procedure for gold-catalyzed annulation reaction.



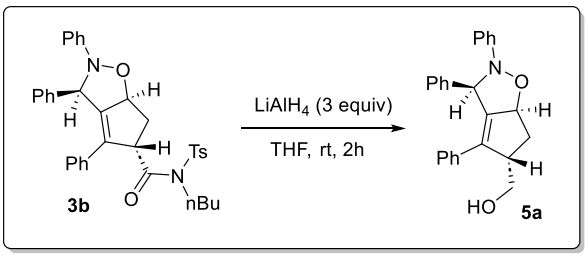
A Schlenk tube was charged with JohnPhos gold chloride (5.31 mg, 0.01 mmol) and $AgNTf_2$ (3.88 mg, 0.01 mmol), and to this mixture was added dry DCE (2 mL). The resulting mixture was stirred at room temperature for 5 minutes, and to this mixture was added a dry DCE solution (2 mL) of (*Z*)-*N*,1-diphenylmethanimine oxide **2a** (47.3 mg, 0.24 mmol). After stirring it for 2 minutes, DCE solution (1 mL) of *N*-butyl-*N*-(4-hydroxy-6-phenylhexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide **(1b)** (79 mg, 0.2 mmol) was dropwise slowly added to this mixture. After stirring for 30 minutes at room temperature, the reaction mixture was filtered through a short celite bed and concentrated to crude products **3b**. Flash column chromatography on a silica column (5% EA/hexane) afforded the desired (3*R*,5*S*,6a*S*)-*N*-butyl-2,3,4-triphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide **3b** (77 mg, 0.129 mmol, 65%) as a white sticky solid. All the other products were prepared similarly.

(4) Standard procedure for scale-up reaction and chemical functionalizations.

4.1. Standard procedure for scale-up reaction.

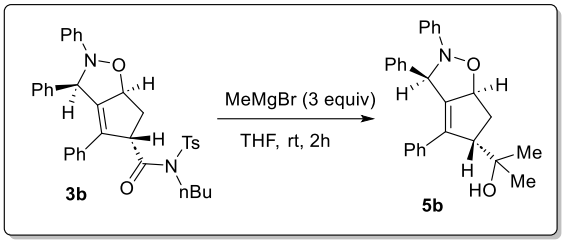
A scale-up reaction was performed between *N*-butyl-*N*-(4-hydroxy-6-phenylhexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide **1b** (1.2 g, 3.00 mmol) and nitrone **2a** (710 mg, 3.6 mmol) in dichloroethane (DCE, 20.0 mL) under the standard conditions to afford **3b** (1.04 g, 58 %) as white sticky solid.

4.2. Synthesis of (2,3,4-triphenyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazol-5-yl)methanol (5a):



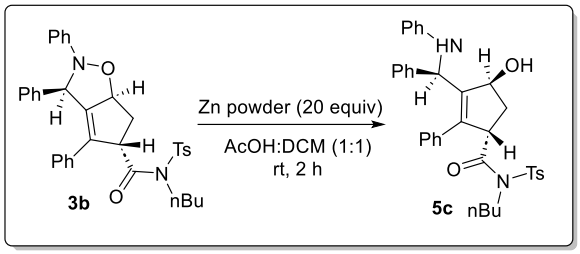
To a dry THF (3 mL) solution of **3b** (118.5 mg, 0.20 mmol) was added $LiAlH_4$ (22.8 mg, 0.60 mmol) and the reaction was stirred at room temperature for 2 h. Upon completion of the reaction, the reaction mixture was quenched with a saturated NH_4Cl and extracted with DCM and brine solution. The organic layer was dried with $MgSO_4$ and concentrated under reduced pressure and purified by column chromatography over silica gel with 15% EtOAc/Hexane to afford **5a** (39.0 mg, 0.105 mmol, 53%) as a white solid.

4.3. Synthesis of 2-(2,3,4-triphenyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazol-5-yl)propan-2-ol (5b):

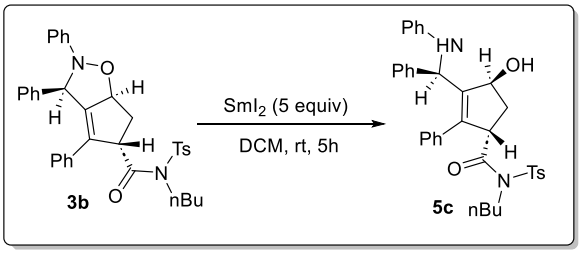


To a dry THF (3 mL) solution of **3b** (118.5 mg, 0.20 mmol) was added MeMgBr (3M in diethyl ether) (0.2 mL, 0.60 mmol) at 0 °C and the reaction was stirred at room temperature for 2 h. Upon completion of the reaction, the reaction mixture was quenched with a saturated NH_4Cl and extracted with DCM and brine solution. The organic layer was dried with $MgSO_4$ and concentrated under reduced pressure and purified by column chromatography over silica gel with 15% EtOAc/Hexane to afford **5b** (50.8 mg, 0.127 mmol, 64%) as a white solid.

4.4. Synthesis of *N*-butyl-4-hydroxy-2-phenyl-3-((*R*)-phenyl(phenylamino)methyl)-*N*-tosylcyclopent-2-ene-1-carboxamide (5c):



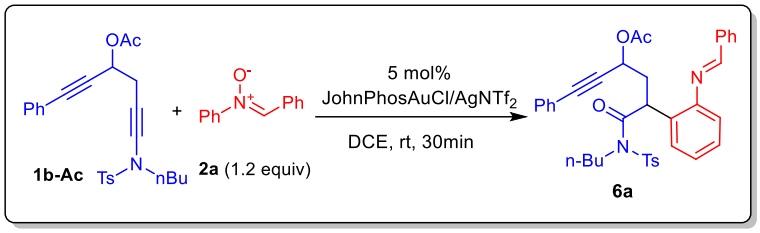
To a DCM (3 mL) solution of **3b** (118.5 mg, 0.20 mmol) was added a Zn powder (261.5.0 mg, 4.0 mmol) followed by HOAc (3 mL), and the reaction was stirred at room temperature for 2 h. Upon completion of the reaction, the reaction mixture was extracted with DCM and brine solution. The organic layer was dried with $MgSO_4$ and concentrated under reduced pressure and purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **5c** (48.7 mg, 0.082 mmol, 41%) as a white solid.



To a DCM (3 mL) solution of **3b** (118.5 mg, 0.20 mmol) was added a SmI_2 (404.0 mg, 1.0 mmol) and the reaction was stirred at room temperature for 5 h. Upon completion of the reaction, the reaction mixture was extracted with DCM and brine solution. The organic layer was dried with $MgSO_4$ and concentrated under reduced pressure and purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **5c** (45.1 mg, 0.076 mmol, 38%) as a white solid.

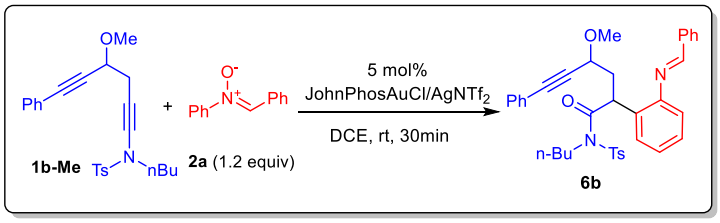
(5) Control experiments.

5.1.a. Synthesis of (*E*)-5-(2-(benzylideneamino)phenyl)-6-((*N*-butyl-4-methylphenyl)sulfonamido)-6-oxo-1-phenylhex-1-yn-3-yl acetate (6a):



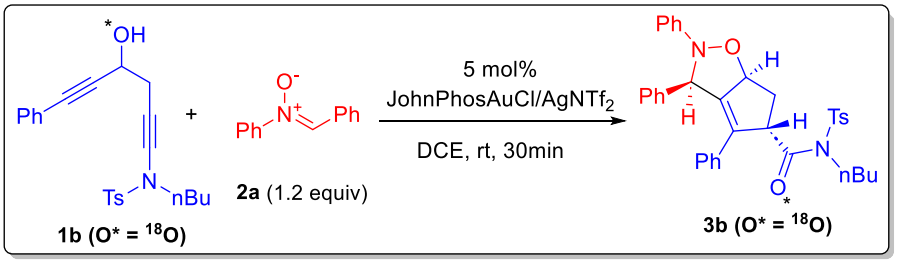
A Schlenk tube was charged with JohnPhos gold chloride (5.31 mg, 0.01 mmol) and $AgNTf_2$ (3.88 mg, 0.01 mmol), and to this mixture was added dry DCE (2 mL). The resulting mixture was stirred at room temperature for 5 minutes, and to this mixture was added a dry DCE solution (2 mL) of (*Z*)-*N*,1-diphenylmethanimine oxide **2a** (47.3 mg, 0.24 mmol). After stirring it for 2 minutes, DCE solution (1 mL) of 6-((*N*-butyl-4-methylphenyl)sulfonamido)-1-phenylhexa-1,5-diyn-3-yl acetate **(1b-Ac)** (87.5 mg, 0.2 mmol) was dropwise slowly added to this mixture. After stirring for 30 minutes at room temperature, the reaction mixture was filtered through a short celite bed and concentrated to crude products **6a**. Flash column chromatography on a silica column (5% EA/hexane) afforded the desired (*E*)-5-(2-(benzylideneamino)phenyl)-6-((*N*-butyl-4-methylphenyl)sulfonamido)-6-oxo-1-phenylhex-1-yn-3-yl acetate **6a** (82 mg, 0.129 mmol, 65%) as a white solid.

5.1.b. Synthesis of (*E*)-2-(2-(benzylideneamino)phenyl)-*N*-butyl-4-methoxy-6-phenyl-*N*-tosylhex-5-ynamide (6b):

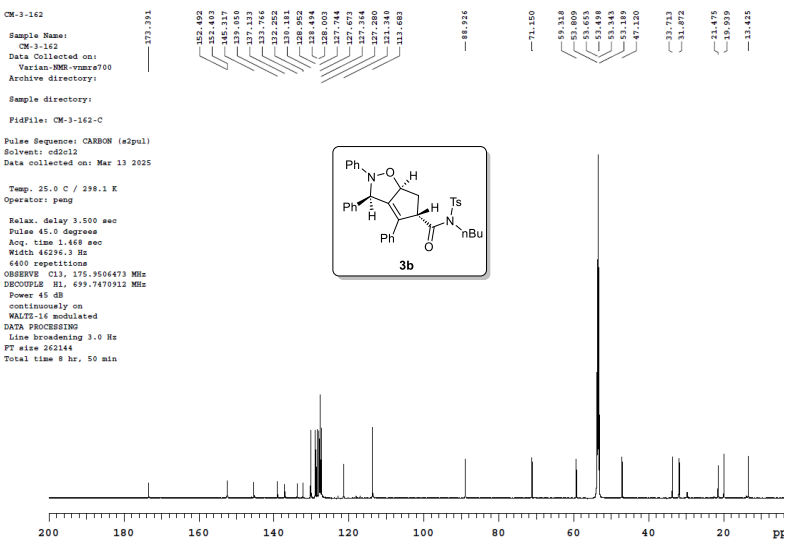


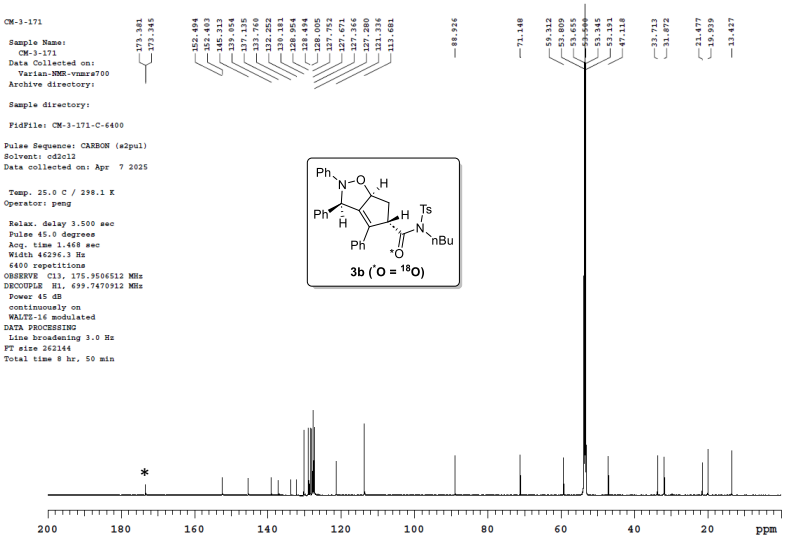
A Schlenk tube was charged with JohnPhos gold chloride (5.31 mg, 0.01 mmol) and $AgNTf_2$ (3.88 mg, 0.01 mmol), and to this mixture was added dry DCE (2 mL). The resulting mixture was stirred at room temperature for 5 minutes, and to this mixture was added a dry DCE solution (2 mL) of (*Z*)-*N*,1-diphenylmethanimine oxide **2a** (47.3 mg, 0.24 mmol). After stirring it for 2 minutes, DCE solution (1 mL) of *N*-butyl-*N*-(4-methoxy-6-phenylhexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide **(1b-Me)** (82.0 mg, 0.2 mmol) was dropwise slowly added to this mixture. After stirring for 30 minutes at room temperature, the reaction mixture was filtered through a short celite bed and concentrated to crude products **6b**. Flash column chromatography on a silica column (5% EA/hexane) afforded the desired (*E*)-2-(2-(benzylideneamino)phenyl)-*N*-butyl-4-methoxy-6-phenyl-*N*-tosylhex-5-ynamide **6b** (86 mg, 0.141 mmol, 71%) as a white solid.

5.3. ^{18}O labeling experiment:



A Schlenk tube was charged with JohnPhos gold chloride (5.31 mg, 0.01 mmol) and $AgNTf_2$ (3.88 mg, 0.01 mmol), and to this mixture was added dry DCE (2 mL). The resulting mixture was stirred at room temperature for 5 minutes, and to this mixture was added a dry DCE solution (2 mL) of (*Z*)-*N*,1-diphenylmethanimine oxide **2a** (47.3 mg, 0.24 mmol). After stirring it for 2 minutes, DCE solution (1 mL) of ^{18}O-substituted *N*-butyl-*N*-(4-hydroxy-6-phenylhexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide **1b (O* = ^{18}O)** (79 mg, 0.2 mmol) was dropwise slowly added to this mixture. After stirring for 30 minutes at room temperature, the reaction mixture was filtered through a short celite bed and concentrated to crude products **3b (O* = ^{18}O)**. Flash column chromatography on a silica column (5% EA/hexane) afforded the desired (3*R*,5*S*,6a*S*)-*N*-butyl-2,3,4-triphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5 carboxamide **3b (O* = ^{18}O)** (75 mg, 0.125 mmol, 63%) as white sticky solid.





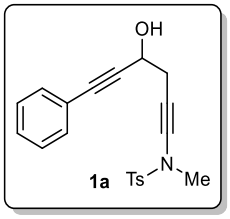
(6) References

(1) Tanpure, S. D.; Dhole, M. D.; Liu, R.-S. Gold-Catalyzed Cyclizations and [3 + 2]-Annulation Cascades between 1,5-Diyn-3-ols and Nitrones to Construct Carbazole Frameworks. *Adv. Synth. Catal.* **2023**, *365* (17), 2936– 2942.

(2) (a) Hosseini, A.; Schreiner, P. R. Synthesis of Exclusively 4-Substituted β-Lactams through the Kinugasa Reaction Utilizing Calcium Carbide. *Org. Lett*. **2019**, *21*, 3746– 3749. (b) Barik, D; Liu, R.-S. Gold(I)-Catalyzed [4 + 2] Annulation between Arylynes and C,N-Diaryl Nitrones for Chemoselective Synthesis of Quinoline Scaffolds via Gold Acetylide Intermediates. *J. Org. Chem.* **2022**, *87*, 11, 7097–7105.

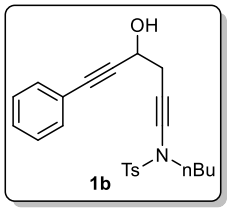
(7) Spectral data for key compounds:

Spectral data for *N*-(4-hydroxy-6-phenylhexa-1,5-diyn-1-yl)-*N*,4-dimethylbenzenesulfonamide (1a):



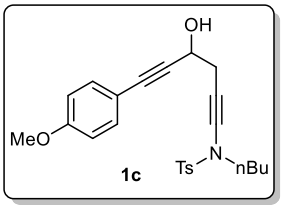
Purified by column chromatography over silica gel with 30% EtOAc/Hexane to afford **1a** as a yellow liquid (680 mg, 1.92 mmol, 90%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 – 7.77 (m, 2H), 7.44 – 7.42 (m, 2H), 7.32 – 7.27 (m, 3H), 7.24 – 7.21 (m, 2H), 4.70 – 4.66 (m, 1H), 3.03 (s, 3H), 2.79 – 2.76 (m, 2H), 2.37 – 2.34 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.5, 132.8, 131.6, 129.6, 128.4, 128.1, 127.6, 122.2, 88.6, 84.9, 77.5, 63.9, 61.4, 38.9, 28.4, 21.4; HRMS-ESI+ calcd for $C_{20}H_{19}NO_3SNa$ $[M+Na]^+$: 376.0983, found: 376.0984.

Spectral data for *N*-butyl-*N*-(4-hydroxy-6-phenylhexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide (1b):



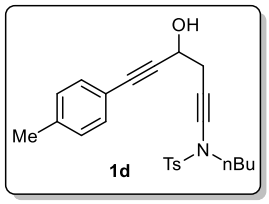
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1b** as a yellow liquid (665 mg, 1.68 mmol, 86%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 – 7.75 (m, 2H), 7.40 – 7.38 (m, 2H), 7.29 – 7.22 (m, 3H), 7.19 (d, J = 8.4 Hz, 2H), 4.71 – 4.67 (m, 1H), 3.23 (t, J = 7.2 Hz, 2H), 2.80 – 2.72 (m, 3H), 2.32 (s, 3H), 1.60 – 1.55 (m, 2H), 1.39 – 1.23 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.3, 134.3, 131.7, 129.6, 128.4, 128.1, 127.4, 122.2, 88.7, 84.9, 76.1, 65.3, 61.5, 50.9, 29.6, 28.7, 21.4, 19.3, 13.4; HRMS-ESI+ calcd for $C_{23}H_{25}NO_3SNa$ $[M+Na]^+$: 418.1452, found: 418.1458.

Spectral data for *N*-butyl-*N*-(4-hydroxy-6-(4-methoxyphenyl)hexa-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1c):



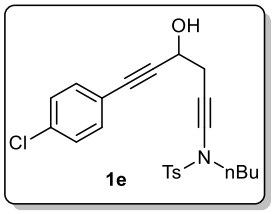
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1c** as a yellow liquid (717.0 mg, 1.68 mmol, 91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 2H), 4.68 – 4.63 (m, 1H), 3.77 (s, 3H), 3.23 (t, *J* = 7.6 Hz, 2H), 2.78 – 2.76 (m, 2H), 2.42 (s, 1H), 2.35 (s, 3H), 1.63 – 1.54 (m, 2H), 1.32 – 1.23 (m, 2H), 0.83 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 144.3, 134.4, 133.2, 129.6, 127.5, 114.3, 113.8, 87.2, 85.0, 76.2, 65.4, 61.6, 55.2, 50.9, 29.7, 28.8, 21.5, 19.4, 13.4; HRMS-ESI+ calcd for $C_{24}H_{27}NO_4SNa$ $[M+H]^+$: 448.1558, found: 448.1552.

Spectral data for *N*-butyl-*N*-(4-hydroxy-6-(p-tolyl)hexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide (1d):



Purified by column chromatography over silica gel with 25 % EtOAc/Hexane to afford **1d** as a yellow liquid (680 mg, 1.66 mmol, 87%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 4.69 – 4.64 (m, 1H), 3.23 (t, *J* = 7.2 Hz, 2H), 2.79 – 2.77 (m, 2H), 2.61 (d, *J* = 7.2 Hz, 1H), 2.34 (s, 3H), 2.31 (s, 3H), 1.61 – 1.54 (m, 2H), 1.30 – 1.23 (m, 2H), 0.82 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.3, 138.6, 134.4, 131.6, 129.6, 128.9, 127.5, 119.2, 87.9, 85.1, 76.1, 65.3, 61.6, 50.9, 29.6, 28.8, 21.4, 21.3, 19.3, 13.4; HRMS-ESI+ calcd for $C_{24}H_{27}NO_3SNa$ $[M+Na]^+$: 432.1609, found: 432.1611.

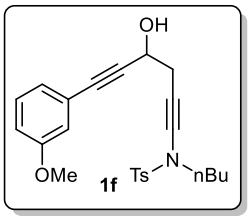
Spectral data for *N*-butyl-*N*-(6-(4-chlorophenyl)-4-hydroxyhexa-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1e):



Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1e** as a yellow liquid (650 mg, 1.51 mmol, 82%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 – 7.75 (m, 2H), 7.35 – 7.32 (m, 2H), 7.26 – 7.21 (m, 4H), 4.69 – 4.64 (m, 1H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.84 – 2.73 (m, 2H), 2.50 (d, *J* = 7.2 Hz, 1H), 2.36 (s, 3H), 1.65 – 1.53 (m, 2H), 1.30 – 1.25 (m, 2H), 0.83 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz,

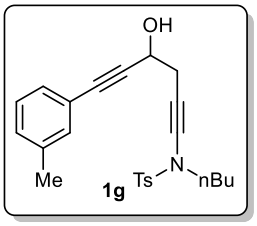
$CDCl_3$): δ 144.4, 134.6, 134.5, 133.0, 129.6, 128.6, 127.5, 120.8, 89.6, 84.0, 76.4, 65.1, 61.6, 50.9, 29.7, 28.7, 21.5, 19.4, 13.4; HRMS-ESI+ calcd for $C_{23}H_{24}ClNO_3SNa$ $[M+Na]^+$: 452.1063, found: 452.1059.

Spectral data for *N*-butyl-*N*-(4-hydroxy-6-(3-methoxyphenyl)hexa-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1f):



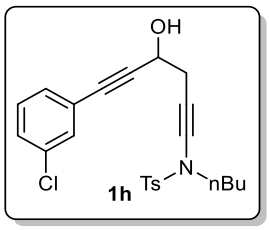
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1f** as a yellow liquid (701.2 mg, 1.64 mmol, 89%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.24 – 7.14 (m, 3H), 7.00 – 6.95 (m, 2H), 6.86 – 6.83 (m, 1H), 4.70 – 4.65 (m, 1H), 3.73 (s, 3H), 3.23 (t, *J* = 7.2 Hz, 2H), 2.84 – 2.69 (m, 3H), 2.33 (s, 3H), 1.60 – 1.53 (m, 2H), 1.31 – 1.20 (m, 2H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 144.3, 134.3, 129.6, 129.2, 127.4, 124.2, 123.2, 116.5, 115.1, 88.4, 84.9, 76.1, 65.2, 61.5, 55.1, 50.9, 29.6, 28.7, 21.4, 19.3, 13.4; HRMS-ESI+ calcd for $C_{24}H_{27}NO_4SNa$ $[M+Na]^+$: 448.1558, found: 448.1554.

Spectral data for *N*-butyl-*N*-(4-hydroxy-6-(m-tolyl)hexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide (1g):



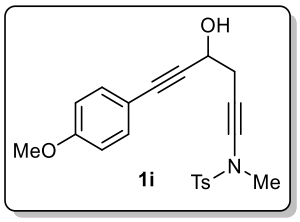
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1g** as a yellow liquid (665 mg, 1.62 mmol, 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.21 – 7.10 (m, 6H), 4.69 – 4.65 (m, 1H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.84 – 2.71 (m, 2H), 2.46 (d, *J* = 7.2 Hz, 1H), 2.35 (s, 3H), 2.28 (s, 3H), 1.67 – 1.54 (m, 2H), 1.32 – 1.23 (m, 2H), 0.84 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.3, 137.9, 134.4, 132.3, 129.6, 129.4, 128.8, 128.1, 127.5, 122.1, 88.2, 85.2, 76.3, 65.3, 61.6, 50.9, 29.7, 28.8, 21.5, 21.1, 19.4, 13.4; HRMS-ESI+ calcd for $C_{24}H_{27}NO_3SNa$ $[M+Na]^+$: 432.1609, found: 432.1610.

Spectral data for *N*-butyl-*N*-(6-(3-chlorophenyl)-4-hydroxyhex-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1h):



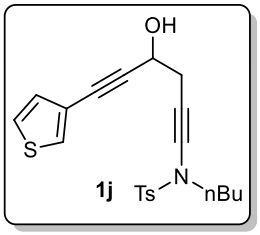
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1h** as a yellow liquid (615 mg, 1.43 mmol, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.20 (m, 6H), 4.71 – 4.66 (m, 1H), 3.25 (t, *J* = 7.2 Hz, 2H), 2.90 – 2.74 (m, 2H), 2.55 (d, *J* = 6.8 Hz, 1H), 2.37 (s, 3H), 1.68 – 1.55 (m, 2H), 1.32 – 1.26 (m, 2H), 0.84 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.4, 134.5, 134.0, 131.6, 129.9, 129.6, 129.5, 128.8, 127.5, 124.0, 89.9, 83.6, 76.4, 65.1, 61.5, 50.9, 29.7, 28.7, 21.5, 19.4, 13.4; HRMS-ESI+ calcd for $C_{23}H_{24}ClNO_3SNa$ $[M+Na]^+$: 452.1063, found: 452.1063.

Spectral data for *N*-(4-hydroxy-6-(4-methoxyphenyl)hexa-1,5-diyn-1-yl)-*N*,4-dimethylbenzene sulfonamide (1i):



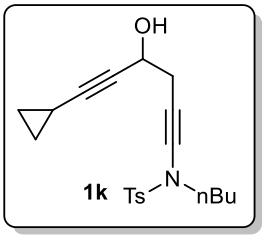
Purified by column chromatography over silica gel with 30% EtOAc/Hexane to afford **1i** as a yellow liquid (655 mg, 1.71 mmol, 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.76 (m, 2H), 7.37 – 7.34 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 6.81 – 6.79 (m, 2H), 4.65 (t, *J* = 5.6 Hz, 1H), 3.77 (s, 3H), 3.00 (s, 3H), 2.76 – 2.74 (m, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 144.6, 133.2, 132.9, 129.7, 127.7, 114.3, 113.8, 87.2, 85.1, 77.7, 64.0, 61.5, 55.2, 39.0, 29.6, 28.7, 21.5.

Spectral data for *N*-butyl-*N*-(4-hydroxy-6-(thiophen-3-yl)hexa-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1j):



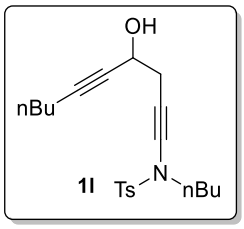
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1j** as a yellow liquid (590 mg, 1.47 mmol, 76%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.76 (m, 2H), 7.45 – 7.44 (m, 1H), 7.24 – 7.21 (m, 3H), 7.09 – 7.08 (m, 1H), 4.68 – 4.63 (m, 1H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.83 – 2.73 (m, 2H), 2.41 – 2.37 (m, 4H), 1.69 – 1.54 (m, 2H), 1.41 – 1.21 (m, 2H), 0.84 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.4, 134.4, 129.8, 129.6, 129.3, 127.5, 125.3, 121.3, 88.2, 80.3, 76.4, 65.2, 61.6, 50.9, 29.7, 28.8, 21.5, 19.4, 13.4; HRMS-ESI- calcd for $C_{21}H_{23}NO_3S_2Na$ $[M+Na]^+$: 424.1017, found: 424.1018.

Spectral data for *N*-butyl-*N*-(6-cyclopropyl-4-hydroxyhexa-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1k):



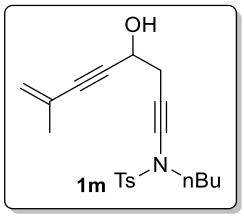
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1k** as a yellow liquid (600 mg, 1.67 mmol, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 4.39 – 4.35 (m, 1H), 3.22 (t, *J* = 7.2 Hz, 2H), 2.68 – 2.57 (m, 2H), 2.41 (s, 3H), 2.31 (d, *J* = 6.4 Hz, 1H), 1.61 – 1.50 (m, 2H), 1.34 – 1.18 (m, 3H), 0.86 (t, *J* = 7.2 Hz, 3H), 0.75 – 0.63 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.4, 134.4, 129.6, 127.5, 88.9, 75.9, 74.9, 65.5, 61.3, 50.9, 29.6, 29.0, 21.5, 19.3, 13.5, 8.1, -0.6; HRMS-ESI+ calcd for $C_{20}H_{25}NO_3SNa$ $[M+Na]^+$: 382.1452, found: 382.1450.

Spectral data for *N*-butyl-*N*-(4-hydroxydeca-1,5-diyn-1-yl)-4-methylbenzenesulfonamide (1l):



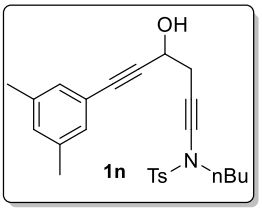
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1l** as a yellow liquid (675 mg, 1.80 mmol, 88%). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.79 – 7.76 (m, 2H), 7.37 – 7.35 (m, 2H), 4.44 – 4.39 (m, 1H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.70 – 2.59 (m, 2H), 2.44 (s, 3H), 2.34 (d, *J* = 6.4 Hz, 1H), 2.21 – 2.17 (m, 2H), 1.62 – 1.55 (m, 2H), 1.50 – 1.27 (m, 6H), 0.91 – 0.86 (m, 6H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 144.7, 134.5, 129.7, 127.6, 85.8, 80.0, 75.8, 65.8, 61.4, 51.1, 30.7, 29.7, 29.0, 21.9, 21.4, 19.5, 18.3, 13.4; HRMS-ESI+ calcd for $C_{21}H_{29}NO_3SNa$ $[M+Na]^+$: 398.1765, found: 398.1766.

Spectral data for *N*-butyl-*N*-(4-hydroxy-7-methylocta-7-en-1,5-diyn-1-yl)-4-methyl benzene sulfonamide (1m):



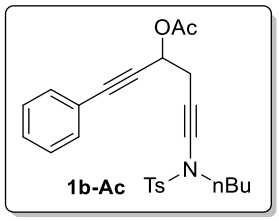
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1m** as a yellow liquid (600 mg, 1.67 mmol, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 5.29 (s, 1H), 5.22 (s, 1H), 4.58 – 4.53 (m, 1H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.79 – 2.65 (m, 2H), 2.41 (s, 3H), 2.34 (d, *J* = 6.8 Hz, 1H), 1.85 (s, 3H), 1.65 – 1.54 (m, 2H), 1.33 – 1.27 (m, 2H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.4, 134.5, 129.6, 127.6, 126.0, 122.6, 87.5, 86.2, 76.2, 65.3, 61.5, 50.9, 29.7, 28.8, 23.2, 21.5, 19.4, 13.5; HRMS-ESI+ calcd for $C_{20}H_{25}NO_3SNa$ $[M+Na]^+$: 382.1452, found: 382.1450.

Spectral data for *N*-butyl-*N*-(6-(3,5-dimethylphenyl)-4-hydroxyhexa-1,5-diyn-1-yl)-4-methylbenzene sulfonamide (1n):



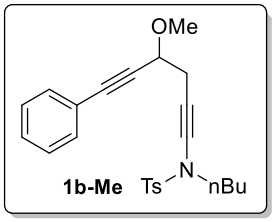
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1n** as a yellow liquid (652 mg, 1.54 mmol, 83%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.60 (m, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.03 (s, 2H), 6.93 (t, *J* = 0.8 Hz, 1H), 4.69 – 4.64 (m, 1H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.83 – 2.73 (m, 2H), 2.58 (d, *J* = 6.8 Hz, 1H), 2.34 (s, 3H), 2.23 (s, 6H), 1.62 – 1.54 (m, 2H), 1.39 – 1.20 (m, 2H), 0.83 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.3, 137.7, 134.4, 130.3, 129.6, 129.4, 127.5, 121.9, 87.9, 85.3, 76.1, 65.3, 61.6, 50.9, 29.6, 28.8, 21.4, 20.9, 19.3, 13.4; HRMS-ESI+ calcd for $C_{25}H_{29}NO_3SNa$ $[M+Na]^+$: 446.1765, found: 446.1765.

Spectral data for 6-((*N*-butyl-4-methylphenyl)sulfonamido)-1-phenylhexa-1,5-diyn-3-yl acetate (1b-Ac):



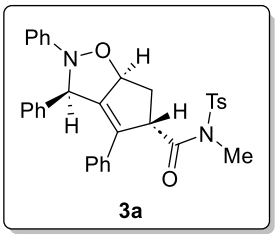
Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1b-Ac** as a yellow liquid (430 mg, 0.98 mmol, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 – 7.45 (m, 2H), 7.39 – 7.37 (m, 2H), 7.30 – 7.19 (m, 5H), 5.63 (t, *J* = 6.4 Hz, 1H), 3.27 – 3.16 (m, 2H), 2.88 – 2.83 (m, 2H), 2.33 (s, 3H), 2.08 (s, 3H), 1.59 – 1.51 (m, 2H), 1.28 – 1.23 (m, 2H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.6, 144.2, 134.6, 131.8, 129.5, 128.7, 128.1, 127.4, 121.8, 85.6, 85.3, 75.6, 64.5, 62.9, 51.0, 29.6, 25.7, 21.4, 20.8, 19.3, 13.4; HRMS-ESI+ calcd for $C_{25}H_{27}NO_4SNa$ $[M+Na]^+$: 460.1558, found: 460.1561.

Spectral data for *N*-butyl-*N*-(4-methoxy-6-phenylhexa-1,5-diyn-1-yl)-4-methylbenzenesulfonamide (1b-Me):



Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **1b-Me** as a yellow liquid (410 mg, 1.00 mmol, 79%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.76 (m, 2H), 7.41 – 7.39 (m, 2H), 7.29 – 7.27 (m, 3H), 7.21 – 7.18 (m, 2H), 4.27 (t, *J* = 6.8 Hz, 1H), 3.46 (s, 3H), 3.22 (t, *J* = 7.2 Hz, 2H), 2.78 – 2.76 (m, 2H), 2.34 (s, 3H), 1.62 – 1.55 (m, 2H), 1.29 – 1.23 (m, 2H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.1, 134.6, 131.8, 129.5, 128.4, 128.2, 127.5, 122.4, 86.7, 86.2, 75.0, 70.6, 65.6, 56.5, 51.0, 29.6, 26.2, 21.5, 19.3, 13.4; HRMS-ESI+ calcd for $C_{24}H_{27}NO_3SNa$ $[M+Na]^+$: 432.1609, found: 432.1609.

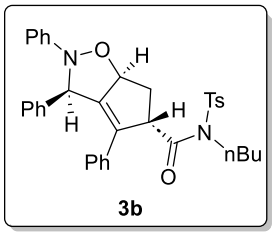
Spectral data for *N*-methyl-2,3,4-triphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (3a):



3a

Purified by column chromatography over silica gel with 10% EtOAc/Hexane to afford **3a** as a white solid (67 mg, 0.121 mmol, 61%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.31 (m, 4H), 7.27 – 7.23 (m, 2H), 7.11 – 6.99 (m, 6H), 6.94 – 6.89 (m, 3H), 6.75 – 6.73 (m, 2H), 5.56 – 5.53 (m, 1H), 5.36 (s, 1H), 5.23 (d, *J* = 9.2 Hz, 1H), 3.22 (s, 3H), 2.50 – 2.40 (m, 4H), 2.34 – 2.29 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.6, 152.5, 152.3, 145.5, 139.0, 136.5, 133.7, 132.3, 130.2, 128.9, 128.5, 128.0, 127.78, 127.71, 127.3, 127.2, 121.3, 113.7, 88.9, 71.1, 59.1, 33.8, 33.4, 21.4; HRMS-ESI+ calcd for $C_{33}H_{30}N_2O_4SNa$ $[M+Na]^+$: 573.1824, found: 573.1822.

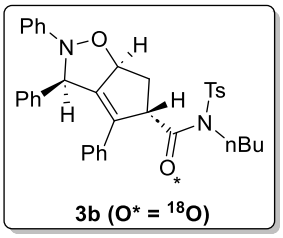
Spectral data for *N*-butyl-2,3,4-triphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (3b):



3b

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3b** as a white sticky solid (77 mg, 0.129 mmol, 65%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 7.7 Hz, 2H), 7.32 (d, *J* = 7.0 Hz, 2H), 7.27 – 7.23 (m, 2H), 7.09 (d, *J* = 7.0 Hz, 2H), 7.08 – 7.00 (m, 4H), 6.92 – 6.91 (m, 3H), 6.69 (d, *J* = 7.7 Hz, 2H), 5.53 (t, *J* = 7.0 Hz, 1H), 5.35 (s, 1H), 5.12 (d, *J* = 9.1 Hz, 1H), 3.75 – 3.71 (m, 2H), 2.47 (s, 3H), 2.45 – 2.39 (m, 1H), 2.27 – 2.24 (m, 1H), 1.55 – 1.50 (m, 2H, merged with water peak), 1.26 – 1.22 (m, 2H), 0.85 (t, *J* = 7.7 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.3, 152.49, 152.40, 145.3, 139.0, 137.1, 133.7, 132.2, 130.1, 128.9, 128.4, 128.0, 127.7, 127.6, 127.3, 127.2, 121.3, 113.6, 88.9, 71.1, 59.3, 47.1, 33.7, 31.8, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{36}H_{36}N_2O_4SNa$ $[M+Na]^+$: 615.2293, found: 615.2292.

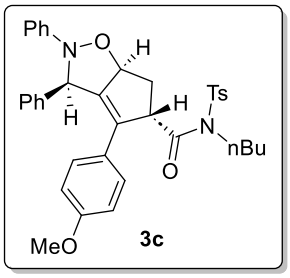
Spectral data for ^{18}O-substituted *N*-butyl-2,3,4-triphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (3b (O* = ^{18}O)):



3b (O* = ^{18}O)

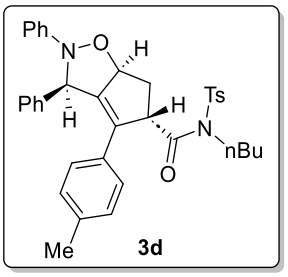
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3b** (O* = ^{18}O) as a white sticky solid (77 mg, 0.129 mmol, 65%). ^1H NMR (700 MHz, CD_2Cl_2): δ 7.71 (d, J = 7.7 Hz, 2H), 7.37 (d, J = 7.7 Hz, 2H), 7.32 (d, J = 7.7 Hz, 2H), 7.26 – 7.24 (m, 2H), 7.09 (d, J = 7.0 Hz, 2H), 7.03 – 7.00 (m, 4H), 6.92 – 6.90 (m, 3H), 6.69 (d, J = 7.7 Hz, 2H), 5.53 (t, J = 7.0 Hz, 1H), 5.35 (s, 1H), 5.11 (d, J = 9.1 Hz, 1H), 3.75 – 3.71 (m, 2H), 2.47 (s, 3H), 2.43 – 2.38 (m, 1H), 2.27 – 2.24 (m, 1H), 1.55 – 1.51 (m, 2H, merged with water peak), 1.26 – 1.22 (m, 2H), 0.85 (t, J = 7.7 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.38, 173.34, 152.49, 152.40, 145.3, 139.0, 137.1, 133.7, 132.2, 130.1, 128.9, 128.4, 128.0, 127.7, 127.6, 127.3, 127.2, 121.3, 113.6, 88.9, 71.1, 59.3, 47.1, 33.7, 31.8, 21.4, 19.9, 13.4. HRMS-FD+ calcd for $C_{36}H_{36}N_2O_3S^{18}O$ $[M]^+$: 594.2427, found: 594.2426.

Spectral data for *N*-butyl-4-(4-methoxyphenyl)-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetra hydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3c):



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3c** as a white sticky solid (87.1 mg, 0.139 mmol, 70%). ^1H NMR (400 MHz, CD_2Cl_2): δ 7.74 (d, J = 6.8 Hz, 2H), 7.39 – 7.32 (m, 4H), 7.27 – 7.23 (m, 2H), 7.14 – 7.06 (m, 3H), 7.02 – 6.99 (m, 2H), 6.92 – 6.88 (m, 1H), 6.65 – 6.63 (m, 2H), 6.46 – 6.43 (m, 2H), 5.51 – 5.47 (m, 1H), 5.34 (s, 1H), 5.10 – 5.07 (m, 1H), 3.77 – 3.73 (m, 2H), 3.66 (s, 3H), 2.47 (s, 3H), 2.37 – 2.30 (m, 1H), 2.19 – 2.14 (m, 1H), 1.55 – 1.49 (m, 2H, merged with water peak), 1.29 – 1.21 (m, 2H), 0.85 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.5, 159.2, 152.4, 150.3, 145.3, 139.2, 137.2, 133.2, 130.2, 129.1, 128.9, 128.5, 128.0, 127.4, 127.3, 124.7, 121.3, 113.7, 113.0, 88.9, 71.2, 59.0, 55.1, 47.1, 33.4, 31.9, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{38}N_2O_5SNa$ $[M+Na]^+$: 645.2399, found: 645.2395.

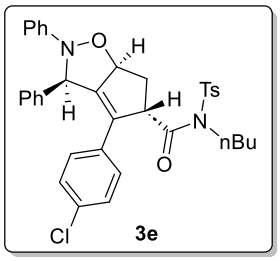
Spectral data for *N*-butyl-2,3-diphenyl-4-(*p*-tolyl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (3d):



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3d** as a white sticky solid (82.4 mg, 0.135 mmol, 68%). ^1H NMR (400 MHz, $CDCl_3$): 7.70 (d, J = 8.0 Hz, 2H), 7.30 (t, J = 8.4 Hz, 5H), 7.24 – 7.20 (m, 1H), 7.08 – 7.00 (m, 5H), 6.88 (t, J = 7.2 Hz, 1H), 6.68 (d, J = 8.0 Hz, 2H), 6.58 (d, J = 8.0 Hz, 2H), 5.57 (t, J = 6.8 Hz, 1H), 5.28 (s, 1H), 5.14 (d, J = 9.2 Hz, 1H), 3.74 – 3.66 (m, 2H), 2.45 (s, 3H), 2.42 – 2.33 (m, 1H), 2.26 – 2.13 (m, 4H), 1.53 – 1.49 (m, 2H, merged with water peak), 1.24

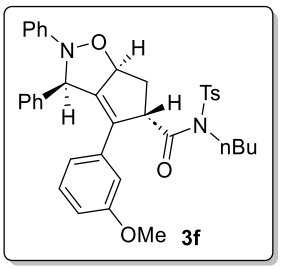
– 1.18 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H);^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.4, 152.3, 151.4, 145.3, 139.2, 137.8, 137.1, 133.4, 130.1, 129.3, 128.9, 128.5, 128.4, 128.0, 127.6, 127.57, 127.51, 127.37, 127.33, 121.3, 113.7, 88.9, 71.1, 59.1, 47.1, 33.5, 31.9, 21.4, 20.8, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{39}N_2O_4S$ $[M+H]^+$: 607.2630, found: 607.2627.

Spectral data for *N*-butyl-4-(4-chlorophenyl)-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3e):



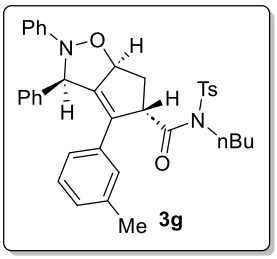
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3e** as a white sticky solid (64.0 mg, 0.102 mmol, 51%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.70 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 7.7 Hz, 2H), 7.25 (t, J = 7.7 Hz, 2H), 7.11 (t, J = 7.7 Hz, 2H), 7.09 (d, J = 7.7 Hz, 1H), 7.00 (d, J = 7.7 Hz, 2H), 6.92 – 6.88 (m, 3H), 6.64 (d, J = 8.4 Hz, 2H), 5.53 (t, J = 6.8 Hz, 1H), 5.32 (s, 1H), 5.09 (d, J = 9.8 Hz, 1H), 3.75 – 3.70 (m, 2H), 2.47 (s, 3H), 2.40 – 2.36 (m, 1H), 2.23 – 2.20 (m, 1H), 1.53 – 1.50 (m, 2H, merged with water peak), 1.26 – 1.21 (m, 2H), 0.85 (t, J = 7.7 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.2, 153.3, 152.3, 145.4, 138.8, 137.0, 133.4, 132.8, 130.9, 130.2, 129.0, 128.9, 128.4, 128.1, 127.8, 127.5, 127.2, 121.4, 113.6, 88.9, 71.0, 59.4, 47.1, 33.6, 31.8, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{36}H_{36}ClN_2O_4S$ $[M+H]^+$: 627.2084, found: 627.2077.

Spectral data for *N*-butyl-4-(3-methoxyphenyl)-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetra hydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3f):



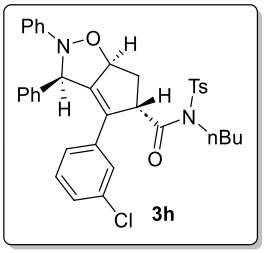
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3f** as a white sticky solid (83.4 mg, 0.134 mmol, 67%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.71 (d, J = 8.4 Hz, 2H), 7.36 – 7.31 (m, 4H), 7.27 – 7.23 (m, 2H), 7.13 – 7.06 (m, 3H), 7.02 – 6.99 (m, 2H), 6.90 (t, J = 7.2 Hz, 1H), 6.83 (t, J = 8.0 Hz, 1H), 6.57- 6.55 (m, 1H), 6.38 – 6.37 (m, 1H), 6.28 (d, J = 7.0 Hz, 1H), 5.52 (t, J = 6.8 Hz, 1H), 5.32 (s, 1H), 5.13 (d, J = 9.2 Hz, 1H), 3.72 (t, J = 7.2 Hz, 2H), 3.64 (s, 3H), 2.45 (s, 3H), 2.39 – 2.31 (m, 1H), 2.20 – 2.15 (m, 1H), 1.54 – 1.45 (m, 2H, merged with water peak), 1.38 – 1.18 (m, 2H), 0.84 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.4, 159.0, 152.5, 152.3, 145.3, 139.0, 137.0, 133.8, 133.6, 130.1, 128.9, 128.7, 128.4, 128.0, 127.4, 127.2, 121.3, 120.1, 113.7, 113.3, 88.9, 71.1, 59.3, 55.1, 47.0, 33.6, 31.8, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{38}N_2O_5SNa$ $[M+Na]^+$: 645.2399, found: 645.2393.

Spectral data for *N*-butyl-2,3-diphenyl-4-(*m*-tolyl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3g):



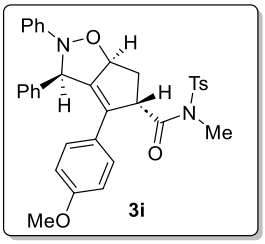
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3g** as a white sticky solid (66.7 mg, 0.110 mmol, 55%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.32 (m, 4H), 7.27 – 7.23 (m, 2H), 7.13 – 7.09 (m, 2H), 7.06 – 7.00 (m, 3H), 6.93 – 6.89 (m, 1H), 6.83 – 6.79 (m, 2H), 6.65 (s, 1H), 6.43 (d, *J* = 7.0 Hz, 1H), 5.52 (t, *J* = 7.2 Hz, 1H), 5.31 (s, 1H), 5.13 (d, *J* = 9.2 Hz, 1H), 3.75 – 3.71 (m, 2H), 2.46 (s, 3H), 2.43 – 2.36 (m, 1H), 2.26 – 2.21 (m, 1H), 2.08 (s, 3H), 1.56 – 1.50 (m, 2H, merged with water peak), 1.30 – 1.21 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.4, 152.4, 152.1, 145.3, 139.1, 137.2, 137.1, 133.8, 131.9, 130.1, 129.1, 128.9, 128.5, 127.9, 127.6, 127.37, 127.31, 124.2, 121.3, 113.6, 88.8, 71.2, 59.1, 47.1, 33.6, 31.8, 21.4, 20.8, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{39}N_2O_4S$ $[M+H]^+$: 607.2630, found: 607.2628.

Spectral data for *N*-butyl-4-(3-chlorophenyl)-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*] isoxazole-5-carboxamide (3h):



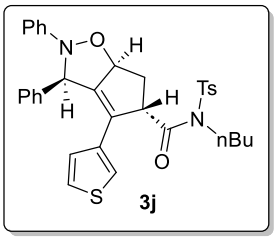
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3h** as a white sticky solid (41.3 mg, 0.065 mmol, 33%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 7.0 Hz, 2H), 7.25 (t, *J* = 7.7 Hz, 2H), 7.11 (t, *J* = 7.7 Hz, 2H), 7.05 (t, *J* = 7.7 Hz, 1H), 7.00 – 6.96 (m, 3H), 6.91 (t, *J* = 7.0 Hz, 1H), 6.85 (t, *J* = 7.7 Hz, 1H), 6.76 (s, 1H), 6.57 (d, *J* = 7.7 Hz, 1H), 5.54 (t, *J* = 7.2 Hz, 1H), 5.33 (s, 1H), 5.09 (d, *J* = 8.4 Hz, 1H), 3.74 – 3.70 (m, 2H), 2.45 (s, 3H), 2.42 – 2.38 (m, 1H), 2.27 – 2.24 (m, 1H), 1.53 – 1.50 (m, 2H), 1.26 – 1.22 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.1, 154.2, 152.4, 145.4, 138.6, 136.9, 134.1, 133.4, 132.8, 130.2, 128.9, 128.4, 128.1, 128.0, 127.6, 127.5, 127.1, 125.6, 121.4, 113.6, 88.7, 71.1, 59.4, 47.1, 33.8, 31.7, 21.5, 19.9, 13.4; HRMS-ESI+ calcd for $C_{36}H_{36}ClN_2O_4S$ $[M+H]^+$: 627.2084, found: 627.2086.

Spectral data for 4-(4-methoxyphenyl)-*N*-methyl-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetra hydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3i):



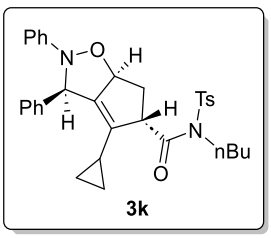
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3i** as a white solid (73.0 mg, 0.125 mmol, 63%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.33 – 7.28 (m, 4H), 7.24 – 7.20 (m, 3H), 7.10 – 7.00 (m, 5H), 6.88 (t, *J* = 7.2 Hz, 1H), 6.69 (d, *J* = 8.4 Hz, 2H), 6.43 (d, *J* = 8.4 Hz, 2H), 5.58 (t, *J* = 6.8 Hz, 1H), 5.27 – 5.24 (m, 2H), 3.65 (s, 3H), 3.19 (s, 3H), 2.45 (s, 3H), 2.41 – 2.36 (m, 1H), 2.25 – 2.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.0, 159.0, 152.5, 150.4, 145.1, 138.7, 136.4, 133.5, 130.1, 129.1, 128.8, 128.2, 128.0, 127.4, 127.2, 124.7, 121.4, 113.8, 113.0, 88.9, 71.4, 59.0, 55.0, 33.8, 33.5, 21.6; HRMS-ESI+ calcd for $C_{34}H_{32}N_2O_5SNa$ $[M+Na]^+$: 603.1929, found: 603.1927.

Spectral data for *N*-butyl-2,3-diphenyl-4-(thiophen-3-yl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3j):



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3j** as a white sticky solid (80.2 mg, 0.134 mmol, 67%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.41 – 7.38 (m, 4H), 7.27 – 7.15 (m, 5H), 7.02 – 7.00 (m, 2H), 6.92 – 6.89 (m, 2H), 6.57 – 6.56 (m, 1H), 6.46 – 6.44 (m, 1H), 5.47 (t, *J* = 7.0 Hz, 1H), 5.31 (s, 1H, merged with CD_2Cl_2), 5.10 (d, *J* = 8.0 Hz, 1H), 3.83 – 3.79 (m, 2H), 2.47 (s, 3H), 2.31 – 2.16 (m, 1H), 2.05 – 2.00 (m, 1H), 1.65 – 1.52 (m, 2H, merged with water peak), 1.38 – 1.13 (m, 2H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.3, 152.2, 150.6, 145.5, 139.4, 137.2, 133.9, 130.3, 128.9, 128.56, 128.52, 128.3, 128.2, 128.1, 127.3, 127.2, 125.0, 123.8, 121.4, 113.7, 88.8, 70.9, 59.7, 47.1, 33.4, 31.9, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{34}H_{35}N_2O_4S_2$ $[M+H]^+$: 599.2038, found: 599.2040.

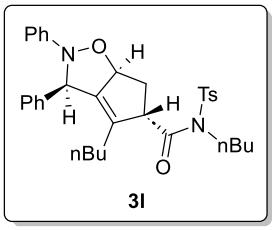
Spectral data for *N*-butyl-4-cyclopropyl-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (3k):



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3k** as a white sticky solid (72.5 mg, 0.130 mmol, 65%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.51 – 7.49

(m, 2H), 7.37 – 7.34 (m, 4H), 7.30 – 7.26 (m, 1H), 7.23 – 7.19 (m, 2H), 6.97 – 6.92 (m, 2H), 6.88 – 6.85 (m, 1H), 5.31 – 5.27 (m, 1H, merged with CD_2Cl_2), 5.08 (s, 1H), 4.21 (d, J = 8.0 Hz, 1H), 3.88 – 3.76 (m, 2H), 2.43 (s, 3H), 2.06 – 1.99 (m, 1H), 1.92 – 1.87 (m, 1H), 1.68 – 1.58 (m, 2H), 1.40 – 1.30 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H), 0.68 – 0.61 (m, 1H), 0.22 – 0.15 (m, 1H), 0.07 – 0.01 (m, 1H), -0.01 - -0.06 (m, 1H), -0.07 - -0.12 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.8, 152.9, 150.5, 145.3, 140.9, 137.0, 136.3, 130.0, 128.8, 128.5, 128.3, 127.6, 127.4, 121.1, 113.5, 87.9, 70.7, 56.7, 47.1, 34.5, 32.0, 21.4, 20.0, 13.4, 9.2, 5.6, 4.3; HRMS-ESI+ calcd for $C_{33}H_{36}N_2O_4SNa$ $[M+Na]^+$: 579.2293, found: 579.2292.

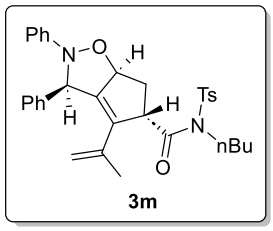
Spectral data for *N*,4-dibutyl-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[d]isoxazole-5-carboxamide (3l):



3l

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3l** as a white sticky solid (69 mg, 0.120 mmol, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.4 Hz, 2H), 7.49 – 7.47 (m, 2H), 7.35 – 7.25 (m, 5H), 7.20 – 7.16 (m, 2H), 6.91 (d, J = 8.0 Hz, 2H), 6.84 (t, J = 7.2 Hz, 1H), 5.38 (t, J = 6.4 Hz, 1H), 5.00 (s, 1H), 4.47 (d, J = 8.4 Hz, 1H), 3.83 – 3.79 (m, 2H), 2.41 (s, 3H), 2.10 – 1.96 (m, 2H), 1.67 – 1.59 (m, 2H), 1.40 – 1.27 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H), 0.75 – 0.64 (m, 4H), 0.53 (t, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.4, 153.0, 150.4, 144.9, 140.3, 137.2, 135.5, 129.9, 128.8, 128.6, 127.8, 127.7, 127.2, 121.2, 113.4, 88.1, 70.7, 59.3, 47.0, 34.7, 31.9, 29.2, 26.8, 22.4, 21.6, 20.0, 13.6, 13.4; HRMS-ESI+ calcd for $C_{34}H_{40}N_2O_4SNa$ $[M+Na]^+$: 595.2606, found: 595.2606.

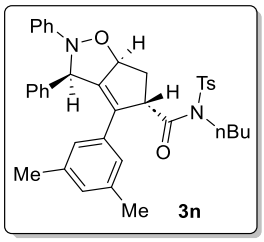
Spectral data for *N*-butyl-2,3-diphenyl-4-(prop-1-en-2-yl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3m):



3m

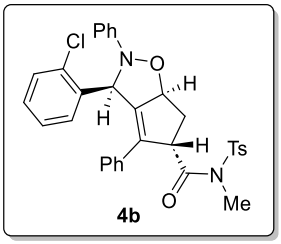
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3m** as a white sticky solid (68 mg, 0.122 mmol, 61%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 – 7.73 (m, 2H), 7.39 – 7.36 (m, 2H), 7.34 – 7.26 (m, 4H), 7.25 – 7.19 (m, 3H), 6.99 – 6.97 (m, 2H), 6.89 – 6.85 (m, 1H), 5.42 (t, J = 6.8 Hz 1H), 5.20 (s, 1H), 4.90 (d, J = 9.2 Hz, 1H), 4.59 (s, 1H), 4.52 (s, 1H), 3.79 – 3.75 (m, 2H), 2.43 (s, 3H), 2.25 – 2.17 (m, 1H), 2.02 – 1.97 (m, 1H), 1.64 – 1.56 (m, 2H), 1.32 – 1.24 (m, 7H), 0.89 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.6, 152.5, 152.0, 145.0, 140.7, 137.3, 137.0, 134.8, 130.0, 128.8, 128.4, 128.3, 127.6, 127.3, 121.4, 116.9, 113.7, 88.7, 71.0, 58.4, 47.1, 33.5, 31.7, 21.6, 21.4, 19.9, 13.5; HRMS-ESI+ calcd for $C_{33}H_{36}N_2O_4SNa$ $[M+Na]^+$: 579.2293, found: 579.2295.

Spectral data for *N*-butyl-4-(3,5-dimethylphenyl)-2,3-diphenyl-*N*-tosyl-3,5,6,6a-tetra hydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (3n):



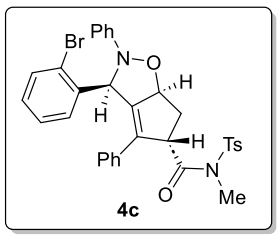
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3n** as a white sticky solid (89.3 mg, 0.143 mmol, 72%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.34 (m, 4H), 7.30 – 7.23 (m, 2H), 7.15 – 7.11 (m, 2H), 7.08 – 7.00 (m, 3H), 6.92 – 6.88 (m, 1H), 6.65 (s, 1H), 6.44 (s, 2H), 5.52 – 5.48 (m, 1H), 5.36 (s, 1H), 5.15 (d, *J* = 9.2 Hz, 1H), 3.72 (t, *J* = 7.6 Hz, 2H), 2.44 (s, 3H), 2.42 – 2.35 (m, 1H), 2.30 – 2.21 (m, 1H), 2.04 (s, 6H), 1.57 – 1.51 (m, 2H, merged with water peak), 1.32 – 1.19 (m, 2H), 0.85 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 152.5, 151.8, 145.3, 139.2, 137.2, 137.0, 133.7, 131.8, 130.1, 129.4, 128.9, 128.5, 127.9, 127.37, 127.34, 125.7, 121.3, 113.6, 88.8, 71.4, 59.0, 47.1, 33.6, 31.8, 21.4, 20.7, 19.9, 13.4; HRMS-ESI+ calcd for $C_{38}H_{40}N_2O_4NaS$ $[M+Na]^+$: 643.2606, found: 643.2639.

Spectral data for 3-(2-chlorophenyl)-*N*-methyl-2,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4b):



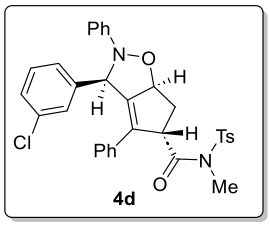
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4b** as a white solid (64.6 mg, 0.110 mmol, 55%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 – 7.70 (m, 2H), 7.42 – 7.35 (m, 3H), 7.28 – 7.24 (m, 2H), 7.09 – 6.91 (m, 9H), 6.82 – 6.80 (m, 2H), 5.97 (s, 1H), 5.57 – 5.54 (m, 1H), 5.24 (d, *J* = 8.0 Hz, 1H), 3.20 (s, 3H), 2.53 – 2.46 (m, 4H), 2.38 – 2.33 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.5, 152.4, 151.9, 145.5, 137.0, 136.4, 134.4, 133.3, 132.3, 130.2, 129.0, 128.7, 128.4, 127.9, 127.7, 127.4, 127.2, 127.1, 121.5, 113.8, 88.8, 66.5, 59.0, 33.9, 33.5, 21.4; HRMS-ESI+ calcd for $C_{33}H_{29}ClN_2O_4NaS$ $[M+Na]^+$: 607.1434, found: 607.1433.

Spectral data for 3-(2-bromophenyl)-*N*-methyl-2,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4c):



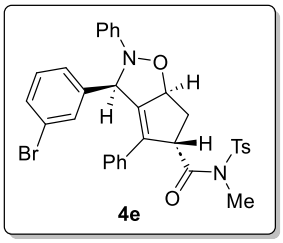
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4c** as a white solid (60.6 mg, 0.096 mmol, 48%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.70 – 7.68 (m, 2H), 7.43 – 7.41 (m, 1H), 7.36 – 7.34 (m, 2H), 7.28 – 7.24 (m, 3H), 7.09 – 7.07 (m, 2H), 7.05 – 7.01 (m, 2H), 6.99 – 6.95 (m, 2H), 6.93 – 6.81 (m, 4H), 5.91 (s, 1H), 5.58 – 5.54 (m, 1H), 5.22 (d, *J* = 8.0 Hz, 1H), 3.19 (s, 3H), 2.53 – 2.45 (m, 4H), 2.40 – 2.33 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.6, 152.6, 151.8, 145.5, 138.7, 136.4, 134.6, 132.3, 131.7, 130.5, 130.2, 128.9, 127.9, 127.76, 127.71, 127.5, 127.2, 124.1, 121.5, 114.0, 88.8, 69.1, 59.2, 33.9, 33.4, 21.4; HRMS-ESI+ calcd for $C_{33}H_{29}BrN_2O_4NaS$ $[M+Na]^+$: 651.0929, found: 651.0926.

Spectral data for 3-(3-chlorophenyl)-*N*-methyl-2,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4d):



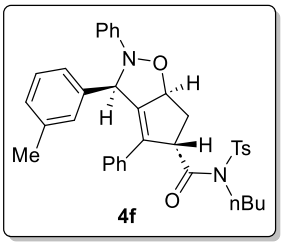
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4d** as a white solid (71.6 mg, 0.122 mmol, 61%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.29 – 7.25 (m, 3H), 7.21 (d, *J* = 7.0 Hz, 1H), 7.06 (t, *J* = 7.0 Hz, 1H), 7.02 – 6.97 (m, 6H), 6.92 (t, *J* = 7.0 Hz, 1H), 6.76 – 6.74 (m, 2H), 5.56 – 5.54 (m, 1H), 5.30 (s, 1H), 5.20 (d, *J* = 9.8 Hz, 1H), 3.19 (s, 3H), 2.49 – 2.44 (m, 4H), 2.35 – 2.32 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 152.2, 152.0, 145.4, 141.0, 136.4, 134.7, 133.7, 132.2, 130.1, 129.2, 129.0, 128.4, 128.0, 127.7, 127.4, 127.2, 126.7, 121.5, 113.6, 88.9, 70.4, 59.4, 33.9, 33.4, 21.4; HRMS-ESI+ calcd for $C_{33}H_{30}ClN_2O_4S$ $[M+H]^+$: 585.1614, found: 585.1613.

Spectral data for 3-(3-bromophenyl)-*N*-methyl-2,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4e):



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4e** as a white solid (73.3 mg, 0.116 mmol, 58%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.44 – 7.43 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.28 – 7.23 (m, 3H), 7.17 – 7.13 (m, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 7.00 – 6.91 (m, 6H), 6.76 (d, *J* = 8.0 Hz, 2H), 5.57 – 5.53 (m, 1H), 5.28 (s, 1H), 5.21 (d, *J* = 9.2 Hz, 1H), 3.19 (s, 3H), 2.50 – 2.33 (m, 5H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 152.2, 152.0, 145.4, 141.3, 136.4, 134.7, 132.2, 131.4, 130.3, 130.1, 129.5, 129.0, 128.0, 127.7, 127.2, 127.1, 121.9, 121.5, 113.6, 88.9, 70.4, 59.5, 33.9, 33.4, 21.4; HRMS-ESI+ calcd for $C_{33}H_{29}BrN_2O_4NaS$ $[M+Na]^+$: 651.0929, found: 651.0929.

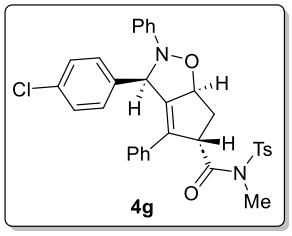
Spectral data for *N*-butyl-2,4-diphenyl-3-(*m*-tolyl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (4f):



4f

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4f** as a white sticky solid (64.1 mg, 0.105 mmol, 53%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.34 (m, 2H), 7.28 – 7.24 (m, 2H), 7.15 – 7.10 (m, 2H), 7.04 – 7.00 (m, 4H), 6.97 – 6.91 (m, 3H), 6.89 – 6.83 (m, 1H), 6.70 – 6.68 (m, 2H), 5.54 – 5.50 (m, 1H), 5.29 (s, 1H), 5.11 (d, *J* = 9.2 Hz, 1H), 3.74 -3.69 (m, 2H), 2.46 (s, 3H), 2.44 – 2.37 (m, 1H), 2.31 – 2.22 (m, 1H), 2.17 (s, 3H), 1.55 – 1.50 (m, 2H, merged with water peak), 1.28 – 1.21 (m, 2H), 0.85 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.4, 152.5, 152.4, 145.2, 138.8, 137.7, 137.1, 133.7, 132.3, 130.1, 129.2, 128.9, 128.0, 127.9, 127.8, 127.7, 127.5, 127.3, 125.4, 121.3, 113.6, 88.9, 71.1, 59.4, 47.1, 33.7, 31.8, 21.4, 20.9, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{38}N_2O_4NaS$ $[M+Na]^+$: 629.2450, found: 629.2455.

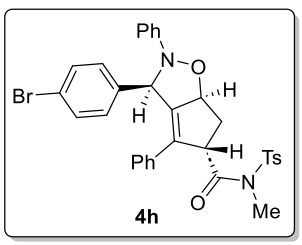
Spectral data for 3-(4-chlorophenyl)-*N*-methyl-2,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4g):



4g

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4g** as a white solid (77.5 mg, 0.132 mmol, 66%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 – 7.70 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.27 (m, 2H), 7.21 – 7.19 (m, 2H), 7.09 – 6.99 (m, 4H), 6.96 – 6.90 (m, 4H), 6.74 – 6.71 (m, 2H), 5.54 – 5.51 (m, 1H), 5.32 (s, 1H), 5.22 (d, *J* = 8.8 Hz, 1H), 3.21 (s, 3H), 2.50 – 2.43 (m, 4H), 2.35 – 2.30 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 151.9, 150.8, 145.5, 138.5, 136.4, 134.1, 132.1, 130.2, 128.8, 128.5, 128.3, 128.0, 127.8, 127.78, 127.73, 127.5, 127.2, 126.0, 115.1, 88.9, 71.0, 59.1, 33.7, 33.5, 21.4; HRMS-ESI- calcd for $C_{33}H_{28}ClN_2O_4S$ $[M-H]^-$: 583.1458, found: 583.1464.

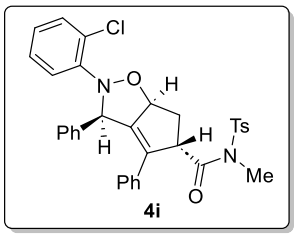
Spectral data for 3-(4-bromophenyl)-*N*-methyl-2,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4h):



4h

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4h** as a white solid (77.1 mg, 0.122 mmol, 61%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.08 (t, *J* = 7.7 Hz, 2H), 7.04 – 7.00 (m, 2H), 6.96 – 6.91 (m, 4H), 6.74 (d, *J* = 8.4 Hz, 2H), 5.53 (t, *J* = 7.0 Hz, 1H), 5.33 (s, 1H), 5.23 (d, *J* = 9.8 Hz, 1H), 3.22 (s, 3H), 2.49 – 2.42 (m, 4H), 2.35 – 2.32 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 151.9, 150.8, 145.5, 138.5, 136.5, 134.2, 130.2, 128.8, 128.5, 128.0, 127.8, 127.79, 127.73, 127.5, 127.2, 126.0, 115.1, 89.0, 71.0, 59.1, 53.8, 33.8, 33.5, 21.4. HRMS-ESI+ calcd for $C_{33}H_{29}BrN_2O_4NaS$ $[M+Na]^+$: 651.0929, found 651.0923

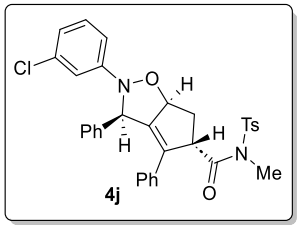
Spectral data for 2-(2-chlorophenyl)-*N*-methyl-3,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4i):



4i

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4i** as a white solid (60.0 mg, 0.102 mmol, 51%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.41 – 7.40 (m, 1H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.26 (t, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 7.7 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.03 – 7.00 (m, 2H), 6.97 – 6.94 (m, 3H), 6.91 (t, *J* = 7.7 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 2H), 5.96 (s, 1H), 5.55 (t, *J* = 7.0 Hz, 1H), 5.22 (d, *J* = 9.8 Hz, 1H), 3.21 (s, 3H), 2.50 – 2.47 (m, 3H), 2.46 (s, 1H), 2.36 – 2.33 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.4, 153.0, 145.6, 145.5, 136.8, 136.5, 132.7, 132.4, 130.2, 129.8, 129.4, 129.0, 128.1, 127.8, 127.7, 127.4, 127.27, 127.20, 127.1, 126.8, 124.1, 122.7, 120.0, 87.7, 68.0, 57.7, 33.8, 33.6, 21.4; HRMS-ESI+ calcd for $C_{33}H_{29}ClN_2O_4SNa$ $[M+Na]^+$: 607.1434, found: 607.1431.

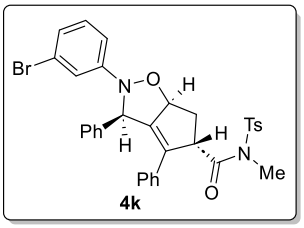
Spectral data for 2-(3-chlorophenyl)-*N*-methyl-3,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4j):



4j

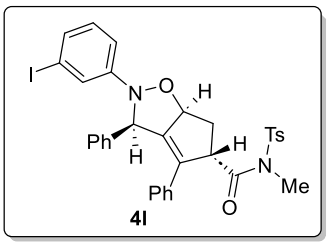
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4j** as a white solid (74.0 mg, 0.126 mmol, 63%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 7.2 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 2H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.11 – 7.00 (m, 5H), 6.93 (d, *J* = 6.8 Hz, 2H), 6.88 – 6.83 (m, 2H), 6.75 (d, *J* = 8.0 Hz, 2H), 5.52 (t, *J* = 6.8 Hz, 1H), 5.35 (s, 1H), 5.23 (d, *J* = 9.2 Hz, 1H), 3.21 (s, 3H), 2.49 – 2.41 (m, 4H), 2.34 – 2.29 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 153.4, 151.8, 145.5, 138.4, 136.4, 134.7, 134.2, 132.1, 130.2, 130.1, 128.4, 128.0, 127.8, 127.79, 127.74, 127.5, 127.2, 121.0, 113.6, 111.9, 89.1, 70.9, 59.1, 33.7, 33.5, 21.4; HRMS-ESI+ calcd for $C_{33}H_{30}ClN_2O_4S$ $[M+H]^+$: 585.1614, found: 585.1612.

Spectral data for 2-(3-bromophenyl)-*N*-methyl-3,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4k):



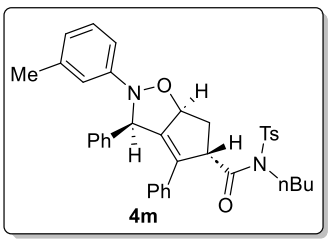
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4k** as a white solid (74.5 mg, 0.118 mmol, 59%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.31 – 7.29 (m, 2H) 7.22 (t, *J* = 2.0 Hz, 1H), 7.13 – 7.00 (m, 6H), 6.95 – 6.89 (m, 3H), 6.75 (d, *J* = 7.6 Hz, 2H), 5.52 (t, *J* = 6.8 Hz, 1H), 5.34 (s, 1H), 5.23 (d, *J* = 9.2 Hz, 1H), 3.21 (s, 3H), 2.49 – 2.40 (m, 4H), 2.34 – 2.29 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.4, 153.4, 151.7, 145.5, 138.4, 136.4, 134.1, 132.0, 130.3, 130.2, 128.4, 128.0, 127.8, 127.73, 127.71, 127.5, 127.1, 123.9, 122.8, 116.3, 112.3, 89.1, 70.9, 58.9, 33.6, 33.4, 21.4; HRMS-ESI+ calcd for $C_{33}H_{29}BrN_2O_4NaS$ $[M+Na]^+$: 651.0929, found: 651.0928.

Spectral data for 2-(3-iodophenyl)-*N*-methyl-3,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4l):



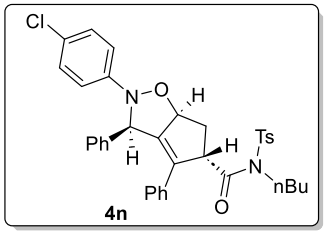
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4l** as a white solid (76.1 mg, 0.112 mmol, 56%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.42 (s, 1H), 7.38 (d, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.09 (t, *J* = 7.7 Hz, 2H), 7.05 – 7.01 (m, 2H), 6.98 – 6.91 (m, 4H), 6.75 (d, *J* = 7.0 Hz, 2H), 5.51 (t, *J* = 6.3 Hz, 1H), 5.33 (s, 1H), 5.23 (d, *J* = 9.8 Hz, 1H), 3.21 (s, 3H), 2.47 – 2.40 (m, 4H), 2.33 – 2.30 (m, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.5, 153.3, 151.8, 145.5, 138.4, 136.4, 134.2, 132.1, 130.4, 130.2, 130.1, 128.4, 128.0, 127.8, 127.79, 127.74, 127.5, 127.2, 122.3, 113.0, 94.6, 89.1, 70.8, 59.1, 33.7, 33.5, 21.4; HRMS-ESI+ calcd for $C_{33}H_{29}IN_2O_4NaS$ $[M+Na]^+$: 699.0790, found: 699.0793.

Spectral data for *N*-butyl-3,4-diphenyl-2-(*m*-tolyl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (4m):



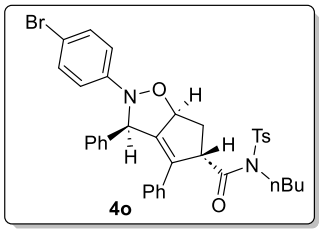
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4m** as a white sticky solid (66.7 mg, 0.110 mmol, 55%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.30 (m, 4H), 7.15 – 6.98 (m, 5H), 6.91 (t, *J* = 7.7 Hz, 2H), 6.85 (s, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 6.74 – 6.67 (m, 3H), 5.54 – 5.51 (m, 1H), 5.34 (s, 1H), 5.11 (d, *J* = 8.8 Hz, 1H), 3.77 – 3.70 (m, 2H), 2.47 (s, 3H), 2.43 – 2.36 (m, 1H), 2.31 (s, 3H), 2.27 – 2.22 (m, 1H), 1.54 – 1.51 (m, 2H, merged with water peak), 1.26 – 1.21 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.4, 152.7, 152.4, 145.3, 139.2, 138.9, 137.1, 130.1, 128.8, 128.4, 128.0, 127.7, 127.6, 127.3, 122.2, 114.2, 110.8, 88.9, 71.1, 59.3, 47.1, 33.7, 31.8, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{39}N_2O_4S$ $[M+H]^+$: 607.2630, found: 607.2636.

Spectral data for *N*-butyl-2-(4-chlorophenyl)-3,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4n):



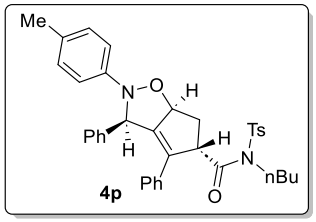
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4n** as a white sticky solid (85.0 mg, 0.135 mmol, 68%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 – 7.69 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.27 (m, 2H), 7.21 – 7.19 (m, 2H), 7.10 – 6.89 (m, 8H), 6.68 – 6.65 (m, 2H), 5.52 – 5.49 (m, 1H), 5.33 (s, 1H), 5.12 (d, *J* = 9.6 Hz, 1H), 3.79 – 3.66 (m, 2H), 2.66 – 2.34 (m, 4H), 2.32 – 2.23 (m, 1H), 1.53 – 1.34 (m, 2H, merged with water peak), 1.29 – 1.12 (m, 2H), 0.85 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.3, 151.9, 150.9, 145.3, 138.5, 137.1, 134.2, 132.1, 130.1, 128.8, 128.4, 128.0, 127.8, 127.7, 127.6, 127.5, 127.2, 125.9, 115.1, 89.0, 71.0, 59.3, 47.1, 33.7, 31.8, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{36}H_{35}ClN_2O_4SNa$ $[M+Na]^+$: 649.1903, found: 649.1903.

Spectral data for 2-(4-bromophenyl)-*N*-butyl-3,4-diphenyl-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazole-5-carboxamide (4o):



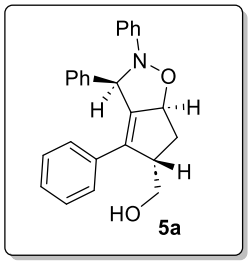
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4o** as a white sticky solid (88.0 mg, 0.131 mmol, 66%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.33 (m, 4H), 7.29 – 7.27 (m, 2H), 7.10 – 6.99 (m, 4H), 6.93 – 6.88 (m, 4H), 6.68 (d, *J* = 7.6 Hz, 2H), 5.50 (t, *J* = 6.4 Hz, 1H), 5.32 (s, 1H, merged with CD_2Cl_2), 5.12 (d, *J* = 9.2 Hz, 1H), 3.88 – 3.59 (m, 2H), 2.47 – 2.33 (m, 4H), 2.28 – 2.23 (m, 1H), 1.54 – 1.40 (m, 2H, merged with water peak), 1.35 – 1.14 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.3, 151.8, 151.3, 145.3, 138.5, 137.1, 134.3, 132.1, 131.7, 130.1, 128.4, 128.0, 127.8, 127.7, 127.6, 127.5, 127.4, 127.2, 115.5, 113.3, 89.0, 70.9, 59.3, 47.1, 33.6, 31.8, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{36}H_{35}BrN_2O_4SNa$ $[M+Na]^+$: 693.1398, found: 693.1398.

Spectral data for *N*-butyl-3,4-diphenyl-2-(*p*-tolyl)-*N*-tosyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta [*d*]isoxazole-5-carboxamide (4p):



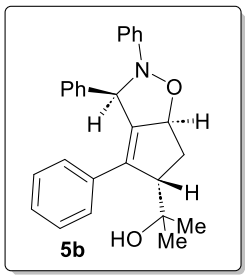
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4p** as a white sticky solid (76.0 mg, 0.125 mmol, 63%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.29 (m, 2H), 7.10 – 6.98 (m, 6H), 6.92 – 6.89 (m, 4H), 6.68 – 6.66 (m, 2H), 5.52 (t, *J* = 6.2 Hz, 1H), 5.33 (s, 1H), 5.11 (d, *J* = 9.2 Hz, 1H), 3.85 – 3.67 (m, 2H), 2.46 (s, 3H), 2.43 – 2.31 (m, 2H), 2.26 (s, 3H), 1.55 – 1.45 (m, 2H, merged with water peak), 1.31 – 1.16 (m, 2H), 0.90 – 0.83 (m, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.4, 152.7, 150.1, 145.3, 139.1, 137.1, 133.6, 132.3, 130.9, 130.1, 129.4, 128.5, 127.9, 127.7, 127.6, 127.3, 113.9, 88.8, 71.2, 59.3, 47.1, 33.7, 31.8, 21.4, 20.2, 19.9, 13.4; HRMS-ESI+ calcd for $C_{37}H_{38}N_2O_4SNa$ $[M+Na]^+$: 629.2450, found: 629.2452.

Spectral data for (2,3,4-triphenyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazol-5-yl)methanol (5a):



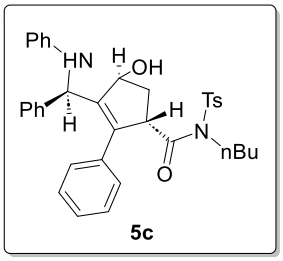
Purified by column chromatography over silica gel with 20% EtOAc/Hexane to afford **5a** as a white solid (39.0 mg, 0.105 mmol, 53%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.36 – 7.34 (m, 2H), 7.29 – 7.25 (m, 2H), 7.11 – 7.00 (m, 10H), 6.92 – 6.88 (m, 1H), 5.62 – 5.58 (m, 1H), 5.34 – 5.33 (m, 1H), 3.89 – 3.86 (m, 1H), 2.68 – 2.55 (m, 2H), 2.61 – 2.20 (m, 2H), 1.41 (s, 1H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 152.6, 149.7, 139.3, 136.0, 132.7, 128.9, 128,6, 128.1, 127.9, 127.7, 127.6, 127.2, 121.1, 113.7, 89.4, 71.3, 64.2, 56.5, 32.7; HRMS-ESI+ calcd for $C_{25}H_{23}NO_2Na$ $[M+Na]^+$: 392.1626, found: 392.1619.

Spectral data for 2-(2,3,4-triphenyl-3,5,6,6a-tetrahydro-2*H*-cyclopenta[*d*]isoxazol-5-yl)propan-2-ol (5b):



Purified by column chromatography over silica gel with 20% EtOAc/Hexane to afford **5b** as a white solid (50.8 mg, 0.127 mmol, 64%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.27 – 7.23 (m, 4H), 7.04 – 6.95 (m, 10H), 6.89 (t, *J* = 7.7 Hz, 1H), 5.57 (t, *J* = 6.3 Hz, 1H), 5.28 (s, 1H), 3.75 (d, *J* = 7.7 Hz, 1H), 2.49 – 2.46 (m, 1H), 2.40 – 2.36 (m, 1H), 1.25 (s, 1H), 1.09 (s, 3H), 1.02 (s, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 152.7, 151.1, 138.9, 138.8, 135.5, 128.9, 128,5, 127.9, 127.7, 127.5, 127.2, 127.0, 121.0, 113.6, 89.1, 73.7, 71.3, 65.6, 33.0, 28.5, 28.4; HRMS-ESI+ calcd for $C_{27}H_{27}NO_2Na$ [M+Na]$^+$: 420.1939, found: 420.1940.

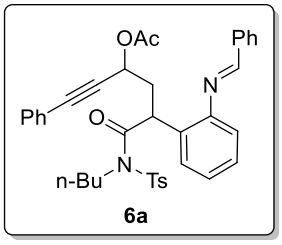
Spectral data for *N*-butyl-4-hydroxy-2-phenyl-3-((*R*)-phenyl(phenylamino)methyl)-*N*-tosylcyclopent-2-ene-1-carboxamide (5c):



5c

Purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **5c** as a white solid (48.7 mg, 0.082 mmol, 41%). ^{1}H NMR (700 MHz, CD_2Cl_2): δ 7.62 (d, *J* = 7.7 Hz, 2H), 7.35 (d, *J* = 7.7 Hz, 2H), 7.30 – 7.27 (m, 4H), 7.24 (t, *J* = 7.7 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.12 (t, *J* = 7.7 Hz, 2H), 7.06 (t, *J* = 7.7 Hz, 2H), 6.82 (d, *J* = 7.0 Hz, 2H), 6.67 (t, *J* = 7.7 Hz, 1H), 6.48 (d, *J* = 7.7 Hz, 2H), 5.33 (s, 1H), 5.02 (s, 1H), 4.64 (s, 1H), 4.19 (br s, 1H), 3.69 – 3.63 (m, 2H), 2.43 (s, 3H), 2.25 – 2.22 (m, 1H), 1.98 – 1.95 (m, 1H), 1.68 (br s, 1H), 1.46 – 1.45 (m, 2H), 1.26 – 1.19 (m, 2H), 0.85 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 174.4, 147.1, 144.9, 144.3, 141.7, 140.7, 137.0, 135.6, 129.8, 129.0, 128.7, 128.2, 127.7, 127.5, 127.3, 117.8, 113.5, 77.4, 56.1, 53.9, 46.7, 38.6, 32.0, 21.4, 19.9, 13.4; HRMS-ESI+ calcd for $C_{36}H_{38}N_2O_4SNa$ [M+Na]$^+$: 617.2450, found: 617.2445.

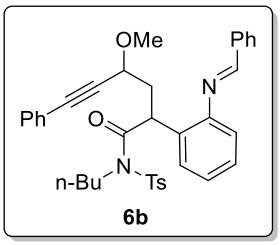
Spectral data for (*E*)-5-(2-(benzylideneamino)phenyl)-6-((*N*-butyl-4-methylphenyl)sulfonamido)-6-oxo-1-phenylhex-1-yn-3-yl acetate (6a):



6a

Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **6a** as a white solid (82 mg, 0.129 mmol, 65%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.51 (s, 1H), 7.91 – 7.89 (m, 2H), 7.70 – 7.68 (m, 2H), 7.46 – 7.42 (m, 1H), 7.36 – 7.22 (m, 10H), 7.09 – 7.05 (m, 2H), 6.81 – 6.79 (m, 1H), 5.38 – 5.35 (m, 1H), 4.91 – 4.87 (m, 1H), 3.86 – 3.65 (m, 2H), 2.58 – 2.49 (m, 1H), 2.39 (s, 3H), 2.04 – 1.94 (m, 1H), 1.89 (s, 3H), 1.74 – 1.70 (m, 1H), 1.60 – 1.49 (m, 1H), 1.28 – 1.23 (m, 2H), 0.80 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 172.7, 169.6, 161.0, 149.0, 144.5, 136.6, 136.1, 132.0, 131.7, 129.1, 129.0, 128.8, 128.6, 128.3, 128.2, 127.0, 126.8, 122.0, 118.2, 86.3, 85.2, 62.5, 46.2, 41.0, 39.2, 33.2, 21.4, 20.6, 20.1, 13.5.

Spectral data for (*E*)-2-(2-(benzylideneamino)phenyl)-*N*-butyl-4-methoxy-6-phenyl-*N*-tosylhex-5-ynamide (6b):



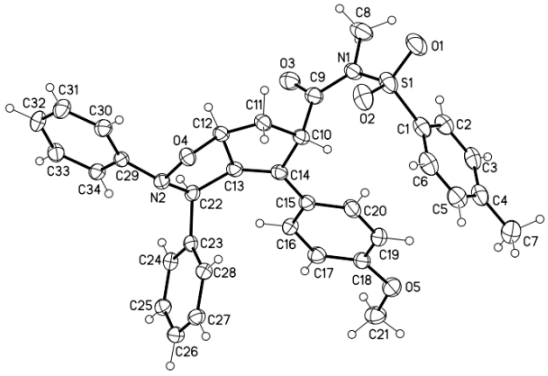
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **6b** as a white solid (86 mg, 0.141 mmol, 71%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.51 (s, 1H), 7.94 – 7.92 (m, 2H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.39 (m, 3H), 7.33 – 7.23 (m, 8H), 7.11 – 7.05 (m, 2H), 6.87 (d, *J* = 7.6 Hz, 1H), 5.03 – 4.99 (m, 1H), 4.01 – 3.97 (m, 1H), 3.89 – 3.63 (m, 2H), 3.25 (s, 3H), 2.45 – 2.25 (m, 4H), 1.94 – 1.87 (m, 1H), 1.81 – 1.78 (m, 1H), 1.72 – 1.55 (m, 1H), 1.30 – 1.21 (m, 2H), 0.83 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (175 MHz, CD_2Cl_2): δ 173.2, 160.6, 148.8, 144.5, 136.8, 136.2, 132.5, 131.6, 129.1, 129.0, 128.79, 128.78, 128.2, 127.0, 126.8, 122.6, 118.0, 87.6, 85.9, 69.1, 55.8, 46.3, 40.8, 40.0, 33.3, 21.4, 20.0, 13.5; HRMS-ESI+ calcd for $C_{37}H_{38}N_2O_4SNa$ $[M+Na]^+$: 629.2450, found: 629.2449.

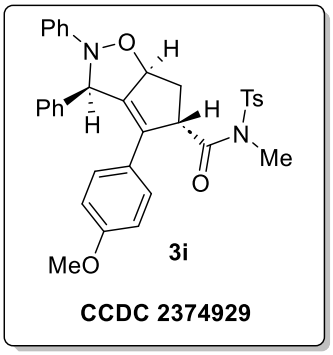
(8) X-ray crystallographic structure and data for 3i, 4i and 6a.

8.1. X-ray Crystallographic data for compound 3i:

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **3i** was dissolved in acetonitrile and kept for slow evaporation (3 days).





Crystal data and structure refinement for 230803lt.

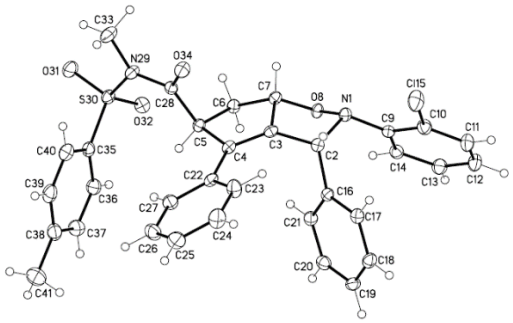
Identification code	230803lt
Empirical formula	$C_{272}H_{256}N_{16}O_{40}S_8$
Formula weight	4645.39
Temperature/K	100.00(10)
Crystal system	monoclinic

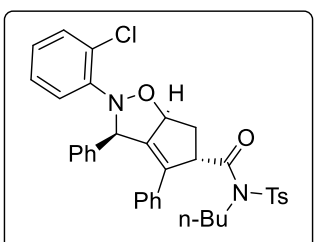
Space group	Cc
a/Å	5.68660(10)
b/Å	20.2872(3)
c/Å	48.7011(7)
α/°	90
β/°	93.3130(10)
γ/°	90
Volume/Å^3	5609.02(15)
Z	1
ρ_{calc}g/cm^3	1.375
μ/mm^{-1}	1.414
F(000)	2448.0
Crystal size/mm^3	0.09 × 0.02 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	3.634 to 150.024
Index ranges	-3 ≤ h ≤ 6, -25 ≤ k ≤ 25, -60 ≤ l ≤ 60
Reflections collected	33611
Independent reflections	8552 [R_{int} = 0.0404, R_{sigma} = 0.0274]
Data/restraints/parameters	8552/2/763
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0431, wR_2 = 0.1057
Final R indexes [all data]	R_1 = 0.0463, wR_2 = 0.1077
Largest diff. peak/hole / e Å^{-3}	0.20/-0.30
Flack parameter	-0.020(12)

8.2. X-ray Crystallographic data for compound 4i:

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **4i** was dissolved in acetonitrile and kept for slow evaporation (3 days).





4i

CCDC 2389031

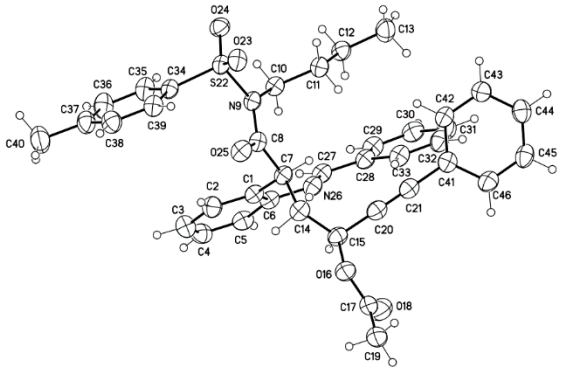
Crystal data and structure refinement for 240644lt_auto.

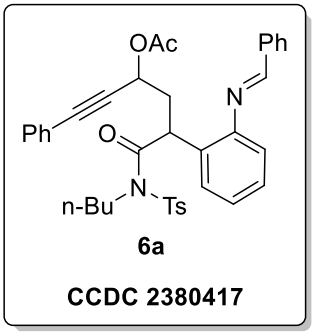
Identification code	240644lt_auto
Empirical formula	$C_{33}H_{29}ClN_2O_4S$
Formula weight	585.09
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	13.71300(10)
b/Å	14.02180(10)
c/Å	18.2490(2)
α/°	110.3010(10)
β/°	109.5870(10)
γ/°	94.9160(10)
Volume/Å^3	3018.42(5)
Z	4
ρ_{calc}g/cm^3	1.288
μ/mm^{-1}	2.088
F(000)	1224.0
Crystal size/mm^3	0.18 × 0.15 × 0.14
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.904 to 154.466
Index ranges	$-15 \leq h \leq 17$, $-17 \leq k \leq 17$, $-22 \leq l \leq 22$
Reflections collected	43959
Independent reflections	12106 [R_{int} = 0.0243, R_{sigma} = 0.0218]
Data/restraints/parameters	12106/0/744
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0339, wR_2 = 0.0819
Final R indexes [all data]	R_1 = 0.0357, wR_2 = 0.0831
Largest diff. peak/hole / e Å^{-3}	0.38/-0.42

8.3. X-ray Crystallographic data for compound 6a:

Ellipsoid contour % probability level = 50%

Sample Preparation for Crystal Growth: The compound **6a** was dissolved in acetonitrile and kept for slow evaporation (3 days).





Crystal data and structure refinement for 240218LT_auto.

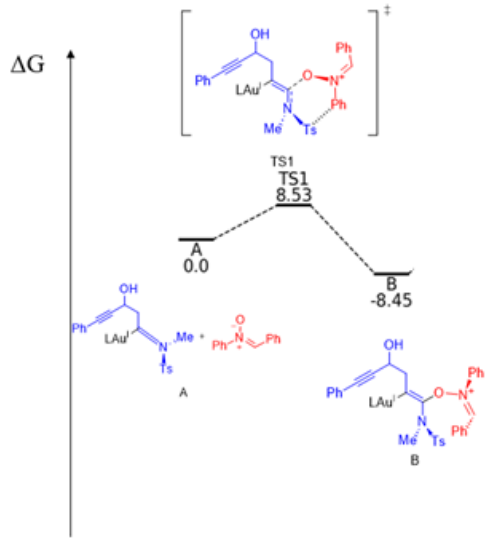
Identification code	240218LT_auto
Empirical formula	$C_{38}H_{38}N_2O_5S$
Formula weight	634.76
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.1231(2)
b/Å	10.6595(3)
c/Å	19.4826(7)
α/°	76.205(2)
β/°	81.449(2)
γ/°	76.849(2)
Volume/Å^3	1782.78(9)
Z	2
ρ_{calc}g/cm^3	1.182
μ/mm^{-1}	1.153
F(000)	672.0
Crystal size/mm^3	0.2 × 0.16 × 0.06
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.718 to 149.296
Index ranges	$-11 \le h \le 11$, $-13 \le k \le 10$, $-24 \le l \le 23$
Reflections collected	21575
Independent reflections	6878 [R_{int} = 0.0279, R_{sigma} = 0.0285]
Data/restraints/parameters	6878/0/418
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0430, wR_2 = 0.1170
Final R indexes [all data]	R_1 = 0.0477, wR_2 = 0.1205

Largest diff. peak/hole / e Å^{-3} 0.37/-0.45

9. Computational details:

9.1. Potential energy diagram of nitrone addition for alkyne oxidation:

We have explicitly computed the potential energy surface for the nitrone attacking the gold-activated alkyne. The calculated activation free energy for this pathway is 8.53 kcal/mol, which is higher than the barrier of the proposed transition state TS1. This suggests that the direct nitrone addition to the Au-activated alkyne is less favorable.



9.2. Computational details for the DFT calculations:

I. Computational methods

All DFT calculations were performed using Orca (version 6.0.1).[1] Geometry optimization calculations utilized the TPSS[2] functional with D4[3] dispersion correction, along with the def2-TZVPP[4,5] basis set for gold atom and the def2-SVP[4,5] basis set for the other atoms. Analytical frequency calculations utilized the B3LYP6,7 functional with D43 dispersion correction along with the def2-TZVPP4,5 basis set for the gold atom and the def2-SVP[4,5] basis set for the other atoms. Single-point calculations utilized the wB97X[8] functional, along with the def2-TZVPP basis set for all atoms. Solvent effects were accounted for using the SMD[9] method for DCE.

The free energy of each state in the chemical progress and the free energy differences (relative to A) were defined by the following equation:

$$\mathbf{G_i = E_{sp} + E_{disp} + E_{solv} + E_{thermo} + E_{ZPV} - TS_i}\ ;\ \mathbf{\Delta G_i = G_i - G_A}$$

G: Gibbs free energies; SP: single point energies; disp: dispersion corrections; solv: solvent corrections; thermo: thermal corrections; ZPV: zero-point vibrational corrections; TS: entropic energies at 298.15 K; i: each state in the chemical progress

II. Computational results

Table S1. Absolute single point energies (SPE), zeroth point vibrational energies (ZPVE), thermal corrections (thermo), entropic energy (TS), enthalpies (H), and Gibbs free energies (G) of. Entropic energy was calculated at 298.15 K. Numbers are in Eh

State	SPE	ZPVE	thermo	TS	H	G
A	-3418.104	0.997	0.065	0.153	-3417.042	-3417.195
TS1	-3418.097	0.998	0.063	0.150	-3417.036	-3417.187
B	-3418.104	0.998	0.064	0.151	-3417.042	-3417.193
TS2	-3418.072	0.998	0.063	0.150	-3417.011	-3417.161
C	-3418.123	1.001	0.062	0.147	-3417.060	-3417.207
TS3	-3418.099	0.998	0.062	0.147	-3417.039	-3417.185
D	-3418.208	1.004	0.061	0.143	-3417.144	-3417.287
E	-2085.511	0.560	0.033	0.092	-2084.918	-2085.010
LAu+	-1256.194	0.418	0.023	0.072	-1255.753	-1255.826
Water	-76.485	0.021	0.003	0.021	-76.461	-76.483

Table S2. Relative enthalpies (ΔH) and Gibbs free energies (ΔG). Numbers are referenced to A and are in kcal/mol

state	ΔH	ΔG
A	0.00	0.00
TS1	3.24	5.10
B	-0.54	1.30
TS2	19.20	21.07
C	-11.40	-7.22
TS3	1.93	6.09
D	-64.17	-57.75
E	-56.98	-77.54

III. References

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IV. Coordination

A

C	-3.64329195524533	4.47832104553508	-14.65698283112377
C	-3.71660994815555	5.69962877419668	-14.74394878260483
C	-3.76095751969761	7.16065926711601	-14.86706089809873
C	-2.45317308071123	7.79818745509427	-14.30396298281523
O	-5.15677826616529	6.03904031222321	-12.09432534070737
H	-3.84946264774362	7.41068295691979	-15.94222260285645
C	-2.65100180240617	9.27054858275309	-14.12481069990580
H	-1.60339998235652	7.57576824209391	-14.96938861502589
H	-2.21220116369397	7.36350488206742	-13.31468971493080
C	-3.78084925790538	9.86073088846004	-13.90076432763051
N	-4.69964603122600	10.66939333384924	-13.50670810566533
P	0.26493904129715	12.52966236530066	-13.71406557310456
Au	-1.23225712483605	10.79471144091445	-14.05693593009892
O	-4.91215375001184	7.72758904995714	-14.23837885839971
H	-5.04395649955942	7.24754346001319	-13.37593229826182
O	-4.46629975236353	7.47052344679843	-18.01215403849865
N	-3.60499728290822	7.38054806676180	-18.96727774394650
C	-3.61095358374782	8.14140239057933	-20.06019359853154
C	-4.52275592527329	9.22422861959075	-20.35081898456234
C	-5.66135794341888	9.55972624121766	-19.57002111344033
C	-6.46366089416533	10.64456603081137	-19.93763991693504

H	-7.34488690683975	10.88881534763962	-19.33439076587925
C	-6.16149948682926	11.41270545693193	-21.07273575288483
H	-6.79788335433330	12.25934749591519	-21.35056617419290
C	-5.04533593643901	11.08270606741754	-21.85892332508510
H	-4.80786060369959	11.67083550366373	-22.75126196124330
H	-5.89575824189205	8.94841581786703	-18.69785825398560
C	-4.23964348804385	10.00012952684783	-21.50599974035064
H	-3.37037025765400	9.74444683516871	-22.12226513915222
H	-2.83501995677584	7.90196817283274	-20.78949875758885
C	-2.57148404819770	6.36546659134886	-18.79361677242413
C	-2.93019600080051	5.20195777043772	-18.09986384569412
H	-3.95547744548251	5.10209212342680	-17.73739773058979
C	-1.96743903117149	4.20894834413229	-17.88976270320747
H	-2.24435364897821	3.29366419107005	-17.35778361090652
C	-0.65561508657241	4.38547895777521	-18.35527104008325
C	-0.30490044536559	5.56266139709997	-19.03295895836850
H	0.72151722201373	5.71156226304086	-19.38318935292786
H	0.09594158474274	3.60828370504835	-18.18448691442532
C	-1.26070966438373	6.56270063235942	-19.25504489129000
H	-0.97914267135629	7.49199394510237	-19.75847650807455
O	-4.88829468969953	12.62222855719672	-11.77897960993789
S	-4.66393416540375	11.16813408759549	-11.73405856123166
O	-3.43632391253690	10.54625062133753	-11.22043349326260
H	-2.45932485102779	13.59607594442455	-16.76165947102148
H	-4.21947598278149	11.91258207625030	-17.30868267793613
C	1.67139232559588	14.88691066901641	-17.48971595836754
C	-2.18888985316817	12.54424455480210	-16.89923108905738
H	3.08735413576066	15.82686239572274	-16.13604632538763
C	2.28437512280352	15.09151871850525	-16.24741719027852
C	0.65437286429792	13.93515328646848	-17.60895162313344

C	-3.17664061112895	11.59610710557488	-17.20168971984148
H	0.17928258454573	13.76033821094192	-18.57959376493493
C	0.22353985931625	13.16916065608769	-16.50577326013232
C	-0.84231997665688	12.15450981060799	-16.76916334186258
C	-2.83534774763910	10.24998809004671	-17.38588545733680
H	-3.61217060303224	9.50787046474827	-17.59001835148906
C	-0.50072383822918	10.80152805666915	-16.98517920240347
C	-1.49241478342789	9.85854510648608	-17.29204614070718
H	0.54940110884596	10.49824587958740	-16.92049046505178
H	-1.21486605256899	8.81058537561541	-17.44599174365148
H	1.98798326351039	15.46213796966951	-18.36573172927610
C	-0.64772825829820	13.86309454839099	-12.70532253737311
C	1.85825052876838	14.35414419825588	-15.13921888123392
H	2.33619078704968	14.53600068809085	-14.17500975584465
C	0.82855916539459	13.39215110946230	-15.23957594991776
C	1.80635387462243	11.80610898091613	-12.85166661937943
H	-5.77543118520996	10.75034007893260	-15.29499718588876
H	-5.39668543591727	12.36567228969074	-14.56932308580278
C	-5.69945306782462	11.32713906003454	-14.36321989975969
H	-6.67368639422673	11.31733461608499	-13.84864034980747
C	-6.08528384929978	10.33984615993549	-11.08426890770497
C	-5.99255822774327	8.96637672164381	-10.81364369028546
H	-5.06551855724054	8.41680557016076	-10.99164991327245
C	-7.26345115800548	11.06805199929753	-10.86222533185505
C	-7.12021886662722	8.31403936126764	-10.31171508978112
H	-7.29369318845340	12.14107028399400	-11.07161343072546
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H	-7.05692848029455	7.24165354216961	-10.09932695998978
H	-9.30078281305609	10.94635706558389	-10.16867236637206

C	-3.57830382615133	3.04971495130958	-14.64465021828571
C	-2.64917389400404	2.36899377471316	-13.82152537804041
H	-1.98073579929596	2.94674563514359	-13.17579571219885
C	-4.43658246022608	2.29635014063026	-15.48356353920609
C	-2.58287117793381	0.97238321414761	-13.84107621776507
H	-5.15521084808571	2.82057589262328	-16.12098990077617
C	-4.36072547825755	0.90035699581154	-15.49635437067422
C	-3.43586355612082	0.23486238298124	-14.67668827963180
H	-1.86000622615639	0.45500254350366	-13.20199980150964
H	-3.37978091204445	-0.85835132102069	-14.68921756391664
H	-5.02697942223215	0.32695685029161	-16.14903201125626
C	-9.52115112676394	8.30141304311277	-9.48486564116314
H	-9.49659124201829	7.22051534104788	-9.69851276728756
H	-10.46559823597120	8.71828983494592	-9.87209818807580
H	-9.53545592109789	8.42215111699883	-8.38499556529473
C	0.13400634812288	15.17832779915634	-12.53540102876242
H	1.08964610978573	15.03927913015997	-12.00614623079123
H	-0.48115112441114	15.87127667140421	-11.93281808958563
H	0.33109673217524	15.66672314136501	-13.50327259234312
C	-1.01431183070652	13.27171592994072	-11.32928825271114
H	-0.12542318782303	13.14813203857991	-10.68836208300727
H	-1.52931095529298	12.30022539190772	-11.42069043440298
H	-1.70190834325812	13.96782780021896	-10.81597737132374
C	-1.93732446640505	14.14984947759535	-13.50705863072264
H	-2.56443952219994	13.24690201646774	-13.60174702442218
H	-1.70795490474293	14.53013149863079	-14.51749654585747
H	-2.52734100306289	14.91793185990565	-12.97555311421711
C	1.31668420193630	10.71594526117068	-11.86934283606816
H	0.69213690977924	11.12846853388917	-11.06192686092218
H	2.19768250106391	10.23454386396816	-11.40711493459584

H	0.72760335684817	9.94034551469650	-12.38999597153251
C	2.67979642670553	12.80935199886353	-12.07524452675556
H	2.12622077616090	13.28336884110566	-11.24844078077344
H	3.10415909861360	13.59826359666277	-12.71556736512538
H	3.53028450240889	12.26088373899596	-11.63073663511845
C	2.62285823966646	11.13043778571465	-13.97499505361919
H	1.99487269528430	10.43083490768808	-14.55654743209055
H	3.44728277831211	10.55083660686353	-13.52149269833198
H	3.05948583639743	11.86505948886598	-14.67121491286690
H	-5.99805303613613	5.59342923124771	-12.31048732059018
H	-4.48840369277945	5.44003293858419	-12.49285428422306

TS1

C	-3.55607695628011	4.41041569359688	-14.72170549686074
C	-3.57557269534301	5.62885807333783	-14.86459564800160
C	-3.51006173701513	7.06136187721883	-15.11126818523363
C	-2.17005996036566	7.72558259248726	-14.68542947224640
O	-4.89192578979202	6.28490557833011	-12.24779643681024
H	-3.72437462546123	7.26416969684694	-16.17961325959742
C	-2.50200954662543	9.14180971368367	-14.31007633382299
H	-1.44221799806620	7.66509594208342	-15.51007562886424
H	-1.72076062129253	7.20835754167476	-13.81647415808228
C	-3.77964230932591	9.36248386708716	-14.04296246512522
N	-4.66507632381995	10.21628033536765	-13.55538388827861
P	0.19751588640856	12.52983167579786	-13.66515565563676
Au	-1.21124319617271	10.72840106510612	-14.09382670781943
O	-4.57838058040130	7.77157456485541	-14.38775025879378
H	-4.73079659734828	7.29485730730828	-13.49882691639735
O	-4.45814397131651	7.46566276528492	-18.08696350535503
N	-3.61378493552997	7.35484914450153	-19.05844300962369

C	-3.63163369038844	8.10040875930012	-20.16075643773348
C	-4.53563157365494	9.18903119372904	-20.45280794988997
C	-5.65027991105218	9.55627897209131	-19.65227658341511
C	-6.44709353265184	10.64338000944754	-20.02407478221444
H	-7.30907939150407	10.91415885926208	-19.40480379963963
C	-6.16223928940001	11.38217809264232	-21.18287949432417
H	-6.79364570746168	12.23158337843585	-21.46344275735315
C	-5.06944801240608	11.02126222611525	-21.98802144569349
H	-4.84548171523471	11.58774534178051	-22.89759696564712
H	-5.87012822788807	8.96862195389012	-18.76043120586226
C	-4.26933795827888	9.93607220368936	-21.63084301004745
H	-3.41791657584140	9.65608382601014	-22.26129063881783
H	-2.87156680040200	7.84012159513392	-20.89986700464654
C	-2.58924435048744	6.33157645270962	-18.88931251585472
C	-2.95640181498465	5.16621745737095	-18.20263702738646
H	-3.98393581923859	5.06789931599082	-17.84554982174022
C	-1.99948450396416	4.16777586616018	-17.99252195919149
H	-2.28246841293083	3.25146965422153	-17.46507846520419
C	-0.68522428979381	4.33934452186468	-18.45332822966097
C	-0.32707182887732	5.51643226943431	-19.12708352181258
H	0.70084532761039	5.66081292566420	-19.47459218291226
H	0.06205693966484	3.55804904361911	-18.28278793764420
C	-1.27687130087300	6.52258452534653	-19.34811258977675
H	-0.99068747669745	7.45169026766084	-19.84936255612737
O	-4.49629886676902	12.21829899018022	-11.92854104618213
S	-4.48058457509841	10.74546466482355	-11.86283037926956
O	-3.34859486184351	9.96994786521291	-11.33530310591874
H	-2.54502026862502	13.58839174271041	-16.60381342158493
H	-4.22705072362796	11.86501650854719	-17.25937240799752
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TS2

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TS3

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C	4.82101794413412	-0.86918725302400	2.72426317717371
C	4.32898423306986	-0.70668870914632	-1.59204974552300

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C	5.79837777043484	0.11618407523709	-3.37962625866319
C	5.39472446255879	-0.93657308575947	-4.20805227780878
C	4.46512529224069	-1.86978062593165	-3.73659042407424
C	3.91130350774886	-1.77653144216415	-2.44500626091102
C	2.94209598484374	-2.83836240874713	-2.03139551480127
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C	2.51003843604038	-5.07183801569305	-1.12595137603775
C	1.17358081566469	-4.74416571522058	-0.88286614266547
C	0.67594723822413	-3.47952426015955	-1.28464131583278
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H	2.78021802029042	1.02704009814818	2.56374588760104
H	1.40618327170286	0.72100810400562	1.46289321404052
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H	1.98604685435396	2.71722815482587	-0.67304604187029
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H	6.12032101309104	-3.03139996519242	1.57632196647782
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H	7.31654345081730	-0.82507574595669	1.58732148555265
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H	4.14436815213831	-2.69286804154171	-4.38297883201070
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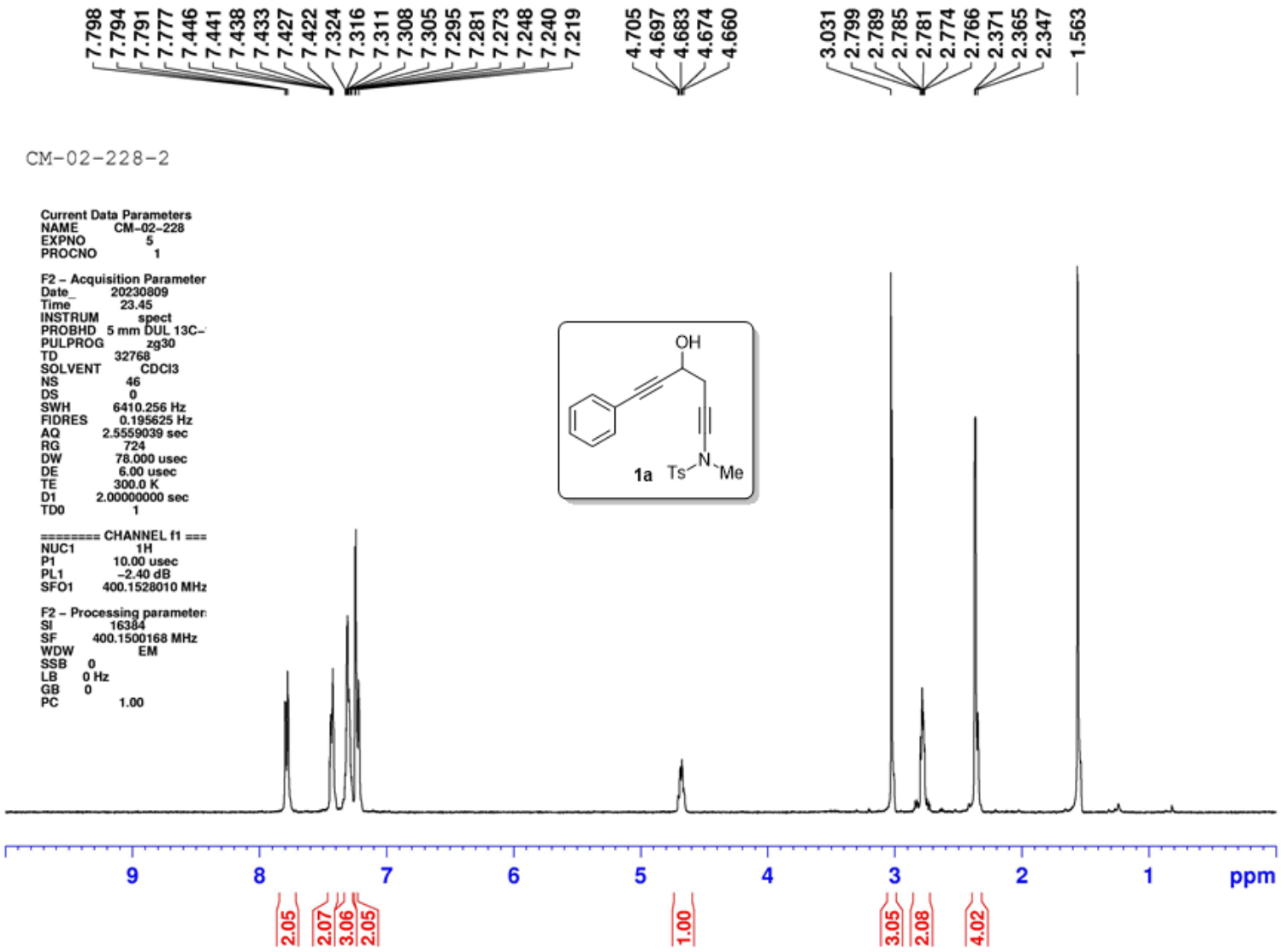
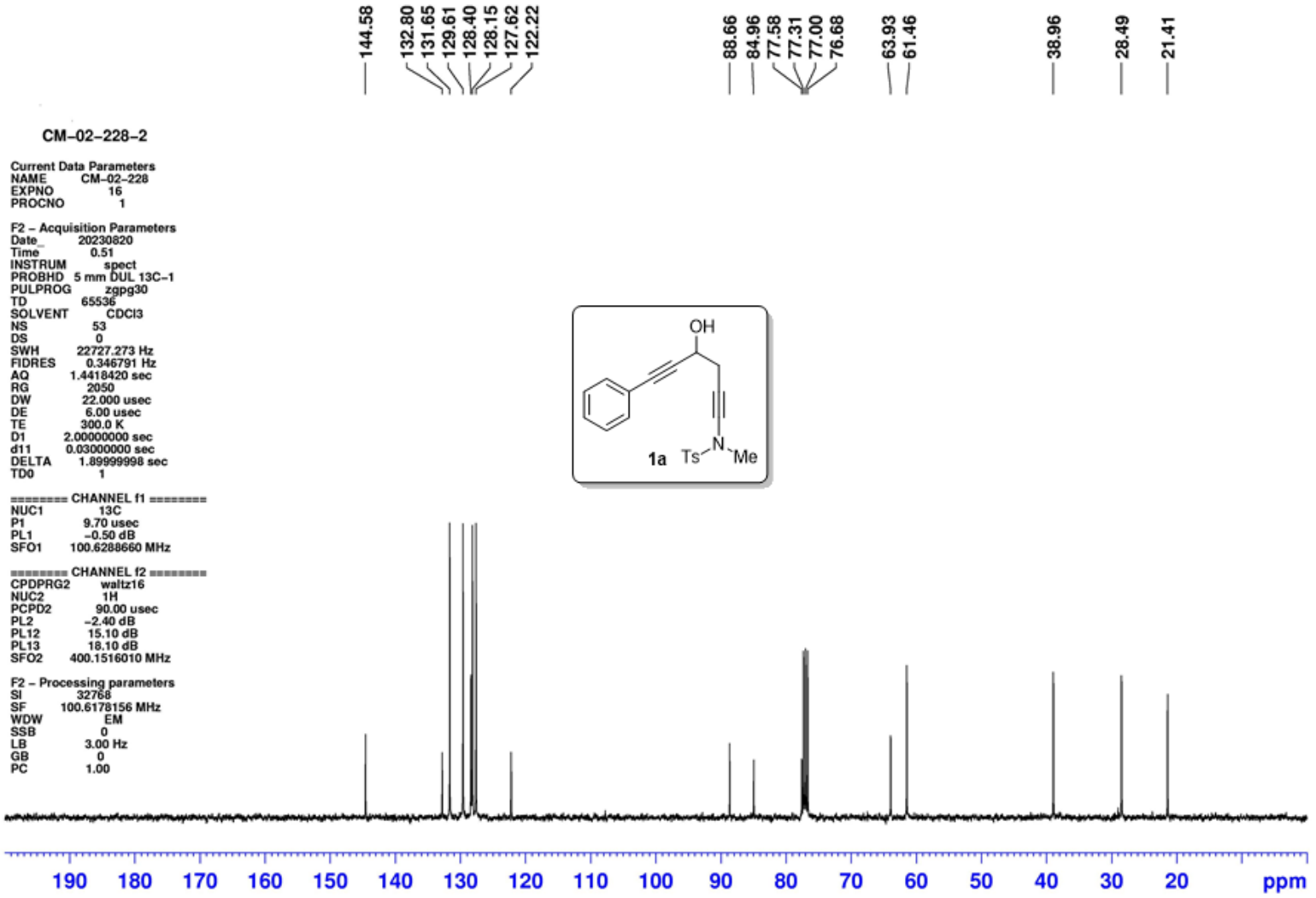
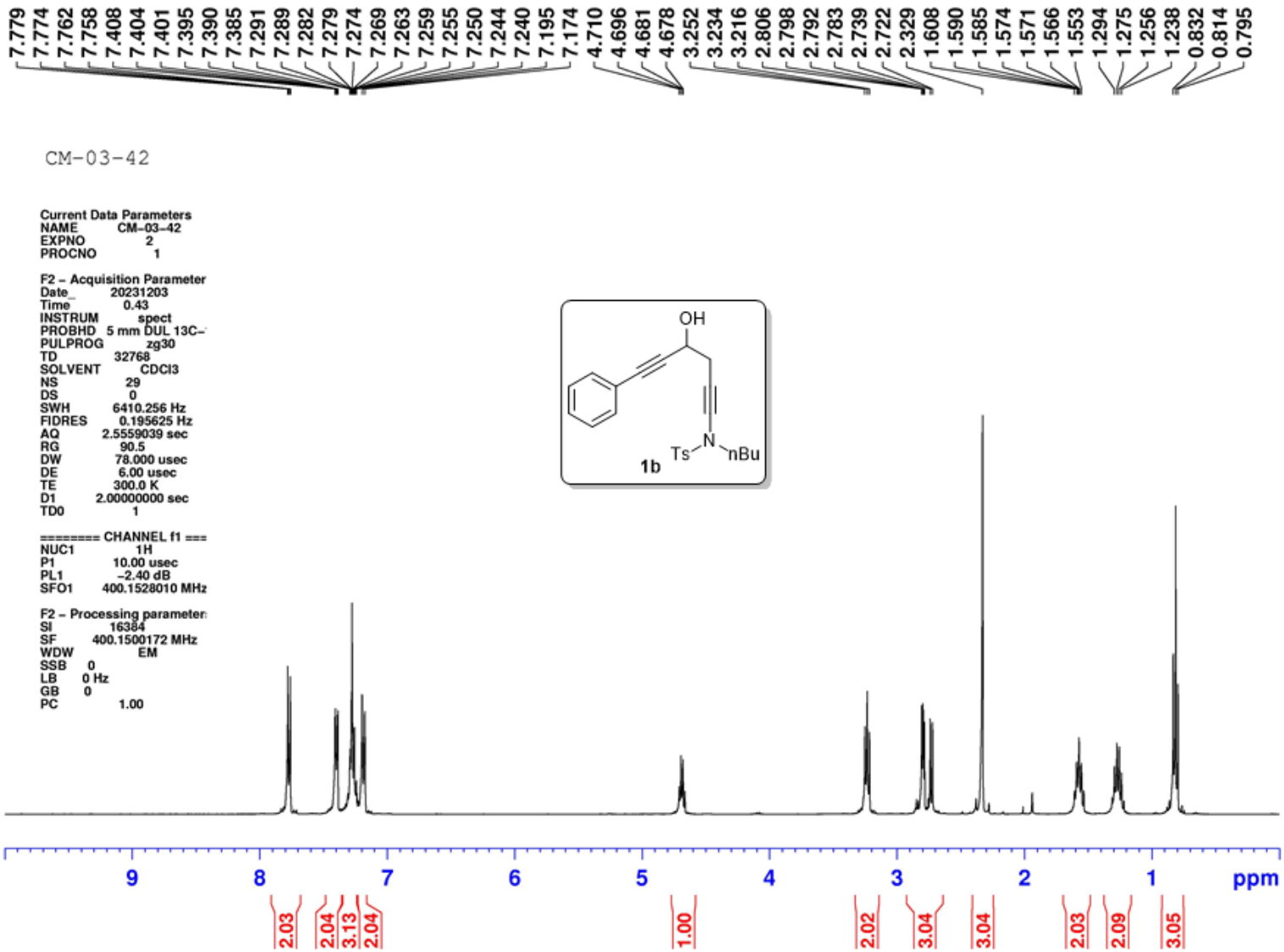
^{1}H NMR ($CDCl_3$, 400 MHz)



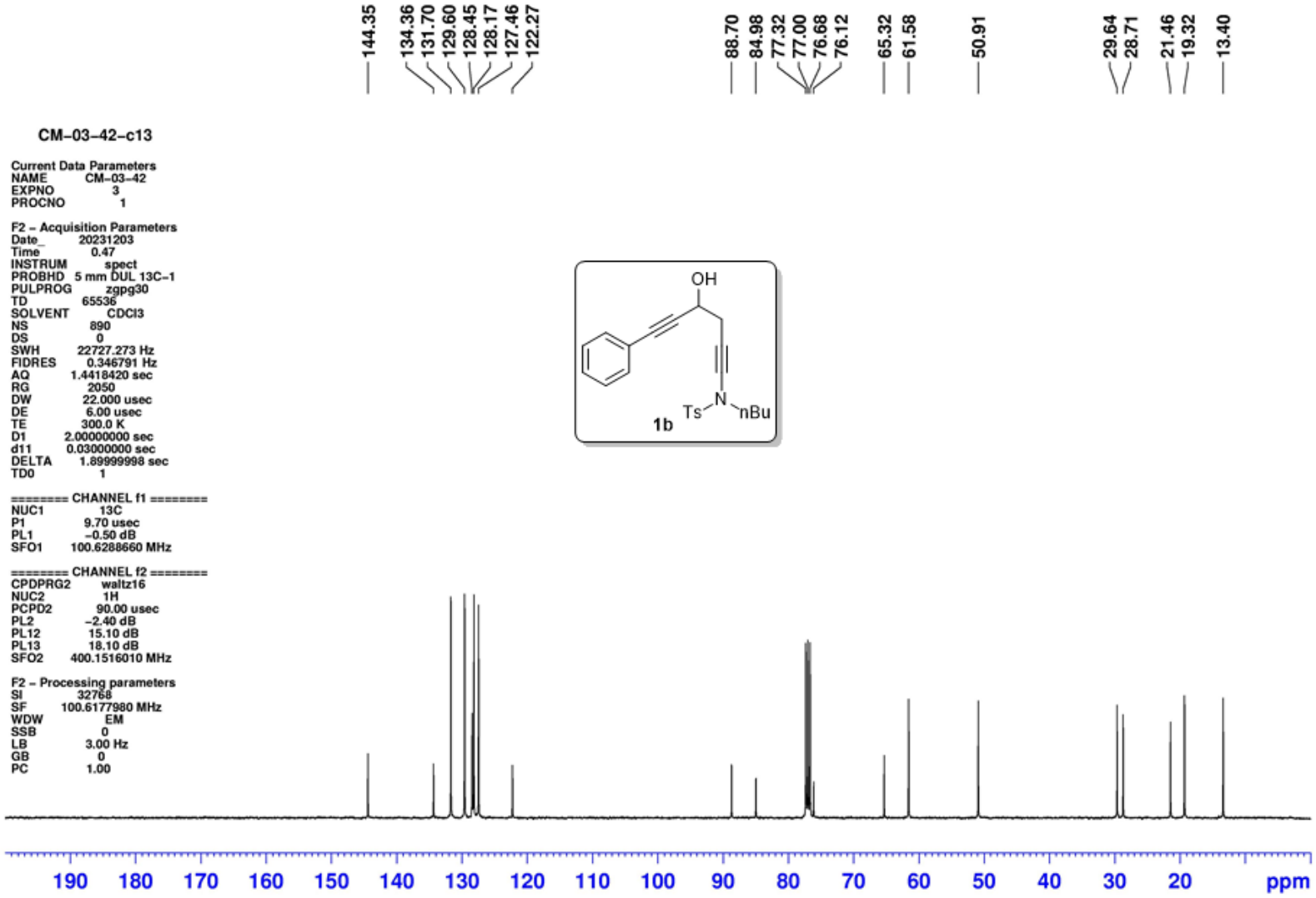
^{13}C NMR ($CDCl_3$, 100 MHz)



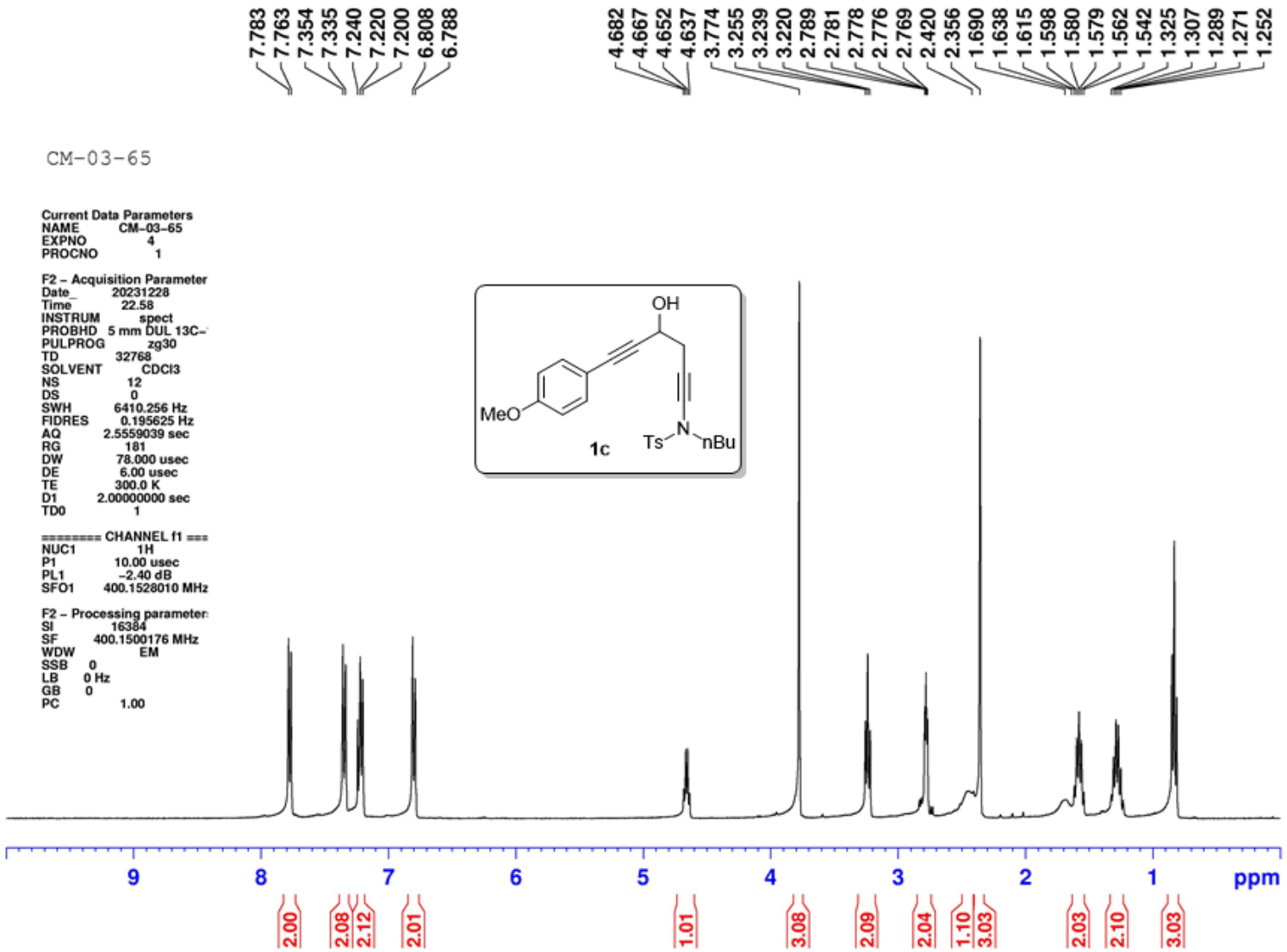
^{1}H NMR ($CDCl_3$, 400 MHz)



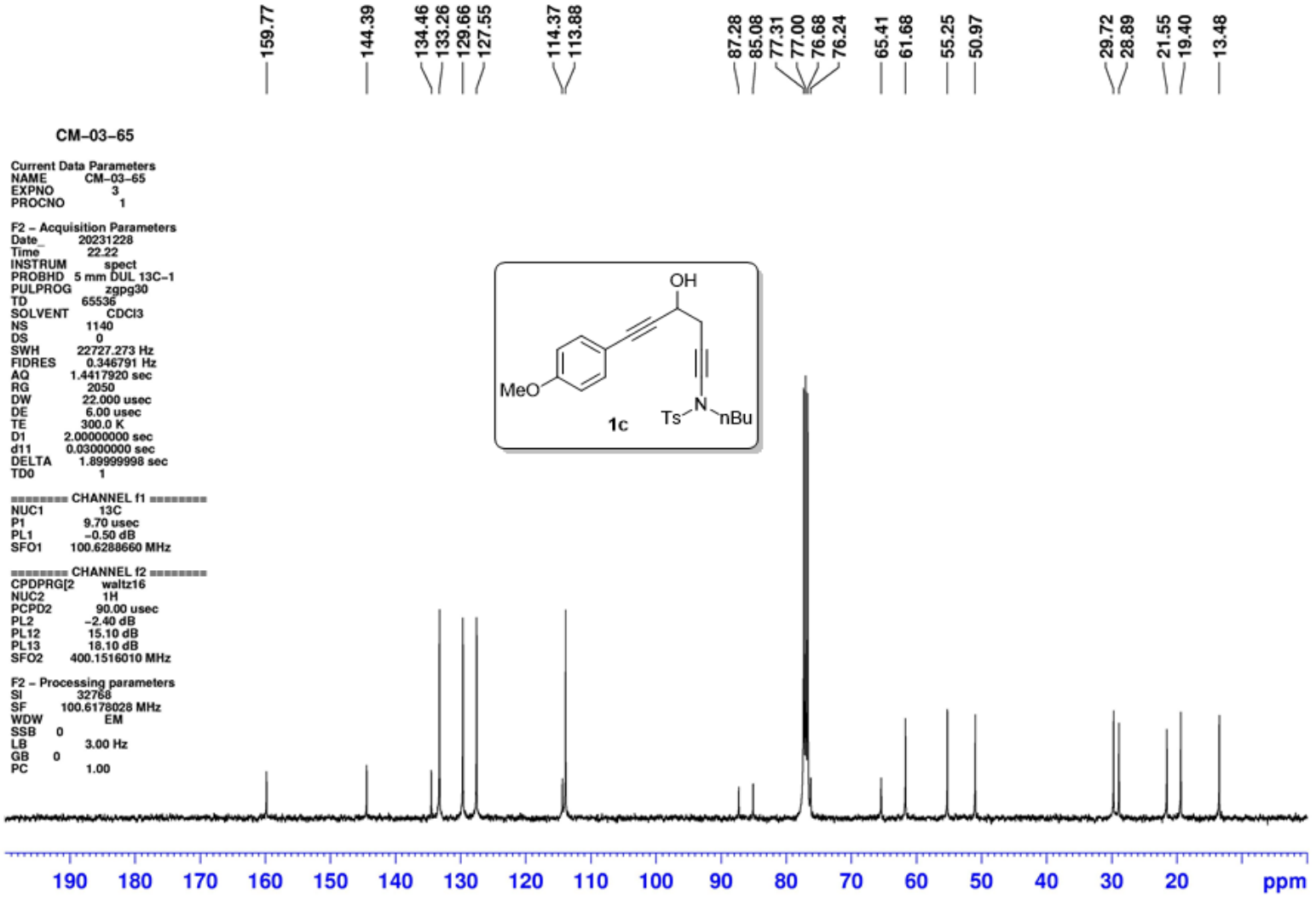
^{13}C NMR ($CDCl_3$, 100 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



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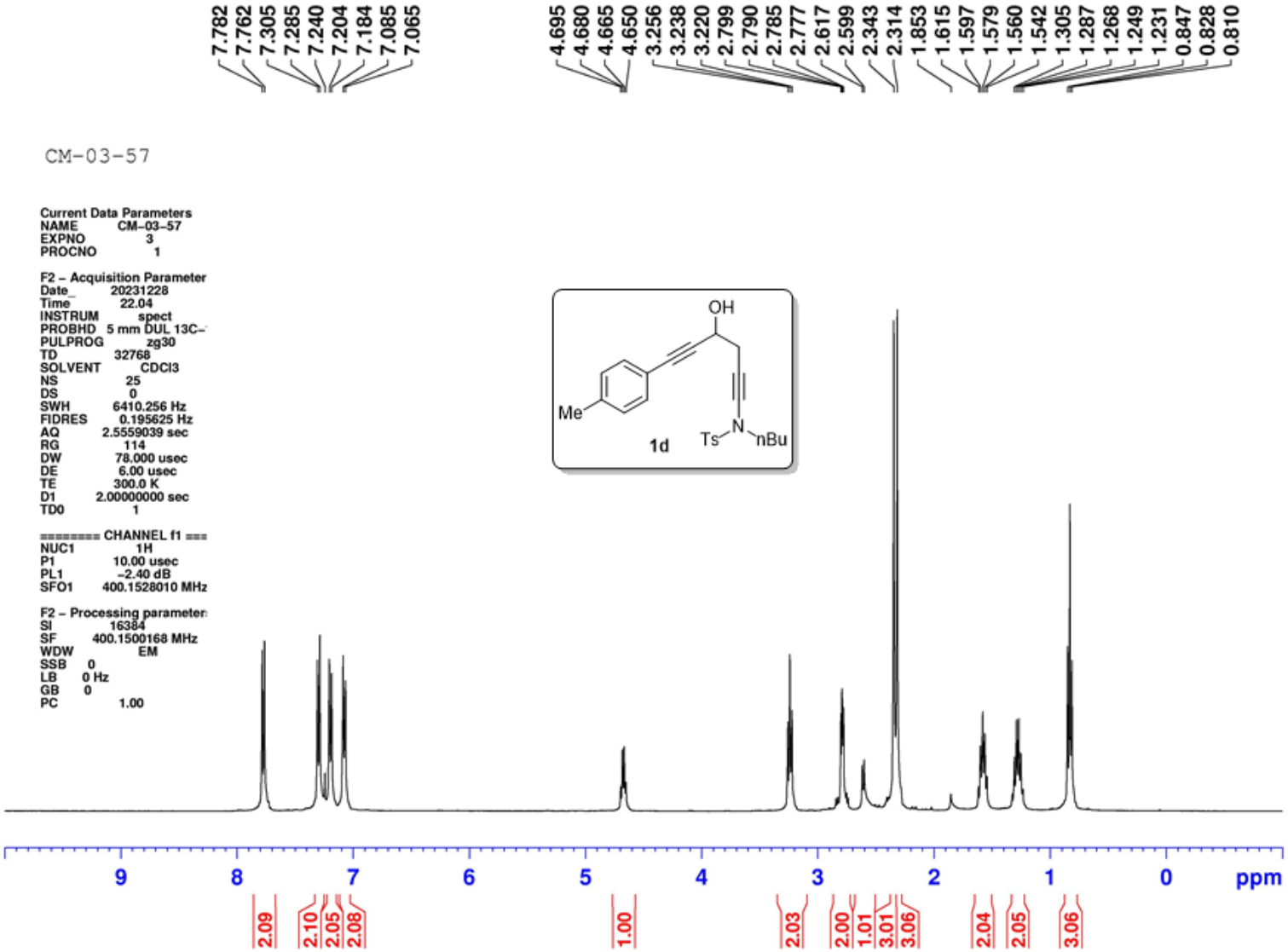
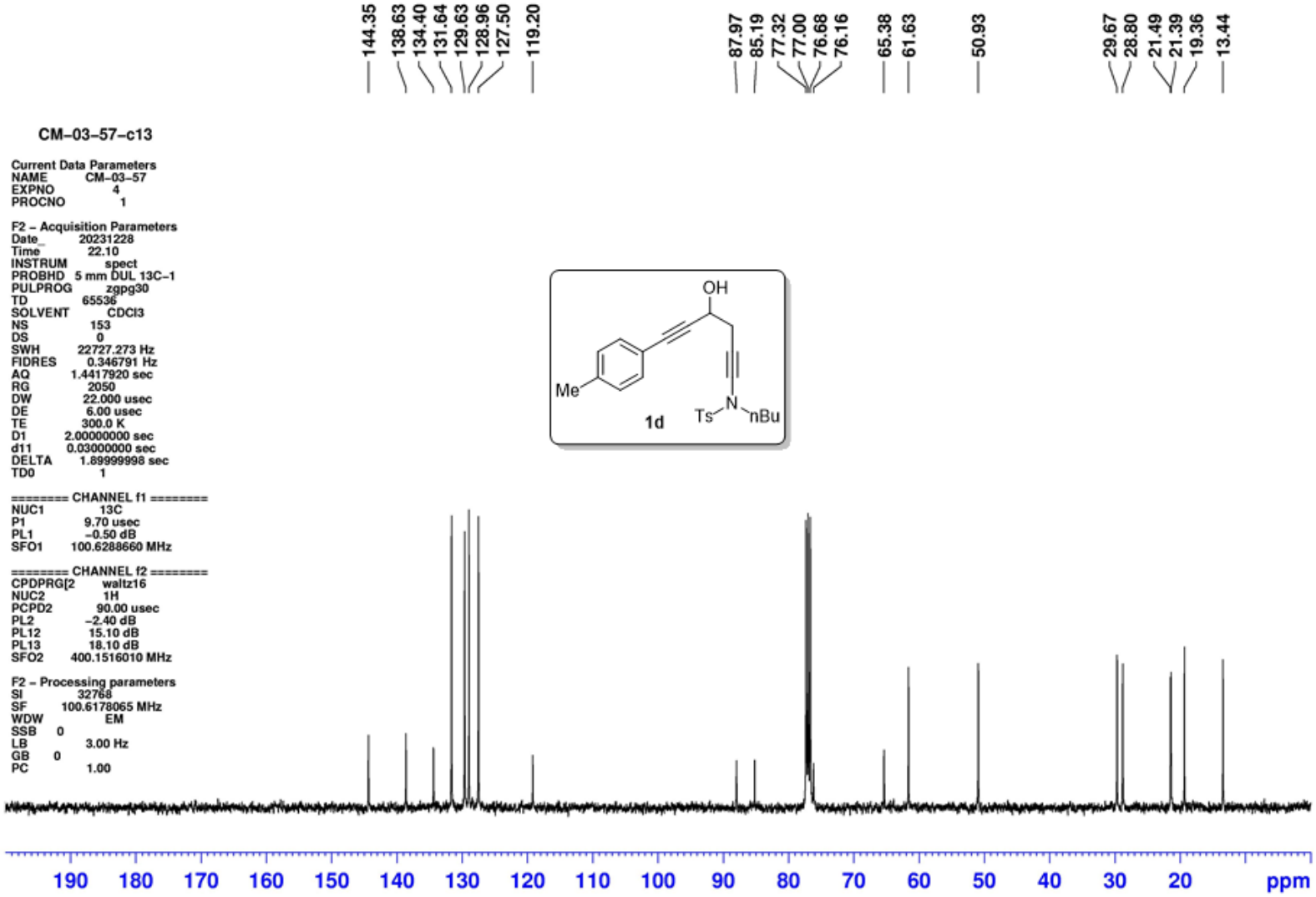


^{13}C NMR ($CDCl_3$, 100 MHz)



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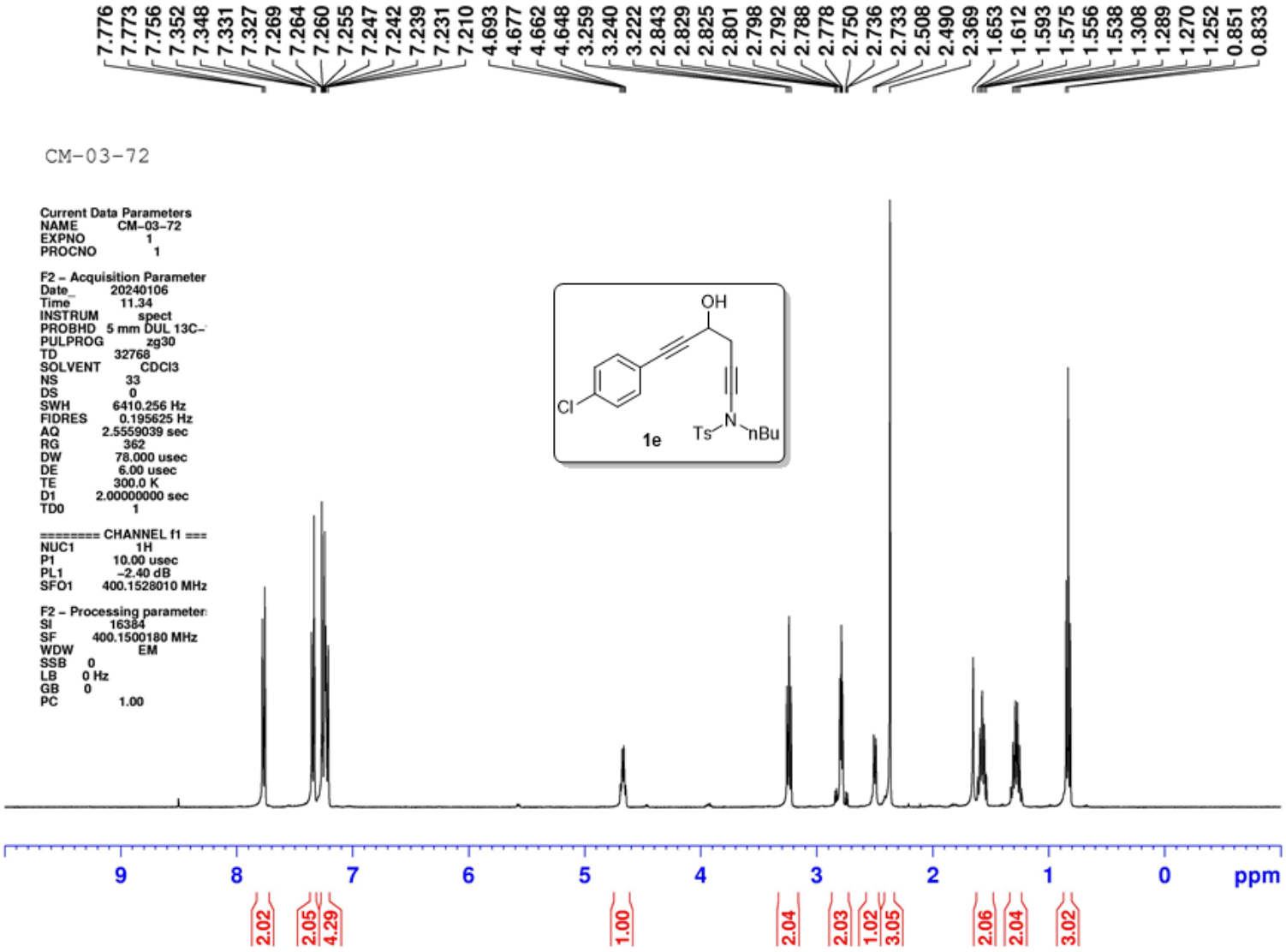
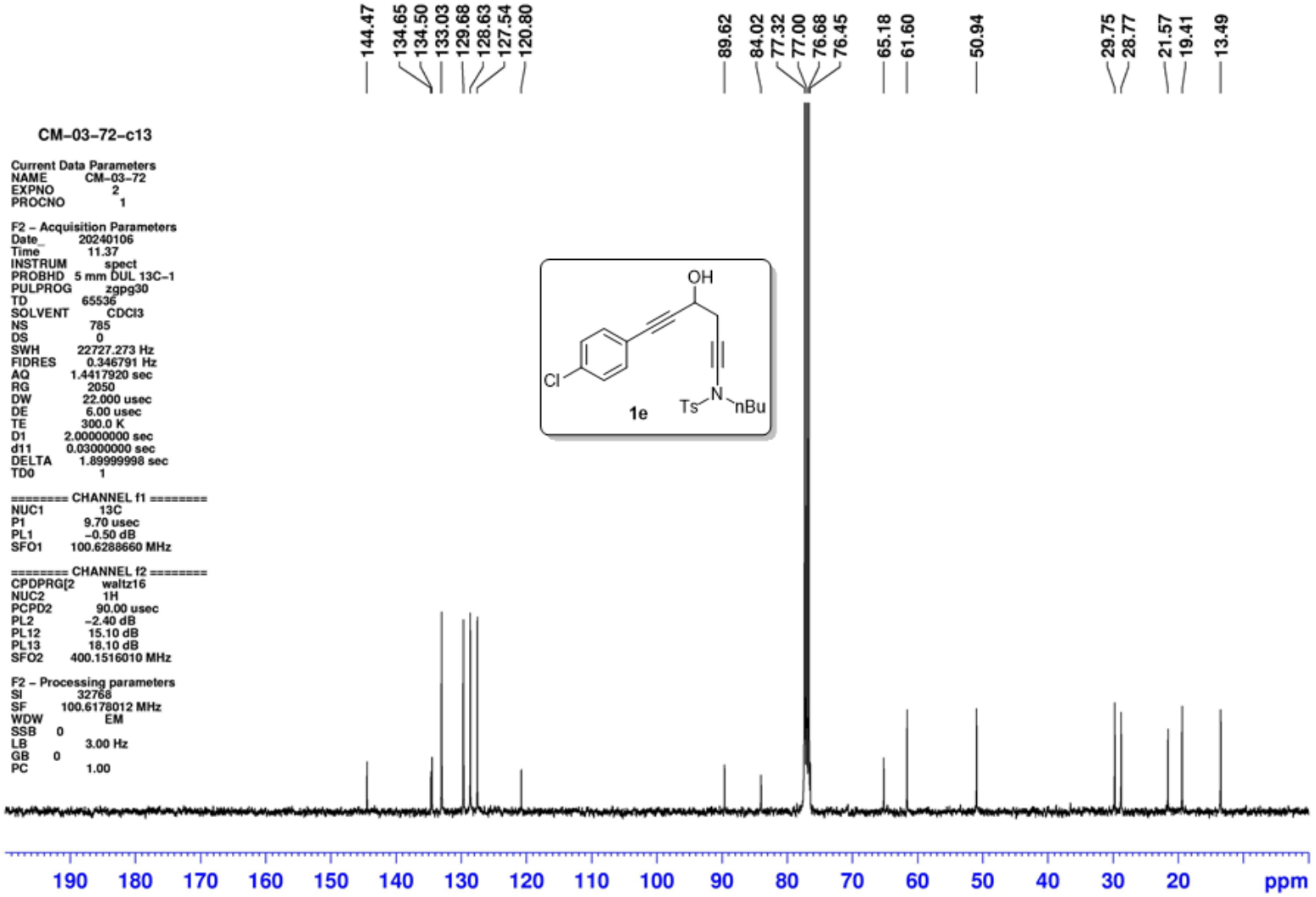


^{13}C NMR ($CDCl_3$, 100 MHz)



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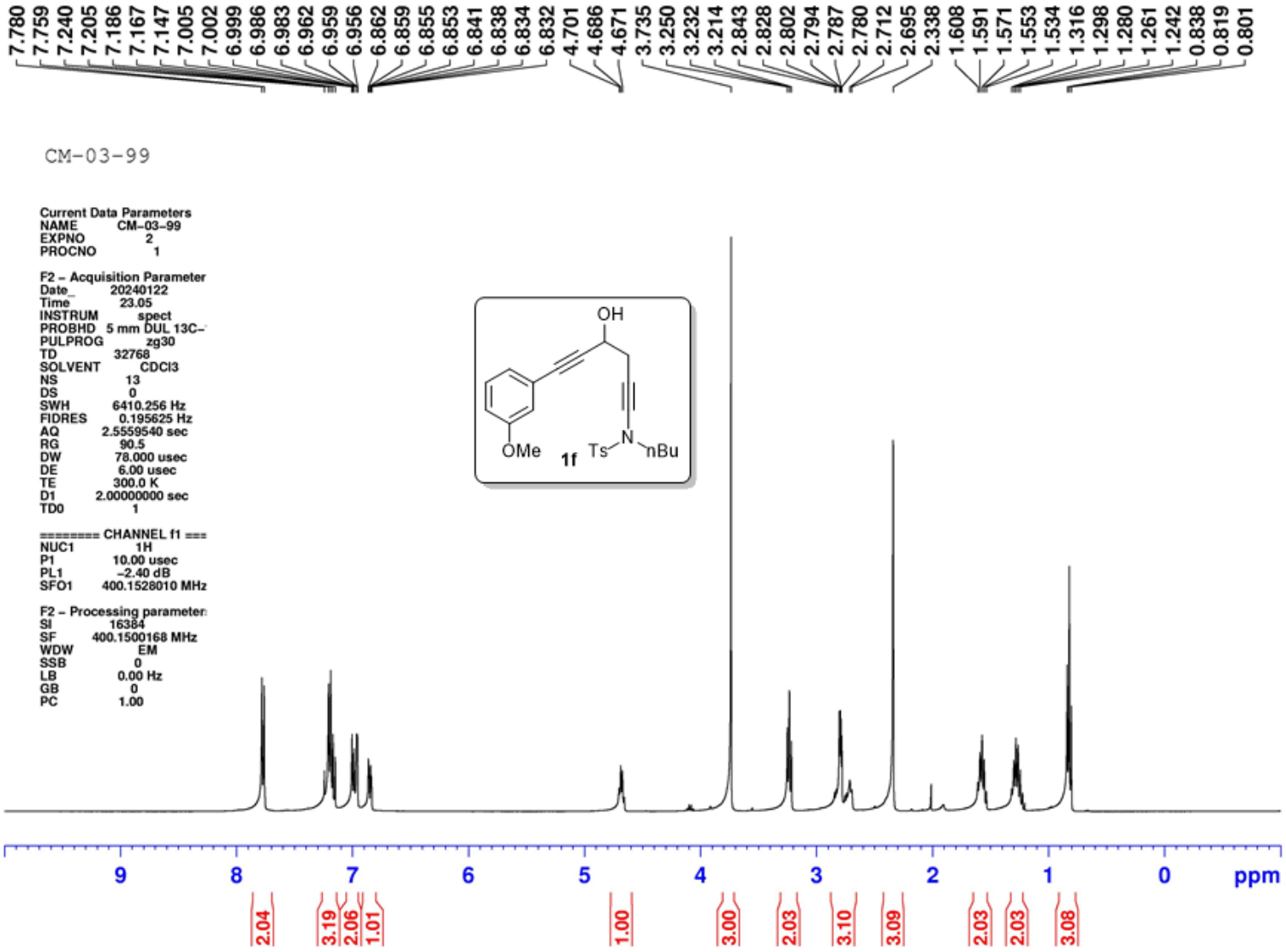
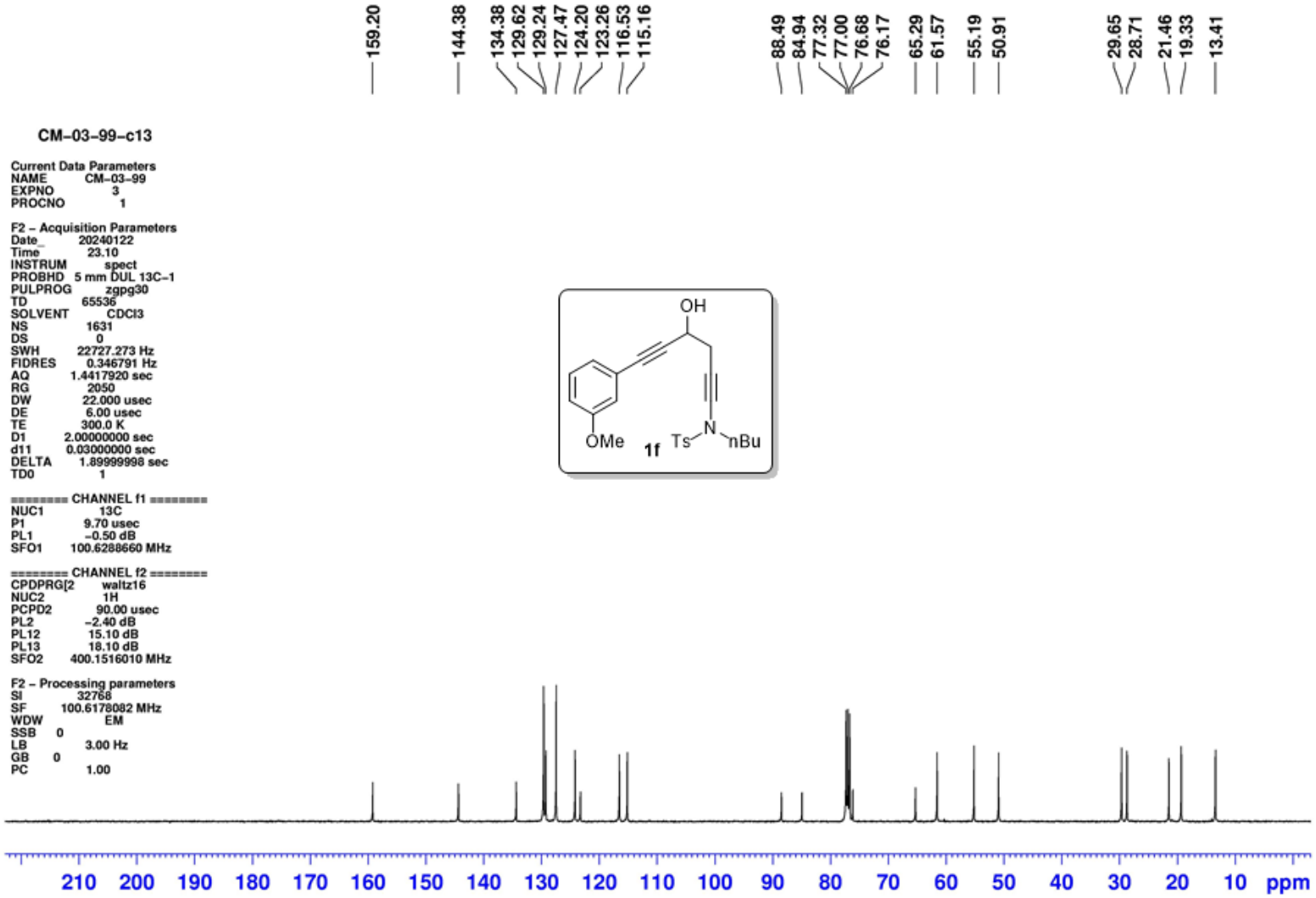


^{13}C NMR ($CDCl_3$, 100 MHz)



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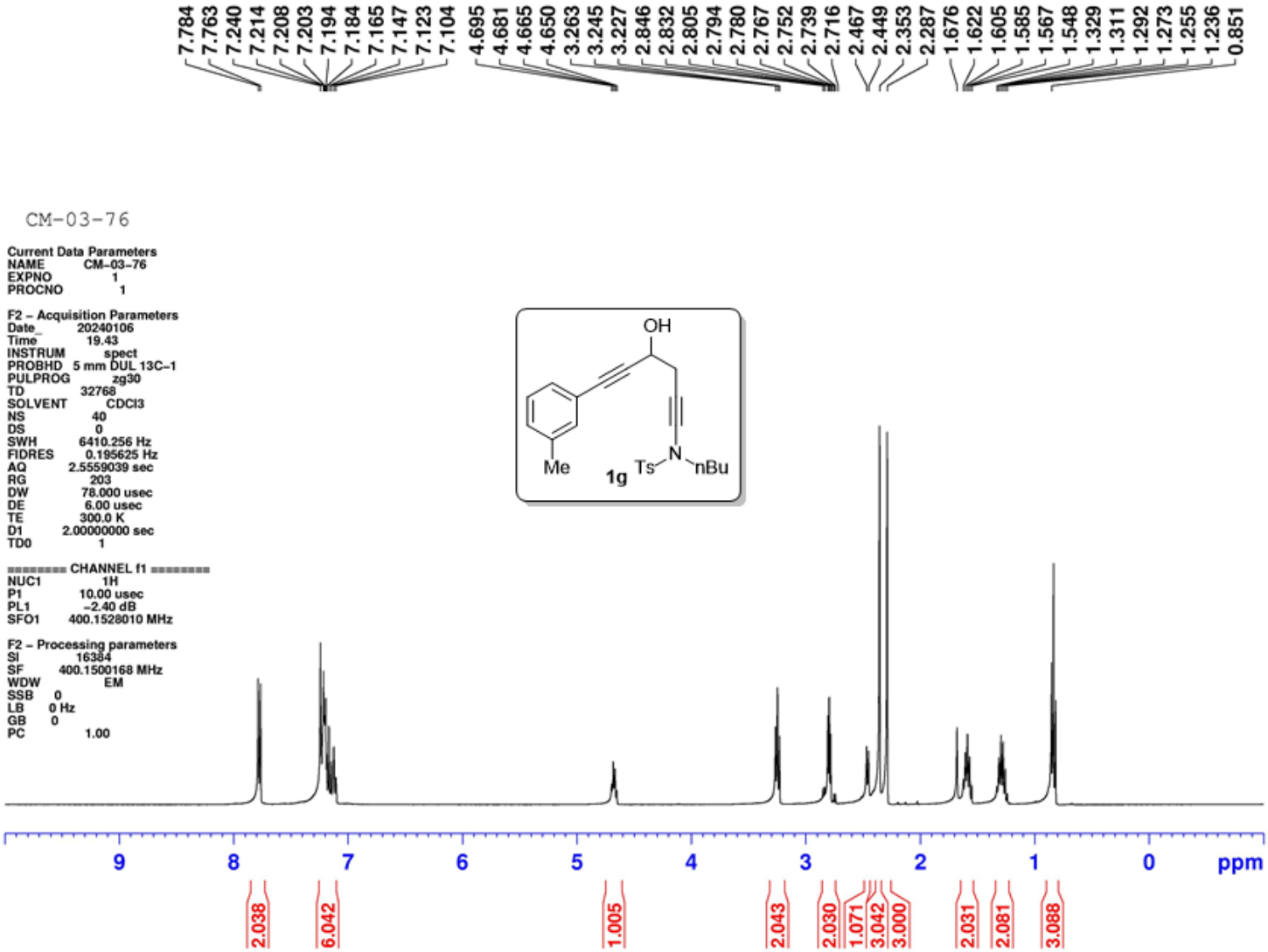
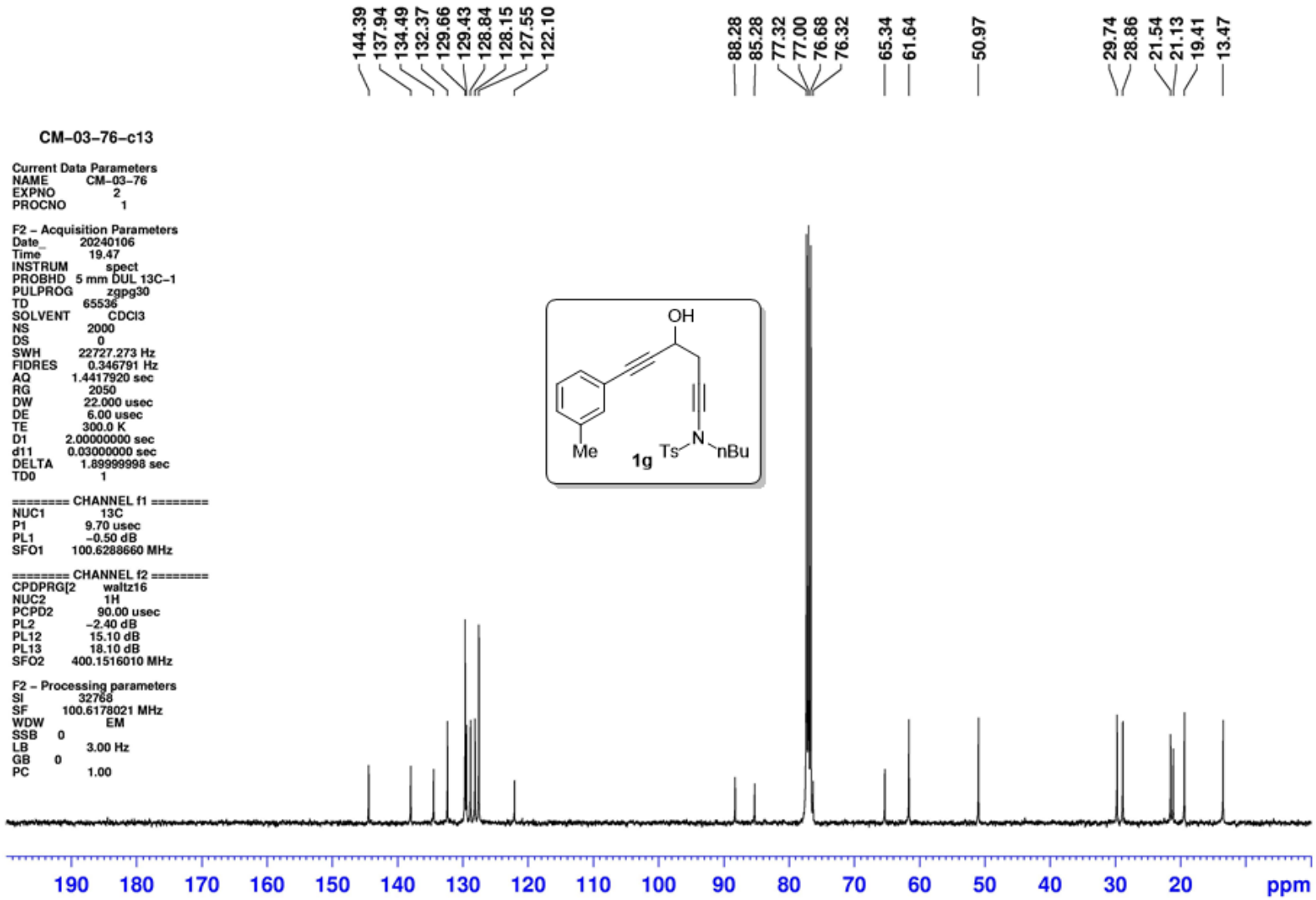
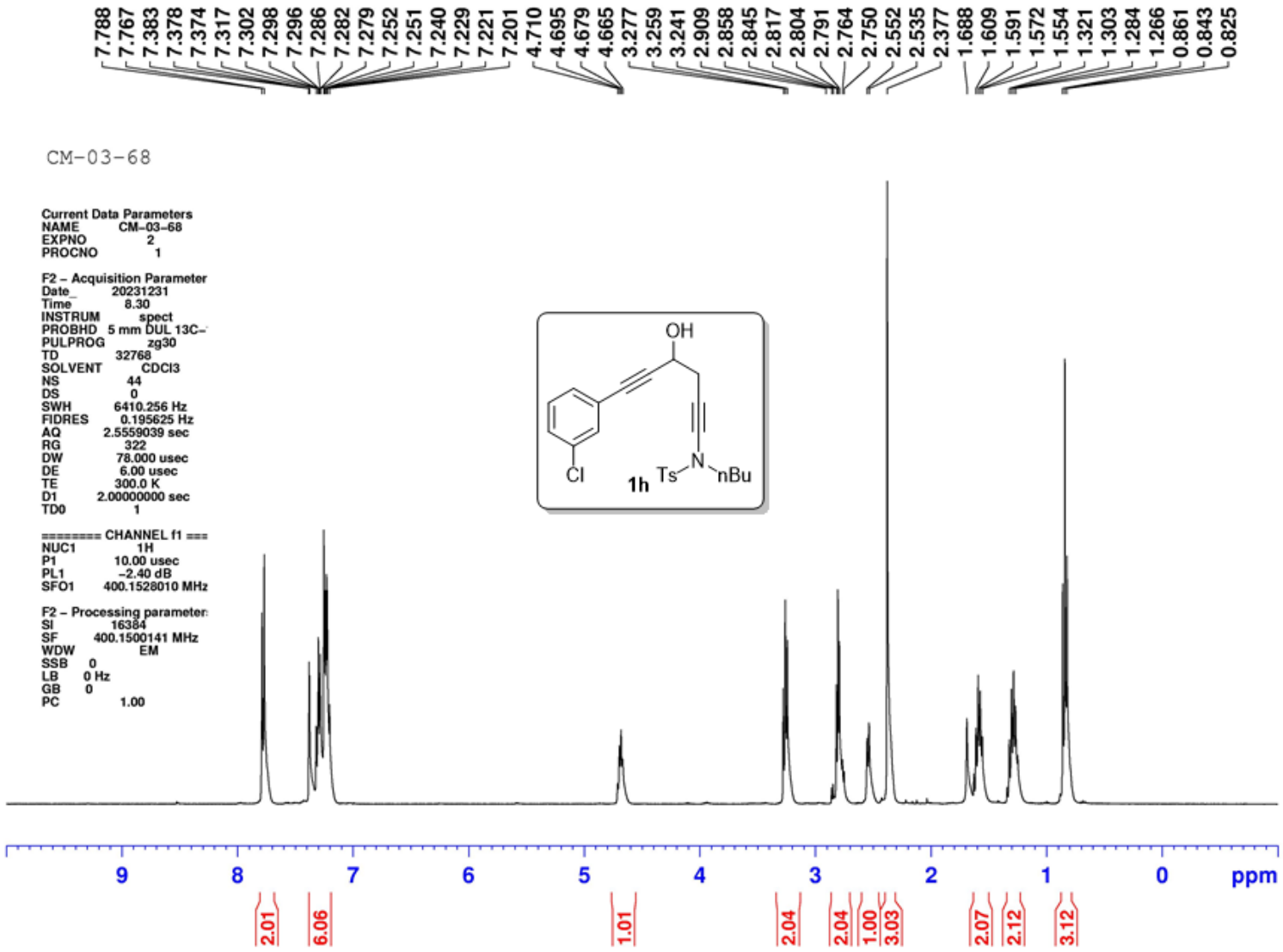


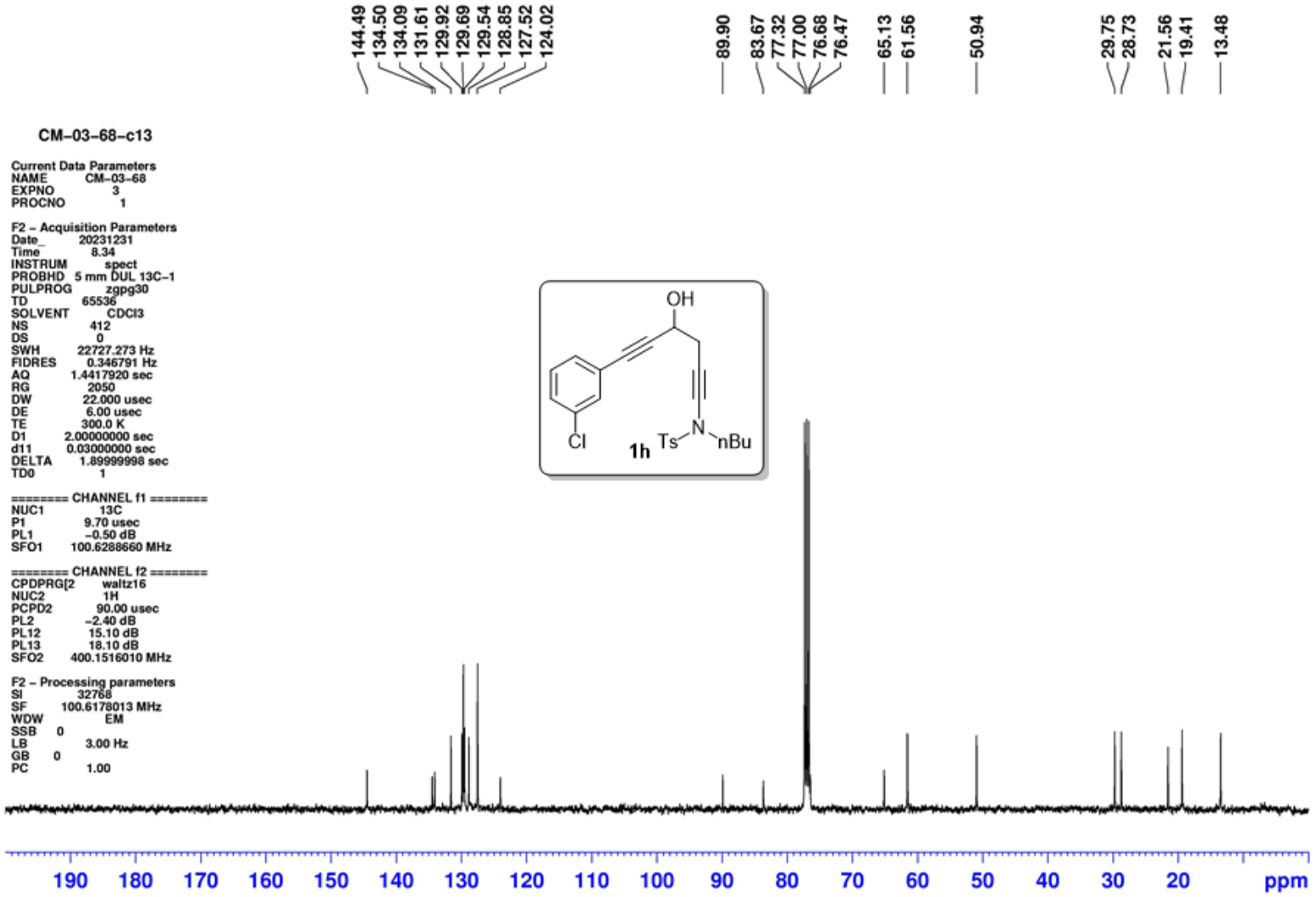
^{13}C NMR ($CDCl_3$, 100 MHz)



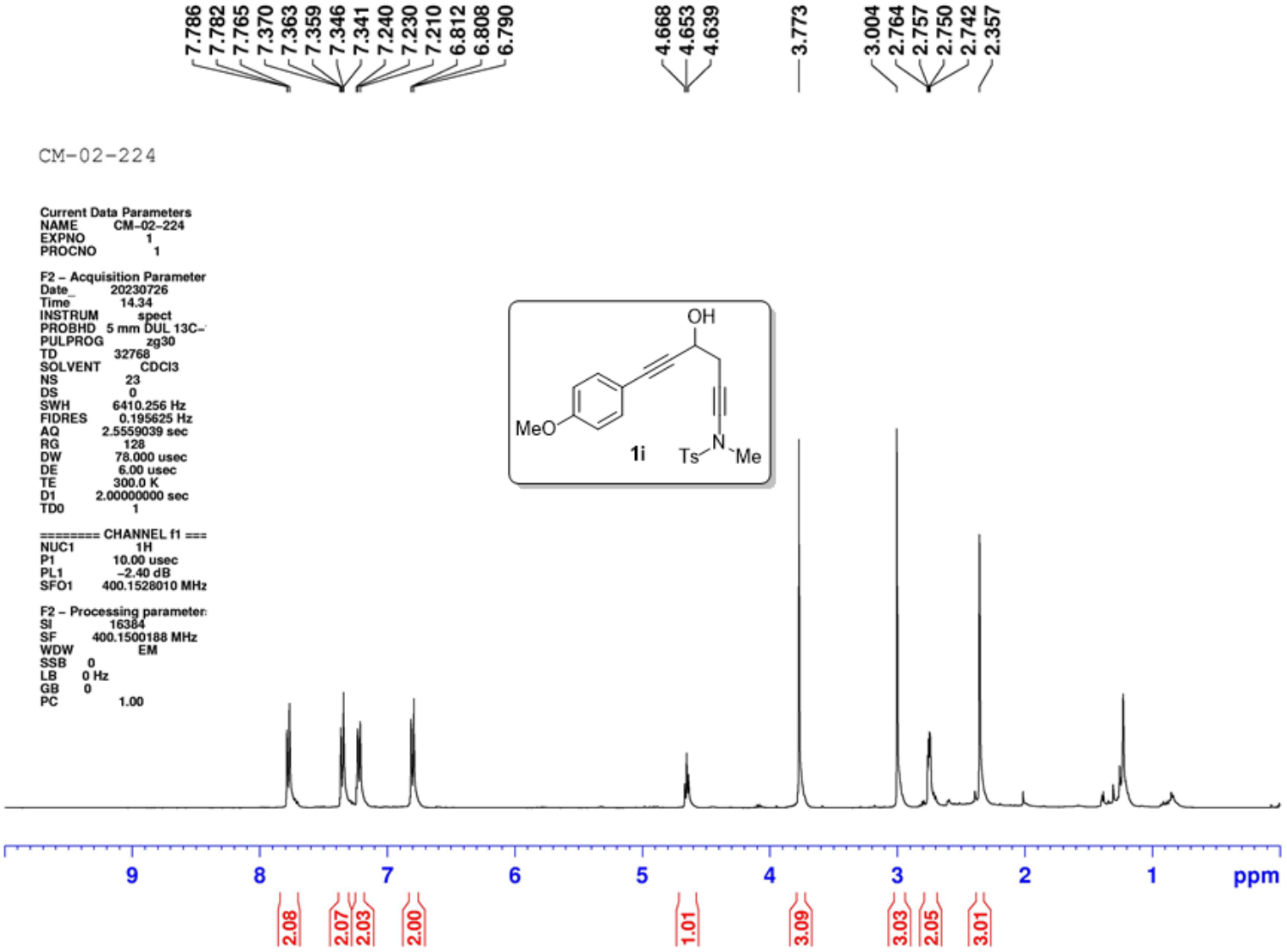
^{1}H NMR ($CDCl_3$, 400 MHz)



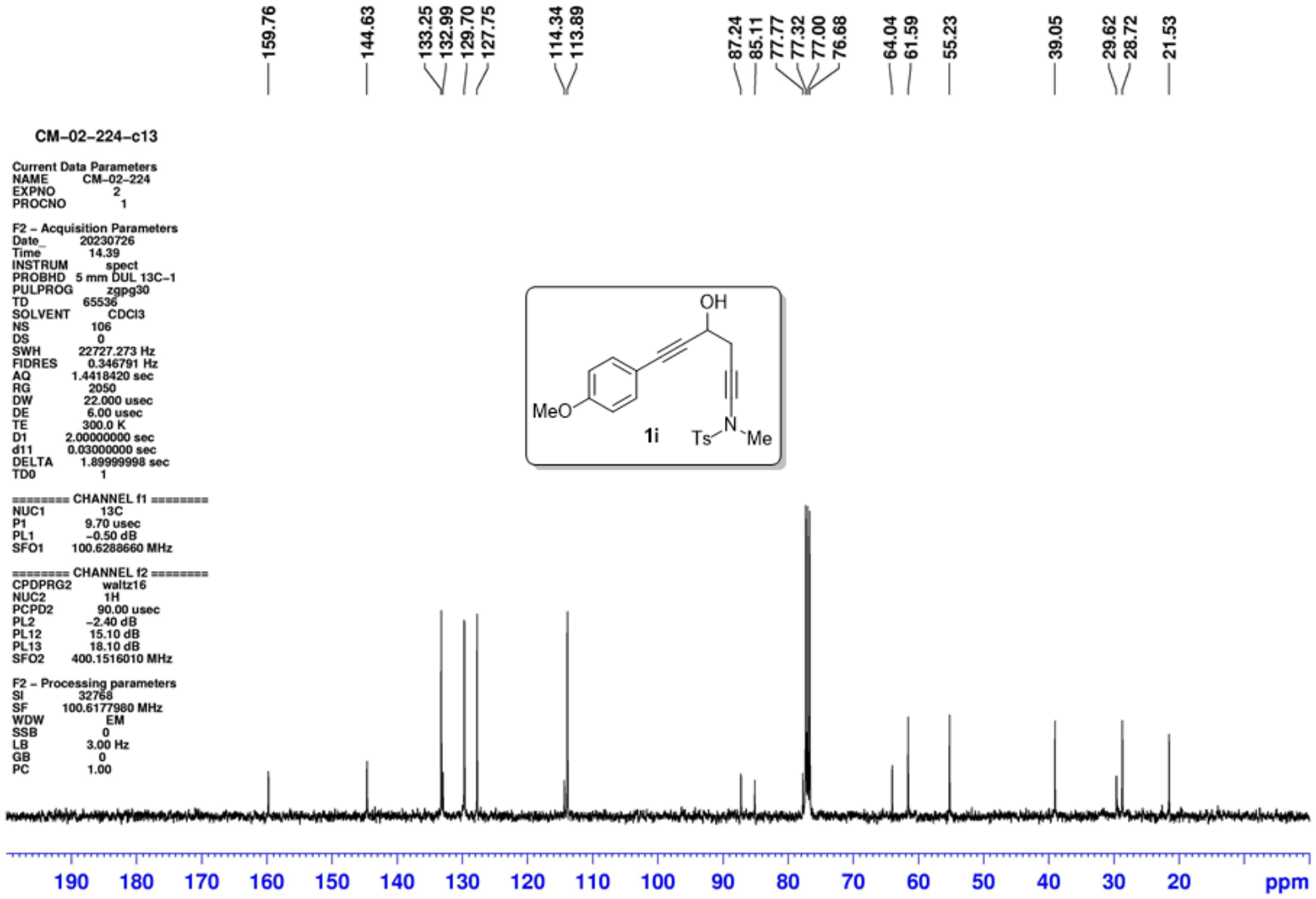
^{13}C NMR ($CDCl_3$, 100 MHz)



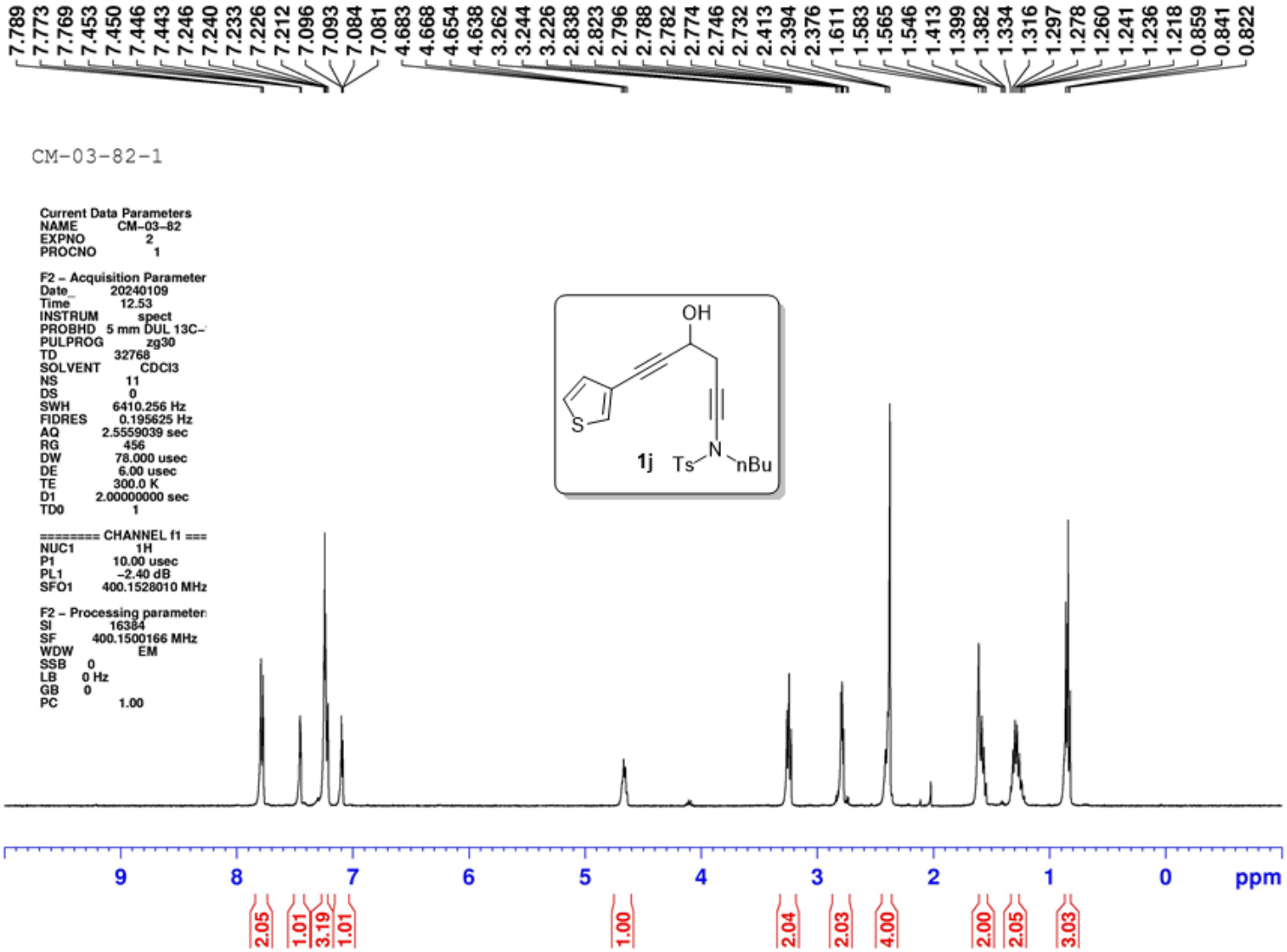
^{1}H NMR ($CDCl_3$, 400 MHz)



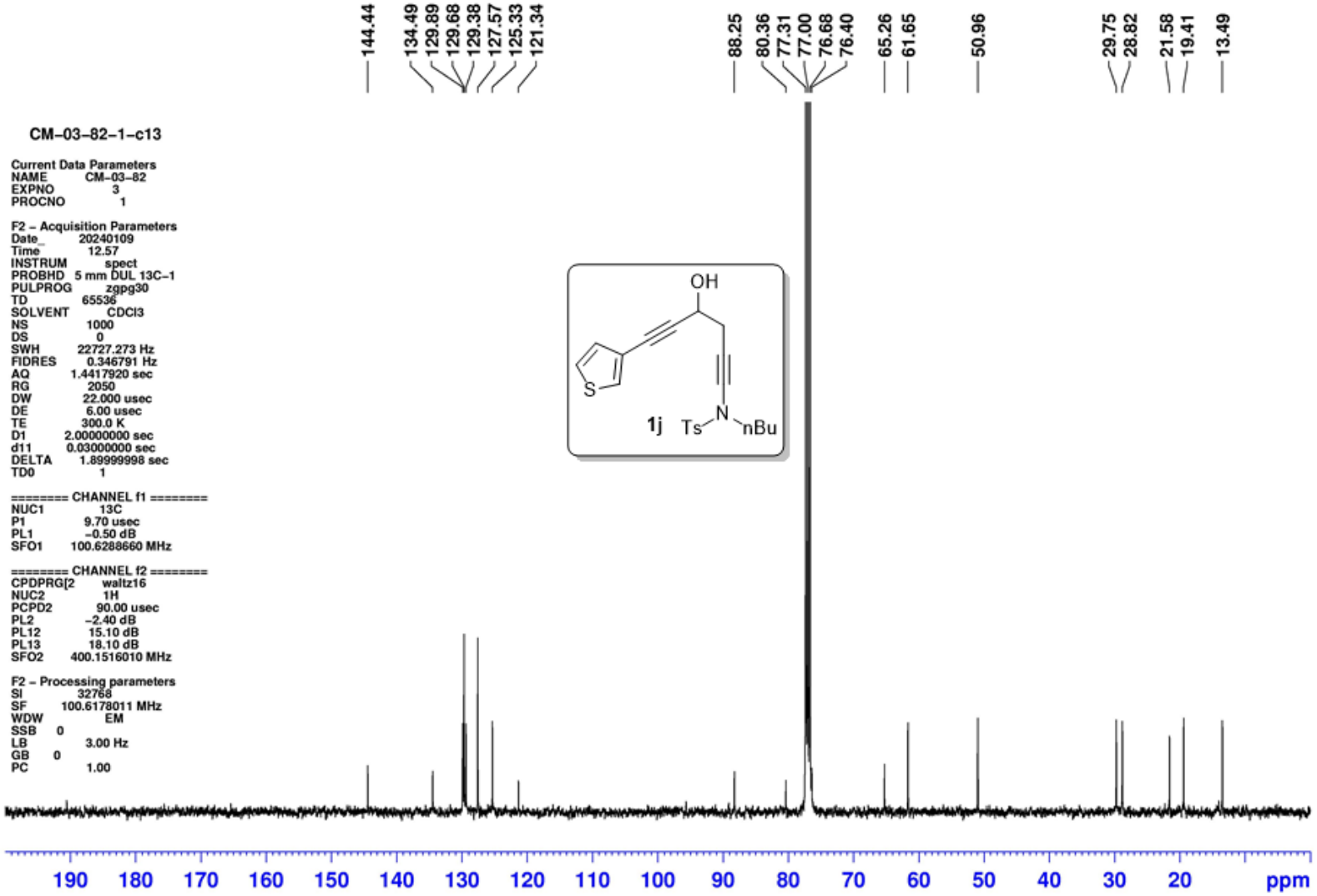
^{13}C NMR ($CDCl_3$, 100 MHz)



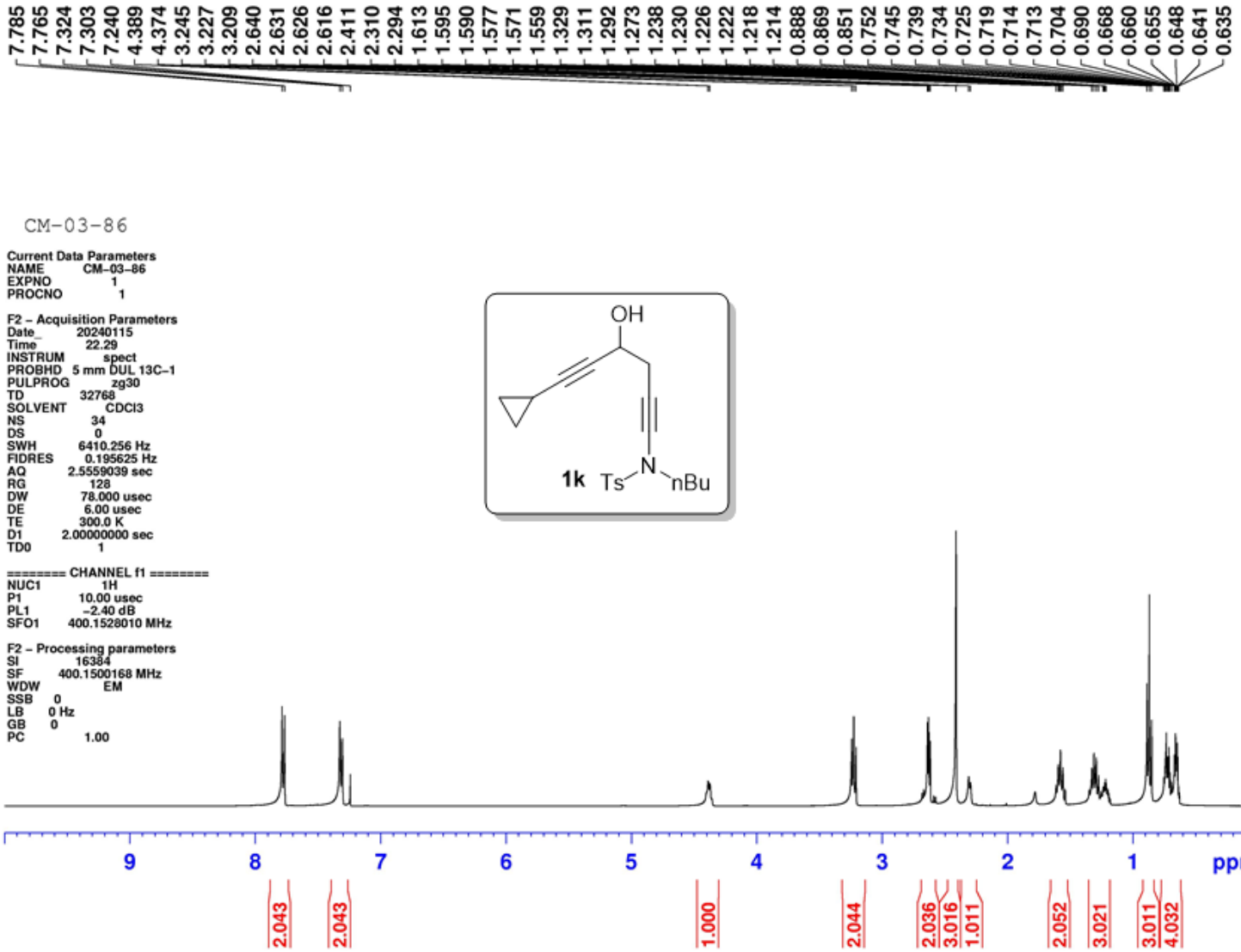
^{1}H NMR ($CDCl_3$, 400 MHz)



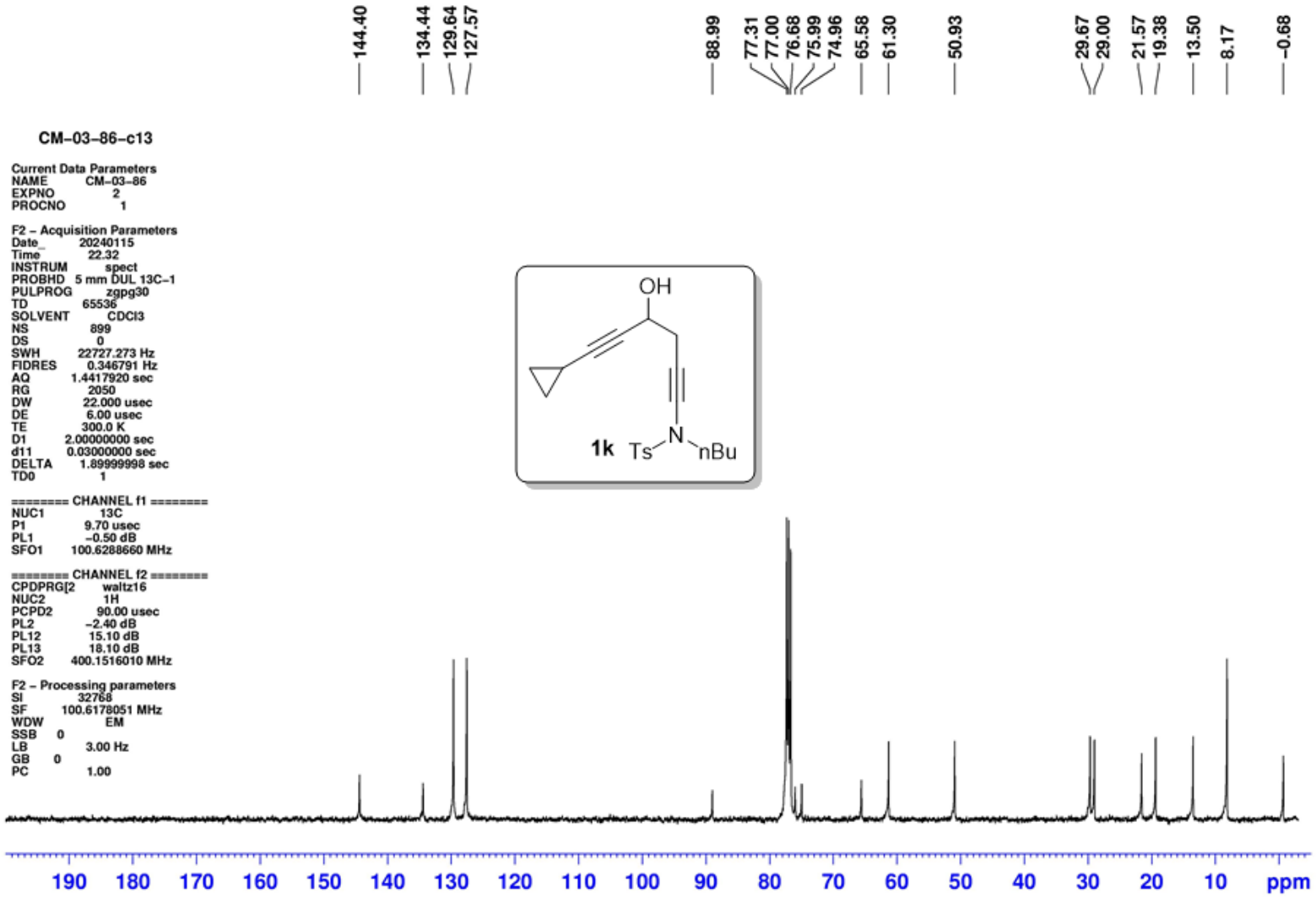
^{13}C NMR ($CDCl_3$, 100 MHz)



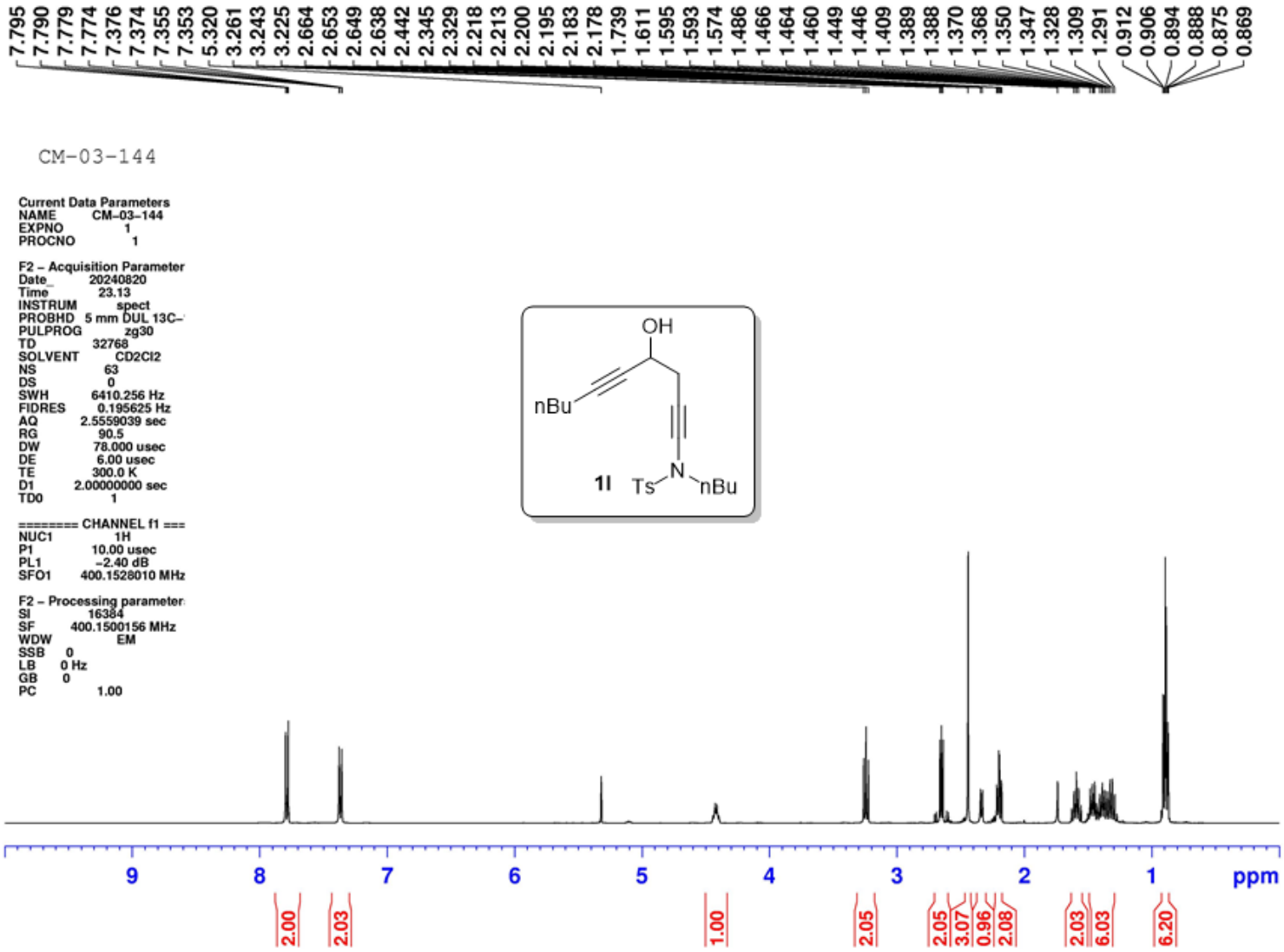
^{1}H NMR ($CDCl_3$, 400 MHz)



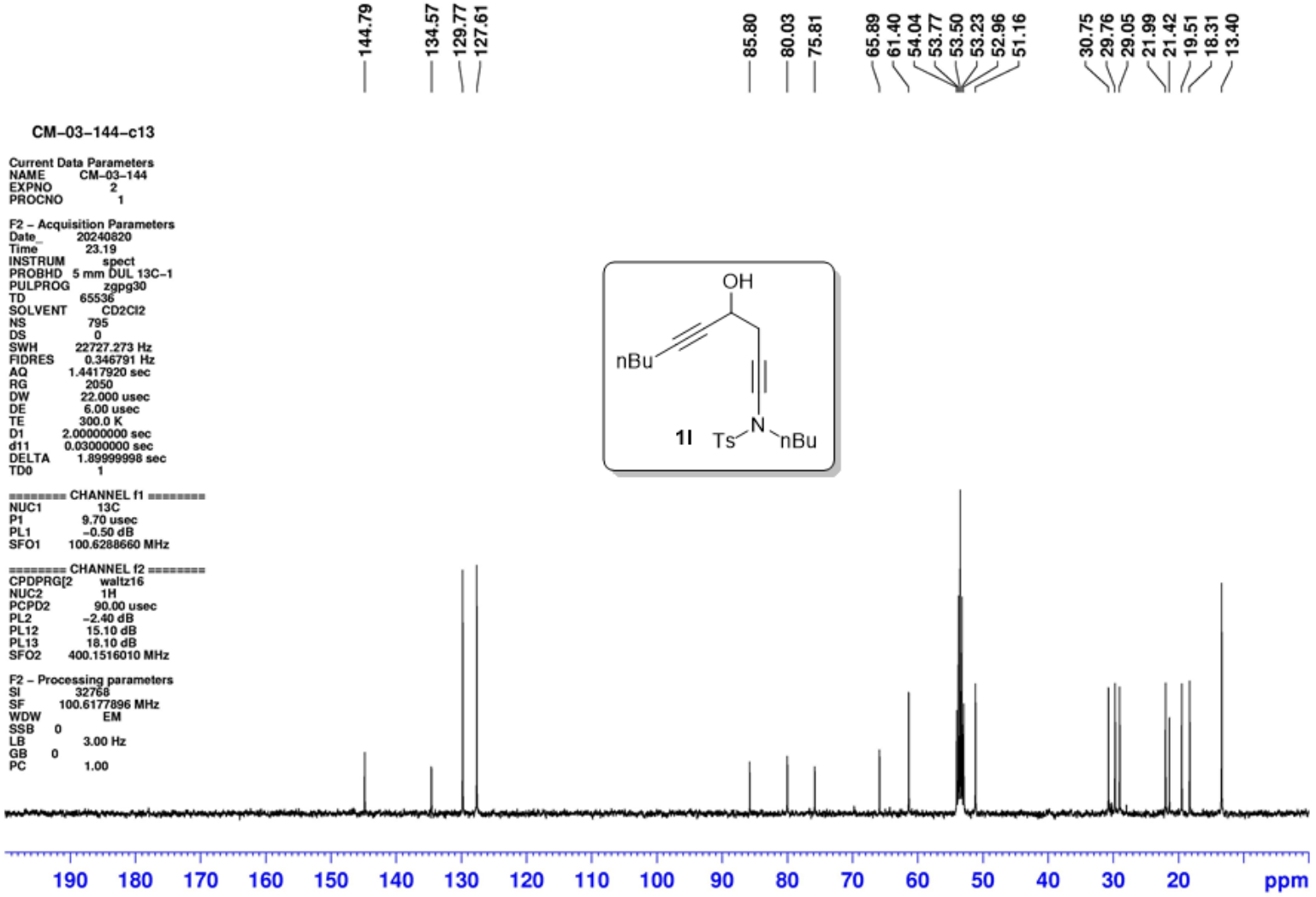
^{13}C NMR ($CDCl_3$, 100 MHz)



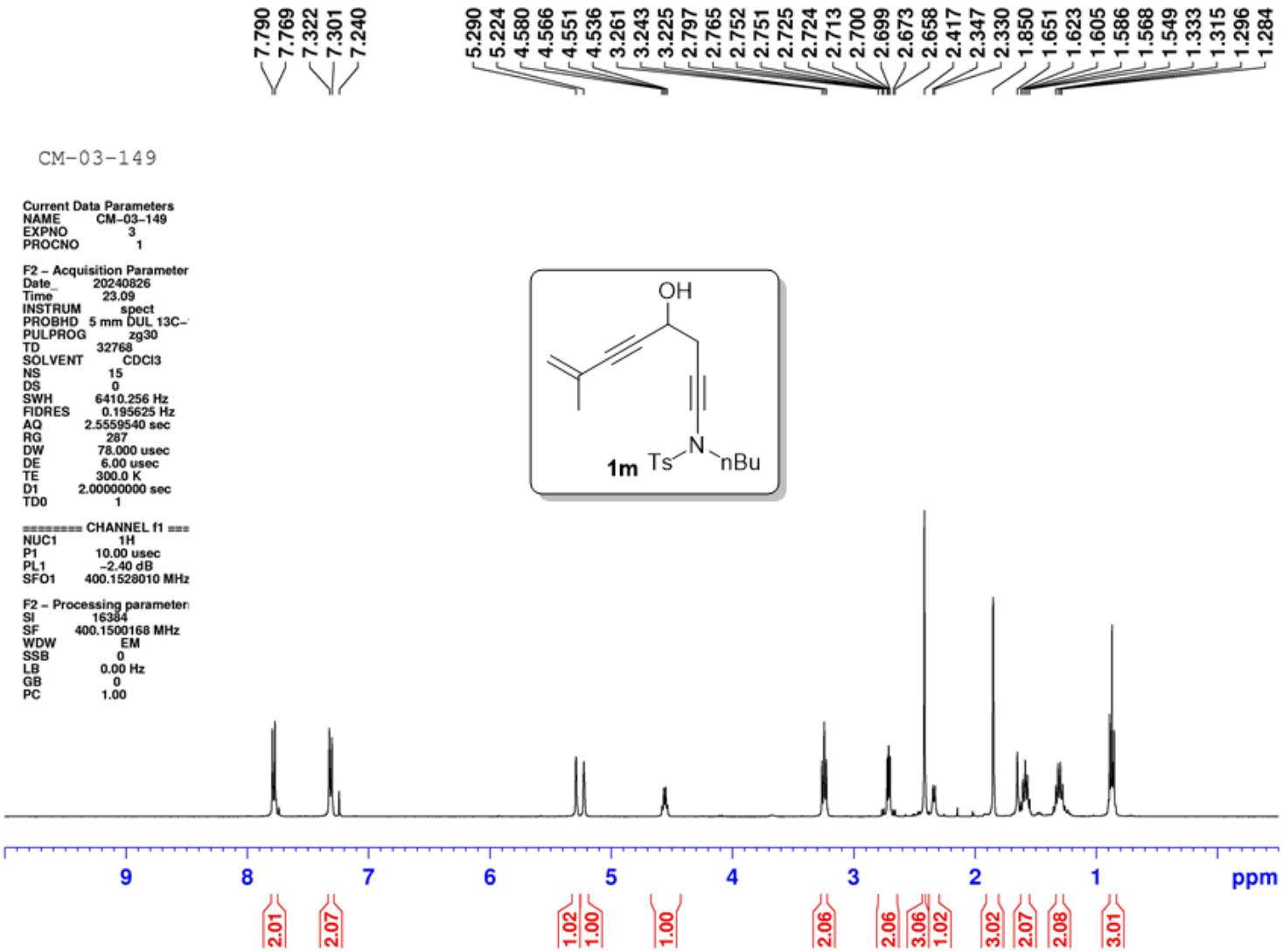
^{1}H NMR (CD_2Cl_2, 400 MHz)



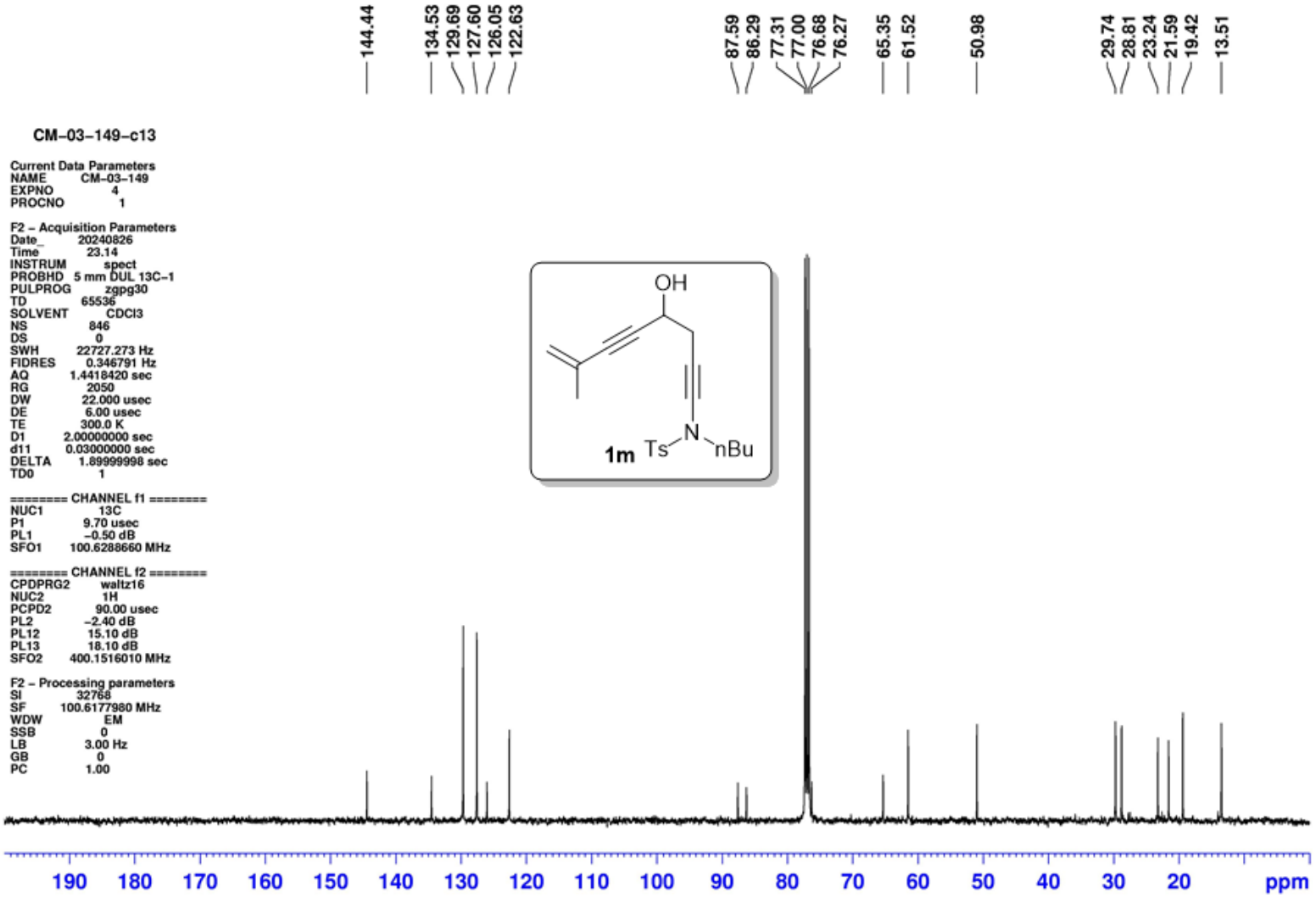
^{13}C NMR (CD_2Cl_2, 100 MHz)



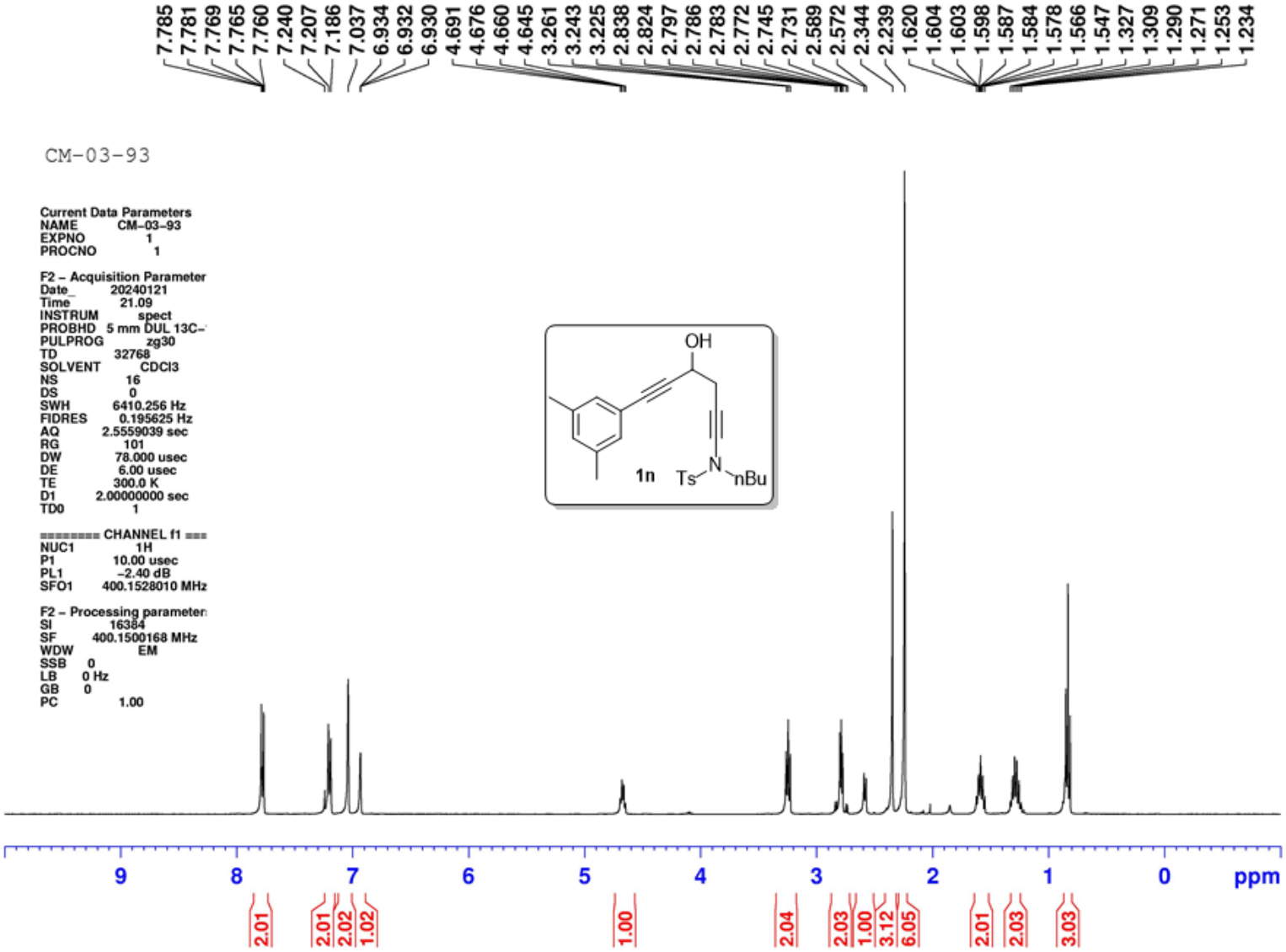
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



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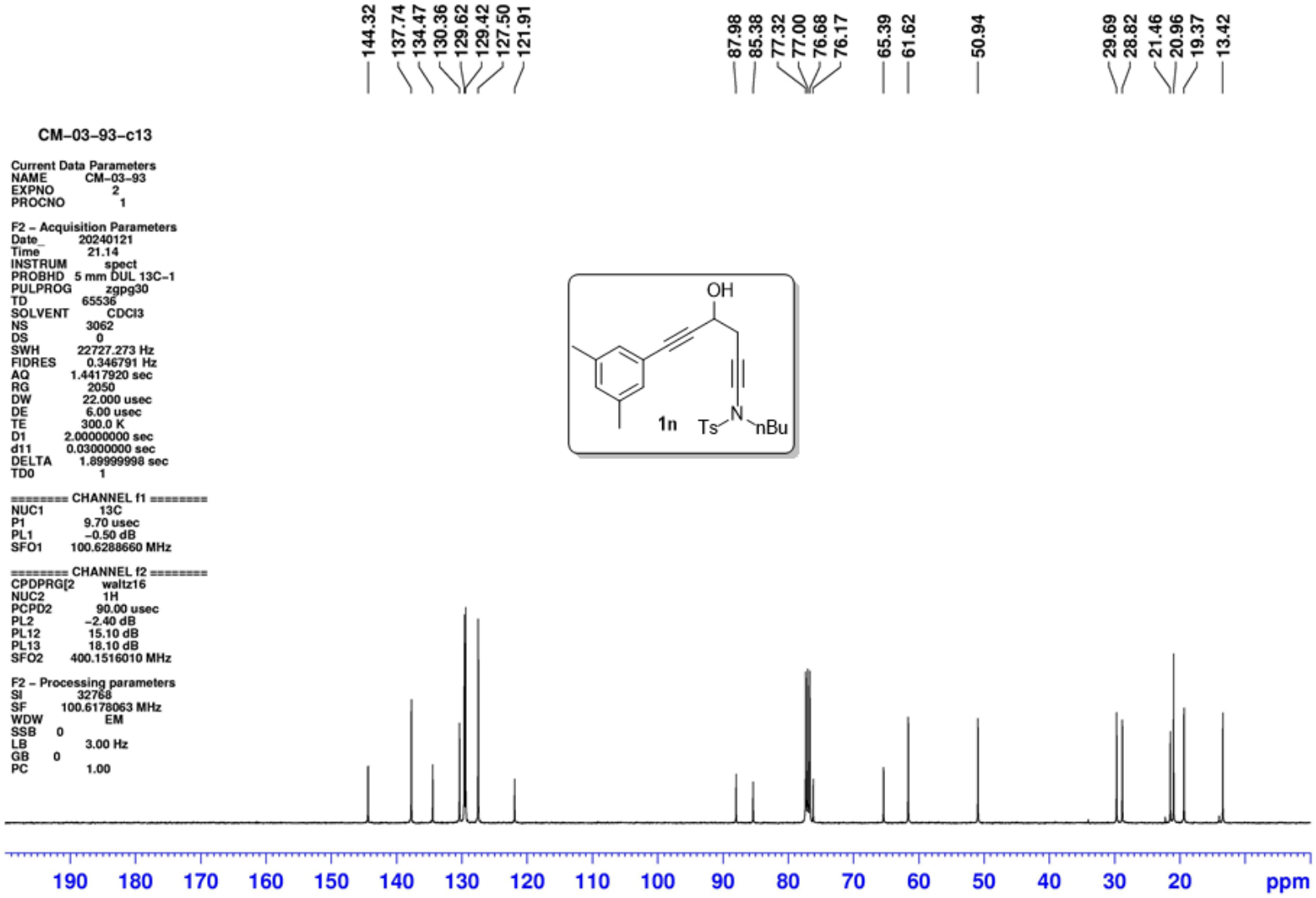
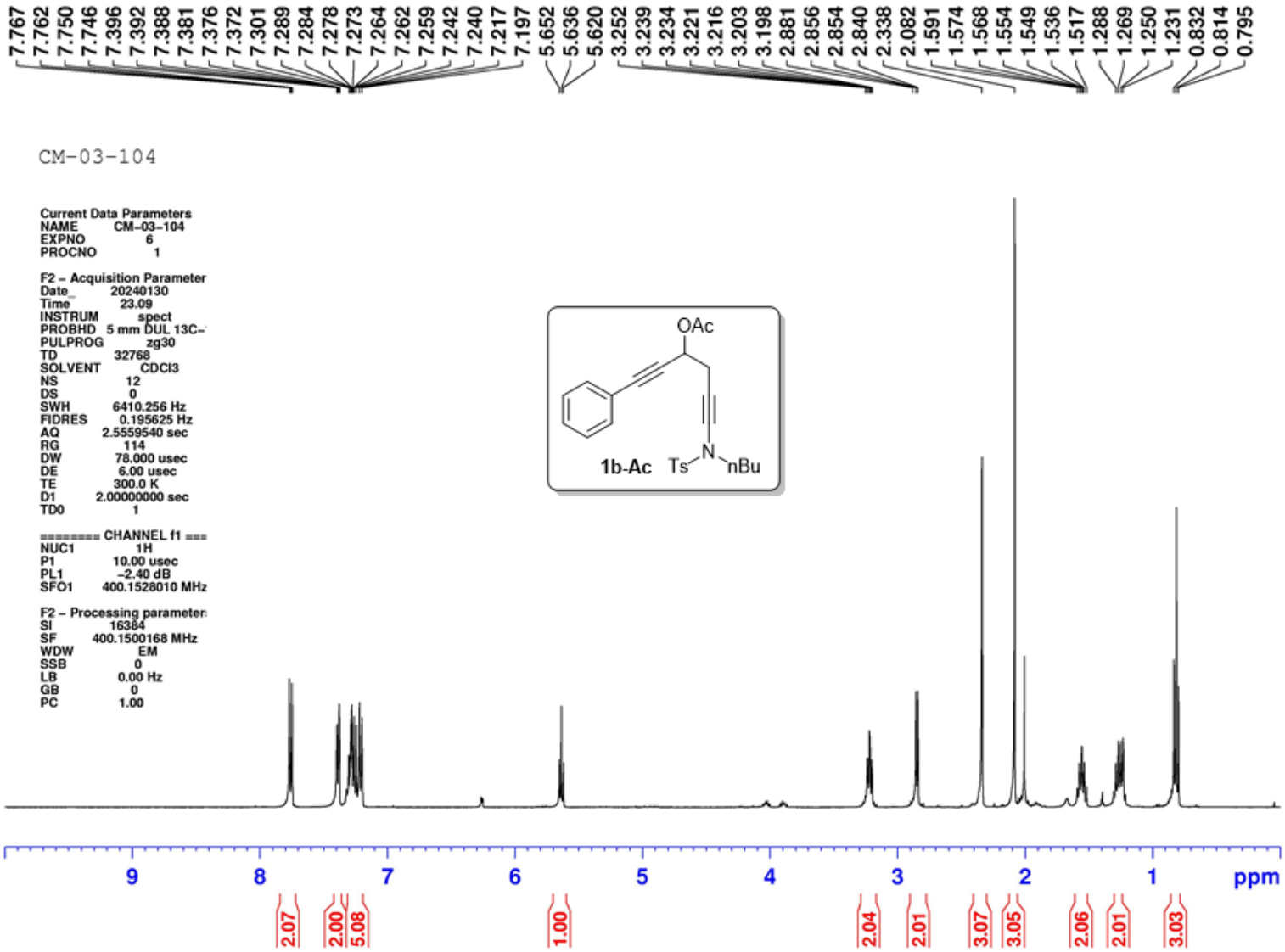


^{1}H NMR ($CDCl_3$, 400 MHz)



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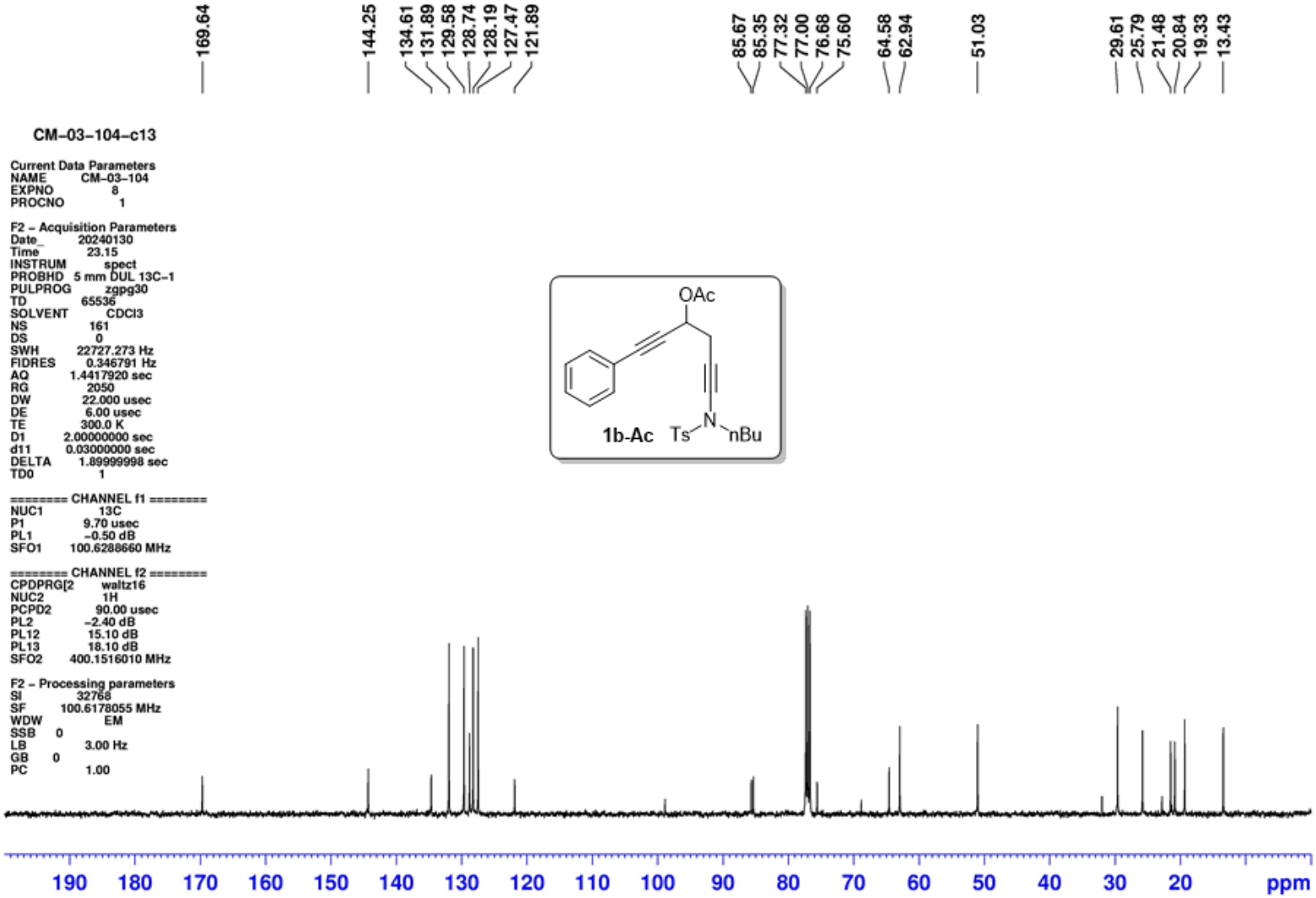
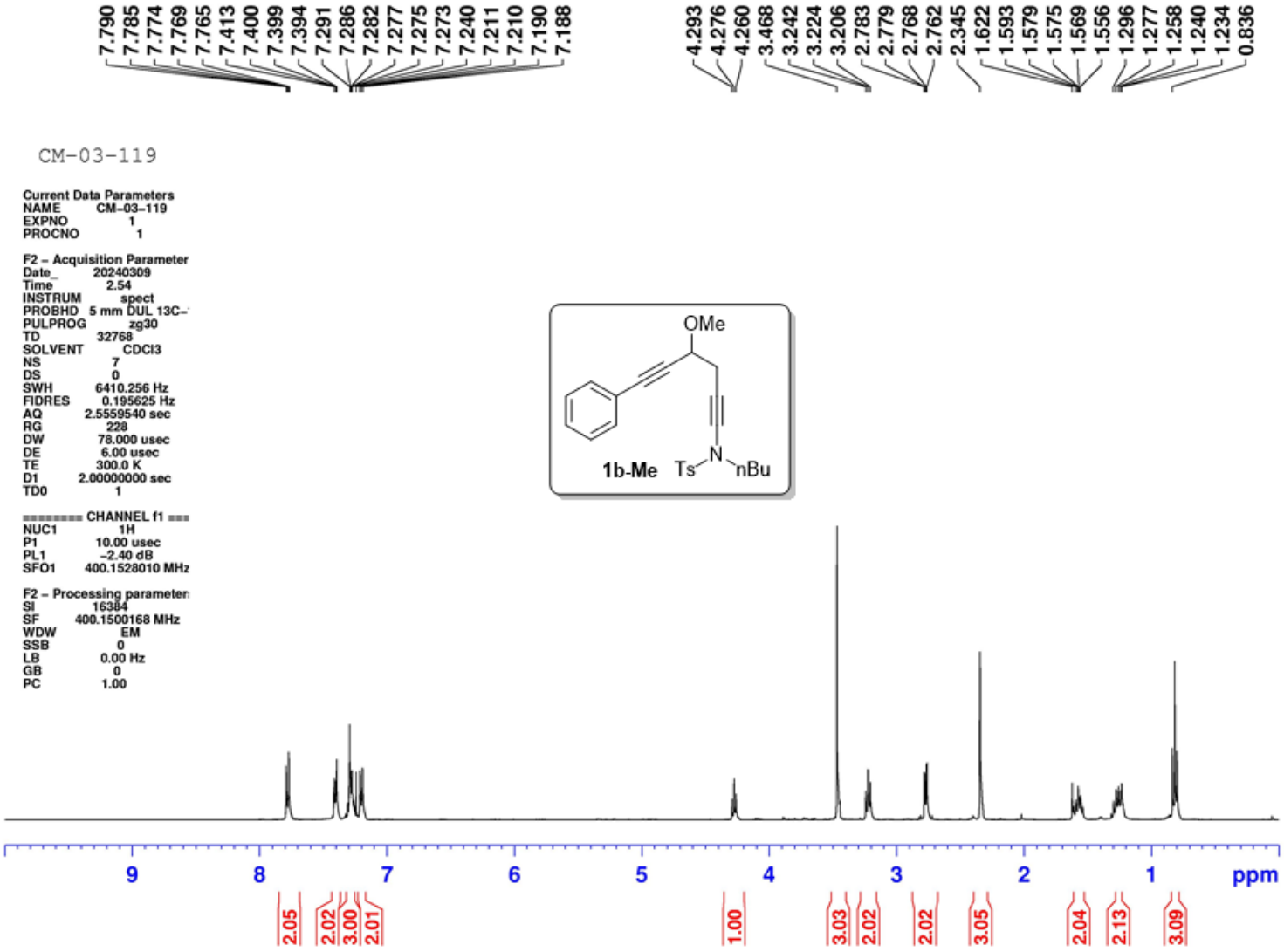
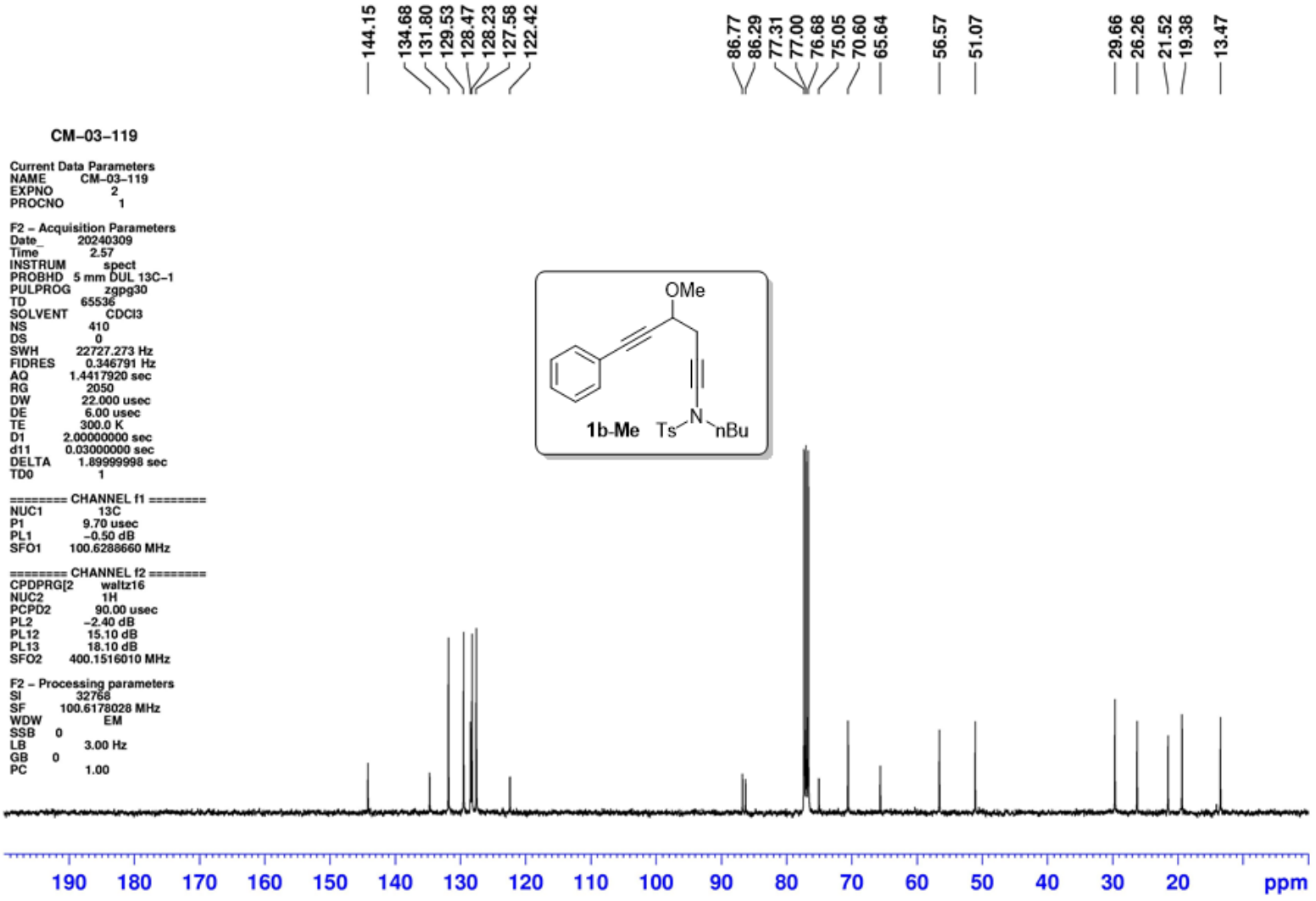


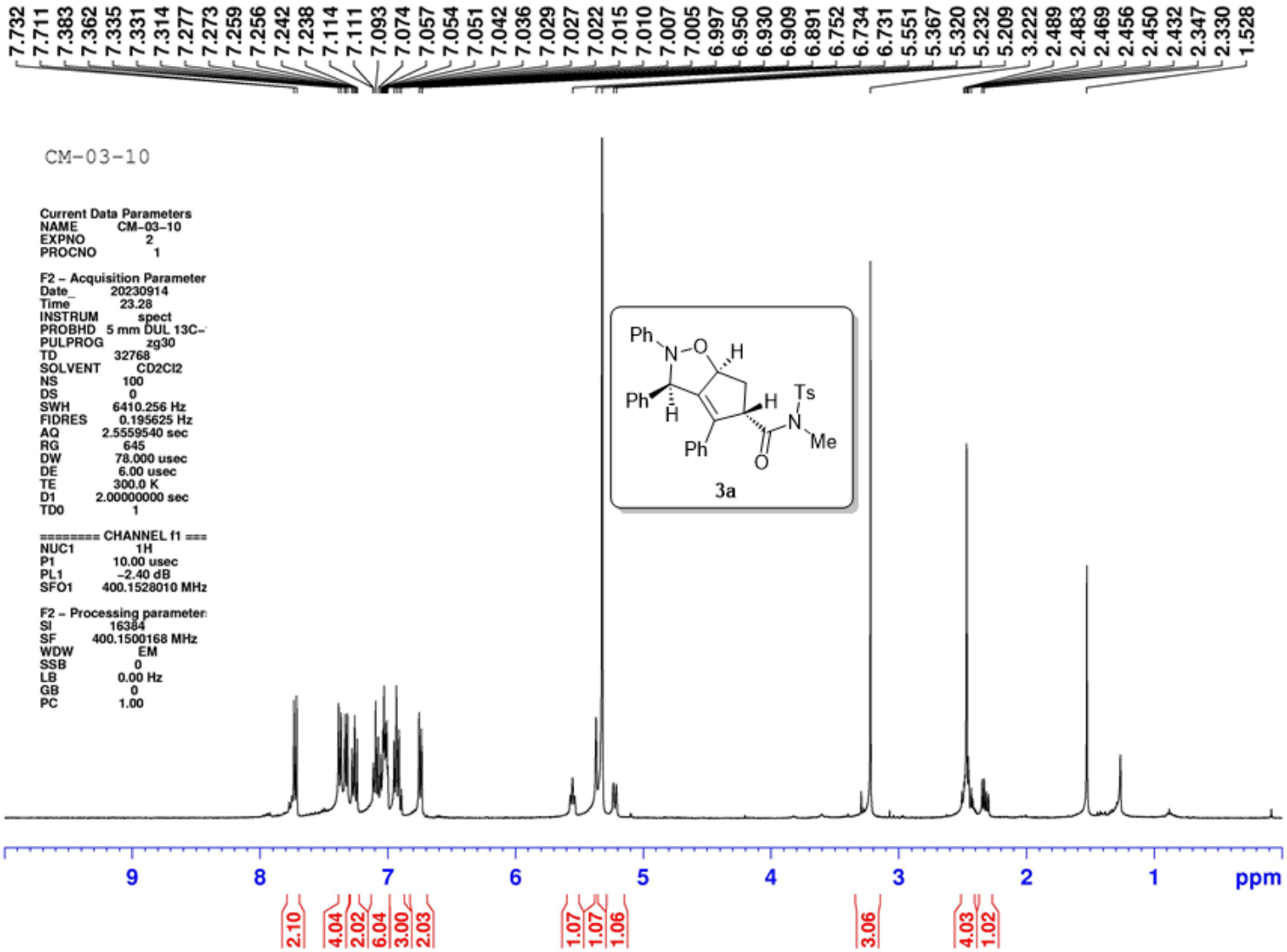
^{1}H NMR ($CDCl_3$, 400 MHz)



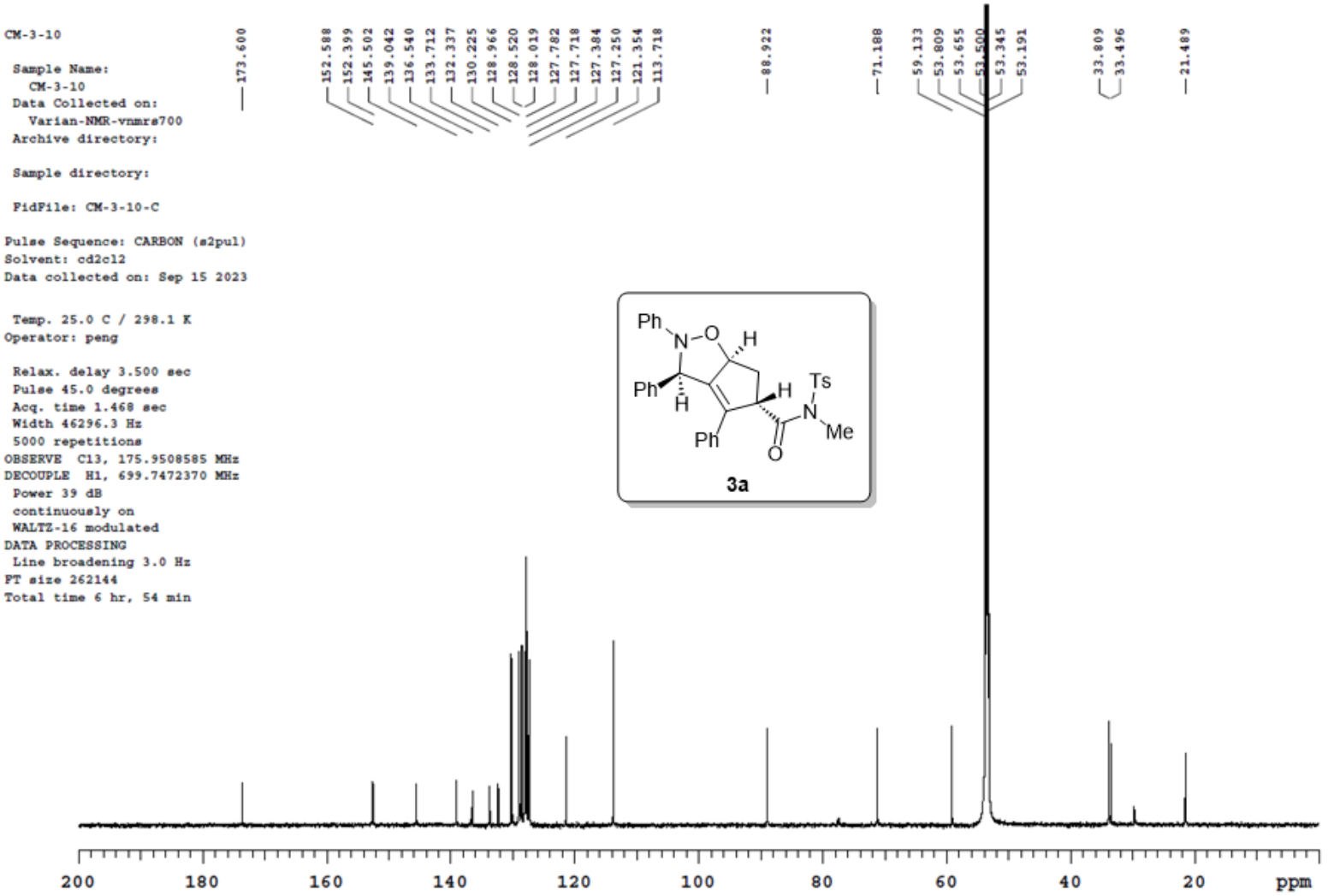
^{13}C NMR ($CDCl_3$, 100 MHz)



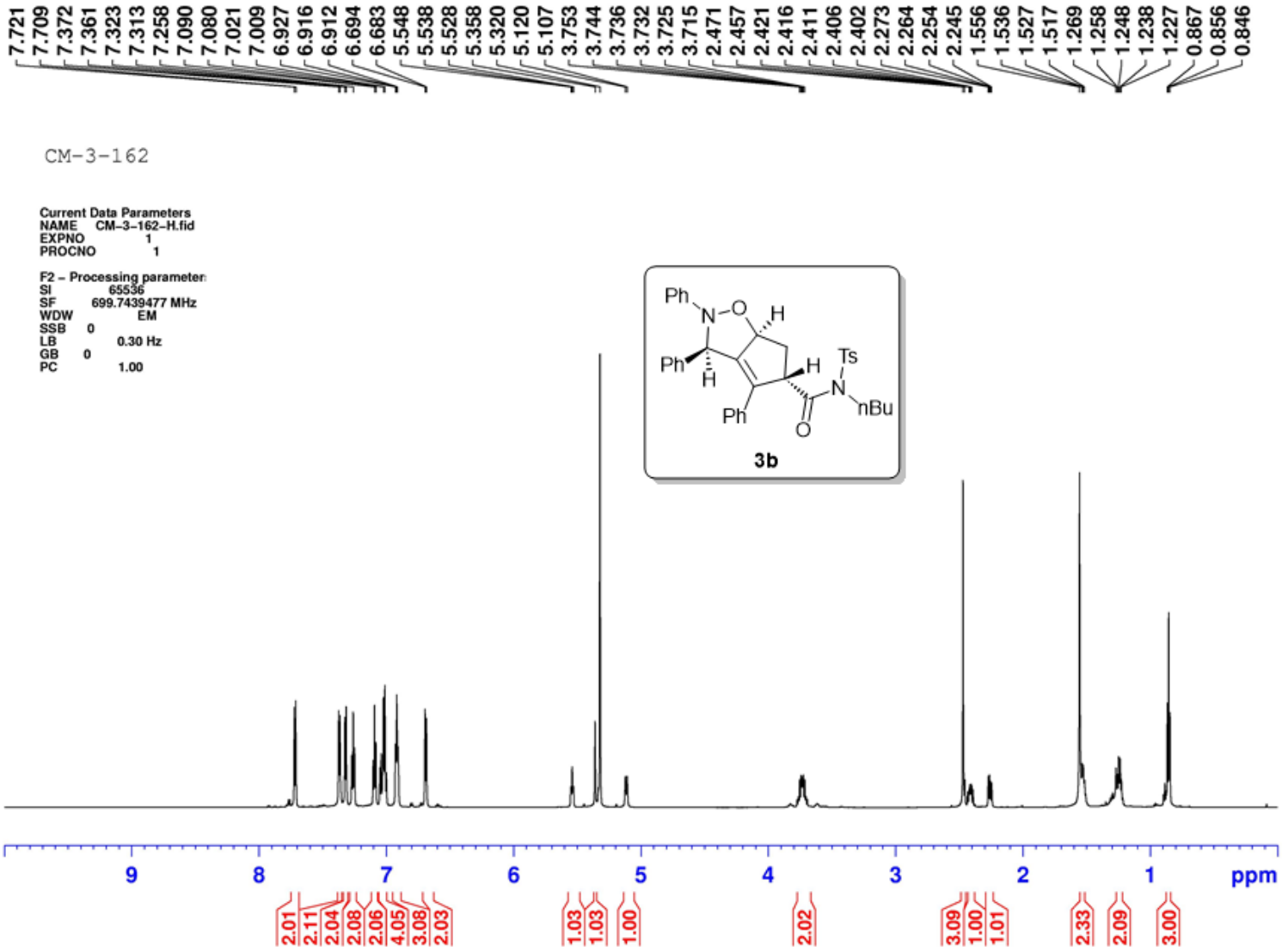
^{1}H NMR (CD_2Cl_2, 400 MHz)



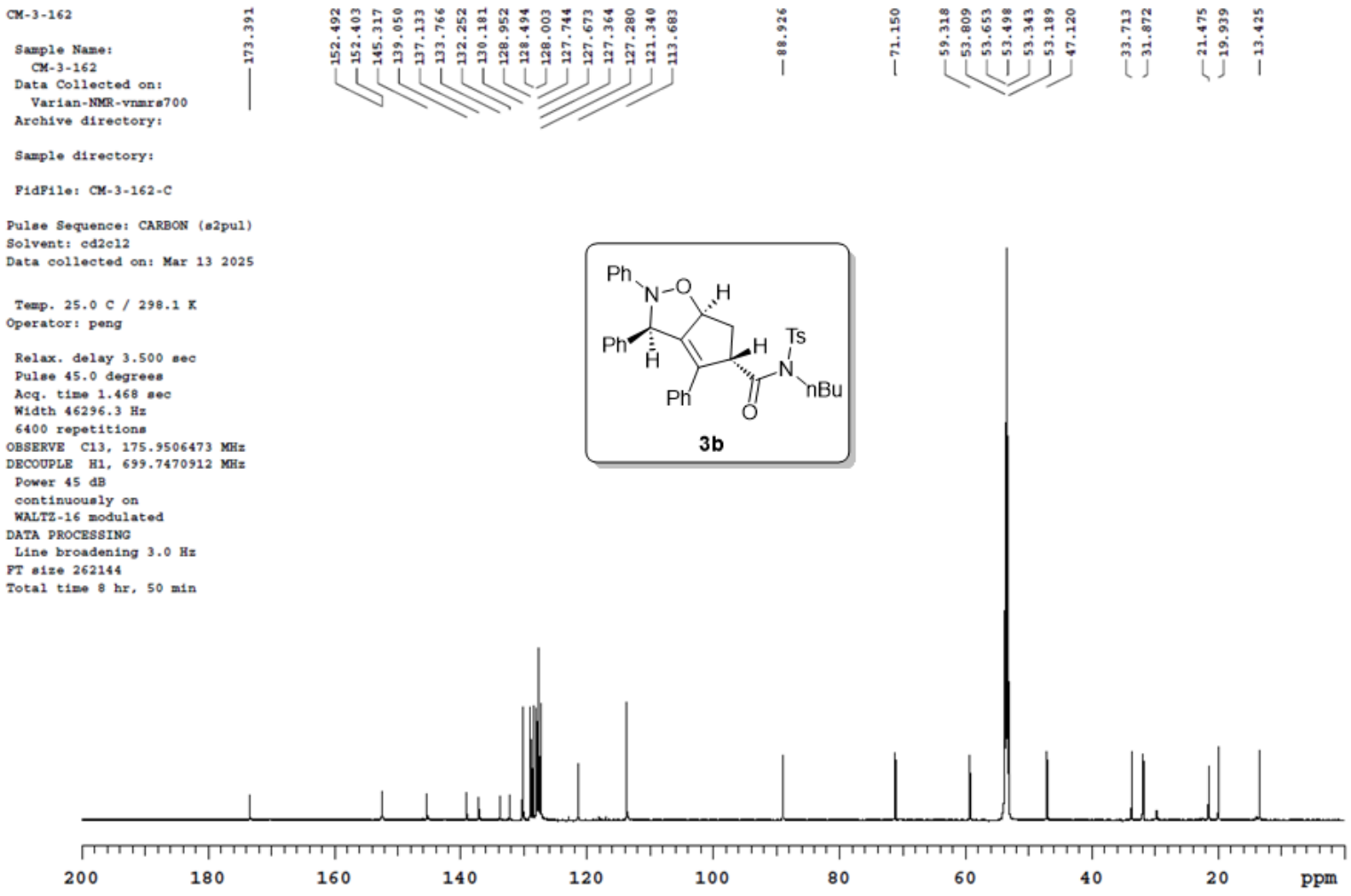
^{13}C NMR (CD_2Cl_2, 175 MHz)



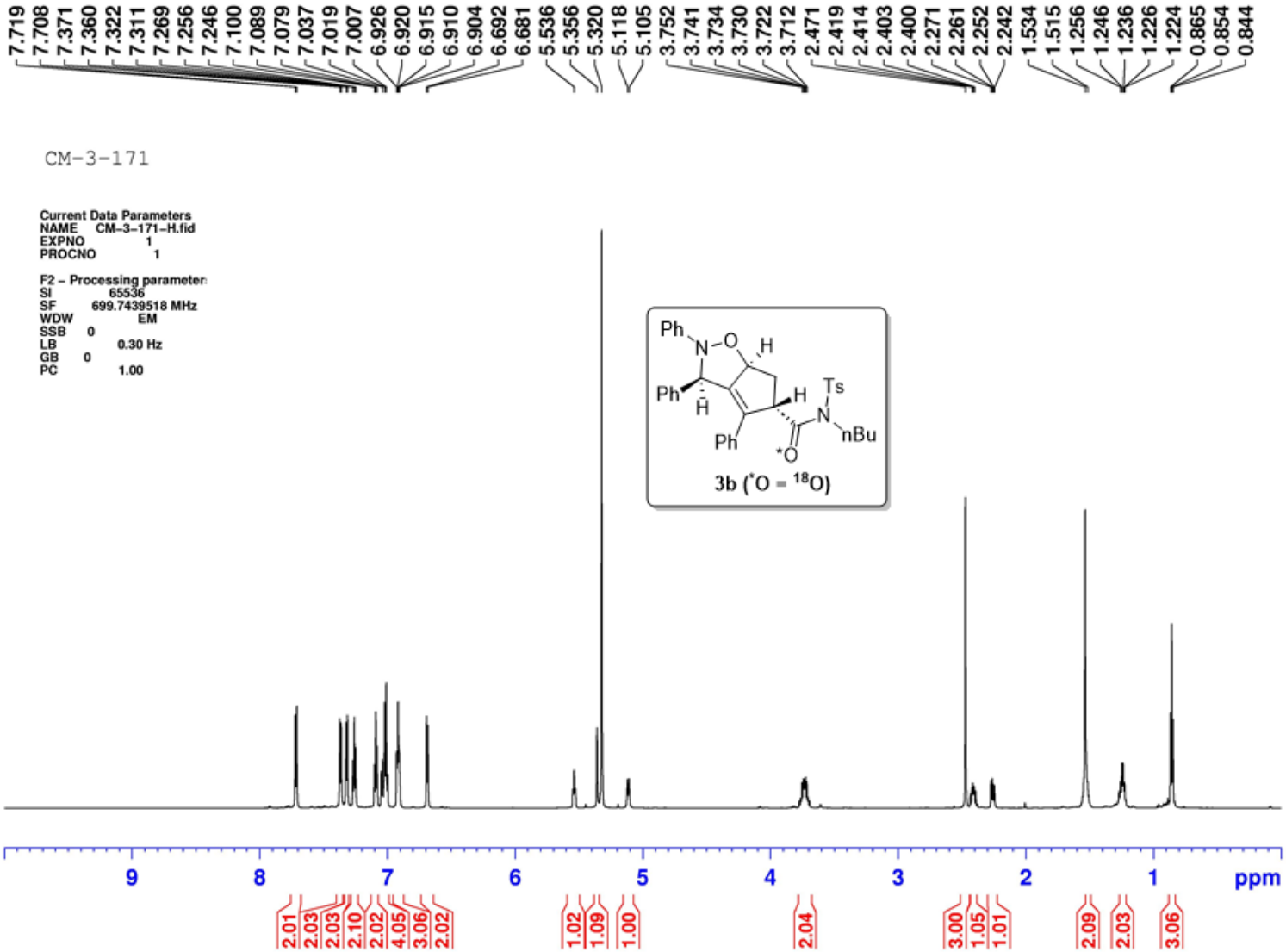
^{1}H NMR (CD_2Cl_2, 700 MHz)



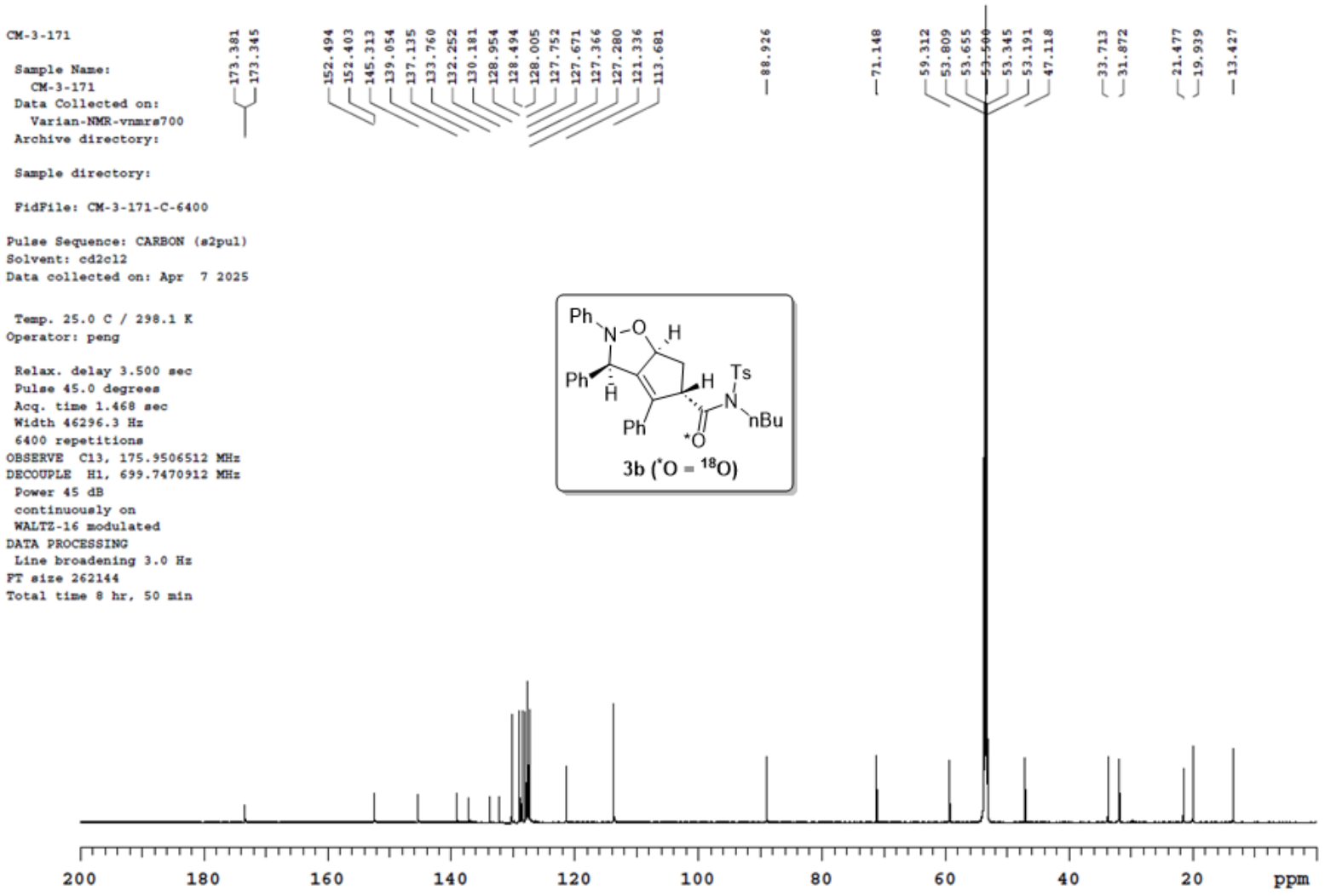
^{13}H NMR (CD_2Cl_2, 175 MHz)



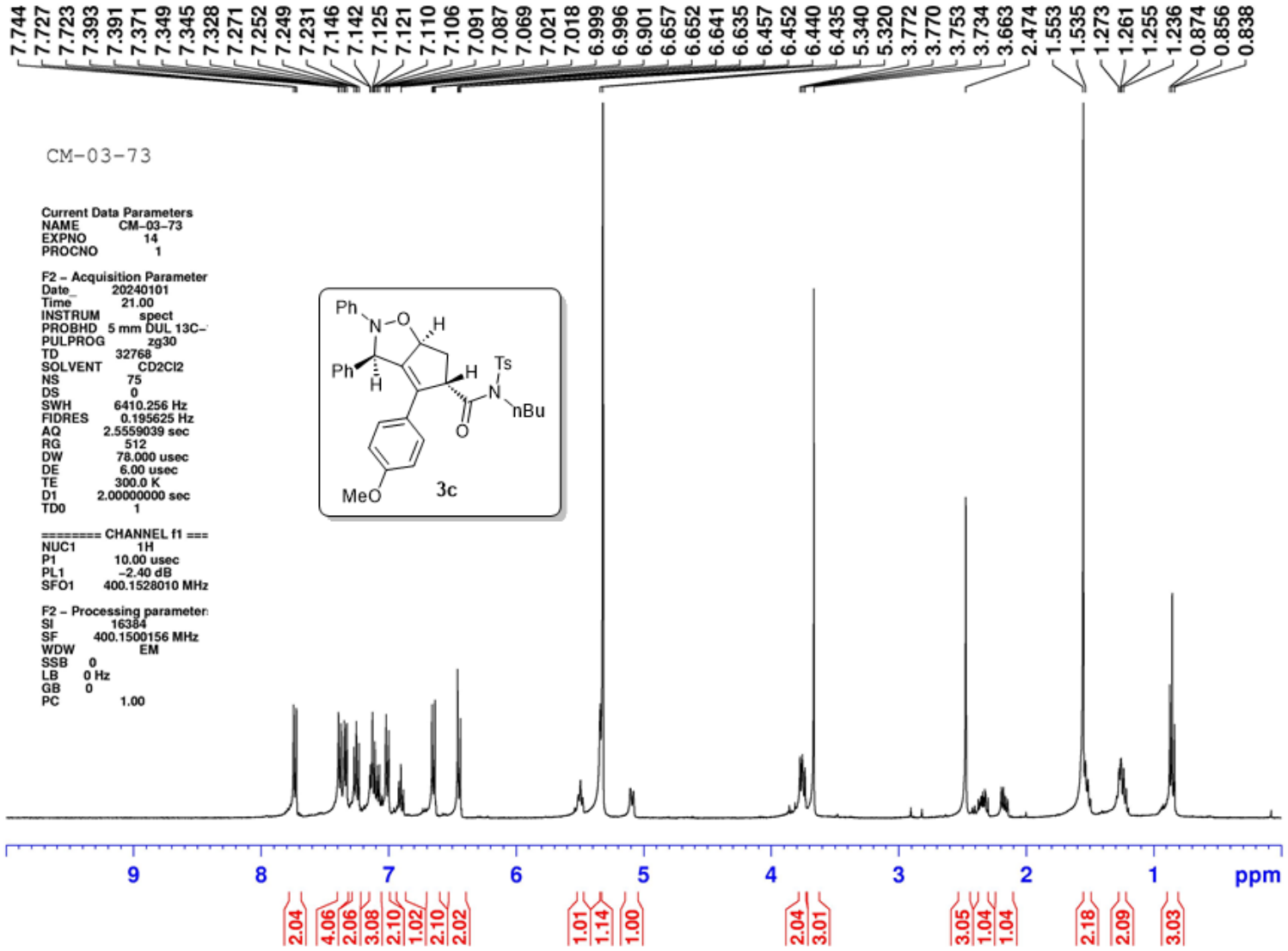
^{1}H NMR (CD_2Cl_2, 700 MHz)



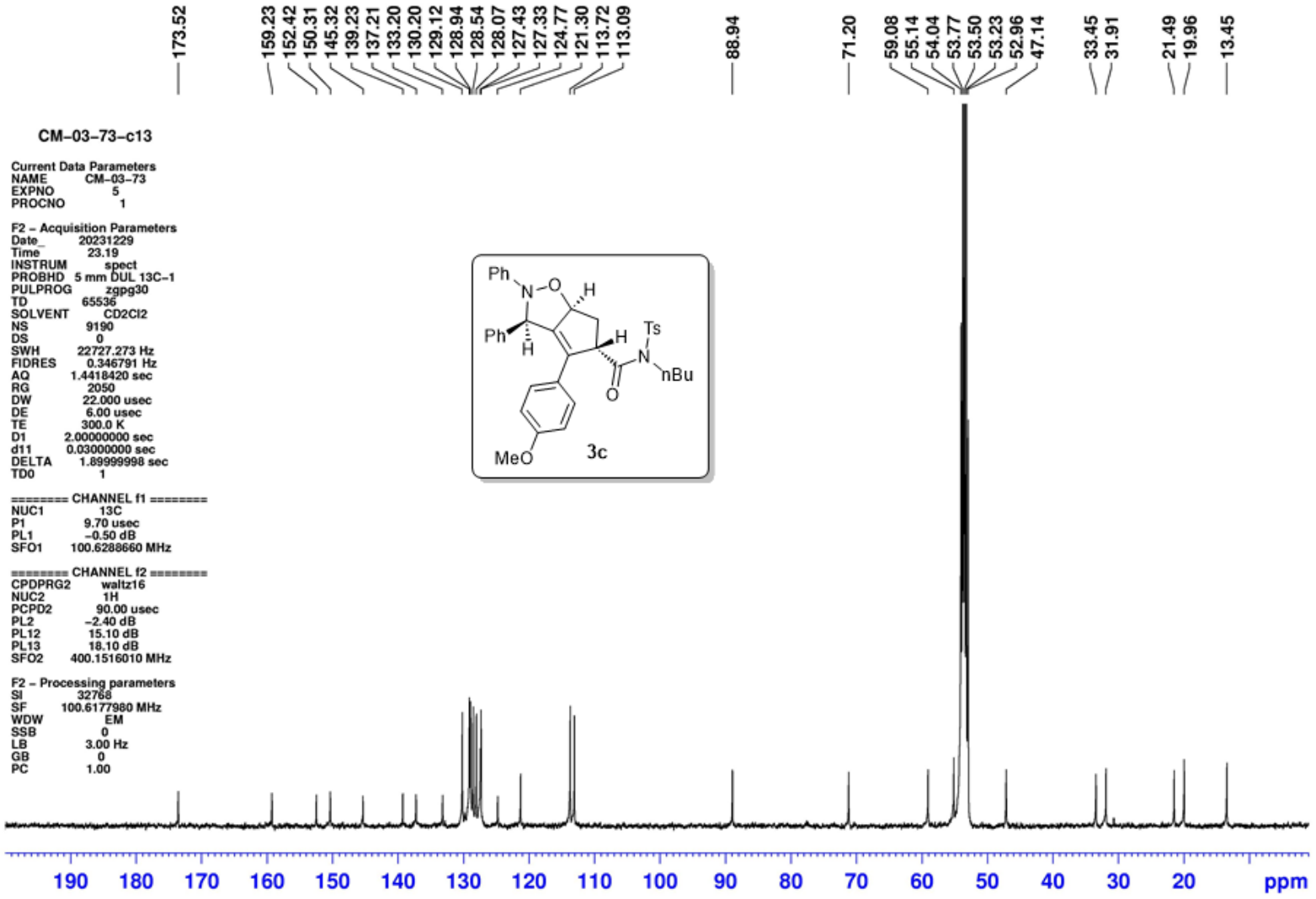
^{13}H NMR (CD_2Cl_2, 175 MHz)



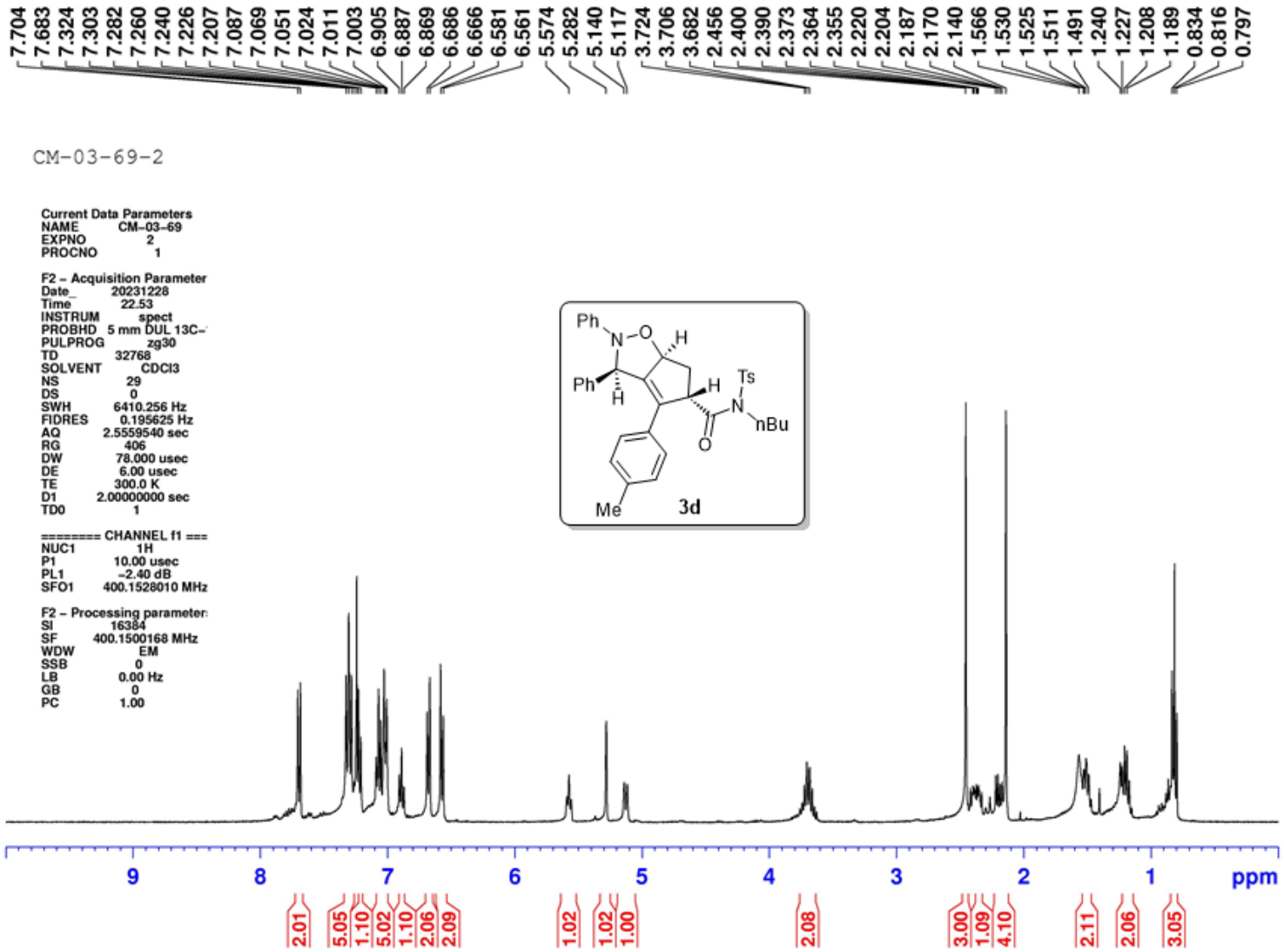
^{1}H NMR (CD_2Cl_2, 400 MHz)



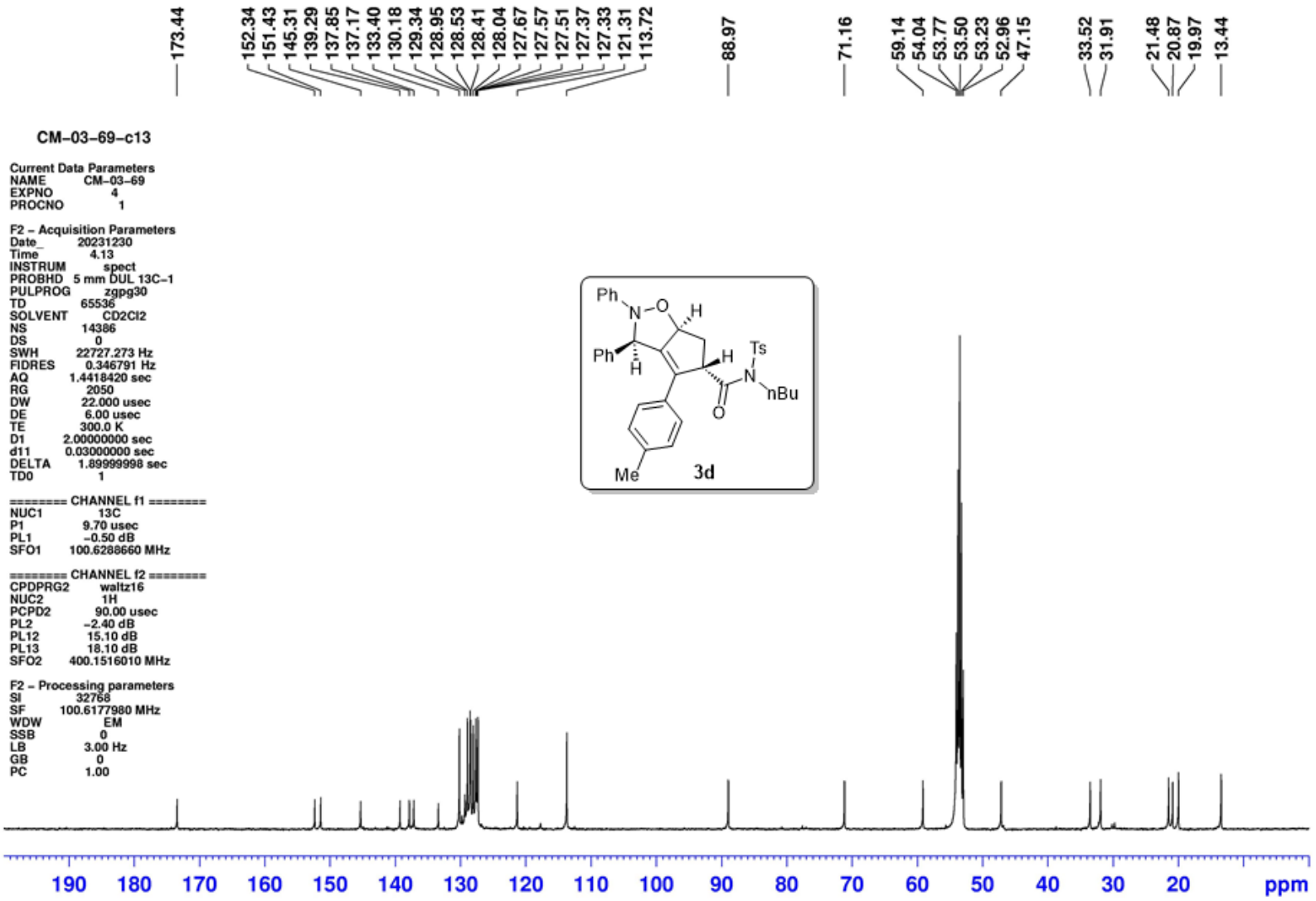
^{13}C NMR (CD_2Cl_2, 100 MHz)



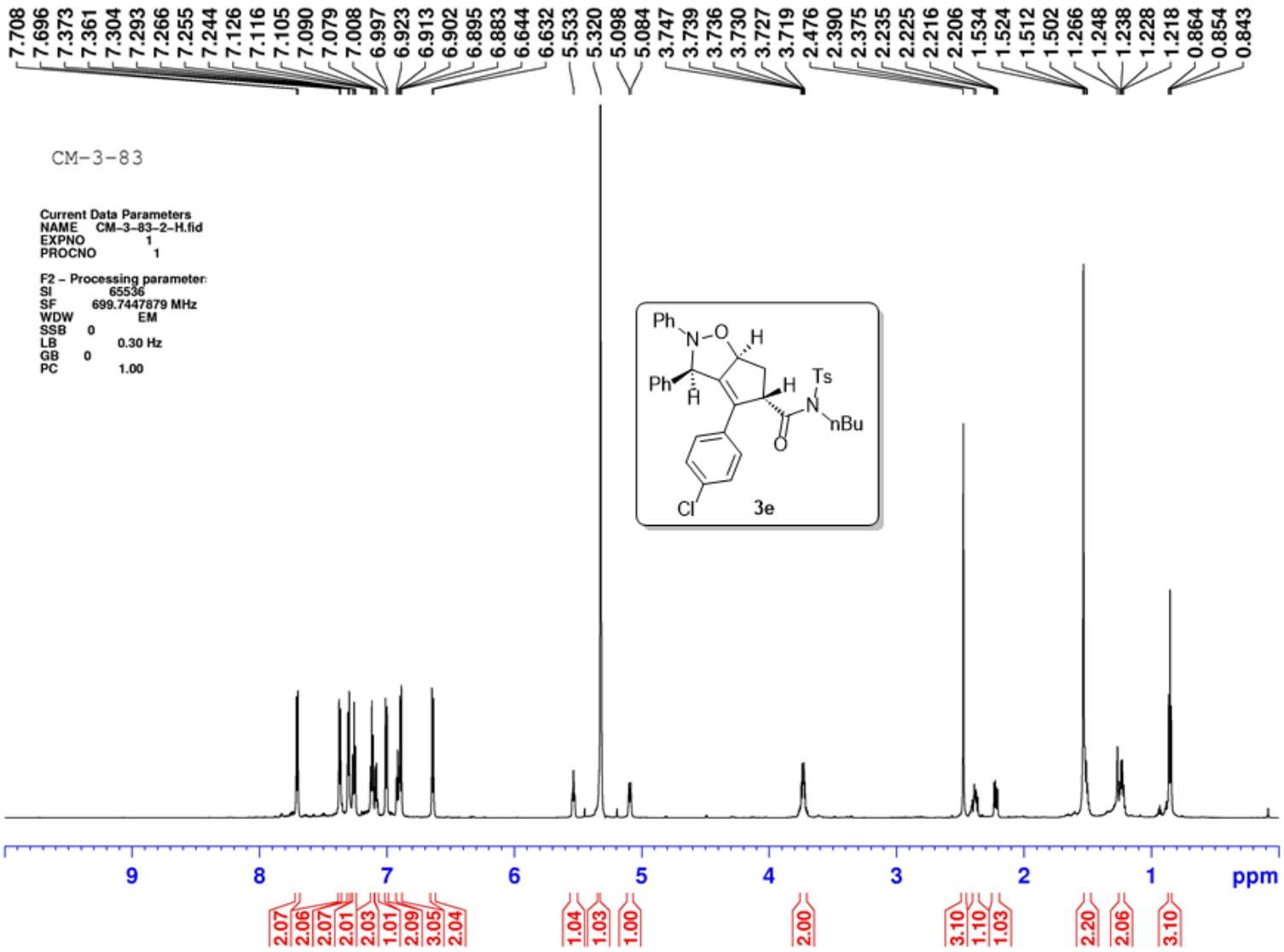
^{1}H NMR ($CDCl_3$, 400 MHz)



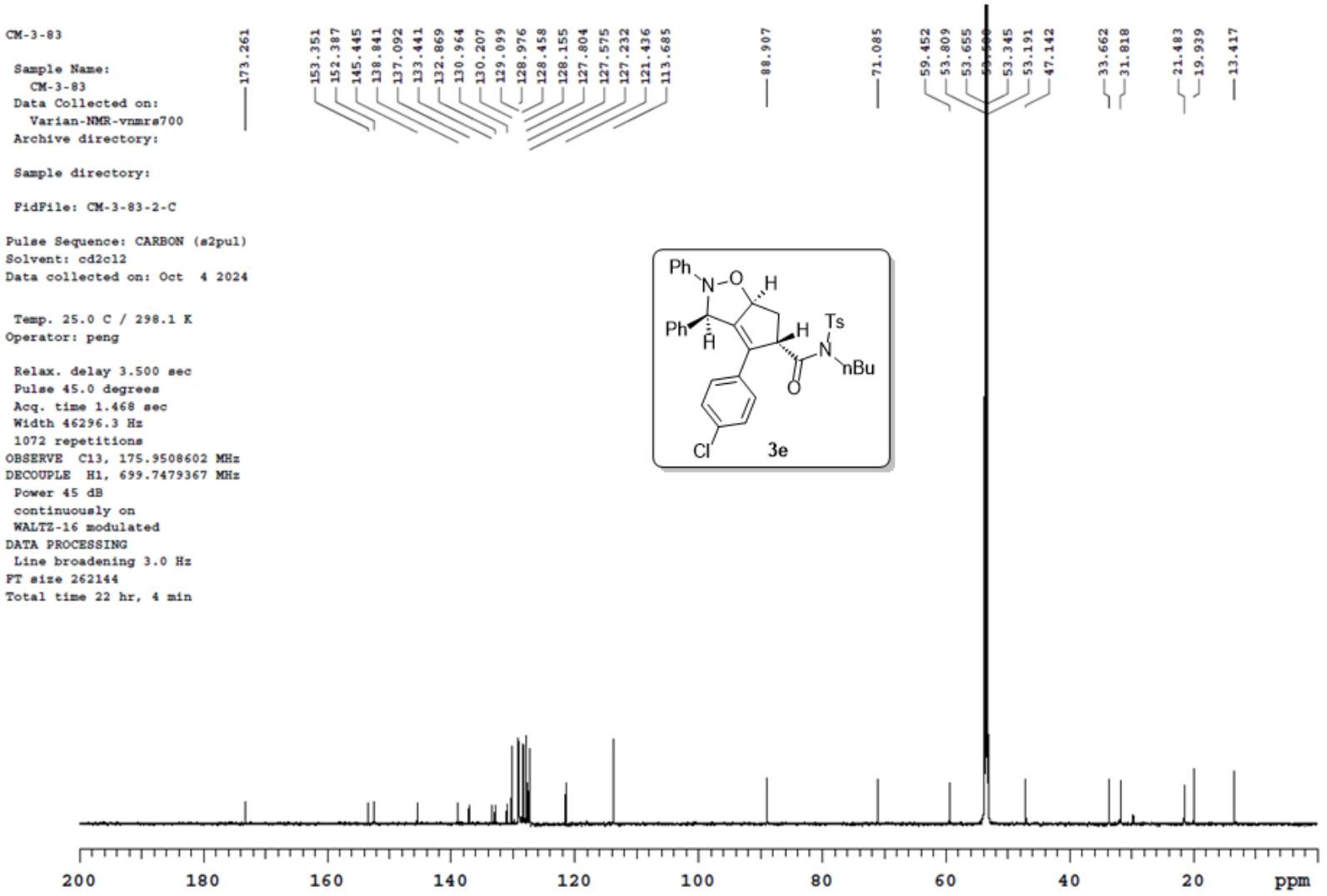
^{13}C NMR (CD_2Cl_2, 100 MHz)



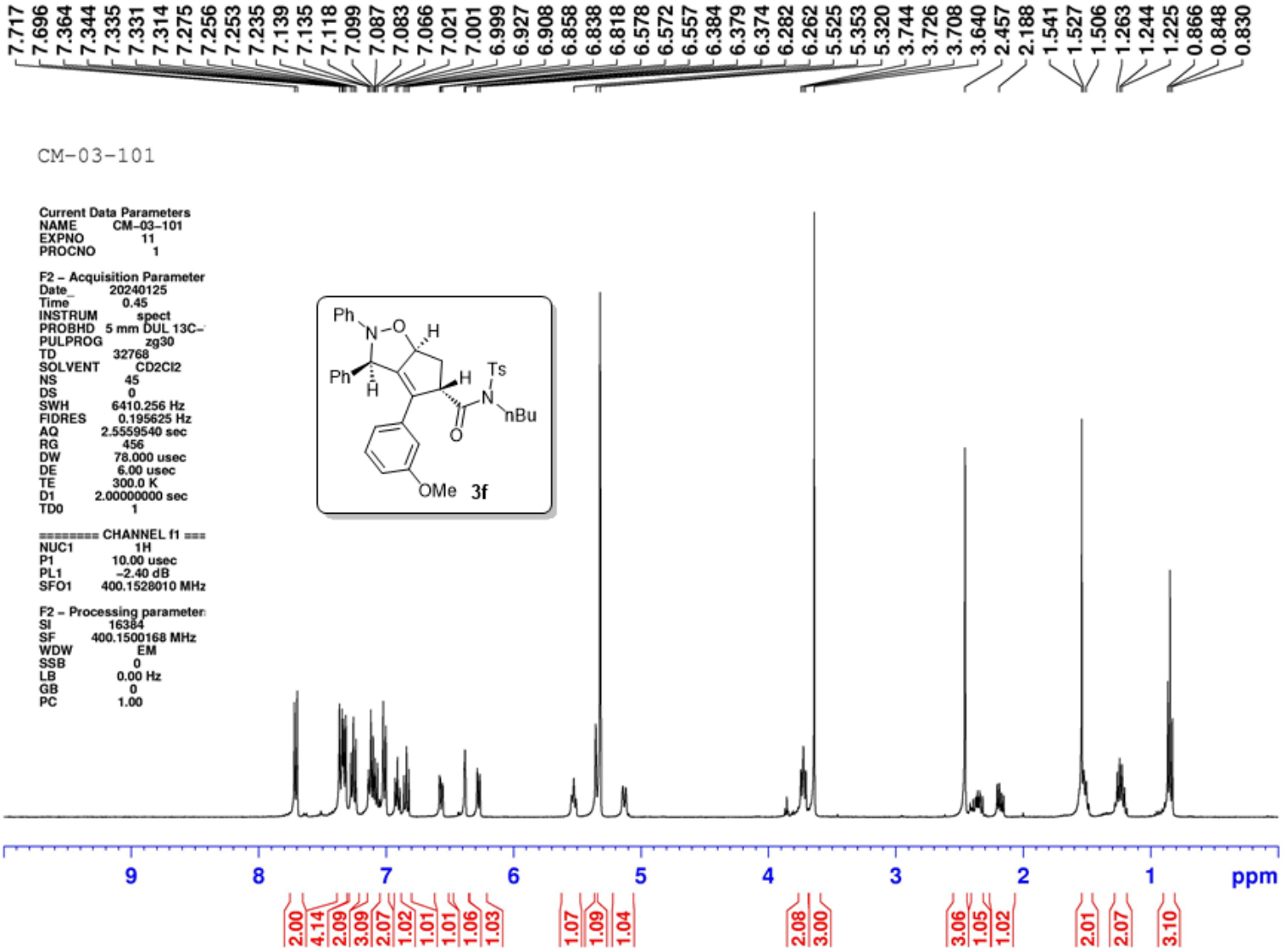
^{1}H NMR (CD_2Cl_2, 700 MHz)



^{13}C NMR (CD_2Cl_2, 175 MHz)



^{1}H NMR (CD_2Cl_2, 400 MHz)



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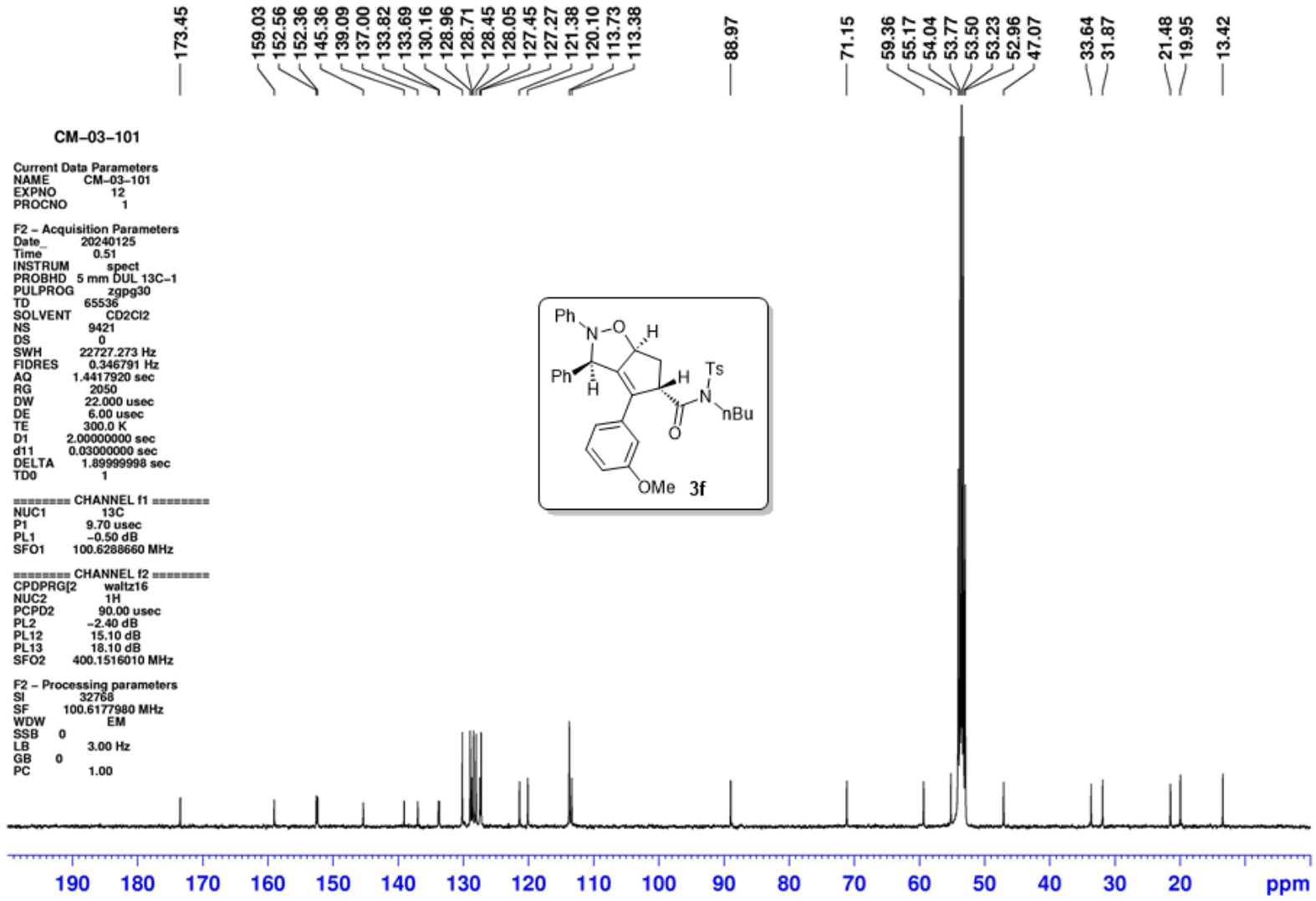

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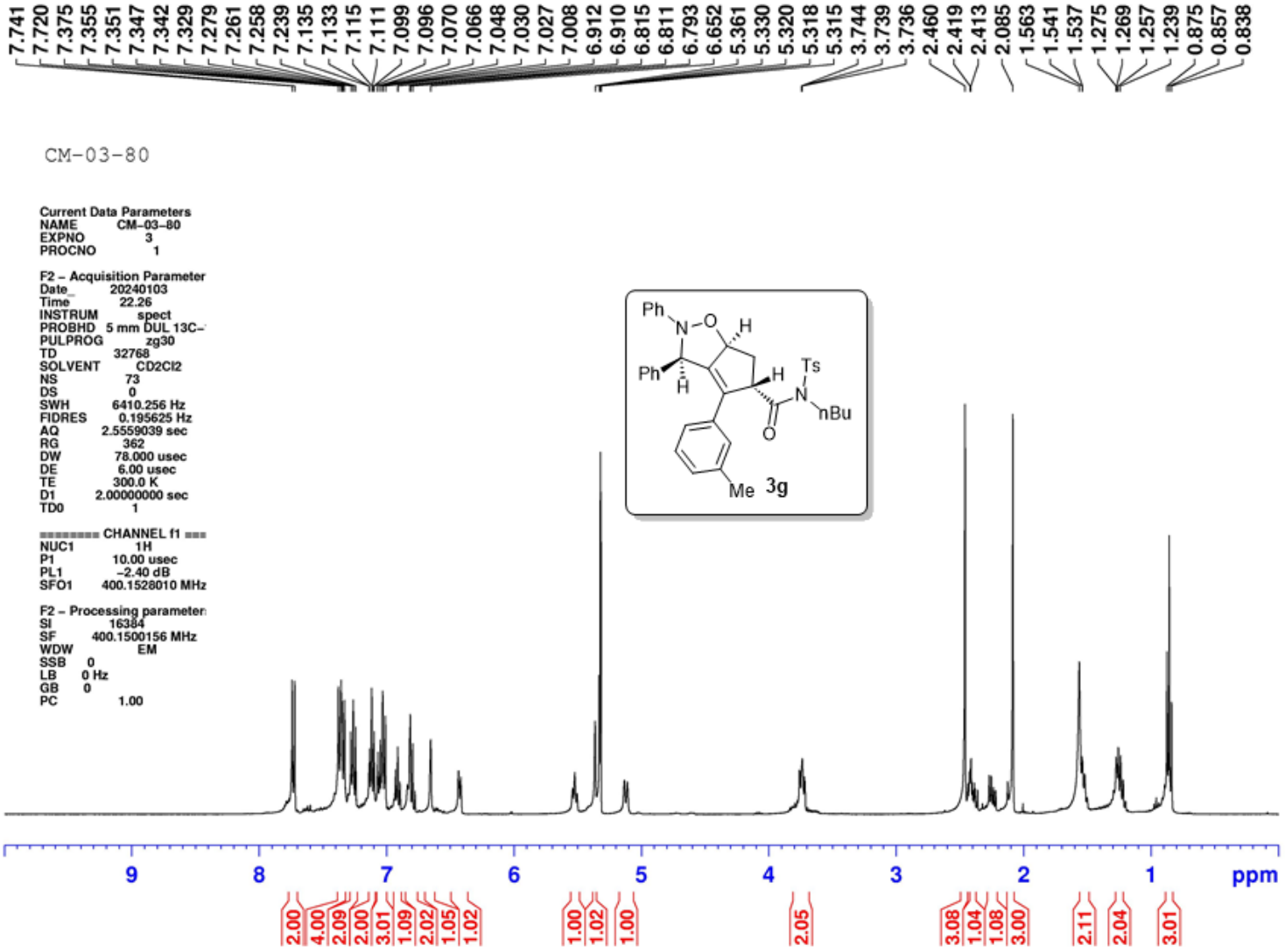
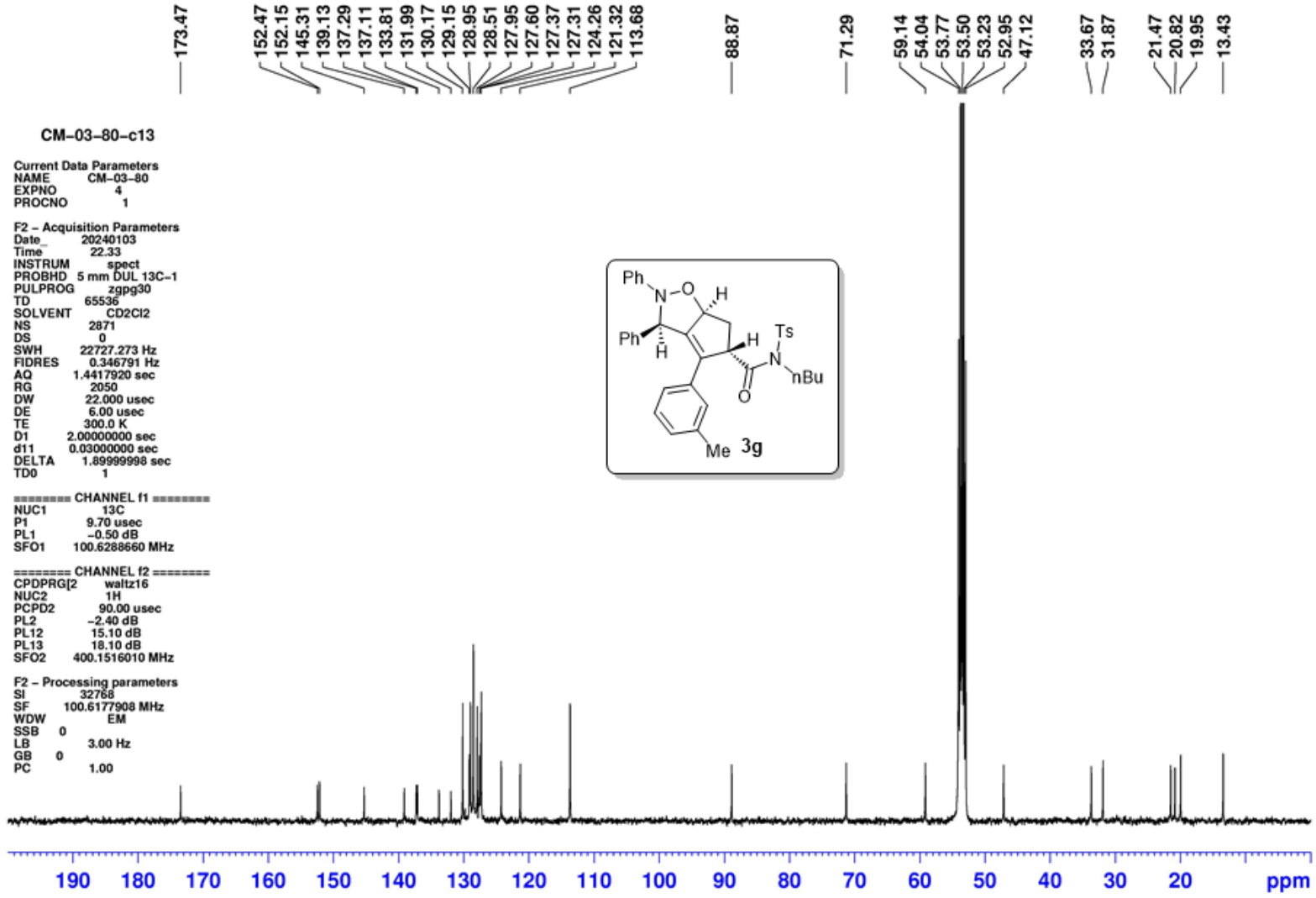
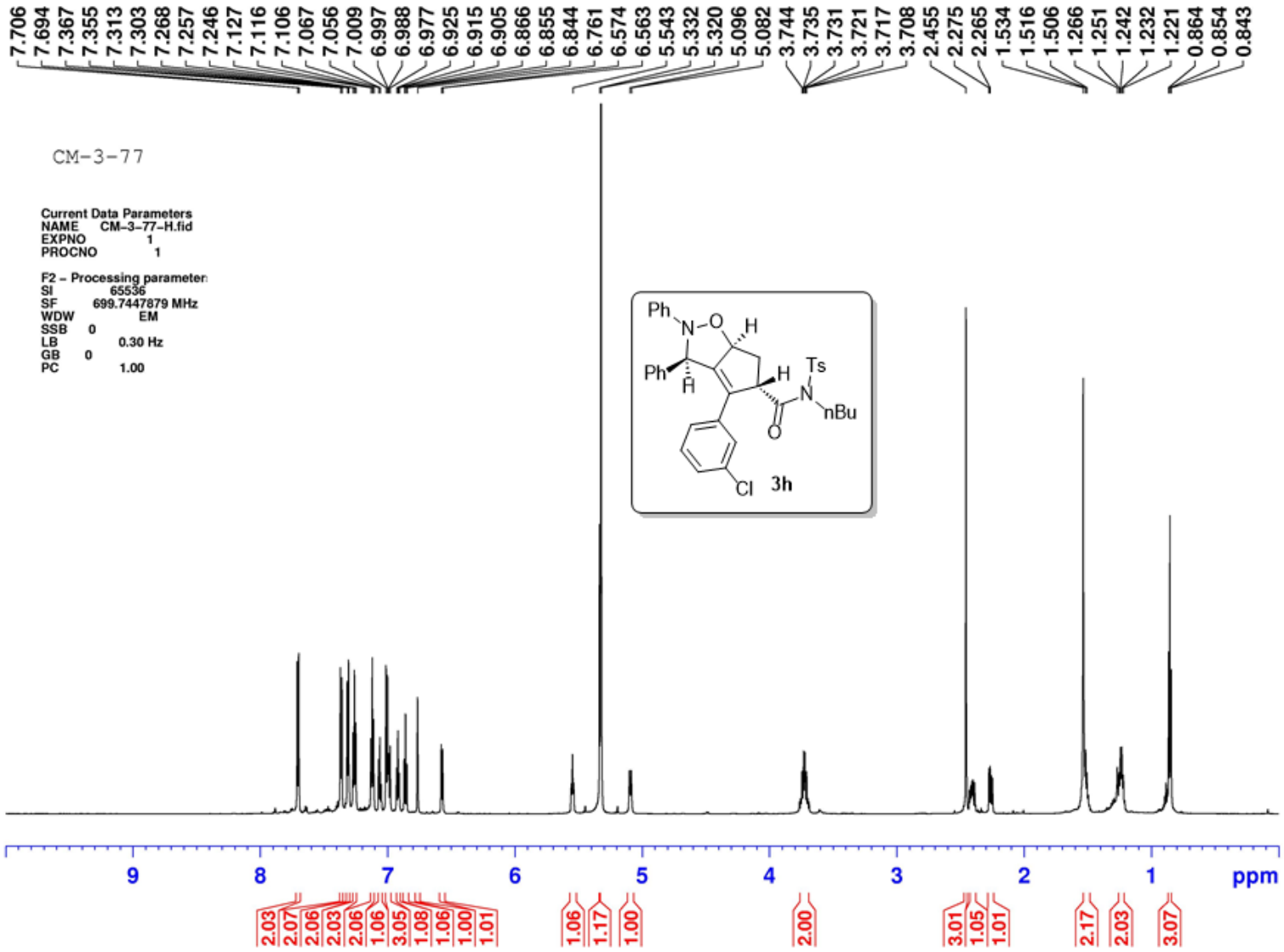


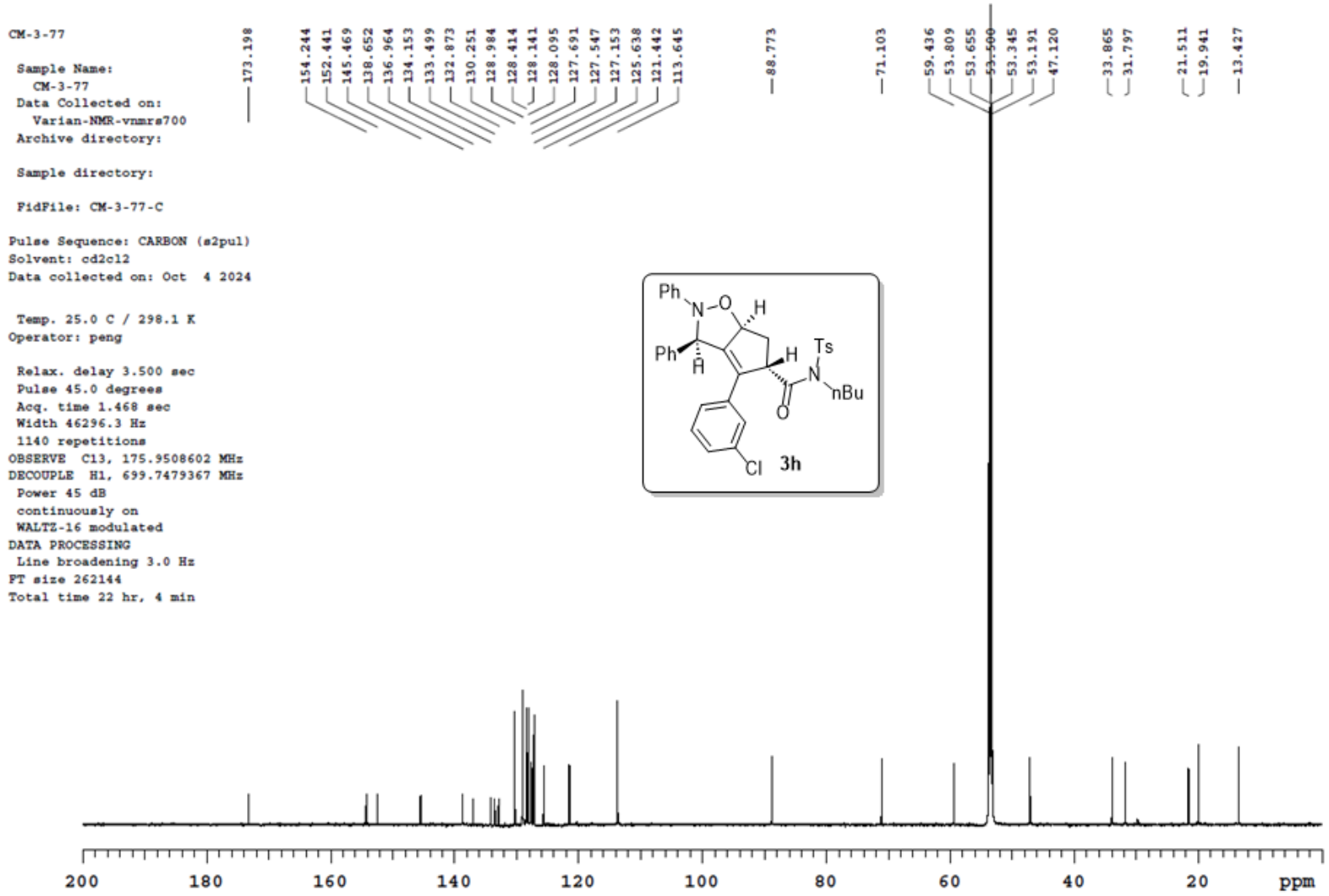
^{13}C NMR (CD_2Cl_2, 100 MHz)



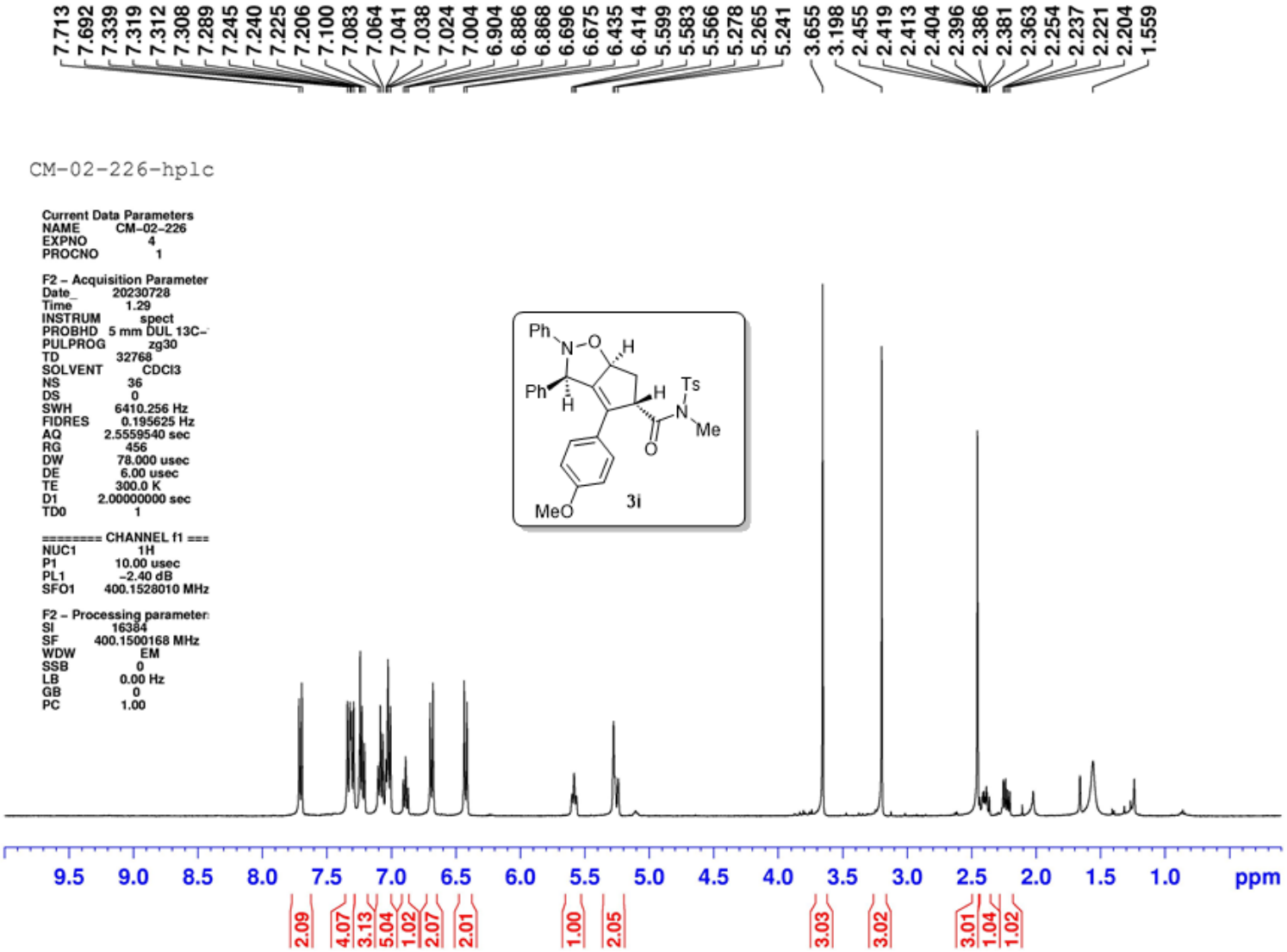
^{1}H NMR (CD_2Cl_2, 700 MHz)



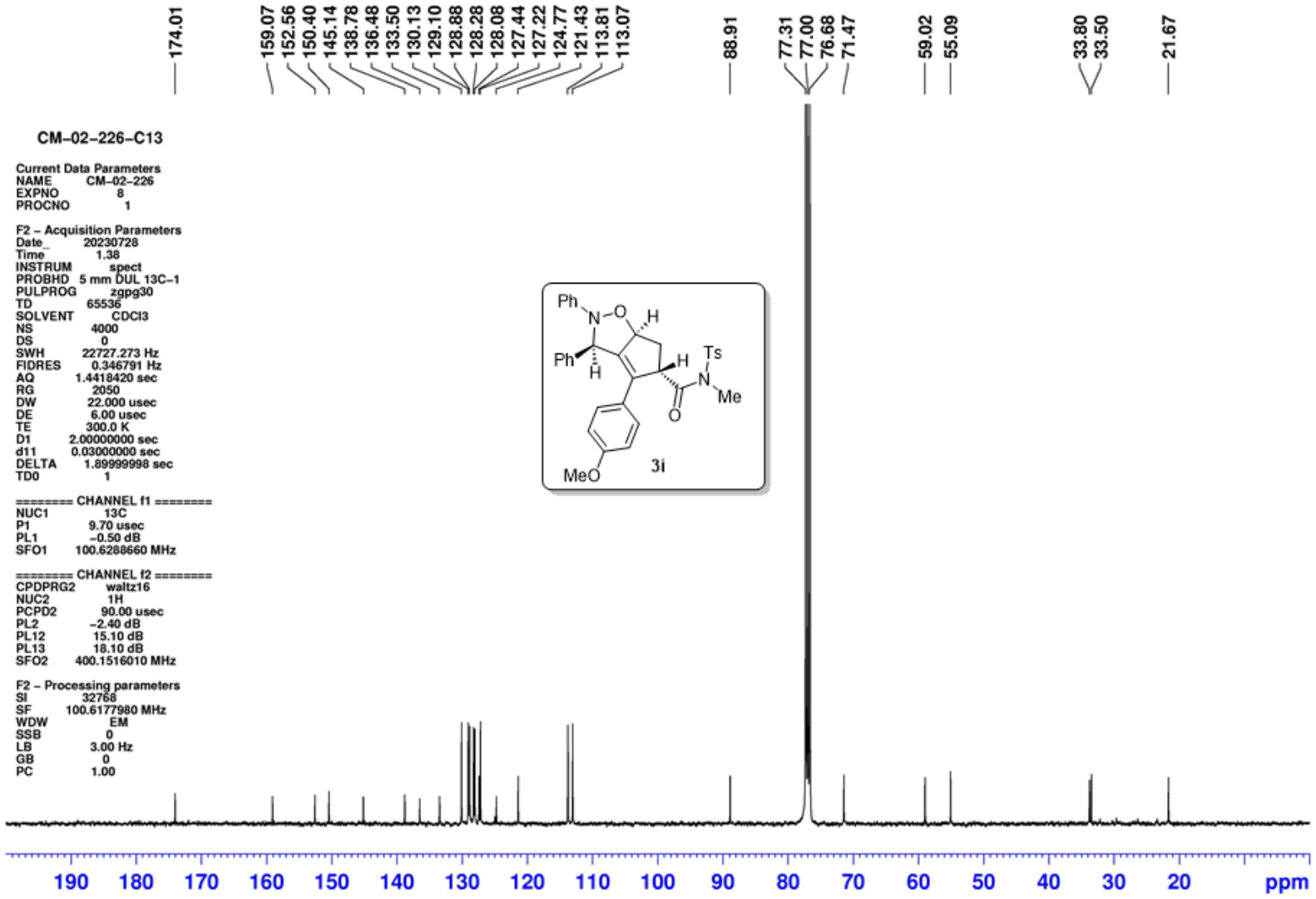
^{13}C NMR (CD_2Cl_2, 175 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



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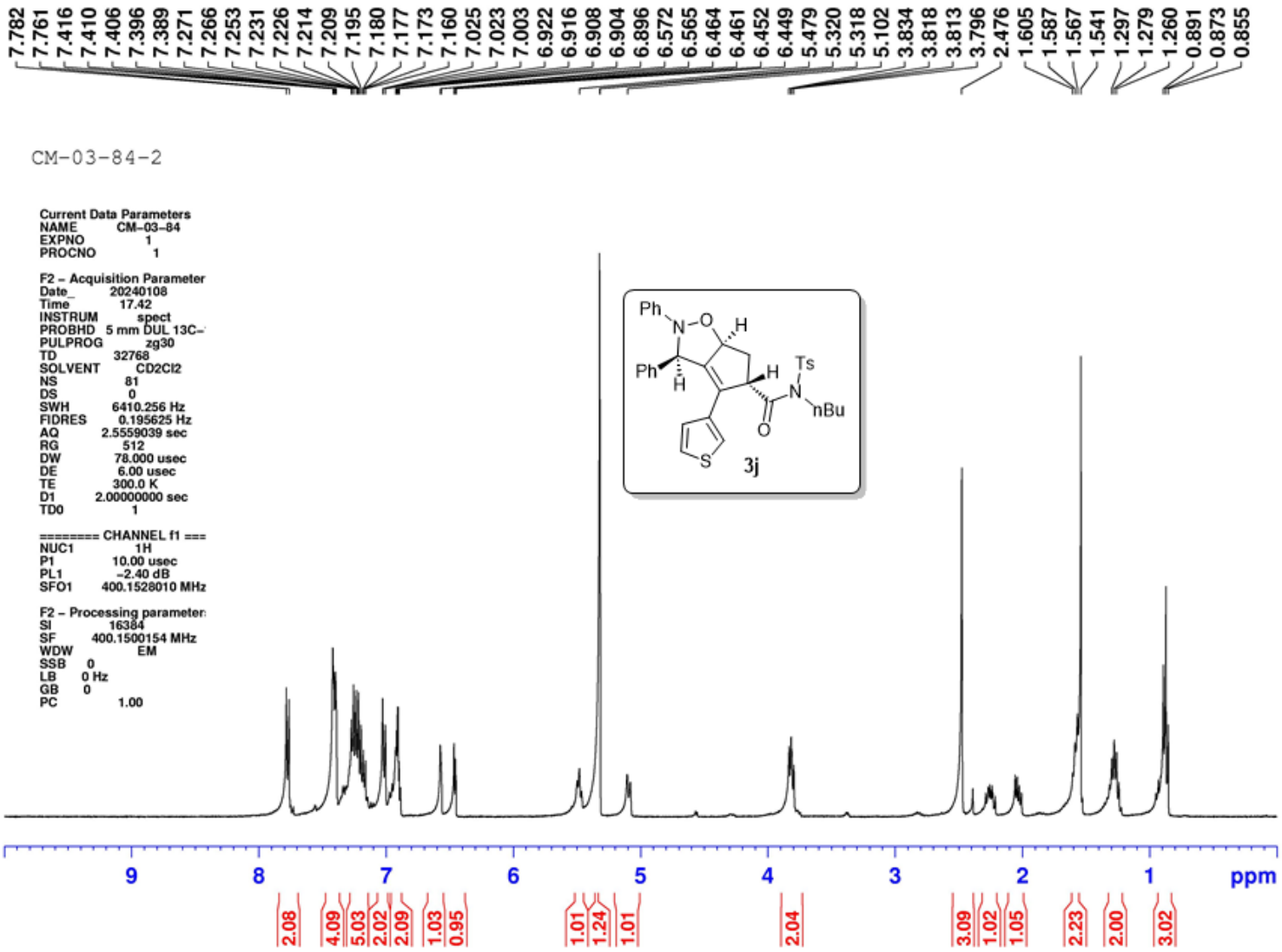
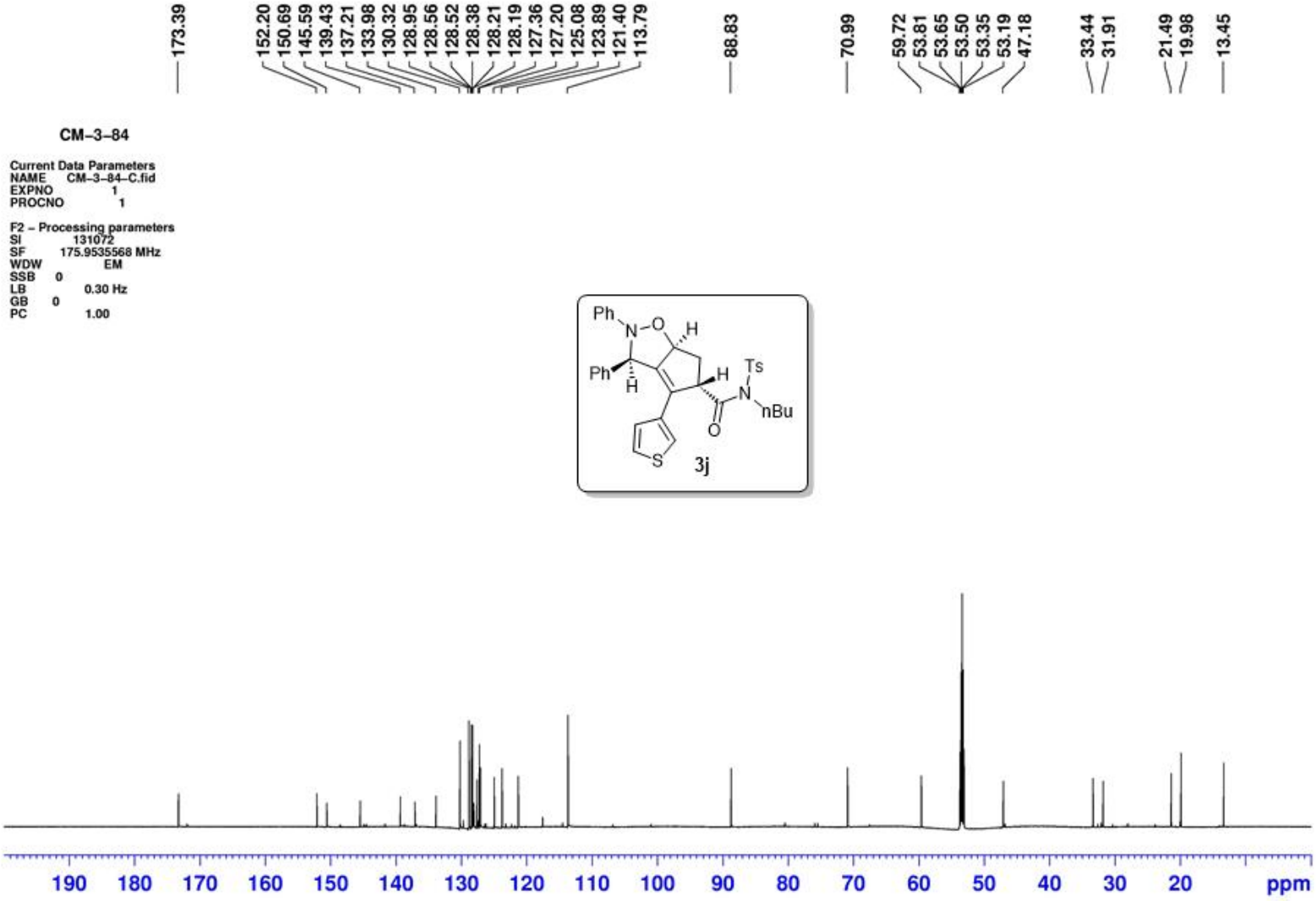
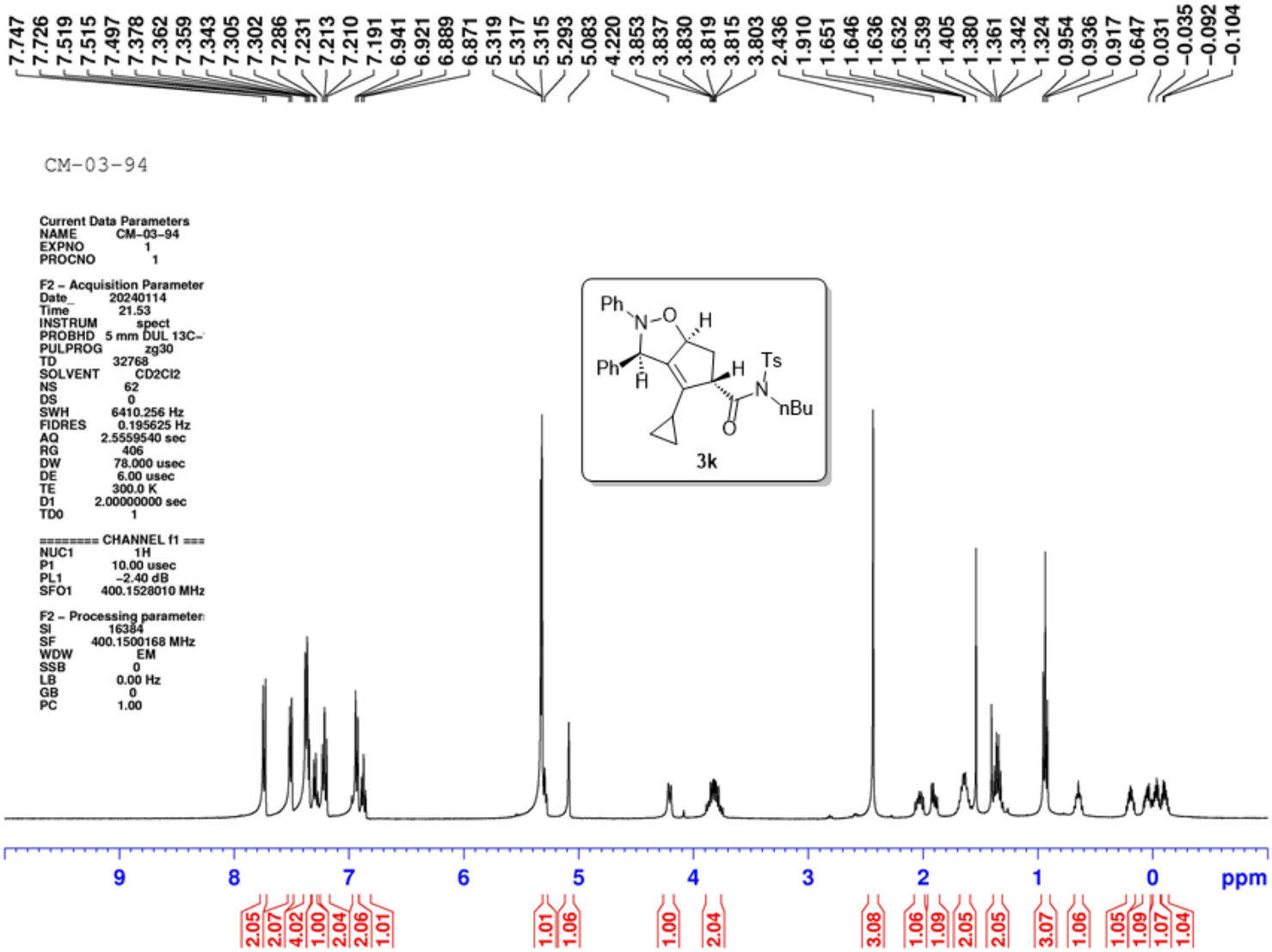


^{13}C NMR (CD_2Cl_2, 175 MHz)



^{1}H NMR (CD_2Cl_2, 400 MHz)



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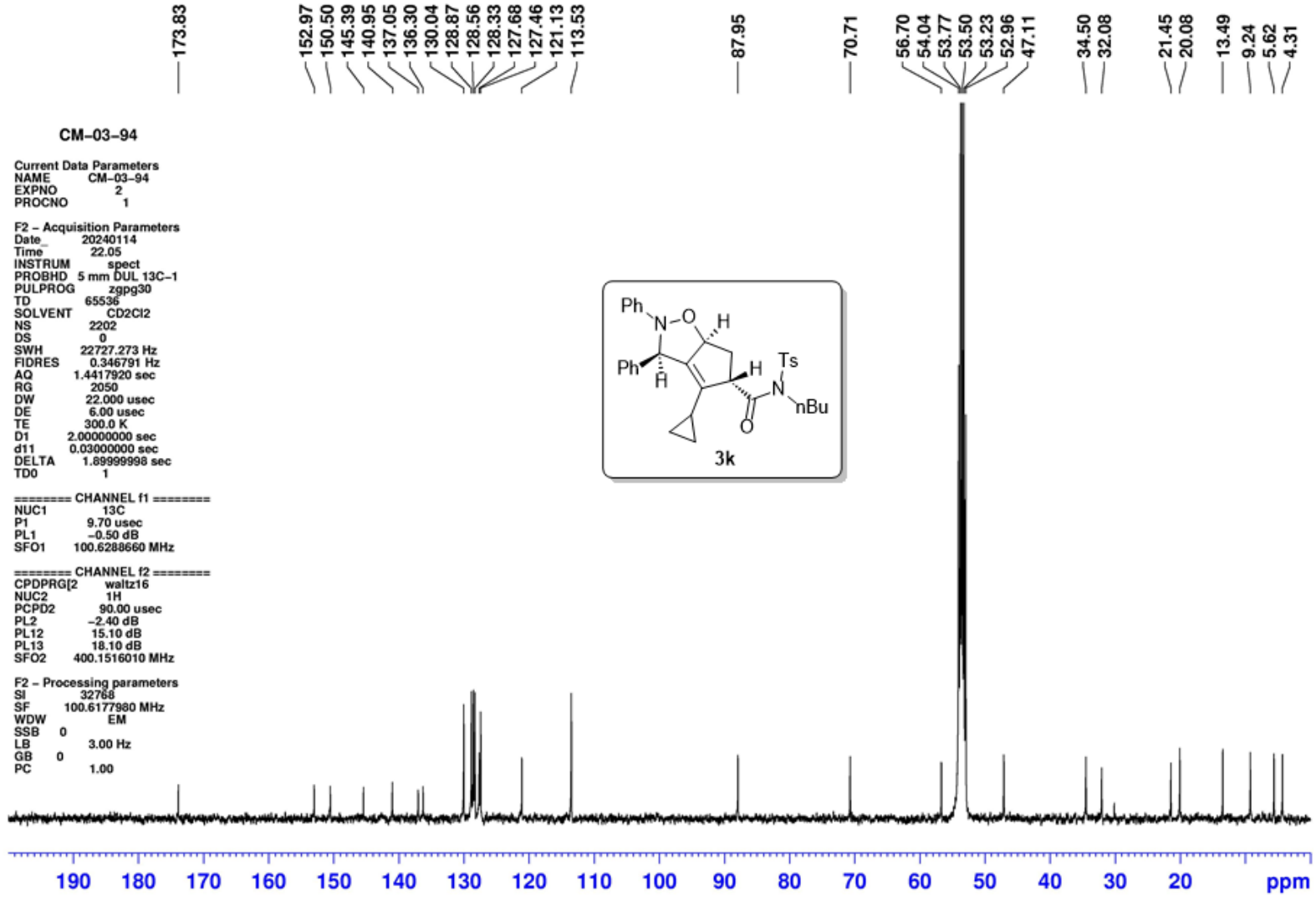
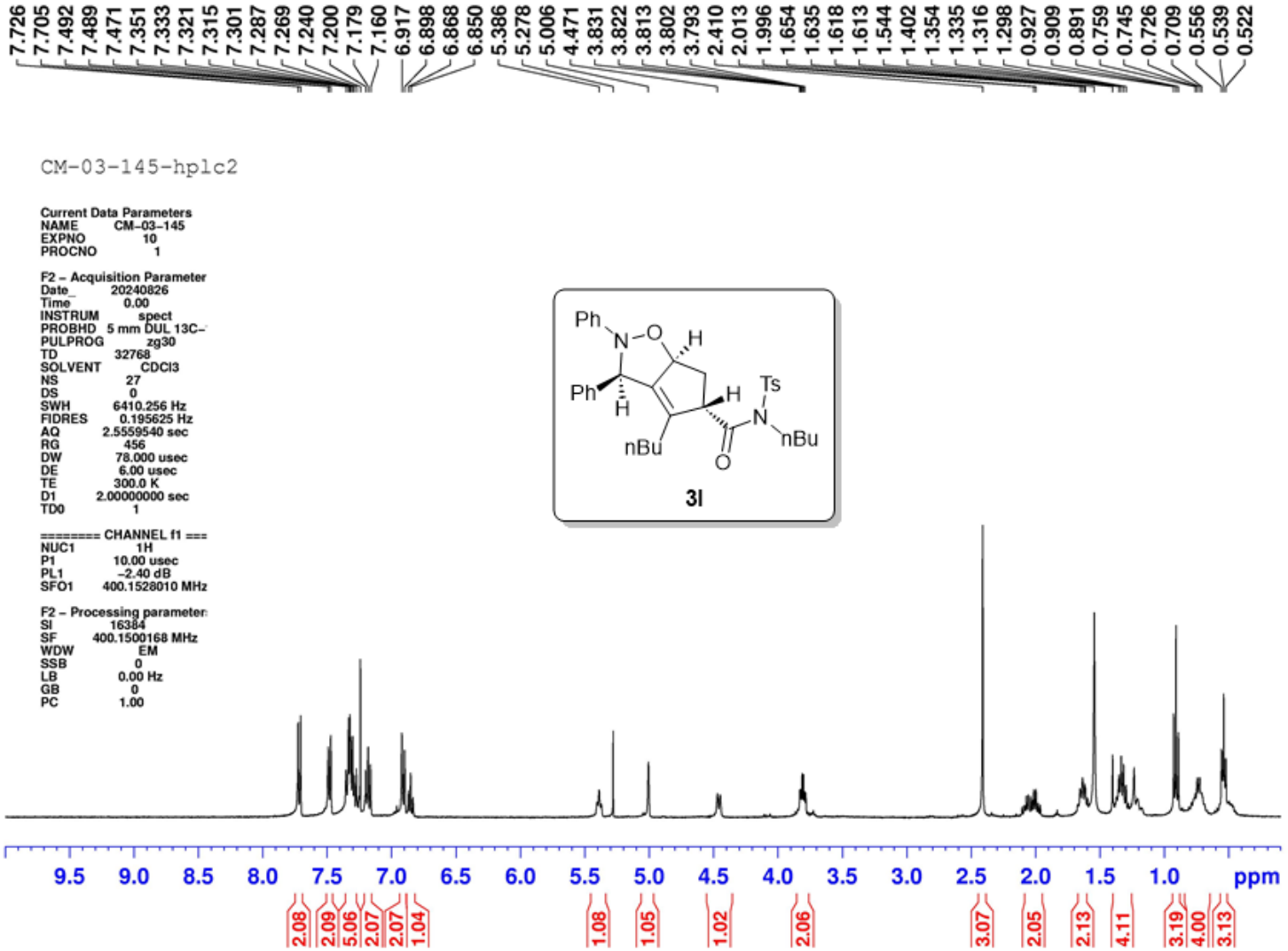


^{1}H NMR ($CDCl_3$, 400 MHz)



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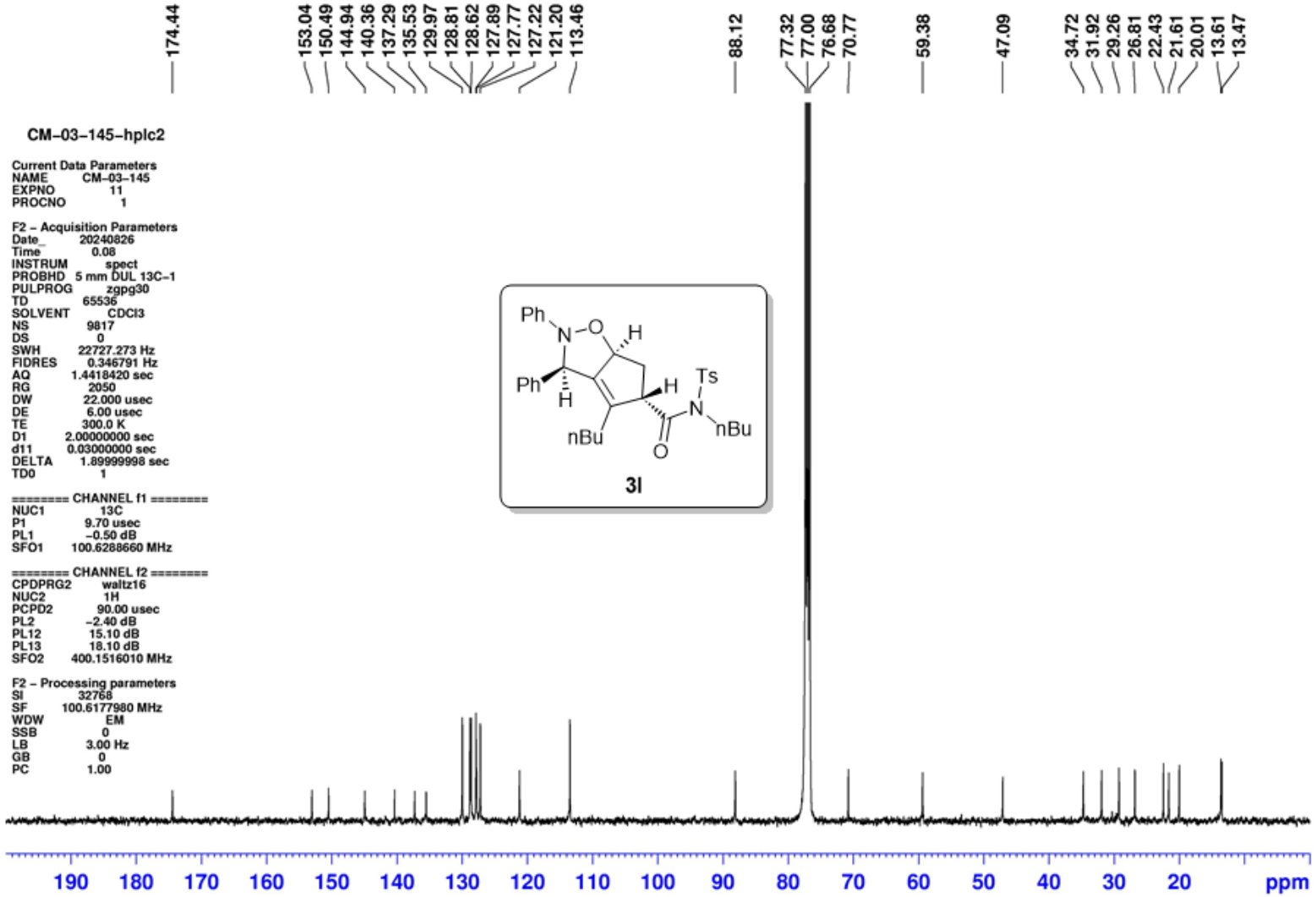

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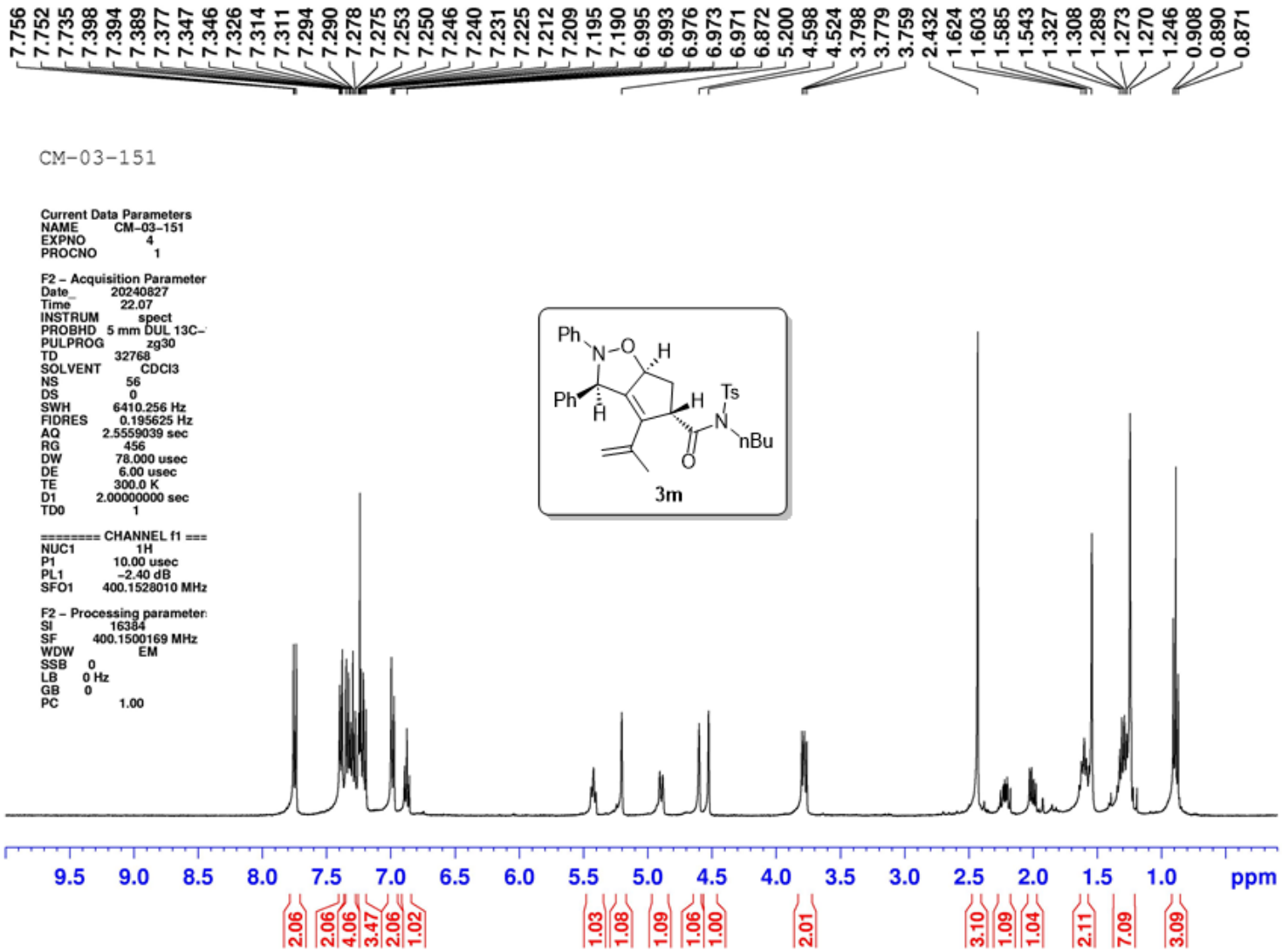

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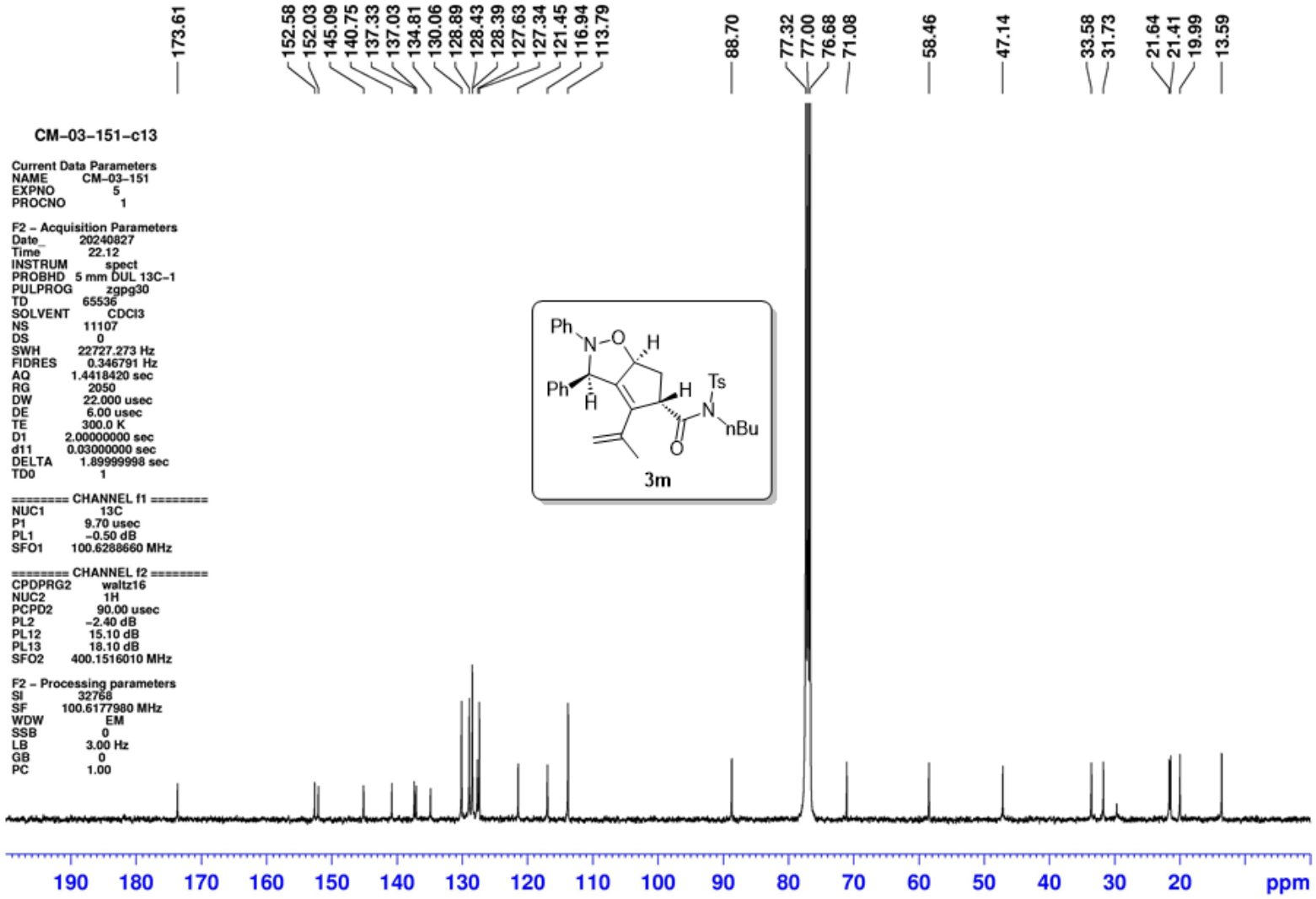

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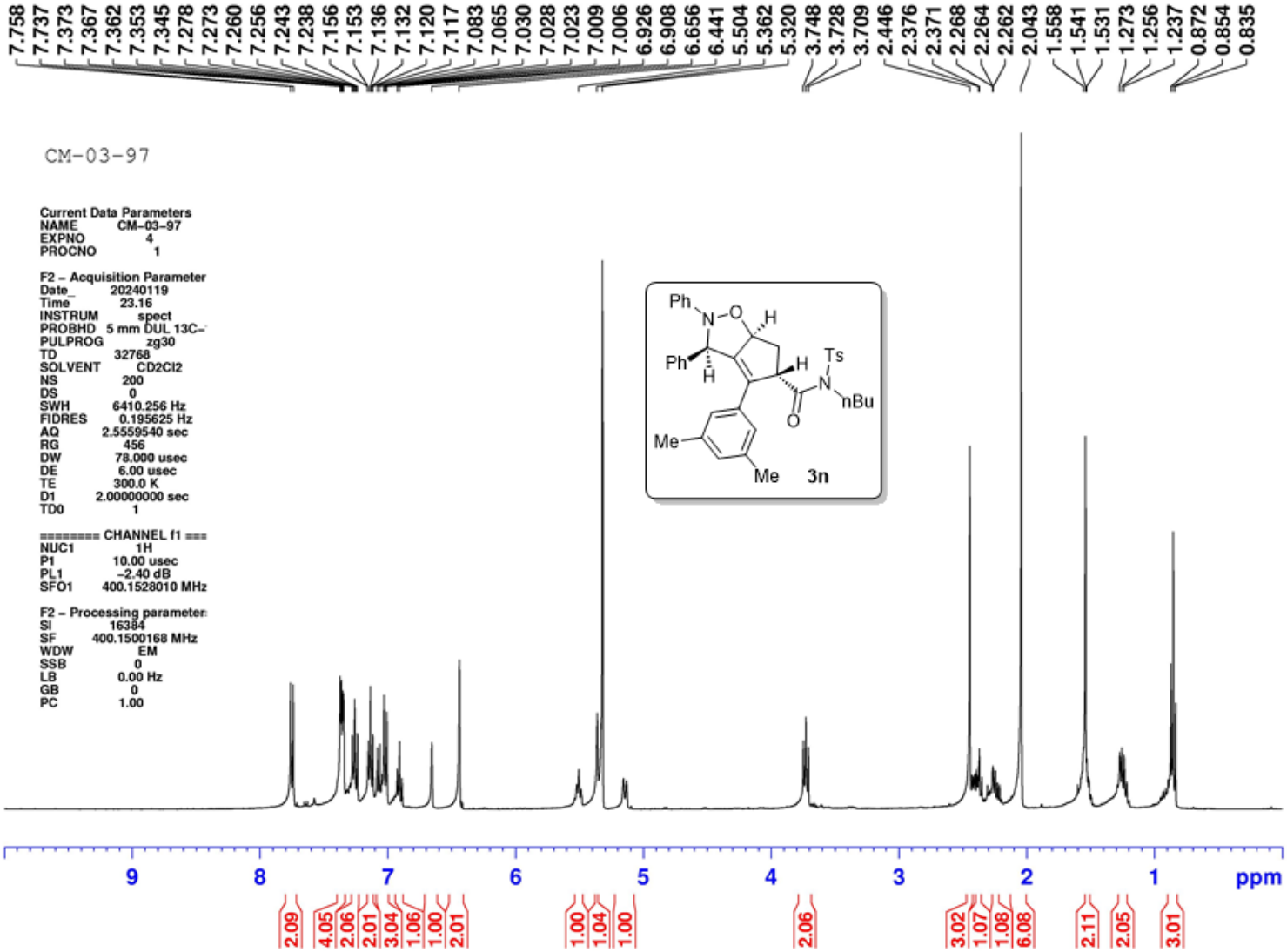
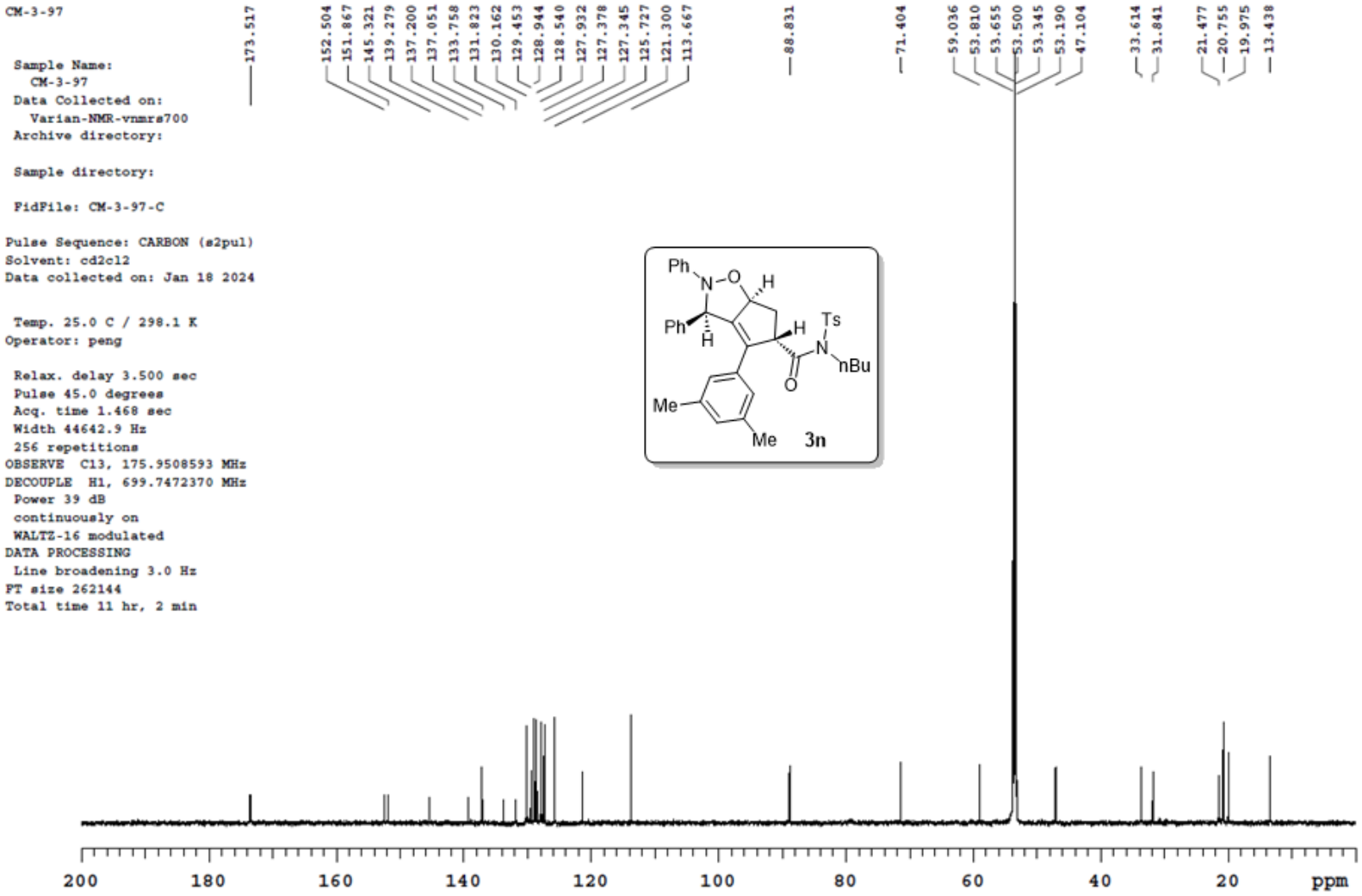


^{13}C NMR (CD_2Cl_2, 175 MHz)



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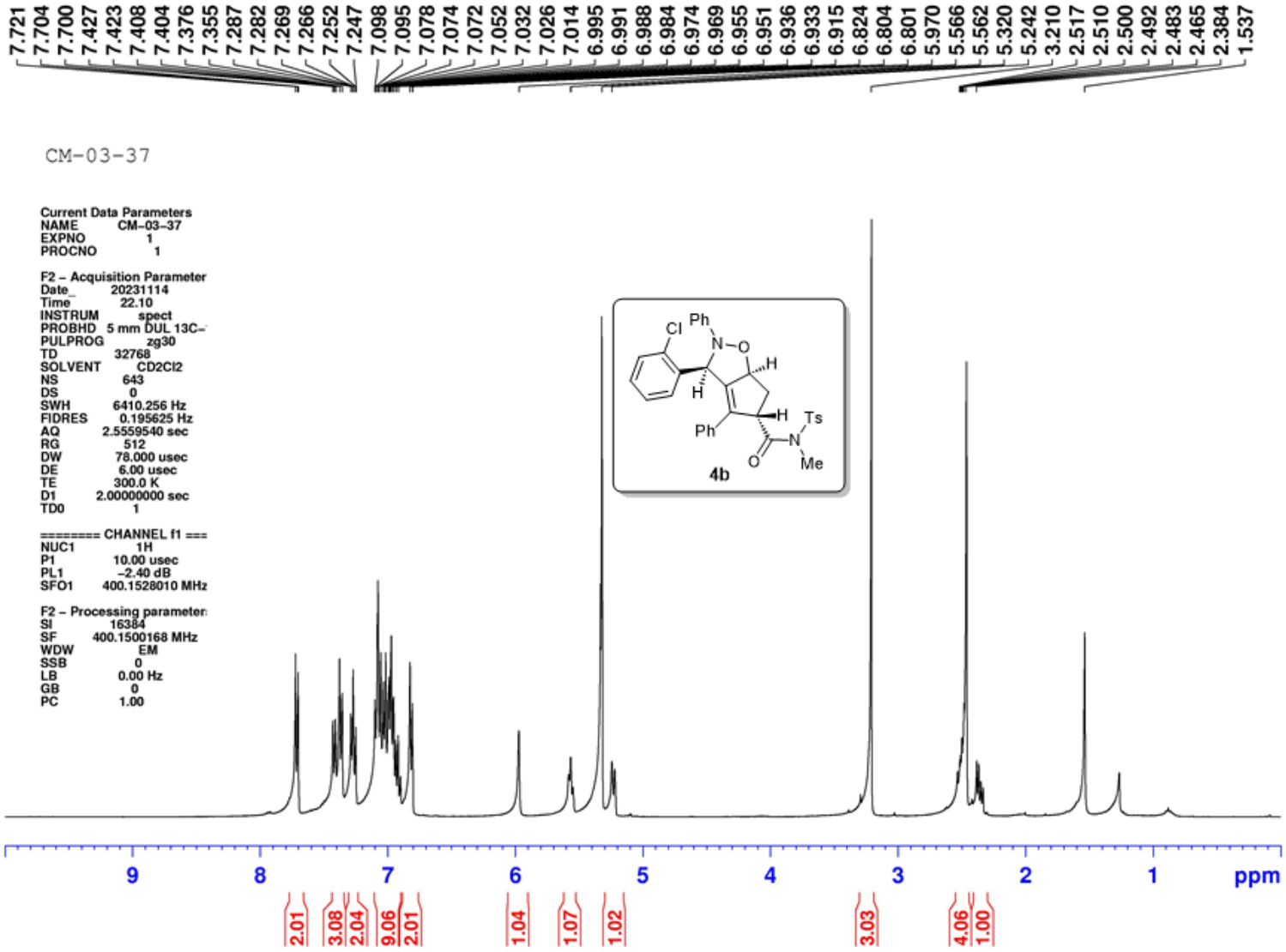

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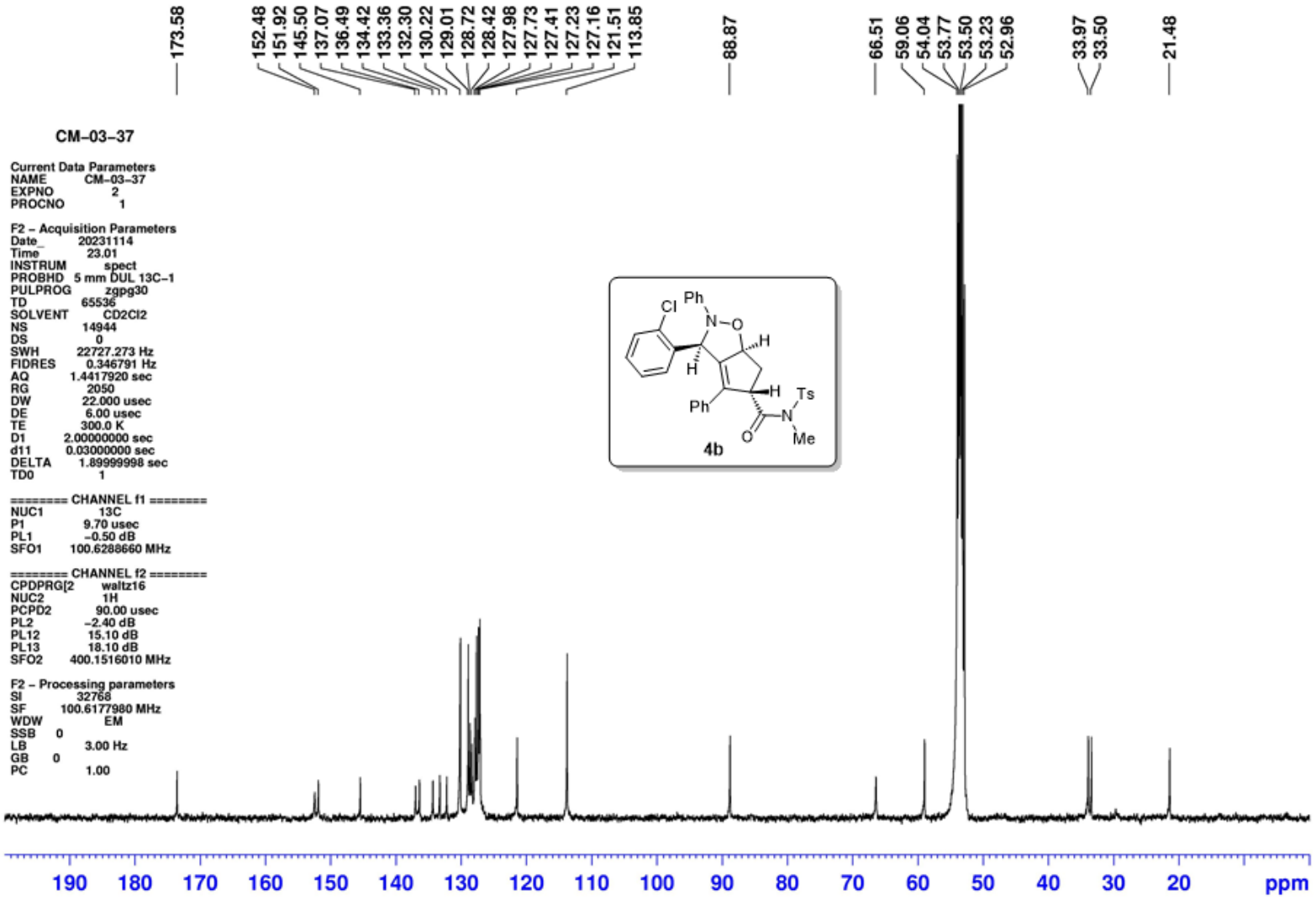

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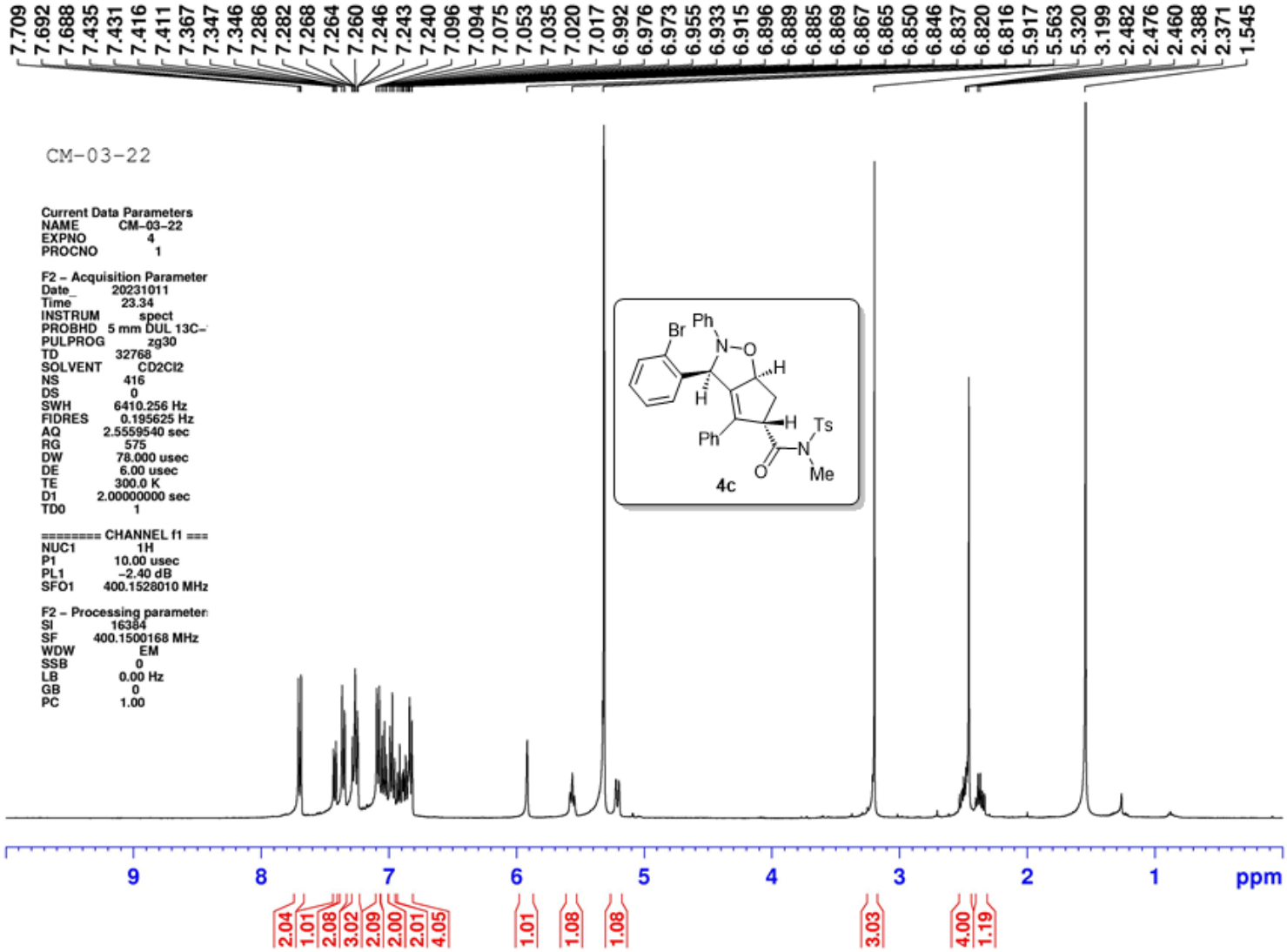

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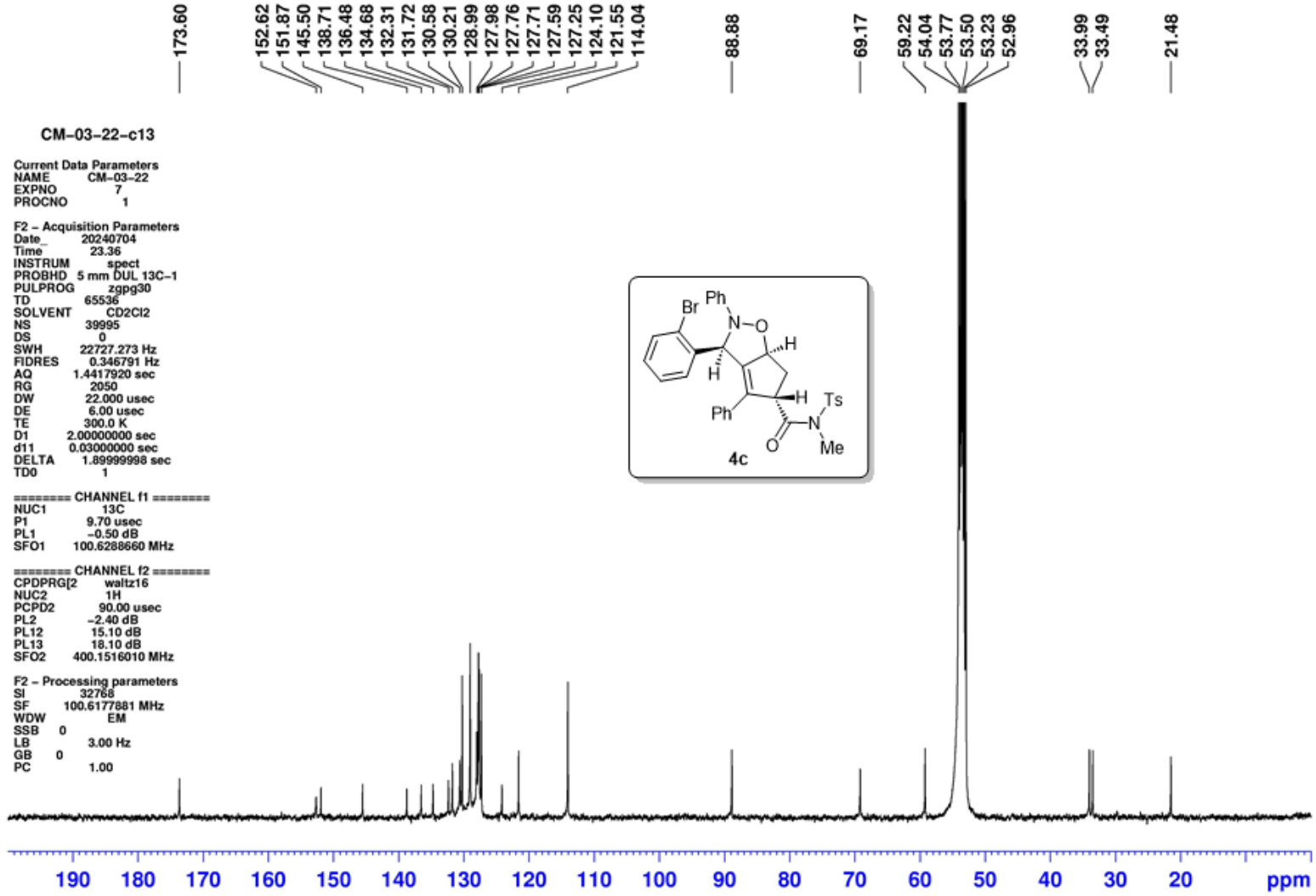

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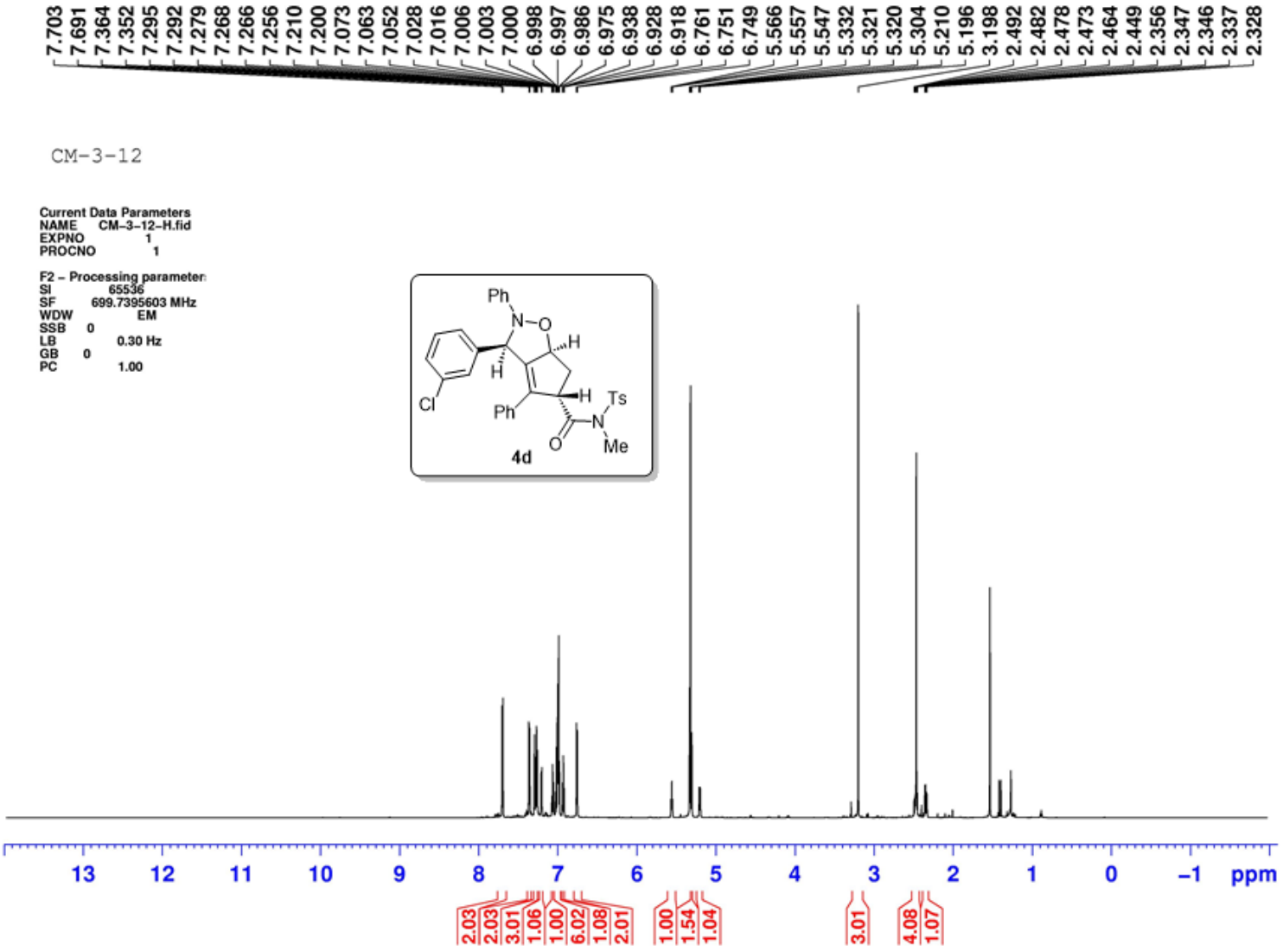

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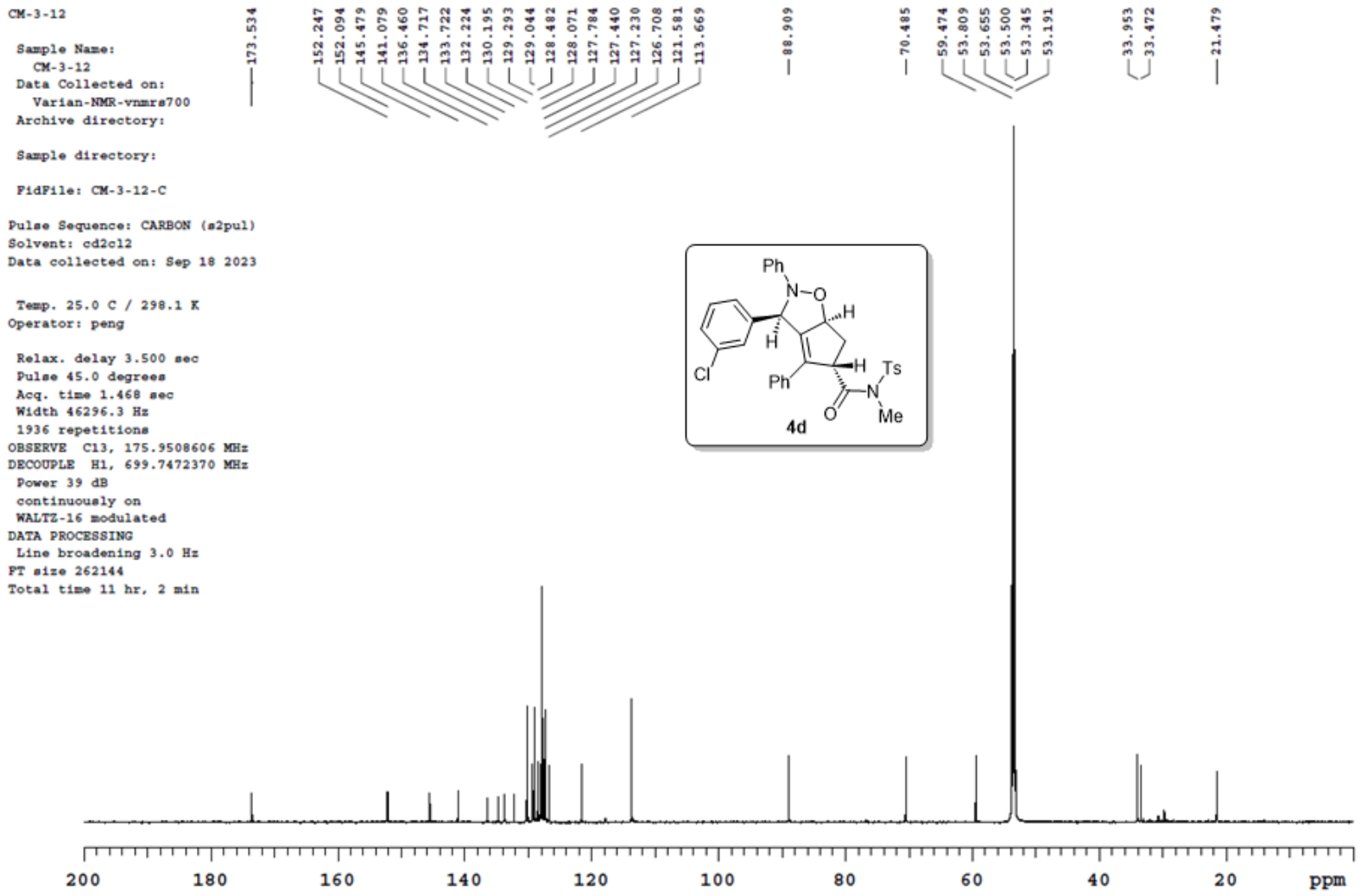

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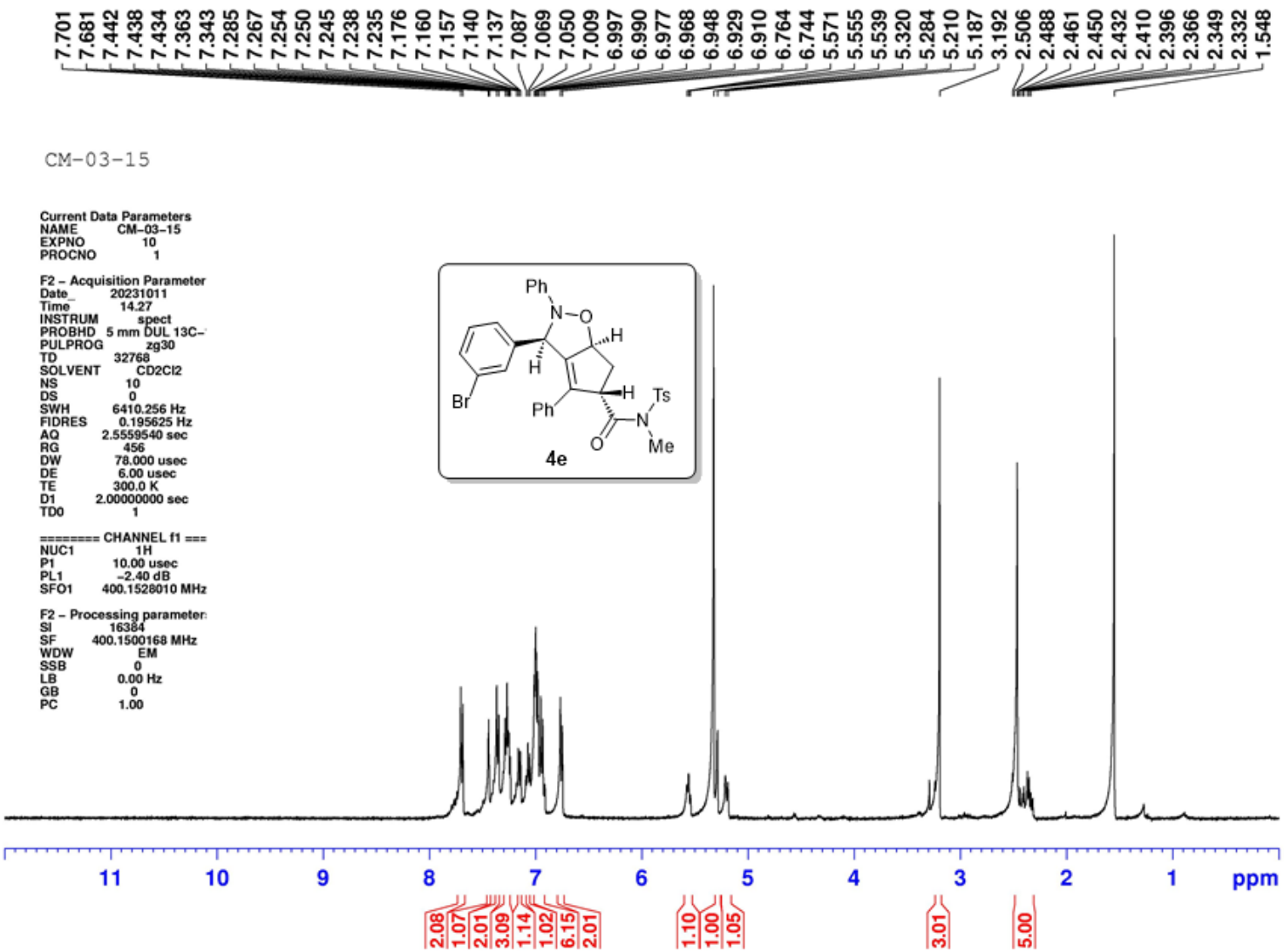

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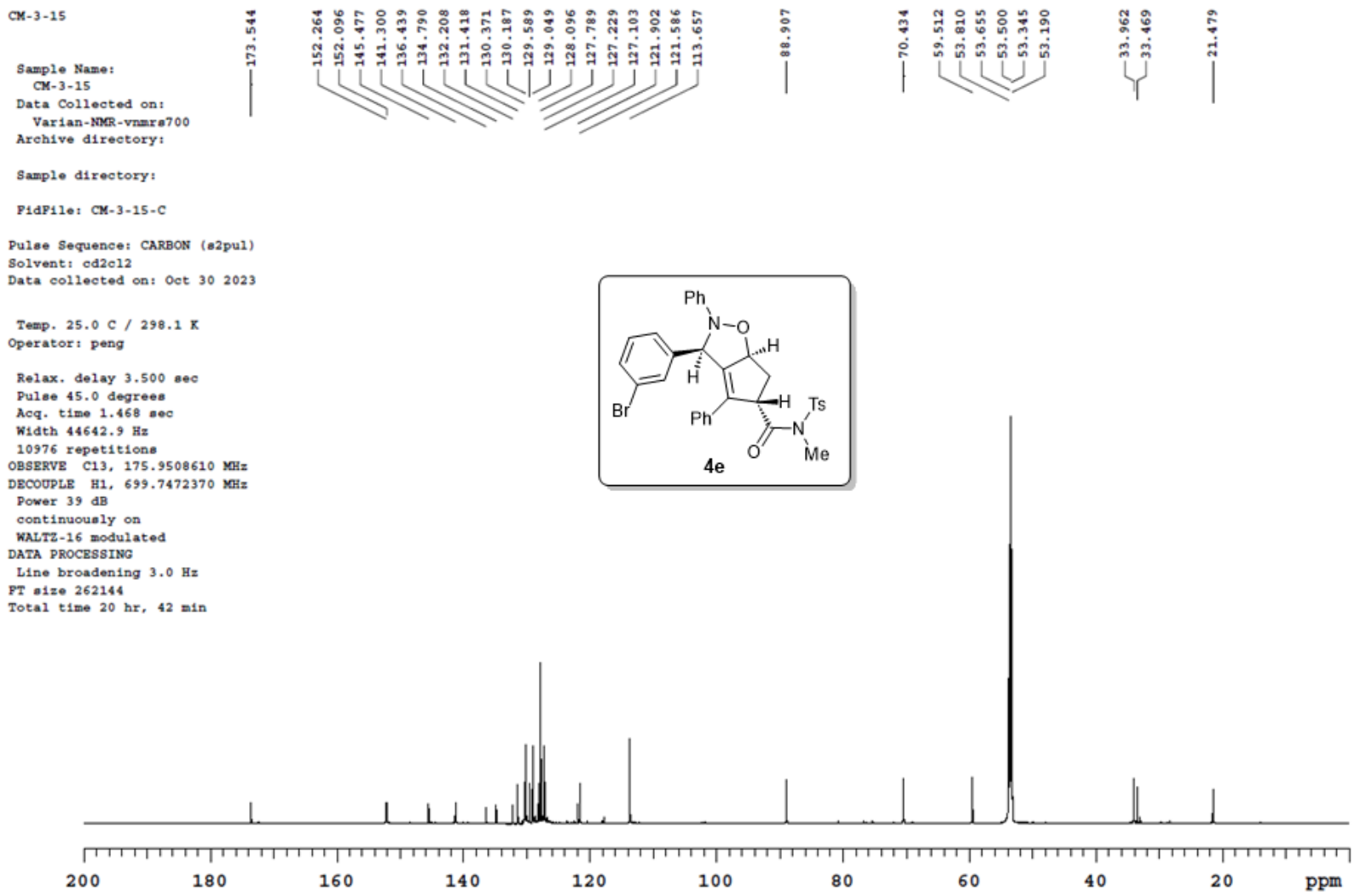

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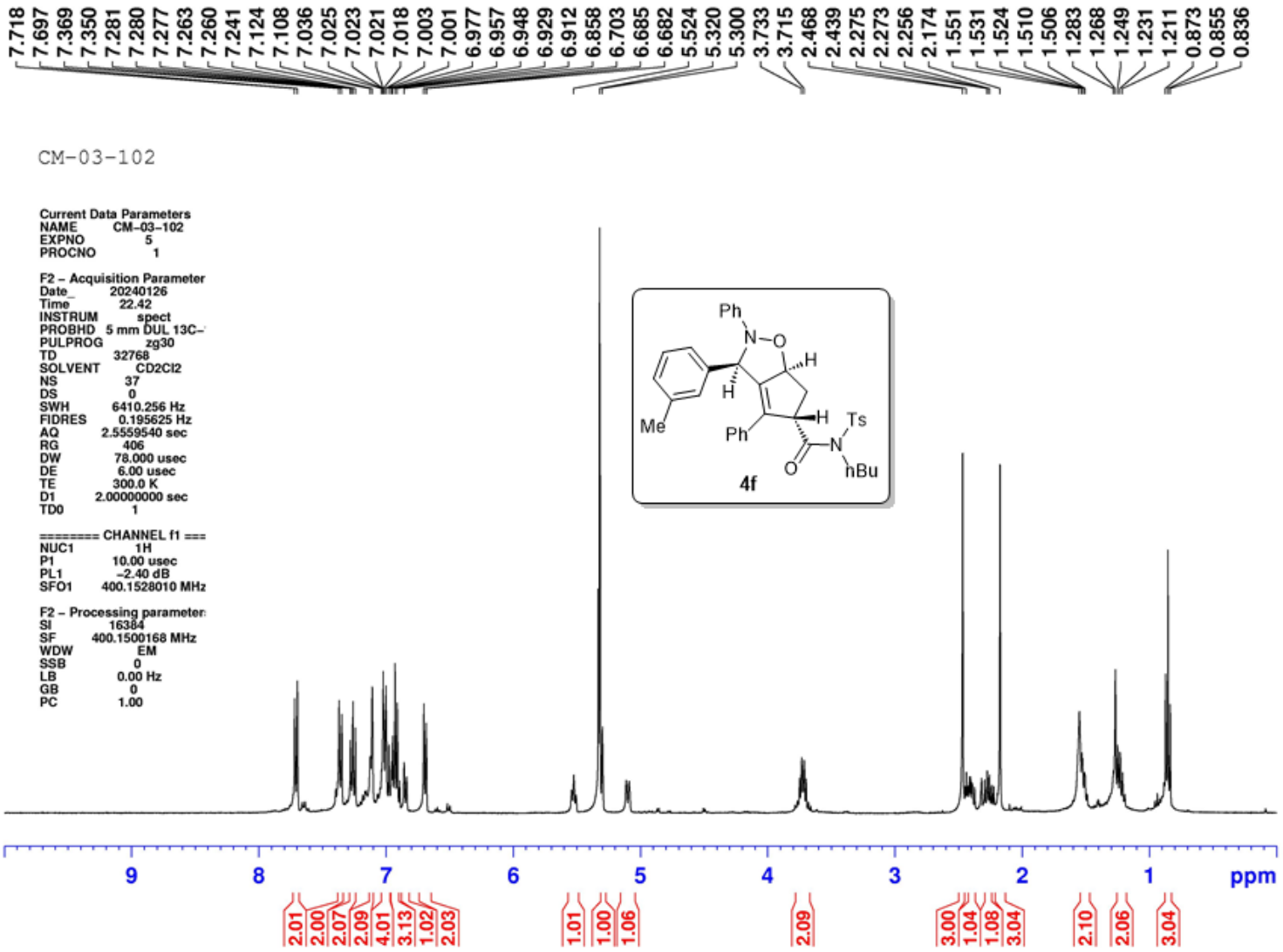

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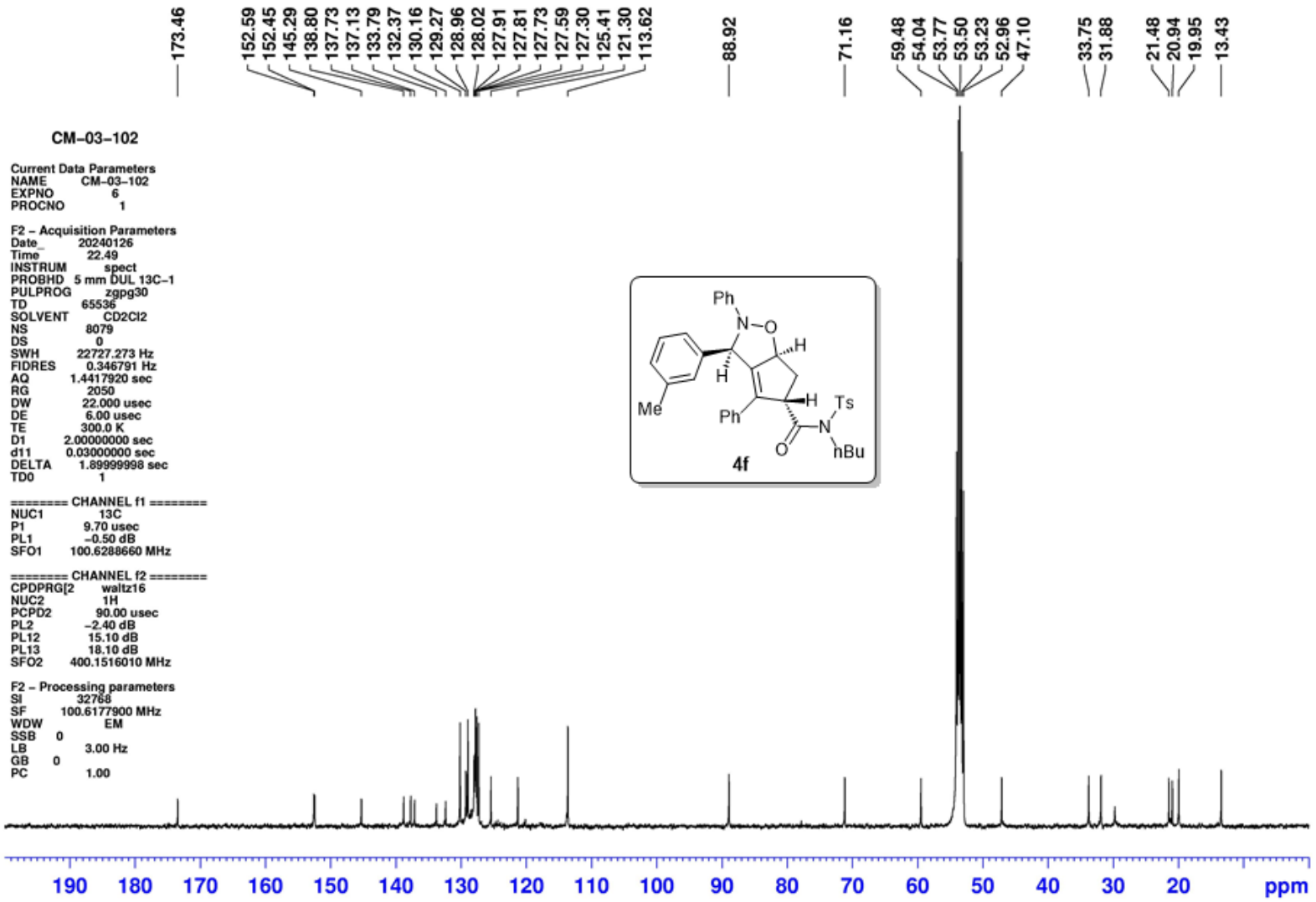

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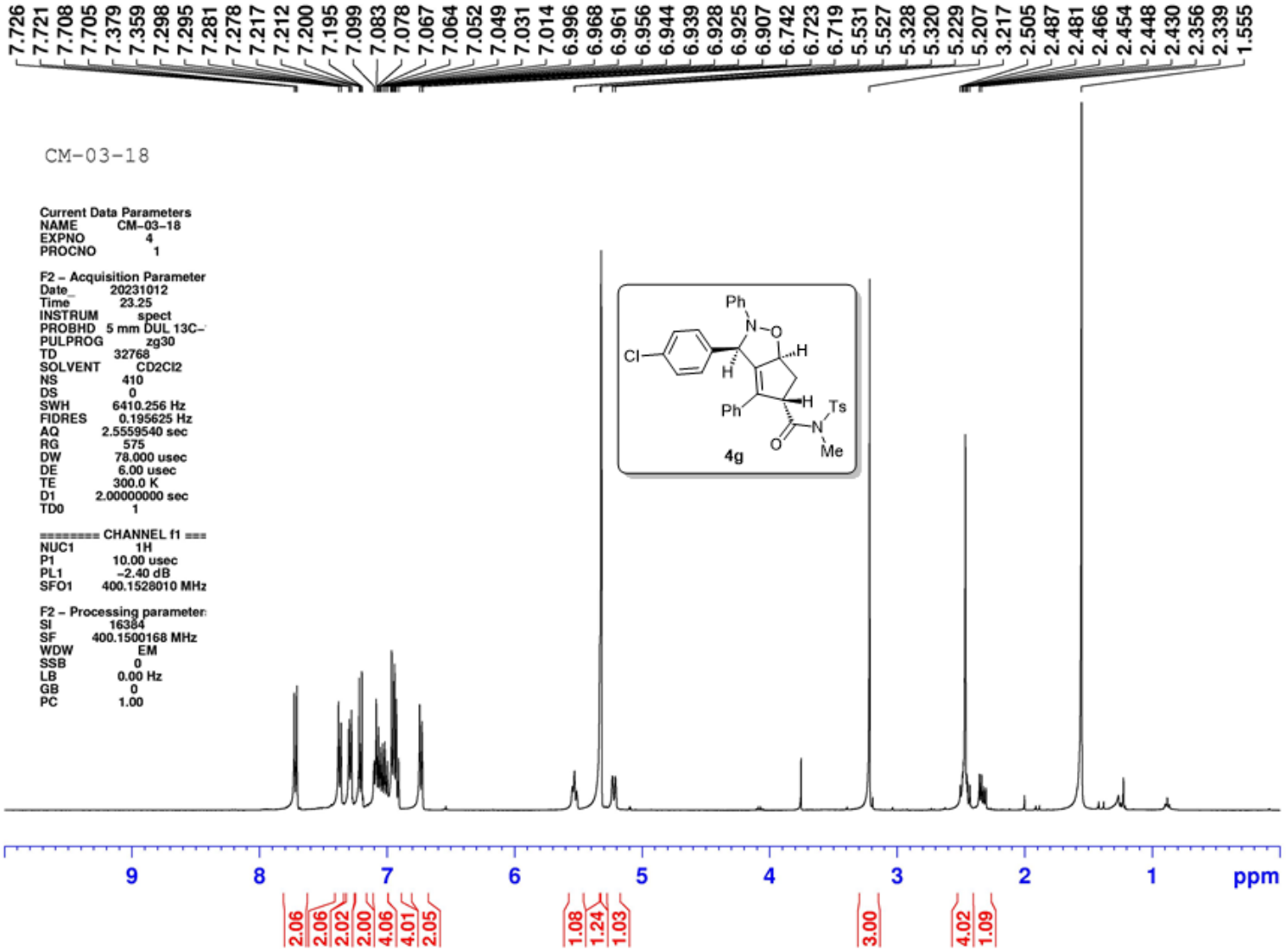

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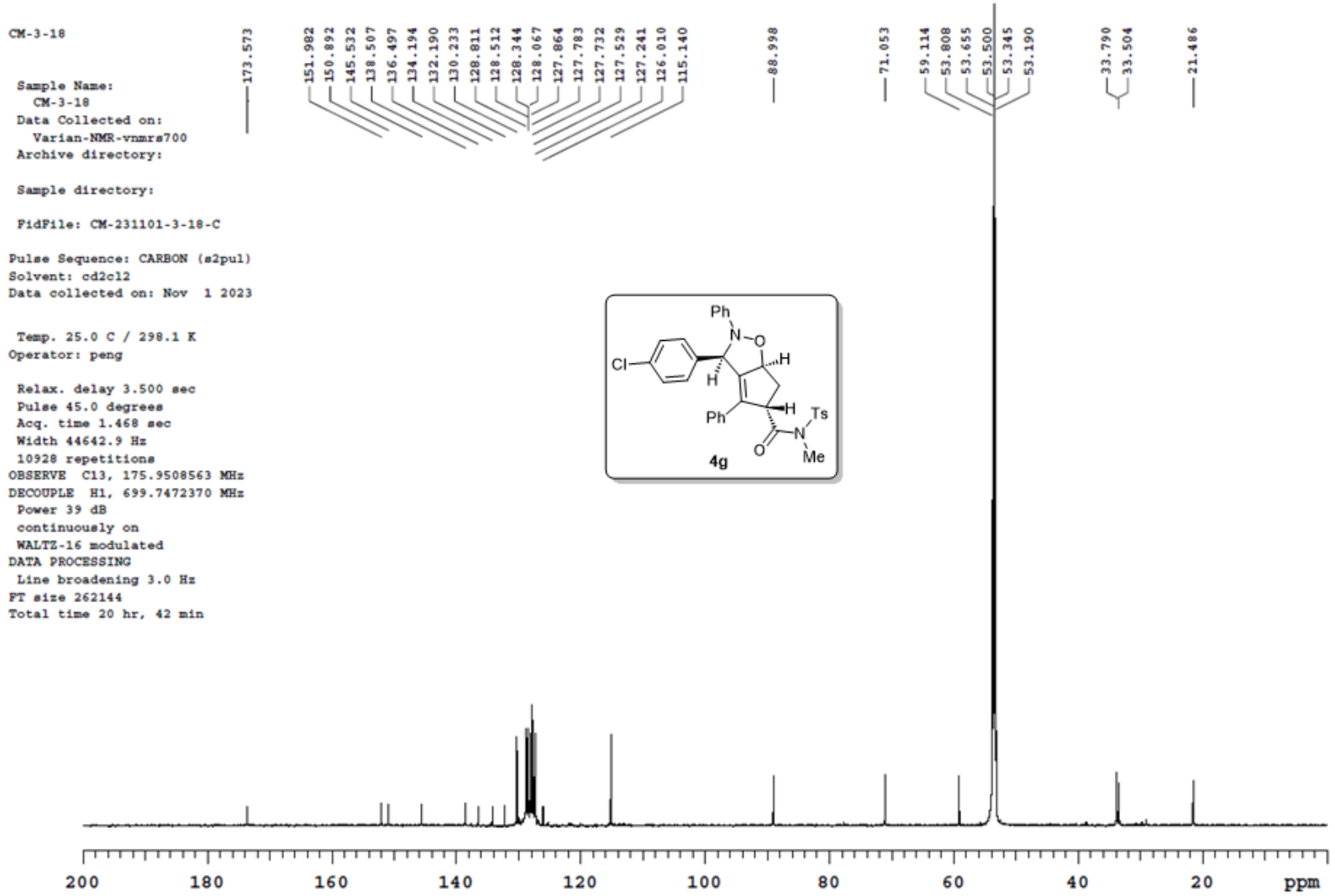

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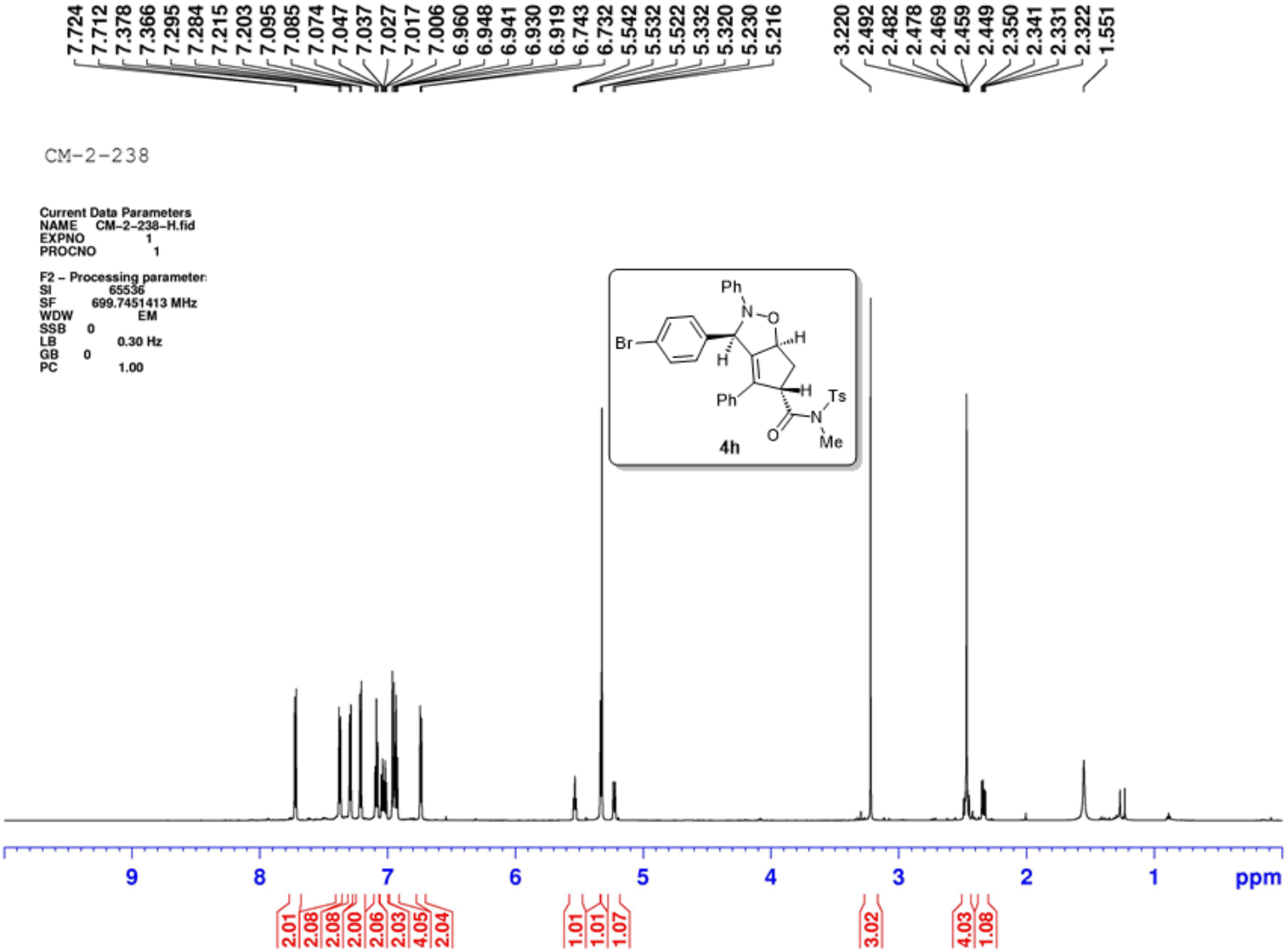

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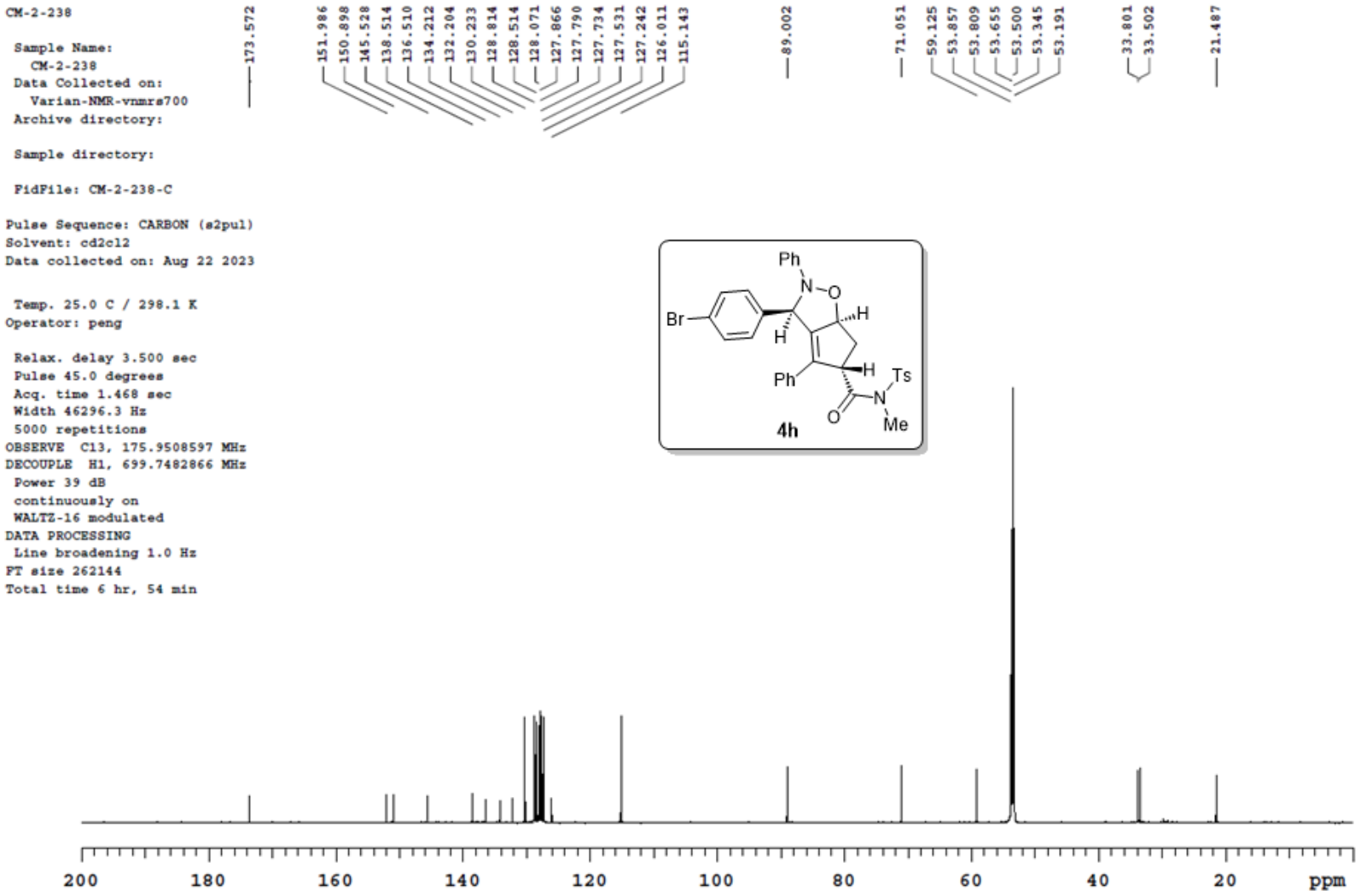

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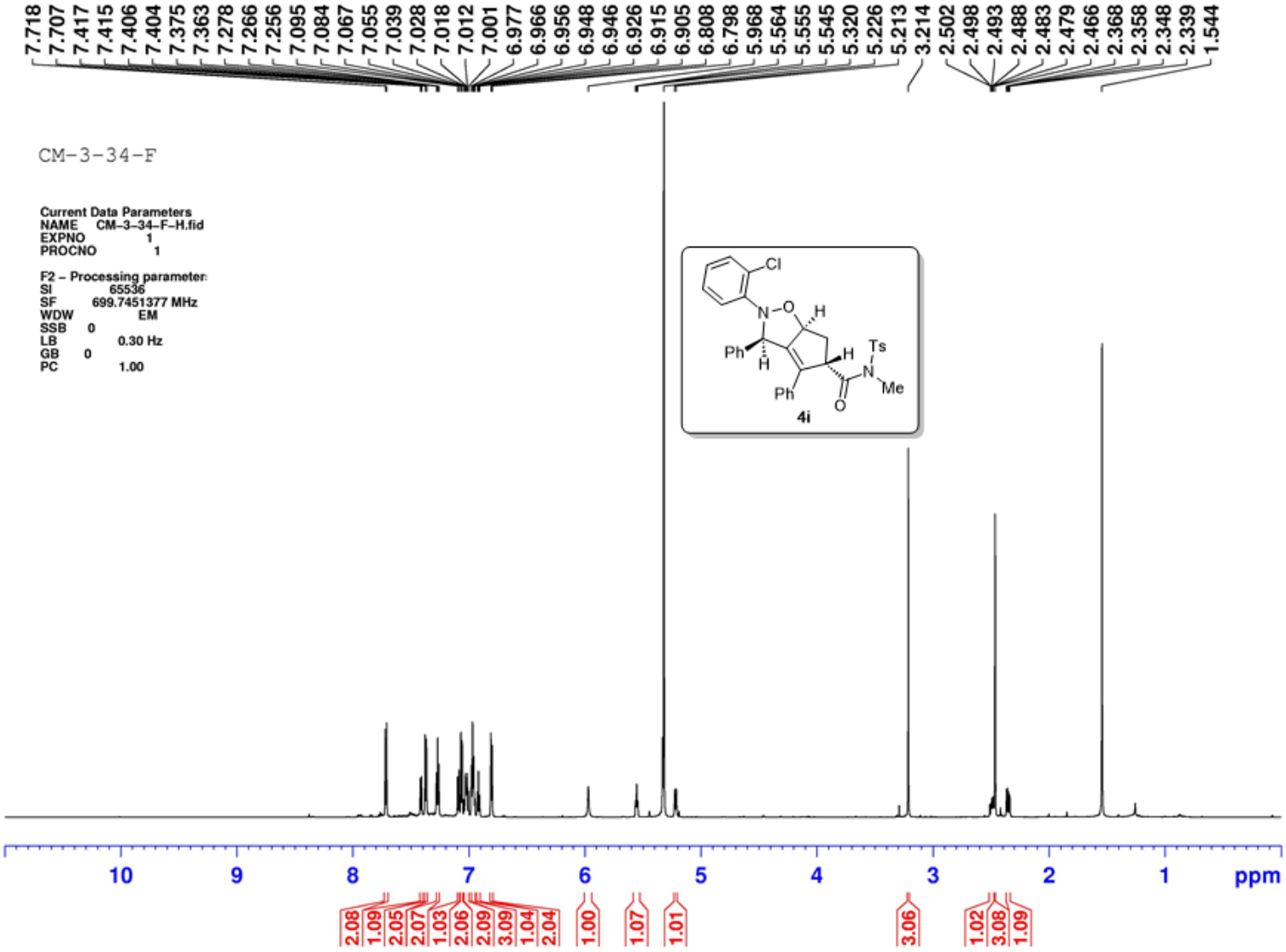

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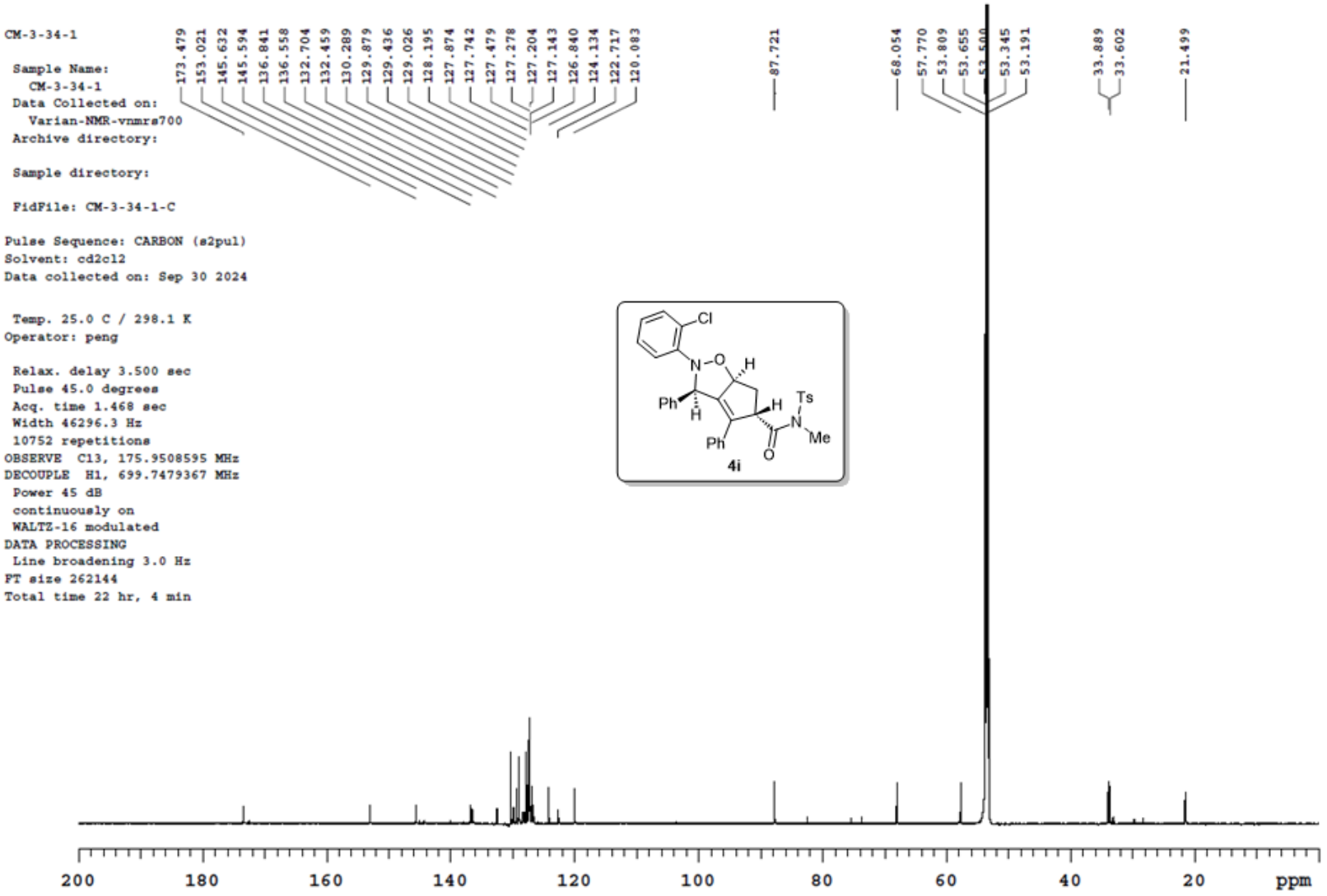

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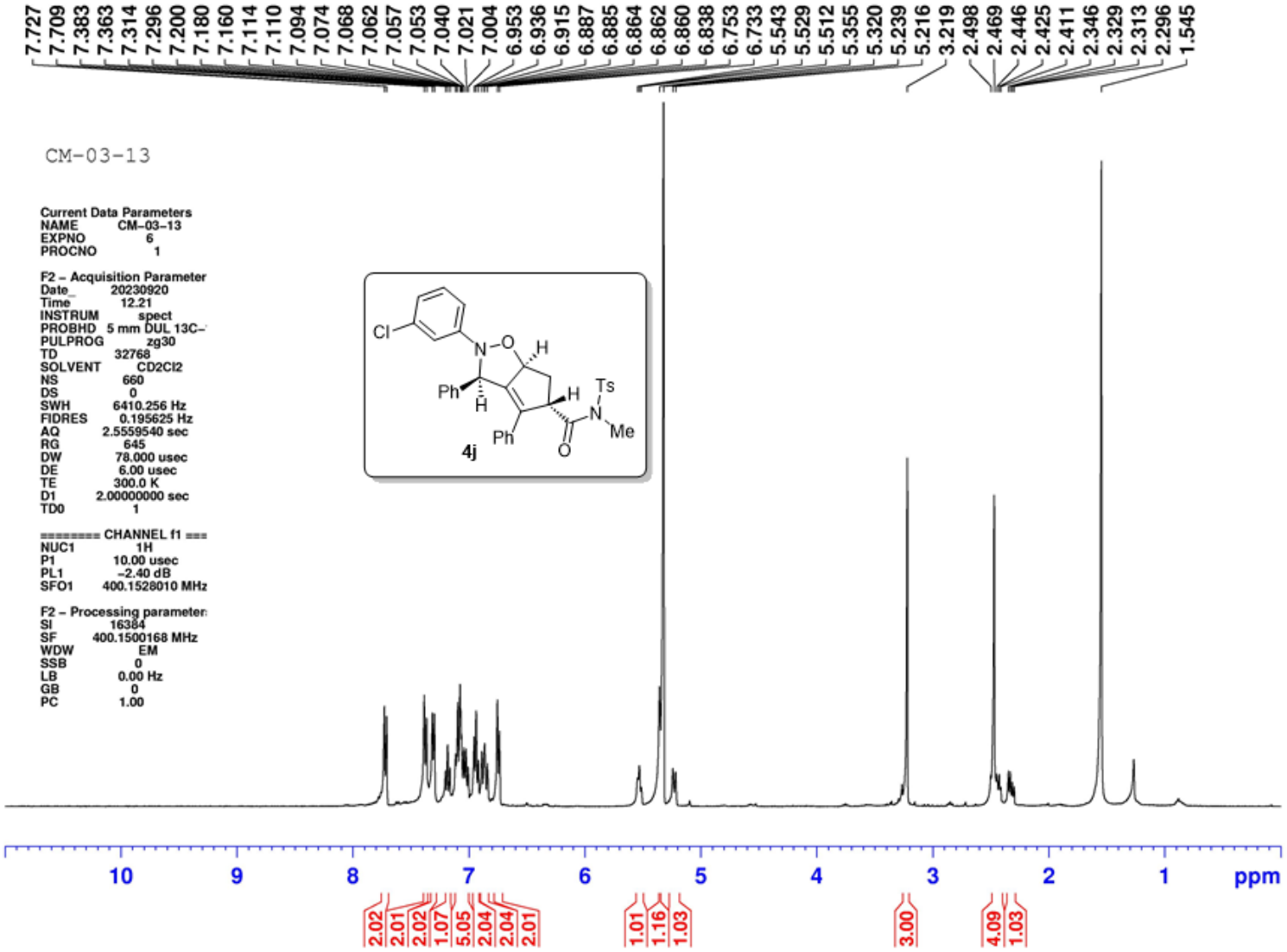

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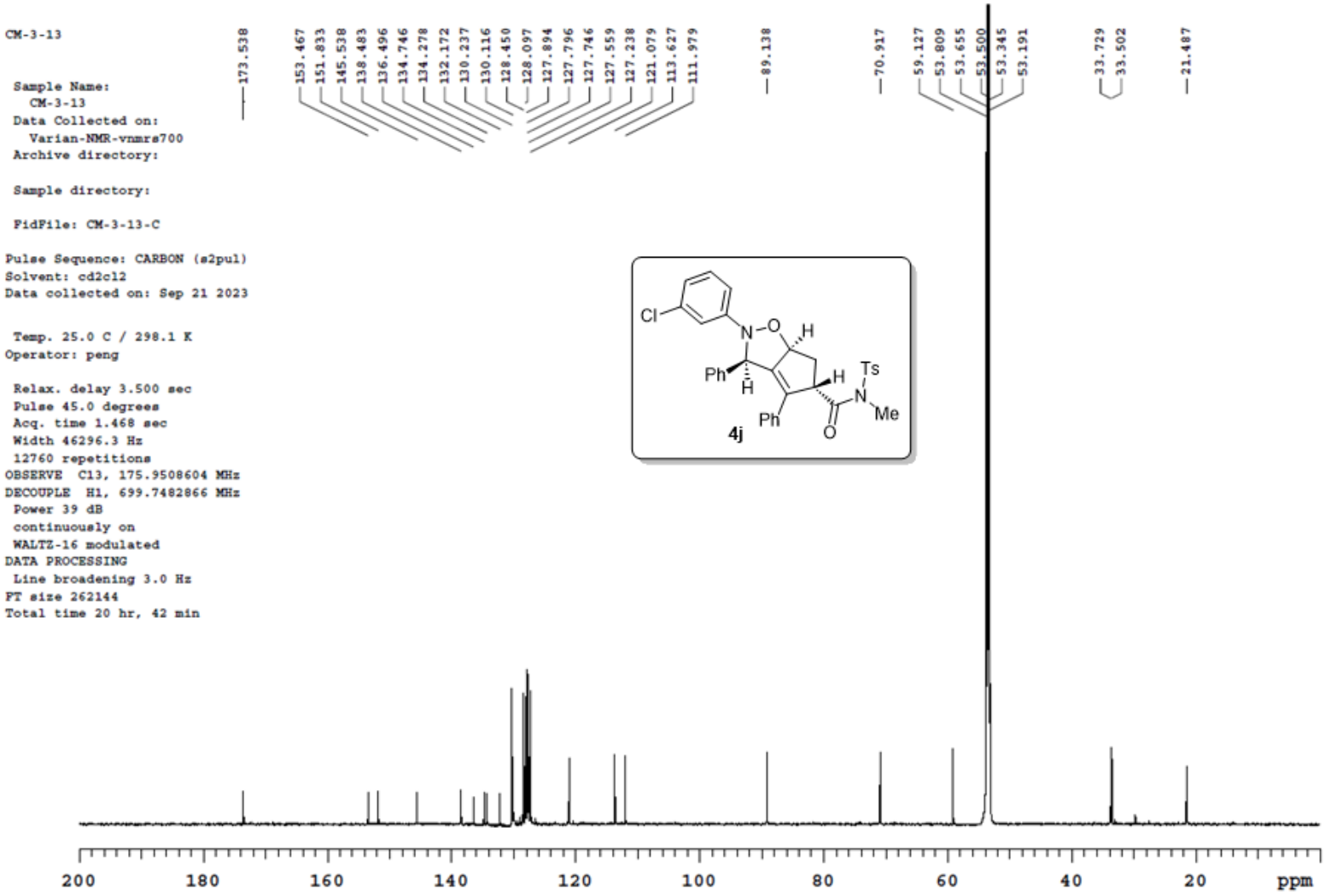

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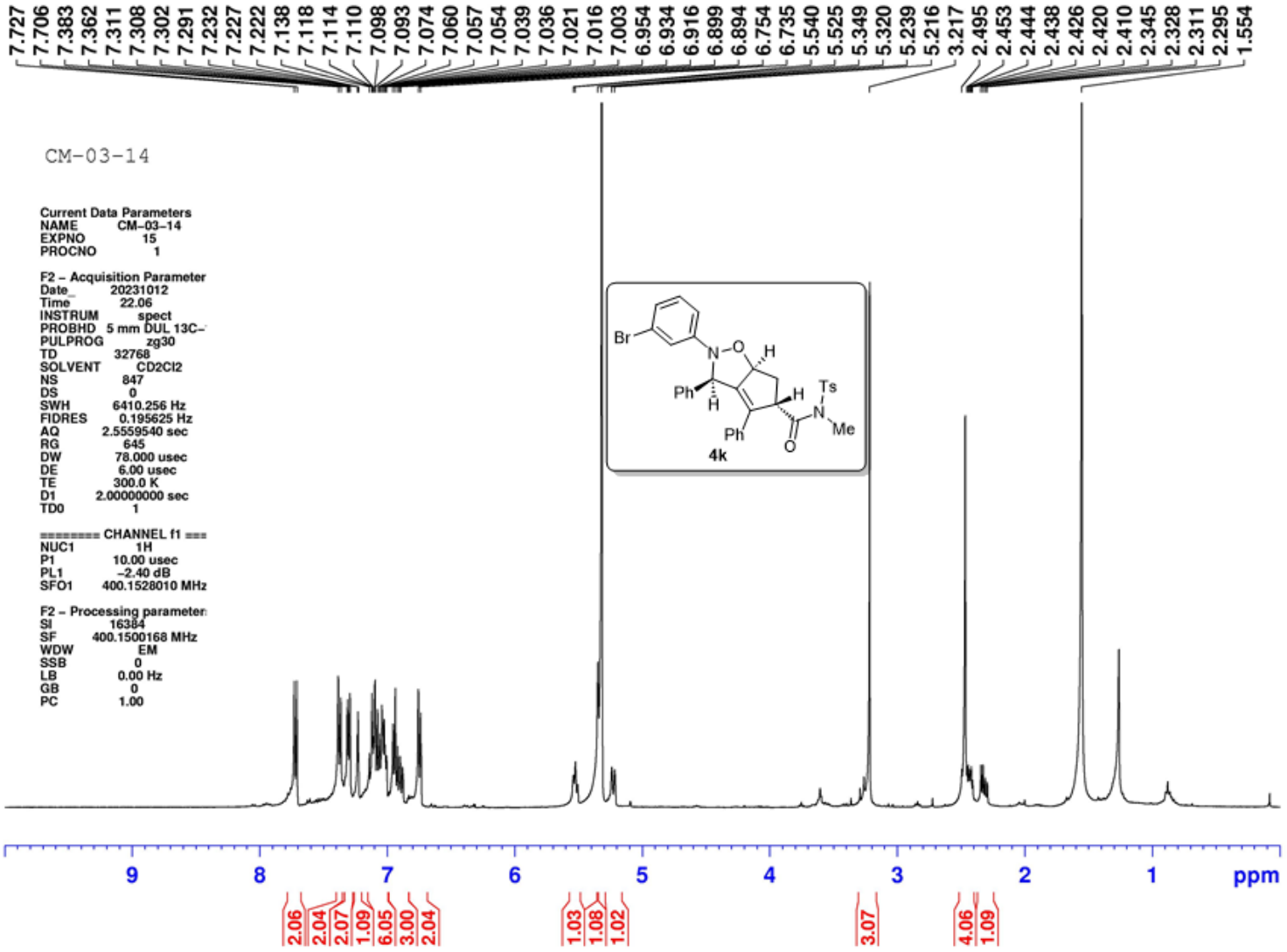

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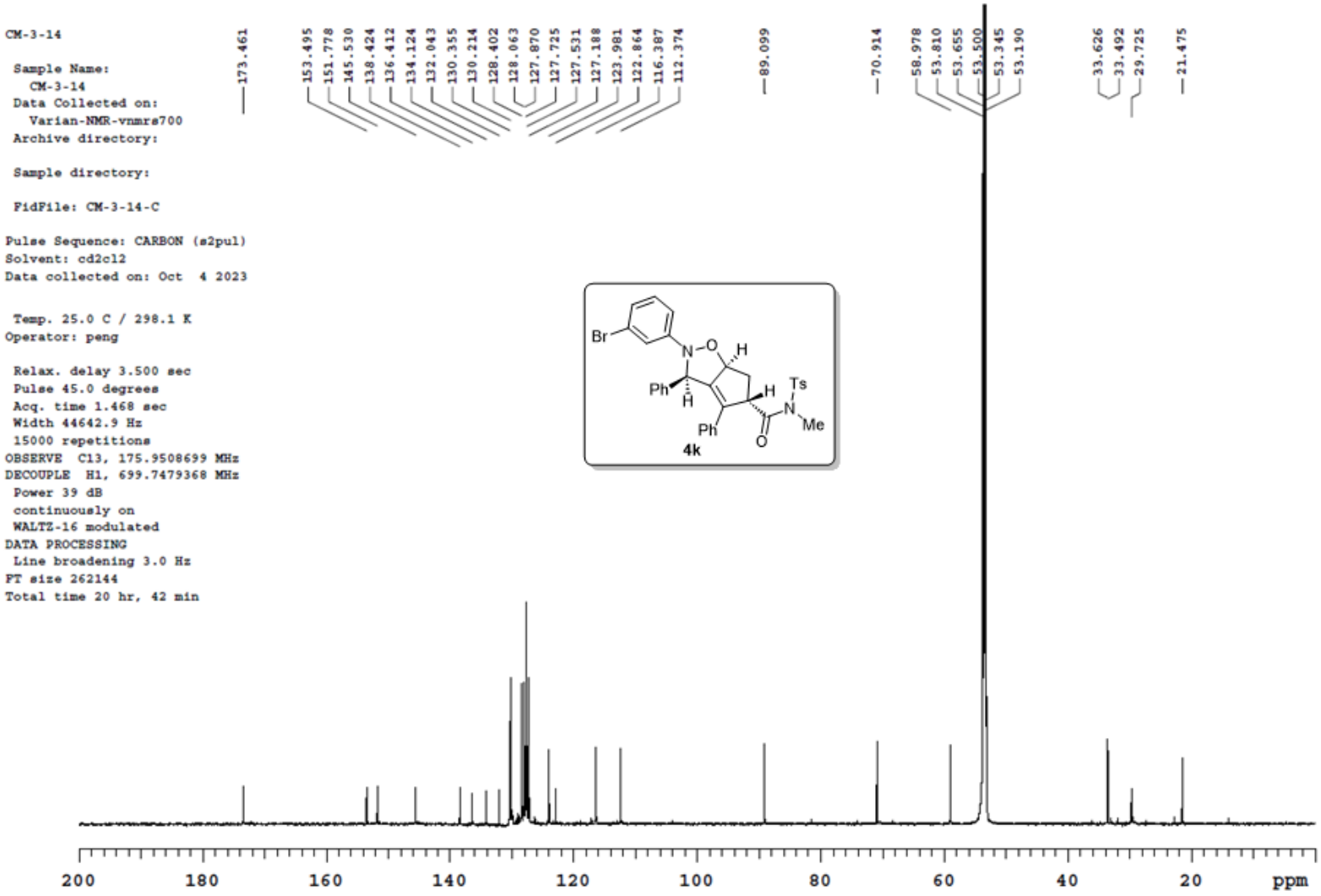

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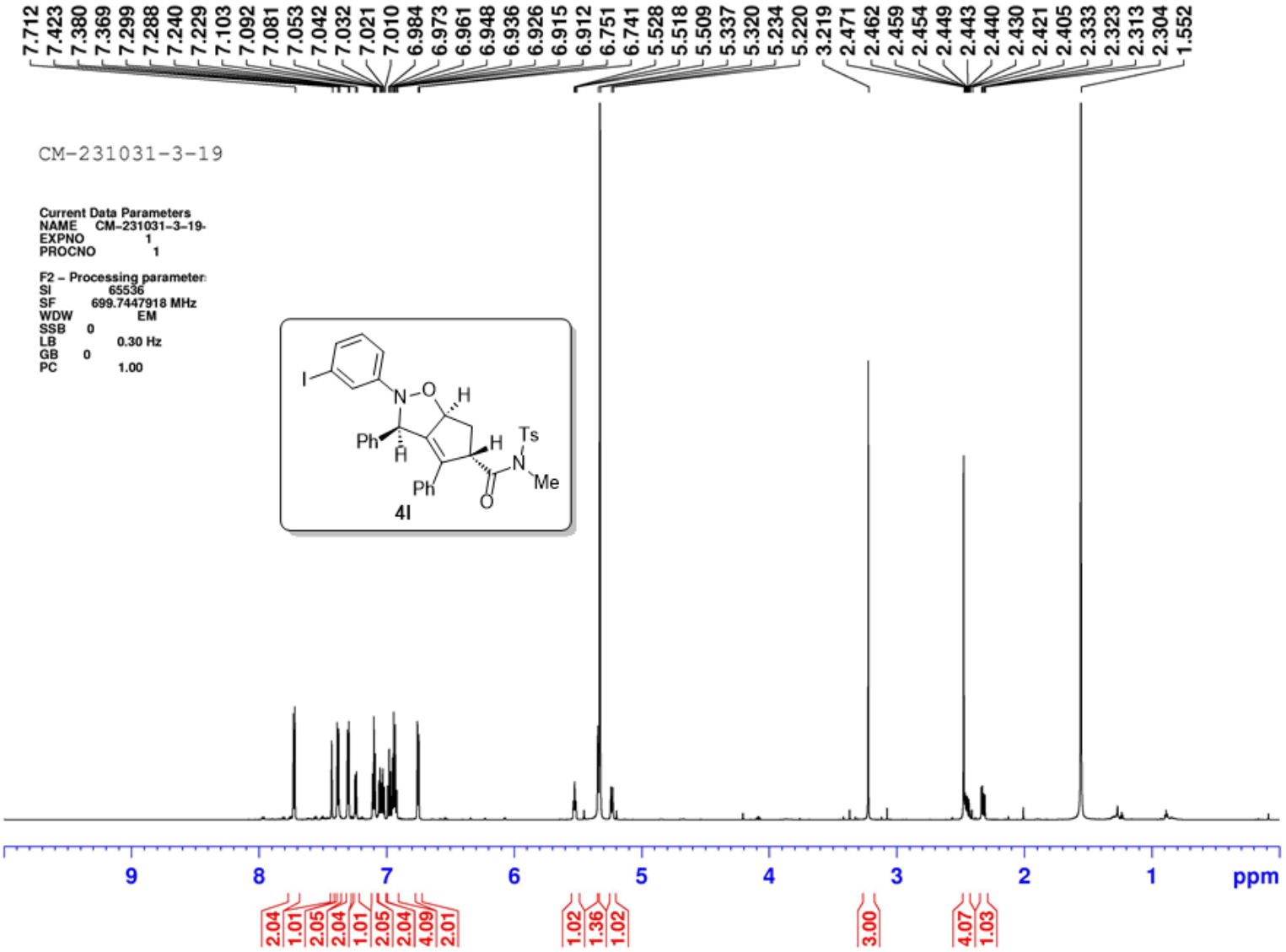

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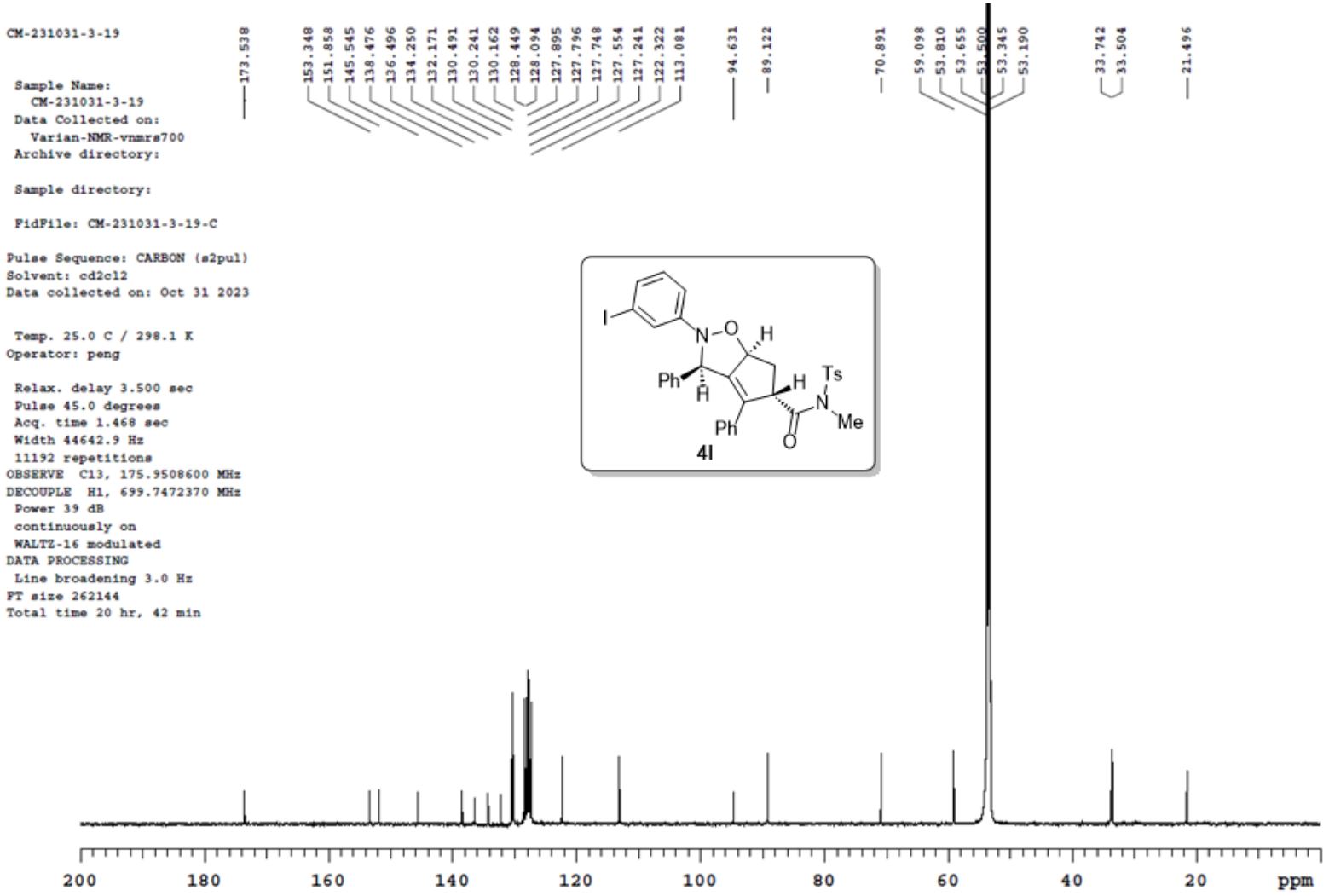

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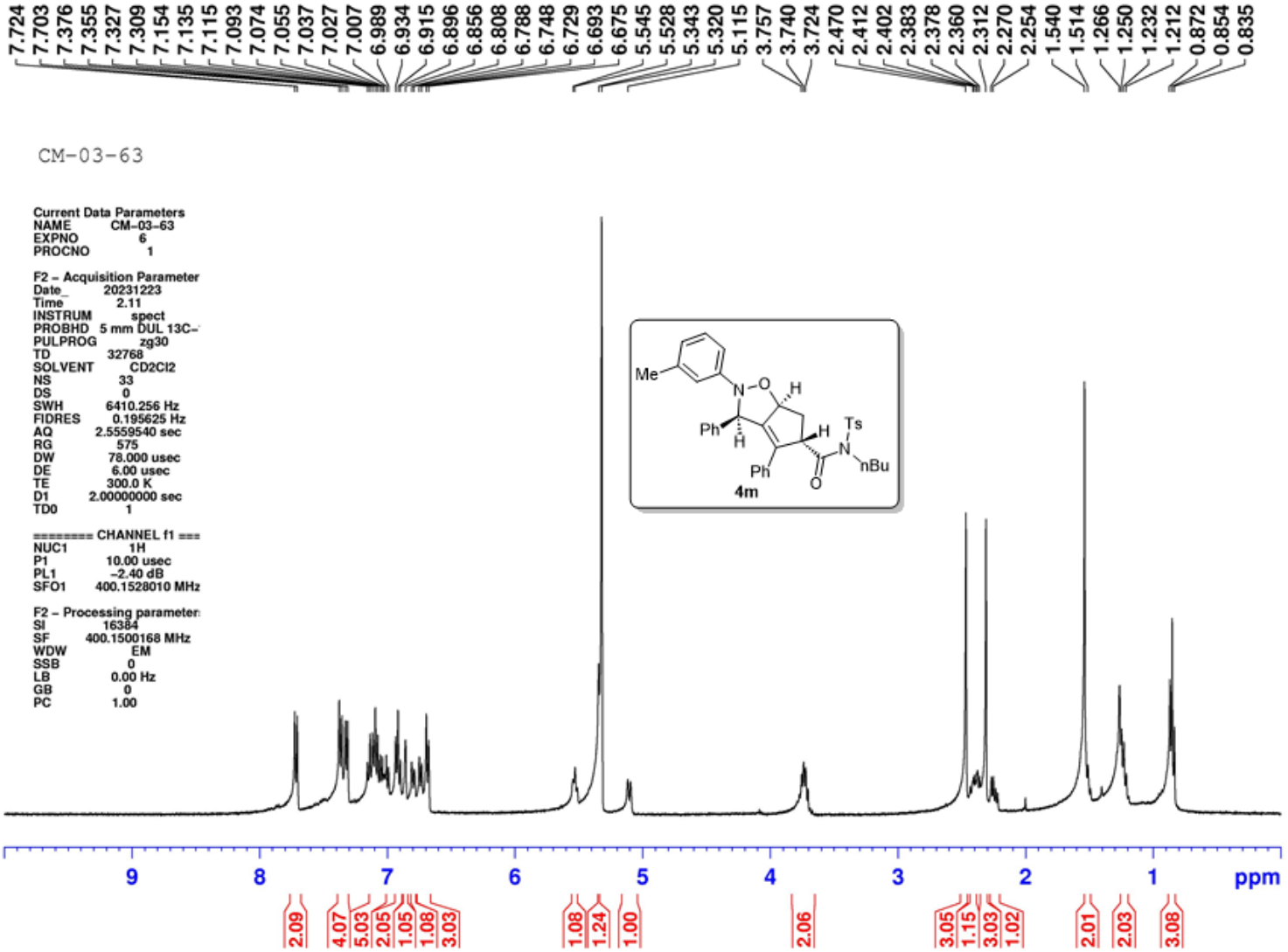

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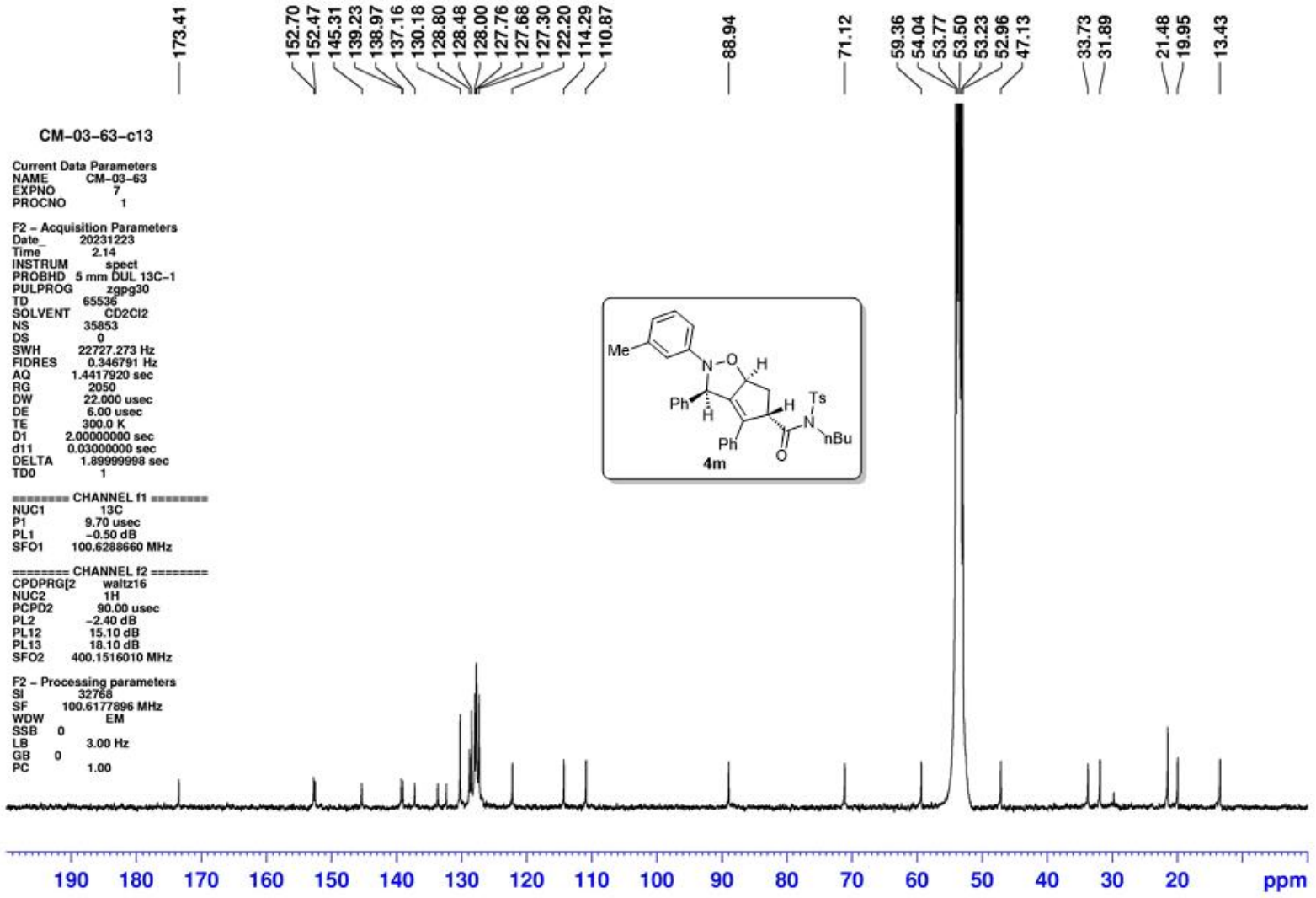

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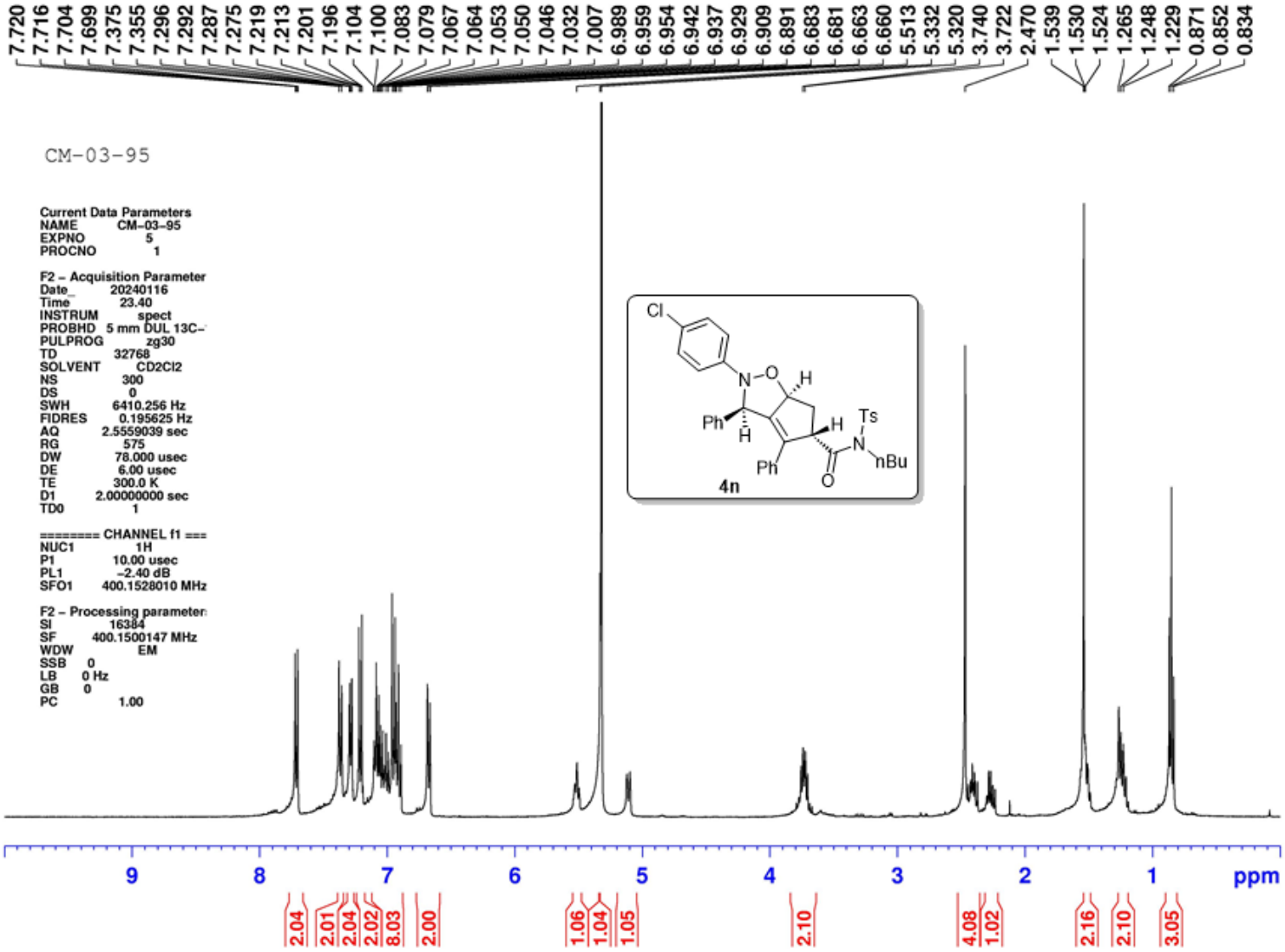

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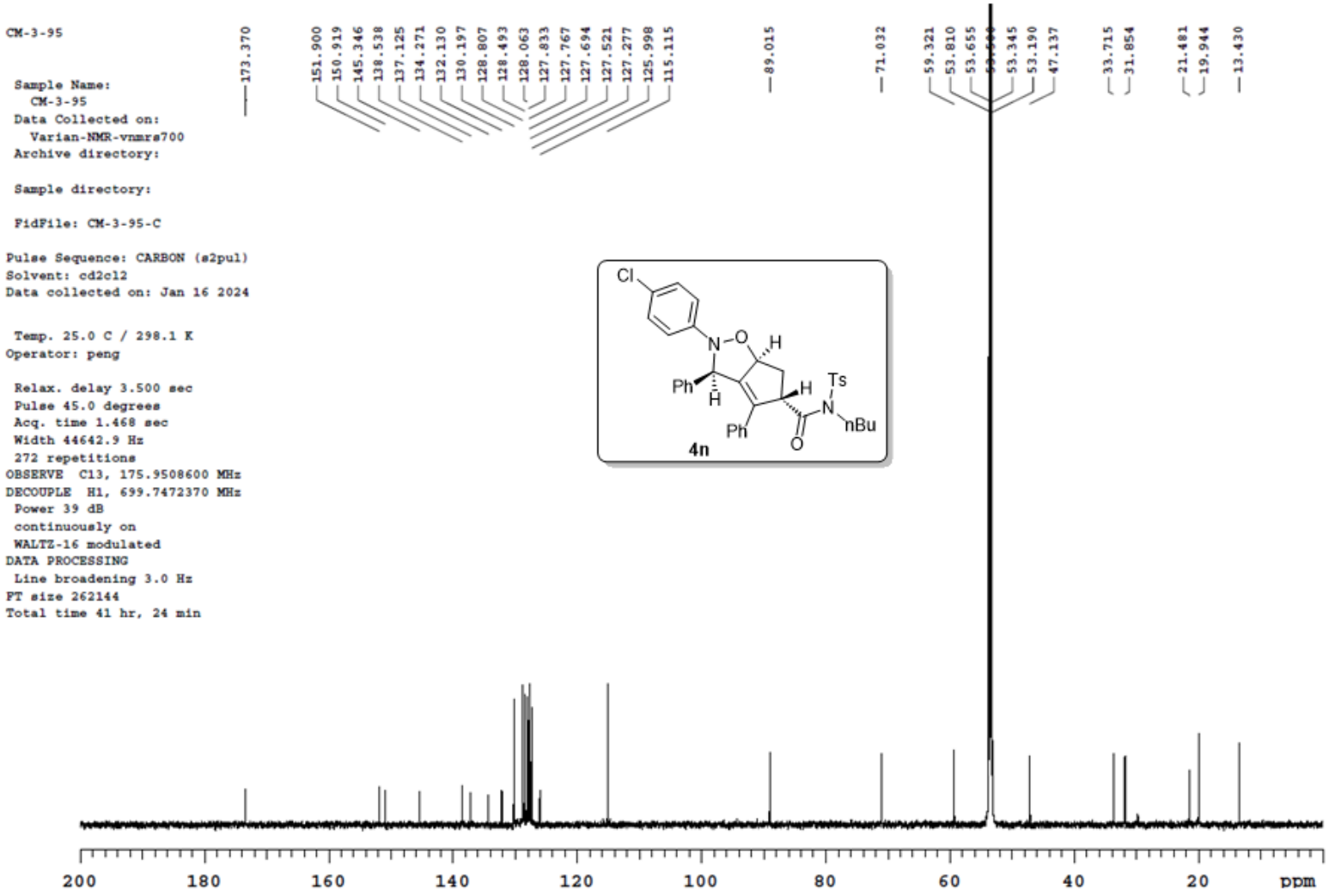

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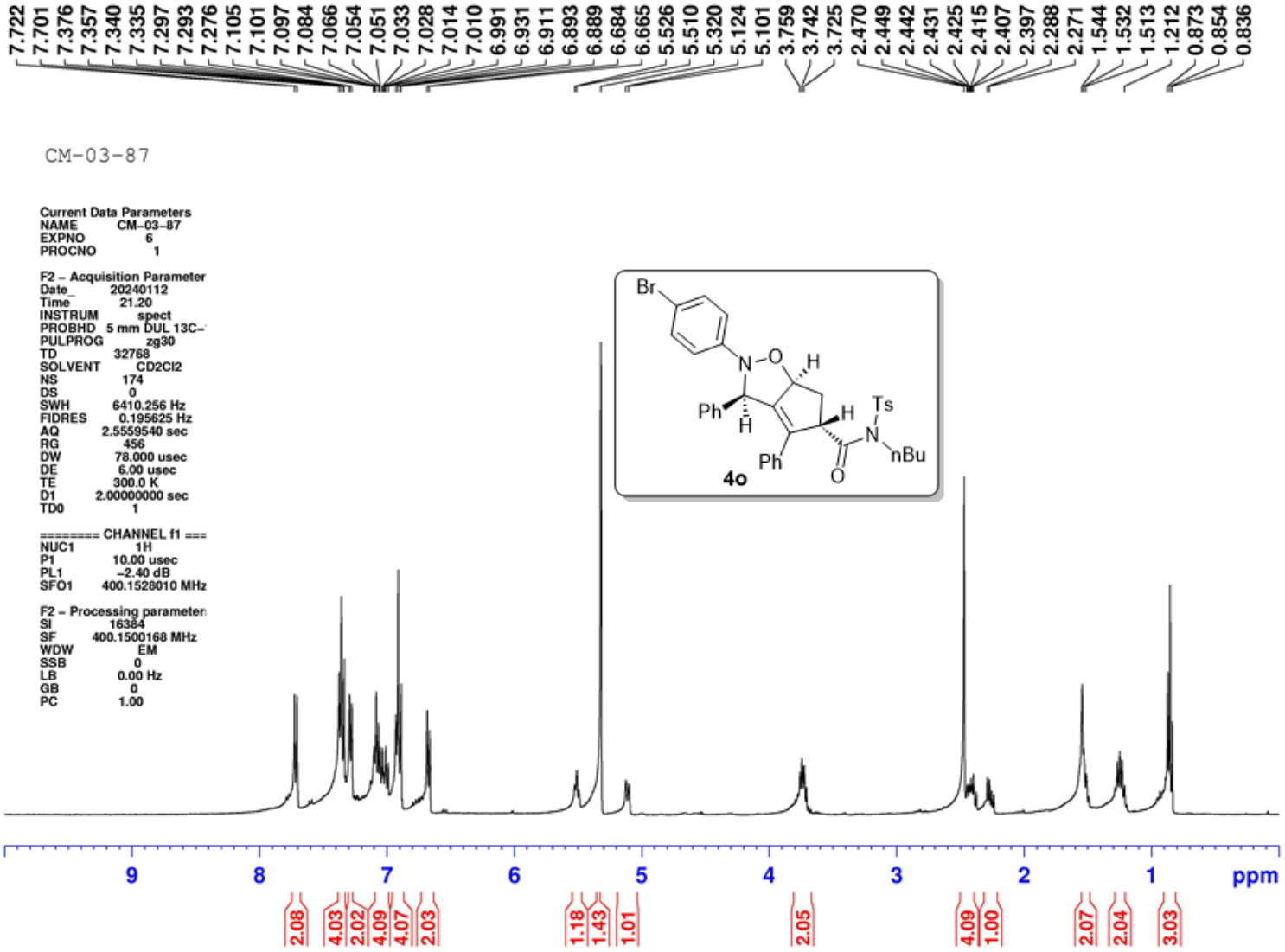

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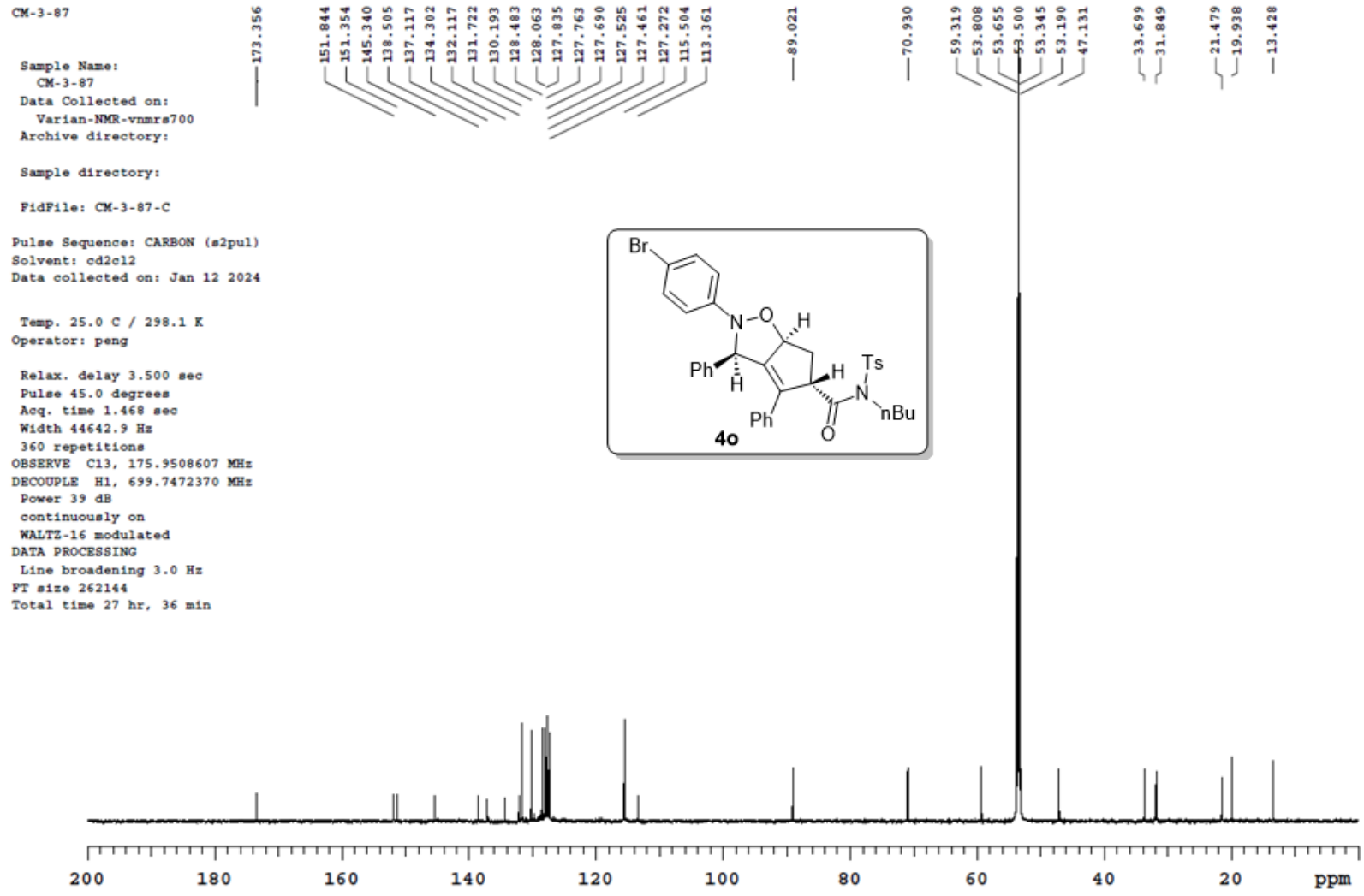

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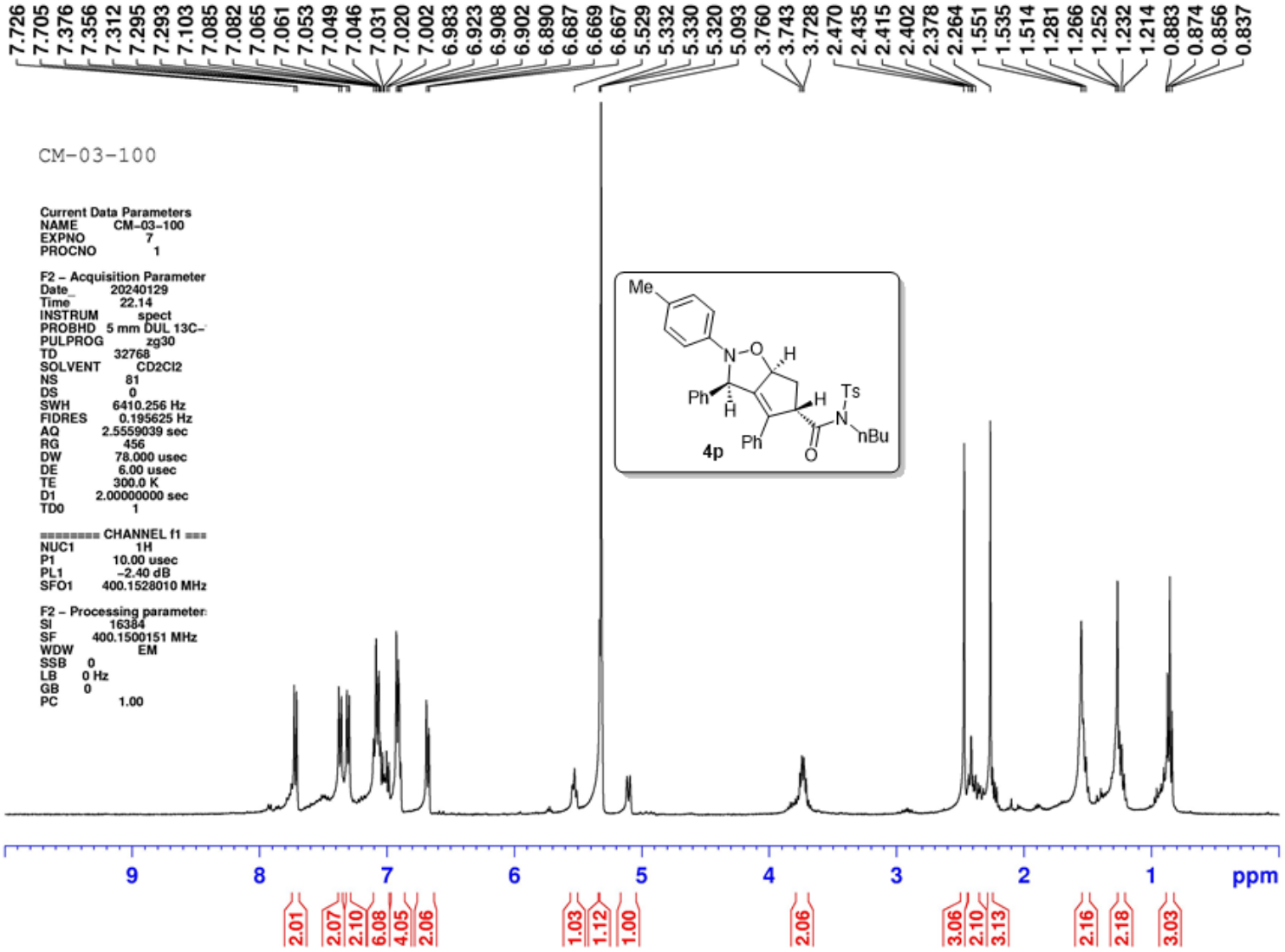

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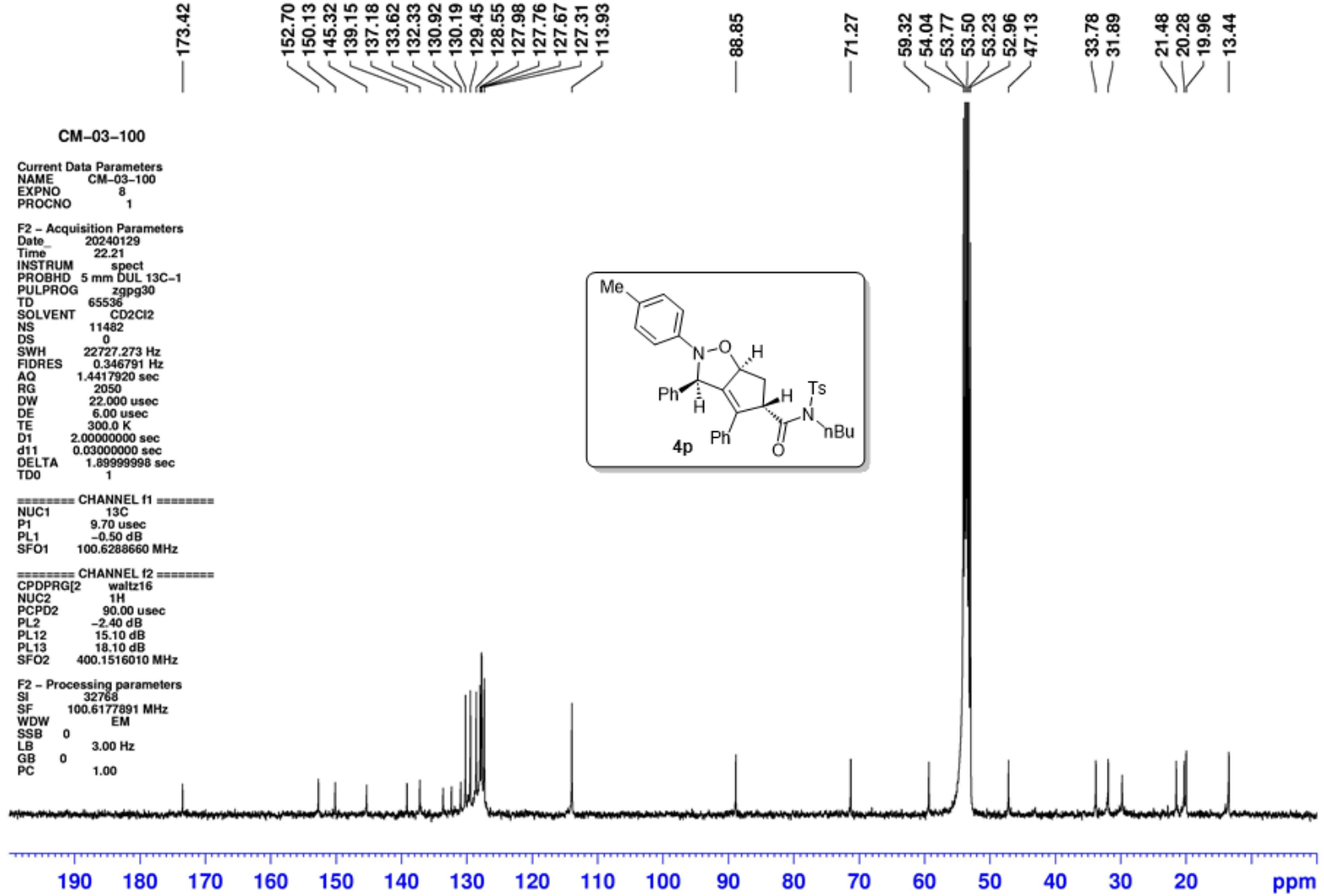

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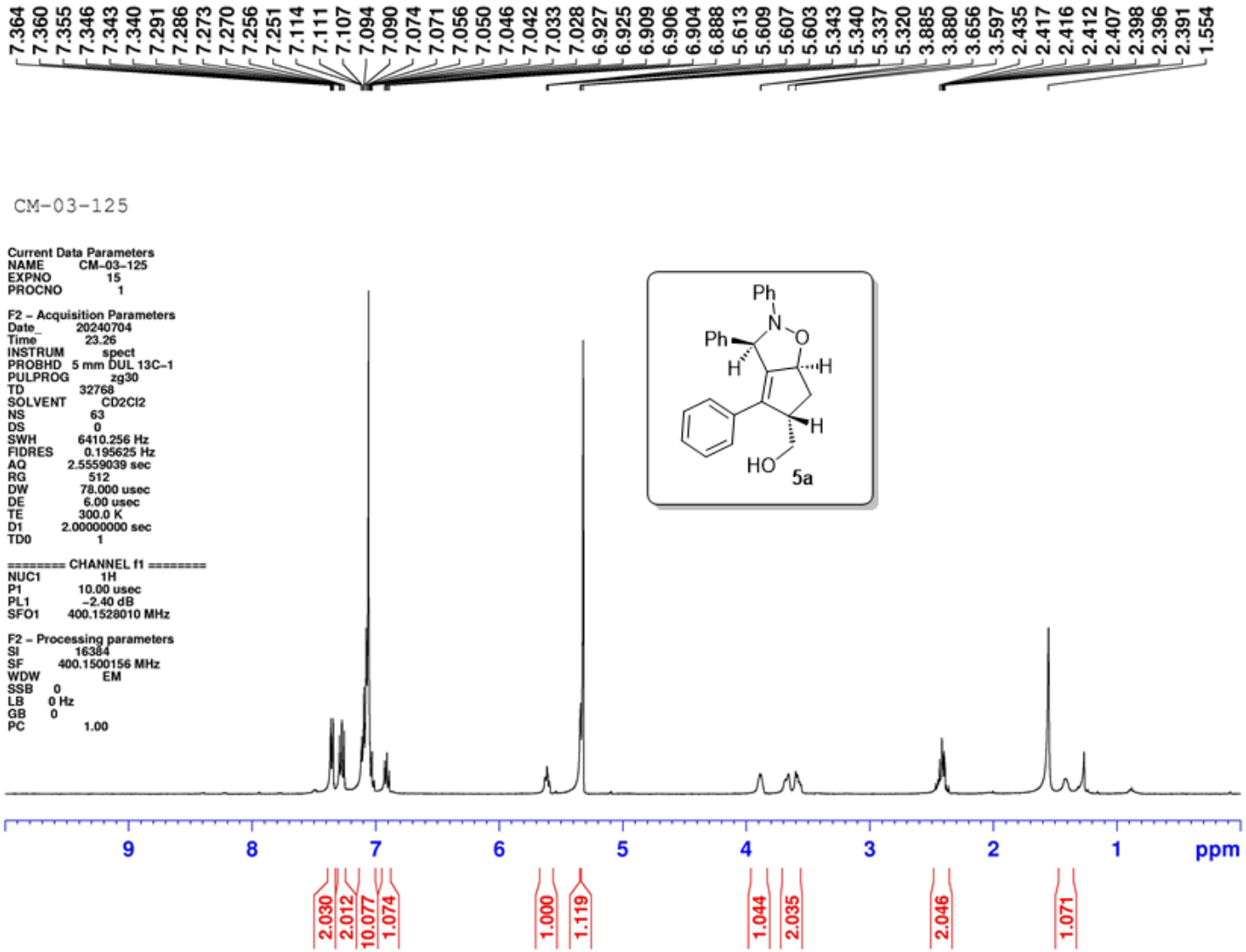

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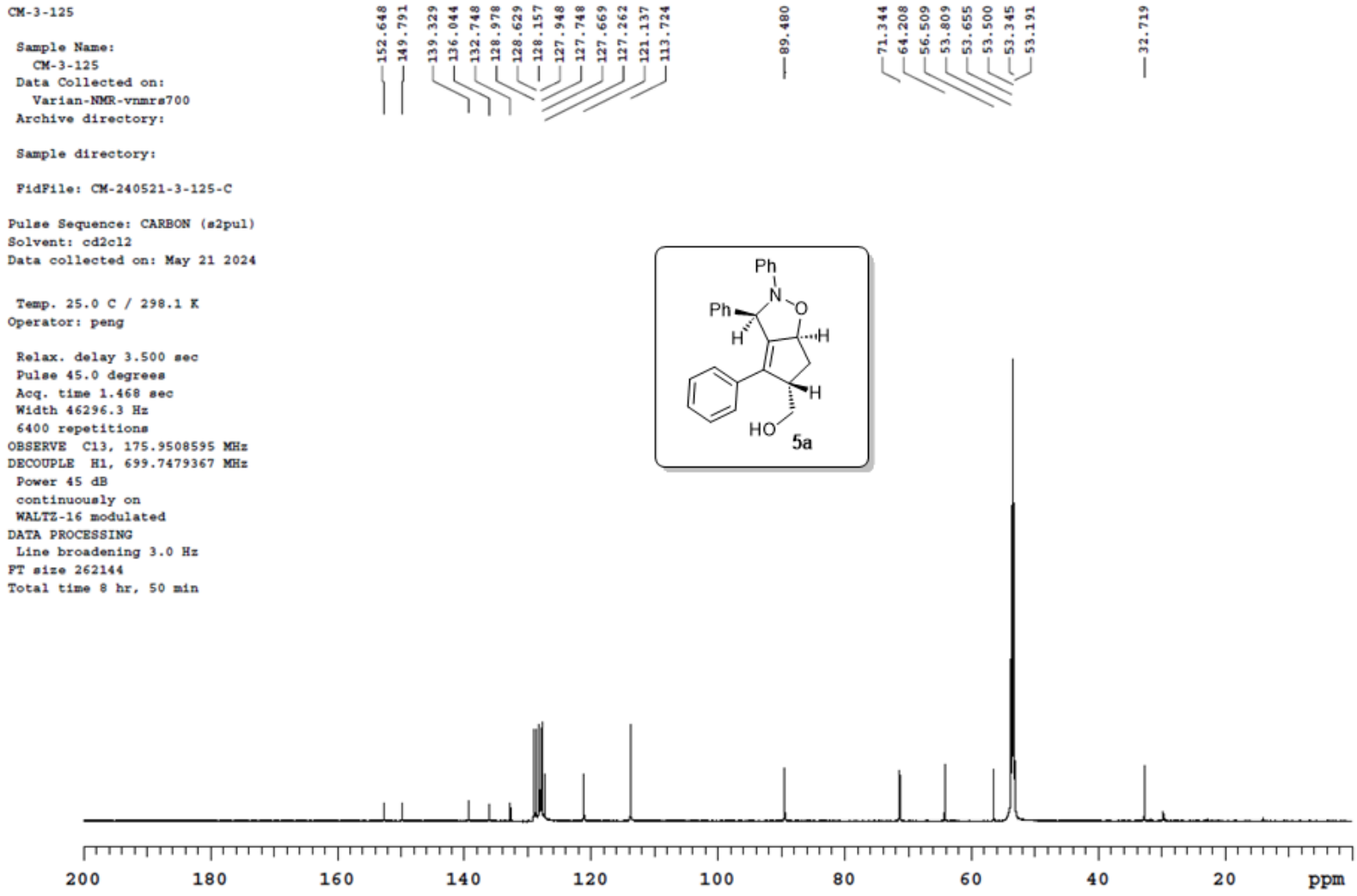

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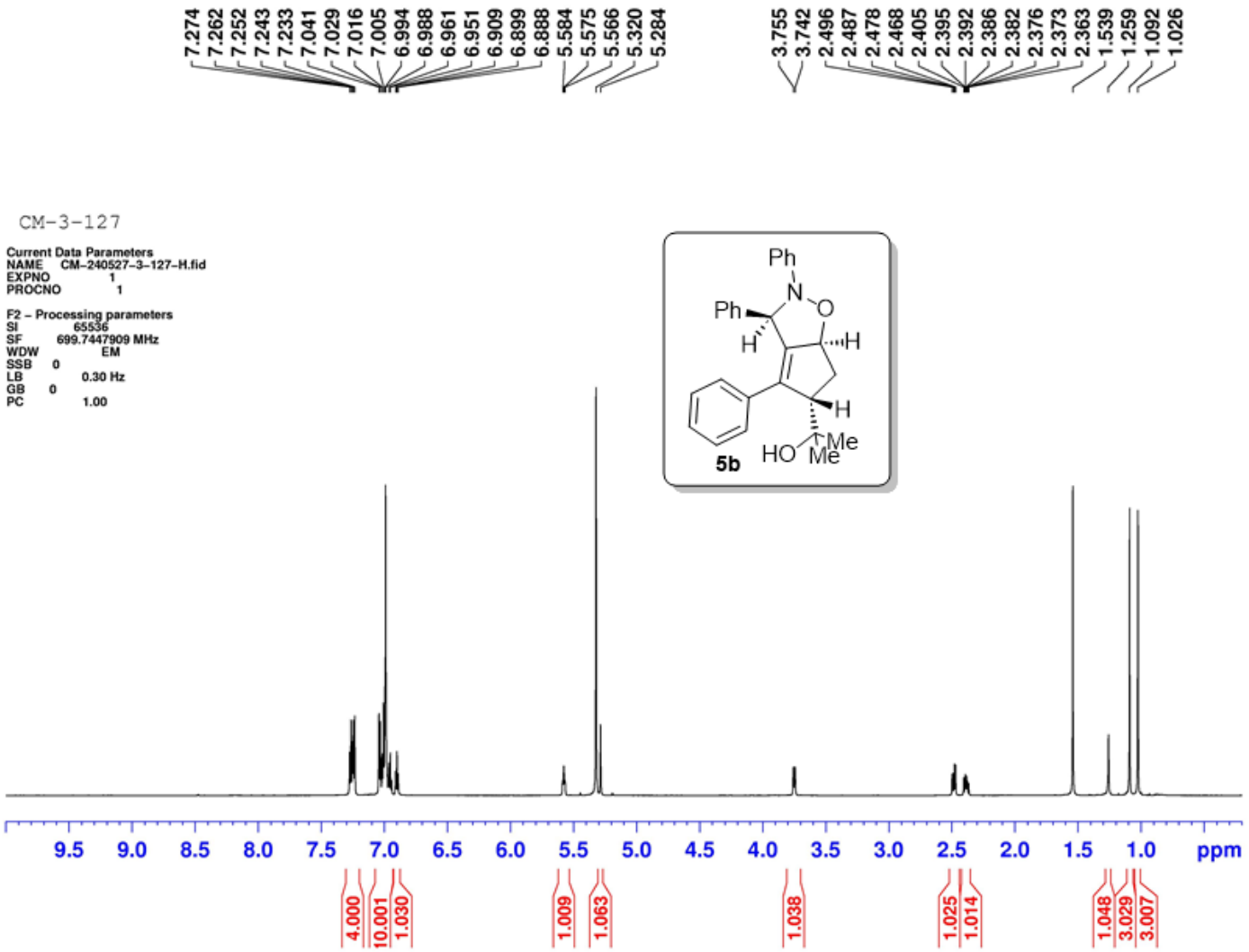

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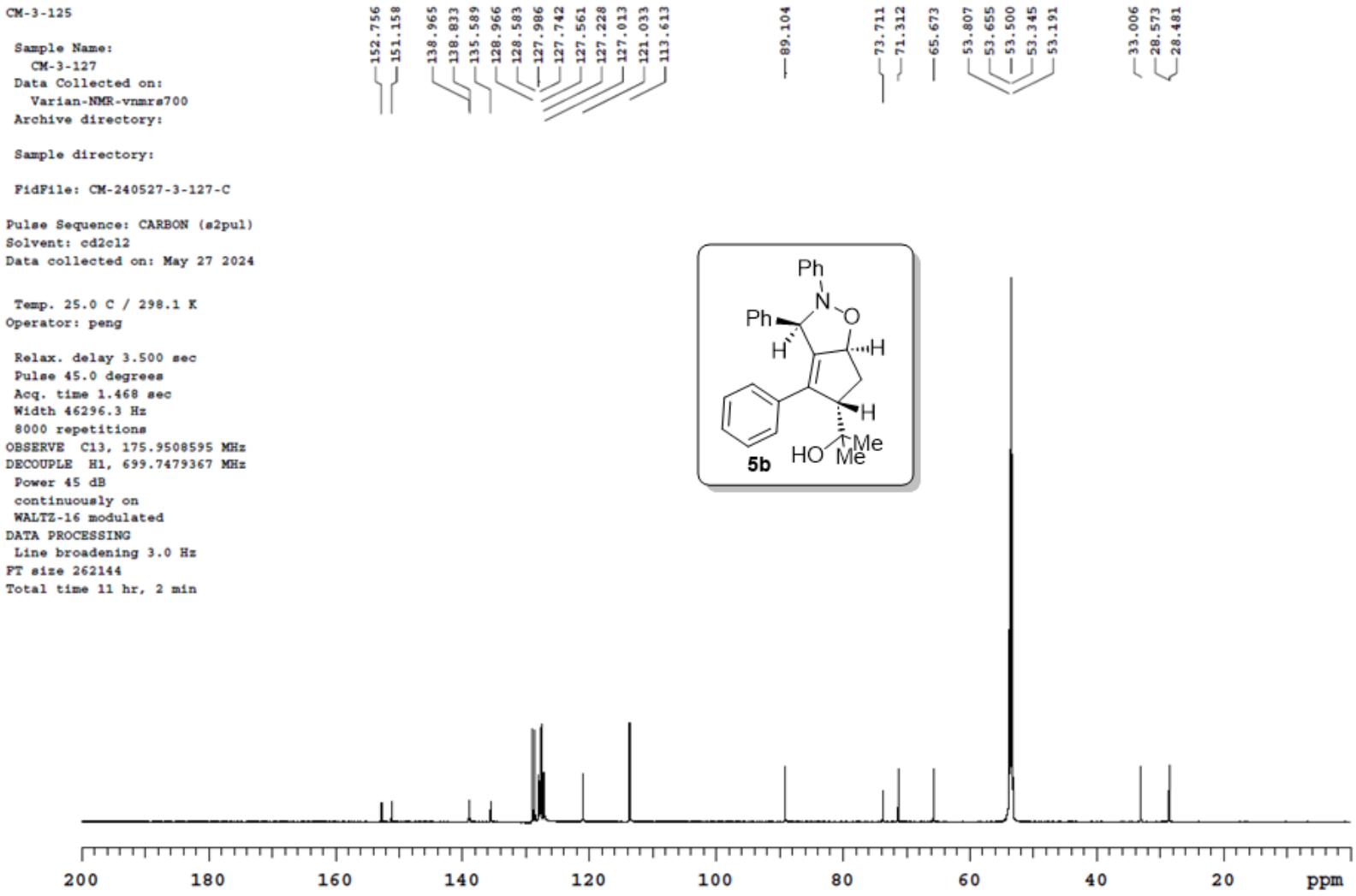

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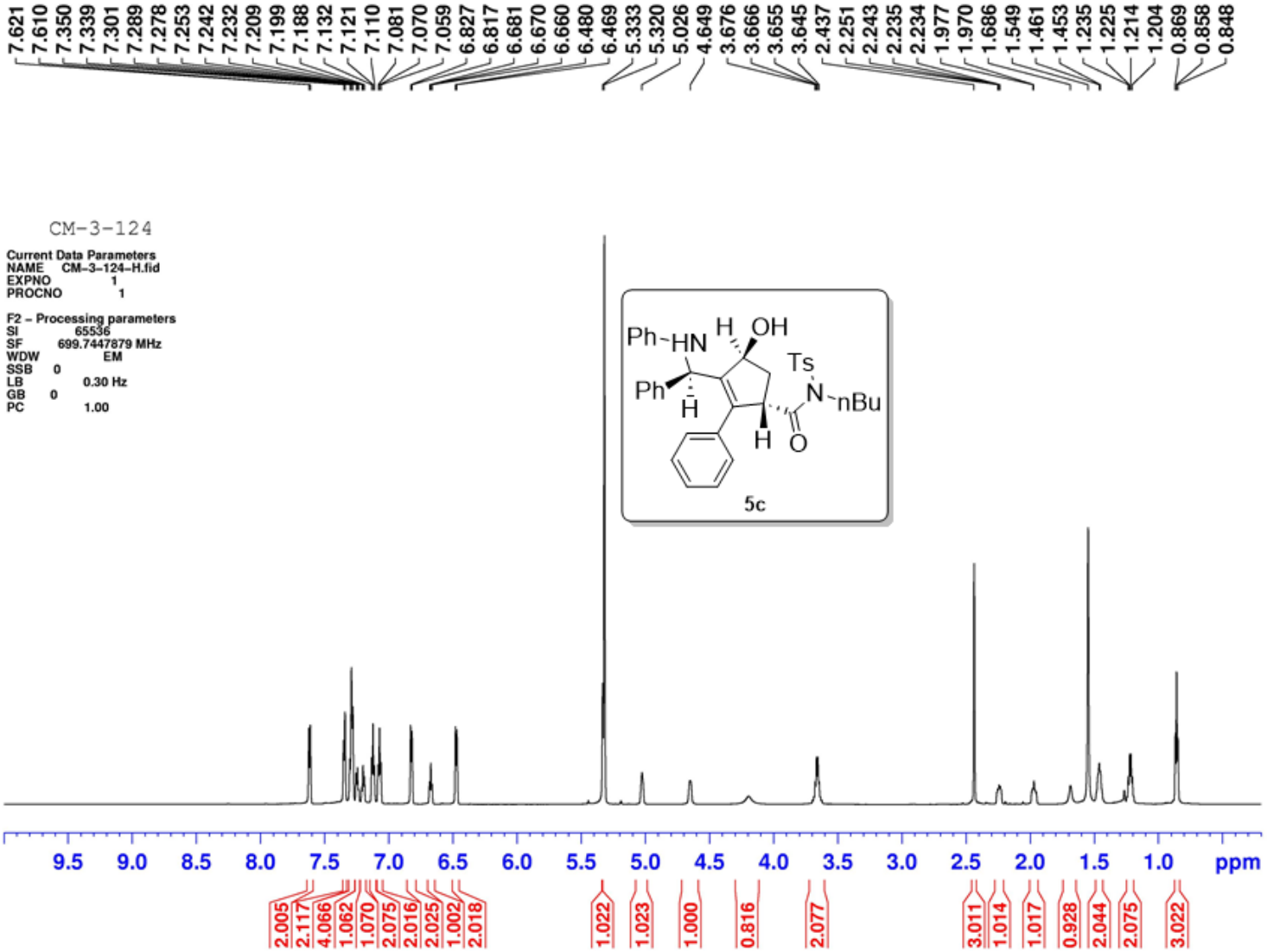

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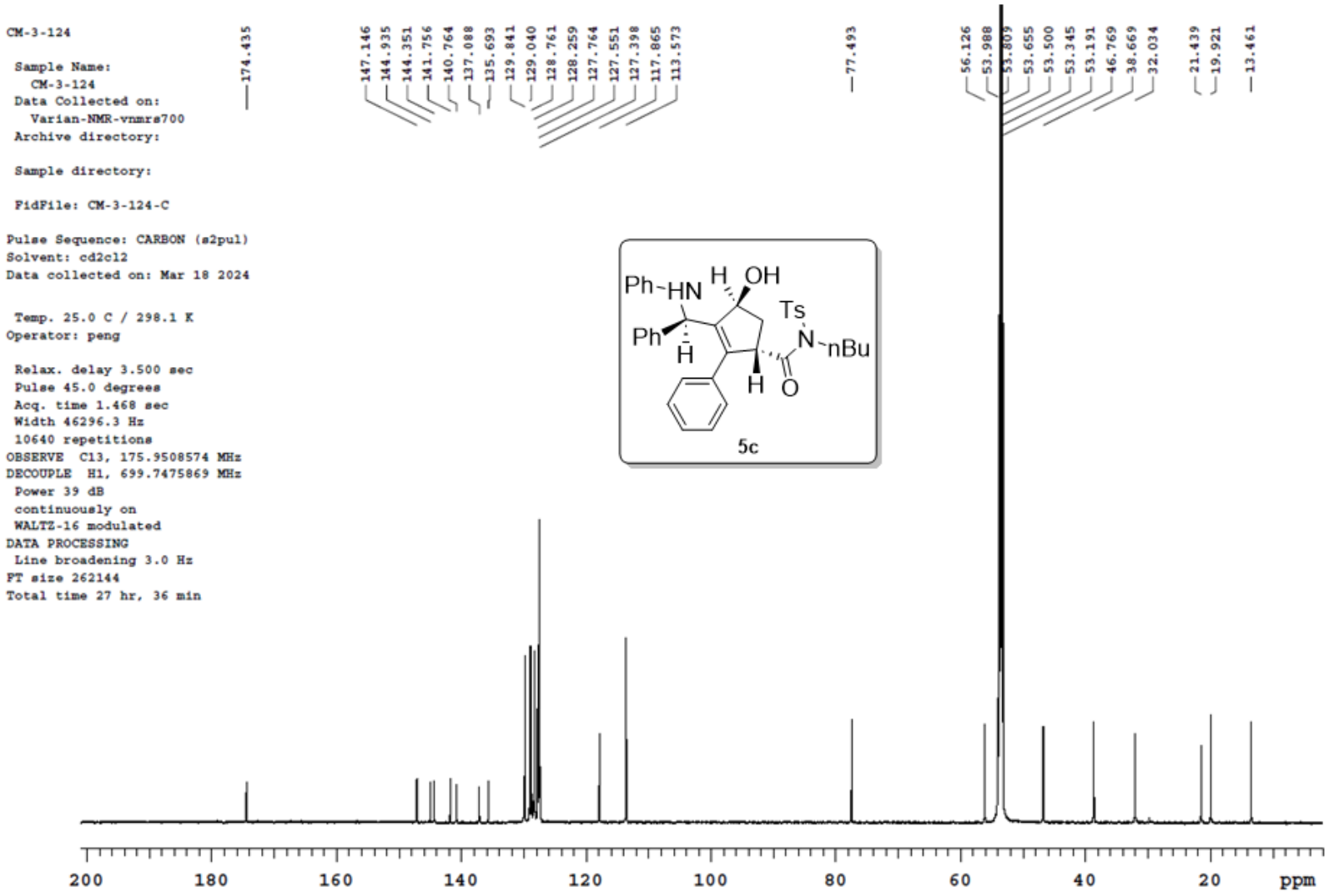

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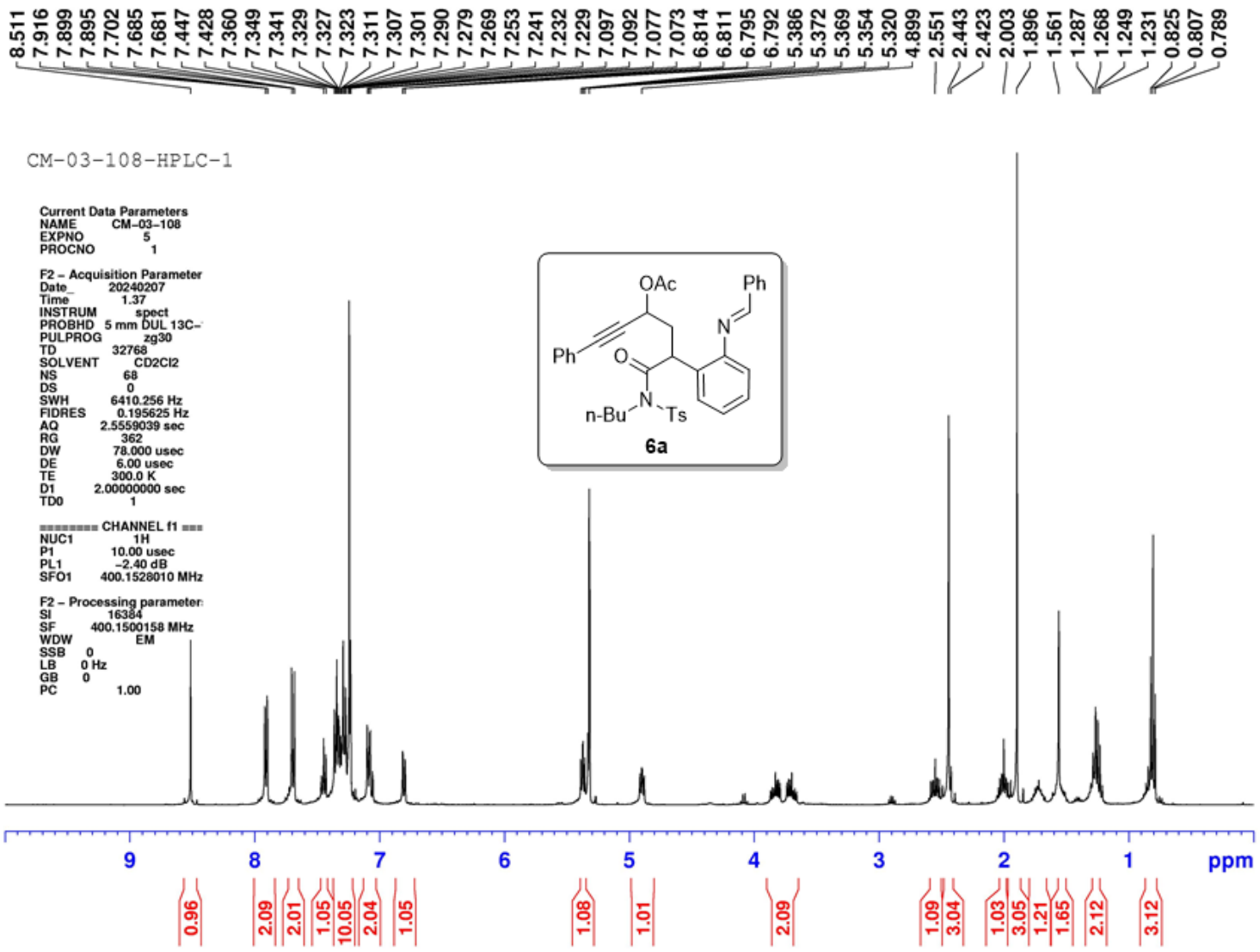
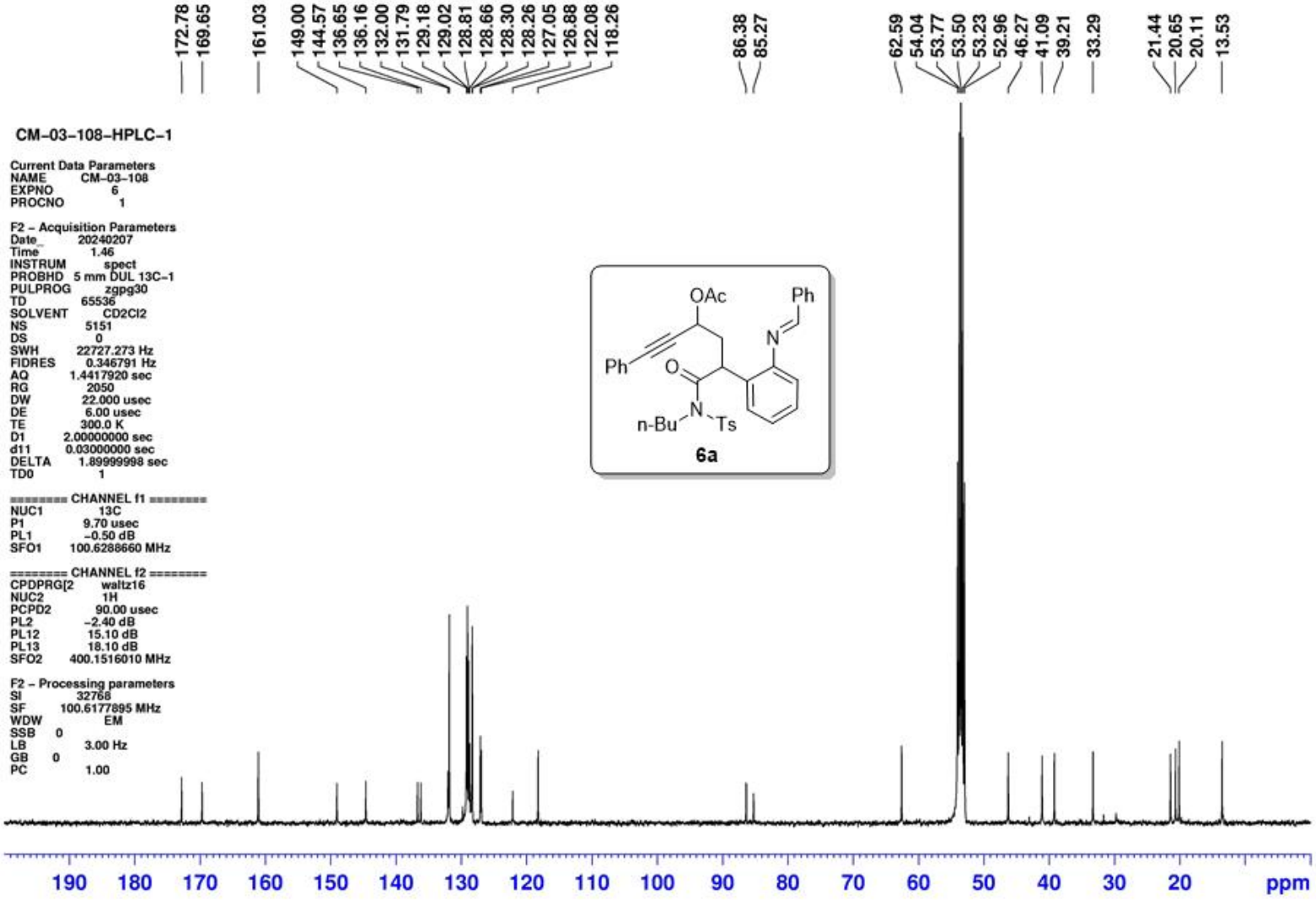


^{13}C NMR (CD_2Cl_2, 100 MHz)



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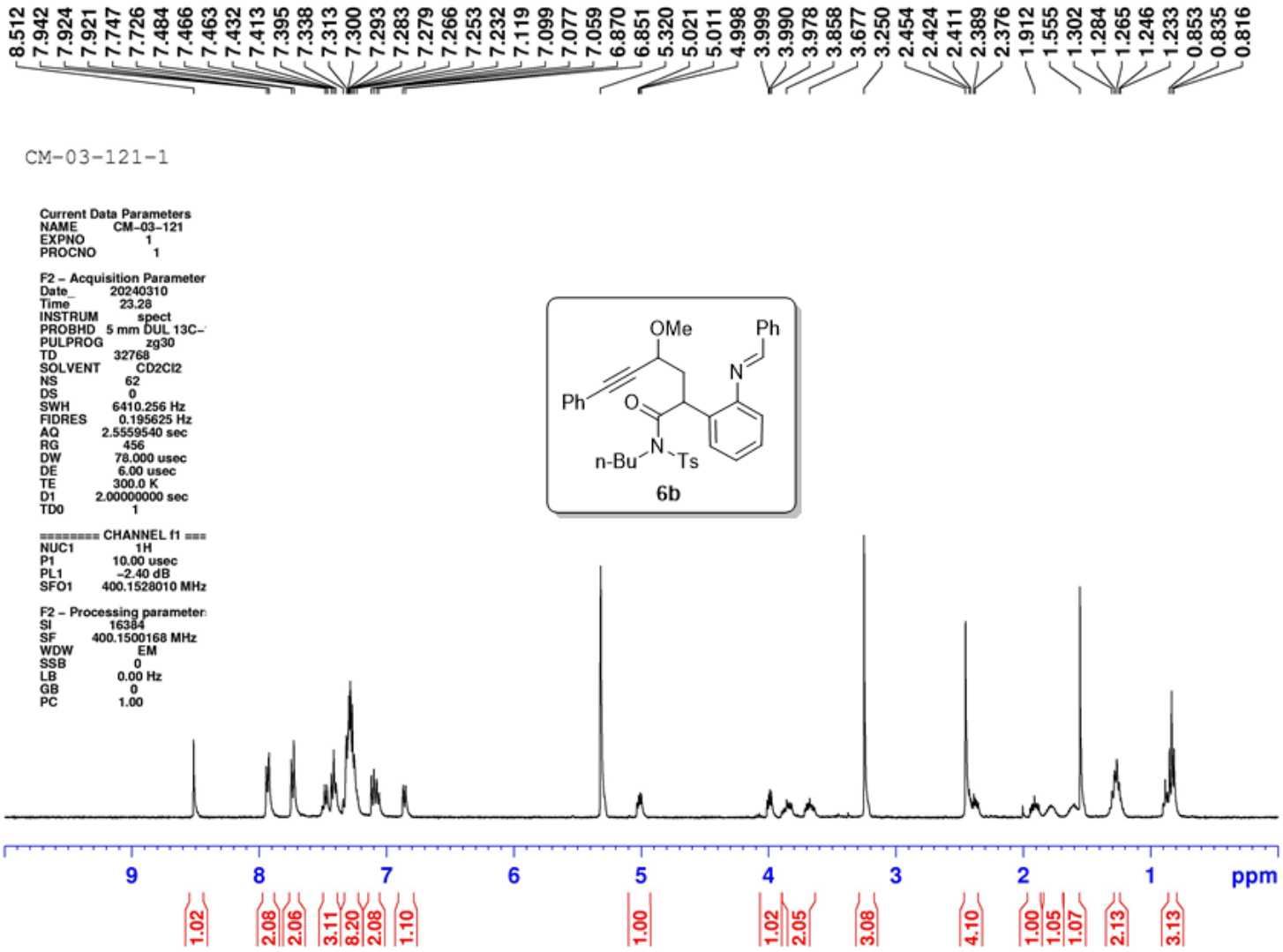

^{13}C NMR (CD_2Cl_2, 175 MHz)