

Reactions of Thioalkynes with Diarylketenes via [3+2]-Annulation Versus Benzannulation using Au and P(C₆F₅)₃ Catalysts.

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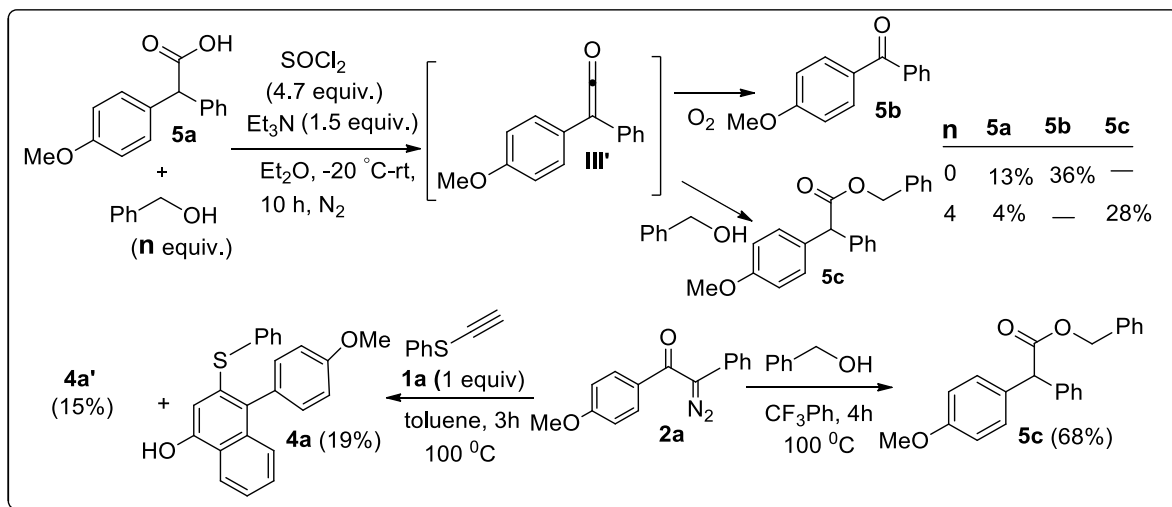
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1. Representative synthetic procedures:

General procedure:

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. DCM, diethyl ether and toluene were distilled from CaH₂ under nitrogen. THF was distilled from Na metal under nitrogen. Other solvents like Acetonitrile, Trifluoromethyl benzene and DMSO were used from commercial sources without further distillation. All other commercial reagents were used without further purification, unless otherwise indicated. ¹H NMR and ¹³C NMR spectra were recorded on a Varian 700 and 500 MHz, Bruker 400 MHz spectrometers using chloroform-*d* (CDCl₃) as the internal standard. High-resolution mass spectral analysis (HRMS) data were measured on JMST100LP4G (JEOL) mass spectrometer or a TOF mass analyzer equipped with the ESI source, JEOL Model: JMS-T200GC AccuTOF GCx equipped with FD (field desorption) source and Magnetic Sector Mass Analyzer (MStation) equipped with the EI source. Single-crystal X-ray diffraction intensity data were collected on a Bruker X8 APEX diffractometer equipped with a CCD area detector and Mo K α radiation ($\lambda = 0.71073$ Å) at 100 K; all data calculations were performed by using the PC version of the APEX2 program package.

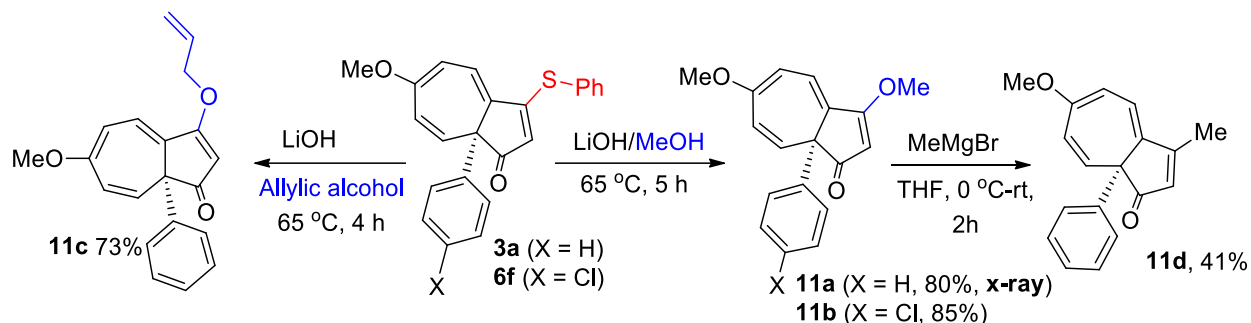
(a) Scheme s1: Ketene precursors from acyl chlorides



We attempted the authentic ketene **III** from a standard procedure, via treatment of diarylacetic acid **5a** with SOCl₂ (4.7 equiv) and Et₃N (1.5 equiv) under N₂, and after the workup, we obtained diaryl ketone **5b** in 36% yield from the oxidation with residual air.^{s5} To examine the efficiency of ketene formation, we treated the solution with benzyl alcohol, but affording the desired ester **5c** only in 28% yield. Accordingly, this procedure is inappropriate for further investigation. We sought an alternative method with α -diazo ketone **2a** through a thermal treatment in hot toluene. This method is more efficient to generate ketene (**III**) because the trap with benzyl alcohol afforded the ester **5c**

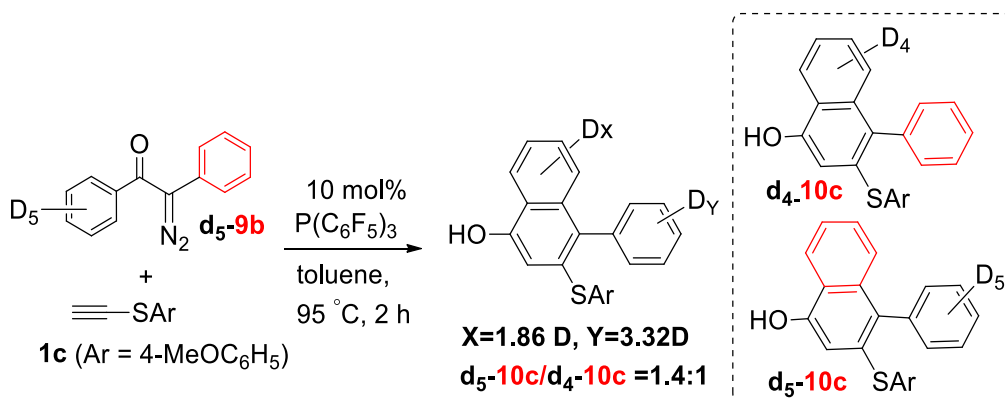
in 68% yield. Treatment of a mixture of thioalkyne **1a** with diazo ketone **2a** in hot toluene yielded **1** in 19% yield together with an unknown byproduct **4a'** in 15% yield. Byproduct **4a'** arose from two discrete diazoketones **2a** and one thioalkyne **1a**. The structure of compound **4a** was inferred from its relative **4b**; improved yield of compound **4a** is achieved with phosphine catalysts that also leads to disappearance of byproduct **4a'** (vide infra).

(b) Scheme s2: Chemical functionalization of compounds 3a and 6f



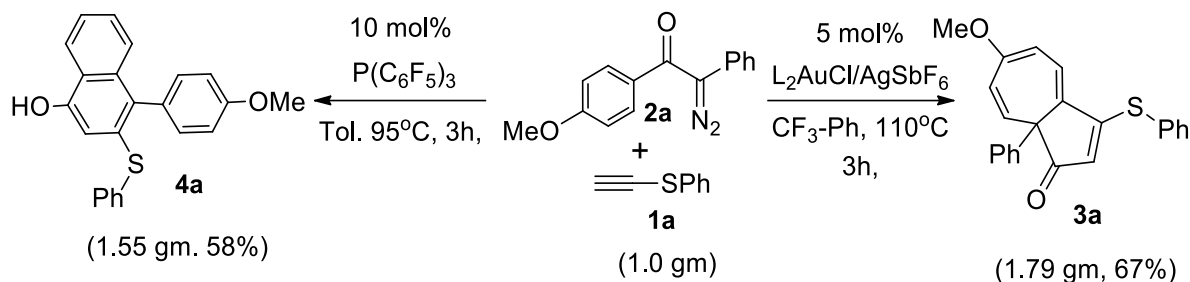
Scheme S2 shows subsequent functionalizations of two selected azulene-1-ones **3a** and **6f**. We first removed the phenylsulfide moiety via treatment with LiOH/MeOH to afford methoxy-derived products **11a** and **11b** in 80% and 85% yields respectively. Further treatment of compound **11a** with MeMgBr yielded species **11d** in 41% yield. We also prepared allyloxy derivative **11c** in 73% yield from species **3a** using a LiOH/allylic alcohol mixture.

(c) Equation s1: Deuterium labeling experiment:



We prepared substrate **d5-9b** bearing a d₅-benzene adjacent to the ketone; this sample afforded two deuterated samples **d5-10c** and **d4-10c** with a respective ratio of 1.4:1 after ¹H and ¹³C NMR analysis.

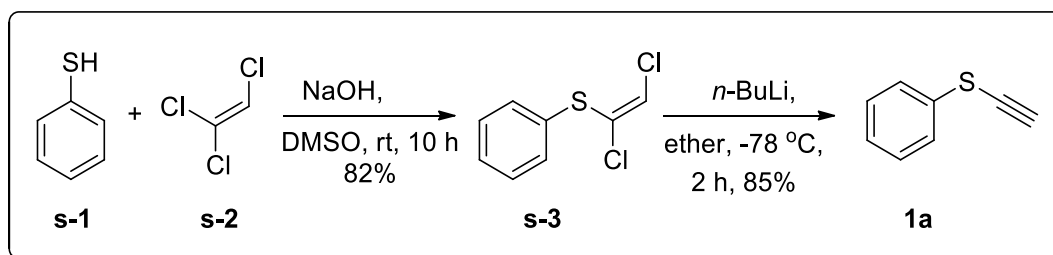
(d) Gram scale reaction for synthesis of Azulene and Naphthol derivatives:



For the azulene **3a** and naphthol **4a**, we follow the same procedure as used in section 3. (a) and (b). we observed desired product **3a** (1.79gm, 67%) and **4a** (1.55gm, 58%) respectively.

2. General procedure for Preparation of Substrates:

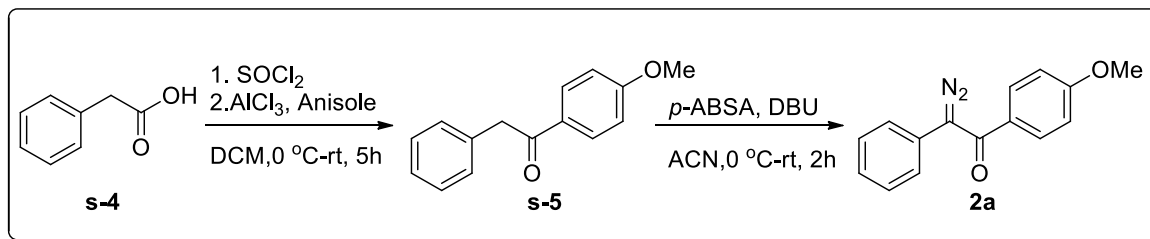
(a) Preparation of Ethynyl(phenyl)sulfane (1a):



In a 100 ml flask was added thiophenol (**s-1**) (3.0 g, 27.3 mmol), DMSO and NaOH (1.65 g, 41 mmol) and the mixture was stirred at room temperature for 8 h before cooling to 0 °C. To this solution was added trichloroethylene **s-2** (5.38 g, 41 mmol). The solution was stirred for 2 h at room temperature. The resulting mixture was diluted with water, extracted with ether and dried over $MgSO_4$. The solution was concentrated and purified on a silica column with hexane, affording (*E*)-(1,2-dichlorovinyl (phenyl) sulfane (**s-3**) as light yellow oil (4.56 g, 22.3 mmol, 82 %). To a ether solution (100 ml) of compound **s-3** (3.6 g, 17.7 mmol) was added *n*-BuLi (28.3 mL, 70.6 mmol) at -78 °C, and the mixture was stirred at the same temperature for 2 h. The reaction mixture was quenched with aq. NH_4Cl solution, extracted with ether, washed with H_2O and dried over $MgSO_4$. After evaporation to dryness, the crude product was purified on a silica column with hexane to afford the desired ethynyl(phenyl)sulfane (**1a**) as light yellow color oil (2.01 g, 15.0 mmol, 85%)^[s1].

Other substrates (**1b-1m**) were synthesized according to reported literature.^[s1]

(b) Preparation of 2-diazo-1-(4-methoxyphenyl)-2-phenylethanone (2a):



To a DCM (60 ml) solution of phenylacetic acid (**s-4**) (3.0 g, 22.03 mmol) was added SOCl_2 (1.91 ml, 26.44 mmol) dropwise at 0 °C. The mixture was warm to room temperature and stirred for 2 h. The resulting solution was cooled to 0 °C, followed by addition of AlCl_3 (2.93 g, 22.03 mmol) and Anisole (2.39 ml, 22.03 mmol). The mixture was stirred at room temperature for 3h. After completion of the reaction. The reaction was quenched with H_2O , extracted with ethyl acetate (2 x 50 mL) and washed with brine (25 mL). The combined organic layers were dried over MgSO_4 , concentrated under reduced pressure, and purified by a silica column (EA/Hexane = 15/85) to afford 1-(4-methoxyphenyl)-2-phenylethanone (**s-5**) white solid (4.0 g, 17.67 mmol, 80%).

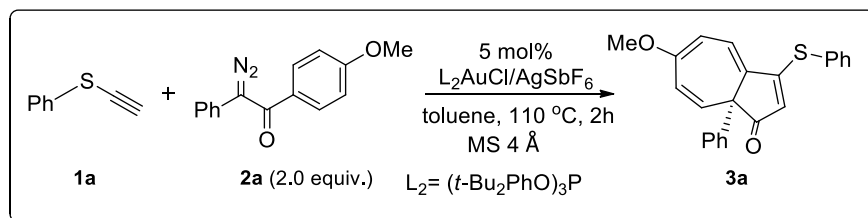
To an acetonitrile (23 ml) solution of 1-(4-methoxyphenyl)-2-phenylethanone (1.0 g, 44.19 mmol) was added *p*-ABSA (1.27 g, 53.03 mmol). The solution was cooled to 0 °C and DBU (0.86 ml, 57.45 mmol) was added dropwise to above mixture and stirred at room temperature for 2 h. The reaction was quenched with H_2O , followed by extraction with ether (2 x 50 mL) and washed with brine (25 mL). The combined organic layers were dried over MgSO_4 , concentrated under reduced pressure, and purified by a silica column (EA/Hexane = 15/85) to afford 2-diazo-1,2-diphenylethan-1-one (**2a**) (0.836 g, 33.14 mmol, 76%) as yellow solid^[s2].

Substrates (**2b-2n**) and (**ds-9a**) were synthesized using above procedure.^[s2-a] Substrates **9b** and **9b'** were synthesized according to reported literature.^[s2-b]

Product **2a-O** was reported in literature.^[s3]

3. Standard procedure for catalytic Operation:

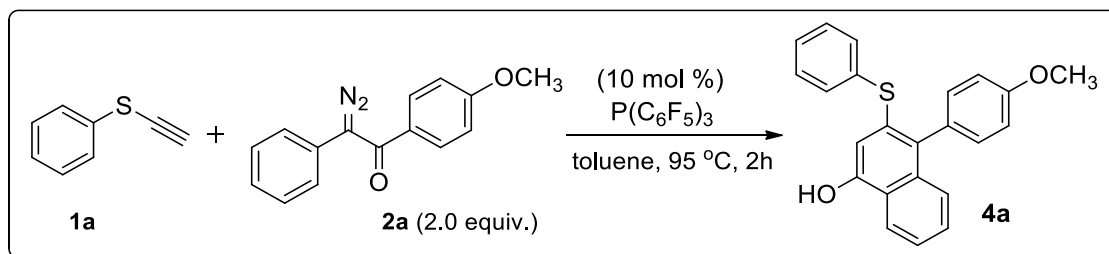
(a) Typical procedure for the synthesis of (R)-6-methoxy-8a-phenyl-3-(phenylthio)azulen-1(8aH)-one (**3a**):



A 15mL flask was charged with L_2AuCl (43.9.3 mg, 0.05 mmol) and AgSbF_6 (17.1 mg, 0.05 mmol), and to this mixture was added dry toluene (2.0 mL). The resulting mixture was stirred at room temperature for 5 min. To this mixture was added a dry toluene (6.0 mL) solution of ethynyl(phenyl)sulfane (**1a**) (134.20 mg, 1.0 mmol) and 2-diazo-1,2-diphenylethan-1-one (**2a**)

(504.5 mg, 2.0 mmol) at room temperature. After addition the reaction mixture stirred in pre-heated oil bath at 110 °C for 2h, the reaction mixture was filtered over a short celite bed, concentrated under reduced pressure, and purified by silica column eluting with (EA/Hexane = 15/85) to afford (R)-6-methoxy-8a-phenyl-3-(phenylthio)azulen-1(8aH)-one (**3a**) (272.5 mg, 0.76 mmol, 76%) as yellow solid.

(b) Typical procedure for synthesis of 4-(4-methoxyphenyl)-3-(phenylthio)naphthalen-1-ol (4a**):**

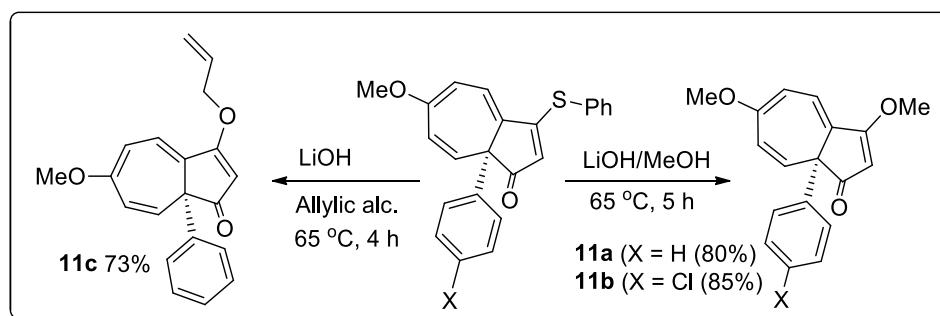


A 15 ml flask was charged with $P(C_6F_5)_3$ (53.2 mg, 0.1 mmol) and to this was added dry toluene (0.6 ml). The resulting mixture was stirred at room temperature for 5 min. To this mixture was added dropwise toluene solution of ethynyl(phenyl)sulfane (**1a**) (3.0 ml) (134.2 mg, 1.0 mmol) and stirred for 5 min. Later was added dropwise toluene solution of 2-diazo-1,2-diphenylethan-1-one (**2a**) (3.0 mL) (504 mg, 2.0 mmol) at room temperature. Later reaction mixture was purged with Argon gas for 10 min. The resulting mixture was heated at 95 °C in oil bath for 2h before filtration over a short celite bed. The solvent was evaporated under reduced pressure, and eluted through a silica column with ethyl acetate/hexane (10:90) to afford 4-(4-methoxyphenyl)-3-(phenylthio)naphthalen-1-ol (**4a**) (233 mg, 0.65 mmol, 65%) as white solid.

Compound **10a**, **10b** and **10c** were synthesized using same procedure (3-b) as described above.

4. Synthetic procedure for chemical functionalizations of (3a**) and (**6f**):**

(a) Typical procedure for the synthesis of (R)-3,6-dimethoxy-8a-phenylazulen-1(8aH)-one (11a**):**

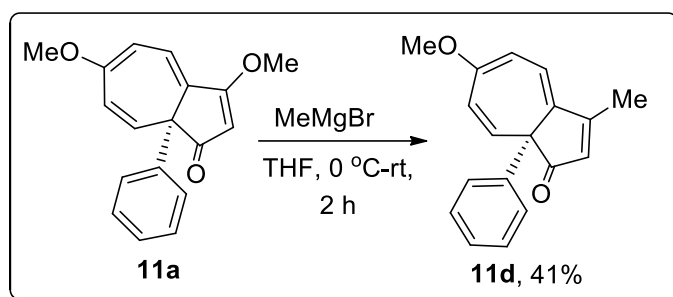


To a methanol solution of (R)-6-methoxy-8a-phenyl-3-(phenylthio)azulen-1(8aH)-one (**3a**) (30 mg, 0.083 mmol) was added LiOH (6.0 mg, 0.251 mmol) and heated at 65 °C in oil bath for 5h.

After completion of reaction, this mixture was quenched with water, extracted with ethyl acetate, dried over MgSO_4 , concentrated and purified on a silica column (EA/Hexane = 30/70) to afford (R)-3,6-dimethoxy-8a-phenylazulen-1(8aH)-one (**7a**) (18.8 mg, 0.067 mmol, 80%) as yellow solid.

Compound **11b** and **11c** were synthesized using same procedure (3-a) as described above, it delivered **11b** (85%) with Methanol and **11c** (73%) with allylic alcohol.

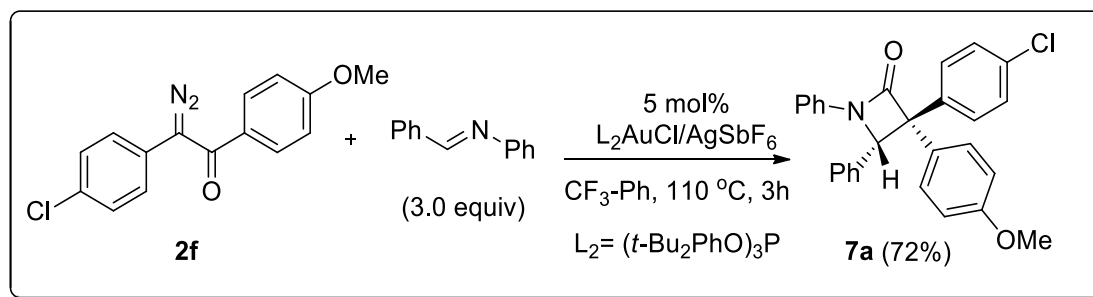
(b) Typical procedure for the synthesis of (R)-6-methoxy-3-methyl-8a-phenylazulen-1(8aH)-one (11d):



To a THF solution of (R)-3,6-dimethoxy-8a-phenylazulen-1(8aH)-one (**11a**) (30 mg, 0.107 mmol) was added methyl magnesium bromide (0.107 ml, 0.321 mmol.) at $0\text{ }^{\circ}\text{C}$ and the reaction was stirred at room temperature for 2 h. After completion of reaction, the solution was concentrated and purified by a silica column (EA/hexane = 10/90) to afford (R)-6-methoxy-3-methyl-8a-phenylazulen-1(8aH)-one (**11d**) (11.5 mg, 0.043 mmol, 41%) as colorless oil.

5. Identification of ketene intermediates:

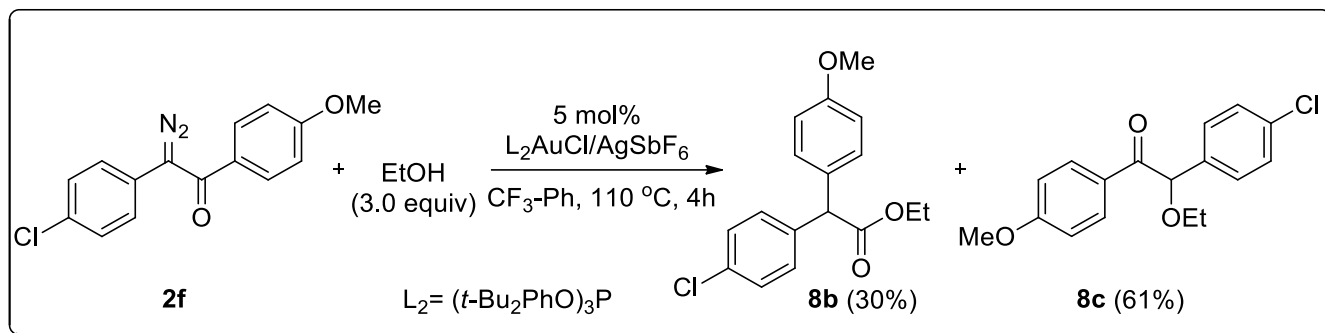
(a) Typical procedure for the synthesis of (3S,4S)-3-(4-chlorophenyl)-3-(4-methoxyphenyl)-1,4-diphenylazetidin-2-one (7a):



A suspension of L_2AuCl (7.66 mg, 0.008 mmol) and AgSbF_6 (2.99 mg, 0.008 mmol) in dry (trifluoromethyl)benzene (1 mL) was fitted with N_2 balloon and stirred at room temperature for 5 min. To this mixture was added dry (trifluoromethyl)benzene (2 mL) solution of 2-(4-chlorophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone **2f** (50 mg, 0.173 mmol) and (E)-N-benzylideneaniline (94.8 mg, 0.523 mmol). After addition the reaction mixture was stirred in pre-heated oil bath at $110\text{ }^{\circ}\text{C}$ for 3h. The solution was filtered over a short celite bed and evaporated

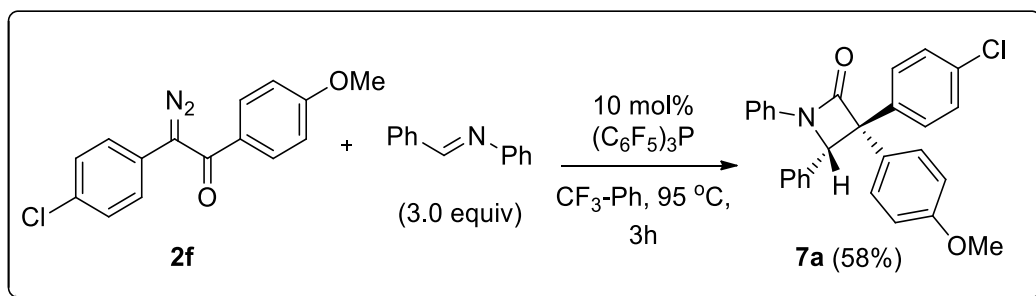
under reduced pressure. The residue was purified on a silica gel column using (EA/hexane = 14/86) as eluent to give compound (3S,4S)-3-(4-chlorophenyl)-3-(4-methoxyphenyl)-1,4-diphenylazetidin-2-one (**7a**) as yellow solid (55.3 mg, 0.12 mmol, 72%).

(b) Typical procedure for the synthesis of ethyl 2-(4-chlorophenyl)-2-(4-methoxyphenyl)acetate (8b**) and 2-(4-chlorophenyl)-2-ethoxy-1-(4-methoxyphenyl)ethanone (**8c**):**



8b and **8c** were synthesized by using above procedure [4-a]. Compound **8b** is reported and the spectroscopic data is identical to authentic sample found in the literature. ^[s4]

(c) Typical procedure for the synthesis of (3S,4S)-3-(4-chlorophenyl)-3-(4-methoxyphenyl)-1,4-diphenylazetidin-2-one (7a**):**



A 15 ml flask was charged with $\text{P}(\text{C}_6\text{F}_5)_3$ (9.3 mg, 0.1 mmol) and to this was added dry (trifluoromethyl)benzene (1 mL). The resulting mixture was stirred at room temperature for 5 min. To this mixture was added dry (trifluoromethyl)benzene (2 mL) solution of 2-(4-chlorophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone **2f** (50 mg, 0.173 mmol) and (*E*)-*N*-benzylideneaniline (94.8 mg, 0.523 mmol) at room temperature. The resulting mixture was heated at 95 °C in oil bath for 3h before filtration over a short celite bed. The residue was purified on a silica gel column using (EA/hexane = 14/86) as eluent to give compound (3S,4S)-3-(4-chlorophenyl)-3-(4-methoxyphenyl)-1,4-diphenylazetidin-2-one (**7a**) as yellow solid (44.5 mg, 0.10 mmol, 58%).

6. References:

[s1] a) P. Sharma, R. R. Singh, S. S. Giri, L.Y. Chen, M.J. Cheng, R. S. Liu, *Org. Lett.* 2019, **21**, 5475-5479; b) E. F. Lopes, B. T. Dalberto, G. Perin, D. Alves, T. Barcellos, E. J. Lenardao,

Chem. Eur.J. 2017, **23**, 13760-13765; c) K. Kang, K. Sakamoto, Y. Nishimoto, M. Yasuda, *Chemistry letter*, 2020, **49**, 1136-1139.

[s2] a) B. Xu, S. F. Zhu, X. D. Zuo, Z. C. Zhang, Q. L. Zhou, *Angew. Chem. Int. Ed.* 2014, **53**, 3913-3916; b) C. N. Chen, W. M. Cheng, J. K. Wang, T. H. Chao, M. J. Cheng, R. S. Liu, *Angew. Chem. Int. Ed.*, 2021, **60**, 4479-4448.

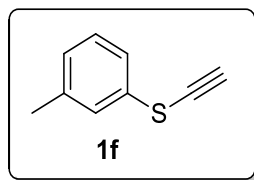
[s3] R. Chebolu, A. Bahuguna, R. Sharma, V. K. Mishra, P. C. Ravikumar, *Chem. Commun.*, 2015, **51**, 15438-15441.

[s4] R. B. Kothapalli, R. Niddana, R. Balamurugan, *Org. Lett.* 2014, **16**, 1278-1281.

[s5] P. D. Bartlett, R. E. McCluney, *J. Org. Chem.* 1983, **48**, 4165-4168.

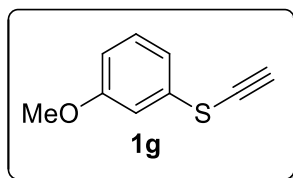
7. Spectral data of key compound:

Spectral data for Ethynyl(m-tolyl)sulfane (1f):



Compound **1f** was purified on silica gel column using hexane: as the eluent; Brown oil (514.4 mg, 3.4 mmol, 76%); ^1H NMR (400 MHz, CDCl_3): δ 7.24 (s, 1H), 7.23 ~ 7.19 (m, 2H), 7.04 ~ 7.02 (m, 1H), 3.22 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 139.2, 131.1, 129.0, 127.7, 127.0, 123.6, 86.7, 71.2, 21.3; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_9\text{H}_8\text{S}$: 148.0347; found: 148.0338.

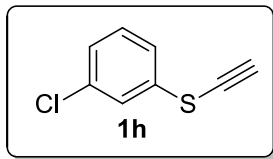
Spectral data for Ethynyl(3-methoxyphenyl)sulfane (1g):



Compound **1g** was purified on silica gel column using ethyl acetate/hexane: (1: 99) as the eluent; Brown oil (565.7 mg, 3.4 mmol, 81%); ^1H NMR (400 MHz, CDCl_3): δ 7.24 ~ 7.20 (m, 1H), 7.00 (s, 1H), 6.99 ~ 6.97 (m, 1H), 6.76 ~ 6.74 (m, 1H), 3.79 (s, 3H), 3.25 (s, 1H); ^{13}C NMR (100 MHz,

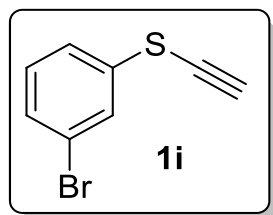
CDCl₃): δ ; 160.2, 132.7, 130.0, 118.7, 112.6, 111.9, 87.2, 70.8, 55.3; HRMS (EI-MS) m/z : [M]⁺ calcd for C₉H₈OS: 164.0296; found: 164.0294.

Spectral data for (3-chlorophenyl)(ethynyl)sulfane (1h):



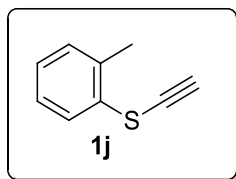
Compound **1h** was purified on silica gel column using hexane: as the eluent; Brown oil (443.5 mg, 2.6 mmol, 63%); ¹H NMR (400 MHz, CDCl₃): δ 7.44 (s, 1H), 7.29 ~ 7.17 (m, 3H), 3.31 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ ; 135.2, 133.6, 130.1, 126.9, 126.0, 124.3, 88.1, 69.8; HRMS (EI-MS) m/z : [M]⁺ calcd for C₈H₅ClS: 167.9800; found: 167.9797.

Spectral data for (3-bromophenyl)(ethynyl)sulfane (1i):



Compound **1i** was purified on silica gel column using hexane: as the eluent; Brown liquid (233 mg, 1.10 mmol, 62%); ¹H NMR (400 MHz, CDCl₃): δ 7.45 - 7.42 (m, 1H), 7.35-7.31 (m, 2H), 7.24-7.20 (m, 1H), 3.23 (s, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 131.4, 129.2, 126.7, 126.5, 86.8, 70.9, two carbons are merged with other peaks; HRMS (ESI-TOF) m/z : [M+H]⁺ calcd. for C₈H₆BrS: 212.9373, found 212.9377.

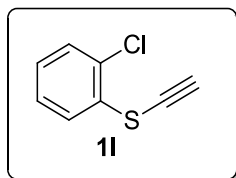
Spectral data for Ethynyl(o-tolyl)sulfane (1j):



Compound **1j** was purified on silica gel column using hexane: as the eluent; Light yellow oil (460 mg, 3.1 mmol, 68%); ¹H NMR (400 MHz, CDCl₃): δ 7.66 (d, J = 7.6 Hz, 1H), 7.25 ~ 7.19 (m, 1H), 7.18 ~ 7.14 (m, 2H), 3.19 (s, 1H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ ; 135.6, 130.5,

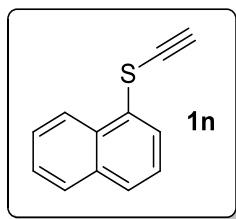
130.2, 127.1, 126.97, 126.91, 86.4, 71.1, 19.4; HRMS (EI-MS) m/z : $[M]^+$ calcd for C_9H_8S : 148.0347; found: 148.0337.

Spectral data for (2-chlorophenyl)(ethynyl)sulfane (1l):



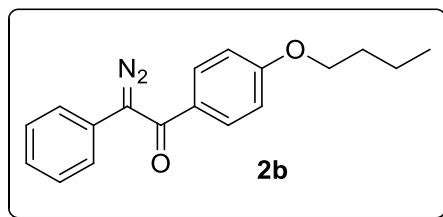
Compound **1l** was purified on silica gel column using hexane: as the eluent; Yellow oil (373.1 mg, 2.2 mmol, 53%); 1H NMR (500 MHz, $CDCl_3$): δ 7.71 ~ 7.67 (m, 1H), 7.32 ~ 7.28 (m, 2H), 7.17 ~ 7.14 (m, 1H), 3.34 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ ; 131.2, 130.4, 129.4, 127.5, 127.4, 127.0, 88.7, 69.8; HRMS (EI-MS) m/z : $[M]^+$ calcd for C_8H_5ClS : 167.9800; found: 167.9798.

Spectral data for Ethynyl(naphthalen-1-yl)sulfane (1n):



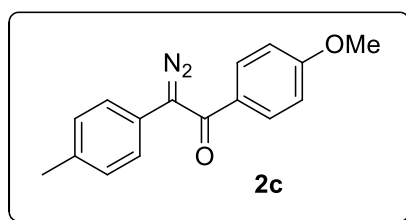
Compound **1n** was purified on silica gel column using hexane: as the eluent; Light brown oil (572.8 mg, 3.1 mmol, 70%); 1H NMR (400 MHz, $CDCl_3$): δ 8.10 ~ 8.08 (m, 1H), 7.90 ~ 7.85 (m, 2H), 7.78 ~ 7.76 (m, 1H), 7.59 ~ 7.52 (m, 2H), 7.49 ~ 7.45 (m, 1H), 3.21 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ ; 133.8, 130.8, 128.6, 128.1, 128.0, 126.7, 126.5, 126.4, 125.8, 123.5, 86.3, 71.2; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{12}H_8S$: 184.0347; found: 184.0344.

Spectral data for 1-(4-butoxyphenyl)-2-diazo-2-phenylethanone (2b):



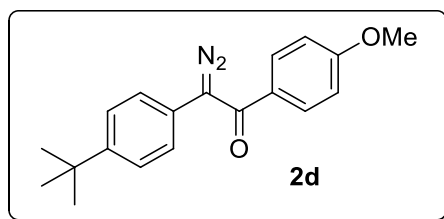
Compound **2b** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow oil (620 mg, 2.14 mmol, 57%); ^1H NMR (400 MHz, CDCl_3): δ 7.58 (d, J = 8.8 Hz, 2H), 7.43 ~ 7.35 (m, 4H), 7.24 ~ 7.21 (m, 1H), 6.85 (d, J = 8.7 Hz, 2H), 3.98 (t, J = 6.4 Hz, 2H), 1.78 ~ 1.72 (m, 2H), 1.50 ~ 1.45 (m, 2H), 0.96 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 187.3, 162.0, 130.0, 128.9, 126.8, 126.5, 126.1, 114.1, 72.3, 67.8, 31.1, 19.1, 13.7, one carbon merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_2$: 294.1362; found: 294.1359.

Spectral data for 2-diazo-1-(4-methoxyphenyl)-2-(p-tolyl)ethanone (2c):



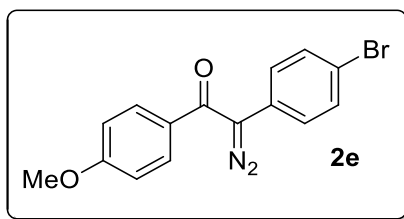
Compound **2c** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow oil (0.326 g, 1.22 mmol, 59%); ^1H NMR (500 MHz, CDCl_3): δ 7.57 (d, J = 8.7 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 8.1 Hz, 2H), 6.86 (d, J = 8.7 Hz, 2H), 3.82 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 187.3, 162.2, 136.8, 130.3, 130.0, 129.6, 126.3, 123.2, 113.5, 55.2, 21.0, one carbons are merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_2$: 266.1055, found 266.1051.

Spectral data for 2-(4-(tert-butyl)phenyl)-2-diazo-1-(4-methoxyphenyl)ethanone (2d):



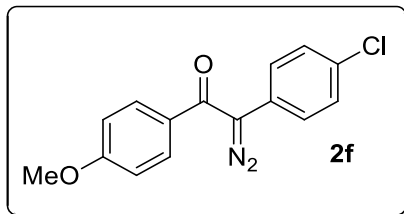
Compound **2d** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow Liquid (535.1 mg, 1.7 mmol, 49%); ^1H NMR (500 MHz, CDCl_3): δ 7.58 (d, J = 8.7 Hz, 2H), 7.40 (d, J = 8.5 Hz, 2H), 7.34 (d, J = 8.5 Hz, 2H), 6.87 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 187.4, 162.3, 150.1, 130.5, 130.0, 129.8, 126.0, 123.1, 113.6, 55.3, 34.5, 31.2, one carbon merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2$: 308.1519; found: 308.1916.

Spectral data for 2-(4-bromophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone (2e):



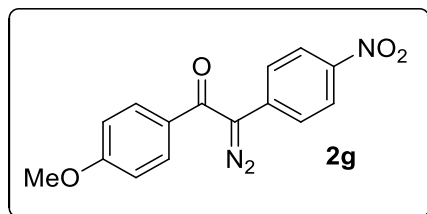
Compound **2e** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (868 mg, 2.6 mmol, 80%); ^1H NMR (400 MHz, CDCl_3): δ 7.58 (d, J = 8.8 Hz, 2H), 7.49 (d, J = 8.6 Hz, 2H), 7.32 (d, J = 8.6 Hz, 2H), 6.89 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 186.9, 162.5, 132.1, 130.1, 129.9, 127.3, 125.6, 120.4, 113.7, 55.3, one carbon merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{15}\text{H}_{11}\text{BrN}_2\text{O}_2$: 330.0004; found: 330.0003.

Spectral data for 2-(4-chlorophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone (2f):



Compound **2f** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (357 mg, 1.25 mmol, 65%); ^1H NMR (500 MHz, CDCl_3): δ 7.58 (d, J = 8.6 Hz, 2H), 7.36 (q, J = 17.9, 8.7 Hz, 4H), 6.89 (d, J = 8.6 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 186.9, 162.5, 132.4, 130.0, 129.9, 129.1, 127.0, 125.0, 113.7, 55.3, one carbon is merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{15}\text{H}_{11}\text{ClN}_2\text{O}_2$: 286.0509, found 286.0511.

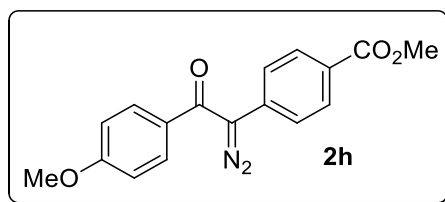
Spectral data for 2-diazo-1-(4-methoxyphenyl)-2-(4-nitrophenyl)ethanone (2g):



Compound **2g** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow solid (400 mg, 1.34 mmol, 73%); ^1H NMR (500 MHz, CDCl_3): δ 8.22 (d, J = 8.8 Hz, 2H),

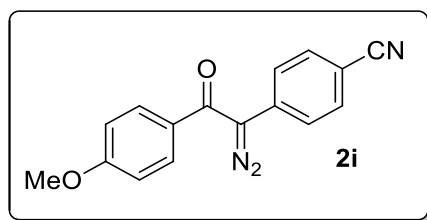
7.64 (t, $J = 8.8$ Hz, 4H), 6.93 (d, $J = 8.3$ Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 186.2, 162.9, 145.4, 134.5, 129.8, 124.7, 124.1, 113.9, 72.5, 55.4, one carbon is merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{15}\text{H}_{11}\text{N}_3\text{O}_4$: 297.0750, found 297.0742.

Spectral data for Methyl 4-(1-diazo-2-(4-methoxyphenyl)-2-oxoethyl)benzoate (2h):



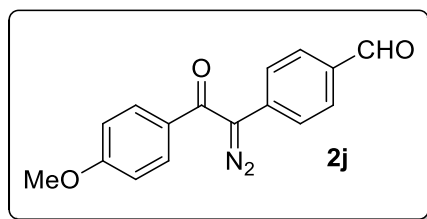
Compound **2h** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow solid (700 mg, 2.26 mmol, 64%); ^1H NMR (400 MHz, CDCl_3): δ 8.02 (d, $J = 8.4$ Hz, 2H), 7.60 (d, $J = 8.4$ Hz, 2H), 7.51 (d, $J = 8.4$ Hz, 2H), 6.89 (d, $J = 8.5$ Hz, 2H), 3.89 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 186.8, 166.5, 162.6, 131.8, 130.1, 130.0, 129.9, 127.8, 124.8, 113.8, 72.6, 55.4, 52.1; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{17}\text{H}_{14}\text{N}_2\text{O}_4$: 310.0959, found 310.0954.

Spectral data for 4-(1-diazo-2-(4-methoxyphenyl)-2-oxoethyl)benzonitrile (2i):



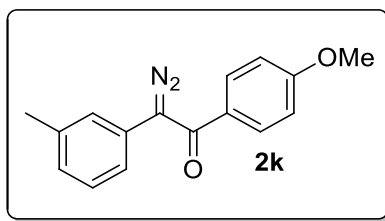
Compound **2i** was purified on silica gel column using ethyl acetate/hexane: (20: 80) as the eluent; Yellow solid (680 mg, 2.45 mmol, 62%); ^1H NMR (400 MHz, CDCl_3): δ 7.64 ~ 7.58 (m, 6H), 6.91 (d, $J = 8.5$ Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 186.4, 162.8, 132.5, 132.2, 129.8, 129.7, 125.0, 118.6, 113.9, 109.4, 72.3, 55.4; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O}_2$: 277.0856, found 277.0862.

Spectral data for 4-(1-diazo-2-(4-methoxyphenyl)-2-oxoethyl)benzaldehyde (2j)



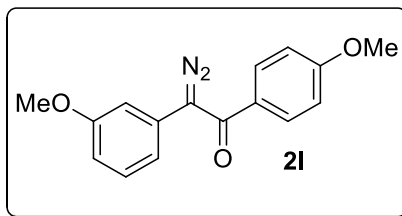
Compound **2j** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow solid (770 mg, 2.75 mmol, 70%); ^1H NMR (400 MHz, CDCl_3): δ 9.96 (s, 1H), 7.88 (d, J = 8.4 Hz, 2H), 7.65 ~ 7.61 (m, 4H), 6.92 (d, J = 8.7 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 191.2, 186.7, 162.8, 134.1, 133.7, 130.2, 130.0, 125.1, 113.0, 72.8, 55.5, one carbon is merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_3$: 280.0853, found 280.0859.

Spectral data for 2-diazo-1-(4-methoxyphenyl)-2-(m-tolyl)ethanone (2k):



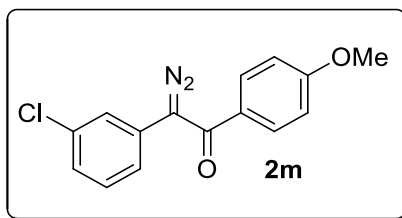
Compound **2k** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow oil (665 mg, 2.4 mmol, 60%); ^1H NMR (400 MHz, CDCl_3): δ 7.58 (d, J = 8.8 Hz, 2H), 7.28 ~ 7.24 (m, 2H), 7.19 (d, J = 8.4 Hz, 1H), 7.04 (d, J = 7.4 Hz, 1H), 6.87 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ : 187.3, 162.4, 138.8, 130.5, 130.0, 128.8, 127.7, 126.7, 126.3, 123.4, 113.6, 72.3, 55.4, 21.5; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_2$: 266.1049; found: 266.1041.

Spectral data for 2-diazo-2-(3-methoxyphenyl)-1-(4-methoxyphenyl)ethanone (2l):



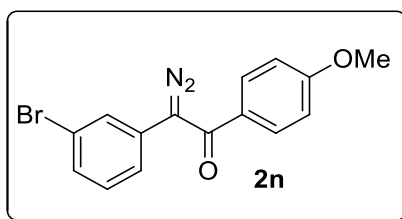
Compound **2l** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow oil (727 mg, 2.5 mmol, 66%); ^1H NMR (400 MHz, CDCl_3): δ 7.59 (d, J = 8.8 Hz, 2H), 7.27 (t, J = 8.0 Hz, 1H), 7.07 ~ 7.06 (m, 1H), 6.95 ~ 6.92 (m, 1H), 6.88 (d, J = 8.6 Hz, 2H), 6.78 ~ 6.75 (m, 1H), 3.82 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ : 187.2, 162.4, 159.9, 130.3, 130.0, 129.8, 127.9, 118.1, 113.6, 112.5, 111.6, 72.4, 55.3, 55.2; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_3$: 282.0998; found: 282.0992.

Spectral data for 2-(3-chlorophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone (2m):



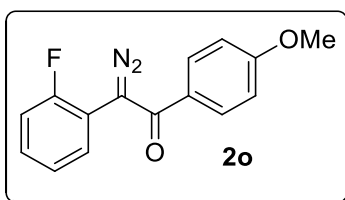
Compound **2m** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow oil (516.9 g, 1.8 mmol, 47%); ^1H NMR (400 MHz, CDCl_3): δ 7.59 (d, J = 8.9 Hz, 2H), 7.51 ~ 7.50 (m, 1H), 7.32 ~ 7.29 (m, 2H), 7.20 ~ 7.17 (m, 1H), 6.89 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 187.7, 162.6, 134.9, 130.0, 129.9, 128.5, 126.7, 125.4, 123.6, 113.7, 71.7, 55.4, one carbon merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{15}\text{H}_{11}\text{ClN}_2\text{O}_2$: 286.0503; found: 286.0503.

Spectral data for 2-(3-bromophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone (2n):



Compound **2n** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow oil (564.3 mg, 1.7 mmol, 52%); ^1H NMR (400 MHz, CDCl_3): δ 7.65 (s, 1H), 7.59 (d, J = 8.4 Hz, 2H), 7.35 ~ 7.33 (m, 2H), 7.25 ~ 7.21 (m, 1H), 6.89 (d, J = 8.4 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 186.7, 162.6, 130.2, 130.0, 129.9, 129.6, 128.8, 128.2, 124.2, 123.0, 113.8, 71.6, 55.4; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{15}\text{H}_{11}\text{BrN}_2\text{O}_2$: 329.9998; found: 329.9999.

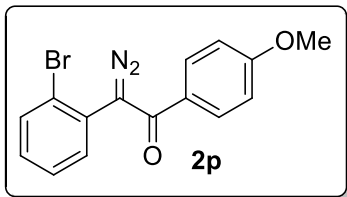
Spectral data for 2-diazo-2-(2-fluorophenyl)-1-(4-methoxyphenyl)ethanone (2o):



Compound **2o** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow liquid (442.6 mg, 1.6 mmol, 40%); ^1H NMR (400 MHz, CDCl_3): δ 7.53 (d, J = 8.7 Hz, 2H), 7.38 ~ 7.33 (m, 1H), 7.27 ~ 7.22 (m, 1H), 7.13 ~ 7.09 (m, 2H), 6.83 (d, J = 8.8 Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 186.7, 162.3, 160.0, 157.5, 132.2, 131.4, 131.0, 130.0,

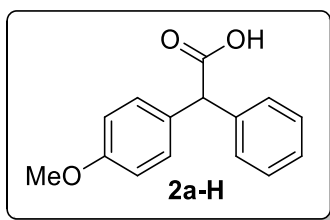
129.6, 124.5, 116.0, 115.8, 114.8, 114.2, 113.5, 67.8, 55.2; HRMS (FD) m/z : $[M]^+$ calcd for $C_{15}H_{11}FN_2O_2$: 270.0799; found: 270.0806.

Spectral data for 2-(2-bromophenyl)-2-diazo-1-(4-methoxyphenyl)ethanone (2p):



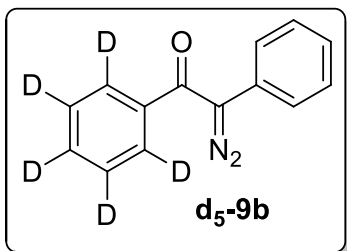
Compound **2p** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow liquid (466.6 mg, 1.4 mmol, 43%); 1H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, J = 7.8 Hz, 1H), 7.46 ~ 7.43 (m, 2H), 7.28 ~ 7.26 (m, 2H), 6.24 ~ 6.20 (m, 1H), 6.78 (d, J = 8.8 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ : 186.7, 162.3, 133.7, 133.4, 131.3, 130.4, 130.3, 129.7, 127.9, 127.8, 125.2, 113.4, 55.3; HRMS (FD) m/z : $[M]^+$ calcd for $C_{15}H_{11}BrN_2O_2$: 329.9998; found: 329.9998.

Spectral data for 2-(4-methoxyphenyl)-2-phenylacetic acid (2a-H):



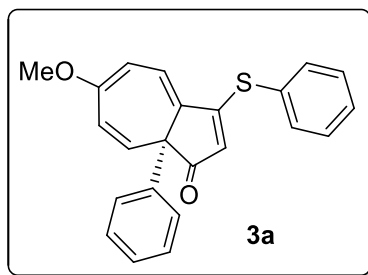
Compound **2a-H** was purified on silica gel column using ethyl acetate/hexane: (30: 70) as the eluent; Brown Solid (79.9mg, 0.33 mmol, 34%); 1H NMR (500 MHz, $CDCl_3$): δ 7.29 (s, 4H), 7.22 (d, J = 9.1 Hz, 3H), 6.83 (d, J = 8.4 Hz, 2H), 4.97 (s, 1H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 179.0, 158.8, 138.1, 129.9, 129.7, 128.5, 128.4, 127.3, 113.9, 56.1, 55.1; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{15}H_{14}O_3$: 242.0943; found: 242.0941.

Spectral data for 2-diazo-2-phenyl-1-(phenyl-d5)ethan-1-one (d5-9b):



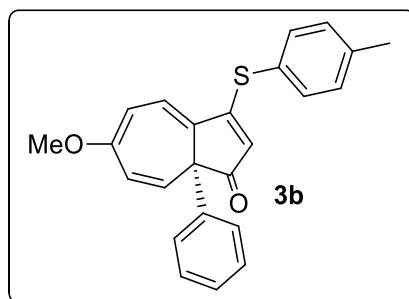
Compound **d5-9b** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (400 mg, 1.34 mmol, 73%); ^1H NMR (500 MHz, CDCl_3): δ 7.60 (s, 1H), 7.48 (t, $J = 2.87$ Hz, 2H), 7.39 (t, $J = 3.3$ Hz, 2H); ^{13}C NMR (175 MHz, CDCl_3): δ 188.3, 137.8, 137.7, 131.5, 131.4, 129.0, 128.9, 128.8, 128.5, 128.4, 128.2, 127.7, 127.6, 126.8, 126.0, 125.9, 125.8; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{14}\text{H}_5\text{D}_5\text{N}_2\text{O}$: 227.1095, found 227.1094.

Spectral data for (R)-6-methoxy-8a-phenyl-3-(phenylthio)azulen-1(8aH)-one (3a):



Compound **3a** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (272.5 mg, 0.76 mmol, 76%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 (d, $J = 7.4$ Hz, 2H), 7.44 ~ 7.41 (m, 3H), 7.21 (d, $J = 7.1$ Hz, 2H), 7.17 (t, $J = 7.2$ Hz, 2H), 7.12 (t, $J = 6.9$ Hz, 1H), 6.71 (d, $J = 7.4$ Hz, 1H), 6.40 (d, $J = 10.7$ Hz, 1H), 6.23 (dd, $J = 10.7, 1.8$ Hz, 1H), 5.55 (d, $J = 7.3$ Hz, 1H), 5.26 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.3, 173.2, 162.2, 138.9, 135.0, 133.1, 133.0, 130.2, 129.9, 128.5, 127.8, 126.9, 126.4, 126.3, 120.7, 119.5, 101.4, 60.5, 54.8; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{18}\text{O}_2\text{S}$: 358.1028; found: 358.1031.

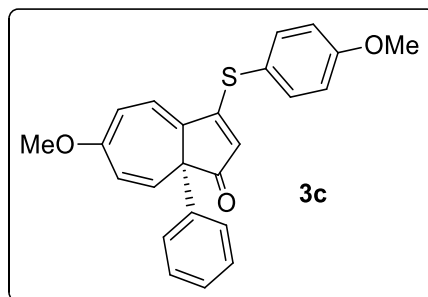
Spectral data for (R)-6-methoxy-8a-phenyl-3-(p-tolylthio)azulen-1(8aH)-one (3b):



Compound **3b** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (85.5 mg, 0.22 mmol, 68%); ^1H NMR (700 MHz, CDCl_3): δ 7.45 (d, $J = 8.0$ Hz, 2H), 7.23 ~ 7.19 (m, 4H), 7.16 (t, $J = 7.2$ Hz, 2H), 7.12 (t, $J = 7.0$ Hz, 1H), 6.69 (d, $J = 7.4$ Hz, 1H), 6.39 (d, $J = 10.7$ Hz, 1H), 6.22 (dd, $J = 10.7, 1.6$ Hz, 1H), 5.54 (d, $J = 7.4$ Hz, 1H), 5.24 (s, 1H), 3.48 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.3, 173.8, 162.1, 140.6, 138.9,

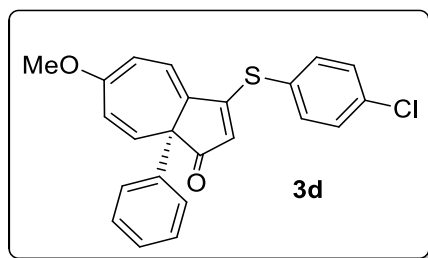
134.9, 133.2, 133.0, 130.6, 127.8, 126.8, 126.3, 124.9, 120.6, 119.4, 101.5, 60.5, 54.8, 21.3, one carbon merged with other peaks; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{24}H_{20}O_2S$: 372.1184; found: 372.1185.

Spectral data for (R)-6-methoxy-3-((4-methoxyphenyl)thio)-8a-phenylazulen-1(8aH)-one (3c):



Compound **3c** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Light yellow solid (71 mg, 0.18 mmol, 60%); 1H NMR (700 MHz, $CDCl_3$): δ 7.48 (d, J = 8.6 Hz, 2H), 7.20 (d, J = 7.2 Hz, 2H), 7.16 (t, J = 7.2 Hz, 2H), 7.12 (t, J = 7.1 Hz, 1H), 6.93 (d, J = 8.7 Hz, 2H), 6.69 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.22 (dd, J = 10.7, 1.8 Hz, 1H), 5.54 (dd, J = 7.4, 1.5 Hz, 1H), 5.22 (s, 1H), 3.82 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 201.2, 174.4, 162.1, 161.2, 138.9, 136.5, 133.1, 133.0, 127.8, 126.8, 126.34, 126.33, 120.6, 119.4, 118.8, 115.4, 101.4, 60.6, 55.4, 54.8; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{24}H_{20}O_3S$: 388.1133; found: 388.1137.

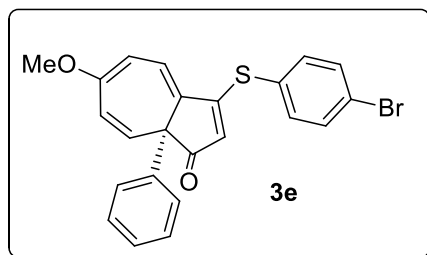
Spectral data for (R)-3-((4-chlorophenyl)thio)-6-methoxy-8a-phenylazulen-1(8aH)-one (3d):



Compound **3d** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (82.7 mg, 0.21 mmol, 71%); 1H NMR (700 MHz, $CDCl_3$): δ 7.52 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 8.2 Hz, 2H), 7.20 ~ 7.13 (m, 5H), 6.68 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.23 (d, J = 10.7 Hz, 1H), 5.55 (d, J = 7.4 Hz, 1H), 5.25 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 201.1, 172.3, 162.3, 138.7, 136.8, 136.2, 133.0, 132.8, 130.2, 127.9, 126.98,

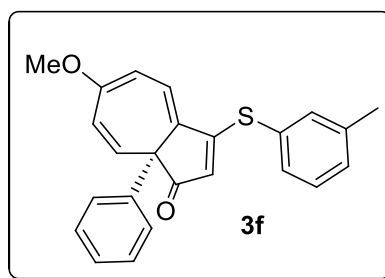
126.95, 126.4, 126.3, 120.6, 119.7, 101.4, 60.4, 54.9; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{23}H_{17}ClO_2S$: 392.0638; found: 392.0625.

Spectral data for (R)-3-((4-bromophenyl)thio)-6-methoxy-8a-phenylazulen-1(8aH)-one (3e):



Compound **3e** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Light yellow solid (62.6 mg, 0.14 mmol, 61%); 1H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, J = 7.8 Hz, 2H), 7.43 (d, J = 7.4 Hz, 2H), 7.21 ~ 7.11 (m, 5H), 6.70 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.23 (dd, J = 10.7, 1.8 Hz, 1H), 5.55 (dd, J = 7.4, 1.3 Hz, 1H), 5.26 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 201.3, 173.2, 162.2, 138.9, 135.0, 133.1, 133.0, 130.2, 129.9, 128.5, 127.8, 126.9, 126.38, 126.32, 120.6, 119.5, 101.4, 60.5, 54.8; HRMS (FD) m/z : $[M]^+$ calcd for $C_{23}H_{17}BrO_2S$: 436.0133; found: 436.0129.

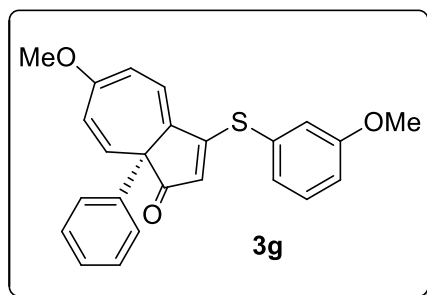
Spectral data for (R)-6-methoxy-8a-phenyl-3-(m-tolylthio)azulen-1(8aH)-one (3f):



Compound **3f** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (95.5 mg, 0.25 mmol, 76%); 1H NMR (700 MHz, $CDCl_3$): δ 7.38 (s, 1H), 7.37 (d, J = 7.9 Hz, 1H), 7.29 (t, J = 7.6 Hz, 1H), 7.23 (d, J = 7.0 Hz, 1H), 7.20 (d, J = 7.0 Hz, 2H), 7.16 (t, J = 7.3 Hz, 2H), 7.13 ~ 7.10 (m, 1H), 6.69 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.22 (t, J = 10.7 Hz, 1H), 5.54 (d, J = 7.4 Hz, 1H), 5.26 (s, 1H), 3.48 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 201.3, 173.5, 162.1, 139.9, 138.9, 135.4, 133.1, 133.0, 131.9, 131.0, 129.7,

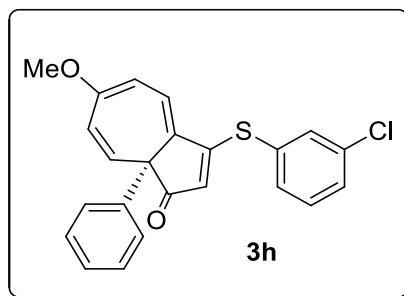
128.1, 127.8, 126.9, 126.37, 126.35, 120.7, 119.5, 101.4, 60.5, 54.8, 21.2; HRMS (ESI-TOF) m/z : $[M+H]^+$ calcd for $C_{24}H_{20}O_2S$: 373.1262; found: 373.1264.

Spectral data for (R)-6-methoxy-3-((3-methoxyphenyl)thio)-8a-phenylazulen-1(8aH)-one (3g):



Compound **3g** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Light yellow solid (97.0 mg, 0.24 mmol, 82%); 1H NMR (700 MHz, $CDCl_3$): δ 7.33 (t, J = 8.0 Hz, 1H), 7.21 ~ 7.20 (m, 2H), 7.17 ~ 7.16 (m, 3H), 7.14 ~ 7.11 (m, 2H), 6.97 (dd, J = 8.3, 1.7 Hz, 1H), 6.69 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.23 (dd, J = 10.7, 1.8 Hz, 1H), 5.55 (d, J = 7.4 Hz, 1H), 5.32 (s, 1H), 3.80 (s, 3H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 201.3, 173.0, 162.2, 160.3, 138.9, 133.1, 133.0, 130.6, 129.3, 127.8, 127.1, 126.9, 126.38, 126.35, 120.7, 120.0, 119.5, 116.1, 101.4, 60.4, 55.4, 54.9; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{24}H_{20}O_3S$: 388.1133; found: 388.1132.

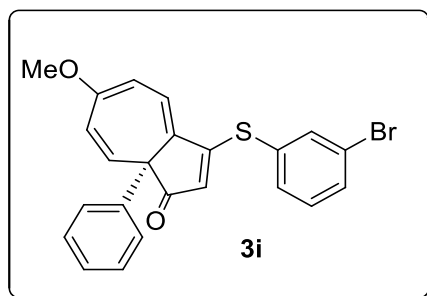
Spectral data for (R)-3-((3-chlorophenyl)thio)-6-methoxy-8a-phenylazulen-1(8aH)-one (3h):



Compound **3h** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (56 mg, 0.14 mmol, 48%); 1H NMR (700 MHz, $CDCl_3$): δ 7.60 (s, 1H), 7.48 (d, J = 7.6 Hz, 1H), 7.43 ~ 7.42 (m, 1H), 7.37 (t, J = 7.9 Hz, 1H), 7.20 ~ 7.16 (m, 4H), 7.13 (t, J = 7.1 Hz,

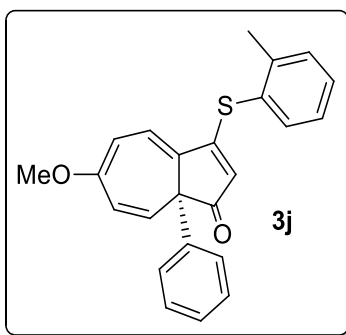
1H), 6.68 (d, $J = 7.4$ Hz, 1H), 6.40 (d, $J = 10.7$ Hz, 1H), 6.24 (d, $J = 10.7$ Hz, 1H), 5.55 (d, $J = 7.4$ Hz, 1H), 5.28 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.2, 171.9, 162.3, 138.7, 135.4, 134.7, 133.1, 133.0, 132.8, 130.9, 130.5, 130.2, 127.9, 127.0, 126.4, 126.3, 120.7, 119.8, 101.4, 60.4, 54.9; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{ClO}_2\text{S}$: 415.0535; found: 415.0540.

Spectral data for (R)-3-((3-bromophenyl)thio)-6-methoxy-8a-phenylazulen-1(8aH)-one (3i):



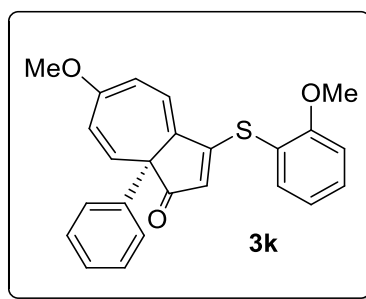
Compound **3i** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Light Yellow solid (60.6 mg, 0.13 mmol, 59%); ^1H NMR (700 MHz, CDCl_3): δ 7.59 ~ 7.58 (m, 2H), 7.44 ~ 7.41 (m, 2H), 7.21 ~ 7.20 (m, 2H), 7.17 (t, $J = 7.3$ Hz, 2H), 7.12 (t, $J = 6.9$ Hz, 1H), 6.71 (d, $J = 7.4$ Hz, 1H), 6.40 (d, $J = 10.7$ Hz, 1H), 6.23 (dd, $J = 10.7, 1.8$ Hz, 1H), 5.55 (dd, $J = 7.4, 1.4$ Hz, 1H), 5.26 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.3, 173.2, 162.2, 138.9, 135.0, 133.1, 133.0, 130.2, 129.9, 128.5, 127.9, 127.8, 126.9, 126.38, 126.33, 126.30, 120.6, 119.5, 101.4, 60.5, 54.8; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{BrO}_2\text{S}$: 436.0127; found: 436.0126.

Spectral data for (R)-6-methoxy-8a-phenyl-3-(o-tolylthio)azulen-1(8aH)-one (3j):



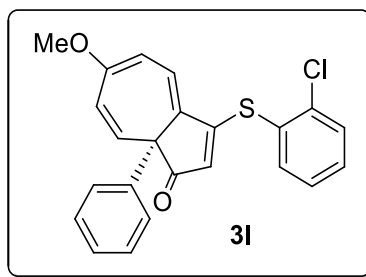
Compound **3j** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow solid (81.7 mg, 0.21 mmol, 65%); ^1H NMR (700 MHz, CDCl_3): δ 7.57 (d, J = 7.6 Hz, 1H), 7.37 ~ 7.32 (m, 2H), 7.25 ~ 7.23 (m, 1H), 7.21 ~ 7.16 (m, 4H), 7.13 (t, J = 7.0 Hz, 1H), 6.74 (d, J = 7.7 Hz, 1H), 6.40 (d, J = 10.7 Hz, 1H), 6.25 (dd, J = 10.7, 1.89 Hz, 1H), 5.56 (d, J = 7.4, 1.54 Hz, 1H), 5.09 (s, 1H), 3.50 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.3, 172.4, 162.1, 142.4, 138.9, 136.2, 133.1, 133.0, 131.3, 130.8, 127.8, 127.7, 127.3, 126.8, 126.3, 126.2, 120.4, 119.6, 101.4, 60.5, 54.8, 20.5; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$: 395.1081; found: 395.1082.

Spectral data for (R)-6-methoxy-3-((2-methoxyphenyl)thio)-8a-phenylazulen-1(8aH)-one (3k):



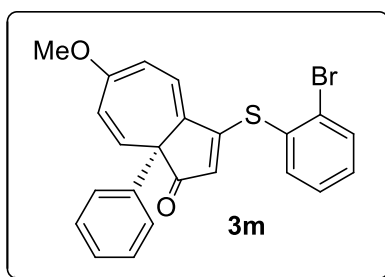
Compound **3k** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow solid (81.6 mg, 0.21 mmol, 69%); ^1H NMR (700 MHz, CDCl_3): δ 7.56 ~ 7.55 (m, 1H), 7.45 ~ 7.42 (m, 1H), 7.23 ~ 7.22 (m, 2H), 7.17 (t, J = 7.2 Hz, 2H), 7.12 (t, J = 7.1 Hz, 1H), 7.0 ~ 6.96 (m, 2H), 6.71 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.24 (dd, J = 10.7, 1.8 Hz, 1H), 5.54 (d, J = 7.5 Hz, 1H), 5.20 (s, 1H), 3.85 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.5, 172.2, 162.0, 159.4, 139.1, 136.9, 133.5, 132.8, 132.4, 127.8, 126.8, 126.3, 121.5, 120.8, 119.5, 116.1, 111.8, 101.5, 60.6, 56.0, 54.8, one carbon merged with other peaks; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{24}\text{H}_{20}\text{O}_3\text{S}$: 388.1133; found: 388.1138.

Spectral data for (R)-3-((2-chlorophenyl)thio)-6-methoxy-8a-phenylazulen-1(8aH)-one (3l):



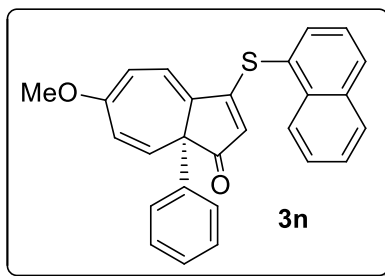
Compound **3l** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (83.4 mg, 0.21 mmol, 72%); ^1H NMR (700 MHz, CDCl_3): δ 7.70 ~ 7.69 (m, 1H), 7.55 ~ 7.53 (m, 1H), 7.42 ~ 7.40 (m, 1H), 7.32 (t, J = 7.6 Hz 1H), 7.22 ~ 7.21 (m, 2H), 7.17 (t, J = 7.7 Hz, 2H), 7.12 (t, J = 7.2 Hz, 1H), 6.70 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.25 (dd, J = 10.7, 1.6 Hz, 1H), 5.55 (d, J = 7.4 Hz, 1H), 5.16 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.3, 170.6, 162.3, 139.1, 138.8, 137.3, 133.0, 132.9, 131.9, 130.9, 127.99, 127.91, 127.8, 126.9, 126.5, 126.3, 121.0, 119.7, 101.4, 60.5, 54.9; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{ClO}_2\text{S}$: 392.0638; found: 392.0637.

Spectral data for (R)-3-((2-bromophenyl)thio)-6-methoxy-8a-phenylazulen-1-one (3m):



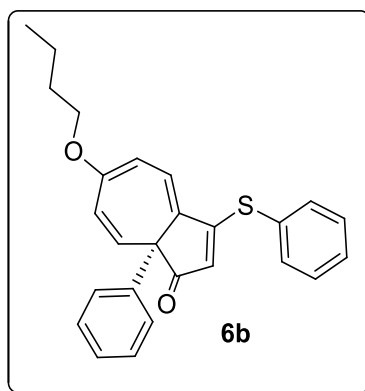
Compound **3m** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow solid (64.7 mg, 0.14 mmol, 63%); ^1H NMR (700 MHz, CDCl_3): δ 7.59 ~ 7.58 (m, 2H), 7.44 ~ 7.42 (m, 2H), 7.20 (d, J = 7.6 Hz, 2H), 7.17 (t, J = 7.2 Hz, 2H), 7.12 (t, J = 7.2 Hz, 1H), 6.70 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.23 (dd, J = 10.7, 1.8 Hz, 1H), 5.55 (dd, J = 7.4, 1.6 Hz, 1H), 5.26 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.3, 173.1, 162.2, 138.9, 135.0, 133.1, 133.0, 130.2, 129.9, 128.5, 127.8, 126.9, 126.39, 126.34, 120.7, 119.5, 101.4, 60.5, 54.9, two carbon merged with other peaks; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{BrO}_2\text{S}$: 436.0127; found: 436.0129.

Spectral data for (R)-6-methoxy-3-(naphthalen-1-ylthio)-8a-phenylazulen-1(8aH)-one (3n):



Compound **3n** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (84.2 mg, 0.20 mmol, 76%); ^1H NMR (700 MHz, CDCl_3): δ 8.28 (d, J = 8.3 Hz, 1H), 7.97 (d, J = 8.2 Hz, 1H), 7.89 (t, J = 6.7 Hz, 2H), 7.58 ~ 7.56 (m, 1H), 7.55 ~ 7.53 (m, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.23 ~ 7.21 (m, 2H), 7.18 (t, J = 7.3 Hz, 2H), 6.13 (t, J = 7.1 Hz, 1H), 6.85 (d, J = 7.4 Hz, 1H), 6.38 (d, J = 10.7 Hz, 1H), 6.26 (dd, J = 10.7, 1.6 Hz, 1H), 5.60 (d, J = 7.4 Hz, 1H), 4.90 (s, 1H), 3.51 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.2, 172.3, 162.2, 138.9, 135.2, 134.4, 133.7, 133.3, 133.0, 131.6, 128.8, 127.91, 127.90, 126.9, 126.4, 126.3, 125.8, 125.6, 125.3, 121.5, 119.6, 101.5, 60.4, 54.9, one carbon merged with other peaks; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{27}\text{H}_{20}\text{O}_2\text{S}$: 408.1184; found: 408.1193.

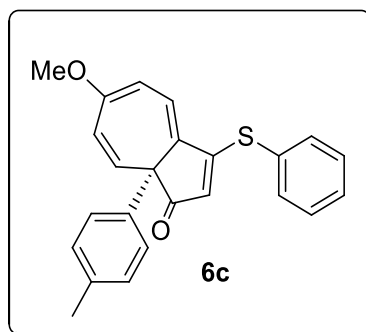
Spectral data for (R)-6-butoxy-8a-phenyl-3-(phenylthio)azulen-1(8aH)-one (6b):



Compound **6b** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow oil (83.6 mg, 0.20 mmol, 56%); ^1H NMR (700 MHz, CDCl_3): δ 7.59 ~ 7.57 (m, 2H), 7.44 ~ 7.41 (m, 3H), 7.21 (d, J = 7.4 Hz, 2H), 7.16 (t, J = 7.2 Hz, 2H), 7.36 (t, J = 6.8 Hz, 1H), 6.89 (d, J = 7.4 Hz, 1H), 6.38 (d, J = 10.7 Hz, 1H), 6.23 (dd, J = 10.7, 1.8 Hz, 1H), 5.56 (dd, J = 7.4, 1.5 Hz, 1H), 5.25 (s, 1H), 3.66 ~ 3.62 (m, 1H), 3.59 ~ 3.56 (m, 1H), 1.55 ~ 1.50 (m, 2H), 1.31 ~

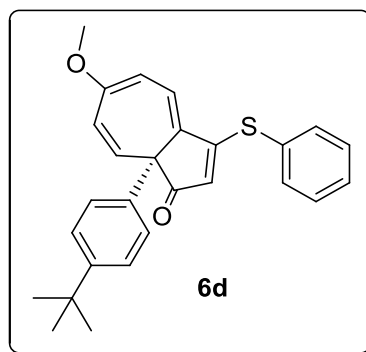
1.23 (m, 2H), 0.84 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.4, 173.2, 161.8, 138.9, 135.0, 132.9, 132.8, 130.1, 129.9, 128.5, 127.8, 126.8, 126.7, 126.3, 120.5, 119.7, 102.5, 67.4, 60.5, 30.7, 19.0, 13.6; HRMS (ESI-MS) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{24}\text{O}_2\text{S}$: 423.1394; found: 423.1396.

Spectral data for (R)-6-methoxy-3-(phenylthio)-8a-(p-tolyl)azulen-1(8aH)-one (6c):



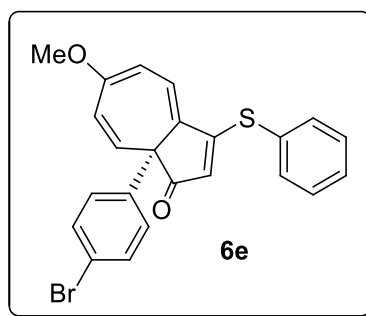
Compound **6c** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (115.2 mg, 0.30 mmol, 83%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 (d, $J = 7.0$ Hz, 2H), 7.44 ~ 7.42 (m, 3H), 7.09 (d, $J = 7.9$ Hz, 2H), 6.98 (d, $J = 7.8$ Hz, 2H), 6.69 (d, $J = 7.4$ Hz, 1H), 6.38 (d, $J = 10.7$ Hz, 1H), 6.22 (d, $J = 10.6$ Hz, 1H), 5.55 (d, $J = 7.2$ Hz, 1H), 5.25 (s, 1H), 3.50 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.5, 173.0, 162.1, 136.4, 135.9, 135.0, 133.1, 133.0, 130.1, 129.8, 128.6, 128.5, 126.2, 126.1, 120.6, 119.4, 101.3, 60.2, 54.8, 21.0; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$: 372.1184; found: 372.1185.

Spectral data for (R)-8a-(4-(tert-butyl)phenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6d):



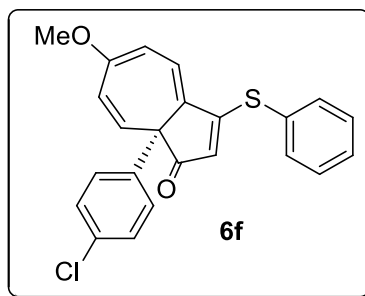
Compound **6d** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (91.2 mg, 0.21 mmol, 59%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 ~ 7.57 (m, 2H), 7.43 ~ 7.41 (m, 3H), 7.17 (d, J = 8.4 Hz, 2H), 7.11 (d, J = 8.4 Hz, 2H), 6.69 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.7 Hz, 1H), 6.21 (dd, J = 10.7, 1.9 Hz, 1H), 5.56 (dd, J = 7.5, 1.7 Hz, 1H), 5.24 (s, 1H), 3.51 (s, 3H), 1.21 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.6, 173.1, 162.1, 149.5, 135.8, 135.0, 133.1, 130.1, 129.8, 128.5, 126.1, 125.7, 124.8, 120.6, 119.4, 101.4, 60.2, 54.9, 34.3, 31.2, one carbon merged with other peaks ; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{26}\text{O}_2\text{S}$: 437.1551; found: 437.1569.

Spectral data for (R)-8a-(4-bromophenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6e):



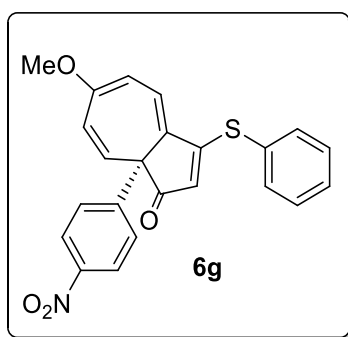
Compound **6e** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow solid (130.4 mg, 0.29 mmol, 80%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 ~ 7.57 (m, 2H), 7.45 ~ 7.42 (m, 3H), 7.28 (d, J = 8.6 Hz, 2H), 7.08 (d, J = 8.6 Hz, 2H), 6.71 (d, J = 7.4 Hz, 1H), 6.35 (d, J = 10.6 Hz, 1H), 6.22 (dd, J = 10.7, 2 Hz, 1H), 5.56 (dd, J = 7.5, 1.8 Hz, 1H), 5.24 (s, 1H), 3.50 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 200.7, 173.4, 162.2, 138.0, 135.0, 132.6, 132.5, 130.9, 130.2, 129.9, 128.3, 128.1, 126.6, 120.9, 120.5, 119.8, 101.5, 59.9, 54.9; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{BrO}_2\text{S}$: 336.0133; found: 336.0132.

Spectral data for (R)-8a-(4-chlorophenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6f):



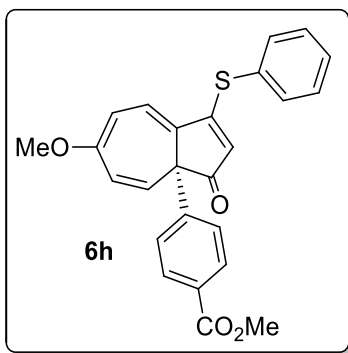
Compound **6f** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Light yellow solid (127.5 mg, 0.32 mmol, 87%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 (d, J = 7.5 Hz, 2H), 7.45 ~ 7.42 (m, 3H), 7.13 (s, 4H), 6.71 (d, J = 7.4 Hz, 1H), 6.35 (d, J = 10.7 Hz, 1H), 6.22 (d, J = 10.6 Hz, 1H), 5.56 (d, J = 7.4 Hz, 1H), 5.25 (s, 1H), 3.50 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 200.8, 173.4, 162.2, 137.4, 135.0, 132.7, 132.68, 132.64, 130.2, 129.9, 128.3, 128.0, 127.7, 126.6, 120.5, 119.7, 101.5, 59.8, 54.9; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{ClO}_2\text{S}$: 392.0638; found: 392.0641.

Spectral data for (R)-6-methoxy-8a-(4-nitrophenyl)-3-(phenylthio)azulen-1-one (6g):



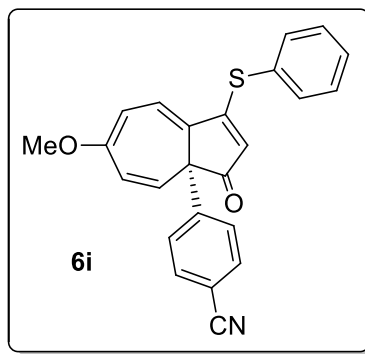
Compound **6g** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow solid (106.8 mg, 0.26 mmol, 71%); ^1H NMR (700 MHz, CDCl_3): δ 8.03 (d, J = 8.8 Hz, 2H), 7.59 ~ 7.58 (m, 2H), 7.47 ~ 7.43 (m, 3H), 7.37 (d, J = 8.8 Hz, 2H), 6.77 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.6 Hz, 1H), 6.27 (d, J = 10.3, 1.8 Hz, 1H), 5.58 (dd, J = 7.4, 1.4 Hz, 1H), 5.27 (s, 1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 199.4, 173.9, 162.3, 146.9, 146.4, 135.0, 132.2, 131.9, 130.4, 130.0, 128.0, 127.4, 127.2, 123.1, 120.5, 120.3, 101.6, 60.4, 54.9; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{NO}_4\text{S}$: 403.0872; found: 403.0874.

Spectral data for (R)-methyl 4-(6-methoxy-3-oxo-1-(phenylthio)-3,3a-dihydroazulen-3a-yl)benzoate (6h)



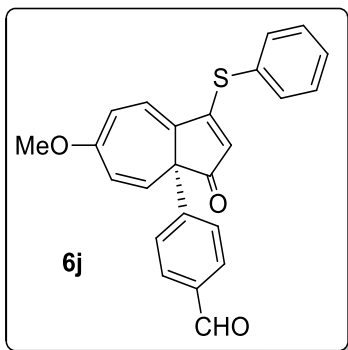
Compound **6h** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; White solid (105 mg, 0.25 mmol, 68%); ^1H NMR (700 MHz, CDCl_3): δ 7.84 (d, J = 8.2 Hz, 2H), 7.58 (d, J = 7.6 Hz, 2H), 7.45 ~ 7.43 (m, 3H), 7.27 (d, J = 8.2 Hz, 2H), 6.73 (d, J = 7.4 Hz, 1H), 6.39 (d, J = 10.6 Hz, 1H), 6.25 (d, J = 10.6 Hz, 1H), 5.55 (d, J = 7.1 Hz, 1H), 5.26 (s, 1H), 3.84 (s, 3H), 3.47 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 200.3, 173.5, 166.9, 162.2, 144.1, 135.0, 132.6, 132.5, 130.3, 129.9, 129.1, 128.7, 128.3, 126.7, 126.4, 120.6, 119.9, 101.5, 60.5, 54.9, 51.9; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{25}\text{H}_{20}\text{O}_4\text{S}$: 416.1087; found: 416.1078.

Spectral data for (R)-4-(6-methoxy-3-oxo-1-(phenylthio)-3,3a-dihydroazulen-3a-yl)benzonitrile (6i):



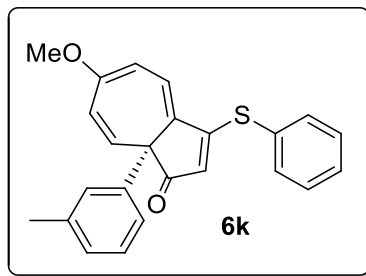
Compound **6i** was purified on silica gel column using ethyl acetate/hexane: (19: 81) as the eluent; White solid (81.45 mg, 0.21 mmol, 57%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 (d, J = 6.65 Hz, 2H), 7.47 ~ 7.42 (m, 5H), 7.31 (d, J = 8.3 Hz, 2H), 6.75 (d, J = 7.4 Hz, 1H), 6.36 (d, J = 10.6 Hz, 1H), 6.25 (dd, J = 10.6, 1.8 Hz, 1H), 5.57 (dd, J = 7.2, 1.4 Hz, 1H), 5.25 (s, 1H), 3.50 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 199.7, 173.8, 162.3, 144.3, 135.0, 132.2, 132.0, 131.7, 130.4, 130.0, 128.1, 127.2, 127.1, 120.5, 120.1, 118.8, 110.7, 101.6, 60.5, 54.9; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{24}\text{H}_{17}\text{NO}_2\text{S}$: 383.0985; found: 383.0983.

Spectral data for (R)-4-(6-methoxy-3-oxo-1-(phenylthio)-3,3a-dihydroazulen-3a-yl)benzaldehyde (6j):



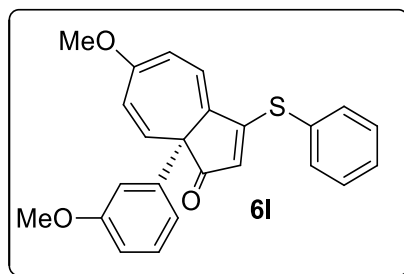
Compound **6j** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Pale yellow solid (76.4 mg, 0.19 mmol, 53%); ^1H NMR (700 MHz, CDCl_3): δ 9.90 (s, 1H), 7.68 (d, J = 8.1 Hz, 2H), 7.58 (d, J = 7.7 Hz, 2H), 7.45 ~ 7.42 (m, 3H), 7.38 (d, J = 8.8 Hz, 2H), 6.75 (d, J = 7.4 Hz, 1H), 6.40 (d, J = 10.7 Hz, 1H), 6.26 (dd, J = 10.6, 1.4 Hz, 1H), 5.57 (d, J = 7.3 Hz, 1H), 5.27 (s, 1H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 199.9, 191.8, 173.7, 162.3, 146.0, 135.1, 135.0, 132.5, 132.3, 130.3, 129.9, 129.3, 128.2, 127.1, 126.9, 120.6, 120.0, 101.6, 60.7, 54.9; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{24}\text{H}_{18}\text{NO}_3\text{S}$: 386.0982; found: 386.0983.

Spectral data for (R)-6-methoxy-3-(phenylthio)-8a-(m-tolyl)azulen-1(8aH)-one (6k):



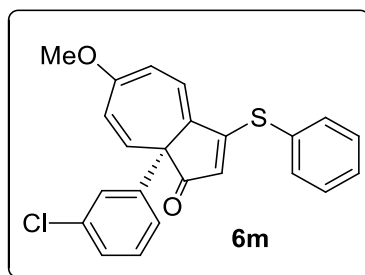
Compound **6k** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow oil (97.2 mg, 0.26 mmol, 70%); ^1H NMR (400 MHz, CDCl_3): δ 7.59 ~ 7.57 (m, 2H), 7.45 ~ 7.42 (m, 3H), 7.07 ~ 6.92 (m, 4H), 6.69 (d, J = 7.5 Hz, 1H), 6.38 (d, J = 10.7 Hz, 1H), 6.22 (dd, J = 10.6, 2 Hz, 1H), 5.55 (dd, J = 7.5, 1.9 Hz, 1H), 5.25 (s, 1H), 3.50 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.4, 173.1, 162.1, 138.8, 137.4, 135.0, 133.1, 133.0, 130.1, 129.9, 128.5, 127.7, 127.6, 127.0, 126.3, 123.2, 120.7, 119.5, 101.4, 60.4, 54.9, 21.6; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$: 395.1081; found: 395.1084.

Spectral data for (R)-6-methoxy-8a-(3-methoxyphenyl)-3-(phenylthio)azulen-1(8aH)-one (6l):



Compound **6l** was purified on silica gel column using ethyl acetate/hexane: (18: 82) as the eluent; Yellow oil (123.1 mg, 0.31 mmol, 85%); ^1H NMR (700 MHz, CDCl_3): δ 7.58 ~ 7.57 (m, 2H), 7.44 ~ 7.41 (m, 3H), 7.09 (t, J = 7.9 Hz, 1H), 6.81 (d, J = 7.9 Hz, 1H), 6.77 ~ 6.75 (m, 1H), 6.69 ~ 6.66 (m, 2H) 6.36 (d, J = 10.7 Hz, 1H), 6.23 (dd, J = 10.7, 2.0 Hz, 1H), 5.56 (dd, J = 7.5, 1.8 Hz, 1H), 5.25 (s, 1H), 3.73 (s, 3H), 3.50 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.1, 173.2, 162.1, 159.0, 140.5, 135.0, 133.0, 132.7, 130.1, 129.9, 128.7, 128.5, 126.4, 120.6, 119.6, 118.9, 112.7, 111.8, 101.5, 60.4, 55.1, 54.9; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{24}\text{H}_{20}\text{O}_3\text{S}$: 388.1133; found: 388.1135.

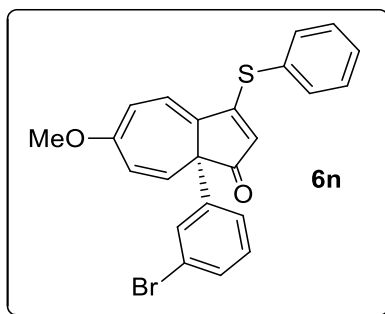
Spectral data for (R)-8a-(3-chlorophenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6m):



Compound **6m** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Light yellow solid (106.9 mg, 0.27 mmol, 73%); ^1H NMR (700 MHz, CDCl_3): δ 7.59 ~ 7.58 (m, 2H), 7.45 ~ 7.42 (m, 3H), 7.14 (s, 1H), 7.12 (m, 3H), 6.72 (d, J = 7.4 Hz, 1H), 6.34 (d, J = 10.7 Hz, 1H), 6.24 (dd, J = 10.7, 1.8 Hz, 1H), 5.58 (dd, J = 7.4, 1.6 Hz, 1H), 5.25 (s, 1H), 3.51 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 200.5, 173.4, 162.2, 140.9, 135.0, 133.6, 132.4, 132.3, 130.3,

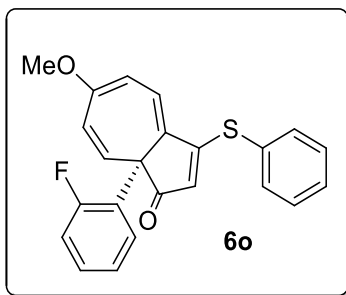
129.9, 129.1, 128.3, 127.2, 126.7, 126.4, 124.8, 120.5, 119.9, 101.6, 60.0, 54.9; HRMS (ESI-TOF) m/z : $[M+Na]^+$ calcd for $C_{23}H_{17}ClO_2S$: 415.0535; found: 415.0522.

Spectral data for (R)-8a-(3-bromophenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6n):



Compound **6n** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Yellow solid (94.6 mg, 0.21 mmol, 58%); 1H NMR (700 MHz, $CDCl_3$): δ 7.59 ~ 7.58 (m, 2H), 7.45 ~ 7.42 (m, 3H), 7.28 ~ 7.25 (m, 2H), 7.17 (d, J = 7.9 Hz, 1H), 7.04 (t, J = 7.9 Hz, 1H), 6.72 (d, J = 7.4 Hz, 1H), 6.33 (d, J = 10.7 Hz, 1H), 6.24 (dd, J = 10.7, 1.82 Hz, 1H), 5.58 (dd, J = 7.4, 1.4 Hz, 1H), 5.25 (s, 1H), 3.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 200.5, 173.4, 162.2, 141.2, 135.0, 132.4, 132.2, 130.3, 130.1, 129.9, 129.4, 129.2, 128.3, 126.7, 125.2, 121.9, 120.5, 119.8, 101.6, 60.0, 54.9; HRMS (ESI-MS) m/z : $[M+Na]^+$ calcd for $C_{23}H_{17}BrO_2S$: 459.0030; found: 459.0030.

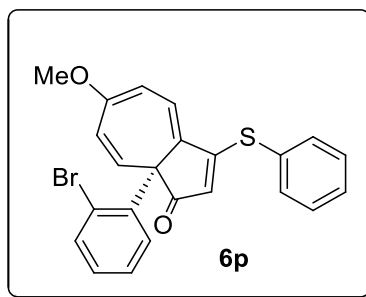
Spectral data for (R)-8a-(2-fluorophenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6o):



Compound **6o** was purified on silica gel column using ethyl acetate/hexane: (15: 85) as the eluent; Light yellow solid (109.4 mg, 0.29 mmol, 78%); 1H NMR (700 MHz, $CDCl_3$): δ 7.59 ~ 7.57 (m, 2H), 7.44 ~ 7.40 (m, 3H), 7.13 ~ 7.09 (m, 2H), 6.94 ~ 6.88 (m, 2H), 6.65 (d, J = 7.3 Hz, 1H), 6.31 (dd, J = 10.5, 3.9 Hz, 1H), 6.24 (dd, J = 10.6, 1.7 Hz, 1H), 5.57 (dd, J = 7.3, 1.5 Hz, 1H), 5.28 (s,

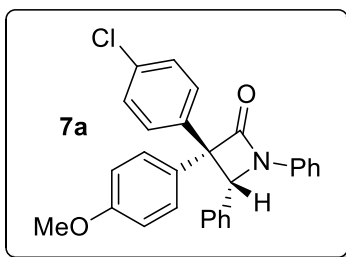
1H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 200.7, 172.9, 162.0, 160.5, 135.0, 131.9, 131.6, 130.1, 129.8, 129.04, 129.02, 128.76, 128.72, 128.5, 125.97, 125.96, 125.0, 124.9, 123.13, 123.11, 120.75, 120.74, 119.2, 116.4, 116.3, 101.4, 58.3, 54.9; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{FO}_2\text{S}$: 376.0933; found: 376.0934.

Spectral data for (S)-8a-(2-bromophenyl)-6-methoxy-3-(phenylthio)azulen-1(8aH)-one (6p):



Compound **6p** was purified on silica gel column using ethyl acetate/hexane: (16: 84) as the eluent; Yellow solid (99.4 mg, 0.22 mmol, 61%); ^1H NMR (400 MHz, CDCl_3): δ 7.58 ~ 7.56 (m, 2H), 7.45 ~ 7.42 (m, 3H), 7.25 ~ 7.23 (m, 2H), 7.13 ~ 7.09 (m, 1H), 7.00 ~ 6.96 (m, 1H), 6.67 (d, J = 7.2 Hz, 1H), 6.37 (d, J = 10.3 Hz, 1H), 6.25 (dd, J = 10.3, 1.8 Hz, 1H), 5.62 (dd, J = 7.2, 1.8 Hz, 1H), 5.29 (s, 1H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 200.8, 172.9, 162.0, 160.5, 135.0, 131.9, 131.6, 130.1, 129.8, 129.0, 128.7, 128.5, 125.9, 124.9, 123.1, 120.7, 119.2, 116.3, 101.4, 58.3, 54.9; HRMS (FD) m/z : $[\text{M}]^+$ calcd for $\text{C}_{23}\text{H}_{17}\text{BrO}_2\text{S}$: 436.0127; found: 436.0124.

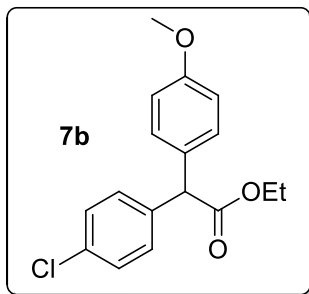
Spectral data for 3-(4-chlorophenyl)-3-(4-methoxyphenyl)-1,4-diphenylazetidin-2-one (7a):



Compound **7a** was purified on silica gel column using ethyl acetate/hexane: (14: 86) as the eluent; White solid (55.3 mg, 0.12 mmol, 72%); ^1H NMR (700 MHz, CDCl_3): δ 7.51 (d, J = 8.8 Hz, 2H), 7.36 (d, J = 7.7 Hz, 2H), 7.23 (t, J = 8.2 Hz, 2H), 7.15 ~ 7.10 (m, 5H), 7.04 ~ 7.01 (m, 3H), 6.97 (d, J = 8.6 Hz, 2H), 6.89 (d, J = 8.7 Hz, 2H), 5.72 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 166.8, 158.9, 137.3, 136.0, 134.6, 132.7, 132.4, 129.6, 129.0, 128.5, 128.39, 128.35,

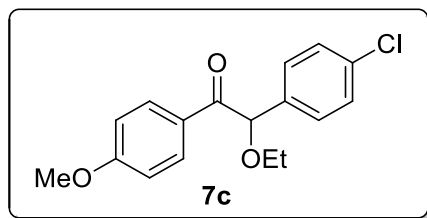
128.0, 127.4, 124.2, 117.4, 114.2, 71.0, 67.2, 55.3; HRMS (ESI-TOF) m/z : $[M+Na]^+$ calcd for $C_{28}H_{22}ClNO_2$: 462.1236; found: 462.1234.

Spectral data for Ethyl 2-(4-chlorophenyl)-2-(4-methoxyphenyl)acetate (7b):



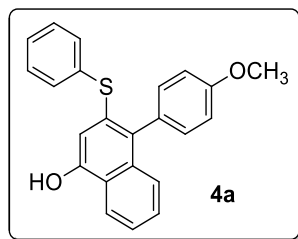
Compound **7b** was purified on silica gel column using ethyl acetate/hexane: (14: 86) as the eluent; Colorless liquid (16 mg, 0.05 mmol, 30%); 1H NMR (700 MHz, $CDCl_3$): δ 7.25 (d, J = 8.4 Hz, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.6 Hz, 2H), 7.83 (d, J = 8.6 Hz, 2H), 4.89 (s, 1H), 4.19 ~ 4.16 (m, 2H), 3.76 (s, 3H), 1.23 (t, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 172.3, 158.8, 137.6, 133.0, 130.4, 129.8, 129.5, 128.6, 114.0, 61.2, 55.6, 55.2, 14.1; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{17}H_{17}ClO_3$: 304.0866; found: 304.0868.

Spectral data for 2-(4-chlorophenyl)-2-ethoxy-1-(4-methoxyphenyl)ethanone (7c):



Compound **7c** was purified on silica gel column using ethyl acetate/hexane: (14: 86) as the eluent; Colorless liquid (32.4 mg, 0.10 mmol, 61%); 1H NMR (700 MHz, $CDCl_3$): δ 8.0 (d, J = 8.9 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 6.84 (d, J = 8.8 Hz, 2H), 5.43 (s, 1H), 3.81 (s, 3H), 3.61 ~ 3.55 (m, 2H), 1.25 (t, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ ; 195.9, 163.6, 135.6, 134.0, 131.6, 128.8, 128.3, 127.5, 113.6, 84.8, 65.6, 55.4, 15.2; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{17}H_{17}ClO_3$: 304.0866; found: 304.0868.

Spectral data for 4-(4-methoxyphenyl)-3-(phenylthio)naphthalen-1-ol (4a):

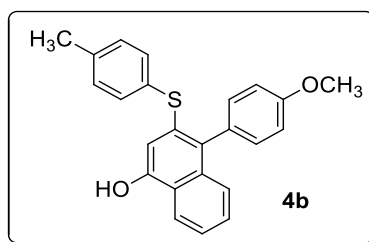


Compound **4a** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (233 mg, 0.65 mmol, 65%); ^1H NMR (500 MHz, CDCl_3): δ 8.13 (d, J = 8.0 Hz, 1H), 7.43-7.36 (m, 3H), 7.34-7.27 (m, 3H), 7.26-7.22 (m, 4H), 7.01 (d, J = 8.5 Hz, 2H), 6.57 (s, 1H), 5.21 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 158.9, 151.0, 135.5, 134.4, 133.3, 132.3, 132.2, 131.9, 130.6, 129.1, 127.2, 127.0, 126.2, 124.9, 123.4, 121.6, 113.7, 109.8, 55.2; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{23}\text{H}_{18}\text{O}_2\text{S}$: 358.1028, found 358.1027.

Spectral data for (4a'):Unknown species

Compound **4a'** was purified on silica gel column using ethyl acetate/hexane: (04: 96) as the eluent; White solid (34 mg, 0.056 mmol, 15%); ^1H NMR (700 MHz, CDCl_3): δ 7.43-7.38 (m, 4H), 7.34-7.31 (m, 5H), 7.29-7.23 (m, 7H), 7.21 (d, J = 8.5 Hz, 2H), 7.00 (d, J = 8.2 Hz, 3H), 6.88 (d, J = 8.6 Hz, 2H), 5.30 (s, 1H), 3.86 (s, 3H), 3.79 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 171.0, 159.1, 159.0, 146.1, 138.3, 137.4, 135.1, 134.4, 133.3, 132.0, 131.6, 130.1, 130.0, 129.8, 129.2, 128.7, 128.5, 127.4, 127.3, 126.9, 126.6, 125.9, 125.7, 121.0, 119.4, 114.1, 113.8, 56.2, 55.2, 55.2; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ found: 605.1783.

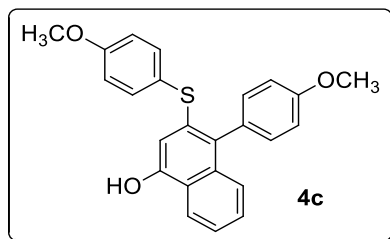
Spectral data for 4-(4-methoxyphenyl)-3-(*p*-tolylthio)naphthalen-1-ol (4b):



Compound **4b** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (92 mg, 0.24 mmol, 73%); ^1H NMR (500 MHz, CDCl_3): δ 8.11 (d, J = 8.1 Hz, 1H), 7.39-7.33 (m, 3H), 7.26 (t, J = 7.3 Hz, 4H), 7.12 (d, J = 7.8 Hz, 2H), 7.02 (d, J = 8.3 Hz, 2H), 6.48 (s, 1H), 5.27 (s, 1H), 3.87 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 158.9, 151.0, 137.8, 134.5, 134.4, 133.3, 132.0, 131.1, 130.9, 130.6, 130.0, 126.9, 126.0, 124.6, 123.0, 121.6,

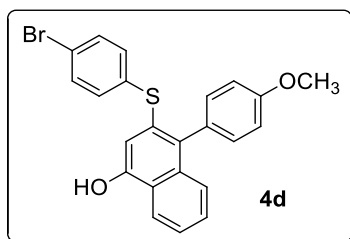
113.8, 108.8, 55.2, 21.1; HRMS (ESI-TOF) m/z : $[M+Na]^+$ calcd. for $C_{24}H_{20}NaO_2S$: 395.1082, found 395.1089.

Spectral data for 4-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)naphthalen-1-ol (4c):



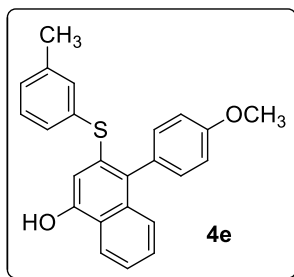
Compound **4c** was purified on silica gel column using ethyl acetate/hexane: (14: 86) as the eluent; White solid (99 mg, 0.25 mmol, 84%); 1H NMR (700 MHz, $CDCl_3$): δ 8.10 (d, J = 8.4 Hz, 1H), 7.39-7.33 (m, 5H), 7.26 (t, J = 8.4 Hz, 2H), 7.05 (d, J = 7.7 Hz, 2H), 6.88 (d, J = 7.7 Hz, 2H), 6.38 (s, 1H), 5.15 (s, 1H), 3.88 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 159.9, 159.0, 151.0, 136.1, 135.8, 134.4, 132.1, 130.5, 129.6, 126.9, 125.8, 124.4, 124.4, 122.7, 121.6, 115.0, 113.8, 107.8, 55.3, 55.2; HRMS (EI-MS) m/z : $[M]^+$ calcd. for $C_{24}H_{20}O_3S$: 388.1133, found 388.1137.

Spectral data for 3-((4-bromophenyl)thio)-4-(4-methoxyphenyl)naphthalen-1-ol (4d):



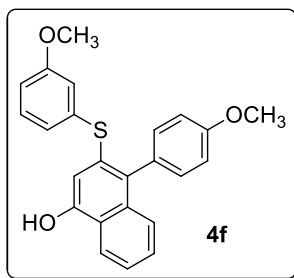
Compound **4d** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (49 mg, 0.11 mmol, 47%); 1H NMR (700 MHz, $CDCl_3$): δ 8.14 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 6.5 Hz, 2H), 7.37-7.35 (m, 1H), 7.32 (d, J = 7.3 Hz, 2H), 7.28-7.22 (m, 4H), 7.01 (d, J = 8.5 Hz, 2H), 6.58 (s, 1H), 5.33 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 158.9, 151.1, 135.6, 134.5, 133.3, 132.3, 132.2, 131.9, 130.6, 129.1, 127.2, 127.0, 126.2, 124.9, 123.4, 121.6, 113.7, 109.8, 55.2; HRMS (ESI-TOF) m/z : $[M+Na]^+$ calcd. for $C_{23}H_{17}BrNaO_2S$: 459.0030, found 459.0029.

Spectral data for 4-(4-methoxyphenyl)-3-(m-tolylthio)naphthalen-1-ol (4e):



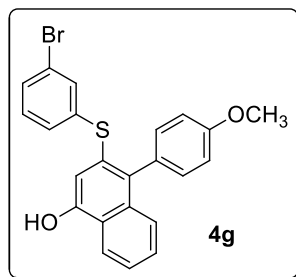
Compound **4e** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (89 mg, 0.23 mmol, 71%); ^1H NMR (700 MHz, CDCl_3): δ 8.15 (d, J = 8.5 Hz, 1H), 7.43-7.36 (m, 3H), 7.25 (d, J = 8.1 Hz, 2H), 7.19-7.14 (m, 3H), 7.07 (d, J = 7.3 Hz, 1H), 7.02 (d, J = 8.3 Hz, 2H), 6.58 (s, 1H), 5.26 (s, 1H), 3.88 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 158.9, 151.0, 139.0, 134.9, 134.4, 133.7, 133.1, 131.9, 131.9, 130.6, 129.6, 129.0, 128.3, 127.0, 126.2, 124.8, 123.2, 121.6, 113.7, 109.6, 55.2, 21.2; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$: 372.1184, found 372.1182.

Spectral data for 4-(4-methoxyphenyl)-3-((3-methoxyphenyl)thio)naphthalen-1-ol (4f):



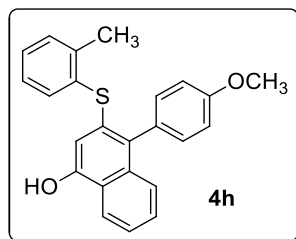
Compound **4f** was purified on silica gel column using ethyl acetate/hexane: (14: 86) as the eluent; White solid (93 mg, 0.24 mmol, 79%); ^1H NMR (500 MHz, CDCl_3): δ 8.17 (d, J = 8.1 Hz, 1H), 7.47-7.38 (m, 3H), 7.27-7.20 (m, 3H), 7.04 (d, J = 8.3 Hz, 2H), 6.93 (d, J = 7.6 Hz, 1H), 6.89 (s, 1H), 6.82 (d, J = 8.1 Hz, 1H), 6.65 (s, 1H), 5.31 (s, 1H), 3.90 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 159.9, 158.9, 151.0, 136.7, 134.4, 133.1, 132.4, 131.9, 130.6, 129.9, 127.0, 126.3, 125.0, 124.5, 123.4, 121.6, 117.2, 113.7, 113.2, 109.9, 55.2, 55.2; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_3\text{S}$: 388.1133, found 388.1130.

Spectral data for 3-((3-bromophenyl)thio)-4-(4-methoxyphenyl)naphthalen-1-ol (4g):



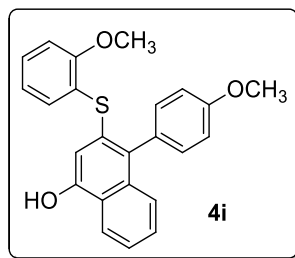
Compound **4g** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (59 mg, 0.13 mmol, 57%); ^1H NMR (500 MHz, CDCl_3): δ 8.13 (d, $J = 7.9$ Hz, 1H), 7.43-7.34 (m, 3H), 7.32-7.22 (m, 6H), 7.01 (d, $J = 8.4$ Hz, 2H), 6.57 (s, 1H), 5.19 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 158.9, 151.1, 135.5, 134.4, 133.3, 132.3, 132.2, 131.9, 130.6, 129.1, 127.2, 127.0, 126.2, 124.9, 123.4, 121.6, 113.7, 109.8, 55.2; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{23}\text{H}_{17}\text{BrO}_2\text{S}$: 436.0133, found 436.0127.

Spectral data for 4-(4-methoxyphenyl)-3-(o-tolylthio)naphthalen-1-ol (4h):



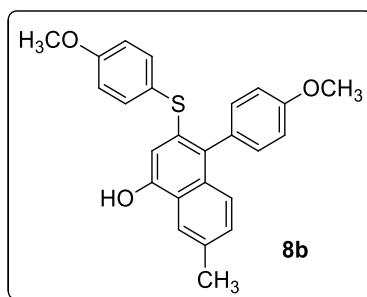
Compound **4h** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (94 mg, 0.25 mmol, 75%); ^1H NMR (500 MHz, CDCl_3): δ 8.09 (d, $J = 8.9$ Hz, 1H), 7.38-7.32 (m, 4H), 7.25-7.20 (m, 4H), 7.14-7.10 (m, 1H), 7.01 (d, $J = 8.5$ Hz, 2H), 6.31 (s, 1H), 5.20 (s, 1H), 3.86 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 158.9, 151.1, 141.2, 134.7, 134.5, 133.9, 133.6, 131.8, 130.9, 130.7, 130.6, 128.3, 126.9, 126.6, 125.9, 124.6, 123.0, 121.6, 113.8, 108.2, 55.2, 20.7; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$: 372.1184, found 372.1189.

Spectral data for 4-(4-methoxyphenyl)-3-((2-methoxyphenyl)thio)naphthalen-1-ol (4i):



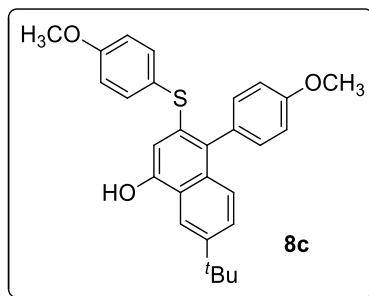
Compound **4i** was purified on silica gel column using ethyl acetate/hexane: (14: 86) as the eluent; White solid (96 mg, 0.24 mmol, 81%); ^1H NMR (500 MHz, CDCl_3): δ 8.13 (d, J = 8.4 Hz, 1H), 7.42-7.33 (m, 3H), 7.26-7.17 (m, 4H), 6.99 (d, J = 8.3 Hz, 2H), 6.85 (t, J = 6.8 Hz, 2H), 6.55 (s, 1H), 5.18 (s, 1H), 3.85 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 158.8, 158.1, 150.9, 134.5, 133.5, 132.6, 132.6, 131.9, 130.7, 128.8, 126.8, 126.2, 124.8, 123.6, 123.4, 121.6, 121.1, 113.7, 111.0, 109.8, 55.8, 55.2; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_3\text{S}$: 388.1133, found 388.1135.

Spectral data for 4-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)-7-methylnaphthalen-1-ol (8b):



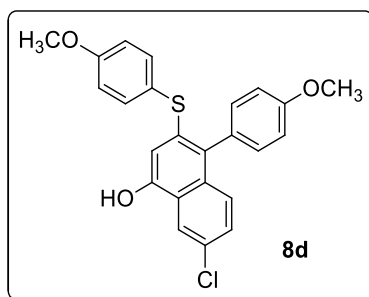
Compound **8b** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (88 mg, 0.21 mmol, 72%); ^1H NMR (700 MHz, CDCl_3): δ 7.88 (s, 1H), 7.35-7.25 (m, 5H), 7.19 (d, J = 8.6 Hz, 1H), 7.04 (d, J = 8.4 Hz, 2H), 6.86 (d, J = 8.6 Hz, 2H), 6.39 (s, 1H), 5.22 (s, 1H), 3.88 (s, 3H), 3.80 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 159.7, 158.9, 150.5, 135.7, 134.3, 134.2, 132.7, 132.0, 130.7, 129.9, 129.1, 125.8, 124.8, 122.9, 120.5, 114.9, 113.7, 108.2, 55.3, 55.2, 21.5; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{25}\text{H}_{22}\text{O}_3\text{S}$: 402.1290, found 402.1297.

Spectral data for 7-(tert-butyl)-4-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)naphthalen-1-ol (8c):



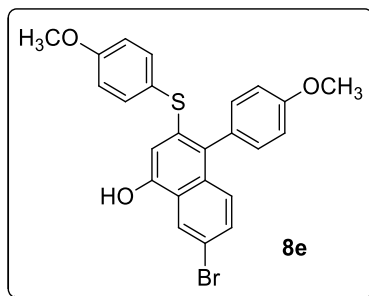
Compound **8c** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; Colorless oil (93 mg, 0.21 mmol, 69%); ^1H NMR (500 MHz, CDCl_3): δ 7.47 (d, J = 7.9 Hz, 2H), 7.39 (s, 1H), 7.29 (d, J = 8.7 Hz, 3H), 7.23 (d, J = 6.7 Hz, 2H), 6.99 (d, J = 9.1 Hz, 1H), 6.83 (d, J = 8.4 Hz, 2H), 6.43 (s, 1H), 5.15 (s, 1H), 3.89 (s, 3H), 3.78 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3): δ 159.5, 156.9, 150.0, 135.4, 135.0, 131.9, 131.1, 130.4, 129.8, 127.8, 125.4, 125.1, 123.8, 119.3, 114.8, 114.7, 109.2, 100.0, 55.3, 34.6, 31.4; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{28}\text{H}_{28}\text{O}_3\text{S}$: 444.1759, found 444.1763.

Spectral data for 7-chloro-4-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)naphthalen-1-ol (8d):



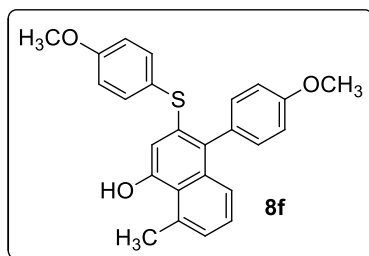
Compound **8d** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (72 mg, 0.17 mmol, 56%); ^1H NMR (500 MHz, CDCl_3): δ 8.08 (s, 1H), 7.36 (d, J = 8.7 Hz, 2H), 7.31-7.24 (m, 4H), 7.04 (d, J = 8.5 Hz, 2H), 6.88 (d, J = 8.7 Hz, 2H), 6.35 (s, 1H), 5.19 (s, 1H), 3.88 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 160.0, 159.1, 150.2, 136.5, 136.3, 132.7, 132.0, 130.4, 129.9, 129.2, 127.7, 127.4, 123.9, 123.3, 120.9, 115.0, 113.9, 108.4, 55.3, 55.2; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{24}\text{H}_{19}\text{O}_3\text{S}$: 422.0743, found 422.0748.

Spectral data for 7-bromo-4-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)naphthalen-1-ol (8e):



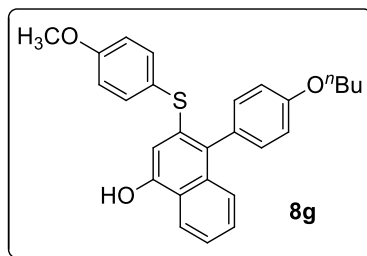
Compound **8e** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (90 mg, 0.19 mmol, 63%); ^1H NMR (500 MHz, CDCl_3): δ 8.26 (s, 1H), 7.37 (t, J = 9.9 Hz, 3H), 7.23 (t, J = 6.0 Hz, 3H), 7.04 (d, J = 7.9 Hz, 2H), 6.88 (d, J = 8.0 Hz, 2H), 6.33 (s, 1H), 5.23 (s, 1H), 3.87 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 160.0, 159.1, 150.1, 136.8, 136.4, 132.8, 132.0, 130.2, 129.8, 129.1, 127.5, 124.2, 123.8, 123.8, 118.5, 115.1, 114.0, 108.3, 55.3, 55.2; HRMS (FD) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{24}\text{H}_{19}\text{BrO}_3\text{S}$: 466.0238, found 466.0233.

Spectral data for 4-(4-methoxyphenyl)-3-((4-methoxyphenyl)thio)-8-methylnaphthalen-1-ol (8f):



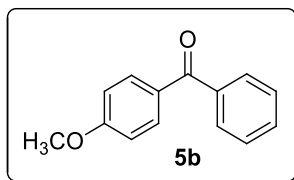
Compound **8f** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (53 mg, 0.13 mmol, 43%); ^1H NMR (500 MHz, CDCl_3): δ 7.40-7.34 (m, 2H), 7.30-7.21 (m, 4H) 7.11 (d, J = 7.5 Hz, 2H), 6.99 (d, J = 9.2 Hz, 1H), 6.83 (d, J = 8.7 Hz, 2H), 6.45 (s, 1H), 5.27 (s, 1H), 3.89 (s, 3H), 3.78 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 159.5, 156.9, 150.1, 138.4, 137.8, 135.3, 131.5, 129.6, 128.2, 128.1, 127.9, 127.8, 125.5, 123.9, 119.4, 114.8, 109.4, 100.0, 55.4, 55.3, 21.5; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{25}\text{H}_{22}\text{O}_3\text{S}$: 402.1290, found 402.1294.

Spectral data for 4-(4-butoxyphenyl)-3-((4-methoxyphenyl)thio)naphthalen-1-ol (8g):



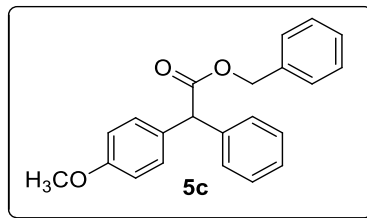
Compound **8g** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (112 mg, 0.26 mmol, 86%); ^1H NMR (700 MHz, CDCl_3): δ 8.07 (d, J = 8.2 Hz, 1H), 7.37-7.30 (m, 5H), 7.22 (t, J = 8.2 Hz, 2H), 7.01 (d, J = 8.3 Hz, 2H), 6.84 (d, J = 8.6 Hz, 2H), 6.36 (s, 1H), 5.26 (s, 1H), 4.01 (s, 2H), 3.77 (s, 3H), 1.80-1.76 (m, 2H), 1.53-1.48 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 159.8, 158.5, 150.9, 136.1, 135.8, 134.4, 132.0, 130.2, 129.7, 126.9, 125.8, 124.4, 124.4, 122.7, 121.5, 114.9, 114.3, 107.7, 67.6, 55.3, 31.4, 19.3, 13.8 ; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{27}\text{H}_{26}\text{O}_3\text{S}$: 430.1603, found 430.1605.

Spectral data for (4-methoxyphenyl)(phenyl)methanone (5b**):**



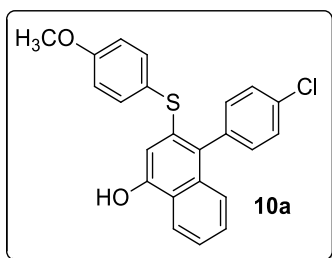
Compound **5b** was purified on silica gel column using ethyl acetate/hexane: (08: 92) as the eluent; Colorless oil (16 mg, 0.075 mmol, 36%); ^1H NMR (500 MHz, CDCl_3): δ 7.81 (d, J = 8.7 Hz, 2H), 7.73 (d, J = 7.1 Hz, 2H), 7.54 (t, J = 7.3 Hz, 1H), 7.45 (t, J = 7.7 Hz, 2H), 6.94 (d, J = 8.7 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 195.5, 163.2, 138.2, 132.5, 131.8, 130.1, 129.7, 128.1, 113.5, 55.4; HRMS (ESI-TOF) m/z : $[\text{M}+\text{H}]^+$ calcd. for $\text{C}_{14}\text{H}_{13}\text{O}_2$: 213.0915, found: 213.0918.

Spectral data for benzyl 2-(4-methoxyphenyl)-2-phenylacetate (5c**):**



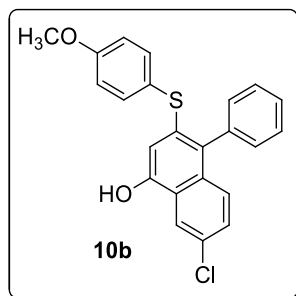
Compound **5c** was purified on silica gel column using ethyl acetate/hexane: (05: 95) as the eluent; Colorless oil (21 mg, 0.059 mmol, 28%); ^1H NMR (700 MHz, CDCl_3): δ 7.32-7.27 (m, 9H), 7.25-7.21 (m, 3H), 6.84 (d, J = 8.6 Hz, 2H), 5.18 (s, 2H), 5.03 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 172.5, 158.7, 138.8, 135.7, 130.6, 129.6, 128.5, 128.4, 128.4, 128.1, 128.1, 127.1, 113.9, 66.8, 56.1, 55.2; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd. for $\text{C}_{22}\text{H}_{20}\text{O}_3\text{Na}$: 355.1310, found: 355.1303.

Spectral data for 4-(4-chlorophenyl)-3-((4-methoxyphenyl)thio)naphthalen-1-ol (10a):



Compound **10a** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (66.9 mg, 0.17 mmol, 28%); ^1H NMR (700 MHz, CDCl_3): δ 8.11 (d, J = 8.2 Hz, 1H), 7.47 (d, J = 8.3 Hz, 2H), 7.40-7.38 (m, 1H), 7.36-7.33 (m, 2H), 7.32-7.27 (m, 4H), 6.87 (d, J = 8.7 Hz, 2H), 6.40 (s, 1H), 5.22 (s, 1H), 3.81 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 159.9, 151.3, 136.8, 135.9, 135.5, 133.9, 133.5, 132.4, 128.8, 128.7, 127.2, 125.4, 124.6, 124.1, 122.7, 121.7, 115.0, 108.0, 55.3; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd. for $\text{C}_{23}\text{H}_{17}\text{ClO}_2\text{S}$: 392.0638, found 392.0634.

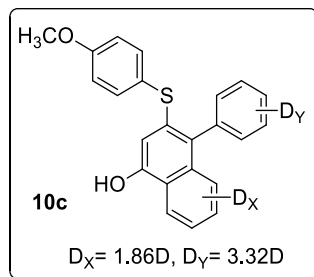
Spectral data for 7-chloro-3-((4-methoxyphenyl)thio)-4-phenylnaphthalen-1-ol (10b):



Compound **10b** was purified on silica gel column using ethyl acetate/hexane: (12: 88) as the eluent; White solid (4.7 mg, 0.01 mmol, 2%); ^1H NMR (700 MHz, CDCl_3): δ 8.09 (s, 1H), 7.52-7.43 (m, 3H), 7.33 (q, J = 16.3, 8.4 Hz, 4H), 7.25 (s, 2H), 6.88 (d, 8.4 Hz, 2H), 6.37 (s, 1H), 5.23 (s, 1H), 3.81 (s, 3H); ^{13}C NMR (175 MHz, CDCl_3): δ 160.0, 150.3, 137.8, 136.3, 136.1, 132.3, 130.9,

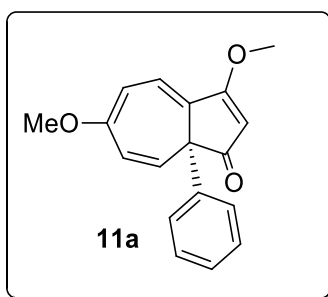
130.5, 129.7, 128.5, 127.8, 127.7, 127.4, 123.8, 123.3, 121.0, 115.0, 108.6, 55.3; HRMS (EI-MS) m/z : $[M]^+$ calcd. for $C_{23}H_{17}ClO_2S$: 392.0638, found 392.0635.

Spectral data for (10c):



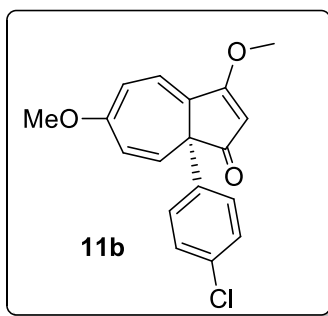
Compound **10c** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (77.2 mg, 0.21 mmol, 35%); 1H NMR (700 MHz, $CDCl_3$): δ 8.10 (d, $J = 4.7$ Hz, 0.4H), 7.50 (t, $J = 4.0$ Hz, 0.8H), 7.45 (d, $J = 3.59$ Hz, 0.4H), 7.38 (d, $J = 4.4$ Hz, 0.4H), 7.35 (d, $J = 8.4$ Hz, 3.6H), 6.87 (d, $J = 8.6$ Hz, 2H), 6.41 (s, 1H), 5.27 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 159.8, 151.1, 138.3, 138.2, 136.0, 135.3, 134.1, 134.0, 131.0, 130.9, 130.1, 128.4, 128.3, 128.2, 127.4, 127.3, 127.0, 126.9, 126.9, 126.8, 125.8, 125.6, 124.5, 124.4, 124.4, 124.4, 124.3, 122.7, 122.6, 121.6, 121.4, 114.9, 108.0, 55.3 ; HRMS (EI-MS) m/z : $[M]^+$ calcd. for $C_{23}H_{13}D_5O_2S$: 363.1341, found 363.1345.

Spectral data for (R)-3,6-dimethoxy-8a-phenylazulen-1(8aH)-one (11a):



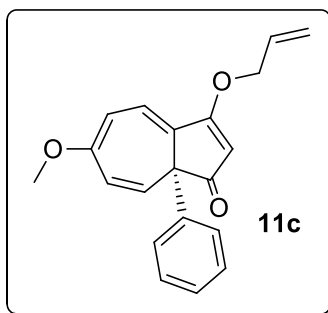
Compound **11a** was purified on silica gel column using ethyl acetate/hexane: (30: 70) as the eluent; White solid (18.8 mg, 0.06 mmol, 80%); 1H NMR (700 MHz, $CDCl_3$): δ 7.23 (d, $J = 8.4$ Hz, 2H), 7.16 (t, $J = 7.4$ Hz, 2H), 7.12 (t, $J = 7.1$ Hz, 1H), 6.71 (d, $J = 7.4$ Hz, 1H), 6.43 (d, $J = 10.7$ Hz, 1H), 6.19 (dd, $J = 10.7$, 1.9 Hz, 1H), 5.51 (dd, $J = 7.4$, 1.5 Hz, 1H), 5.19 (s, 1H), 3.95 (s, 3H), 3.46 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ : 202.0, 180.7, 162.0, 138.9, 133.0, 128.4, 127.7, 126.8, 126.3, 126.2, 118.9, 101.3, 100.2, 58.8, 58.6, 54.8; HRMS (EI-MS) m/z : $[M]^+$ calcd for $C_{18}H_{16}O_3$: 280.1099; found: 280.1095.

Spectral data for (R)-8a-(4-chlorophenyl)-3,6-dimethoxyazulen-1(8aH)-one (11b):



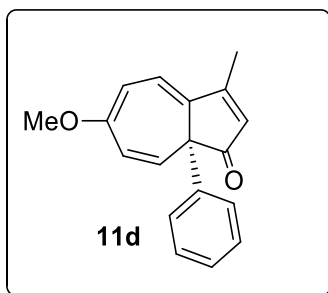
Compound **11b** was purified on silica gel column using ethyl acetate/hexane: (30: 70) as the eluent; White solid (20.5 mg, 0.06 mmol, 85%); ^1H NMR (700 MHz, CDCl_3): δ 7.16 (d, J = 8.5 Hz, 2H), 7.12 (d, J = 8.6 Hz, 2H), 6.71 (d, J = 7.4 Hz, 1H), 6.38 (d, J = 10.7 Hz, 1H), 6.18 (dd, J = 10.7, 1.8 Hz, 1H), 5.52 (dd, J = 7.4, 1.4 Hz, 1H), 5.18 (s, 1H), 3.95 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 201.5, 180.6, 162.0, 137.5, 132.7, 132.5, 127.97, 127.92, 127.8, 126.4, 119.1, 101.3, 100.1, 58.6, 58.2, 54.8; HRMS (ESI-MS) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{18}\text{H}_{15}\text{ClO}_3$: 337.0607; found: 337.0605.

Spectral data for (R)-3-(allyloxy)-6-methoxy-8a-phenylazulen-1(8aH)-one (11c):



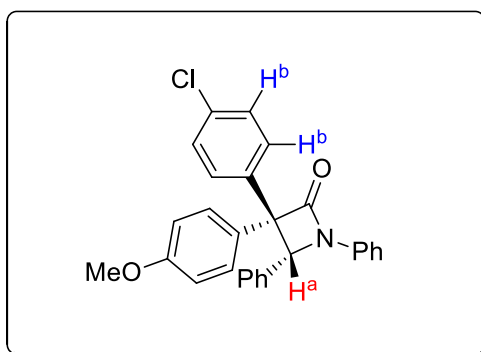
Compound **11c** was purified on silica gel column using ethyl acetate/hexane: (30: 70) as the eluent; Yellow oil (18.7 mg, 0.06 mmol, 73%); ^1H NMR (400 MHz, CDCl_3): δ 7.24 ~ 7.21 (m, 2H), 7.18 ~ 7.10 (m, 3H), 6.76 (d, J = 7.4 Hz, 1H), 6.42 (d, J = 10.7 Hz, 1H), 6.21 ~ 6.17 (m, 1H), 6.08 ~ 5.98 (m, 1H), 5.53 ~ 5.50 (m, 1H), 5.47 ~ 5.42 (m, 1H), 5.38 ~ 5.35 (m, 1H), 5.18 (s, 1H), 4.68 ~ 4.59 (m, 2H), 3.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ ; 202.1, 179.3, 162.0, 138.9, 133.0, 131.0, 128.6, 127.7, 126.8, 126.3, 126.2, 119.4, 119.0, 101.3, 100.9, 72.1, 58.6, 54.8; HRMS (EI-MS) m/z : $[\text{M}]^+$ calcd for $\text{C}_{20}\text{H}_{18}\text{O}_3$: 306.1256; found: 306.1258.

Spectral data for (R)-6-methoxy-3-methyl-8a-phenylazulen-1(8aH)-one (11d):



Compound **11d** was purified on silica gel column using ethyl acetate/hexane: (10: 90) as the eluent; White solid (11.5 mg, 0.04 mmol, 41%); ^1H NMR (700 MHz, CDCl_3): δ 7.15 ~ 7.12 (m, 3H), 7.10 ~ 7.08 (m, 2H), 7.01 (d, J = 7.4 Hz, 1H), 6.33 (dd, J = 10.6, 1.9 Hz, 1H), 6.13 (d, J = 1.2 Hz, 1H), 5.99 (d, J = 10.5 Hz, 1H), 5.59 (dd, J = 7.4, 1.6 Hz, 1H), 3.50 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ ; 194.5, 174.2, 164.0, 139.2, 133.7, 132.3, 131.4, 127.7, 127.0, 126.9, 126.0, 123.0, 101.9, 57.6, 54.9, 14.6; HRMS (ESI-TOF) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{16}\text{O}_2$: 265.1228; found: 265.1228.

8. ^1H -NOE of compound 7a:



Sr. No.	Irradiation	Intensity increase % (Key peaks)
1.	H^a (δ 1.72)	H^b (δ 7.36, 2.18 %)
2.	H^b (δ 7.36)	H^a (δ 1.72, 1.30 %)

9. Computational Details:

Geometries were optimized using the B3LYP functional combined with the 6-31G** basis set for light atoms and a double- ζ contraction of the Los Alamos valence functions and pseudopotentials for gold. Hessians at these geometries were computed to provide the zero-point energy and vibrational enthalpy. Solvation energies, H_{solv} s, were computed with the CPCM solvation model. The electronic energy E_{elec} was evaluated with the same functional but with better basis sets (the 6-311++G** basis set for light atoms and a triple- ζ contraction of the Los Alamos valence functions augmented with diffuse s and p functions for gold). Enthalpy of all species were calculated as $H = E_{\text{elec}} + H_{\text{solv}} + \text{ZPE} + H_{\text{vib}} + 4RT$, where the $4RT$ term is to account for the translational and rotational thermal corrections as well as PV.

a) The enthalpy reaction profile for the formation of 3a from 2a:

Species	E_{elec}	H_{solv}	$\text{ZPE} + H_{\text{vib}} + 4kT$	$H_{\text{total}}(\text{hartree})$
1a	-706.67711	-0.00283	0.11852	-706.56142
2a	-838.93415	-0.00510	0.25606	-838.68319
3a	-1436.15137	-0.00671	0.36823	-1435.78986
N ₂	-109.55942	-0.00024	0.00890	-109.55076
LAu	-1633.50121	-0.04025	0.48533	-1633.05614
A	-2472.49068	-0.03215	0.74298	-2471.77984
B	-2362.96523	-0.03139	0.73184	-2362.26478
C	-2362.97845	-0.03128	0.73142	-2362.27832
D	-3069.69079	-0.03548	0.85549	-3068.87078
E	-1436.13822	-0.00760	0.36799	-1435.77783
F	-729.34962	-0.00454	0.24276	-729.11140
G	-729.42532	-0.00353	0.24411	-729.18475
TS ₁	-2472.48583	-0.03151	0.74130	-2471.77605
TS ₂	-2362.93852	-0.03124	0.72963	-2362.24013
TS ₃	-3069.64459	-0.02986	0.85160	-3068.82285
TS ₄	-1436.13237	-0.00753	0.36634	-1435.77357
TS ₅	-838.88747	-0.00644	0.25243	-838.64148
TS ₆	-729.33654	-0.00831	0.24141	-729.10345

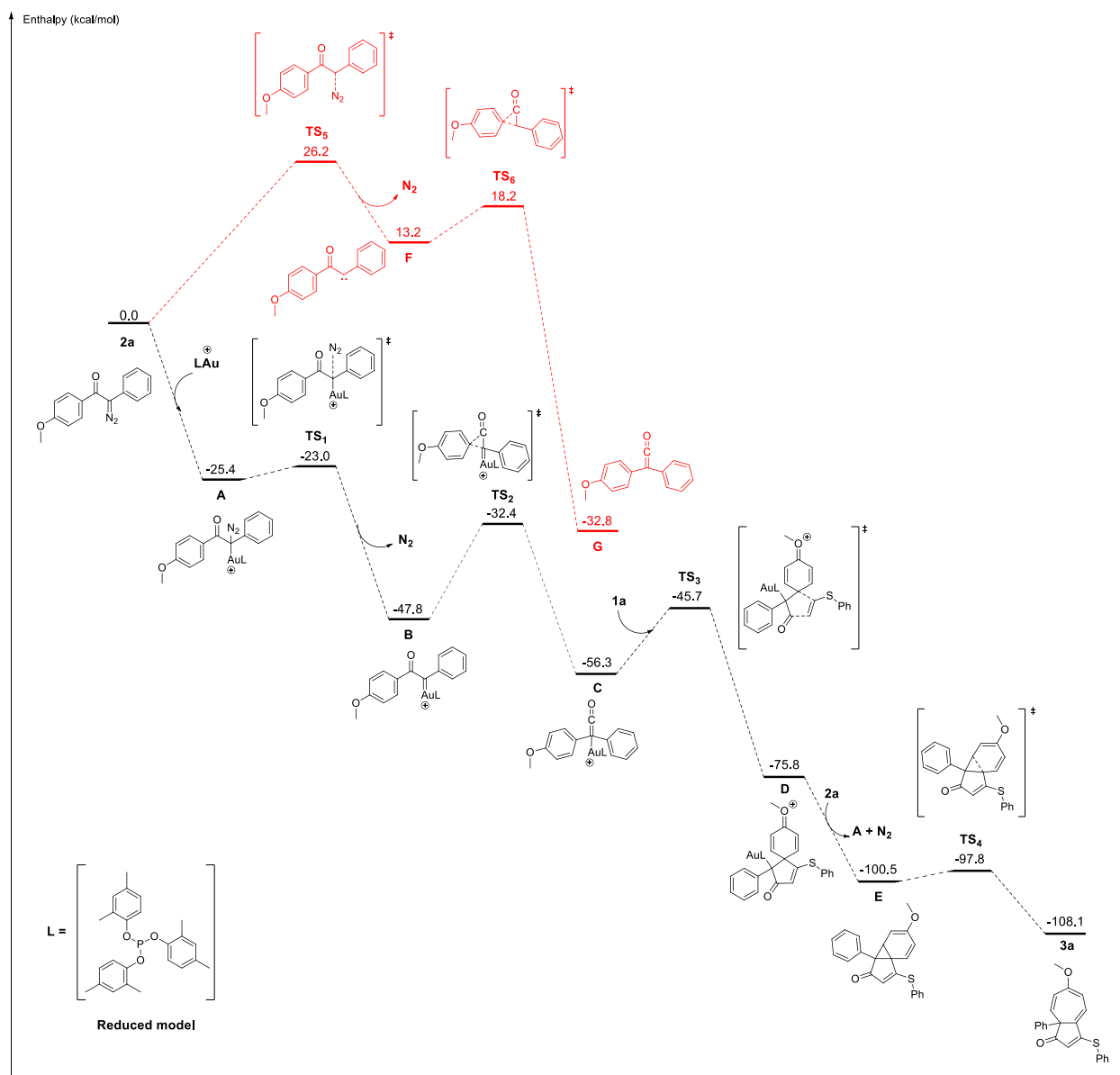


Figure S1. The enthalpy reaction profile for the formation of **3a** from **2a**.

1a

S	-1.56007900	-0.00347600	-0.99662200
C	0.14254000	-0.00128100	-0.37947000
C	0.80608200	-1.21396900	-0.16945900
C	0.80519200	1.21291300	-0.17542900
C	2.13460400	-1.20830400	0.25762700

H	0.28394400	-2.14999300	-0.33766400
C	2.13370400	1.21032100	0.25171200
H	0.28238100	2.14771800	-0.34825700
C	2.79789600	0.00177700	0.46871900
H	2.65043600	-2.14942300	0.42334200
H	2.64884000	2.15262300	0.41280900
H	3.83238900	0.00296900	0.79906700
C	-2.46177700	0.00132400	0.44447600
C	-3.18121400	0.00459000	1.41998100
H	-3.79888600	0.00749900	2.28771600

2a

C	1.33172300	0.22781000	-0.23536600
C	2.79273000	0.04541900	-0.04570800
C	3.65523800	1.15844700	-0.05187400
C	3.34873400	-1.23059900	0.15893400
C	5.02491500	1.00257700	0.13901300
H	3.25994400	2.15916700	-0.19871000
C	4.72171500	-1.37320400	0.35533500
H	2.70128900	-2.09569200	0.15404900
C	5.56897700	-0.26579500	0.34549800
H	5.66639600	1.87899600	0.12992100
H	5.12919400	-2.36793600	0.51196100
H	6.63747500	-0.38753600	0.49507000
C	0.27762100	-0.81257900	-0.13002500
C	-1.15371300	-0.40068600	0.00371600
C	-2.12555300	-1.23512800	-0.56353100
C	-1.58045400	0.72087200	0.73710800

C	-3.48278400	-0.95008100	-0.44890100
H	-1.79867400	-2.11961600	-1.09988200
C	-2.92979700	1.00852700	0.87379700
H	-0.85772800	1.35930500	1.23493600
C	-3.89181800	0.18115400	0.27263600
H	-4.20716800	-1.60779900	-0.91358000
H	-3.26881600	1.86332800	1.44890500
O	0.57171600	-2.00523600	-0.16994600
O	-5.18551800	0.55557300	0.45432600
C	-6.21172600	-0.24792500	-0.11408400
H	-7.15206600	0.23381800	0.15576000
H	-6.12905200	-0.29335000	-1.20686000
H	-6.19715600	-1.26661500	0.29212000
N	0.93805600	1.42605100	-0.61381800
N	0.64079100	2.46943300	-0.96589700

3a

C	-3.13091600	1.93037000	-0.18651100
C	-2.89660300	1.50129300	1.18002100
C	-1.94518900	0.64722500	1.60821800
C	-2.17935500	2.02009800	-1.17055600
C	-1.02992300	-0.16691400	0.72486100
C	-0.80139500	1.65715900	-1.06382900
C	-0.25605600	0.75144600	-0.20635000
H	-3.53049400	1.95829800	1.93560700
H	-1.82992400	0.49429200	2.67923500
H	-2.49825300	2.51641400	-2.08294600
H	-0.13016500	2.16434100	-1.75586100

C	0.11551500	-0.79694800	1.58446500
C	1.38572100	-0.43125700	0.97210600
H	2.34186200	-0.77918500	1.33703500
C	1.16885600	0.47676000	-0.02399300
O	-4.35039600	2.44986300	-0.52321800
C	-5.47886900	2.18571900	0.30345300
H	-6.35332500	2.43671400	-0.29946000
H	-5.52861600	1.13135200	0.59645500
H	-5.48282400	2.81249500	1.20373700
C	-1.78241400	-1.32268500	0.03200300
C	-2.53541100	-2.20379000	0.82400200
C	-1.71317400	-1.55163200	-1.34568900
C	-3.21151100	-3.27685600	0.24758400
H	-2.56727500	-2.05856900	1.89826300
C	-2.39294800	-2.62710900	-1.92265000
H	-1.13123200	-0.88697500	-1.97359800
C	-3.14689700	-3.49149000	-1.13096500
H	-3.78556000	-3.95017200	0.87803300
H	-2.33133800	-2.78429200	-2.99595500
H	-3.67641400	-4.32625100	-1.58117300
O	-0.07046000	-1.43784100	2.60698200
S	2.36766200	1.30855100	-1.01721400
C	3.91378000	0.57282700	-0.47144500
C	4.37608800	-0.60770000	-1.06547000
C	4.68215800	1.21687000	0.50518800
C	5.60111500	-1.14658000	-0.67185900
H	3.77794200	-1.09642800	-1.82740200
C	5.90825800	0.67346600	0.89115900

H	4.31914100	2.13451200	0.95617000
C	6.36722500	-0.50717800	0.30485200
H	5.95745800	-2.06382600	-1.13084900
H	6.50313800	1.17327500	1.64965300
H	7.32180800	-0.92755300	0.60679700

N₂

N	0.00000000	0.00000000	0.55274900
N	0.00000000	0.00000000	-0.55274900

LAu

Au	-1.17535300	-0.02057700	1.75651300
P	0.39277700	-0.16829400	0.08682400
O	-0.29777100	-0.89098100	-1.17356200
O	0.96772300	1.21664300	-0.45149200
O	1.66327200	-0.98731500	0.54954900
C	2.97508300	-0.95193400	-0.03881100
C	3.13863500	-1.23314300	-1.38763400
C	4.03373700	-0.68629700	0.83007300
C	4.43132400	-1.24332300	-1.91023000
H	2.28201900	-1.44562500	-2.01840700
C	5.31412800	-0.71349800	0.26416900
C	5.53903600	-0.98720100	-1.09193000
H	4.57528200	-1.45834400	-2.96485400
H	6.16440400	-0.51120900	0.91051400
C	0.12230100	2.31277200	-0.79424200
C	-0.58060300	2.28070300	-1.99374400
C	0.11161200	3.41209800	0.07081700

C	-1.35411000	3.38643700	-2.34426300
H	-0.50634600	1.41781800	-2.64611000
C	-0.67905200	4.49964900	-0.31943500
C	-1.41606200	4.51266800	-1.51211400
H	-1.90433200	3.37495800	-3.28049200
H	-0.70998700	5.37128000	0.32937100
C	-1.52728100	-1.59960900	-1.10764400
C	-2.71118100	-0.86957000	-1.19335300
C	-1.49577400	-2.99689100	-1.02482700
C	-3.92673400	-1.55544700	-1.19224900
H	-2.67350300	0.21109100	-1.28652900
C	-2.73702600	-3.64260600	-1.03142800
C	-3.95715200	-2.95303300	-1.11526500
H	-4.85443600	-0.99573700	-1.26418100
H	-2.74978000	-4.72800800	-0.97259100
C	3.81151100	-0.38948200	2.29115400
H	3.20054600	0.50972100	2.43042500
H	3.29333200	-1.21370000	2.79273200
H	4.76390300	-0.22860700	2.80009400
C	6.94194900	-1.03199600	-1.64729000
H	7.60314400	-0.33765500	-1.12165700
H	7.37154200	-2.03539100	-1.54106000
H	6.95936100	-0.78034600	-2.71105200
C	-0.20031800	-3.76570600	-0.95434800
H	0.41147700	-3.59429800	-1.84659900
H	0.40340300	-3.47392400	-0.08886900
H	-0.39444600	-4.83745200	-0.88113900
C	-5.26280100	-3.70884800	-1.15155500

H	-5.45154300	-4.10931000	-2.15463700
H	-5.25304700	-4.55742700	-0.46133300
H	-6.10648400	-3.06531600	-0.89033500
C	-2.22298100	5.72548400	-1.90664600
H	-1.61266500	6.42359600	-2.49204700
H	-3.08394700	5.45106800	-2.52208300
H	-2.58757600	6.26778700	-1.03013600
C	0.93430800	3.43979200	1.33536800
H	0.68989300	2.60716000	2.00522100
H	2.00398100	3.36634100	1.11150200
H	0.76594600	4.36860500	1.88396600

A

Au	-0.18562000	0.63628800	-0.79536400
P	1.84275800	-0.05724200	0.15422800
O	2.38019600	0.91154300	1.34278100
O	1.93765700	-1.52866700	0.80205100
O	2.96457800	-0.11305000	-0.97994600
C	4.23336900	-0.76008600	-0.93083400
C	5.07705300	-0.60764200	0.16207700
C	4.58523900	-1.49836800	-2.06421800
C	6.32748900	-1.22528000	0.13475200
H	4.76816500	-0.02160600	1.02006300
C	5.85060600	-2.09569000	-2.05321700
C	6.73624000	-1.97537300	-0.97382400
H	6.99067600	-1.11625600	0.98804800
H	6.15098400	-2.67783300	-2.92108700
C	1.03045400	-1.97979300	1.79264300

C	1.17681000	-1.54258300	3.10583100
C	0.06965700	-2.92430700	1.41538700
C	0.31761200	-2.04196600	4.08419400
H	1.96233500	-0.83823400	3.35516800
C	-0.77240200	-3.40196300	2.42722900
C	-0.67097600	-2.97997900	3.75969800
H	0.42907200	-1.70688200	5.11155100
H	-1.53077000	-4.13467000	2.16233100
C	1.81685600	2.18035600	1.61156300
C	0.70146100	2.24800300	2.43976000
C	2.44744800	3.32416300	1.10282500
C	0.18167800	3.49904300	2.78026500
H	0.26472100	1.33324900	2.82759400
C	1.89464100	4.55734400	1.46510900
C	0.77223400	4.67324200	2.29937200
H	-0.67865100	3.55640100	3.44127600
H	2.36702600	5.46181200	1.08926400
C	-2.05490600	1.21825500	-1.78693000
C	-3.02712700	2.09215900	-0.99847500
C	-2.60595300	2.85215900	0.10057100
C	-4.36508400	2.16182700	-1.41854000
C	-3.51905500	3.65818100	0.78147800
H	-1.57184300	2.81390800	0.42989800
C	-5.27299800	2.96589900	-0.73197300
H	-4.69889100	1.58553900	-2.27684000
C	-4.85135300	3.71479600	0.36925600
H	-3.18560300	4.24152900	1.63389800
H	-6.30682400	3.00974200	-1.05951600

H	-5.55936700	4.34182700	0.90216100
C	-2.56464600	-0.12872000	-2.40023200
C	-3.18239200	-1.11894200	-1.49853300
C	-3.71696800	-2.27361800	-2.09948100
C	-3.24585000	-1.00057200	-0.09315600
C	-4.29110300	-3.28357600	-1.34001100
H	-3.66622700	-2.36418900	-3.17909800
C	-3.80902100	-2.00366100	0.67398100
H	-2.85931900	-0.12100100	0.40891500
C	-4.33624600	-3.15684100	0.06033800
H	-4.69419100	-4.15902400	-1.83396300
H	-3.85763100	-1.92556300	1.75416000
O	-2.40883400	-0.31353200	-3.59715700
O	-4.85348600	-4.07655700	0.89843400
C	-5.44728700	-5.25841800	0.35577800
H	-5.80621500	-5.82791100	1.21258900
H	-6.29074800	-5.01261100	-0.29846100
H	-4.71245800	-5.85435100	-0.19694600
C	3.64812500	-1.64227000	-3.23646500
H	2.70280300	-2.11031900	-2.94005100
H	3.40051500	-0.66866100	-3.67313100
H	4.09955900	-2.25851800	-4.01694100
C	8.10258200	-2.61649600	-1.02128300
H	8.08080000	-3.56571000	-1.56444700
H	8.82417800	-1.96673100	-1.53120500
H	8.48921500	-2.80887100	-0.01681300
C	3.67355100	3.23300900	0.22910200
H	4.48766700	2.71013200	0.74174400

H	3.47719300	2.68329100	-0.69726200
H	4.02855100	4.22990600	-0.04021400
C	0.24464100	6.03424600	2.68682200
H	0.93314500	6.54067600	3.37297800
H	0.12792100	6.68272000	1.81252500
H	-0.72410400	5.96189200	3.18814200
C	-1.57639900	-3.55360600	4.82369600
H	-1.11186000	-4.42220900	5.30582500
H	-1.78617100	-2.82167600	5.60899300
H	-2.52973600	-3.88620000	4.40348000
C	-0.03499100	-3.41886900	-0.00541600
H	-0.29588200	-2.61260900	-0.70046100
H	0.91441500	-3.84416800	-0.34678000
H	-0.80527700	-4.18825700	-0.08961300
N	-1.61355600	1.97403100	-2.89061600
N	-1.27549800	2.56469200	-3.77389000

B

Au	-0.29199900	0.51468400	-0.52533700
P	1.85433400	-0.30117300	0.12191500
O	2.71453400	0.73234600	1.04537500
O	1.93704000	-1.67586600	0.96645200
O	2.73133200	-0.64025800	-1.16981700
C	3.93873500	-1.38361600	-1.27188700
C	4.92368900	-1.32013500	-0.29400800
C	4.08089300	-2.13814200	-2.44083300
C	6.10058200	-2.04643100	-0.47891400
H	4.78153000	-0.72019100	0.59721600

C	5.27822600	-2.84621400	-2.58884600
C	6.29915500	-2.81771400	-1.62917700
H	6.87184900	-2.00665400	0.28494800
H	5.41374000	-3.44300600	-3.48771500
C	1.13052100	-1.87206500	2.11311500
C	1.50153800	-1.28514300	3.31928000
C	0.02536000	-2.72375700	2.00054000
C	0.73507800	-1.53313900	4.45766400
H	2.38626200	-0.65992700	3.36322300
C	-0.71633300	-2.94984300	3.16637900
C	-0.38596300	-2.37074300	4.39901200
H	1.02260200	-1.07978900	5.40215300
H	-1.57714000	-3.61183200	3.10818700
C	2.36119000	2.09367900	1.16729900
C	1.36827000	2.44600900	2.07634700
C	3.07009700	3.04664700	0.42343900
C	1.05625600	3.79529900	2.25729600
H	0.86457600	1.67135200	2.64590100
C	2.73016600	4.38770000	0.63448600
C	1.73732400	4.78728600	1.54163800
H	0.29143700	4.07395900	2.97702200
H	3.26933600	5.14813900	0.07455000
C	-2.13587800	1.15473200	-1.14472800
C	-2.62586200	2.48487600	-1.07929800
C	-1.83758900	3.51288700	-0.48307400
C	-3.92151300	2.82521400	-1.57612100
C	-2.32448900	4.80542000	-0.37992900
H	-0.85206000	3.26661100	-0.10069800

C	-4.39554300	4.12068100	-1.47646800
H	-4.53154300	2.06097900	-2.04533700
C	-3.59858500	5.10925300	-0.87833800
H	-1.72007300	5.58085600	0.07826200
H	-5.37810300	4.37459600	-1.85981800
H	-3.97544800	6.12521700	-0.80280200
C	-2.91386800	0.13134300	-1.89433800
C	-3.86470000	-0.79527000	-1.29923400
C	-4.48990000	-1.75543000	-2.11468100
C	-4.18203900	-0.74688700	0.07500200
C	-5.41110100	-2.64687500	-1.58555000
H	-4.23877900	-1.78636700	-3.17032400
C	-5.09660000	-1.63111500	0.61353300
H	-3.70617800	-0.01230100	0.71957700
C	-5.72158800	-2.58958500	-0.21225300
H	-5.88207000	-3.37783200	-2.23092300
H	-5.35716700	-1.61119500	1.66592200
O	-2.58723600	0.18039300	-3.08491800
O	-6.59629200	-3.40167100	0.40662300
C	-7.28834500	-4.39721200	-0.35163700
H	-7.93309200	-4.91219300	0.35974800
H	-7.90105400	-3.94098700	-1.13669000
H	-6.58869500	-5.11346400	-0.79608600
C	2.99523600	-2.18396900	-3.48602500
H	2.05666800	-2.56985300	-3.07308900
H	2.78071200	-1.18686900	-3.88531700
H	3.28905100	-2.82729200	-4.31829300
C	7.58497100	-3.57900800	-1.84749300

H	7.40450200	-4.53334600	-2.35106500
H	8.27963400	-3.00742500	-2.47495000
H	8.09295900	-3.78556700	-0.90161800
C	4.15458100	2.64755400	-0.54551200
H	4.92630600	2.04767300	-0.05280900
H	3.76086100	2.04335300	-1.36961600
H	4.63186100	3.53108600	-0.97455300
C	1.44763200	6.25312700	1.76507200
H	2.20621700	6.70774000	2.41314700
H	1.45383600	6.81310000	0.82460500
H	0.47791500	6.40272500	2.24846700
C	-1.19233000	-2.67657200	5.63879300
H	-0.76696000	-3.52895800	6.18215000
H	-1.20534300	-1.82731200	6.32801000
H	-2.22693600	-2.93166200	5.39274200
C	-0.33201100	-3.38183700	0.69116500
H	-0.61880300	-2.64634500	-0.07020300
H	0.51477200	-3.94591100	0.28724400
H	-1.17089900	-4.06912900	0.82168400
C			
Au	0.30566000	-0.48542100	-0.73011600
P	-1.77941800	0.09089600	0.14922800
O	-1.86705300	-0.12835500	1.75494100
O	-2.33066600	1.58645200	-0.07751700
O	-2.92241600	-0.79145500	-0.53208700
C	-4.32703300	-0.54370000	-0.50640600
C	-5.00424200	-0.43757400	0.70147400

C	-4.96912300	-0.48134700	-1.74575600
C	-6.38631900	-0.25093600	0.68068400
H	-4.46522300	-0.49729300	1.64010100
C	-6.35660900	-0.30044000	-1.72193700
C	-7.08501200	-0.18358400	-0.53039200
H	-6.92349900	-0.16123200	1.62047200
H	-6.88416400	-0.24666500	-2.67117700
C	-1.61307900	2.73628300	0.33792100
C	-1.64008400	3.10841900	1.67818700
C	-0.97639100	3.50290100	-0.64462100
C	-0.98512400	4.27627800	2.06858500
H	-2.17822000	2.49949700	2.39579700
C	-0.33258700	4.66842700	-0.21219000
C	-0.32047200	5.07456600	1.12909100
H	-1.00462700	4.57316200	3.11334300
H	0.16813200	5.28513400	-0.95468000
C	-0.82749600	-0.75351300	2.48566500
C	0.23652800	0.02865500	2.92487300
C	-0.94180200	-2.11401600	2.79787000
C	1.23433700	-0.55853500	3.70456300
H	0.26491700	1.08447400	2.67529700
C	0.08022900	-2.66468300	3.58033400
C	1.16990200	-1.91509500	4.04605400
H	2.06022400	0.05042300	4.06164900
H	0.01634900	-3.71848100	3.84029500
C	2.33270700	-1.08355800	-1.53647500
C	2.57146000	-2.54880200	-1.16199400
C	1.59093200	-3.52469700	-1.39910800

C	3.80443900	-2.92801100	-0.61761800
C	1.84307800	-4.86204400	-1.09673000
H	0.62521800	-3.24275400	-1.81232000
C	4.04284500	-4.26616300	-0.30161400
H	4.57290700	-2.18404700	-0.44153900
C	3.06850100	-5.23614800	-0.54216300
H	1.07788900	-5.60801500	-1.28737200
H	4.99954200	-4.54940300	0.12639000
H	3.26197900	-6.27610800	-0.29902500
C	1.92389300	-0.94475100	-2.84507000
C	3.30104600	-0.00533900	-1.07997700
C	4.17447500	0.61934500	-1.97721000
C	3.35915100	0.35966000	0.27935600
C	5.07085900	1.60131600	-1.55296000
H	4.17787800	0.33714100	-3.02726400
C	4.25609000	1.32171700	0.71346000
H	2.71013300	-0.12689600	1.00191300
C	5.11654000	1.96075400	-0.19889700
H	5.73164800	2.06196400	-2.27673200
H	4.31371400	1.60323200	1.75939200
O	1.59452500	-0.84617000	-3.94665500
O	5.94460600	2.88855500	0.32844200
C	6.85760000	3.56711900	-0.53272500
H	7.41192300	4.25461700	0.10575700
H	7.55593600	2.86611600	-1.00442000
H	6.32840100	4.13549300	-1.30650000
C	-4.20443400	-0.60054700	-3.03954100
H	-3.46516600	0.20188600	-3.14325100

H	-3.65998600	-1.54924700	-3.09710200
H	-4.88199000	-0.54562600	-3.89429300
C	-8.58563900	-0.01754700	-0.55614400
H	-8.91038800	0.55413300	-1.43020000
H	-9.08783700	-0.99164500	-0.59935600
H	-8.94658900	0.49611200	0.33907600
C	-2.11523800	-2.94034500	2.33415900
H	-3.05746100	-2.55024600	2.73386900
H	-2.20967700	-2.94351300	1.24340200
H	-2.01171300	-3.97538200	2.66646400
C	2.22149700	-2.54988500	4.92418100
H	1.90117300	-2.55840100	5.97291700
H	2.41176800	-3.58762400	4.63550100
H	3.16737400	-2.00359100	4.87646900
C	0.35487300	6.36080000	1.54090100
H	1.19871000	6.59845600	0.88711900
H	-0.34488300	7.20365400	1.48942700
H	0.72426100	6.30791500	2.56886100
C	-1.00774600	3.10877800	-2.10033700
H	-0.51516200	2.14436100	-2.27365800
H	-2.03662300	3.01172000	-2.46250700
H	-0.50004800	3.85675100	-2.71331800

D

Au	0.16339700	0.26804500	-0.52113200
P	2.29342100	-0.27417200	0.33620800
O	3.23546100	0.96973400	0.81281300
O	2.32212000	-1.21844400	1.66301400

O	3.13989300	-1.14706200	-0.70258300
C	4.36579600	-1.84148500	-0.55063800
C	5.26992300	-1.55362600	0.46504700
C	4.61012200	-2.82131900	-1.52041900
C	6.46473300	-2.27299500	0.52539800
H	5.05565100	-0.78789600	1.20055100
C	5.82003800	-3.51556600	-1.42430700
C	6.76162600	-3.26211300	-0.41737400
H	7.17196300	-2.05470500	1.32052100
H	6.03110700	-4.28329600	-2.16509000
C	1.43991800	-0.97346200	2.73059000
C	1.70619700	0.06021300	3.62422700
C	0.35027800	-1.83993900	2.89716500
C	0.85374100	0.26050500	4.71060900
H	2.58237400	0.68168800	3.47625700
C	-0.48296500	-1.60748500	3.99863300
C	-0.25393900	-0.57111000	4.91573500
H	1.06713500	1.06053700	5.41427800
H	-1.32788200	-2.27443700	4.15572100
C	3.02150300	2.29362500	0.36597700
C	2.17922700	3.10949200	1.11538200
C	3.72340100	2.76714400	-0.74940800
C	2.01120600	4.44310900	0.74418400
H	1.68127200	2.70101800	1.98885600
C	3.52642700	4.11072800	-1.09100100
C	2.67862100	4.96285000	-0.37130400
H	1.36669900	5.08680500	1.33691600
H	4.06444300	4.50529100	-1.94955700

C	-1.76129900	0.69911300	-1.38475300
C	-1.77861400	2.12971700	-1.88406600
C	-1.35689000	3.18153400	-1.05236000
C	-2.25561800	2.45632400	-3.16665900
C	-1.42767800	4.51010100	-1.47275400
H	-0.95001900	2.95453100	-0.07096300
C	-2.31287200	3.78407000	-3.59162600
H	-2.55350800	1.66836400	-3.84824500
C	-1.90862100	4.81824500	-2.74586700
H	-1.08900800	5.30157200	-0.81023700
H	-2.67190200	4.00830900	-4.59185600
H	-1.95534800	5.85013400	-3.08065800
C	-1.85031500	-0.41871500	-2.41881300
C	-3.02067400	0.32514100	-0.38496500
C	-2.62215500	0.55354300	1.02023100
C	-4.19446500	1.13829500	-0.79890200
C	-3.16468200	1.52588500	1.81012900
H	-1.83979300	-0.08248100	1.42310900
C	-4.75522900	2.09035500	-0.01397500
H	-4.57762500	0.96563500	-1.79964700
C	-4.23482400	2.31545600	1.29847900
H	-2.80020000	1.67507400	2.81862300
H	-5.58631500	2.70334500	-0.34386700
O	-1.31177800	-0.40014300	-3.51325600
O	-4.83155400	3.27125800	1.97282200
C	-4.42469400	3.61392200	3.31651200
H	-5.07213500	4.43944200	3.60522600
H	-4.57802300	2.76474600	3.98690300

H	-3.37992800	3.93378100	3.32678300
C	-2.65715200	-1.52850500	-1.87060200
H	-2.73191100	-2.48921500	-2.36231300
C	-3.26734000	-1.16023400	-0.73370800
S	-4.33251300	-2.04863400	0.34793700
C	-4.46130600	-3.65695000	-0.44113900
C	-3.53936800	-4.66393300	-0.12939700
C	-5.51939300	-3.90911700	-1.32319900
C	-3.67245100	-5.92310900	-0.71531500
H	-2.73022200	-4.46218900	0.56491700
C	-5.64500500	-5.17244800	-1.90226200
H	-6.23610900	-3.12631000	-1.54909100
C	-4.72301200	-6.17697700	-1.60018400
H	-2.95924400	-6.70600500	-0.47662500
H	-6.46429100	-5.37138400	-2.58607200
H	-4.82578500	-7.15931700	-2.05076200
C	3.61242000	-3.11037900	-2.61330200
H	2.64592400	-3.42152100	-2.20199900
H	3.42281200	-2.22428500	-3.22852200
H	3.97678200	-3.90646400	-3.26639500
C	8.06618600	-4.02168100	-0.37206900
H	7.92381300	-5.07711700	-0.62369600
H	8.78679200	-3.61222900	-1.09038300
H	8.52530800	-3.96894600	0.61877200
C	4.65521600	1.88332600	-1.54020100
H	5.32371700	1.31720800	-0.88522200
H	4.10380600	1.15391900	-2.14404300
H	5.26517500	2.48145800	-2.22065600

C	2.48084300	6.39666300	-0.80177100
H	3.39415000	6.81513700	-1.23413000
H	1.69689800	6.47093100	-1.56550300
H	2.18342700	7.03039600	0.03862600
C	-1.14697700	-0.39637600	6.12200900
H	-0.79276100	-1.00494300	6.96262900
H	-1.16422700	0.64304200	6.46300400
H	-2.17507500	-0.70705900	5.91232000
C	0.10993400	-2.98569000	1.94548200
H	0.99996900	-3.61637800	1.85631700
H	-0.71755300	-3.60783900	2.29567600
H	-0.13185900	-2.63280100	0.93564300

E

C	2.60439500	-2.09852200	-0.11447600
C	2.12537800	-1.63874500	1.07040600
C	0.95366600	-0.75401100	1.12402800
C	1.89444600	-1.87382000	-1.36299900
C	0.96623000	0.64747200	0.49970300
C	0.74577100	-1.16943200	-1.40998900
C	0.22259000	-0.46301500	-0.23241200
H	2.55661200	-1.95140300	2.01378600
H	0.31486400	-0.86512900	1.99818700
H	2.29147100	-2.36436800	-2.24555200
H	0.17483000	-1.11405700	-2.33251400
C	-0.13510800	1.55237600	1.06464500
C	-1.43282800	0.96938100	0.68049100
H	-2.38022900	1.37993700	1.00165900

C	-1.23715400	-0.13713400	-0.07323300
O	3.70122300	-2.89166000	-0.27747400
C	4.45626700	-3.21585600	0.87931100
H	5.31702700	-3.78793600	0.53073500
H	4.79996900	-2.31023600	1.39484400
H	3.87406700	-3.82762600	1.58043800
C	2.22745300	1.30413500	0.04404800
C	3.22637100	1.60653500	0.97902300
C	2.40079400	1.71176400	-1.28392600
C	4.37685200	2.29223600	0.59293300
H	3.09132000	1.30885300	2.01413200
C	3.55301600	2.39562400	-1.67325500
H	1.62975000	1.49175600	-2.01579000
C	4.54508600	2.68565800	-0.73612700
H	5.14021200	2.52371100	1.33035000
H	3.67340900	2.70398900	-2.70788800
H	5.44220700	3.21842300	-1.03825200
O	0.05730800	2.56534300	1.71410000
S	-2.40676700	-1.24344100	-0.78298300
C	-3.98012500	-0.49078500	-0.34707200
C	-4.54190000	0.48919200	-1.17405300
C	-4.66633300	-0.92844300	0.79162300
C	-5.78443100	1.03624300	-0.85307500
H	-4.00731600	0.81785900	-2.05916200
C	-5.91051500	-0.37917400	1.10401300
H	-4.22661800	-1.69254500	1.42420500
C	-6.46894800	0.60279200	0.28404000
H	-6.21801400	1.79845600	-1.49339000

H	-6.44197600	-0.71917200	1.98773000
H	-7.43739200	1.02824500	0.52933600
F			
C	1.40695500	-0.21389500	-0.00022300
C	2.81533400	-0.21368100	-0.00011600
C	3.51218900	-1.45422100	0.00066300
C	3.58158400	0.98998100	-0.00077300
C	4.89857800	-1.48986600	0.00068000
H	2.93791700	-2.37533900	0.00118500
C	4.96790800	0.93362000	-0.00073100
H	3.05083100	1.93379100	-0.00125400
C	5.63408300	-0.29823300	-0.00003700
H	5.41355700	-2.44598500	0.00123800
H	5.53976500	1.85717500	-0.00122500
H	6.71952200	-0.32966300	-0.00004300
C	0.36200700	0.77982100	0.00016600
C	-1.05214800	0.33497100	0.00007500
C	-2.07118000	1.29527900	0.00048100
C	-1.40631400	-1.02558700	-0.00042800
C	-3.41185900	0.92284300	0.00041300
H	-1.79022700	2.34333200	0.00086300
C	-2.73625500	-1.41254300	-0.00049700
H	-0.62360500	-1.77886300	-0.00075200
C	-3.75011200	-0.43942700	-0.00007400
H	-4.17945900	1.68723200	0.00074900
H	-3.02379200	-2.45847900	-0.00088000
O	0.67509300	1.98550300	0.00054700

O	-5.02292000	-0.91808700	-0.00016300
C	-6.09851600	0.01120200	-0.00006700
H	-7.01040700	-0.58698700	-0.00040800
H	-6.08266400	0.64616200	0.89419900
H	-6.08234600	0.64671100	-0.89393400

G

C	-0.93043900	0.93537000	0.02736100
C	-2.12222600	0.05182500	-0.04396900
C	-3.37070400	0.46223200	0.45694400
C	-2.02613500	-1.21939500	-0.63553200
C	-4.48792700	-0.36267600	0.35216700
H	-3.46318700	1.43101400	0.94124600
C	-3.14304700	-2.04879600	-0.72104700
H	-1.07274200	-1.55236800	-1.03196300
C	-4.38045100	-1.62559900	-0.23334900
H	-5.44218900	-0.02264700	0.74424300
H	-3.04528500	-3.02850200	-1.18023900
H	-5.24911300	-2.27306600	-0.30434600
C	-1.10046600	2.25361400	0.05753100
C	0.47531000	0.43592900	0.07198700
C	1.48151700	1.00609500	-0.71634100
C	0.83323800	-0.61439000	0.93990500
C	2.80643900	0.56880200	-0.64228700
H	1.22874000	1.80346300	-1.40961700
C	2.13969300	-1.07301100	1.00616800
H	0.07334300	-1.07139900	1.56573900
C	3.14062800	-0.48038800	0.21962500

H	3.55485800	1.03942900	-1.26835600
H	2.41673000	-1.88442400	1.67111300
O	-1.24249900	3.41715300	0.08239900
O	4.39357000	-1.00021800	0.36604900
C	5.44780700	-0.43502300	-0.39771300
H	6.34782800	-0.98683300	-0.12326200
H	5.27173400	-0.54562400	-1.47536000
H	5.59128300	0.62795000	-0.16548500

TS₁

Au	-0.19954900	0.61126100	-0.73897500
P	1.85864300	-0.12226300	0.15875200
O	2.45511400	0.82612200	1.33958700
O	1.93375800	-1.59811200	0.80556900
O	2.95686800	-0.20493900	-0.99888400
C	4.21382800	-0.87317000	-0.98027200
C	5.06811100	-0.77767500	0.11118700
C	4.54518200	-1.57609900	-2.14226700
C	6.30616400	-1.41763800	0.05204300
H	4.77683800	-0.21832900	0.99269500
C	5.79865800	-2.19763900	-2.16251700
C	6.69345800	-2.13416000	-1.08597300
H	6.97663500	-1.35294000	0.90420700
H	6.08185100	-2.75323000	-3.05329700
C	1.01987800	-2.02050500	1.80176100
C	1.19583300	-1.59591400	3.11567600
C	0.01764900	-2.92390400	1.43092100
C	0.32815600	-2.06592300	4.10089800

H	2.01045000	-0.92329400	3.35936100
C	-0.83194000	-3.37339600	2.44957000
C	-0.69980500	-2.96298600	3.78277700
H	0.46338800	-1.74043200	5.12853200
H	-1.61987600	-4.07598900	2.18934600
C	1.93606400	2.11090400	1.61571800
C	0.81987100	2.21453200	2.43915300
C	2.60868600	3.23481600	1.11633700
C	0.34268000	3.48150600	2.78380200
H	0.34951300	1.31377600	2.82052300
C	2.09895900	4.48506700	1.48300000
C	0.97733200	4.63643100	2.31265200
H	-0.51815300	3.56581000	3.44135100
H	2.60525500	5.37408000	1.11440600
C	-2.05479500	1.17385400	-1.61033700
C	-2.93209400	2.18463900	-0.96567400
C	-2.44502700	3.02121700	0.05674400
C	-4.27252700	2.32280000	-1.38522000
C	-3.28192400	3.96068600	0.65351300
H	-1.41475500	2.92833400	0.38697200
C	-5.10435000	3.26116200	-0.78464900
H	-4.65828700	1.69349200	-2.18187700
C	-4.60958500	4.08083200	0.23537600
H	-2.89857000	4.59817100	1.44358400
H	-6.13497400	3.35773800	-1.11040100
H	-5.26029800	4.81380300	0.70255800
C	-2.68310800	-0.04048900	-2.28787300
C	-3.32845800	-1.05657100	-1.43366100

C	-3.89473300	-2.17169900	-2.07741700
C	-3.40116500	-0.98261100	-0.02505100
C	-4.51043700	-3.18585800	-1.35707000
H	-3.83878600	-2.22586100	-3.15928500
C	-4.00841100	-1.98884100	0.70327700
H	-2.98546200	-0.13482000	0.50882200
C	-4.56825000	-3.10236800	0.04612800
H	-4.93857200	-4.03018300	-1.88307200
H	-4.06795700	-1.94427200	1.78493400
O	-2.59211700	-0.15736300	-3.50709500
O	-5.12966200	-4.02829500	0.84784300
C	-5.75019800	-5.17456500	0.26115500
H	-6.13835000	-5.75863600	1.09511800
H	-6.57641000	-4.88400000	-0.39683300
H	-5.02528600	-5.77532300	-0.29938900
C	3.59805400	-1.65899400	-3.31240600
H	2.64455800	-2.11638100	-3.02582700
H	3.36886400	-0.66559900	-3.71317600
H	4.03135500	-2.25711400	-4.11694300
C	8.04689300	-2.79902900	-1.16643500
H	8.00525200	-3.72234200	-1.75145600
H	8.78022000	-2.14136600	-1.64882200
H	8.43191900	-3.04384600	-0.17276900
C	3.83390700	3.10382300	0.24654200
H	4.62640000	2.54890500	0.75931900
H	3.62068900	2.56557100	-0.68281600
H	4.22583300	4.08844700	-0.01680400
C	0.49776000	6.01348700	2.70651000

H	1.20169400	6.49115000	3.39762400
H	0.40719500	6.67125100	1.83595400
H	-0.47420100	5.97313400	3.20555400
C	-1.61464100	-3.50615800	4.85474400
H	-1.16529700	-4.37602600	5.34880700
H	-1.81093500	-2.75999000	5.63024800
H	-2.57405700	-3.82745900	4.43975800
C	-0.12284100	-3.40688600	0.00912900
H	-0.36516200	-2.58833200	-0.67853400
H	0.80681300	-3.86213100	-0.34752100
H	-0.92030000	-4.14893400	-0.06839300
N	-1.51435200	1.95721100	-3.04227200
N	-1.07607200	2.67594800	-3.76223900

TS₂

Au	0.25424900	-0.39685900	-0.70478500
P	-1.82138900	0.24997600	0.19037400
O	-2.00640600	-0.07661900	1.77602600
O	-2.17484400	1.82726700	0.12731500
O	-3.04143900	-0.41653600	-0.59431900
C	-4.42510100	-0.08869300	-0.57394400
C	-5.04294900	0.43531100	0.55472700
C	-5.11960900	-0.36932000	-1.75528400
C	-6.41192000	0.70173600	0.50711300
H	-4.47594000	0.63723100	1.45584100
C	-6.49052800	-0.09183000	-1.75800100
C	-7.15853700	0.44020500	-0.64661700
H	-6.89981800	1.11761100	1.38394500

H	-7.05378100	-0.29805400	-2.66500800
C	-1.18390900	2.79072400	0.41892100
C	-0.86190300	3.06319500	1.74491200
C	-0.61420900	3.49163200	-0.65261400
C	0.07216400	4.06084700	2.02565300
H	-1.35376900	2.51439500	2.54052200
C	0.31908100	4.48501100	-0.32993300
C	0.67413200	4.78996100	0.99253300
H	0.31814800	4.28366400	3.06015000
H	0.76726700	5.05291100	-1.14202200
C	-1.24202200	-1.07910000	2.41740400
C	0.05194600	-0.76958900	2.82623500
C	-1.83327000	-2.32181900	2.67667100
C	0.80049300	-1.72941900	3.50968300
H	0.45621600	0.21688900	2.62257200
C	-1.05289600	-3.25501100	3.36956700
C	0.25606300	-2.98730400	3.79557700
H	1.80804000	-1.48818100	3.83690800
H	-1.48965400	-4.22636500	3.58884700
C	2.05368400	-1.00808400	-1.59346700
C	2.47689700	-2.41825100	-1.52638200
C	2.23751700	-3.18025400	-0.36567900
C	3.07546600	-3.03673300	-2.64365100
C	2.59310700	-4.52450000	-0.32524900
H	1.77965900	-2.70923200	0.49933400
C	3.41528500	-4.38687600	-2.60054700
H	3.24831400	-2.46441400	-3.55076400
C	3.17987100	-5.13041000	-1.44117700

H	2.40691000	-5.10449100	0.57310000
H	3.86185700	-4.85835800	-3.47019800
H	3.44887900	-6.18168900	-1.40835700
C	2.60574900	-0.12718100	-2.52321300
C	3.46262900	0.23285500	-1.20292700
C	3.15433800	1.41696300	-0.49419300
C	4.76511100	-0.31868100	-1.09919200
C	4.12271500	2.06338300	0.25387900
H	2.15851600	1.84560800	-0.55663400
C	5.73035500	0.31795800	-0.35342800
H	5.00175900	-1.24709500	-1.60905700
C	5.42319100	1.51893000	0.32926900
H	3.86945000	2.97772300	0.77557000
H	6.73538200	-0.07988300	-0.26662800
O	2.66367200	0.35851100	-3.61201500
O	6.43005700	2.05340600	1.02592000
C	6.23048900	3.27320700	1.75120800
H	7.19075400	3.49681800	2.21365800
H	5.94886200	4.08763000	1.07599500
H	5.46878200	3.14695200	2.52751200
C	1.63940800	5.91314900	1.29194900
H	1.11137000	6.87100800	1.37000400
H	2.15941800	5.75481600	2.24135000
H	2.38812800	6.02414700	0.50168900
C	-1.01072600	3.20593800	-2.07981300
H	-0.75537600	2.18189200	-2.37739000
H	-2.09092100	3.31708800	-2.21818300
H	-0.50526200	3.88862900	-2.76631200

C	-8.64562900	0.69882100	-0.69165800
H	-9.21151800	-0.22342300	-0.51258400
H	-8.94897000	1.42233400	0.06973100
H	-8.95531900	1.08376800	-1.66786500
C	-4.42160200	-0.94142400	-2.96309100
H	-3.61617900	-0.28483400	-3.30990100
H	-3.96680800	-1.91273500	-2.74017400
H	-5.12629800	-1.07755300	-3.78626000
C	-3.24242100	-2.63750700	2.24224300
H	-3.95087100	-1.89108500	2.61457800
H	-3.33704000	-2.64967500	1.15133000
H	-3.54987000	-3.61615700	2.61672100
C	1.03644800	-4.01687100	4.57803300
H	2.11418100	-3.84844300	4.50072900
H	0.77585500	-3.97913500	5.64253900
H	0.82309200	-5.03210400	4.23058500

TS₃

Au	0.40027700	0.44482800	-0.46942900
P	2.38506900	-0.58614000	0.22885200
O	3.59016900	0.42627500	0.63408000
O	2.29701700	-1.54915400	1.52424700
O	2.93620500	-1.58298100	-0.89467700
C	3.93561800	-2.58875700	-0.79922400
C	5.01558800	-2.47996400	0.06860000
C	3.77425700	-3.67208500	-1.66913000
C	5.97283600	-3.49491700	0.07993700
H	5.11478900	-1.62544600	0.72720100

C	4.75908800	-4.66461800	-1.62947600
C	5.86372200	-4.60110900	-0.76968400
H	6.81547000	-3.41791700	0.76109000
H	4.65487400	-5.51845900	-2.29474600
C	1.64987700	-1.12714700	2.70834300
C	2.28231600	-0.21959800	3.55447700
C	0.41768300	-1.71168800	3.02177400
C	1.66106100	0.13993900	4.74926900
H	3.25292600	0.18103500	3.28467600
C	-0.17209000	-1.32780600	4.23349900
C	0.42348000	-0.41036900	5.10886800
H	2.15311500	0.84499500	5.41342200
H	-1.12400100	-1.77725700	4.50686400
C	3.62246800	1.77808800	0.21269700
C	2.84749400	2.70879200	0.90034100
C	4.48399700	2.13863600	-0.82774900
C	2.91481700	4.05173100	0.53526500
H	2.21433200	2.38134300	1.71884000
C	4.52856500	3.49952800	-1.15976500
C	3.76018900	4.46788800	-0.50165900
H	2.30801800	4.77989700	1.06562500
H	5.19385800	3.81006500	-1.96164800
C	-1.48693900	1.44884200	-1.04463500
C	-1.11413900	2.92759200	-1.27424000
C	-1.70645100	3.92785000	-0.49048400
C	-0.17301800	3.30156600	-2.24789100
C	-1.36398800	5.26836500	-0.68053600
H	-2.43536400	3.66564000	0.26637000

C	0.15357000	4.64125200	-2.44332300
H	0.31126300	2.54752000	-2.86178200
C	-0.44104400	5.63313000	-1.65963100
H	-1.83499600	6.02821000	-0.06401100
H	0.87615300	4.90774800	-3.20843100
H	-0.19011400	6.67793800	-1.81492300
C	-1.64323900	0.80602600	-2.30568000
C	-2.60491700	1.18744300	-0.05633500
C	-2.37406500	0.91343900	1.29537400
C	-3.94044300	1.32792100	-0.48112700
C	-3.42795100	0.74600400	2.19712500
H	-1.35700400	0.82659800	1.66666100
C	-4.99772800	1.16594600	0.40018100
H	-4.15416800	1.57883800	-1.51699000
C	-4.75047400	0.85962100	1.74908400
H	-3.20408500	0.52614800	3.23381100
H	-6.02530200	1.27225500	0.06986800
O	-1.59793500	0.79258900	-3.46814000
O	-5.85201400	0.69021900	2.52347300
C	-5.67823100	0.44292000	3.91597300
H	-6.68241600	0.36925500	4.33363400
H	-5.14207600	-0.49745700	4.09273900
H	-5.14212900	1.26582900	4.40314000
C	-1.88029600	-1.44580100	-1.92710700
H	-1.09366600	-1.71294800	-2.60606000
C	-2.82800100	-1.86108900	-1.24466000
S	-4.00375400	-2.35752200	-0.18710900
C	-5.51532000	-2.39253300	-1.17818900

C	-5.53304100	-2.88223800	-2.48637100
C	-6.68744900	-1.97535200	-0.54077300
C	-6.74720600	-2.93485300	-3.17066500
H	-4.61687900	-3.21396600	-2.96369300
C	-7.89753300	-2.05155100	-1.23365600
H	-6.65774100	-1.58510700	0.47197600
C	-7.92817100	-2.52551100	-2.54594400
H	-6.77034100	-3.30795500	-4.18986200
H	-8.81317400	-1.73045400	-0.74693900
H	-8.87060800	-2.57814200	-3.08179900
C	2.59380800	-3.76262900	-2.60290600
H	1.64683000	-3.75836700	-2.05135200
H	2.56652700	-2.91465400	-3.29617700
H	2.63851100	-4.68115800	-3.19218900
C	6.91616100	-5.68396500	-0.78201500
H	6.47732400	-6.66675600	-0.97755700
H	7.66185400	-5.49957500	-1.56491800
H	7.44927800	-5.73419800	0.17127200
C	5.33531000	1.12136900	-1.54570700
H	5.97760100	0.57485700	-0.84764300
H	4.72660300	0.37541300	-2.06757100
H	5.97493600	1.60877600	-2.28463200
C	3.85403800	5.92684500	-0.87997200
H	4.38956100	6.06379000	-1.82290400
H	2.85947600	6.37213200	-0.98525700
H	4.38579300	6.50035500	-0.11178200
C	-0.22804500	-0.05172600	6.42342000
H	0.26852300	-0.55951000	7.25862500

H	-0.16887300	1.02340700	6.61978800
H	-1.28148600	-0.34379700	6.44344600
C	-0.22812900	-2.72234400	2.10739000
H	0.44601700	-3.56100200	1.90577400
H	-1.14228400	-3.11902400	2.55526000
H	-0.49058700	-2.28191000	1.13830300

TS₄

C	-2.77771700	-1.97785300	0.16974300
C	-2.26985200	-1.68614900	-1.08725500
C	-1.17117400	-0.81628500	-1.29048200
C	-2.01196700	-1.79175400	1.35507200
C	-0.96410700	0.47339500	-0.55619300
C	-0.74463600	-1.26410400	1.35537600
C	-0.19846500	-0.51081400	0.27935400
H	-2.62241300	-2.24768700	-1.94625100
H	-0.56221800	-0.96696800	-2.17932500
H	-2.40031900	-2.26647000	2.25047000
H	-0.10231100	-1.45175100	2.21268800
C	0.13909700	1.33461400	-1.23338200
C	1.43263000	0.80063900	-0.79893700
H	2.37961100	1.17830000	-1.15859200
C	1.23883100	-0.23998200	0.05538700
O	-3.92678100	-2.68550700	0.37632000
C	-4.75002600	-2.97093800	-0.74384600
H	-5.68510500	-3.36289200	-0.34083000
H	-4.95001600	-2.06597300	-1.33056400
H	-4.29875100	-3.72913300	-1.39702300

C	-2.13233100	1.26792200	-0.04218600
C	-3.15034400	1.64352600	-0.92740400
C	-2.17417100	1.73508100	1.27569500
C	-4.19592200	2.46001300	-0.49938000
H	-3.11526000	1.29843800	-1.95571400
C	-3.22090500	2.55109000	1.70593300
H	-1.38728600	1.45429000	1.96861000
C	-4.23624400	2.91368900	0.82037000
H	-4.97716300	2.74602200	-1.19790700
H	-3.24195000	2.90325600	2.73335700
H	-5.05222300	3.54772900	1.15514700
O	-0.07382800	2.25940700	-1.99739000
S	2.42863100	-1.27833700	0.83642100
C	3.98657400	-0.50545500	0.38185700
C	4.49389000	0.55443100	1.14312800
C	4.71757400	-1.00694300	-0.70115600
C	5.72611700	1.11720200	0.81068800
H	3.92503100	0.93228600	1.98622100
C	5.95195600	-0.44169800	-1.02460800
H	4.32011700	-1.83249700	-1.28238800
C	6.45546100	0.61990700	-0.27130600
H	6.11720100	1.94142200	1.39948200
H	6.51817100	-0.83132000	-1.86519700
H	7.41605300	1.05794600	-0.52517500

TS₅

C	1.50510000	0.87507500	-0.46422800
C	2.18796300	-0.34232400	-0.09104700

C	3.15825300	-0.88105000	-0.96847200
C	1.89231000	-1.05170700	1.09830900
C	3.81618100	-2.06694700	-0.66550100
H	3.37482500	-0.34258900	-1.88585200
C	2.52477600	-2.25682200	1.38234400
H	1.15485000	-0.64569500	1.78321600
C	3.49251700	-2.75913700	0.50641100
H	4.56525900	-2.46522900	-1.34293200
H	2.28006000	-2.79959000	2.29032100
H	3.99432400	-3.69473900	0.73644300
C	0.40086900	1.48355600	0.22715800
C	-0.92013400	0.79779700	-0.02738700
C	-1.98938100	1.14985700	0.80342900
C	-1.13828400	-0.16251700	-1.03208100
C	-3.24314500	0.55919800	0.66049200
H	-1.81727500	1.90506900	1.56287800
C	-2.38136000	-0.75782700	-1.18597400
H	-0.33603400	-0.42777400	-1.71309200
C	-3.44298300	-0.40353100	-0.33828500
H	-4.04938800	0.85348200	1.32176200
H	-2.56354900	-1.49155000	-1.96409300
O	0.44443600	2.52511600	0.89593500
O	-4.62228100	-1.04501200	-0.57104500
C	-5.74292700	-0.71105500	0.23497800
H	-6.56669200	-1.32828100	-0.12592200
H	-5.56114600	-0.93498100	1.29363000
H	-6.01281900	0.34745800	0.13331900
N	2.82037500	2.35282500	-0.18679500

N	3.49988400	3.12548700	-0.60316000
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TS₆

C	-1.40802700	1.31093000	0.62177200
C	-2.33740800	0.26329000	0.33769500
C	-2.87452100	-0.49457500	1.40787000
C	-2.82325400	0.01505900	-0.97399200
C	-3.83239900	-1.47367700	1.17697600
H	-2.51179200	-0.28557800	2.40881200
C	-3.80992200	-0.93735200	-1.19606600
H	-2.42663700	0.60390300	-1.79580200
C	-4.30413300	-1.68860000	-0.12310900
H	-4.22889900	-2.05807700	2.00147800
H	-4.18985400	-1.10815500	-2.19877700
H	-5.06653500	-2.44185900	-0.30098800
C	-0.53140600	1.96746700	-0.23401100
C	0.72580500	1.08314500	-0.03292900
C	0.85940100	-0.17385500	-0.62850300
C	1.82175600	1.62530400	0.66679500
C	2.06402100	-0.87713900	-0.56598300
H	0.01840000	-0.61643900	-1.15383500
C	3.01881600	0.93750100	0.74017700
H	1.72357400	2.60185100	1.12993900
C	3.14927800	-0.32089400	0.12162200
H	2.14343400	-1.84402300	-1.04784700
H	3.87608800	1.34473800	1.26594600
O	-0.49344400	3.04027400	-0.83356400
O	4.36607300	-0.91327300	0.25506000

C	4.57232500	-2.18265800	-0.34920600
H	5.60270300	-2.45856300	-0.12224000
H	3.89539900	-2.94065500	0.06403100
H	4.44109500	-2.13681900	-1.43732300

b) The enthalpy reaction profile for the formation of 4a:

Species	E _{elec}	H _{solv}	ZPE + H _{vib} + 4kT	H _{total} (hartree)
1a	-706.67882	-0.00411	0.11940	-706.56353
4a	-1436.21346	-0.01091	0.36946	-1435.85491
4a'	-1436.21206	-0.01078	0.36943	-1435.85341
G	-729.42507	-0.00566	0.24410	-729.18663
H	-1436.08114	-0.01189	0.36653	-1435.72650
H'	-1436.07463	-0.01442	0.36543	-1435.72362
I	-1436.15713	-0.01110	0.36833	-1435.79989
I'	-1436.15686	-0.01129	0.36828	-1435.79986
J	-1436.15838	-0.00921	0.36737	-1435.80022
J'	-1436.15839	-0.00924	0.36732	-1435.80030
K	-1436.16128	-0.01141	0.36800	-1435.80470
K'	-1436.15579	-0.01168	0.36764	-1435.79984
TS ₁	-1436.06980	-0.01181	0.36407	-1435.71754
TS ₂	-1436.07186	-0.01404	0.36468	-1435.72122
TS ₂ '	-1436.07424	-0.01385	0.36462	-1435.72346
TS ₃	-1436.12623	-0.00949	0.36557	-1435.77015
TS ₃ '	-1436.12503	-0.00949	0.36554	-1435.76898
TS ₄	-1436.13363	-0.00963	0.36577	-1435.77750
TS ₄ '	-1436.13035	-0.01016	0.36561	-1435.77490
TS ₅	-2872.31303	-0.01801	0.73111	-2871.59993
TS ₅ '	-2872.30219	-0.01739	0.73033	-2871.58925



C	3.34272600	1.13364700	-0.00012800
H	4.06215700	1.91945600	-0.00020200
C	2.51936500	0.24342300	-0.00004600
S	1.47080500	-1.08253300	0.00008200
C	-0.16929300	-0.33329600	0.00003200
C	-1.24715200	-1.22666700	-0.00006300
C	-0.39257600	1.04442800	0.00009100
C	-2.55058600	-0.73327700	-0.00008400

H	-1.07109500	-2.29882000	-0.00014000
C	-1.70320800	1.52468500	0.00005400
H	0.44722500	1.73041700	0.00015100
C	-2.78450300	0.64323000	-0.00001800
H	-3.38416900	-1.42936800	-0.00016800
H	-1.87477600	2.59723800	0.00008900
H	-3.80085400	1.02456500	-0.00006700

4a

C	1.67856000	-0.11876300	0.04452900
C	2.25474100	-0.72109400	-1.07916300
C	3.38302900	-1.53942000	-0.97600100
C	3.95915700	-1.76490600	0.27845700
C	3.39799000	-1.16538400	1.41589600
C	2.27640200	-0.35676400	1.29563800
H	1.81570800	-0.54863800	-2.05749400
H	3.79736900	-1.98768000	-1.87106300
H	3.85750400	-1.35335000	2.38070400
H	1.84764200	0.09823600	2.18368500
O	5.05947400	-2.54234500	0.50113800
C	5.66137500	-3.18623100	-0.61051300
H	6.50403100	-3.75232300	-0.21092300
H	4.96558200	-3.87597200	-1.10509700
H	6.03140900	-2.46214800	-1.34783300
C	0.47103700	0.75455100	-0.07993600
C	0.60209800	2.18095800	-0.02552600
C	1.86816900	2.81361200	0.13212100
C	-0.55544900	3.02388000	-0.12293300

C	1.98373300	4.18276900	0.21860500
C	-0.40454100	4.43018700	-0.00624600
C	0.83577300	5.00400400	0.16020000
C	-1.82365100	2.40224800	-0.33525400
O	-2.97247700	3.13087900	-0.47796500
H	-2.74887800	4.04626700	-0.68688400
H	-1.27930500	5.07670300	-0.01867200
H	0.93108200	6.08161300	0.25145900
H	2.75446100	2.19206100	0.18570000
H	2.96383500	4.63499800	0.33890000
C	-1.93774200	1.03313400	-0.39735800
H	-2.91750200	0.60489500	-0.56672500
C	-0.79832200	0.20835300	-0.24828100
S	-0.94041300	-1.58362200	-0.33473700
C	-2.68239400	-1.88593000	-0.02218600
C	-3.48099000	-2.40878100	-1.04646400
C	-3.22960200	-1.69389600	1.25460300
C	-4.81526800	-2.73628100	-0.79573300
H	-3.05463300	-2.55564000	-2.03353700
C	-4.56649300	-2.00658600	1.49449900
H	-2.60595300	-1.30035700	2.05063700
C	-5.36057300	-2.53183800	0.47167500
H	-5.42823500	-3.14363100	-1.59443900
H	-4.98606600	-1.85023400	2.48401900
H	-6.39965900	-2.78205600	0.66419800

4a'

C	-0.36614700	2.16887800	-0.05195800
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C	-0.22852100	3.00300000	-1.17153600
C	-0.21301600	4.39127500	-1.02952500
C	-0.33946900	4.96763800	0.23477500
C	-0.48169600	4.14862000	1.35652000
C	-0.49640900	2.76135000	1.21375300
H	-0.13404400	2.55626800	-2.15701400
H	-0.10331000	5.02148700	-1.90744300
H	-0.57808100	4.58998600	2.34447300
H	-0.60222600	2.12522000	2.08770800
C	-0.38302400	0.68072400	-0.20446700
C	-1.62665800	-0.03306600	-0.13108200
C	-2.86702100	0.62731100	0.07017900
C	-1.65840600	-1.46196300	-0.25197200
C	-4.05801900	-0.05949900	0.17643000
C	-2.88364500	-2.15236700	-0.11585000
C	-4.06999200	-1.47208000	0.09276400
C	-0.42641200	-2.14055900	-0.51352200
O	-0.37564300	-3.49722500	-0.68204000
H	-1.25617300	-3.82453100	-0.90535000
H	-2.93468400	-3.23700900	-0.14039500
H	-2.87538700	1.70871000	0.14285200
H	-4.97733400	0.49327900	0.32825400
C	0.75476800	-1.44535300	-0.59990300
H	1.66343500	-1.99583000	-0.80997000
C	0.78546100	-0.03914300	-0.42151400
S	2.34082700	0.85395600	-0.56458700
C	3.56083200	-0.34441500	-0.02159200
C	4.62373400	-0.65694900	-0.87757200

C	3.52258000	-0.89752400	1.26666500
C	5.64146500	-1.51099700	-0.44702700
H	4.64799600	-0.23348900	-1.87659500
C	4.52924200	-1.76693200	1.68153400
H	2.70461300	-0.64727600	1.93425500
C	5.59387300	-2.07174000	0.82890000
H	6.46388800	-1.74609700	-1.11639400
H	4.48916900	-2.19772800	2.67783800
H	6.38108200	-2.74276900	1.15946500
H	-0.32684400	6.04801600	0.34603800
O	-5.19514200	-2.23871500	0.21051600
C	-6.43591500	-1.59072400	0.44537800
H	-7.17998900	-2.38555900	0.51412400
H	-6.42818700	-1.02417700	1.38515500
H	-6.70650000	-0.91719200	-0.37768900

G

C	0.47377600	0.59613600	-0.03193900
C	0.96139600	-0.49498100	0.70020600
C	2.30920600	-0.85349300	0.66230900
C	3.20880200	-0.10039600	-0.10260200
C	2.73792300	0.99883500	-0.83398200
C	1.39041400	1.33070100	-0.80620800
H	0.27712900	-1.07613400	1.31020900
H	2.64466200	-1.70767900	1.23826900
H	3.44417400	1.56677900	-1.43033500
H	1.03729300	2.16885000	-1.40048100
O	4.54551900	-0.35517800	-0.20633100

C	5.07729700	-1.45633400	0.51376200
H	6.14478300	-1.47490600	0.29005600
H	4.93793200	-1.33853300	1.59596300
H	4.62587300	-2.40485000	0.19568200
C	-0.96762800	0.97425600	0.03692100
C	-2.08633000	-0.00287400	-0.01558900
C	-3.31427400	0.25490800	0.61933500
C	-1.94207100	-1.20777700	-0.72482100
C	-4.36786500	-0.65207900	0.53117900
H	-3.43955600	1.16847000	1.19482800
C	-2.99276400	-2.12075800	-0.79406300
H	-1.00384100	-1.42242600	-1.22547100
C	-4.21234800	-1.84792500	-0.17202900
H	-5.30795500	-0.42959800	1.02784100
H	-2.85880200	-3.04664800	-1.34637800
H	-5.02986700	-2.56000900	-0.23079500
C	-1.25224400	2.26788200	0.15378500
O	-1.49696400	3.41018800	0.25170900

H

C	2.08543300	0.47748700	-0.02522000
C	1.44677400	1.58352200	0.58061200
C	1.98353700	2.86924100	0.52943600
C	3.19110600	3.08792900	-0.14276900
C	3.85051100	2.00508500	-0.75815300
C	3.31343900	0.73556200	-0.69398800
H	0.53108100	1.41991800	1.13685900
H	1.46329900	3.68071900	1.02355300

H	4.77580200	2.20039400	-1.28991600
H	3.82290700	-0.08230500	-1.19170100
O	3.80865300	4.29147100	-0.25836300
C	3.19082900	5.43091800	0.32709900
H	3.84577000	6.27371800	0.10412900
H	2.19998800	5.61669000	-0.10469100
H	3.09688700	5.32259400	1.41443800
C	1.49943700	-0.85561000	0.01493900
C	2.35547000	-2.03345100	0.15810800
C	1.97188000	-3.31283300	-0.31283000
C	3.60186000	-1.93424300	0.82683700
C	2.79802900	-4.41750300	-0.13647400
C	4.41604300	-3.04559000	1.00888100
C	4.02319600	-4.29531100	0.52275900
C	0.08023800	-1.04582700	-0.20925600
O	-0.55168300	-2.09122300	0.02813700
H	3.90756100	-0.97938300	1.23944200
H	5.35657800	-2.93842800	1.54181200
H	4.66081700	-5.16329700	0.66272800
H	1.02293200	-3.42440700	-0.81896700
H	2.48154600	-5.38384100	-0.51852400
C	-0.61226800	0.09617000	-0.91978700
H	0.01051400	0.85957400	-1.37875700
C	-1.94802500	0.19427900	-0.92574600
S	-3.08954700	-0.99354700	-0.79711200
C	-4.56401900	-0.15783200	-0.17778100
C	-5.69489100	-0.95913600	0.01200200
C	-4.60150800	1.20638400	0.12106000

C	-6.86834400	-0.38914800	0.50587300
H	-5.65797400	-2.01987600	-0.22145300
C	-5.77901500	1.76602700	0.61270100
H	-3.71293200	1.80762900	-0.04500800
C	-6.91318500	0.97271900	0.80761700
H	-7.74647800	-1.01068400	0.65340400
H	-5.81270800	2.82722500	0.84235600
H	-7.82775300	1.41550300	1.19037100

H'

C	-2.36834600	-0.07873500	0.29145000
C	-3.20845900	-1.17324600	-0.01010500
C	-4.49309900	-0.99938400	-0.51869900
C	-4.99597800	0.28965500	-0.73350400
C	-4.19176300	1.39513100	-0.42306800
C	-2.91426000	1.21165100	0.08078700
H	-2.84613900	-2.17616900	0.17488000
H	-5.09326900	-1.87522300	-0.73679900
H	-4.59509400	2.39077500	-0.57785300
H	-2.32189000	2.08744400	0.31985600
O	-6.24013500	0.57302600	-1.22301000
C	-7.09368800	-0.51181200	-1.54746600
H	-8.01976800	-0.06787800	-1.91630400
H	-6.66209600	-1.14820700	-2.33084700
H	-7.31580100	-1.13086800	-0.66871300
C	-0.99388600	-0.25786000	0.79062000
C	-0.07941500	0.91266400	0.78219600
C	0.20508000	1.59688700	-0.41680500

C	0.48505300	1.42109700	1.96801700
C	1.02264900	2.72427600	-0.43103400
C	1.31915900	2.54126700	1.95383800
C	1.58940200	3.20257700	0.75471000
C	-0.64884000	-1.45209800	1.44139800
O	-1.25878100	-2.51533400	1.64283200
H	0.23918200	0.94772600	2.91367300
H	1.73400800	2.91316200	2.88697900
H	2.21853400	4.08816800	0.74510400
H	-0.22785500	1.23207500	-1.34335600
H	1.22368800	3.22940700	-1.37178900
C	0.82080900	-1.63784400	1.99548600
H	0.91739600	-1.85127800	3.05796500
C	1.71252400	-1.79285400	1.07955300
S	2.61263200	-2.33215800	-0.16696600
C	3.73092500	-0.99649000	-0.64074500
C	4.65691000	-1.32247300	-1.63718600
C	3.70380900	0.27036500	-0.05856300
C	5.57283000	-0.35738500	-2.05373200
H	4.66630800	-2.31374000	-2.08192500
C	4.62798200	1.22283600	-0.48660600
H	2.97375200	0.51576800	0.70456800
C	5.56122500	0.91466200	-1.47854700
H	6.29417600	-0.60271400	-2.82702300
H	4.60471900	2.21305200	-0.04299500
H	6.27563900	1.66415600	-1.80450000

I

C	1.53984900	-0.33780100	0.28884600
C	2.82511600	0.06059800	-0.08910100
C	3.85190200	-0.86541100	-0.29282400
C	3.60143400	-2.22943000	-0.11921600
C	2.31864200	-2.64777800	0.26351000
C	1.31248300	-1.71547300	0.46642500
H	3.04111600	1.11366600	-0.22941300
H	4.83260700	-0.50926600	-0.58481500
H	2.13732400	-3.70911900	0.39768900
H	0.33118000	-2.06490600	0.77225600
O	4.52245100	-3.22179400	-0.29564700
C	5.84026200	-2.85260600	-0.66971800
H	6.40331900	-3.78371000	-0.74874400
H	5.85766600	-2.33762300	-1.63888300
H	6.31075200	-2.20957200	0.08500900
C	0.43286300	0.67366300	0.57008000
C	0.71395400	2.07147700	0.03583000
C	0.58484900	2.35611900	-1.33233300
C	1.13085500	3.09671400	0.89677600
C	0.84213100	3.63525200	-1.82377900
C	1.39260100	4.37647000	0.40264000
C	1.24521300	4.65226200	-0.95627700
C	-0.09068400	0.64271500	2.07801300
O	0.43198700	0.91773100	3.13327000
H	1.25254200	2.88719500	1.95371300
H	1.71276800	5.15810300	1.08574400
H	1.44698200	5.64877600	-1.33842200
H	0.28689100	1.57205400	-2.02198900

H	0.72966800	3.83601300	-2.88544900
C	-1.39825800	0.14980500	1.63228600
H	-2.31896900	-0.11274300	2.13803000
C	-1.01358300	0.15806100	0.32663100
S	-1.75988400	-0.27730000	-1.17942700
C	-3.40159900	-0.79355600	-0.64853700
C	-4.39549400	0.16323100	-0.41105400
C	-3.68978100	-2.15709500	-0.52515000
C	-5.67424300	-0.24905700	-0.03584100
H	-4.16585800	1.21816800	-0.51959500
C	-4.97367900	-2.56106500	-0.15590800
H	-2.91492700	-2.89195900	-0.71766400
C	-5.96420000	-1.60922100	0.09076300
H	-6.44464100	0.49273400	0.15180900
H	-5.19757300	-3.61920200	-0.06012600
H	-6.96201000	-1.92654400	0.37834200

I'

C	-0.63137000	2.16410900	0.00936200
C	-0.57469100	2.39800000	-1.37367000
C	-0.70981900	3.68662200	-1.88699600
C	-0.91745300	4.76614200	-1.02567700
C	-0.99289600	4.54304000	0.34838500
C	-0.85177100	3.25246400	0.86432900
H	-0.43245800	1.56451900	-2.05558100
H	-0.65647800	3.84681500	-2.96007600
H	-1.16400300	5.37399600	1.02682400
H	-0.92182700	3.08627200	1.93344200

C	-0.46661100	0.75098500	0.55376200
C	-1.63989800	-0.17306700	0.24578000
C	-1.49371800	-1.56466200	0.28083400
C	-2.92454000	0.33886600	-0.00406000
C	-2.57125400	-2.42470900	0.06119500
C	-4.00789800	-0.50230300	-0.21842800
C	-3.84045900	-1.89324400	-0.19100600
C	0.01737400	0.66868800	2.07217500
O	-0.50574100	0.97663500	3.11789200
H	-3.07862200	1.41178700	-0.03082300
H	-4.99820000	-0.10261500	-0.41032500
H	-0.52078100	-1.99980600	0.48692100
H	-2.40847500	-3.49545500	0.09117200
C	1.29590700	0.08457300	1.65057200
H	2.18416100	-0.24680100	2.17369200
C	0.94613900	0.14060100	0.33655500
S	1.70472100	-0.29647700	-1.16316300
C	3.30907600	-0.89917300	-0.60972000
C	3.54718400	-2.27665300	-0.55471000
C	4.32677400	0.00699000	-0.28852100
C	4.80430500	-2.74596600	-0.17058100
H	2.75455500	-2.97189100	-0.81141800
C	5.57769700	-0.47063600	0.10231500
H	4.13690300	1.07383100	-0.34510000
C	5.81767400	-1.84520600	0.16017200
H	4.98919500	-3.81508800	-0.12831600
H	6.36613400	0.23184400	0.35503600
H	6.79437300	-2.21315600	0.45962600

H	-1.02557500	5.77060000	-1.42457200
O	-4.96434500	-2.63408600	-0.42087000
C	-4.85286200	-4.04767400	-0.38996300
H	-4.51714900	-4.40691900	0.59134100
H	-5.85363200	-4.43361800	-0.58936200
H	-4.16430800	-4.41780600	-1.16065800

J

C	1.55851100	-0.22493600	-0.02048200
C	1.93443900	-1.16231600	-0.99222700
C	3.04946000	-1.98786900	-0.82897300
C	3.82573100	-1.87942400	0.32862700
C	3.48102500	-0.93034700	1.30456600
C	2.37559800	-0.11543300	1.12445100
H	1.36434800	-1.23580400	-1.91293800
H	3.30300500	-2.69498500	-1.60956100
H	4.09904600	-0.85360900	2.19308300
H	2.12662900	0.61737300	1.88579400
O	4.93287500	-2.63018200	0.59778400
C	5.32582900	-3.60938300	-0.35111800
H	6.21153000	-4.09260600	0.06374400
H	4.54201300	-4.36198800	-0.50441700
H	5.58166700	-3.15725000	-1.31795300
C	0.38180600	0.66469600	-0.18632800
C	0.62624800	2.11599100	0.08772400
C	1.59751900	2.82684500	-0.63716700
C	-0.06463000	2.78504000	1.11307600
C	1.85204500	4.16945700	-0.36289400

C	0.19471700	4.12652500	1.39111700
C	1.15105300	4.82421000	0.65165400
C	-1.94036200	2.38708100	-1.27560000
O	-1.99962400	3.51650400	-1.57476300
H	-0.80742700	2.24312600	1.69067100
H	-0.34727900	4.62544600	2.18935100
H	1.35168800	5.86953500	0.86708600
H	2.15251000	2.31664700	-1.41878200
H	2.60014200	4.70475300	-0.94052500
C	-1.97825700	1.10082900	-0.95789900
H	-2.96807800	0.66415400	-1.05373000
C	-0.85006400	0.23550300	-0.58742400
S	-1.18517300	-1.52726300	-0.81849300
C	-2.80873300	-1.69946800	-0.07145600
C	-3.81493400	-2.35212600	-0.79536600
C	-3.06396800	-1.27371100	1.24029700
C	-5.06105200	-2.58304700	-0.20913100
H	-3.61903200	-2.67338300	-1.81362300
C	-4.31769100	-1.48630200	1.81031800
H	-2.27987300	-0.77991100	1.80528400
C	-5.31748700	-2.14621800	1.09056500
H	-5.83448200	-3.09314200	-0.77596900
H	-4.51041900	-1.14809100	2.82441500
H	-6.29005500	-2.31820000	1.54182900

J'

C	-0.27981300	2.14483500	-0.01406800
C	0.28071700	3.03840400	-0.94315900

C	0.24053300	4.41648800	-0.72933200
C	-0.37078600	4.93291300	0.41247200
C	-0.95271500	4.05950600	1.33515400
C	-0.91683500	2.68489900	1.11938400
H	0.72471200	2.65264300	-1.85524100
H	0.67931000	5.08589500	-1.46370000
H	-1.43784800	4.45153500	2.22461700
H	-1.37849900	2.01382500	1.83712100
C	-0.26222200	0.67437700	-0.22395000
C	-1.56129500	-0.03481500	-0.00768900
C	-2.66418600	0.20195400	-0.83893700
C	-1.73139100	-0.92667100	1.06979600
C	-3.88664000	-0.43850500	-0.63382200
C	-2.94286700	-1.56552600	1.29186200
C	-4.02959400	-1.33033200	0.43662200
C	-0.21777100	-2.24789500	-1.20109900
O	-1.05421400	-3.03594200	-1.42191600
H	-0.89520000	-1.11777700	1.73589900
H	-3.07545100	-2.25191000	2.12150900
H	-2.56476300	0.89953700	-1.66543900
H	-4.71187800	-0.23605400	-1.30586400
C	0.82725100	-1.45716600	-0.98964200
H	1.77459400	-1.95408300	-1.17776800
C	0.83339500	-0.03878600	-0.61466700
S	2.44539200	0.75634600	-0.80633600
C	3.55336800	-0.44580100	-0.06443400
C	4.69464400	-0.83372800	-0.77800300
C	3.34779200	-0.93495800	1.23369200

C	5.62433700	-1.69711900	-0.19477400
H	4.84854800	-0.46084000	-1.78583700
C	4.26778200	-1.81504100	1.79999600
H	2.47011600	-0.62381500	1.79101100
C	5.41084900	-2.19421300	1.09085900
H	6.50855400	-1.99004600	-0.75337800
H	4.09876400	-2.19557900	2.80325600
H	6.12985300	-2.87303700	1.53955500
H	-0.40390000	6.00575200	0.57835900
O	-5.17406100	-2.00802200	0.73467700
C	-6.30405500	-1.82379100	-0.10483300
H	-6.09473900	-2.13046900	-1.13731200
H	-7.09007500	-2.45885600	0.30591500
H	-6.64514200	-0.78071200	-0.10198500

K

C	1.66073300	-0.15780200	0.16118800
C	2.16446400	-0.71811000	-1.01824000
C	3.24953000	-1.59742300	-1.00609100
C	3.85492200	-1.93074000	0.21095300
C	3.36561700	-1.37560900	1.40260100
C	2.28544300	-0.50421800	1.37282300
H	1.70228700	-0.46312700	-1.96732800
H	3.60975200	-2.00879800	-1.94129100
H	3.84774600	-1.64502800	2.33643600
H	1.91379700	-0.08211800	2.30194600
O	4.91774000	-2.77546400	0.34445800
C	5.44915800	-3.37756000	-0.82591900

H	6.27265000	-4.00990000	-0.49140700
H	4.70212000	-3.99809700	-1.33684200
H	5.83343900	-2.62756700	-1.52900900
C	0.50685600	0.79693500	0.13653500
C	0.71140400	2.15662600	0.15487300
C	2.02092700	2.76382400	0.11274400
C	-0.46399800	3.09996600	0.28310100
C	2.17332200	4.10107500	-0.08729400
C	-0.21694000	4.51031300	-0.15340400
C	1.03768300	4.97991800	-0.28626000
C	-1.83066200	2.54188000	-0.14020600
O	-2.76003300	3.29899200	-0.40703500
H	-0.62653200	3.16107000	1.38347500
H	-1.09796400	5.12208900	-0.31308300
H	1.21649500	6.01458100	-0.56410900
H	2.89028000	2.11953900	0.18022700
H	3.17396300	4.51948100	-0.15195000
C	-1.95280400	1.10041000	-0.09107000
H	-2.94291800	0.69618100	-0.26191800
C	-0.85847500	0.28779600	0.04865500
S	-0.98013700	-1.49750200	0.08211000
C	-2.74936500	-1.80073500	0.03259900
C	-3.38096500	-2.05272900	-1.19158300
C	-3.48386700	-1.86511300	1.22367300
C	-4.74221100	-2.35866000	-1.22248400
H	-2.80581600	-2.00767300	-2.11062300
C	-4.84446200	-2.16980800	1.18608800
H	-2.98748200	-1.67728000	2.17012100

C	-5.47423300	-2.41650500	-0.03551000
H	-5.22915000	-2.55155000	-2.17371700
H	-5.41138800	-2.21690000	2.11107100
H	-6.53321100	-2.65547800	-0.06177900

K'

C	-0.38488200	2.18651800	0.02435200
C	-0.22382800	2.85274600	-1.20038600
C	-0.18025500	4.24591400	-1.25178300
C	-0.29767800	4.99482900	-0.07973300
C	-0.45956400	4.34406600	1.14420400
C	-0.50306600	2.95054800	1.19536400
H	-0.13502300	2.27154700	-2.11333900
H	-0.05730600	4.74595600	-2.20805600
H	-0.55141400	4.92032000	2.06029500
H	-0.62775300	2.44457700	2.14831100
C	-0.44963200	0.69012700	0.08160300
C	-1.65817000	0.03709900	0.13366700
C	-2.92985400	0.71548900	0.04378800
C	-1.70477000	-1.46073200	0.34071500
C	-4.08986100	0.02529900	-0.11382800
C	-2.98145400	-2.13986800	-0.04360800
C	-4.10832300	-1.42473900	-0.21435100
C	-0.43894900	-2.23381300	-0.05819600
O	-0.48266600	-3.44079300	-0.27506700
H	-1.63128400	-1.56514300	1.44774200
H	-2.96197900	-3.21778400	-0.15123600
H	-2.93782700	1.79954100	0.02951300

H	-5.02699100	0.55836600	-0.24482200
C	0.78756800	-1.46247500	-0.04059900
H	1.70589600	-2.01854800	-0.18342400
C	0.78045200	-0.09499800	0.03325400
S	2.28078400	0.88111000	0.02520300
C	3.58648400	-0.35109500	0.02879000
C	4.16297100	-0.76109400	-1.17977500
C	4.08305900	-0.84324600	1.24262500
C	5.22511400	-1.66619300	-1.17193900
H	3.77845400	-0.37144100	-2.11664000
C	5.14405200	-1.74865700	1.24356900
H	3.63795900	-0.51532500	2.17631400
C	5.71522700	-2.16059100	0.03783100
H	5.66858900	-1.98371500	-2.11087000
H	5.52564500	-2.12990900	2.18601900
H	6.54238600	-2.86414700	0.04150200
H	-0.26368900	6.07961400	-0.12020300
O	-5.28681300	-2.03667100	-0.59188100
C	-6.29188000	-2.06171300	0.41723900
H	-6.56039800	-1.05252000	0.75860900
H	-7.17132600	-2.52940300	-0.02947500
H	-5.96722700	-2.65056100	1.28528100

TS₁

C	2.55295800	-0.16093700	0.05353400
C	2.95785800	-1.43719100	-0.37441300
C	4.24713600	-1.91932600	-0.14800100
C	5.18517500	-1.12512000	0.51900800

C	4.80515100	0.14952500	0.95759100
C	3.51884900	0.61743000	0.73103200
H	2.25194500	-2.07660800	-0.89203100
H	4.50478700	-2.91094900	-0.50140900
H	5.53330900	0.75604500	1.48671700
H	3.24977300	1.60089900	1.09987600
O	6.47523200	-1.49474700	0.79116300
C	6.89849400	-2.78216800	0.37802700
H	7.93881900	-2.87529800	0.69431600
H	6.30618900	-3.57672400	0.85068900
H	6.84269800	-2.89927700	-0.71237100
C	1.17793500	0.36332100	-0.15663500
C	0.91754500	1.81705700	-0.13525500
C	-0.15442900	2.35788900	0.60161600
C	1.72470700	2.71286500	-0.86681300
C	-0.41933300	3.72799500	0.59567600
C	1.46546200	4.08146500	-0.86589200
C	0.38998200	4.59677500	-0.13641800
C	0.19750100	-0.56894400	-0.42298000
O	-0.04458700	-1.74402800	-0.32837100
H	2.55685800	2.32024300	-1.44281500
H	2.09959800	4.74840400	-1.44337600
H	0.18953800	5.66416300	-0.13664600
H	-0.76658100	1.68903900	1.19882000
H	-1.25119800	4.11773900	1.17597400
C	-1.16879800	0.35475000	-1.45329400
H	-0.75777900	1.24359700	-1.89999900
C	-2.26325400	-0.26808300	-1.45084700

S	-3.24699900	-1.57869600	-1.31809900
C	-4.54674600	-1.08009700	-0.16648800
C	-5.63340900	-1.95260100	-0.05792500
C	-4.47860900	0.08309900	0.60164300
C	-6.66295600	-1.65288700	0.83416000
H	-5.67869100	-2.85449600	-0.66180700
C	-5.51794600	0.37306500	1.48495700
H	-3.62879900	0.75060200	0.50552400
C	-6.60847200	-0.49102100	1.60512100
H	-7.50864500	-2.32804200	0.92118300
H	-5.47150600	1.27780100	2.08351200
H	-7.41230000	-0.25898000	2.29667200

TS₂

C	-0.76683700	0.71897400	0.62710100
C	-0.23654900	1.29402900	-0.54208400
C	0.81002400	2.21359700	-0.50932600
C	1.37004400	2.58684500	0.71891400
C	0.84584800	2.04876200	1.90142100
C	-0.21119500	1.14657600	1.85235600
H	-0.64407700	1.00038300	-1.50429200
H	1.19069600	2.61406200	-1.44150900
H	1.26162700	2.37432000	2.84975000
H	-0.63368500	0.78015400	2.78248600
O	2.41665400	3.45858700	0.86659300
C	2.89456000	4.12807400	-0.28972000
H	3.67742600	4.80531000	0.05531600
H	3.32136500	3.42774100	-1.01958700

H	2.10196000	4.70992400	-0.77697400
C	-1.88096600	-0.25332100	0.56273600
C	-3.07807800	0.09953300	-0.22054800
C	-3.98155400	-0.89461800	-0.66734300
C	-3.35995700	1.43746600	-0.57977200
C	-5.08160200	-0.56539200	-1.45054700
C	-4.46853000	1.76309600	-1.35609700
C	-5.33473000	0.76374700	-1.80229000
C	-1.95079100	-1.37262400	1.45117000
O	-2.90833300	-2.11303400	1.71828800
H	-2.70551600	2.22920200	-0.23320300
H	-4.65978300	2.80279800	-1.60738300
H	-6.20006400	1.01664100	-2.40826100
H	-3.81385900	-1.92332200	-0.37725200
H	-5.75158500	-1.35221500	-1.78615500
C	-0.63107800	-1.89194800	2.04918300
H	-0.59100600	-2.17765800	3.10112900
C	0.19970200	-2.19956900	1.10316300
S	1.15240200	-3.05553400	0.08380300
C	2.47906800	-1.95584900	-0.45057100
C	3.24606200	-2.41176700	-1.52815900
C	2.78793700	-0.76308000	0.20416500
C	4.34054700	-1.65795800	-1.95022000
H	2.99265300	-3.33949800	-2.03339200
C	3.88129800	-0.01697400	-0.23445700
H	2.17891700	-0.41181400	1.02969400
C	4.66047600	-0.46183400	-1.30477400
H	4.93876600	-2.00565300	-2.78683200

H	4.11561100	0.91691300	0.26731900
H	5.51334600	0.12224100	-1.63656800

TS₂'

C	-2.28747300	-0.04238800	0.33274100
C	-3.09313600	-1.15997400	0.01677600
C	-4.35198200	-1.02230900	-0.55959100
C	-4.86526900	0.25323300	-0.82928600
C	-4.09720500	1.38158000	-0.50643500
C	-2.84339400	1.23332000	0.06215700
H	-2.72415500	-2.15056200	0.24693800
H	-4.92540700	-1.91325800	-0.78761100
H	-4.51130200	2.36513700	-0.70358900
H	-2.27875700	2.12440500	0.31110100
O	-6.08610300	0.50173000	-1.38580400
C	-6.90845200	-0.60475100	-1.72198200
H	-7.82215600	-0.18382800	-2.14431300
H	-6.43117200	-1.25264400	-2.46822000
H	-7.16190500	-1.20439400	-0.83861500
C	-0.93928700	-0.19352400	0.89846200
C	-0.02748700	0.97564600	0.86718200
C	0.24319000	1.65027700	-0.34149900
C	0.55079100	1.49637800	2.04215100
C	1.06398600	2.77390200	-0.37589700
C	1.38896500	2.61240600	2.00620600
C	1.64856500	3.26092200	0.79792300
C	-0.64271400	-1.34442000	1.67623000
O	-1.33861200	-2.33102100	1.96690700

H	0.31327900	1.03608200	2.99601800
H	1.81559000	2.99174000	2.93095900
H	2.28162700	4.14330500	0.77223400
H	-0.19716600	1.27644100	-1.26072200
H	1.25558200	3.26840600	-1.32424500
C	0.81479800	-1.55382400	2.16658900
H	0.97950400	-1.78973500	3.21793700
C	1.63577500	-1.70726200	1.17908700
S	2.56941700	-2.37719300	0.01904700
C	3.59527400	-1.06571400	-0.67535800
C	4.39055500	-1.44268300	-1.76283300
C	3.64532900	0.22654100	-0.15297600
C	5.25047100	-0.50507200	-2.33302800
H	4.33953900	-2.45204200	-2.16166800
C	4.50820900	1.15279300	-0.73765000
H	3.01601500	0.51149300	0.68285300
C	5.31167300	0.79249800	-1.82139200
H	5.86884000	-0.79050900	-3.17846500
H	4.54097100	2.16276900	-0.34164600
H	5.98103400	1.52116000	-2.26798300

TS₃

C	1.43636900	-0.38518900	0.11485300
C	2.61534000	-0.35293100	-0.64712600
C	3.49385000	-1.43578600	-0.69320600
C	3.20801900	-2.59408700	0.03861500
C	2.03933100	-2.64780500	0.81354400
C	1.17866800	-1.56288700	0.84886700

H	2.84995900	0.53460800	-1.22507200
H	4.38752100	-1.36611500	-1.30195400
H	1.83800100	-3.54692700	1.38654500
H	0.28954900	-1.61535900	1.47059200
O	3.99397000	-3.70911500	0.07159000
C	5.19173600	-3.70860000	-0.68930000
H	5.65757700	-4.68015300	-0.51840100
H	4.99075100	-3.58873200	-1.76153200
H	5.87845300	-2.91694400	-0.36348600
C	0.48697400	0.75719600	0.17137300
C	1.01975500	2.12946100	-0.08972900
C	0.41657600	2.99252000	-1.02209200
C	2.16405800	2.58956600	0.58987400
C	0.92357100	4.27114500	-1.25028500
C	2.67463900	3.86359000	0.35266600
C	2.05597700	4.71479300	-0.56600700
C	-0.65505000	1.37840900	1.94104700
O	-0.20544100	1.52586600	3.02102500
H	2.64336500	1.94200900	1.31728800
H	3.55404600	4.19704700	0.89676600
H	2.45432300	5.70839700	-0.74878200
H	-0.45331500	2.65235400	-1.57610200
H	0.43877800	4.91709000	-1.97733400
C	-1.65021100	1.20485900	1.00033800
H	-2.68075000	1.53947800	1.04875100
C	-0.92878400	0.51782600	0.01316800
S	-1.58053000	-0.63705200	-1.14972500
C	-3.27495300	-0.88912500	-0.60509800

C	-4.32535100	-0.36995000	-1.37088500
C	-3.55075700	-1.65084400	0.53828600
C	-5.64682400	-0.60846700	-0.98958200
H	-4.10601000	0.21653000	-2.25728500
C	-4.87306100	-1.87163000	0.92091300
H	-2.73455600	-2.06647300	1.11989300
C	-5.92210500	-1.35374300	0.15753300
H	-6.45935300	-0.20605300	-1.58713200
H	-5.08395200	-2.45759900	1.81052700
H	-6.95072300	-1.53427800	0.45479300

TS₃'

C	-0.38396600	2.03895700	-0.11620000
C	-1.35770500	2.66889000	-0.91438600
C	-1.29593500	4.03603900	-1.17710200
C	-0.26413500	4.81182400	-0.64594300
C	0.70690400	4.20590800	0.15446200
C	0.64430700	2.84049900	0.41738900
H	-2.16152400	2.07590400	-1.33718400
H	-2.05556700	4.49618700	-1.80284900
H	1.50824100	4.80078900	0.58360100
H	1.39148400	2.38327700	1.05981100
C	-0.42631400	0.58251500	0.18565700
C	-1.74956900	-0.11114800	0.11626400
C	-1.94526500	-1.26257200	-0.65769000
C	-2.86028800	0.38711000	0.82884700
C	-3.18082800	-1.91354900	-0.71261300
C	-4.09529700	-0.24078400	0.77360400

C	-4.26623700	-1.40181000	0.00458100
C	0.14344100	-0.32689500	2.10374600
O	-0.21367800	0.04935600	3.16237300
H	-2.74234600	1.27514800	1.44184200
H	-4.94501300	0.14257600	1.32912600
H	-1.11784100	-1.66220700	-1.23667100
H	-3.28404600	-2.80064700	-1.32644800
C	0.92883300	-1.02362700	1.20853000
H	1.47367100	-1.94664000	1.37502100
C	0.77758600	-0.20772100	0.07749800
S	1.94753900	0.00428000	-1.22555800
C	3.42254000	-0.82937000	-0.62503100
C	3.82508600	-2.02735300	-1.22667300
C	4.20101000	-0.25887400	0.39088500
C	5.00036500	-2.65396000	-0.80870700
H	3.21989600	-2.46315400	-2.01510600
C	5.36520500	-0.89899400	0.81335100
H	3.89538300	0.67874300	0.84328600
C	5.76793000	-2.09462900	0.21356300
H	5.31101100	-3.58202600	-1.27924300
H	5.96372200	-0.45765000	1.60470600
H	6.67936300	-2.58607200	0.54032400
H	-0.21996300	5.87799000	-0.84809700
O	-5.52067100	-1.94654000	0.01956700
C	-5.74552500	-3.12420000	-0.73634700
H	-6.79233400	-3.38910500	-0.57964900
H	-5.57297300	-2.95903500	-1.80799200
H	-5.10984800	-3.95262600	-0.39718500

TS₄

C	1.67249800	-0.14940300	0.13867400
C	2.09934200	-0.91903200	-0.95097700
C	3.22870400	-1.73844500	-0.87608100
C	3.96555300	-1.79231500	0.31171700
C	3.56354200	-1.01736600	1.41024800
C	2.43864900	-0.21076600	1.31860700
H	1.54383800	-0.87558700	-1.88293000
H	3.52225600	-2.31736700	-1.74350700
H	4.14817700	-1.06954800	2.32283100
H	2.13647200	0.38206100	2.17704100
O	5.08238000	-2.55358000	0.50111800
C	5.52889300	-3.36846500	-0.57140200
H	6.41321500	-3.89130200	-0.20441600
H	4.76958300	-4.10479000	-0.86393300
H	5.80321800	-2.76942600	-1.44924100
C	0.48128300	0.74858200	0.05959400
C	0.68341900	2.17194900	0.08454800
C	1.90304900	2.77605500	-0.31933200
C	-0.39586600	3.03764400	0.45332500
C	2.01086500	4.14885100	-0.42019600
C	-0.25435900	4.45084400	0.34244600
C	0.92169200	4.99996600	-0.10916800
C	-2.12558000	2.39253800	-0.37134500
O	-2.92871700	3.27085200	-0.44701800
H	-1.03017600	2.67939200	1.26894600
H	-1.09994200	5.07897500	0.60572100

H	1.02636600	6.07495700	-0.21654000
H	2.74133800	2.14222400	-0.58586700
H	2.94448400	4.58476300	-0.76533000
C	-1.96944100	1.02721400	-0.46854300
H	-2.79026100	0.54412400	-0.99150900
C	-0.80249100	0.26067900	-0.18224300
S	-0.97644900	-1.52944500	-0.29710900
C	-2.72976100	-1.82085500	-0.03573300
C	-3.48344600	-2.39325000	-1.06710600
C	-3.32469800	-1.58351100	1.21159500
C	-4.82423500	-2.72169300	-0.85356600
H	-3.01943200	-2.57667500	-2.03088800
C	-4.66717400	-1.89708200	1.41251900
H	-2.73470500	-1.15367400	2.01424900
C	-5.41863300	-2.46961200	0.38242800
H	-5.40328500	-3.16649800	-1.65749100
H	-5.12541900	-1.70423800	2.37811200
H	-6.46269400	-2.71960600	0.54565100

TS₄'

C	-0.42643000	2.17962900	0.08652400
C	-0.09490400	2.95032700	-1.04002400
C	-0.14283300	4.34416100	-0.99338700
C	-0.53292500	4.99425700	0.17785000
C	-0.87823300	4.24157500	1.30219400
C	-0.82825800	2.84927600	1.25476000
H	0.19440300	2.45034400	-1.95938000
H	0.11856700	4.92110200	-1.87585900

H	-1.18408300	4.73930600	2.21808600
H	-1.09456400	2.26643300	2.13176000
C	-0.40599100	0.68583100	0.05214400
C	-1.65243400	-0.02310800	0.14687500
C	-2.89205200	0.55569000	-0.22141600
C	-1.66826500	-1.39995700	0.54602800
C	-4.05440700	-0.19014200	-0.25696900
C	-2.87545400	-2.15135100	0.51254400
C	-4.05218300	-1.56711500	0.09278500
C	-0.15180300	-2.38307400	-0.28478000
O	-0.34989000	-3.55996300	-0.32568300
H	-0.97963600	-1.65436000	1.35833900
H	-2.86963700	-3.19729900	0.79929200
H	-2.92118000	1.59860100	-0.51663900
H	-4.97207000	0.28815800	-0.57954900
C	0.84564600	-1.44045800	-0.44294200
H	1.70818000	-1.81979400	-0.98403200
C	0.75688800	-0.03948800	-0.20778000
S	2.28026200	0.90182200	-0.41270500
C	3.58153600	-0.29350700	-0.09037900
C	4.50179600	-0.58039500	-1.10523500
C	3.75033800	-0.85795500	1.18199800
C	5.58174300	-1.42878000	-0.84988700
H	4.36798900	-0.14202000	-2.08898400
C	4.81886200	-1.71827100	1.42448700
H	3.04412300	-0.62296700	1.97137400
C	5.73870000	-2.00266000	0.41119600
H	6.29287300	-1.64637100	-1.64135100

H	4.94059500	-2.15935300	2.40948100
H	6.57459000	-2.66764400	0.60682600
H	-0.57089500	6.07912100	0.21400100
O	-5.16128100	-2.36426900	0.05966900
C	-6.39516900	-1.79940700	-0.35500500
H	-6.34802700	-1.42724300	-1.38648100
H	-7.12594400	-2.60749400	-0.30204000
H	-6.71509200	-0.98430300	0.30706900

TS₅

C	4.34587400	-0.18252300	-0.33772300
C	5.32633500	-0.43729200	-1.30302300
C	6.43913800	-1.23395800	-1.02382400
C	6.58551900	-1.79343100	0.25084700
C	5.61420500	-1.54483900	1.23185200
C	4.51319400	-0.75123100	0.93804400
H	5.21999400	-0.00734300	-2.29470200
H	7.17562600	-1.40811600	-1.79899900
H	5.74827900	-1.98245200	2.21566900
H	3.76622200	-0.56698800	1.70470500
O	7.62763900	-2.58441200	0.63708100
C	8.63840200	-2.87793300	-0.31532900
H	9.35735800	-3.51864300	0.19696600
H	8.23340400	-3.41254200	-1.18386800
H	9.14737500	-1.96856900	-0.65949200
C	3.16133900	0.68457600	-0.63361800
C	3.20501800	2.05968000	-0.39308100
C	4.39802100	2.74056800	0.01662100

C	1.98072300	2.88586800	-0.53543500
C	4.45698300	4.10689600	0.04915900
C	2.15397800	4.34891600	-0.63882300
C	3.33682000	4.92660600	-0.32001000
C	0.79944800	2.27395400	-1.23831900
O	-0.22831400	3.00296500	-1.44755300
H	1.45864700	2.83890600	0.51003600
H	1.27182500	4.92094700	-0.90112100
H	3.45071100	6.00579900	-0.34371400
H	5.27861400	2.15158000	0.24553200
H	5.38791600	4.58985700	0.33348400
C	0.84354500	0.89296600	-1.49226400
H	-0.02664400	0.44490300	-1.95444800
C	1.97799200	0.13191000	-1.21044000
S	2.03662800	-1.61846700	-1.55803800
C	0.57077700	-1.92459900	-2.55379800
C	0.67258300	-1.86951300	-3.95031900
C	-0.63605700	-2.30451600	-1.95396100
C	-0.43183200	-2.18599200	-4.74100200
H	1.61326300	-1.58235000	-4.40873800
C	-1.73787400	-2.61903300	-2.75189200
H	-0.72381200	-2.34318000	-0.87325300
C	-1.63665300	-2.56096400	-4.14291500
H	-0.34976600	-2.14131800	-5.82293100
H	-2.67366700	-2.90238000	-2.28042700
H	-2.49460700	-2.80952600	-4.76068900
C	-4.29770000	-0.12725900	0.24215900
C	-5.24946100	-0.52304900	1.18983100

C	-6.33355400	-1.33607100	0.84992100
C	-6.48640700	-1.76673000	-0.47246900
C	-5.54932600	-1.37446900	-1.43928800
C	-4.47449100	-0.56988500	-1.08203200
H	-5.14264100	-0.18980000	2.21765100
H	-7.04546000	-1.61900600	1.61610600
H	-5.68783300	-1.71114700	-2.46172000
H	-3.75362200	-0.27493700	-1.83877700
O	-7.50447800	-2.55986500	-0.92052600
C	-8.48015100	-2.98981400	0.01532200
H	-9.18479900	-3.60584300	-0.54528900
H	-8.03491500	-3.59121600	0.81823700
H	-9.01749700	-2.14230600	0.45999300
C	-3.14613200	0.75551500	0.60734100
C	-3.15827200	2.12216300	0.27638900
C	-4.29692600	2.76699900	-0.30755200
C	-1.98025300	2.96196900	0.52534700
C	-4.34307400	4.12742300	-0.46769900
C	-2.13476300	4.40882900	0.45589800
C	-3.26376400	4.96998300	-0.05735000
C	-0.85624100	2.41725200	1.34998200
O	0.14696600	3.14474500	1.60094400
H	-1.24693000	2.86066000	-0.54814400
H	-1.28362900	4.99800100	0.77907600
H	-3.35809100	6.04787000	-0.14619200
H	-5.15461200	2.16177400	-0.57812900
H	-5.23603000	4.58103600	-0.88990200
C	-0.93358400	1.03893100	1.67695700

H	-0.10960100	0.62767400	2.24623800
C	-2.02869100	0.25452200	1.33034200
S	-2.08908400	-1.49394900	1.75759900
C	-0.67031800	-1.73073500	2.83499300
C	-0.78760300	-1.47823500	4.20855600
C	0.52642100	-2.24845900	2.32435500
C	0.28736800	-1.73240600	5.05995600
H	-1.71872500	-1.08337100	4.60157800
C	1.59740000	-2.50740300	3.18224800
H	0.62430900	-2.44287200	1.26160100
C	1.48000900	-2.24872200	4.54874900
H	0.19135200	-1.53130600	6.12285800
H	2.52121900	-2.91013100	2.77739400
H	2.31376000	-2.45128800	5.21465400

TS₅'

C	4.35548600	-1.01545700	-0.38784800
C	5.35013500	-1.18318500	-1.36330400
C	6.45907100	-1.99246500	-1.11619000
C	6.59048400	-2.64541500	0.11060700
C	5.60827600	-2.48512400	1.08897900
C	4.49862700	-1.67548400	0.84234700
H	5.24795400	-0.67599400	-2.31818200
H	7.22051600	-2.11197600	-1.88142800
H	5.70719000	-2.98728000	2.04712500
H	3.73419100	-1.55148700	1.60402300
C	3.16897600	-0.13461300	-0.63744400
C	3.22216400	1.23011700	-0.34692800

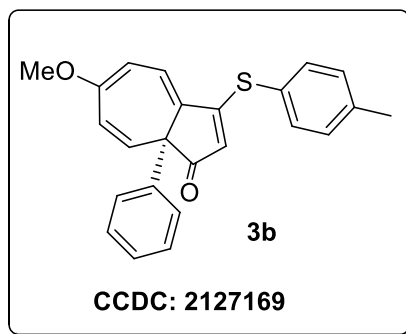
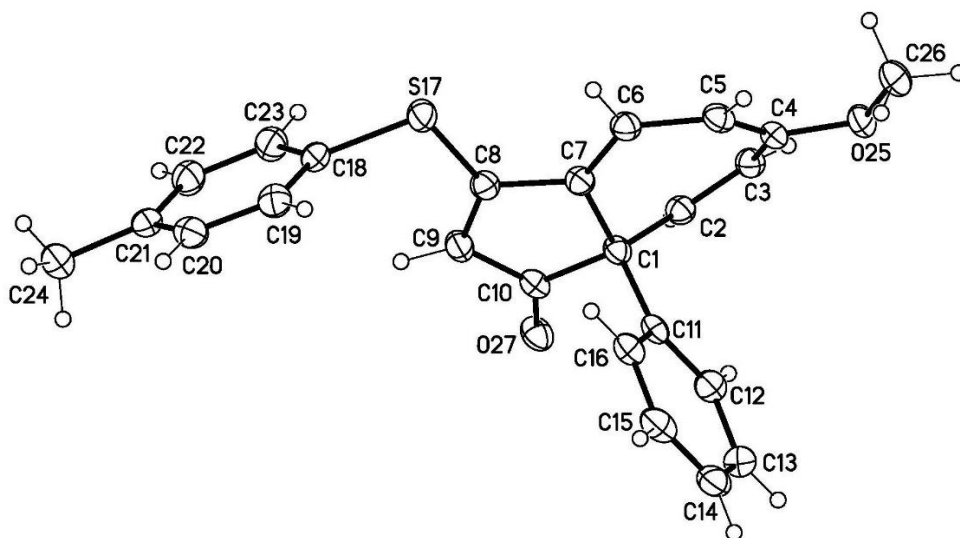
C	4.42148200	1.88871000	0.08136300
C	2.00180600	2.06724800	-0.45068800
C	4.48430900	3.25026700	0.18039900
C	2.17321700	3.53347200	-0.48784300
C	3.35878100	4.08780500	-0.14009000
C	0.81591900	1.48854300	-1.17288500
O	-0.20770200	2.23021300	-1.35499600
H	1.48235400	1.96668000	0.59158400
H	1.30494000	4.13602700	-0.72339100
H	5.30540200	1.29044000	0.26983500
H	5.41411200	3.73576800	0.46279800
C	0.84848800	0.11519600	-1.46938500
H	-0.02735100	-0.31104700	-1.94140500
C	1.97929000	-0.66284200	-1.22310400
S	2.02320100	-2.40105000	-1.62994600
C	0.55795000	-2.65876500	-2.63971800
C	0.66947200	-2.57499400	-4.03395800
C	-0.65959000	-3.02762400	-2.05473700
C	-0.43639100	-2.85224300	-4.83736500
H	1.61836900	-2.29680700	-4.48074300
C	-1.76293800	-3.30119700	-2.86533800
H	-0.75418600	-3.08887000	-0.97563900
C	-1.65216000	-3.21505000	-4.25421000
H	-0.34686200	-2.78619800	-5.91757300
H	-2.70680700	-3.57595000	-2.40491200
H	-2.51109000	-3.43265200	-4.88223700
C	-4.32167300	-0.88863500	0.22617400
C	-5.26668500	-1.31117200	1.17483700

C	-6.36369000	-2.08543700	0.79659100
C	-6.54041800	-2.44717200	-0.53987300
C	-5.61272800	-2.02985600	-1.49571300
C	-4.51305300	-1.25909700	-1.11508600
H	-5.13565600	-1.02620300	2.21420800
H	-7.08379900	-2.40142000	1.54598600
H	-5.74589800	-2.30177600	-2.53928000
H	-3.79086100	-0.93702000	-1.85956900
C	-3.15159800	-0.04196200	0.62000800
C	-3.14487600	1.33745500	0.34573400
C	-4.28008600	2.02300300	-0.19790500
C	-1.95431600	2.14908400	0.62185400
C	-4.30586400	3.38736500	-0.30972600
C	-2.07816200	3.60103800	0.60289300
C	-3.20136300	4.19297600	0.11523000
C	-0.83725000	1.55544600	1.42116000
O	0.17582000	2.25744100	1.70162600
H	-1.22412000	2.06243300	-0.45460700
H	-1.22802000	4.18181600	0.94037100
H	-5.15541300	1.44565300	-0.47268700
H	-5.19438300	3.88811100	-0.68410400
C	-0.93088600	0.16399500	1.68420600
H	-0.10951900	-0.28255300	2.23024800
C	-2.03934800	-0.59053400	1.31487100
S	-2.11866700	-2.35490500	1.66802300
C	-0.71269900	-2.64802600	2.74762600
C	-0.82796500	-2.41484800	4.12484500
C	0.47069400	-3.19046200	2.23181600

C	0.23698400	-2.71168000	4.97480700
H	-1.74932100	-2.00153000	4.52179400
C	1.53091000	-3.49342200	3.08878800
H	0.56611600	-3.37067000	1.16633900
C	1.41647400	-3.25302000	4.45875800
H	0.14296200	-2.52527900	6.04051800
H	2.44396700	-3.91677400	2.68051500
H	2.24184000	-3.48960000	5.12387000
H	7.45439500	-3.27483000	0.30311600
H	-7.39645600	-3.04727000	-0.83467900
O	3.53890600	5.45515900	-0.15183900
O	-3.32551100	5.56973400	0.09345200
C	3.42449400	6.06856000	1.13282500
H	4.17240500	5.67841700	1.83654200
H	3.59604300	7.13634400	0.98425800
H	2.42566800	5.91170200	1.55866300
C	-3.14207100	6.15015700	-1.19518400
H	-3.87368400	5.77122700	-1.92211100
H	-3.28269700	7.22673800	-1.07727900
H	-2.13302100	5.95280500	-1.58029800

10. X-ray crystallographic data:

a) X-ray structure of 3b:



211216LT_auto

Table S1 Crystal data and structure refinement for 211216LT_auto.

Identification code	211216LT_auto
Empirical formula	C ₂₄ H ₂₀ O ₂ S
Formula weight	372.46
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	13.9643(3)

b/Å	10.0272(2)
c/Å	13.3690(3)
$\alpha/^\circ$	90
$\beta/^\circ$	96.154(2)
$\gamma/^\circ$	90
Volume/Å ³	1861.18(7)
Z	4
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.329
μ/mm^{-1}	1.665
F(000)	784.0
Crystal size/mm ³	0.129 × 0.075 × 0.049
Radiation	Cu K α (λ = 1.54184)
2 Θ range for data collection/ $^\circ$	6.366 to 134.128
Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 6, -15 ≤ l ≤ 15
Reflections collected	14032
Independent reflections	3307 [R_{int} = 0.0214, R_{sigma} = 0.0207]
Data/restraints/parameters	3307/0/246
Goodness-of-fit on F ²	1.072
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0320, wR_2 = 0.0821
Final R indexes [all data]	R_1 = 0.0366, wR_2 = 0.0844
Largest diff. peak/hole / e Å ⁻³	0.22/-0.28

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	$U(\text{eq})$
C1	2742.1(10)	958.6(13)	7421.5(10)	20.0(3)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
C2	2385.3(10)	-310.9(13)	6914.0(10)	20.9(3)
C3	2632.2(10)	-742.4(14)	6027.5(10)	21.9(3)
C4	3214.6(10)	-38.0(15)	5355.3(10)	21.9(3)
C5	3274.2(10)	1300.7(14)	5242.4(10)	23.0(3)
C6	2789.9(10)	2279.0(14)	5796.3(10)	22.4(3)
C7	2518.1(10)	2137.0(14)	6727.4(10)	20.6(3)
C8	1977.7(10)	3110.9(14)	7259.9(11)	21.8(3)
C9	1804.8(10)	2653.4(14)	8178.9(11)	23.4(3)
C10	2162.9(10)	1305.1(14)	8317.1(10)	21.6(3)
C11	3801.0(10)	873.3(14)	7869.5(10)	21.4(3)
C12	4159.1(11)	-313.4(15)	8302.2(11)	27.2(3)
C13	5095.5(12)	-374.2(17)	8777.8(12)	32.2(4)
C14	5676.3(11)	742.9(18)	8831.6(11)	32.6(4)
C15	5322.4(11)	1925.4(17)	8410.1(11)	30.5(4)
C16	4388.0(10)	1991.5(15)	7928.1(10)	24.7(3)
C18	1191.1(10)	5526.5(14)	7668.1(11)	23.6(3)
C19	1731.0(11)	6584.8(14)	8087.1(11)	26.2(3)
C20	1397.8(11)	7340.1(15)	8850.1(11)	26.7(3)
C21	530.5(11)	7031.0(15)	9219.6(11)	25.4(3)
C22	-7.2(11)	5968.9(16)	8786.0(12)	29.4(3)
C23	306.6(11)	5230.6(16)	8005.8(12)	28.8(3)
C24	198.0(12)	7810.8(16)	10080.9(12)	33.2(4)
C26	4093.4(12)	-426.5(16)	3935.4(11)	30.8(4)
O25	3636.3(7)	-936.5(10)	4767.7(7)	26.3(2)
O27	2047.7(8)	531.7(10)	8999.6(7)	26.9(2)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
S17	1637.4(3)	4615.0(3)	6675.6(3)	26.73(12)

Table S3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	24.0(7)	20.5(7)	16.1(6)	0.0(5)	4.4(5)	0.3(6)
C2	22.7(7)	19.7(7)	20.0(7)	1.6(5)	1.9(5)	0.0(6)
C3	24.8(7)	19.5(7)	21.2(7)	-0.7(6)	0.8(6)	0.2(6)
C4	23.4(7)	26.2(7)	16.0(7)	-3.1(5)	1.1(5)	3.8(6)
C5	24.7(7)	27.9(8)	16.8(7)	0.7(6)	3.8(5)	-1.0(6)
C6	25.9(7)	21.2(7)	19.8(7)	1.1(5)	1.0(5)	0.5(6)
C7	22.8(7)	19.4(7)	19.5(7)	0.2(5)	1.9(5)	-0.6(6)
C8	23.4(7)	20.3(7)	21.2(7)	-1.5(6)	0.3(5)	-0.3(6)
C9	25.1(7)	24.4(7)	21.0(7)	-3.9(6)	4.1(6)	0.6(6)
C10	24.0(7)	24.5(7)	16.6(7)	-2.2(6)	3.0(5)	-1.9(6)
C11	25.0(7)	25.7(7)	14.2(6)	-3.1(5)	5.0(5)	1.5(6)
C12	31.4(8)	25.9(8)	23.8(7)	-1.6(6)	1.5(6)	2.1(6)
C13	34.5(8)	37.2(9)	24.0(8)	-1.6(7)	-0.6(6)	11.3(7)
C14	25.5(7)	50.5(10)	21.6(8)	-7.4(7)	1.5(6)	5.2(7)
C15	28.1(8)	40.7(9)	23.3(8)	-7.0(7)	5.1(6)	-6.5(7)
C16	27.7(7)	27.7(7)	19.3(7)	-2.9(6)	5.2(6)	-1.3(6)
C18	28.1(7)	20.2(7)	22.1(7)	1.5(6)	0.4(6)	6.0(6)
C19	30.7(8)	22.4(7)	25.8(8)	4.7(6)	4.7(6)	0.5(6)
C20	34.4(8)	20.7(7)	24.3(8)	1.4(6)	-0.7(6)	-1.6(6)
C21	30.3(7)	23.4(7)	21.6(7)	1.8(6)	-1.5(6)	6.3(6)

Table S3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C22	23.7(7)	32.3(8)	32.1(8)	-2.9(7)	2.9(6)	2.1(6)
C23	26.0(7)	26.7(8)	32.8(8)	-5.5(7)	-0.7(6)	0.1(6)
C24	40.2(9)	32.7(8)	26.5(8)	-3.9(7)	2.3(7)	5.2(7)
C26	35.3(8)	37.4(9)	21.3(7)	-2.5(6)	10.1(6)	3.3(7)
O25	32.2(5)	28.1(5)	19.4(5)	-2.8(4)	6.7(4)	4.8(5)
O27	36.5(6)	25.1(5)	20.3(5)	1.0(4)	8.2(4)	-1.5(4)
S17	36.1(2)	22.2(2)	22.23(19)	1.64(14)	4.80(15)	6.39(15)

Table S4 Bond Lengths for 211216LT_auto.

Atom	Atom	Length/ $\text{\AA}$	Atom	Atom	Length/ $\text{\AA}$
C1	C2	1.5022(19)	C11	C12	1.392(2)
C1	C7	1.5142(18)	C11	C16	1.386(2)
C1	C10	1.5544(18)	C12	C13	1.393(2)
C1	C11	1.5370(19)	C13	C14	1.380(2)
C2	C3	1.341(2)	C14	C15	1.381(2)
C3	C4	1.458(2)	C15	C16	1.394(2)
C4	C5	1.354(2)	C18	C19	1.385(2)
C4	O25	1.3692(16)	C18	C23	1.392(2)
C5	C6	1.4407(19)	C18	S17	1.7781(15)
C6	C7	1.3473(19)	C19	C20	1.390(2)
C7	C8	1.4646(19)	C20	C21	1.391(2)
C8	C9	1.357(2)	C21	C22	1.393(2)
C8	S17	1.7409(14)	C21	C24	1.506(2)
C9	C10	1.446(2)	C22	C23	1.388(2)

Table S4 Bond Lengths for 211216LT_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C10	O27	1.2212(17)	C26	O25	1.4349(17)

Table S5 Bond Angles for 211216LT_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C7	110.35(11)	O27	C10	C9	128.14(13)
C2	C1	C10	111.26(11)	C12	C11	C1	119.81(13)
C2	C1	C11	112.80(11)	C16	C11	C1	121.02(13)
C7	C1	C10	101.96(11)	C16	C11	C12	118.94(13)
C7	C1	C11	114.15(11)	C11	C12	C13	120.32(14)
C11	C1	C10	105.69(10)	C14	C13	C12	120.40(15)
C3	C2	C1	124.64(13)	C13	C14	C15	119.53(14)
C2	C3	C4	127.00(13)	C14	C15	C16	120.38(15)
C5	C4	C3	126.44(13)	C11	C16	C15	120.42(14)
C5	C4	O25	123.56(13)	C19	C18	C23	119.72(14)
O25	C4	C3	109.74(12)	C19	C18	S17	118.47(11)
C4	C5	C6	125.43(13)	C23	C18	S17	121.78(12)
C7	C6	C5	126.67(13)	C18	C19	C20	120.25(14)
C6	C7	C1	126.06(13)	C19	C20	C21	120.79(14)
C6	C7	C8	126.12(13)	C20	C21	C22	118.26(14)
C8	C7	C1	107.80(11)	C20	C21	C24	120.49(14)
C7	C8	S17	119.32(10)	C22	C21	C24	121.23(14)
C9	C8	C7	111.45(12)	C23	C22	C21	121.40(14)
C9	C8	S17	129.23(11)	C22	C23	C18	119.52(14)
C8	C9	C10	109.81(12)	C4	O25	C26	117.70(11)
C9	C10	C1	108.17(11)	C8	S17	C18	102.19(7)

Table S5 Bond Angles for 211216LT_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O27	C10	C1	123.69(12)				

Table S6 Torsion Angles for 211216LT_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	-5.4(2)	C10	C1	C2	C3	168.40(13)
C1	C7	C8	C9	-2.68(16)	C10	C1	C7	C6	-174.66(13)
C1	C7	C8	S17	178.16(10)	C10	C1	C7	C8	6.95(14)
C1	C11	C12	C13	-175.14(13)	C10	C1	C11	C12	85.19(15)
C1	C11	C16	C15	174.70(12)	C10	C1	C11	C16	-89.28(14)
C2	C1	C7	C6	-56.38(18)	C11	C1	C2	C3	-73.02(17)
C2	C1	C7	C8	125.24(12)	C11	C1	C7	C6	71.88(18)
C2	C1	C10	C9	-126.59(12)	C11	C1	C7	C8	-106.50(13)
C2	C1	C10	O27	53.09(18)	C11	C1	C10	C9	110.64(12)
C2	C1	C11	C12	-36.59(17)	C11	C1	C10	O27	-69.67(16)
C2	C1	C11	C16	148.94(12)	C11	C12	C13	C14	0.5(2)
C2	C3	C4	C5	-30.4(2)	C12	C11	C16	C15	0.2(2)
C2	C3	C4	O25	155.36(14)	C12	C13	C14	C15	0.0(2)
C3	C4	C5	C6	2.1(2)	C13	C14	C15	C16	-0.4(2)
C3	C4	O25	C26	168.87(12)	C14	C15	C16	C11	0.3(2)
C4	C5	C6	C7	27.3(2)	C16	C11	C12	C13	-0.6(2)
C5	C4	O25	C26	-5.6(2)	C18	C19	C20	C21	1.4(2)
C5	C6	C7	C1	5.6(2)	C19	C18	C23	C22	-2.5(2)
C5	C6	C7	C8	-176.30(14)	C19	C18	S17	C8	108.39(12)
C6	C7	C8	C9	178.94(14)	C19	C20	C21	C22	-1.8(2)
C6	C7	C8	S17	-0.2(2)	C19	C20	C21	C24	176.95(13)

Table S6 Torsion Angles for 211216LT_auto.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C7	C1	C2	C3	55.97(18)	C20	C21	C22	C23	0.0(2)
C7	C1	C10	C9	-8.96(14)	C21	C22	C23	C18	2.1(2)
C7	C1	C10	O27	170.72(13)	C23	C18	C19	C20	0.8(2)
C7	C1	C11	C12	-163.59(12)	C23	C18	S17	C8	-73.76(14)
C7	C1	C11	C16	21.94(17)	C24	C21	C22	C23	-178.67(14)
C7	C8	C9	C10	-3.39(17)	O25	C4	C5	C6	175.56(13)
C7	C8	S17	C18	-171.16(11)	S17	C8	C9	C10	175.66(11)
C8	C9	C10	C1	7.96(16)	S17	C18	C19	C20	178.65(11)
C8	C9	C10	O27	-171.70(14)	S17	C18	C23	C22	179.73(12)
C9	C8	S17	C18	9.85(15)					

Table S7 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto.

Atom	x	y	z	U(eq)
H2	1954.22	-845.95	7244.47	25
H3	2402.74	-1599.35	5814.71	26
H5	3668.19	1621.25	4757.55	28
H6	2647.56	3109.36	5471.71	27
H9	1494.88	3145.03	8659.37	28
H12	3762.68	-1085.45	8272.89	33
H13	5335.91	-1189.45	9066.89	39
H14	6314.85	698.76	9156.19	39
H15	5718.32	2698.07	8449.08	37
H16	4151.86	2808.15	7637.71	30
H19	2331.33	6795.42	7852.25	31

Table S7 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 211216LT_auto.

Atom	x	y	z	U(eq)
H20	1766.71	8076.21	9122.38	32
H22	-601.34	5745.32	9029.57	35
H23	-79.58	4528.33	7704.33	35
H24A	-506.41	7873.83	9996.36	50
H24B	475.8	8708.83	10090.75	50
H24C	408.05	7357.36	10716	50
H26A	3616.1	39.22	3470.08	46
H26B	4370.69	-1166.6	3584.02	46
H26C	4605.41	196.11	4183.78	46

Experimental

Single crystals of $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$ [211216LT_auto] were [1]. A suitable crystal was selected and [1] on a **XtaLAB Synergy R, DW system, HyPix-Arc 150** diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J., Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [211216LT_auto]

Crystal Data for $\text{C}_{24}\text{H}_{20}\text{O}_2\text{S}$ ($M = 372.46$ g/mol): monoclinic, space group $P2_1/c$ (no. 14), $a = 13.9643(3)$ Å, $b = 10.0272(2)$ Å, $c = 13.3690(3)$ Å, $\beta = 96.154(2)^\circ$, $V = 1861.18(7)$ Å³, $Z = 4$, $T = 100.00(10)$ K, $\mu(\text{Cu K}\alpha) = 1.665$ mm⁻¹, $D_{\text{calc}} = 1.329$ g/cm³, 14032 reflections measured ($6.366^\circ \leq 2\theta \leq 134.128^\circ$), 3307 unique ($R_{\text{int}} = 0.0214$, $R_{\text{sigma}} = 0.0207$) which were used in all calculations. The final R_1 was 0.0320 ($I > 2\sigma(I)$) and wR_2 was 0.0844 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
At 1.2 times of:
All C(H) groups
At 1.5 times of:
All C(H,H,H) groups
- 2.a Aromatic/amide H refined with riding coordinates:
C2(H2), C3(H3), C5(H5), C6(H6), C9(H9), C12(H12), C13(H13), C14(H14),
C15(H15), C16(H16), C19(H19), C20(H20), C22(H22), C23(H23)
- 2.b Idealised Me refined as rotating group:
C24(H24A,H24B,H24C), C26(H26A,H26B,H26C)

This report has been created with Olex2, compiled on 2021.11.18 svn.ra9532c28 for OlexSys. Please [let us know](#) if there are any errors or if you would like to have additional features.

b) X-ray structure of 4b:

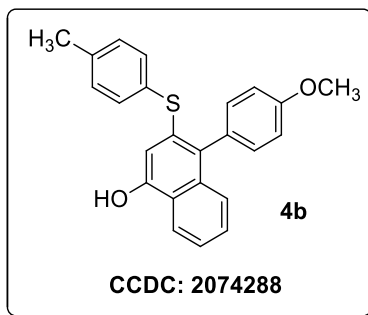
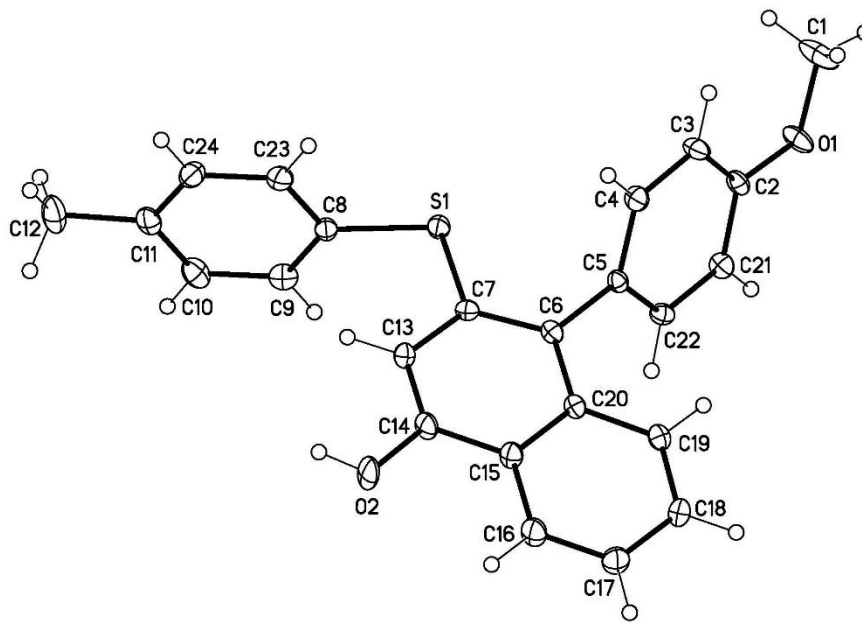


Table S8. Crystal data and structure refinement for 210340lt_0m.

Identification code	210340LT_0m	
Empirical formula	C ₂₄ H ₂₀ O ₂ S	
Formula weight	372.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 5.8791(3) Å	α = 90°.
	b = 14.5329(6) Å	β = 96.175(3)°.
	c = 22.0105(9) Å	γ = 90°.
Volume	1869.67(14) Å ³	

Z	4
Density (calculated)	1.323 Mg/m ³
Absorption coefficient	0.189 mm ⁻¹
F(000)	784
Crystal size	0.20 x 0.19 x 0.07 mm ³
Theta range for data collection	1.682 to 28.290°.
Index ranges	-7<=h<=7, -19<=k<=16, -29<=l<=29
Reflections collected	18659
Independent reflections	4627 [R(int) = 0.0360]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6881
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4627 / 0 / 249
Goodness-of-fit on F ²	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0876
R indices (all data)	R1 = 0.0523, wR2 = 0.0953
Extinction coefficient	n/a
Largest diff. peak and hole	0.304 and -0.282 e.Å ⁻³

Table S9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 210340lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7364(1)	3212(1)	91(1)	16(1)
O(1)	3225(2)	1241(1)	-2190(1)	19(1)
O(2)	5135(2)	2451(1)	2251(1)	25(1)
C(1)	4967(3)	767(1)	-2476(1)	30(1)
C(2)	3596(3)	1375(1)	-1564(1)	14(1)
C(3)	5545(3)	1093(1)	-1204(1)	16(1)
C(4)	5737(2)	1272(1)	-577(1)	15(1)
C(5)	4016(2)	1725(1)	-304(1)	12(1)
C(6)	4296(2)	1924(1)	366(1)	12(1)
C(7)	5892(2)	2562(1)	611(1)	12(1)
C(8)	8859(2)	4071(1)	553(1)	14(1)
C(9)	7871(3)	4929(1)	629(1)	18(1)
C(10)	9121(3)	5614(1)	949(1)	20(1)
C(11)	11378(3)	5473(1)	1193(1)	18(1)
C(12)	12759(3)	6234(1)	1519(1)	27(1)
C(13)	6244(2)	2730(1)	1248(1)	15(1)
C(14)	4897(3)	2304(1)	1632(1)	16(1)
C(15)	3123(3)	1694(1)	1405(1)	15(1)
C(16)	1582(3)	1310(1)	1789(1)	20(1)
C(17)	-155(3)	745(1)	1558(1)	19(1)
C(18)	-415(3)	525(1)	931(1)	16(1)
C(19)	1066(2)	879(1)	550(1)	14(1)
C(20)	2860(2)	1488(1)	767(1)	12(1)
C(21)	1834(2)	1813(1)	-1302(1)	14(1)
C(22)	2052(2)	1982(1)	-679(1)	13(1)
C(23)	11093(3)	3915(1)	800(1)	18(1)
C(24)	12331(3)	4610(1)	1119(1)	19(1)

Table S10. Bond lengths [Å] and angles [°] for 210340lt_0m.

S(1)-C(7)	1.7796(14)
S(1)-C(8)	1.7798(14)
O(1)-C(2)	1.3856(16)
O(1)-C(1)	1.4341(18)
O(2)-C(14)	1.3723(16)
O(2)-H(7)	0.85(2)
C(1)-H(10)	0.9800
C(1)-H(9)	0.9800
C(1)-H(1)	0.9800
C(2)-C(3)	1.383(2)
C(2)-C(21)	1.3925(19)
C(3)-C(4)	1.3982(19)
C(3)-H(8)	0.9500
C(4)-C(5)	1.3946(19)
C(4)-H(13)	0.9500
C(5)-C(22)	1.396(2)
C(5)-C(6)	1.4950(18)
C(6)-C(7)	1.3863(19)
C(6)-C(20)	1.4333(18)
C(7)-C(13)	1.4160(18)
C(8)-C(23)	1.385(2)
C(8)-C(9)	1.393(2)
C(9)-C(10)	1.385(2)
C(9)-H(5)	0.9500
C(10)-C(11)	1.392(2)
C(10)-H(4)	0.9500
C(11)-C(24)	1.390(2)
C(11)-C(12)	1.508(2)
C(12)-H(2)	0.9800
C(12)-H(20)	0.9800
C(12)-H(3)	0.9800
C(13)-C(14)	1.3666(19)
C(13)-H(6)	0.9500
C(14)-C(15)	1.419(2)

C(15)-C(16)	1.4174(19)
C(15)-C(20)	1.4282(18)
C(16)-C(17)	1.366(2)
C(16)-H(17)	0.9500
C(17)-C(18)	1.409(2)
C(17)-H(16)	0.9500
C(18)-C(19)	1.3732(19)
C(18)-H(15)	0.9500
C(19)-C(20)	1.420(2)
C(19)-H(14)	0.9500
C(21)-C(22)	1.3864(19)
C(21)-H(12)	0.9500
C(22)-H(11)	0.9500
C(23)-C(24)	1.390(2)
C(23)-H(18)	0.9500
C(24)-H(19)	0.9500

C(7)-S(1)-C(8)	104.46(6)
C(2)-O(1)-C(1)	117.37(12)
C(14)-O(2)-H(7)	110.2(14)
O(1)-C(1)-H(10)	109.5
O(1)-C(1)-H(9)	109.5
H(10)-C(1)-H(9)	109.5
O(1)-C(1)-H(1)	109.5
H(10)-C(1)-H(1)	109.5
H(9)-C(1)-H(1)	109.5
C(3)-C(2)-O(1)	124.05(12)
C(3)-C(2)-C(21)	120.40(13)
O(1)-C(2)-C(21)	115.54(13)
C(2)-C(3)-C(4)	118.96(13)
C(2)-C(3)-H(8)	120.5
C(4)-C(3)-H(8)	120.5
C(5)-C(4)-C(3)	121.83(13)
C(5)-C(4)-H(13)	119.1
C(3)-C(4)-H(13)	119.1
C(4)-C(5)-C(22)	117.68(12)

C(4)-C(5)-C(6)	120.50(13)
C(22)-C(5)-C(6)	121.82(12)
C(7)-C(6)-C(20)	118.33(12)
C(7)-C(6)-C(5)	120.77(12)
C(20)-C(6)-C(5)	120.86(12)
C(6)-C(7)-C(13)	121.44(12)
C(6)-C(7)-S(1)	117.43(10)
C(13)-C(7)-S(1)	121.02(10)
C(23)-C(8)-C(9)	119.22(13)
C(23)-C(8)-S(1)	119.96(11)
C(9)-C(8)-S(1)	120.62(12)
C(10)-C(9)-C(8)	120.00(14)
C(10)-C(9)-H(5)	120.0
C(8)-C(9)-H(5)	120.0
C(9)-C(10)-C(11)	121.42(14)
C(9)-C(10)-H(4)	119.3
C(11)-C(10)-H(4)	119.3
C(24)-C(11)-C(10)	117.91(14)
C(24)-C(11)-C(12)	120.94(15)
C(10)-C(11)-C(12)	121.14(14)
C(11)-C(12)-H(2)	109.5
C(11)-C(12)-H(20)	109.5
H(2)-C(12)-H(20)	109.5
C(11)-C(12)-H(3)	109.5
H(2)-C(12)-H(3)	109.5
H(20)-C(12)-H(3)	109.5
C(14)-C(13)-C(7)	120.09(13)
C(14)-C(13)-H(6)	120.0
C(7)-C(13)-H(6)	120.0
C(13)-C(14)-O(2)	122.71(13)
C(13)-C(14)-C(15)	121.25(13)
O(2)-C(14)-C(15)	116.03(12)
C(16)-C(15)-C(14)	121.95(13)
C(16)-C(15)-C(20)	119.70(13)
C(14)-C(15)-C(20)	118.32(12)
C(17)-C(16)-C(15)	121.02(13)

C(17)-C(16)-H(17)	119.5
C(15)-C(16)-H(17)	119.5
C(16)-C(17)-C(18)	119.90(13)
C(16)-C(17)-H(16)	120.0
C(18)-C(17)-H(16)	120.0
C(19)-C(18)-C(17)	120.36(13)
C(19)-C(18)-H(15)	119.8
C(17)-C(18)-H(15)	119.8
C(18)-C(19)-C(20)	121.62(13)
C(18)-C(19)-H(14)	119.2
C(20)-C(19)-H(14)	119.2
C(19)-C(20)-C(15)	117.36(12)
C(19)-C(20)-C(6)	122.24(12)
C(15)-C(20)-C(6)	120.33(12)
C(22)-C(21)-C(2)	119.77(13)
C(22)-C(21)-H(12)	120.1
C(2)-C(21)-H(12)	120.1
C(21)-C(22)-C(5)	121.33(13)
C(21)-C(22)-H(11)	119.3
C(5)-C(22)-H(11)	119.3
C(8)-C(23)-C(24)	120.24(14)
C(8)-C(23)-H(18)	119.9
C(24)-C(23)-H(18)	119.9
C(23)-C(24)-C(11)	121.19(15)
C(23)-C(24)-H(19)	119.4
C(11)-C(24)-H(19)	119.4

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 210340lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	18(1)	19(1)	12(1)	-2(1)	4(1)	-6(1)
O(1)	25(1)	25(1)	8(1)	-1(1)	1(1)	9(1)
O(2)	32(1)	36(1)	9(1)	-4(1)	1(1)	-18(1)
C(1)	36(1)	41(1)	14(1)	-5(1)	4(1)	18(1)
C(2)	20(1)	14(1)	8(1)	-1(1)	2(1)	0(1)
C(3)	16(1)	19(1)	14(1)	-2(1)	4(1)	4(1)
C(4)	14(1)	18(1)	13(1)	-1(1)	-2(1)	2(1)
C(5)	15(1)	10(1)	11(1)	0(1)	2(1)	-1(1)
C(6)	14(1)	12(1)	10(1)	0(1)	0(1)	2(1)
C(7)	12(1)	13(1)	12(1)	0(1)	2(1)	1(1)
C(8)	17(1)	15(1)	11(1)	0(1)	4(1)	-4(1)
C(9)	18(1)	19(1)	17(1)	3(1)	2(1)	2(1)
C(10)	30(1)	12(1)	19(1)	1(1)	4(1)	2(1)
C(11)	26(1)	17(1)	11(1)	0(1)	5(1)	-5(1)
C(12)	41(1)	24(1)	15(1)	-2(1)	0(1)	-11(1)
C(13)	14(1)	16(1)	14(1)	-2(1)	-1(1)	-2(1)
C(14)	19(1)	20(1)	9(1)	-1(1)	-1(1)	-2(1)
C(15)	18(1)	16(1)	12(1)	1(1)	0(1)	-2(1)
C(16)	25(1)	22(1)	12(1)	0(1)	3(1)	-6(1)
C(17)	22(1)	20(1)	16(1)	2(1)	5(1)	-5(1)
C(18)	16(1)	14(1)	17(1)	0(1)	-1(1)	-3(1)
C(19)	17(1)	12(1)	13(1)	0(1)	-1(1)	2(1)
C(20)	14(1)	12(1)	11(1)	0(1)	-1(1)	2(1)
C(21)	15(1)	16(1)	12(1)	2(1)	-2(1)	3(1)
C(22)	14(1)	12(1)	14(1)	1(1)	3(1)	2(1)
C(23)	16(1)	17(1)	21(1)	-2(1)	4(1)	1(1)
C(24)	16(1)	23(1)	18(1)	-1(1)	2(1)	-4(1)

Table S12. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 210340lt_0m.

	x	y	z	U(eq)
H(7)	6210(40)	2835(14)	2349(9)	38
H(10)	6375	1133	-2434	45
H(9)	4455	675	-2910	45
H(1)	5263	168	-2278	45
H(8)	6733	781	-1381	19
H(13)	7076	1081	-329	18
H(5)	6341	5044	461	22
H(4)	8422	6193	1004	24
H(2)	13278	6661	1217	40
H(20)	14089	5971	1765	40
H(3)	11808	6566	1785	40
H(6)	7418	3139	1408	18
H(17)	1761	1449	2213	23
H(16)	-1187	500	1821	23
H(15)	-1622	130	772	19
H(14)	885	712	130	17
H(12)	486	1996	-1550	17
H(11)	840	2278	-503	16
H(18)	11781	3332	752	22
H(19)	13857	4493	1290	23

c) X-ray structure of 8b:

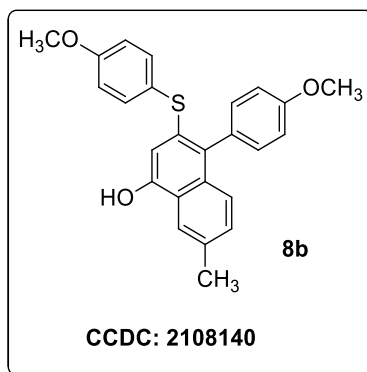
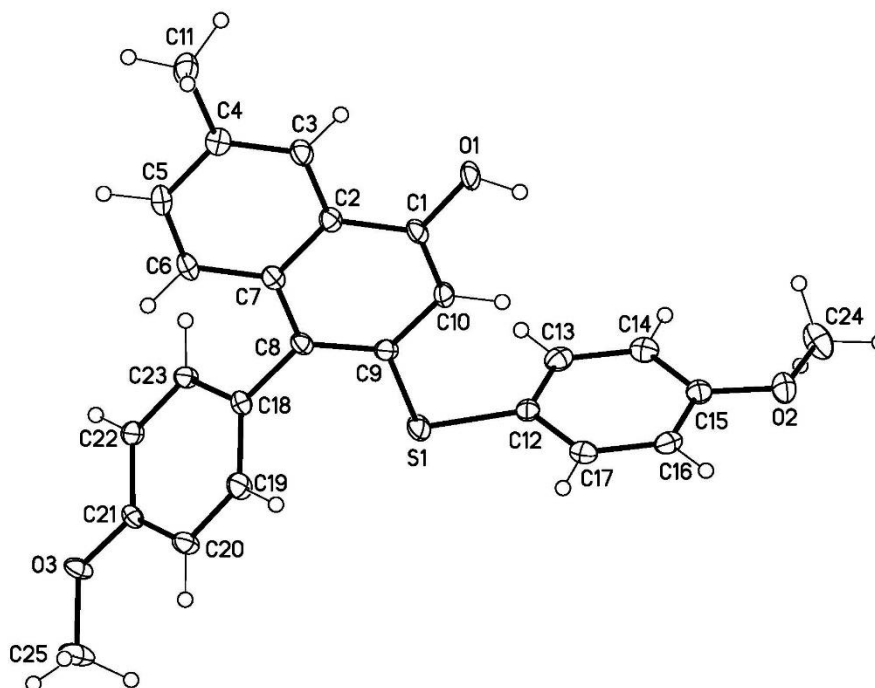


Table S13. Crystal data and structure refinement for 210903lt_0m_a.

Identification code	210903LT_0m_a	
Empirical formula	C ₂₅ H ₂₂ O ₃ S	
Formula weight	402.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 18.1663(11) Å	α = 90°.
	b = 15.0546(9) Å	β = 98.161(2)°.
	c = 22.1448(14) Å	γ = 90°.

Volume	5995.0(6) Å ³
Z	12
Density (calculated)	1.338 Mg/m ³
Absorption coefficient	0.186 mm ⁻¹
F(000)	2544
Crystal size	0.15 x 0.13 x 0.06 mm ³
Theta range for data collection	1.132 to 26.673°.
Index ranges	-20<=h<=22, -18<=k<=18, -27<=l<=27
Reflections collected	53102
Independent reflections	12370 [R(int) = 0.0378]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6982
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12370 / 0 / 796
Goodness-of-fit on F ²	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0930
R indices (all data)	R1 = 0.0560, wR2 = 0.1022
Extinction coefficient	n/a
Largest diff. peak and hole	0.336 and -0.236 e.Å ⁻³

Table S14. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 210903lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2525(1)	1720(1)	4930(1)	19(1)
S(2)	9216(1)	1774(1)	4960(1)	18(1)
S(3)	4027(1)	7875(1)	5134(1)	19(1)
O(1)	967(1)	2297(1)	2818(1)	21(1)
O(2)	3888(1)	-890(1)	3424(1)	22(1)
O(3)	1980(1)	3598(1)	7217(1)	17(1)
O(4)	7781(1)	2420(1)	2817(1)	22(1)
O(5)	10137(1)	-1229(1)	3511(1)	29(1)
O(6)	8698(1)	3709(1)	7229(1)	15(1)
O(7)	5634(1)	7488(1)	7237(1)	23(1)
O(8)	4677(1)	6402(1)	2815(1)	16(1)
O(9)	3493(1)	11260(1)	6355(1)	25(1)
C(1)	1124(1)	2474(1)	3427(1)	15(1)
C(2)	644(1)	3095(1)	3665(1)	14(1)
C(3)	31(1)	3481(1)	3291(1)	16(1)
C(4)	-430(1)	4074(1)	3524(1)	17(1)
C(5)	-266(1)	4312(1)	4144(1)	18(1)
C(6)	329(1)	3958(1)	4514(1)	16(1)
C(7)	800(1)	3319(1)	4293(1)	14(1)
C(8)	1399(1)	2905(1)	4678(1)	13(1)
C(9)	1829(1)	2287(1)	4426(1)	14(1)
C(10)	1699(1)	2086(1)	3797(1)	15(1)
C(11)	-1098(1)	4476(1)	3137(1)	23(1)
C(12)	2889(1)	929(1)	4455(1)	15(1)
C(13)	2606(1)	72(1)	4394(1)	18(1)
C(14)	2923(1)	-561(1)	4054(1)	17(1)
C(15)	3528(1)	-330(1)	3769(1)	17(1)
C(16)	3811(1)	531(1)	3823(1)	17(1)
C(17)	3498(1)	1151(1)	4169(1)	17(1)
C(18)	1547(1)	3118(1)	5344(1)	13(1)
C(19)	2185(1)	3575(1)	5586(1)	18(1)

C(20)	2347(1)	3758(1)	6205(1)	17(1)
C(21)	1863(1)	3471(1)	6594(1)	13(1)
C(22)	1213(1)	3020(1)	6362(1)	14(1)
C(23)	1059(1)	2851(1)	5744(1)	14(1)
C(24)	3649(1)	-1794(1)	3388(1)	26(1)
C(25)	2641(1)	4063(1)	7470(1)	24(1)
C(26)	7904(1)	2584(1)	3431(1)	16(1)
C(27)	7415(1)	3203(1)	3655(1)	15(1)
C(28)	6814(1)	3581(1)	3263(1)	16(1)
C(29)	6335(1)	4171(1)	3473(1)	17(1)
C(30)	6472(1)	4422(1)	4093(1)	16(1)
C(31)	7052(1)	4075(1)	4483(1)	15(1)
C(32)	7541(1)	3434(1)	4283(1)	13(1)
C(33)	8121(1)	3012(1)	4687(1)	13(1)
C(34)	8554(1)	2377(1)	4448(1)	14(1)
C(35)	8458(1)	2186(1)	3817(1)	15(1)
C(36)	5683(1)	4552(1)	3059(1)	24(1)
C(37)	9487(1)	899(1)	4503(1)	15(1)
C(38)	9021(1)	173(1)	4341(1)	20(1)
C(39)	9250(1)	-515(1)	4005(1)	22(1)
C(40)	9959(1)	-508(1)	3836(1)	20(1)
C(41)	10432(1)	203(1)	4000(1)	18(1)
C(42)	10188(1)	906(1)	4328(1)	17(1)
C(43)	8263(1)	3237(1)	5350(1)	14(1)
C(44)	8946(1)	3584(1)	5607(1)	18(1)
C(45)	9114(1)	3762(1)	6226(1)	16(1)
C(46)	8584(1)	3595(1)	6604(1)	13(1)
C(47)	7885(1)	3278(1)	6357(1)	14(1)
C(48)	7730(1)	3098(1)	5740(1)	14(1)
C(49)	10893(1)	-1318(1)	3421(1)	32(1)
C(50)	9386(1)	4106(1)	7495(1)	21(1)
C(51)	5491(1)	7294(1)	6629(1)	15(1)
C(52)	4886(1)	7604(1)	6255(1)	14(1)
C(53)	4785(1)	7403(1)	5626(1)	14(1)
C(54)	5269(1)	6849(1)	5376(1)	13(1)
C(55)	5900(1)	6509(1)	5767(1)	13(1)

C(56)	6445(1)	5968(1)	5548(1)	14(1)
C(57)	7074(1)	5703(1)	5921(1)	15(1)
C(58)	7206(1)	5952(1)	6541(1)	17(1)
C(59)	6678(1)	6459(1)	6768(1)	17(1)
C(60)	6026(1)	6743(1)	6395(1)	14(1)
C(61)	5144(1)	6656(1)	4709(1)	13(1)
C(62)	4562(1)	6117(1)	4454(1)	16(1)
C(63)	4392(1)	5999(1)	3827(1)	15(1)
C(64)	4815(1)	6436(1)	3445(1)	13(1)
C(65)	5414(1)	6960(1)	3689(1)	16(1)
C(66)	5578(1)	7064(1)	4313(1)	16(1)
C(67)	3858(1)	8870(1)	5520(1)	15(1)
C(68)	4364(1)	9569(1)	5546(1)	19(1)
C(69)	4230(1)	10354(1)	5831(1)	21(1)
C(70)	3577(1)	10457(1)	6084(1)	18(1)
C(71)	3064(1)	9768(1)	6056(1)	17(1)
C(72)	3210(1)	8972(1)	5777(1)	16(1)
C(73)	7907(1)	5664(1)	6940(1)	21(1)
C(74)	4053(1)	5891(1)	2542(1)	22(1)
C(75)	2799(1)	11429(1)	6560(1)	26(1)

Table S15. Bond lengths [Å] and angles [°] for 210903lt_0m_a.

S(1)-C(12)	1.7767(16)
S(1)-C(9)	1.7813(16)
S(2)-C(37)	1.7735(16)
S(2)-C(34)	1.7815(15)
S(3)-C(67)	1.7736(16)
S(3)-C(53)	1.7773(16)
O(1)-C(1)	1.3654(18)
O(1)-H(1)	0.8400
O(2)-C(15)	1.3654(19)
O(2)-C(24)	1.4276(19)
O(3)-C(21)	1.3787(18)
O(3)-C(25)	1.4332(18)
O(4)-C(26)	1.3695(18)
O(4)-H(4)	0.8400
O(5)-C(40)	1.3660(19)
O(5)-C(49)	1.423(2)
O(6)-C(46)	1.3801(18)
O(6)-C(50)	1.4350(18)
O(7)-C(51)	1.3660(18)
O(7)-H(7)	0.8400
O(8)-C(64)	1.3824(18)
O(8)-C(74)	1.4317(18)
O(9)-C(70)	1.3663(19)
O(9)-C(75)	1.423(2)
C(1)-C(10)	1.365(2)
C(1)-C(2)	1.427(2)
C(2)-C(3)	1.416(2)
C(2)-C(7)	1.419(2)
C(3)-C(4)	1.372(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.410(2)
C(4)-C(11)	1.509(2)
C(5)-C(6)	1.370(2)
C(5)-H(5)	0.9500

C(6)-C(7)	1.420(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.428(2)
C(8)-C(9)	1.381(2)
C(8)-C(18)	1.496(2)
C(9)-C(10)	1.412(2)
C(10)-H(10)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.388(2)
C(12)-C(17)	1.393(2)
C(13)-C(14)	1.391(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.386(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.394(2)
C(16)-C(17)	1.378(2)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.389(2)
C(18)-C(23)	1.399(2)
C(19)-C(20)	1.387(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.385(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.395(2)
C(22)-C(23)	1.381(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

C(26)-C(35)	1.362(2)
C(26)-C(27)	1.424(2)
C(27)-C(28)	1.414(2)
C(27)-C(32)	1.421(2)
C(28)-C(29)	1.370(2)
C(28)-H(28)	0.9500
C(29)-C(30)	1.412(2)
C(29)-C(36)	1.505(2)
C(30)-C(31)	1.369(2)
C(30)-H(30)	0.9500
C(31)-C(32)	1.424(2)
C(31)-H(31)	0.9500
C(32)-C(33)	1.431(2)
C(33)-C(34)	1.388(2)
C(33)-C(43)	1.494(2)
C(34)-C(35)	1.413(2)
C(35)-H(35)	0.9500
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(42)	1.383(2)
C(37)-C(38)	1.396(2)
C(38)-C(39)	1.374(2)
C(38)-H(38)	0.9500
C(39)-C(40)	1.391(2)
C(39)-H(39)	0.9500
C(40)-C(41)	1.388(2)
C(41)-C(42)	1.391(2)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
C(43)-C(44)	1.391(2)
C(43)-C(48)	1.401(2)
C(44)-C(45)	1.387(2)
C(44)-H(44)	0.9500
C(45)-C(46)	1.387(2)
C(45)-H(45)	0.9500

C(46)-C(47)	1.394(2)
C(47)-C(48)	1.382(2)
C(47)-H(47)	0.9500
C(48)-H(48)	0.9500
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-C(52)	1.361(2)
C(51)-C(60)	1.429(2)
C(52)-C(53)	1.413(2)
C(52)-H(52)	0.9500
C(53)-C(54)	1.382(2)
C(54)-C(55)	1.430(2)
C(54)-C(61)	1.492(2)
C(55)-C(60)	1.420(2)
C(55)-C(56)	1.421(2)
C(56)-C(57)	1.371(2)
C(56)-H(56)	0.9500
C(57)-C(58)	1.411(2)
C(57)-H(57)	0.9500
C(58)-C(59)	1.375(2)
C(58)-C(73)	1.509(2)
C(59)-C(60)	1.411(2)
C(59)-H(59)	0.9500
C(61)-C(62)	1.389(2)
C(61)-C(66)	1.401(2)
C(62)-C(63)	1.389(2)
C(62)-H(62)	0.9500
C(63)-C(64)	1.387(2)
C(63)-H(63)	0.9500
C(64)-C(65)	1.391(2)
C(65)-C(66)	1.381(2)
C(65)-H(65)	0.9500

C(66)-H(66)	0.9500
C(67)-C(72)	1.387(2)
C(67)-C(68)	1.392(2)
C(68)-C(69)	1.377(2)
C(68)-H(68)	0.9500
C(69)-C(70)	1.392(2)
C(69)-H(69)	0.9500
C(70)-C(71)	1.389(2)
C(71)-C(72)	1.390(2)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
C(73)-H(73A)	0.9800
C(73)-H(73B)	0.9800
C(73)-H(73C)	0.9800
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800
C(75)-H(75C)	0.9800

C(12)-S(1)-C(9)	104.01(7)
C(37)-S(2)-C(34)	103.42(7)
C(67)-S(3)-C(53)	102.38(7)
C(1)-O(1)-H(1)	109.5
C(15)-O(2)-C(24)	117.09(13)
C(21)-O(3)-C(25)	117.49(12)
C(26)-O(4)-H(4)	109.5
C(40)-O(5)-C(49)	117.03(14)
C(46)-O(6)-C(50)	117.43(12)
C(51)-O(7)-H(7)	109.5
C(64)-O(8)-C(74)	117.72(12)
C(70)-O(9)-C(75)	117.23(13)
C(10)-C(1)-O(1)	122.92(14)
C(10)-C(1)-C(2)	120.97(14)
O(1)-C(1)-C(2)	116.11(13)

C(3)-C(2)-C(7)	120.32(14)
C(3)-C(2)-C(1)	121.64(14)
C(7)-C(2)-C(1)	118.04(14)
C(4)-C(3)-C(2)	121.33(15)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	118.37(15)
C(3)-C(4)-C(11)	122.13(15)
C(5)-C(4)-C(11)	119.50(14)
C(6)-C(5)-C(4)	121.63(14)
C(6)-C(5)-H(5)	119.2
C(4)-C(5)-H(5)	119.2
C(5)-C(6)-C(7)	121.25(15)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(2)-C(7)-C(6)	117.05(14)
C(2)-C(7)-C(8)	120.64(14)
C(6)-C(7)-C(8)	122.31(14)
C(9)-C(8)-C(7)	118.68(14)
C(9)-C(8)-C(18)	120.62(14)
C(7)-C(8)-C(18)	120.68(13)
C(8)-C(9)-C(10)	121.17(14)
C(8)-C(9)-S(1)	117.53(12)
C(10)-C(9)-S(1)	121.24(12)
C(1)-C(10)-C(9)	120.41(14)
C(1)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(4)-C(11)-H(11A)	109.5
C(4)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(4)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-C(17)	119.09(14)
C(13)-C(12)-S(1)	121.10(12)
C(17)-C(12)-S(1)	119.69(12)

C(12)-C(13)-C(14)	120.91(15)
C(12)-C(13)-H(13)	119.5
C(14)-C(13)-H(13)	119.5
C(15)-C(14)-C(13)	119.36(14)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
O(2)-C(15)-C(14)	124.92(14)
O(2)-C(15)-C(16)	115.01(14)
C(14)-C(15)-C(16)	120.07(15)
C(17)-C(16)-C(15)	120.09(15)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(12)	120.47(15)
C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(19)-C(18)-C(23)	117.81(14)
C(19)-C(18)-C(8)	120.74(14)
C(23)-C(18)-C(8)	121.43(14)
C(20)-C(19)-C(18)	121.93(15)
C(20)-C(19)-H(19)	119.0
C(18)-C(19)-H(19)	119.0
C(21)-C(20)-C(19)	119.21(14)
C(21)-C(20)-H(20)	120.4
C(19)-C(20)-H(20)	120.4
O(3)-C(21)-C(20)	123.87(14)
O(3)-C(21)-C(22)	116.06(13)
C(20)-C(21)-C(22)	120.07(14)
C(23)-C(22)-C(21)	119.85(14)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(18)	121.12(14)
C(22)-C(23)-H(23)	119.4
C(18)-C(23)-H(23)	119.4
O(2)-C(24)-H(24A)	109.5
O(2)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5

O(2)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(3)-C(25)-H(25A)	109.5
O(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(3)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(35)-C(26)-O(4)	123.00(14)
C(35)-C(26)-C(27)	120.80(14)
O(4)-C(26)-C(27)	116.19(13)
C(28)-C(27)-C(32)	120.39(14)
C(28)-C(27)-C(26)	121.02(14)
C(32)-C(27)-C(26)	118.59(14)
C(29)-C(28)-C(27)	121.69(15)
C(29)-C(28)-H(28)	119.2
C(27)-C(28)-H(28)	119.2
C(28)-C(29)-C(30)	118.05(15)
C(28)-C(29)-C(36)	121.65(15)
C(30)-C(29)-C(36)	120.30(14)
C(31)-C(30)-C(29)	121.72(14)
C(31)-C(30)-H(30)	119.1
C(29)-C(30)-H(30)	119.1
C(30)-C(31)-C(32)	121.38(14)
C(30)-C(31)-H(31)	119.3
C(32)-C(31)-H(31)	119.3
C(27)-C(32)-C(31)	116.68(14)
C(27)-C(32)-C(33)	120.34(14)
C(31)-C(32)-C(33)	122.96(14)
C(34)-C(33)-C(32)	118.32(14)
C(34)-C(33)-C(43)	120.20(14)
C(32)-C(33)-C(43)	121.47(13)
C(33)-C(34)-C(35)	121.34(14)
C(33)-C(34)-S(2)	118.40(12)
C(35)-C(34)-S(2)	120.22(11)

C(26)-C(35)-C(34)	120.41(14)
C(26)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8
C(29)-C(36)-H(36A)	109.5
C(29)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(29)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(42)-C(37)-C(38)	118.85(14)
C(42)-C(37)-S(2)	119.70(12)
C(38)-C(37)-S(2)	121.35(12)
C(39)-C(38)-C(37)	120.61(15)
C(39)-C(38)-H(38)	119.7
C(37)-C(38)-H(38)	119.7
C(38)-C(39)-C(40)	120.25(15)
C(38)-C(39)-H(39)	119.9
C(40)-C(39)-H(39)	119.9
O(5)-C(40)-C(41)	124.49(16)
O(5)-C(40)-C(39)	115.67(15)
C(41)-C(40)-C(39)	119.84(15)
C(40)-C(41)-C(42)	119.43(15)
C(40)-C(41)-H(41)	120.3
C(42)-C(41)-H(41)	120.3
C(37)-C(42)-C(41)	121.00(15)
C(37)-C(42)-H(42)	119.5
C(41)-C(42)-H(42)	119.5
C(44)-C(43)-C(48)	117.22(14)
C(44)-C(43)-C(33)	120.39(14)
C(48)-C(43)-C(33)	122.39(14)
C(45)-C(44)-C(43)	122.41(15)
C(45)-C(44)-H(44)	118.8
C(43)-C(44)-H(44)	118.8
C(46)-C(45)-C(44)	119.13(14)
C(46)-C(45)-H(45)	120.4
C(44)-C(45)-H(45)	120.4

O(6)-C(46)-C(45)	124.43(14)
O(6)-C(46)-C(47)	115.76(13)
C(45)-C(46)-C(47)	119.80(14)
C(48)-C(47)-C(46)	120.11(14)
C(48)-C(47)-H(47)	119.9
C(46)-C(47)-H(47)	119.9
C(47)-C(48)-C(43)	121.28(14)
C(47)-C(48)-H(48)	119.4
C(43)-C(48)-H(48)	119.4
O(5)-C(49)-H(49A)	109.5
O(5)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
O(5)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
O(6)-C(50)-H(50A)	109.5
O(6)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
O(6)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-O(7)	123.35(14)
C(52)-C(51)-C(60)	120.63(14)
O(7)-C(51)-C(60)	116.01(14)
C(51)-C(52)-C(53)	120.50(14)
C(51)-C(52)-H(52)	119.8
C(53)-C(52)-H(52)	119.8
C(54)-C(53)-C(52)	121.48(14)
C(54)-C(53)-S(3)	118.54(12)
C(52)-C(53)-S(3)	119.97(12)
C(53)-C(54)-C(55)	118.36(14)
C(53)-C(54)-C(61)	119.85(14)
C(55)-C(54)-C(61)	121.72(13)
C(60)-C(55)-C(56)	117.00(14)
C(60)-C(55)-C(54)	120.49(14)
C(56)-C(55)-C(54)	122.44(14)

C(57)-C(56)-C(55)	121.48(14)
C(57)-C(56)-H(56)	119.3
C(55)-C(56)-H(56)	119.3
C(56)-C(57)-C(58)	121.39(14)
C(56)-C(57)-H(57)	119.3
C(58)-C(57)-H(57)	119.3
C(59)-C(58)-C(57)	118.23(15)
C(59)-C(58)-C(73)	121.38(15)
C(57)-C(58)-C(73)	120.39(14)
C(58)-C(59)-C(60)	121.66(15)
C(58)-C(59)-H(59)	119.2
C(60)-C(59)-H(59)	119.2
C(59)-C(60)-C(55)	120.20(14)
C(59)-C(60)-C(51)	121.35(14)
C(55)-C(60)-C(51)	118.41(14)
C(62)-C(61)-C(66)	117.75(14)
C(62)-C(61)-C(54)	121.10(14)
C(66)-C(61)-C(54)	121.00(13)
C(63)-C(62)-C(61)	121.95(14)
C(63)-C(62)-H(62)	119.0
C(61)-C(62)-H(62)	119.0
C(64)-C(63)-C(62)	119.03(14)
C(64)-C(63)-H(63)	120.5
C(62)-C(63)-H(63)	120.5
O(8)-C(64)-C(63)	124.17(14)
O(8)-C(64)-C(65)	115.61(13)
C(63)-C(64)-C(65)	120.21(14)
C(66)-C(65)-C(64)	119.94(14)
C(66)-C(65)-H(65)	120.0
C(64)-C(65)-H(65)	120.0
C(65)-C(66)-C(61)	121.07(14)
C(65)-C(66)-H(66)	119.5
C(61)-C(66)-H(66)	119.5
C(72)-C(67)-C(68)	119.54(14)
C(72)-C(67)-S(3)	120.42(12)
C(68)-C(67)-S(3)	120.00(12)

C(69)-C(68)-C(67)	120.61(15)
C(69)-C(68)-H(68)	119.7
C(67)-C(68)-H(68)	119.7
C(68)-C(69)-C(70)	119.76(15)
C(68)-C(69)-H(69)	120.1
C(70)-C(69)-H(69)	120.1
O(9)-C(70)-C(71)	124.37(15)
O(9)-C(70)-C(69)	115.47(14)
C(71)-C(70)-C(69)	120.16(15)
C(70)-C(71)-C(72)	119.68(15)
C(70)-C(71)-H(71)	120.2
C(72)-C(71)-H(71)	120.2
C(67)-C(72)-C(71)	120.24(14)
C(67)-C(72)-H(72)	119.9
C(71)-C(72)-H(72)	119.9
C(58)-C(73)-H(73A)	109.5
C(58)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(58)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
O(8)-C(74)-H(74A)	109.5
O(8)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
O(8)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
O(9)-C(75)-H(75A)	109.5
O(9)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
O(9)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 210903lt_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	20(1)	26(1)	11(1)	-3(1)	-1(1)	7(1)
S(2)	18(1)	24(1)	11(1)	-2(1)	-2(1)	6(1)
S(3)	18(1)	24(1)	14(1)	-5(1)	-4(1)	5(1)
O(1)	22(1)	30(1)	10(1)	-6(1)	1(1)	11(1)
O(2)	24(1)	19(1)	22(1)	-4(1)	6(1)	3(1)
O(3)	18(1)	22(1)	9(1)	-1(1)	0(1)	-7(1)
O(4)	26(1)	31(1)	10(1)	-4(1)	0(1)	15(1)
O(5)	37(1)	22(1)	26(1)	-8(1)	-5(1)	9(1)
O(6)	17(1)	20(1)	8(1)	-1(1)	-1(1)	-5(1)
O(7)	26(1)	33(1)	9(1)	-5(1)	0(1)	14(1)
O(8)	20(1)	20(1)	9(1)	-1(1)	0(1)	-4(1)
O(9)	25(1)	18(1)	32(1)	-5(1)	-2(1)	2(1)
C(1)	18(1)	18(1)	9(1)	-2(1)	3(1)	-1(1)
C(2)	16(1)	16(1)	12(1)	0(1)	4(1)	-2(1)
C(3)	19(1)	18(1)	12(1)	-1(1)	3(1)	1(1)
C(4)	18(1)	15(1)	17(1)	3(1)	4(1)	0(1)
C(5)	22(1)	14(1)	18(1)	-2(1)	8(1)	2(1)
C(6)	22(1)	14(1)	13(1)	-3(1)	6(1)	-2(1)
C(7)	16(1)	13(1)	13(1)	-1(1)	4(1)	-3(1)
C(8)	15(1)	15(1)	11(1)	-2(1)	3(1)	-3(1)
C(9)	12(1)	18(1)	12(1)	0(1)	1(1)	-2(1)
C(10)	16(1)	18(1)	12(1)	-2(1)	4(1)	2(1)
C(11)	25(1)	25(1)	20(1)	0(1)	4(1)	10(1)
C(12)	13(1)	19(1)	11(1)	0(1)	-2(1)	4(1)
C(13)	15(1)	24(1)	14(1)	4(1)	0(1)	1(1)
C(14)	19(1)	15(1)	18(1)	3(1)	-1(1)	0(1)
C(15)	17(1)	19(1)	13(1)	1(1)	-2(1)	4(1)
C(16)	12(1)	23(1)	16(1)	3(1)	1(1)	-1(1)
C(17)	17(1)	18(1)	16(1)	0(1)	-2(1)	-1(1)
C(18)	16(1)	14(1)	11(1)	-1(1)	3(1)	0(1)
C(19)	19(1)	23(1)	14(1)	-2(1)	7(1)	-5(1)

C(20)	17(1)	19(1)	14(1)	-2(1)	2(1)	-6(1)
C(21)	17(1)	13(1)	9(1)	-1(1)	0(1)	1(1)
C(22)	14(1)	18(1)	12(1)	0(1)	4(1)	-2(1)
C(23)	14(1)	15(1)	14(1)	-1(1)	1(1)	-2(1)
C(24)	41(1)	16(1)	19(1)	1(1)	2(1)	5(1)
C(25)	23(1)	35(1)	13(1)	-1(1)	-1(1)	-13(1)
C(26)	19(1)	18(1)	10(1)	-1(1)	2(1)	1(1)
C(27)	18(1)	14(1)	13(1)	1(1)	4(1)	0(1)
C(28)	21(1)	19(1)	10(1)	-1(1)	2(1)	3(1)
C(29)	19(1)	16(1)	16(1)	1(1)	2(1)	1(1)
C(30)	20(1)	13(1)	16(1)	-1(1)	6(1)	3(1)
C(31)	21(1)	14(1)	11(1)	-2(1)	5(1)	-1(1)
C(32)	15(1)	13(1)	12(1)	0(1)	4(1)	-3(1)
C(33)	15(1)	15(1)	10(1)	0(1)	3(1)	-3(1)
C(34)	14(1)	16(1)	11(1)	2(1)	1(1)	-1(1)
C(35)	16(1)	16(1)	13(1)	-2(1)	4(1)	3(1)
C(36)	27(1)	27(1)	17(1)	-1(1)	2(1)	12(1)
C(37)	16(1)	16(1)	12(1)	2(1)	-1(1)	3(1)
C(38)	14(1)	24(1)	20(1)	5(1)	-1(1)	-1(1)
C(39)	24(1)	17(1)	23(1)	2(1)	-6(1)	-5(1)
C(40)	27(1)	16(1)	13(1)	1(1)	-5(1)	5(1)
C(41)	17(1)	22(1)	15(1)	2(1)	0(1)	4(1)
C(42)	16(1)	17(1)	16(1)	1(1)	-2(1)	-2(1)
C(43)	16(1)	14(1)	10(1)	-1(1)	1(1)	2(1)
C(44)	17(1)	23(1)	14(1)	-1(1)	7(1)	-3(1)
C(45)	14(1)	20(1)	15(1)	-2(1)	1(1)	-4(1)
C(46)	18(1)	11(1)	9(1)	0(1)	1(1)	1(1)
C(47)	13(1)	17(1)	14(1)	2(1)	4(1)	-1(1)
C(48)	12(1)	17(1)	14(1)	-1(1)	1(1)	-2(1)
C(49)	48(1)	27(1)	22(1)	0(1)	10(1)	14(1)
C(50)	19(1)	28(1)	15(1)	-3(1)	-3(1)	-7(1)
C(51)	20(1)	16(1)	10(1)	-1(1)	4(1)	0(1)
C(52)	16(1)	16(1)	12(1)	-1(1)	5(1)	1(1)
C(53)	13(1)	16(1)	13(1)	1(1)	1(1)	-2(1)
C(54)	16(1)	13(1)	11(1)	0(1)	3(1)	-4(1)
C(55)	16(1)	11(1)	13(1)	1(1)	4(1)	-3(1)

C(56)	19(1)	12(1)	12(1)	-2(1)	5(1)	-3(1)
C(57)	18(1)	12(1)	18(1)	-2(1)	7(1)	1(1)
C(58)	19(1)	15(1)	16(1)	3(1)	2(1)	0(1)
C(59)	22(1)	18(1)	10(1)	0(1)	1(1)	2(1)
C(60)	18(1)	13(1)	12(1)	1(1)	3(1)	0(1)
C(61)	16(1)	12(1)	11(1)	-1(1)	2(1)	1(1)
C(62)	18(1)	17(1)	14(1)	1(1)	6(1)	-3(1)
C(63)	16(1)	14(1)	15(1)	-2(1)	1(1)	-4(1)
C(64)	16(1)	13(1)	10(1)	-1(1)	1(1)	3(1)
C(65)	17(1)	19(1)	13(1)	1(1)	3(1)	-4(1)
C(66)	15(1)	17(1)	14(1)	-2(1)	2(1)	-4(1)
C(67)	15(1)	17(1)	10(1)	2(1)	-2(1)	2(1)
C(68)	14(1)	23(1)	20(1)	7(1)	2(1)	2(1)
C(69)	15(1)	18(1)	29(1)	5(1)	-1(1)	-4(1)
C(70)	19(1)	16(1)	16(1)	2(1)	-5(1)	4(1)
C(71)	14(1)	23(1)	15(1)	2(1)	0(1)	1(1)
C(72)	14(1)	19(1)	14(1)	2(1)	-1(1)	-3(1)
C(73)	20(1)	24(1)	20(1)	1(1)	2(1)	7(1)
C(74)	23(1)	26(1)	14(1)	-2(1)	-3(1)	-9(1)
C(75)	34(1)	26(1)	18(1)	-2(1)	3(1)	9(1)

Table S17. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 210903lt_0m_a.

	x	y	z	U(eq)
H(1)	1316	2001	2707	31
H(4)	8100	2058	2727	33
H(7)	5294	7814	7334	35
H(3)	-64	3327	2871	20
H(5)	-577	4727	4309	21
H(6)	430	4144	4928	19
H(10)	2015	1678	3630	18
H(11A)	-943	5003	2927	35
H(11B)	-1468	4645	3397	35
H(11C)	-1315	4040	2834	35
H(13)	2189	-83	4587	21
H(14)	2728	-1147	4017	21
H(16)	4219	692	3622	21
H(17)	3701	1733	4212	21
H(19)	2520	3769	5321	22
H(20)	2785	4076	6360	20
H(22)	878	2830	6628	17
H(23)	614	2547	5588	17
H(24A)	3720	-2057	3797	38
H(24B)	3943	-2126	3125	38
H(24C)	3122	-1821	3216	38
H(25A)	3079	3720	7399	36
H(25B)	2643	4142	7910	36
H(25C)	2652	4646	7275	36
H(28)	6742	3423	2844	20
H(30)	6152	4842	4243	19
H(31)	7131	4266	4896	18
H(35)	8781	1776	3660	18
H(36A)	5767	5186	2996	36
H(36B)	5229	4474	3246	36

H(36C)	5627	4244	2665	36
H(38)	8542	155	4465	24
H(39)	8924	-997	3888	27
H(41)	10918	210	3888	22
H(42)	10508	1398	4434	20
H(44)	9309	3703	5349	21
H(45)	9587	3995	6388	20
H(47)	7514	3185	6613	17
H(48)	7253	2877	5578	17
H(49A)	11042	-796	3203	48
H(49B)	10950	-1853	3179	48
H(49C)	11208	-1367	3817	48
H(50A)	9799	3709	7439	32
H(50B)	9378	4203	7932	32
H(50C)	9451	4676	7295	32
H(52)	4529	7957	6419	17
H(56)	6373	5786	5133	17
H(57)	7429	5343	5759	18
H(59)	6754	6621	7187	20
H(62)	4271	5819	4715	19
H(63)	3992	5625	3663	18
H(65)	5711	7247	3427	20
H(66)	5992	7418	4477	19
H(68)	4805	9504	5366	23
H(69)	4583	10822	5855	25
H(71)	2617	9840	6226	21
H(72)	2864	8497	5762	19
H(73A)	8061	6125	7244	32
H(73B)	8302	5570	6688	32
H(73C)	7815	5108	7148	32
H(74A)	4109	5275	2685	33
H(74B)	4029	5905	2097	33
H(74C)	3595	6142	2657	33
H(75A)	2401	11414	6212	39
H(75B)	2812	12015	6753	39
H(75C)	2706	10974	6857	39

d) X-ray structure of 11a:

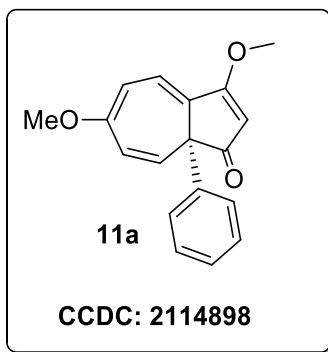
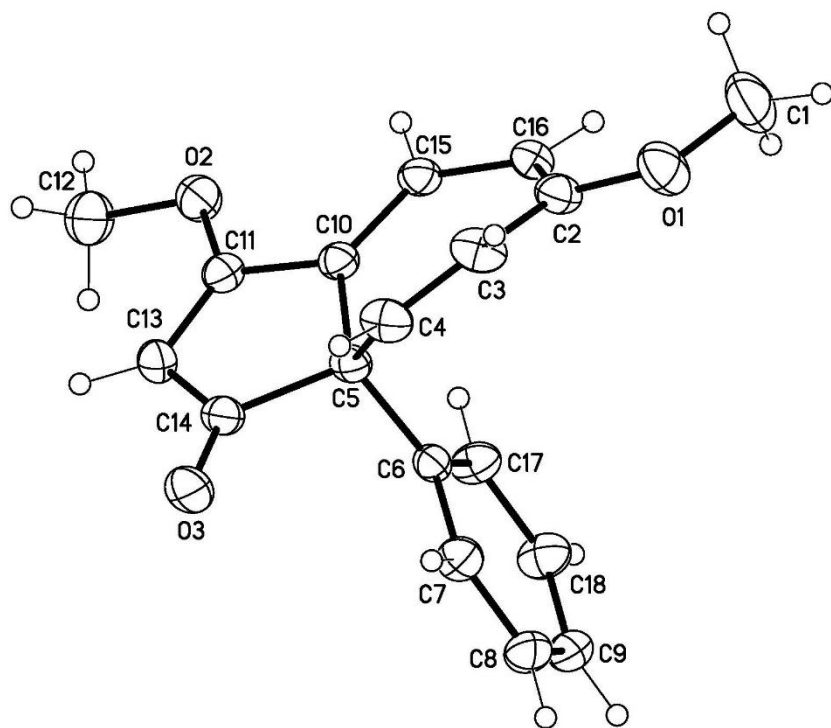


Table S18. Crystal data and structure refinement for 210919_0m.

Identification code	210919_0m
Empirical formula	C ₁₈ H ₁₆ O ₃
Formula weight	280.31
Temperature	296(2) K
Wavelength	0.71073 Å

Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5967(8) Å	$\alpha = 82.083(5)^\circ$.
	b = 8.8188(8) Å	$\beta = 74.736(5)^\circ$.
	c = 11.0107(11) Å	$\gamma = 63.889(4)^\circ$.
Volume	722.89(12) Å ³	
Z	2	
Density (calculated)	1.288 Mg/m ³	
Absorption coefficient	0.087 mm ⁻¹	
F(000)	296	
Crystal size	0.20 x 0.15 x 0.15 mm ³	
Theta range for data collection	1.918 to 26.442°.	
Index ranges	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -13 ≤ l ≤ 13	
Reflections collected	11911	
Independent reflections	2949 [R(int) = 0.0261]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6927	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2949 / 0 / 192	
Goodness-of-fit on F ²	1.060	
Final R indices [I > 2σ(I)]	R1 = 0.0401, wR2 = 0.0969	
R indices (all data)	R1 = 0.0510, wR2 = 0.1046	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.179 and -0.169 e.Å ⁻³	

Table S19. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 210919_0m. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2726(2)	10702(1)	5167(1)	62(1)
O(2)	2224(1)	9538(1)	-429(1)	51(1)
O(3)	3483(1)	4555(1)	2122(1)	56(1)
C(1)	2987(3)	12209(2)	5061(2)	78(1)
C(2)	2671(2)	10109(2)	4103(1)	44(1)
C(3)	2217(2)	8682(2)	4436(1)	50(1)
C(4)	2552(2)	7443(2)	3705(1)	46(1)
C(5)	3615(2)	7207(2)	2365(1)	36(1)
C(6)	5625(2)	6488(2)	2280(1)	33(1)
C(7)	6431(2)	5099(2)	3020(1)	44(1)
C(8)	8254(2)	4387(2)	2902(2)	49(1)
C(9)	9295(2)	5051(2)	2056(2)	49(1)
C(10)	2926(2)	8807(2)	1584(1)	35(1)
C(11)	2657(2)	8345(2)	462(1)	40(1)
C(12)	2133(2)	9025(2)	-1584(2)	65(1)
C(13)	2904(2)	6713(2)	507(1)	45(1)
C(14)	3340(2)	5946(2)	1682(1)	41(1)
C(15)	2666(2)	10353(2)	1842(1)	38(1)
C(16)	2852(2)	10865(2)	2957(1)	42(1)
C(17)	6688(2)	7144(2)	1436(1)	44(1)
C(18)	8507(2)	6433(2)	1327(2)	51(1)

Table S20. Bond lengths [Å] and angles [°] for 210919_0m.

O(1)-C(2)	1.3666(17)
O(1)-C(1)	1.427(2)
O(2)-C(11)	1.3310(16)
O(2)-C(12)	1.4392(18)
O(3)-C(14)	1.2202(16)
C(1)-H(1)	0.9800
C(1)-H(16)	0.9800
C(1)-H(3)	0.9800
C(2)-C(16)	1.3487(19)
C(2)-C(3)	1.449(2)
C(3)-C(4)	1.330(2)
C(3)-H(4)	0.9500
C(4)-C(5)	1.5040(19)
C(4)-H(5)	0.9500
C(5)-C(10)	1.5101(17)
C(5)-C(6)	1.5369(17)
C(5)-C(14)	1.5542(19)
C(6)-C(17)	1.3802(18)
C(6)-C(7)	1.3855(18)
C(7)-C(8)	1.385(2)
C(7)-H(12)	0.9500
C(8)-C(9)	1.373(2)
C(8)-H(13)	0.9500
C(9)-C(18)	1.371(2)
C(9)-H(2)	0.9500
C(10)-C(15)	1.3402(18)
C(10)-C(11)	1.4543(19)
C(11)-C(13)	1.3552(19)

C(12)-H(7)	0.9800
C(12)-H(8)	0.9800
C(12)-H(6)	0.9800
C(13)-C(14)	1.436(2)
C(13)-H(9)	0.9500
C(15)-C(16)	1.4340(19)
C(15)-H(10)	0.9500
C(16)-H(11)	0.9500
C(17)-C(18)	1.3823(19)
C(17)-H(15)	0.9500
C(18)-H(14)	0.9500
C(2)-O(1)-C(1)	118.22(13)
C(11)-O(2)-C(12)	116.73(12)
O(1)-C(1)-H(1)	109.5
O(1)-C(1)-H(16)	109.5
H(1)-C(1)-H(16)	109.5
O(1)-C(1)-H(3)	109.5
H(1)-C(1)-H(3)	109.5
H(16)-C(1)-H(3)	109.5
C(16)-C(2)-O(1)	123.74(13)
C(16)-C(2)-C(3)	126.64(14)
O(1)-C(2)-C(3)	109.34(12)
C(4)-C(3)-C(2)	128.14(13)
C(4)-C(3)-H(4)	115.9
C(2)-C(3)-H(4)	115.9
C(3)-C(4)-C(5)	125.18(13)
C(3)-C(4)-H(5)	117.4
C(5)-C(4)-H(5)	117.4
C(4)-C(5)-C(10)	111.08(11)

C(4)-C(5)-C(6)	112.23(11)
C(10)-C(5)-C(6)	113.34(10)
C(4)-C(5)-C(14)	111.52(11)
C(10)-C(5)-C(14)	101.85(10)
C(6)-C(5)-C(14)	106.26(10)
C(17)-C(6)-C(7)	118.12(12)
C(17)-C(6)-C(5)	121.63(11)
C(7)-C(6)-C(5)	120.19(11)
C(8)-C(7)-C(6)	120.62(13)
C(8)-C(7)-H(12)	119.7
C(6)-C(7)-H(12)	119.7
C(9)-C(8)-C(7)	120.61(13)
C(9)-C(8)-H(13)	119.7
C(7)-C(8)-H(13)	119.7
C(18)-C(9)-C(8)	119.14(13)
C(18)-C(9)-H(2)	120.4
C(8)-C(9)-H(2)	120.4
C(15)-C(10)-C(11)	126.02(12)
C(15)-C(10)-C(5)	126.99(12)
C(11)-C(10)-C(5)	106.96(11)
O(2)-C(11)-C(13)	130.24(13)
O(2)-C(11)-C(10)	117.24(12)
C(13)-C(11)-C(10)	112.52(12)
O(2)-C(12)-H(7)	109.5
O(2)-C(12)-H(8)	109.5
H(7)-C(12)-H(8)	109.5
O(2)-C(12)-H(6)	109.5
H(7)-C(12)-H(6)	109.5
H(8)-C(12)-H(6)	109.5
C(11)-C(13)-C(14)	108.97(13)

C(11)-C(13)-H(9)	125.5
C(14)-C(13)-H(9)	125.5
O(3)-C(14)-C(13)	128.47(13)
O(3)-C(14)-C(5)	123.11(13)
C(13)-C(14)-C(5)	108.42(11)
C(10)-C(15)-C(16)	127.45(12)
C(10)-C(15)-H(10)	116.3
C(16)-C(15)-H(10)	116.3
C(2)-C(16)-C(15)	125.19(13)
C(2)-C(16)-H(11)	117.4
C(15)-C(16)-H(11)	117.4
C(6)-C(17)-C(18)	120.99(13)
C(6)-C(17)-H(15)	119.5
C(18)-C(17)-H(15)	119.5
C(9)-C(18)-C(17)	120.52(13)
C(9)-C(18)-H(14)	119.7
C(17)-C(18)-H(14)	119.7

Symmetry transformations used to generate equivalent atoms:

Table S21. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 210919_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	82(1)	54(1)	47(1)	-9(1)	-15(1)	-26(1)
O(2)	62(1)	44(1)	49(1)	1(1)	-24(1)	-18(1)
O(3)	56(1)	36(1)	84(1)	4(1)	-20(1)	-27(1)
C(1)	112(2)	61(1)	72(1)	-15(1)	-33(1)	-38(1)
C(2)	44(1)	37(1)	45(1)	-6(1)	-7(1)	-10(1)
C(3)	50(1)	42(1)	45(1)	-1(1)	4(1)	-17(1)
C(4)	43(1)	38(1)	52(1)	4(1)	1(1)	-20(1)
C(5)	33(1)	29(1)	44(1)	1(1)	-6(1)	-15(1)
C(6)	34(1)	29(1)	36(1)	-3(1)	-7(1)	-14(1)
C(7)	47(1)	38(1)	47(1)	10(1)	-13(1)	-21(1)
C(8)	50(1)	37(1)	61(1)	9(1)	-25(1)	-14(1)
C(9)	35(1)	43(1)	66(1)	-3(1)	-16(1)	-12(1)
C(10)	30(1)	32(1)	43(1)	1(1)	-8(1)	-13(1)
C(11)	33(1)	38(1)	48(1)	-2(1)	-10(1)	-12(1)
C(12)	73(1)	68(1)	52(1)	-8(1)	-27(1)	-21(1)
C(13)	39(1)	41(1)	58(1)	-10(1)	-12(1)	-18(1)
C(14)	31(1)	33(1)	61(1)	-4(1)	-6(1)	-15(1)
C(15)	38(1)	29(1)	46(1)	4(1)	-13(1)	-12(1)
C(16)	44(1)	30(1)	51(1)	-1(1)	-14(1)	-14(1)
C(17)	38(1)	40(1)	49(1)	10(1)	-9(1)	-16(1)
C(18)	37(1)	50(1)	62(1)	7(1)	-5(1)	-20(1)

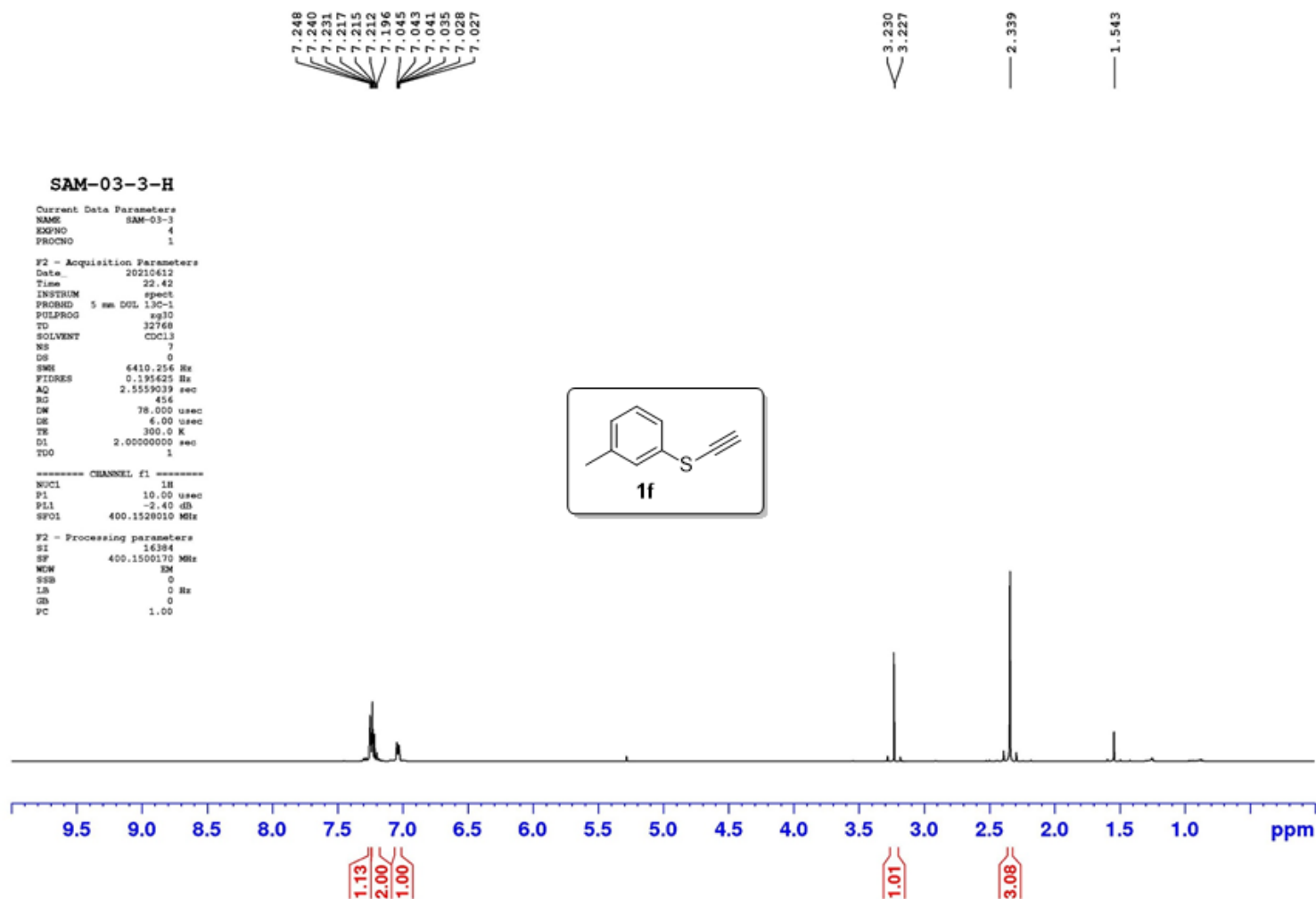
Table S22. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$)

for 210919_0m.

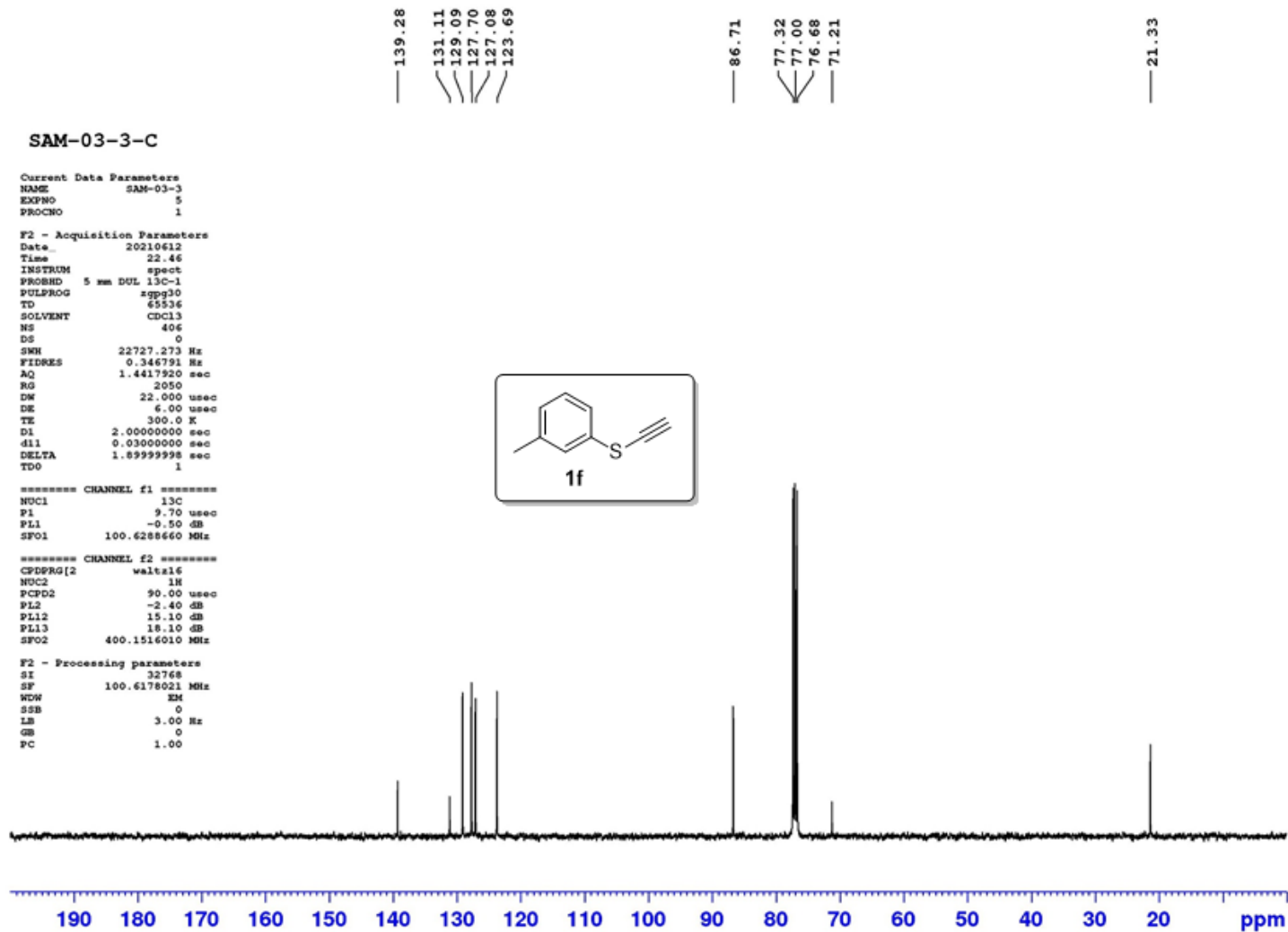
	x	y	z	U(eq)
H(1)	4101	12053	4448	116
H(16)	3048	12459	5883	116
H(3)	1992	13150	4780	116
H(4)	1602	8625	5283	60
H(5)	2083	6644	4056	55
H(12)	5726	4632	3615	52
H(13)	8790	3429	3411	59
H(2)	10546	4559	1976	58
H(7)	3273	8101	-1940	97
H(8)	1879	9984	-2185	97
H(6)	1185	8640	-1415	97
H(9)	2806	6164	-135	54
H(10)	2319	11209	1214	46
H(11)	3124	11813	2882	50
H(15)	6162	8100	922	53
H(14)	9216	6905	742	62

11. ^1H and ^{13}C spectra of key compounds:

Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz



Solvent: CDCl_3
SFO1: 400 MHz

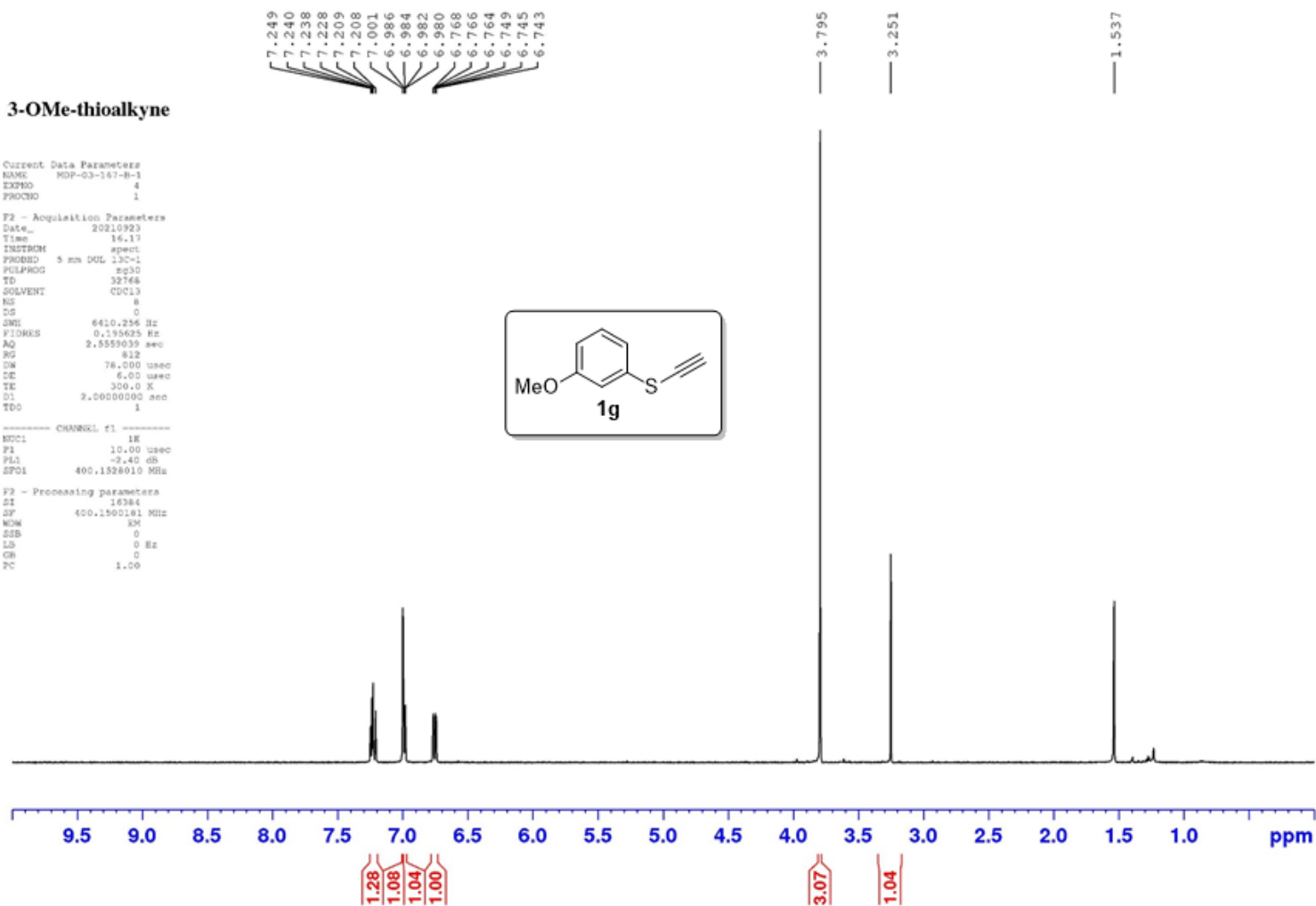
3-OMe-thioalkyne

Current Data Parameters
NAME: MDP-03-167-B-1
EXPNO: 4
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20210923
Time: 16.17
INSTRUM: spect
PROBHD: 5 mm DUL 13C-1
PULPROG: zgpg
TD: 32768
SOLVENT: CDCl_3
RG: 812
SWH: 6410.256 Hz
FIDRES: 0.195625 Hz
AQ: 2.5559039 sec
RG: 812
DM: 78.000 used
DE: 6.00 used
TE: 300.0 K
D1: 2.00000000 sec
TD0: 1

CHANNEL f1
NUC1: ^{13}C
P1: 10.00 used
PL1: -2.40 dB
SFO1: 400.1528010 MHz

F2 - Processing parameters
SI: 16384
SF: 400.1500181 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0
PC: 1.00



Solvent: CDCl_3
SFO1: 100 MHz

3-OMe Thioalkyne

```

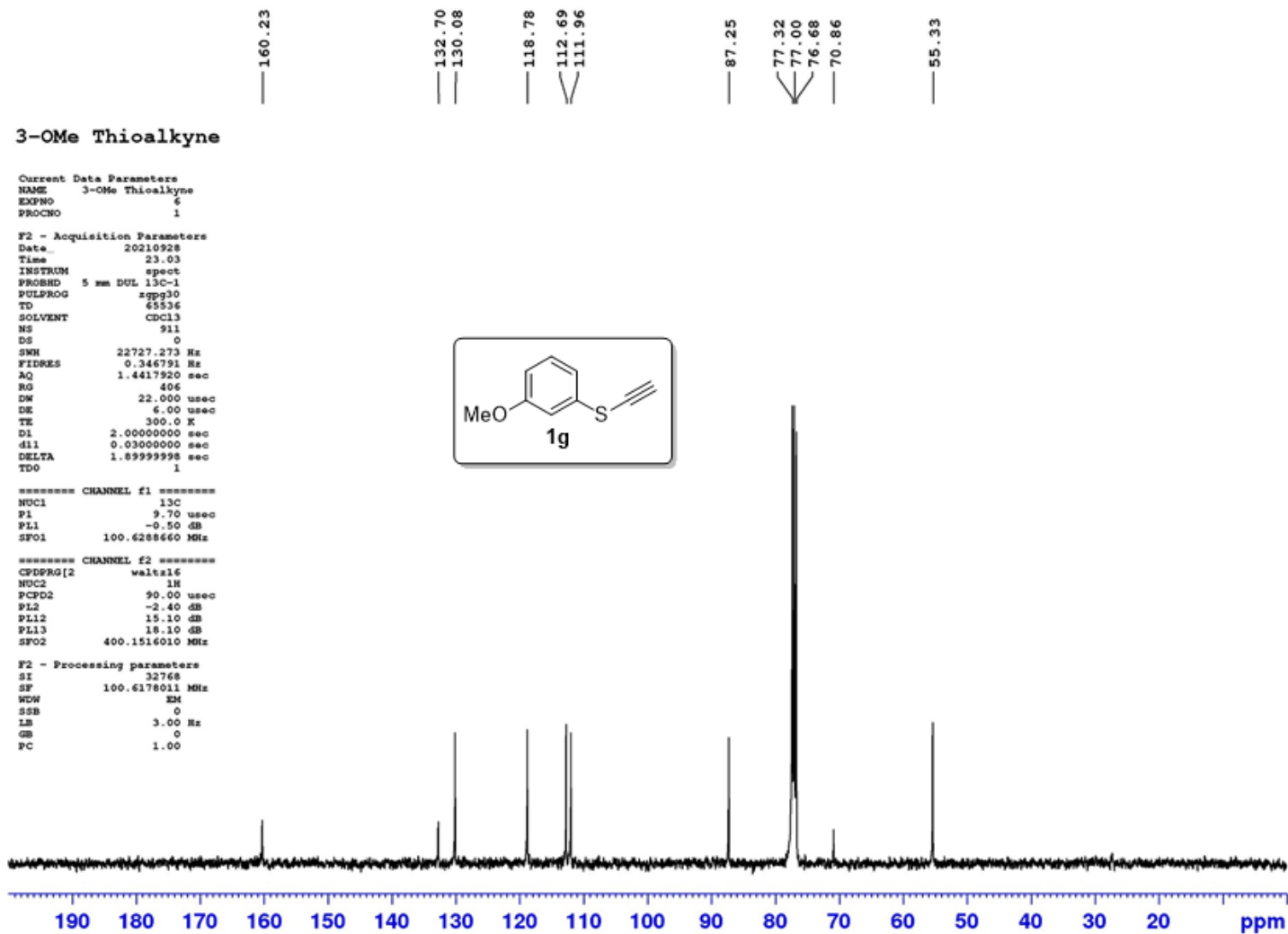
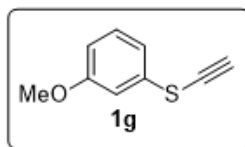
Current Data Parameters
NAME      3-OMe Thioalkyne
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
Date_     20210928
Time      23.03
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        911
DS        0
SWH       22727.273 Hz
FIDRES    0.346791 Hz
AQ        1.4417920 sec
RG        406
DW        22.000 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA     1.89999998 sec
TD0       1

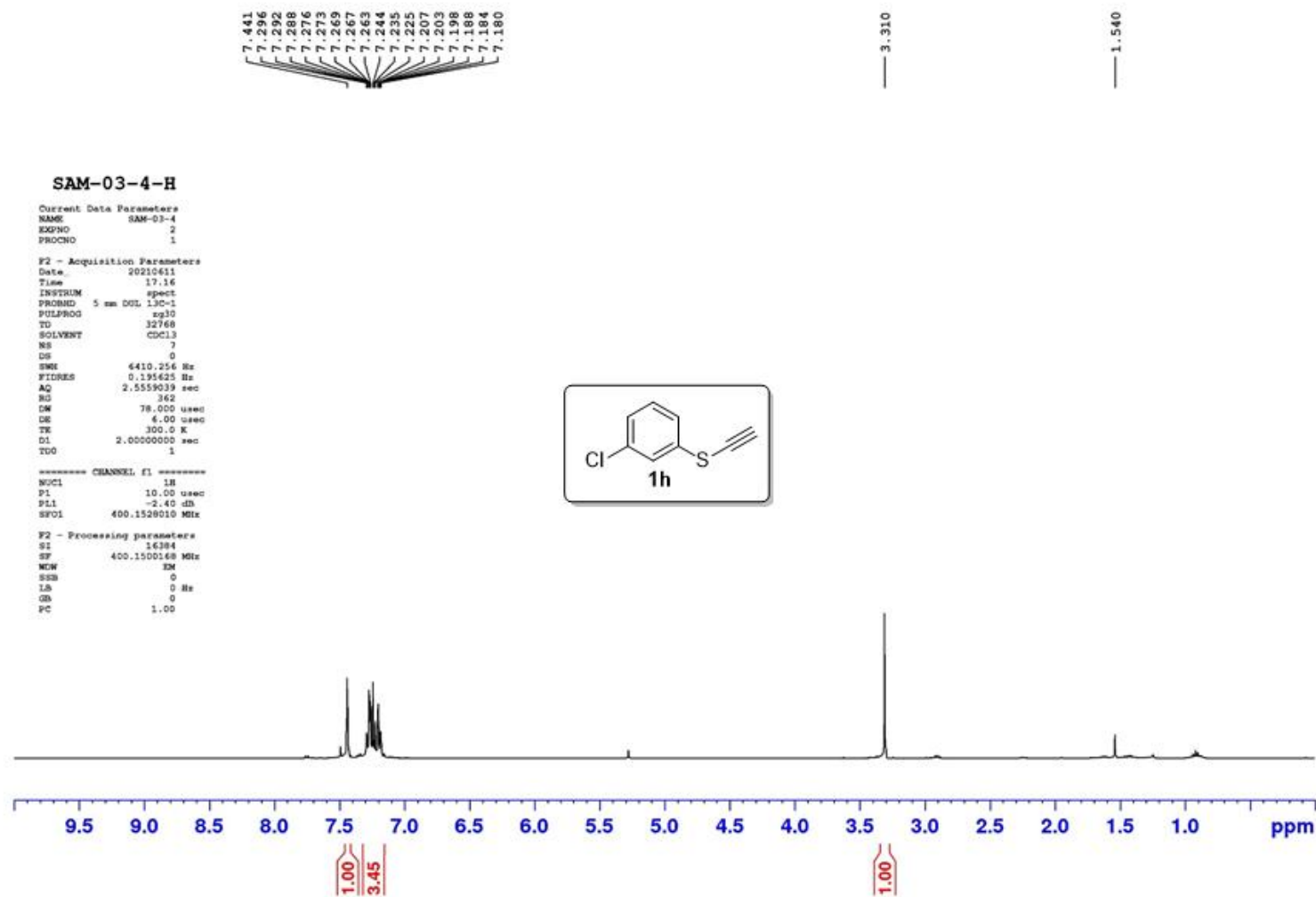
===== CHANNEL f1 =====
NUC1      13C
P1        9.70 usec
PL1       -0.50 dB
SFO1      100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.40 dB
PL12      15.10 dB
PL13      18.10 dB
SFO2      400.1516010 MHz

F2 - Processing parameters
SI        32768
SF        100.6178011 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.00
  
```



Solvent: CDCl₃
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-4-C

```

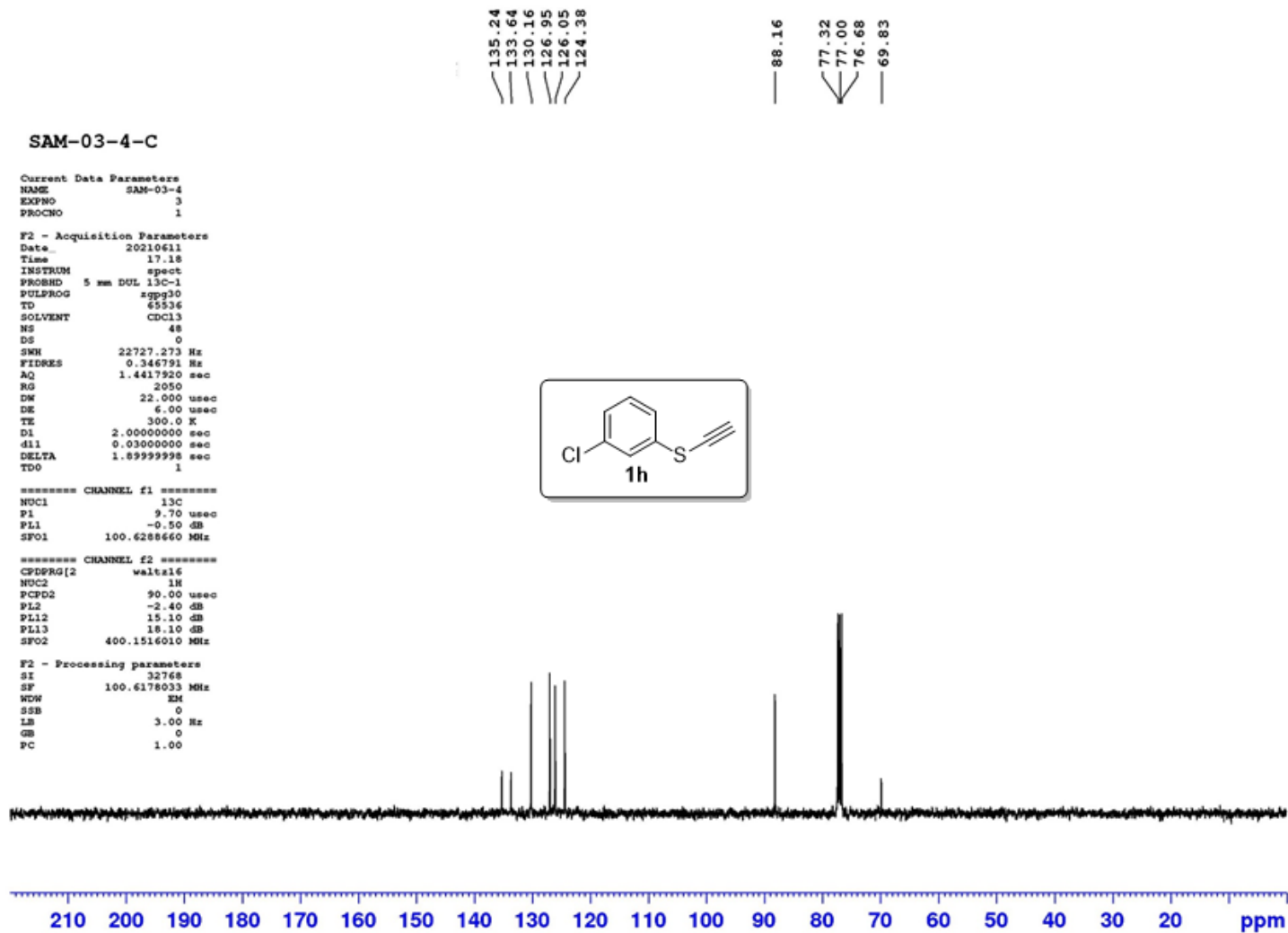
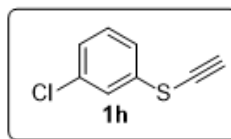
Current Data Parameters
NAME          SAM-03-4
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20210611
Time          17.18
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            48
DS            0
SWH           22727.273 Hz
FIDRES        0.346791 Hz
AQ            1.4417920 sec
RG            2050
DM            22.000 usec
DE            6.00 usec
TE            300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

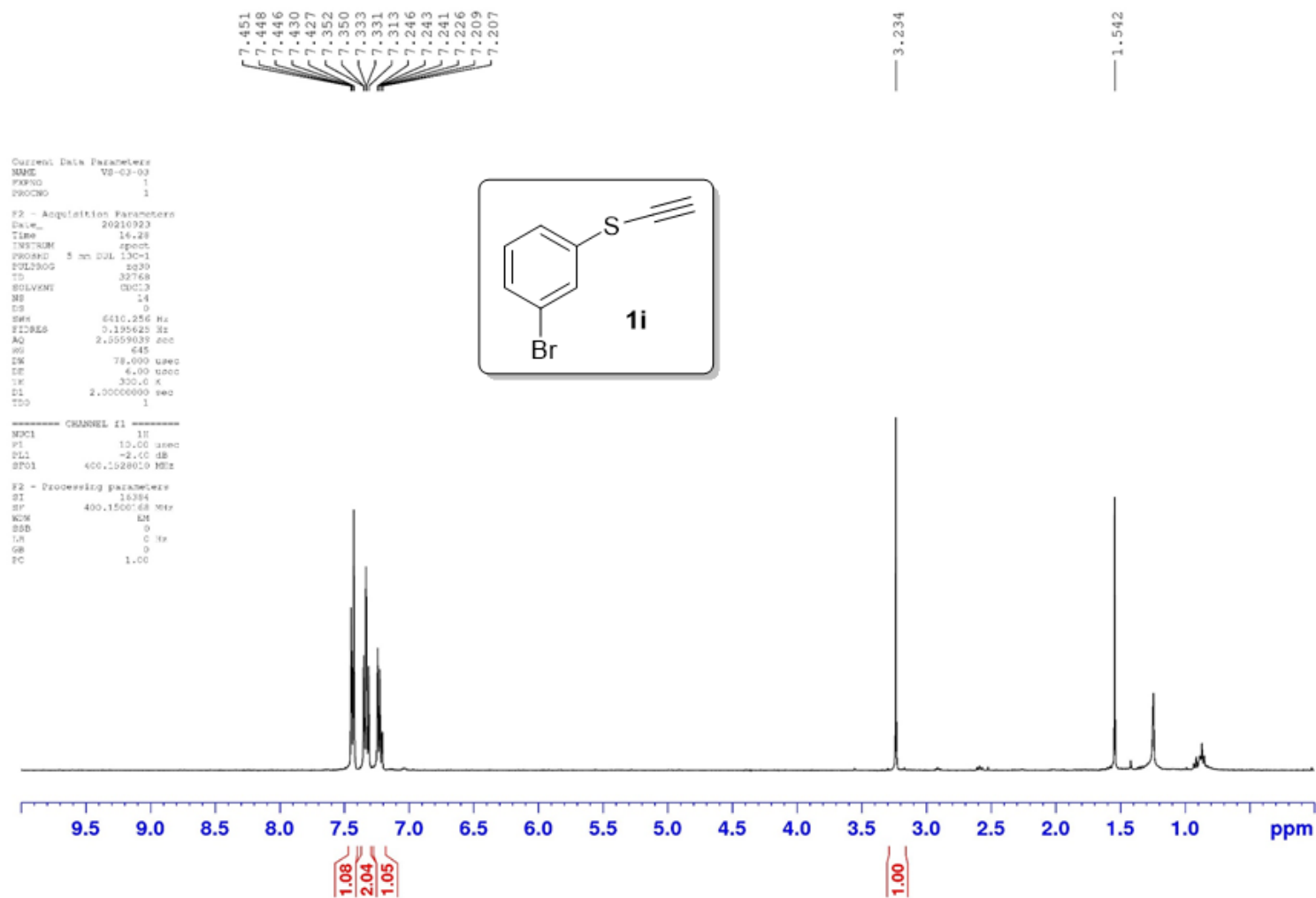
===== CHANNEL f1 =====
NUC1          13C
P1            9.70 usec
PL1           -0.50 dB
SFO1          100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         90.00 usec
PL2           -2.40 dB
PL12          15.10 dB
PL13          18.10 dB
SFO2          400.1516010 MHz

F2 - Processing parameters
SI            32768
SF            100.6178033 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.00
  
```



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 125 MHz

VS-03-03

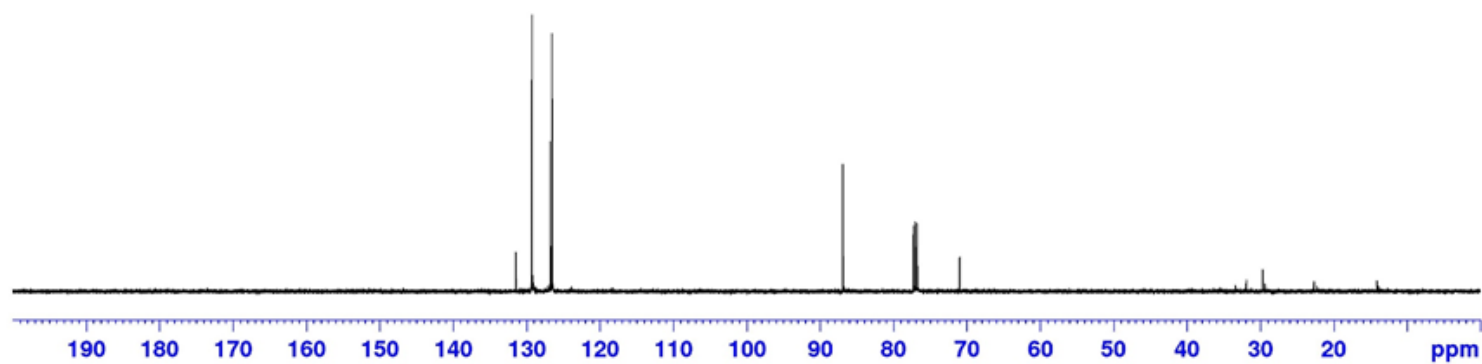
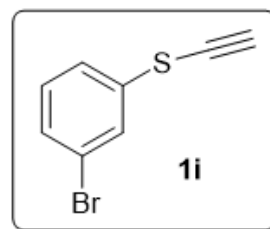
Current Data Parameters
NAME VS-03-03-12C-1
EXPNO 1
PROCNO 1

F2 - Processing parameter
SI 65536
SF 125.669751
SCW 28
SRR 1
LB 0.30
GB 0
PC 1.00

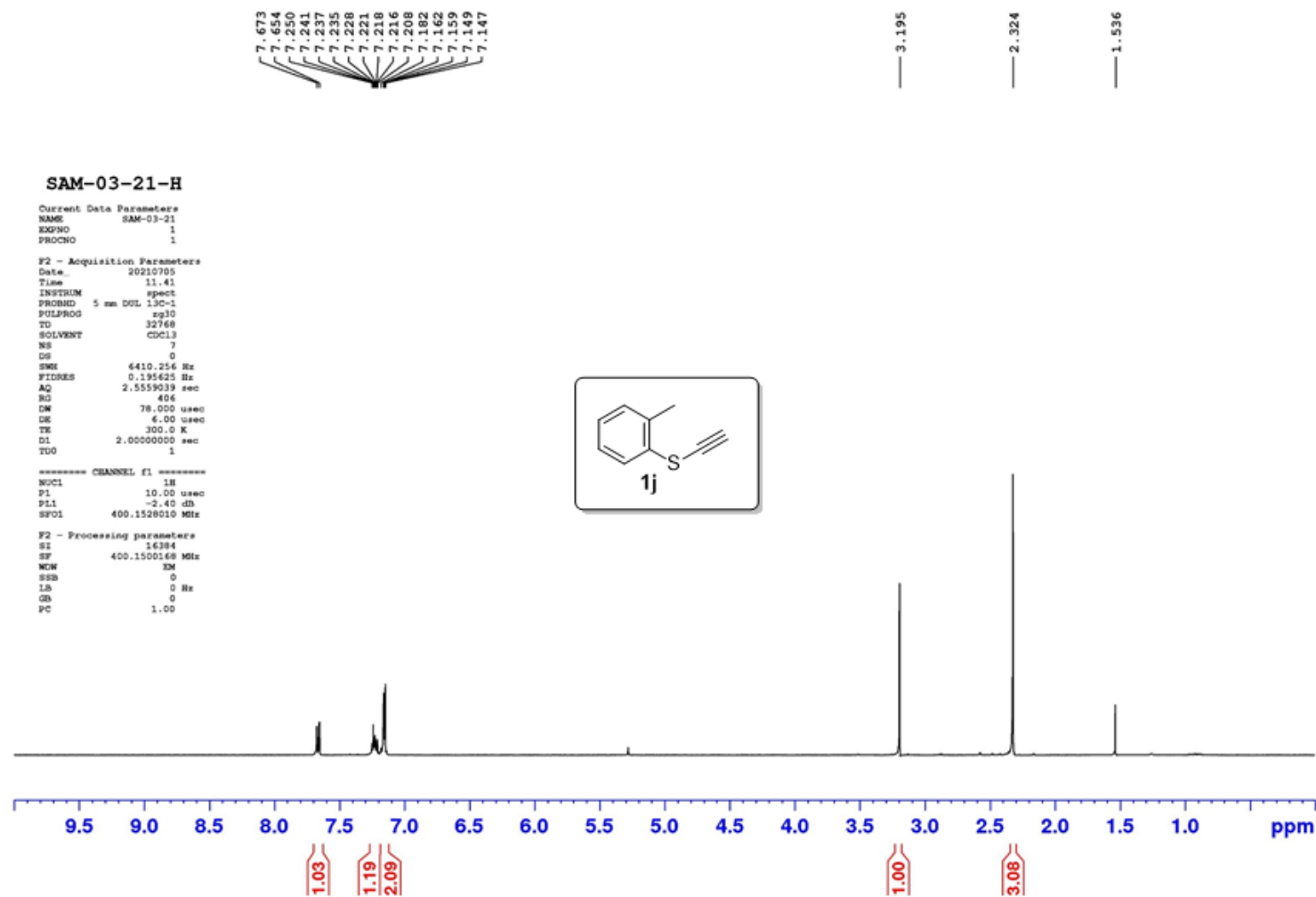
131.422
129.237
126.754
126.513

86.889

77.254
77.000
76.746
70.961



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-21-C

```

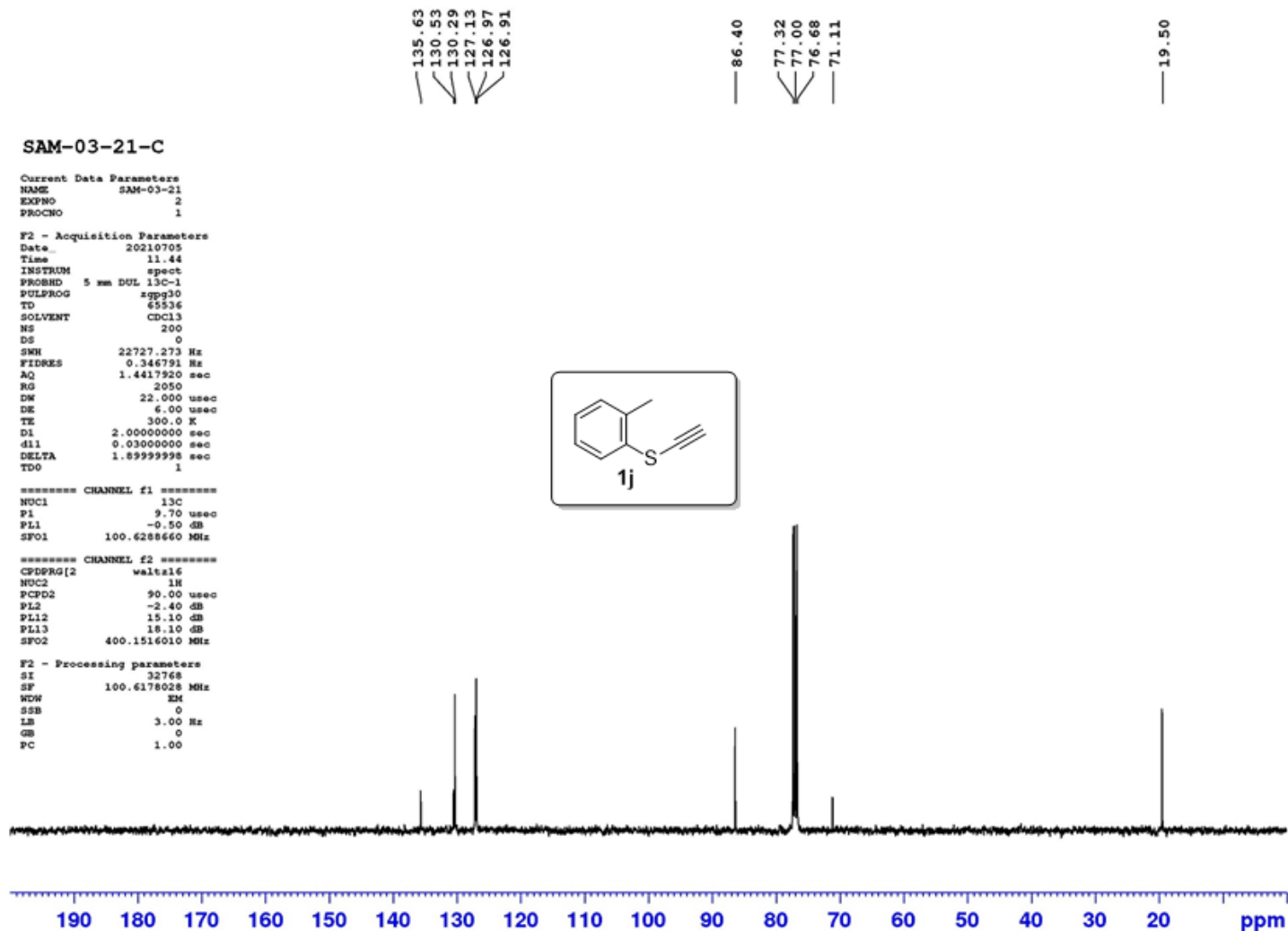
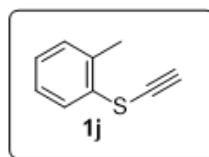
Current Data Parameters
NAME      SAM-03-21
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20210705
Time      11.44
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         200
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4417920 sec
RG         2050
DM         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

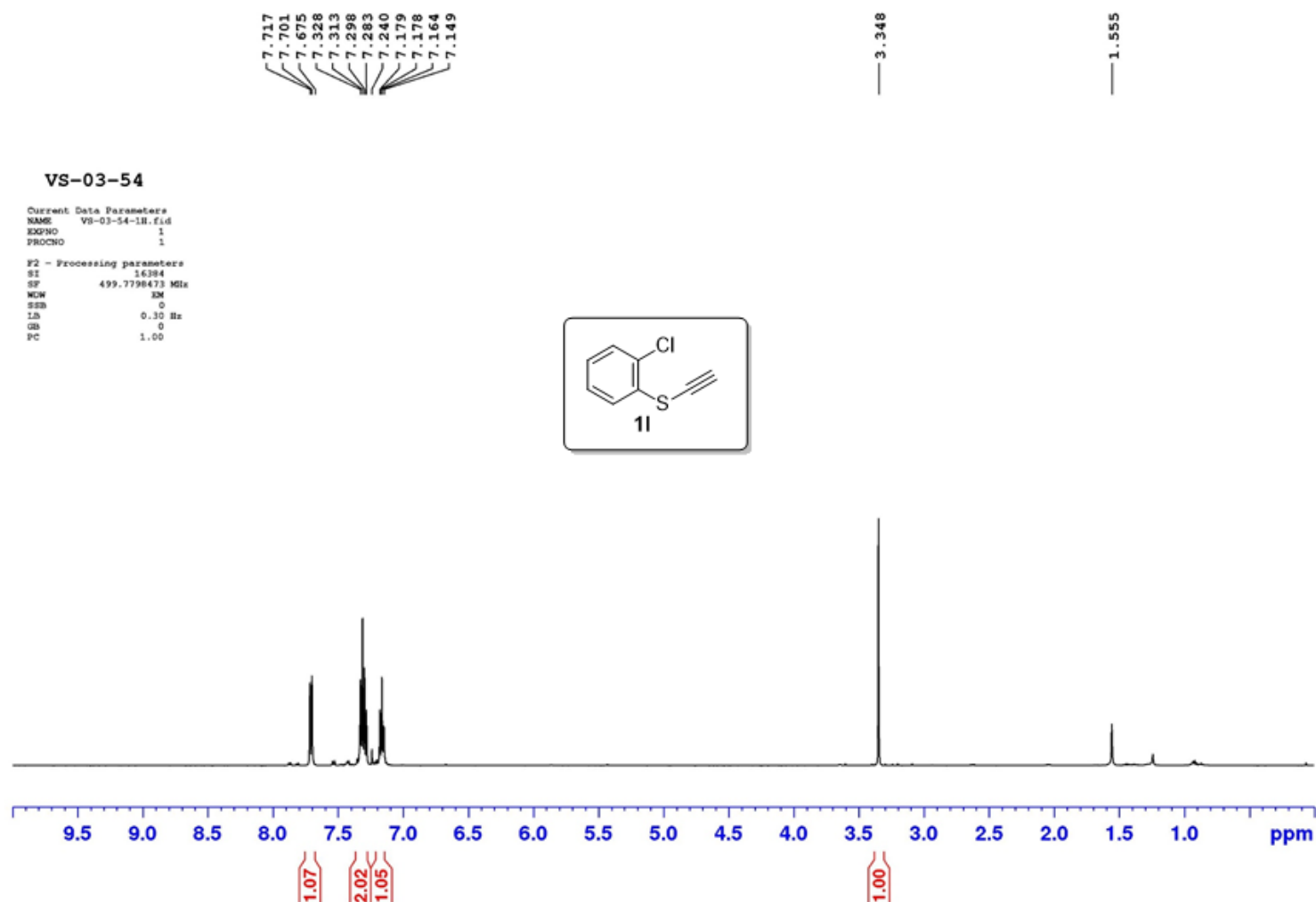
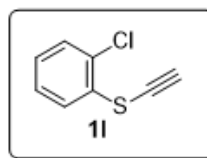
F2 - Processing parameters
SI         32768
SF         100.6178028 MHz
WDW        EM
SSB         0
LB         3.00 Hz
GB         0
PC         1.00
  
```



Solvent: CDCl_3
SFO1: 500 MHz

VS-03-54

Current Data Parameters
NAME VS-03-54-1B.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 16384
SF 499.7798473 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 100 MHz

2-Cl-thioalkyne

Current Data Parameters
NAME 2-Cl-S-alkyne
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210802
Time 21.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 89
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4417920 sec
RG 57
DM 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{13}C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz

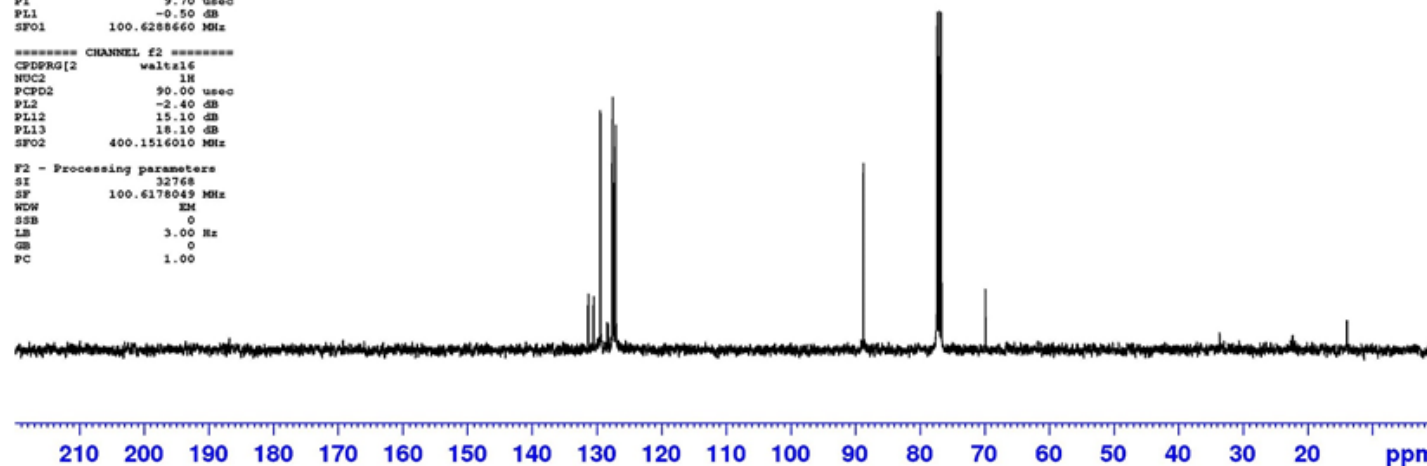
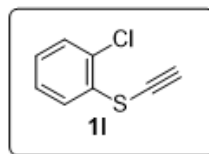
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178049 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

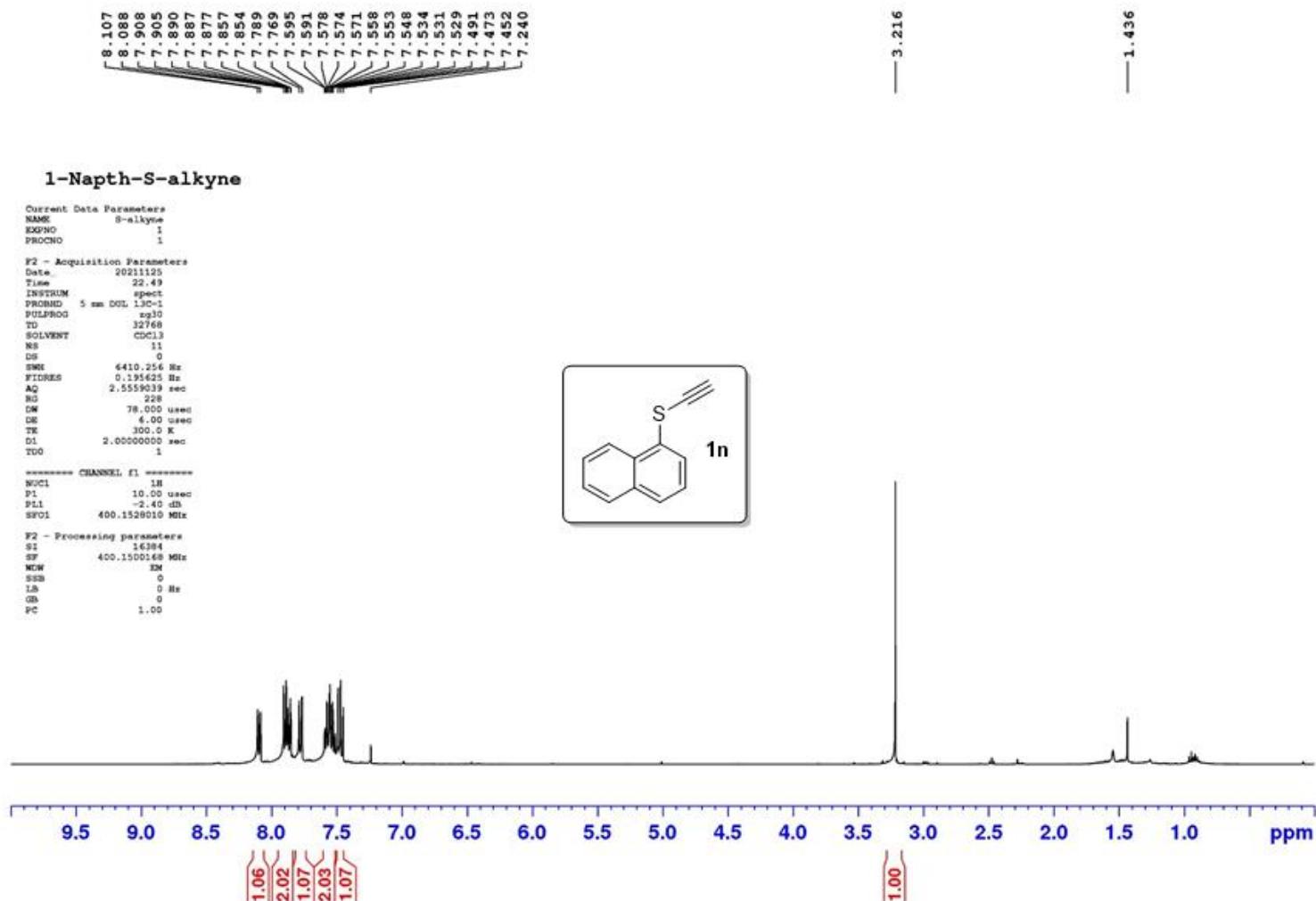
131.29
130.46
129.43
127.58
127.47
127.06

88.76

77.32
77.00
76.68
69.84



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

1-Naphth-S-alkyne

```

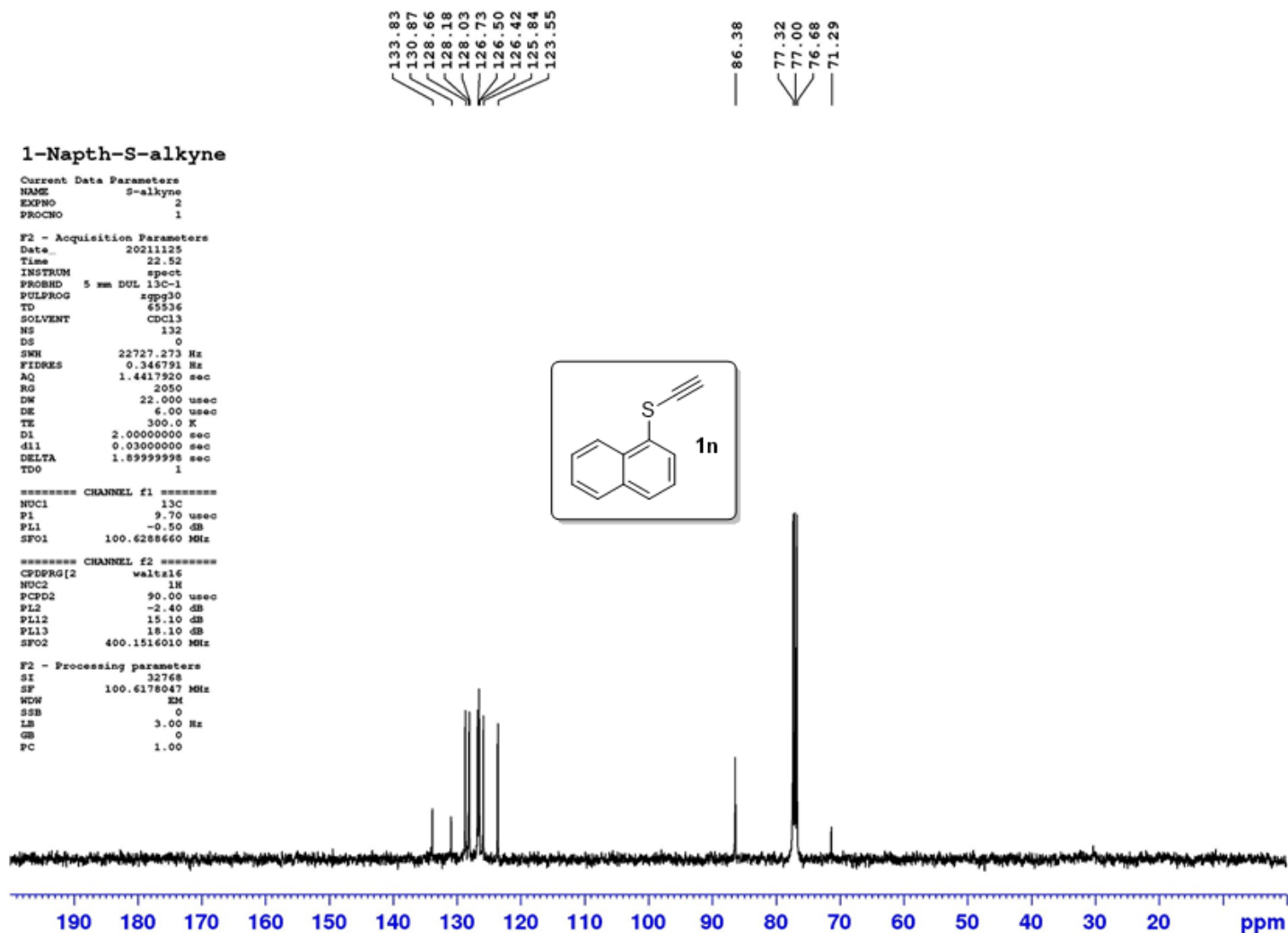
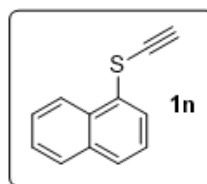
Current Data Parameters
NAME      S-alkyne
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20211125
Time      22.52
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        132
DS        0
SWH       22727.273 Hz
FIDRES    0.346791 Hz
AQ        1.4417920 sec
RG        2050
DM        22.000 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA     1.89999998 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.70 usec
PL1       -0.50 dB
SFO1      100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.40 dB
PL12      15.10 dB
PL13      18.10 dB
SFO2      400.1516010 MHz

F2 - Processing parameters
SI        32768
SF        100.6178047 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.00
  
```



Solvent: CDCl_3
SFO1: 400 MHz

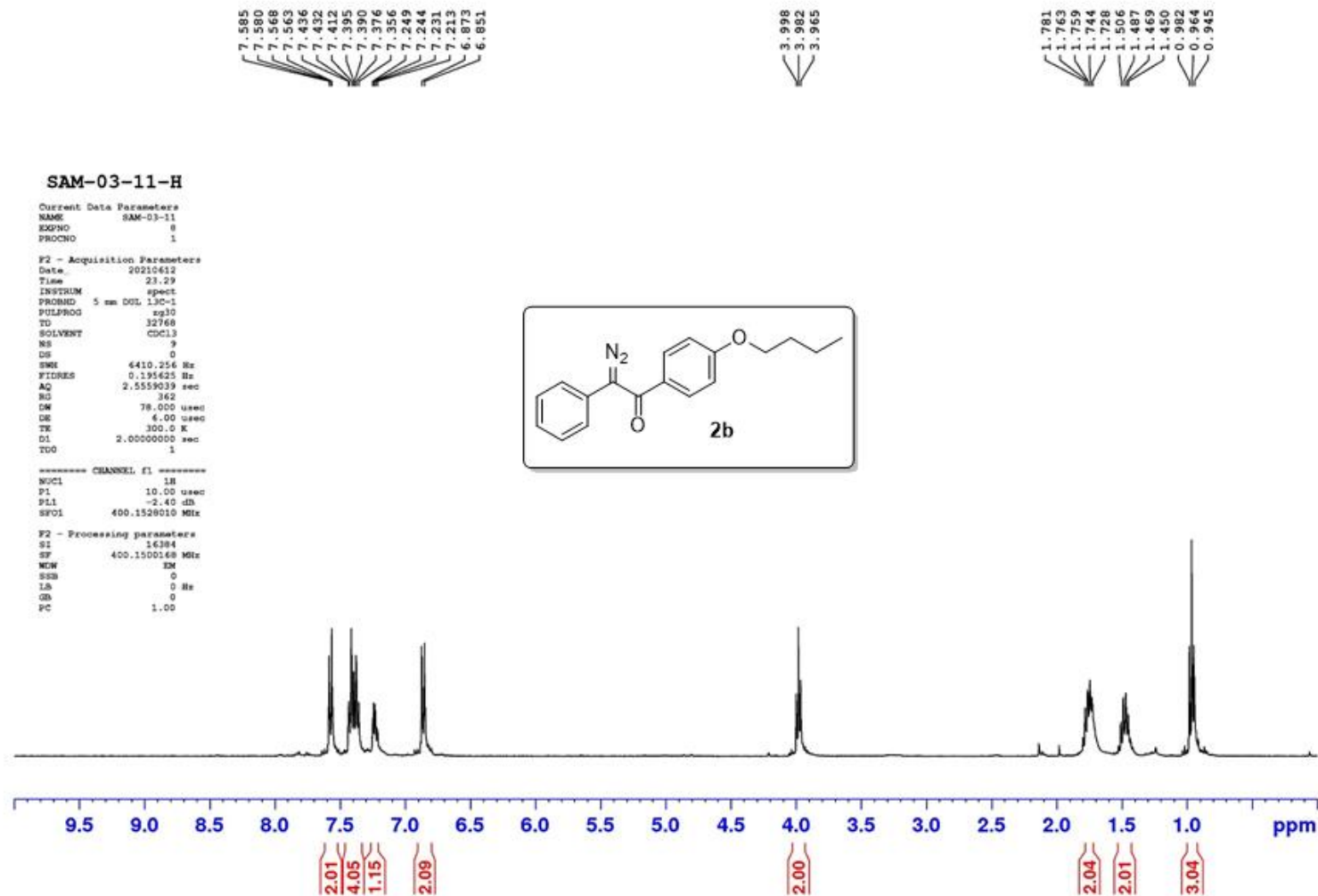
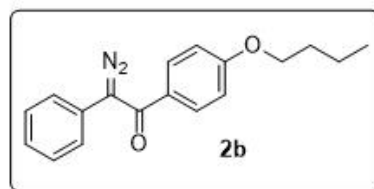
SAM-03-11-H

Current Data Parameters
NAME SAM-03-11
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210612
Time 23.29
INSTRUM spect
PROBHD 5 mm DOL 130-1
PULPROG zg30
TD 32768
SOLVENT CDCl_3
NS 9
DS 0
SWH 6410.256 Hz
FIDRES 0.195425 Hz
AQ 2.5559039 sec
RG 362
DM 78.000 used
DE 6.00 used
TE 300.2 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 ^{13}C
P1 10.00 used
PL1 -2.40 dB
SFO1 400.1526010 MHz

F2 - Processing parameters
SI 32768
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-11-C

```

Current Data Parameters
NAME      SAM-03-11
EXPNO     9
PROCNO    1

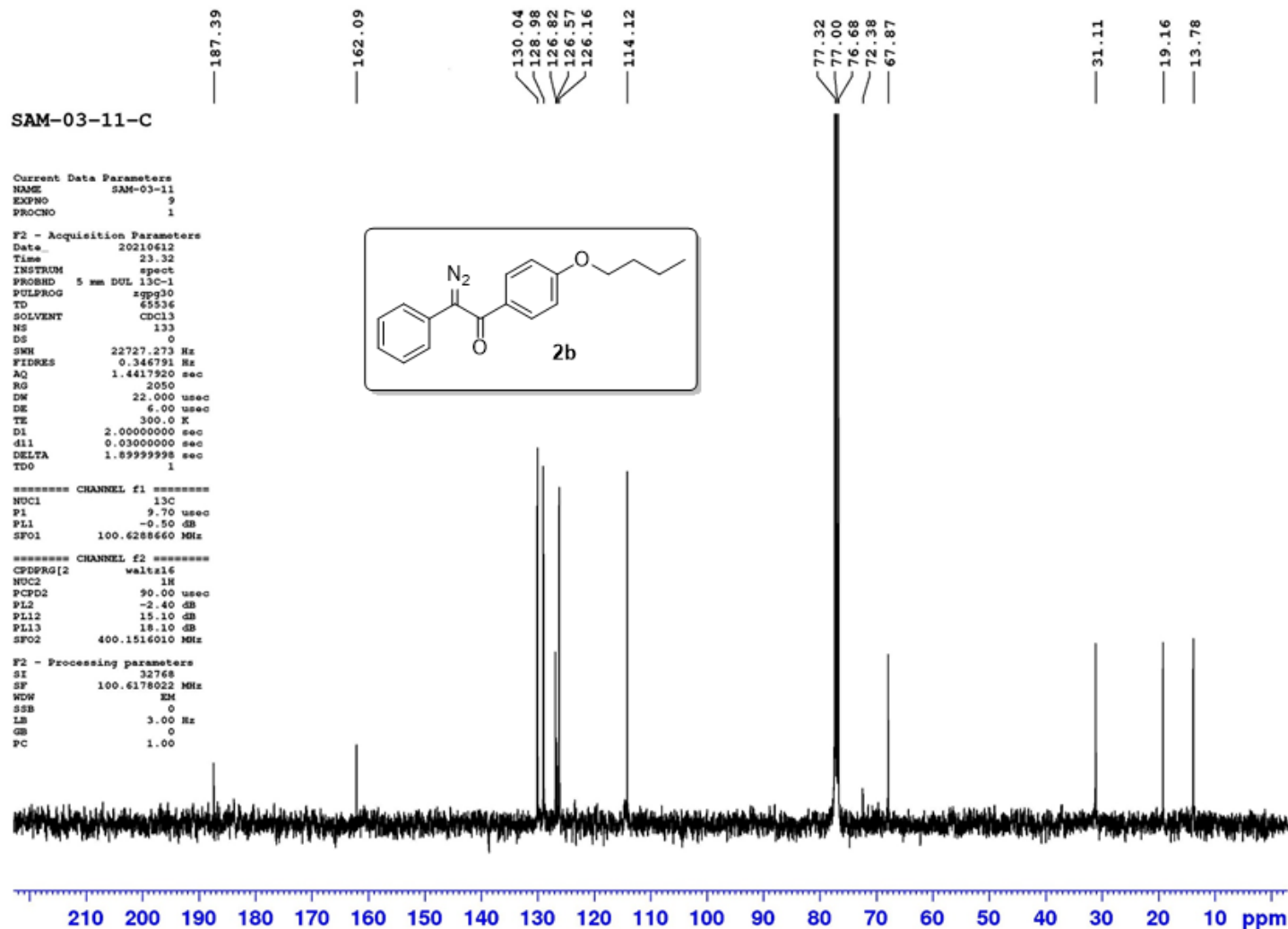
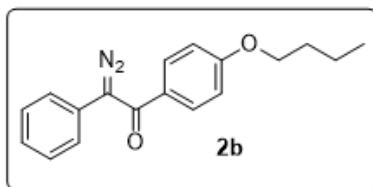
F2 - Acquisition Parameters
Date_     20210612
Time      23.32
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         133
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4417920 sec
RG         2050
DM         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6178022 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00

```



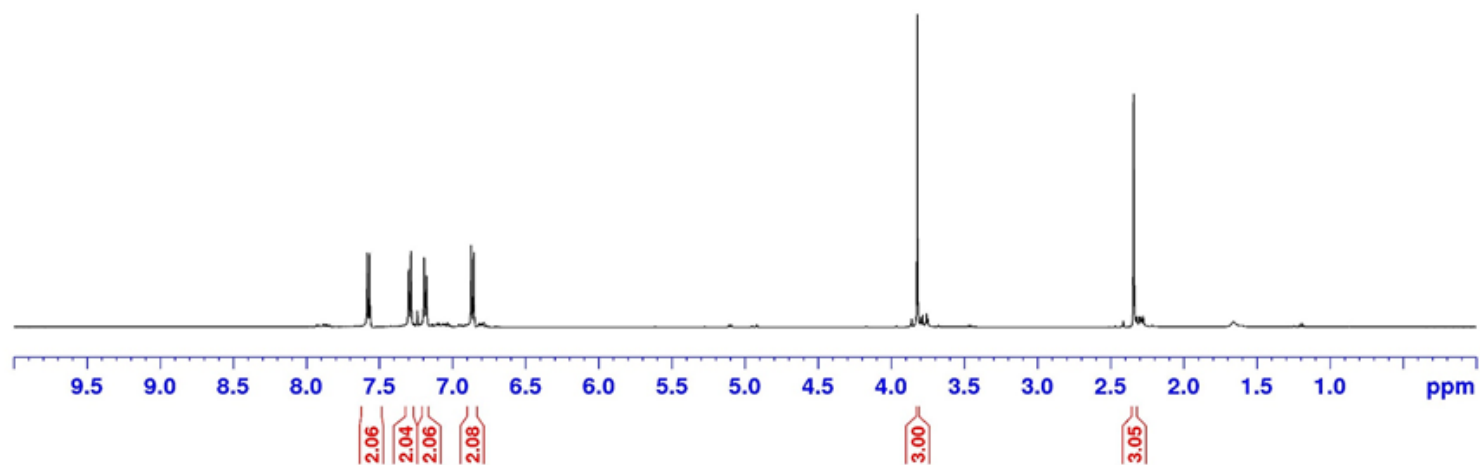
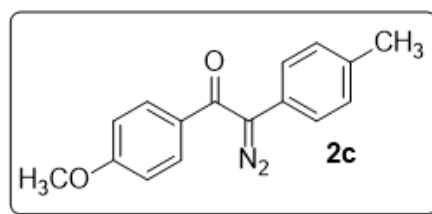
Solvent: CDCl₃
SFO1: 500 MHz

7.583
7.566
7.301
7.284
7.240
7.194
7.177
6.872
6.855

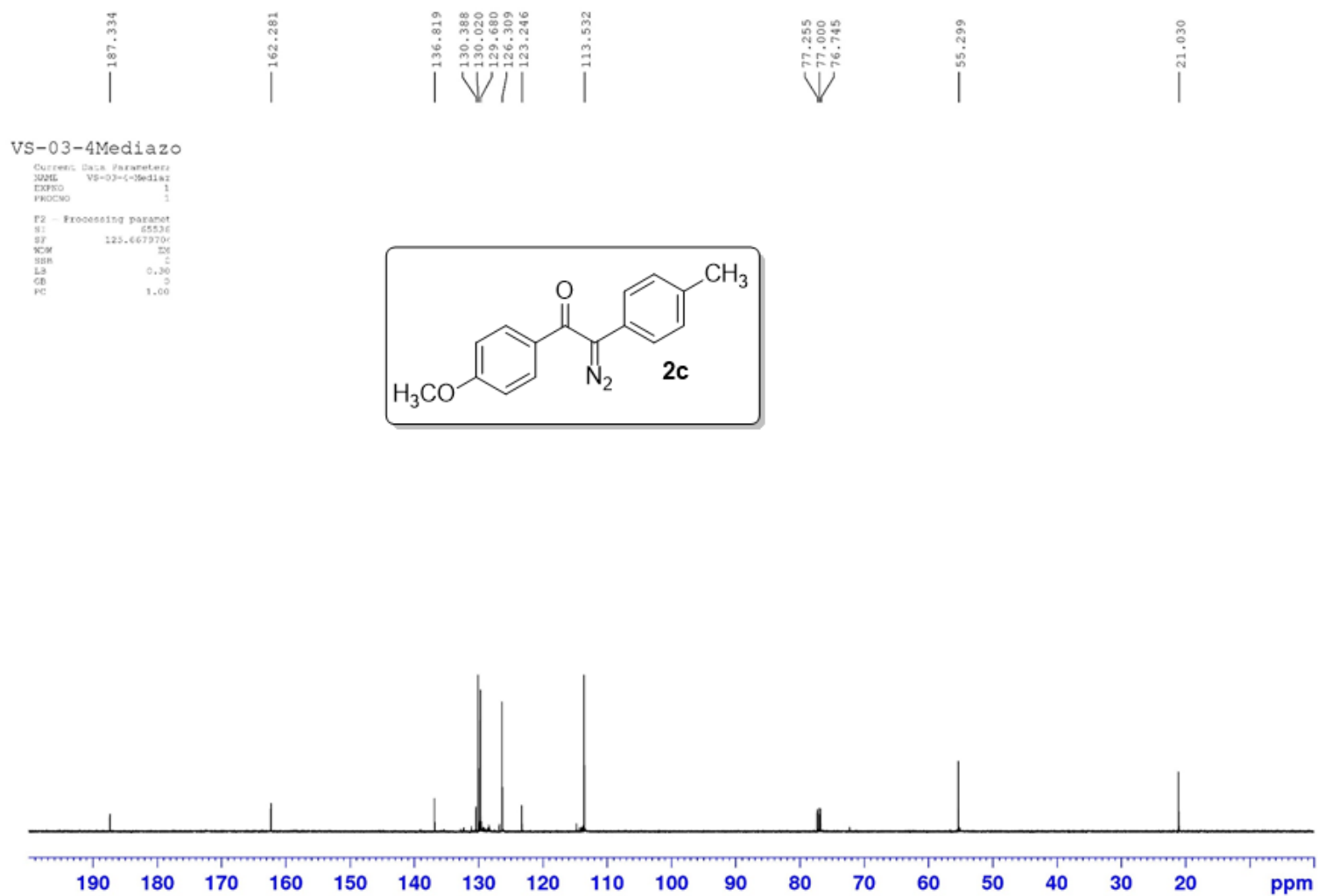
3.821

2.341

Current Data Parameters
NAME: VS-03-4-Mediazo-1h.fid
EXPNO: 1
PROCNO: 1
F2 - Processing parameters
SI: 32768
SF: 499.727654 MHz
RG: 64
SD: 0
LB: 0.30 Hz
GB: 0
PC: 1.00



Solvent: CDCl₃
SFO1: 125 MHz



Solvent: CDCl₃
SFO1: 400 MHz

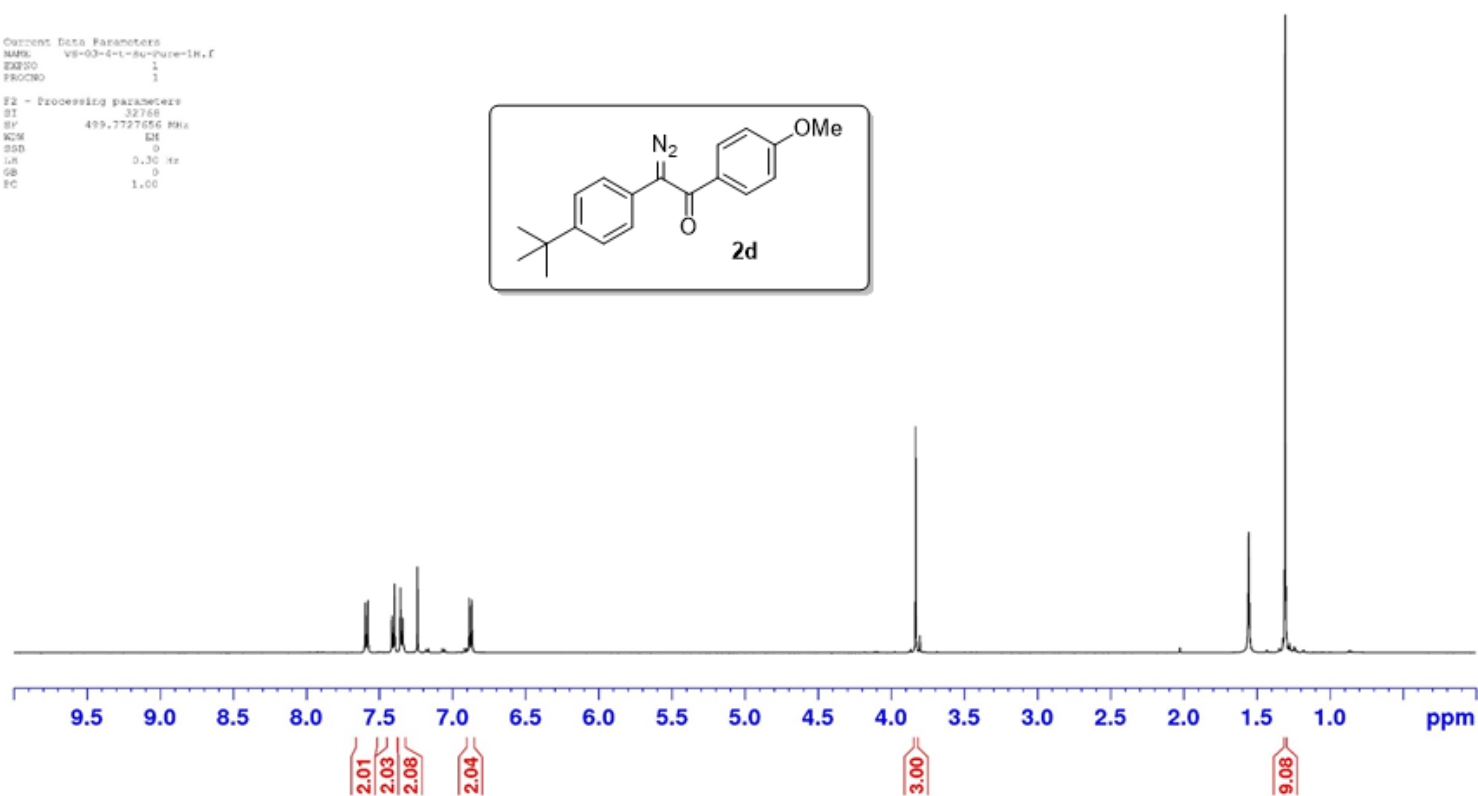
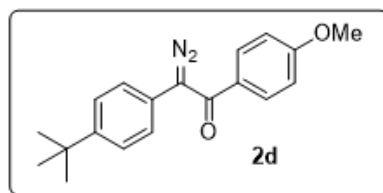
7.597
7.580
7.414
7.397
7.357
7.340
7.240
6.885
6.868

3.832

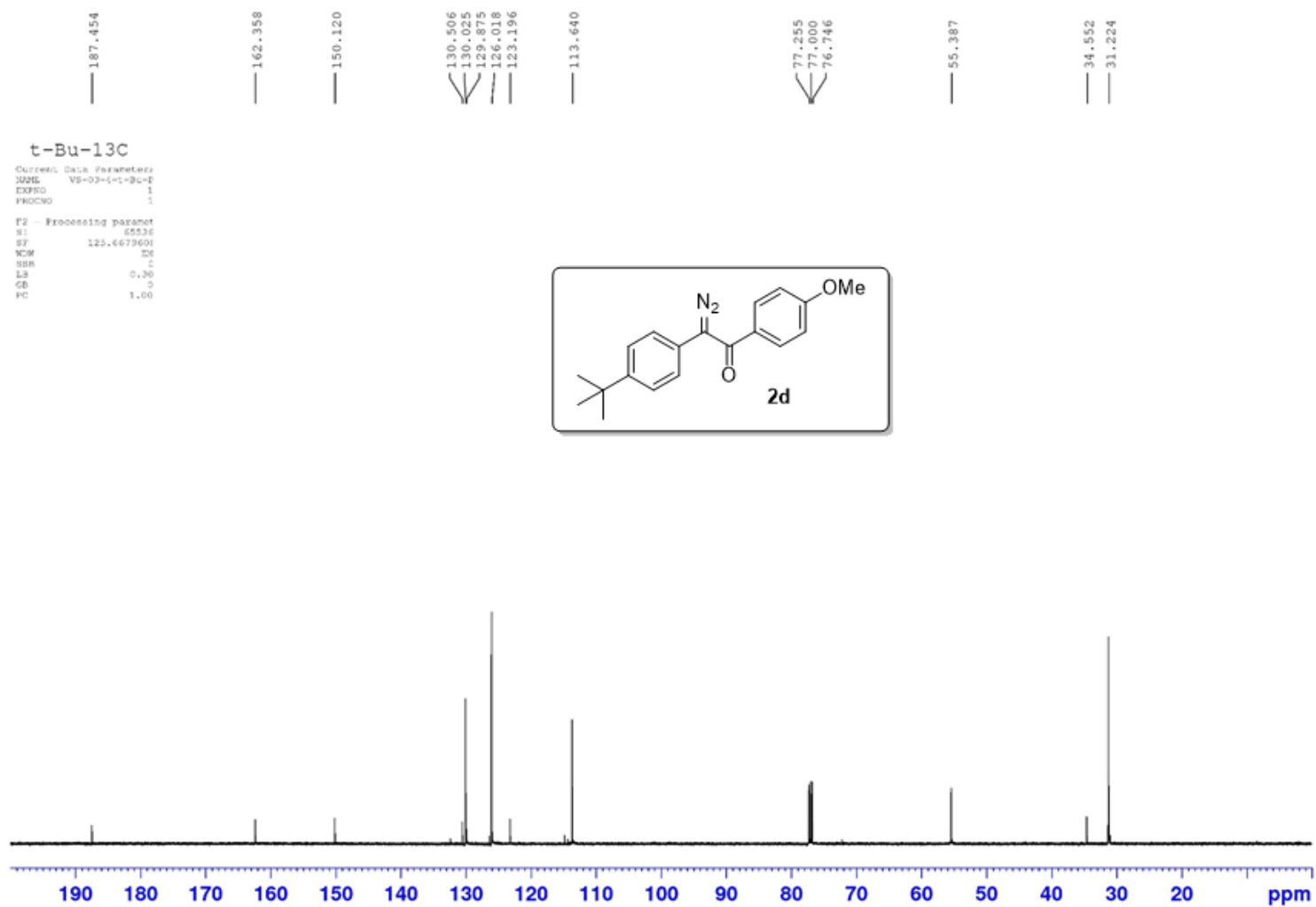
1.554

1.305

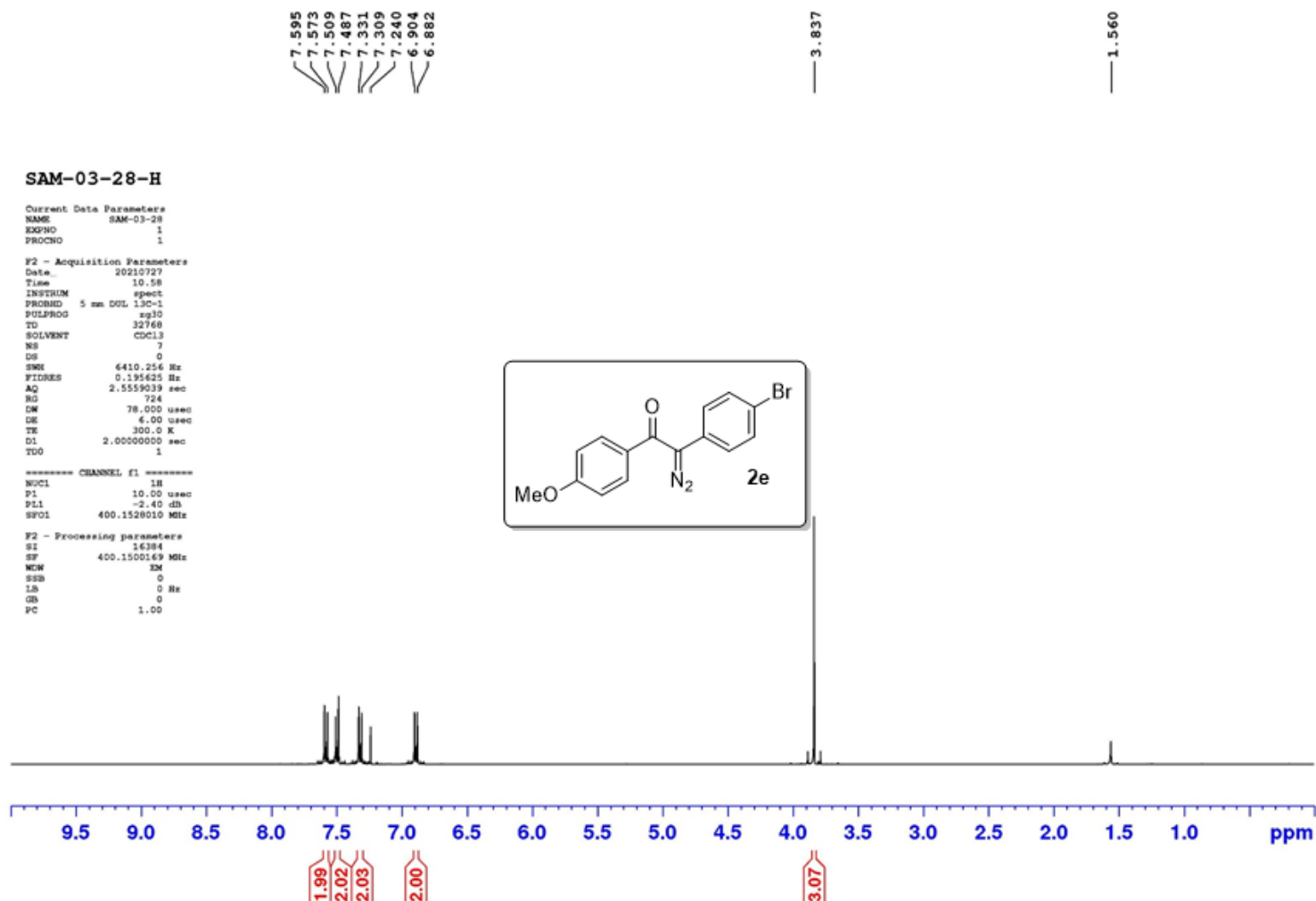
Current Data Parameters
NAME: VS-03-4-1-8u-pure-1H.f
EXPNO: 1
PROCNO: 1
F2 - Processing parameters
SI: 32768
SF: 499.7727656 MHz
RG: 64
SD: 0
LB: 0.30 Hz
GB: 0
PC: 1.00



Solvent: CDCl₃
SFO1: 100 MHz



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-28-C

```

Current Data Parameters
NAME      SAM-03-28
EXPNO     2
PROCNO    1

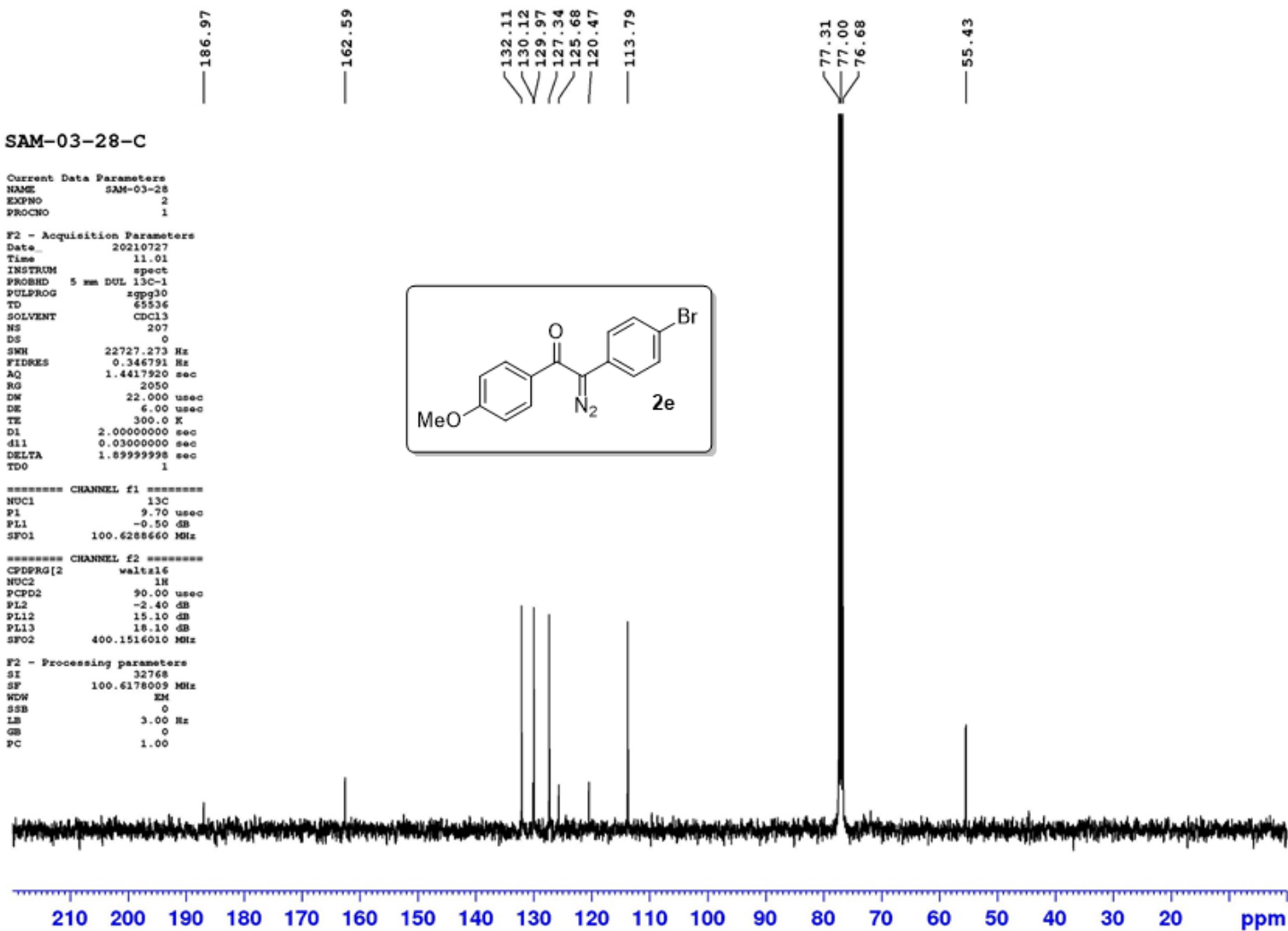
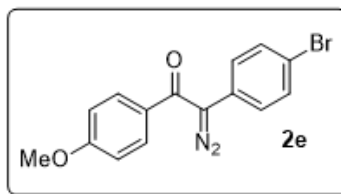
F2 - Acquisition Parameters
Date_     20210727
Time      11.01
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         207
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4417920 sec
RG         2050
DM         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

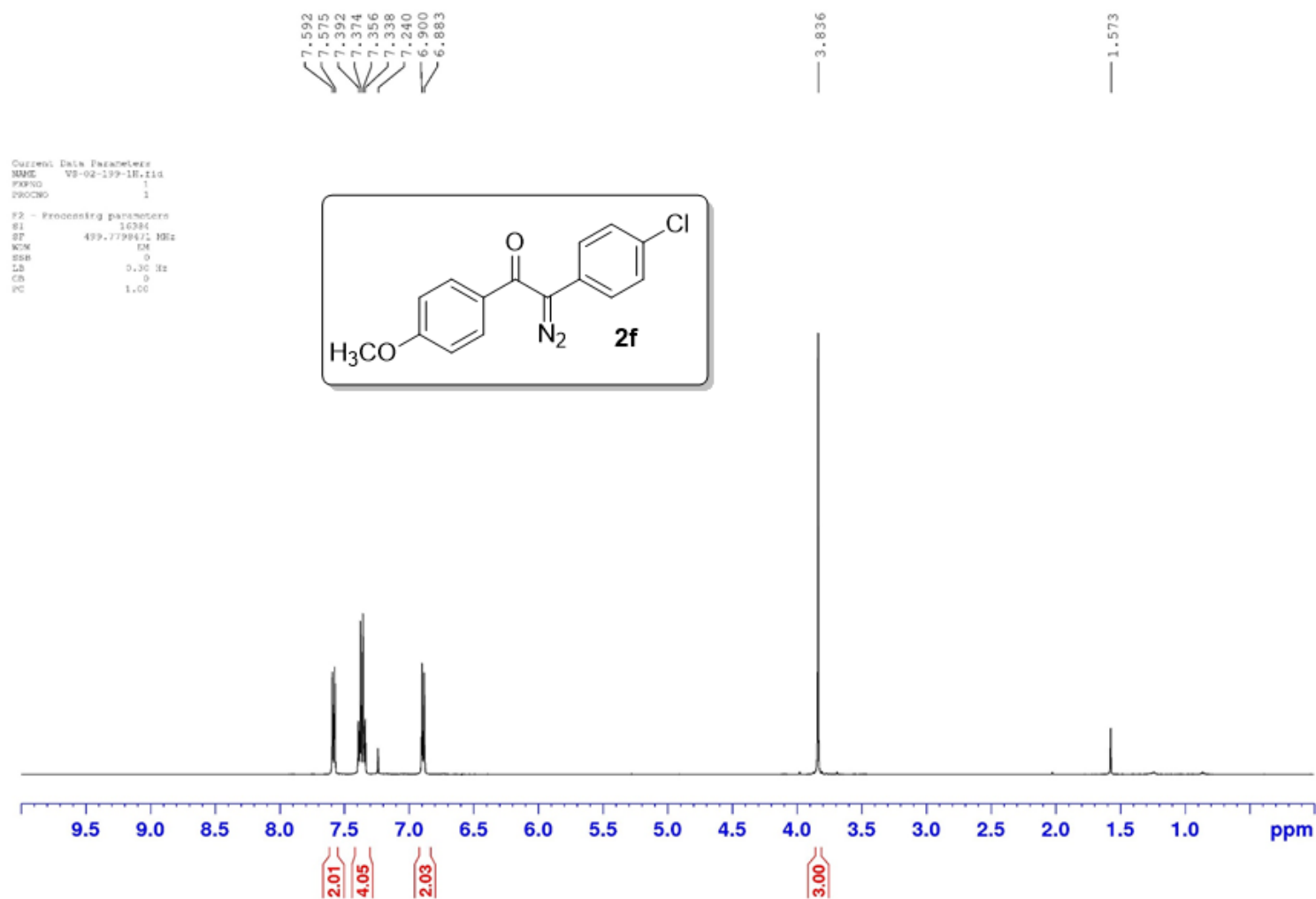
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6178009 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00

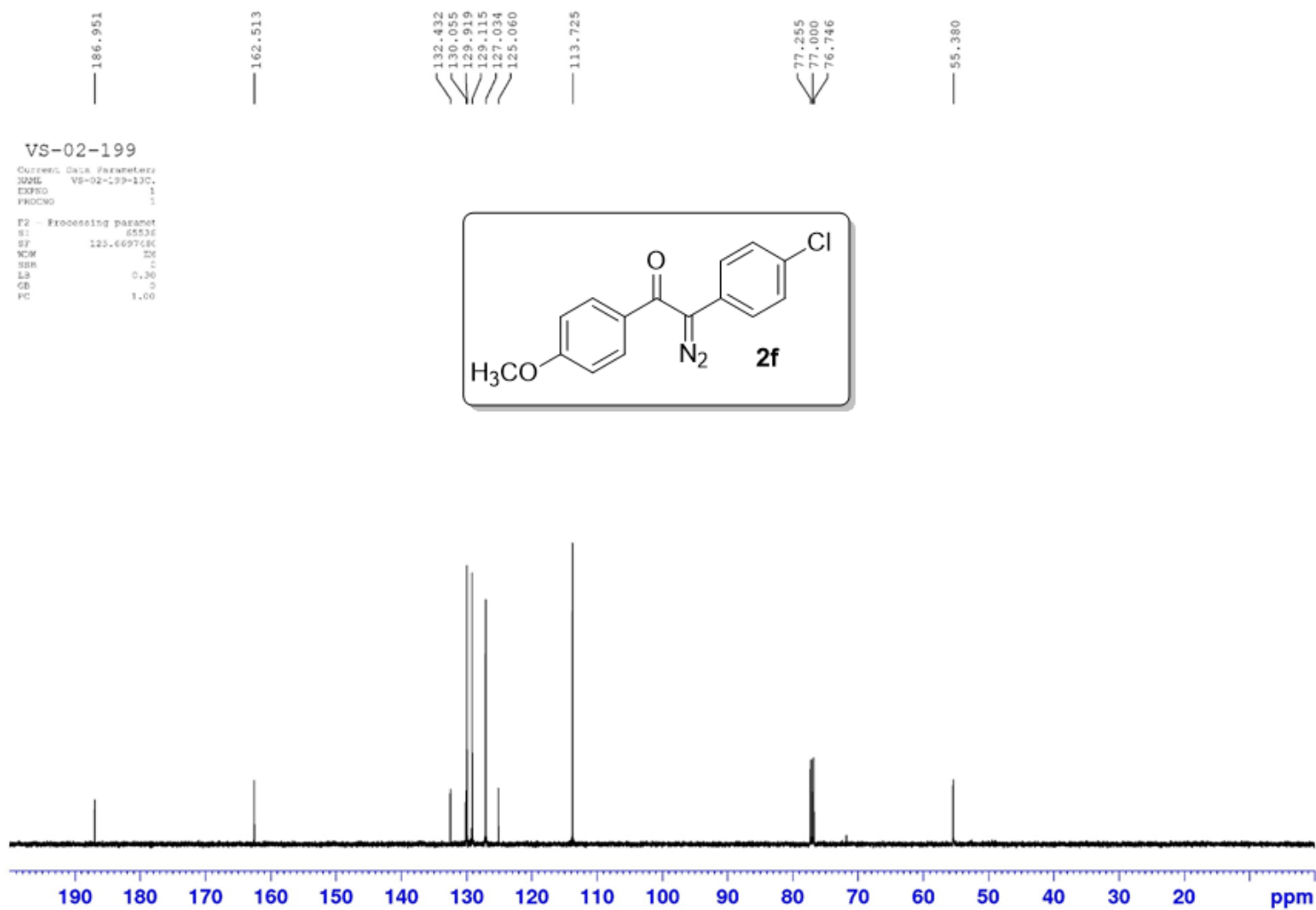
```



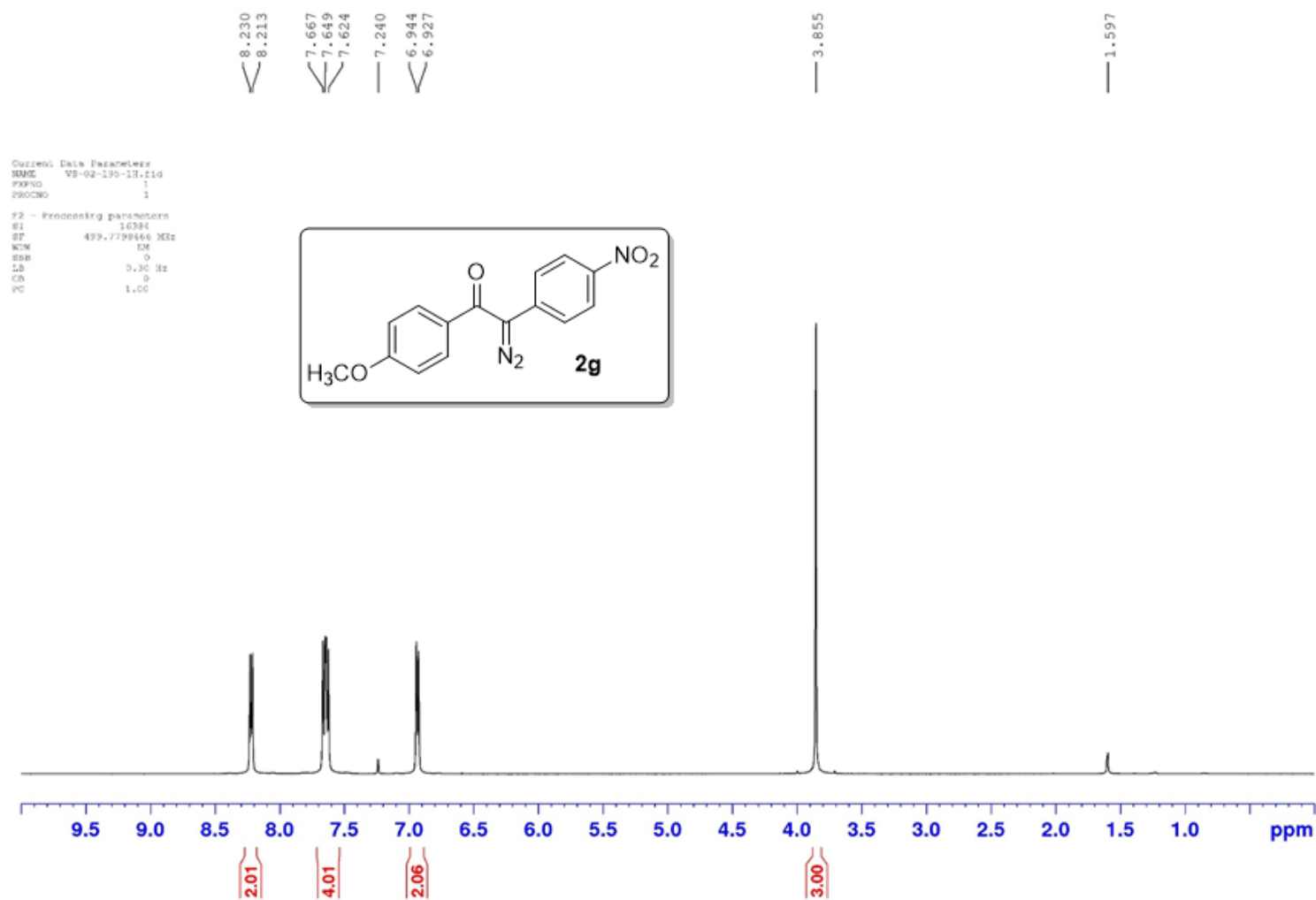
Solvent: CDCl_3
SFO1: 500 MHz



Solvent: CDCl_3
SFO1: 125 MHz



Solvent: CDCl₃
SFO1: 500 MHz



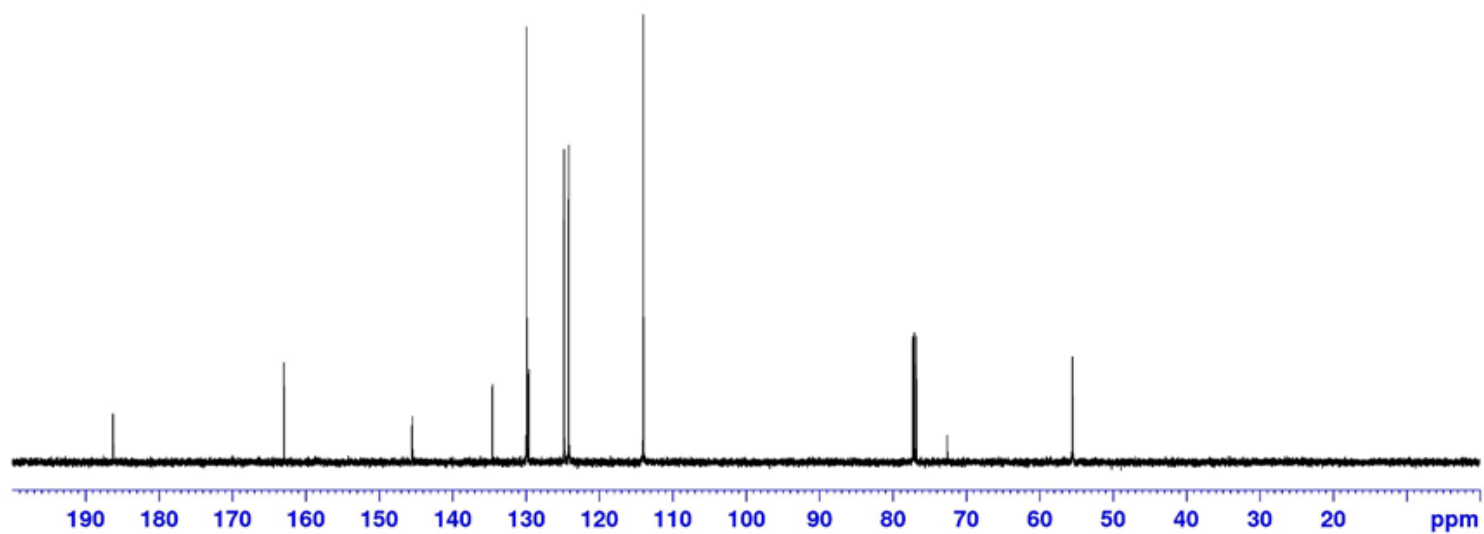
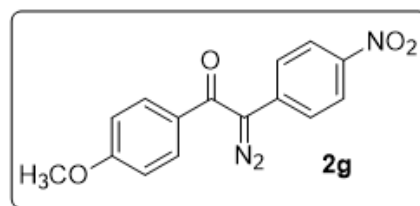
Solvent: CDCl₃
SFO1: 125 MHz



VS-02-195

Current Data Parameters
NAME VS-02-195-13C
EXPNO 1
PROCNO 1

F2 - Processing parameter
SI 65536
SF 125.669709
SCW 126
SRB 1
LB 0.30
GB 0
PC 1.00



Solvent: CDCl₃
SFO1: 400 MHz

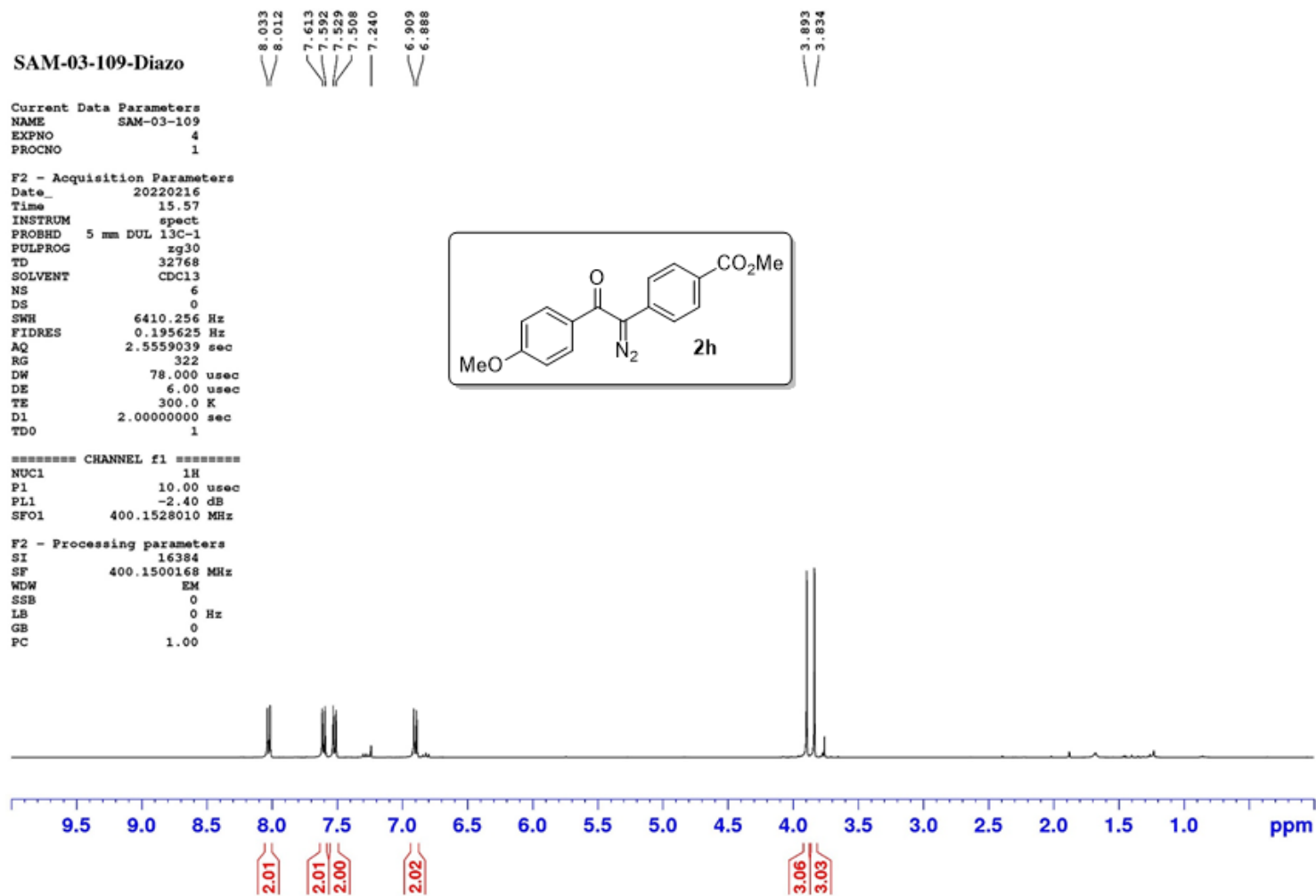
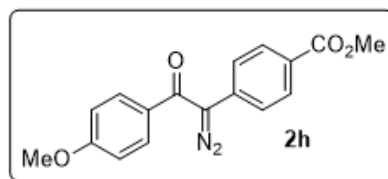
SAM-03-109-Diazo

Current Data Parameters
NAME SAM-03-109
EXPNO 4
PROCNO 1

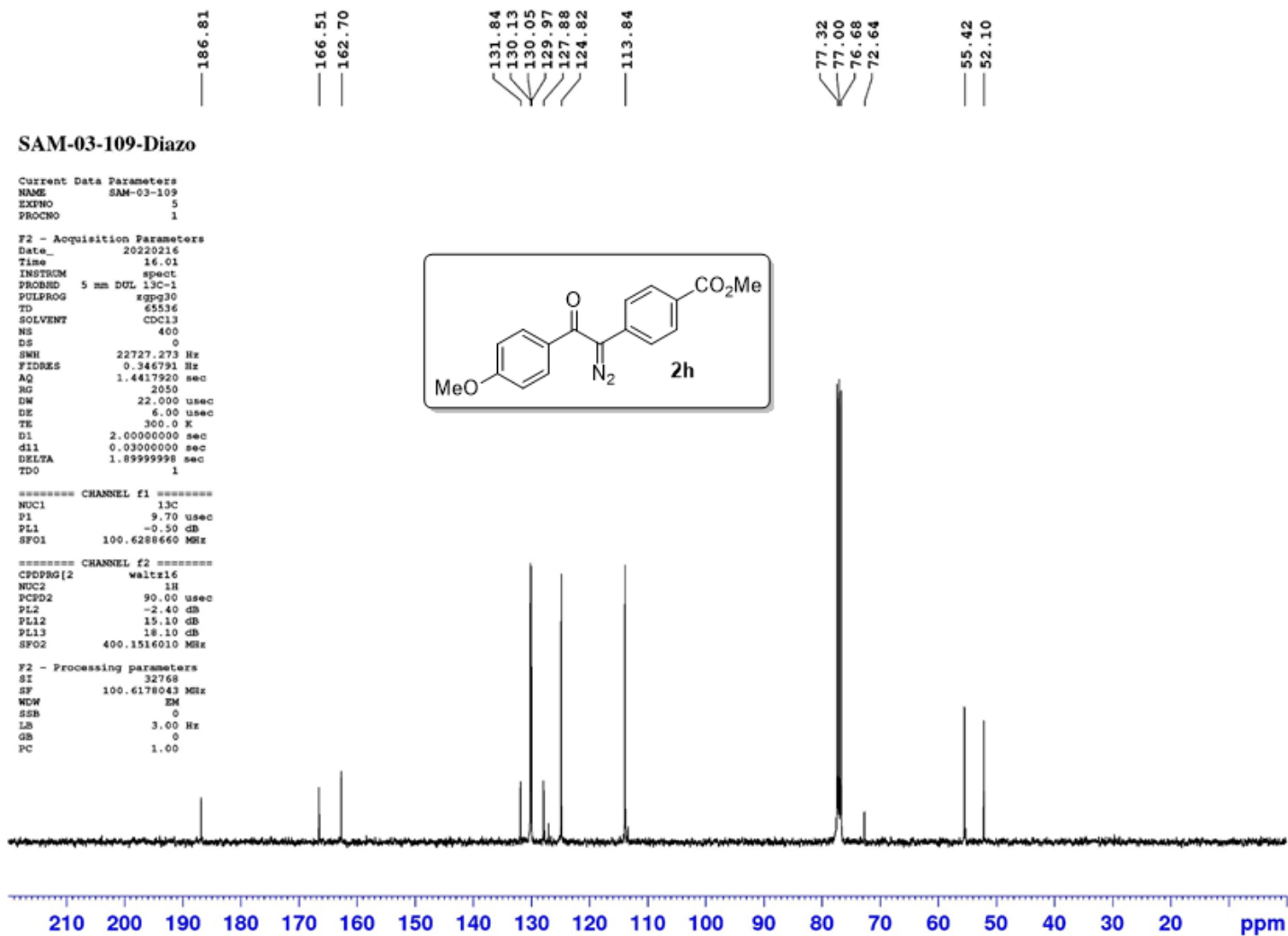
F2 - Acquisition Parameters
Date_ 20220216
Time 15.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 100 MHz



Solvent: CDCl_3
SFO1: 400 MHz

7.648
7.627
7.622
7.604
7.600
7.583
7.240
6.931
6.909

3.844

1.656

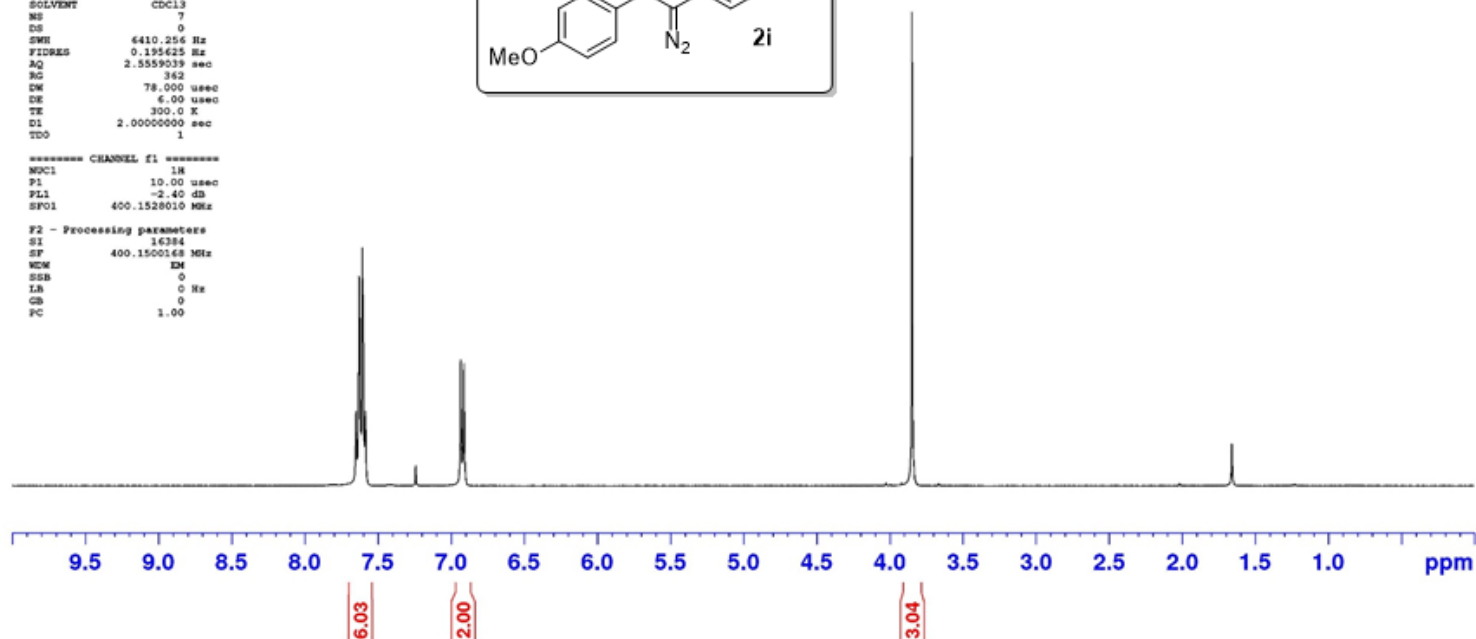
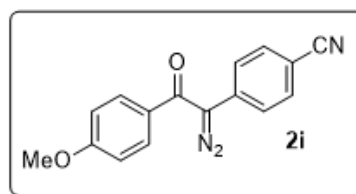
SAM-03-112-C-diazo

Current Data Parameters
NAME SAM-03-112
EXPNO 2
PROCNO 1

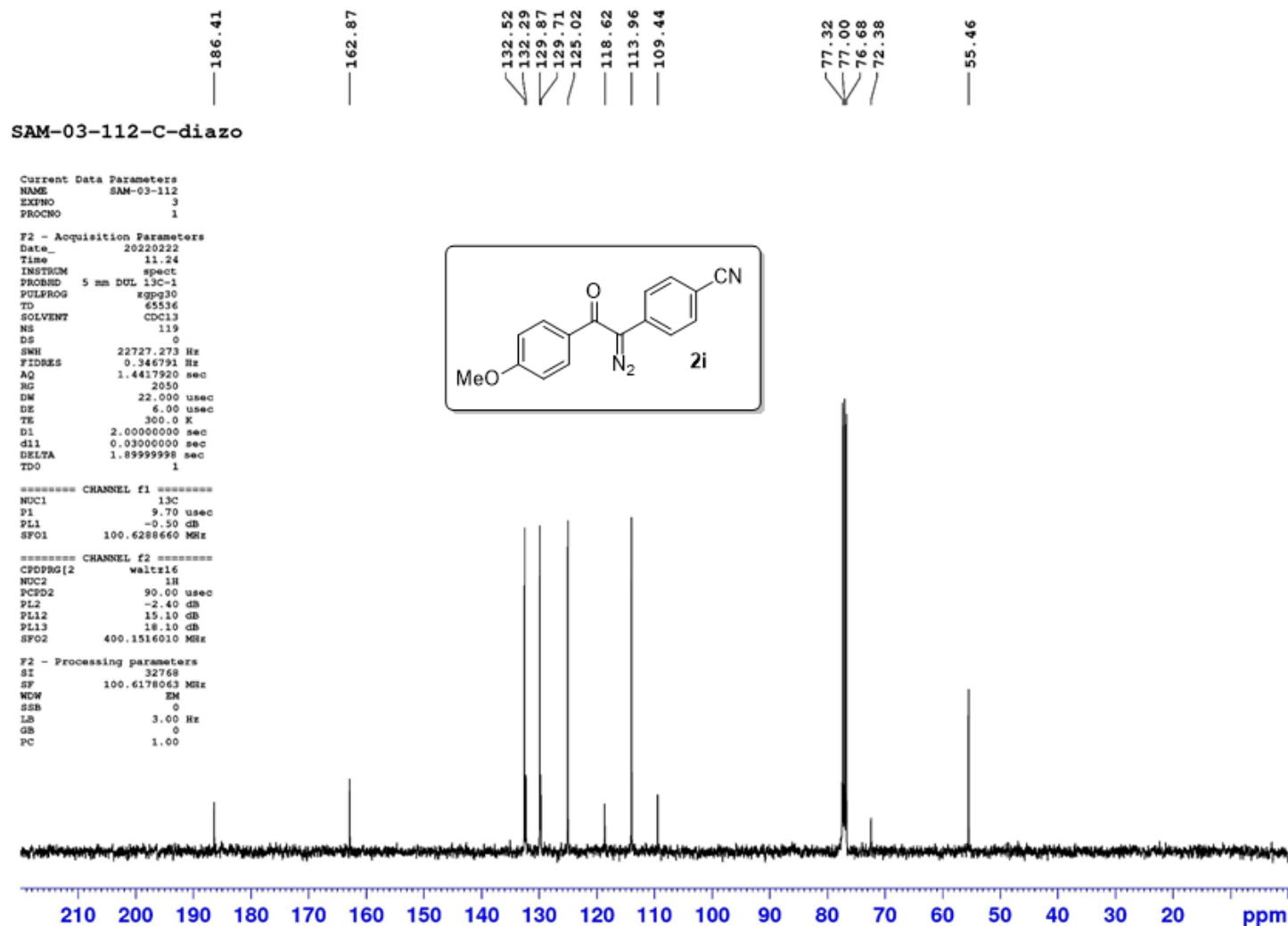
F2 - Acquisition Parameters
Date_ 20220222
Time 11.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl_3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 362
DM 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

***** CHANNEL f1 *****
NUC1 ^{13}C
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

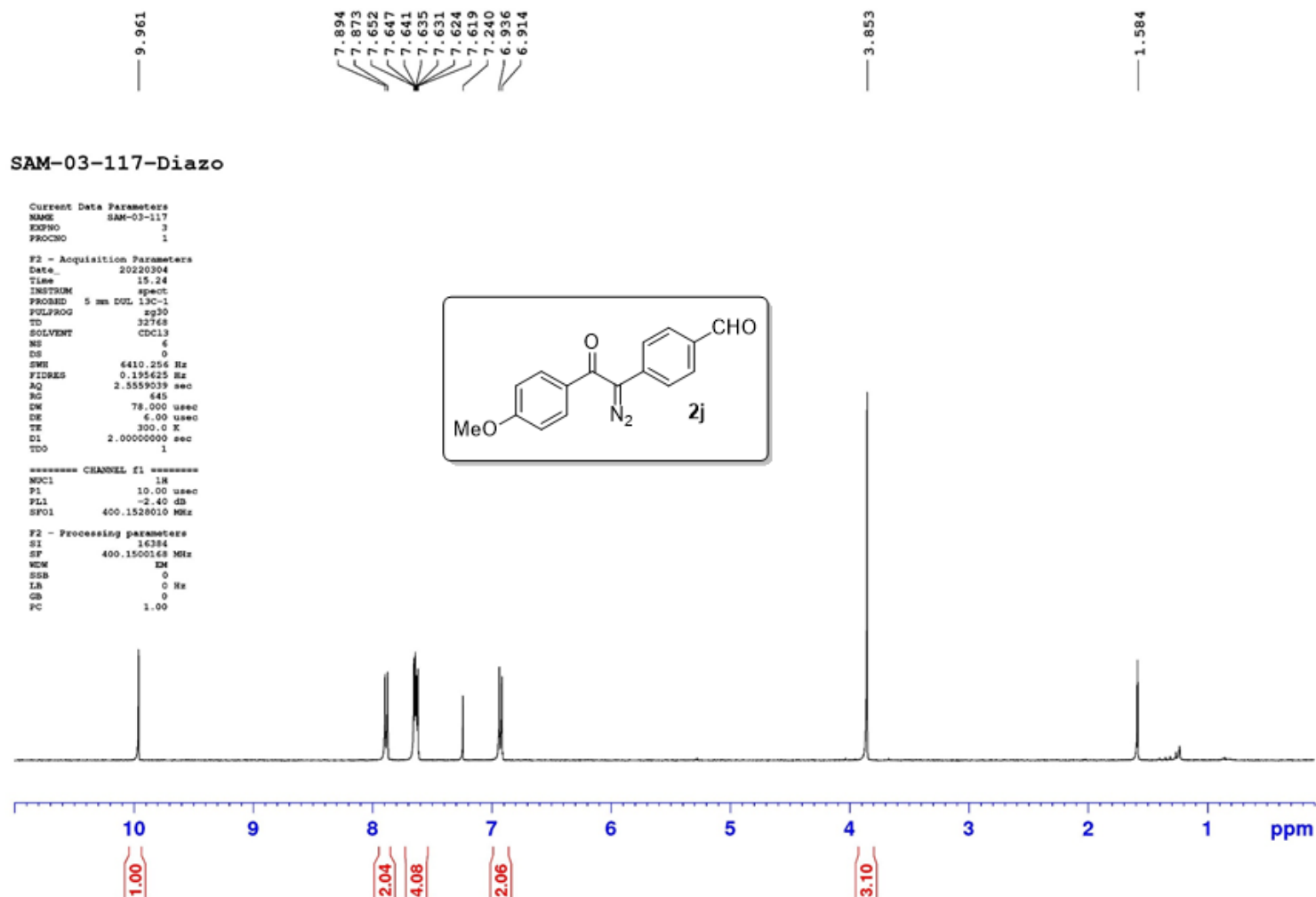
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 100 MHz



Solvent: CDCl₃
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-117-Diazo

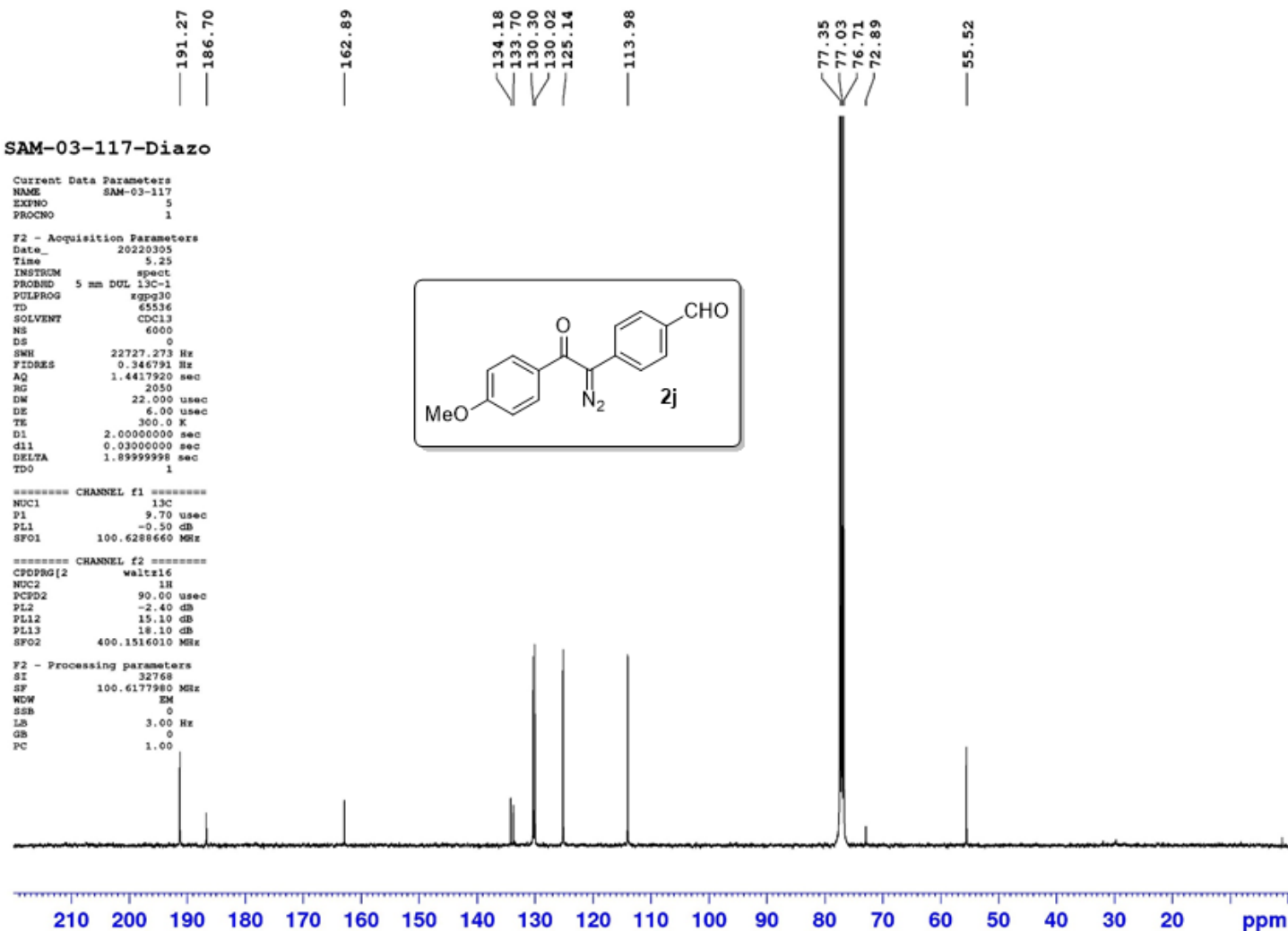
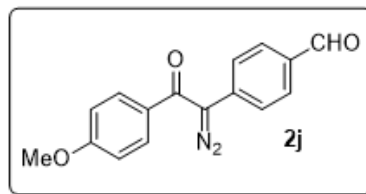
Current Data Parameters
NAME SAM-03-117
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220305
Time 5.25
INSTRUM spect
PROBHD 5 mm DOL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 6000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4417920 sec
RG 2050
DM 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

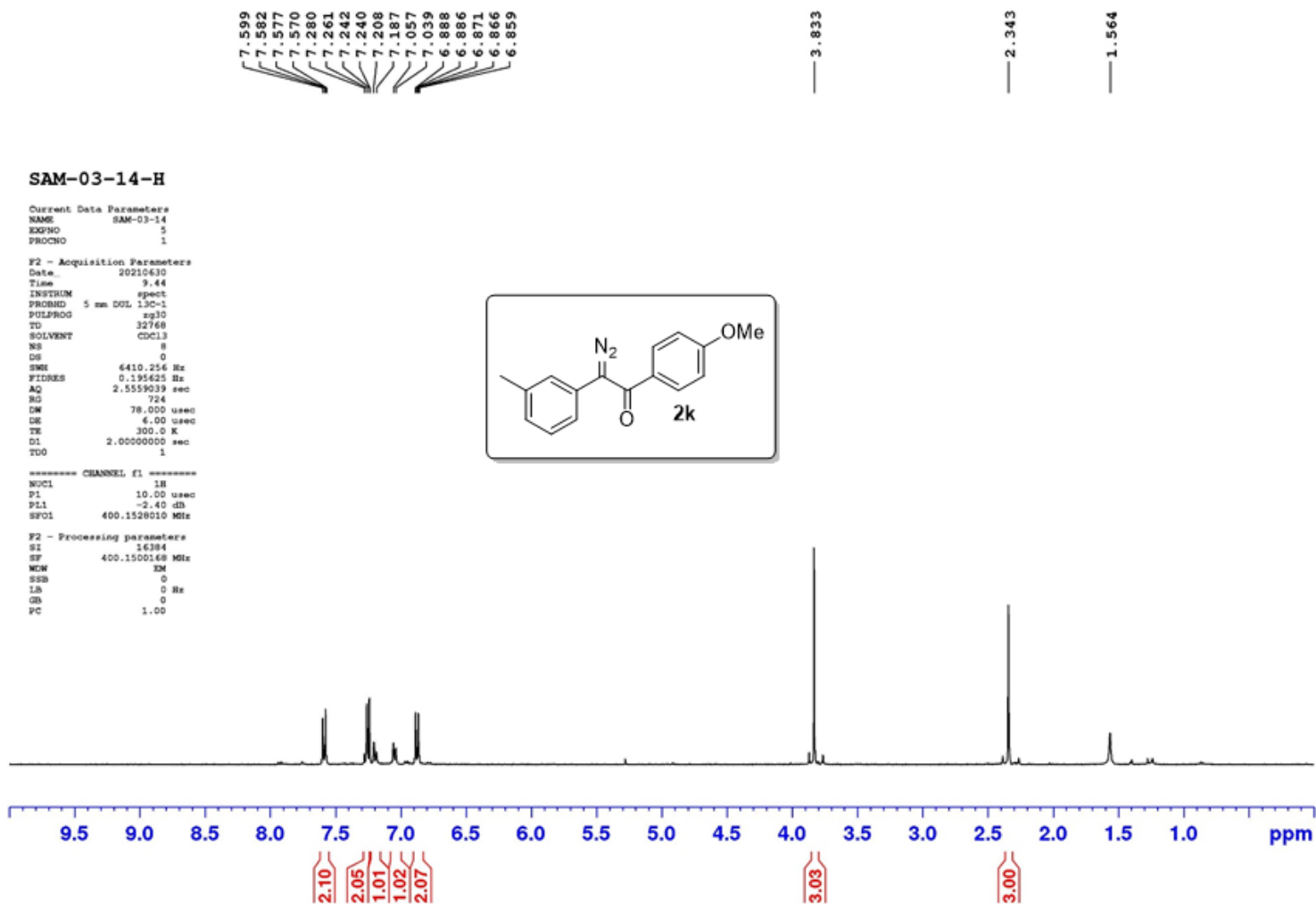
===== CHANNEL f1 =====
NUC1 ^{13}C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz

===== CHANNEL f2 =====
CPCPRG2 waltz16
NUC2 ^1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 16.10 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-14-C

```

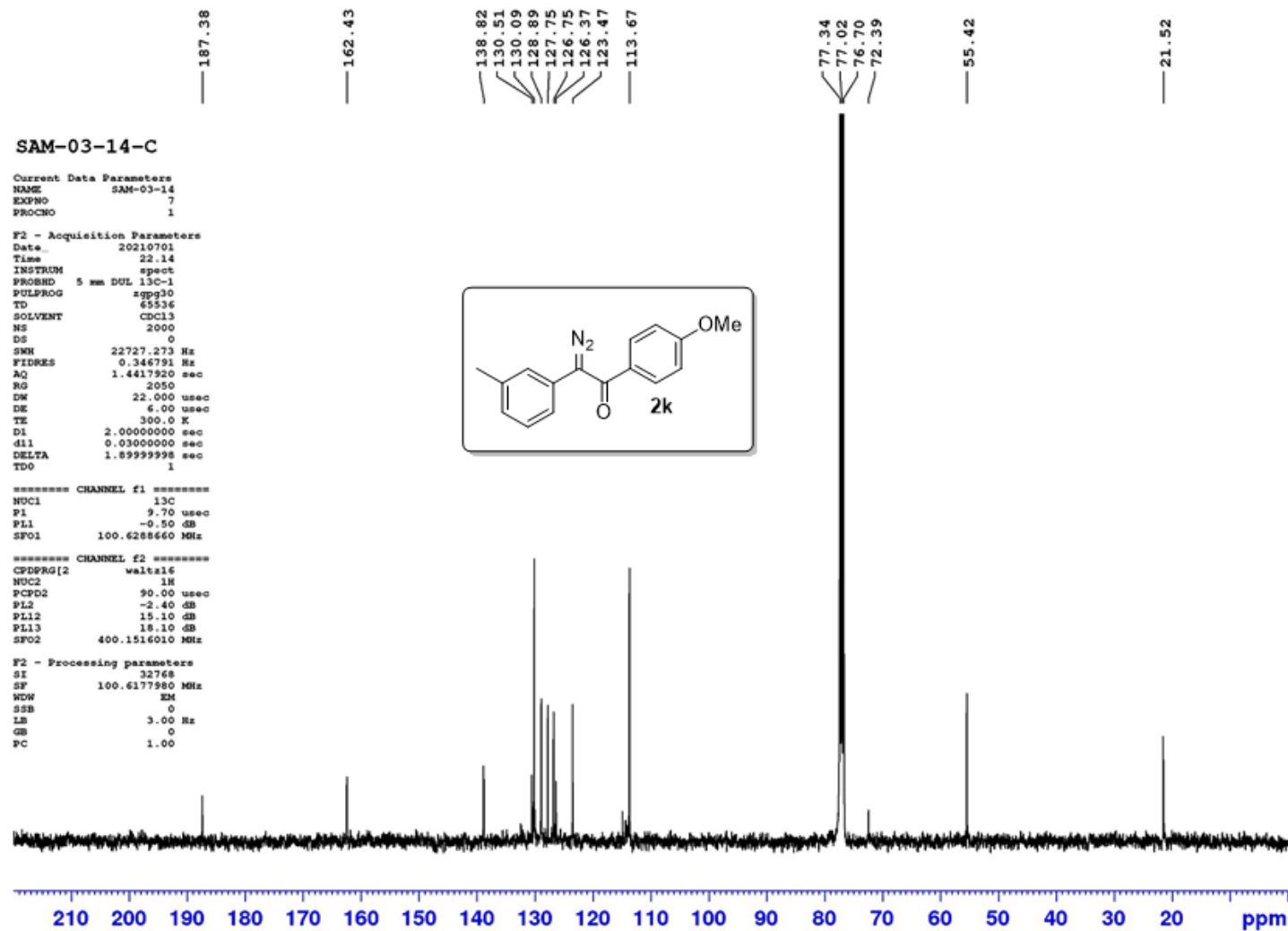
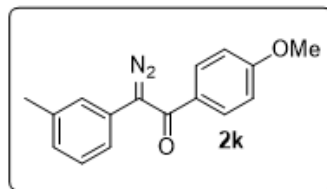
Current Data Parameters
NAME      SAM-03-14
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20210701
Time      22.14
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        2000
DS        0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4417920 sec
RG         2050
DM         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

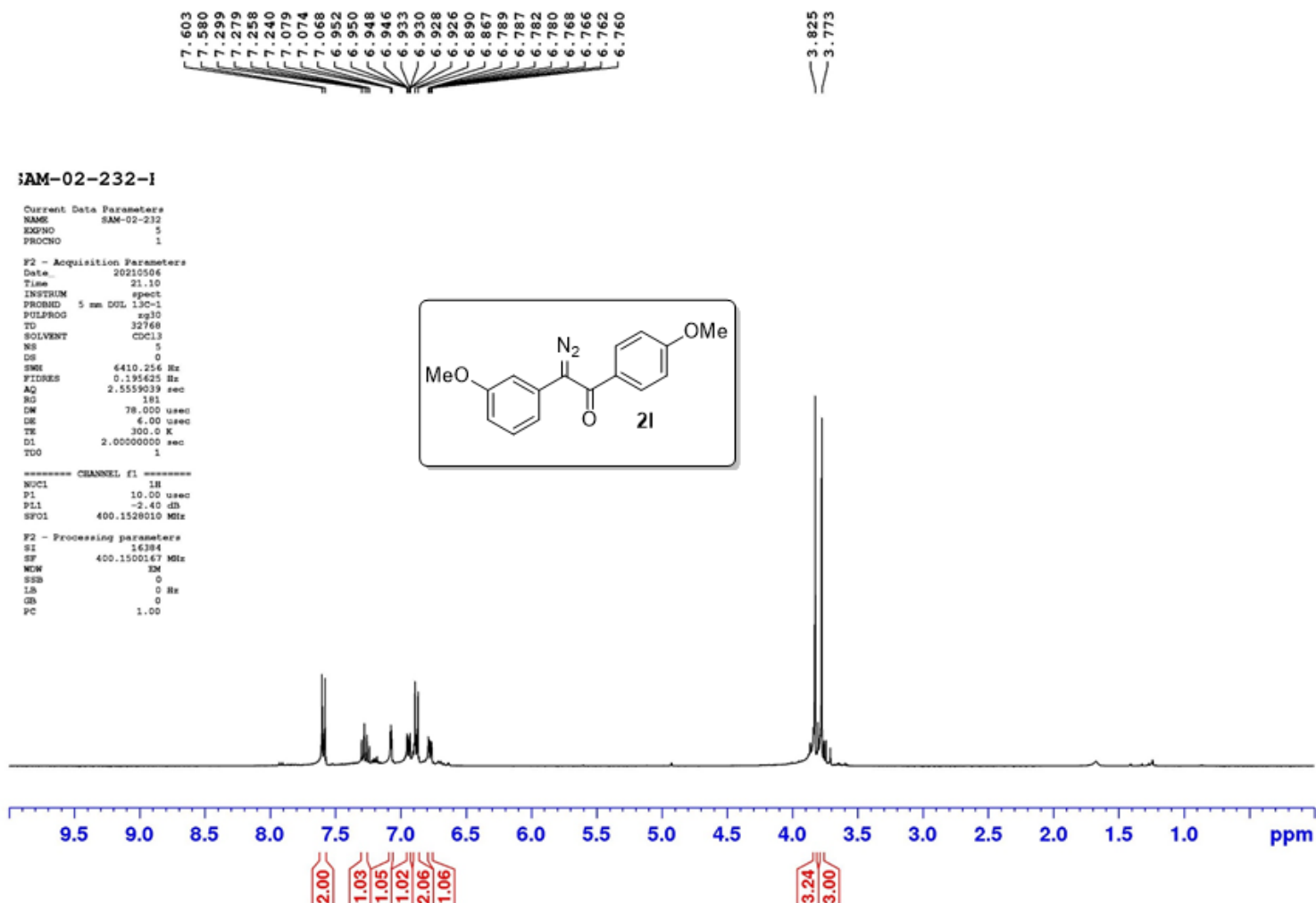
===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
  
```



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-02-232-DEPT

```

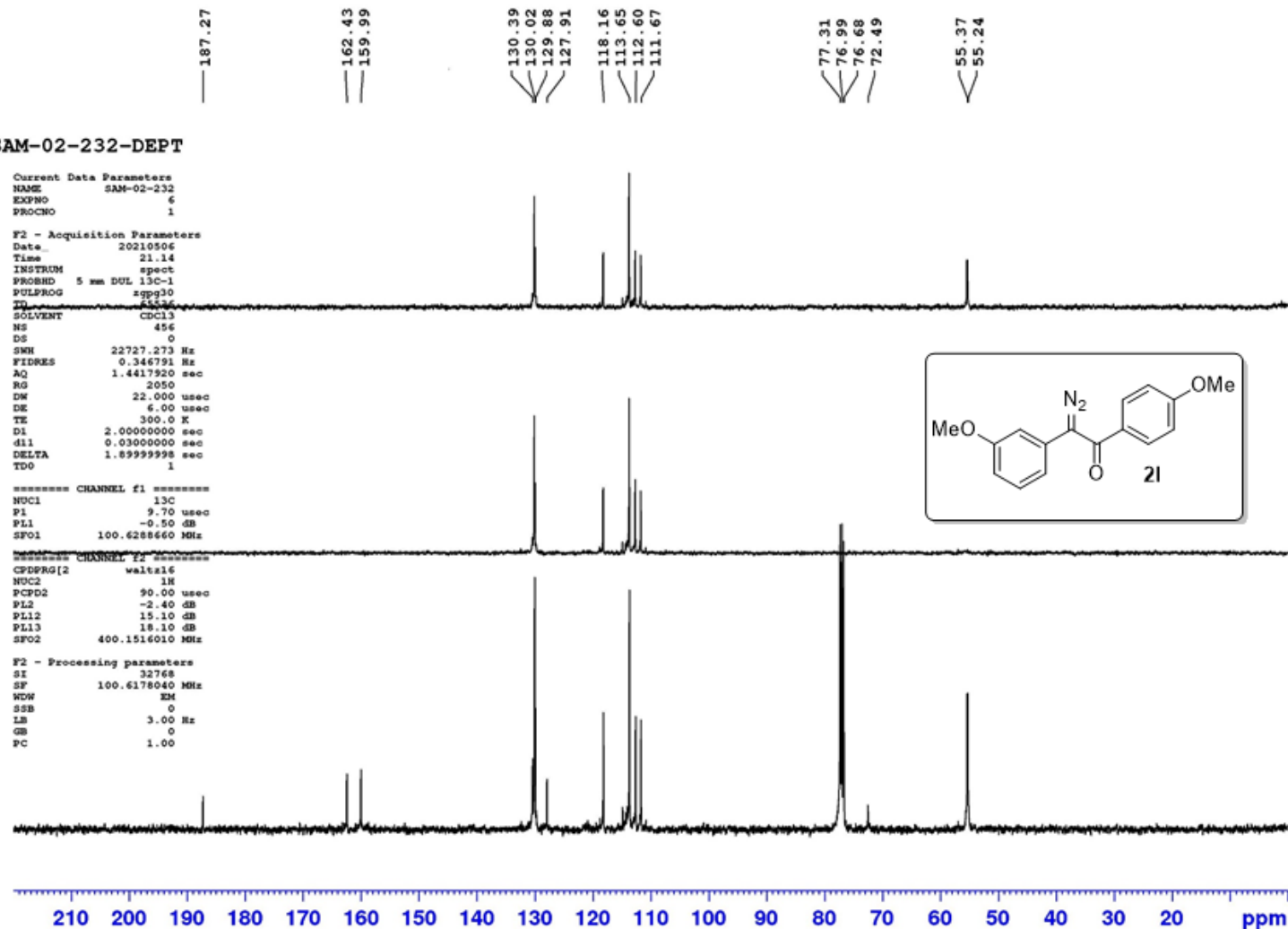
Current Data Parameters
NAME      SAM-02-232
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
Date_     20210506
Time      21.14
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT    CDCl3
NS         456
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4417920 sec
RG         2050
DM         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

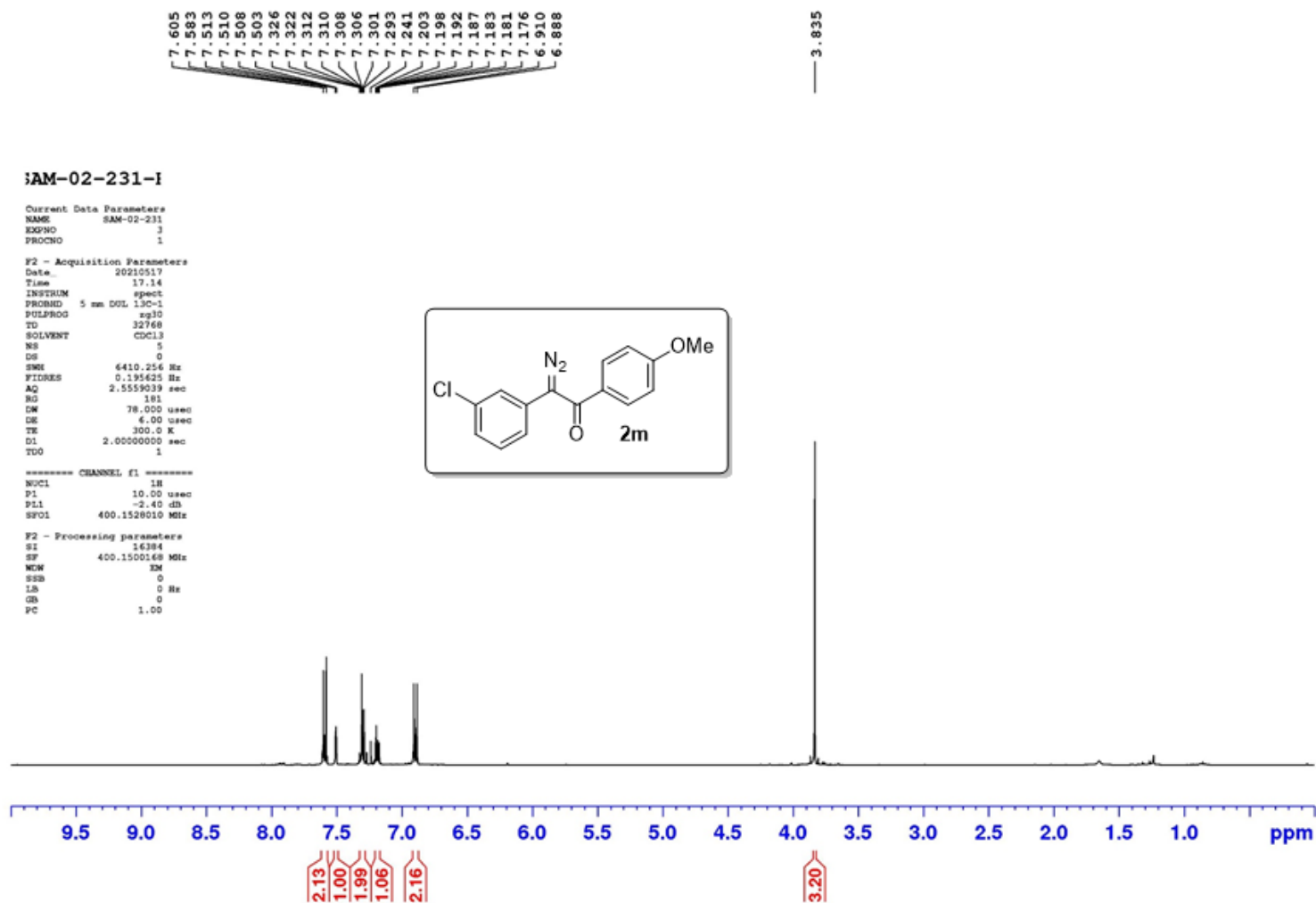
===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6178040 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
  
```



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-02-231-C

```

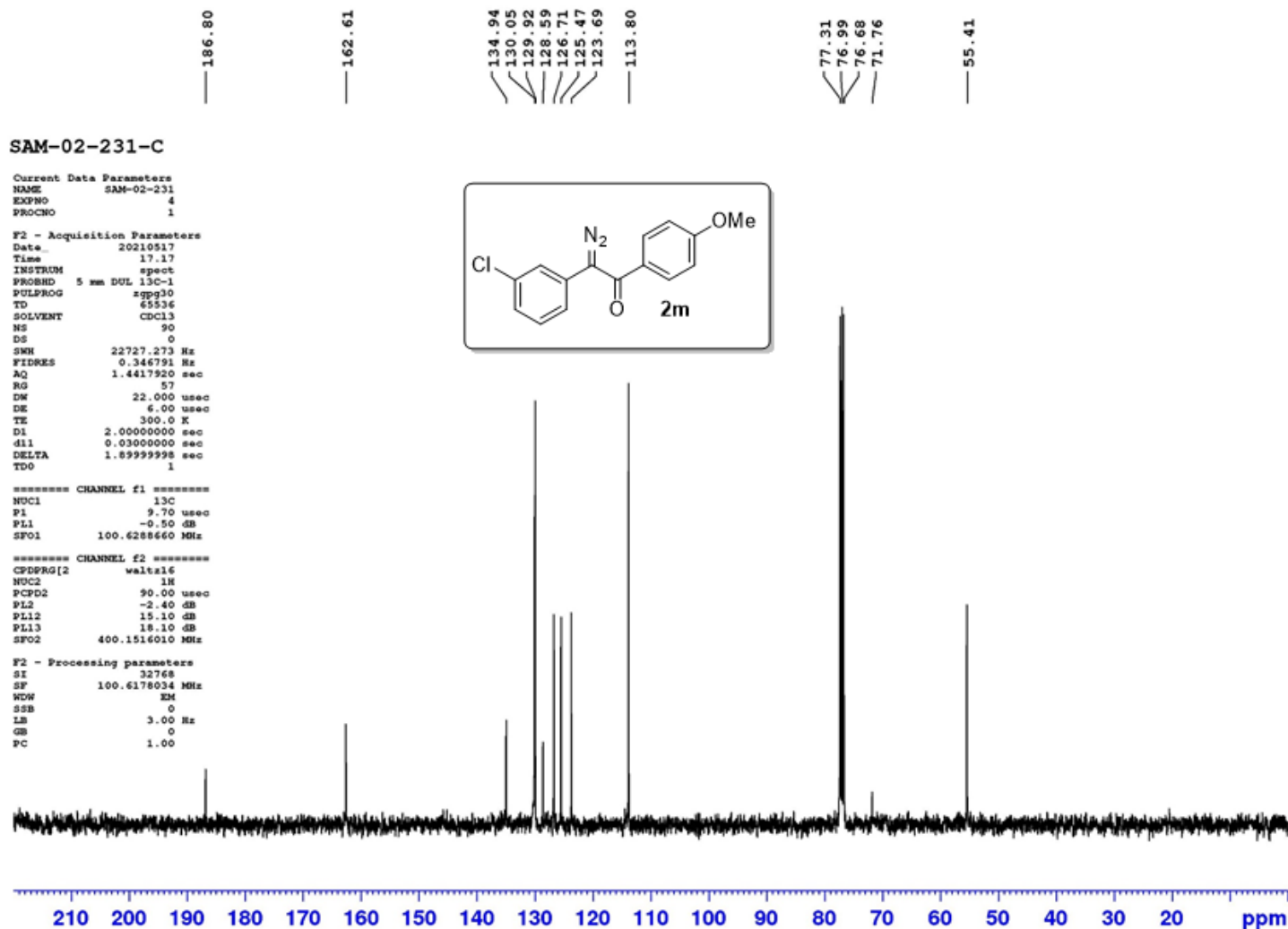
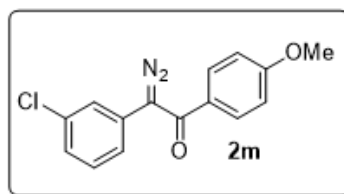
Current Data Parameters
NAME      SAM-02-231
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20210517
Time      17.17
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        90
DS        0
SWH       22727.273 Hz
FIDRES    0.346791 Hz
AQ        1.4417920 sec
RG        57
DM        22.000 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA     1.89999998 sec
TD0       1

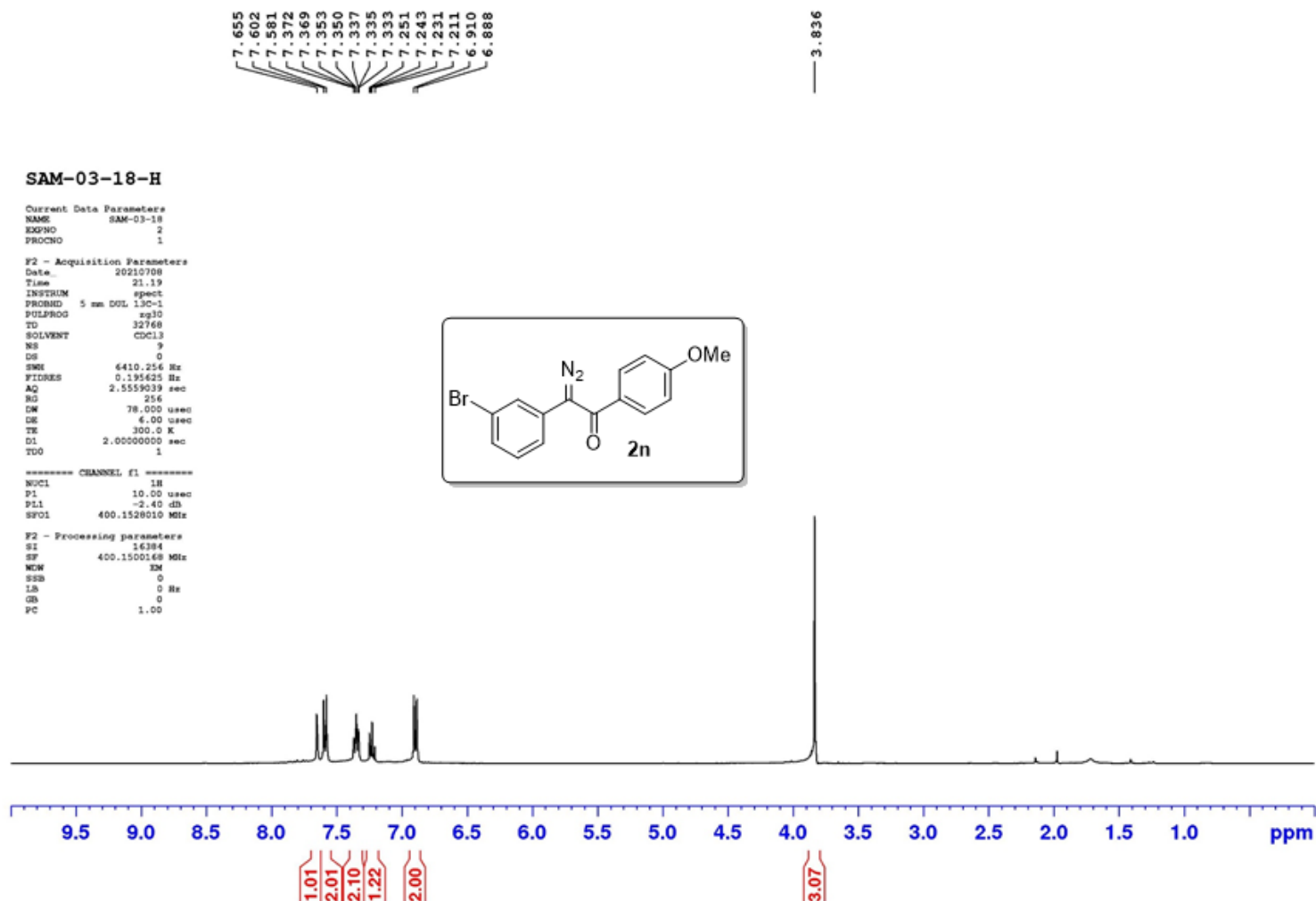
===== CHANNEL f1 =====
NUC1      13C
P1        9.70 usec
PL1       -0.50 dB
SFO1      100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.40 dB
PL12      15.10 dB
PL13      18.10 dB
SFO2      400.1516010 MHz

F2 - Processing parameters
SI        32768
SF        100.6178034 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.00
  
```



Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
SFO1: 100 MHz

SAM-03-18-C

```

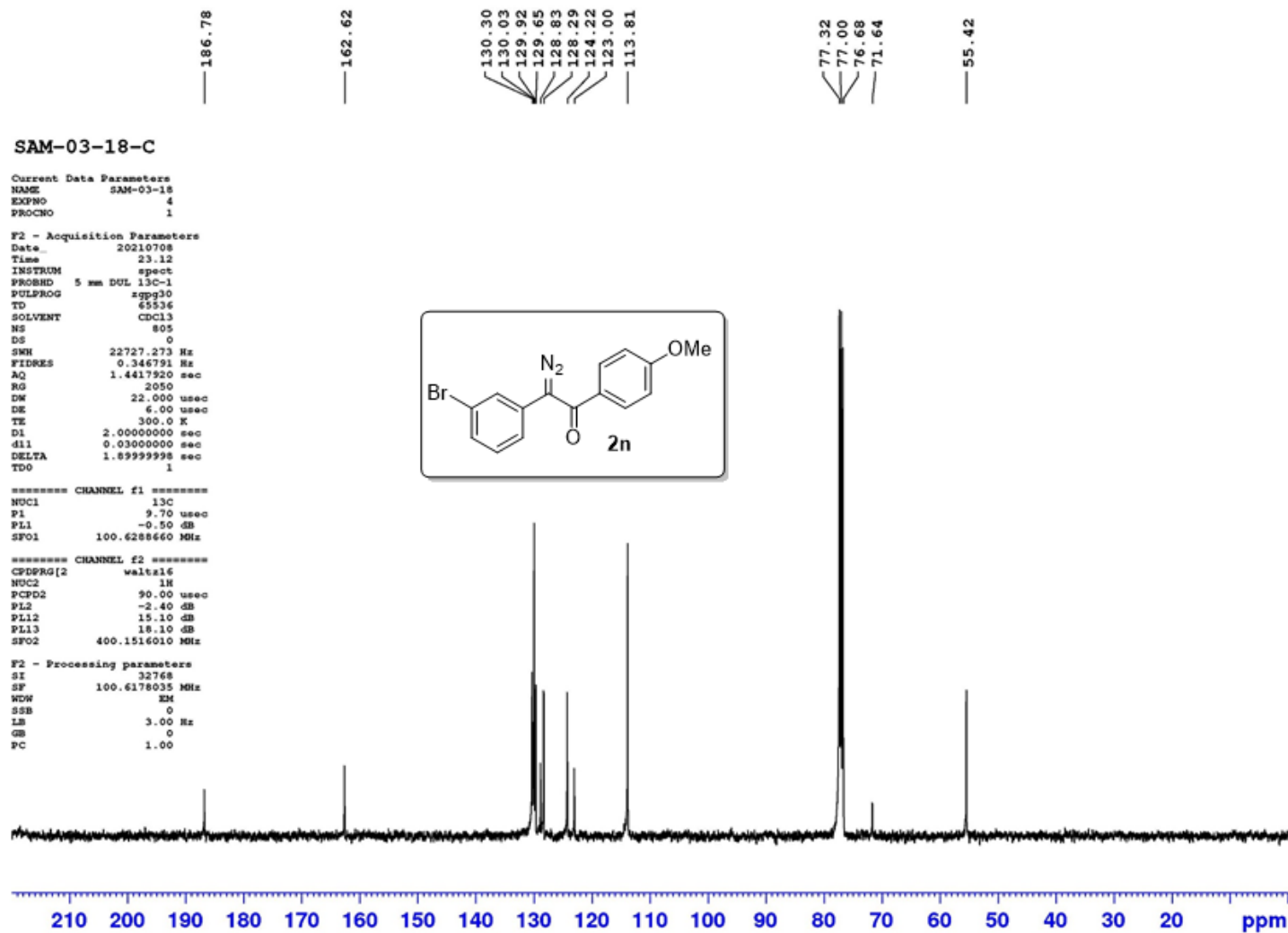
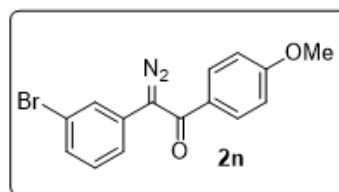
Current Data Parameters
NAME      SAM-03-18
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20210708
Time      23.12
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        805
DS        0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4417920 sec
RG         2050
DM         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

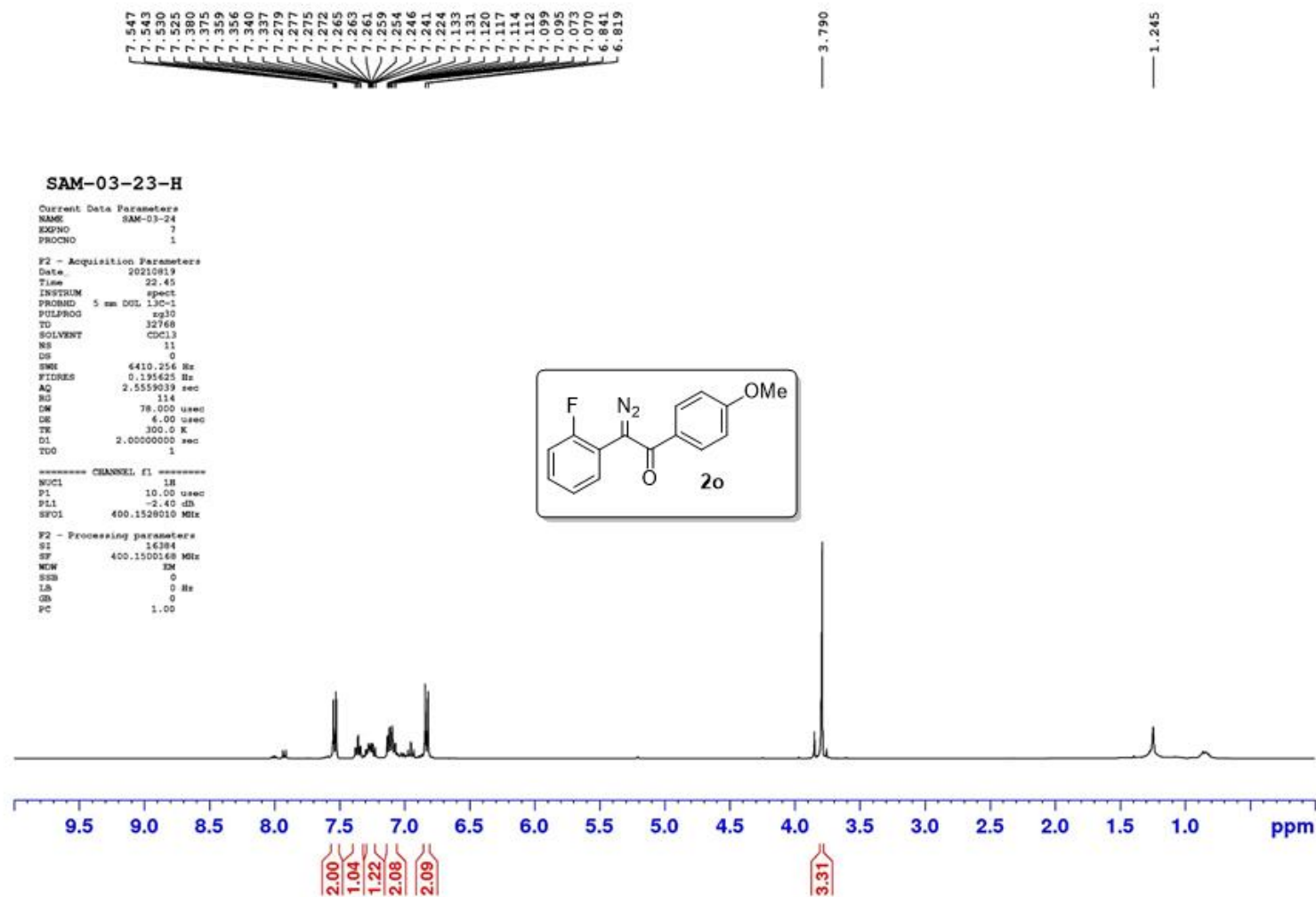
===== CHANNEL f1 =====
NUC1       13C
P1         9.70 usec
PL1        -0.50 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2       400.1516010 MHz

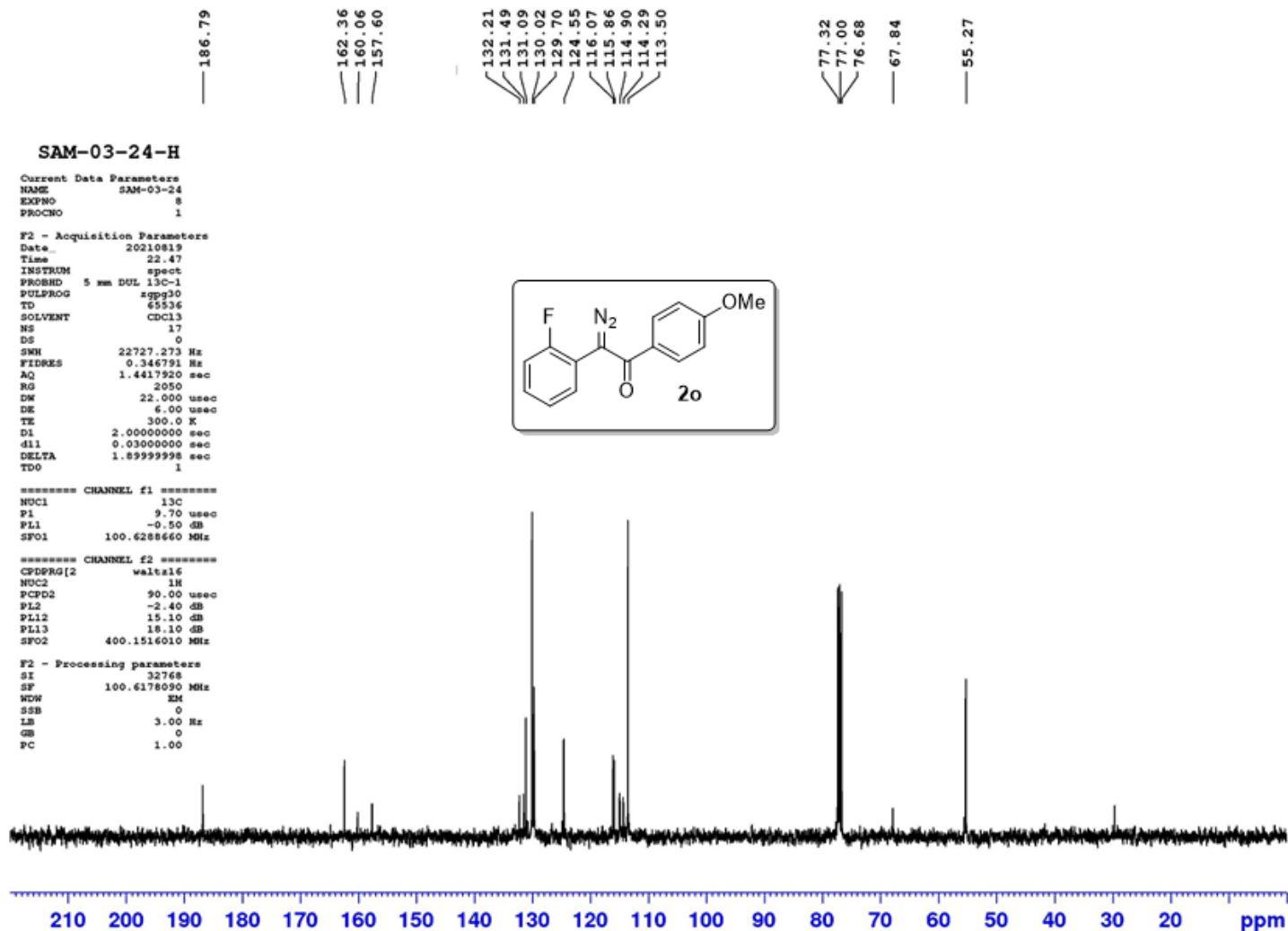
F2 - Processing parameters
SI         32768
SF         100.6178035 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
  
```



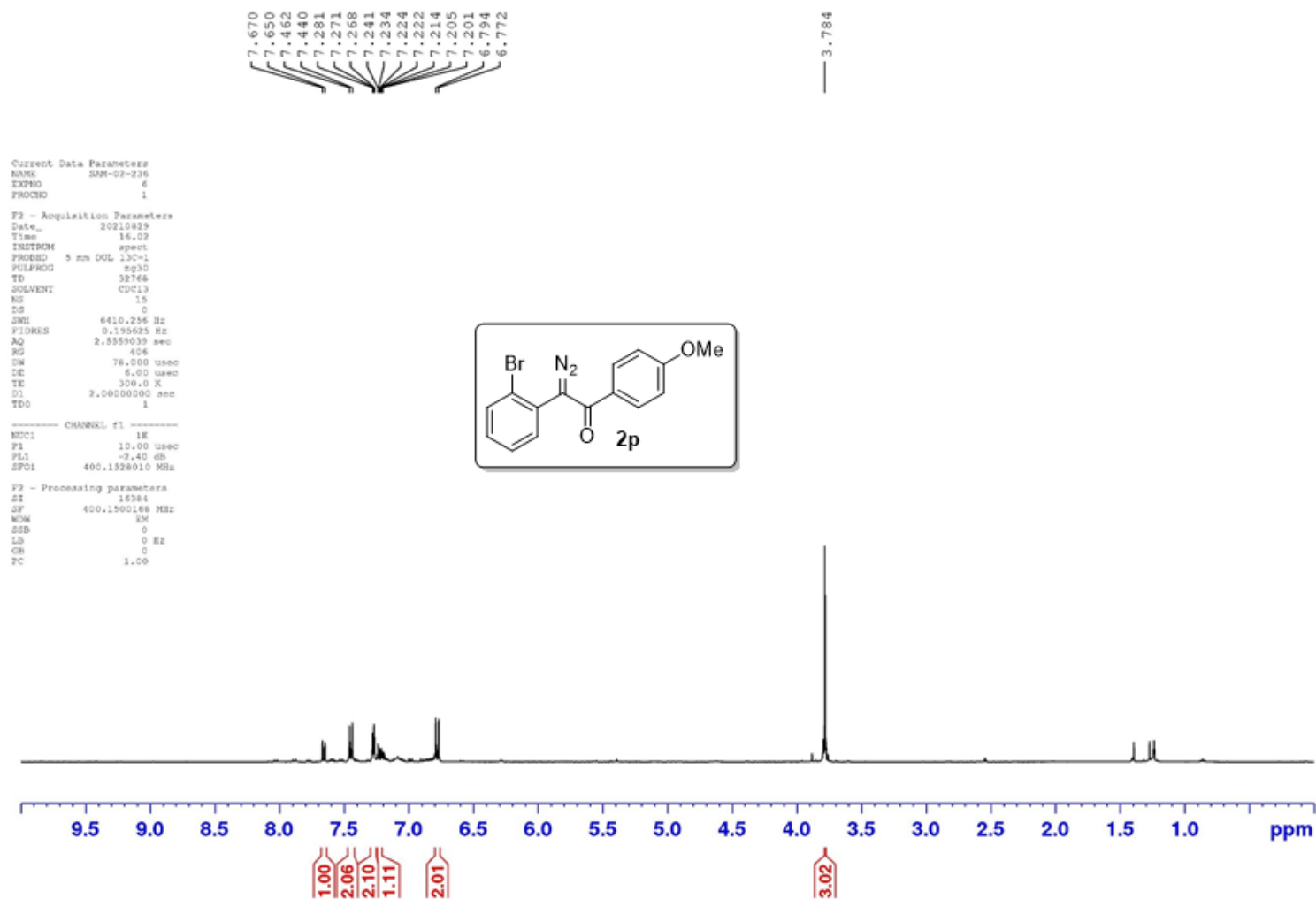
Solvent: CDCl₃
SFO1: 400 MHz



Solvent: CDCl₃
SFO1: 100 MHz



Solvent: CDCl₃
SFO1: 400 MHz



Solvent: CDCl₃
SFO1: 100 MHz

SAM-02-235

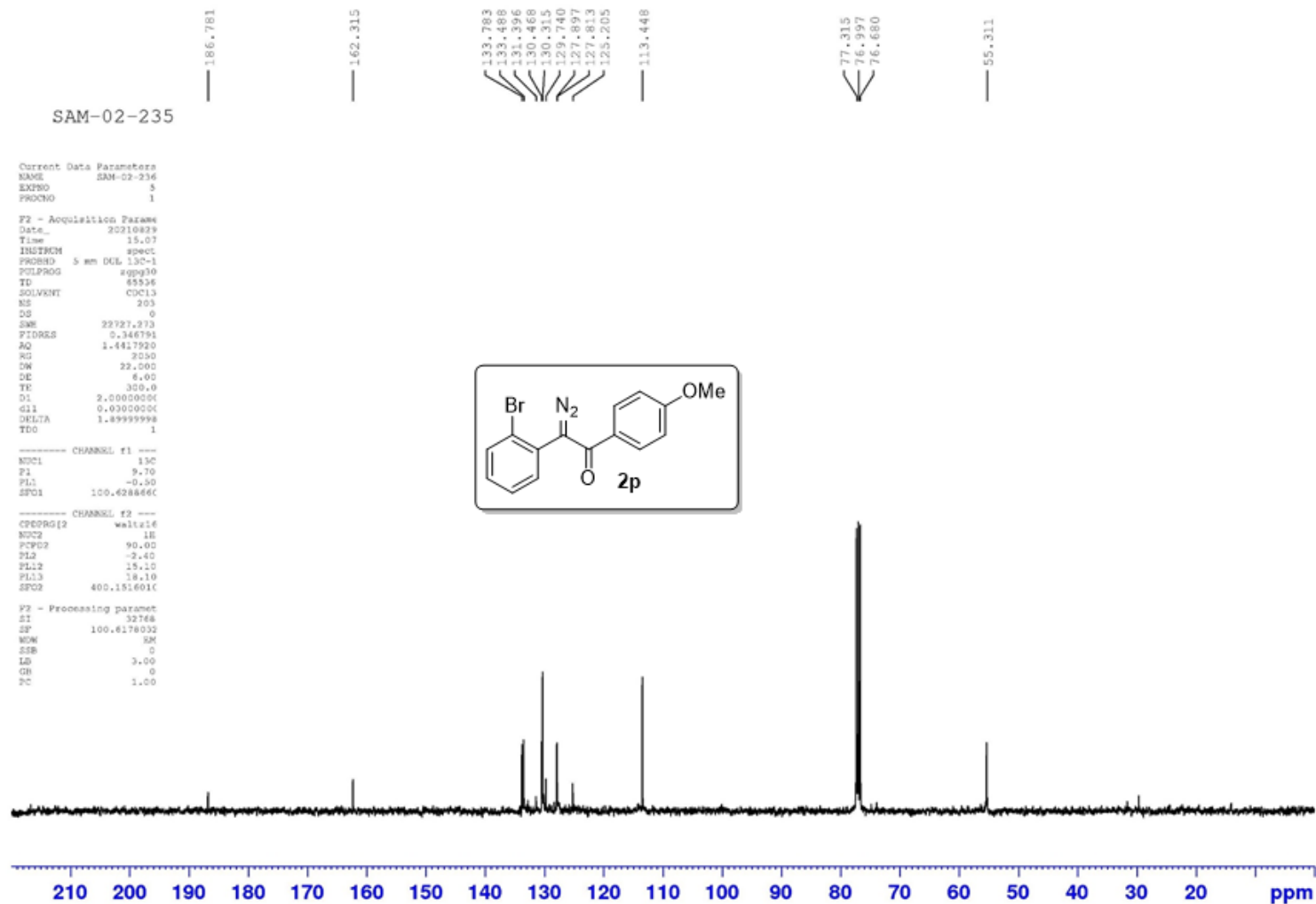
Current Data Parameters
NAME SAM-02-236
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210829
Time 15:07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 203
DS 0
SWH 22727.273
FIDRES 0.346791
AQ 1.4417920
RG 3050
OW 22.000
DE 6.00
TE 300.0
D1 2.0000000
d11 0.0300000
DELTA 1.8999999
TD0 1

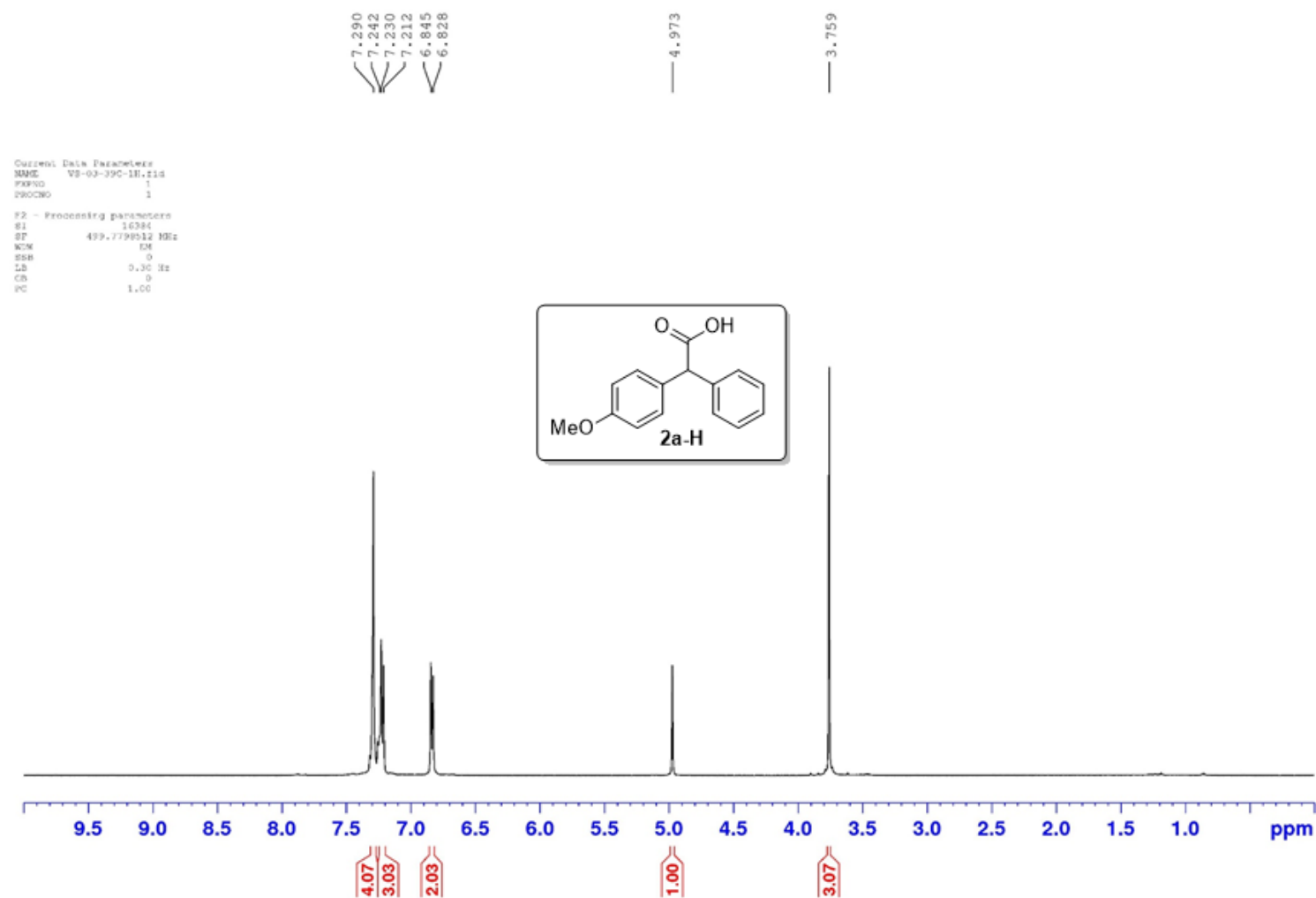
----- CHANNEL f1 -----
NUC1 13C
P1 9.70
PL1 -0.50
SFO1 100.628466C

----- CHANNEL f2 -----
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00
PL2 -2.00
PL12 15.15
PL13 18.10
SFO2 400.151601C

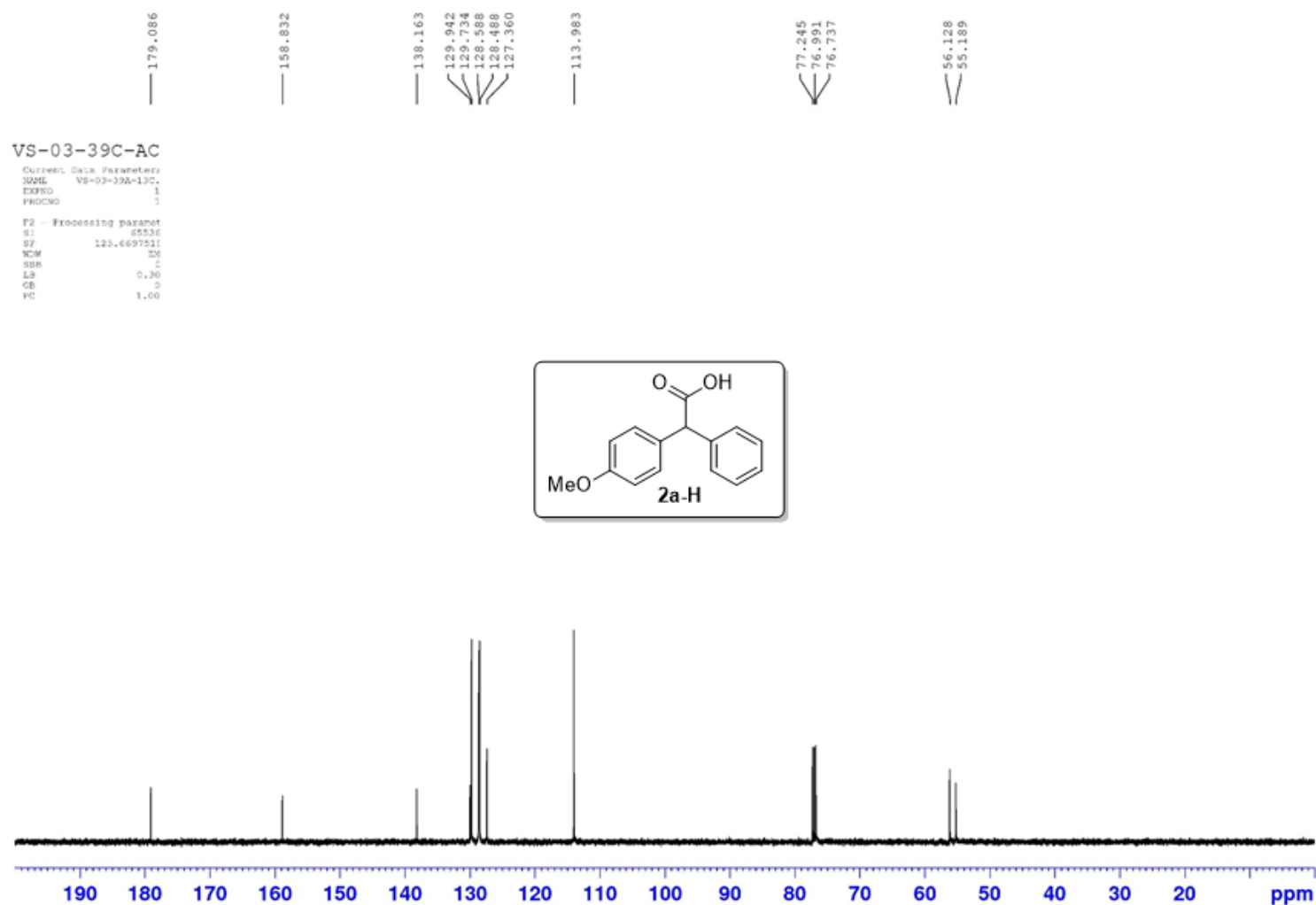
F2 - Processing parameters
SI 32768
SF 100.6178032
WOM RM
SGB 0
LB 3.00
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 500 MHz



Solvent: CDCl_3
SFO1: 125 MHz

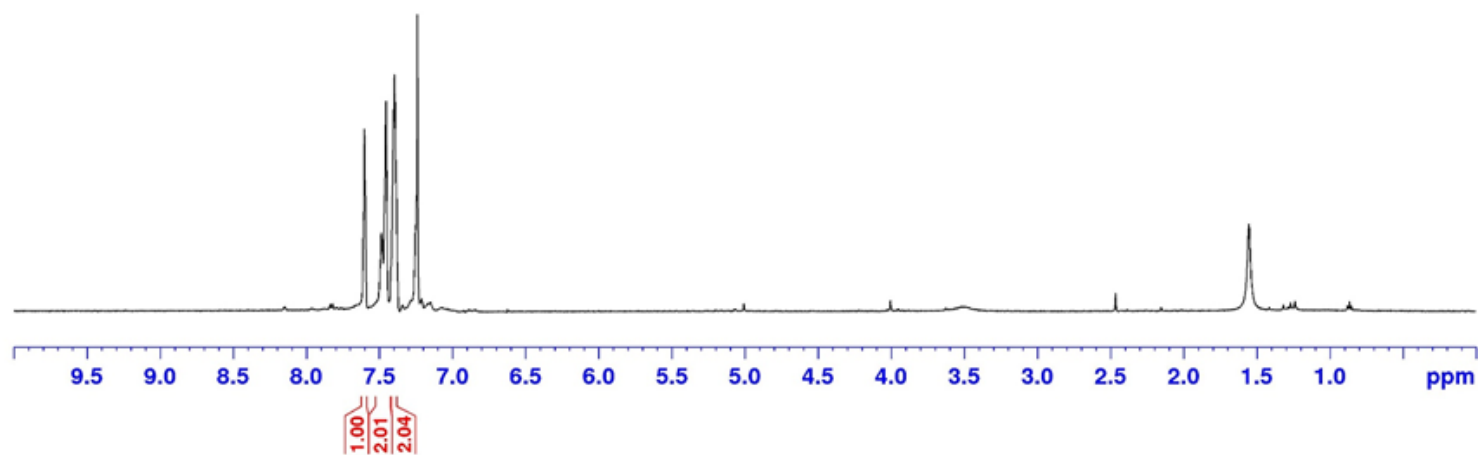
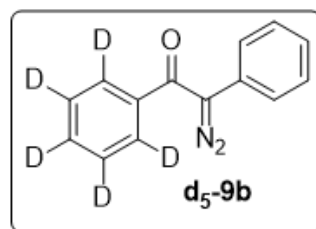


Solvent: CDCl₃
SFO1: 500 MHz

7.602
7.486
7.481
7.455
7.404
7.398
7.391
7.240

1.552

Current Data Parameters
NAME V8-03-20-1H.f16
PROCNO 3
PROCNO 1
F2 - Processing parameters
SI 16384
SF 499.7798474 MHz
WIDEN EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



VS-03-20

Current Data Parameters
NAME VS-03-20-C-116
EXPNO 3
PROCNO 1

F2 - Processing parameter
SI 131.072
SF 175.950397
KCM 26
SR 0
LB 0.30
GB 0
PC 1.00

137.866
137.775
137.775
131.589
131.483
129.030
129.030
128.919
128.808
128.524
128.408
128.296
127.724
127.619
126.669
126.037
125.923
125.867

77.182
77.000
76.818

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

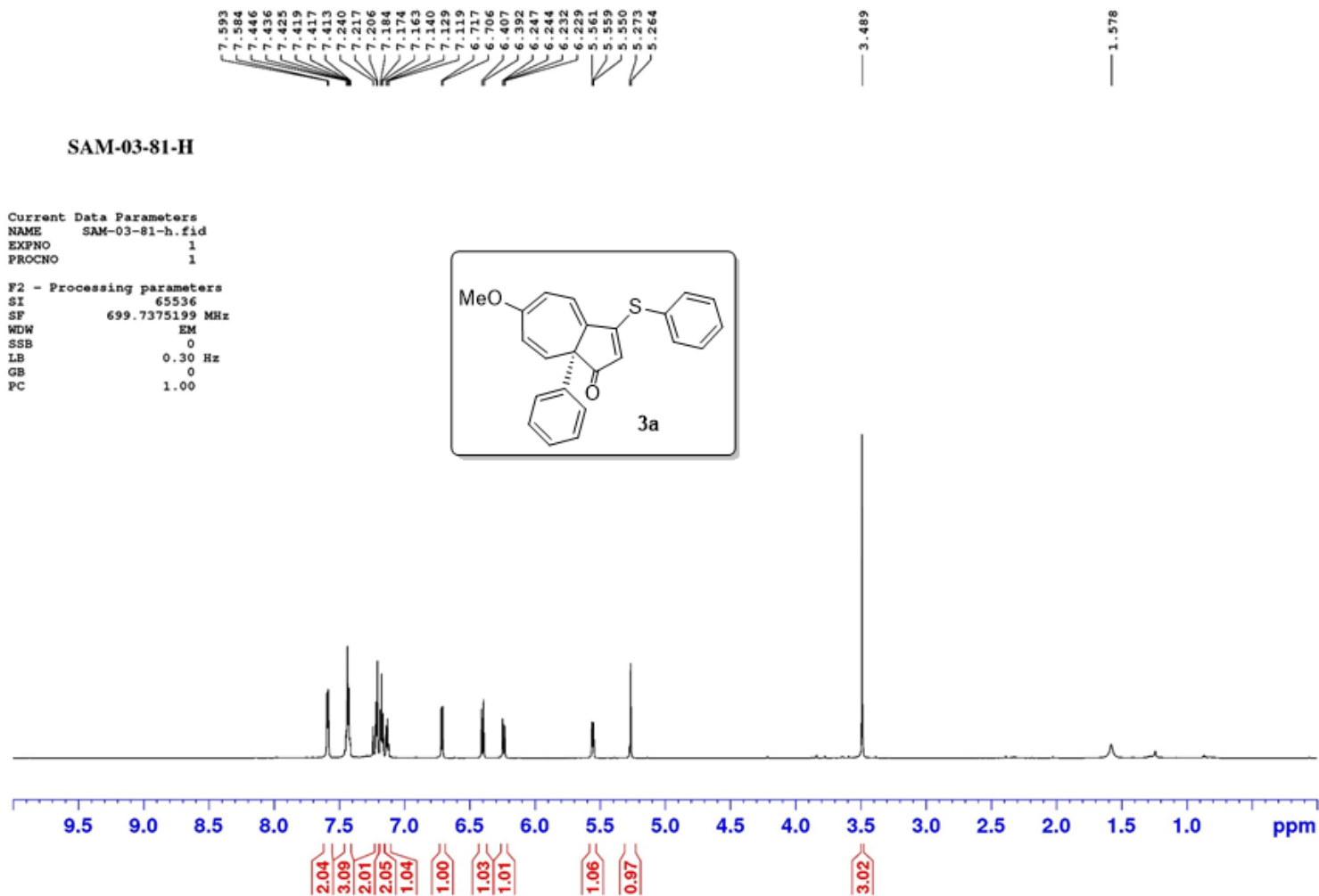
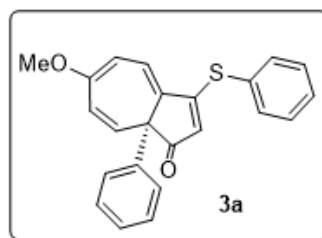
N=[N]C(=O)c1ccccc1C2=CC(=C(C(=C2)D)D)D
d₅-9b

Solvent: CDCl₃
SFO1: 700 MHz

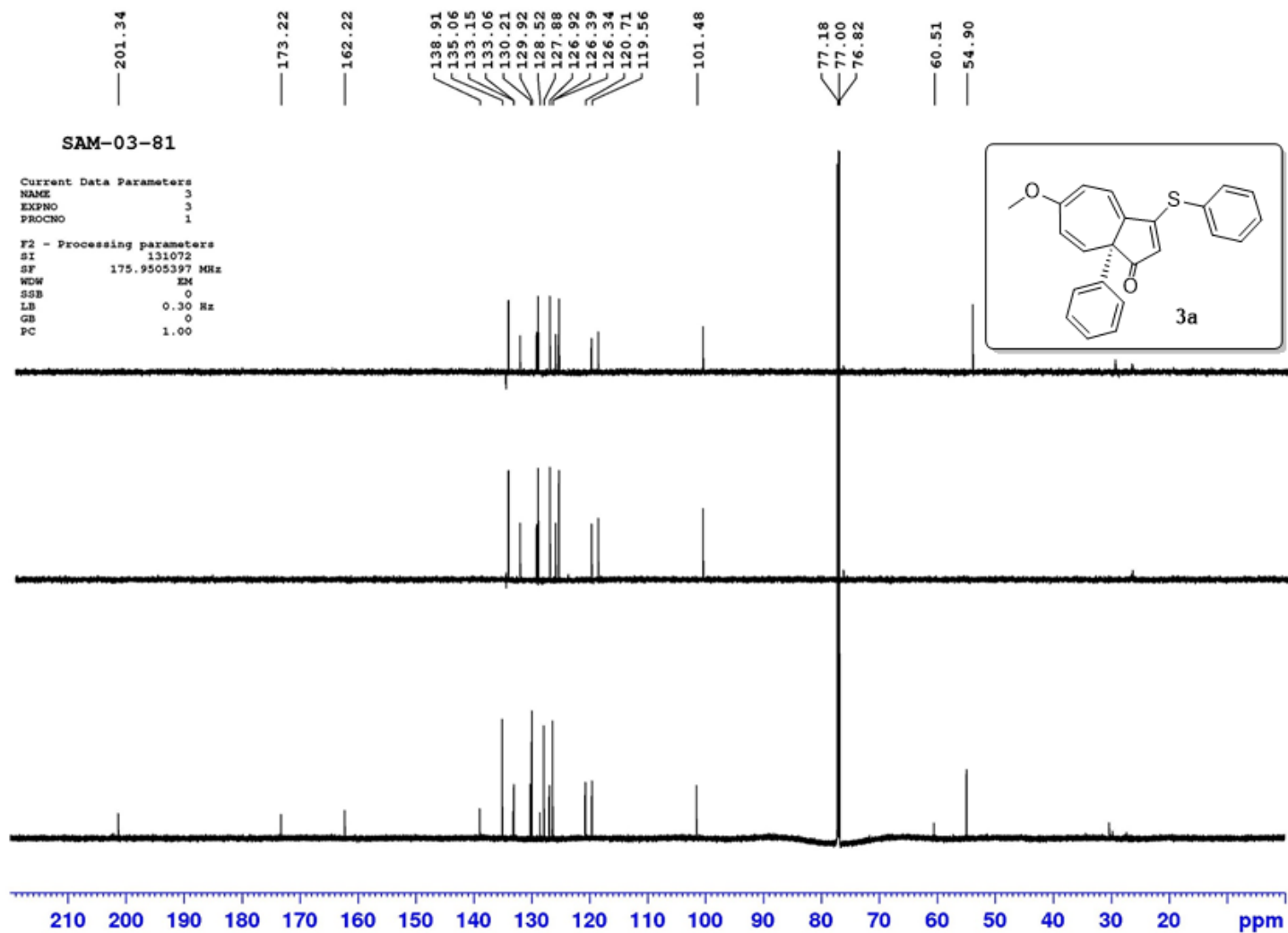
SAM-03-81-H

Current Data Parameters
NAME SAM-03-81-h.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7375199 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
 SFO1: 175 MHz

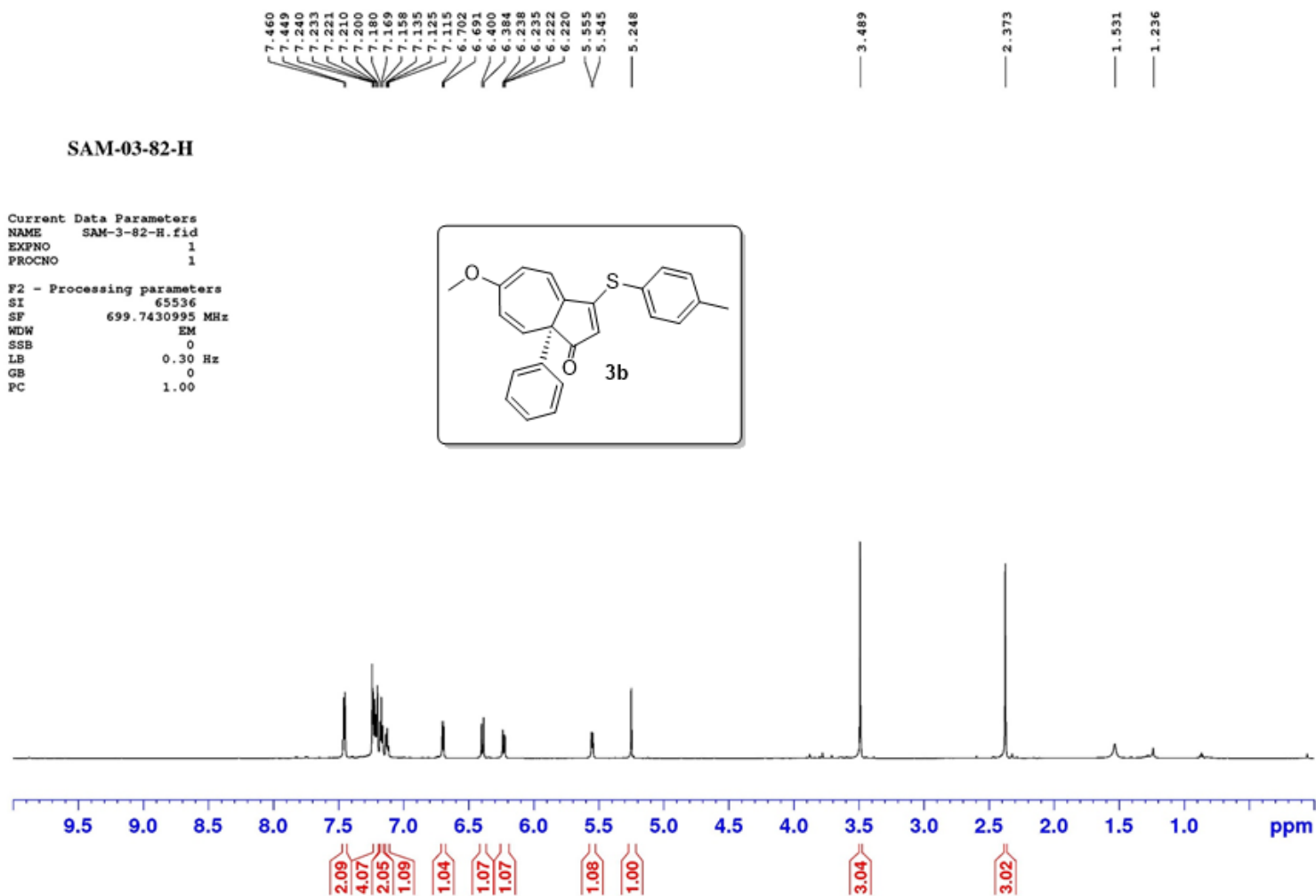
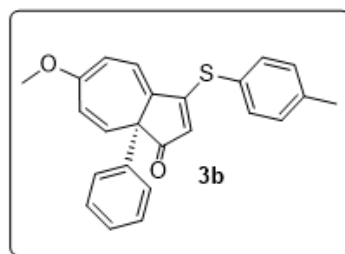


Solvent: CDCl₃
SFO1: 700 MHz

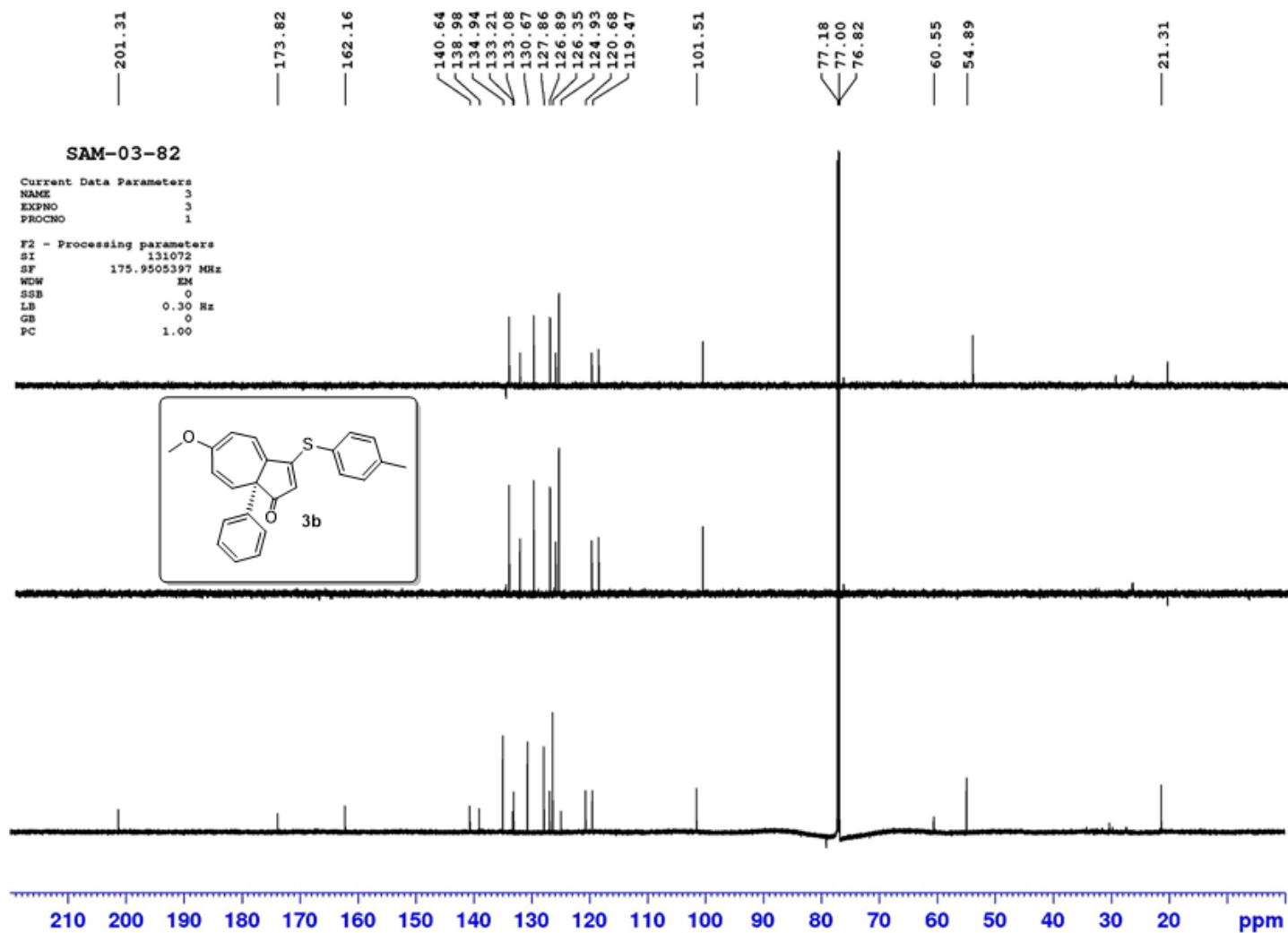
SAM-03-82-H

Current Data Parameters
NAME SAM-3-82-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7430995 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
 SFO1: 175 MHz



Solvent: CDCl₃
SFO1: 700 MHz

SAM-03-83-H

Current Data Parameters
NAME SAM-03-83-H.fid
EXPNO 1
PROCNO 1

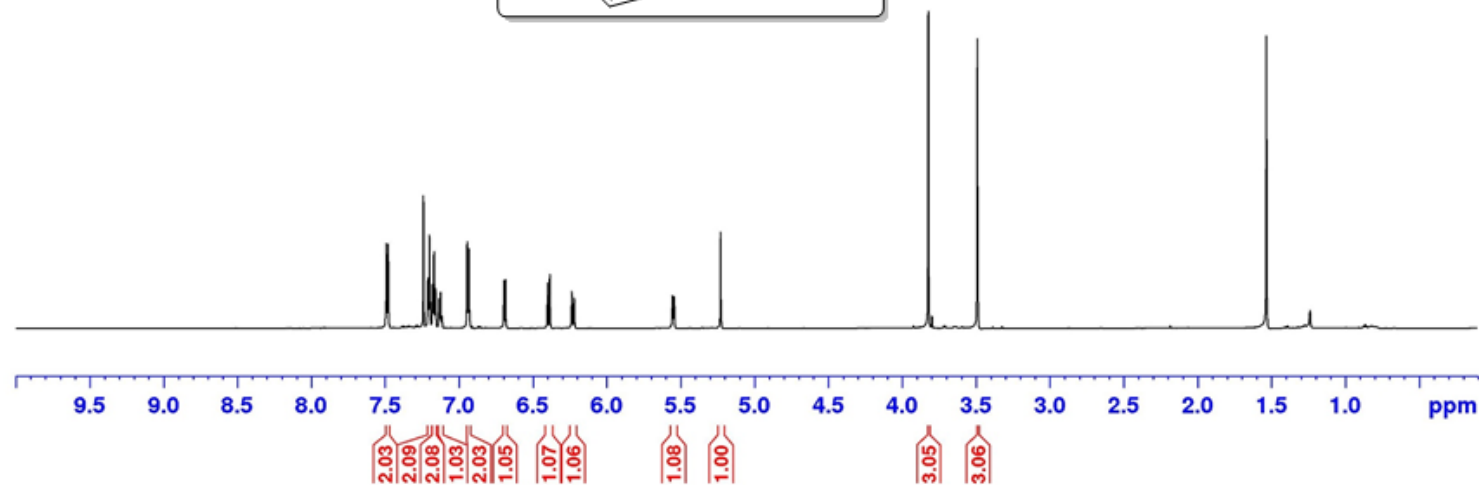
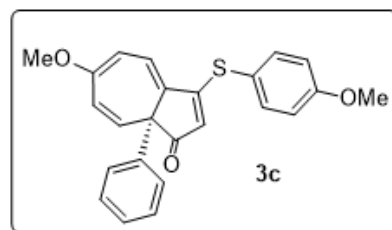
F2 - Processing parameters
SI 65536
SF 699.7431023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.491
7.479
7.240
7.209
7.198
7.179
7.168
7.157
7.134
7.124
7.114
6.944
6.931
6.895
6.884
6.899
6.884
6.884
6.835
6.833
6.820
6.818
5.554
5.543
5.227

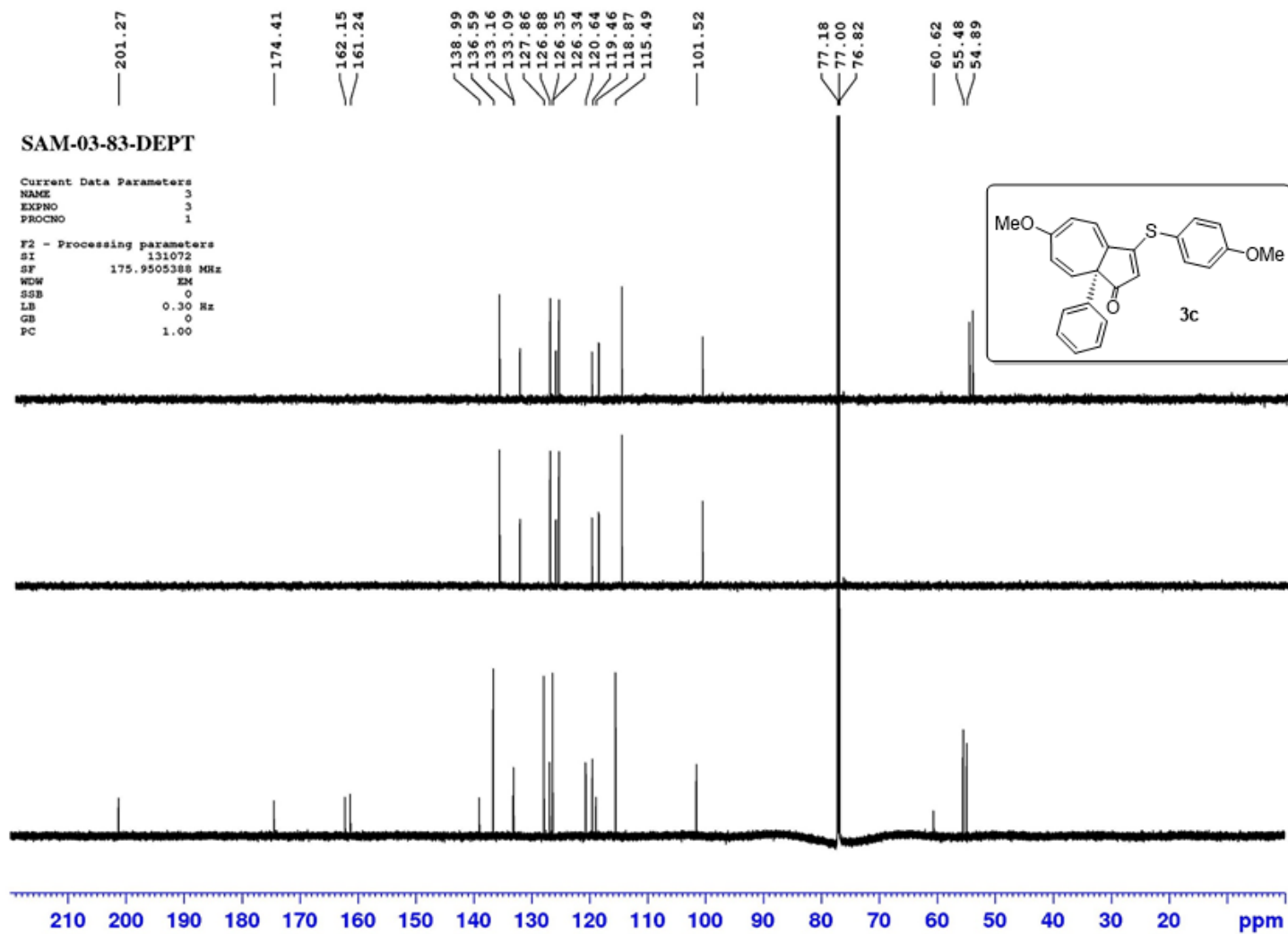
3.821

3.488

1.531



Solvent: CDCl_3
 SFO1: 175 MHz



Solvent: CDCl₃
SFO1: 700 MHz

SAM-03-84-H

Current Data Parameters
NAME SAM-3-84-H.fid
EXPNO 1
PROCNO 1

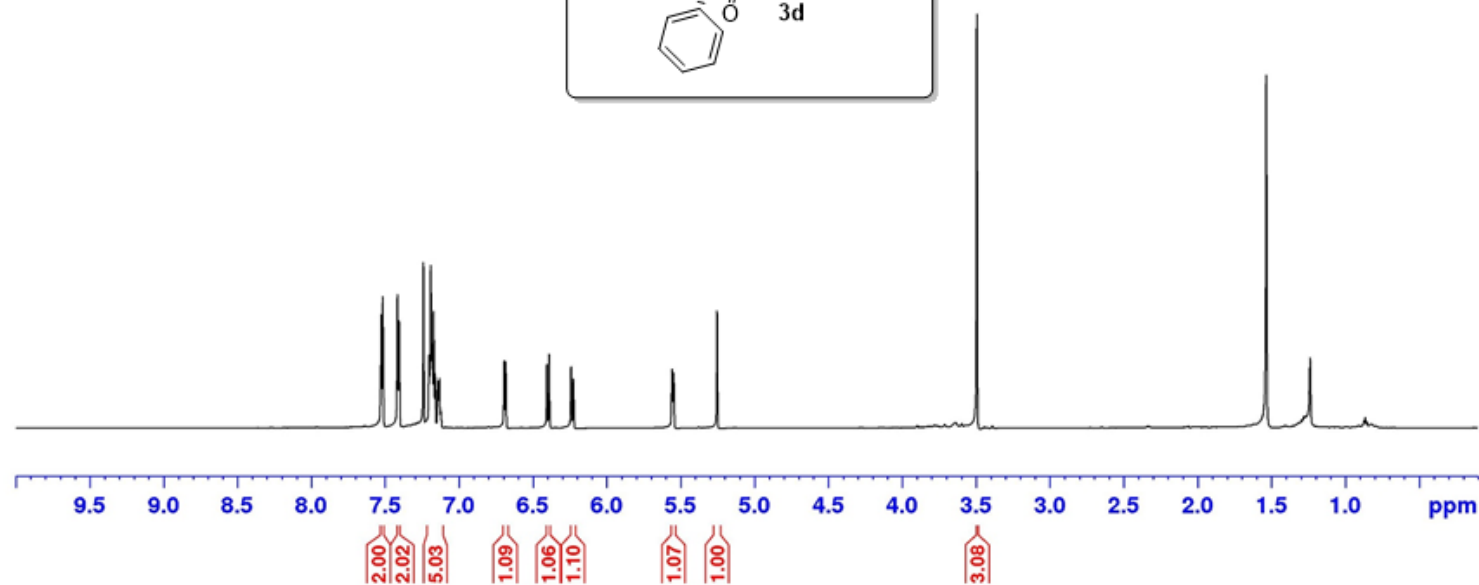
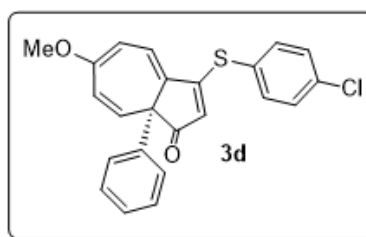
F2 - Processing parameters
SI 65536
SF 699.7430984 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.526
7.515
7.516
7.416
7.404
7.240
7.201
7.190
7.182
7.171
7.160
7.141
7.132
6.693
6.682
6.404
6.389
6.239
6.224

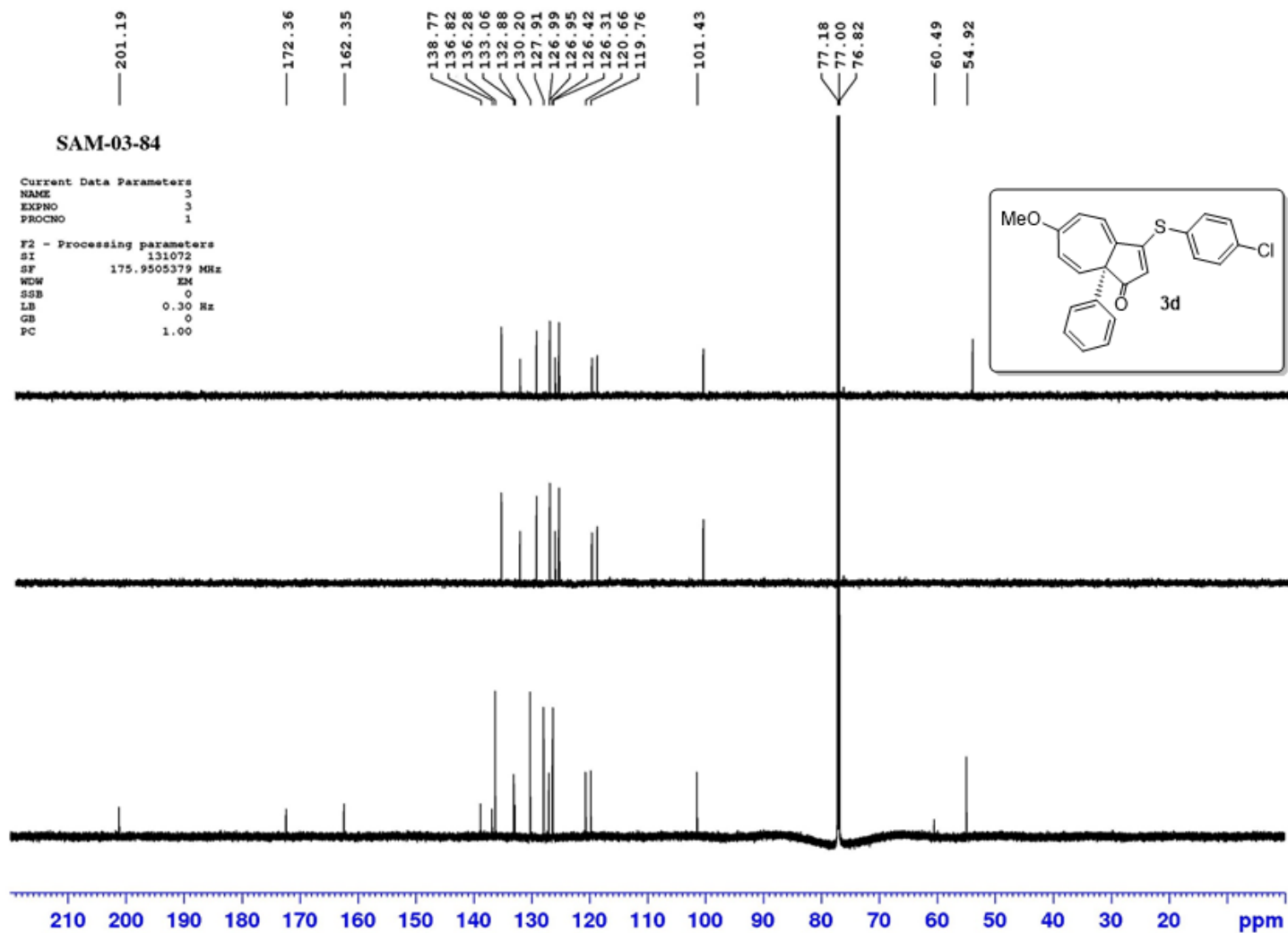
5.556
5.545
5.251

3.492

1.532



Solvent: CDCl_3
 SFO1: 175 MHz



Solvent: CDCl₃
SFO1: 700 MHz

SAM-03-88-H

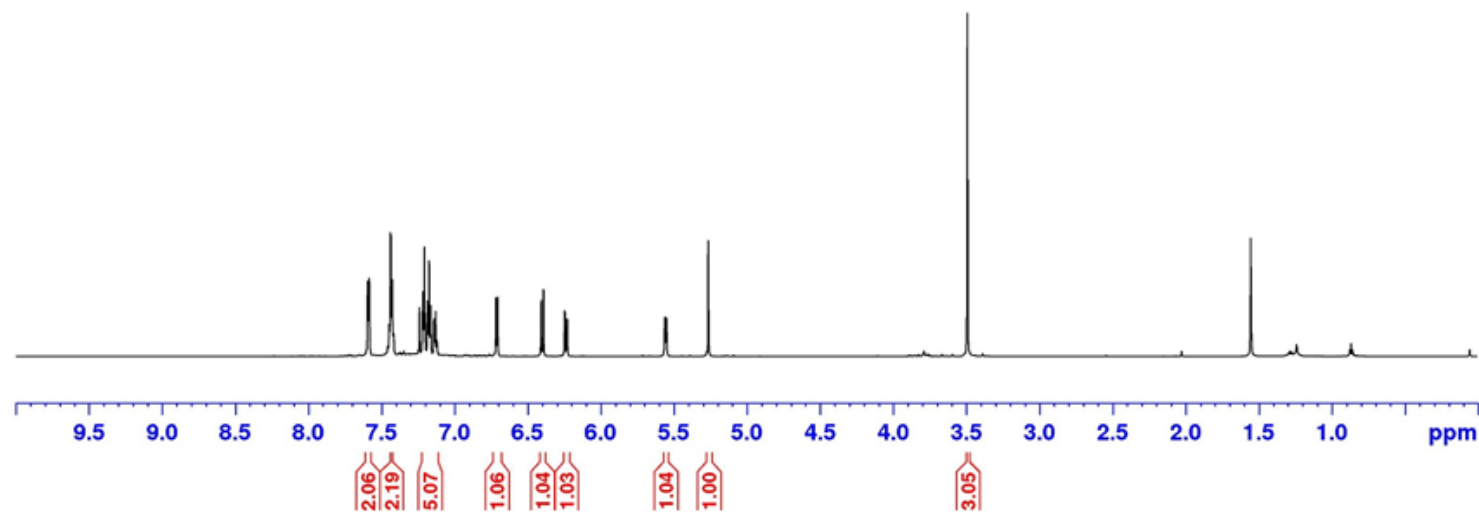
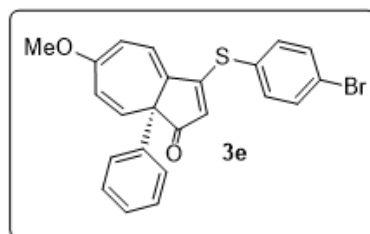
Current Data Parameters
NAME SAM-03-88-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7430981 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

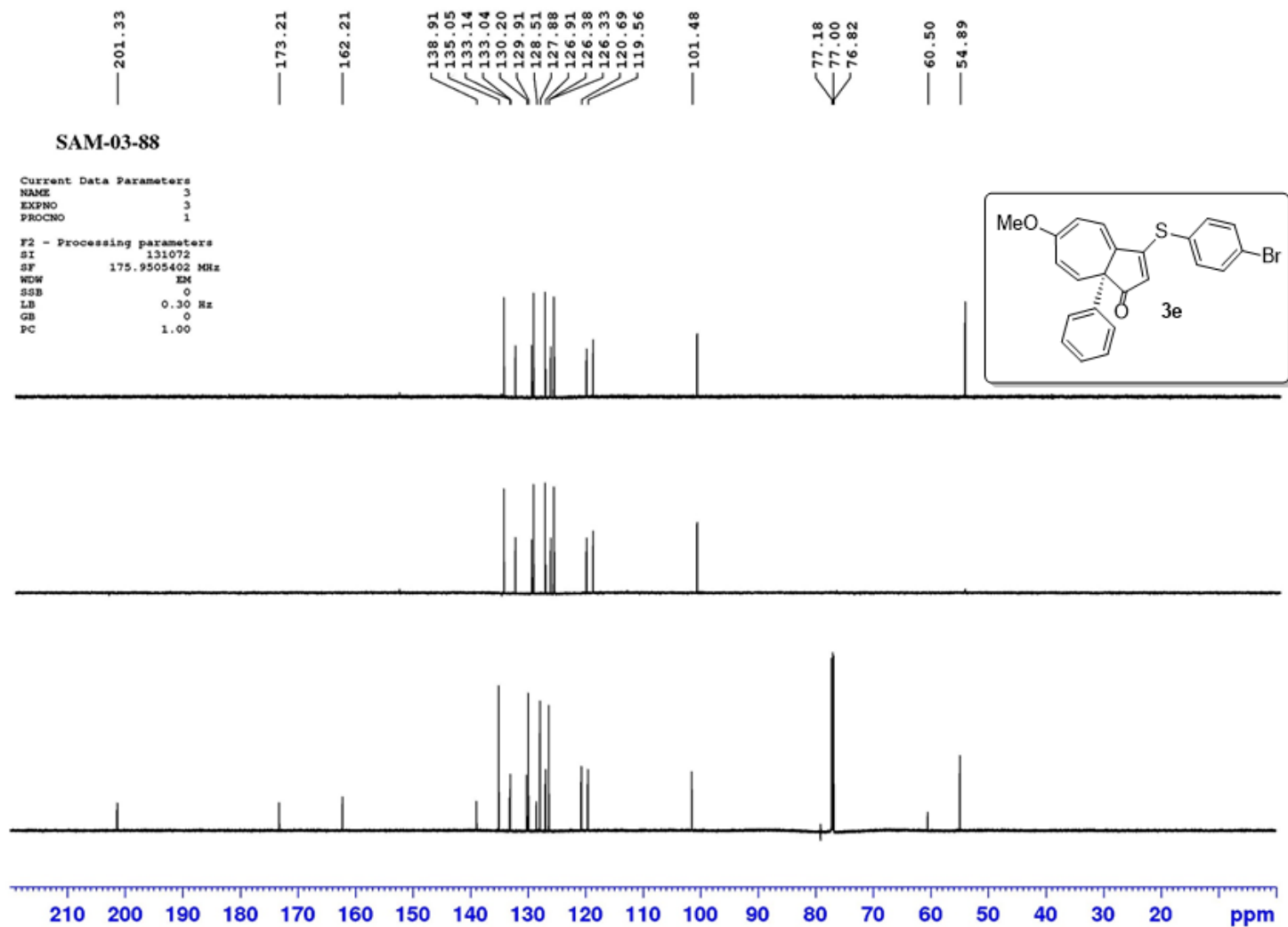
7.593
7.581
7.436
7.426
7.240
7.216
7.205
7.184
7.173
7.162
7.139
7.129
7.119
6.716
6.705
6.406
6.391
6.246
6.244
6.231
6.228
5.561
5.559
5.551
5.549
5.263

3.491

1.552



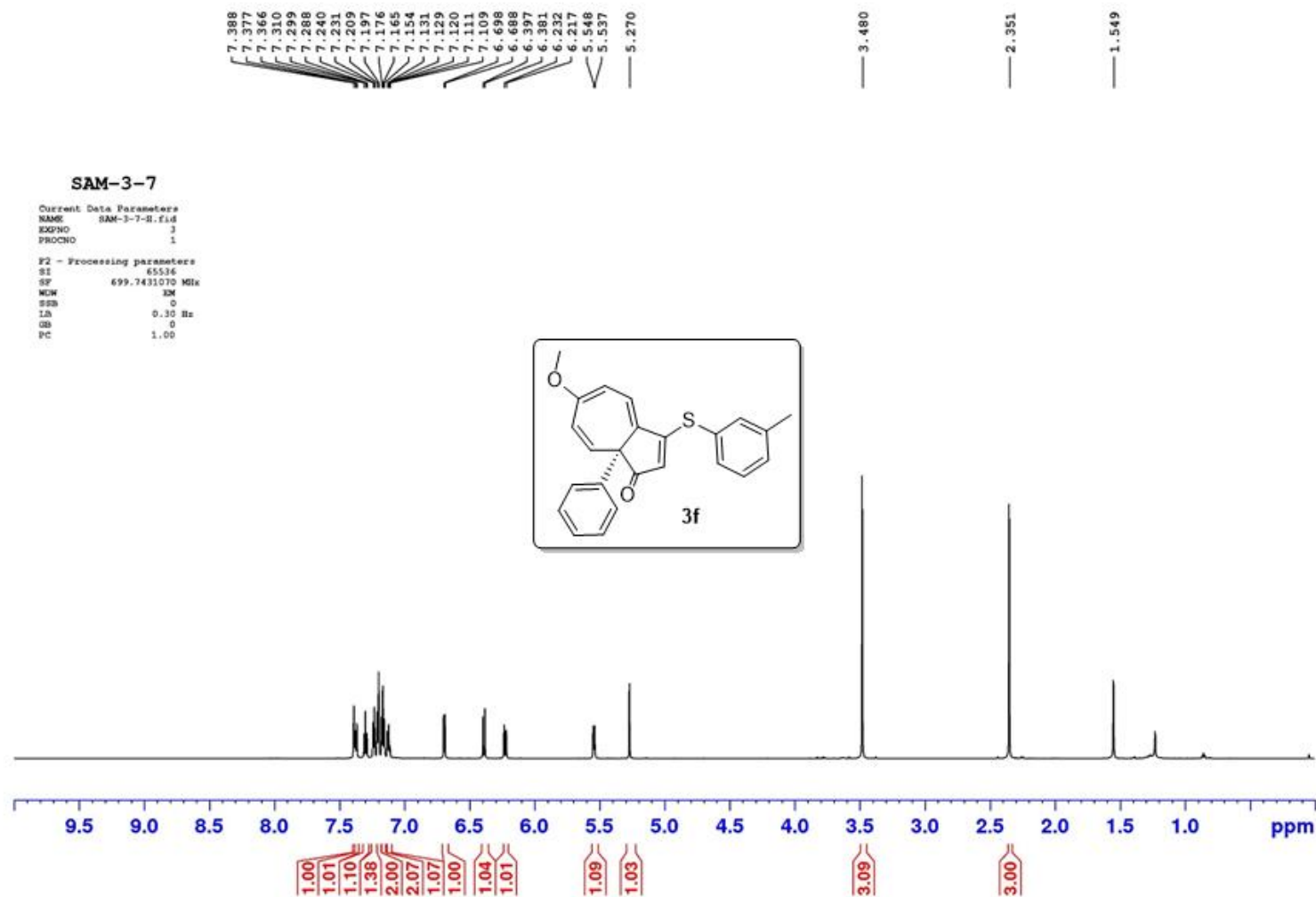
Solvent: CDCl_3
 SFO1: 175 MHz



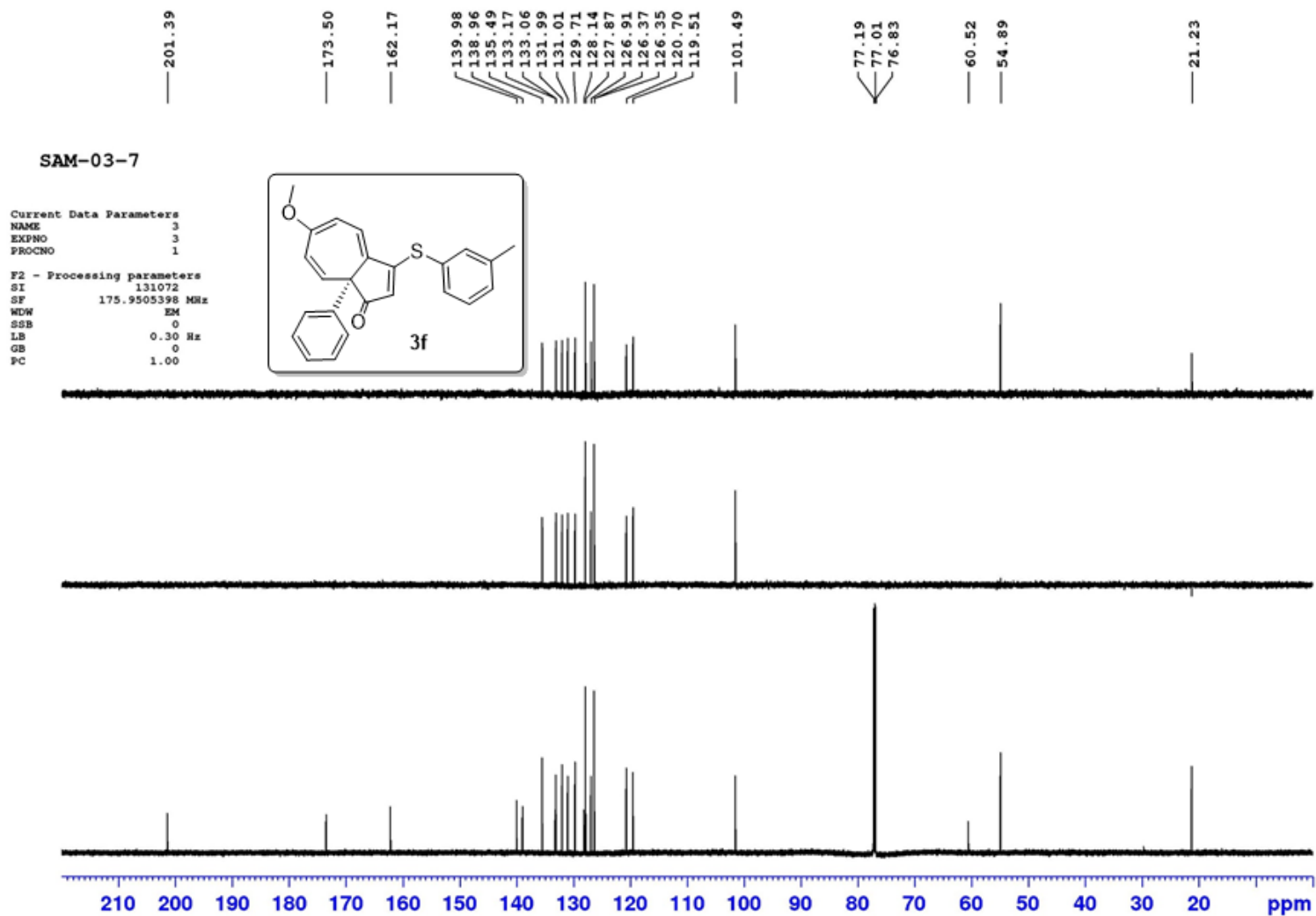
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-7

Current Data Parameters
NAME SAM-3-7-8.fid
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431070 MHz
WDW EM
SSB 0
LA 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl₃
SFO1: 175 MHz

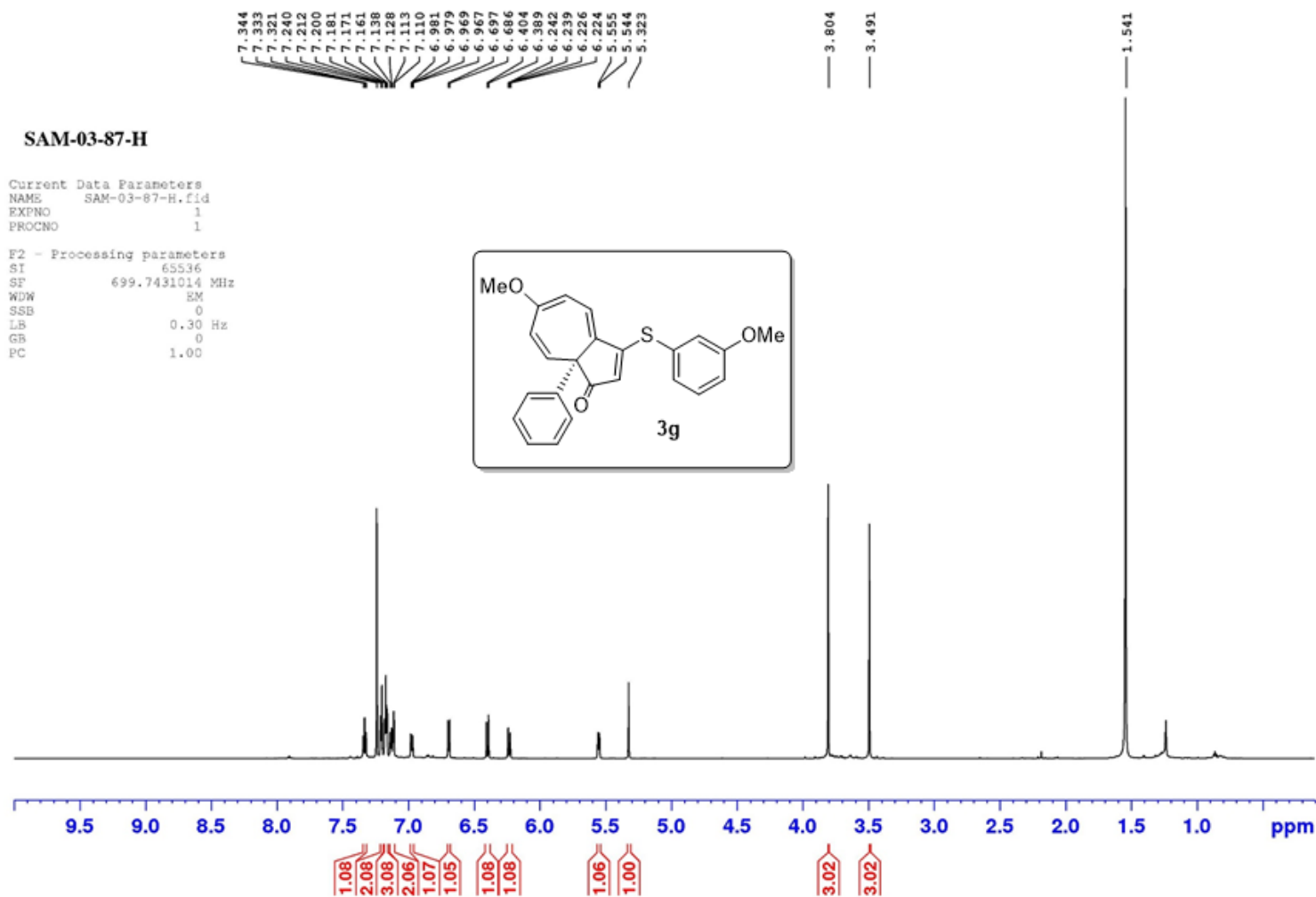
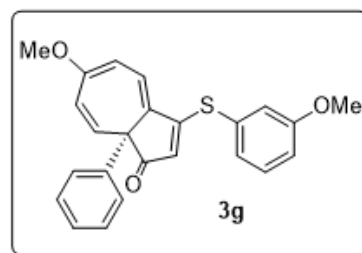


Solvent: CDCl₃
SFO1: 700 MHz

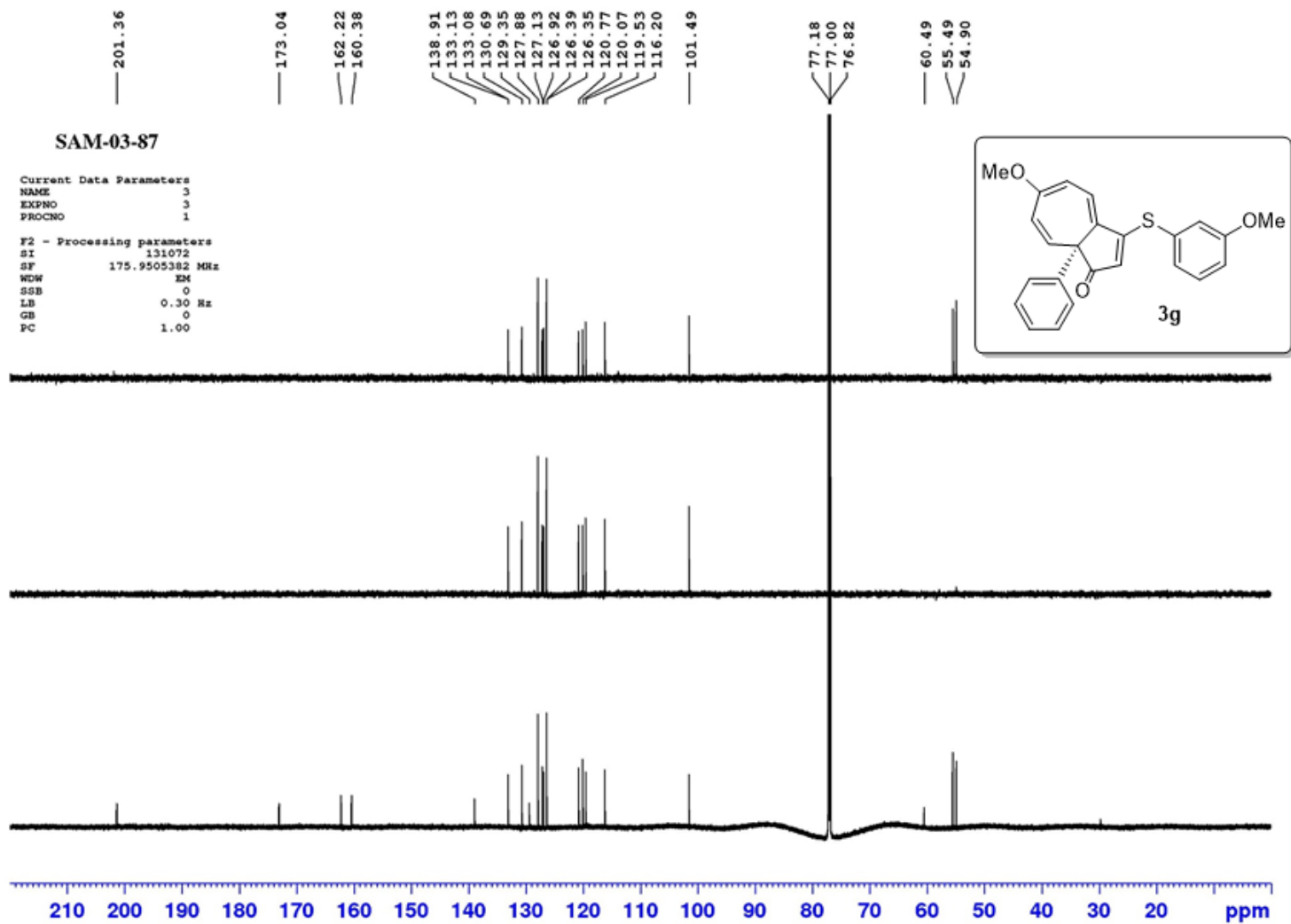
SAM-03-87-H

Current Data Parameters
NAME SAM-03-87-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7431014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



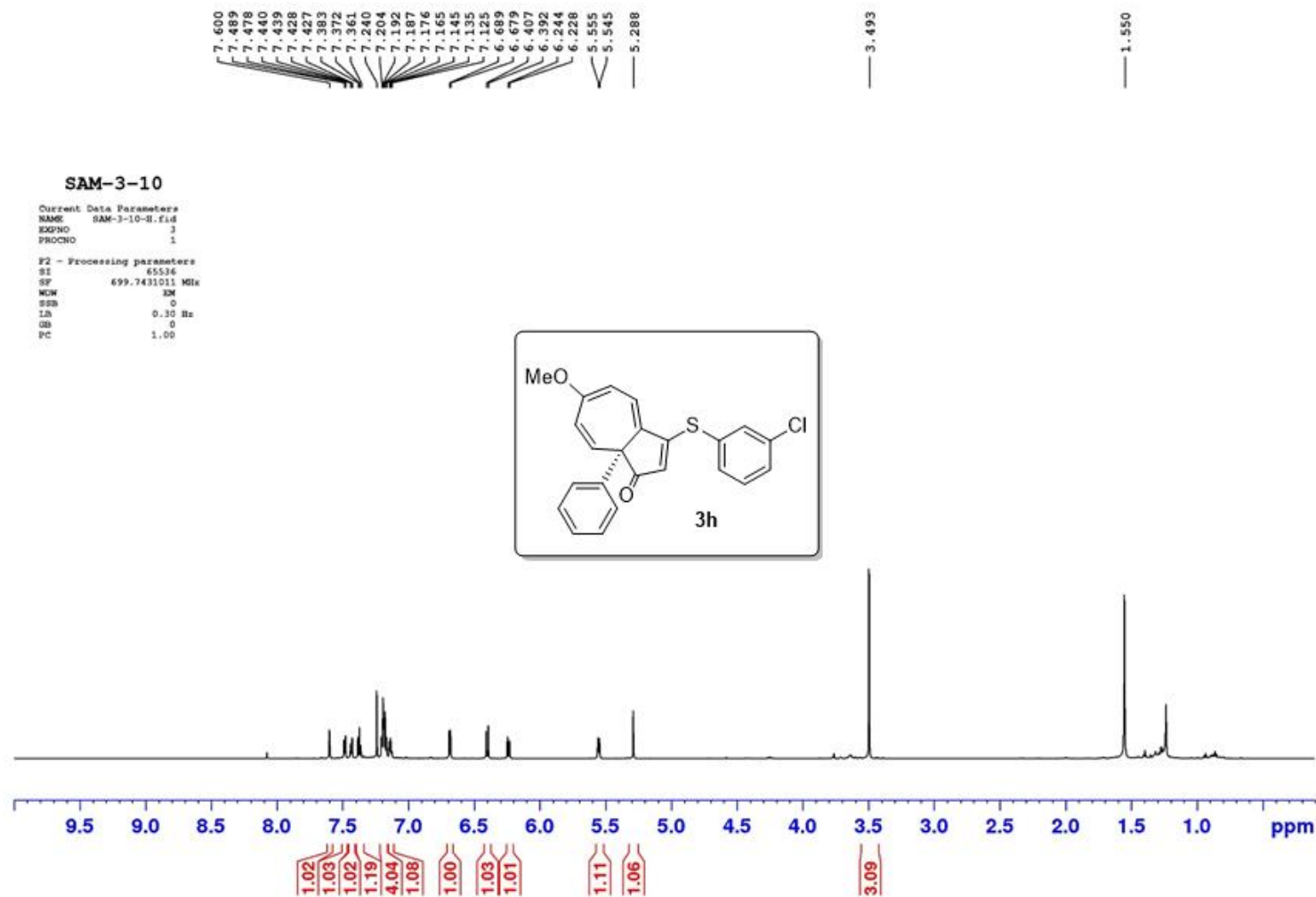
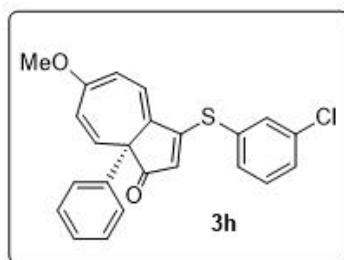
Solvent: CDCl_3
SFO1: 175 MHz



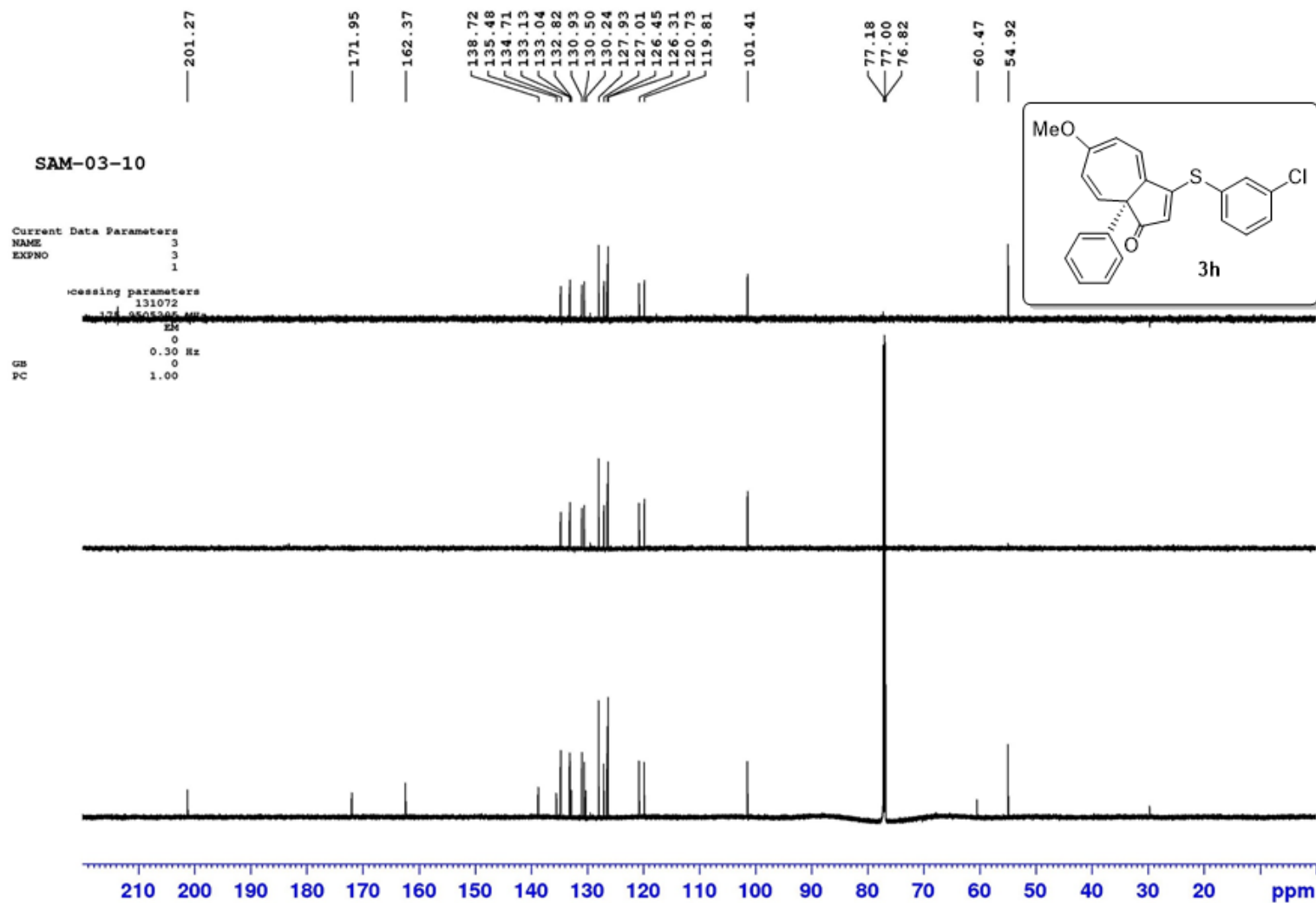
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-10

Current Data Parameters
NAME SAM-3-10-8.fid
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431011 MHz
RG 328
SFO 0
LA 0.30 Hz
GB 0
PC 1.00



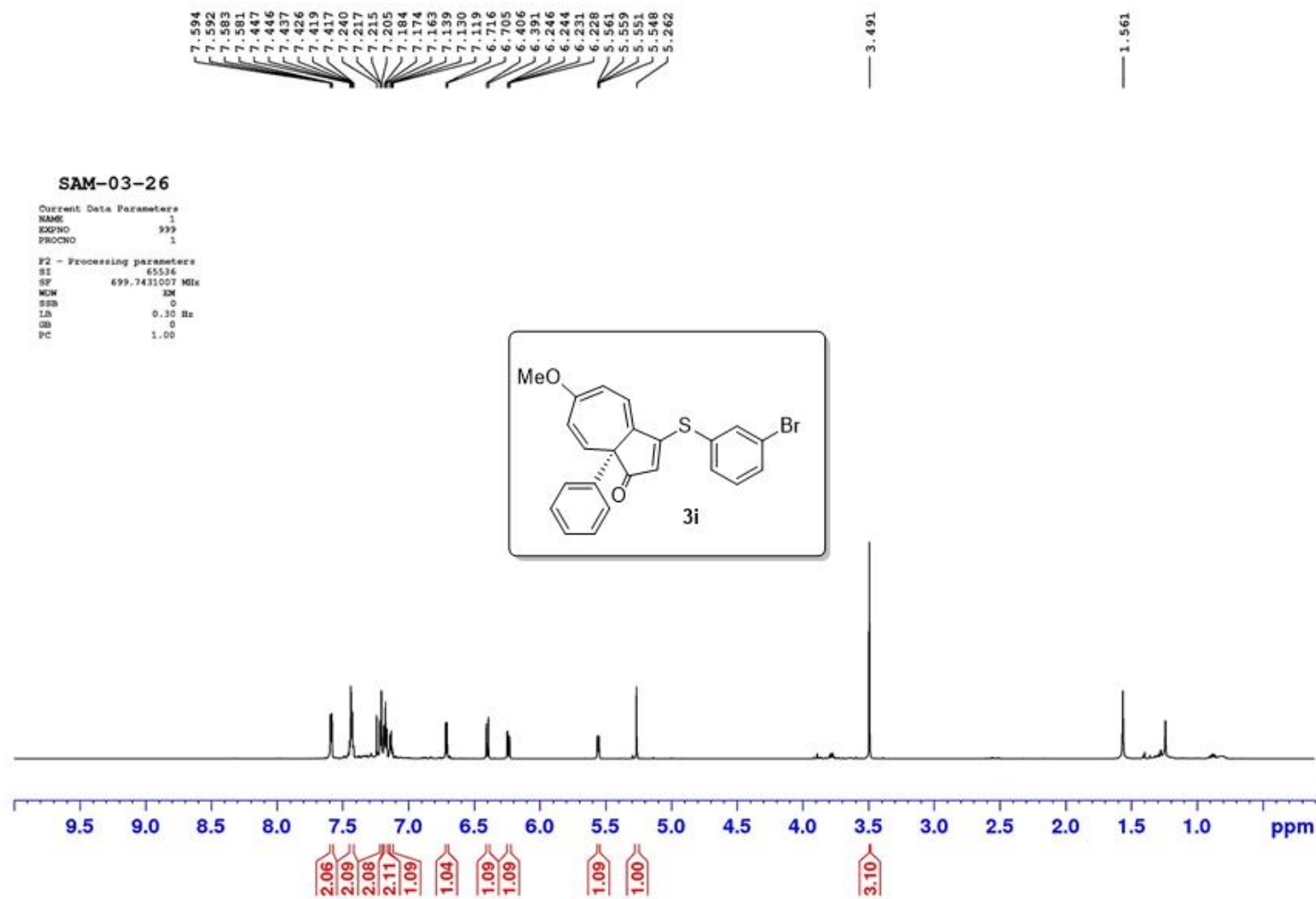
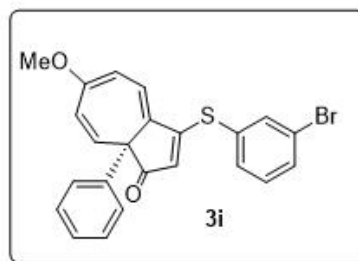
Solvent: CDCl_3
SFO1: 175 MHz



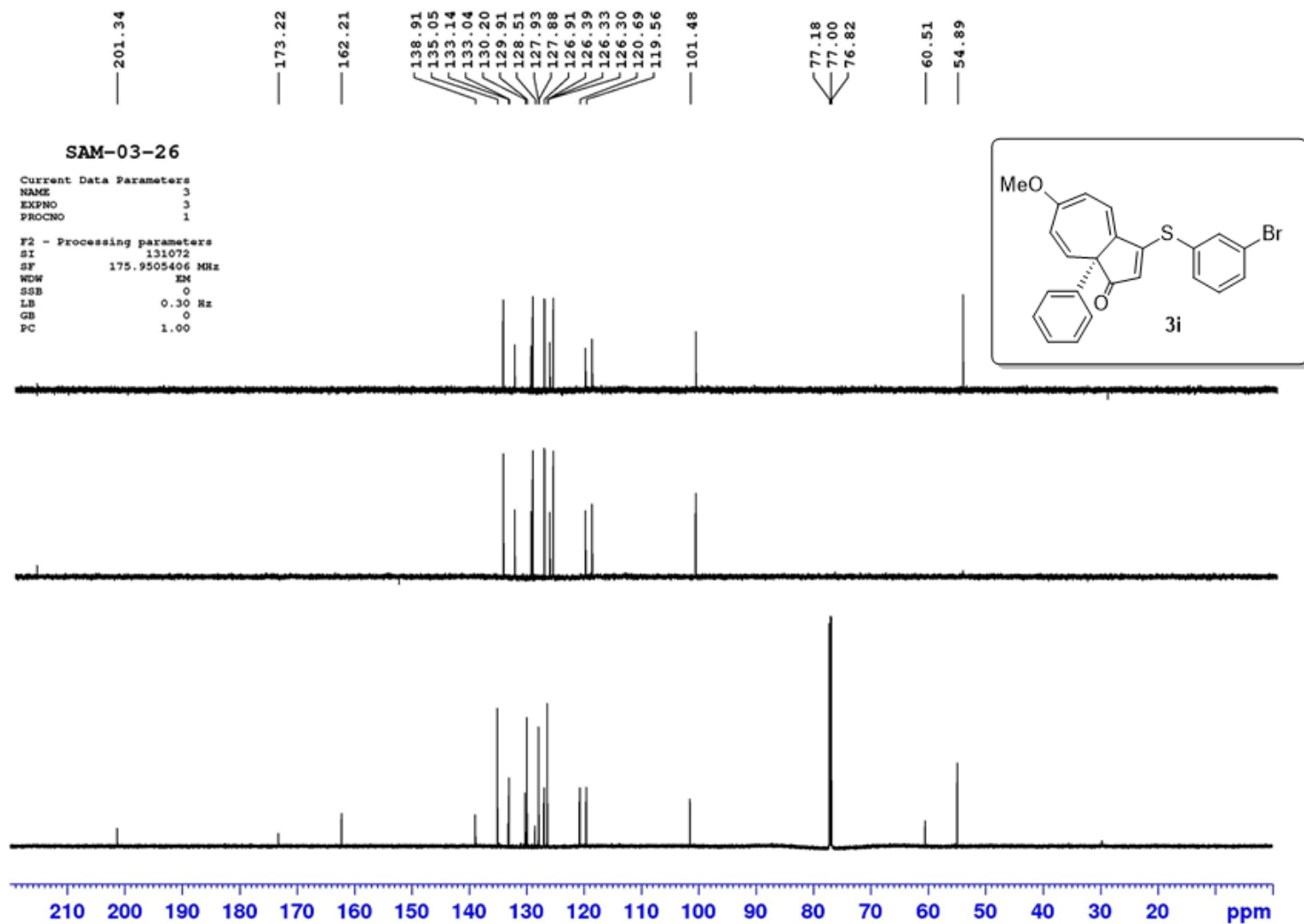
Solvent: CDCl₃
SFO1: 700 MHz

SAM-03-26

Current Data Parameters
NAME 1
EXPNO 999
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431007 MHz
WDW 32M
SSB 0
LA 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl₃
SFO1: 175 MHz



Solvent: CDCl_3
SFO1: 700 MHz

7.581
7.570
7.378
7.377
7.367
7.357
7.356
7.339
7.329
7.255
7.249
7.235
7.218
7.216
7.205
7.190
7.180
7.169
7.146
7.136
7.126
6.743
6.733
6.417
6.401
6.258
6.255
6.243
6.240
5.577
5.575
5.566
5.564
5.095

— 3.504

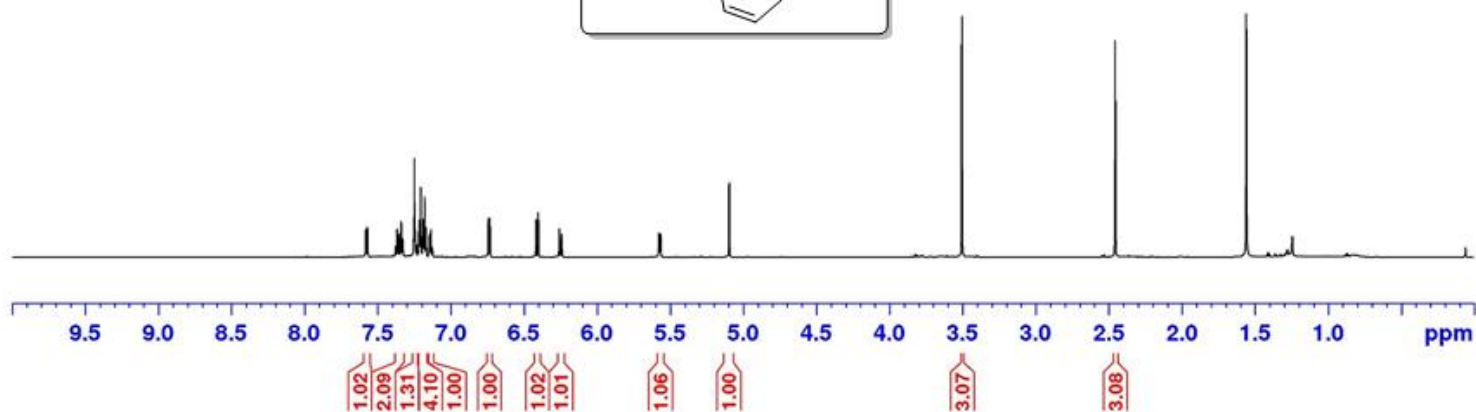
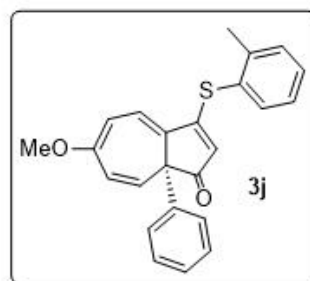
— 2.455

— 1.558

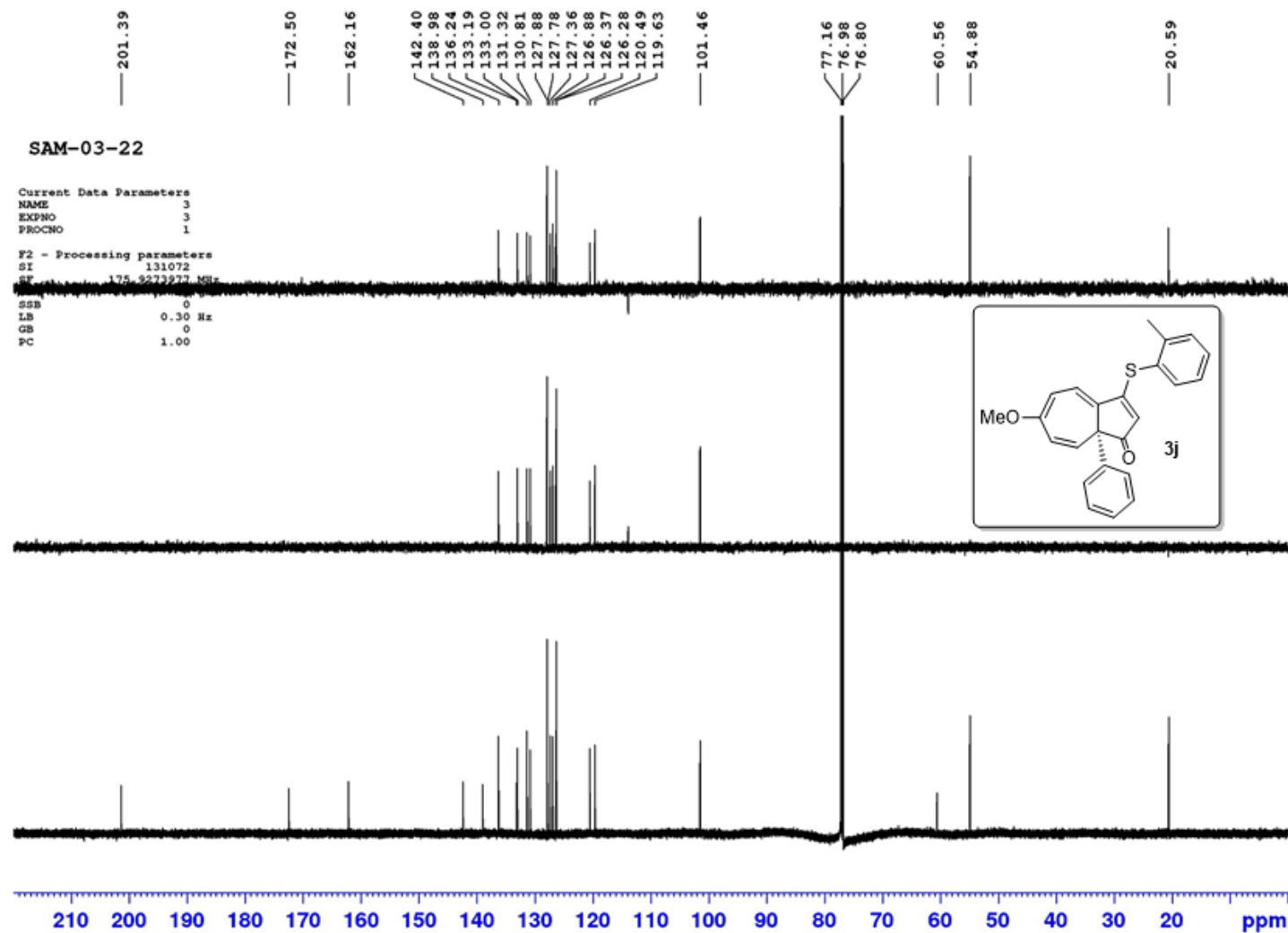
SAM-03-22

Current Data Parameters
NAME SAM-3-22-H.f16
EXPNO 1
PROCNO 1

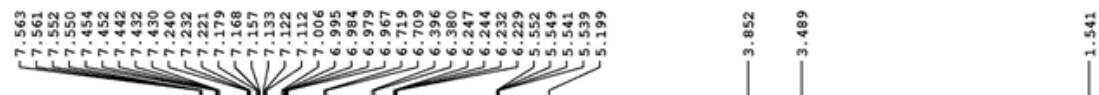
F2 - Processing parameters
SI 65536
SF 699.7430945 MHz
RG 328
SF2 0
LA 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
 SFO1: 175 MHz



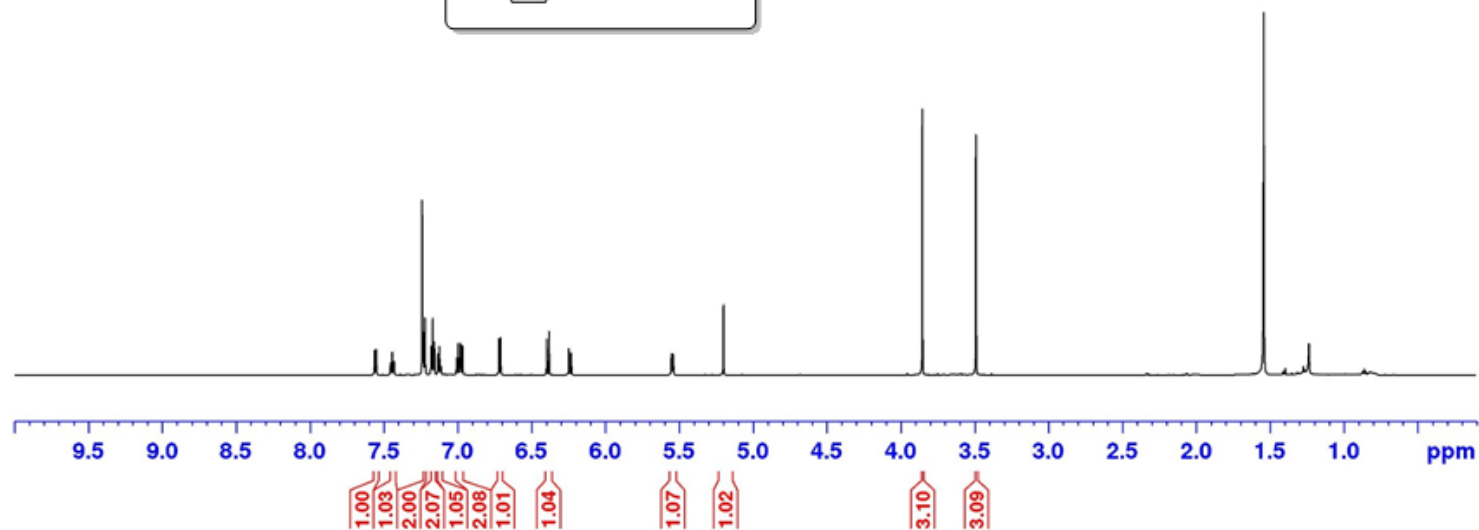
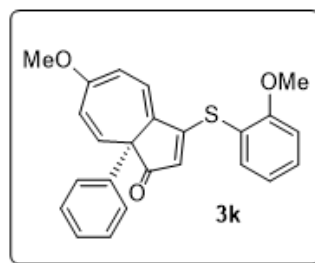
Solvent: CDCl₃
SFO1: 700 MHz



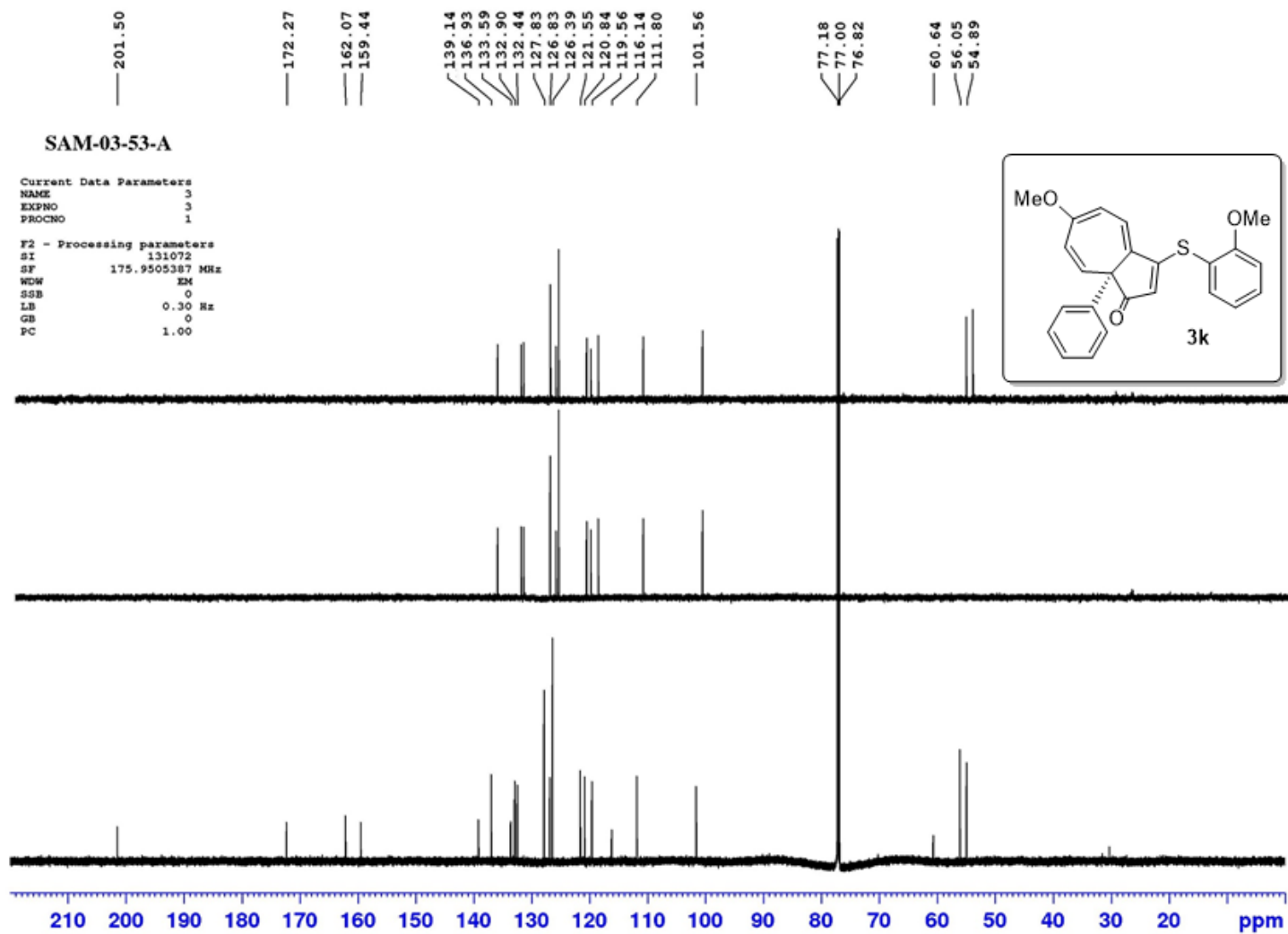
SAM-03-53-P

Current Data Parameters
NAME SAM-03-53-P-H.fid
EXPNO 1
PROCNO 1

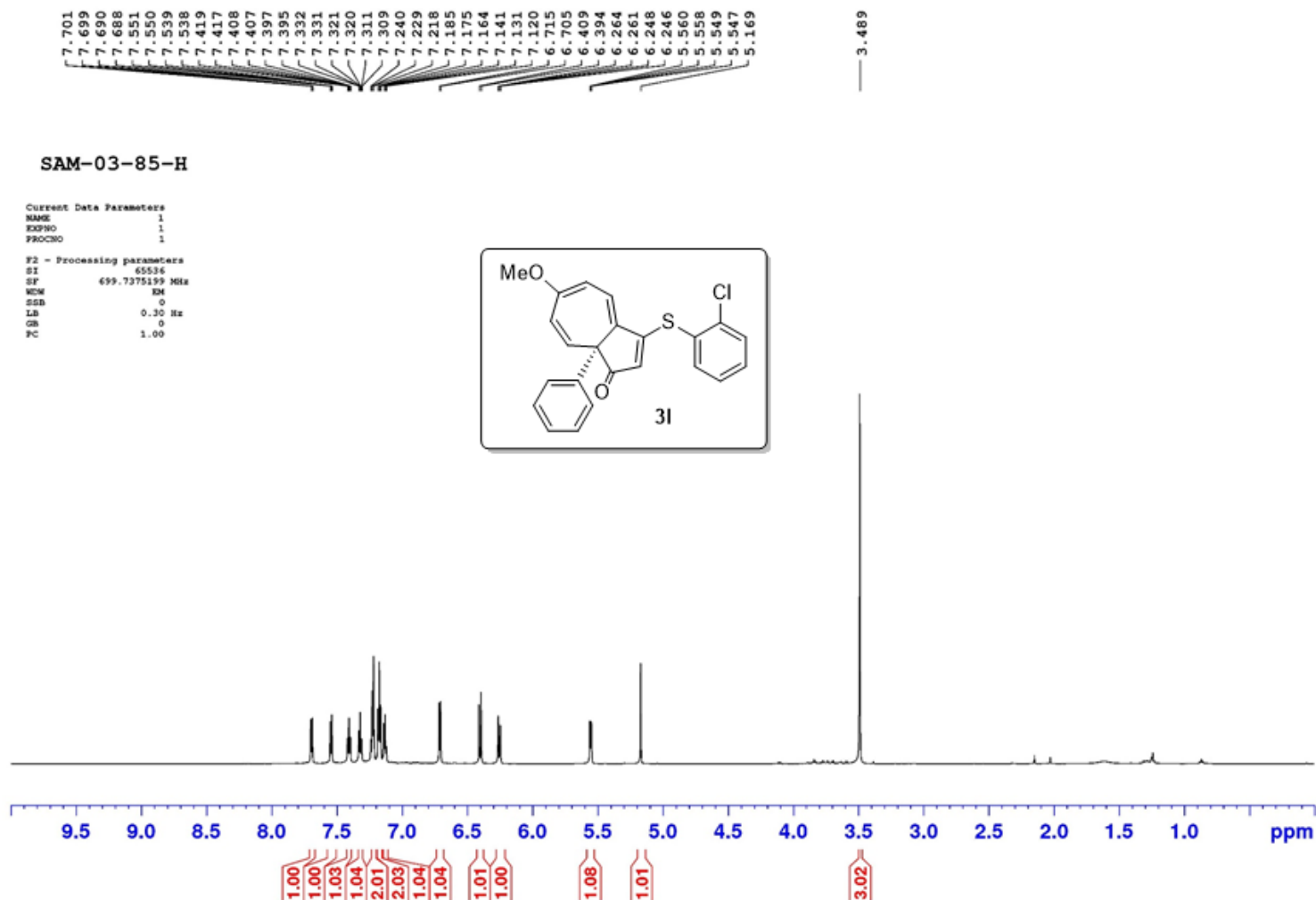
F2 - Processing parameters
SI 65536
SF 699.7431024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



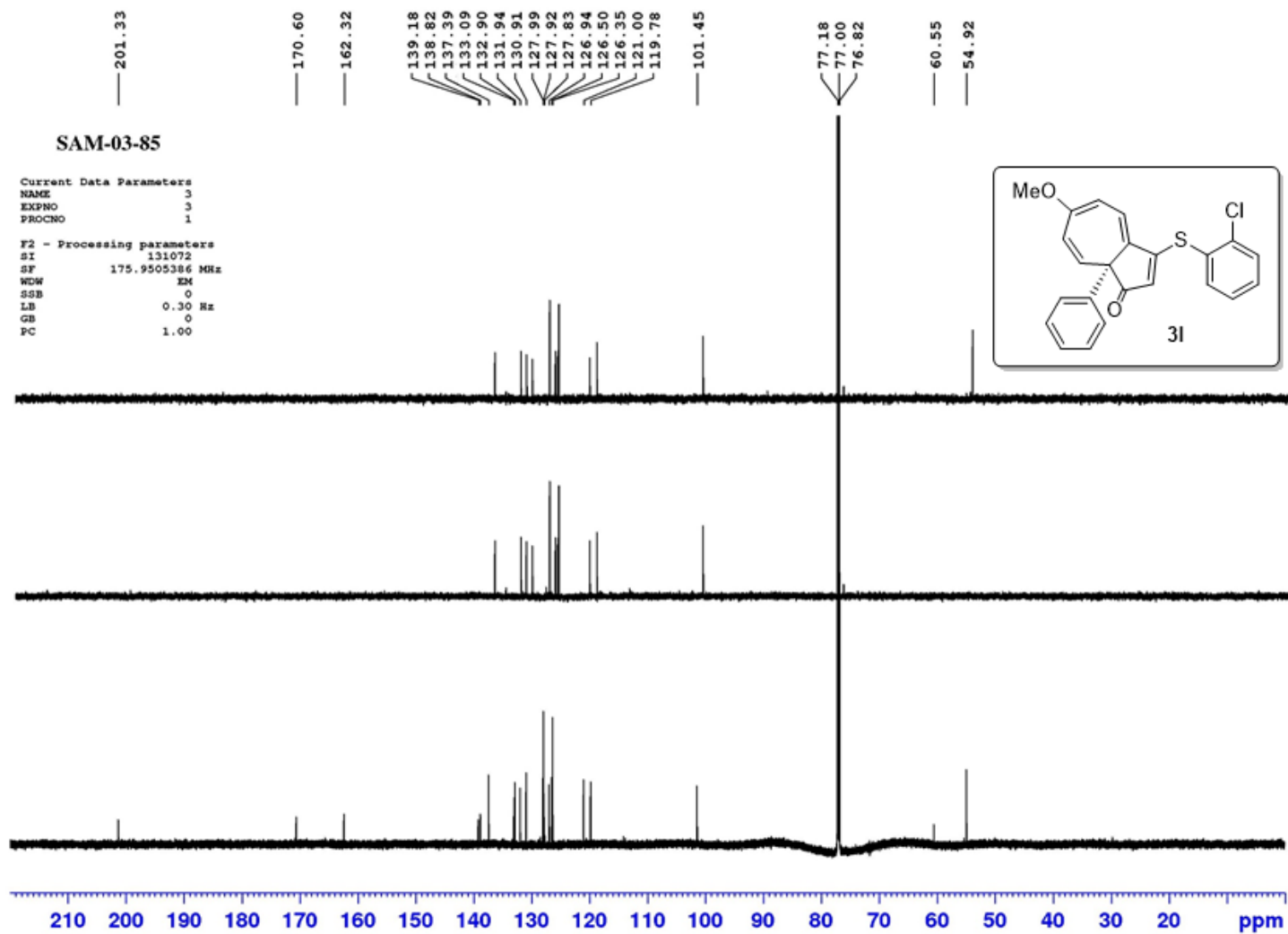
Solvent: CDCl_3
 SFO1: 175 MHz



Solvent: CDCl_3
SFO1: 700 MHz



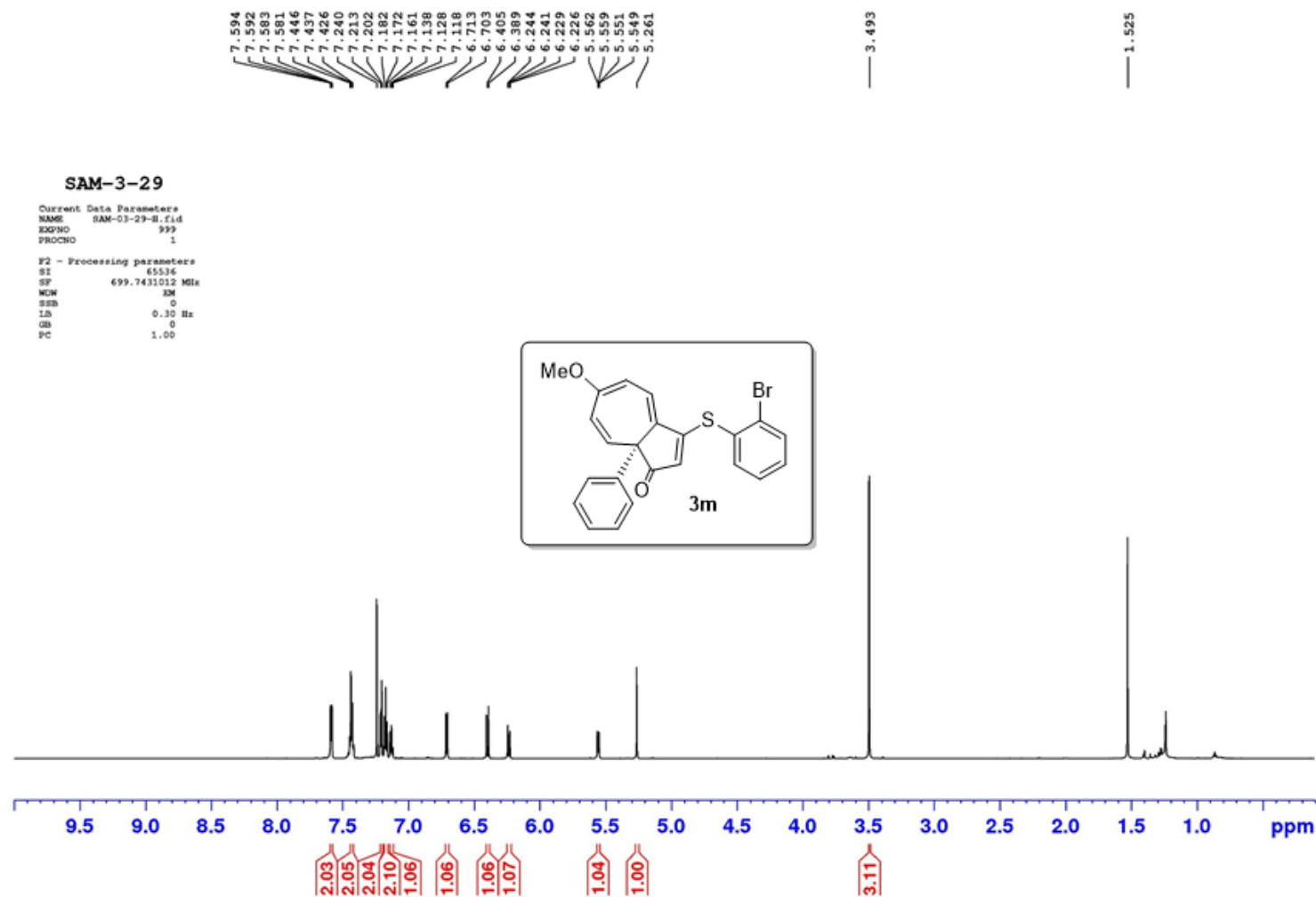
Solvent: CDCl_3
SFO1: 175 MHz



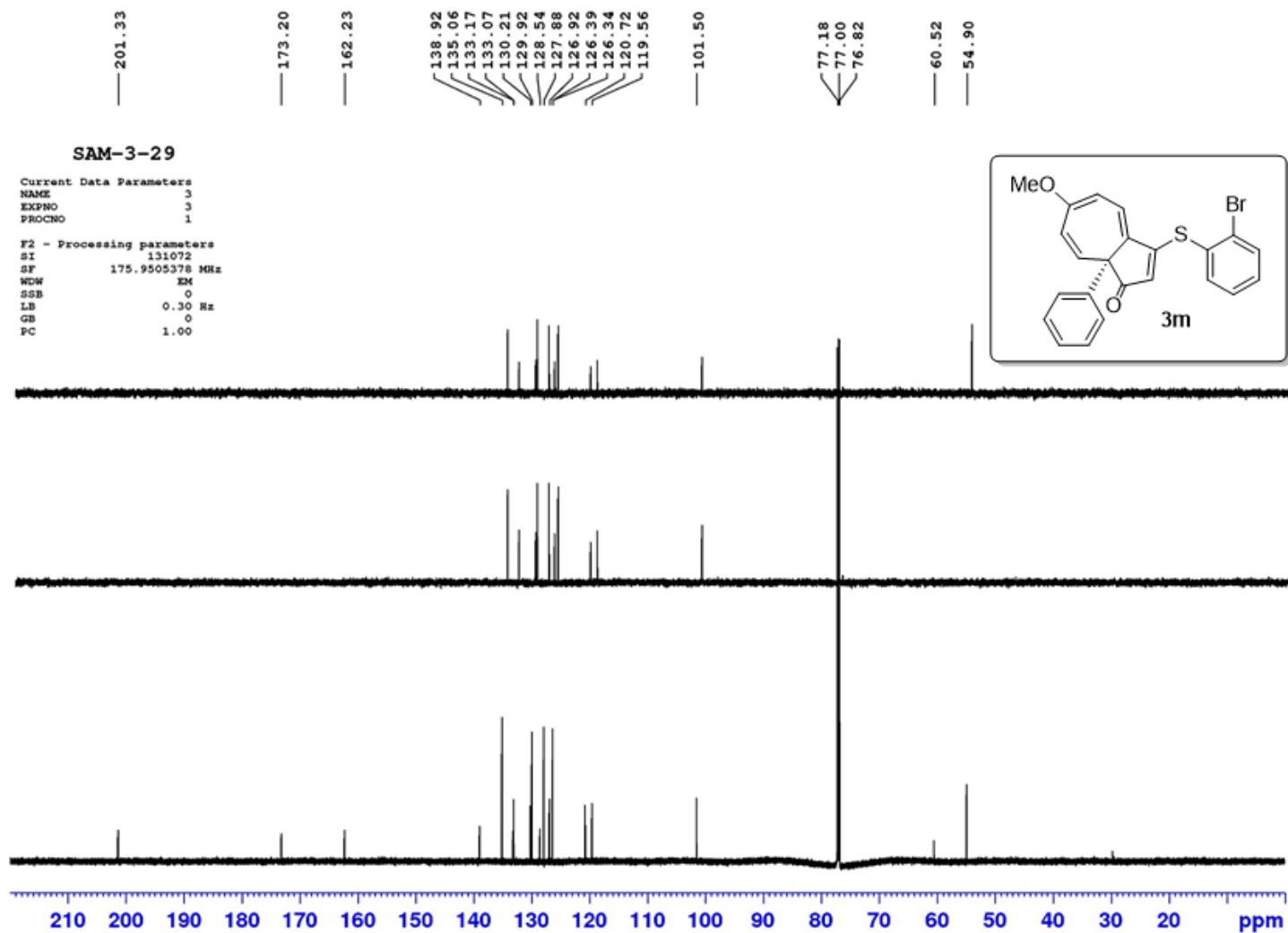
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-29

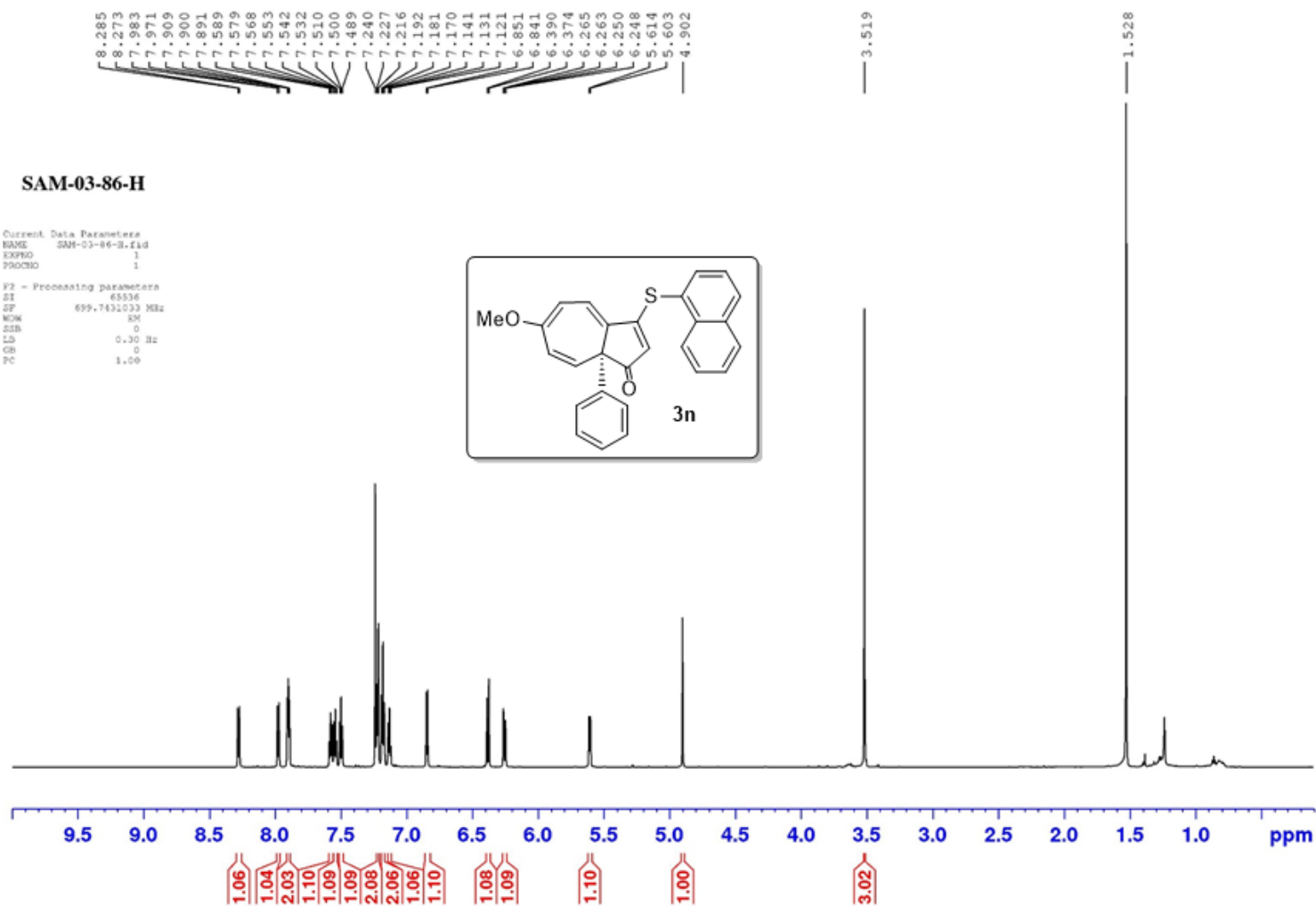
Current Data Parameters
NAME SAM-03-29-B.f16
EXPNO 999
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



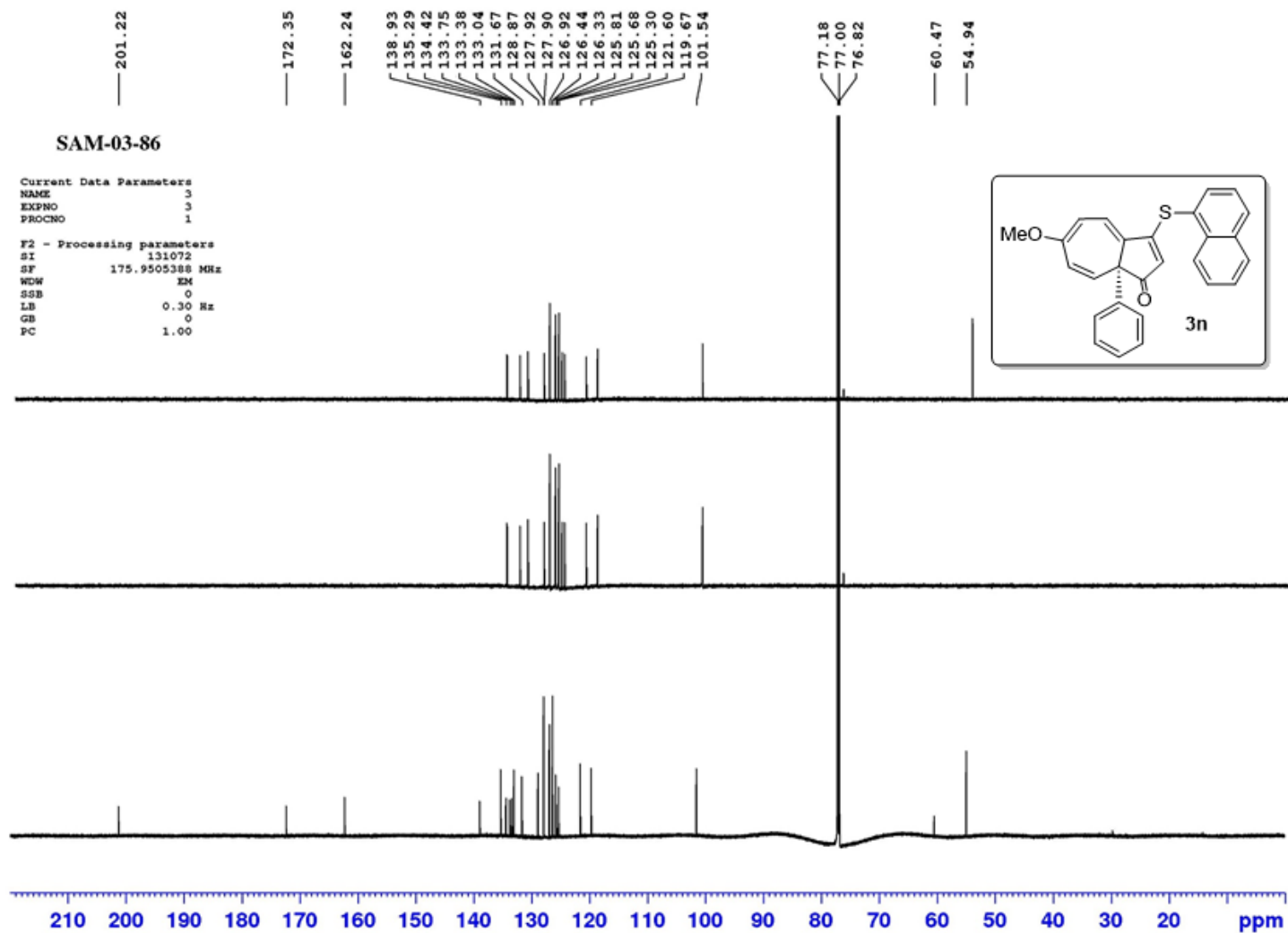
Solvent: CDCl_3
 SFO1: 175 MHz



Solvent: CDCl₃
SFO1: 700 MHz



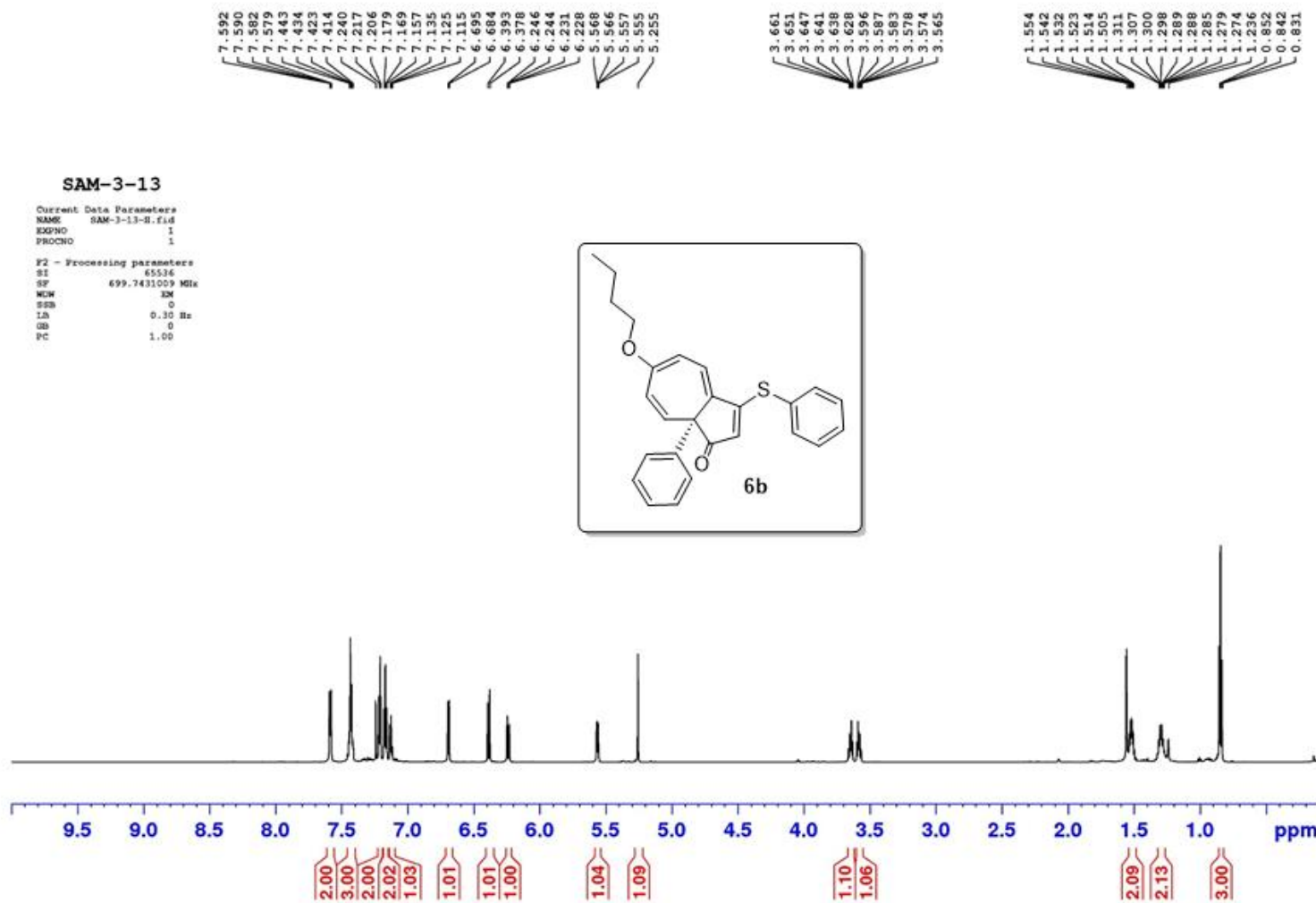
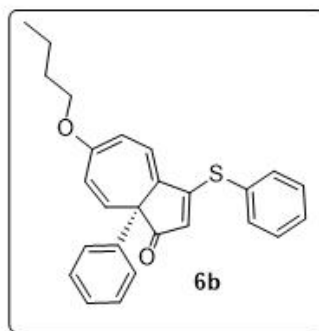
Solvent: CDCl_3
 SFO1: 175 MHz



Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-13

Current Data Parameters
NAME SAM-3-13-B.f16
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431009 MHz
RG 328
SFO 0
LA 0.30 Hz
GB 0
PC 1.00

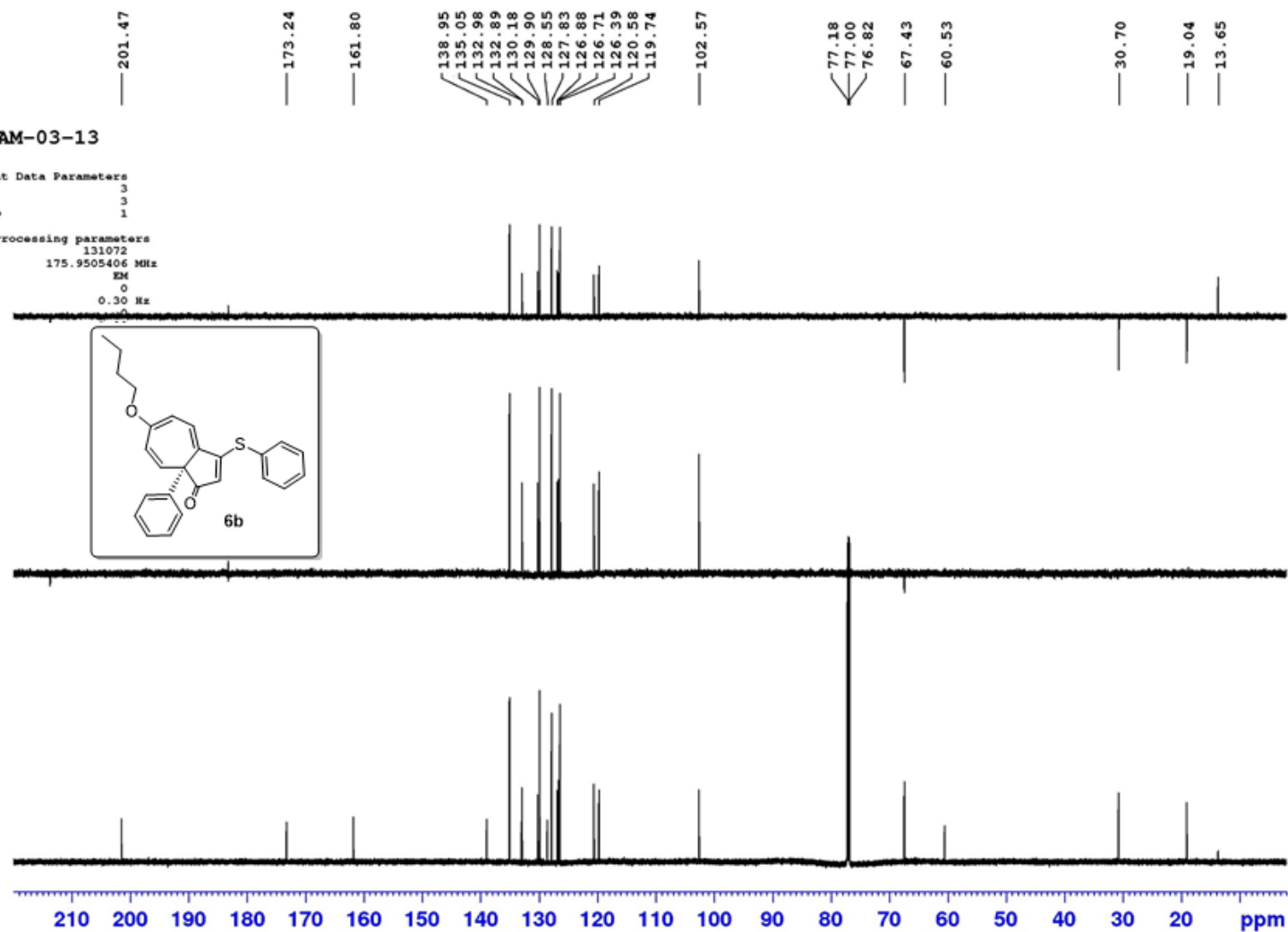


Solvent: CDCl₃
SFO1: 175 MHz

SAM-03-13

Current Data Parameters
NAME 3
EXPNO 3
PROCNO 1

F2 - Processing parameters
SI 131072
175.9505406 MHz
EM
0
0.30 Hz



Solvent: CDCl_3
SFO1: 700 MHz

7.588
7.578
7.441
7.432
7.422
7.240
7.101
7.090
6.988
6.977
6.701
6.691
6.395
6.380
6.233
6.218

5.560
5.550
5.257

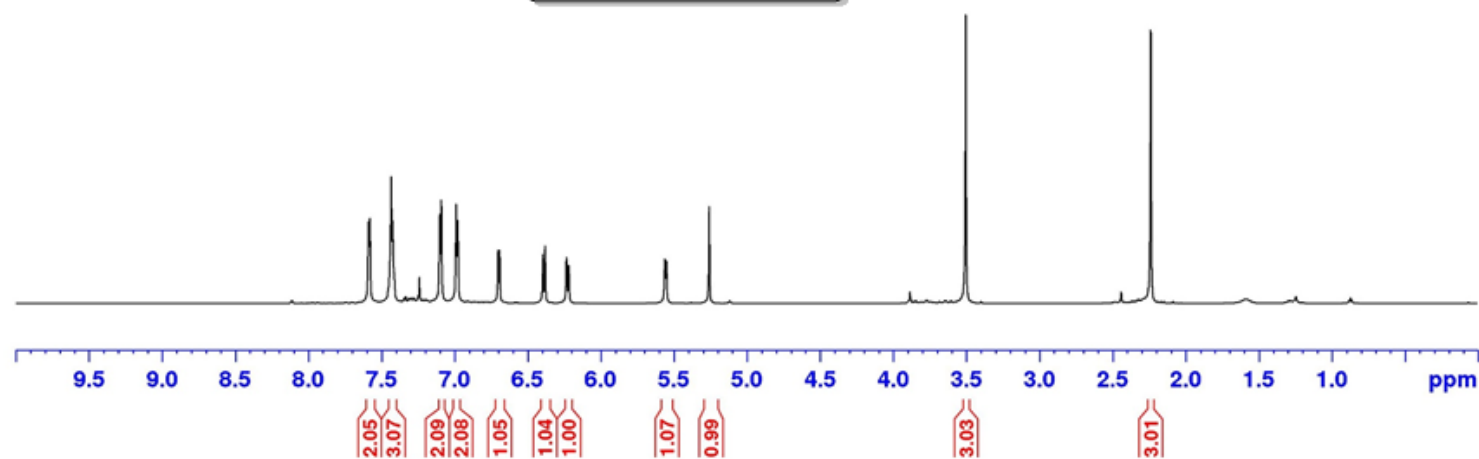
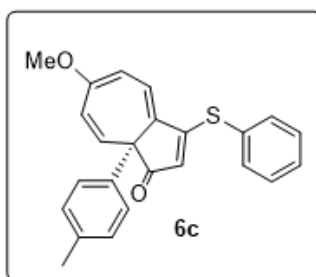
3.502

2.237

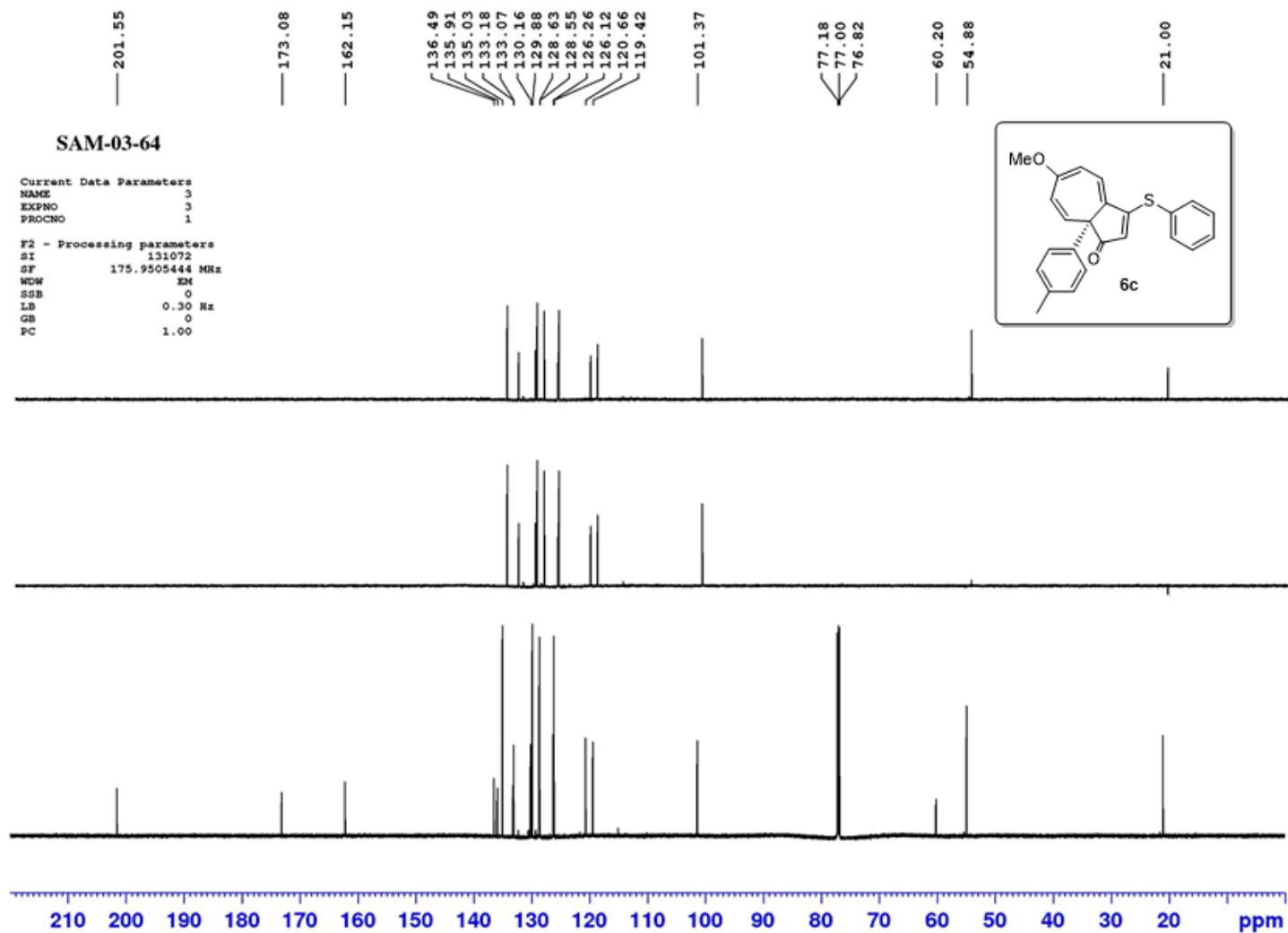
SAM-03-64-H

Current Data Parameters
NAME 1
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7431024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00



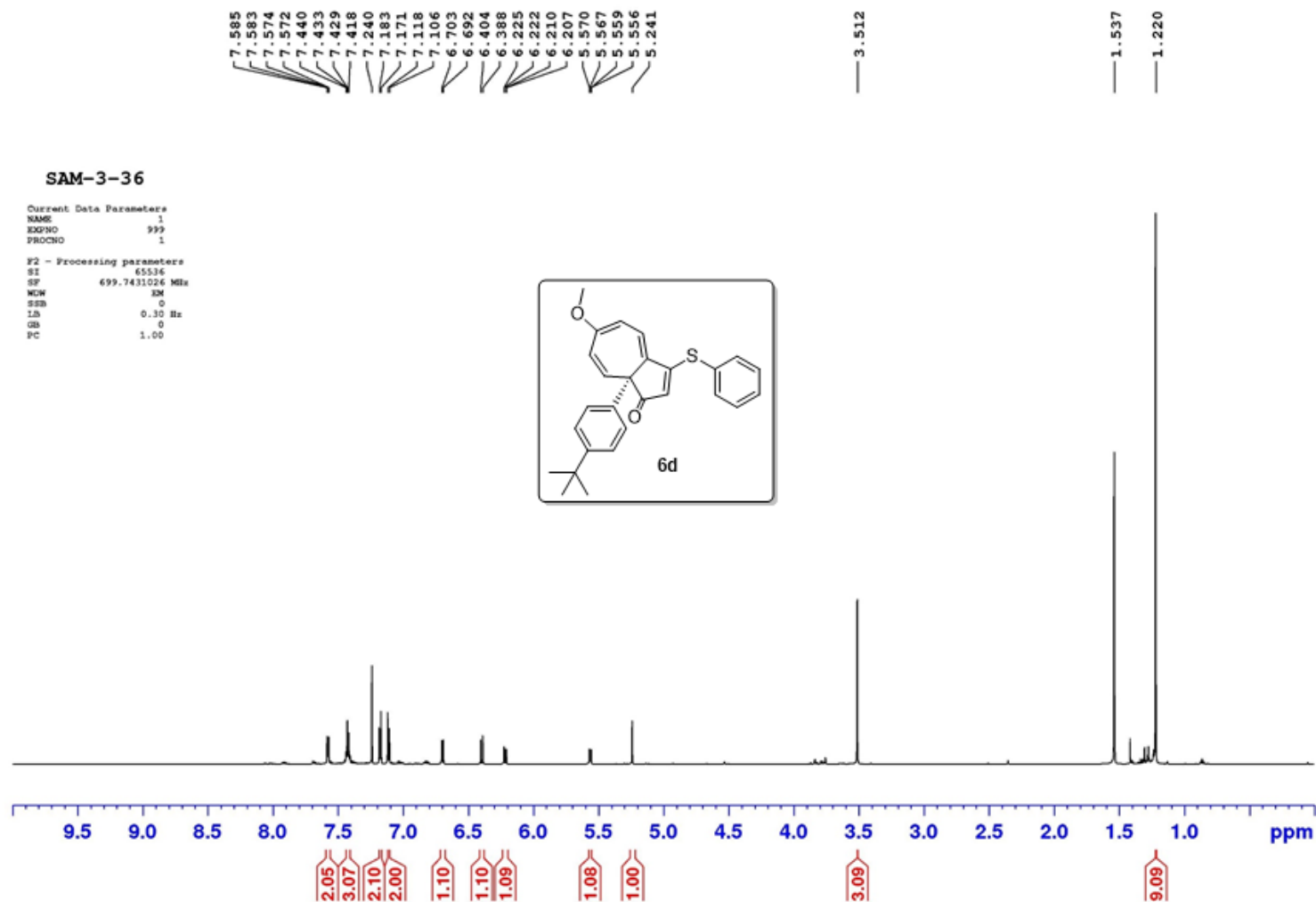
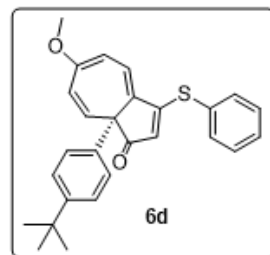
Solvent: CDCl_3
SFO1: 175 MHz



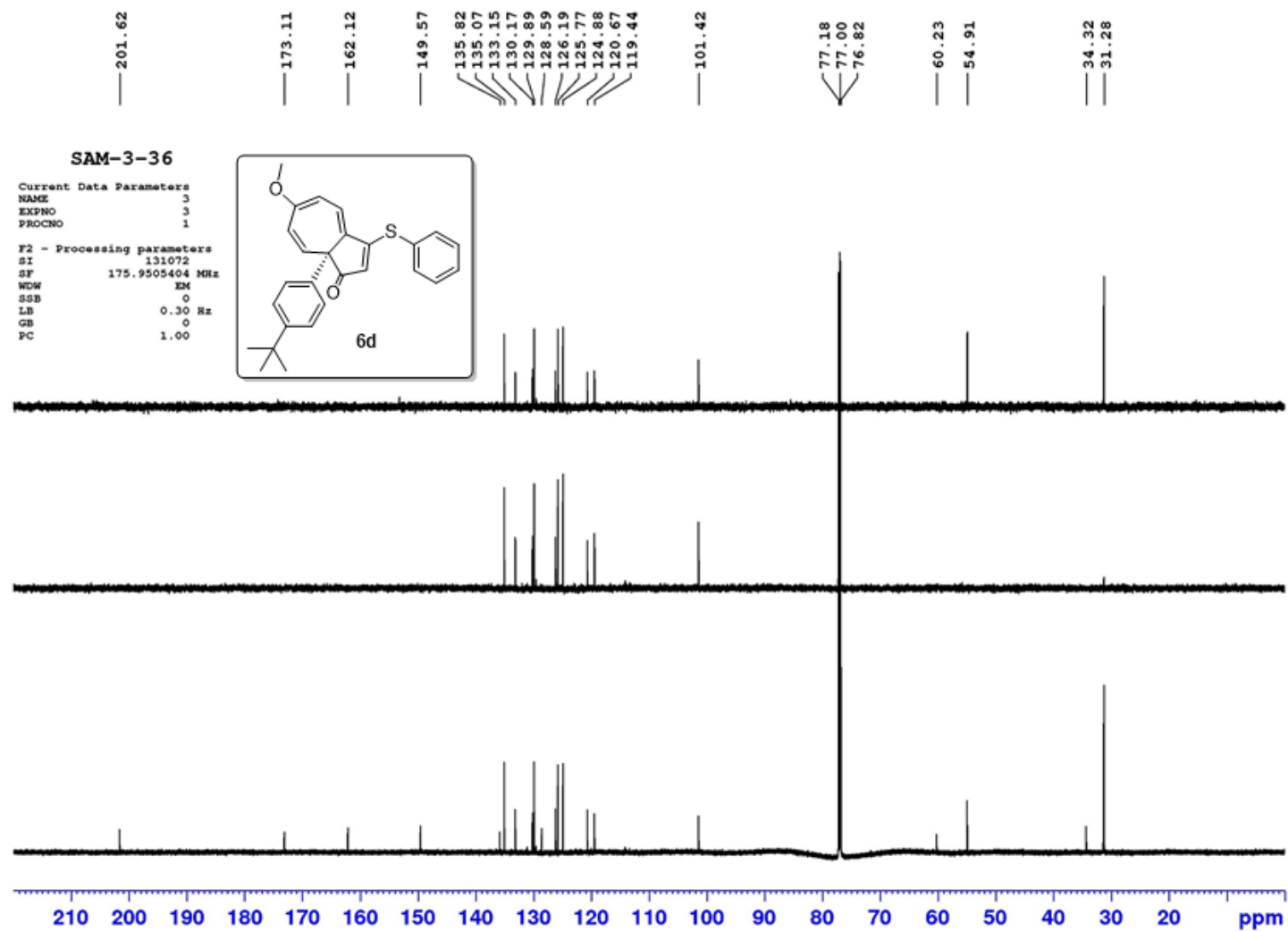
Solvent: CDCl₃
SFO1: 700 MHz

SAM-3-36

Current Data Parameters
NAME 1
EXPNO 999
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



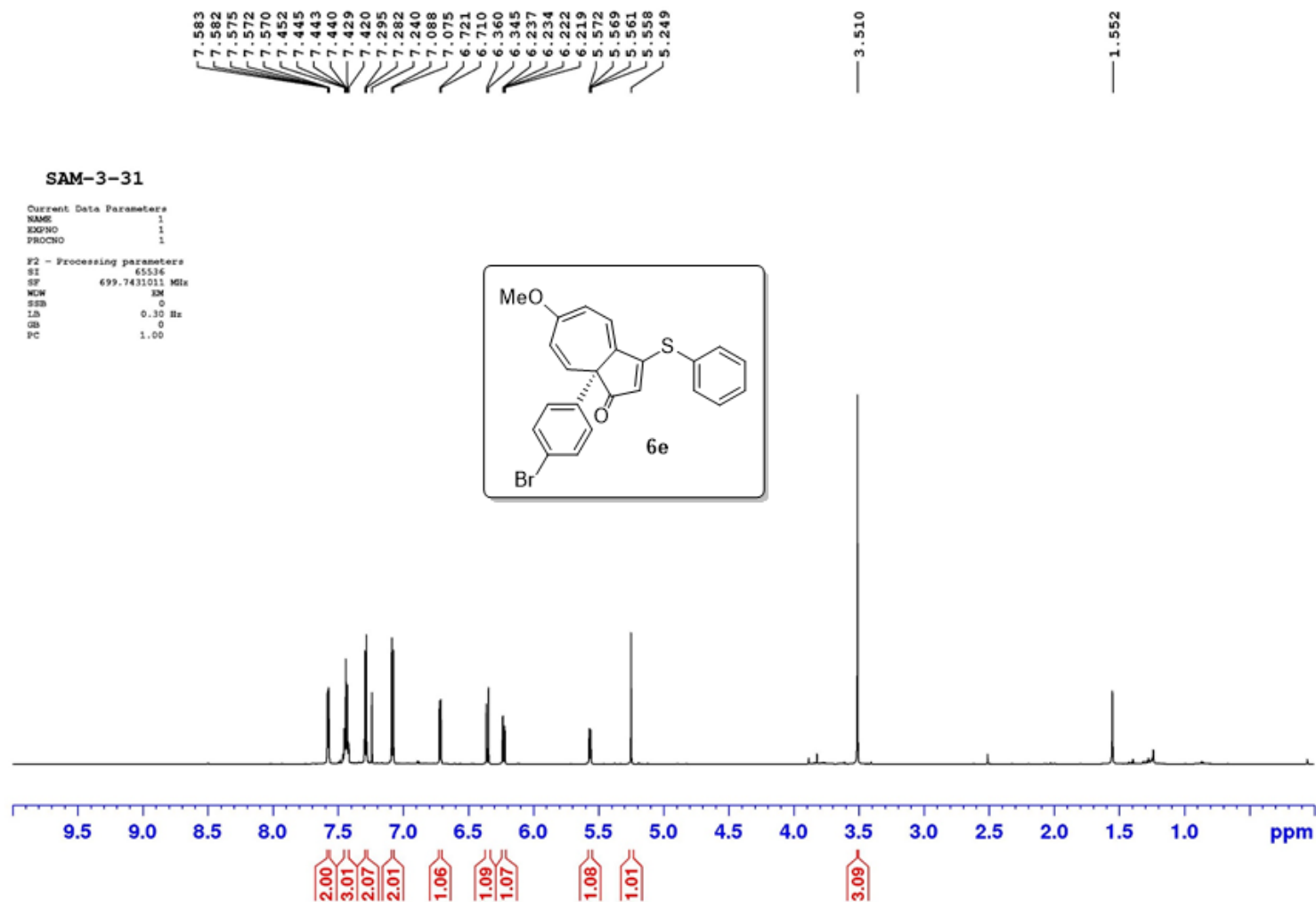
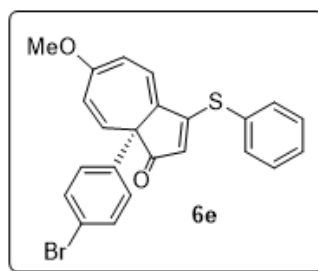
Solvent: CDCl₃
SFO1: 175 MHz



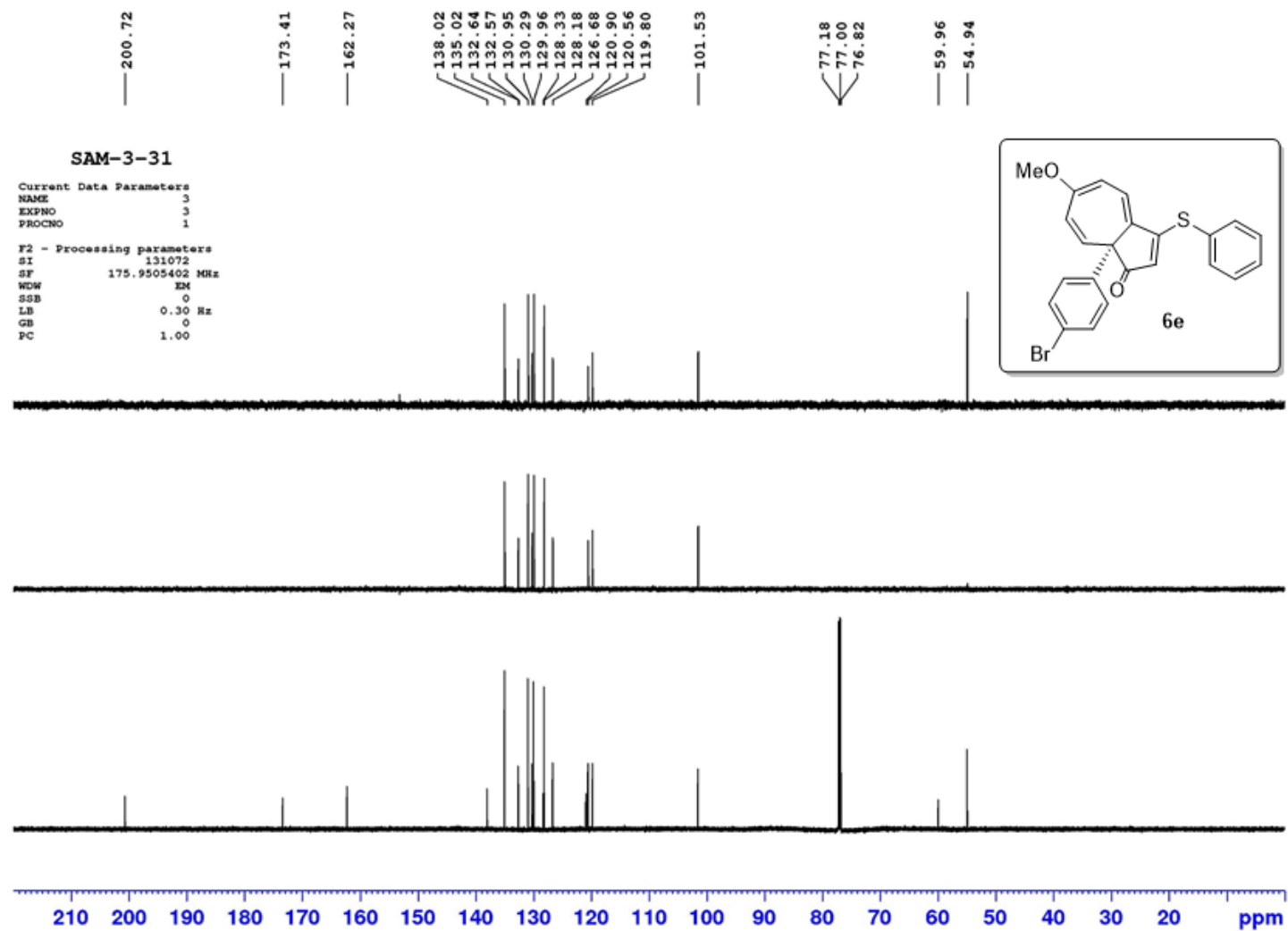
Solvent: CDCl₃
SFO1: 700 MHz

SAM-3-31

Current Data Parameters
NAME 1
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431011 MHz
WDW RM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



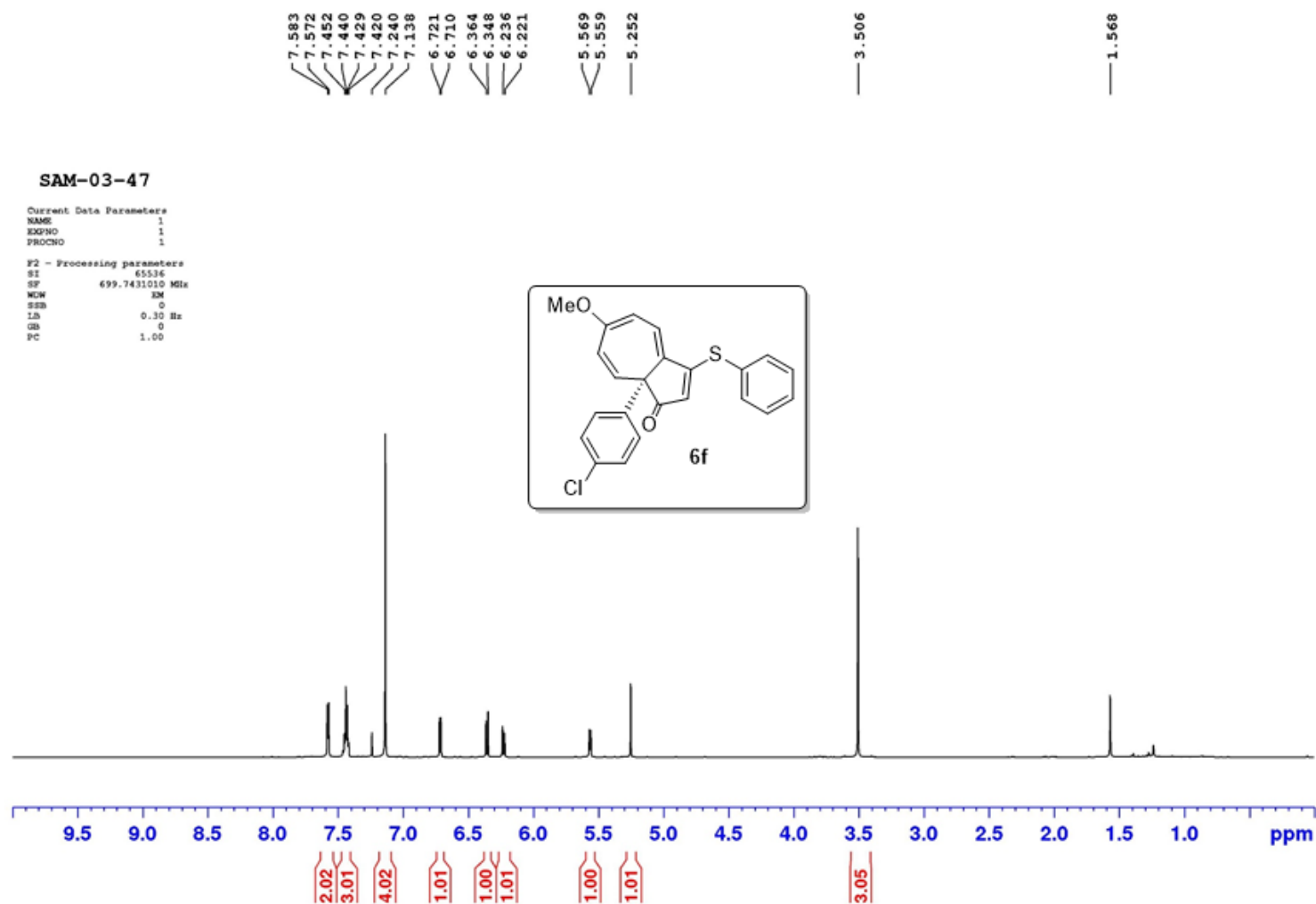
Solvent: CDCl_3
SFO1: 175 MHz



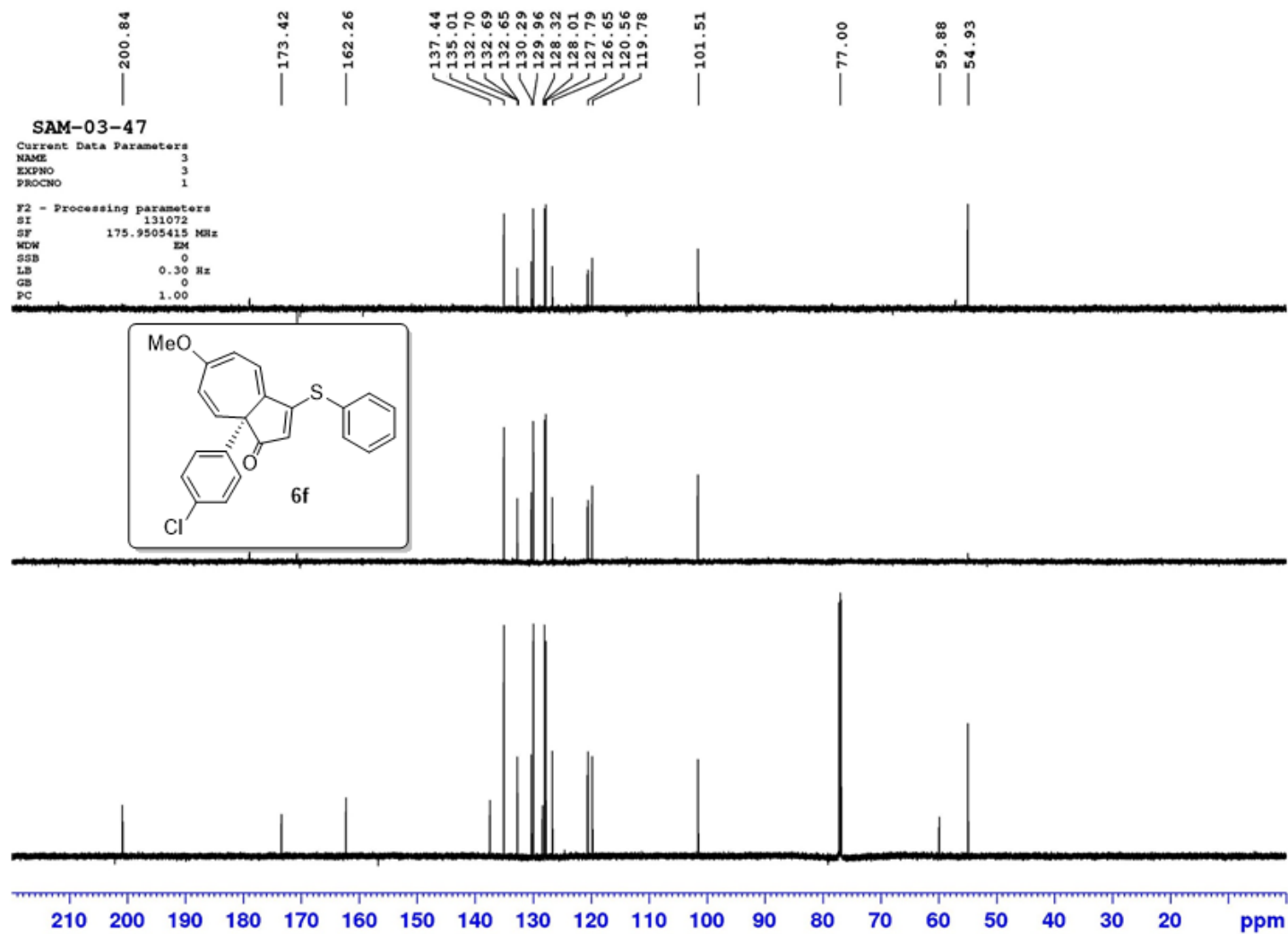
Solvent: CDCl_3
SFO1: 700 MHz

SAM-03-47

Current Data Parameters
NAME 1
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431010 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



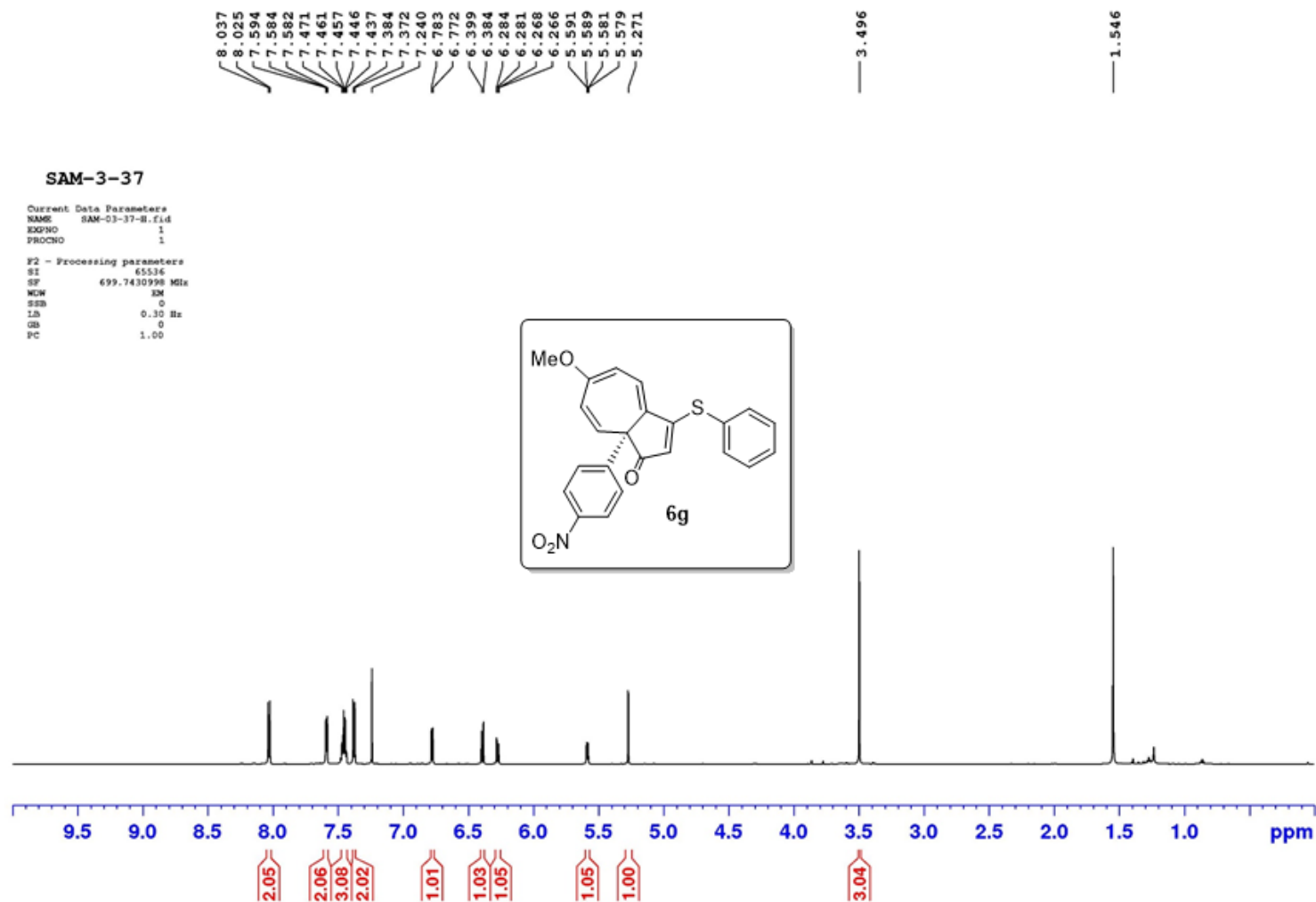
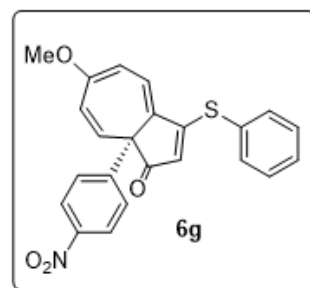
Solvent: CDCl_3
 SFO1: 175 MHz



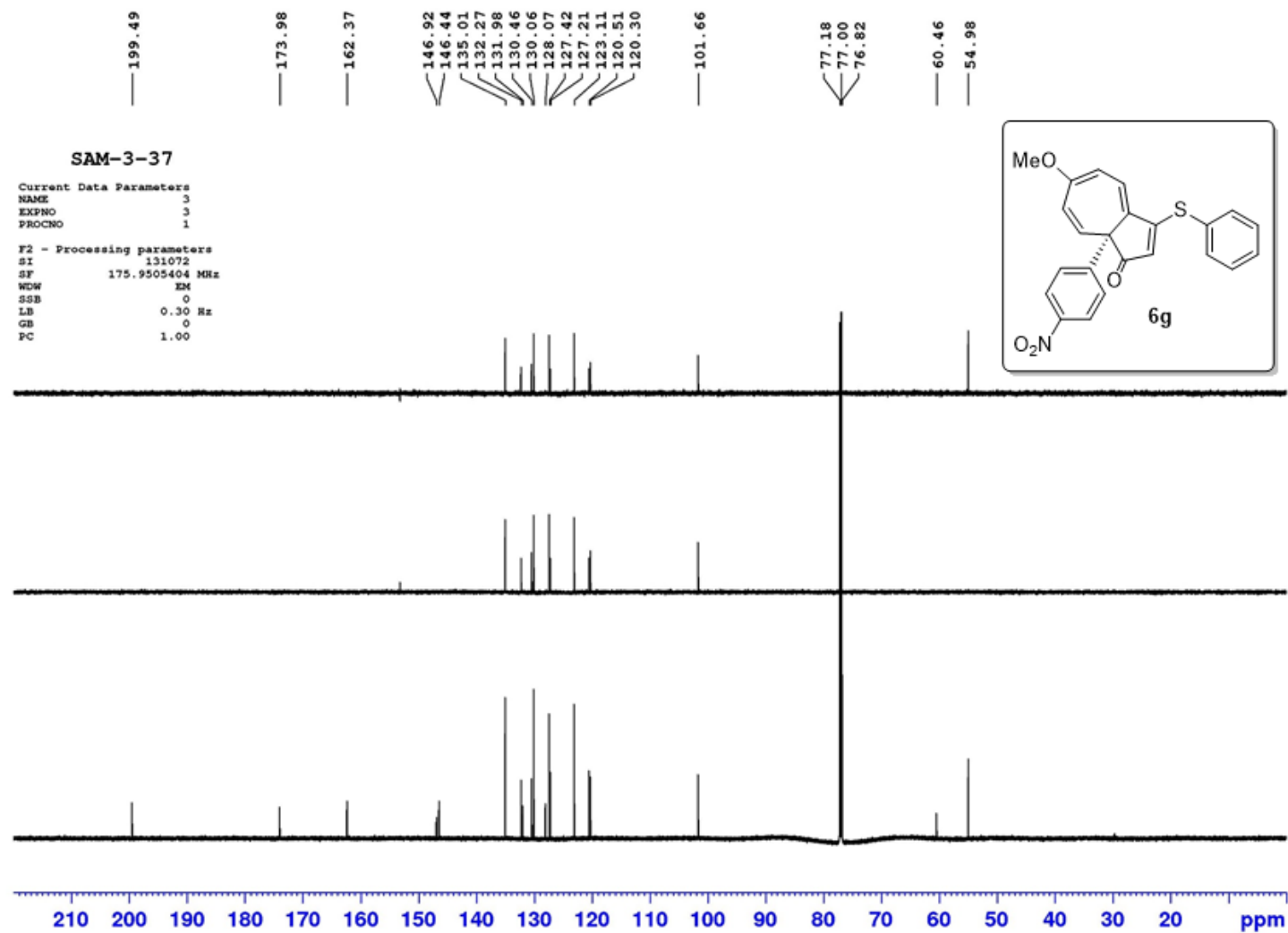
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-37

Current Data Parameters
NAME SAM-03-37-8.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7430998 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



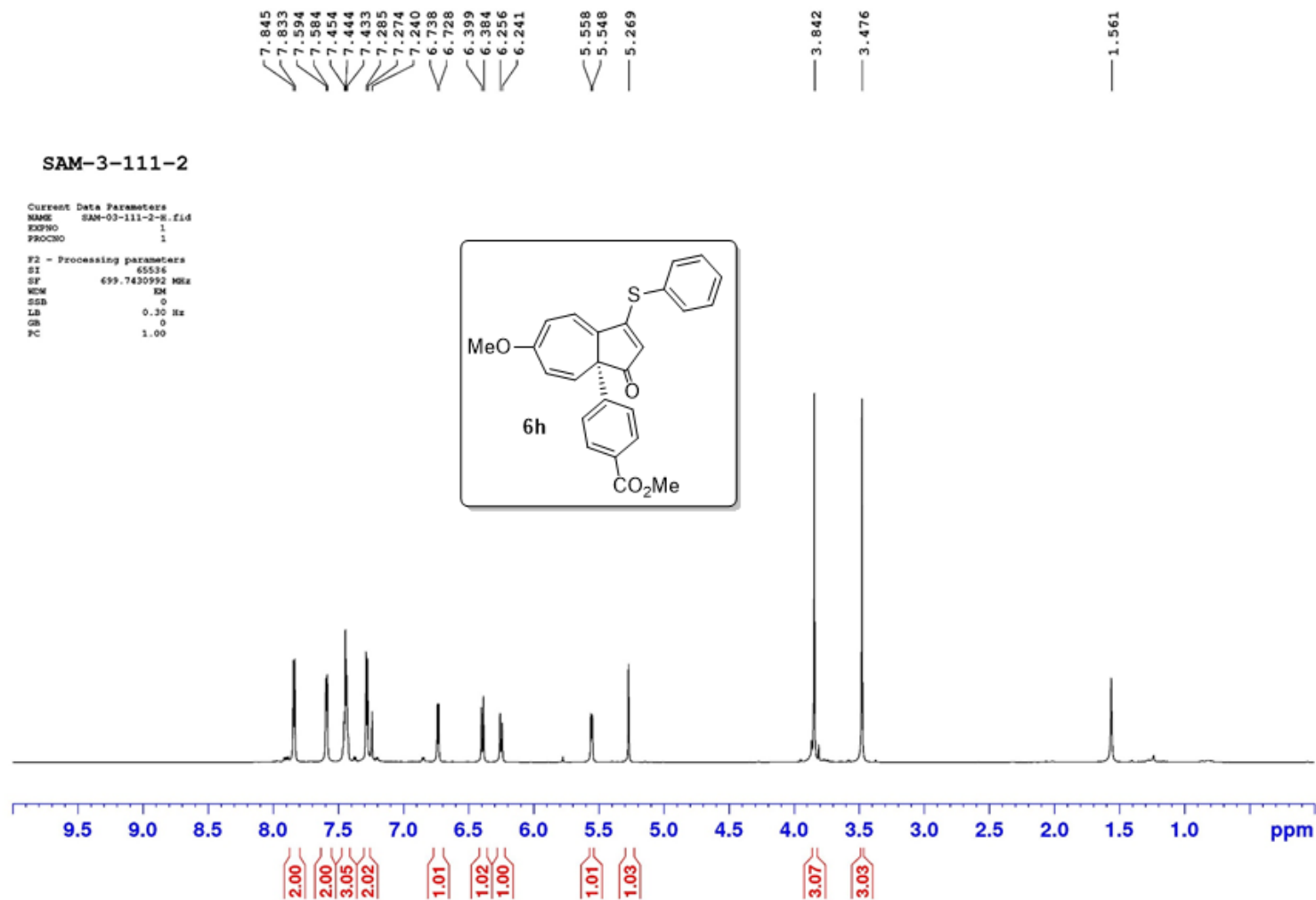
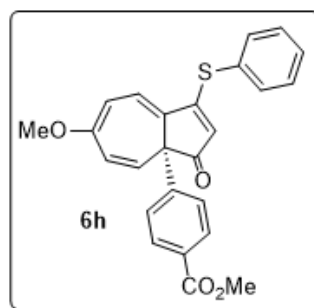
Solvent: CDCl_3
SFO1: 175 MHz



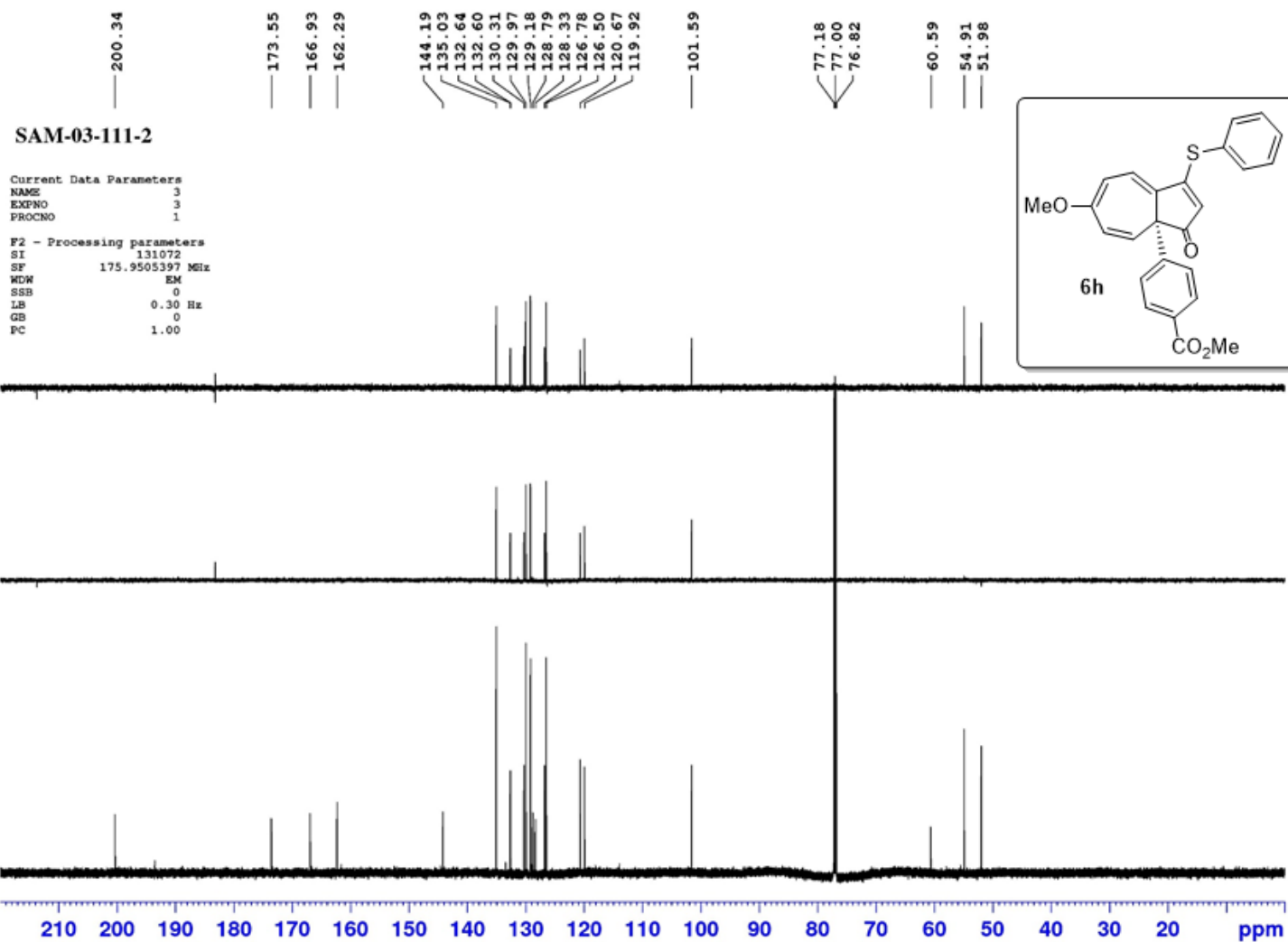
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-111-2

Current Data Parameters
NAME SAM-03-111-2-H.Eid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7430992 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
 SFO1: 175 MHz

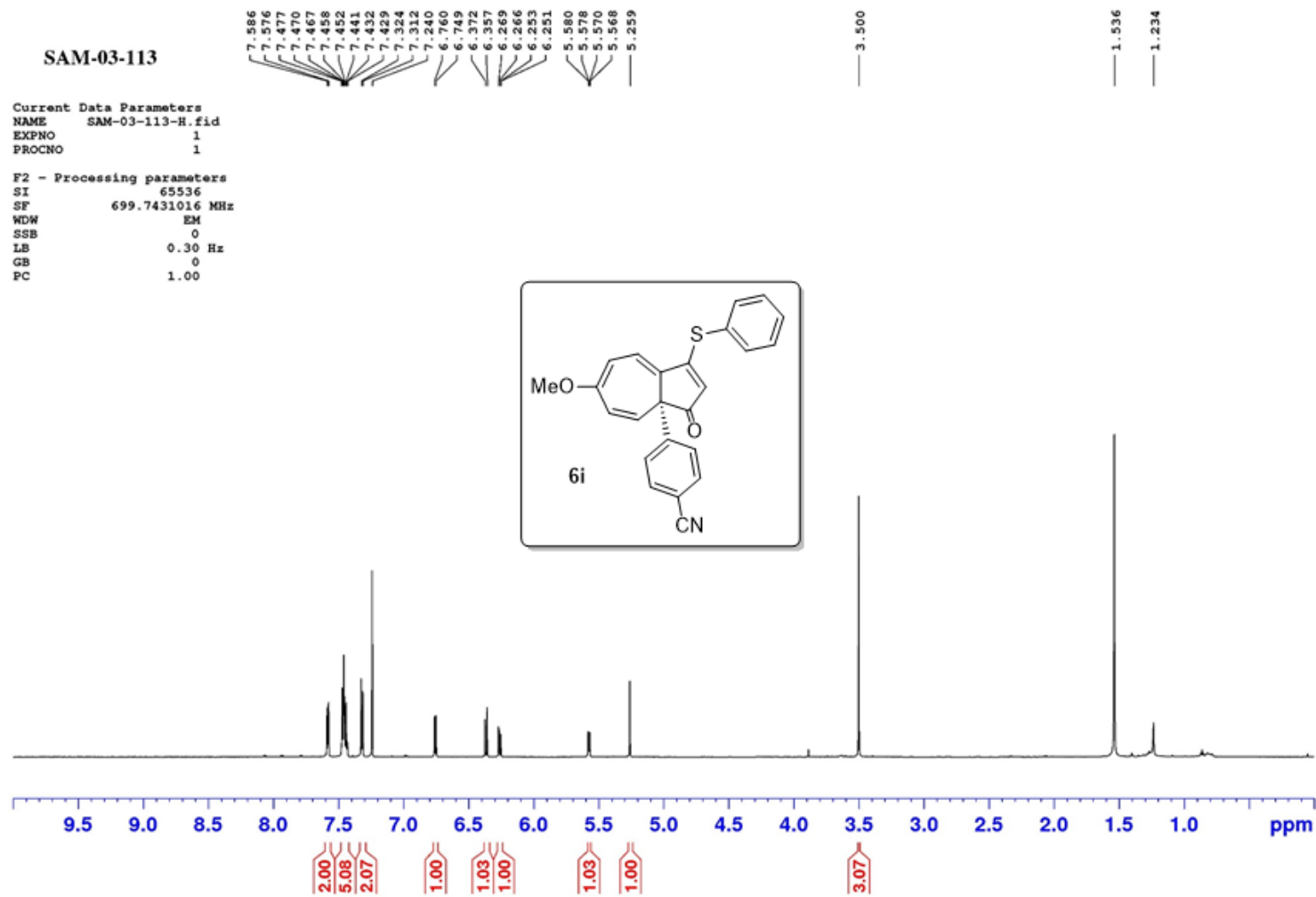


Solvent: CDCl₃
SFO1: 700 MHz

SAM-03-113

Current Data Parameters
NAME SAM-03-113-H.fid
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7431016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

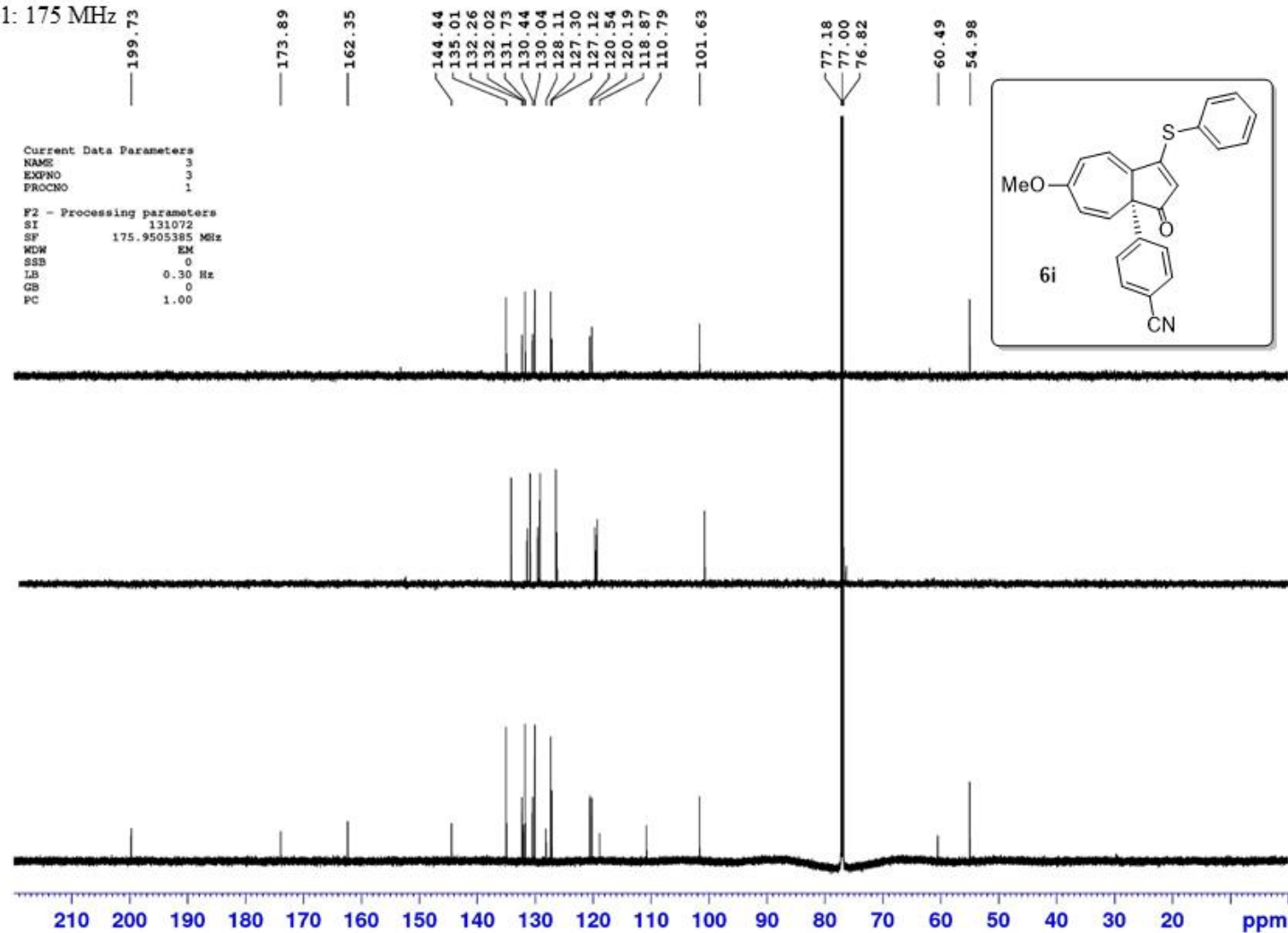


SAM-03-113

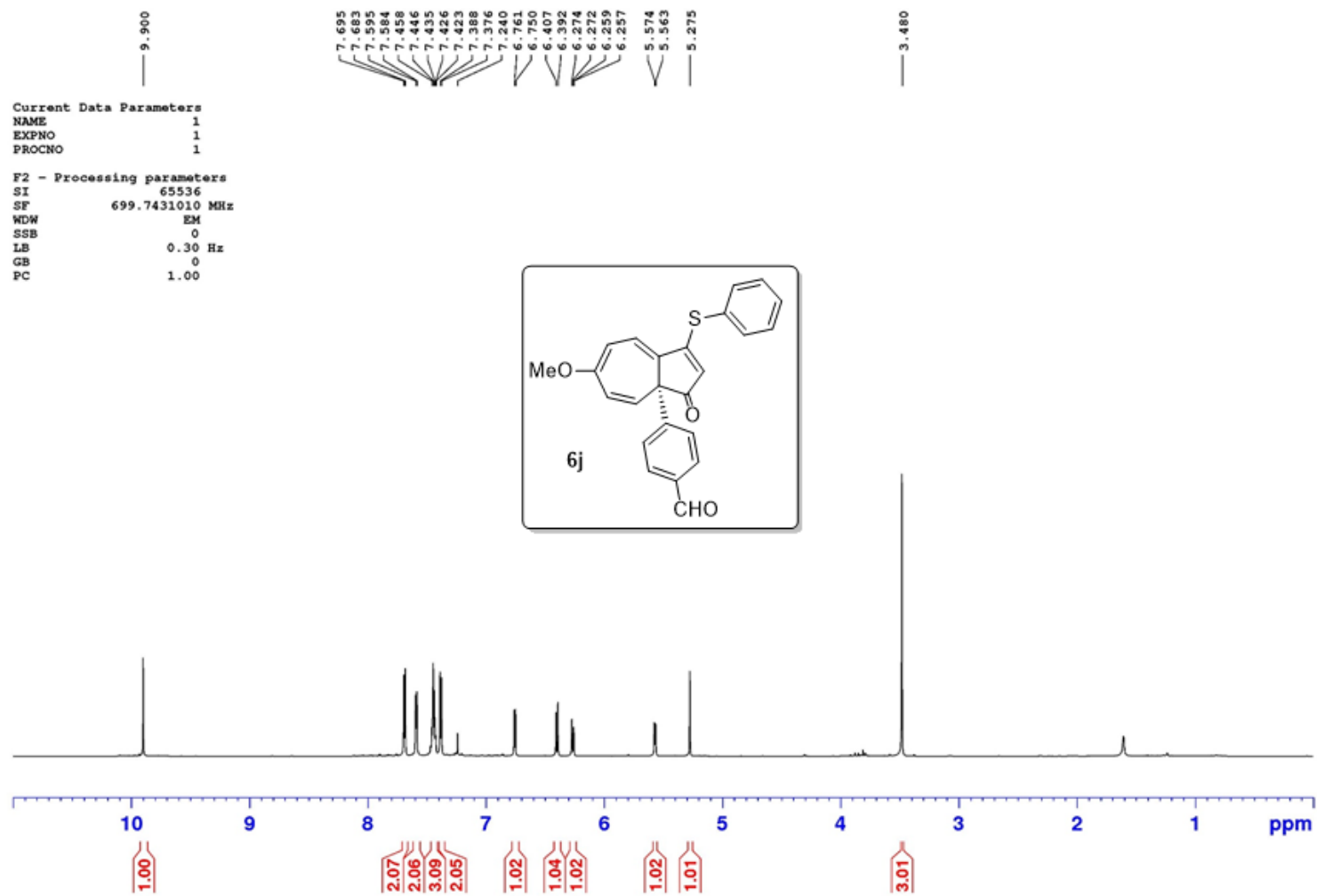
Solvent: CDCl₃

SFO1: 175 MHz

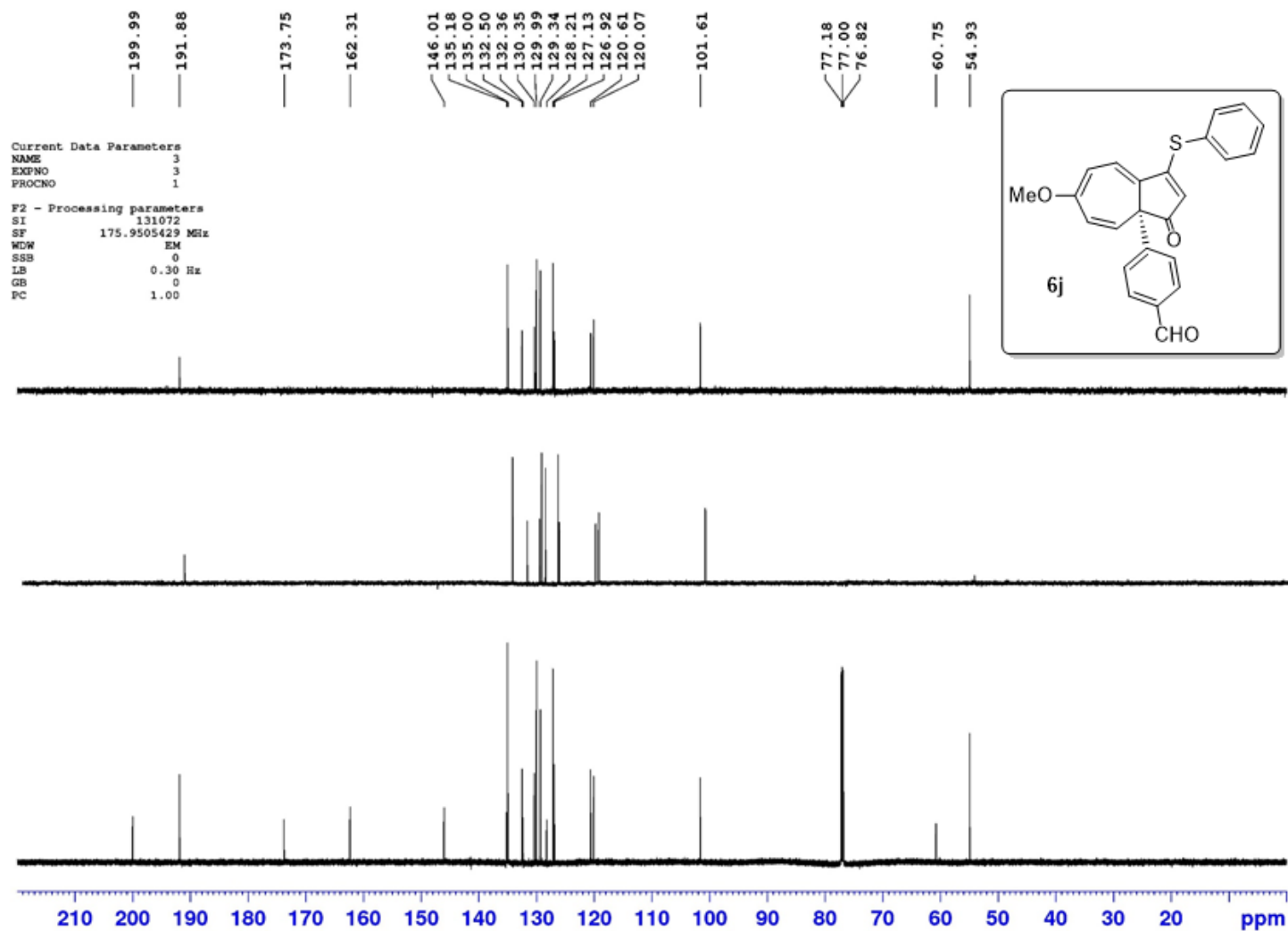
Current Data Parameters
 NAME 3
 EXPNO 3
 PROCNO 1
 F2 - Processing parameters
 SI 131072
 SF 175.9505385 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



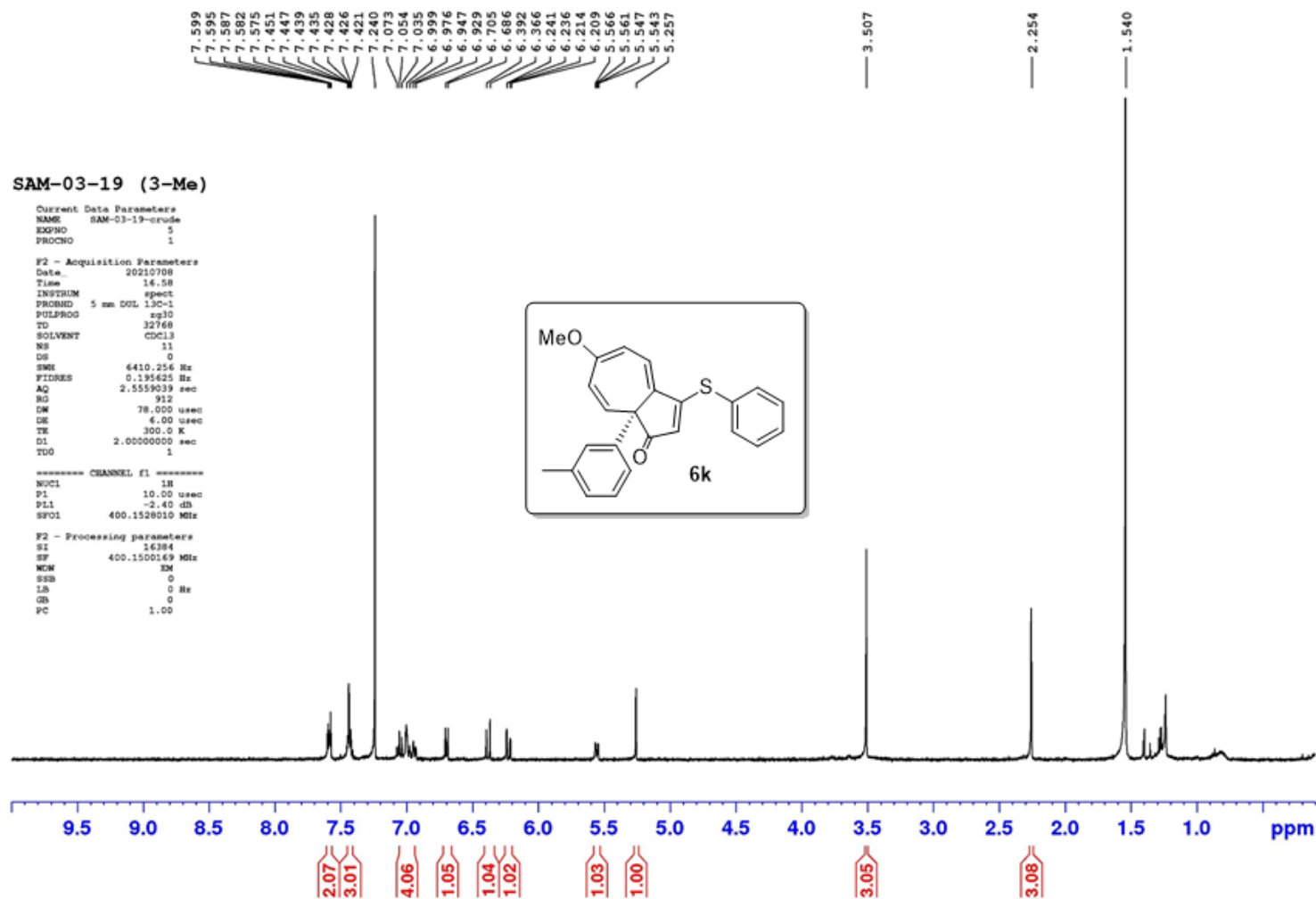
Solvent: CDCl₃
SFO1: 700 MHz



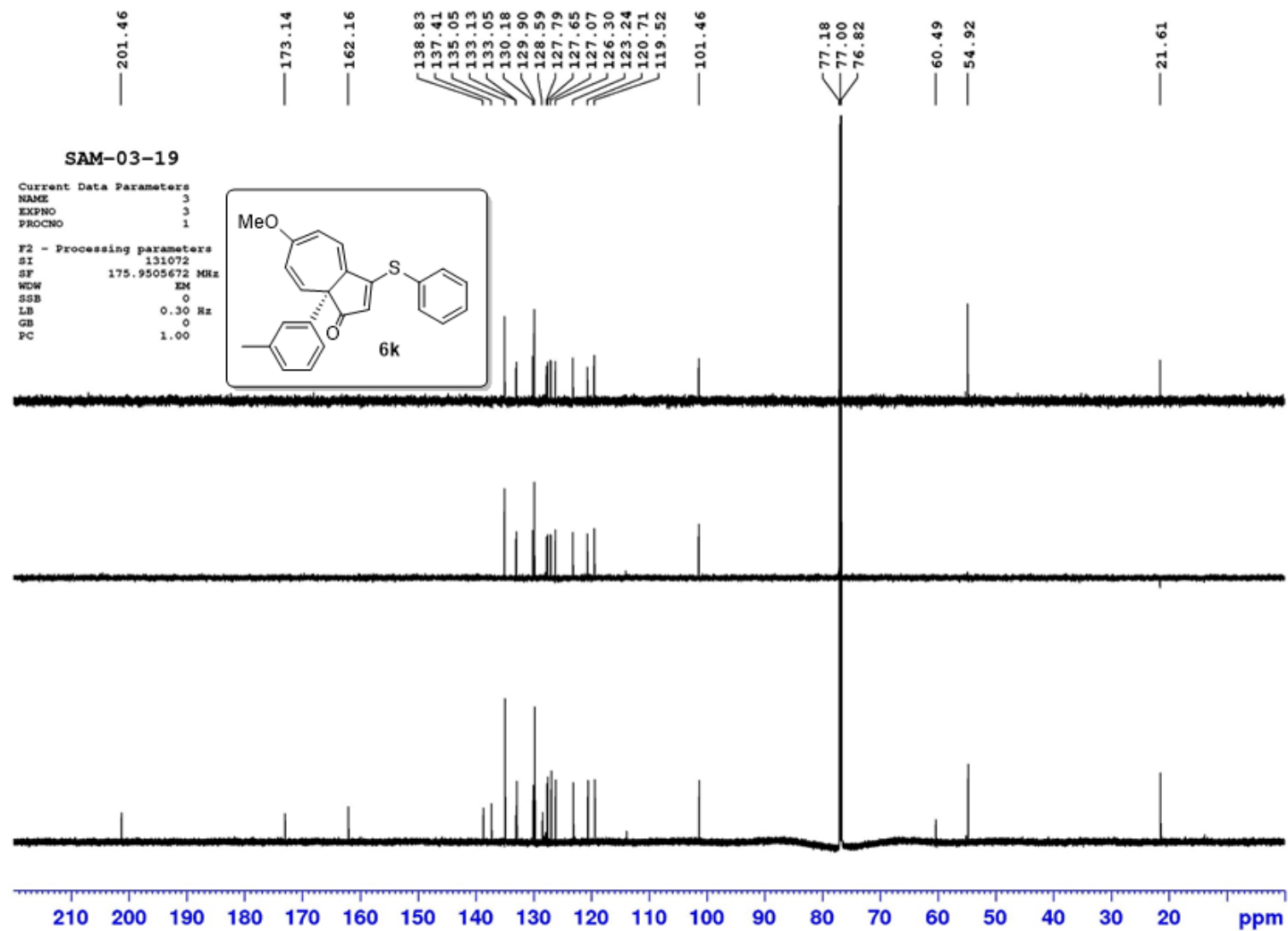
Solvent: CDCl₃
SFO1: 175 MHz



Solvent: CDCl_3
SFO1: 400 MHz



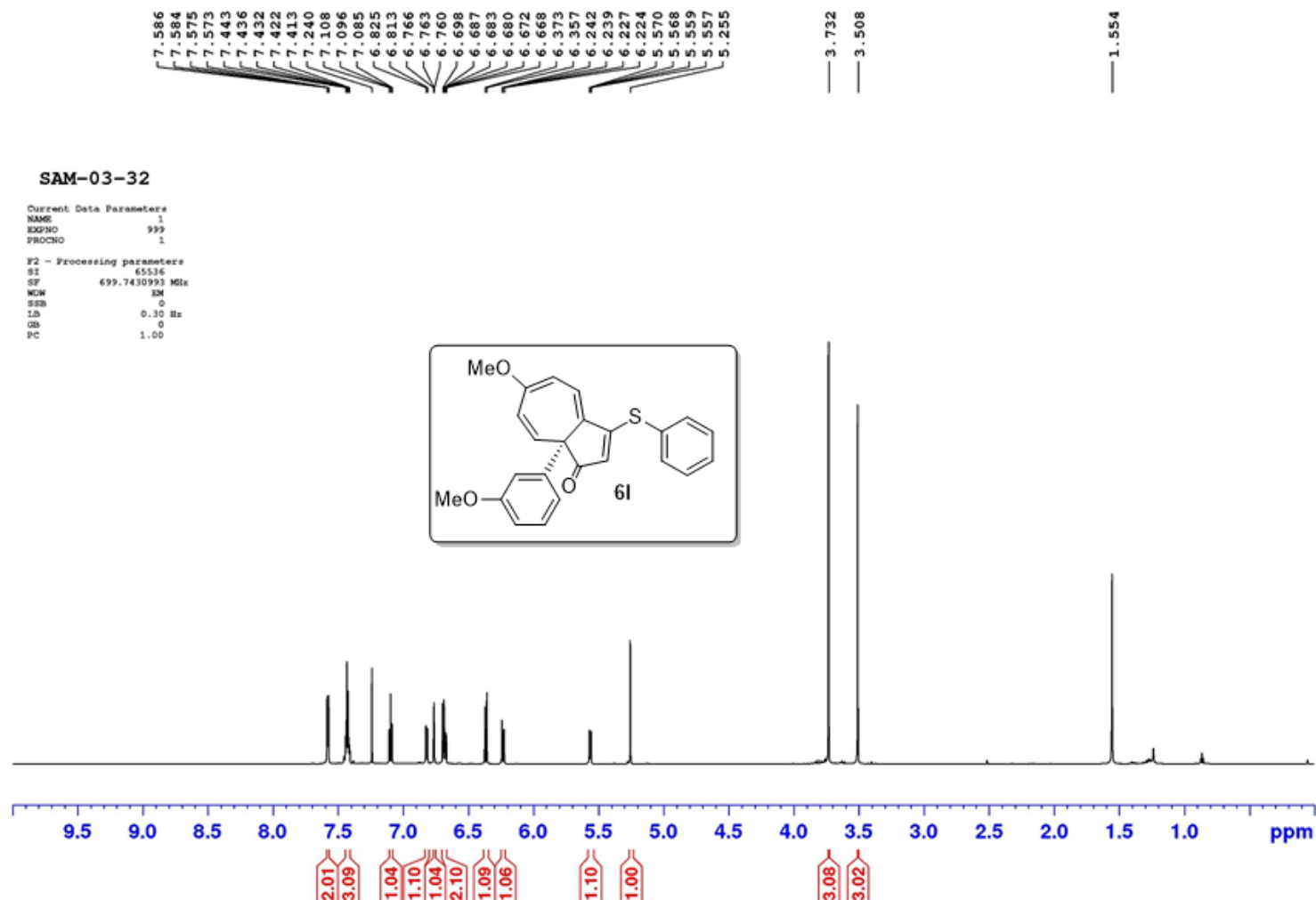
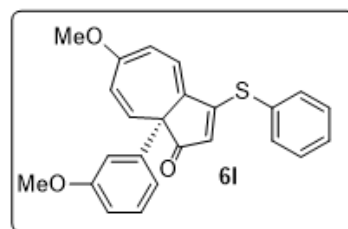
Solvent: CDCl_3
 SFO1: 175 MHz



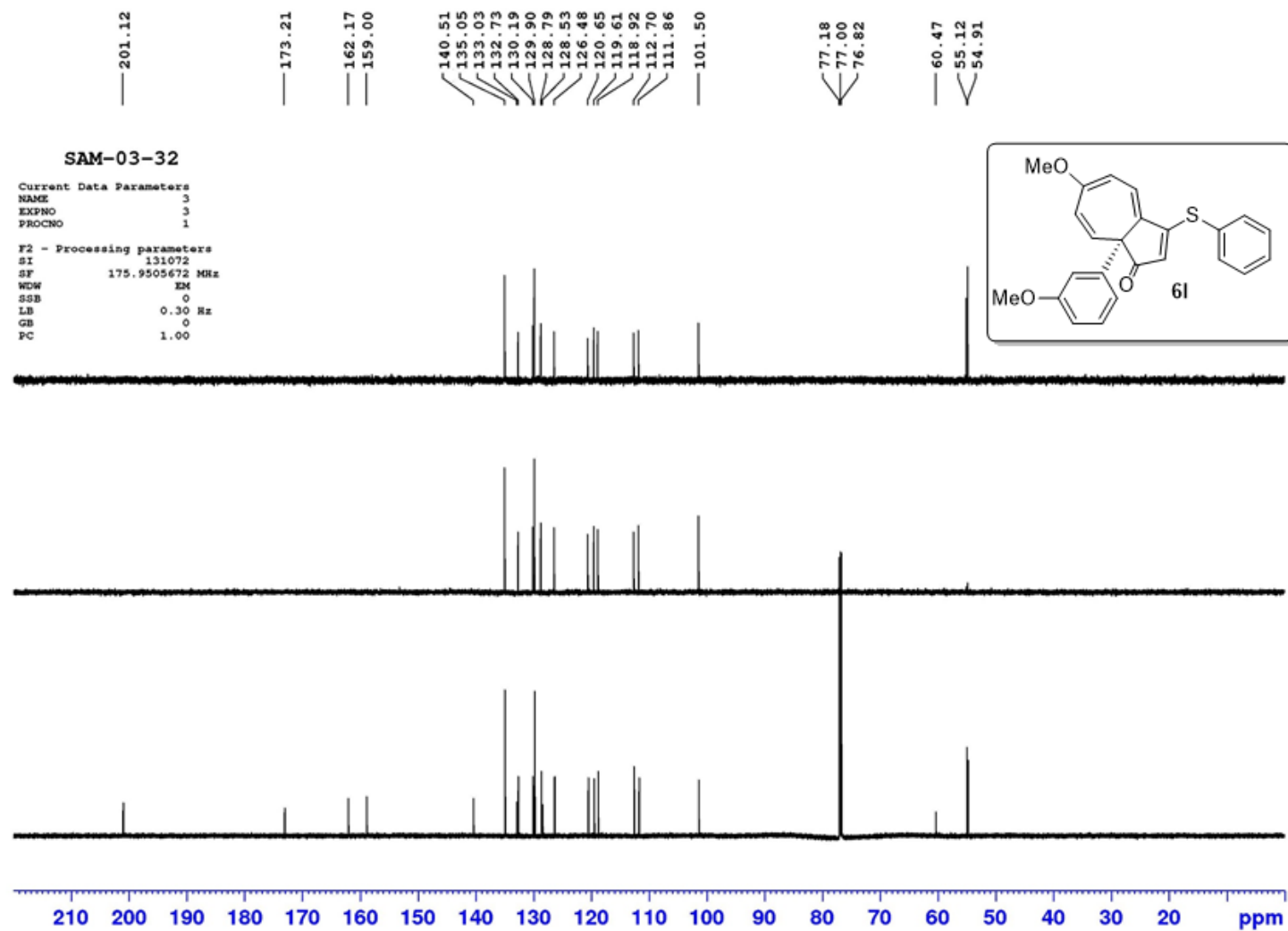
Solvent: CDCl_3
SFO1: 700 MHz

SAM-03-32

Current Data Parameters
NAME 1
EXPNO 999
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7430993 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



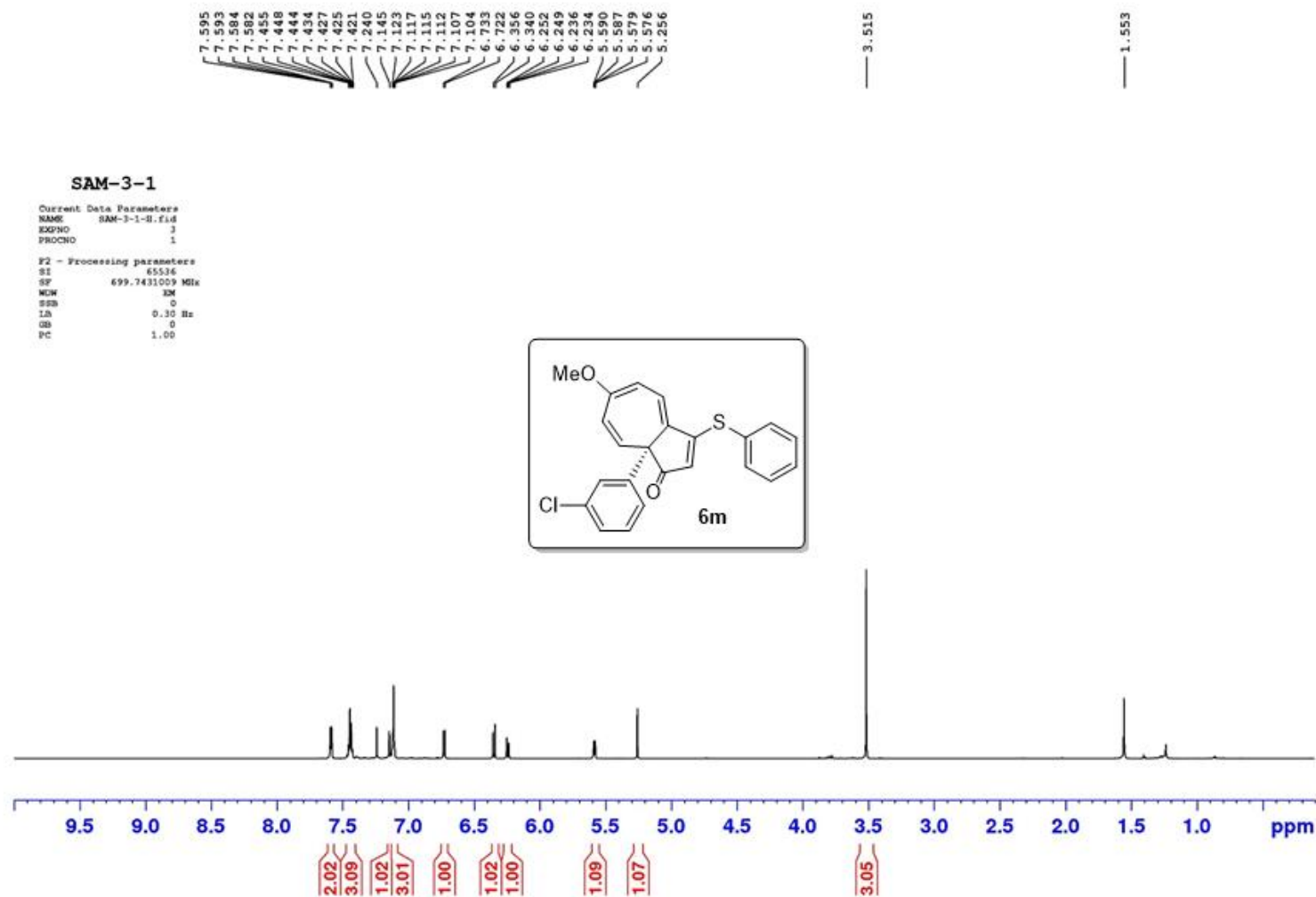
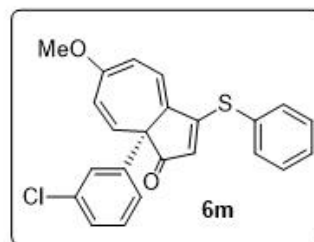
Solvent: CDCl₃
SFO1: 175 MHz



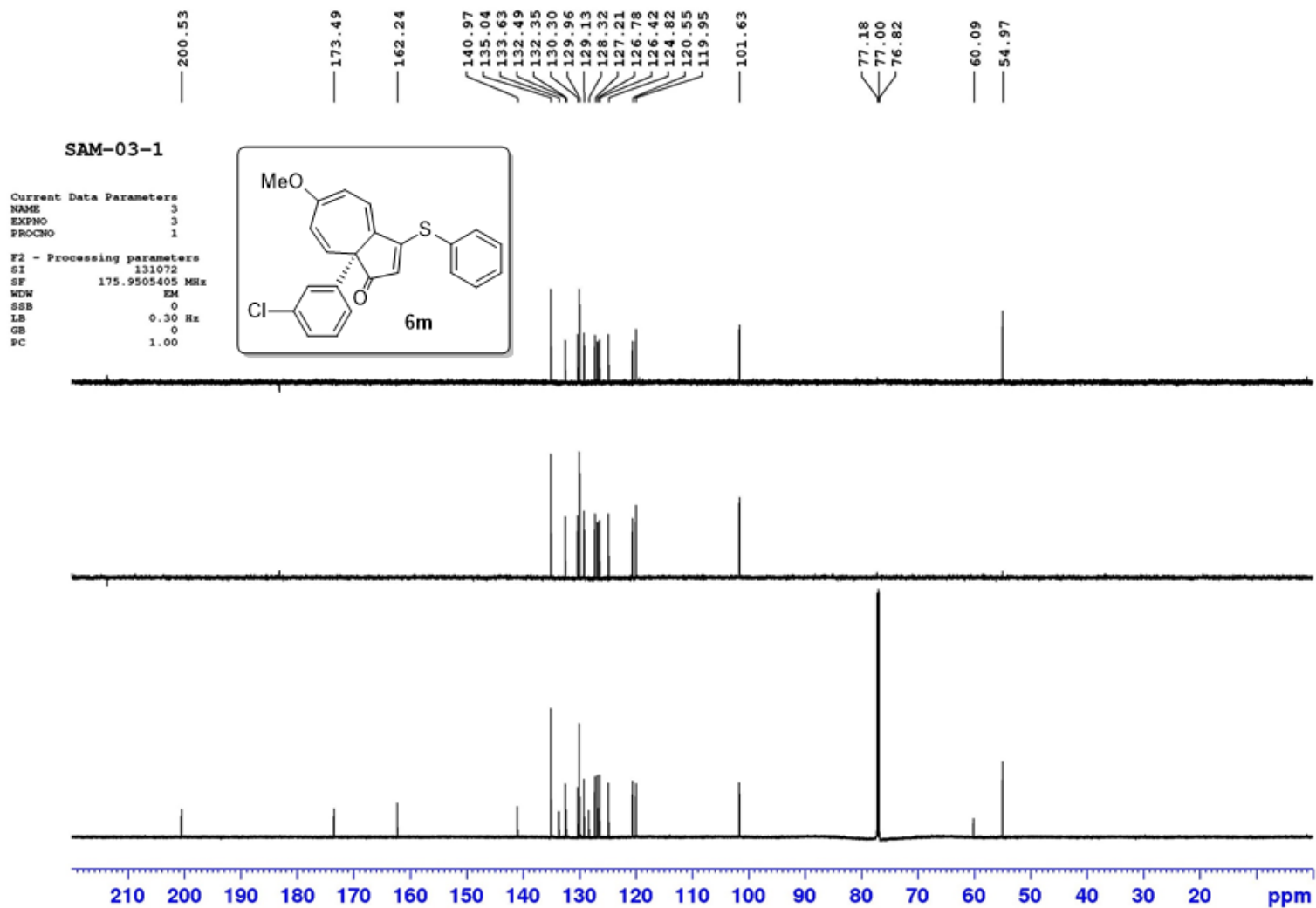
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-1

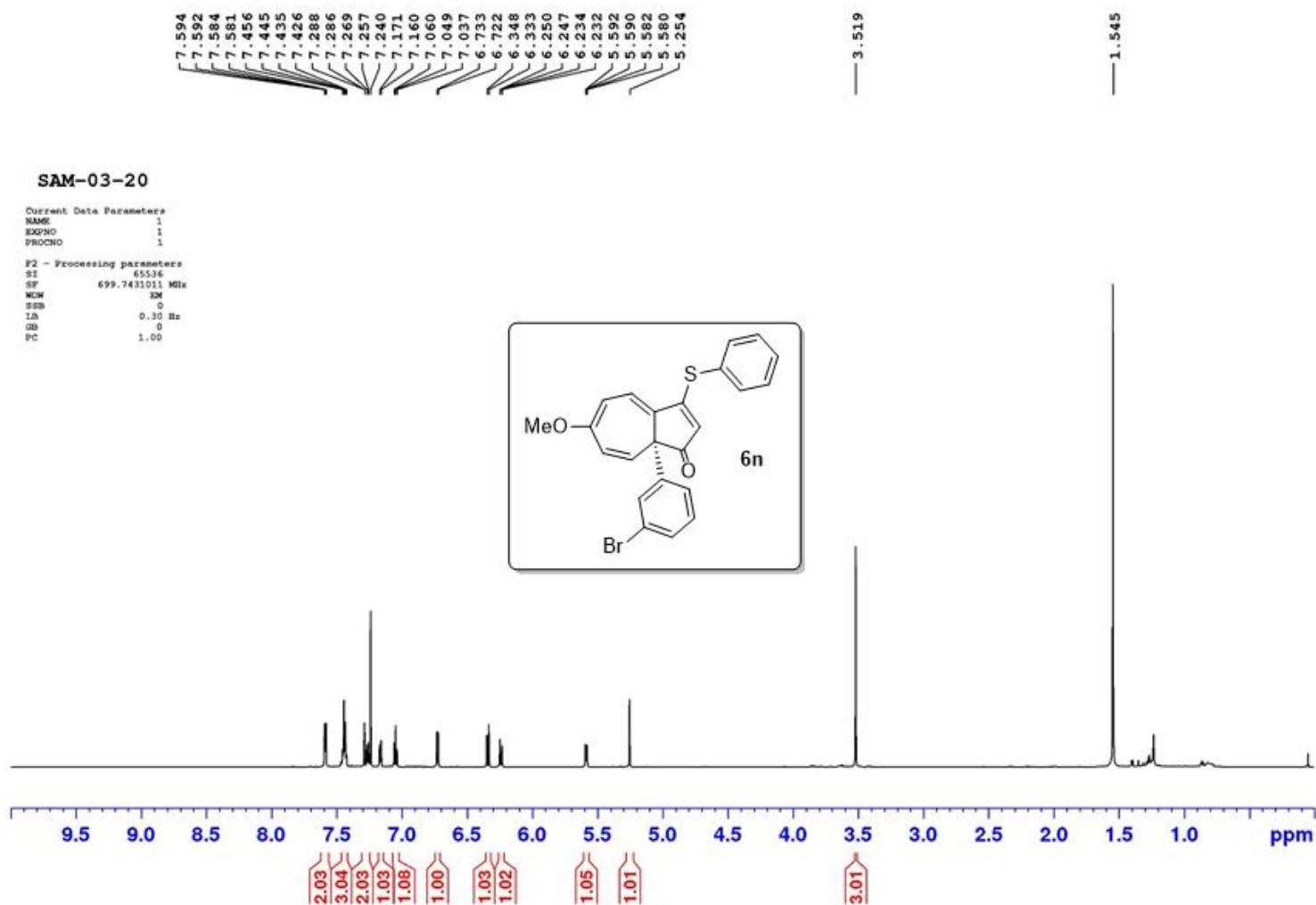
Current Data Parameters
NAME SAM-3-1-8.fid
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431009 MHz
RGW 32M
SFB 0
LA 0.30 Hz
GB 0
PC 1.00



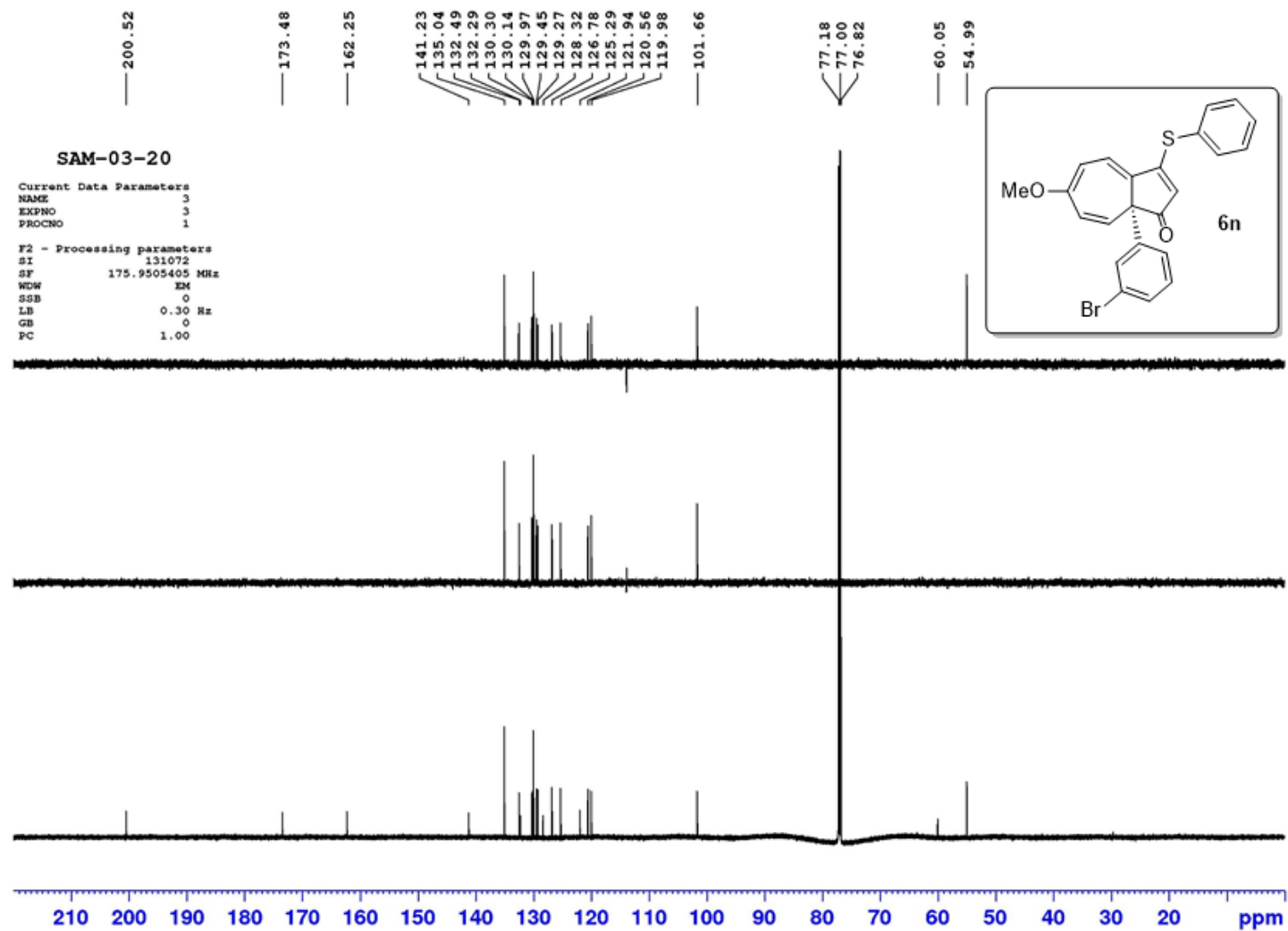
Solvent: CDCl₃
SFO1: 175 MHz



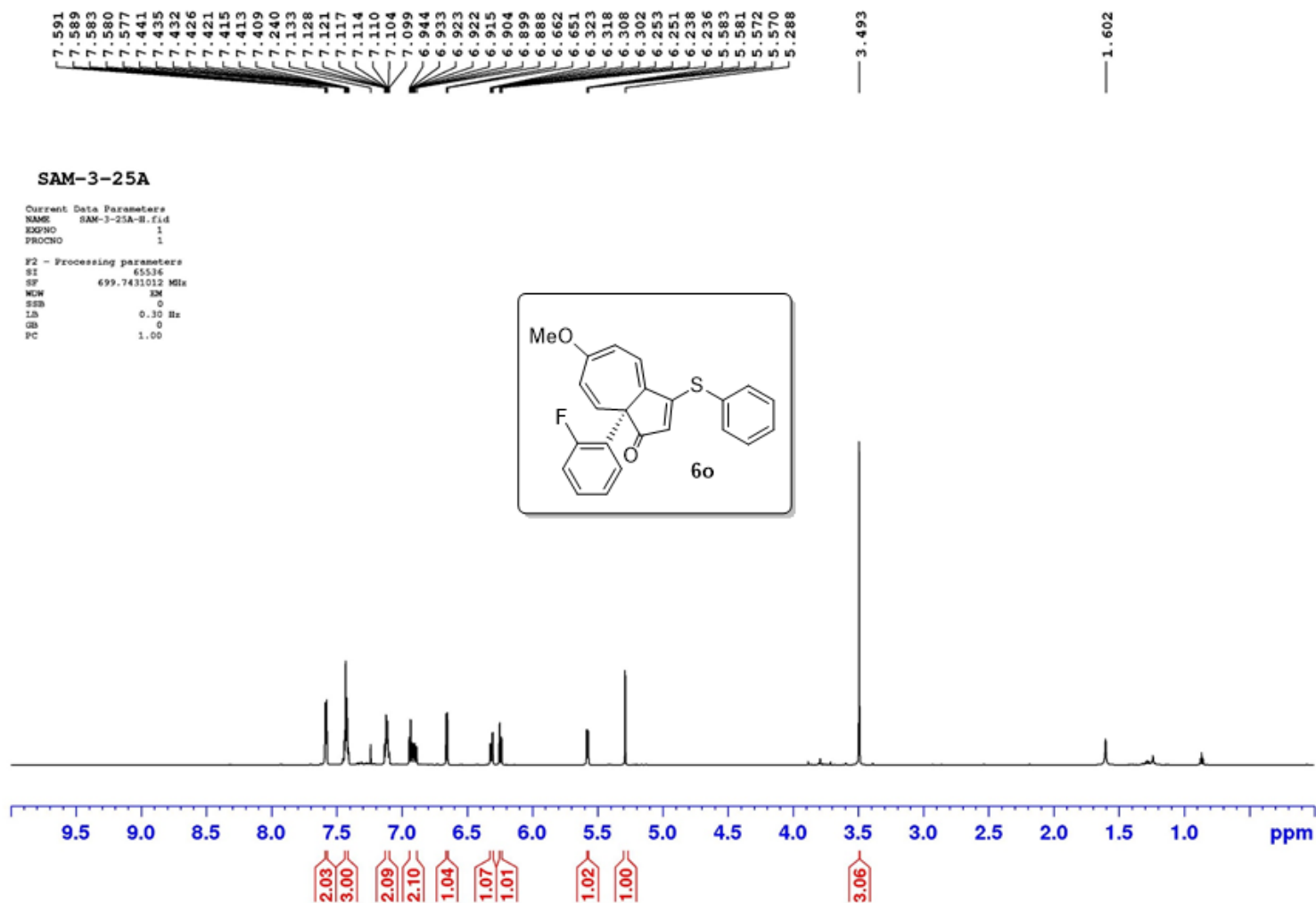
Solvent: CDCl₃
SFO1: 700 MHz



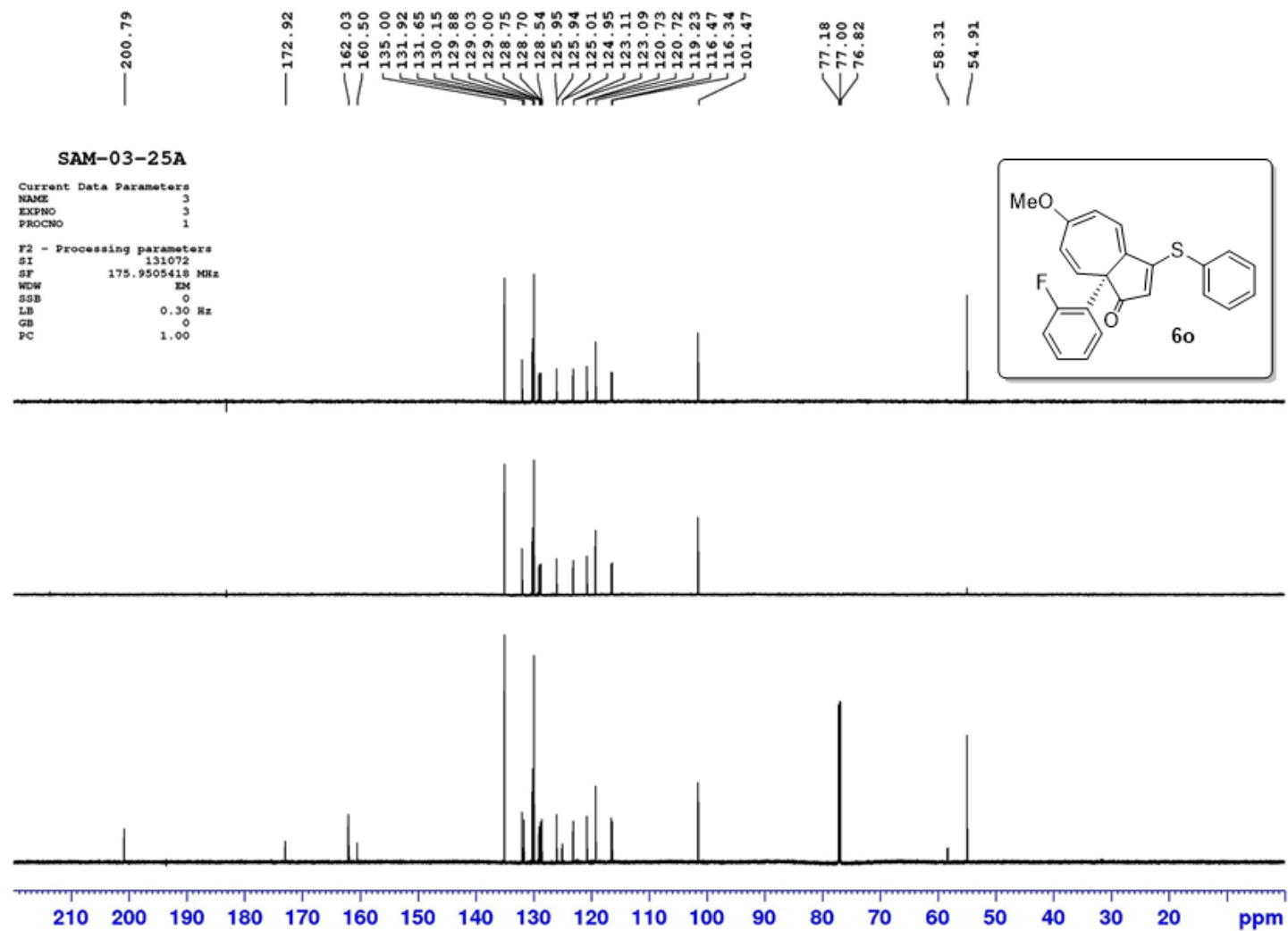
Solvent: CDCl_3
SFO1: 175 MHz



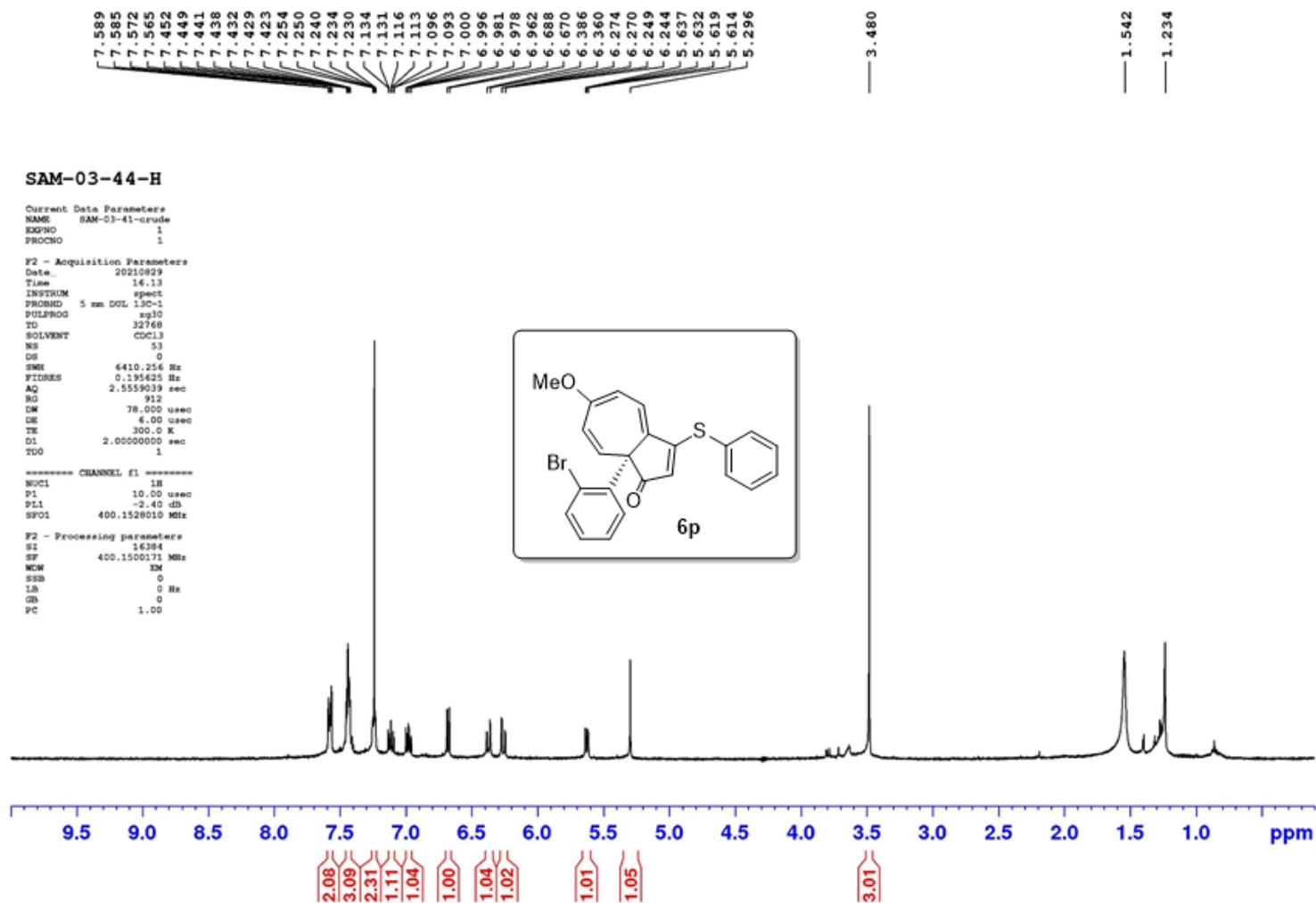
Solvent: CDCl₃
SFO1: 700 MHz



Solvent: CDCl₃
SFO1: 175 MHz



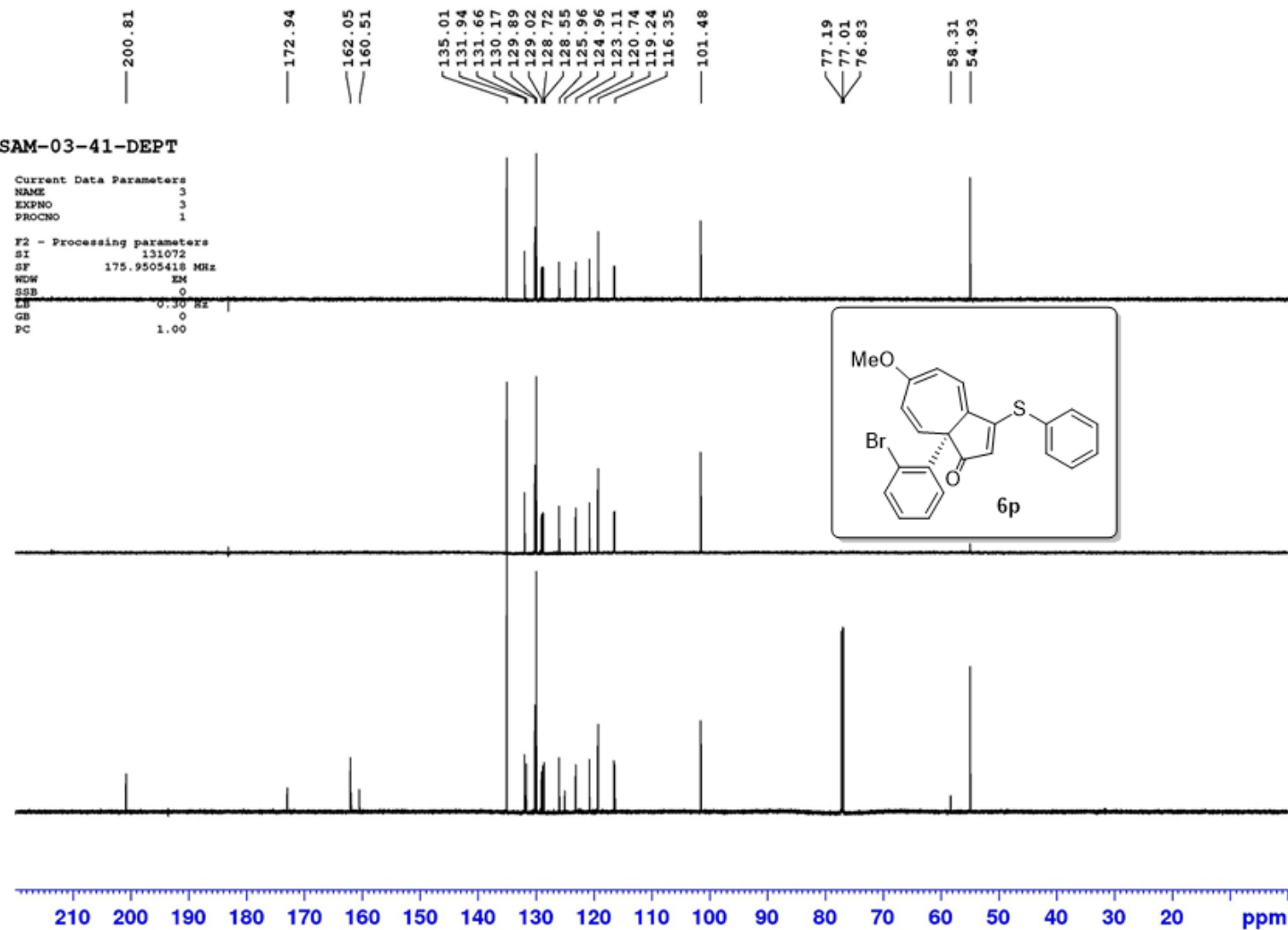
Solvent: CDCl_3
SFO1: 400 MHz



Solvent: CDCl_3
 SFO1: 175 MHz

SAM-03-41-DEPT

Current Data Parameters
 NAME 3
 EXPNO 3
 PROCNO 1
 F2 - Processing parameters
 SI 131072
 SF 175.9505418 MHz
 WDW EM
 SSB 0
 GB 0
 PC 1.00

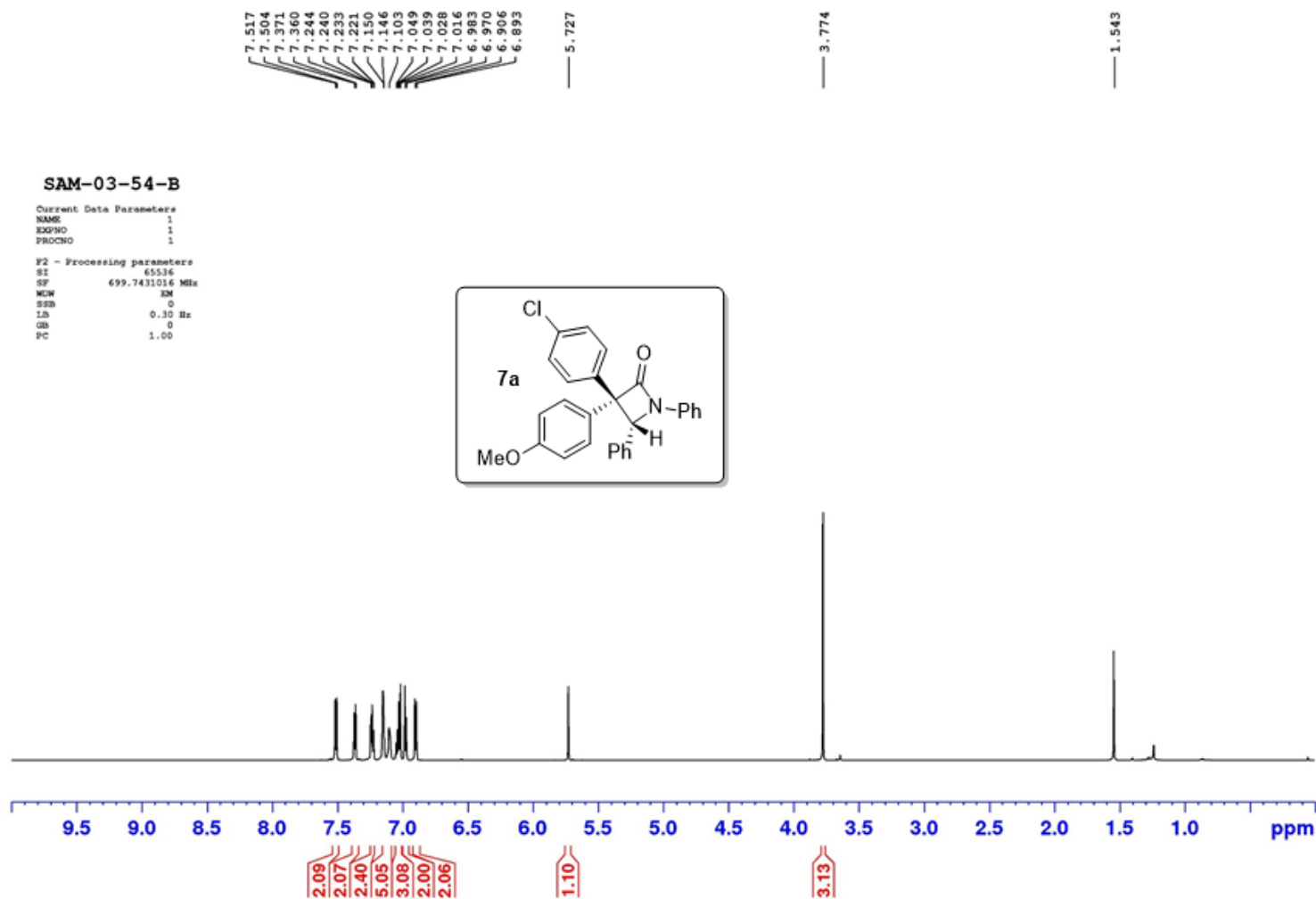
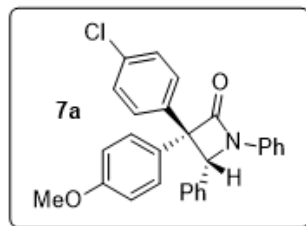


Solvent: CDCl_3
SFO1: 700 MHz

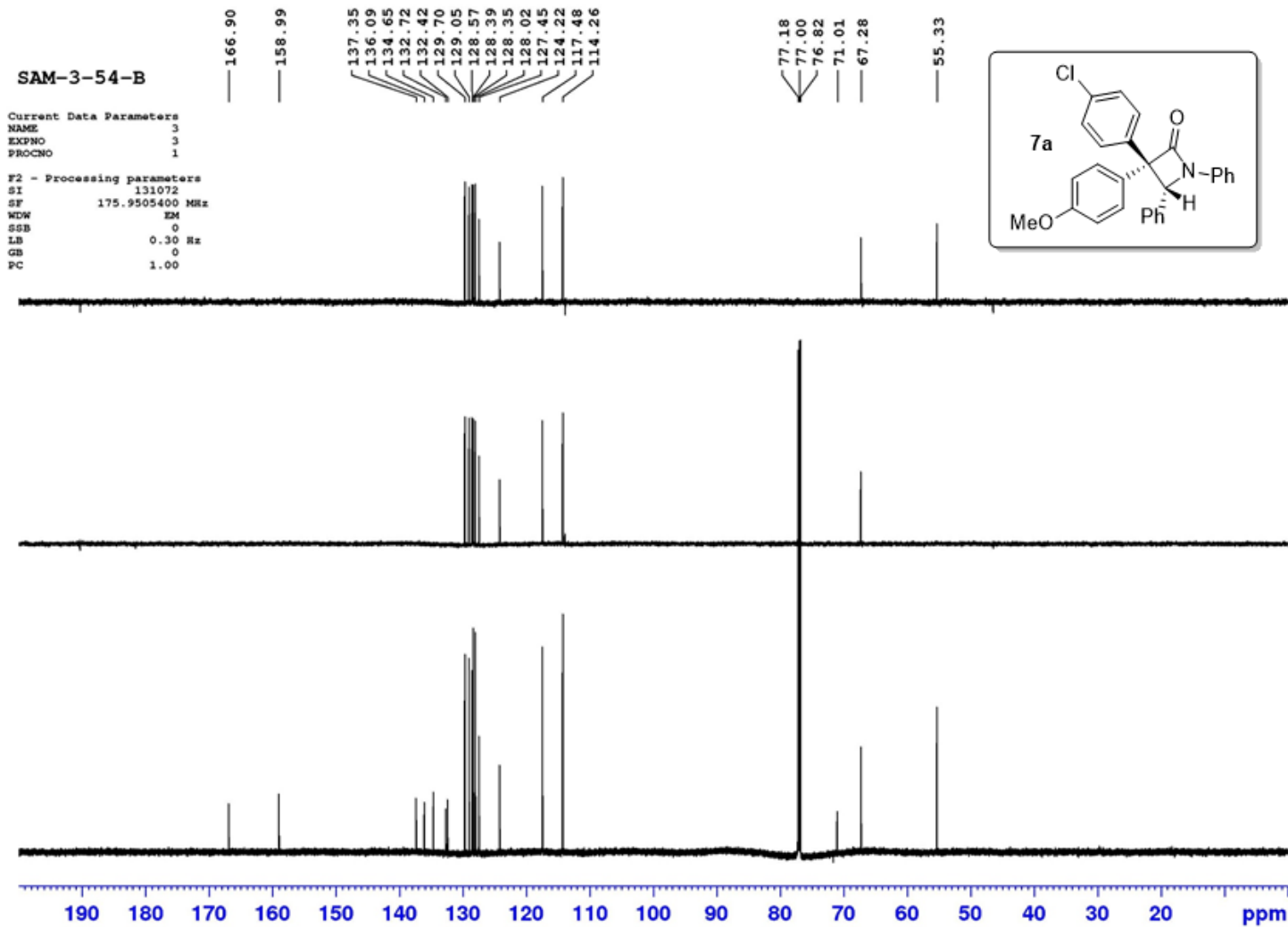
SAM-03-54-B

Current Data Parameters
NAME 1
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7431016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

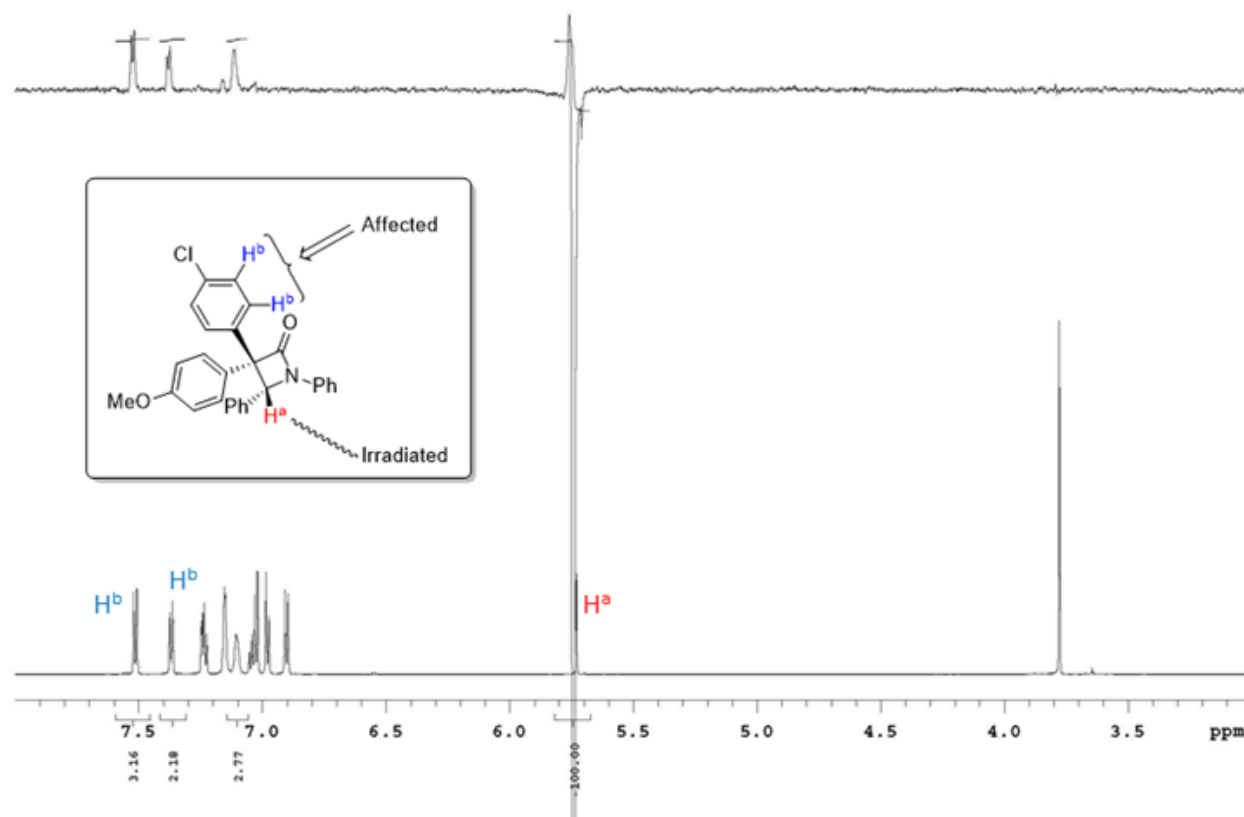


Solvent: CDCl_3
 SFO1: 175 MHz



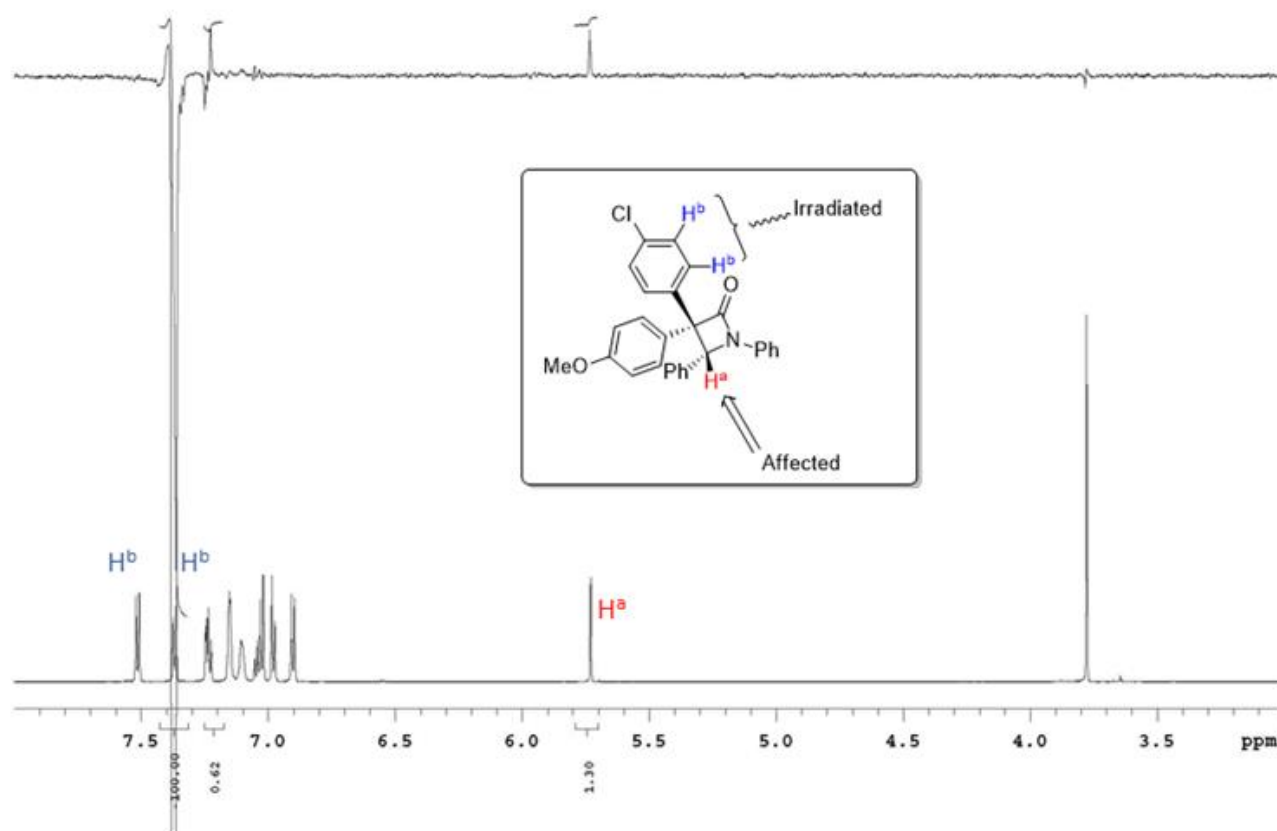
Solvent: CDCl_3
SFO1: 700 MHz

NOE of compound (**7a**):



Solvent: CDCl_3
SFO1: 700 MHz

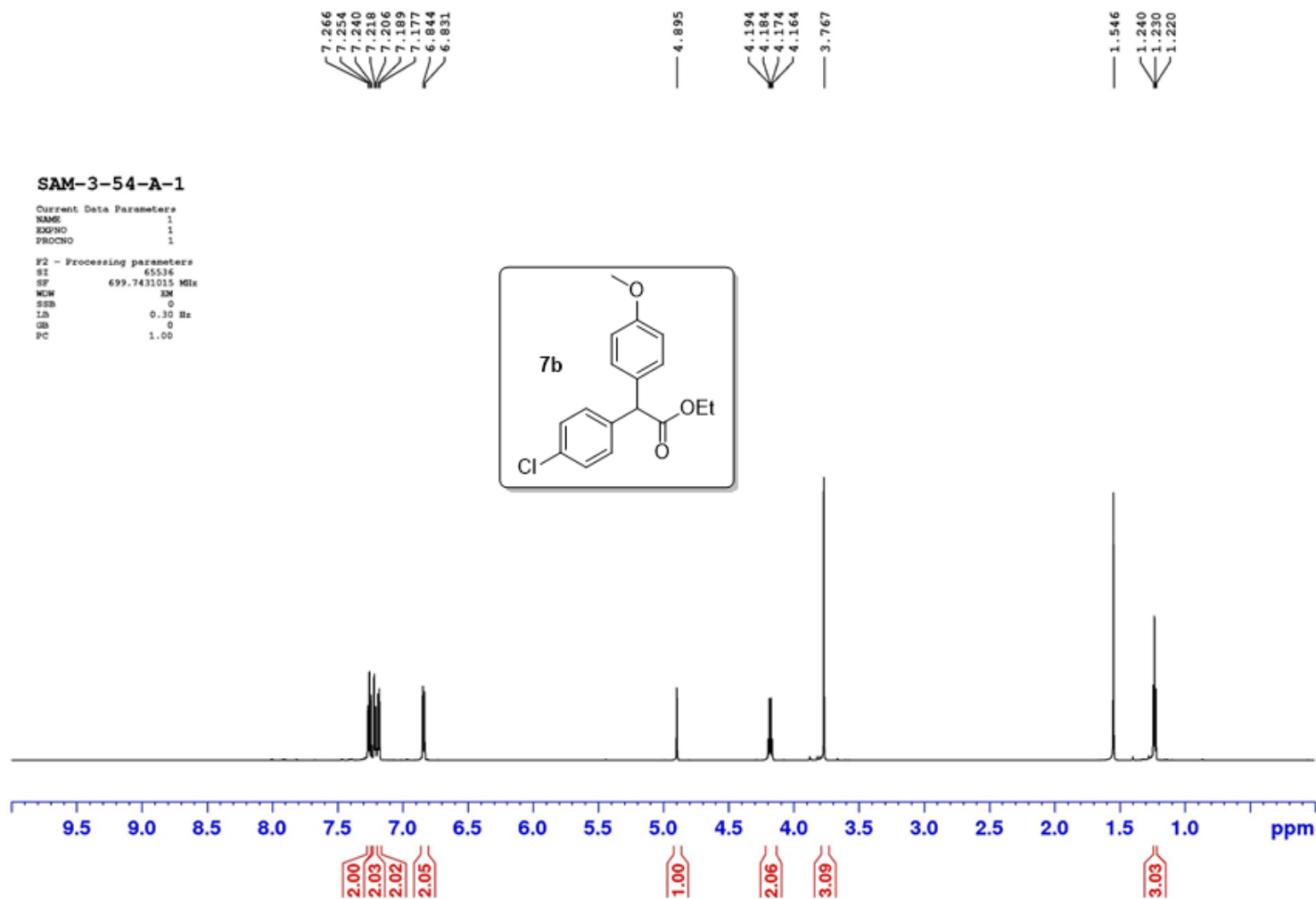
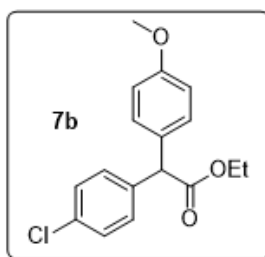
NOE of compound (**7a**):



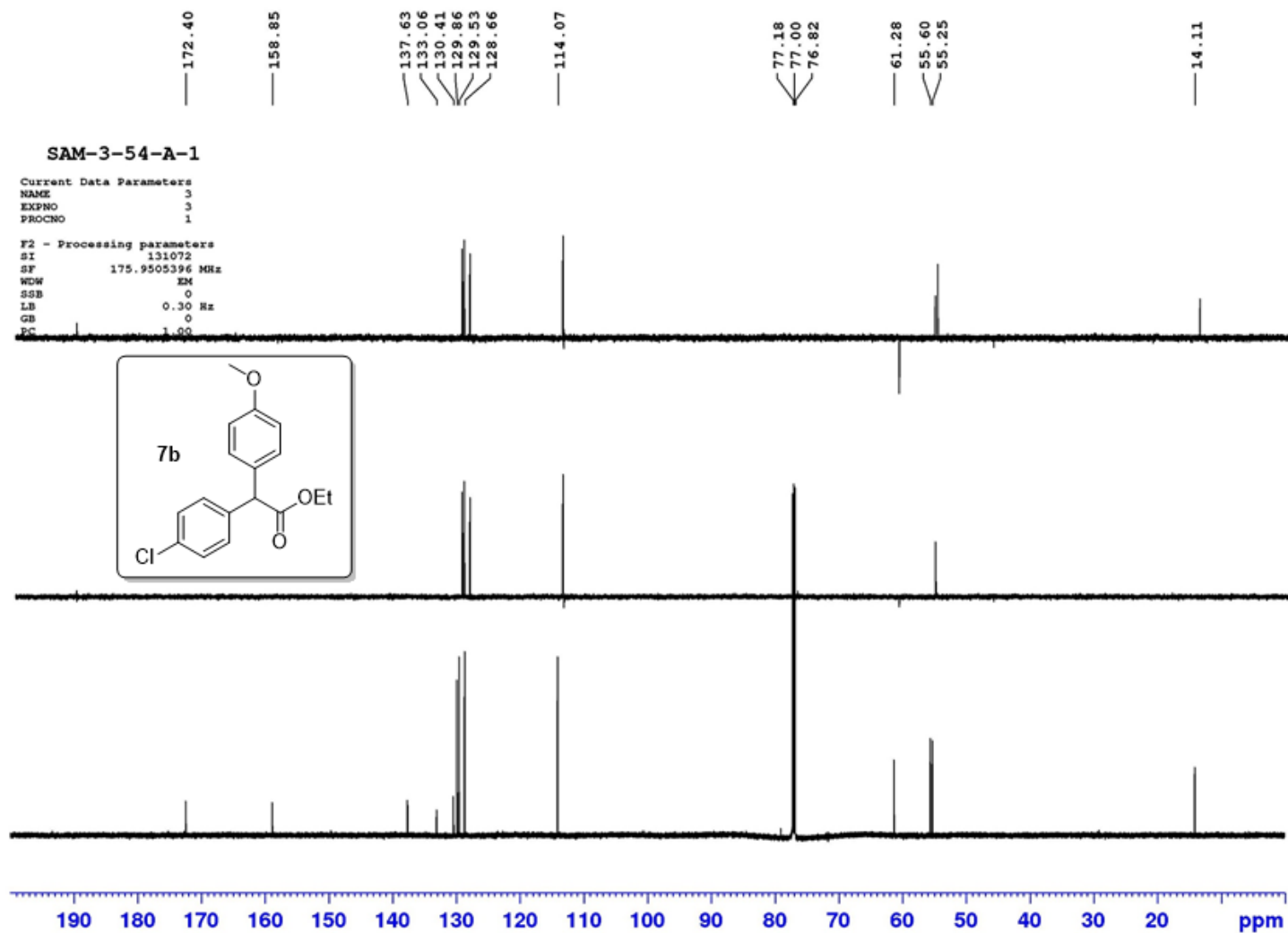
Solvent: CDCl_3
SFO1: 700 MHz

SAM-3-54-A-1

Current Data Parameters
NAME 1
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 175 MHz

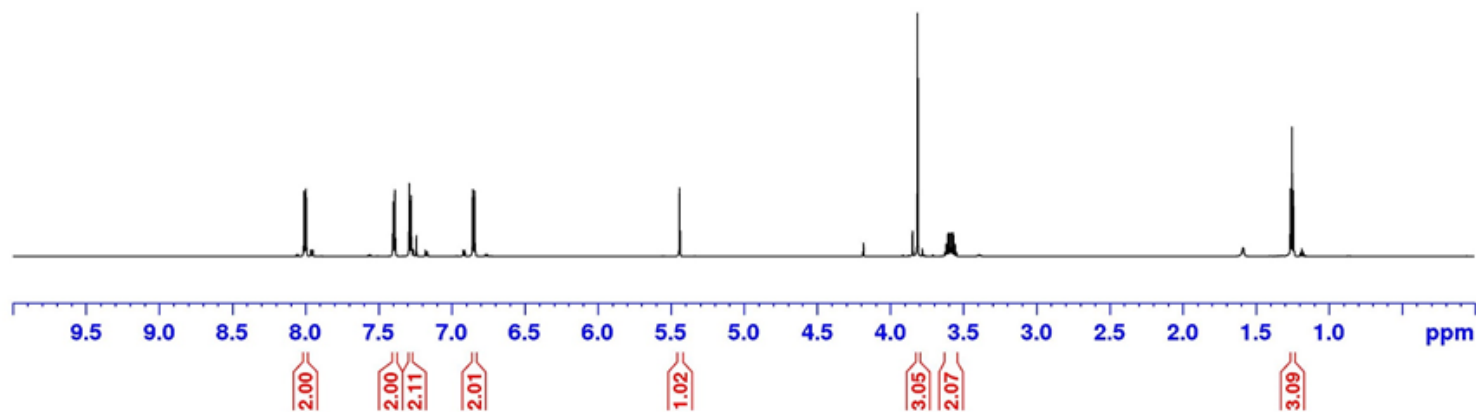
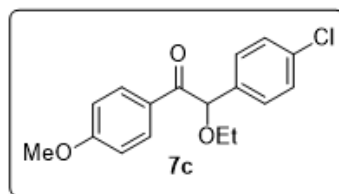


Solvent: CDCl₃
SFO1: 700 MHz

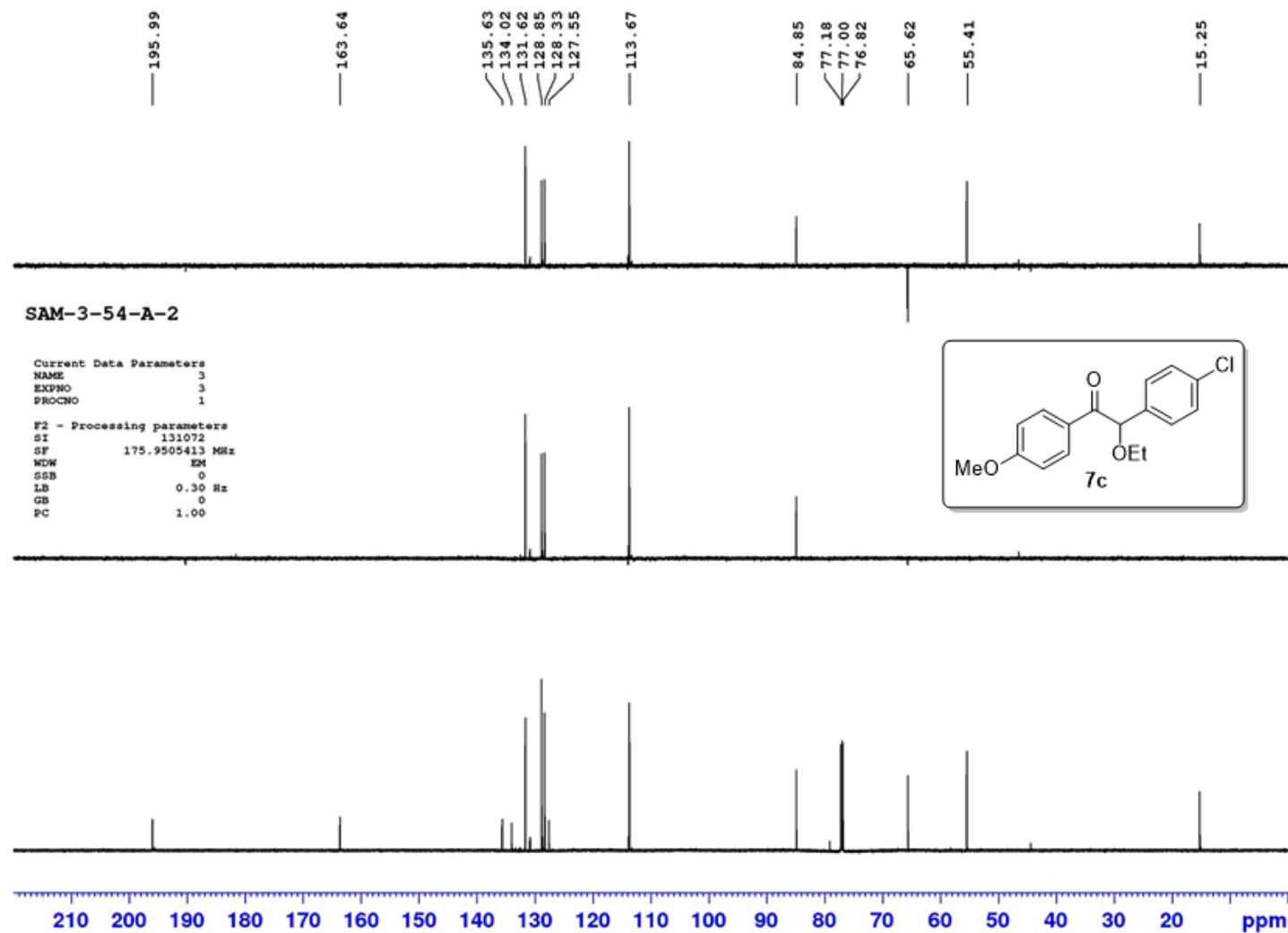


SAM-3-54-A-2

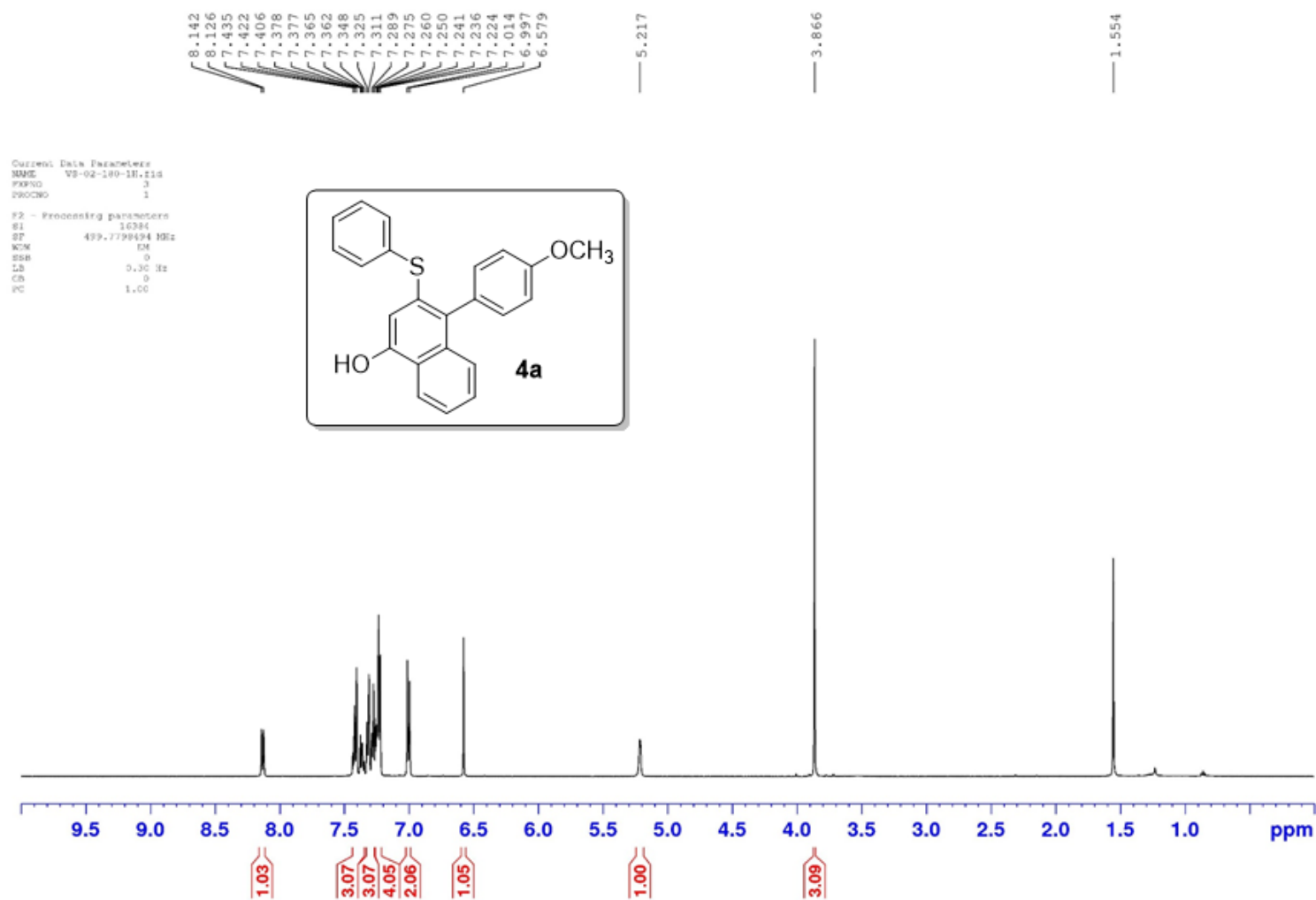
Current Data Parameters
NAME 1
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431014 MHz
RG 328
SFB 0
LB 0.30 Hz
GB 0
PC 1.00



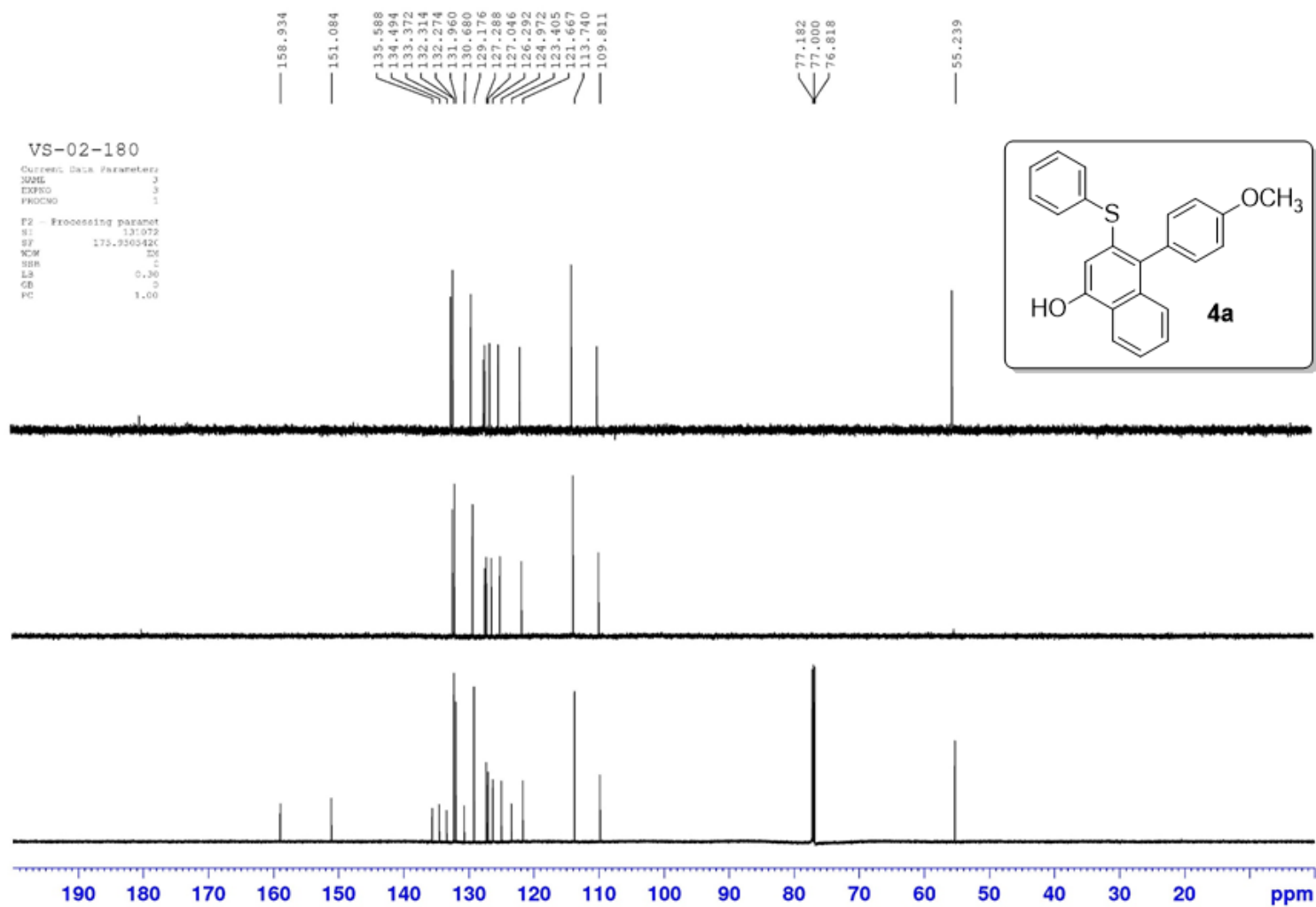
Solvent: CDCl_3
 SFO1: 175 MHz



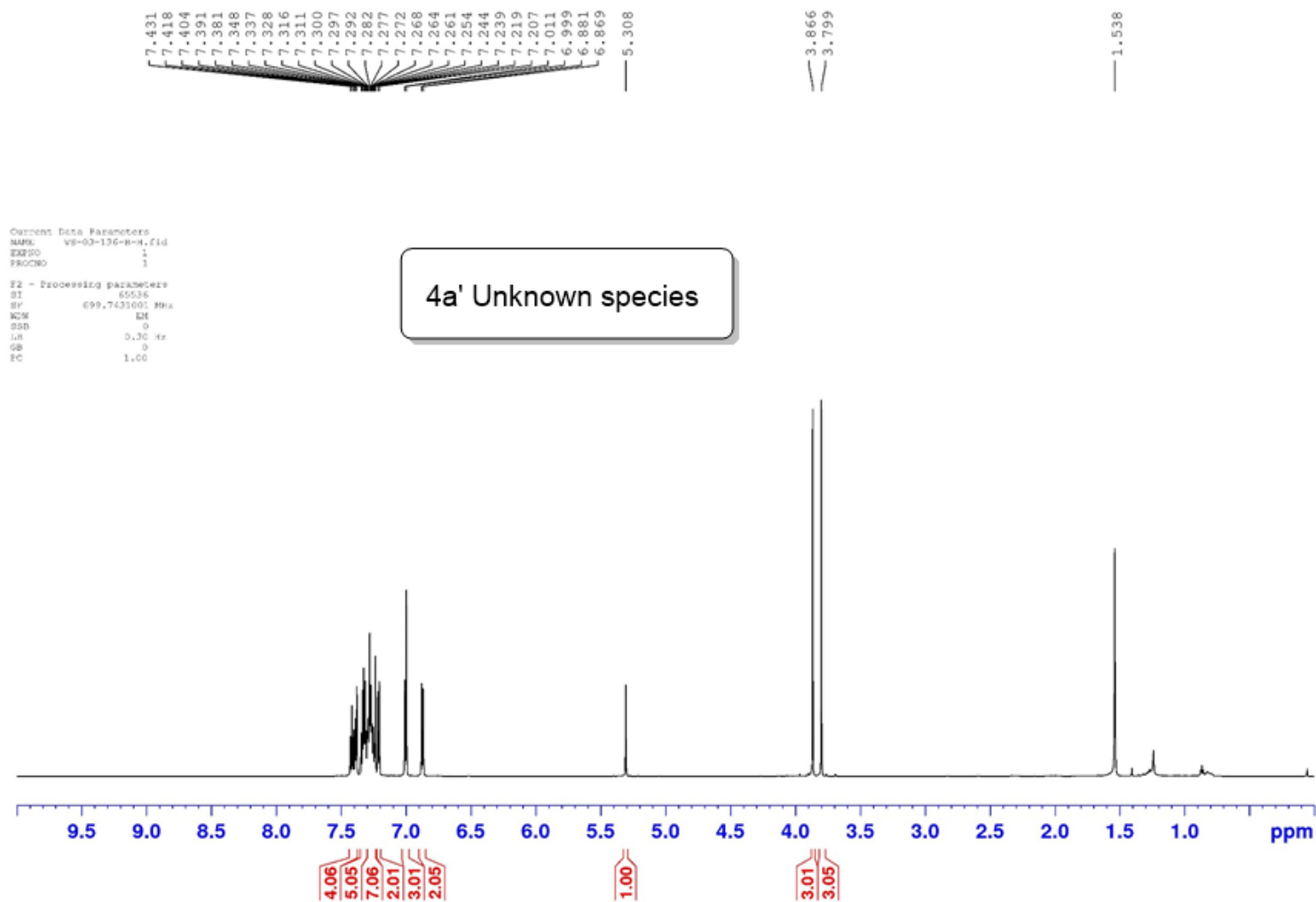
Solvent: CDCl_3
SFO1: 500 MHz



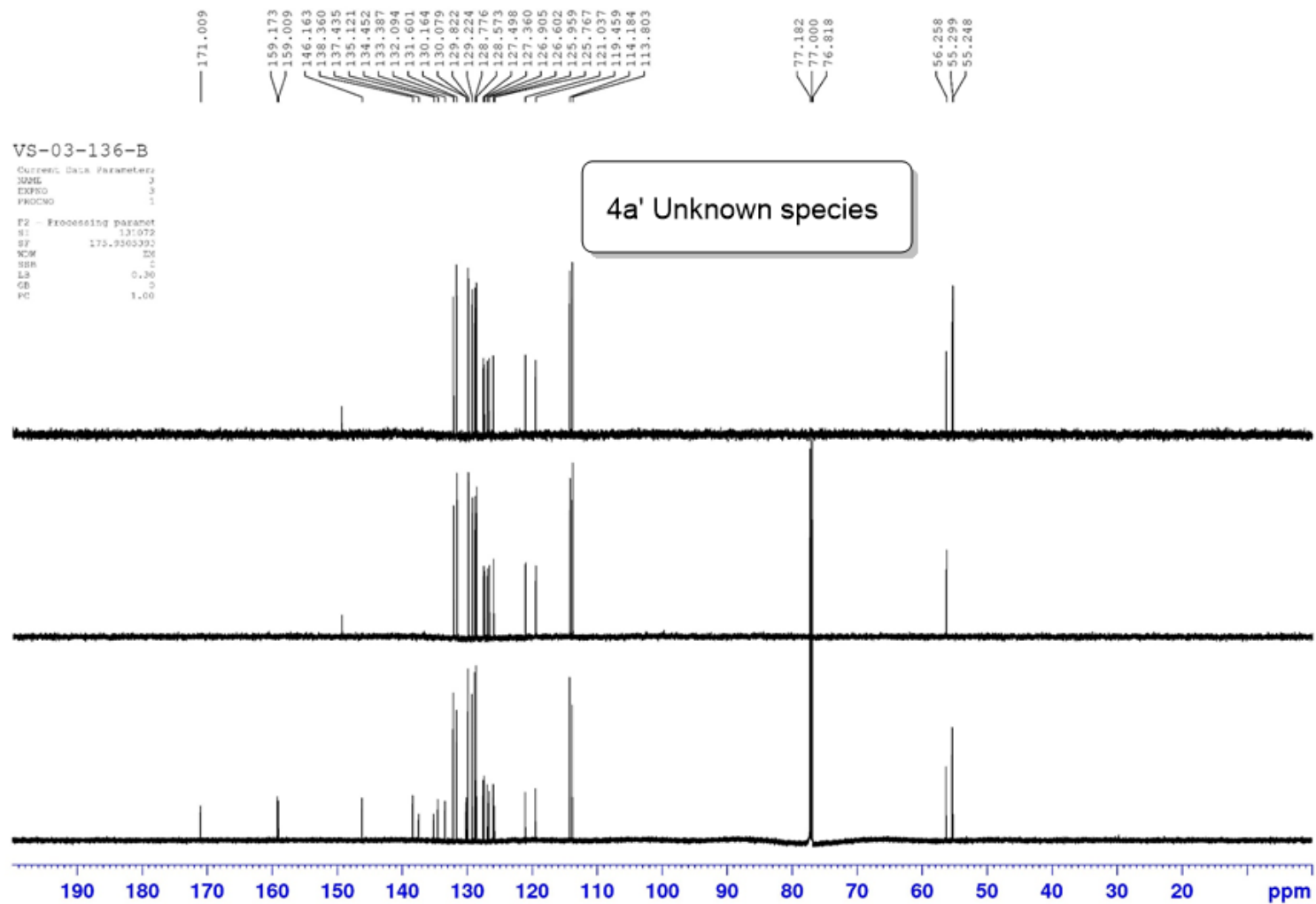
Solvent: CDCl₃
SFO1: 175 MHz



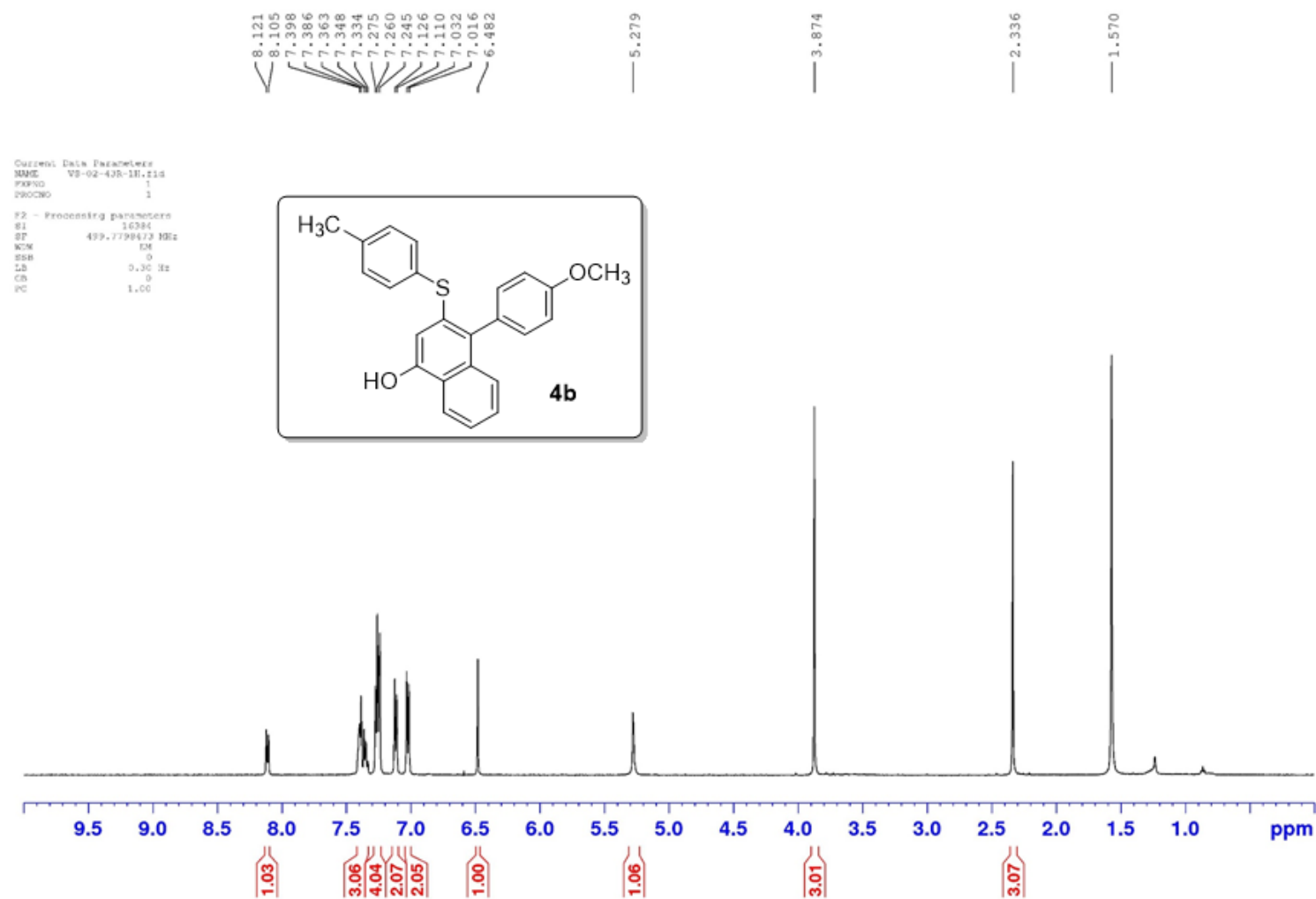
Solvent: CDCl_3
SFO1: 700 MHz



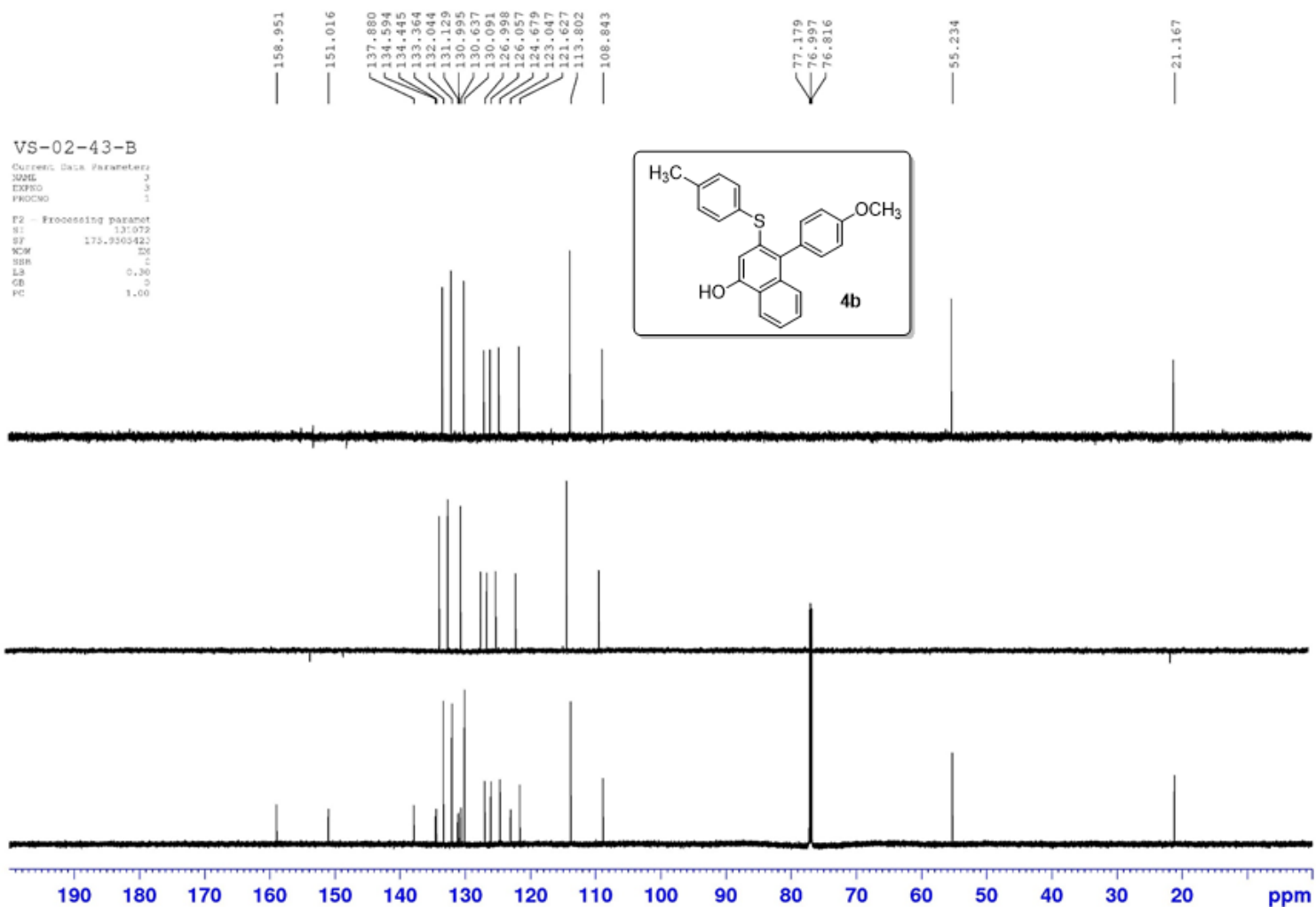
Solvent: CDCl_3
SFO1: 175 MHz



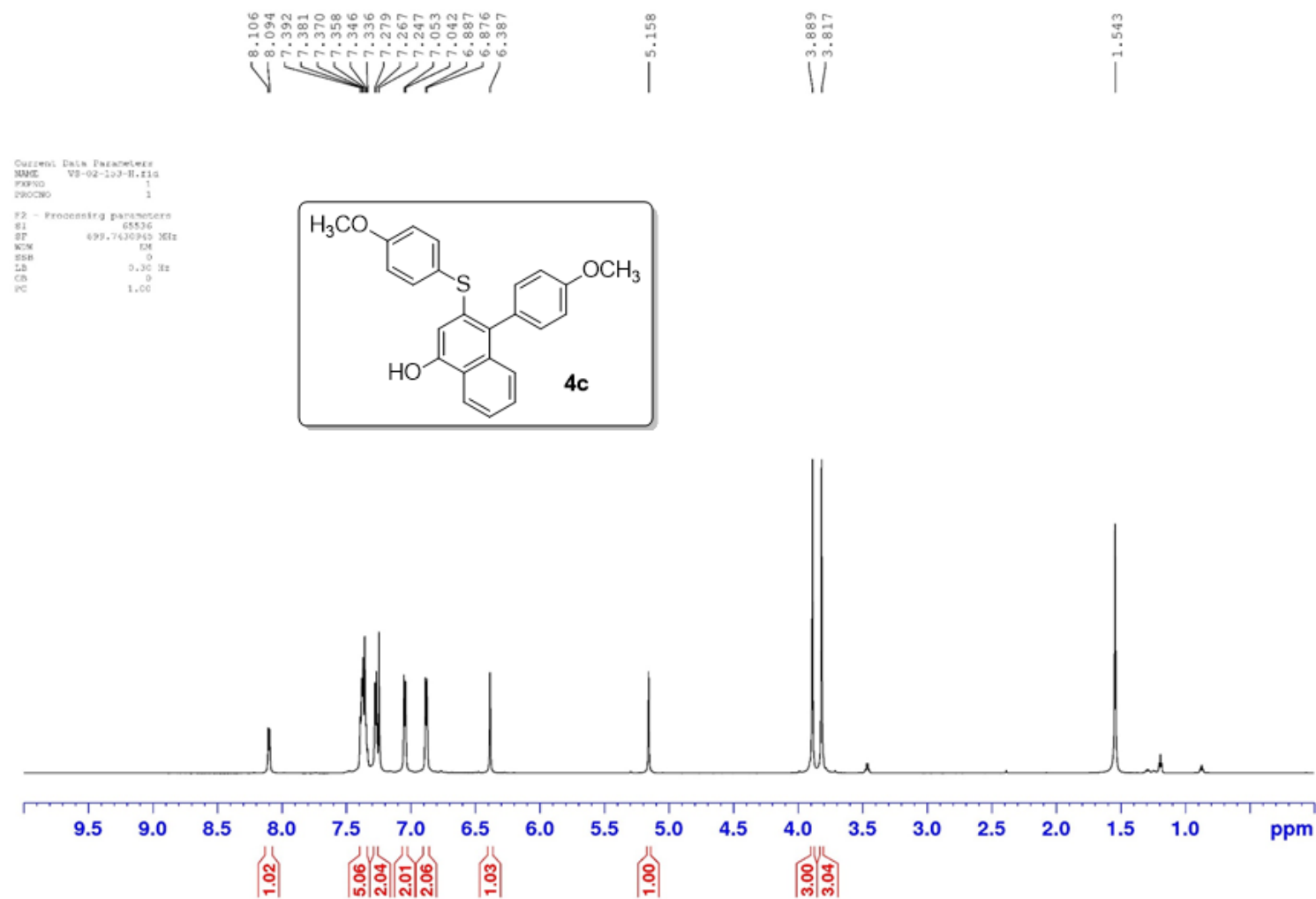
Solvent: CDCl_3
SFO1: 500 MHz



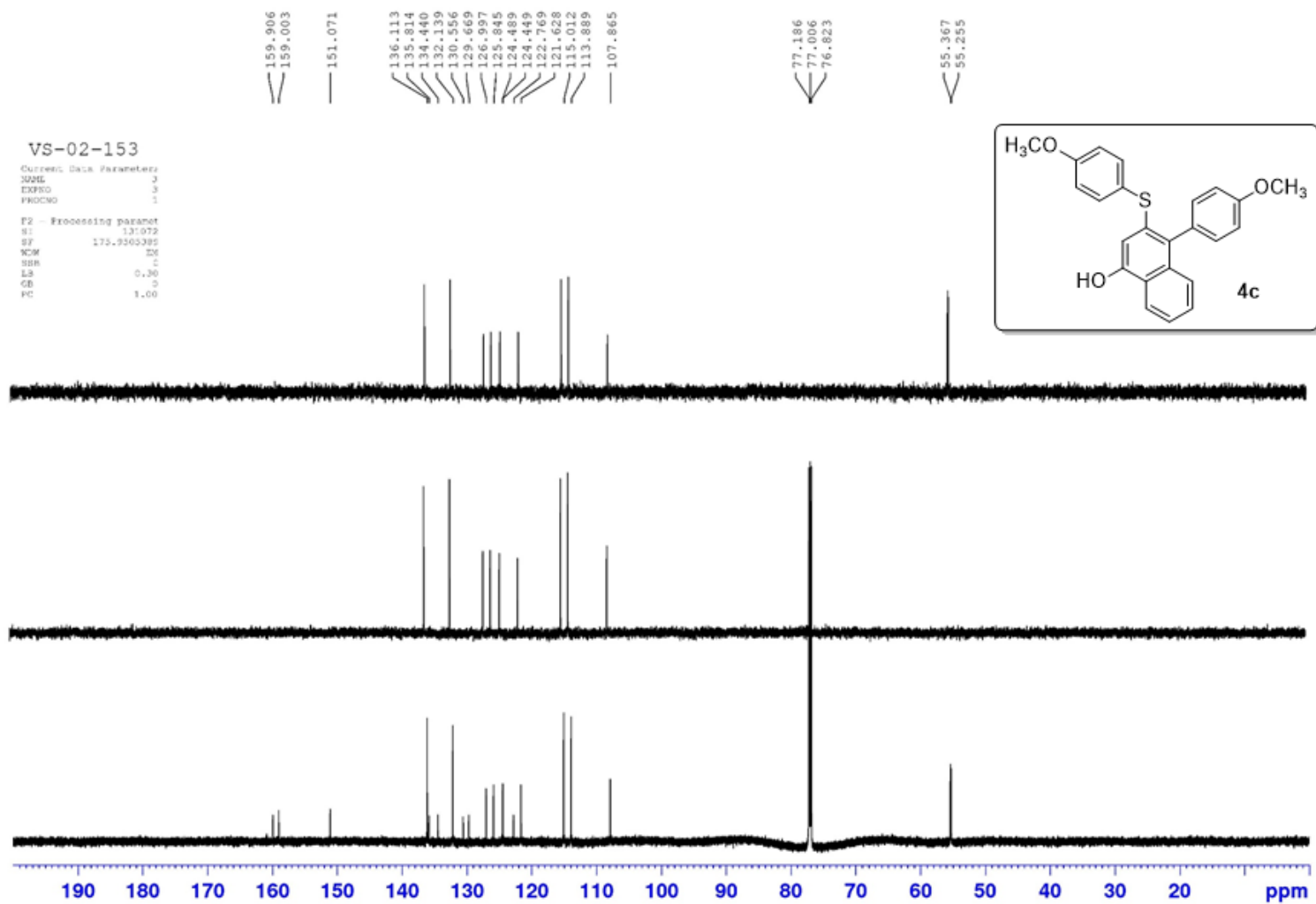
Solvent: CDCl₃
SFO1: 175 MHz



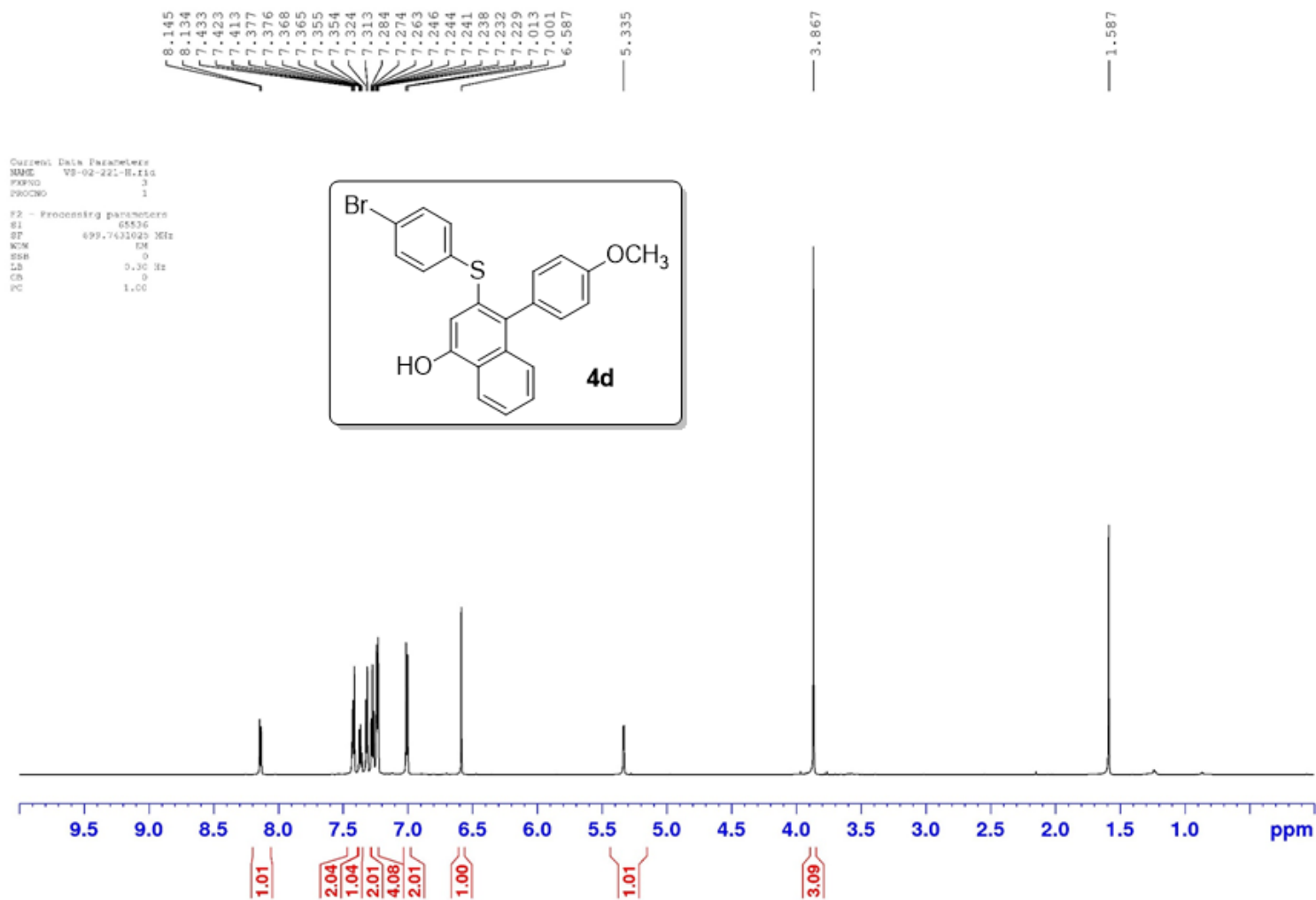
Solvent: CDCl_3
SFO1: 700 MHz



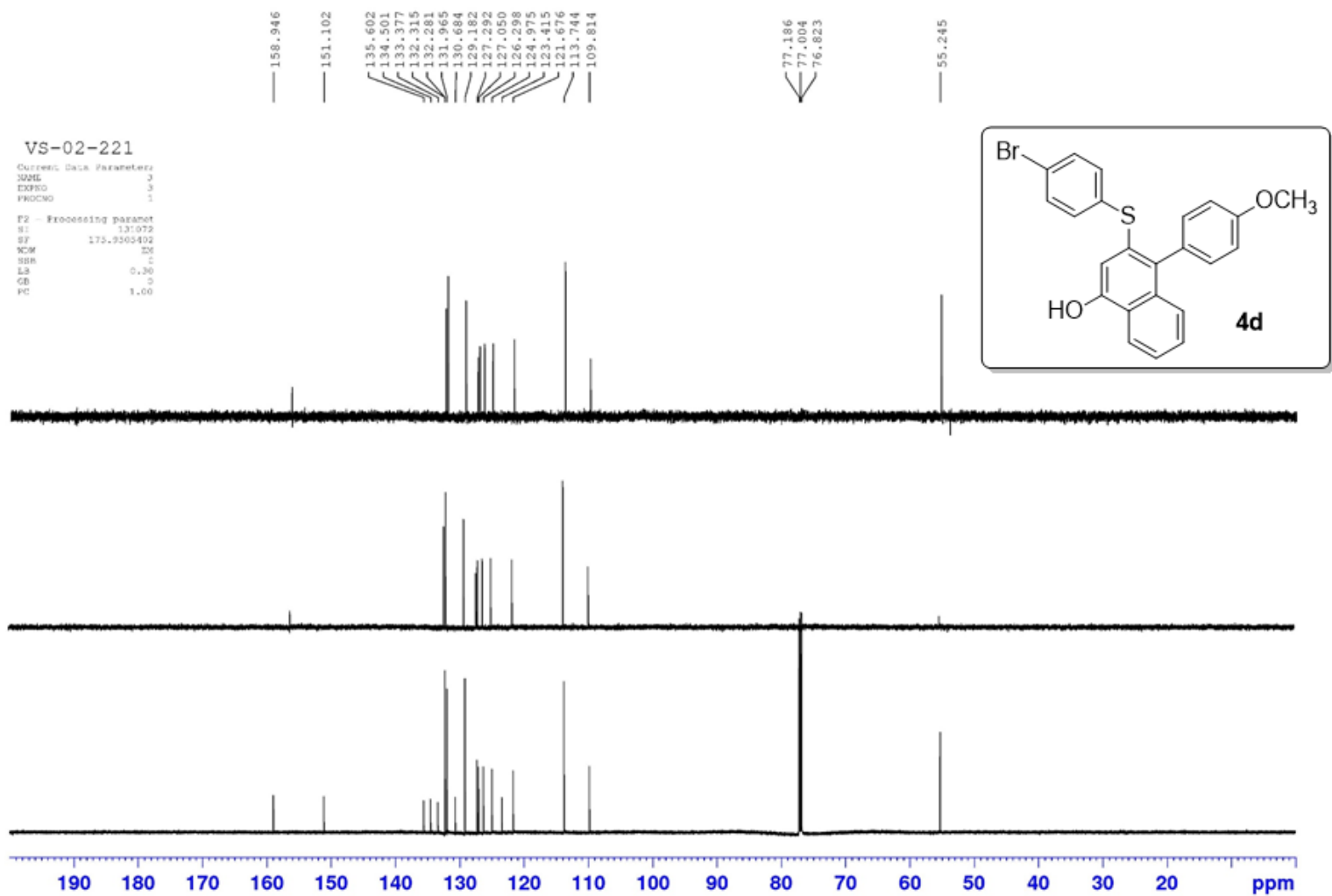
Solvent: CDCl₃
SFO1: 175 MHz



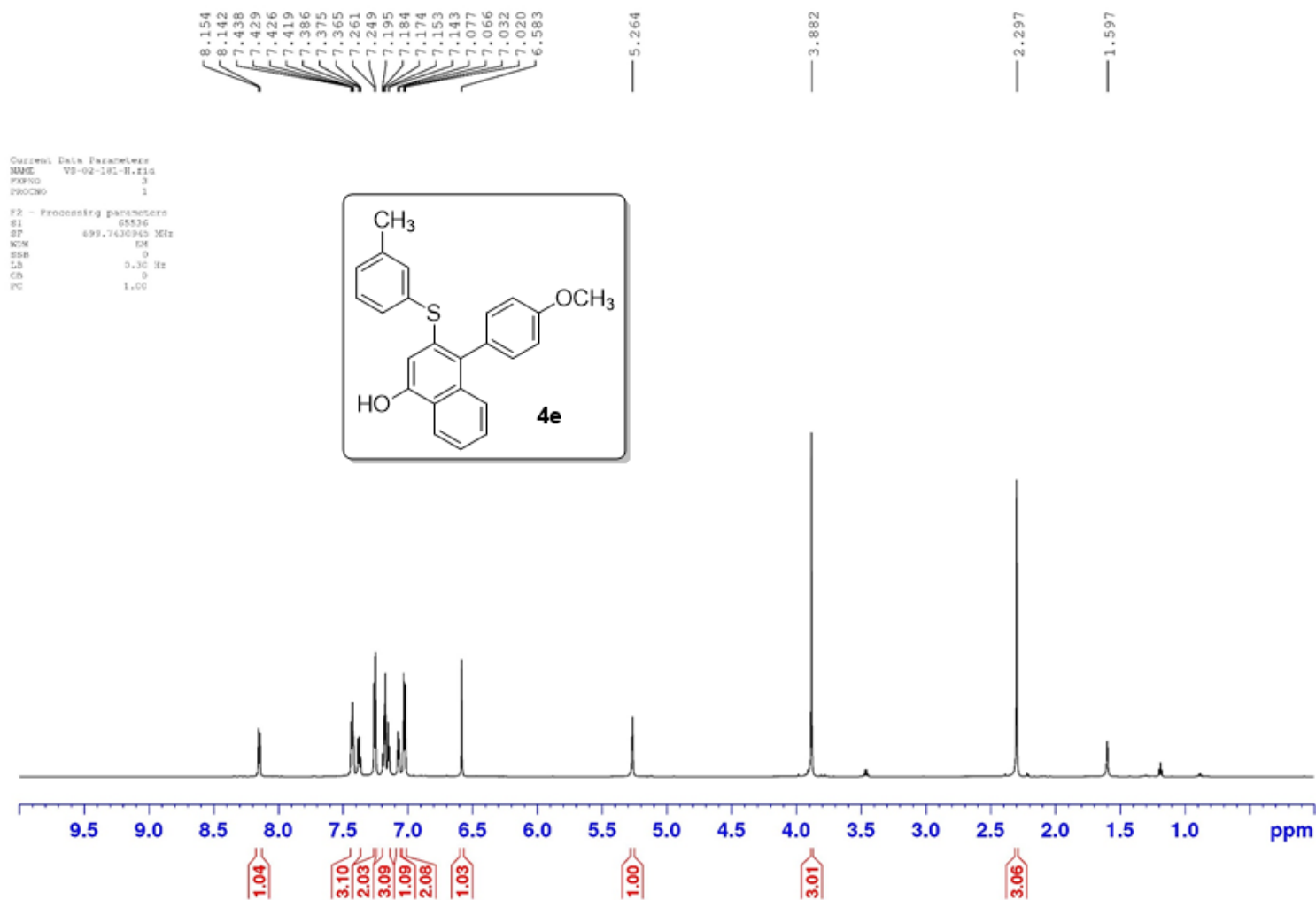
Solvent: CDCl_3
SFO1: 700 MHz



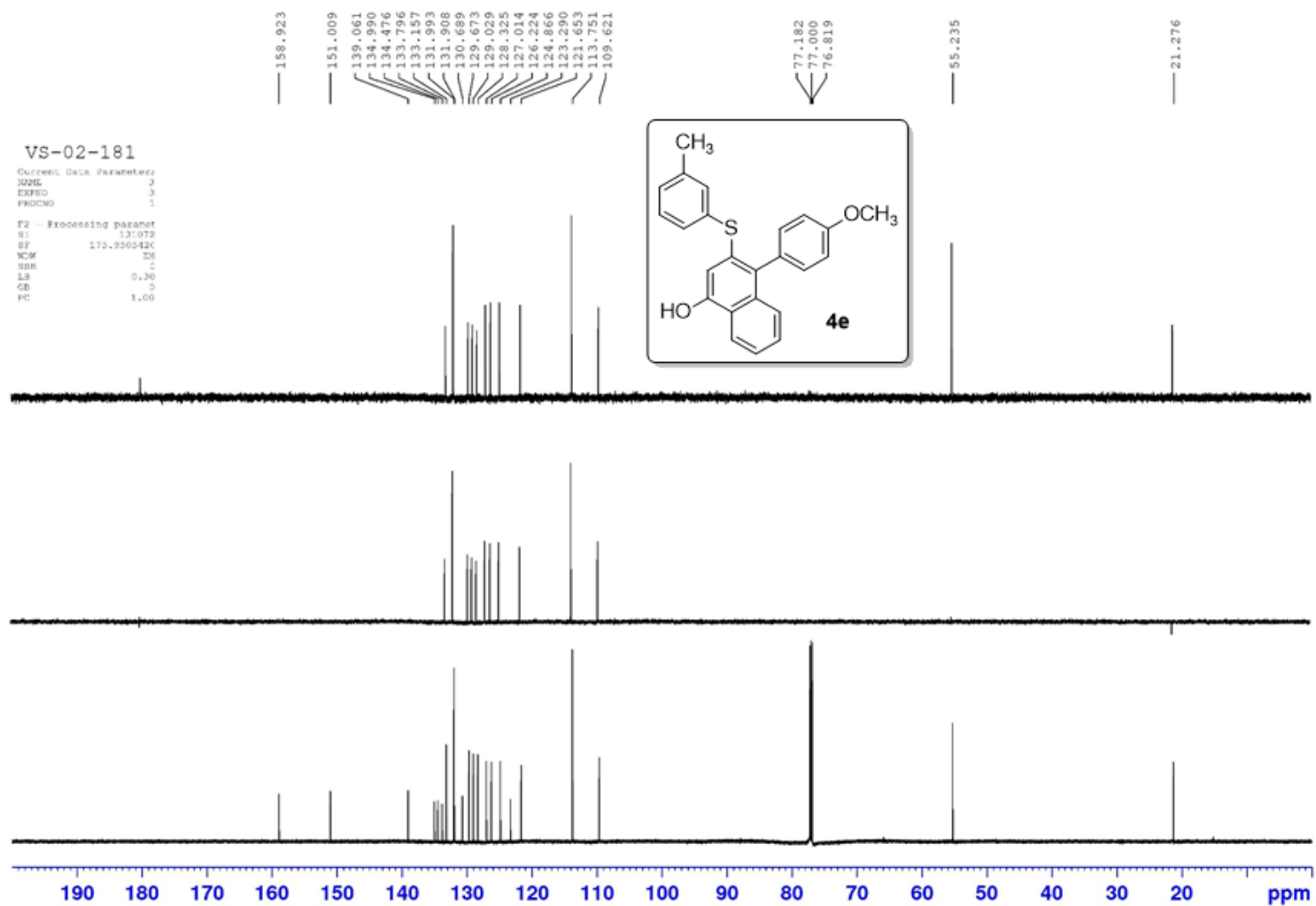
Solvent: CDCl_3
SFO1: 175 MHz



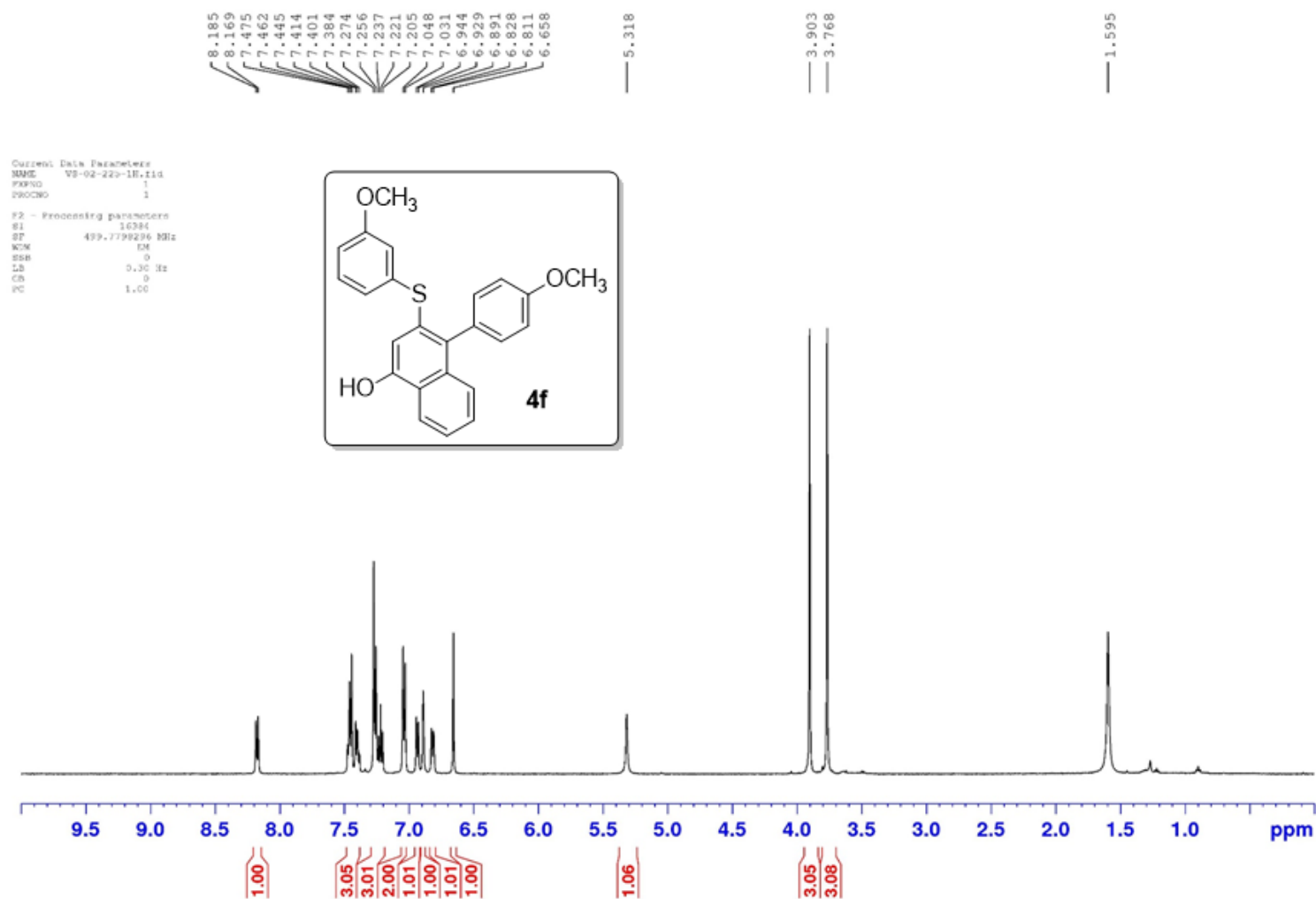
Solvent: CDCl_3
SFO1: 700 MHz



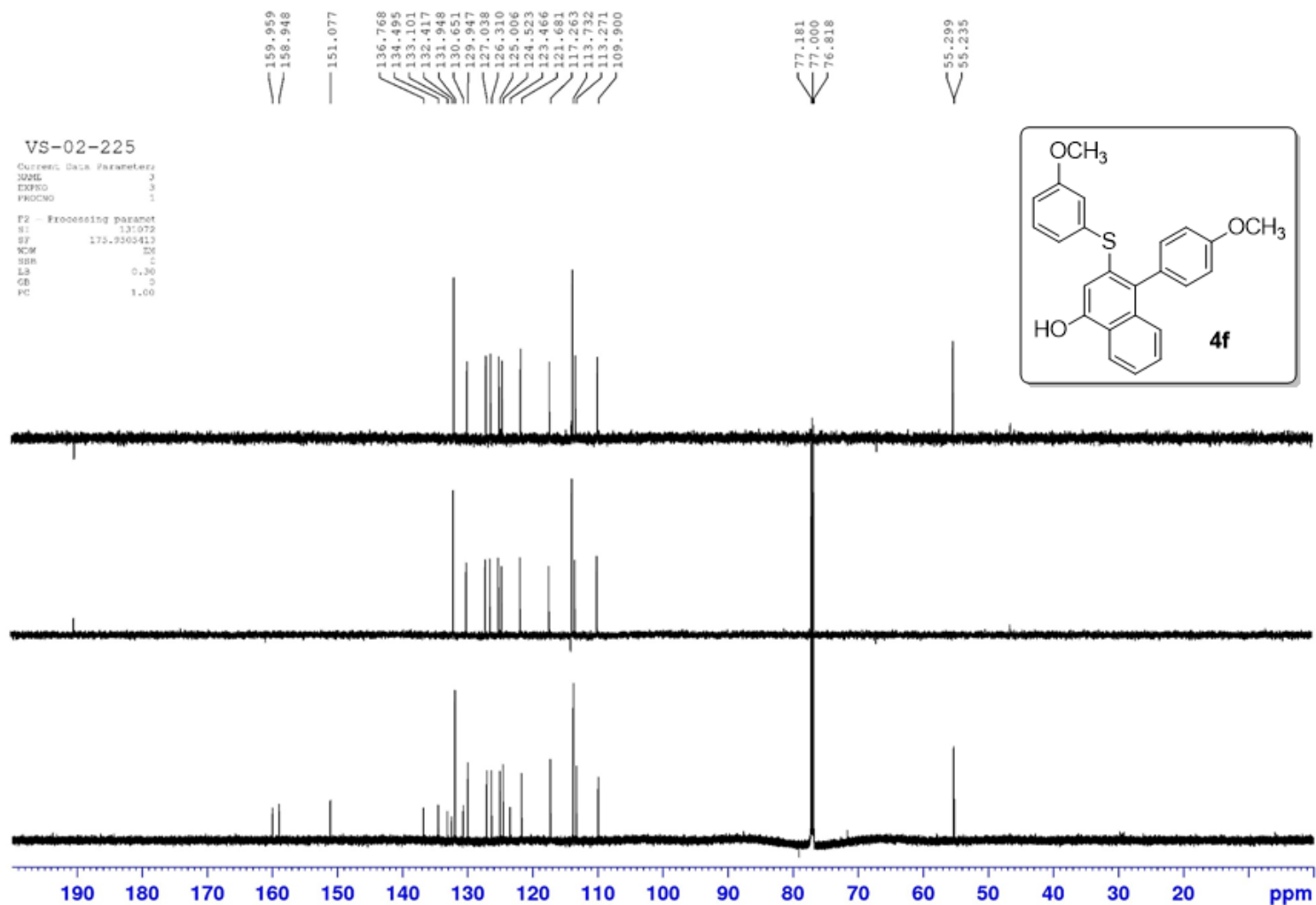
Solvent: CDCl₃
SFO1: 175 MHz



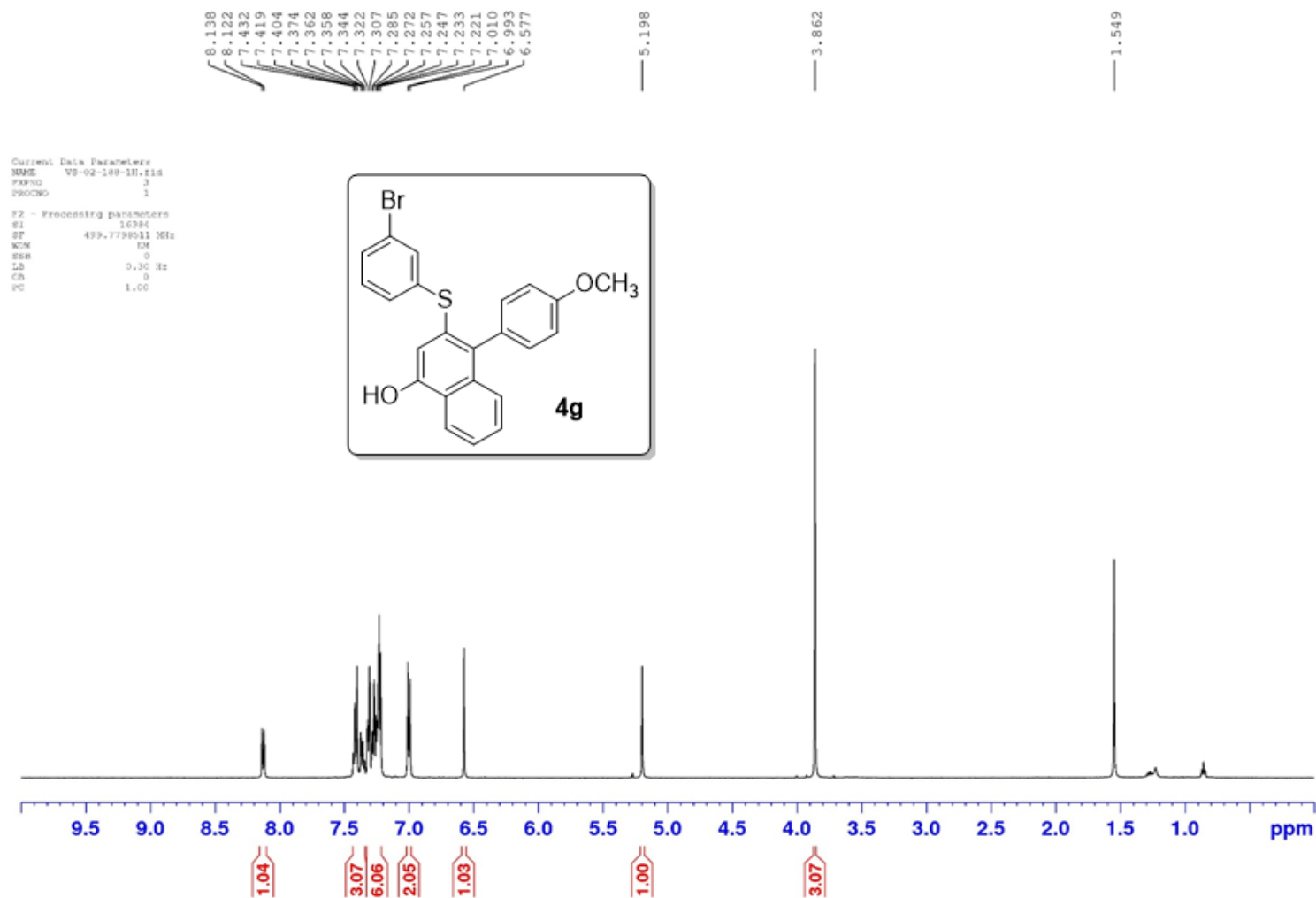
Solvent: CDCl_3
SFO1: 500 MHz



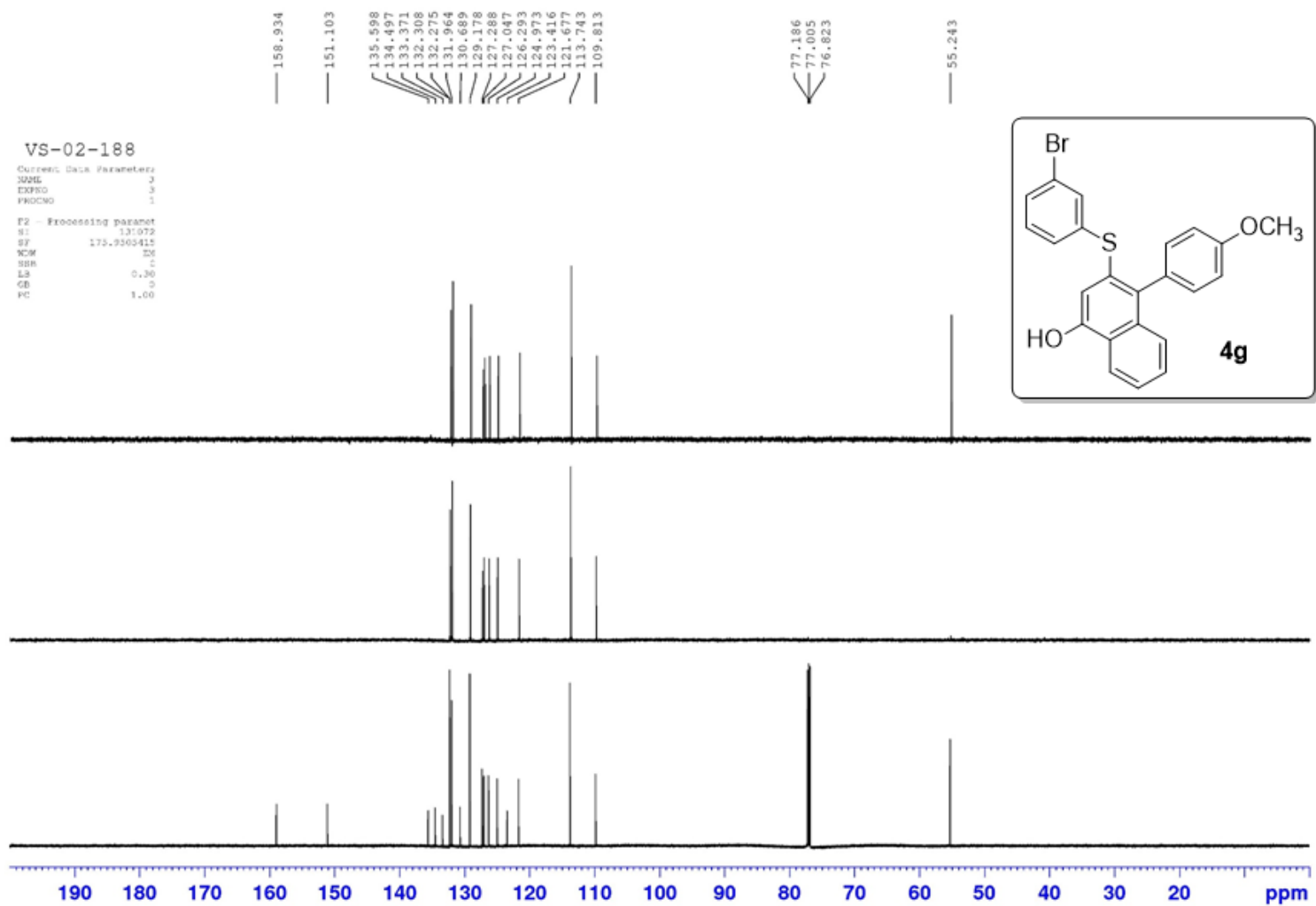
Solvent: CDCl₃
SFO1: 175 MHz



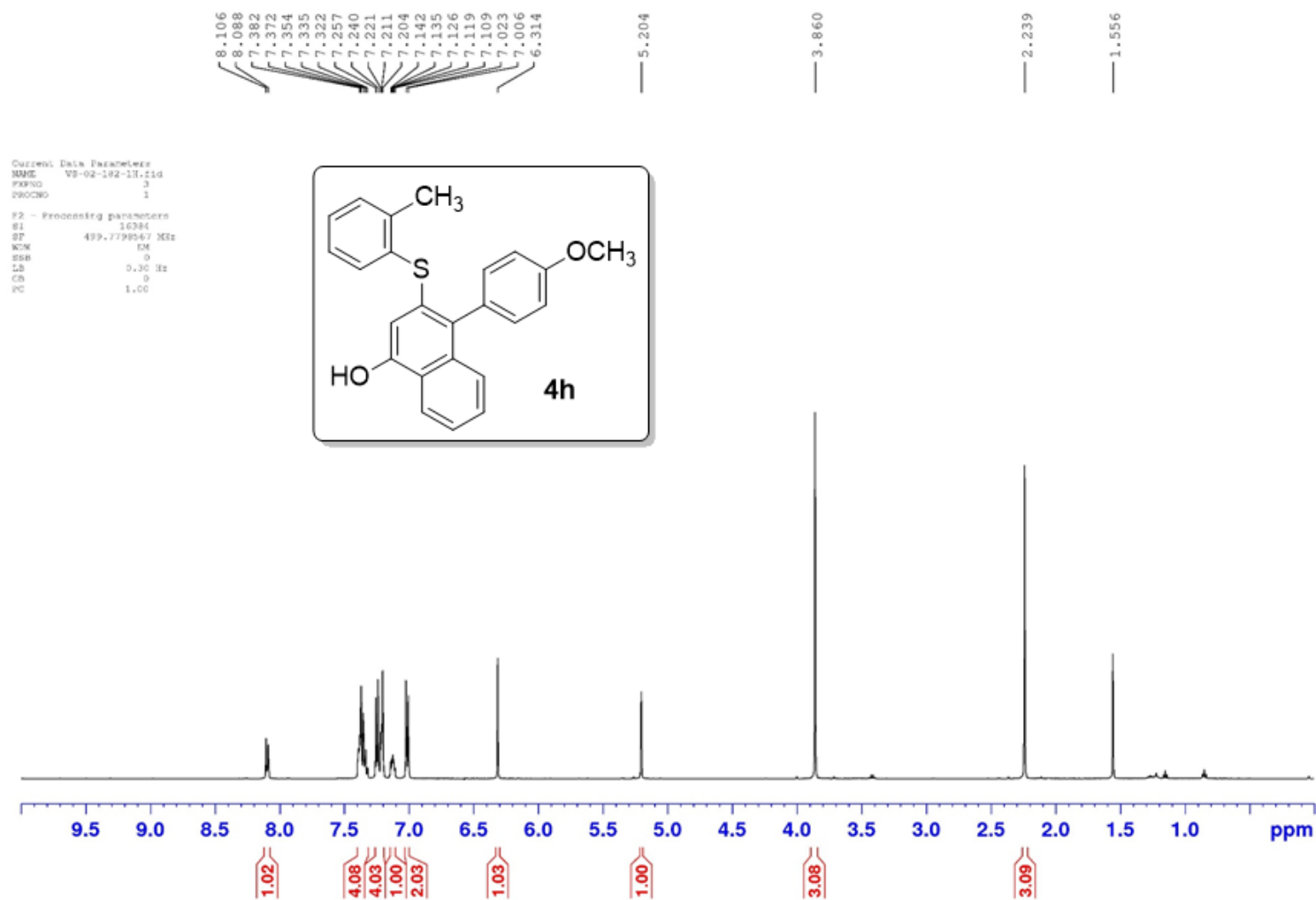
Solvent: CDCl_3
SFO1: 500 MHz



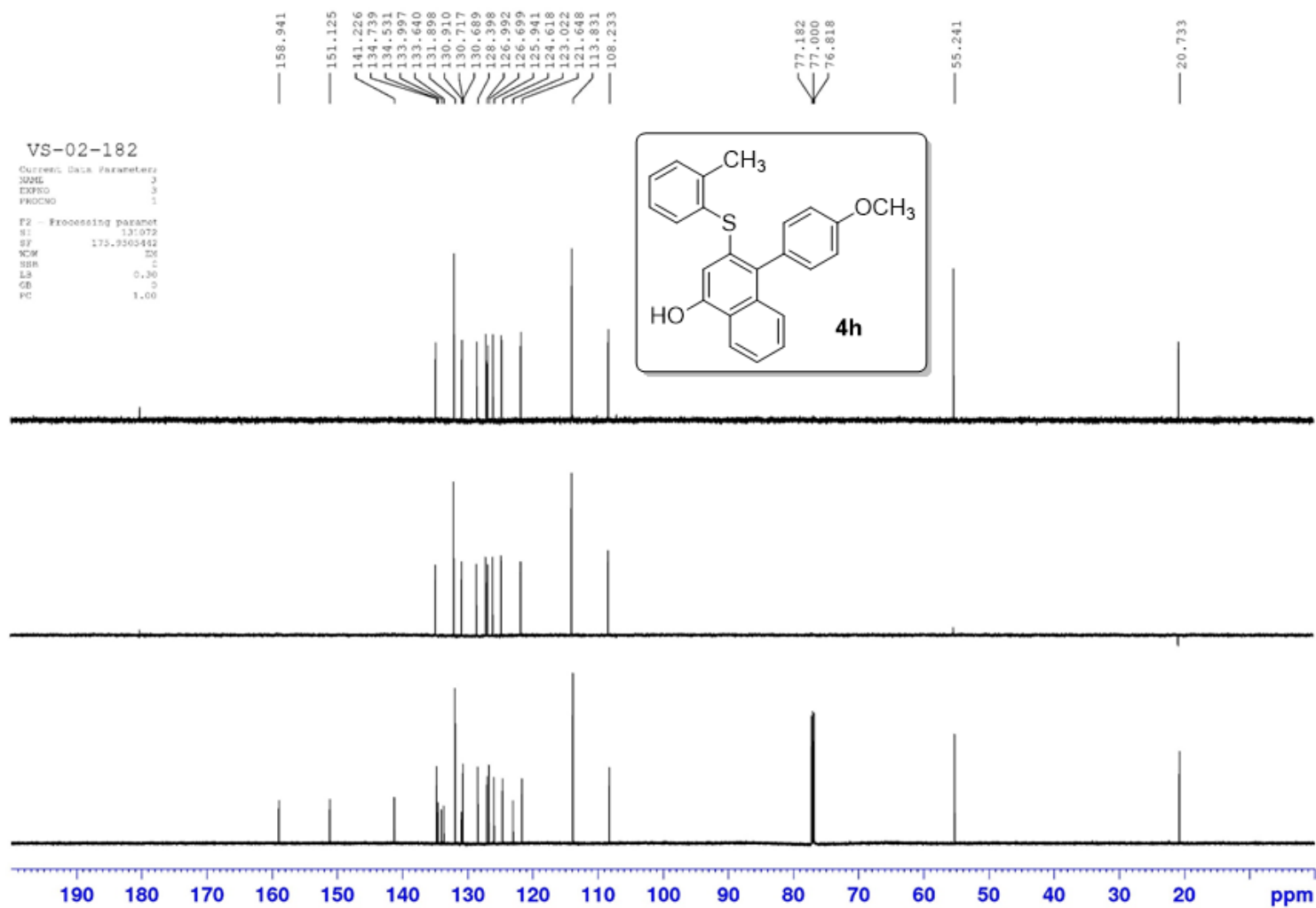
Solvent: CDCl₃
SFO1: 175 MHz



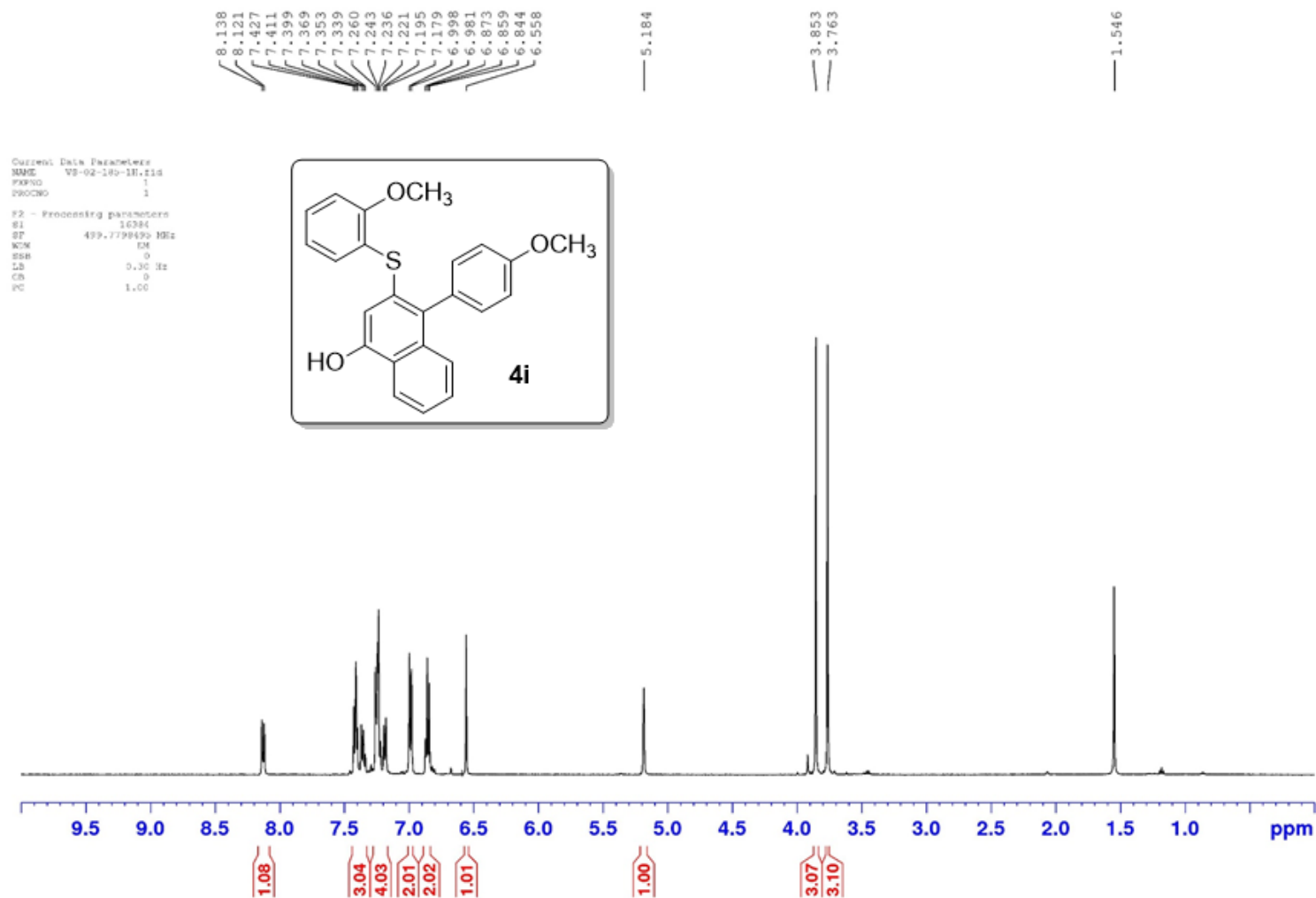
Solvent: CDCl_3
SFO1: 500 MHz



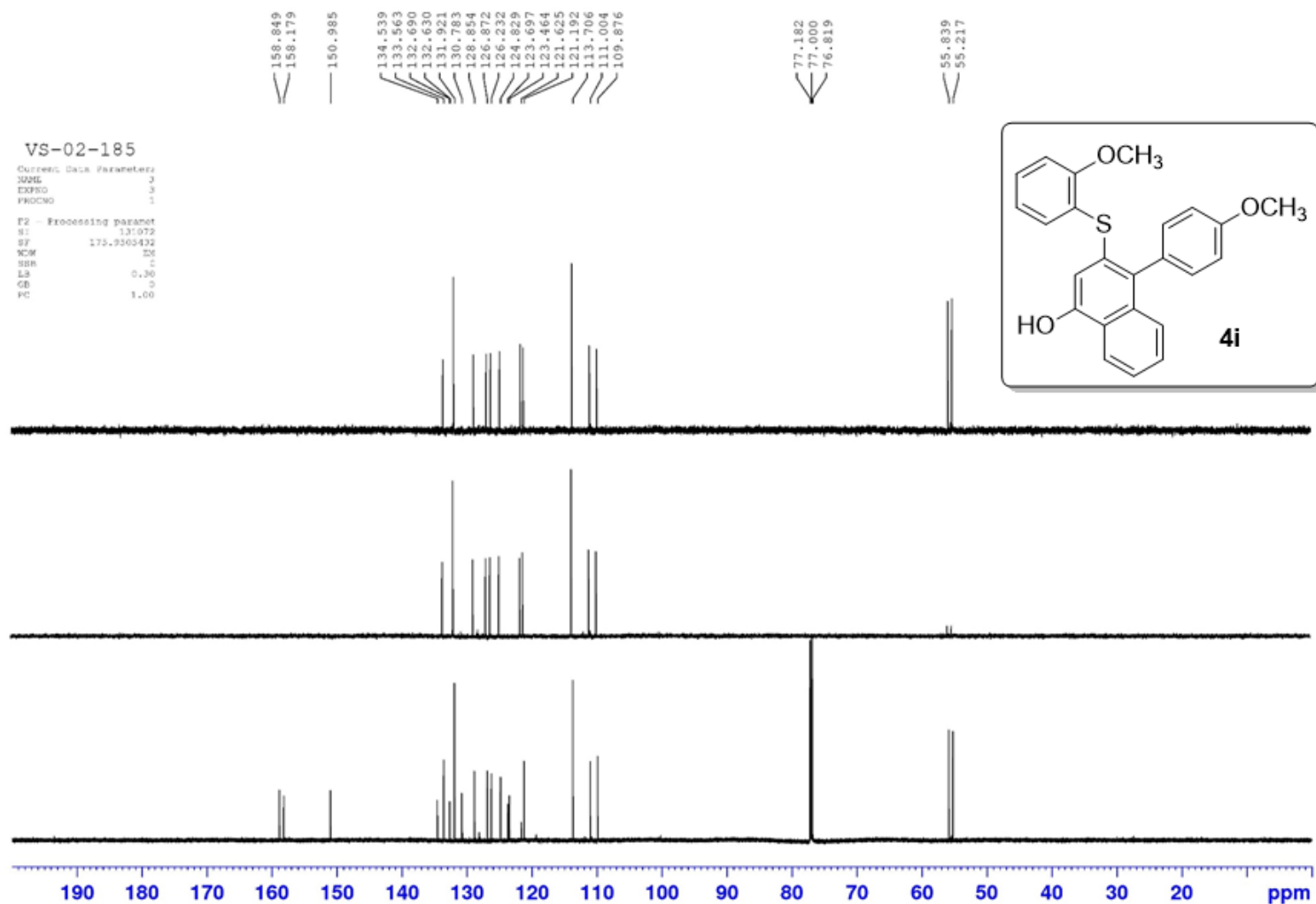
Solvent: CDCl₃
SFO1: 175 MHz



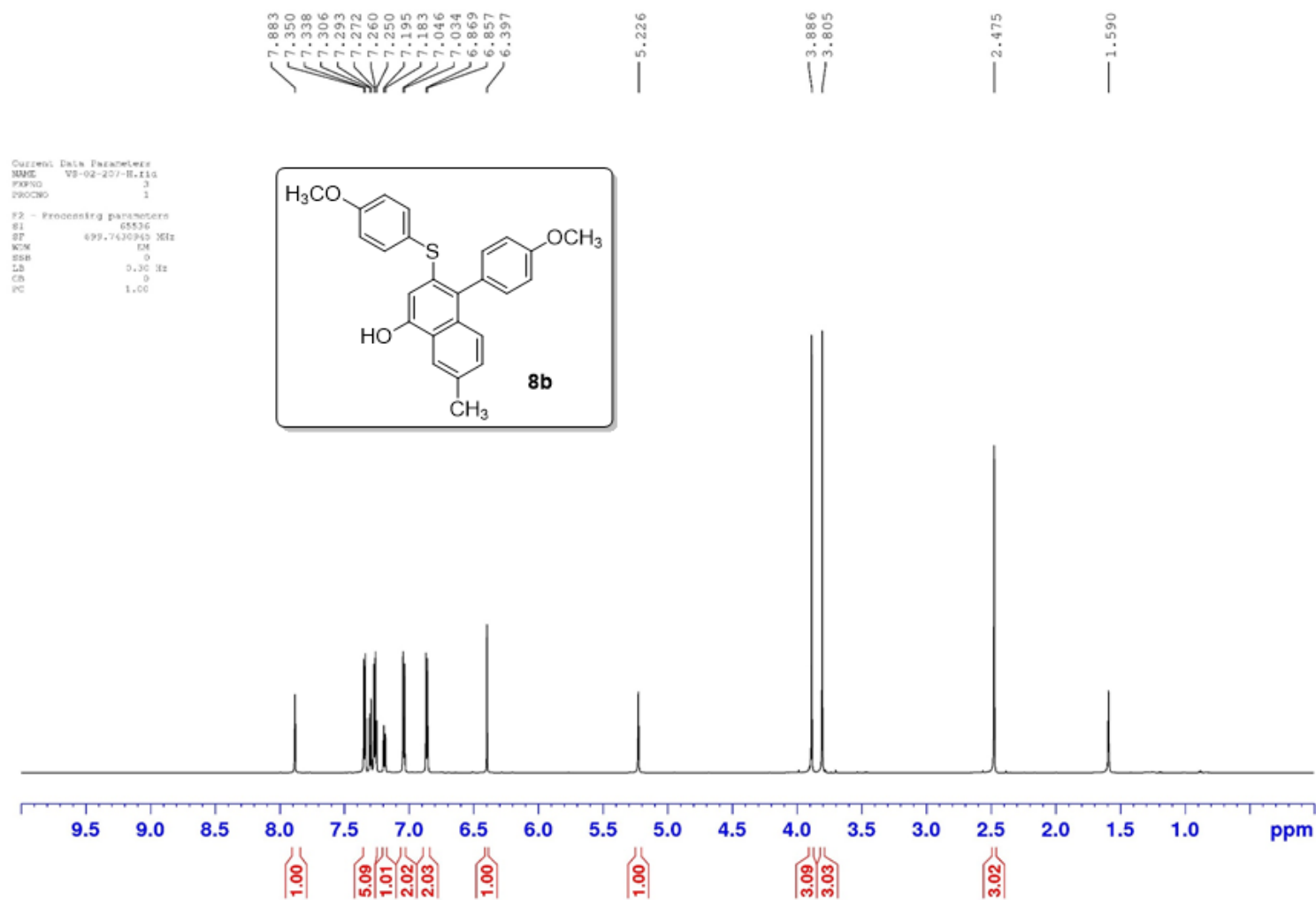
Solvent: CDCl_3
SFO1: 500 MHz



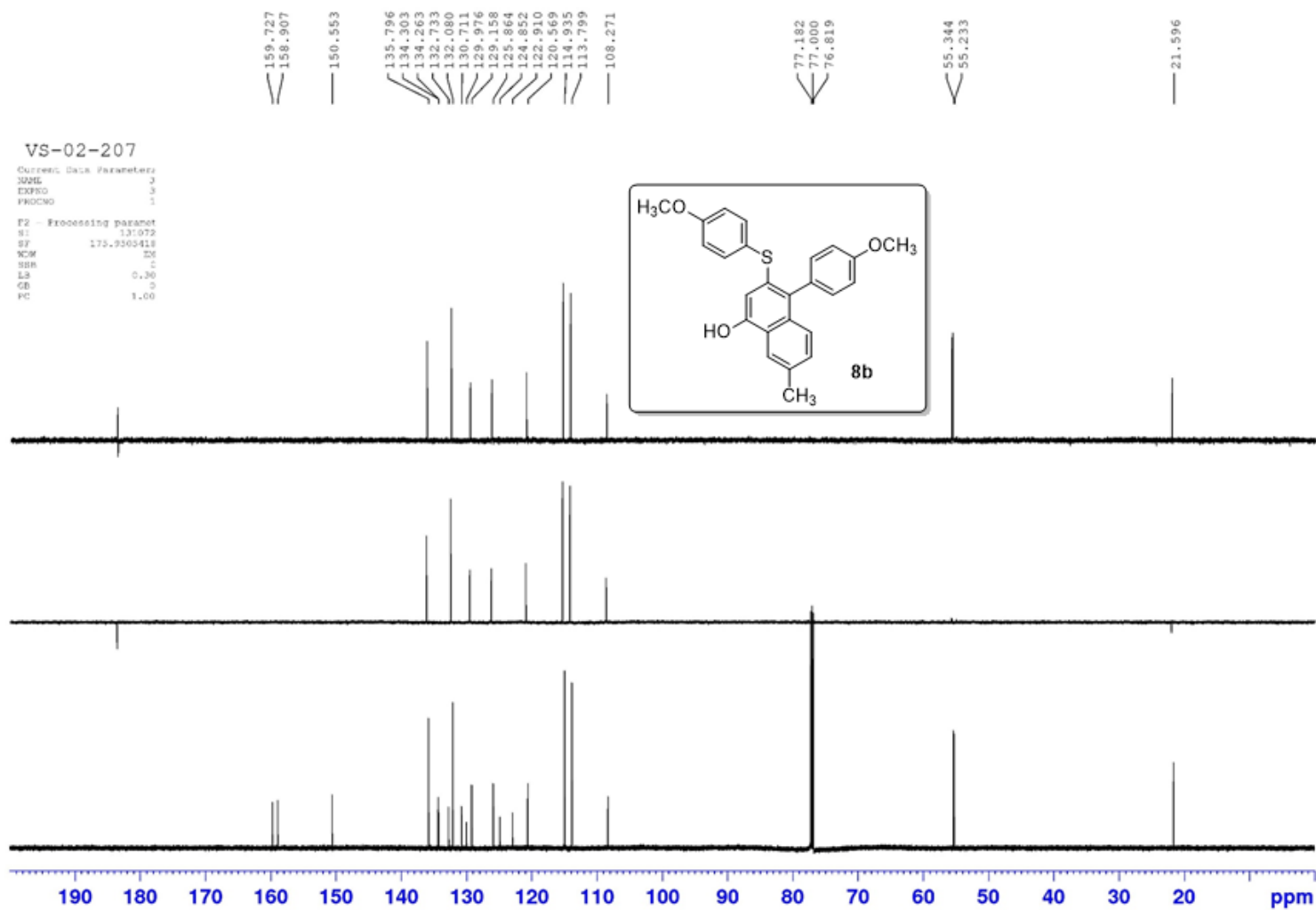
Solvent: CDCl_3
SFO1: 175 MHz



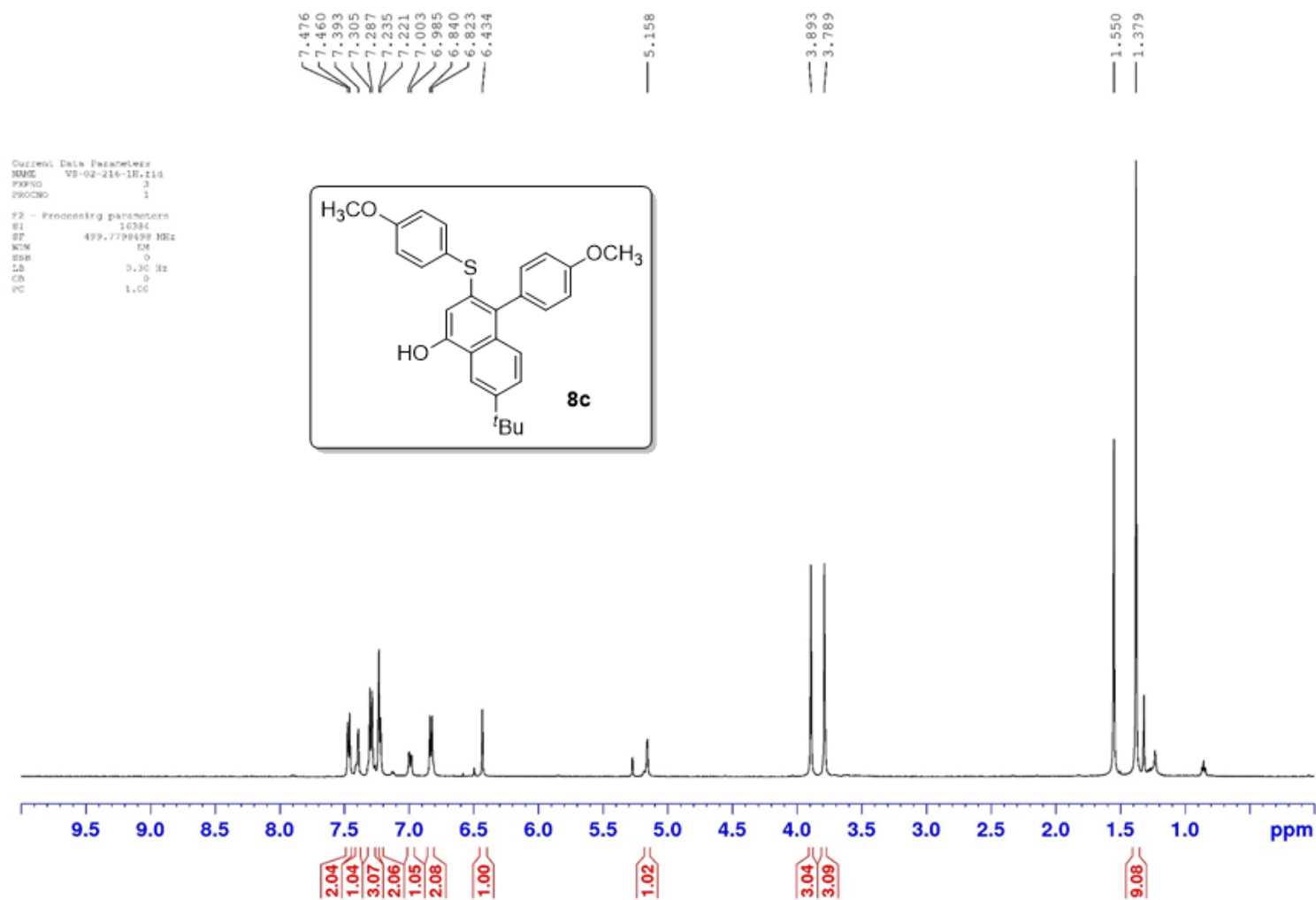
Solvent: CDCl₃
SFO1: 700 MHz



Solvent: CDCl₃
SFO1: 175 MHz



Solvent: CDCl₃
SFO1: 500 MHz

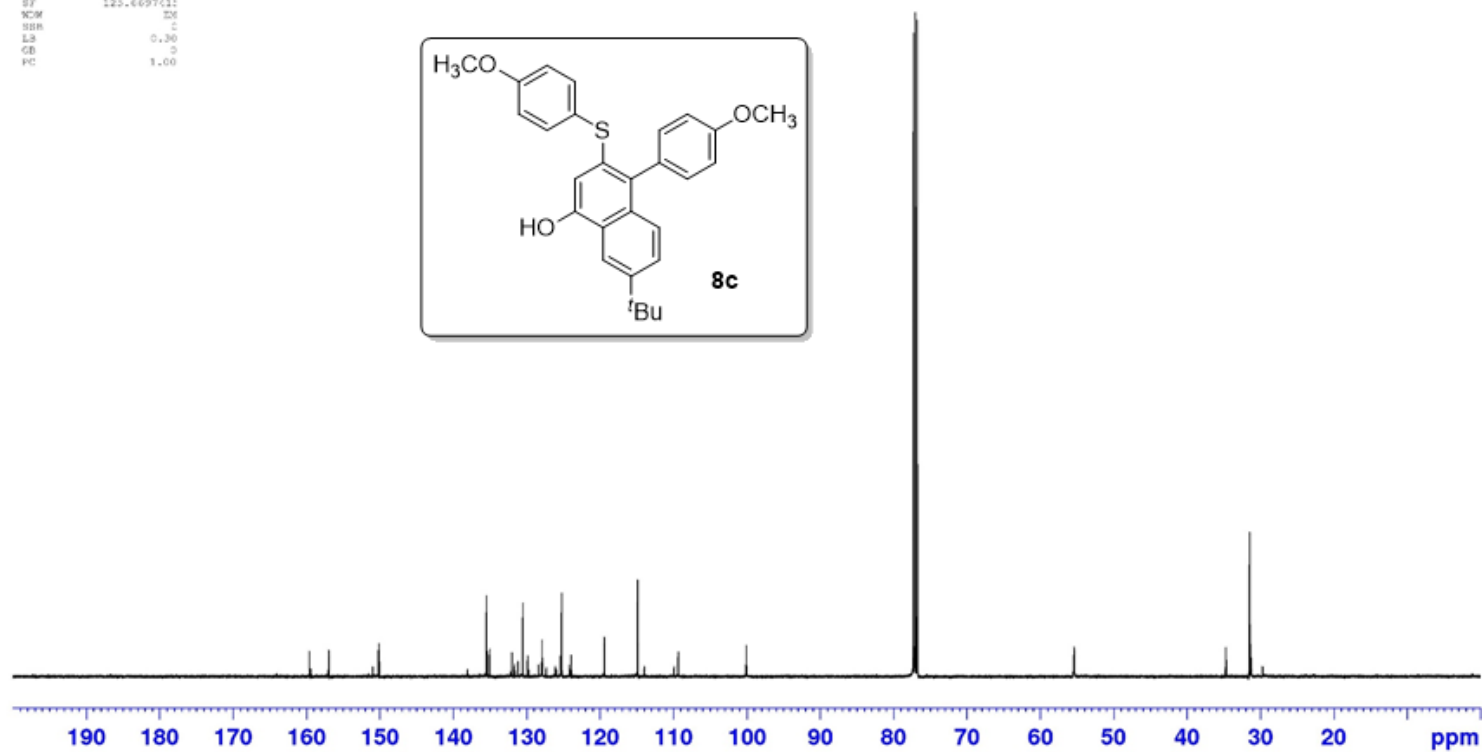
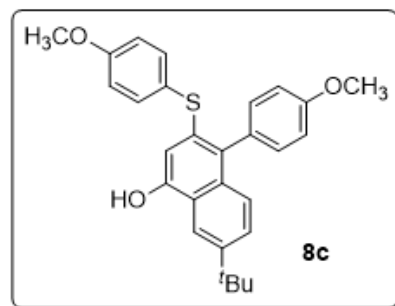


Solvent: CDCl_3
SFO1: 125 MHz

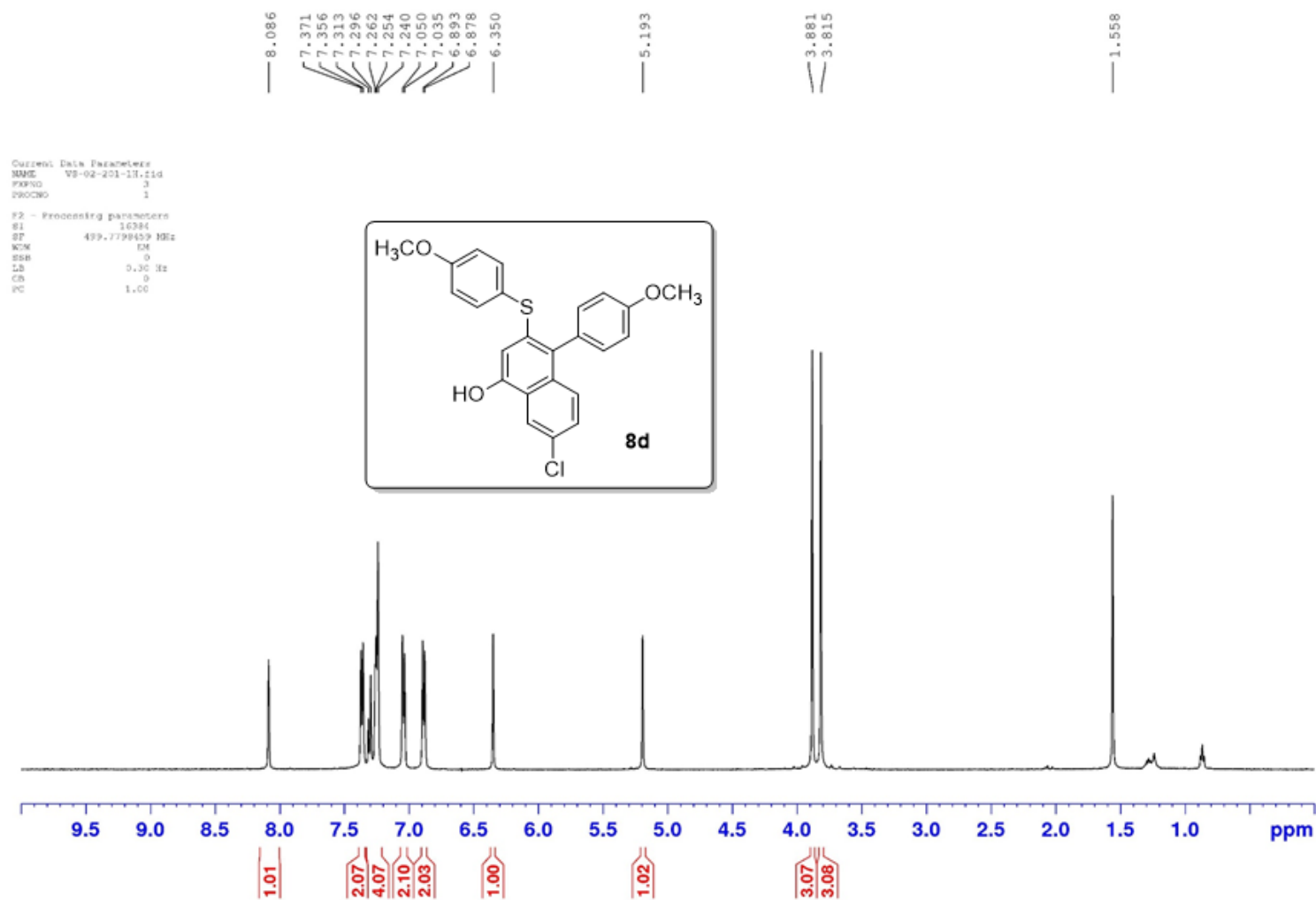
VS-02-216

Current Data Parameters
NAME VS-02-216A-13C
EXPNO 1
PROCNO 1

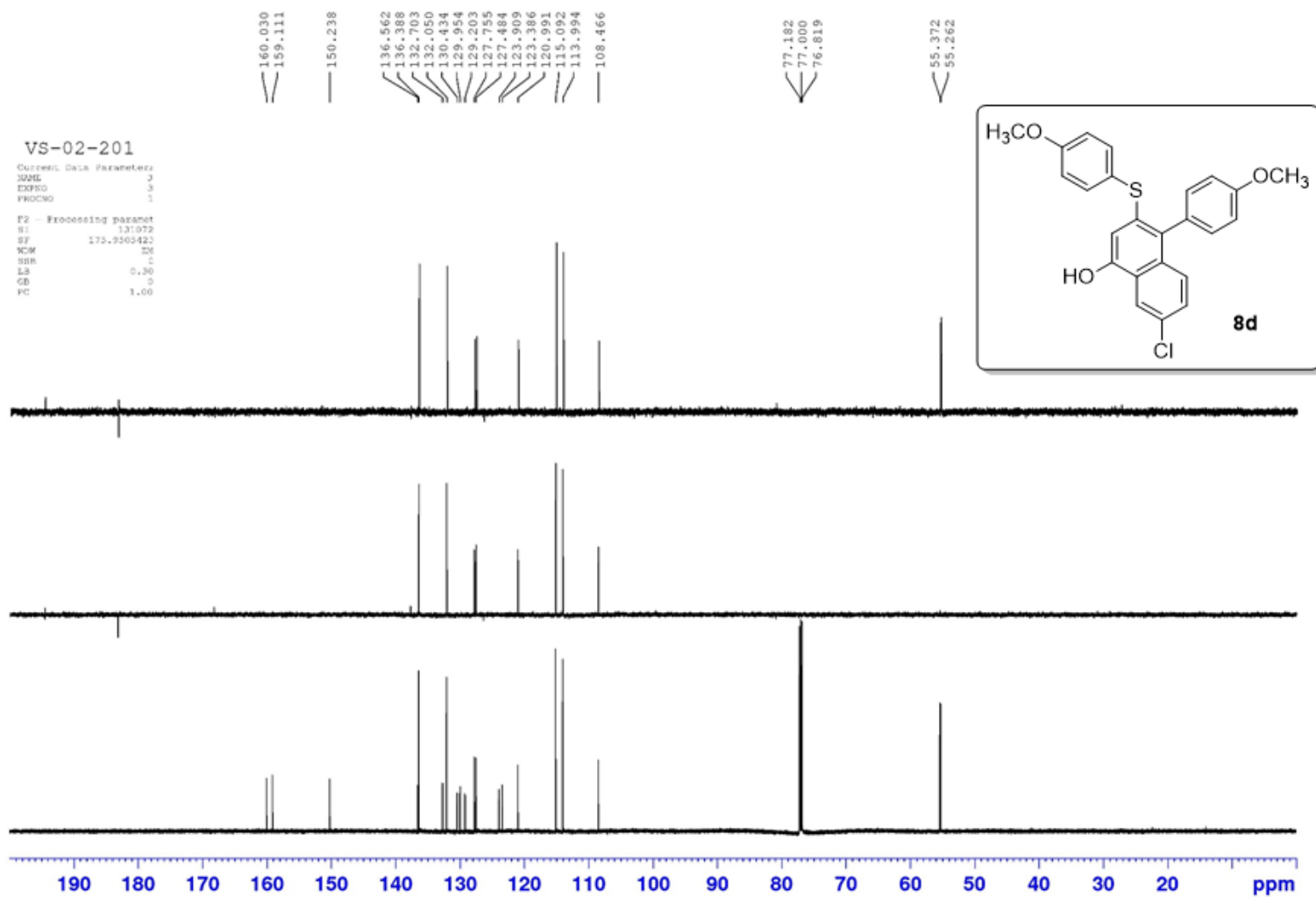
F2 - Processing parameters
SI 65536
SF 125.6697011
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00



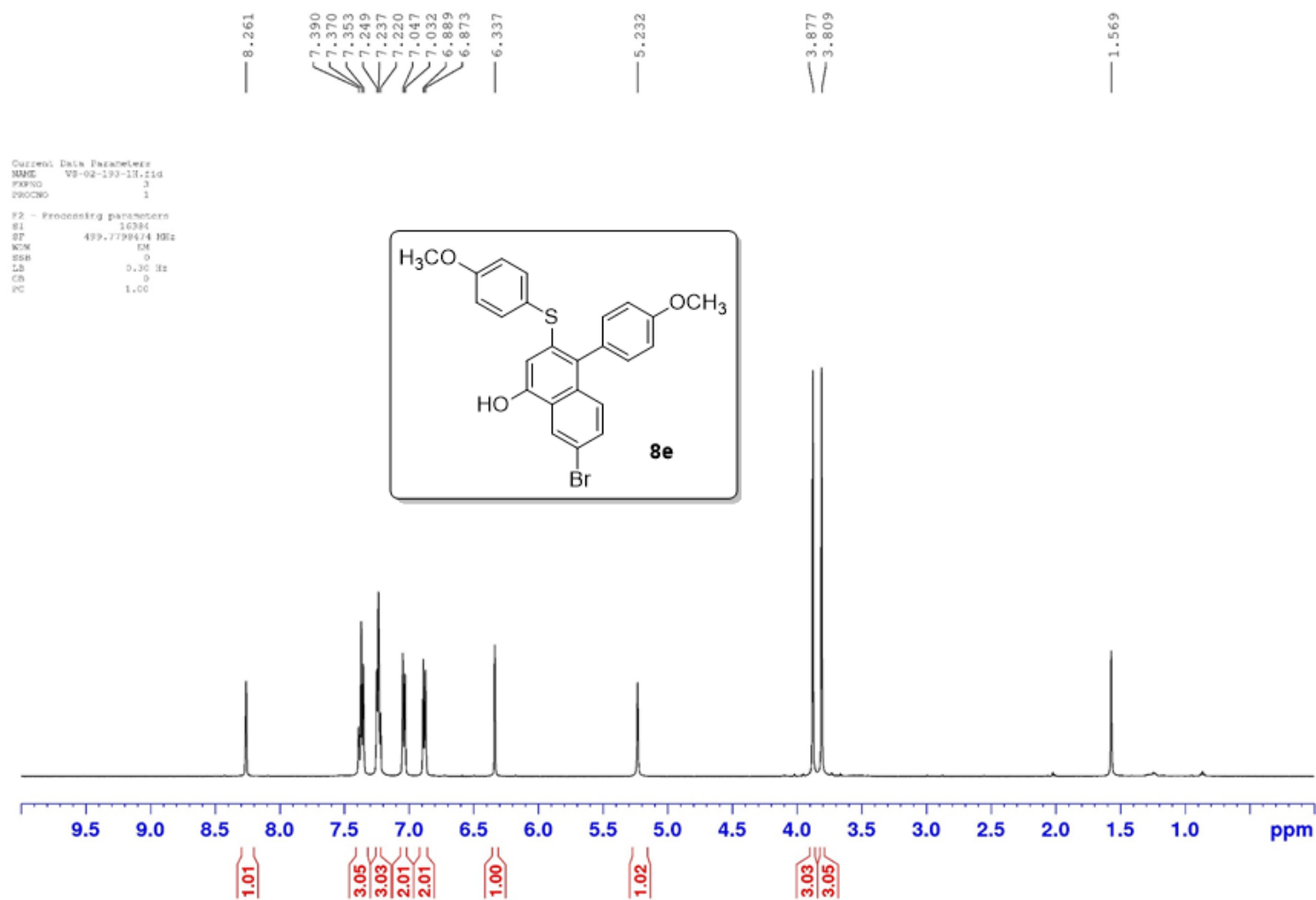
Solvent: CDCl_3
SFO1: 500 MHz



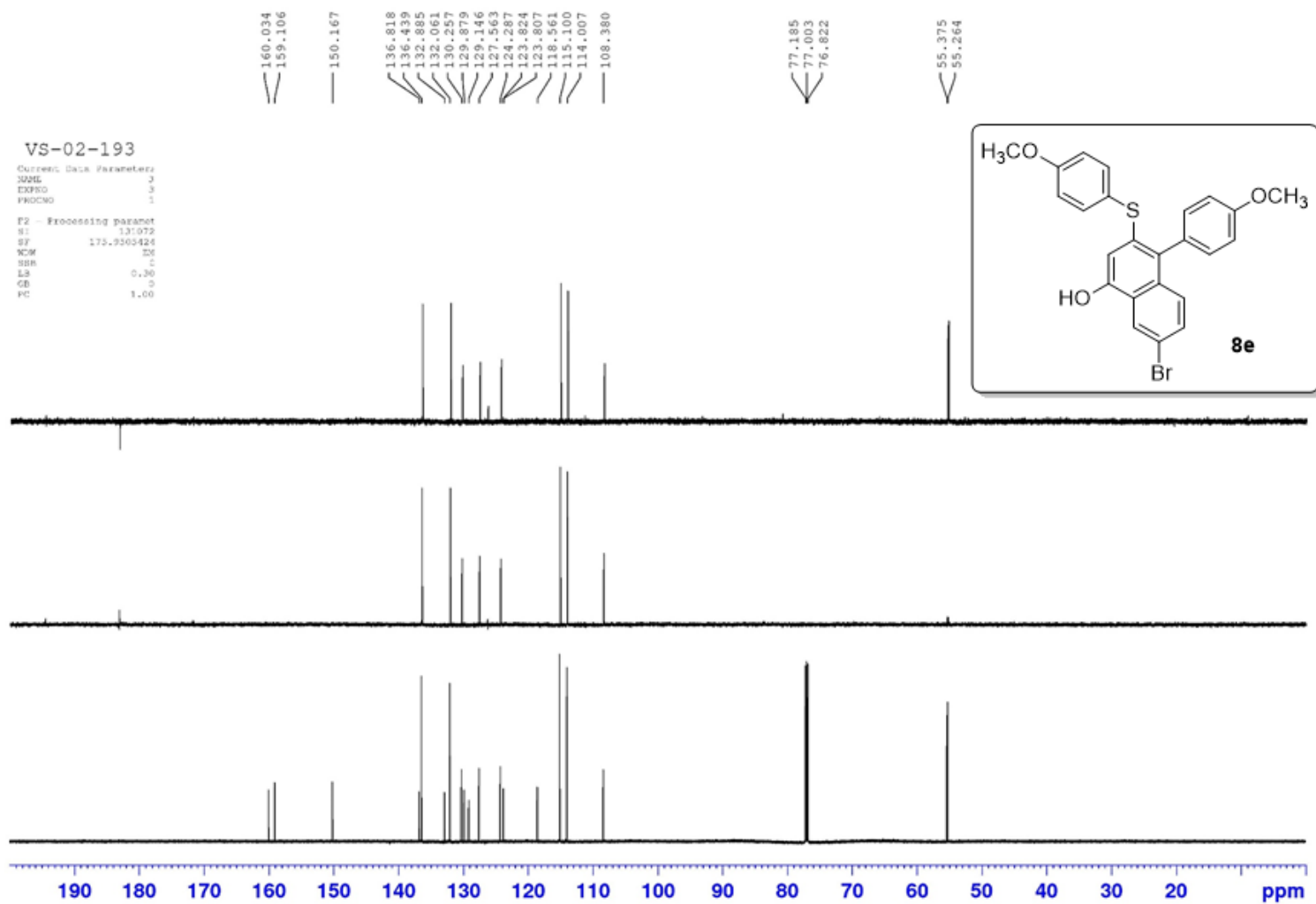
Solvent: CDCl₃
SFO1: 175 MHz



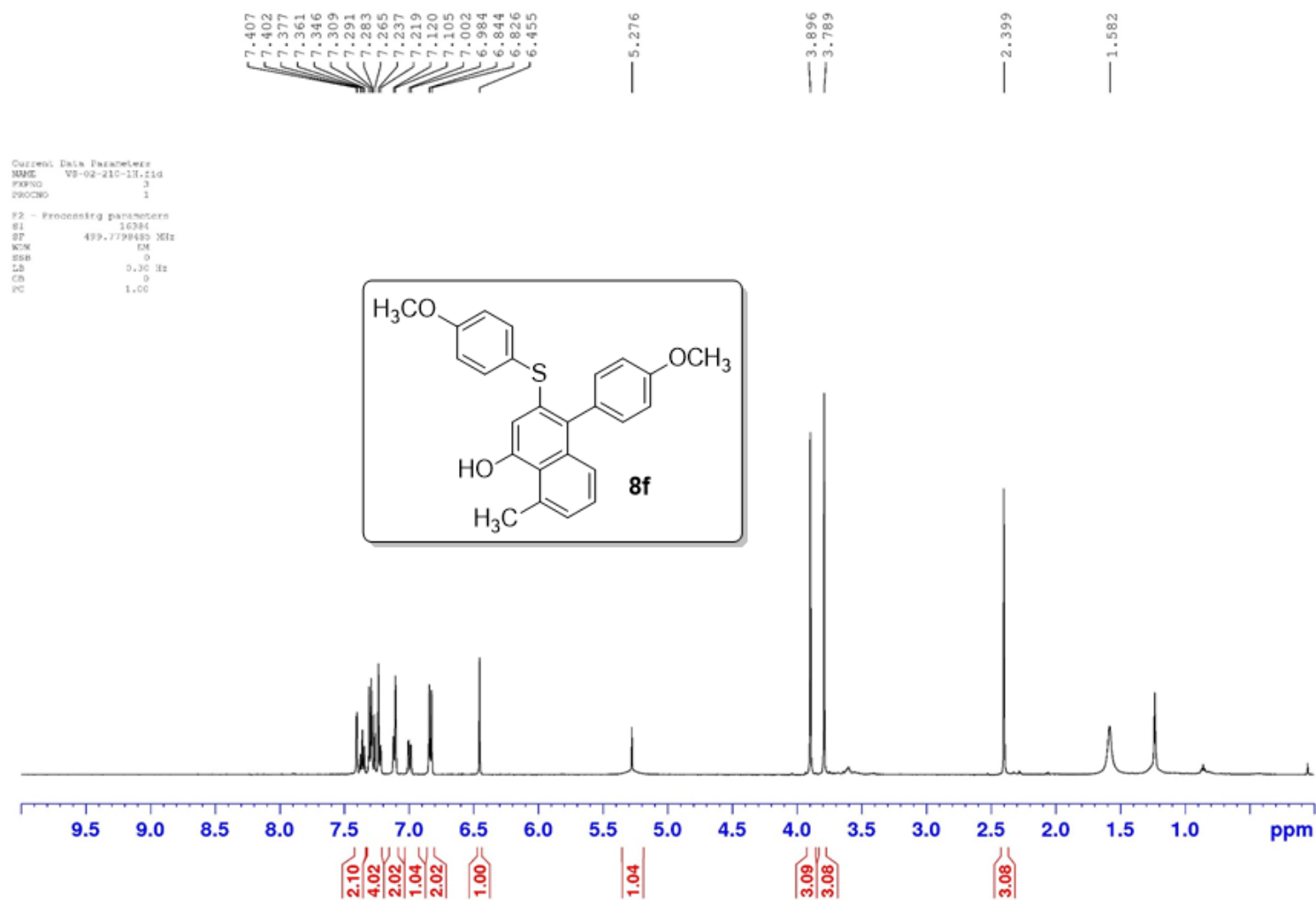
Solvent: CDCl_3
SFO1: 500 MHz



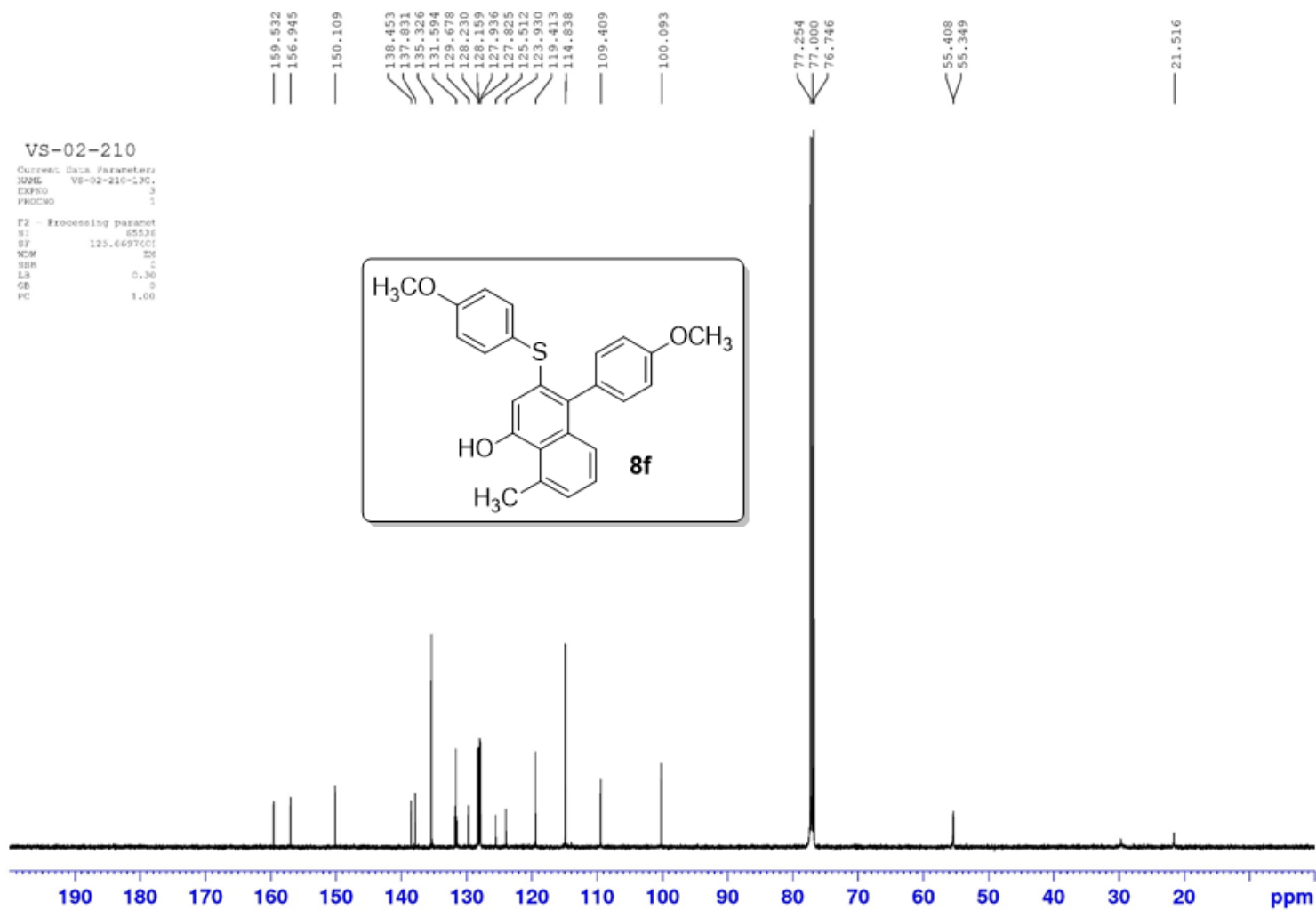
Solvent: CDCl₃
SFO1: 175 MHz



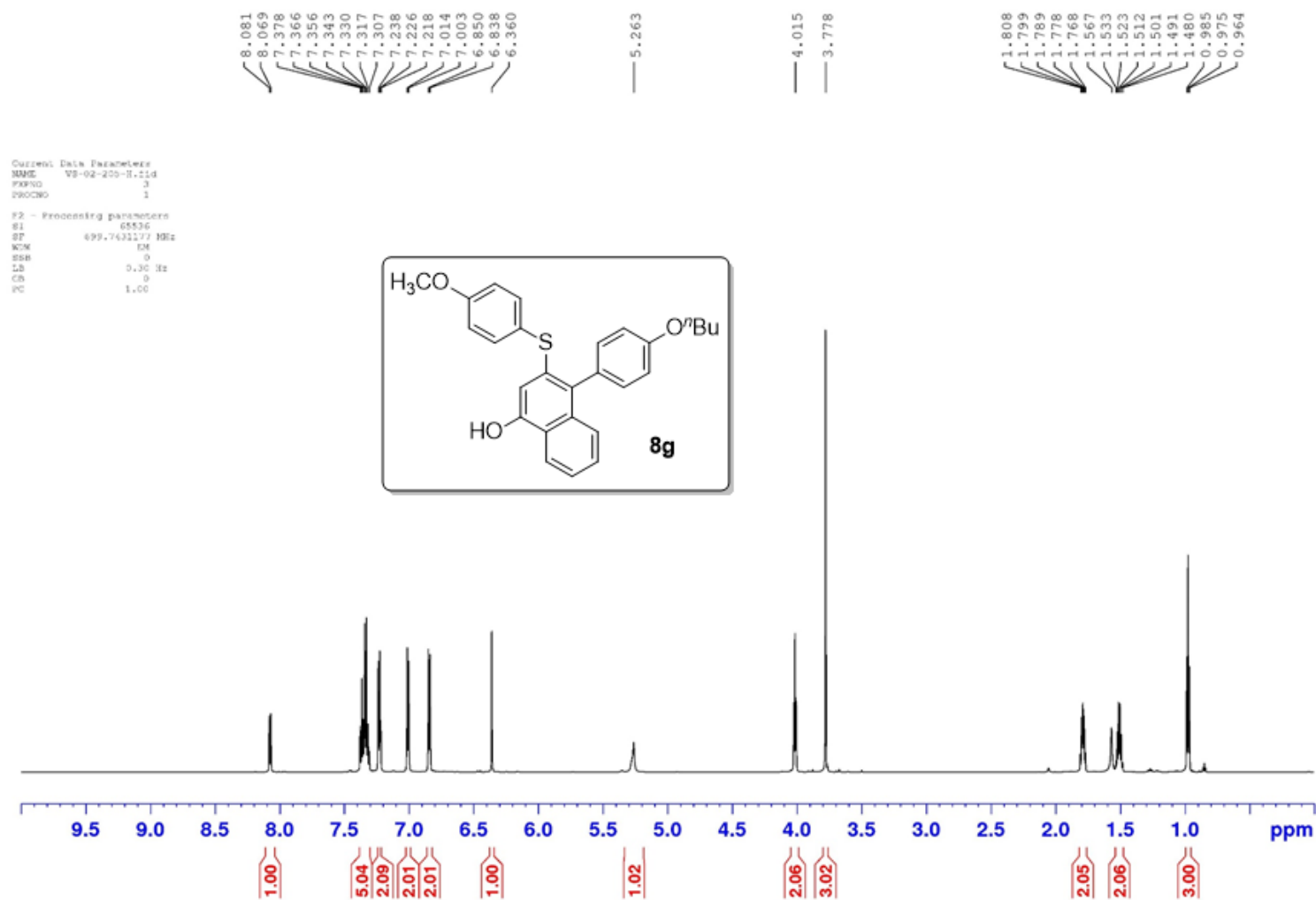
Solvent: CDCl_3
SFO1: 500 MHz



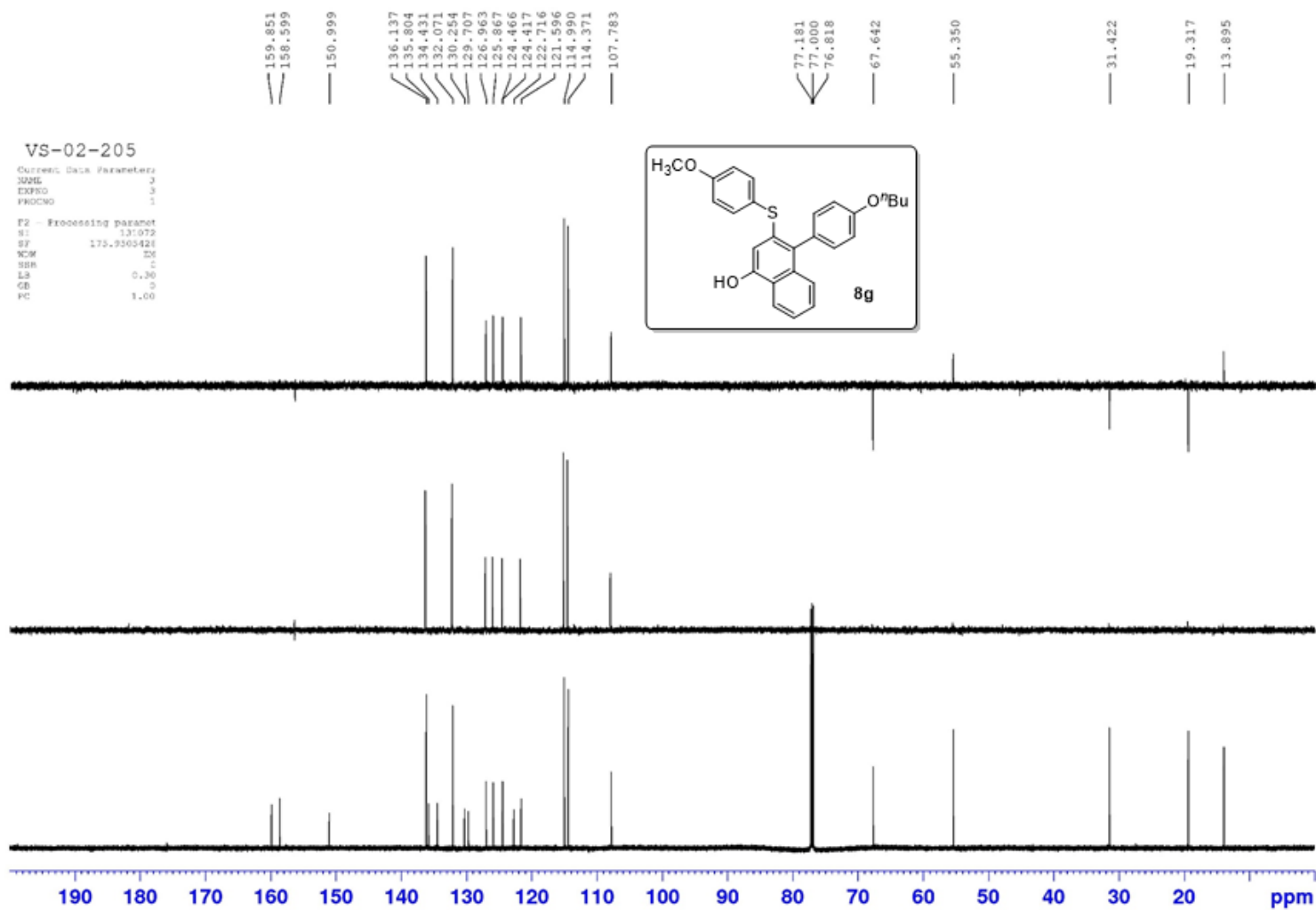
Solvent: CDCl_3
SFO1: 125 MHz



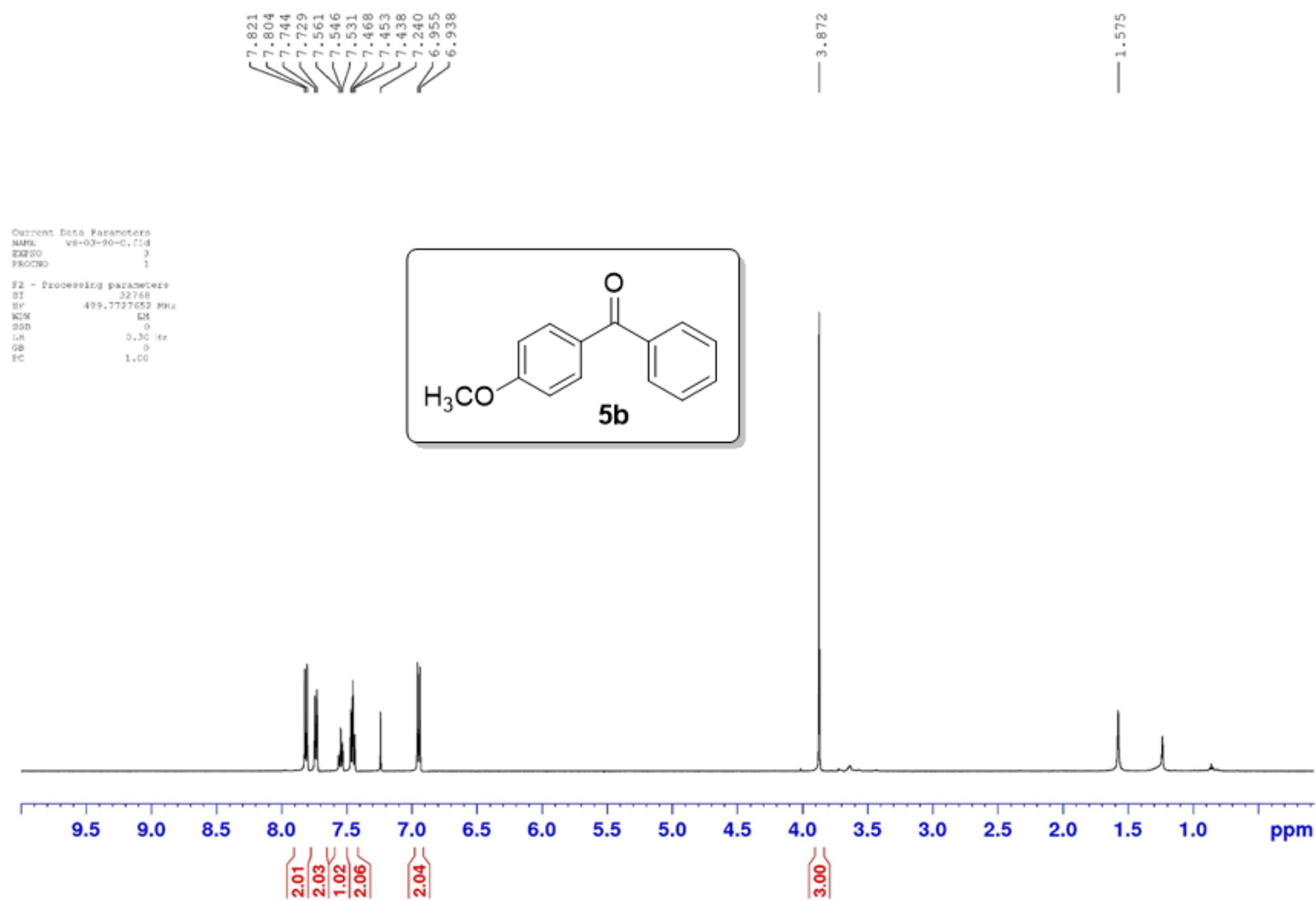
Solvent: CDCl₃
SFO1: 700 MHz



Solvent: CDCl₃
SFO1: 175 MHz



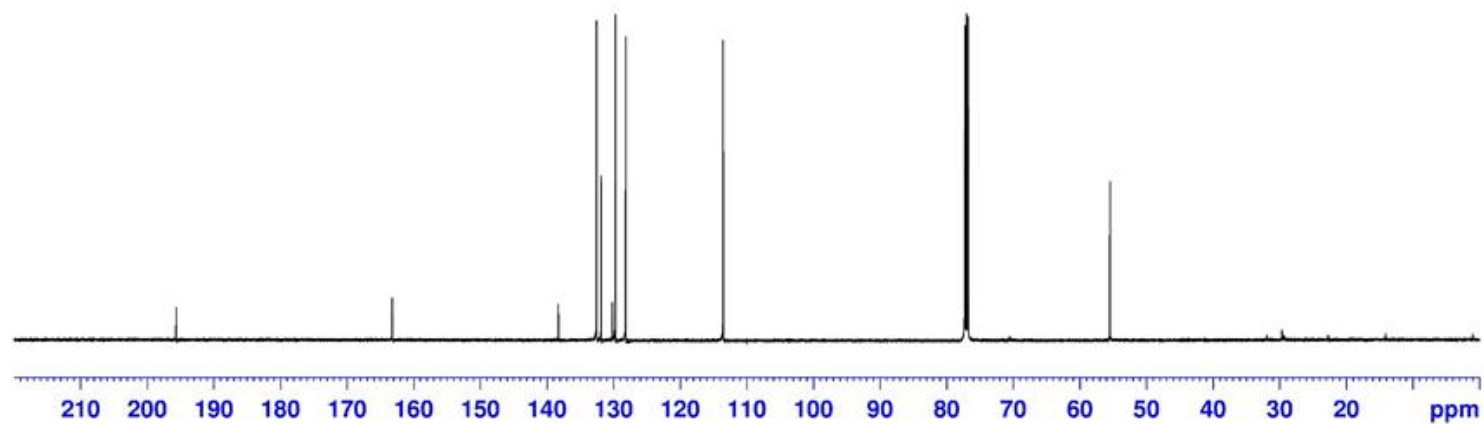
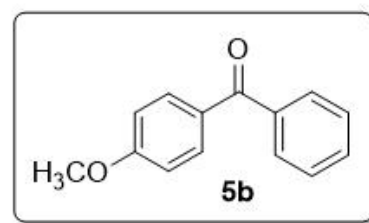
Solvent: CDCl_3
SFO1: 500 MHz



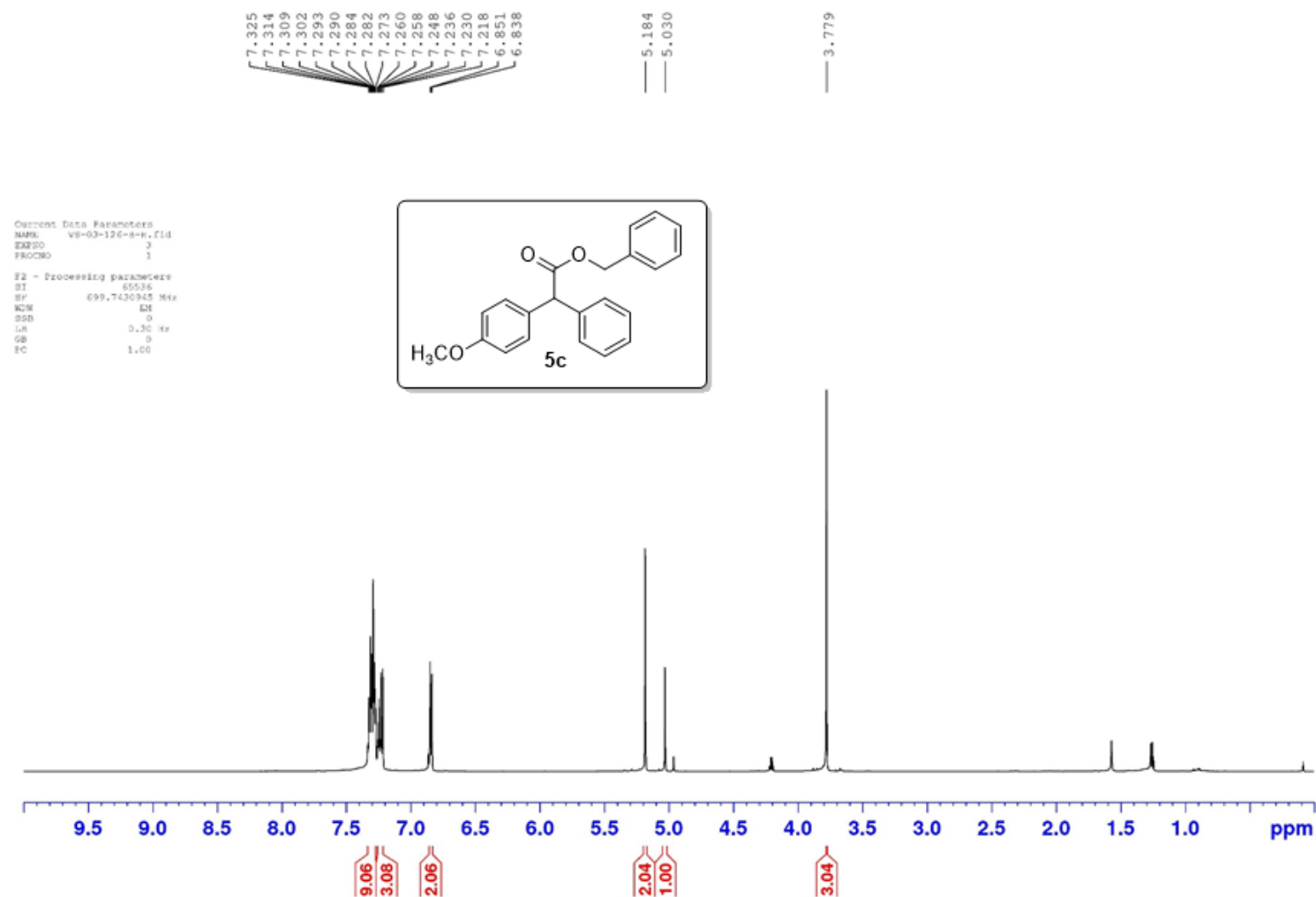
Solvent: CDCl_3
SFO1: 125 MHz

Current Data Parameters
NAME VS-03-90C-13C-1d
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 125.6698725 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

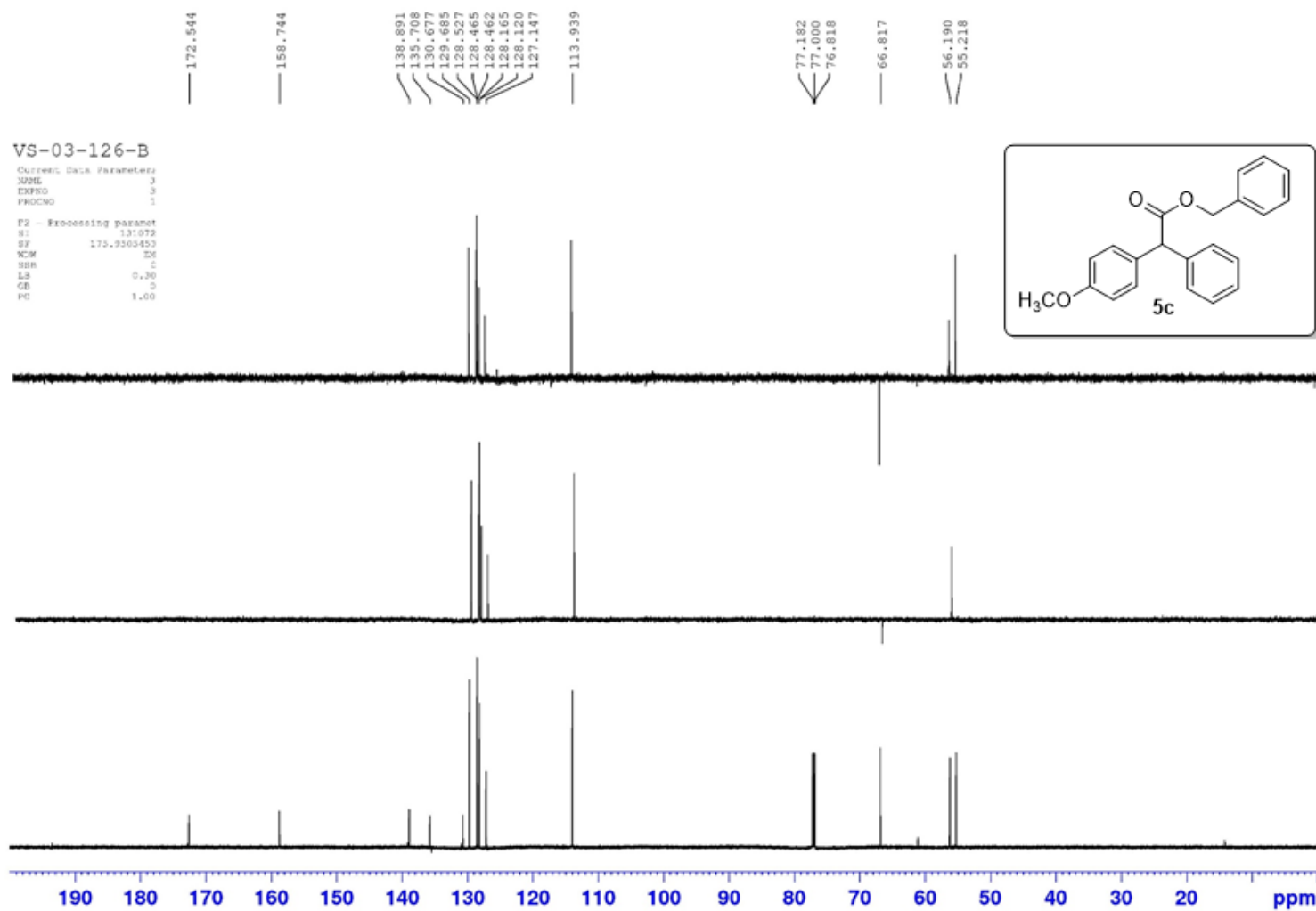
163.214
136.285
132.551
131.872
130.161
129.717
128.171
113.544
77.259
77.005
76.751
55.485



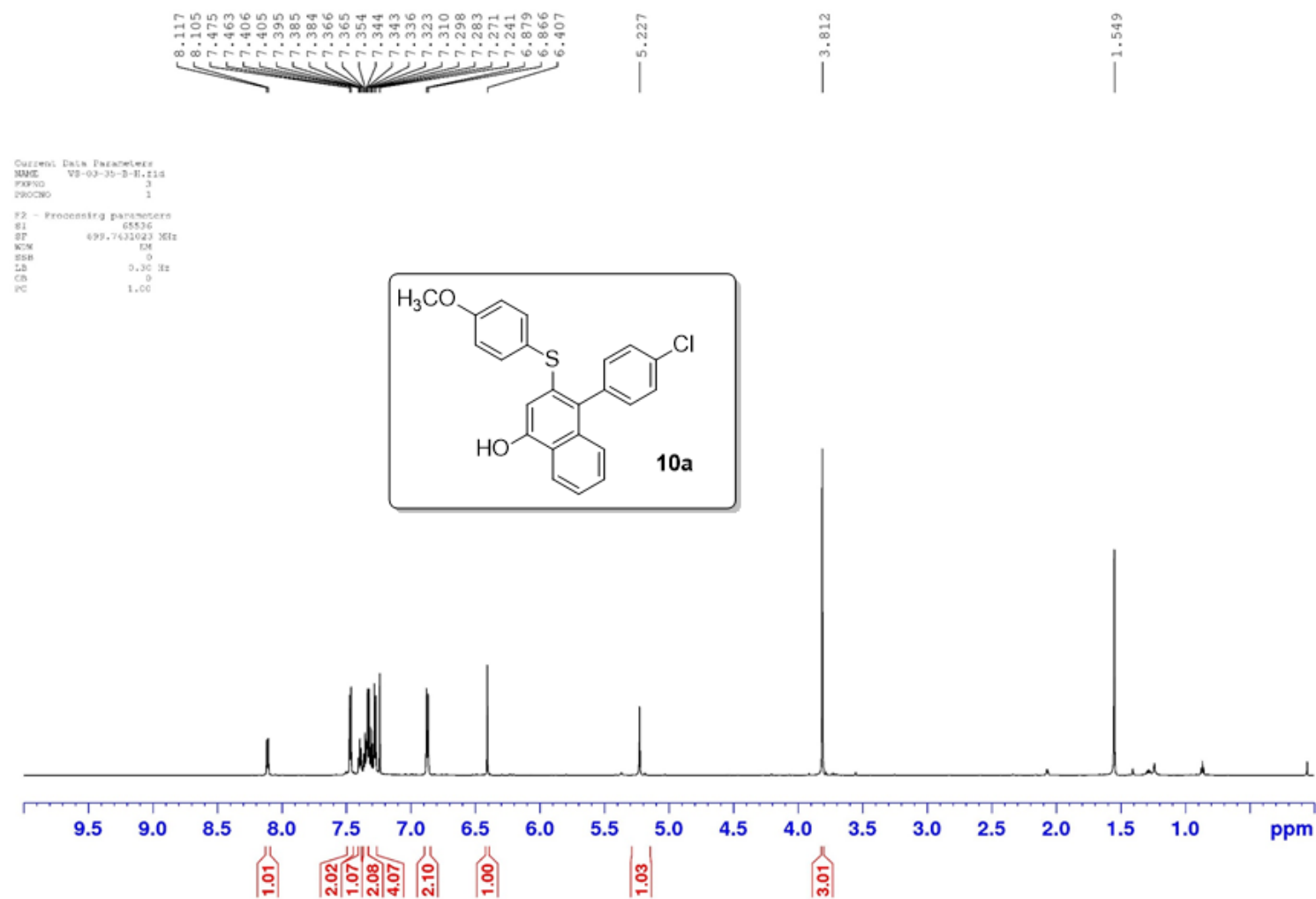
Solvent: CDCl_3
SFO1: 700 MHz



Solvent: CDCl₃
SFO1: 175 MHz



Solvent: CDCl_3
SFO1: 700 MHz

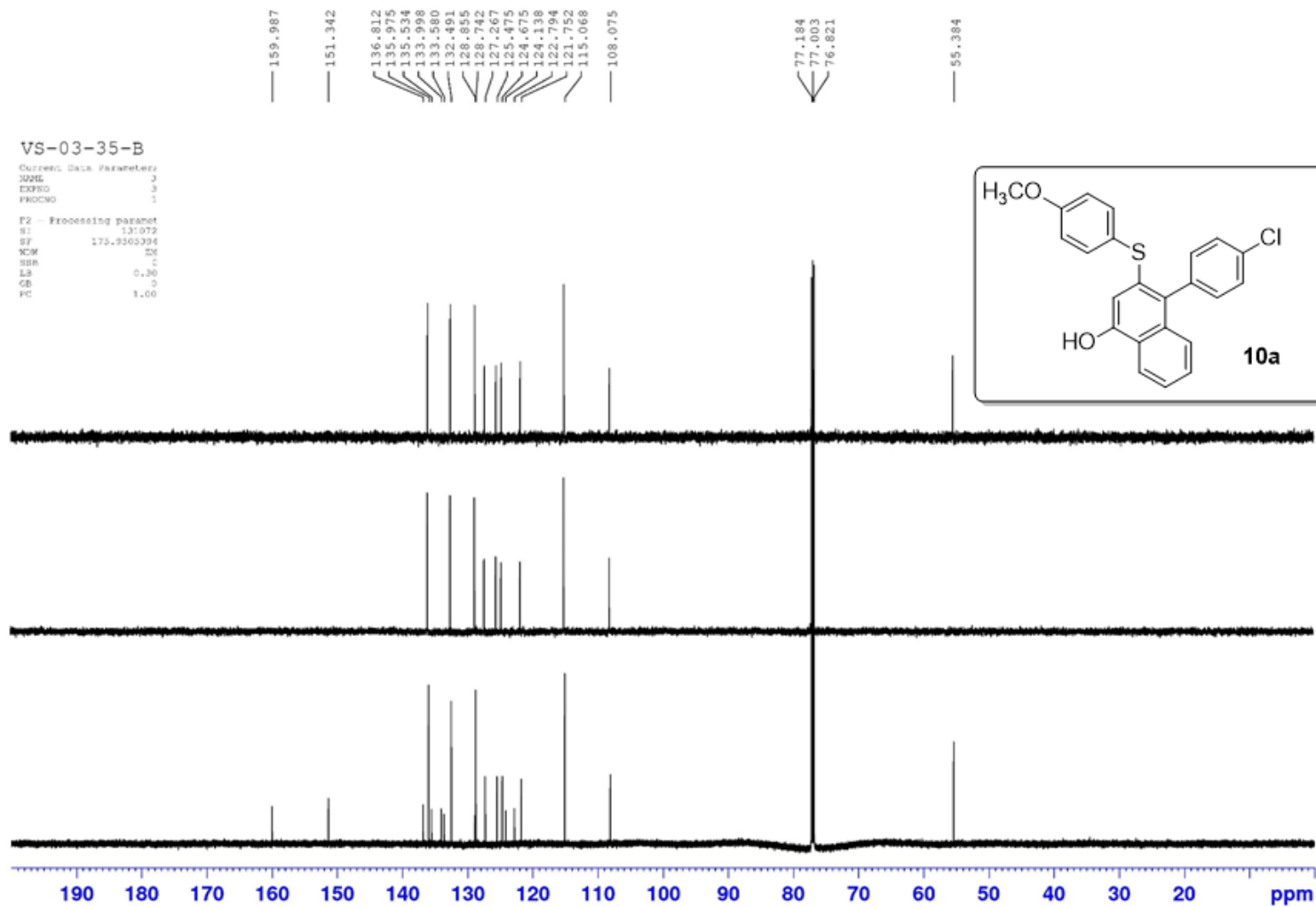


Solvent: CDCl₃
SFO1: 175 MHz

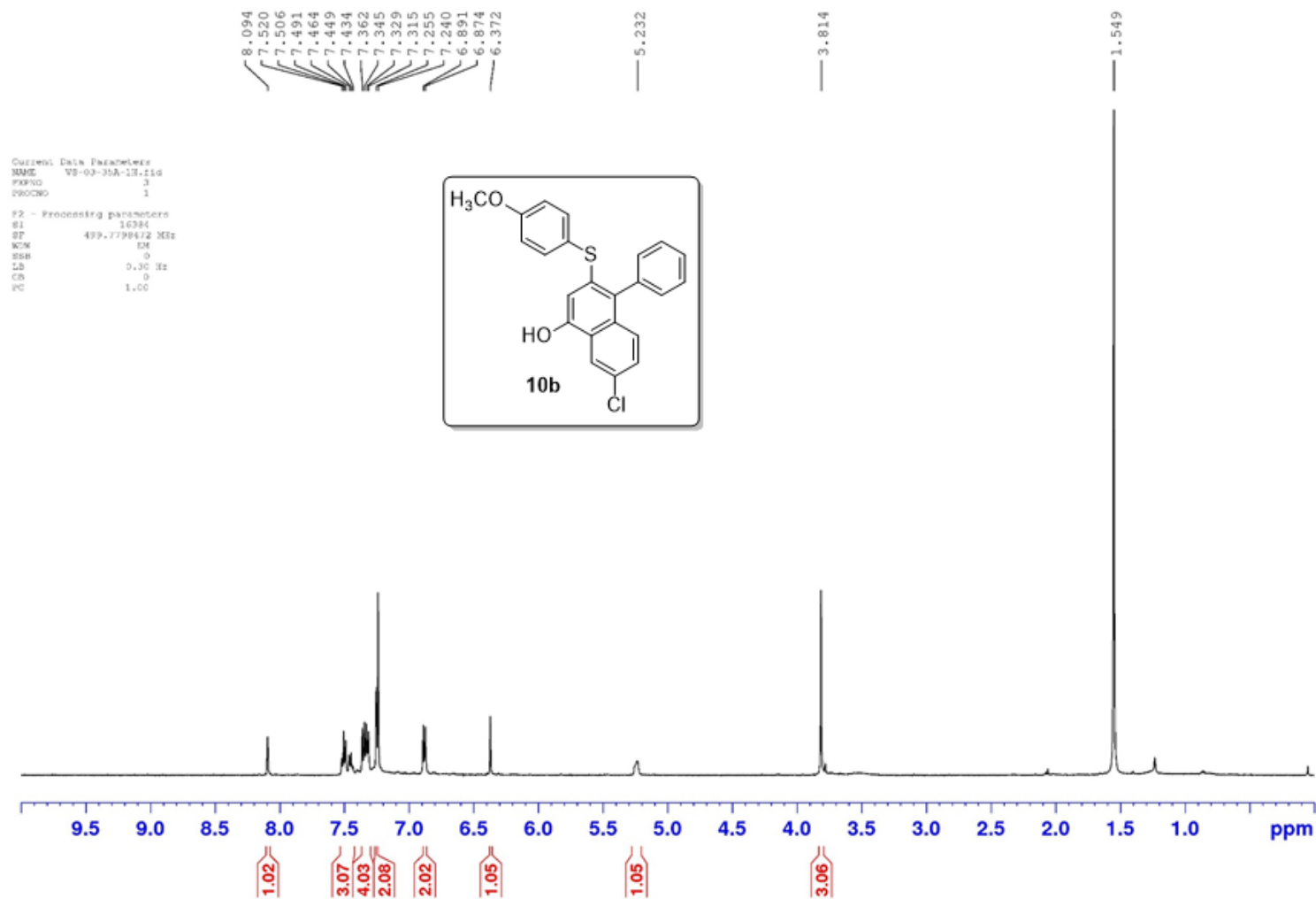
VS-03-35-B

Current Data Parameters
NAME 3
EXPNO 3
PROCNO 1

F2 - Processing parameter
SI 13:072
SF 175.906394
SCW 26
SRR 4
LB 0.30
GB 0
PC 1.00



Solvent: CDCl₃
SFO1: 500 MHz

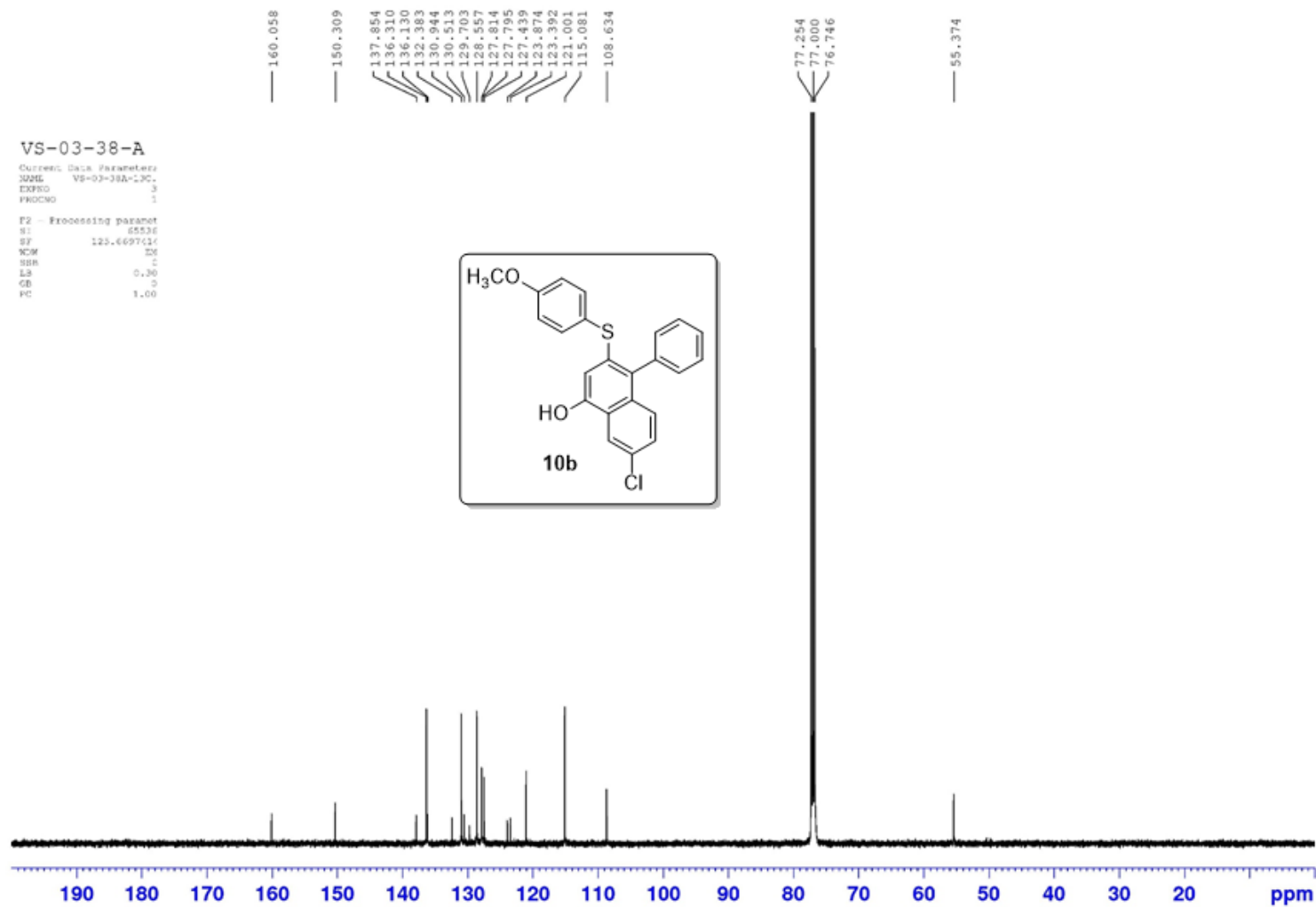
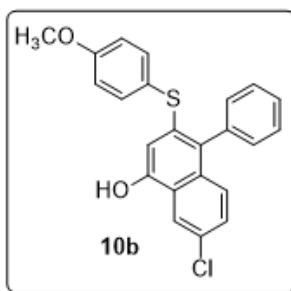


Solvent: CDCl_3
SFO1: 125 MHz

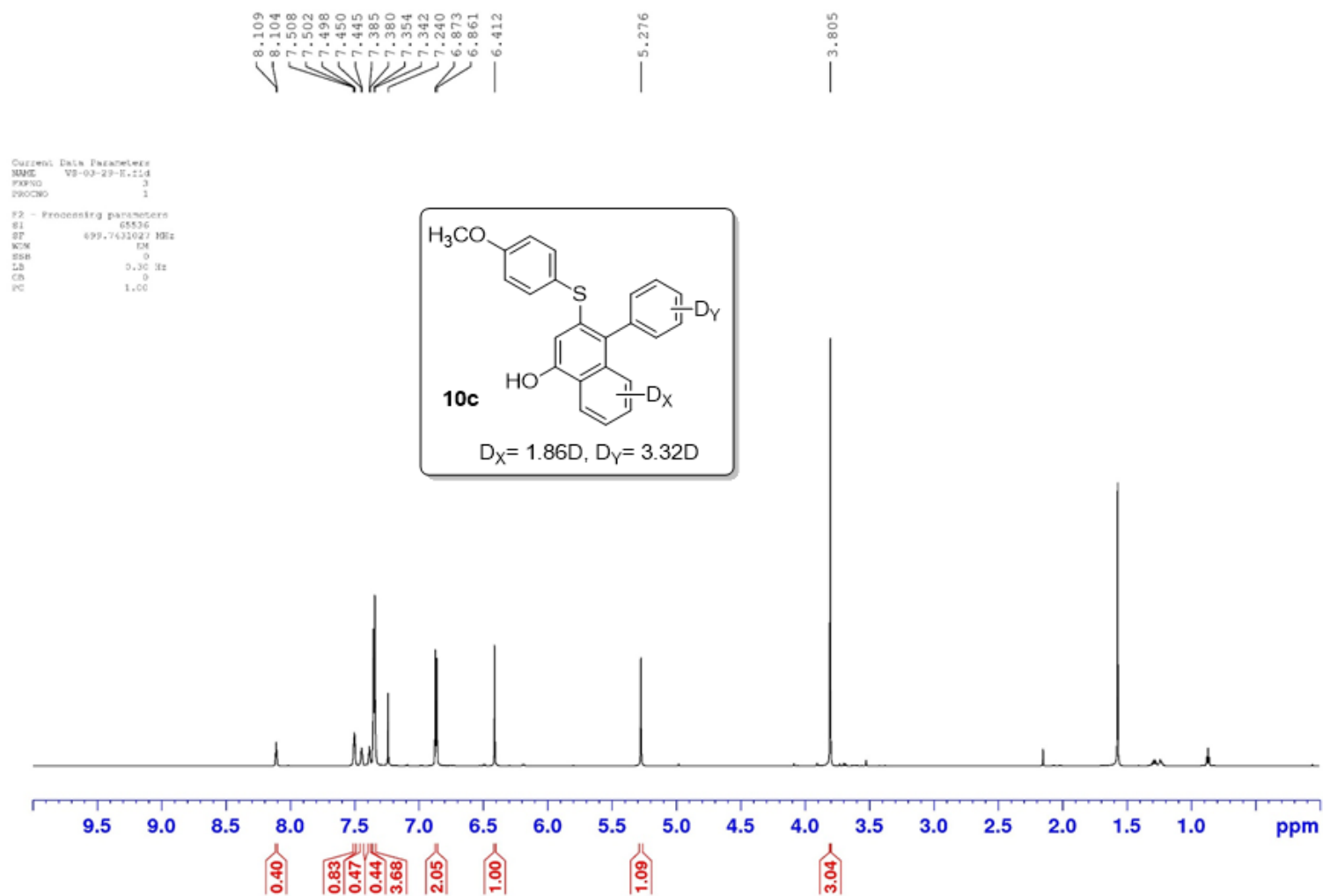
VS-03-38-A

Current Data Parameters
NAME VS-03-38A-13C
EXPNO 3
PROCNO 1

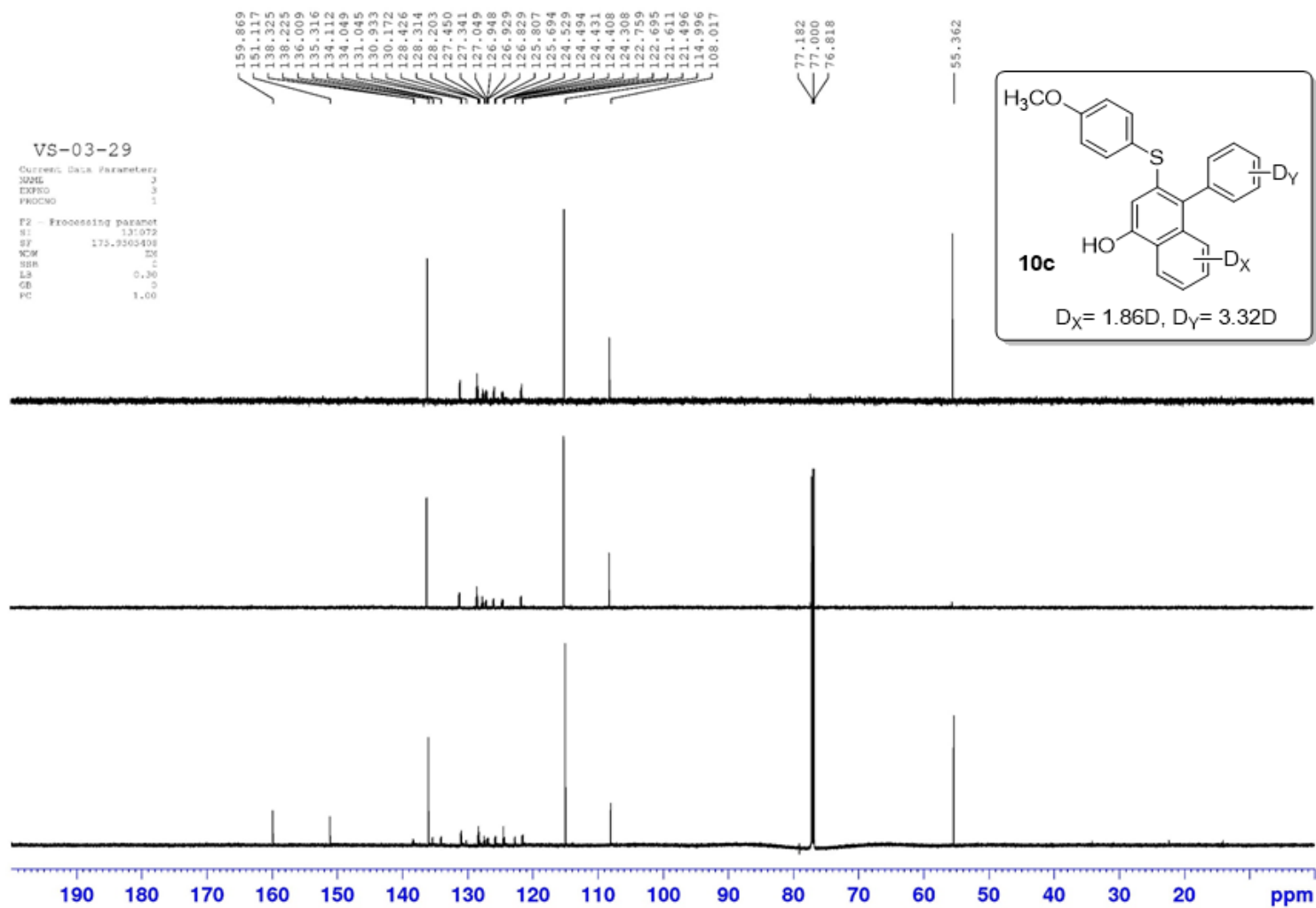
F2 - Processing parameters
SI 65536
SF 125.6697034
NCM 128
SRR 1
LB 0.30
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 700 MHz



Solvent: CDCl₃
SFO1: 175 MHz

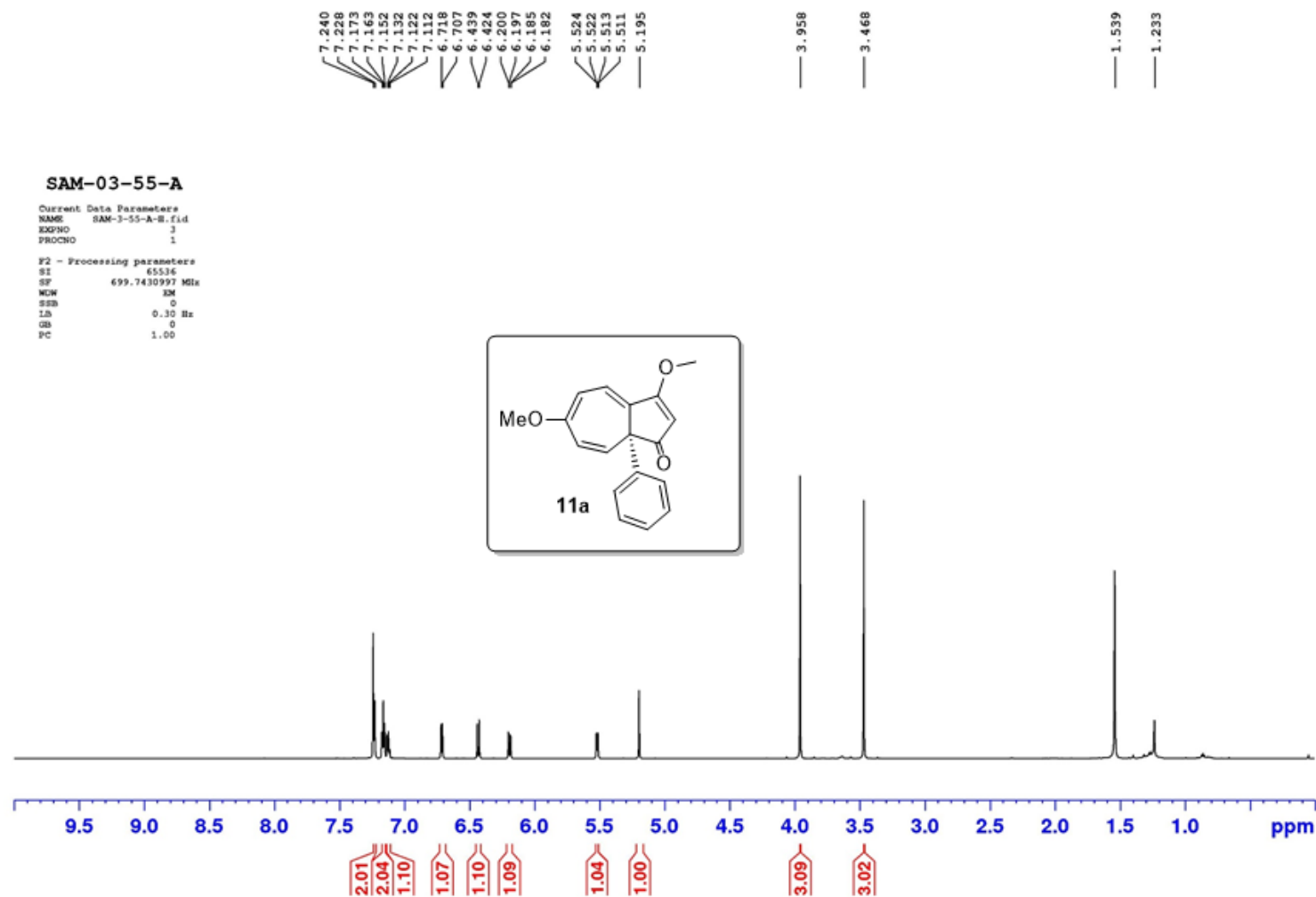
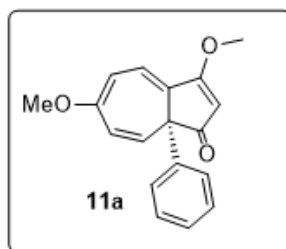


Solvent: CDCl_3
SFO1: 700 MHz

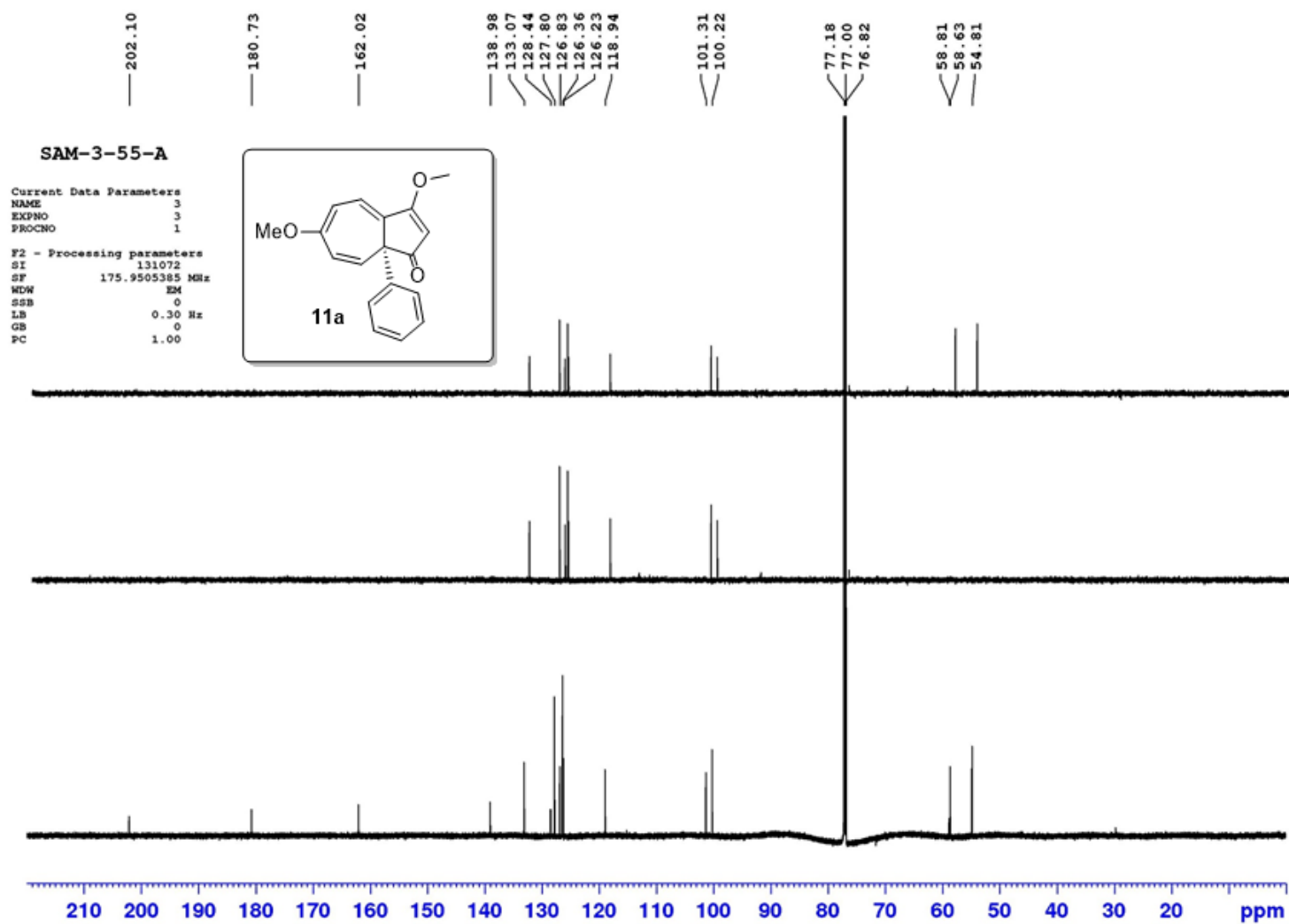
SAM-03-55-A

Current Data Parameters
NAME SAM-3-55-A-S.Fid
EXPNO 3
PROCNO 1

F2 - Processing parameters
SI 65536
SF 699.7430997 MHz
WDW HM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
SFO1: 175 MHz

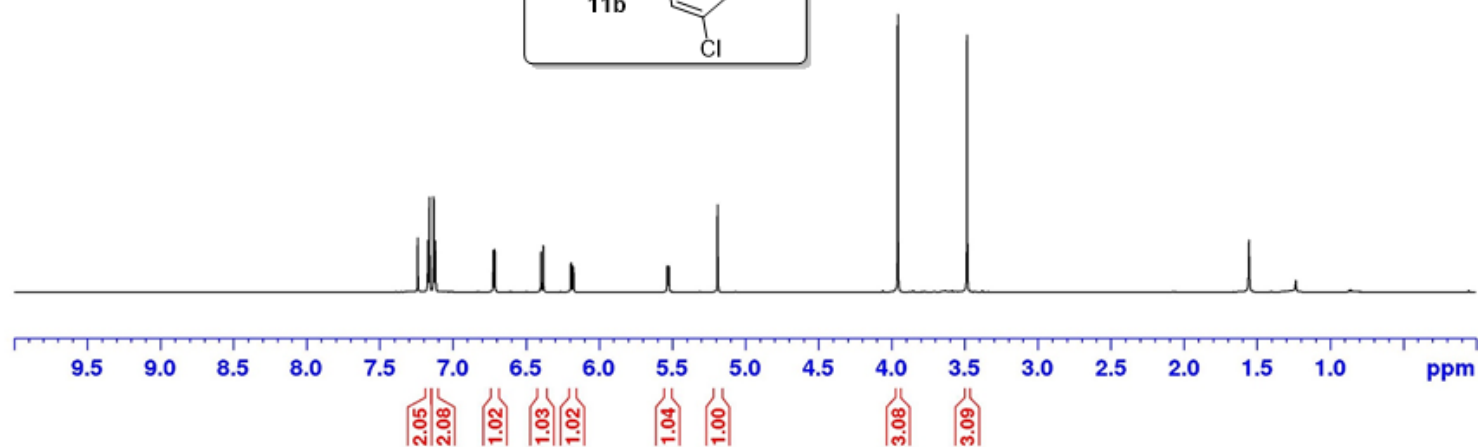
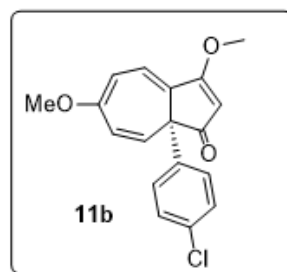


Solvent: CDCl_3
SFO1: 700 MHz

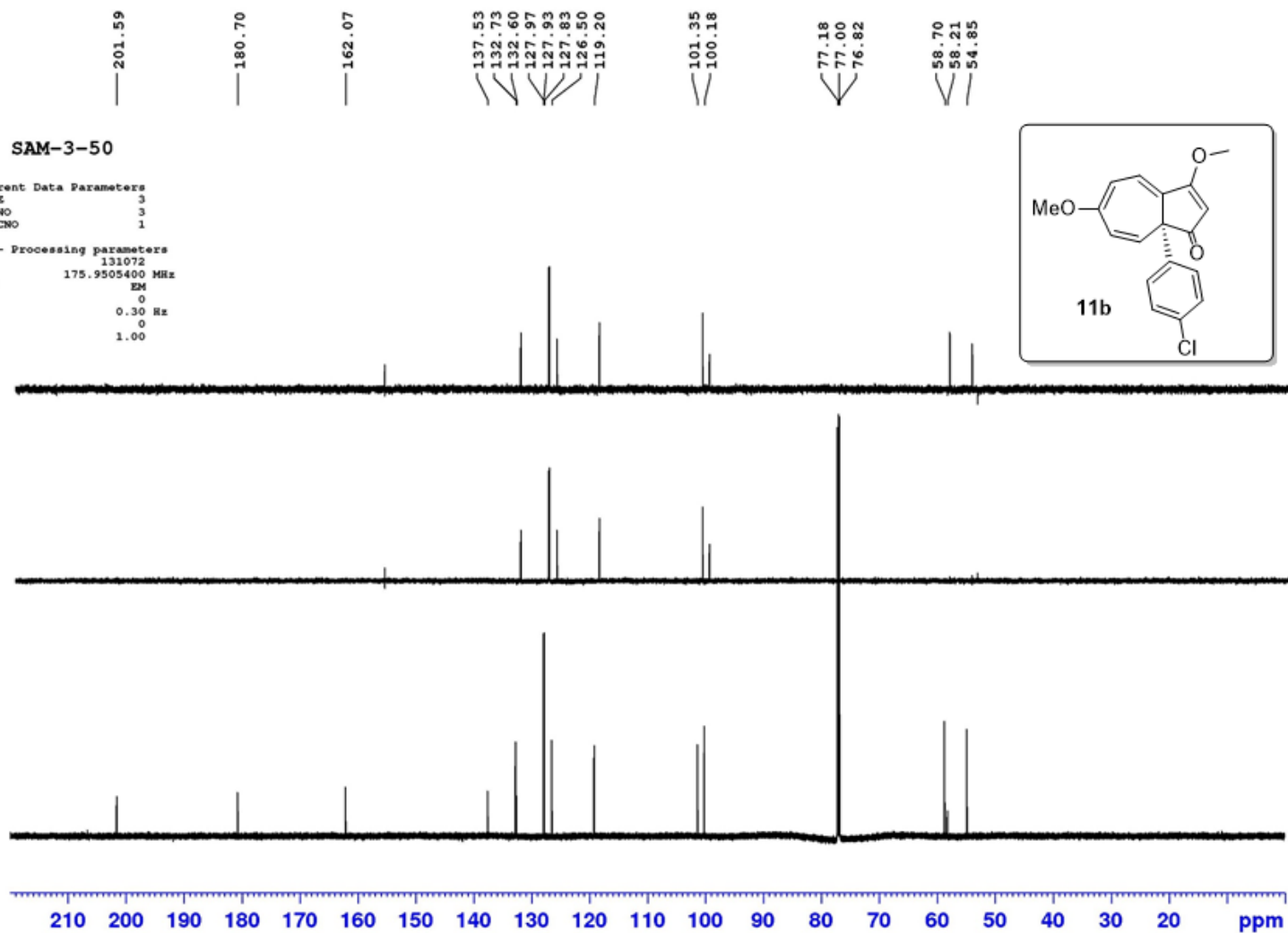
SAM-3-50

Current Data Parameters
NAME SAM-3-50-H.Eid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

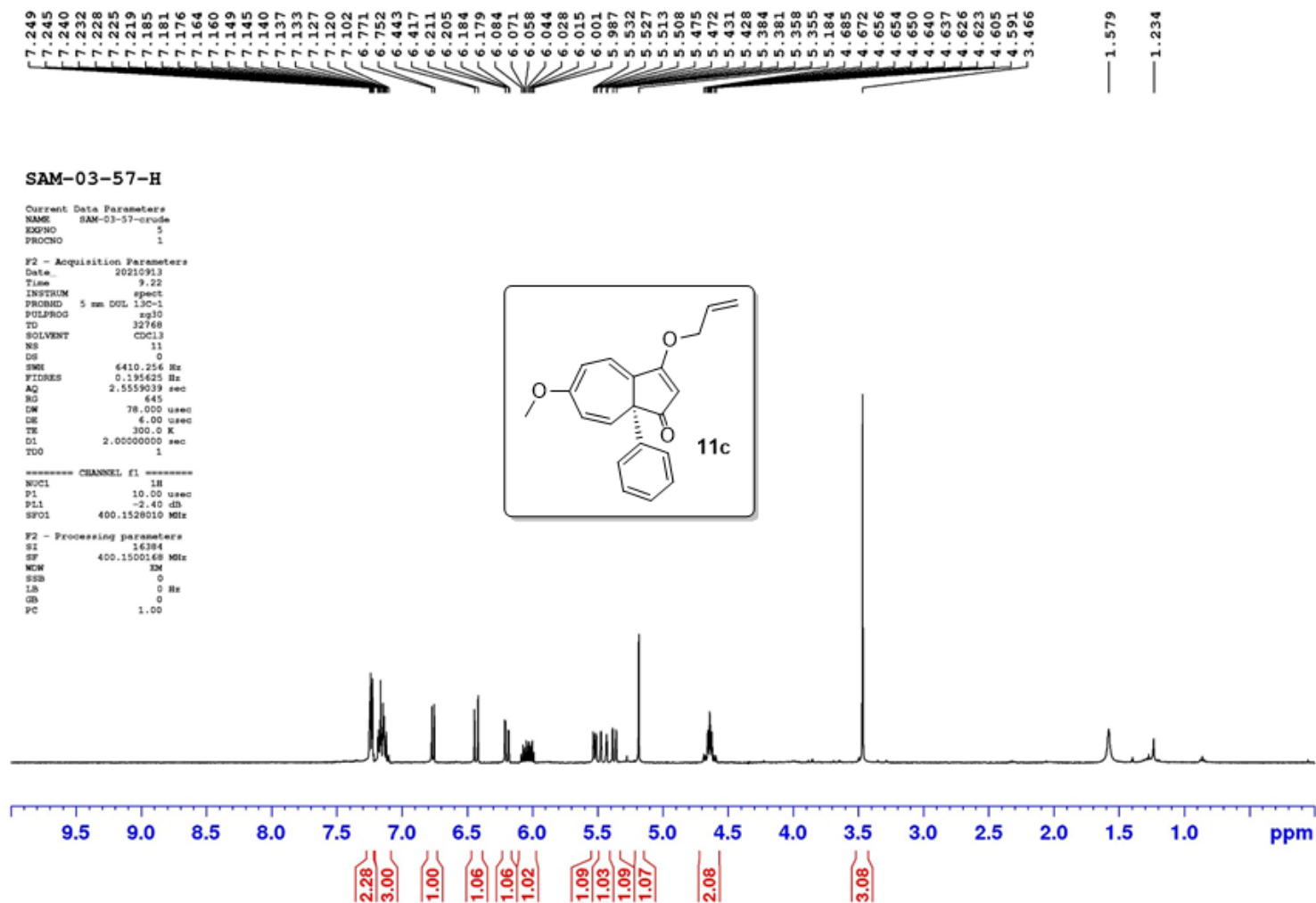
7.240
7.171
7.159
7.131
7.119
6.723
6.713
6.397
6.381
6.192
6.190
6.177
6.174
5.533
5.531
5.523
5.521
5.188
3.956
3.482
1.553



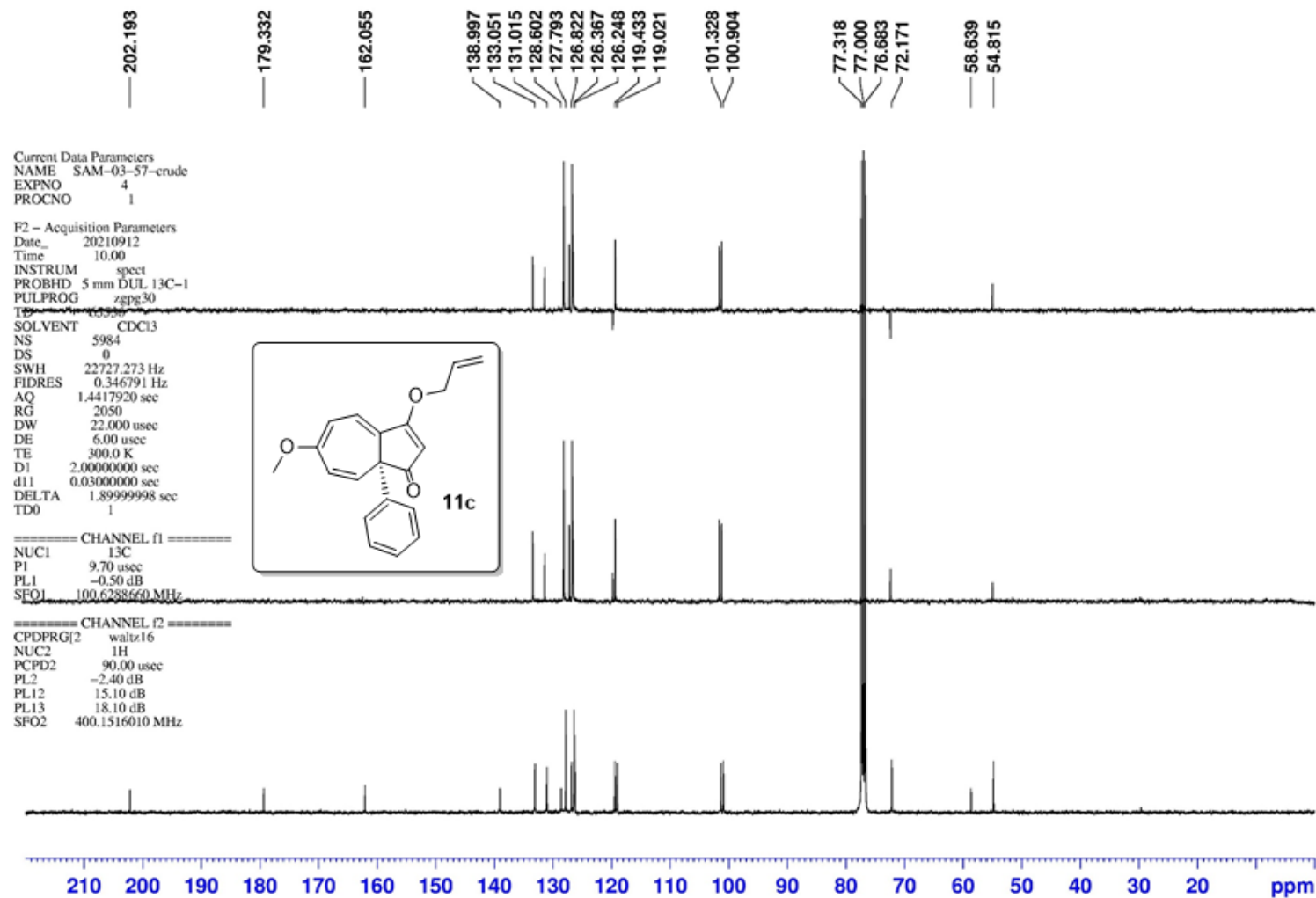
Solvent: CDCl_3
SFO1: 175 MHz



Solvent: CDCl_3
SFO1: 400 MHz



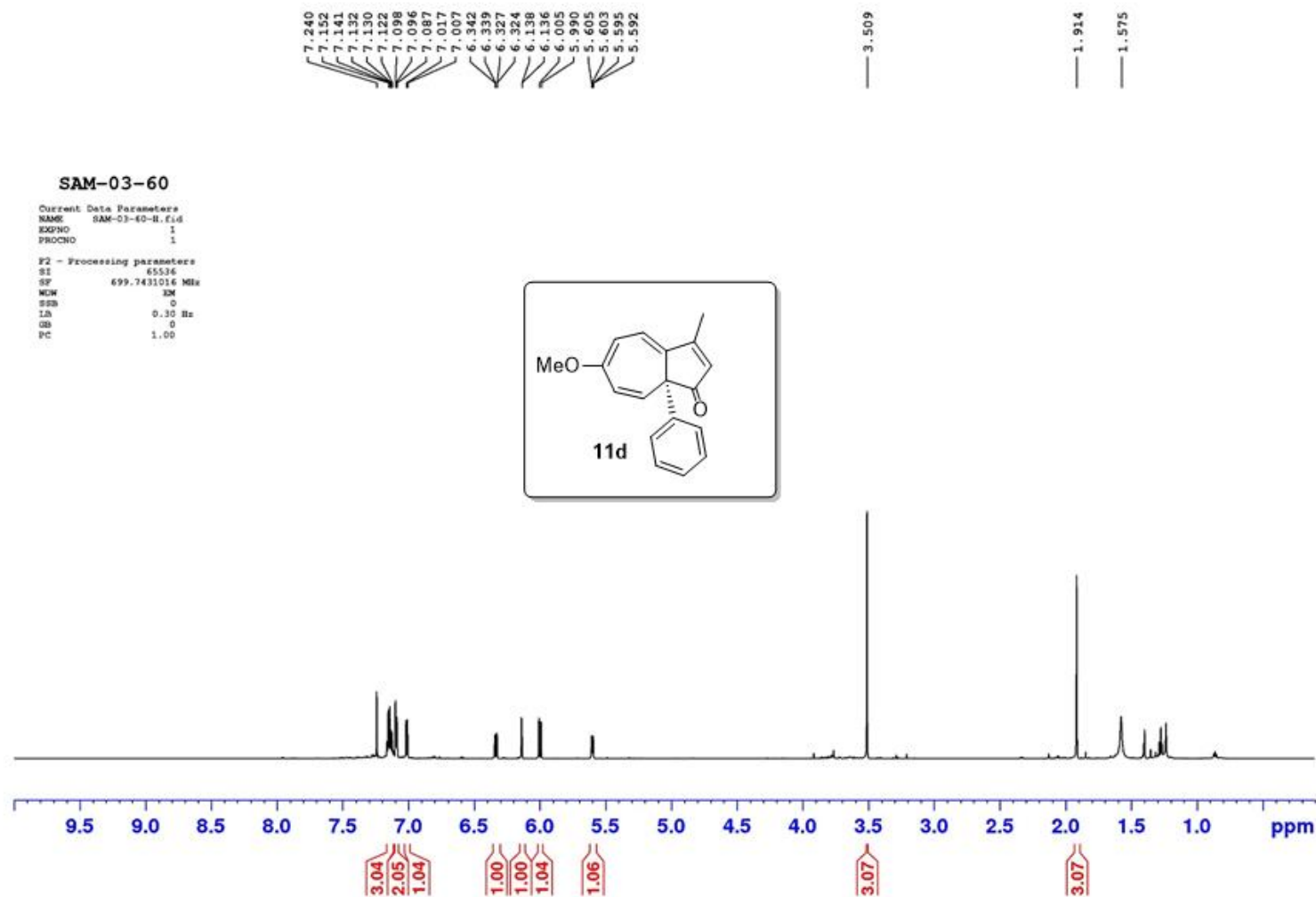
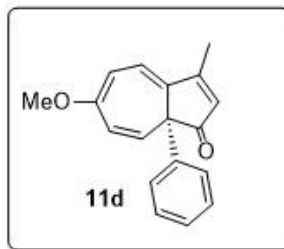
Solvent: CDCl_3
SFO1: 100 MHz



Solvent: CDCl₃
SFO1: 700 MHz

SAM-03-60

Current Data Parameters
NAME SAM-03-60-R.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7431016 MHz
RGW 32M
SFB 0
LA 0.30 Hz
GB 0
PC 1.00



Solvent: CDCl_3
 SFO1: 175 MHz

