

## **Aerobic oxidation/metal-free cyclization cascades of nitrosoarenes, allenynes with TEMPO/O<sub>2</sub>: A switch of diradical to single radical intermediates**

Chandrima Maitra,<sup>a</sup> Debashis Barik,<sup>a</sup> Yeu-Shiuan Ho,<sup>b</sup> Mu-Jeng Cheng,<sup>\*b</sup> and Rai-Shung Liu<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, Tsing-Hua University, Hsinchu, Taiwan, China

<sup>b</sup>Department of Chemistry, Cheng-Kung University, Tainan City, Taiwan, China

E-mail: [rsliu@mx.nthu.edu.tw](mailto:rsliu@mx.nthu.edu.tw) and [mjcheng@mail.ncku.edu.tw](mailto:mjcheng@mail.ncku.edu.tw)

### **Contents:**

#### **Experimental section**

<b>(1) General methods .....</b>	<b>S2</b>
<b>(2) General procedure for synthesis of substrates .....</b>	<b>S2</b>
<b>2.1. General procedure for synthesis of 1,2-bis(alkynyl)diynes.....</b>	<b>S2</b>
<b>2.2. General procedure the for synthesis of Allenynes .....</b>	<b>S3</b>
<b>2.3. General procedure for synthesis of nitrosoarenes .....</b>	<b>S3</b>
<b>(3) Standard procedure for TEMPO promoted single radical cascade reaction .....</b>	<b>S3</b>
<b>(4) Standard procedure for chemical functionalizations .....</b>	<b>S4</b>
<b>(5) References .....</b>	<b>S5</b>
<b>(6) Spectral data for key compounds .....</b>	<b>S6</b>
<b>(7) <sup>1</sup>H-NOE data for compounds 5c, 5d and 5d'.....</b>	<b>S26</b>
<b>(8) X-ray crystallographic structure and data for 4i, 4v', 5a and 5d.....</b>	<b>S27</b>
<b>(9) Computational details.....</b>	<b>S32</b>
<b>(10) <sup>1</sup>H and <sup>13</sup>C spectra of key compounds .....</b>	<b>S73</b>

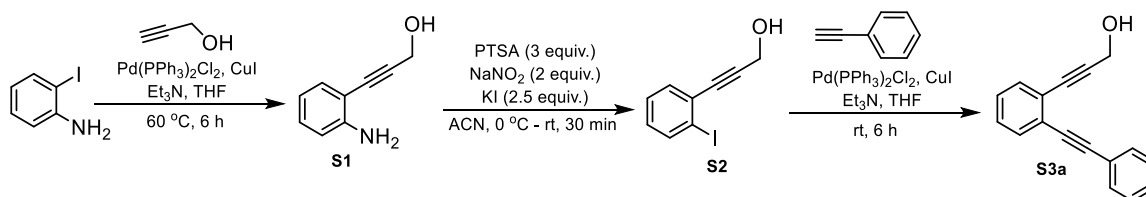
## Experimental section.

### (1) General methods:

Unless otherwise noted, all the reactions for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed under nitrogen atmosphere. Toluene and DCE were distilled from  $\text{CaH}_2$  under nitrogen. THF was distilled from Na metal under nitrogen. All other commercial reagents were used without further purification unless otherwise indicated.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a Varian 700 MHz and Bruker 400 MHz Spectrometers using chloroform-d ( $\text{CDCl}_3$ ;  $\delta_{\text{H}} = 7.24$  ppm,  $\delta_{\text{C}} = 77.00$  as a solvent and  $\text{Me}_4\text{Si}$  as an internal standard. Chemical Shift ( $\delta$ ) and Spin-Spin coupling constant (J). The following abbreviations were used to show the multiplicities: s: singlet, bs: broad singlet, d: doublet, t: triplet, q: quadruplet, dd: doublet of doublet, tt: triplet of triplet, qt: quadruplet of triplet, tq: triplet of quadruplet, m: multiplet. Mass spectrometry was performed in the positive electrospray ionization (ESI+) mode, positive electron ionization (EI+) mode and positive field ionization (FI+) mode. All heating reactions were carried out with oil bath as heat source. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f - 254) using UV light as visualizing agents. Single-crystal X-ray diffraction intensity data were collected on a Bruker X8 APEX diffractometer equipped with a CCD area detector and Mo  $K\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 100 K; all data calculations were performed by using the PC version of the APEX2 program package. All the substrate 1-Alkenyl-2-alkynylbenzenes and nitrosoarenes were prepared according to the literature procedures which are described below.

### (2) General procedure for synthesis of substrates:

#### 2.1. General procedure for synthesis of 1,2-bis(alkynyl)diynes.

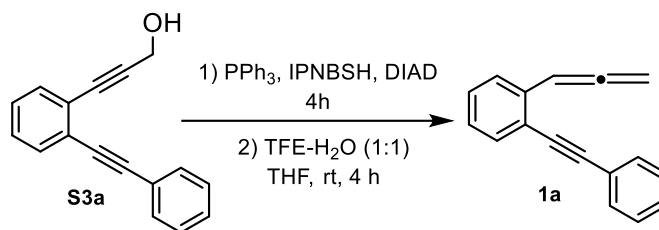


To a solution of 2-iodoaniline (3.0 gm, 13.69 mmol),  $\text{PdCl}_2(\text{PPh}_3)_2$  (480.5 mg, 0.684 mmol),  $\text{CuI}$  (260.7 mg, 1.369 mmol) and  $\text{Et}_3\text{N}$  (15 ml) in dry THF (20 mL) was degassed well under  $\text{N}_2$  and added prop-2-yn-1-ol (876  $\mu\text{L}$ , 15.059 mmol) dropwise. After the reaction mixture was stirred at 60  $^\circ\text{C}$  for 6 h, the reaction mixture was cooled down to room temperature. The solvent was then removed under reduced pressure. The residue was purified by column chromatography over silica gel with 30%  $\text{EtOAc}/\text{Hexane}$  to give **S1** (brown liquid, 1.8 g, 89%).

To a solution of p-TsOH· $\text{H}_2\text{O}$  (3.51 gm, 20.37 mmol) in MeCN (50 mL) was added the **S1** (1 g, 6.794 mmol). The resulting suspension of amine salt was cooled to 0 – 5  $^\circ\text{C}$  and to this was added, gradually, an aqueous solution of  $\text{NaNO}_2$  (900 mg, 13.58 mmol) and  $\text{KI}$  (2.81 gm, 16.98 mmol) in  $\text{H}_2\text{O}$ . The reaction mixture was stirred for 10 min then allowed to come to 20  $^\circ\text{C}$  and stirred for 30 minutes. To the reaction mixture was then added saturated  $\text{NaHCO}_3$  (until pH = 9–10) and saturated  $\text{Na}_2\text{S}_2\text{O}_3$  solution. Then extracted with  $\text{EtOAc}$  and dried over  $\text{Na}_2\text{SO}_4$ . The crude was purified by column chromatography over silica gel with 10%  $\text{EtOAc}/\text{Hexane}$  to afford **S2** (brown liquid, 1.5 g, 86%).

To a solution of **S2** (3.0 gm, 11.625 mmol), PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub> (407.8 mg, 0.581 mmol), CuI (221.5 mg, 1.163 mmol), and Et<sub>3</sub>N (15 ml) in dry THF (20 mL) was degassed well under N<sub>2</sub> and ethynylbenzene (1.4 mL, 12.788 mmol) dropwise. After the reaction mixture was stirred for 6 h, the solvent was removed under reduced pressure. The residue was purified by column chromatography over silica gel with 30% EtOAc/Hexane to give **S3a** (brown liquid, 2.3 g, 85%). The spectral data were in agreement with those previously reported.<sup>[1]</sup>

## 2.2. General procedure for the synthesis of Allenynes.



To a solution of **S3a** (2.0 g, 8.6 mmol, 1 equiv.) in dry THF (20 mL) were added PPh<sub>3</sub> (9.0 g, 34.4 mmol, 4 equiv.), and dry THF solution of *N*-isopropylidene-*N'*-2-nitrobenzenesulfonyl hydrazine (IPNBSH; 8.85 g, 34.4 mmol, 4 equiv.) and stirred well for 10 minutes at 0 °C. Then DIAD (ca. 1.9 M in THF, 20 mL) was added dropwise at 0 °C. After the reaction mixture was stirred at room temperature for 4 hours, a mixture of TFE–H<sub>2</sub>O (1:1, 50 mL) was added to the reaction mixture. After 4 hours, water was added to the mixture, and the whole mixture was extracted with Et<sub>2</sub>O. The organic layer was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated in vacuo. The residue was purified by column chromatography on silica gel with hexane to give **1a** (1.2 g, 64%) as a yellow oil. The spectral data were in agreement with those previously reported.<sup>[2]</sup>

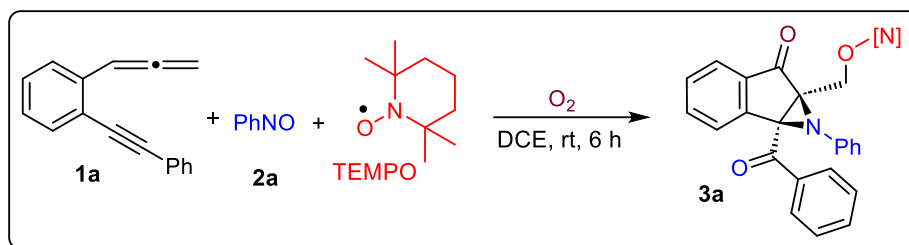
All other allenynes were prepared according to the procedure reported in the literatures.<sup>[2],[3],[4]</sup>

## 2.3. General procedure for the synthesis of nitrosoarenes.

All the nitrosoarenes were prepared according to the procedure reported in the literatures.<sup>[5]</sup>

### (3) Standard procedure for TEMPO promoted single radical cascade reaction:

#### 3.1 Synthesis of (1aS,6aR)-1a-benzoyl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3a).

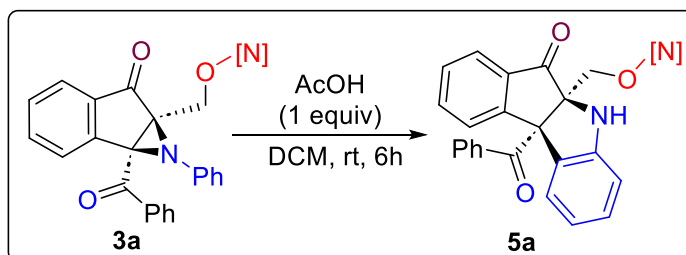


A mixture of the 1-Allenyl-2-alkynylbenzene **1a** (43.3 mg, 0.20 mmol), nitrosoarene **2a** (42.8 mg, 0.40 mmol) and TEMPO (46.8 mg, 0.30 mmol) in dichloroethane (DCE, 3.0 mL) was stirred at rt for 6 h under

O<sub>2</sub> atmosphere. After complete consumption of the starting materials, the solvent was then removed under reduced pressure. The residue was purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **3a** (65.2 mg, 0.132 mmol, 66%) as a yellow solid.

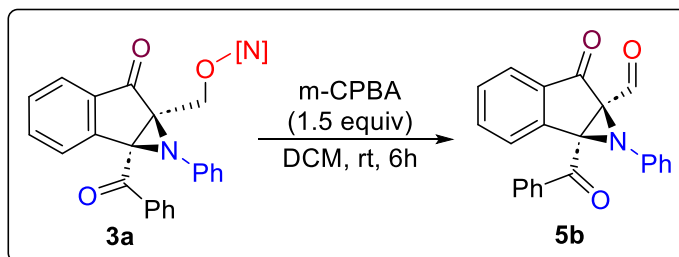
#### (4) Standard procedure for chemical functionalizations:

##### 4.1. Synthesis of (5aR,10bS)-10b-benzoyl-5a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-5a,10b-dihydroindeno[2,1-b]indol-6(5H)-one (**5a**).



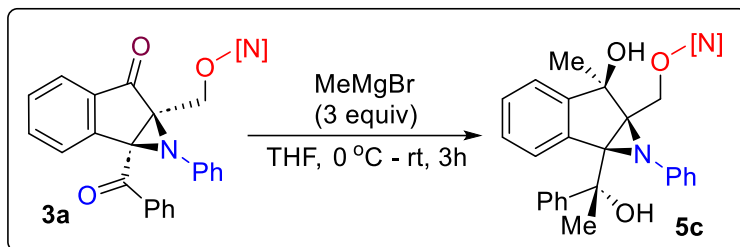
To a dry DCM (3 mL) solution of **3a** (99 mg, 0.20 mmol) was added AcOH (1 equiv, 0.20 mmol) and the reaction was stirred at room temperature for 6 h. Upon completion of the reaction, the reaction mixture was quenched with a saturated NaHCO<sub>3</sub> and extracted with DCM and brine solution. The organic layer was dried with MgSO<sub>4</sub> and concentrated under reduced pressure and purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **5a** (50.5 mg, 0.102 mmol, 51%) as a yellow solid.

##### 4.2. Synthesis of (1aS,6aR)-1a-benzoyl-6-oxo-1-phenyl-1a,6-dihydroindeno[1,2-b]azirine-6a(1H)-carbaldehyde (**5b**).



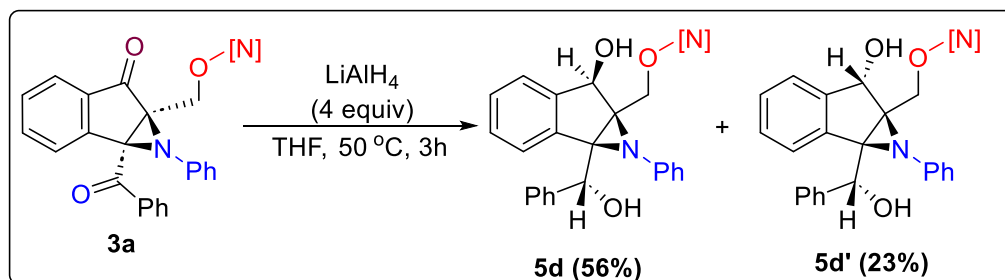
To a dry DCM (3 mL) solution of **3a** (99 mg, 0.20 mmol) was added m-CPBA (1.5 equiv, 52.0 mg, 0.30 mmol) and the reaction was stirred at room temperature for 6 h. Upon completion of the reaction, the reaction mixture was quenched with a saturated NaHCO<sub>3</sub> and extracted with DCM and brine solution. The organic layer was dried with MgSO<sub>4</sub> and concentrated under reduced pressure and purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **5a** (36.7 mg, 0.103 mmol, 52%) as a yellow oil.

##### 4.3 Synthesis of (1aS,6R,6aR)-1a-((R)-1-hydroxy-1-phenylethyl)-6-methyl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1,1a,6,6a-tetrahydroindeno[1,2-b]azirin-6-ol (**5c**).



To a dry THF (3 mL) solution of **3a** (99 mg, 0.20 mmol) was added MeMgBr (3M in diethyl ether) (0.2 mL, 0.60 mmol) at 0 °C and the reaction was stirred at room temperature for 3 h. Upon completion of the reaction, the reaction mixture was quenched with a saturated NH<sub>4</sub>Cl and extracted with DCM and brine solution. The organic layer was dried with MgSO<sub>4</sub> and concentrated under reduced pressure and purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **5c** (45.3 mg, 0.086 mmol, 43%) as a white sticky solid.

**4.4 Synthesis of (1aS,6R,6aR)-1a-((R)-hydroxy(phenyl)methyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1,1a,6,6a-tetrahydroindeno[1,2-b]azirin-6-ol (5d) and (1aS,6S,6aR)-1a-((R)-hydroxy(phenyl)methyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1,1a,6,6a-tetrahydroindeno[1,2-b]azirin-6-ol (5d').**



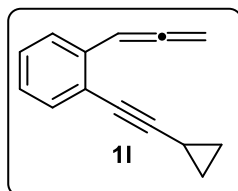
To a dry THF (3 mL) solution of **3a** (99 mg, 0.20 mmol) was added LiAlH<sub>4</sub> (30.4 mg, 0.80 mmol) and the reaction was stirred under reflux condition for 3 h. Upon completion of the reaction, the reaction mixture was quenched with a saturated NH<sub>4</sub>Cl and extracted with DCM and brine solution. The organic layer was dried with MgSO<sub>4</sub> and concentrated under reduced pressure and purified by column chromatography over silica gel with 25% EtOAc/Hexane to afford **5d** (55.8 mg, 0.112 mmol, 56%) and **5d'** (22.9 mg, 0.046 mmol, 23%) as a white solid.

#### (5) References:

- Pandit, Y; Liu, R.-S. *Adv. Synth. Catal.* **2020**, *362*, 3183– 3189.
- Maitra, C; Jadhav, P. J; Barik, D; Ho, Y.-S; Cheng, C. -C; Cheng, M. -J; Chiang, Y. -W; Liu, R.-S. *Org. Lett.* **2023**, *25*, 1, 82–86.
- Ikeuchi, T.; Inuki, S.; Oishi, S.; Ohno, H. *Angew. Chem., Int. Ed.* **2019**, *58*, 7792– 7796.
- Hughes, T. S.; Carpenter, B. K. *J. Chem. Soc., Perkin Trans. 2* **1999**, 2291– 2298.
- (a) H.-P. Wang, S. Sun, J. Cheng, *Tetrahedron Lett.* 2017, **58**, 3875; (b) F. G. Bordwell, W.-Z. Liu, *J. Am. Chem. Soc.* 1996, **118**, 8777-8781; (c) B. Priewisch, K. Rück-Braun, *J. Org. Chem.* 2005, **70**, 2350– 2352.

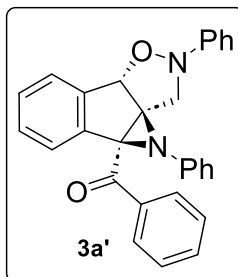
**(6) Spectral data for key compounds:**

**Spectral data for 1-(cyclopropylethynyl)-2-(propa-1,2-dien-1-yl)benzene (11):**



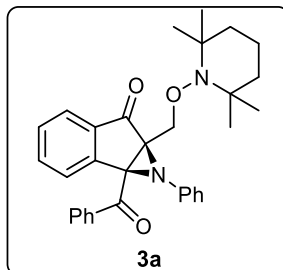
Prepared by general procedure from **S31** (500 mg, 2.55 mmol, 1 equiv.). Purified by silica gel column, hexane as eluent; Yellow oil (250 mg, 1.39 mmol, 54%);  $^1\text{H NMR}$  (700 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.41 (d,  $J = 8.4$  Hz, 1H), 7.33 (d,  $J = 7.7$  Hz, 1H), 7.18 (t,  $J = 7.7$  Hz, 1H), 7.07 (t,  $J = 7.7$  Hz, 1H), 6.67 (t,  $J = 7.0$  Hz, 1H), 5.13 (d,  $J = 6.3$  Hz, 2H), 1.53 – 1.45 (m, 1H), 0.88 – 0.86 (m, 2H), 0.81 – 0.79 (m, 2H);  $^{13}\text{C NMR}$  (175 MHz,  $\text{CDCl}_3$ )  $\delta$ : 210.3, 135.3, 132.3, 127.6, 126.4, 126.3, 121.6, 98.3, 92.1, 78.6, 73.7, 8.7, 0.33. HRMS- $\text{EI}^+$  calcd for  $\text{C}_{14}\text{H}_{12}$   $[\text{M}]^+$ : 180.0939, found: 180.0937.

**Spectral data for ((3aS,4aS,8bS)-2,4-diphenyl-2,3-dihydro-4H-azirino[2',3':2,3]indeno[2,1-d]isoxazol-4a(8bH)-yl)(phenyl) methanone (3a')**



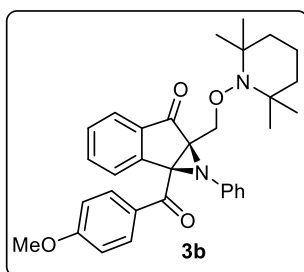
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3a'** as a yellow solid.  $^1\text{H NMR}$  (700 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.92 (d,  $J = 8.4$  Hz, 2H), 7.43 (t,  $J = 7.7$  Hz, 1H), 7.40 (d,  $J = 7.0$  Hz, 1H), 7.31 (t,  $J = 7.7$  Hz, 2H), 7.27 (t,  $J = 7.7$  Hz, 3H), 7.23 (d,  $J = 7.7$  Hz, 1H), 7.20 (t,  $J = 7.7$  Hz, 1H), 7.09 (d,  $J = 8.4$  Hz, 2H), 7.00 – 6.97 (m, 3H), 6.78 (t,  $J = 7.7$  Hz, 1H), 6.71 (d,  $J = 7.7$  Hz, 2H), 5.42 (s, 1H), 4.32 (d,  $J = 10.5$  Hz, 1H), 3.69 (d,  $J = 10.5$  Hz, 1H).  $^{13}\text{C NMR}$  (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  193.2, 150.7, 144.2, 141.2, 138.6, 135.5, 133.5, 130.0, 129.9, 129.0, 128.7, 128.6, 128.5, 128.0, 127.6, 122.7, 122.4, 120.0, 115.0, 77.5, 67.8, 62.9, 54.6; HRMS-ESI+ calcd for  $\text{C}_{29}\text{H}_{22}\text{N}_2\text{O}_2\text{Na}$   $[\text{M}+\text{Na}]^+$ : 453.1581, found: 453.1581.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3a):**



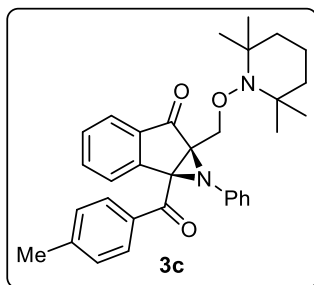
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3a** as a yellow solid (65.2 mg, 0.132 mmol, 66%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.01 – 7.99 (m, 2H), 7.52 – 7.48 (m, 1H), 7.47 – 7.45 (m, 1H), 7.37 – 7.33 (m, 3H), 7.24 – 7.22 (m, 1H), 7.20 – 7.16 (m, 1H), 6.97 (t, *J* = 7.6 Hz, 2H), 6.78 – 6.76 (m, 1H), 6.68 – 6.66 (m, 2H), 4.63 (d, *J* = 10.4 Hz, 1H), 4.24 (d, *J* = 10.4 Hz, 1H), 1.40 – 1.31 (m, 4H), 1.27 – 1.23 (m, 2H), 1.17 (s, 3H), 0.96 (s, 3H), 0.85 (s, 3H), 0.65 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.3, 192.1, 145.4, 144.6, 135.4, 134.6, 133.6, 133.4, 130.0, 129.1, 128.6, 128.4, 127.6, 124.8, 122.8, 120.1, 71.6, 60.9, 60.09, 60.07, 59.5, 39.85, 39.82, 32.56, 32.51, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>35</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 495.2647, found: 495.2642.

**Spectral data for (1aS,6aR)-1a-(4-methoxybenzoyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3b):**



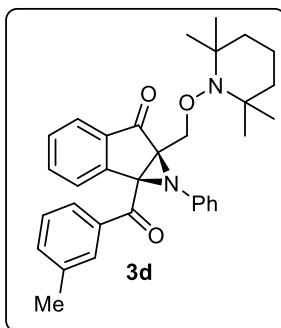
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3b** as a yellow solid (64.7 mg, 0.123 mmol, 62%, contains some impurities). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 8.00 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 7.2 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.97 (t, *J* = 7.6 Hz, 2H), 6.84 (d, *J* = 9.2 Hz, 2H), 6.78 – 6.71 (m, 1H), 6.68 – 6.66 (m, 2H), 4.59 (d, *J* = 10.4 Hz, 1H), 4.22 (d, *J* = 10.4 Hz, 1H), 3.80 (s, 3H), 1.47 – 1.35 (m, 4H), 1.33 – 1.26 (m, 2H), 1.20 (s, 3H), 0.97 (s, 3H), 0.89 (s, 3H), 0.70 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 195.4, 190.3, 163.9, 145.7, 144.7, 134.5, 133.4, 132.4, 129.0, 128.6, 128.5, 127.5, 124.7, 122.7, 120.1, 113.6, 71.7, 60.8, 60.1, 60.0, 59.2, 55.5, 55.3, 39.8, 32.56, 32.53, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>Na [M+Na]<sup>+</sup>: 547.2572, found: 547.2575.

**Spectral data for (1aS,6aR)-1a-(4-methylbenzoyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3c):**



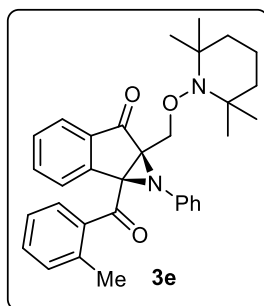
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3c** as a yellow solid (66 mg, 0.129 mmol, 65%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.89 (d, *J* = 7.7 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.36 – 7.34 (m, 1H), 7.23 (s, 1H), 7.18 – 7.14 (m, 3H), 6.96 (t, *J* = 7.7 Hz, 2H), 6.76 (t, *J* = 7.7 Hz, 1H), 6.68 (d, *J* = 7.7 Hz, 2H), 4.58 (d, *J* = 10.4 Hz, 1H), 4.23 (d, *J* = 10.4 Hz, 1H), 2.34 (s, 3H), 1.45 – 1.31 (m, 4H), 1.28 – 1.20 (m, 2H), 1.18 (s, 3H), 0.97 (s, 3H), 0.88 (s, 3H), 0.69 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.4, 191.6, 145.5, 144.7, 144.6, 134.5, 133.4, 132.9, 130.1, 129.12, 129.10, 128.6, 127.5, 124.8, 122.7, 120.2, 71.6, 60.9, 60.1, 60.0, 59.3, 39.85, 39.82, 32.57, 32.51, 21.7, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>37</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 509.2804, found: 509.2809.

**Spectral data for (1a*S*,6a*R*)-1a-(3-methylbenzoyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1*H*)-one (3d):**



Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3d** as a yellow sticky solid (51.8 mg, 0.102 mmol, 51%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.82 (s, 1H), 7.75 (d, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.23 – 7.20 (m, 2H), 7.17 (t, *J* = 7.7 Hz, 1H), 6.97 (t, *J* = 7.7 Hz, 2H), 6.76 (t, *J* = 7.7 Hz, 1H), 6.67 (d, *J* = 7.7 Hz, 2H), 4.63 (d, *J* = 10.4 Hz, 1H), 4.23 (d, *J* = 10.4 Hz, 1H), 2.29 (s, 3H), 1.45 – 1.31 (m, 4H), 1.28 – 1.21 (m, 2H), 1.19 (s, 3H), 0.97 (s, 3H), 0.87 (s, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.4, 192.3, 145.5, 144.6, 138.2, 135.4, 134.5, 134.4, 133.3, 130.3, 129.0, 128.5, 128.2, 127.6, 127.4, 124.8, 122.7, 120.1, 71.6, 61.0, 60.09, 60.07, 59.5, 39.84, 39.81, 32.5, 32.4, 21.2, 19.9, 19.5, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>37</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 509.2804, found: 509.2805.

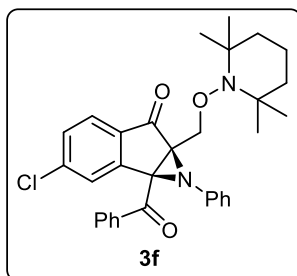
**Spectral data for (1a*S*,6a*R*)-1a-(2-methylbenzoyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1*H*)-one (3e):**





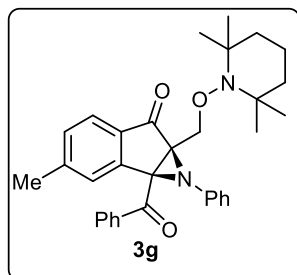
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3e** as a yellow sticky solid (39.6 mg, 0.078 mmol, 39%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 7.72 (d, *J* = 7.7 Hz, 1H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.17 – 7.12 (m, 2H), 7.05 (t, *J* = 7.7 Hz, 1H), 6.97 (t, *J* = 7.7 Hz, 2H), 6.76 (t, *J* = 7.7 Hz, 1H), 6.68 (d, *J* = 8.4 Hz, 2H), 4.50 (d, *J* = 10.4 Hz, 1H), 4.31 (d, *J* = 10.4 Hz, 1H), 2.65 (s, 3H), 1.42 – 1.23 (m, 6H), 1.12 (s, 3H), 1.08 (s, 3H), 0.93 (s, 3H), 0.86 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.3, 194.6, 145.0, 144.7, 139.6, 135.1, 134.4, 133.4, 132.07, 132.02, 131.3, 128.9, 128.6, 127.6, 125.3, 124.7, 122.7, 120.1, 71.3, 61.7, 60.1, 60.0, 39.8, 32.6, 32.4, 21.4, 20.1, 19.9, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>37</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 509.2804, found: 509.2803.

**Spectral data for (1a*S*,6a*R*)-1a-benzoyl-3-chloro-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1*H*)-one (3f):**



Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3f** as a yellow solid (53.8 mg, 0.102 mmol, 51%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 8.04 (d, *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.42 – 7.39 (m, 3H), 7.26 (s, 1H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.04 (t, *J* = 7.7 Hz, 2H), 6.83 (t, *J* = 7.7 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 2H), 4.57 (d, *J* = 10.4 Hz, 1H), 4.27 (d, *J* = 10.4 Hz, 1H), 1.44 – 1.21 (m, 6H), 1.13 (s, 3H), 0.99 (s, 3H), 0.86 (s, 3H), 0.72 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 193.5, 191.1, 146.4, 143.8, 140.7, 134.8, 133.5, 131.4, 129.6, 129.3, 128.4, 128.2, 127.4, 125.4, 122.6, 119.6, 70.9, 59.8, 59.7, 59.3, 39.41, 39.40, 32.1, 32.0, 19.6, 19.2, 16.5; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>ClN<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 551.2077, found: 551.2071.

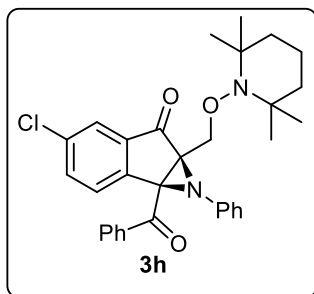
**Spectral data for (1a*S*,6a*R*)-1a-benzoyl-3-methyl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1*H*)-one (3g):**



Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3g** as a yellow sticky solid (56.9 mg, 0.112 mmol, 56%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 7.99 (d, *J* = 7.7 Hz, 2H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.25 (s, 1H), 7.15 (d, *J* = 7.7 Hz, 2H), 6.98 (t, *J* = 7.7 Hz, 2H), 6.77 (t, *J*

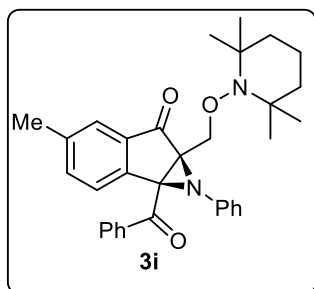
= 7.0 Hz, 1H), 6.68 (d,  $J = 7.7$  Hz, 2H), 4.64 (d,  $J = 10.4$  Hz, 1H), 4.22 (d,  $J = 10.4$  Hz, 1H), 2.21 (s, 3H), 1.36 – 1.23 (m, 4H), 1.18 (s, 3H), 0.94 (s, 3H), 0.85 (s, 3H), 0.62 (s, 3H);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  195.5, 192.3, 144.7, 142.8, 139.3, 135.49, 135.47, 133.6, 133.5, 130.0, 128.6, 128.3, 127.3, 125.1, 122.7, 120.1, 71.7, 60.7, 60.07, 60.05, 59.9, 39.86, 39.82, 32.55, 32.51, 21.1, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for  $\text{C}_{33}\text{H}_{37}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ : 509.2804, found: 509.2807.

**Spectral data for (1aS,6aR)-1a-benzoyl-4-chloro-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3h):**



Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3h** as a yellow solid (62 mg, 0.117 mmol, 59%).  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ ): 7.99 (d,  $J = 7.7$  Hz, 2H), 7.52 (t,  $J = 7.7$  Hz, 1H), 7.42 (d,  $J = 1.4$  Hz, 1H), 7.37 (t,  $J = 7.7$  Hz, 2H), 7.32 – 7.31 (m, 1H), 7.18 (d,  $J = 7.7$  Hz, 1H), 7.01 (t,  $J = 7.7$  Hz, 2H), 6.81 (t,  $J = 7.7$  Hz, 1H), 6.66 (d,  $J = 7.7$  Hz, 2H), 4.61 (d,  $J = 10.5$  Hz, 1H), 4.21 (d,  $J = 10.5$  Hz, 1H), 1.40 – 1.32 (m, 4H), 1.27 – 1.18 (m, 2H), 1.15 (s, 3H), 0.94 (s, 3H), 0.85 (s, 3H), 0.65 (s, 3H);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  194.0, 191.6, 144.2, 143.6, 135.33, 135.32, 135.0, 134.4, 133.8, 130.0, 128.8, 128.6, 128.5, 124.8, 123.1, 120.0, 71.4, 60.4, 60.14, 60.11, 60.0, 39.84, 39.81, 32.5, 32.4, 20.0, 19.6, 16.8; HRMS-ESI+ calcd for  $\text{C}_{32}\text{H}_{33}\text{N}_2\text{O}_3\text{ClNa}$   $[\text{M}+\text{Na}]^+$ : 551.2077, found: 551.2074.

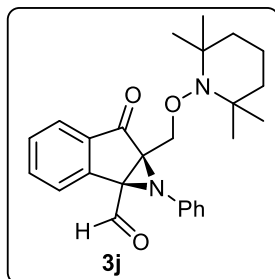
**Spectral data for (1aS,6aR)-1a-benzoyl-4-methyl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3i):**



Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3i** as a yellow sticky solid (63 mg, 0.124 mmol, 62%).  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ ): 8.02 (d,  $J = 7.7$  Hz, 2H), 7.51 (t,  $J = 7.7$  Hz, 1H), 7.37 – 7.33 (m, 3H), 7.04 (s, 1H), 6.99 – 6.96 (m, 3H), 6.77 (t,  $J = 7.7$  Hz, 1H), 6.69 (d,  $J = 7.7$  Hz, 2H), 4.56 (d,  $J = 10.5$  Hz, 1H), 4.25 (d,  $J = 10.5$  Hz, 1H), 2.24 (s, 3H) 1.49 – 1.31 (m, 4H), 1.28 – 1.17 (m, 2H), 1.13 (s, 3H), 0.97 (s, 3H), 0.83 (s, 3H), 0.68 (s, 3H);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  194.9, 192.2, 146.0, 145.8, 144.7, 135.4, 133.6, 131.1, 130.1, 130.0, 128.6, 128.4, 128.0, 124.7, 122.7, 120.1, 71.6, 60.7,

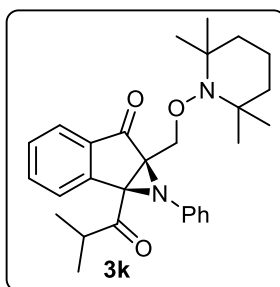
60.0, 59.5, 39.84, 39.81, 32.54, 32.50, 22.0, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>36</sub>N<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 531.2623, found: 531.2630.

**Spectral data for (1aS,6aR)-6-oxo-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-6,6a-dihydroindeno[1,2-b]azirine-1a(1H)-carbaldehyde (3j):**



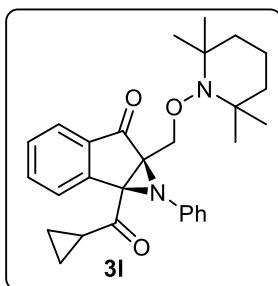
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3j** as a yellow solid (51.7 mg, 0.123 mmol, 62%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 9.74 (s, 1H), 7.87 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 6.98 (t, *J* = 7.7 Hz, 2H), 6.79 (t, *J* = 7.7 Hz, 1H), 6.58 (d, *J* = 7.7 Hz, 2H), 4.92 (d, *J* = 10.5 Hz, 1H), 4.42 (d, *J* = 10.5 Hz, 1H), 1.53 – 1.41 (m, 4H), 1.32 – 1.21 (m, 2H), 1.29 (s, 6H), 1.06 (s, 3H), 0.97 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.4, 194.3, 144.0, 141.6, 134.6, 134.0, 129.2, 128.8, 128.3, 124.6, 123.4, 120.2, 71.9, 60.2, 60.0, 59.7, 39.8, 39.7, 33.1, 32.7, 20.1, 16.9; HRMS-ESI+ calcd for C<sub>26</sub>H<sub>31</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 419.0432, found: 419.0433.

**Spectral data for (1aS,6aR)-1a-isobutyryl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3k):**



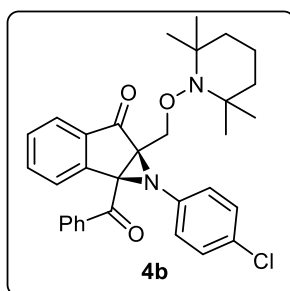
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3k** as a yellow liquid (46.9 mg, 0.102 mmol, 51%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.48 – 7.45 (m, 2H), 7.34 (d, *J* = 7.7 Hz, 1H), 7.18 – 7.15 (m, 1H), 6.98 (t, *J* = 7.7 Hz, 2H), 6.78 (t, *J* = 7.7 Hz, 1H), 6.64 (d, *J* = 7.7 Hz, 2H), 4.39 (s, 2H), 3.36 – 3.33 (m, 1H), 1.46 – 1.43 (m, 4H), 1.34 (d, *J* = 7.0 Hz, 3H), 1.29 (s, 4H), 1.22 (s, 4H), 1.17 – 1.16 (m, 6H), 1.06 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 208.2, 194.9, 144.6, 144.2, 134.3, 133.9, 129.0, 128.7, 127.4, 124.6, 122.9, 120.2, 71.9, 60.3, 60.29, 60.25, 59.7, 39.86, 39.83, 37.2, 33.0, 32.7, 20.2, 20.1, 19.2, 17.0, 16.5; HRMS-ESI+ calcd for C<sub>29</sub>H<sub>36</sub>N<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 483.2623, found: 483.2628.

**Spectral data for (1aS,6aR)-1a-(cyclopropanecarbonyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (3l):**



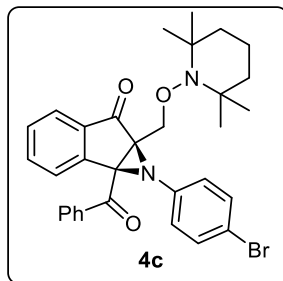
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **3I** as a yellow liquid (52 mg, 0.113 mmol, 57%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.54 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 6.38 (d, *J* = 7.7 Hz, 1H), 7.17 (t, *J* = 7.7 Hz, 1H), 6.98 (t, *J* = 7.7 Hz, 2H), 6.77 (t, *J* = 7.7 Hz, 1H), 6.65 (d, *J* = 7.7 Hz, 2H), 4.59 (d, *J* = 10.5 Hz, 1H), 4.35 (d, *J* = 10.5 Hz, 1H), 2.73 – 2.70 (m, 1H), 1.48 – 1.42 (m, 4H), 1.39 – 1.35 (m, 2H), 1.29 (s, 3H), 1.28 (s, 3H), 1.16 (s, 3H), 1.06 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 203.5, 194.9, 144.6, 143.8, 134.3, 134.1, 129.0, 128.6, 127.8, 124.5, 122.9, 120.1, 71.5, 61.8, 60.2, 59.6, 39.8, 32.9, 32.6, 20.1, 20.0, 19.0, 17.0, 13.4, 13.3; HRMS-ESI+ calcd for C<sub>29</sub>H<sub>34</sub>N<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 481.2467, found: 481.2463.

**Spectral data for (1a*S*,6a*R*)-1a-benzoyl-1-(4-chlorophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1H)-one (4b):**



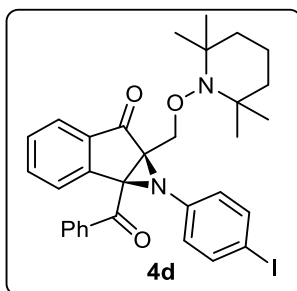
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4b** as a yellow solid (60 mg, 0.11 mmol, 57%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.97 (d, *J* = 7.7 Hz, 2H), 7.52 – 7.49 (m, 2H), 7.38 – 7.34 (m, 3H), 7.23 (d, *J* = 7.7 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.61 (d, *J* = 8.4 Hz, 2H), 4.57 (d, *J* = 10.5 Hz, 1H), 4.24 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.19 (m, 6H), 1.14 (s, 3H), 0.96 (s, 3H), 0.84 (s, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.0, 191.7, 145.1, 143.4, 135.2, 134.8, 133.7, 133.2, 129.9, 129.5, 128.7, 128.5, 128.0, 127.5, 125.1, 121.3, 71.4, 61.0, 60.1, 59.5, 39.83, 39.80, 32.51, 32.50, 20.0, 19.6, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>ClNa [M+Na]<sup>+</sup>: 551.2077, found: 551.2095.

**Spectral data for (1a*S*,6a*R*)-1a-benzoyl-1-(4-bromophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1H)-one (4c):**



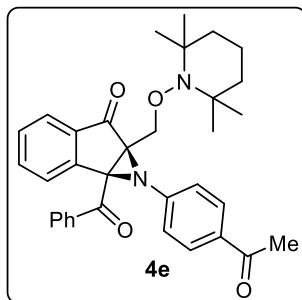
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4c** as a yellow solid (56 mg, 0.097 mmol, 49%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.96 (d, *J* = 8.4 Hz, 2H), 7.52 – 7.49 (m, 2H), 7.39 – 7.34 (m, 3H), 7.24 – 7.21 (m, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 8.4 Hz, 2H), 4.57 (d, *J* = 10.5 Hz, 1H), 4.24 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.19 (m, 6H), 1.14 (s, 3H), 0.96 (s, 3H), 0.83 (s, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.9, 191.7, 145.1, 143.9, 135.2, 134.8, 133.7, 133.2, 131.6, 129.9, 129.5, 128.5, 127.5, 125.1, 121.7, 115.6, 71.3, 60.9, 60.0, 59.4, 39.8, 39.7, 32.5, 32.4, 20.0, 19.6, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>BrNa [M+Na]<sup>+</sup>: 595.1572, found: 595.1578.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(4-iodophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4d):**



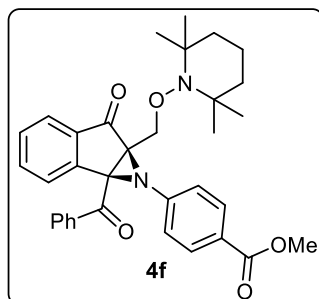
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4d** as a yellow solid (69.4 mg, 0.111 mmol, 56%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.96 (d, *J* = 7.7 Hz, 2H), 7.52 – 7.50 (m, 2H), 7.39 – 7.34 (m, 3H), 7.27 (d, *J* = 7.7 Hz, 2H), 7.24 – 7.21 (m, 2H, merged with CDCl<sub>3</sub>), 6.45 (d, *J* = 8.4 Hz, 2H), 4.56 (d, *J* = 10.5 Hz, 1H), 4.24 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.32 (m, 4H), 1.28 – 1.16 (m, 2H), 1.13 (s, 3H), 0.96 (s, 3H), 0.83 (s, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.9, 191.7, 145.1, 144.6, 137.5, 135.2, 134.8, 133.7, 133.2, 129.9, 129.5, 128.5, 127.5, 125.2, 122.2, 86.1, 71.3, 60.8, 60.1, 59.4, 39.82, 39.80, 32.5, 32.4, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>34</sub>N<sub>2</sub>O<sub>3</sub>I [M+H]<sup>+</sup>: 621.1614, found: 621.1615.

**Spectral data for (1aS,6aR)-1-(4-acetylphenyl)-1a-benzoyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4e):**



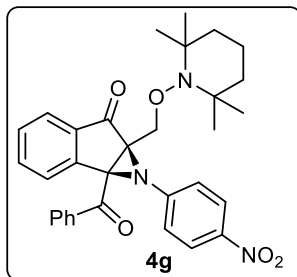
Purified by column chromatography over silica gel with 10% EtOAc/Hexane to afford **4e** as a yellow solid (69.5 mg, 0.129 mmol, 65%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.96 – 7.95 (m, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.39 – 7.35 (m, 3H), 7.26 (d, *J* = 7.7 Hz, 1H), 7.22 – 7.19 (m, 1H), 6.74 (d, *J* = 8.4 Hz, 2H), 4.59 (d, *J* = 10.5 Hz, 1H), 4.30 (d, *J* = 10.5 Hz, 1H), 2.41 (s, 3H), 1.44 – 1.30 (m, 4H), 1.28 – 1.19 (m, 2H), 1.13 (s, 3H), 0.98 (s, 3H), 0.82 (s, 3H), 0.68 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 196.8, 194.6, 191.3, 149.5, 145.1, 135.0, 134.9, 133.8, 132.7, 132.0, 129.9, 129.5, 129.4, 128.5, 127.5, 125.2, 119.9, 71.1, 60.8, 60.1, 60.0, 59.3, 39.8, 39.7, 32.4, 26.2, 20.0, 19.6, 16.8; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>37</sub>N<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup>: 537.2753, found: 537.2747.

**Spectral data for methyl 4-((1aS,6aR)-1a-benzoyl-6-oxo-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-6,6a-dihydroindeno[1,2-b]azirin-1(1aH)-yl)benzoate (4f):**



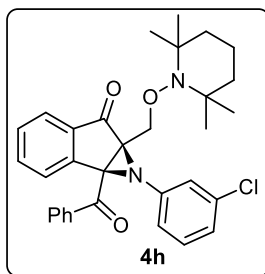
Purified by column chromatography over silica gel with 10% EtOAc/Hexane to afford **4f** as a yellow solid (76 mg, 0.137 mmol, 69%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.96 (d, *J* = 7.7 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.52 – 7.50 (m, 1H), 7.47 (d, *J* = 7.7 Hz, 1H), 7.37 – 7.34 (m, 3H), 7.25 (s, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.72 (d, *J* = 8.4 Hz, 2H), 4.60 (d, *J* = 10.5 Hz, 1H), 4.28 (d, *J* = 10.5 Hz, 1H), 3.76 (s, 3H), 1.41 – 1.32 (m, 4H), 1.27 – 1.19 (m, 2H), 1.14 (s, 3H), 0.97 (s, 3H), 0.82 (s, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.6, 191.4, 166.6, 149.3, 145.1, 135.1, 134.8, 133.8, 132.8, 130.4, 129.9, 129.55, 129.53, 128.5, 127.5, 126.6, 125.2, 124.6, 119.8, 71.2, 60.8, 60.1, 60.0, 59.3, 51.8, 39.8, 39.7, 32.4, 19.9, 19.6, 16.8; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>37</sub>N<sub>2</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 553.2702, found: 553.2700.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(4-nitrophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4g):**



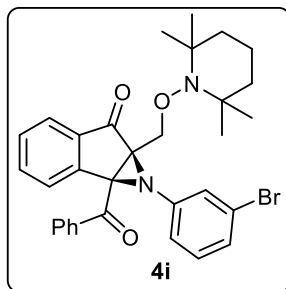
Purified by column chromatography over silica gel with 10% EtOAc/Hexane to afford **4g** as a yellow solid (76.6 mg, 0.141 mmol, 71%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.94 (d, *J* = 7.7 Hz, 2H), 7.90 (d, *J* = 9.1 Hz, 2H), 7.54 – 7.51 (m, 2H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.26 – 7.24 (m, 1H, merged with CDCl<sub>3</sub>), 6.80 (d, *J* = 9.1 Hz, 2H), 4.55 (d, *J* = 10.5 Hz, 1H), 4.34 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.20 (m, 6H), 1.10 (s, 3H), 1.00 (s, 3H), 0.80 (s, 3H), 0.71 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.1, 190.7, 151.3, 144.9, 143.2, 135.1, 134.7, 134.1, 132.4, 129.9, 129.8, 128.6, 127.4, 125.6, 124.7, 120.1, 70.9, 60.9, 60.19, 60.11, 59.3, 39.77, 39.76, 32.49, 32.43, 19.9, 19.7, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>3</sub>O<sub>5</sub>Na [M+Na]<sup>+</sup>: 562.2317, found: 562.2313.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(3-chlorophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4h):**



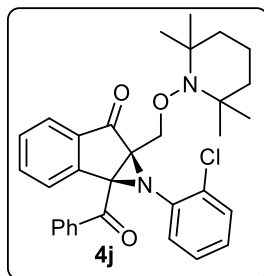
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4h** as a yellow solid (53 mg, 0.10 mmol, 51%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.97 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.25 (s, 1H), 7.22 (s, 1H), 6.91 (t, *J* = 7.7 Hz, 1H), 6.75 (d, *J* = 7.7 Hz, 1H), 6.66 (s, 1H), 6.58 (d, *J* = 7.7 Hz, 1H), 4.57 (d, *J* = 10.5 Hz, 1H), 4.26 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.18 (m, 6H), 1.14 (s, 3H), 0.98 (s, 3H), 0.83 (s, 3H), 0.67 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.8, 191.5, 146.1, 145.0, 135.2, 134.8, 134.3, 133.8, 133.0, 129.9, 129.7, 129.5, 128.5, 127.5, 125.1, 123.0, 120.3, 118.4, 71.3, 60.9, 60.1, 60.0, 59.4, 39.8, 32.5, 19.9, 19.6, 16.9, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>ClNa [M+Na]<sup>+</sup>: 551.2077, found: 551.2074.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(3-bromophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4i):**



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4i** as a yellow solid (68 mg, 0.118 mmol, 59%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.96 (t, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.41 – 7.39 (m, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.25 – 7.22 (m, 2H), 6.90 – 6.89 (m, 1H), 6.85 (t, *J* = 7.7 Hz, 1H), 6.81 (s, 1H), 6.63 (dd, *J*<sub>1</sub> = 7.7 Hz, *J*<sub>2</sub> = 0.7 Hz, 1H), 4.56 (d, *J* = 10.5 Hz, 1H), 4.26 (d, *J* = 10.5 Hz, 1H), 1.43 – 1.31 (m, 4H), 1.29 – 1.18 (m, 2H), 1.13 (s, 3H), 0.98 (s, 3H), 0.83 (s, 3H), 0.68 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.8, 191.5, 146.2, 145.0, 135.1, 134.8, 133.8, 133.0, 129.97, 129.96, 129.5, 128.5, 127.5, 125.9, 125.1, 123.2, 122.3, 118.9, 71.3, 60.9, 60.1, 60.0, 59.4, 39.82, 39.80, 32.5, 19.9, 19.6, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>BrNa [M+Na]<sup>+</sup>: 595.1572, found: 595.1570.

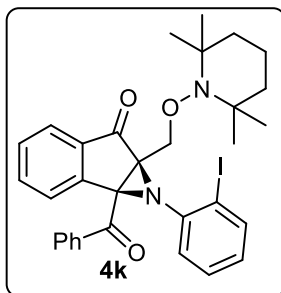
**Spectral data for (1aS,6aR)-1a-benzoyl-1-(2-chlorophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4j):**



Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4j** as a yellow solid (51 mg, 0.096 mmol, 49%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.96 (d, *J* = 7.7 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.32 (t, *J* = 7.7 Hz, 3H), 7.28 (d, *J* = 7.0 Hz, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 7.04 (d, *J* = 7.7 Hz, 1H), 6.89 (t, *J* = 7.7 Hz, 1H), 6.74 – 6.70 (m, 2H), 4.90 (d, *J* = 9.8 Hz, 1H), 4.18 (d, *J* = 10.5 Hz, 1H), 1.40 – 1.31 (m, 4H), 1.28 (s, 3H), 1.26 – 1.18 (m, 2H), 0.88 (s, 3H), 0.85 (s, 3H), 0.45 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 195.0, 191.7, 145.3, 141.3, 135.9, 134.2, 133.3, 133.0, 130.1, 130.0, 129.1, 128.9, 128.1, 128.0, 126.8, 125.2, 124.3, 124.0, 121.9, 71.3, 60.08, 60.02, 59.8, 39.9, 32.6, 32.5, 20.0, 19.3, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>ClNa [M+Na]<sup>+</sup>: 551.2077, found: 551.2077.

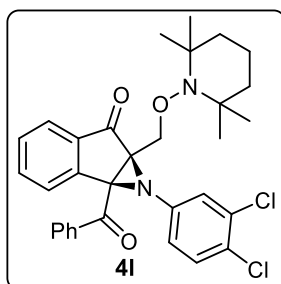
**Spectral data for (1aS,6aR)-1a-benzoyl-1-(2-iodophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4k):**





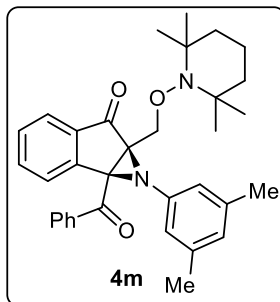
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4k** as a yellow solid (42 mg, 0.067 mmol, 34%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.93 (d, *J* = 7.7 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.31 (t, *J* = 7.7 Hz, 3H), 7.19 (t, *J* = 7.0 Hz, 1H), 6.98 (t, *J* = 7.7 Hz, 1H), 6.66 (d, *J* = 7.7 Hz, 1H), 6.51 (t, *J* = 7.0 Hz, 1H), 5.00 (d, *J* = 9.8 Hz, 1H), 4.18 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.31 (m, 7H), 1.23 – 1.17 (m, 2H), 0.87 (d, *J* = 6.3 Hz, 6H), 0.40 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.2, 192.1, 145.5, 145.0, 140.1, 136.3, 133.9, 133.18, 133.10, 130.2, 130.1, 129.1, 128.2, 128.0, 124.8, 124.2, 122.0, 88.0, 71.6, 60.6, 60.1, 60.0, 40.0, 39.9, 32.7, 32.5, 20.0, 19.2, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>34</sub>N<sub>2</sub>O<sub>3</sub>I [M+H]<sup>+</sup>: 621.1614, found: 621.1613.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(3,4-dichlorophenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4l):**



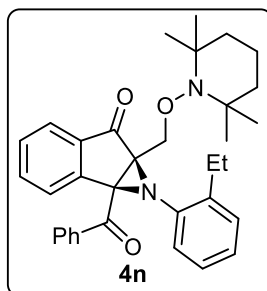
Purified by column chromatography over silica gel with 5% EtOAc/Hexane to afford **4l** as a yellow solid (77.6 mg, 0.137 mmol, 69%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.94 (d, *J* = 7.7 Hz, 2H), 7.54 – 7.51 (m, 2H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 2H), 7.28 – 7.25 (m, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.77 (d, *J* = 8.4 Hz, 1H), 6.55 – 6.54 (m, 1H), 4.52 (d, *J* = 10.5 Hz, 1H), 4.26 (d, *J* = 10.5 Hz, 1H), 1.42 – 1.19 (m, 6H), 1.11 (s, 3H), 0.98 (s, 3H), 0.81 (s, 3H), 0.69 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 194.6, 191.2, 144.8, 144.6, 135.02, 135.01, 133.9, 132.9, 132.4, 130.3, 129.9, 129.8, 128.6, 127.4, 126.4, 125.4, 121.9, 119.6, 71.1, 61.0, 60.15, 60.11, 59.3, 39.81, 39.80, 32.5, 32.4, 20.0, 19.6, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>Cl<sub>2</sub> [M+H]<sup>+</sup>: 563.1868, found: 563.1870.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(3,5-dimethylphenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4m):**



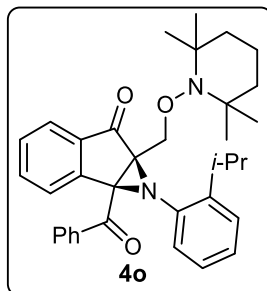
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4m** as a yellow solid (64.8 mg, 0.123, 62%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 8.00 (d, *J* = 7.7 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.36 – 7.33 (m, 3H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 1H), 6.39 (s, 1H), 6.28 (s, 2H), 4.60 (d, *J* = 10.5 Hz, 1H), 4.22 (d, *J* = 10.5 Hz, 1H), 2.04 (s, 6H), 1.42 – 1.32 (m, 4H), 1.27 – 1.19 (m, 2H), 1.16 (s, 3H), 0.96 (s, 3H), 0.85 (s, 3H), 0.65 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.4, 192.3, 145.4, 144.4, 138.1, 135.5, 134.2, 133.5, 133.4, 130.0, 129.0, 128.3, 127.5, 124.7, 124.6, 118.0, 71.6, 60.8, 60.0, 59.5, 39.84, 39.81, 32.55, 32.51, 20.9, 19.9, 19.6, 19.5, 16.9; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>38</sub>N<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 545.2780, found: 545.2787.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(2-ethylphenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4n):**



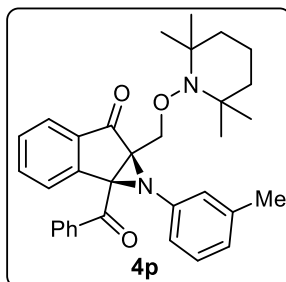
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4n** as a yellow solid (55 mg, 0.105 mmol, 53%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.94 (d, *J* = 7.7 Hz, 2H), 7.49 – 7.46 (m, 2H), 7.33 – 7.29 (m, 3H), 7.19 – 7.15 (m, 2H), 6.92 (d, *J* = 7.7 Hz, 1H), 6.79 – 6.74 (m, 2H), 6.57 (d, *J* = 7.7 Hz, 1H), 4.90 (d, *J* = 10.5 Hz, 1H), 4.14 (d, *J* = 10.5 Hz, 1H), 2.72 – 2.67 (m, 1H), 2.41 – 2.36 (m, 1H), 1.45 – 1.32 (m, 5H), 1.29 (s, 3H), 1.20 – 1.18 (m, 4H), 0.86 (s, 3H), 0.84 (s, 3H), 0.45 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.8, 192.1, 145.5, 141.7, 135.7, 134.8, 134.3, 133.5, 133.3, 130.1, 129.0, 128.2, 128.1, 127.9, 125.6, 124.5, 123.2, 120.5, 71.7, 60.9, 60.00, 60.01, 39.96, 39.90, 32.6, 32.5, 23.4, 20.0, 19.3, 16.8, 13.3; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>39</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 523.2960, found: 523.2962.

**(1aS,6aR)-1a-benzoyl-1-(2-isopropylphenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4o):**



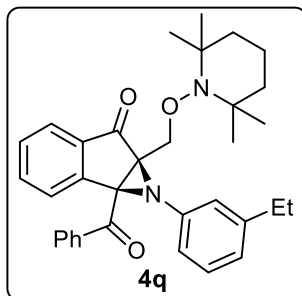
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4o** as a yellow solid (54.7 mg, 0.102 mmol, 51%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 7.96 – 7.94 (m, 2H), 7.49 (d, *J* = 7.2 Hz, 2H), 7.34 – 7.31 (m, 3H), 7.20 – 7.14 (m, 2H), 6.98 – 6.96 (m, 1H), 6.79 (t, *J* = 3.6 Hz, 2H), 6.64 – 6.61 (m, 1H), 4.81 (d, *J* = 10.4 Hz, 1H), 4.21 (d, *J* = 10.4 Hz, 1H), 3.12 – 3.05 (m, 1H), 1.36 (br s, 4H), 1.29 – 1.06 (m, 8H), 1.04 (s, 3H), 0.90 (s, 3H), 0.83 (s, 3H), 0.54 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.9, 191.6, 145.0, 140.7, 139.6, 135.5, 134.1, 133.4, 133.3, 129.9, 128.9, 128.2, 127.7, 125.6, 125.4, 124.4, 123.3, 121.0, 71.6, 61.3, 59.9, 59.5, 39.8, 39.7, 32.4, 32.3, 27.0, 23.6, 22.4, 19.9, 19.4, 16.8; HRMS-ESI+ calcd for C<sub>35</sub>H<sub>41</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 537.3117, found: 537.3125.

**(1a*S*,6a*R*)-1a-benzoyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1-(*m*-tolyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1H)-one (4p):**



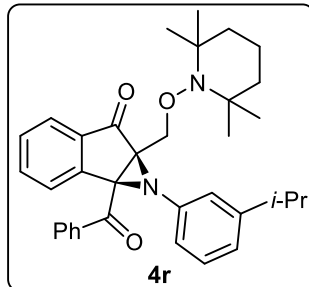
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4p** as a yellow solid (65 mg, 0.127 mmol, 64%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 8.02 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 3H), 7.25 (d, *J* = 2.8 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.86 (t, *J* = 7.7 Hz, 1H), 6.59 (d, *J* = 7.7 Hz, 1H), 6.49 – 6.48 (m, 2H), 4.62 (d, *J* = 10.5 Hz, 1H), 4.25 (d, *J* = 10.5 Hz, 1H), 2.10 (s, 3H), 1.45 – 1.33 (m, 4H), 1.29 – 1.20 (m, 2H), 1.18 (s, 3H), 0.98 (s, 3H), 0.87 (s, 3H), 0.67 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.3, 192.2, 145.4, 144.5, 138.4, 135.5, 134.4, 133.6, 133.4, 130.0, 129.1, 128.43, 128.41, 127.5, 124.8, 123.6, 120.9, 117.2, 71.6, 60.8, 60.07, 60.06, 59.5, 39.85, 39.82, 32.56, 32.51, 21.1, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>37</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 509.2804, found: 509.2810.

**(1a*S*,6a*R*)-1a-benzoyl-1-(3-ethylphenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-*b*]azirin-6(1H)-one (4q):**



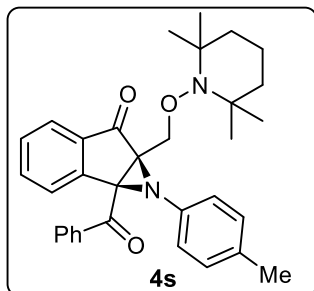
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4q** as a yellow solid (53.3 mg, 0.102 mmol, 51%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 8.01 (d, *J* = 7.0 Hz, 2H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.36 – 7.33 (m, 3H), 7.23 (s, 1H, merged with CDCl<sub>3</sub>), 7.17 (t, *J* = 7.7 Hz, 1H), 7.87 (t, *J* = 7.7 Hz, 1H), 6.59 (d, *J* = 7.7 Hz, 1H), 6.50 (d, *J* = 7.0 Hz, 2H), 4.60 (d, *J* = 10.5 Hz, 1H), 4.24 (d, *J* = 10.5 Hz, 1H), 2.41 – 2.33 (m, 2H), 1.42 – 1.32 (m, 4H), 1.29 – 1.19 (m, 2H), 1.16 (s, 3H), 0.97 (t, *J* = 7.7 Hz, 6H), 0.86 (d, *J* = 3.5 Hz, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.4, 192.3, 145.4, 144.8, 144.5, 135.5, 134.4, 133.6, 133.4, 130.0, 129.0, 128.5, 128.4, 127.5, 124.8, 122.5, 119.8, 117.6, 71.6, 60.9, 60.0, 59.5, 39.84, 39.82, 32.57, 32.51, 28.5, 20.0, 19.6, 16.9, 15.3, 14.1, 14.0; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>38</sub>N<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 545.2780, found: 545.2783.

**(1aS,6aR)-1a-benzoyl-1-(3-isopropylphenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4r):**



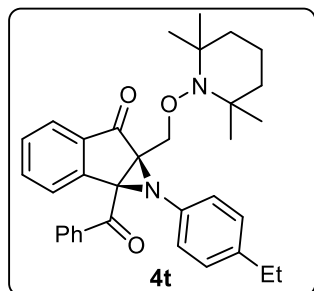
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4r** as a yellow solid (61 mg, 0.113 mmol, 57%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 8.02 (d, *J* = 7.7 Hz, 2H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.43 (d, *J* = 7.0 Hz, 1H), 7.36 – 7.33 (m, 3H), 7.24 (s, 1H, merged with CDCl<sub>3</sub>), 7.16 (t, *J* = 7.7 Hz, 1H), 6.88 (t, *J* = 7.7 Hz, 1H), 6.61 (d, *J* = 7.0 Hz, 1H), 6.51 (d, *J* = 7.0 Hz, 2H), 4.57 (d, *J* = 10.5 Hz, 1H), 4.25 (d, *J* = 10.5 Hz, 1H), 2.64 – 2.60 (m, 1H), 1.43 – 1.31 (m, 4H), 1.28 – 1.18 (m, 2H), 1.15 (s, 3H), 1.02 – 0.98 (m, 9H), 0.87 (s, 3H), 0.69 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.3, 192.3, 149.3, 145.4, 144.5, 135.5, 134.4, 133.6, 133.5, 130.0, 129.0, 128.48, 128.41, 127.5, 124.7, 121.0, 118.4, 117.9, 71.6, 60.9, 60.0, 59.5, 39.8, 33.8, 32.57, 32.50, 23.7, 23.3, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>35</sub>H<sub>41</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 537.3117, found: 537.3118.

**Spectral data for (1aS,6aR)-1a-benzoyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1-(p-tolyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4s):**



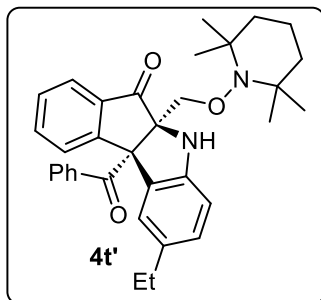
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4s** as a yellow solid (69.1 mg, 0.135 mmol, 68%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 8.00 (d, *J* = 7.7 Hz, 2H), 7.50 – 7.45 (m, 2H), 7.36 – 7.33 (m, 3H), 7.22 (d, *J* = 7.7 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 1H), 6.77 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 8.4 Hz, 2H), 4.61 (d, *J* = 10.5 Hz, 1H), 4.22 (d, *J* = 10.5 Hz, 1H), 2.08 (s, 3H), 1.43 – 1.31 (m, 4H), 1.26 – 1.19 (m, 2H), 1.16 (s, 3H), 0.95 (s, 3H), 0.85 (s, 3H), 0.64 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 195.4, 192.3, 149.4, 145.4, 141.9, 135.5, 134.5, 133.6, 133.5, 132.1, 130.0, 129.2, 129.0, 128.3, 127.5, 124.7, 119.9, 71.6, 61.3, 60.9, 60.07, 60.04, 59.7, 39.84, 39.81, 32.5, 32.4, 20.6, 20.0, 19.6, 16.9; HRMS-ESI+ calcd for C<sub>33</sub>H<sub>37</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 509.2804, found: 509.2802.

**Spectral data for (1aS,6aR)-1a-benzoyl-1-(4-ethylphenyl)-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1a,6a-dihydroindeno[1,2-b]azirin-6(1H)-one (4t):**



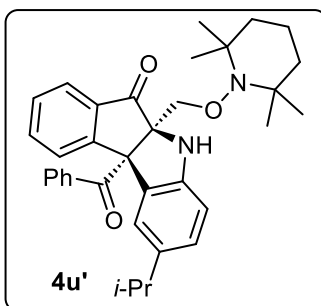
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4t** as a yellow solid (59.5 mg, 0.113 mmol, 57%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 8.02 (d, *J* = 7.6 Hz, 2H), 7.52 – 7.44 (m, 2H), 7.37 – 7.33 (m, 3H), 7.24 – 7.22 (m, 1H, merged with CDCl<sub>3</sub>), 7.18 (t, *J* = 7.7 Hz, 1H), 6.80 (d, *J* = 7.2 Hz, 2H), 6.59 – 6.57 (m, 2H), 4.60 (d, *J* = 10.4 Hz, 1H), 4.24 (d, *J* = 10.4 Hz, 1H), 2.42 – 2.36 (m, 2H), 1.39 – 1.19 (m, 6H), 1.16 (s, 3H), 1.06 – 1.02 (m, 3H), 0.96 (s, 3H), 0.86 (s, 3H), 0.66 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 195.5, 192.3, 145.4, 142.1, 138.5, 135.6, 134.5, 133.6, 133.5, 130.0, 129.0, 128.3, 127.9, 127.5, 124.7, 120.0, 71.6, 60.9, 60.0, 59.6, 39.8, 32.5, 32.4, 27.9, 20.0, 19.6, 16.9, 15.3; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>39</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 523.2960, found: 523.2960.

**Spectral data for (5aR,10bS)-10b-benzoyl-2-ethyl-5a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-5a,10b-dihydroindeno[2,1-b]indol-6(5H)-one (4t')**:



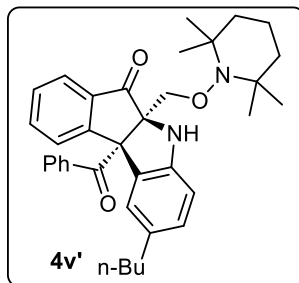
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4t'** as a yellow solid (22 mg, 0.042 mmol, 21%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.87 (d, *J* = 7.7 Hz, 2H), 7.80 – 7.77 (m, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.39 – 7.36 (m, 2H), 7.25 (s, 2H, merged with CDCl<sub>3</sub>), 6.85 (d, *J* = 7.7 Hz, 1H), 6.72 (s, 1H), 6.64 (d, *J* = 8.4 Hz, 1H), 4.93 (s, 1H), 4.24 (d, *J* = 9.8 Hz, 1H), 4.17 (d, *J* = 9.8 Hz, 1H), 2.33 – 2.30 (m, 2H), 1.34 – 1.13 (m, 6H), 0.99 (s, 3H), 0.94 – 0.83 (m, 2H), 0.78 (s, 3H), 0.64 (s, 6H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 207.1, 196.9, 157.8, 145.7, 136.6, 136.4, 135.55, 135.51, 132.5, 132.1, 130.0, 128.5, 127.9, 127.8, 127.3, 124.2, 123.8, 111.1, 78.3, 75.9, 69.3, 60.1, 60.0, 40.04, 40.02, 40.00, 39.9, 32.5, 32.3, 28.0, 19.8, 16.7, 15.7; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>39</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 523.2960, found: 523.2965.

**(5aR,10bS)-10b-benzoyl-2-isopropyl-5a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-5a,10b-dihydroindeno[2,1-b]indol-6(5H)-one (4u')**:



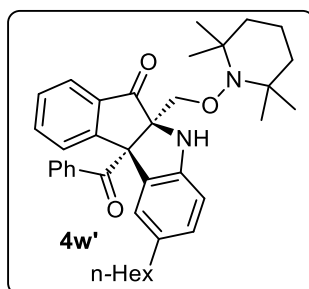
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4u'** as a yellow solid (74 mg, 0.137 mmol, 69%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.83 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 7.7 Hz, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.24 – 7.21 (m, 2H, merged with CDCl<sub>3</sub>), 6.88 (d, *J* = 7.7 Hz, 1H), 6.72 (s, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 4.92 (s, 1H), 4.23 (d, *J* = 9.8 Hz, 1H), 4.17 (d, *J* = 9.8 Hz, 1H), 2.59 – 2.55 (m, 1H), 1.34 – 1.14 (m, 6H), 0.99 (s, 3H), 0.95 – 0.93 (m, 6H), 0.79 (s, 3H), 0.67 (s, 3H), 0.64 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 207.0, 197.4, 157.9, 145.8, 141.2, 136.7, 135.5, 135.4, 132.3, 131.9, 129.9, 127.9, 127.8, 127.2, 126.9, 123.8, 123.0, 111.0, 78.4, 75.8, 69.4, 60.1, 60.0, 40.04, 40.00, 33.3, 32.5, 32.3, 24.1, 23.9, 19.9, 19.8, 16.8; HRMS-ESI+ calcd for C<sub>35</sub>H<sub>41</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 537.3117, found: 537.3113.

**Spectral data for (5aR,10bS)-10b-benzoyl-2-butyl-5a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-5a,10b-dihydroindeno[2,1-b]indol-6(5H)-one (4v')**:



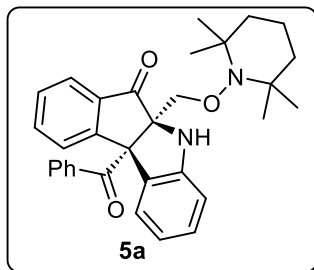
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4v'** as a yellow solid (63.8 mg, 0.116 mmol, 58%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.85 (d, *J* = 7.7 Hz, 2H), 7.78 – 7.77 (m, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.23 (d, *J* = 7.7 Hz, 2H, merged with CDCl<sub>3</sub>), 6.81 (d, *J* = 7.7 Hz, 1H), 6.67 (s, 1H), 6.63 (d, *J* = 8.4 Hz, 1H), 4.93 (s, 1H), 4.24 (d, *J* = 9.8 Hz, 1H), 4.17 (d, *J* = 9.8 Hz, 1H), 2.28 – 2.25 (m, 2H), 1.34 – 1.12 (m, 8H), 1.03 – 0.97 (m, 5H), 0.80 (s, 3H), 0.70 (t, *J* = 7.7 Hz, 3H), 0.67 (s, 3H), 0.64 (s, 3H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 207.1, 197.4, 157.9, 145.7, 136.8, 135.5, 135.4, 134.9, 132.4, 132.0, 129.9, 129.1, 127.86, 127.84, 127.2, 124.8, 123.8, 111.0, 78.4, 75.8, 69.3, 60.2, 60.0, 40.06, 40.01, 35.7, 34.8, 33.6, 32.5, 32.3, 21.7, 19.96, 19.90, 16.8, 13.7; HRMS-ESI+ calcd for C<sub>36</sub>H<sub>43</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 551.3273, found: 551.3271.

**(5aR,10bS)-10b-benzoyl-2-hexyl-5a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-5a,10b-dihydroindeno[2,1-b]indol-6(5H)-one (4w')**:



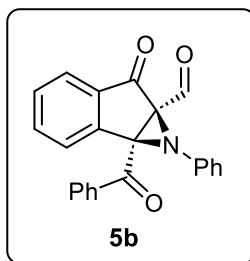
Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **4w'** as a yellow solid (70.5 mg, 0.122 mmol, 61%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.86 – 7.84 (m, 2H), 7.79 – 7.77 (m, 2H), 7.71 – 7.67 (m, 1H), 7.40 – 7.34 (m, 2H), 7.25 – 7.21 (m, 2H, merged with CDCl<sub>3</sub>), 6.82 (d, *J* = 8.0 Hz, 1H), 6.68 – 6.61 (m, 2H), 4.93 (s, 1H), 4.25 (d, *J* = 9.6 Hz, 1H), 4.18 (d, *J* = 9.6 Hz, 1H), 2.28 – 2.24 (m, 2H), 1.29 – 1.23 (m, 5H), 1.14 – 1.06 (m, 6H), 0.99 (br s, 5H), 0.76 (t, *J* = 7.2 Hz, 7H), 0.64 (s, 6H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 207.1, 197.2, 157.9, 145.7, 136.7, 135.5, 135.4, 135.0, 132.4, 132.0, 129.9, 129.1, 127.84, 127.83, 127.2, 124.8, 123.7, 111.0, 78.4, 75.8, 69.3, 60.1, 60.0, 40.06, 40.00, 35.0, 32.5, 32.3, 31.5, 31.3, 29.6, 28.3, 24.8, 22.4, 19.9, 19.8, 16.8, 14.0; HRMS-ESI+ calcd for C<sub>38</sub>H<sub>47</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 579.3586, found: 579.3588.

**Spectral data for (5aR,10bS)-10b-benzoyl-5a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-5a,10b-dihydroindeno[2,1-b]indol-6(5H)-one (5a):**



Purified by column chromatography over silica gel with 5 % EtOAc/Hexane to afford **5a** as a yellow solid (50.5 mg, 0.102 mmol, 51%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.88 (d, *J* = 8.4 Hz, 2H), 6.78 (t, *J* = 6.4 Hz, 2H), 7.71 – 7.67 (m, 1H), 7.40 – 7.35 (m, 2H), 7.26 – 7.22 (m, 2H, merged with CDCl<sub>3</sub>), 7.01 (t, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 6.55 (t, *J* = 7.2 Hz, 1H), 5.04 (s, 1H), 4.27 (d, *J* = 10.0 Hz, 1H), 4.15 (d, *J* = 9.6 Hz, 1H), 1.40 – 1.12 (m, 6H), 0.99 (s, 3H), 0.80 (s, 3H), 0.65 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 206.7, 196.9, 157.8, 147.8, 136.6, 135.6, 135.5, 132.6, 132.0, 129.9, 129.1, 127.9, 127.3, 125.0, 123.8, 120.2, 111.1, 78.1, 75.7, 69.2, 60.2, 40.0, 32.5, 32.3, 19.9, 16.8; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>34</sub>N<sub>2</sub>O<sub>3</sub>Na [M+Na]<sup>+</sup>: 517.2467, found: 517.2442.

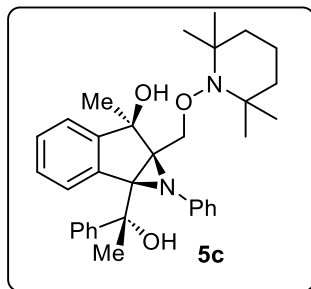
**Spectral data for (1a*S*,6a*R*)-1a-benzoyl-6-oxo-1-phenyl-1a,6-dihydroindeno[1,2-*b*]azirine-6a(1*H*)-carbaldehyde (5b):**



Purified by column chromatography over silica gel with 20 % EtOAc/Hexane to afford **5b** as a yellow liquid (36.7 mg, 0.103 mmol, 52%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 9.63 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H), 7.05 (t, *J* = 7.7 Hz, 2H), 6.87 (t, *J* = 7.7 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 2H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 193.0, 190.9, 190.2, 143.1, 142.9, 135.3, 134.6, 134.4, 133.9, 130.3, 129.5, 129.0, 127.2, 125.3, 124.1, 120.2, 65.0, 61.9; HRFD calcd for C<sub>23</sub>H<sub>15</sub>NO<sub>3</sub> [M]<sup>+</sup>: 353.1057, found: 353.1060.

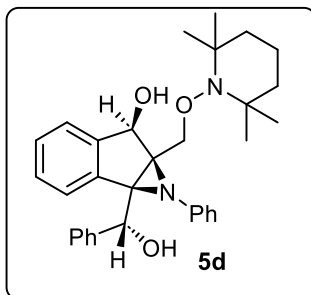
**Spectral data for (1a*S*,6*R*,6a*R*)-1a-((*R*)-1-hydroxy-1-phenylethyl)-6-methyl-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1,1a,6,6a-tetrahydroindeno[1,2-*b*]azirin-6-ol (5c):**





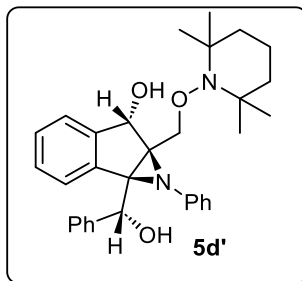
Purified by column chromatography over silica gel with 20 % EtOAc/Hexane to afford **5c** as a yellow sticky solid (45.3 mg, 0.086 mmol, 43%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.93 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.49 (m, 2H), 7.24 – 7.22 (m, 2H, merged with CDCl<sub>3</sub>), 7.20 – 7.18 (m, 2H), 7.11 – 7.09 (m, 1H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.99 – 6.96 (m, 4H), 6.74 – 6.72 (m, 1H), 4.25 (d, *J* = 10.5 Hz, 1H), 4.18 (d, *J* = 10.5 Hz, 1H), 3.83 (s, 1H), 2.77 (s, 1H), 2.18 (s, 3H), 1.52 – 1.28 (m, 6H), 1.26 (s, 9H), 1.17 – 1.15 (m, 6H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 146.7, 145.0, 144.5, 136.5, 128.5, 127.8, 127.7, 127.5, 127.2, 127.1, 125.4, 123.3, 121.7, 121.6, 80.9, 76.7, 72.7, 62.1, 60.4, 59.8, 55.1, 40.0, 39.9, 33.3, 32.1, 32.0, 31.7, 20.4, 20.3, 16.9; HRMS-ESI+ calcd for C<sub>34</sub>H<sub>43</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 527.3273, found: 527.3273.

**Spectral data for (1aS,6R,6aR)-1a-((R)-hydroxy(phenyl)methyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1,1a,6,6a-tetrahydroindeno[1,2-b]azirin-6-ol (5d):**



Purified by column chromatography over silica gel with 20 % EtOAc/Hexane to afford **5d** as a yellow solid (55.8 mg, 0.112 mmol, 56%). <sup>1</sup>H NMR (700 MHz, CDCl<sub>3</sub>): 7.66 (d, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 1H), 7.10 – 7.04 (m, 3H), 6.91 (t, *J* = 7.7 Hz, 3H), 6.72 (t, *J* = 7.0 Hz, 1H), 6.66 (d, *J* = 7.7 Hz, 2H), 5.52 (d, *J* = 9.8 Hz, 1H), 5.31 (s, 1H), 4.86 (d, *J* = 9.8 Hz, 1H), 4.32 (d, *J* = 9.8 Hz, 1H), 3.33 (s, 1H), 2.02 (d, *J* = 9.8 Hz, 1H), 1.54 – 1.46 (m, 6H), 1.41 (s, 3H), 1.35 – 1.23 (m, 3H), 1.17 – 1.16 (m, 6H); <sup>13</sup>C NMR (175 MHz, CDCl<sub>3</sub>): δ 145.1, 142.3, 140.5, 136.3, 128.5, 128.42, 128.40, 127.8, 127.6, 126.6, 126.0, 124.7, 121.9, 120.9, 77.3, 76.4, 71.7, 60.5, 60.1, 59.1, 50.1, 40.1, 40.0, 33.2, 32.9, 20.6, 20.3, 16.9; HRMS-ESI+ calcd for C<sub>32</sub>H<sub>39</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 499.2960, found: 499.2963.

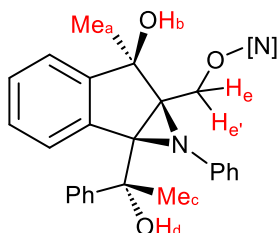
**Spectral data for (1aS,6S,6aR)-1a-((R)-hydroxy(phenyl)methyl)-1-phenyl-6a-(((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-1,1a,6,6a-tetrahydroindeno[1,2-b]azirin-6-ol (5d'):**



Purified by column chromatography over silica gel with 20 % EtOAc/Hexane to afford **5d'** as a yellow solid (22.9 mg, 0.046 mmol, 23%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ): 7.54 (d,  $J = 7.6$  Hz, 2H), 7.40 – 7.38 (m, 1H), 7.29 – 7.24 (m, 2H), 7.19 – 7.16 (m, 1H), 7.06 – 7.03 (m, 1H), 7.01 – 6.99 (m, 2H), 6.98 – 6.95 (m, 2H), 6.90 – 6.88 (m, 2H), 6.75 – 6.71 (m, 1H), 5.52 (d,  $J = 9.2$  Hz, 1H), 5.10 (d,  $J = 3.2$  Hz, 1H), 4.70 (d,  $J = 10.0$  Hz, 1H), 4.41 (d,  $J = 10.0$  Hz, 1H), 2.83 (d,  $J = 3.2$  Hz, 1H), 2.14 (d,  $J = 9.2$  Hz, 1H), 1.55 – 1.46 (m, 6H), 1.41 (s, 3H), 1.24 (s, 6H), 1.14 (s, 3H);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.7, 141.3, 139.8, 136.4, 128.5, 128.2, 128.1, 127.8, 127.4, 127.2, 126.1, 124.3, 121.8, 120.9, 77.4, 76.7, 73.8, 60.4, 60.2, 59.6, 52.6, 39.9, 33.2, 32.8, 20.5, 20.4, 17.0; HRMS-ESI+ calcd for  $\text{C}_{32}\text{H}_{39}\text{N}_2\text{O}_3$   $[\text{M}+\text{H}]^+$ : 499.2960, found: 499.2968.

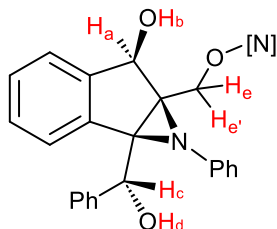
## (7) $^1\text{H}$ -NOE data for compounds **5c**, **5d** and **5d'**:

### 7.1. $^1\text{H}$ -NOE data for compounds **5c**:



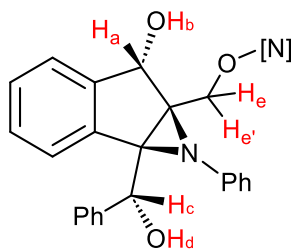
No.	Irradiate	Intensity Enhancement
1.	$\text{Me}_a$ ( $\delta$ : 1.26)	$\text{H}_b$ ( $\delta$ : 2.77, 1.53 %), $\text{H}_e$ ( $\delta$ : 4.18, 2.37 %)
2.	$\text{Me}_c$ ( $\delta$ : 2.18)	$\text{H}_d$ ( $\delta$ : 3.83, 1.15 %)
3.	$\text{H}_e$ ( $\delta$ : 4.18)	$\text{Me}_a$ ( $\delta$ : 1.26, 8.24 %), $\text{H}_b$ ( $\delta$ : 2.77, 0.38 %), $\text{H}_{e'}$ ( $\delta$ : 4.25, 9.98 %)
4.	$\text{H}_{e'}$ ( $\delta$ : 4.25)	$\text{Me}_a$ ( $\delta$ : 1.26, 3.78 %), $\text{Me}_c$ ( $\delta$ : 2.18, 0.27 %), $\text{H}_b$ ( $\delta$ : 2.77, 0.16 %), $\text{H}_d$ ( $\delta$ : 3.83, 4.82 %), $\text{H}_e$ ( $\delta$ : 4.18, 8.74 %)

### 7.2. $^1\text{H}$ -NOE data for compound **5d**:



No.	Irradiate	Intensity Enhancement
1.	H <sub>a</sub> (δ: 5.31)	H <sub>b</sub> (δ: 3.33, 3.42 %), H <sub>e</sub> (δ: 4.31, 2.95 %)
2.	H <sub>c</sub> (δ: 5.52)	H <sub>d</sub> (δ: 2.02, 1.80 %), H <sub>b</sub> (δ: 3.33, 0.37 %), H <sub>e</sub> (δ: 4.31, 0.72 %), H <sub>e'</sub> (δ: 4.86, 0.71 %)

### 7.3. <sup>1</sup>H-NOE data for compound 5d':



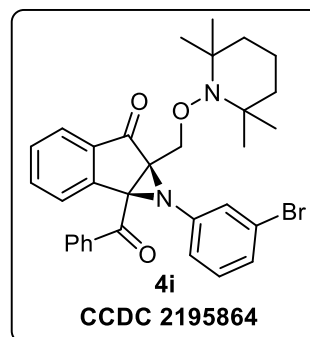
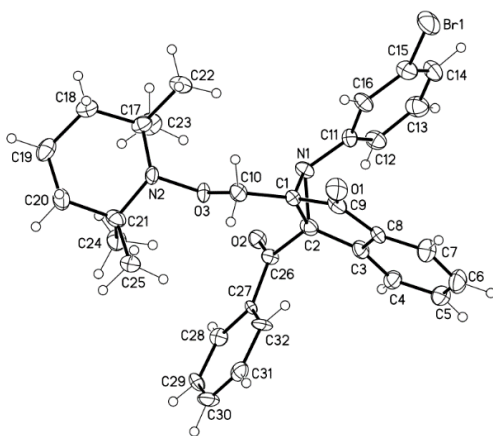
No.	Irradiate	Intensity Enhancement
1.	H <sub>a</sub> (δ: 5.10)	H <sub>b</sub> (δ: 2.83, 2.18 %), H <sub>e</sub> (δ: 4.41, 2.15 %), H <sub>e'</sub> (δ: 4.70, 1.50 %)
2.	H <sub>c</sub> (δ: 5.52)	H <sub>d</sub> (δ: 2.14, 1.53 %), H <sub>e</sub> (δ: 4.41, 1.18 %), H <sub>e'</sub> (δ: 4.70, 0.67 %)

## (8) X-ray Crystallographic Structure and data for compound 4i, 4v', 5a and 5d:

### 8.1. X-ray Crystallographic data for compound 4i:

Ellipsoid contour % probability level = 50%

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



**Table 1 Crystal data and structure refinement for 220159lt2\_auto.**

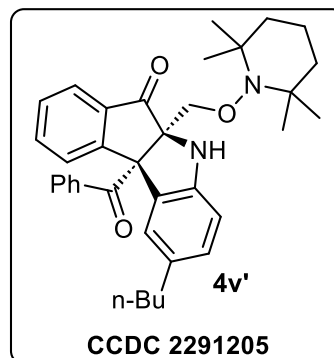
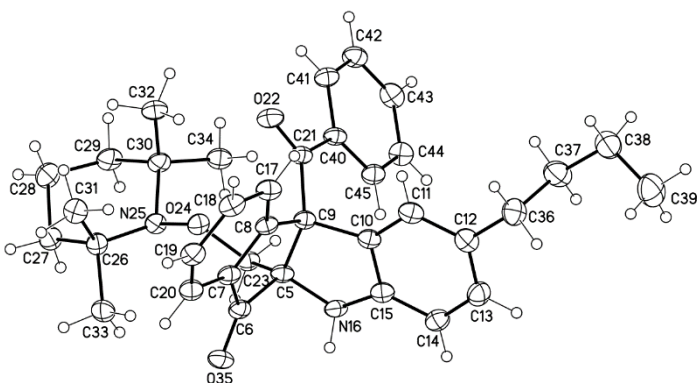
Identification code	220159lt2_auto
Empirical formula	C <sub>64</sub> H <sub>66</sub> Br <sub>2</sub> N <sub>4</sub> O <sub>6</sub>
Formula weight	1147.02

Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	Pna2 <sub>1</sub>
a/Å	15.7300(5)
b/Å	9.1404(3)
c/Å	38.2854(13)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	5504.6(3)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.384
μ/mm <sup>-1</sup>	2.319
F(000)	2384.0
Crystal size/mm <sup>3</sup>	0.08 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	9.24 to 147.518
Index ranges	-17 ≤ h ≤ 19, -11 ≤ k ≤ 11, -47 ≤ l ≤ 42
Reflections collected	74707
Independent reflections	10377 [R <sub>int</sub> = 0.0414, R <sub>sigma</sub> = 0.0249]
Data/restraints/parameters	10377/1/694
Goodness-of-fit on F <sup>2</sup>	1.075
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0664, wR <sub>2</sub> = 0.1877
Final R indexes [all data]	R <sub>1</sub> = 0.0692, wR <sub>2</sub> = 0.1915
Largest diff. peak/hole / e Å <sup>-3</sup>	3.23/-1.06
Flack parameter	0.49(3)

## 8.2. X-ray Crystallographic data for compound 4v':

Ellipsoid contour % probability level = 50%

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



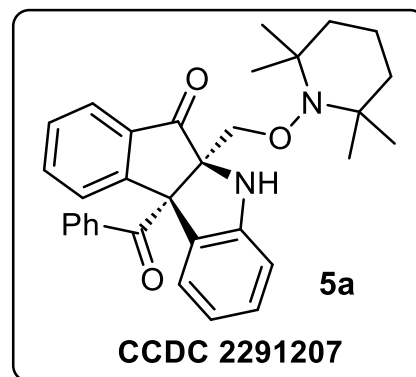
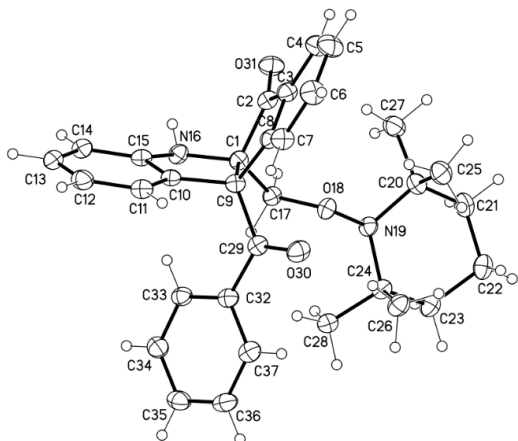
**Table 1 Crystal data and structure refinement for 230124lt\_auto.**

Identification code	230124lt_auto
Empirical formula	C <sub>73</sub> H <sub>85</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>6</sub>
Formula weight	1220.80
Temperature/K	99.99(13)
Crystal system	triclinic
Space group	P-1
a/Å	9.90351(17)
b/Å	16.0833(4)
c/Å	20.5773(4)
α/°	90.8407(16)
β/°	91.3829(14)
γ/°	96.7789(16)
Volume/Å <sup>3</sup>	3253.20(11)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.246
μ/mm <sup>-1</sup>	1.712
F(000)	1300.0
Crystal size/mm <sup>3</sup>	0.07 × 0.03 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	4.296 to 134.16
Index ranges	-11 ≤ h ≤ 11, -19 ≤ k ≤ 19, -23 ≤ l ≤ 24
Reflections collected	47523
Independent reflections	11580 [R <sub>int</sub> = 0.0415, R <sub>sigma</sub> = 0.0339]
Data/restraints/parameters	11580/0/786
Goodness-of-fit on F <sup>2</sup>	1.070
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0635, wR <sub>2</sub> = 0.1931
Final R indexes [all data]	R <sub>1</sub> = 0.0736, wR <sub>2</sub> = 0.1992
Largest diff. peak/hole / e Å <sup>-3</sup>	0.64/-0.57

### 8.3. X-ray Crystallographic data for compound 5a:

Ellipsoid contour % probability level = 50%

**Sample Preparation for Crystal Growth:** The compound **5a** was dissolved in acetonitrile and kept for slow evaporation (3 days).



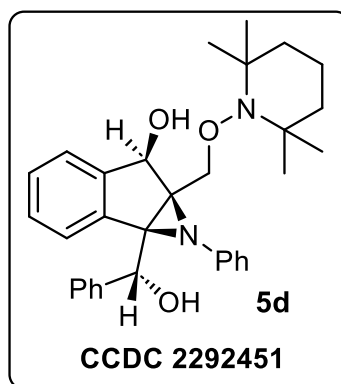
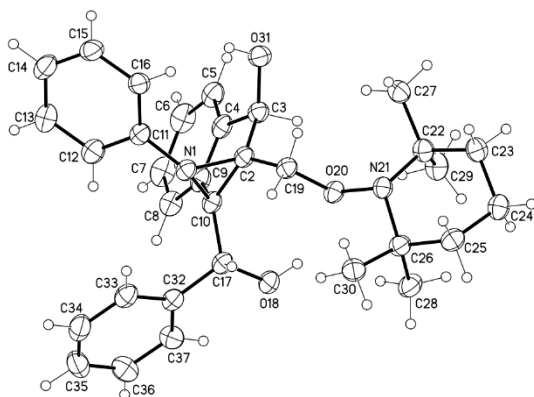
**Table 1 Crystal data and structure refinement for 220727lt\_auto.**

Identification code	220727lt_auto
Empirical formula	C <sub>32</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>
Formula weight	494.61
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	13.4809(2)
b/Å	11.70672(17)
c/Å	17.9878(3)
α/°	90
β/°	110.0432(18)
γ/°	90
Volume/Å <sup>3</sup>	2666.85(8)
Z	4
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.232
μ/mm <sup>-1</sup>	0.624
F(000)	1056.0
Crystal size/mm <sup>3</sup>	0.13 × 0.11 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	7.146 to 134.15
Index ranges	-16 ≤ h ≤ 15, -12 ≤ k ≤ 13, -21 ≤ l ≤ 20
Reflections collected	16106
Independent reflections	4741 [R <sub>int</sub> = 0.0238, R <sub>sigma</sub> = 0.0255]
Data/restraints/parameters	4741/0/339
Goodness-of-fit on F <sup>2</sup>	1.043
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0350, wR <sub>2</sub> = 0.0859
Final R indexes [all data]	R <sub>1</sub> = 0.0412, wR <sub>2</sub> = 0.0893
Largest diff. peak/hole / e Å <sup>-3</sup>	0.27/-0.29

#### 8.4. X-ray Crystallographic data for compound 5d:

Ellipsoid contour % probability level = 50%

**Sample Preparation for Crystal Growth:** The compound **5d** was dissolved in acetonitrile and kept for slow evaporation (3 days).



**Table 1 Crystal data and structure refinement for 230250lt2\_auto.**

Identification code	230250lt2_auto
Empirical formula	C <sub>128</sub> H <sub>152</sub> N <sub>8</sub> O <sub>12</sub>
Formula weight	1994.57
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	32.8040(3)
b/Å	22.73827(19)
c/Å	31.1712(2)
$\alpha$ /°	90
$\beta$ /°	109.6377(10)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	21898.5(3)
Z	8
$\rho_{\text{calc}}$ /cm <sup>3</sup>	1.210
$\mu$ /mm <sup>-1</sup>	0.608
F(000)	8576.0
Crystal size/mm <sup>3</sup>	0.09 × 0.07 × 0.06
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
2 $\theta$ range for data collection/°	4.826 to 134.156
Index ranges	-39 ≤ h ≤ 39, -27 ≤ k ≤ 26, -37 ≤ l ≤ 29
Reflections collected	106756
Independent reflections	19532 [R <sub>int</sub> = 0.0478, R <sub>sigma</sub> = 0.0333]
Data/restraints/parameters	19532/0/1354

Goodness-of-fit on  $F^2$  1.043  
 Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0469$ ,  $wR_2 = 0.1243$   
 Final R indexes [all data]  $R_1 = 0.0582$ ,  $wR_2 = 0.1308$   
 Largest diff. peak/hole /  $e \text{ \AA}^{-3}$  0.41/-0.23

## (9) Computational Details

DFT computations were conducted utilizing the Jaguar software package. For geometry optimization and vibrational frequency calculations, B3LYP-D3 functional with 6-31G\*\* basis set were employed. To attain more accurate electronic energies, single-point energy calculations were performed with same functional but improved 6-311++G\*\* basis set. Examination of open-shell singlet states was carried out using the broken-symmetry methodology [ref. J. Am. Chem. Soc., 1984, 106, 8, 2316; (b) Coord. Chem. Rev. 1995, 144, 199.] To account for solvent effects, the implicitly Poisson-Boltzmann self-consistent polarizable continuum method was applied. This approach was employed to simulate the influence of 1,2-dichloroethane (with a dielectric constant of 10.65 and an effective radius of 2.51 Å). All energy values presented were in the form of enthalpy, having been converted from electronic energies using the equation provided below:

$$H = E_{\text{elec}} + G_{\text{solv}} + \text{ZPE} + 4RT + H_{\text{vib}}.$$

Where  $E_{\text{elec}}$ ,  $G_{\text{solv}}$ , ZPE, and  $H_{\text{vib}}$  are the electronic energy, solvation free energy, zero-point energy correction, and vibrational enthalpy, respectively; And T was the temperature of the standard state which is 298.15K.

Species	$E_{\text{elec}}$	$G_{\text{solv}}$	ZPE+4RT+ $H_{\text{vib}}$	$\langle S^2 \rangle$	$H_{\text{total}}$
1a <sup>CS</sup>	-655.11492	-0.00891	0.24442	0.00	-654.87941
PhNO (2a)	-361.64601	-0.00725	0.10471	0.00	-361.54854
TS <sub>1</sub> <sup>OS</sup>	-1016.74561	-0.01221	0.34948	0.56	-1016.40834
A <sup>OS</sup>	-1016.78376	-0.01383	0.35229	1.03	-1016.44530
TEMPO	-483.88794	-0.00696	0.27615	0.75	-483.61875



TS <sub>2</sub> <sup>D</sup>	-1500.67684	-0.01320	0.62997	1.37	-1500.06007
B <sup>D</sup>	-1500.72375	-0.01229	0.63413	0.76	-1500.10190
O <sub>2</sub>	-150.37031	0.00000	0.00709	2.01	-150.36322
TS <sub>3</sub> <sup>D</sup>	-1651.07722	-0.01640	0.64088	1.05	-1650.45275
C <sup>D</sup>	-1651.09075	-0.01732	0.64436	0.75	-1650.46371
TS <sub>4</sub> <sup>D</sup>	-1651.06156	-0.01404	0.64248	0.75	-1650.43313
D <sup>D</sup>	-1651.11947	-0.01295	0.64576	0.75	-1650.48666
TS <sub>5</sub> <sup>OS</sup>	-3302.22940	-0.01818	1.28584	0.59	-3300.96174
E <sup>CS</sup>	-1651.76015	-0.01551	0.65800	0.00	-1651.11766
F <sup>CS</sup>	-1650.50544	-0.01801	0.63365	0.00	-1649.88980
TS <sub>6</sub> <sup>OS</sup>	-1651.72305	-0.03454	0.65338	0.01	-1651.10422
G <sup>D</sup>	-1576.010462	-0.01553	0.63917	0.77	-1575.38682
OH •	-75.7623994	-0.00790	0.01171	0.75	-75.75858
TS <sub>7</sub> <sup>D</sup>	-3226.508791	-0.02521	1.26983	0.78	-3225.26417
H <sup>CS</sup>	-1575.403513	-0.01436	0.62905	0.00	-1574.78882
TS <sub>8</sub> <sup>OS</sup>	-1575.364255	-0.01391	0.62508	0.96	-1574.75308
I <sup>OS</sup>	-1575.412242	-0.01759	0.62668	1.03	-1574.80315
TS <sub>9</sub> <sup>OS</sup>	-1575.411122	-0.01765	0.62590	0.85	-1574.80287
3a <sup>CS</sup>	-1575.437914	-0.01641	0.62872	0.00	-1574.82560

### Coordinates of optimized structures

#### 1a<sup>CS</sup>

C	-2.093040	-1.066930	-0.308510
C	-0.682880	-1.063370	-0.312370
C	0.011170	0.171980	-0.423090
C	-0.738690	1.354420	-0.525590
C	-2.128460	1.334000	-0.520310
C	-2.810800	0.116900	-0.411170
H	-2.608770	-2.017790	-0.223230
H	-0.209040	2.298530	-0.609830
H	-2.682400	2.264630	-0.600960
H	-3.896470	0.093990	-0.406370
C	1.483570	0.191790	-0.427040
H	1.977330	-0.775020	-0.342760
C	2.231850	1.269150	-0.521920
C	2.971800	2.340470	-0.615240

H	3.297840	2.886890	0.268300
H	3.296940	2.726760	-1.579860
C	0.004640	-2.305580	-0.203290
C	0.555990	-3.384930	-0.106540
C	1.186770	-4.656370	0.009970
C	0.411950	-5.825250	0.152260
C	2.591180	-4.769810	-0.013320
C	1.027650	-7.067890	0.267890
H	-0.670160	-5.742670	0.170820
C	3.197840	-6.017150	0.103110
H	3.193250	-3.873270	-0.122880
C	2.420760	-7.169490	0.244030
H	0.418900	-7.960930	0.377340
H	4.281380	-6.091390	0.084000
H	2.897950	-8.141020	0.334800

**PhNO (2a)**

N	3.109760	0.997260	0.484370
C	4.484950	0.743850	0.133880
C	5.542720	0.795780	1.052920
C	4.709540	0.433180	-1.210880
C	6.832600	0.532760	0.611770
H	5.321060	1.040550	2.086290
C	6.006990	0.170940	-1.647150
H	3.859820	0.404200	-1.886490
C	7.064330	0.220890	-0.735920
H	7.665030	0.567060	1.308500
H	6.195860	-0.071740	-2.688390
H	8.076600	0.015960	-1.073240
O	2.920910	1.274690	1.659660

**TS<sub>1</sub><sup>os</sup>**

C	-0.804620	-0.862080	-1.869880
C	0.069120	-0.927060	-0.770240
C	0.391120	0.271930	-0.054270
C	-0.150060	1.492740	-0.524820
C	-0.996340	1.534800	-1.622630
C	-1.336190	0.351670	-2.294810
H	-1.043000	-1.779490	-2.397910
H	0.105920	2.404820	0.004490
H	-1.399220	2.486030	-1.957430

H	-2.003070	0.379830	-3.151030
C	1.248880	0.241520	1.096160
H	1.589400	-0.731320	1.442620
C	1.845280	1.366440	1.634840
C	1.840830	2.243000	2.615340
H	1.048470	2.232990	3.358230
H	2.639240	2.974720	2.707550
C	0.666040	-2.167720	-0.421390
C	1.222370	-3.215270	-0.155840
C	1.895980	-4.429760	0.159270
C	1.234040	-5.668850	0.055870
C	3.241380	-4.404000	0.578600
C	1.901990	-6.849230	0.369180
H	0.197700	-5.690410	-0.266280
C	3.899900	-5.590410	0.888550
H	3.755190	-3.450390	0.644780
C	3.234550	-6.814880	0.786920
H	1.381260	-7.799150	0.288710
H	4.937030	-5.560910	1.210520
H	3.752030	-7.738090	1.031530
N	3.418470	1.820080	0.565320
C	3.913290	0.679930	-0.182470
C	4.999390	-0.063560	0.287310
C	3.273810	0.340810	-1.376720
C	5.423300	-1.179370	-0.430110
H	5.480730	0.240790	1.210720
C	3.706360	-0.775910	-2.088920
H	2.443750	0.943010	-1.727940
C	4.772200	-1.543090	-1.613580
H	6.259160	-1.770480	-0.065920
H	3.203320	-1.052960	-3.010140
H	5.096120	-2.422220	-2.162970
O	4.270080	2.424120	1.238990

A<sup>os</sup>

C	-1.914970	-0.789390	-1.261320
C	-0.629590	-0.787010	-0.699720
C	0.006750	0.468000	-0.366970
C	-0.683530	1.658860	-0.712810
C	-1.948470	1.627430	-1.278250

C	-2.579300	0.402080	-1.537320
H	-2.380380	-1.742260	-1.490550
H	-0.193850	2.611870	-0.561310
H	-2.446910	2.558750	-1.529980
H	-3.573330	0.378860	-1.973210
C	1.291310	0.428770	0.244870
H	1.720790	-0.561130	0.328770
C	2.099920	1.477910	0.779510
C	1.725920	2.715800	1.202380
H	0.687950	3.012880	1.210920
H	2.460590	3.379030	1.638830
C	0.063300	-2.007760	-0.493260
C	0.751290	-2.996570	-0.324620
C	1.622590	-4.101470	-0.113770
C	1.147940	-5.427280	-0.144750
C	2.991830	-3.867210	0.131230
C	2.023210	-6.488660	0.067430
H	0.094610	-5.609760	-0.332340
C	3.857380	-4.935860	0.339510
H	3.366620	-2.849970	0.150060
C	3.378230	-6.248270	0.310000
H	1.647900	-7.507740	0.044200
H	4.909640	-4.739760	0.524260
H	4.056710	-7.080380	0.474980
N	3.484870	1.103680	1.027500
C	4.197180	0.152460	0.243780
C	5.241620	-0.553630	0.861000
C	3.906980	-0.067790	-1.112170
C	5.967030	-1.490300	0.132110
H	5.459600	-0.350860	1.902370
C	4.639920	-1.013260	-1.826940
H	3.123470	0.498130	-1.601990
C	5.667610	-1.731550	-1.212280
H	6.767800	-2.039830	0.618850
H	4.407330	-1.183510	-2.873680
H	6.230670	-2.469850	-1.774990
O	4.088630	1.643550	2.022040

**TEMPO**

C	-2.797930	-1.634580	-0.197690
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C	-1.269190	-1.679690	-0.242040
C	-0.725120	-0.251310	-0.172550
C	-1.148820	0.505490	1.101790
C	-3.355600	-0.967600	1.075230
H	0.369640	-0.240410	-0.225120
H	-0.874480	-2.286680	0.581340
H	-0.935810	-2.162720	-1.167440
H	-3.155680	-1.077000	-1.073330
H	-3.226970	-2.640660	-0.269250
H	-1.088250	0.302670	-1.048220
N	-2.614600	0.306800	1.359080
O	-3.120230	1.047480	2.279510
C	-3.239750	-1.895660	2.302310
H	-3.510120	-1.336800	3.201640
H	-3.921420	-2.745750	2.195680
H	-2.228620	-2.289610	2.430130
C	-4.830070	-0.592060	0.860190
H	-5.406200	-1.490880	0.618170
H	-5.242530	-0.132070	1.759020
H	-4.929190	0.118620	0.033970
C	-0.356240	0.029600	2.337010
H	0.690850	0.337990	2.252160
H	-0.785660	0.481550	3.234500
H	-0.378530	-1.056870	2.451090
C	-0.926930	2.013540	0.906770
H	-1.207060	2.561400	1.807240
H	0.127550	2.203340	0.682230
H	-1.532920	2.386560	0.075390
C	-2.797930	-1.634580	-0.197690
C	-1.269190	-1.679690	-0.242040
C	-0.725120	-0.251310	-0.172550
C	-1.148820	0.505490	1.101790
C	-3.355600	-0.967600	1.075230
H	0.369640	-0.240410	-0.225120
H	-0.874480	-2.286680	0.581340
H	-0.935810	-2.162720	-1.167440
H	-3.155680	-1.077000	-1.073330
H	-3.226970	-2.640660	-0.269250
H	-1.088250	0.302670	-1.048220
N	-2.614600	0.306800	1.359080

O	-3.120230	1.047480	2.279510
<b>TS<sub>2</sub><sup>D</sup></b>			
C	-3.278190	2.715990	2.396070
C	-2.992740	1.395560	2.067310
C	-1.828320	1.053670	1.351480
C	-0.912470	2.084200	0.974030
C	-1.251620	3.414810	1.286980
C	-2.406370	3.733740	1.993780
H	-4.182180	2.953630	2.948430
H	-3.677360	0.600620	2.345640
H	-0.572590	4.205690	0.978660
H	-2.626350	4.770430	2.231250
C	0.320210	1.849620	0.222620
H	0.535060	2.570440	-0.562190
C	1.256780	0.858810	0.434540
C	1.350810	-0.013100	1.532000
H	0.597400	-0.002120	2.301590
H	2.024710	-0.853610	1.484780
C	-1.616120	-0.297780	0.964610
C	-1.352440	-1.430600	0.615220
C	-0.930530	-2.727610	0.208460
C	0.308960	-2.879990	-0.448590
C	-1.716860	-3.865490	0.470680
C	0.741730	-4.148430	-0.824710
H	0.925970	-2.008410	-0.647890
C	-1.272490	-5.127660	0.086640
H	-2.669410	-3.746400	0.977610
C	-0.043590	-5.273960	-0.561610
H	1.699270	-4.256670	-1.326570
H	-1.885700	-6.000140	0.294080
H	0.300660	-6.260730	-0.858920
N	2.350560	0.753200	-0.498480
O	2.668070	-0.424630	-0.911410
C	3.194530	1.842470	-0.831160
C	3.263180	2.992500	-0.028050
C	4.014900	1.718110	-1.962120
C	4.138150	4.016950	-0.381000
H	2.675960	3.051100	0.879110
C	4.882880	2.751160	-2.297930

H	3.957040	0.808270	-2.546930
C	4.946790	3.907300	-1.515170
H	4.199390	4.901150	0.247170
H	5.513750	2.653260	-3.176890
H	5.627470	4.710650	-1.780990

**B<sup>D</sup>**

C	-3.781410	2.555790	1.883100
C	-3.420110	1.258700	1.539310
C	-2.157040	0.984850	0.976500
C	-1.241570	2.054180	0.773580
C	-1.643240	3.356880	1.100480
C	-2.893050	3.611440	1.658810
H	-4.759110	2.747360	2.315380
H	-4.111070	0.435640	1.689570
H	-0.952260	4.176850	0.922530
H	-3.174910	4.628170	1.916020
C	0.092500	1.855910	0.174920
H	0.340860	2.510920	-0.658570
C	1.029630	0.978950	0.556950
C	1.008490	0.044400	1.733020
H	0.120390	0.213320	2.345430
H	1.003380	-0.996290	1.402000
C	-1.829380	-0.341800	0.584420
C	-1.489230	-1.456220	0.243950
C	-1.002780	-2.736530	-0.142300
C	0.284130	-2.846600	-0.708720
C	-1.775520	-3.896750	0.052820
C	0.781060	-4.098580	-1.059680
H	0.880890	-1.952610	-0.861760
C	-1.267880	-5.141850	-0.306930
H	-2.765750	-3.808160	0.488780
C	0.010530	-5.247290	-0.861380
H	1.775620	-4.175640	-1.489510
H	-1.869360	-6.033220	-0.152500
H	0.404260	-6.221510	-1.137350
N	2.254210	0.908260	-0.205470
O	2.445210	-0.177960	-0.868150
C	3.271210	1.878340	-0.109790
C	3.173720	2.941780	0.803510

C	4.401750	1.750420	-0.932180
C	4.204560	3.872960	0.877570
H	2.315800	3.013270	1.459680
C	5.420050	2.692850	-0.843810
H	4.455440	0.912020	-1.615460
C	5.329150	3.759010	0.056150
H	4.131370	4.689280	1.590350
H	6.293540	2.593450	-1.481940
H	6.129230	4.490270	0.120520
C	2.701240	-1.012060	5.874110
C	4.017770	-1.750030	5.618910
C	3.977490	-2.398920	4.233150
C	3.690890	-1.395420	3.092440
C	2.376760	0.038430	4.788670
H	4.921450	-2.909600	4.009460
H	4.866450	-1.060320	5.696330
H	4.174860	-2.514990	6.388400
H	1.884540	-1.745040	5.900610
H	2.711930	-0.507840	6.847800
H	3.189440	-3.162950	4.224440
N	2.447360	-0.657180	3.470310
O	2.206920	0.340190	2.454800

**O<sub>2</sub>**

O	0.000000	0.000000	0.607080
O	0.000000	0.000000	-0.607080

**TS<sub>3</sub><sup>D</sup>**

C	-2.563070	2.365490	3.248440
C	-2.506170	1.236040	2.436030
C	-1.384460	0.987570	1.628620
C	-0.293070	1.904260	1.651030
C	-0.390680	3.050640	2.448850
C	-1.506220	3.277330	3.253140
H	-3.436500	2.538490	3.869950
H	-3.332370	0.532990	2.411860
H	0.430910	3.761140	2.448570
H	-1.551640	4.164450	3.877360
C	0.895770	1.713580	0.803540
H	1.407920	2.630280	0.532260
C	1.682310	0.513350	0.884760



C	1.565940	-0.455250	2.030790
H	0.530720	-0.614280	2.322020
H	2.015610	-1.413270	1.772090
C	-1.335640	-0.145940	0.771640
C	-1.154330	-1.063570	-0.002410
C	-0.856350	-2.089280	-0.941210
C	0.488240	-2.390000	-1.248000
C	-1.885090	-2.793410	-1.594830
C	0.783190	-3.365990	-2.195530
H	1.294890	-1.872100	-0.738810
C	-1.576530	-3.767850	-2.539690
H	-2.918690	-2.560520	-1.359040
C	-0.244200	-4.055050	-2.845480
H	1.821240	-3.589920	-2.423350
H	-2.377990	-4.302720	-3.041270
H	-0.007720	-4.814340	-3.585340
N	2.678380	0.288270	0.013130
O	3.389780	-0.774830	-0.002280
C	2.989580	1.226480	-1.052600
C	3.696040	2.387670	-0.758600
C	2.599130	0.907150	-2.349650
C	4.001030	3.268430	-1.797670
H	3.995870	2.592960	0.264500
C	2.906140	1.794920	-3.377130
H	2.042190	-0.005660	-2.531660
C	3.602590	2.974960	-3.102320
H	4.547840	4.182110	-1.585650
H	2.591820	1.571140	-4.391880
H	3.832390	3.667100	-3.906970
C	1.867110	-0.937850	6.597020
C	3.344970	-1.186930	6.906790
C	4.018370	-1.816820	5.685560
C	3.871880	-0.968860	4.402810
C	1.646320	-0.054730	5.348540
H	5.087010	-1.984040	5.864300
H	3.843700	-0.249970	7.181590
H	3.441040	-1.850180	7.774350
H	1.374740	-1.904080	6.426550
H	1.358690	-0.464320	7.445230
H	3.566600	-2.800190	5.502110

N	2.415970	-0.676260	4.229600
O	2.294950	0.194830	3.084890
C	1.995570	1.423730	5.634840
H	2.011790	1.985310	4.698370
H	1.229570	1.862450	6.283120
H	2.958110	1.549860	6.131990
C	0.155240	-0.115530	4.966260
H	-0.463470	0.151640	5.829550
H	-0.076920	0.587790	4.164650
H	-0.118070	-1.124060	4.642490
C	4.778010	0.282580	4.450970
H	5.823390	-0.015770	4.321660
H	4.513670	0.961280	3.637400
H	4.707280	0.828090	5.393120
C	4.306470	-1.824700	3.198040
H	4.276820	-1.256420	2.265890
H	5.331090	-2.182560	3.346510
H	3.651280	-2.694990	3.092440
O	0.065240	1.733430	-1.004300
O	-0.156000	2.913540	-1.366770

C<sup>D</sup>

C	-2.506050	2.116640	3.428410
C	-2.492880	1.132700	2.443010
C	-1.372940	0.969190	1.609940
C	-0.254640	1.823930	1.783920
C	-0.289350	2.808260	2.768950
C	-1.404130	2.955500	3.596120
H	-3.377650	2.226570	4.066780
H	-3.344840	0.474250	2.308940
H	0.568220	3.463030	2.892830
H	-1.410370	3.722260	4.364610
C	0.949780	1.715160	0.877520
H	1.626370	2.550440	1.073450
C	1.665160	0.383480	0.946980
C	1.536400	-0.480870	2.165250
H	0.493020	-0.682300	2.412940
H	2.052940	-1.423850	1.999830
C	-1.338740	-0.055070	0.621450
C	-1.187350	-0.915820	-0.221280

C	-0.942670	-1.897870	-1.222690
C	0.356730	-2.420360	-1.392790
C	-1.978960	-2.338890	-2.066930
C	0.602920	-3.352150	-2.397930
H	1.166910	-2.100290	-0.744490
C	-1.719580	-3.273050	-3.065960
H	-2.977940	-1.936370	-1.935600
C	-0.429150	-3.779680	-3.237370
H	1.607670	-3.745170	-2.522620
H	-2.525690	-3.603500	-3.714980
H	-0.229750	-4.505580	-4.020600
N	2.543110	0.019340	0.031420
O	3.135620	-1.120790	0.001700
C	2.918490	0.890330	-1.072760
C	3.646560	2.045400	-0.814840
C	2.571720	0.506070	-2.364510
C	4.012860	2.860600	-1.886830
H	3.920840	2.297990	0.204730
C	2.934660	1.331600	-3.424200
H	2.008960	-0.407790	-2.518350
C	3.650540	2.509000	-3.187350
H	4.577530	3.769560	-1.703110
H	2.652610	1.060390	-4.436970
H	3.925740	3.151670	-4.018390
C	1.991390	-0.900100	6.725920
C	3.497560	-0.945950	6.995290
C	4.218770	-1.474190	5.753400
C	3.923940	-0.651740	4.479140
C	1.620380	-0.051220	5.489290
H	5.304510	-1.494550	5.903860
H	3.871280	0.049150	7.263930
H	3.706310	-1.593000	7.855180
H	1.631020	-1.923880	6.561990
H	1.446170	-0.502960	7.590280
H	3.901000	-2.509470	5.575350
N	2.438610	-0.558350	4.349850
O	2.165360	0.282290	3.209000
C	1.772730	1.459280	5.779960
H	1.700070	2.023870	4.848480
H	0.964310	1.788650	6.441410

H	2.716960	1.709610	6.265330
C	0.145460	-0.318130	5.134290
H	-0.490250	-0.134810	6.007040
H	-0.193510	0.341610	4.333570
H	0.011290	-1.356530	4.817860
C	4.651160	0.711530	4.508170
H	5.724780	0.559580	4.357580
H	4.279000	1.345140	3.700090
H	4.524450	1.245060	5.451210
C	4.440580	-1.441860	3.261620
H	4.306110	-0.895170	2.325780
H	5.509510	-1.647560	3.381360
H	3.915470	-2.397320	3.173110
O	0.479340	1.933090	-0.522470
O	0.478380	3.214970	-0.824660

**TS<sub>4</sub><sup>D</sup>**

C	-3.449940	1.777850	1.707080
C	-2.725970	0.811440	1.012660
C	-1.324100	0.882730	0.973300
C	-0.675160	1.941360	1.643800
C	-1.401500	2.907460	2.332490
C	-2.794560	2.822340	2.368010
H	-4.534030	1.715660	1.738400
H	-3.232750	-0.002910	0.504450
H	-0.879790	3.722560	2.824490
H	-3.369930	3.568200	2.908100
C	0.825060	2.004710	1.467080
H	1.337720	2.444400	2.324290
C	1.276420	0.585120	1.183420
C	1.244980	-0.289140	2.422160
H	0.253000	-0.305930	2.879400
H	1.538700	-1.302820	2.159480
C	-0.497940	-0.097940	0.319260
C	-0.221900	-1.074370	-0.411480
C	-0.406070	-2.176130	-1.306740
C	0.652360	-2.749730	-2.036500
C	-1.711370	-2.681640	-1.492830
C	0.405040	-3.785640	-2.933470
H	1.654540	-2.371950	-1.877570

C	-1.947610	-3.719130	-2.388510
H	-2.531260	-2.247110	-0.928810
C	-0.890470	-4.273540	-3.114830
H	1.230660	-4.216820	-3.492470
H	-2.957730	-4.096050	-2.521960
H	-1.076480	-5.082820	-3.815360
N	2.120630	0.184460	0.206550
O	2.043850	-1.073620	-0.104160
C	2.718000	1.038600	-0.780390
C	3.653890	1.989640	-0.378220
C	2.389560	0.860340	-2.123170
C	4.247030	2.805640	-1.339000
H	3.899170	2.085530	0.675090
C	2.986650	1.683320	-3.074770
H	1.672060	0.095680	-2.396600
C	3.910860	2.656960	-2.685710
H	4.972340	3.554500	-1.036160
H	2.727110	1.567970	-4.122970
H	4.372370	3.295720	-3.433230
C	2.497320	-0.880770	6.802260
C	3.996360	-1.192480	6.781400
C	4.374820	-1.797720	5.427050
C	3.990210	-0.901510	4.228380
C	2.057180	0.053250	5.652900
H	5.450840	-2.000860	5.371740
H	4.580310	-0.284790	6.974020
H	4.245420	-1.891930	7.587800
H	1.939050	-1.821710	6.715030
H	2.202960	-0.419400	7.752110
H	3.860400	-2.760900	5.315380
N	2.542890	-0.563720	4.384650
O	2.195490	0.327410	3.306090
C	2.529440	1.504350	5.898270
H	2.400240	2.097860	4.990590
H	1.926170	1.957880	6.691310
H	3.573790	1.569650	6.205000
C	0.518080	0.062660	5.586720
H	0.102040	0.333650	6.562630
H	0.158160	0.792780	4.856300
H	0.140200	-0.925690	5.309690

C	4.929220	0.321050	4.114680
H	5.909890	-0.000560	3.748990
H	4.518150	1.038670	3.401090
H	5.085900	0.832440	5.065440
C	4.126250	-1.727460	2.935400
H	3.921300	-1.124800	2.047720
H	5.145830	-2.117640	2.849440
H	3.433490	-2.573790	2.943760
O	1.069750	2.913890	0.327080
O	1.153360	4.161790	0.743960

**D<sup>D</sup>**

C	-2.797160	3.058930	1.008630
C	-2.428040	1.716960	0.880280
C	-1.068600	1.391800	0.881390
C	-0.105250	2.413420	1.046430
C	-0.472830	3.745070	1.160370
C	-1.835880	4.065800	1.141600
H	-3.851250	3.322110	1.013290
H	-3.184720	0.943780	0.802320
H	0.284880	4.516230	1.256670
H	-2.149840	5.100770	1.238130
C	1.295370	1.841250	0.981160
H	2.024880	2.347420	1.596640
C	1.055910	0.353590	1.350550
C	0.985490	0.193650	2.898650
H	0.123460	0.765290	3.256030
H	0.781300	-0.863300	3.079510
C	-0.347470	0.132480	0.791770
C	-0.378500	-1.057890	0.167010
C	-1.396630	-1.775880	-0.598950
C	-1.277080	-3.161610	-0.798530
C	-2.481310	-1.091660	-1.173170
C	-2.236910	-3.849050	-1.537530
H	-0.431150	-3.689250	-0.371520
C	-3.433790	-1.785160	-1.914000
H	-2.555940	-0.015790	-1.070420
C	-3.319750	-3.166010	-2.093590
H	-2.136980	-4.920980	-1.681820
H	-4.262540	-1.244510	-2.362060

H	-4.065650	-3.704030	-2.671540
N	1.829350	-0.766950	0.756160
O	0.836130	-1.708250	0.257080
C	2.840680	-0.561440	-0.226050
C	4.058560	-0.053710	0.241380
C	2.676810	-0.876700	-1.577800
C	5.090910	0.196460	-0.657700
H	4.158660	0.128030	1.305360
C	3.728930	-0.643580	-2.462270
H	1.740130	-1.293740	-1.926590
C	4.932360	-0.096250	-2.014030
H	6.029200	0.605910	-0.292640
H	3.600260	-0.881950	-3.514530
H	5.741320	0.091610	-2.713870
C	5.148730	-1.400210	4.043070
C	6.079610	-0.286050	4.512140
C	5.719230	1.001950	3.777520
C	4.236460	1.403360	3.942000
C	3.641140	-1.085390	4.211990
H	6.333630	1.840730	4.125010
H	6.000830	-0.146670	5.596570
H	7.122940	-0.556870	4.313200
H	5.335840	-1.597340	2.979510
H	5.353260	-2.333330	4.580510
H	5.932420	0.875570	2.707990
N	3.390120	0.229980	3.508920
O	2.023520	0.688660	3.744200
C	3.210860	-1.122370	5.693530
H	2.231050	-0.652230	5.804900
H	3.130570	-2.164090	6.020060
H	3.910020	-0.623970	6.365100
C	2.889470	-2.218720	3.479000
H	3.359030	-3.175230	3.732840
H	1.845350	-2.292690	3.792070
H	2.918060	-2.081020	2.397900
C	3.959920	1.913020	5.378280
H	4.387820	2.914030	5.492910
H	2.885130	1.980080	5.554550
H	4.398700	1.284310	6.152370
C	3.971850	2.583100	2.990540

H	2.984900	3.014020	3.170700
H	4.711810	3.369330	3.172950
H	4.055310	2.284760	1.942800
O	1.763180	1.961190	-0.412470
O	2.243160	3.171140	-0.626970

**TS<sub>5</sub><sup>OS</sup>**

C	3.883610	1.864470	4.481330
C	4.612110	1.385990	3.390590
C	3.921440	0.945990	2.256120
C	2.502030	0.991700	2.245090
C	1.785460	1.504540	3.315190
C	2.486680	1.934190	4.445320
H	4.415400	2.213770	5.362070
H	5.695390	1.393220	3.412660
H	0.708390	1.586800	3.255390
H	1.942830	2.337960	5.294250
C	1.985350	0.455530	0.937790
H	0.831270	1.051970	0.664480
C	3.177500	0.680600	-0.017910
C	3.227750	2.158890	-0.500650
H	3.711650	2.751550	0.283750
H	3.845940	2.195220	-1.399770
C	4.359790	0.518020	0.943550
C	5.380130	0.017040	0.227010
C	6.753000	-0.358450	0.550990
C	7.694090	-0.556010	-0.473200
C	7.138060	-0.572190	1.885910
C	8.997120	-0.937180	-0.162230
H	7.393270	-0.412560	-1.505250
C	8.440200	-0.958210	2.188530
H	6.405780	-0.478120	2.678600
C	9.376200	-1.136750	1.166630
H	9.718000	-1.084850	-0.961230
H	8.721960	-1.132500	3.223070
H	10.391820	-1.439770	1.404700
N	3.514900	-0.226890	-1.147930
O	4.993590	-0.233900	-1.086660
C	3.111260	-1.616580	-1.133490
C	2.144760	-2.000480	-2.064890



C	3.689110	-2.579740	-0.293750
C	1.745580	-3.336650	-2.141040
H	1.714560	-1.254280	-2.722440
C	3.282060	-3.906910	-0.373860
H	4.447100	-2.293120	0.424720
C	2.310480	-4.293070	-1.300910
H	1.007100	-3.637830	-2.876260
H	3.728700	-4.644170	0.287440
H	1.997770	-5.331000	-1.368050
C	1.934830	5.645060	-3.047420
C	0.778100	5.208700	-3.951180
C	0.816970	3.689660	-4.144830
C	0.795860	2.916450	-2.808610
C	1.969760	4.908240	-1.686820
H	-0.031400	3.348310	-4.749770
H	-0.181390	5.513100	-3.517160
H	0.849920	5.715780	-4.920700
H	2.881950	5.446120	-3.565680
H	1.896310	6.723360	-2.851180
H	1.731980	3.420170	-4.688370
N	1.931250	3.450110	-2.000810
O	1.944950	2.703100	-0.762890
C	0.860630	5.400790	-0.730690
H	0.749220	4.693180	0.094140
H	1.137920	6.375070	-0.314250
H	-0.107810	5.514950	-1.217740
C	3.326470	5.209990	-1.020870
H	3.493520	6.292050	-0.997190
H	3.352010	4.851770	0.011600
H	4.146040	4.744720	-1.576280
C	-0.592380	3.000920	-2.136030
H	-1.271870	2.306200	-2.632690
H	-0.527210	2.704650	-1.089230
H	-1.039130	3.995340	-2.193110
C	1.103560	1.433690	-3.073790
H	0.925220	0.840140	-2.175110
H	0.443510	1.048450	-3.855280
H	2.145210	1.297330	-3.378410
O	1.541770	-0.865840	0.929890
O	1.036390	-1.310080	2.067220

C	-2.806510	1.662640	4.790510
C	-3.607120	1.702420	3.644760
C	-3.205610	0.972890	2.523380
C	-1.998360	0.235870	2.552560
C	-1.232240	0.163160	3.704060
C	-1.642560	0.890300	4.830080
H	-3.112360	2.217150	5.673560
H	-4.541920	2.252770	3.644520
H	-0.329460	-0.435840	3.721210
H	-1.053070	0.847290	5.741600
C	-1.763530	-0.436790	1.208670
H	-1.157300	-1.333460	1.269150
C	-3.239860	-0.644140	0.742010
C	-3.920280	-1.824310	1.506990
H	-3.933060	-1.573860	2.570230
H	-4.954390	-1.834470	1.155750
C	-3.864020	0.649150	1.272190
C	-4.721170	1.126290	0.357080
C	-5.605920	2.287900	0.313880
C	-6.737470	2.283510	-0.517670
C	-5.337270	3.419280	1.101320
C	-7.602670	3.375580	-0.526370
H	-6.935360	1.418480	-1.141680
C	-6.202960	4.509220	1.083230
H	-4.437000	3.450250	1.703860
C	-7.347780	4.484060	0.282950
H	-8.482680	3.358280	-1.162860
H	-5.983000	5.380290	1.694090
H	-8.027200	5.331910	0.277320
N	-3.676550	-0.635050	-0.668790
O	-4.766810	0.316020	-0.759060
C	-2.888550	-0.609310	-1.836590
C	-2.008870	-1.679630	-2.056360
C	-3.075550	0.351660	-2.839270
C	-1.321560	-1.770280	-3.262150
H	-1.936160	-2.450680	-1.301330
C	-2.387070	0.235300	-4.046080
H	-3.765240	1.168970	-2.676020
C	-1.505770	-0.822080	-4.271360
H	-0.662380	-2.614640	-3.427560

H	-2.543840	0.986290	-4.815490
H	-0.978960	-0.912810	-5.216350
C	-3.796340	-5.283350	-1.523910
C	-2.612120	-6.214910	-1.278650
C	-1.457610	-5.406270	-0.692280
C	-1.840140	-4.631590	0.588930
C	-4.263150	-4.508490	-0.266430
H	-0.605120	-6.051290	-0.448660
H	-2.895280	-7.029830	-0.602180
H	-2.305560	-6.690410	-2.217920
H	-3.518850	-4.547300	-2.289390
H	-4.658370	-5.839220	-1.910710
H	-1.103190	-4.688550	-1.443100
N	-3.050860	-3.785600	0.270680
O	-3.362860	-3.136290	1.537230
C	-4.972540	-5.432180	0.747010
H	-5.051270	-4.926570	1.712300
H	-5.984420	-5.650730	0.391010
H	-4.468180	-6.386450	0.898460
C	-5.303590	-3.479830	-0.760410
H	-5.990530	-3.976750	-1.454210
H	-5.914590	-3.086900	0.055710
H	-4.825690	-2.644130	-1.271050
C	-2.020240	-5.601950	1.783140
H	-1.035740	-5.938470	2.122740
H	-2.508410	-5.090640	2.614420
H	-2.598540	-6.492190	1.536630
C	-0.671130	-3.701950	0.940060
H	-0.825940	-3.217600	1.903500
H	0.253720	-4.280280	1.006490
H	-0.508100	-2.939690	0.176270
O	-1.138310	0.467450	0.240980
O	-0.328870	1.414010	0.842930

**E<sup>CS</sup>**

C	-2.851510	3.024550	0.831360
C	-2.431570	1.695940	0.724300
C	-1.063770	1.412900	0.800060
C	-0.139030	2.460770	1.015460
C	-0.562140	3.778790	1.121990

C	-1.931580	4.059370	1.023790
H	-3.912240	3.253270	0.777410
H	-3.158190	0.899040	0.608530
H	0.161480	4.571120	1.287250
H	-2.282360	5.083480	1.110900
C	1.292680	1.938980	1.033100
H	1.913040	2.430000	1.774240
C	1.072300	0.427260	1.357480
C	0.975840	0.248490	2.898290
H	0.132390	0.847780	3.256910
H	0.734320	-0.801680	3.070840
C	-0.308950	0.174750	0.757990
C	-0.314950	-1.046460	0.195530
C	-1.303230	-1.813930	-0.561480
C	-1.174380	-3.209050	-0.668250
C	-2.362980	-1.171860	-1.224120
C	-2.102220	-3.945440	-1.400550
H	-0.345310	-3.704650	-0.175150
C	-3.283980	-1.914180	-1.957880
H	-2.441360	-0.091600	-1.194070
C	-3.161860	-3.303310	-2.043520
H	-1.995260	-5.024000	-1.472130
H	-4.093600	-1.405970	-2.473980
H	-3.882580	-3.879770	-2.616310
N	1.886660	-0.683110	0.788370
O	0.905600	-1.675220	0.348200
C	2.837640	-0.480630	-0.258070
C	4.117830	-0.091150	0.146370
C	2.556500	-0.695890	-1.609930
C	5.102190	0.144220	-0.809080
H	4.301380	0.016410	1.208810
C	3.557420	-0.479990	-2.555710
H	1.572100	-1.032010	-1.912670
C	4.826210	-0.048140	-2.164560
H	6.092410	0.460830	-0.492320
H	3.340930	-0.644330	-3.607850
H	5.597280	0.124540	-2.909920
C	5.054560	-1.529480	4.063220
C	6.043740	-0.454240	4.502740
C	5.741950	0.835820	3.745660

C	4.281410	1.313960	3.907920
C	3.566970	-1.134390	4.238240
H	6.397920	1.649710	4.076020
H	5.980390	-0.289870	5.584720
H	7.070940	-0.780440	4.302340
H	5.221840	-1.756280	3.002220
H	5.217000	-2.461140	4.617430
H	5.945150	0.681230	2.678110
N	3.375970	0.174900	3.508800
O	2.032460	0.698910	3.746750
C	3.151770	-1.118110	5.724760
H	2.196520	-0.599530	5.834080
H	3.026150	-2.147230	6.076270
H	3.880690	-0.637800	6.377750
C	2.749420	-2.242180	3.536790
H	3.171740	-3.216840	3.804580
H	1.706880	-2.254930	3.863840
H	2.773920	-2.124000	2.453080
C	4.043760	1.872720	5.332990
H	4.518180	2.855900	5.415800
H	2.974830	1.994190	5.515920
H	4.460760	1.245650	6.120720
C	4.070080	2.482590	2.929070
H	3.137440	3.007760	3.143920
H	4.884410	3.205070	3.047820
H	4.064620	2.148100	1.889690
O	1.899900	2.084070	-0.257250
O	2.090260	3.511120	-0.457780
H	1.297730	3.722410	-0.980280

**F<sup>CS</sup>**

C	-2.750610	3.052620	0.411140
C	-2.376200	1.709180	0.506990
C	-1.022350	1.397870	0.636270
C	-0.059530	2.453170	0.700440
C	-0.442690	3.796310	0.584250
C	-1.800070	4.081910	0.441260
H	-3.803550	3.302720	0.314770
H	-3.126630	0.926700	0.497670
H	0.319960	4.561520	0.617000

H	-2.125290	5.114450	0.359970
C	1.251520	1.873990	0.887510
C	1.094240	0.418250	1.280740
C	1.014270	0.246550	2.835240
H	0.165520	0.845130	3.183030
H	0.766730	-0.805550	2.992600
C	-0.304000	0.141690	0.726800
C	-0.299680	-1.107860	0.221940
C	-1.300910	-1.943190	-0.443120
C	-1.171330	-3.342170	-0.418800
C	-2.381040	-1.368440	-1.132130
C	-2.122790	-4.144780	-1.043850
H	-0.326910	-3.789000	0.094670
C	-3.324420	-2.176720	-1.760520
H	-2.462180	-0.290550	-1.202170
C	-3.204820	-3.567670	-1.711890
H	-2.017450	-5.225180	-1.010640
H	-4.150440	-1.718500	-2.296700
H	-3.944360	-4.196170	-2.199010
N	1.919800	-0.664670	0.698740
O	0.942880	-1.699320	0.354990
C	2.728200	-0.358880	-0.444170
C	4.019290	0.092770	-0.155120
C	2.295770	-0.494990	-1.765290
C	4.867250	0.456630	-1.196990
H	4.317760	0.158190	0.886180
C	3.164280	-0.150030	-2.801400
H	1.305100	-0.879280	-1.979030
C	4.442960	0.335010	-2.522580
H	5.864630	0.823890	-0.973800
H	2.835840	-0.256680	-3.831400
H	5.109200	0.609560	-3.335140
C	5.008870	-1.624080	4.151640
C	5.964500	-0.581040	4.721420
C	5.749410	0.734440	3.979630
C	4.290350	1.236490	4.035860
C	3.513580	-1.217030	4.190280
H	6.391480	1.526890	4.380990
H	5.800520	-0.451270	5.797490
H	7.001350	-0.918880	4.608290

H	5.278860	-1.817790	3.105260
H	5.102560	-2.577190	4.685220
H	6.030500	0.600670	2.926620
N	3.404450	0.128650	3.504100
O	2.058740	0.686920	3.678910
C	2.951000	-1.265400	5.626740
H	1.995650	-0.737410	5.670830
H	2.780770	-2.308280	5.913150
H	3.617290	-0.827700	6.370060
C	2.774980	-2.291050	3.358020
H	3.176300	-3.276920	3.617220
H	1.704770	-2.328720	3.574590
H	2.906140	-2.117910	2.290220
C	3.936400	1.727930	5.461490
H	4.444650	2.679650	5.645370
H	2.862080	1.895320	5.550570
H	4.244970	1.040590	6.248930
C	4.181910	2.443780	3.093880
H	3.194130	2.901400	3.127680
H	4.913060	3.201380	3.395580
H	4.391270	2.164730	2.061790
O	2.388790	2.436380	0.825810
O	2.460900	3.785760	0.594460

**TS<sub>6</sub><sup>os</sup>**

C	-3.416560	2.071290	1.476400
C	-2.602930	0.947710	1.349840
C	-1.219100	1.110980	1.211090
C	-0.647640	2.396770	1.249480
C	-1.474420	3.522240	1.324830
C	-2.855100	3.352700	1.441300
H	-4.490450	1.949200	1.585930
H	-3.034480	-0.048580	1.328910
H	-0.997250	4.496870	1.254730
H	-3.500010	4.224560	1.507760
C	0.846790	2.551850	1.213930
H	1.336690	2.586330	2.198080
C	1.005070	-0.078520	1.515710
C	1.117220	0.090420	3.029290
H	0.314000	0.769690	3.322240

H	0.862880	-0.902640	3.419020
C	-0.274240	0.024910	0.905720
C	-0.299220	-0.862580	-0.152750
C	-1.292100	-1.219350	-1.158590
C	-1.287830	-2.519700	-1.697360
C	-2.233780	-0.282220	-1.623200
C	-2.222690	-2.880870	-2.661850
H	-0.554160	-3.239130	-1.348610
C	-3.160920	-0.653370	-2.592000
H	-2.222830	0.730880	-1.243210
C	-3.165270	-1.951630	-3.108290
H	-2.217020	-3.889080	-3.065090
H	-3.879210	0.077630	-2.951500
H	-3.894180	-2.235130	-3.862030
N	1.717210	-1.061510	0.833130
O	0.876130	-1.529830	-0.241480
C	3.050890	-0.958230	0.295530
C	3.433140	0.196430	-0.389090
C	3.889430	-2.068020	0.374830
C	4.708220	0.254440	-0.950150
H	2.749540	1.037750	-0.465830
C	5.159120	-2.002900	-0.197030
H	3.548720	-2.963290	0.883340
C	5.574500	-0.837690	-0.847820
H	5.021700	1.157530	-1.465240
H	5.824660	-2.858570	-0.128990
H	6.567630	-0.785410	-1.283750
C	5.234710	-1.651950	3.810360
C	6.314670	-0.570830	3.777070
C	5.853510	0.589520	2.893880
C	4.494170	1.173870	3.332750
C	3.835360	-1.139100	4.235190
H	6.590390	1.400660	2.901450
H	6.535670	-0.217240	4.791160
H	7.250220	-0.993010	3.391030
H	5.144830	-2.087410	2.808450
H	5.513720	-2.463740	4.492770
H	5.761240	0.245070	1.857480
N	3.520570	0.020490	3.325890
O	2.246440	0.617350	3.691320



C	3.767360	-0.838980	5.749600
H	2.882400	-0.236680	5.968440
H	3.683780	-1.780720	6.302350
H	4.644710	-0.317090	6.130150
C	2.840240	-2.289610	3.964450
H	3.273770	-3.229000	4.322510
H	1.899100	-2.152570	4.504180
H	2.625660	-2.394210	2.899280
C	4.615340	1.933860	4.676860
H	5.084310	2.904780	4.487880
H	3.624200	2.117340	5.097070
H	5.221930	1.423750	5.424710
C	4.039000	2.210610	2.293780
H	3.242360	2.844160	2.683710
H	4.880300	2.864330	2.041110
H	3.687430	1.745320	1.378960
O	1.455860	2.889680	0.192760
O	0.984330	4.985360	0.130330
H	0.531470	4.811100	-0.710320

### G<sup>D</sup>

C	-1.966980	0.921580	3.686350
C	-1.450180	-0.020750	2.796830
C	-0.597670	0.374460	1.759570
C	-0.256320	1.736850	1.632870
C	-0.778160	2.674450	2.534040
C	-1.633500	2.272600	3.554370
H	-2.630530	0.600810	4.484400
H	-1.708810	-1.070250	2.895430
H	-0.487130	3.713140	2.410960
H	-2.036510	3.004510	4.248190
C	0.669360	2.215510	0.573250
H	0.988310	1.455710	-0.163450
C	1.079790	-1.410960	1.148890
C	1.959570	-1.357650	2.348750
H	1.350270	-1.287060	3.254190
H	2.569720	-2.263590	2.415340
C	-0.028030	-0.644960	0.847340
C	-0.443770	-0.971610	-0.451430
C	-1.457510	-0.466220	-1.335140

C	-1.465250	-0.859440	-2.696300
C	-2.458670	0.433050	-0.892740
C	-2.421820	-0.361270	-3.571630
H	-0.708120	-1.549070	-3.052460
C	-3.405720	0.924180	-1.781490
H	-2.494110	0.737290	0.145670
C	-3.396870	0.535920	-3.125980
H	-2.405030	-0.672440	-4.612820
H	-4.162840	1.615890	-1.422080
H	-4.140720	0.925360	-3.814670
N	1.367330	-2.281400	0.072890
O	0.386980	-1.961320	-0.954320
C	2.687540	-2.220240	-0.512650
C	3.264920	-0.994500	-0.858190
C	3.373010	-3.415590	-0.714010
C	4.542000	-0.973160	-1.412820
H	2.720400	-0.076050	-0.669360
C	4.657320	-3.387250	-1.261150
H	2.893770	-4.347860	-0.434160
C	5.238360	-2.168730	-1.611380
H	4.999990	-0.025340	-1.677280
H	5.201300	-4.314150	-1.412100
H	6.238410	-2.147440	-2.035690
C	4.238600	1.270060	5.353430
C	5.713300	1.214810	4.951670
C	5.977140	-0.076290	4.174200
C	5.067330	-0.241580	2.934950
C	3.272060	1.149660	4.152240
H	7.020230	-0.131260	3.840980
H	5.980570	2.089420	4.347640
H	6.348710	1.255010	5.844640
H	4.031390	0.445980	6.048300
H	4.008290	2.202480	5.883190
H	5.808000	-0.931020	4.842120
N	3.656940	-0.086010	3.402050
O	2.796000	-0.188110	2.236820
C	3.262580	2.447210	3.312620
H	2.781920	2.278020	2.349540
H	2.693290	3.221780	3.837010
H	4.261490	2.845540	3.130380

C	1.851250	0.928130	4.701780
H	1.587870	1.737700	5.390800
H	1.112720	0.926050	3.900080
H	1.792010	-0.019970	5.244860
C	5.484460	0.723500	1.801350
H	6.407970	0.366080	1.335210
H	4.708600	0.752640	1.035220
H	5.665640	1.741060	2.149870
C	5.223790	-1.682190	2.411250
H	4.677730	-1.827210	1.477380
H	6.279980	-1.892650	2.213240
H	4.863640	-2.400900	3.153560
O	1.065150	3.365070	0.497240

**OH •**

O	0.000000	0.000000	-0.058070
H	0.000000	0.000000	0.921650

**TS<sub>7</sub><sup>D</sup>**

C	2.532710	3.131950	-2.138040
C	3.724790	2.437750	-1.927670
C	3.769030	1.460670	-0.927800
C	2.582760	1.162900	-0.192790
C	1.396500	1.877130	-0.397840
C	1.385670	2.870820	-1.373890
H	2.493470	3.890400	-2.915210
H	4.592130	2.639620	-2.545100
H	0.534920	1.633270	0.208600
H	0.477640	3.438660	-1.553530
C	2.848550	0.079920	0.755370
C	4.195240	-0.534110	0.322260
C	3.868870	-1.698440	-0.657530
H	3.698900	-1.285860	-1.656390
H	4.734490	-2.368020	-0.692290
C	4.832270	0.603740	-0.446400
C	6.158870	0.550730	-0.213610
C	7.306200	1.361350	-0.609780
C	8.609500	0.874090	-0.405950
C	7.134270	2.645900	-1.152270
C	9.711020	1.647390	-0.761280

H	8.747790	-0.109570	0.028550
C	8.239700	3.416560	-1.495780
H	6.139400	3.056640	-1.261370
C	9.531790	2.917810	-1.310140
H	10.712670	1.256930	-0.604880
H	8.092740	4.413410	-1.900640
H	10.392940	3.520950	-1.581620
N	5.238800	-0.950920	1.289830
O	6.466650	-0.505330	0.636830
C	5.182860	-0.395400	2.616850
C	4.311190	-1.029520	3.510260
C	5.959180	0.688850	3.037180
C	4.181920	-0.547690	4.809880
H	3.725870	-1.874700	3.164380
C	5.838910	1.147000	4.351590
H	6.661740	1.156340	2.357230
C	4.946760	0.541510	5.237270
H	3.488110	-1.031170	5.492590
H	6.445980	1.986740	4.679590
H	4.853240	0.908060	6.256070
C	0.704910	-4.437570	-2.504090
C	0.648460	-5.698650	-1.636360
C	1.994340	-5.897020	-0.932970
C	2.420440	-4.673670	-0.091920
C	1.090190	-3.166630	-1.711720
H	1.972190	-6.776090	-0.276990
H	-0.161900	-5.621690	-0.901900
H	0.416180	-6.572420	-2.256990
H	1.447350	-4.588210	-3.298950
H	-0.258530	-4.254830	-2.994010
H	2.766990	-6.080700	-1.691460
N	2.366450	-3.483310	-0.993380
O	2.706770	-2.344770	-0.172490
C	-0.064280	-2.679960	-0.811660
H	0.288420	-1.903040	-0.128970
H	-0.855440	-2.249550	-1.433750
H	-0.522080	-3.476520	-0.224530
C	1.396130	-2.039810	-2.717520
H	0.546750	-1.911350	-3.396740
H	1.553490	-1.086240	-2.204950

H	2.282690	-2.276760	-3.312900
C	1.565690	-4.550770	1.193650
H	1.896670	-5.293500	1.929690
H	1.686320	-3.555040	1.630810
H	0.504280	-4.721180	1.010890
C	3.891740	-4.842700	0.330080
H	4.207910	-4.031390	0.992250
H	4.021350	-5.789530	0.866310
H	4.544310	-4.849700	-0.549360
O	2.161880	-0.360820	1.685210
O	0.459750	-0.070800	1.605840
C	-3.189440	-3.888120	2.795150
C	-4.146530	-2.885720	2.630420
C	-3.782980	-1.584310	2.264960
C	-2.407460	-1.303530	2.061300
C	-1.450840	-2.309740	2.261770
C	-1.835700	-3.599800	2.621300
H	-3.507090	-4.888160	3.080290
H	-5.195210	-3.104170	2.810000
H	-0.407010	-2.041420	2.132880
H	-1.083820	-4.367490	2.768410
C	-1.897060	0.014590	1.604880
H	-0.793140	-0.073680	1.194240
C	-5.872370	-0.567710	1.203340
C	-6.344630	-1.626210	0.247570
H	-6.290620	-2.599420	0.748070
H	-7.397730	-1.423310	0.043340
C	-4.842910	-0.560950	2.136780
C	-5.011300	0.550190	2.972510
C	-4.254040	1.137010	4.047790
C	-4.431620	2.507830	4.348260
C	-3.318180	0.398790	4.808290
C	-3.679310	3.118140	5.344210
H	-5.150140	3.084390	3.775220
C	-2.570530	1.022520	5.800080
H	-3.189390	-0.660990	4.627370
C	-2.735650	2.385270	6.070420
H	-3.821110	4.176780	5.547720
H	-1.849940	0.440340	6.368820
H	-2.141990	2.868110	6.841790

N	-6.730510	0.545850	1.462440
O	-6.138510	1.248550	2.579530
C	-6.948580	1.520340	0.417160
C	-8.233720	1.676600	-0.087670
C	-5.891180	2.303730	-0.054930
C	-8.458490	2.590220	-1.122090
H	-9.040320	1.081320	0.328870
C	-6.119480	3.211860	-1.083150
H	-4.909240	2.192340	0.392570
C	-7.402110	3.349170	-1.624860
H	-9.458070	2.710470	-1.528020
H	-5.298530	3.811810	-1.466040
H	-7.576150	4.054190	-2.433250
C	-6.675990	0.019800	-4.006930
C	-5.284310	0.303350	-4.576480
C	-4.305220	0.545880	-3.426370
C	-4.274510	-0.610960	-2.403100
C	-6.704670	-1.151310	-2.994390
H	-3.285690	0.697790	-3.801920
H	-4.946100	-0.532790	-5.200670
H	-5.319770	1.179870	-5.234980
H	-7.039440	0.919190	-3.493550
H	-7.388490	-0.206980	-4.809420
H	-4.598180	1.460930	-2.896290
N	-5.686980	-0.821580	-1.940950
O	-5.633110	-1.901330	-0.971870
C	-6.521430	-2.520750	-3.690530
H	-6.263110	-3.278320	-2.946850
H	-7.461250	-2.817500	-4.167740
H	-5.754310	-2.518060	-4.465000
C	-8.103820	-1.163250	-2.350670
H	-8.863220	-1.173800	-3.139850
H	-8.258280	-2.058130	-1.740830
H	-8.259940	-0.273740	-1.738810
C	-3.573620	-1.863070	-2.988090
H	-2.493200	-1.686510	-3.018860
H	-3.758010	-2.727370	-2.345830
H	-3.886240	-2.109820	-4.002520
C	-3.453400	-0.169160	-1.189340
H	-3.331660	-0.998790	-0.494340

H	-2.458630	0.161590	-1.505810
H	-3.934680	0.647850	-0.659170
O	-2.485270	1.060430	1.485150

**H<sup>CS</sup>**

C	2.737460	4.145510	0.415510
C	2.830760	2.836960	-0.059350
C	1.957900	1.870130	0.456710
C	1.025340	2.248590	1.457010
C	0.946000	3.553450	1.935590
C	1.801680	4.511750	1.395550
H	3.407090	4.901500	0.014430
H	3.571950	2.579650	-0.806590
H	0.227440	3.795550	2.712790
H	1.753410	5.541890	1.735080
C	0.271650	1.064210	1.945450
C	0.532080	-0.035290	0.887420
C	-0.596970	-0.018140	-0.178220
H	-0.461120	0.855260	-0.819050
H	-0.460760	-0.920020	-0.787780
C	1.809400	0.445860	0.224190
C	2.536330	-0.645180	-0.095240
C	3.810330	-0.815720	-0.784700
C	4.674540	-1.867350	-0.438660
C	4.180910	0.072020	-1.807880
C	5.900870	-2.001840	-1.083870
H	4.378330	-2.558840	0.342800
C	5.411310	-0.063470	-2.444850
H	3.483450	0.841520	-2.120810
C	6.276150	-1.098050	-2.081190
H	6.569250	-2.811340	-0.805710
H	5.689000	0.627940	-3.235100
H	7.234880	-1.205580	-2.580240
N	0.938700	-1.374930	1.356560
O	1.954180	-1.795880	0.370310
C	-0.047370	-2.395780	1.480550
C	-1.116980	-2.145190	2.352200
C	0.047280	-3.621430	0.814120
C	-2.089620	-3.120780	2.537510
H	-1.184180	-1.186730	2.854890

C	-0.935330	-4.592640	1.020500
H	0.875360	-3.811080	0.144130
C	-2.006750	-4.350400	1.876900
H	-2.921750	-2.914900	3.204650
H	-0.857400	-5.541920	0.497610
H	-2.770170	-5.107580	2.029100
C	-4.790500	-0.139530	-1.840720
C	-5.048940	1.357910	-2.023490
C	-4.701610	2.088720	-0.726070
C	-3.242680	1.864690	-0.248510
C	-3.318670	-0.449400	-1.466670
H	-4.870990	3.167340	-0.823210
H	-4.461900	1.754610	-2.860900
H	-6.101000	1.530390	-2.279630
H	-5.435070	-0.514840	-1.036660
H	-5.044680	-0.697780	-2.749270
H	-5.372040	1.727940	0.063450
N	-3.006390	0.403800	-0.299030
O	-1.873420	-0.006120	0.463620
C	-2.445100	-0.265280	-2.741470
H	-1.391910	-0.483710	-2.567780
H	-2.793830	-0.956720	-3.516990
H	-2.513730	0.743640	-3.152070
C	-3.227730	-1.915590	-1.005250
H	-3.630440	-2.570990	-1.784690
H	-2.201730	-2.227210	-0.799190
H	-3.802480	-2.058380	-0.087340
C	-2.269230	2.752440	-1.067570
H	-2.579690	3.800870	-0.996190
H	-1.252050	2.698200	-0.671060
H	-2.242270	2.487150	-2.125890
C	-3.166660	2.307720	1.225000
H	-2.151240	2.262020	1.616150
H	-3.527160	3.338620	1.314950
H	-3.790440	1.658980	1.845350
O	-0.410060	0.996500	2.948500

**TS<sub>8</sub><sup>OS</sup>**

C	3.196210	3.598130	0.549350
C	3.112490	2.307050	0.035930



C	2.041190	1.479390	0.425400
C	1.102010	2.010400	1.347270
C	1.193920	3.304680	1.863010
C	2.246430	4.111720	1.450940
H	4.024770	4.230340	0.239550
H	3.869470	1.951750	-0.650070
H	0.446000	3.645880	2.572610
H	2.343630	5.127360	1.821960
C	0.099450	1.007640	1.716750
C	0.282490	-0.167080	0.688890
C	-0.723610	0.082480	-0.481740
H	-0.615530	1.110530	-0.832240
H	-0.428690	-0.605940	-1.280400
C	1.681940	0.109110	0.118400
C	2.404530	-0.980580	-0.301140
C	3.734850	-0.882610	-0.974030
C	4.811780	-1.650490	-0.512210
C	3.904170	-0.067030	-2.100500
C	6.053320	-1.563090	-1.140060
H	4.666700	-2.301770	0.343540
C	5.145150	0.012440	-2.731960
H	3.057950	0.501220	-2.473430
C	6.224920	-0.729580	-2.248320
H	6.888970	-2.147250	-0.765490
H	5.267500	0.651200	-3.602250
H	7.192760	-0.664510	-2.737150
N	0.210480	-1.545630	1.007940
O	1.996740	-2.208610	-0.135810
C	-0.307350	-2.273290	1.986150
C	-1.237490	-1.796540	2.969250
C	0.065220	-3.660030	2.004120
C	-1.743800	-2.675930	3.908580
H	-1.537020	-0.757950	2.939680
C	-0.442180	-4.505740	2.968540
H	0.773860	-3.990460	1.253050
C	-1.350920	-4.023880	3.927490
H	-2.457530	-2.312550	4.642260
H	-0.139560	-5.548590	2.984750
H	-1.751850	-4.695620	4.680750
C	-4.653010	0.374410	-2.621820

C	-5.025360	1.820120	-2.290970
C	-4.947290	2.008960	-0.776980
C	-3.562650	1.671090	-0.164650
C	-3.217560	0.012090	-2.162870
H	-5.204190	3.035000	-0.490160
H	-4.359790	2.521790	-2.808150
H	-6.039390	2.040860	-2.644580
H	-5.357290	-0.296670	-2.115120
H	-4.733470	0.177810	-3.696890
H	-5.692180	1.352180	-0.311030
N	-3.144470	0.363380	-0.726210
O	-2.041490	-0.207800	-0.016190
C	-2.210790	0.707720	-3.125720
H	-1.182470	0.384490	-2.965590
H	-2.466900	0.451660	-4.159790
H	-2.238200	1.794940	-3.041010
C	-3.044100	-1.513300	-2.277630
H	-3.233110	-1.829850	-3.308780
H	-2.036750	-1.834570	-2.004760
H	-3.749090	-2.021210	-1.614780
C	-2.582090	2.850790	-0.382460
H	-2.997770	3.759470	0.066780
H	-1.622080	2.669610	0.105780
H	-2.399770	3.059470	-1.438910
C	-3.767670	1.483080	1.350700
H	-2.823120	1.331530	1.868750
H	-4.253710	2.372200	1.767560
H	-4.407380	0.614750	1.533090
O	-0.736490	1.119400	2.599190

**I<sup>os</sup>**

C	2.045300	3.081620	3.192310
C	2.305490	2.188640	2.162570
C	1.401740	1.122270	1.940980
C	0.273840	0.998350	2.798870
C	0.010060	1.907120	3.817720
C	0.907770	2.954800	4.016200
H	2.734320	3.903000	3.368100
H	3.179500	2.308690	1.534500
H	-0.876270	1.783750	4.432260

H	0.737790	3.676820	4.809060
C	-0.548290	-0.143120	2.378720
C	0.238050	-0.878210	1.240190
C	-0.621300	-0.971290	-0.040080
H	-0.126330	-1.663520	-0.726190
H	-1.634070	-1.307840	0.165270
C	1.395800	0.082410	0.969190
C	2.229420	-0.109660	-0.218730
C	2.786040	1.084600	-0.930450
C	4.020060	0.972430	-1.583380
C	2.038500	2.265330	-1.056990
C	4.522940	2.043340	-2.318200
H	4.566090	0.037260	-1.507960
C	2.534900	3.326820	-1.811730
H	1.057500	2.324980	-0.599600
C	3.780850	3.221820	-2.433390
H	5.487530	1.958190	-2.810270
H	1.945210	4.232590	-1.921300
H	4.168780	4.052810	-3.015980
N	0.804550	-2.106760	1.746850
O	2.407460	-1.241410	-0.680770
C	0.093920	-3.248460	1.874450
C	-1.327260	-3.414060	1.829620
C	0.885450	-4.412280	2.131070
C	-1.891380	-4.667790	2.008380
H	-1.964230	-2.545860	1.734720
C	0.305280	-5.658020	2.285770
H	1.960520	-4.273600	2.177290
C	-1.089520	-5.797970	2.222480
H	-2.972820	-4.771080	1.990320
H	0.931350	-6.528100	2.462170
H	-1.546860	-6.774530	2.351700
C	-3.566320	2.110610	-1.955430
C	-3.741850	1.322760	-3.254590
C	-2.364730	0.919000	-3.786560
C	-1.565090	0.051200	-2.782650
C	-2.796390	1.334410	-0.857130
H	-2.450870	0.368120	-4.730180
H	-4.368680	0.438210	-3.088800
H	-4.267190	1.935890	-3.996120

H	-3.005490	3.026820	-2.179600
H	-4.534630	2.419010	-1.544990
H	-1.785150	1.827300	-3.993020
N	-1.578790	0.792950	-1.502880
O	-0.604440	0.375060	-0.559560
C	-3.724300	0.300640	-0.170310
H	-3.229310	-0.170900	0.681570
H	-4.612740	0.808440	0.221190
H	-4.063740	-0.478540	-0.854930
C	-2.345450	2.353190	0.208310
H	-3.212550	2.915200	0.570840
H	-1.878090	1.864290	1.063120
H	-1.625920	3.055580	-0.222570
C	-2.168610	-1.380560	-2.772920
H	-2.101590	-1.804360	-3.781130
H	-1.633750	-2.055860	-2.105980
H	-3.221150	-1.387450	-2.485040
C	-0.100850	-0.025220	-3.255360
H	0.506320	-0.685150	-2.631680
H	-0.066430	-0.405270	-4.281860
H	0.355080	0.968060	-3.230100
O	-1.648230	-0.462110	2.794610

**TS<sub>9</sub><sup>OS</sup>**

C	2.188650	3.128250	3.261780
C	2.377520	2.201550	2.246570
C	1.399220	1.199950	2.051350
C	0.267910	1.168330	2.912970
C	0.077030	2.111920	3.916460
C	1.050980	3.093280	4.094260
H	2.934700	3.901890	3.420280
H	3.250870	2.248040	1.607240
H	-0.810750	2.063280	4.539290
H	0.941060	3.834240	4.880250
C	-0.634400	0.078450	2.507510
C	0.116350	-0.731310	1.404280
C	-0.740090	-0.900480	0.143290
H	-0.297490	-1.675970	-0.487700
H	-1.773070	-1.147790	0.381540
C	1.320700	0.148230	1.094520

C	2.138900	-0.153580	-0.081140
C	2.706740	0.979730	-0.875810
C	3.893570	0.773920	-1.590810
C	2.015040	2.192740	-1.009800
C	4.407590	1.785000	-2.398490
H	4.392160	-0.186460	-1.504920
C	2.522520	3.195210	-1.834390
H	1.063770	2.322370	-0.505960
C	3.722560	2.997160	-2.520690
H	5.335390	1.627510	-2.941160
H	1.976060	4.126930	-1.949610
H	4.118510	3.782050	-3.159340
N	0.736700	-1.841420	2.083460
O	2.283360	-1.318860	-0.464730
C	0.409350	-3.140540	1.870530
C	-0.842710	-3.641540	1.406730
C	1.410310	-4.088320	2.230710
C	-1.053960	-5.007480	1.293240
H	-1.657650	-2.957130	1.212190
C	1.195420	-5.447780	2.080640
H	2.354200	-3.698320	2.596560
C	-0.037290	-5.917940	1.607910
H	-2.021970	-5.372070	0.960820
H	1.983470	-6.150710	2.335890
H	-0.209060	-6.984690	1.498810
C	-3.509260	2.141600	-2.061450
C	-3.702560	1.266570	-3.301150
C	-2.340070	0.754160	-3.775250
C	-1.599180	-0.068930	-2.691610
C	-2.796840	1.413740	-0.893430
H	-2.441800	0.134830	-4.673840
H	-4.376870	0.429960	-3.081420
H	-4.184140	1.846660	-4.097070
H	-2.899620	3.009750	-2.342120
H	-4.468040	2.526390	-1.695680
H	-1.712310	1.613310	-4.041930
N	-1.595870	0.772820	-1.475390
O	-0.649030	0.394270	-0.489860
C	-3.785780	0.477500	-0.152940
H	-3.333050	0.048870	0.744410

H	-4.657390	1.053690	0.177110
H	-4.147950	-0.334850	-0.785470
C	-2.315370	2.483600	0.106330
H	-3.160400	3.109760	0.410990
H	-1.886820	2.034260	1.002760
H	-1.555880	3.119100	-0.358540
C	-2.272930	-1.465290	-2.581610
H	-2.195910	-1.976770	-3.547630
H	-1.793110	-2.105730	-1.841940
H	-3.333050	-1.398050	-2.331340
C	-0.133490	-0.252490	-3.129880
H	0.431160	-0.892570	-2.448380
H	-0.103590	-0.709500	-4.124660
H	0.370990	0.716480	-3.170000
O	-1.756790	-0.169040	2.906010

**3a<sup>CS</sup>**

C	4.683970	2.535210	2.131800
C	4.103730	1.340180	1.692830
C	2.742780	1.332230	1.409280
C	1.982520	2.497040	1.573990
C	2.555280	3.690480	2.006930
C	3.922000	3.701210	2.285860
H	5.746730	2.559520	2.355750
H	4.706480	0.447940	1.562350
H	1.937850	4.576840	2.115510
H	4.401380	4.614430	2.625460
C	0.561770	2.251830	1.221650
C	0.414850	0.746900	0.940920
C	-0.598170	0.273410	-0.069210
H	-0.531680	0.899820	-0.962780
H	-0.368130	-0.759590	-0.334590
C	1.849520	0.191070	0.994980
C	2.248760	-0.878410	0.010240
C	3.395620	-0.629120	-0.918650
C	4.135330	-1.743650	-1.342450
C	3.702860	0.637670	-1.436370
C	5.190050	-1.588720	-2.236710
H	3.864810	-2.721470	-0.957240
C	4.743500	0.786560	-2.351210

H	3.126380	1.505390	-1.136850
C	5.495910	-0.322290	-2.742300
H	5.770240	-2.453270	-2.545650
H	4.968670	1.768760	-2.756040
H	6.315940	-0.201130	-3.444560
N	0.873060	-0.055920	2.059750
O	1.639780	-1.940310	-0.036430
C	0.392570	-1.311890	2.503530
C	-0.972100	-1.523280	2.723970
C	1.322020	-2.293370	2.874120
C	-1.396250	-2.726210	3.288130
H	-1.684010	-0.761700	2.432160
C	0.884180	-3.487430	3.436360
H	2.379710	-2.115130	2.708990
C	-0.478550	-3.714540	3.643910
H	-2.459110	-2.887500	3.445940
H	1.612180	-4.246660	3.708650
H	-0.818460	-4.650010	4.078270
C	-4.625240	-0.863930	-1.694400
C	-5.047030	0.467010	-2.319150
C	-4.915260	1.566710	-1.265970
C	-3.491490	1.699630	-0.668940
C	-3.157880	-0.848700	-1.194610
H	-5.208250	2.542250	-1.670130
H	-4.434090	0.694480	-3.199840
H	-6.083160	0.407260	-2.672540
H	-5.278480	-1.075470	-0.838980
H	-4.740990	-1.691380	-2.403530
H	-5.606910	1.340430	-0.445050
N	-3.043770	0.332390	-0.308710
O	-1.897670	0.356670	0.539790
C	-2.222590	-0.910430	-2.438630
H	-1.174480	-1.051280	-2.176090
H	-2.509260	-1.766740	-3.058870
H	-2.297710	-0.016720	-3.059600
C	-2.926160	-2.104730	-0.334510
H	-3.152250	-3.000260	-0.922970
H	-1.897240	-2.187790	0.020940
H	-3.579190	-2.084000	0.542070
C	-2.566760	2.478660	-1.637180

H	-3.008740	3.456250	-1.859780
H	-1.596450	2.669350	-1.173970
H	-2.415280	1.960670	-2.586790
C	-3.605430	2.506840	0.638770
H	-2.624040	2.693770	1.071950
H	-4.086630	3.469720	0.434400
H	-4.213540	1.957640	1.363670
O	-0.307810	3.093100	1.101790



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.411  
7.399  
7.331  
7.320  
7.240  
7.193  
7.182  
7.171  
7.082  
7.071  
7.061  
6.688  
6.678  
6.668

5.138  
5.128

1.539  
1.494  
1.487  
1.482  
1.475  
1.468  
1.463  
1.456  
0.887  
0.880  
0.876  
0.869  
0.865  
0.860

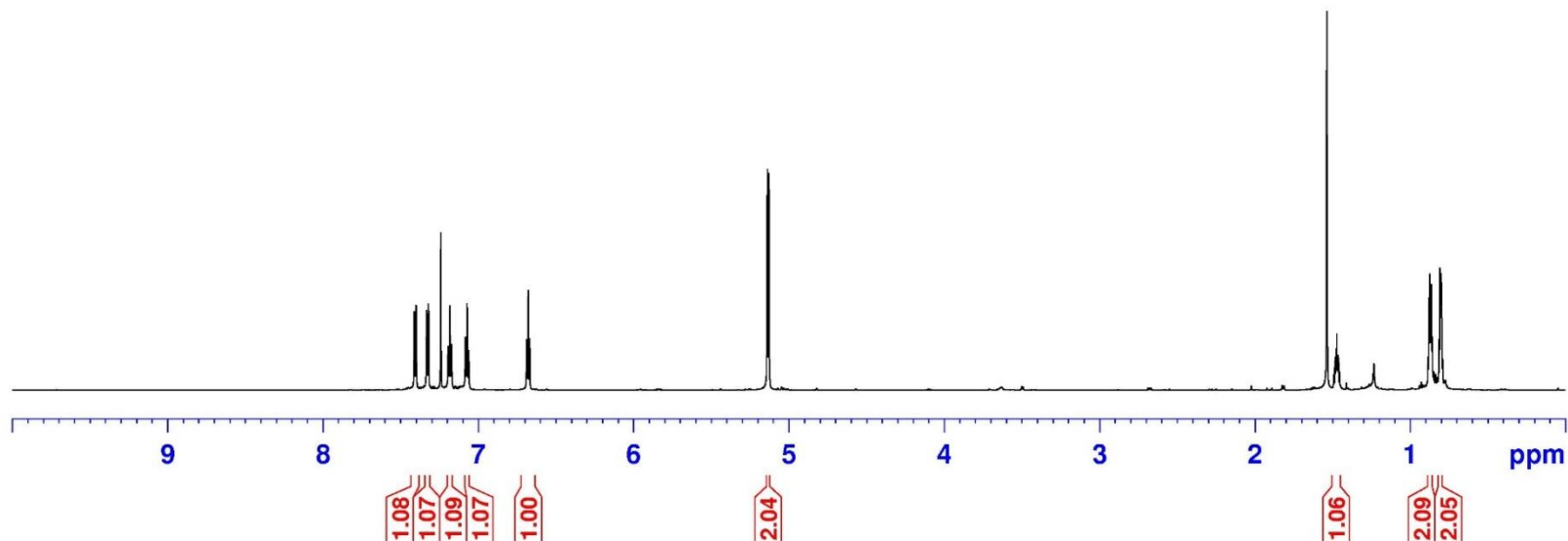
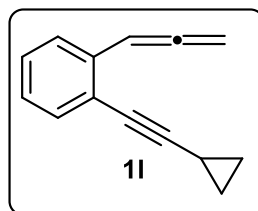
CM-01-101

Current Data Parameters

NAME 1  
EXPNO 1  
PROCNO 1

F2 - Processing parameters

SI 65536  
SF 699.7434520 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

210.39

135.30  
132.35  
127.63  
126.45  
126.32  
121.63

98.36

92.11

78.63  
77.18  
77.00  
76.82  
73.74

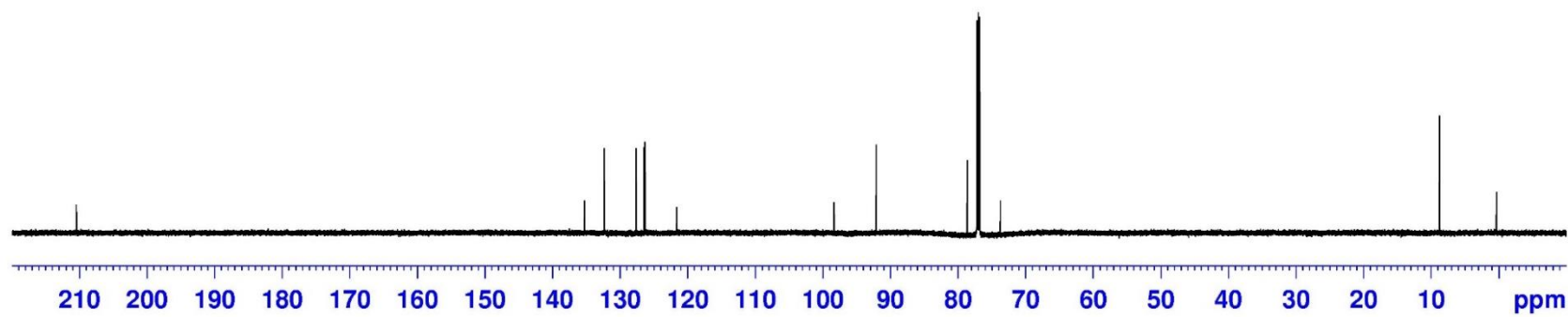
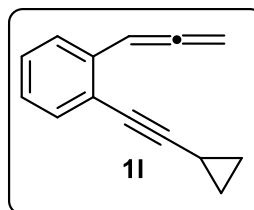
8.77

0.33

CM-01-101

Current Data Parameters  
NAME 3  
EXPNO 3  
PROCNO 1

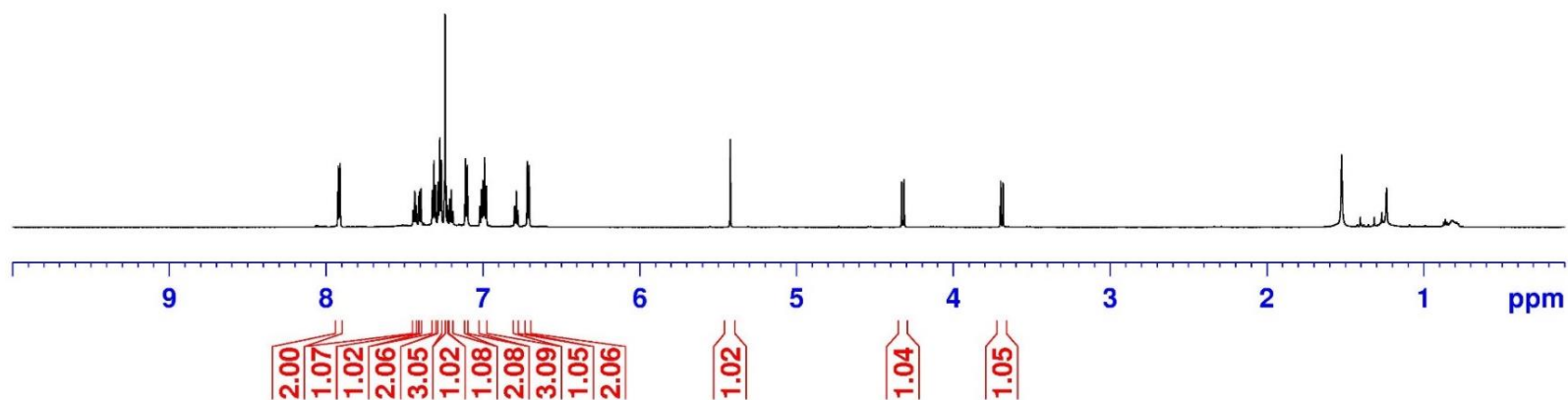
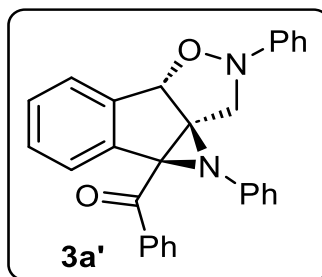
F2 - Processing parameters  
SI 131072  
SF 175.9532178 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



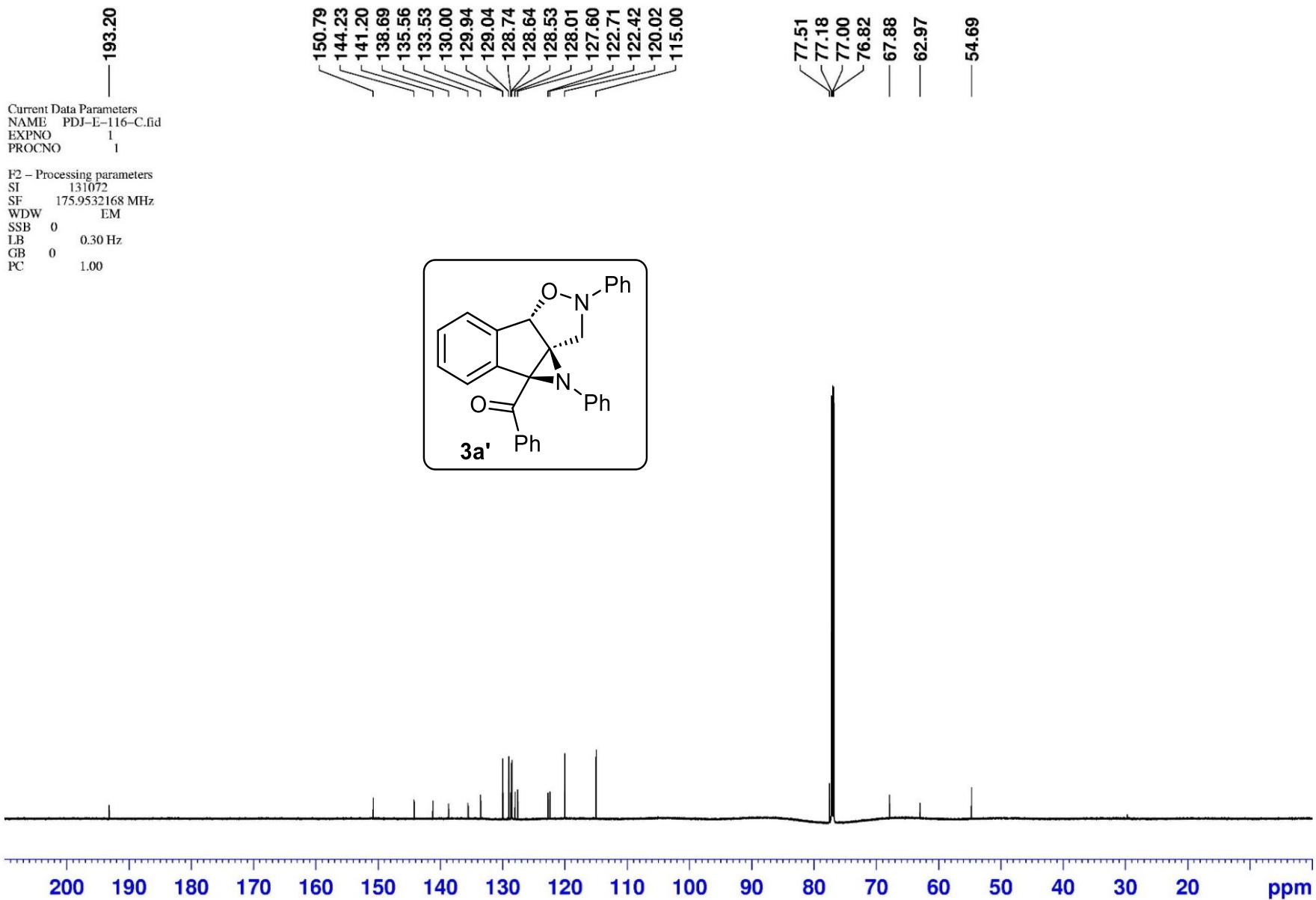
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.922  
7.910  
7.444  
7.433  
7.423  
7.405  
7.395  
7.322  
7.311  
7.300  
7.285  
7.274  
7.264  
7.240  
7.235  
7.224  
7.212  
7.201  
7.191  
7.110  
7.099  
7.018  
7.008  
6.999  
6.988  
6.977  
6.797  
6.787  
6.776  
6.716  
6.705  
5.421  
4.328  
4.313  
3.697  
3.682  
1.522

Current Data Parameters  
NAME PDJ-E-116-H.fid  
EXPNO 1  
PROCNO 1  
F2 - Processing parameters  
SI 65536  
SF 699.7438008 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)



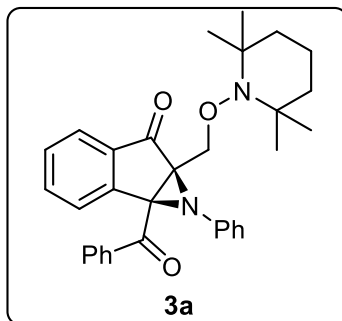
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)

8.014  
8.012  
7.994  
7.528  
7.526  
7.507  
7.491  
7.488  
7.486  
7.470  
7.469  
7.450  
7.379  
7.377  
7.361  
7.358  
7.342  
7.339  
7.243  
7.240  
7.227  
7.225  
7.203  
7.201  
7.185  
7.182  
7.166  
6.995  
6.976  
6.956  
6.789  
6.787  
6.769  
6.683  
6.681  
6.662  
4.636  
4.610  
4.248  
4.222  
1.559  
1.402  
1.378  
1.350  
1.312  
1.277  
1.264  
1.235  
1.174  
0.963  
0.859  
0.653

CM-01-207

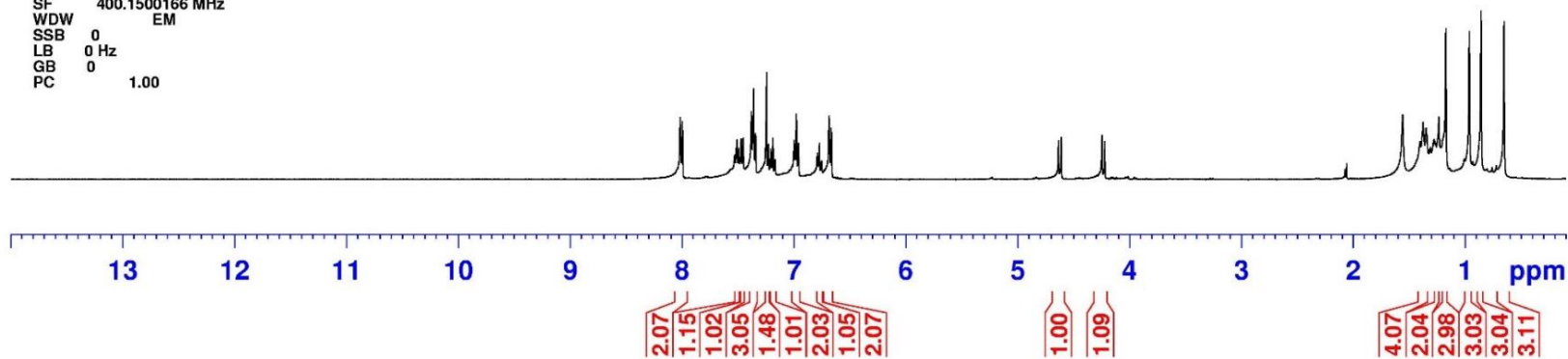
Current Data Parameters  
NAME CM-01-207  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211221  
Time 16.09  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 92  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559039 sec  
RG 512  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 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 400.1500166 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.33  
192.16

145.43  
144.62  
135.47  
134.60  
133.64  
133.44  
130.05  
129.16  
128.63  
128.44  
127.61  
124.86  
122.80  
120.19

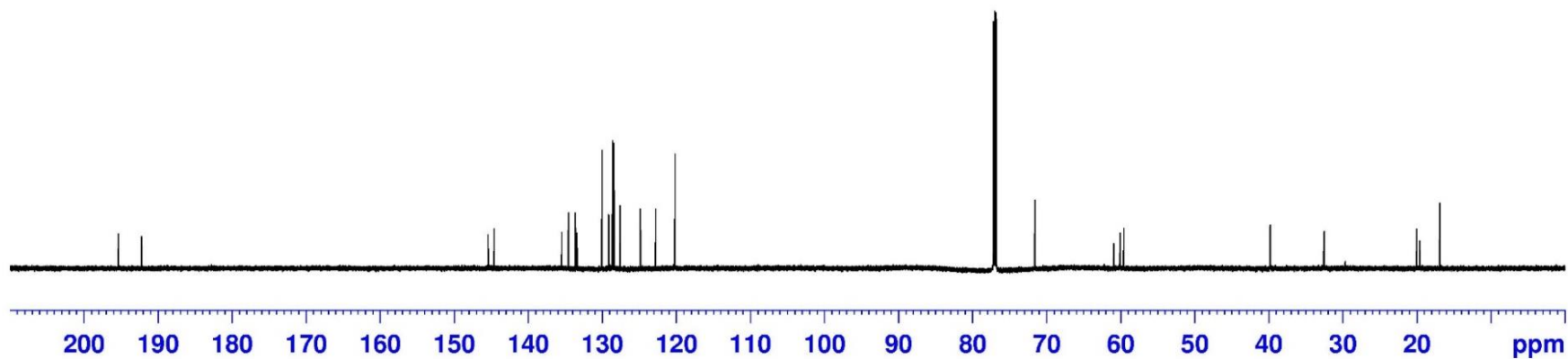
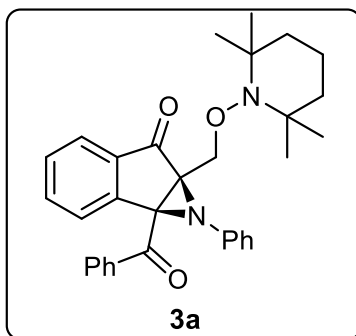
77.18  
77.00  
76.82  
71.60  
60.94  
60.09  
60.07  
59.59

39.85  
39.82  
32.56  
32.51  
20.03  
19.63  
16.92

CM-1-207-down

Current Data Parameters  
NAME CM-1-207-down-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532190 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)

8.006  
7.984  
7.457  
7.439  
7.388  
7.386  
7.370  
7.367  
7.351  
7.272  
7.253  
7.240  
7.198  
7.179  
7.161  
6.991  
6.972  
6.952  
6.842  
6.819  
6.783  
6.781  
6.762  
6.746  
6.744  
6.716  
6.687  
6.685  
6.666  
4.596  
4.570  
4.227  
4.201  
3.809

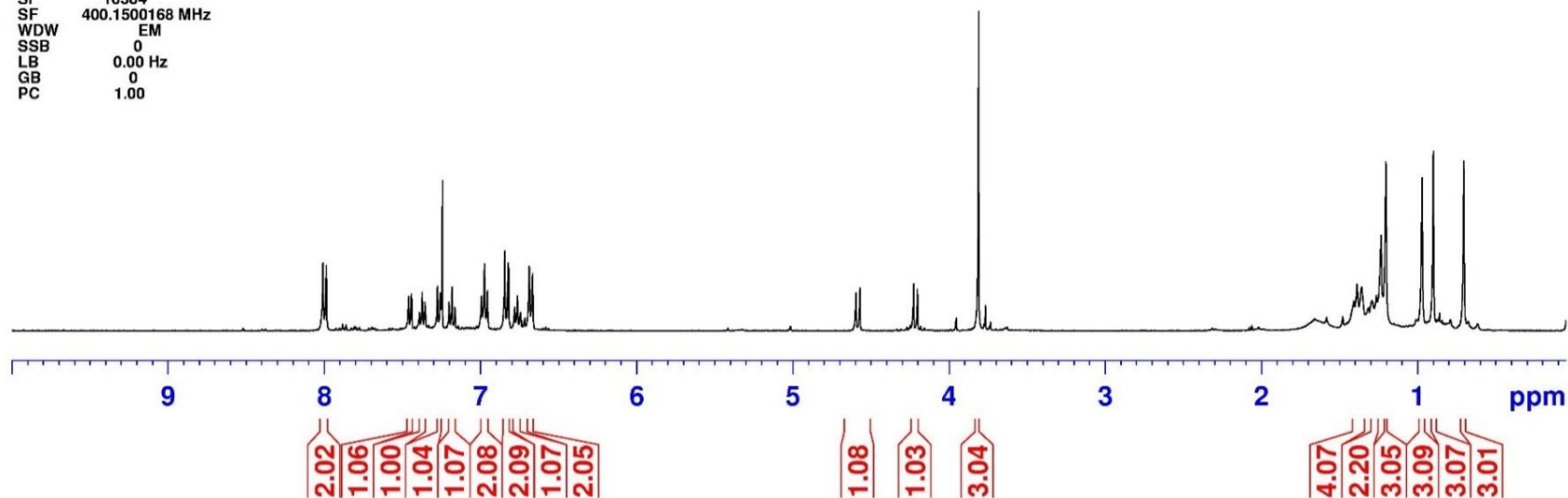
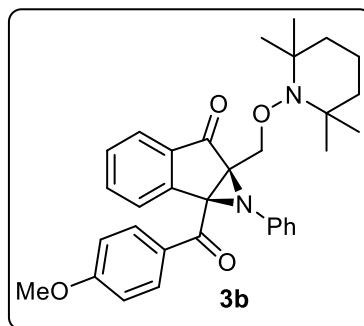
1.581  
1.478  
1.448  
1.407  
1.386  
1.358  
1.334  
1.311  
1.290  
1.262  
1.201  
0.970  
0.897  
0.702

Current Data Parameters  
NAME CM-01-240  
EXPNO 4  
PROCNO 1

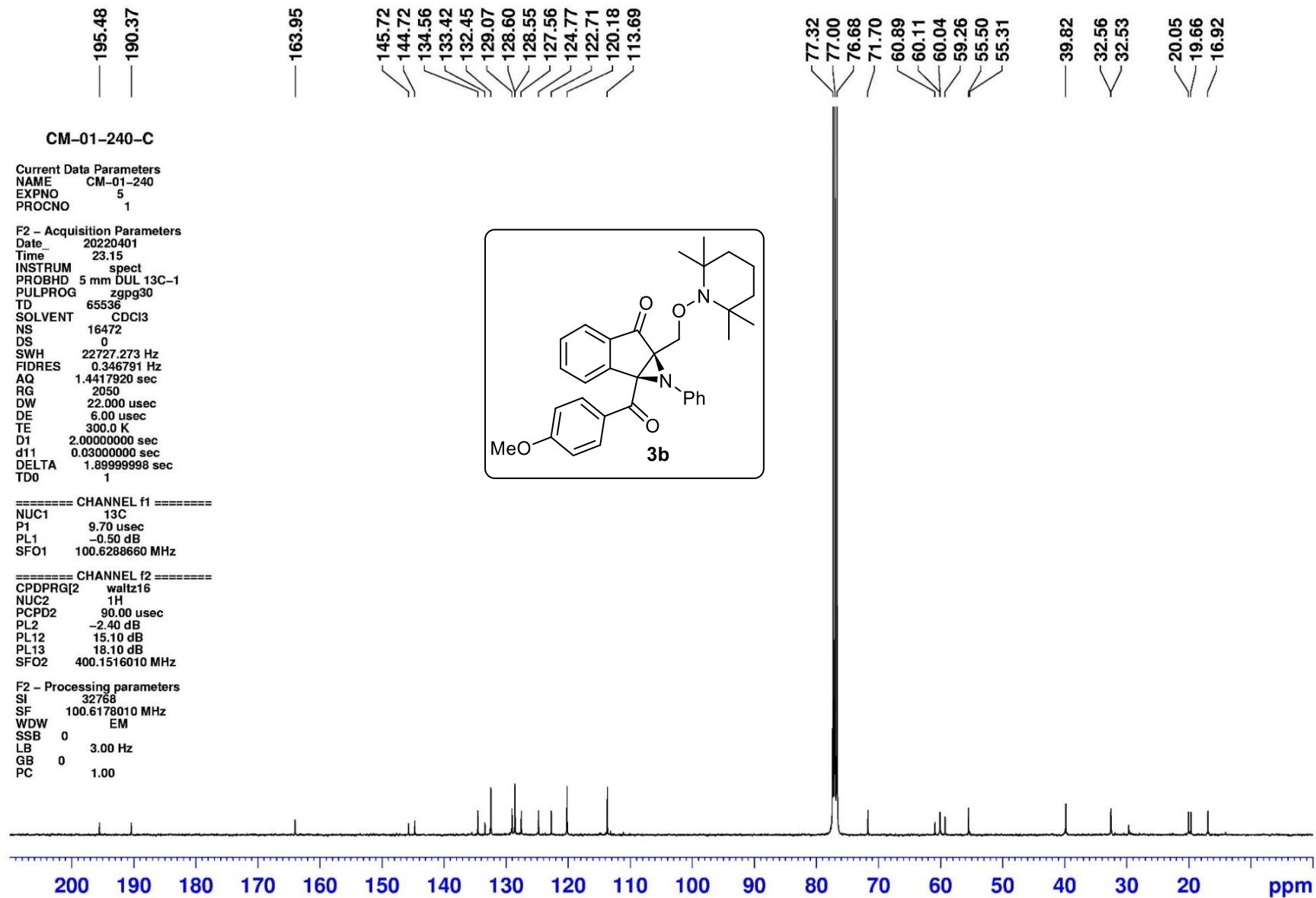
F2 - Acquisition Parameters  
Date 20220401  
Time 16.41  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 42  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 575  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 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 0.00 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 100 MHz)





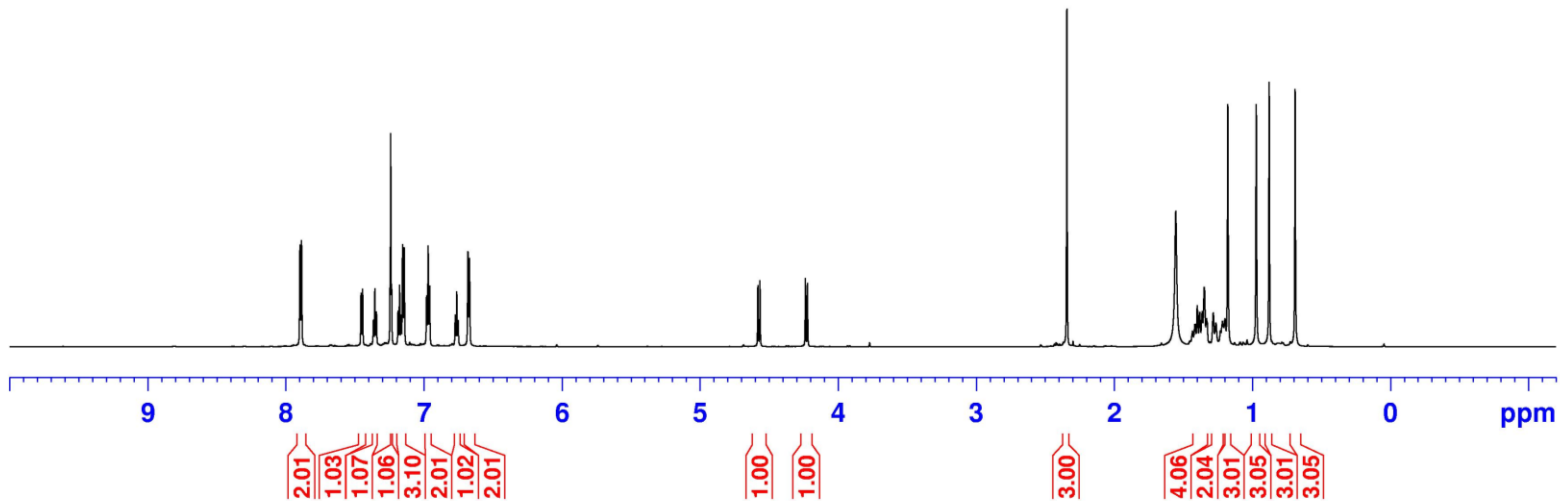
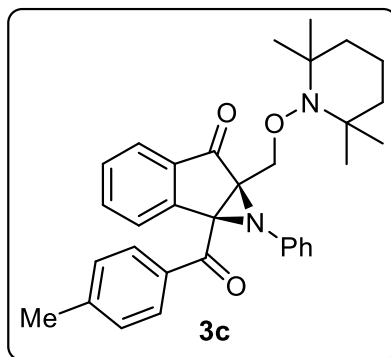
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.897 7.886 7.455 7.444 7.364 7.355 7.354 7.344 7.343 7.240 7.234 7.186 7.176 7.165 7.154 7.142 6.980 6.969 6.958 6.772 6.762 6.751 6.680 6.669 4.581 4.566 4.236 4.221 2.346 1.557 1.455 1.450 1.437 1.419 1.401 1.383 1.365 1.351 1.334 1.329 1.313 1.285 1.269 1.266 1.234 1.219 1.201 1.180 0.975 0.881 0.693

CM-2-67

Current Data Parameters  
NAME CM-2-67-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7437994 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.46  
191.64

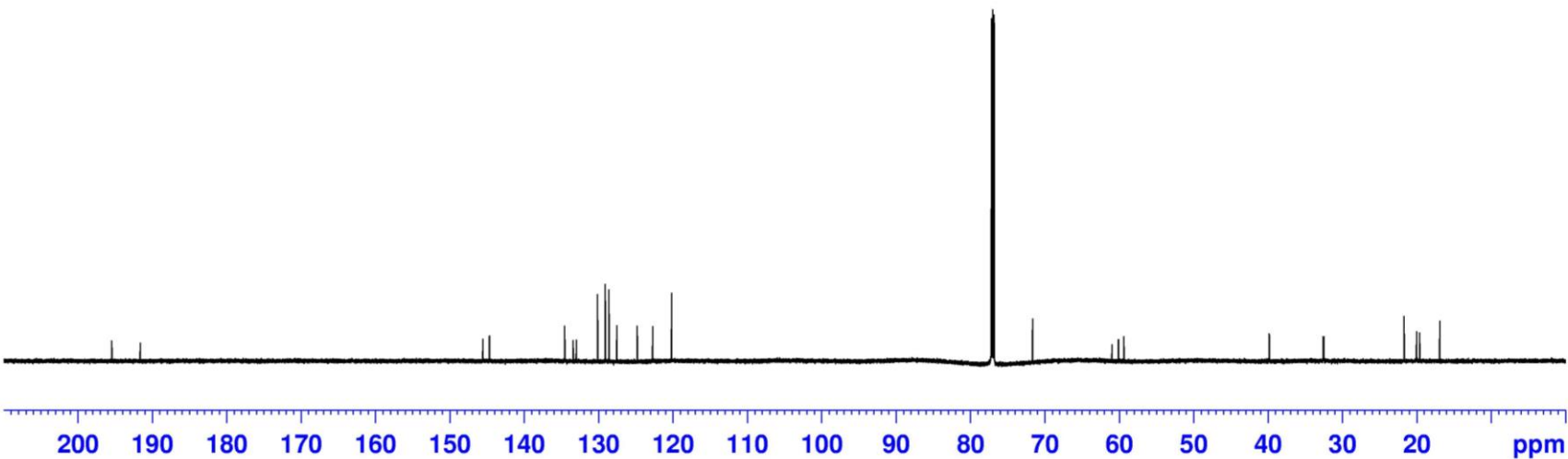
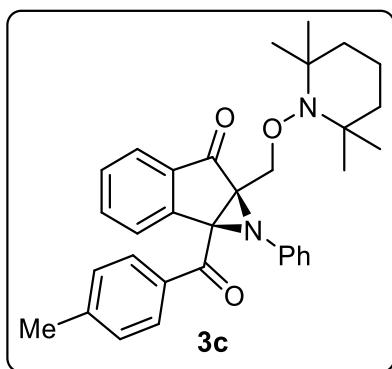
145.58  
144.71  
144.68  
134.57  
133.43  
132.99  
130.16  
129.12  
129.10  
128.60  
127.57  
124.80  
122.74  
120.20

77.18  
77.00  
76.82  
71.66  
60.98  
60.10  
60.06  
59.39

39.85  
39.82  
32.57  
32.51  
21.71  
20.04  
19.61  
16.93

CM-2-67

Current Data Parameters  
NAME CM-2-67-C.fid  
EXPNO 1  
PROCNO 1  
  
F2 - Processing parameters  
SI 131072  
SF 175.9514590 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



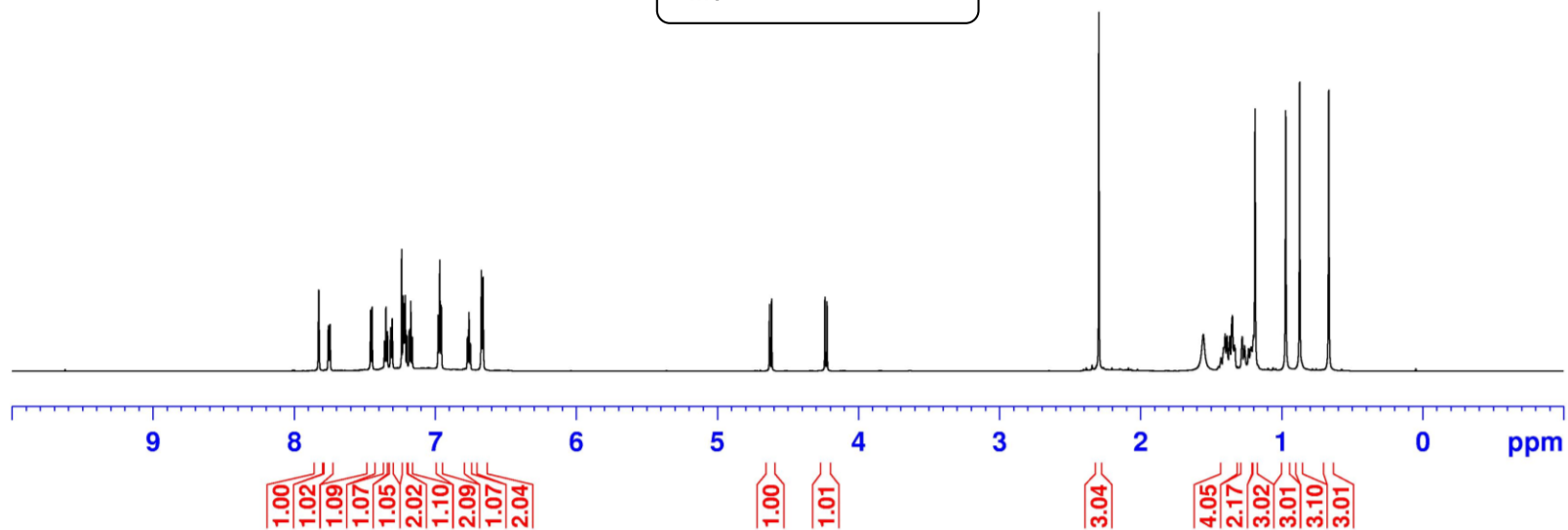
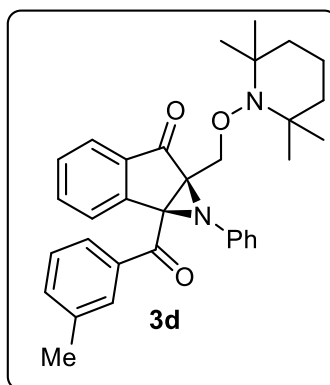
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.827  
7.759  
7.748  
7.460  
7.449  
7.362  
7.351  
7.340  
7.317  
7.307  
7.240  
7.231  
7.225  
7.220  
7.214  
7.203  
7.186  
7.175  
7.165  
6.981  
6.970  
6.959  
6.774  
6.763  
6.753  
6.674  
6.663  
4.632  
4.617  
4.239  
4.225  
2.297  
1.557  
1.432  
1.415  
1.409  
1.403  
1.389  
1.369  
1.351  
1.336  
1.332  
1.314  
1.281  
1.266  
1.235  
1.223  
1.219  
1.191  
0.973  
0.874  
0.668

CM-2-64

Current Data Parameters  
NAME CM-2-64-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7437998 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.41  
192.36

145.52  
144.65  
138.22  
135.48  
134.56  
134.41  
133.36  
130.31  
129.09  
128.59  
128.24  
127.62  
127.46  
124.81  
122.76  
120.18

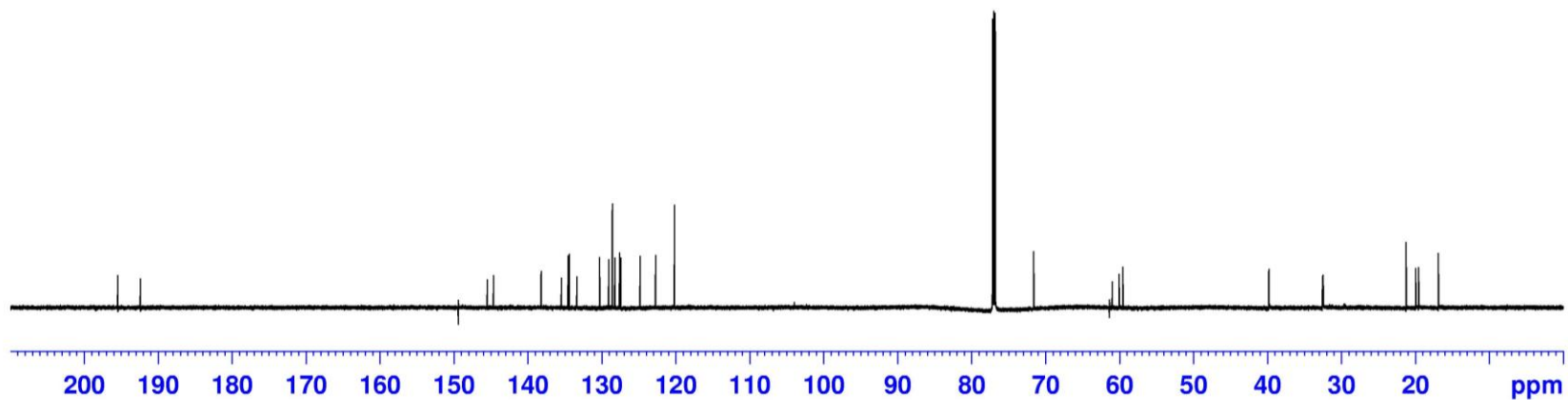
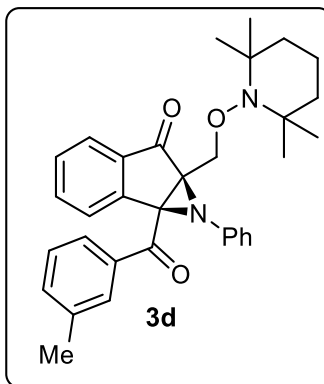
77.18  
77.00  
76.82  
71.63  
61.00  
60.09  
60.07  
59.57

39.84  
39.81  
32.57  
32.48  
21.27  
19.97  
19.57  
16.91

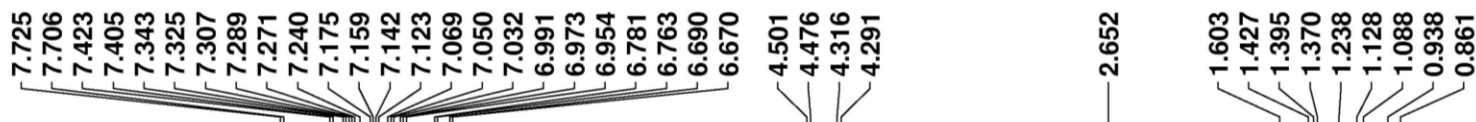
CM-2-64

Current Data Parameters  
NAME CM-2-64-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523419 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



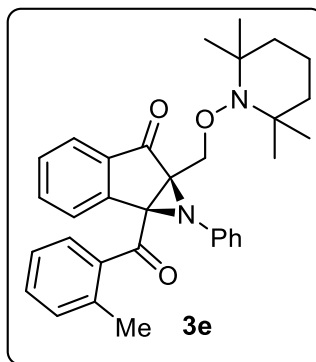
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)



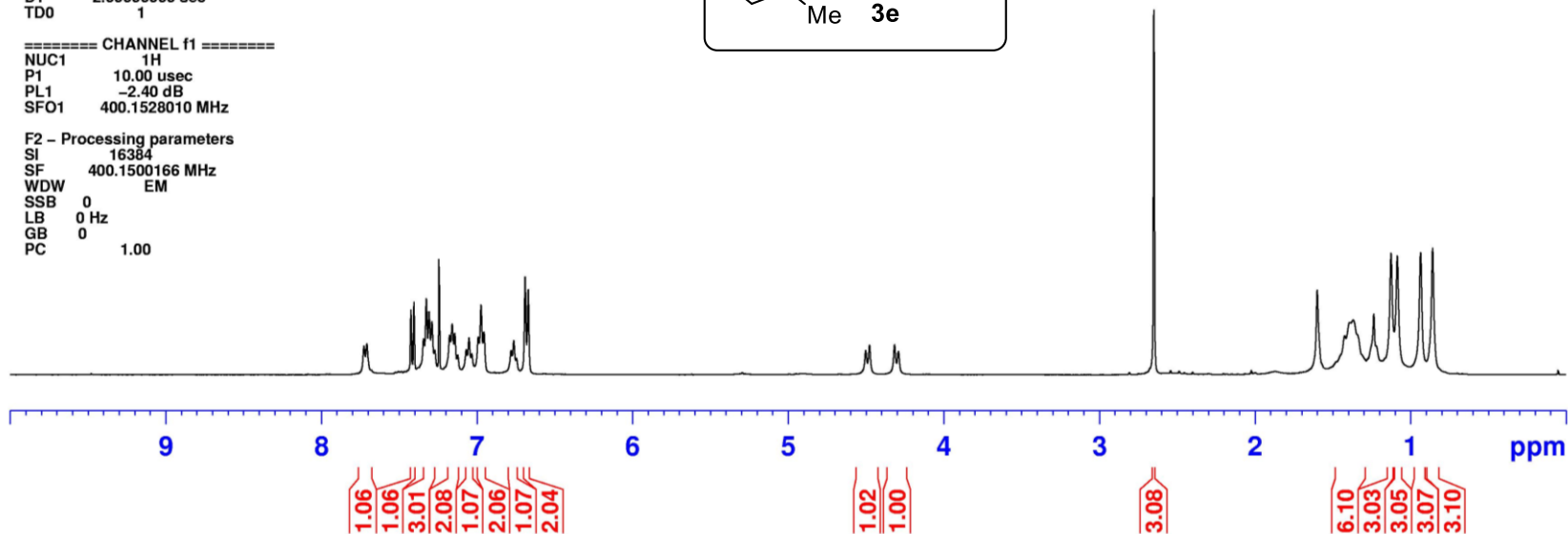
CM-02-70

Current Data Parameters  
NAME CM-02-70  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231011  
Time 23.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 227  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559039 sec  
RG 362  
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 400.1500166 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.30  
194.65

145.08  
144.78  
139.64  
135.17  
134.40  
133.42  
132.07  
132.02  
131.32  
128.96  
128.60  
127.65  
125.39  
124.72  
122.75  
120.17

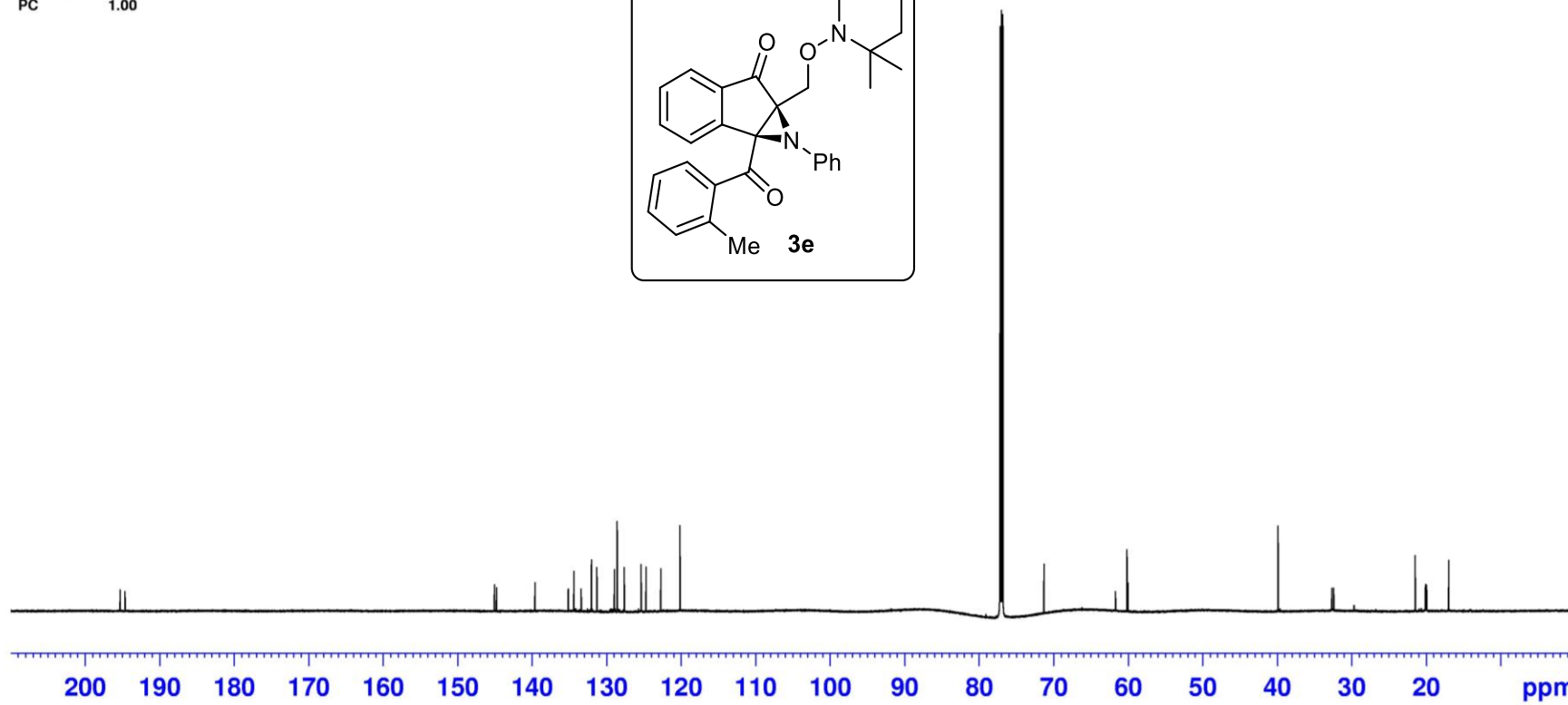
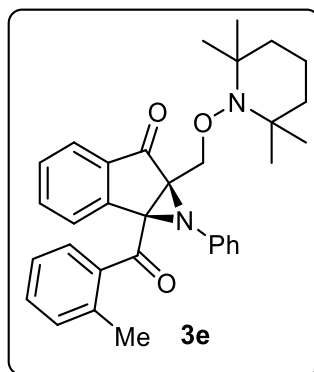
77.18  
77.00  
76.82  
71.32  
61.70  
60.16  
60.02

39.88  
32.67  
32.42  
21.49  
20.11  
19.95  
16.98

CM-2-70

Current Data Parameters  
NAME CM-2-70-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9514587 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



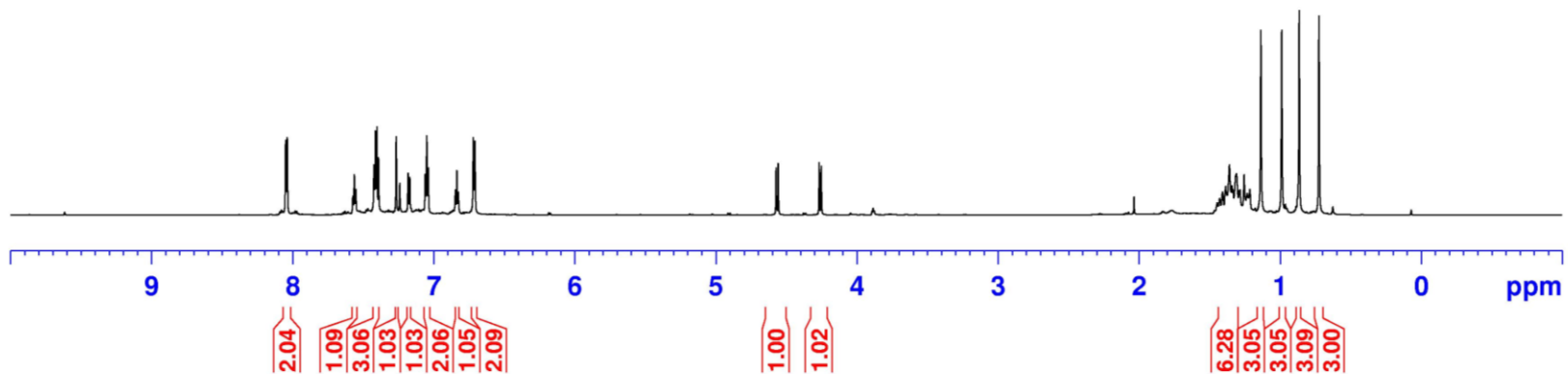
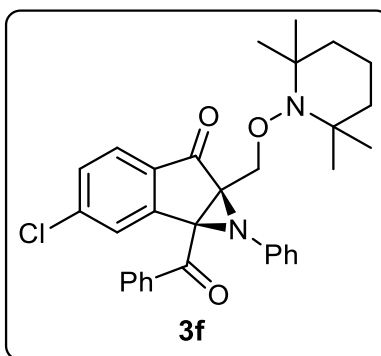
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-63-r

Current Data Parameters  
NAME CM-2-63-r-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7378458 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

193.54  
191.11

146.48  
143.81  
140.77  
134.89  
133.54  
131.41  
129.61  
129.39  
128.48  
128.22  
127.41  
125.49  
122.68  
119.66

77.18  
77.00  
76.82  
70.97  
59.87  
59.70  
59.30

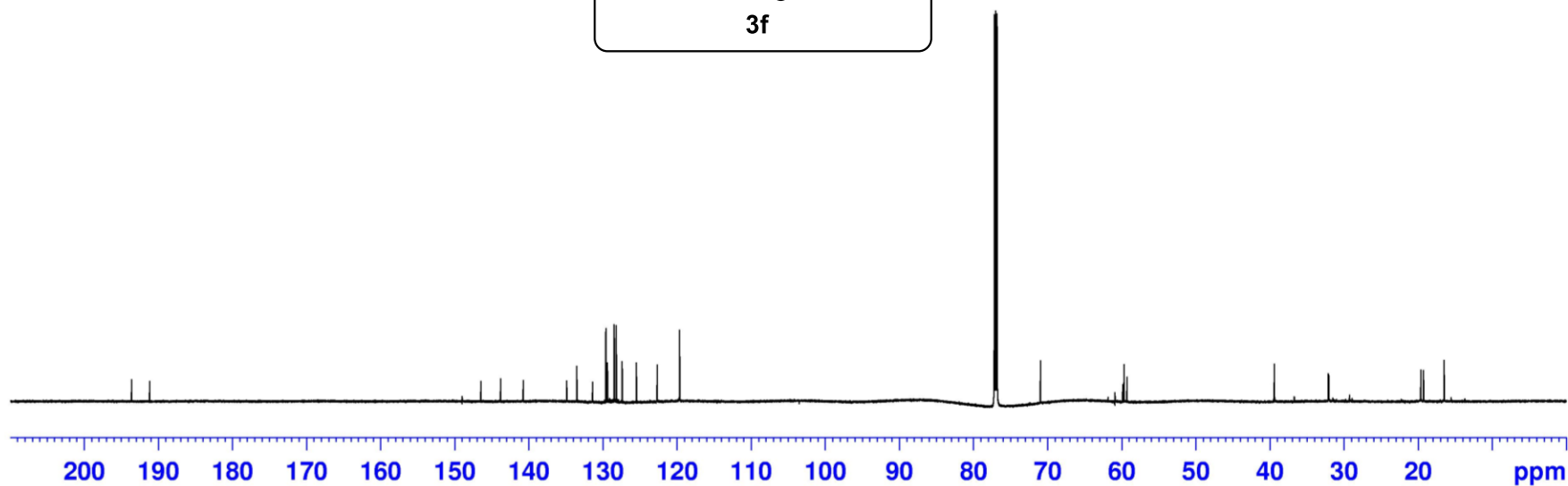
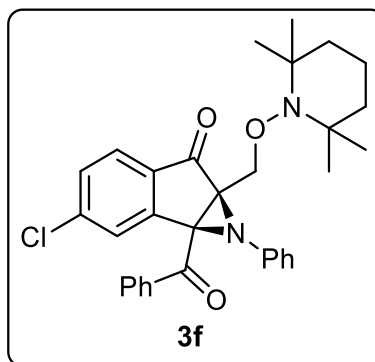
39.41  
39.40  
32.13  
32.06

19.63  
19.27  
16.50

CM-2-63

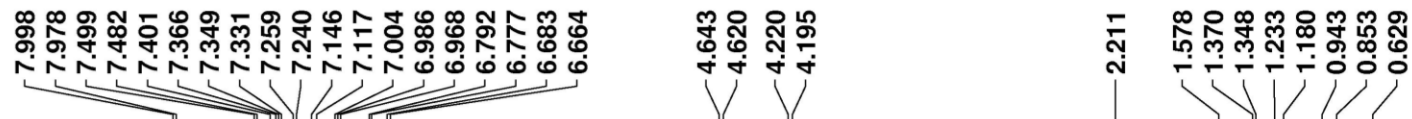
Current Data Parameters  
NAME CM-2-63-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9524156 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)



CM-02-62

Current Data Parameters

NAME CM-02-62  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters

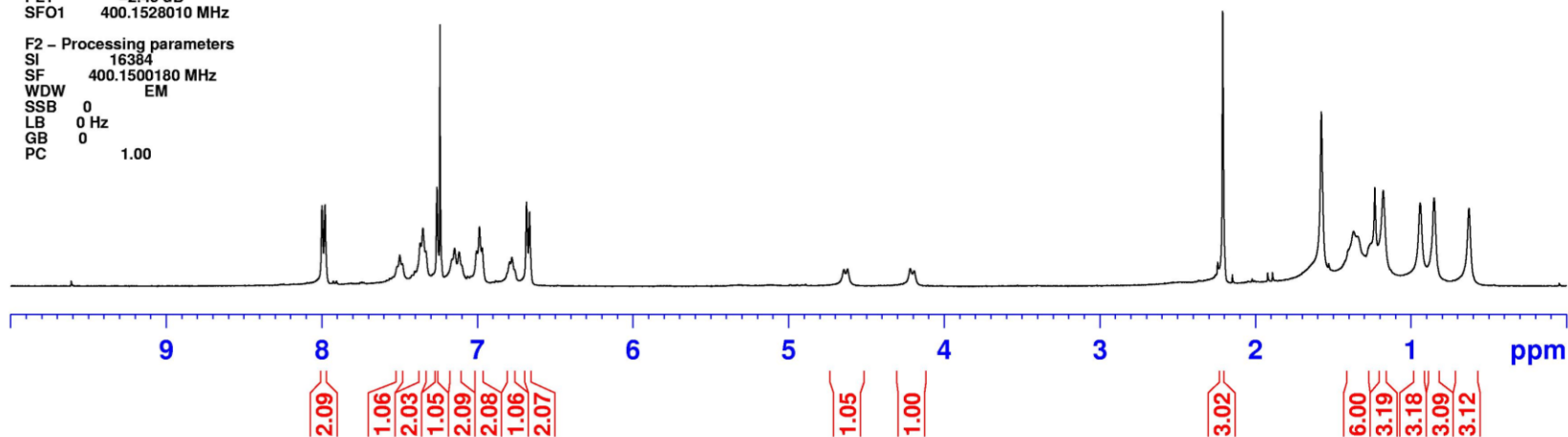
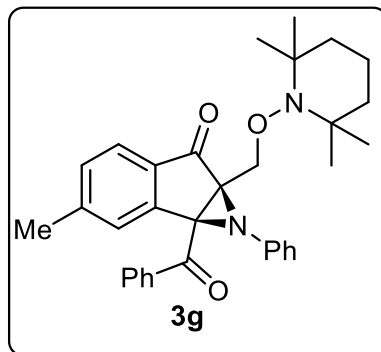
Date\_ 20231003  
Time 23.14  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 119  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559039 sec  
RG 512  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 16384  
SF 400.1500180 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.51  
192.35

144.76  
142.85  
139.35  
135.49  
135.47  
133.66  
133.54  
130.05  
128.61  
128.37  
127.32  
125.14  
122.72  
120.19

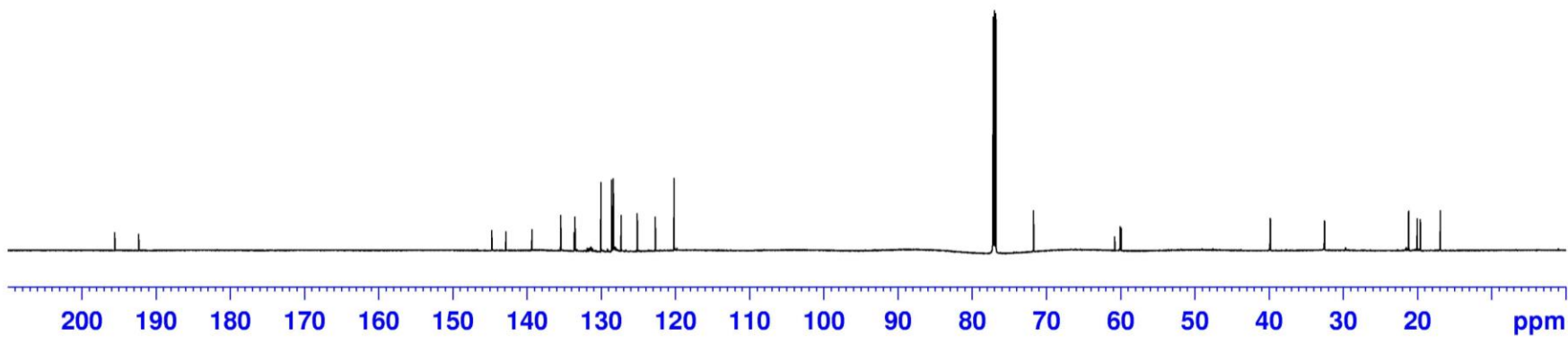
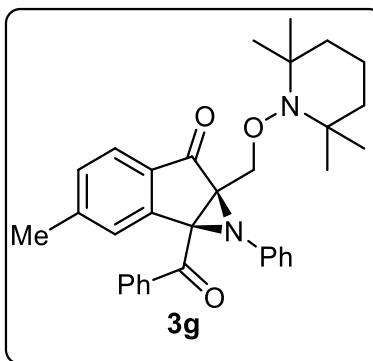
77.18  
77.00  
76.82  
71.73  
60.79  
60.07  
60.05  
59.92

39.86  
39.82  
32.55  
32.51  
21.18  
20.02  
19.60  
16.91

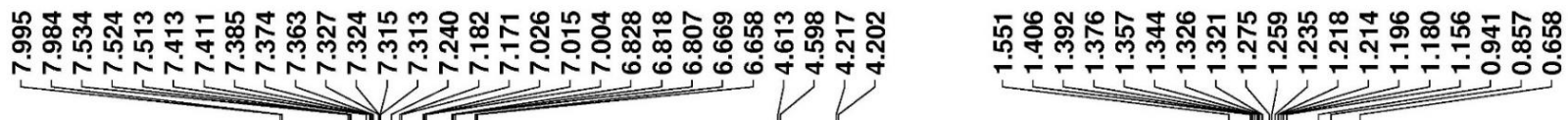
CM-2-62

Current Data Parameters  
NAME CM-2-62-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532190 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



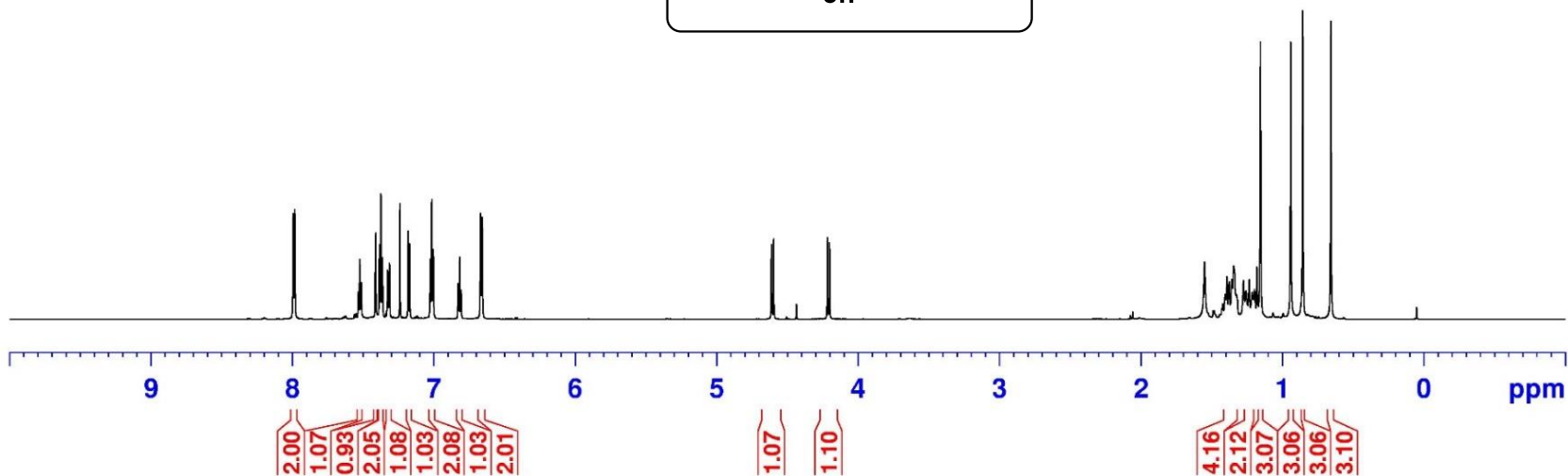
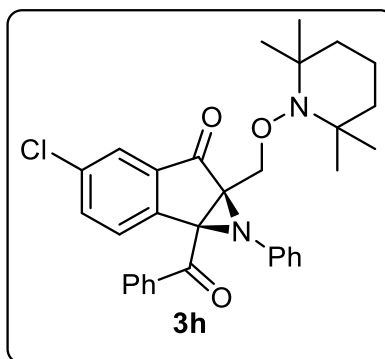
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-1-234

Current Data Parameters  
NAME CM-1-234-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441513 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.06  
191.68

144.20  
143.60  
135.33  
135.32  
135.04  
134.43  
133.80  
130.02  
128.87  
128.66  
128.52  
124.85  
123.16  
120.06

77.18  
77.00  
76.82  
71.47  
60.41  
60.14  
60.11  
60.08

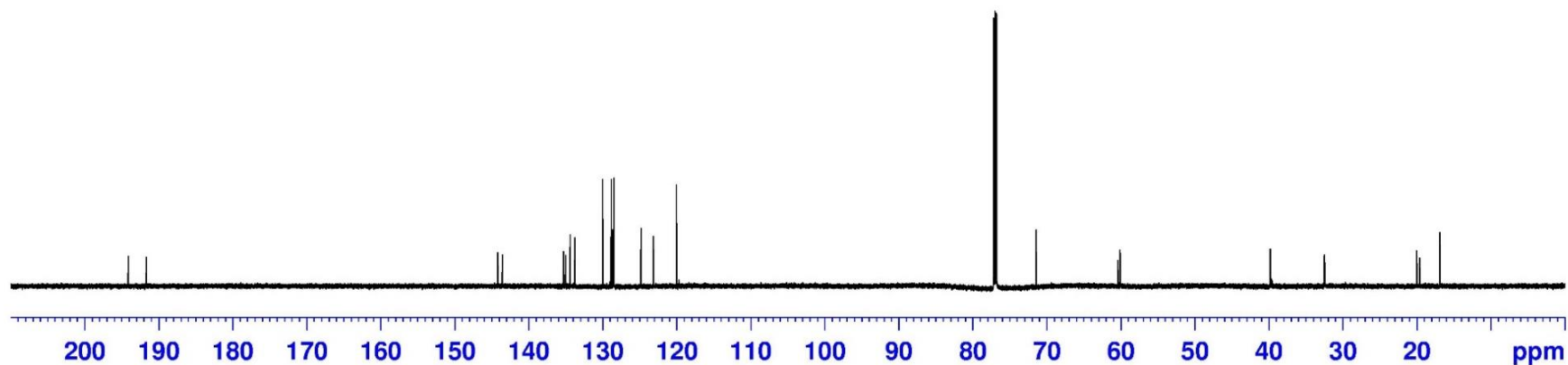
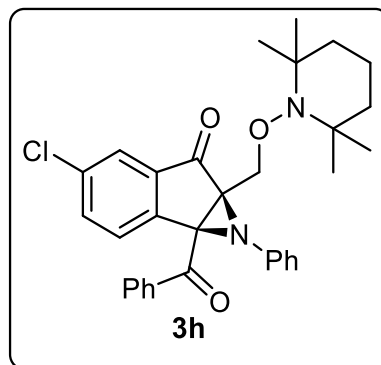
39.84  
39.81  
32.54  
32.47

20.02  
19.62  
16.89

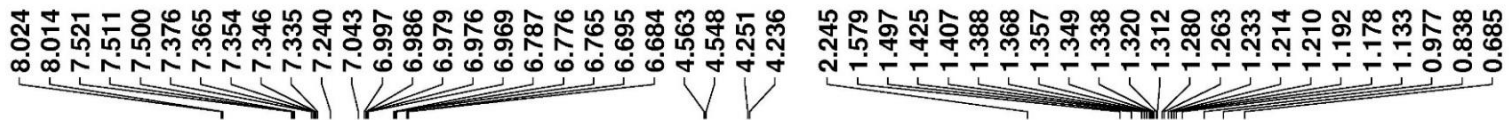
CM-1-234

Current Data Parameters  
NAME CM-1-234-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532211 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



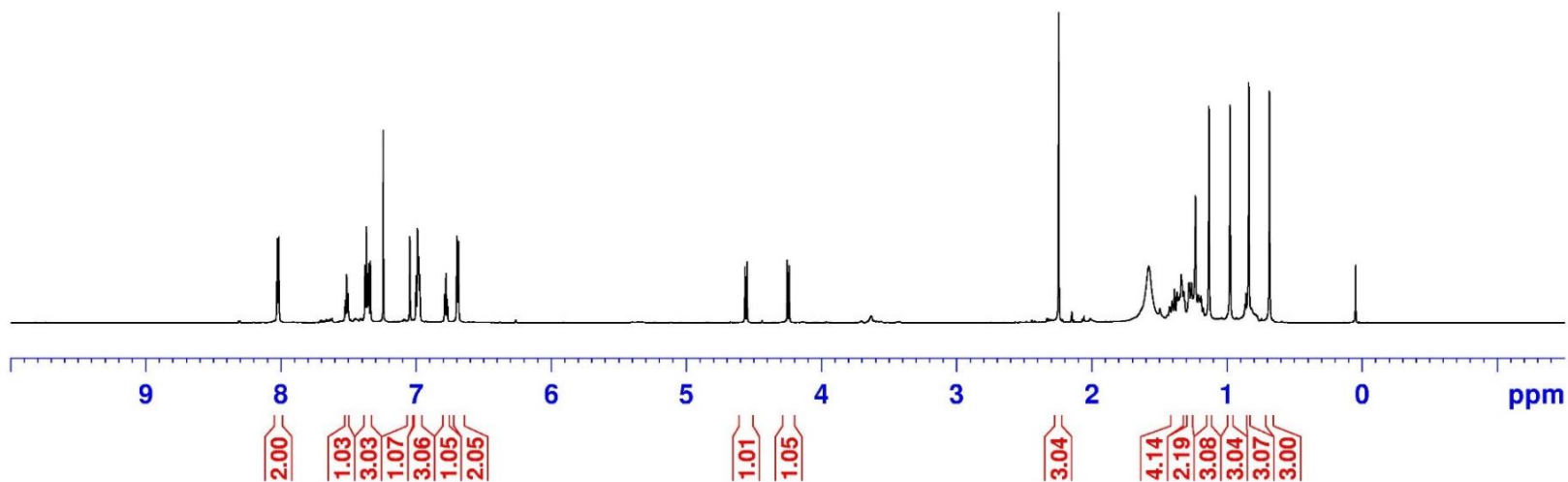
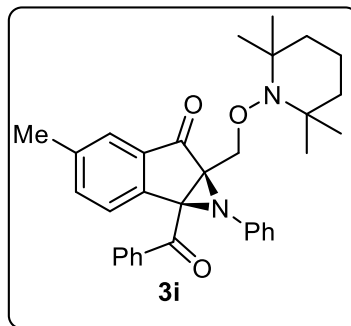
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-1-233-r

Current Data Parameters  
NAME CM-1-233-r-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441504 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.98  
192.27

146.05  
145.81  
144.77  
135.49  
133.63  
131.10  
130.11  
130.04  
128.60  
128.46  
128.06  
124.75  
122.70  
120.17

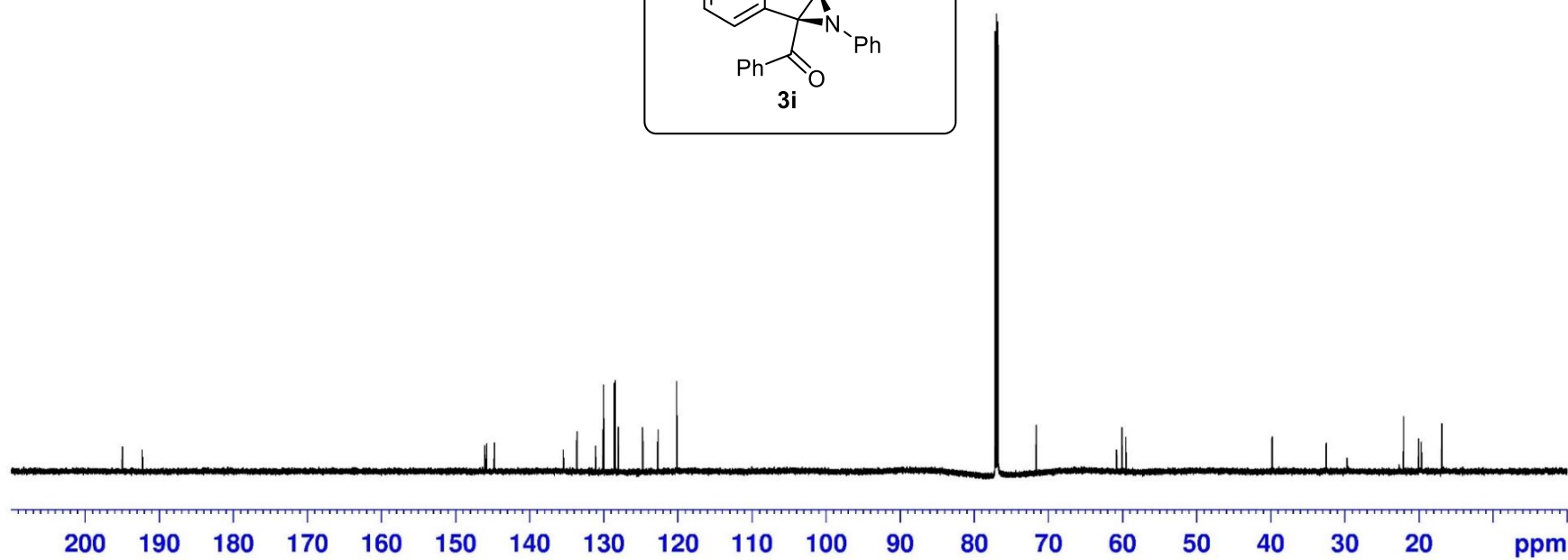
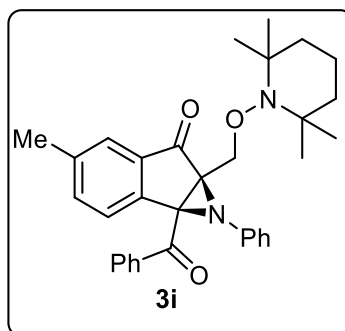
77.18  
77.00  
76.82  
71.66  
60.79  
60.07  
59.57

39.84  
39.81  
32.54  
32.50  
22.07  
20.03  
19.67  
16.93

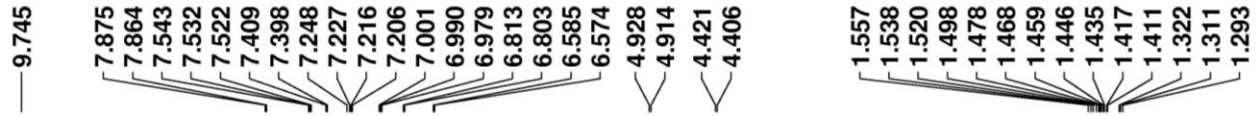
CM-1-233-r

Current Data Parameters  
NAME CM-1-233-r-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532175 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



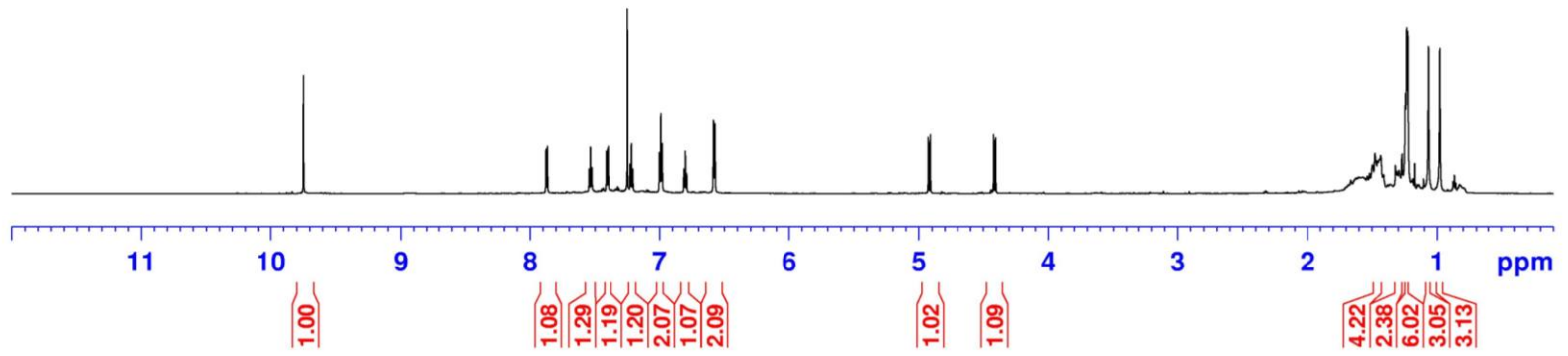
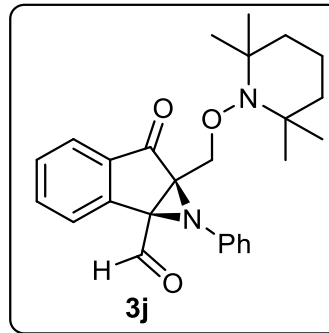
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-1-109

Current Data Parameters  
NAME CM-1-109-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441114 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.40  
194.35

144.04  
141.62  
134.67  
134.03  
129.29  
128.81  
128.33  
124.67  
123.40  
120.27

77.18  
77.00  
76.82  
71.97  
60.27  
60.05  
59.79

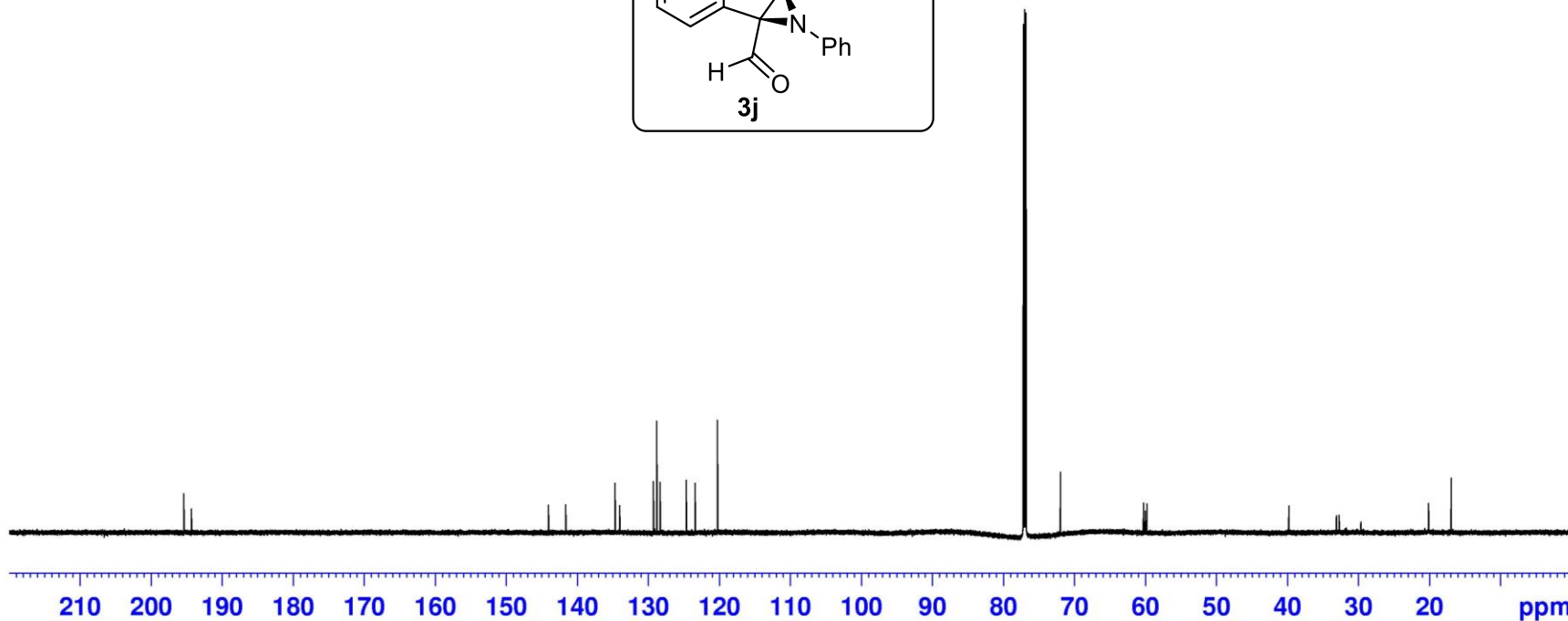
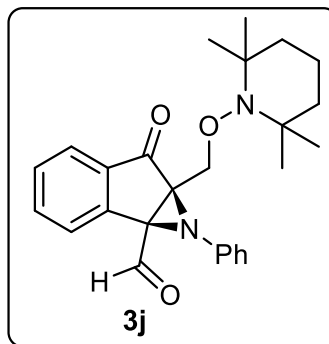
39.80  
39.78  
33.11  
32.72

20.13  
16.95

CM-1-109

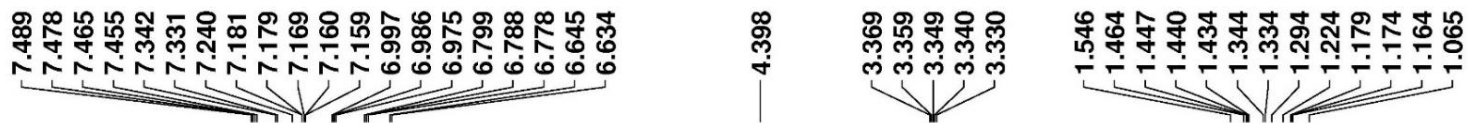
Current Data Parameters  
NAME CM-1-109-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532212 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





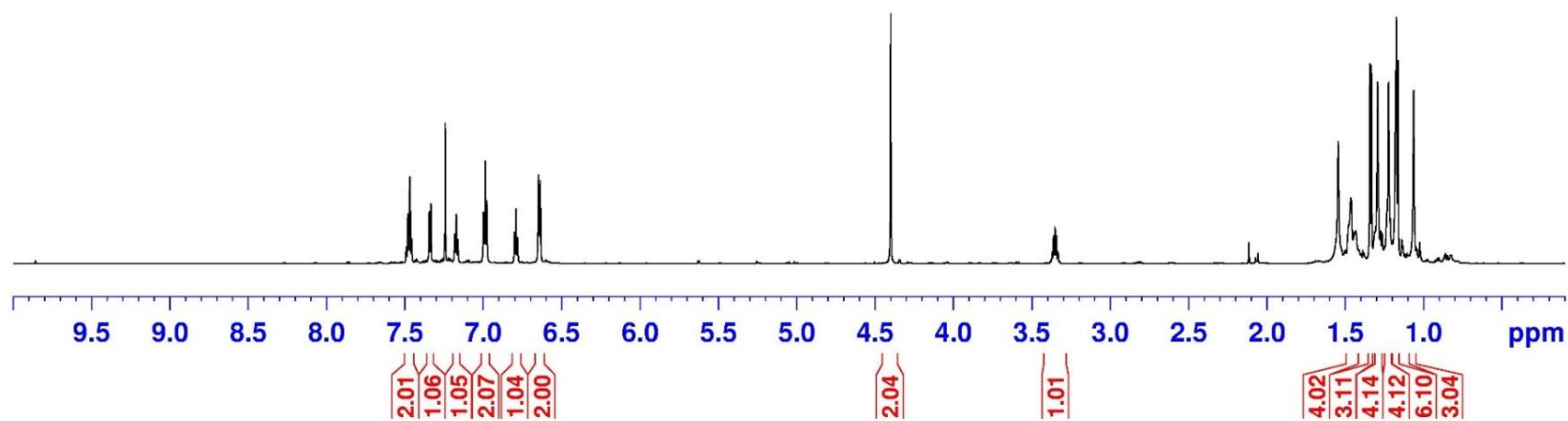
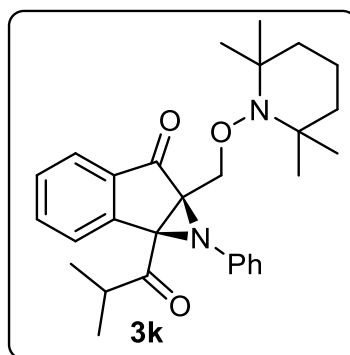
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-1-244

Current Data Parameters  
NAME CM-1-244-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7434153 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

208.22  
194.97

144.62  
144.25  
134.38  
133.98  
129.03  
128.74  
127.42  
124.62  
122.92  
120.24

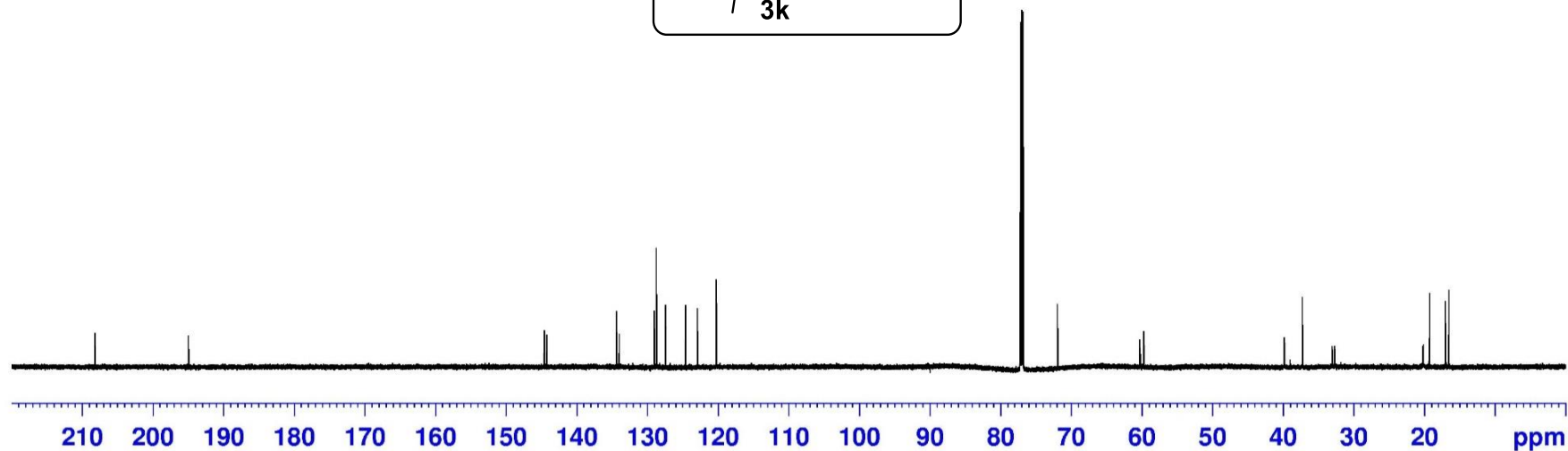
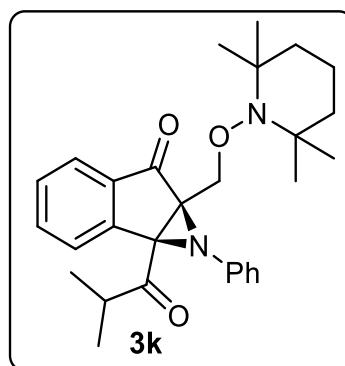
77.18  
77.00  
76.82  
71.94  
60.31  
60.29  
60.25  
59.71

39.86  
39.83  
37.29  
33.06  
32.71  
20.26  
20.15  
19.26  
17.04  
16.53

CM-1-244

Current Data Parameters  
NAME CM-1-244-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532179 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



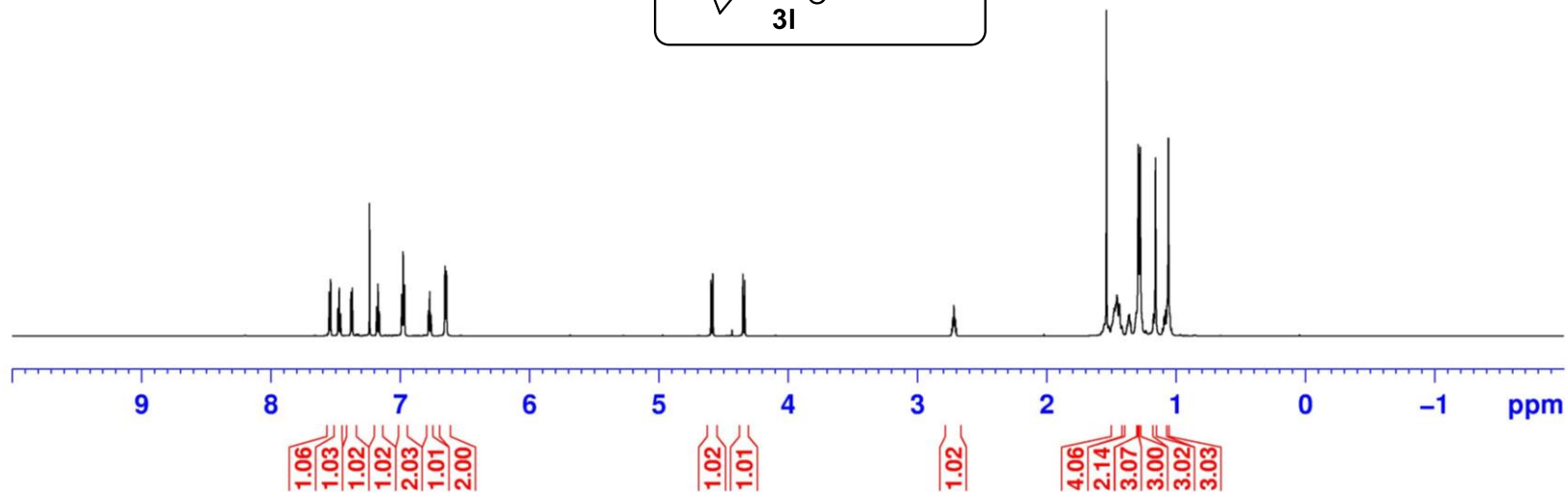
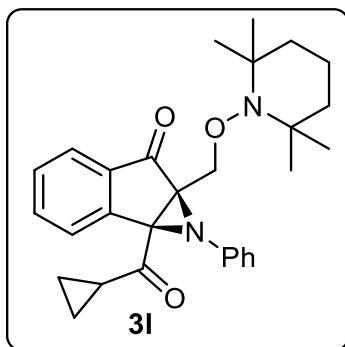
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.548  
7.537  
7.480  
7.470  
7.459  
7.380  
7.369  
7.240  
7.185  
7.174  
7.164  
6.991  
6.980  
6.969  
6.785  
6.774  
6.763  
6.656  
6.645  
4.599  
4.585  
4.352  
4.338  
2.738  
2.731  
2.727  
2.720  
2.714  
2.709  
2.703  
1.541  
1.480  
1.470  
1.459  
1.441  
1.423  
1.394  
1.386  
1.380  
1.375  
1.371  
1.368  
1.365  
1.362  
1.359  
1.356  
1.352  
1.295  
1.280  
1.162  
1.062

CM-2-65

Current Data Parameters  
NAME CM-2-65-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438002 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

203.58  
194.98

144.68  
143.80  
134.32  
134.11  
129.05  
128.68  
127.83  
124.57  
122.91  
120.19

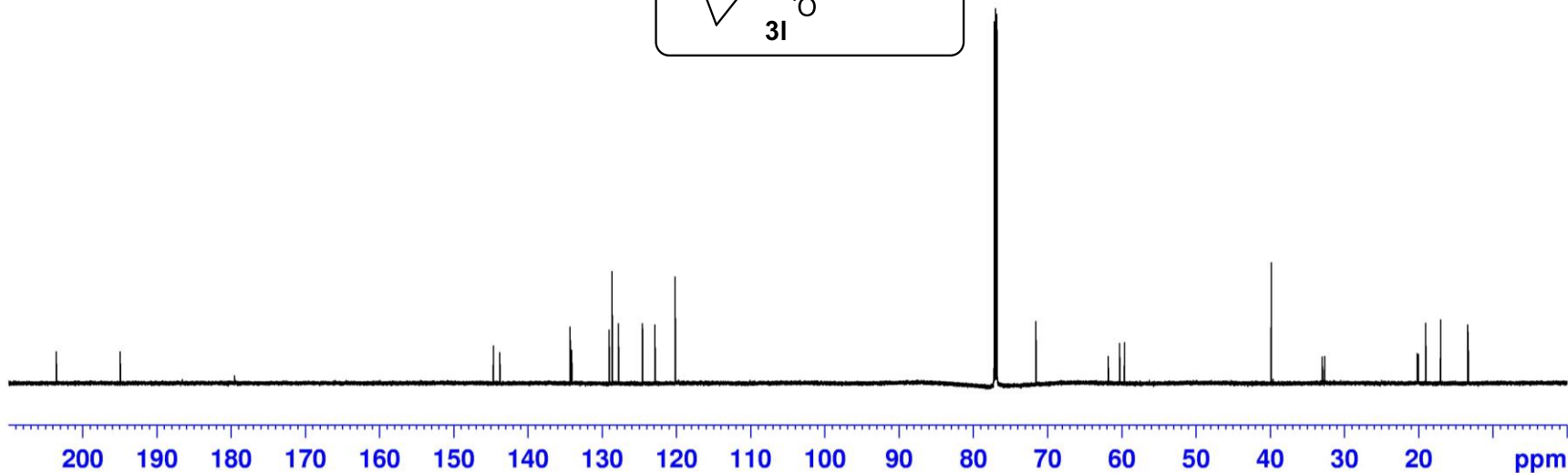
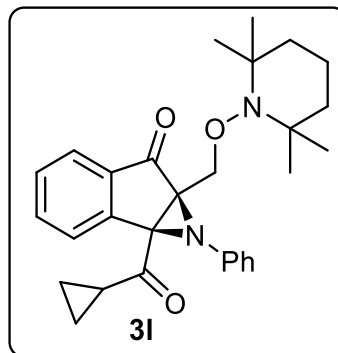
77.18  
77.00  
76.82  
71.55  
61.83  
60.29  
59.64

39.87  
32.99  
32.67  
20.17  
20.04  
19.04  
17.03  
13.40  
13.32

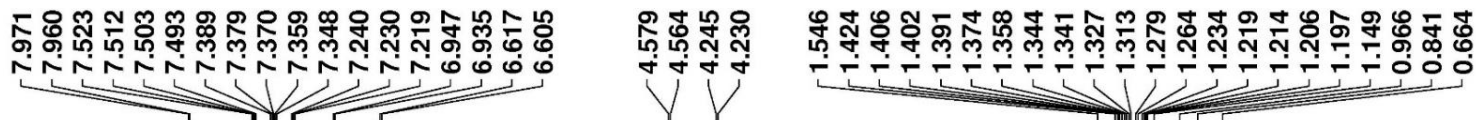
CM-2-65

Current Data Parameters  
NAME CM-2-65-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9514581 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



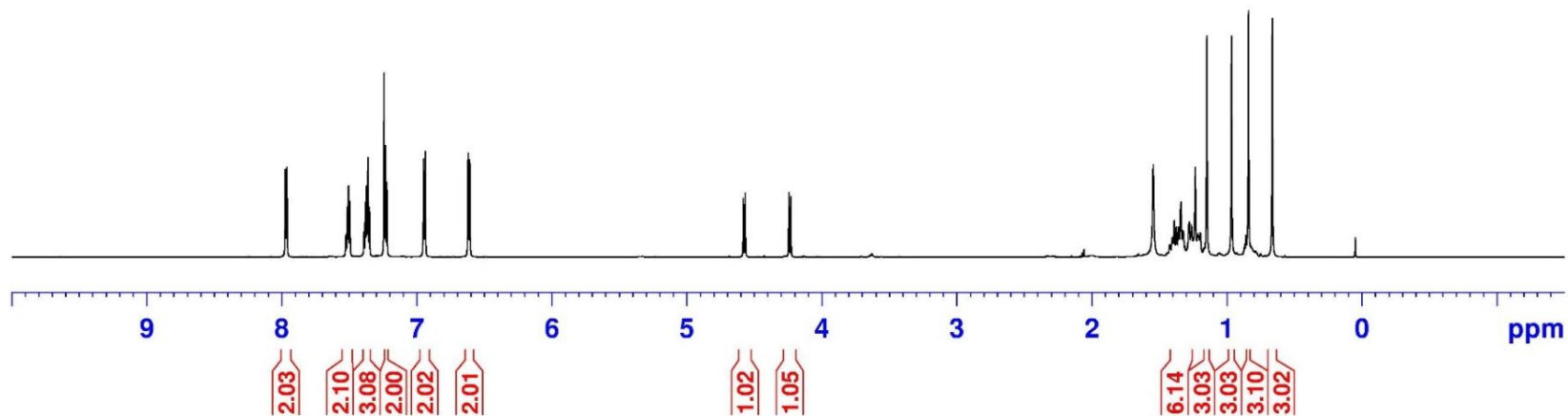
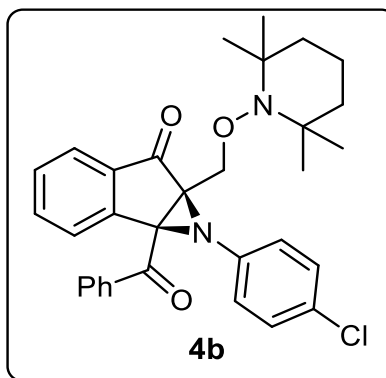
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-1-238-F

Current Data Parameters  
NAME CM-1-238-F-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441497 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.01  
191.73

145.15  
143.43  
135.23  
134.82  
133.78  
133.25  
129.97  
129.50  
128.72  
128.51  
128.06  
127.53  
125.13  
121.35

77.18  
77.00  
76.82  
71.41

61.00  
60.10  
59.54

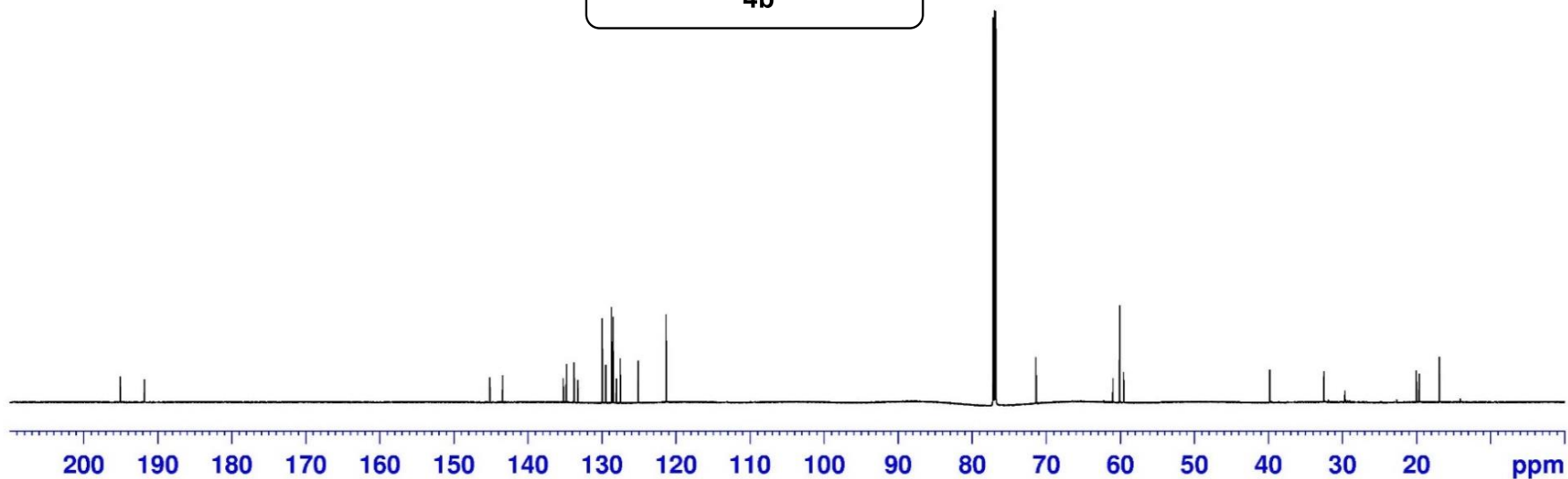
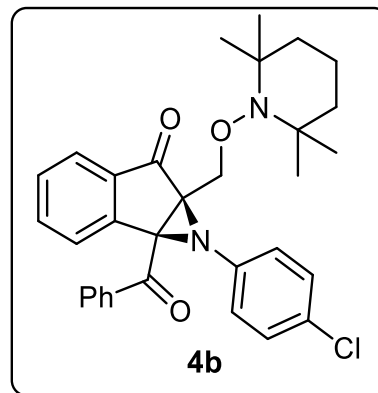
39.83  
39.80  
32.51  
32.50

20.01  
19.64  
16.89

CM-1-238

Current Data Parameters  
NAME CM-1-238-F-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9540990 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.968  
7.956  
7.522  
7.511  
7.509  
7.498  
7.391  
7.380  
7.370  
7.359  
7.348  
7.245  
7.240  
7.235  
7.229  
7.225  
7.218  
7.092  
7.080  
6.567  
6.555

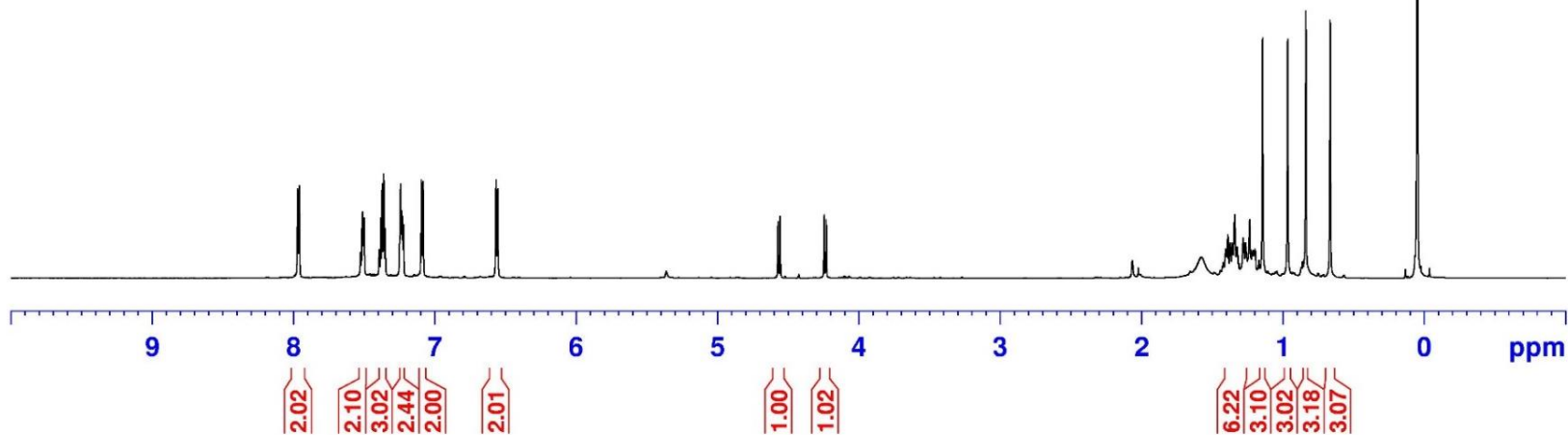
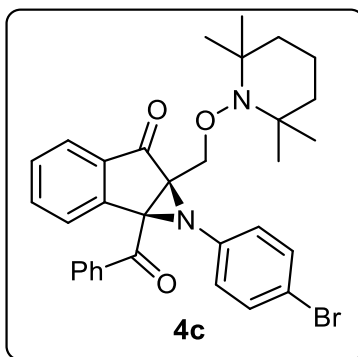
4.572  
4.557  
4.246  
4.231

1.578  
1.423  
1.405  
1.390  
1.373  
1.358  
1.340  
1.325  
1.280  
1.264  
1.235  
1.213  
1.202  
1.196  
1.144  
0.966  
0.838  
0.665

CM-1-215F

Current Data Parameters  
NAME CM-1-215F-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441501 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.97  
191.71

145.12  
143.94  
135.21  
134.83  
133.79  
133.21  
131.63  
129.96  
129.53  
128.51  
127.52  
125.18  
121.77  
115.68

77.18  
77.00  
76.82  
71.38

60.94  
60.09  
59.49

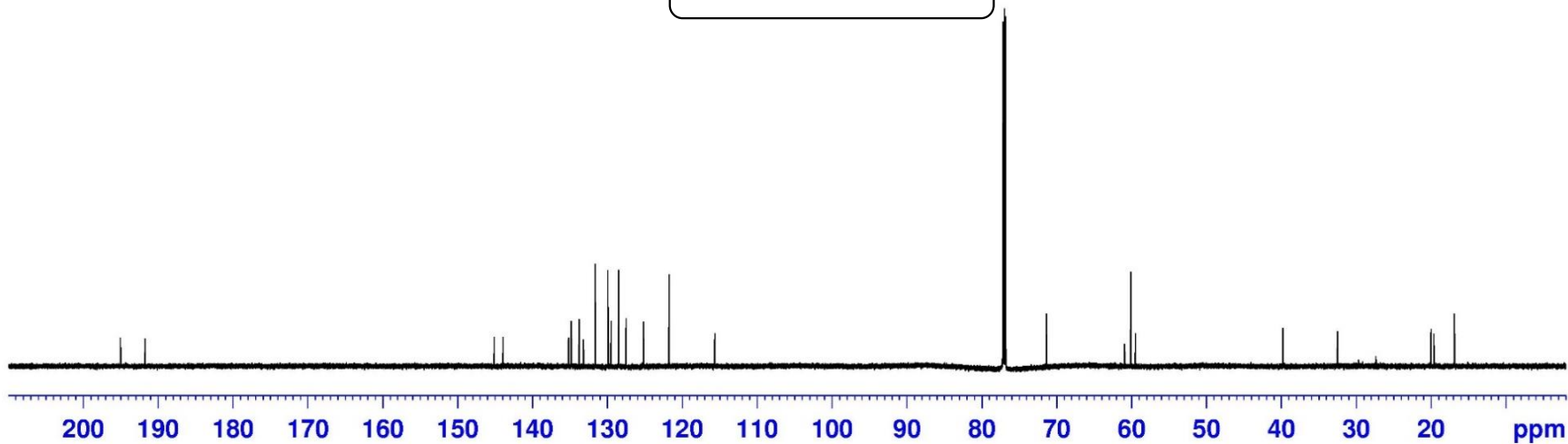
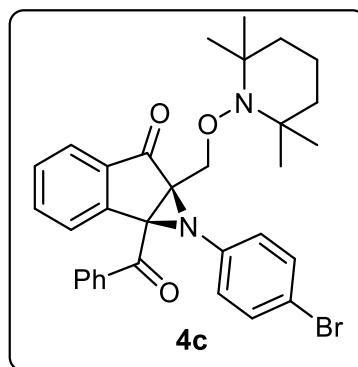
39.82  
39.79  
32.50  
32.49

20.01  
19.63  
16.89

CM-1-215F

Current Data Parameters  
NAME CM-1-215F-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9549796 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.965  
7.954  
7.521  
7.511  
7.500  
7.392  
7.381  
7.369  
7.358  
7.346  
7.277  
7.264  
7.249  
7.240  
7.227  
7.216  
6.457  
6.445

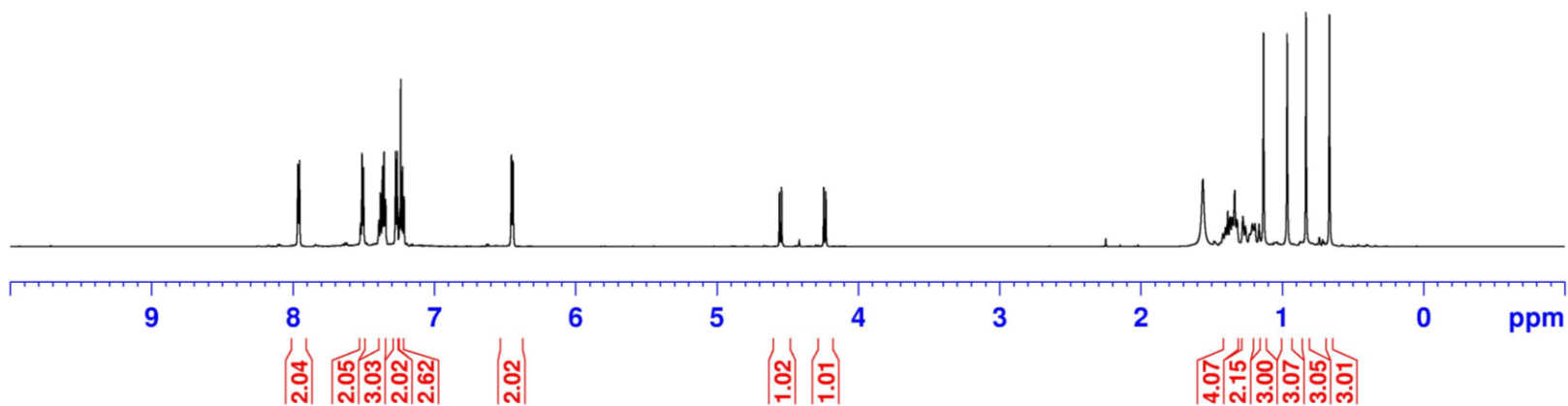
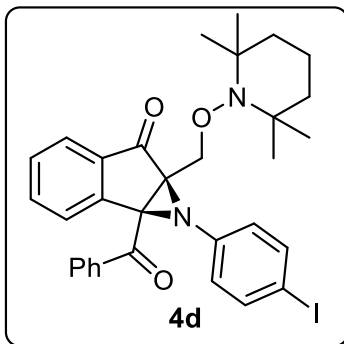
4.560  
4.545  
4.246  
4.231

1.564  
1.422  
1.404  
1.387  
1.370  
1.356  
1.338  
1.323  
1.320  
1.281  
1.264  
1.233  
1.216  
1.212  
1.195  
1.167  
1.135  
0.967  
0.834  
0.668

CM-2-81

Current Data Parameters  
NAME CM-2-81-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438029 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.94  
191.71

145.12  
144.67  
137.53  
135.23  
134.83  
133.79  
133.20  
129.95  
129.54  
128.52  
127.51  
125.22  
122.22

86.15  
77.18  
77.00  
76.82  
71.37  
60.89  
60.10  
59.45

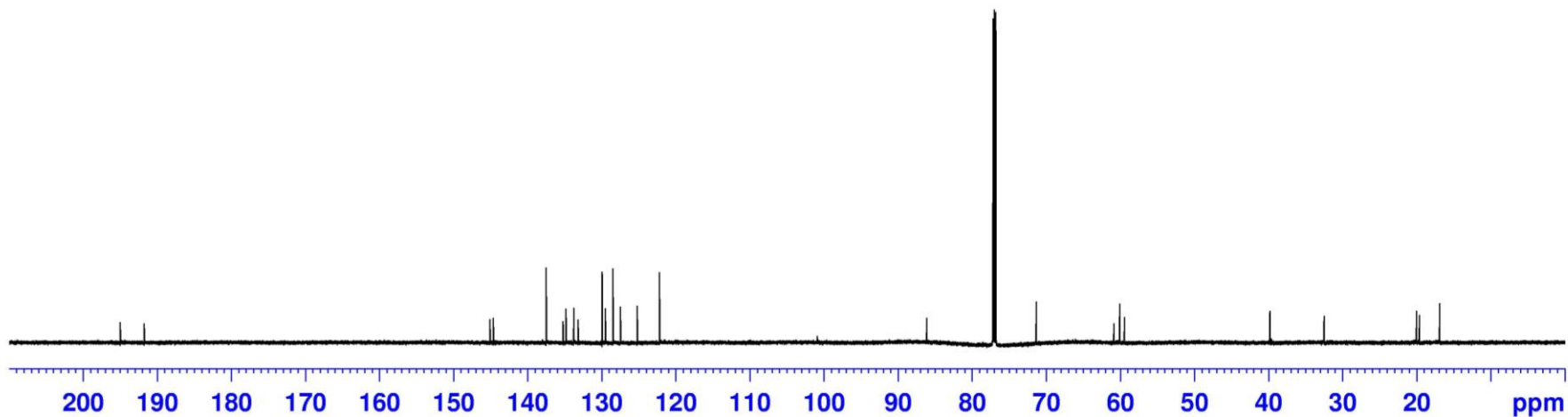
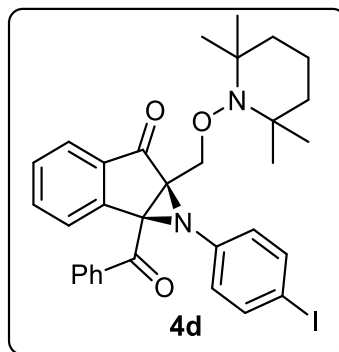
39.82  
39.80  
32.51  
32.49

20.02  
19.64  
16.90

CM-2-81

Current Data Parameters  
NAME CM-2-81-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9514602 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



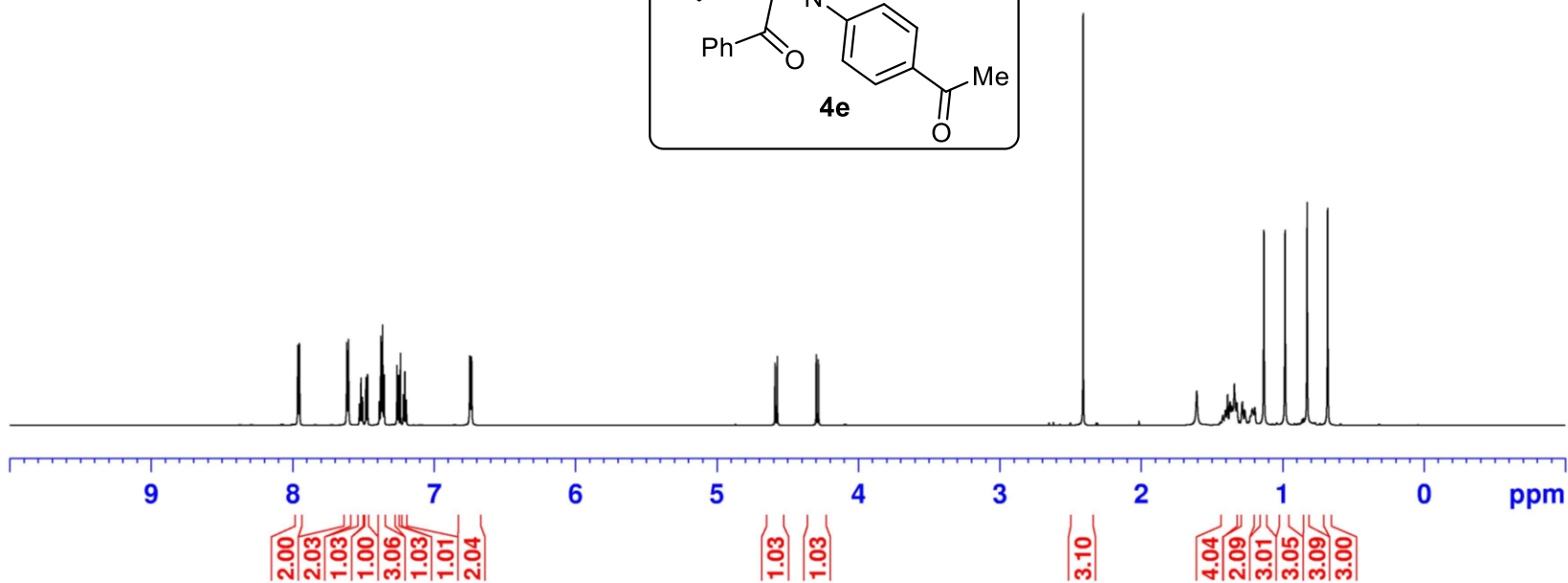
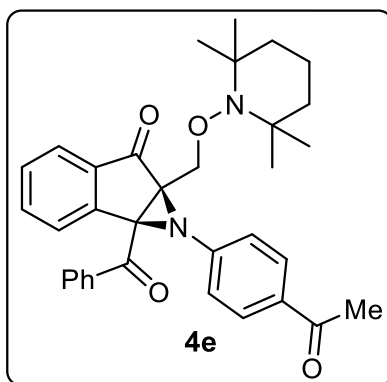
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.965  
7.954  
7.953  
7.619  
7.607  
7.530  
7.519  
7.508  
7.483  
7.472  
7.390  
7.389  
7.379  
7.377  
7.366  
7.354  
7.264  
7.253  
7.240  
7.220  
7.219  
7.209  
7.208  
7.198  
7.197  
6.749  
6.737  
4.590  
4.575  
4.300  
4.285  
2.413  
1.609  
1.407  
1.391  
1.376  
1.373  
1.362  
1.355  
1.343  
1.325  
1.289  
1.286  
1.271  
1.220  
1.216  
1.202  
1.198  
1.135  
0.985  
0.829  
0.684

CM-2-83

Current Data Parameters  
NAME CM-2-83-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441501 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

196.86  
194.68  
191.39

149.55  
145.17  
135.08  
134.90  
133.88  
132.78  
132.09  
129.92  
129.59  
129.41  
128.56  
127.52  
125.28  
119.91

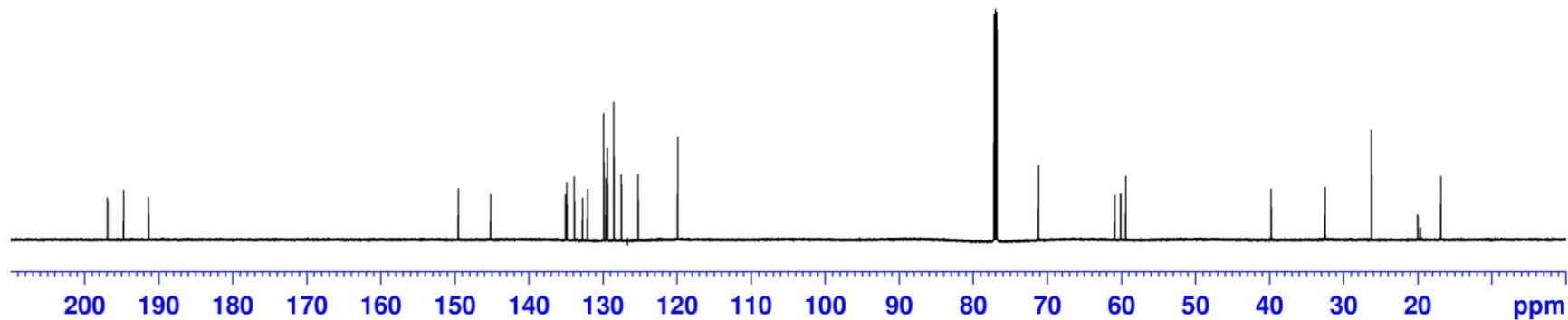
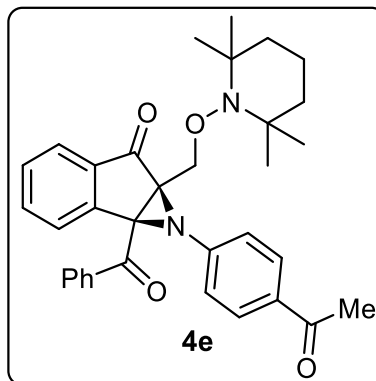
77.18  
77.00  
76.82  
71.19  
60.88  
60.12  
60.09  
59.39

39.80  
39.78  
32.49  
26.25  
20.00  
19.64  
16.87

CM-2-83

Current Data Parameters  
NAME CM-2-83-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523421 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

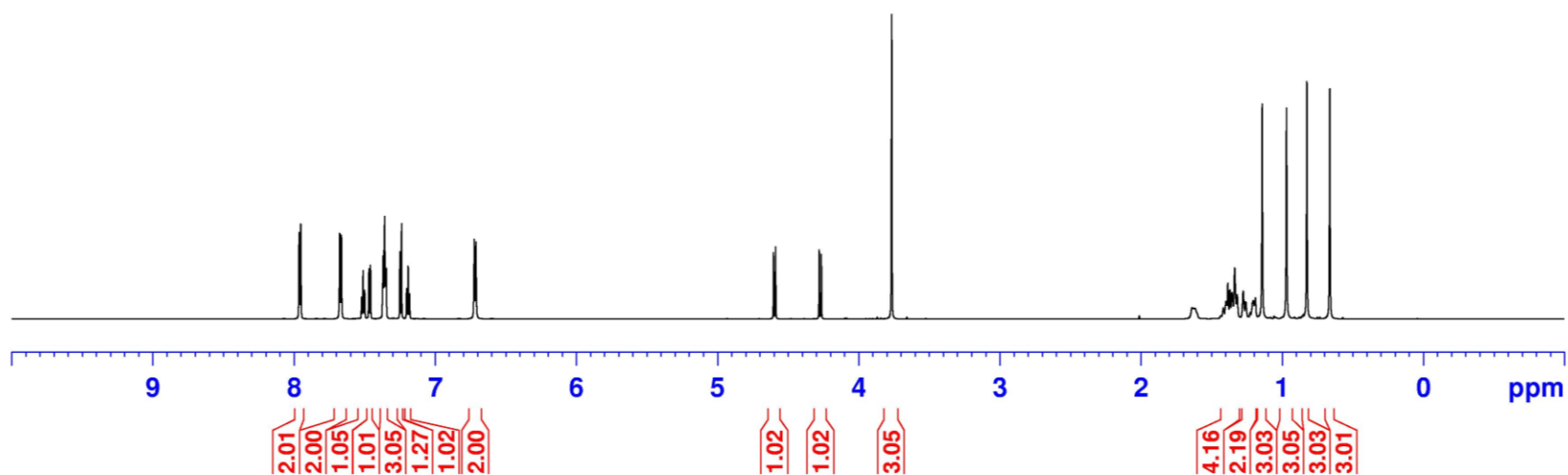
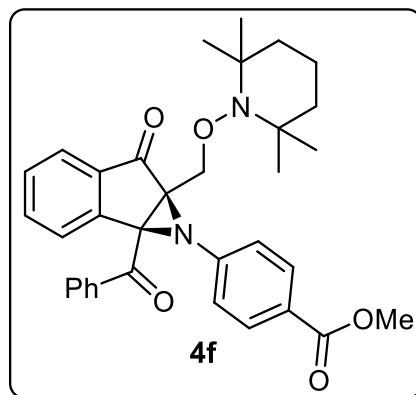
7.965  
7.954  
7.678  
7.666  
7.523  
7.512  
7.503  
7.501  
7.471  
7.460  
7.375  
7.370  
7.364  
7.360  
7.354  
7.352  
7.348  
7.251  
7.240  
7.205  
7.194  
7.183  
6.725  
6.713  
4.605  
4.590  
4.281  
4.266  
3.768

1.623  
1.419  
1.401  
1.387  
1.371  
1.357  
1.338  
1.321  
1.278  
1.261  
1.229  
1.209  
1.192  
1.144  
0.972  
0.827  
0.665

CM-2-86

Current Data Parameters  
NAME CM-2-86-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438027 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



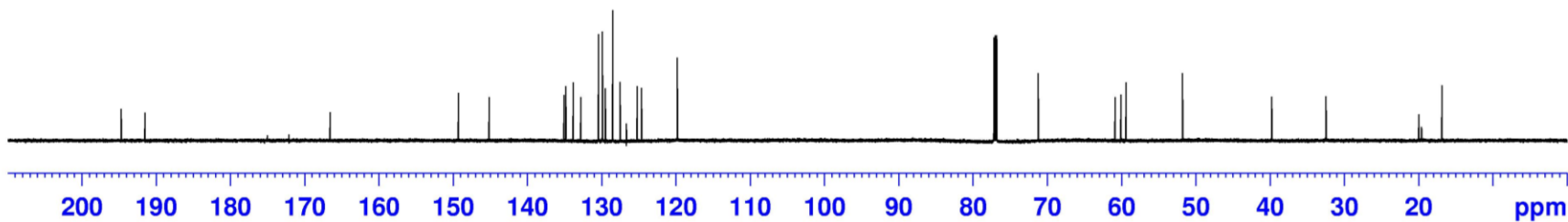
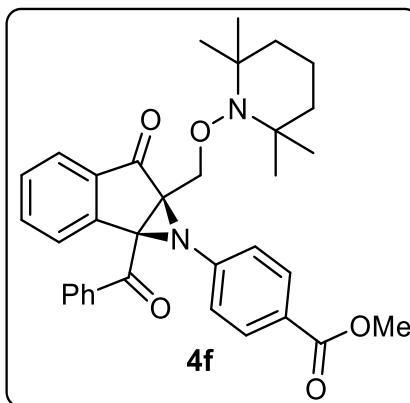
<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)



CM-2-86

Current Data Parameters  
NAME CM-2-86-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523442 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



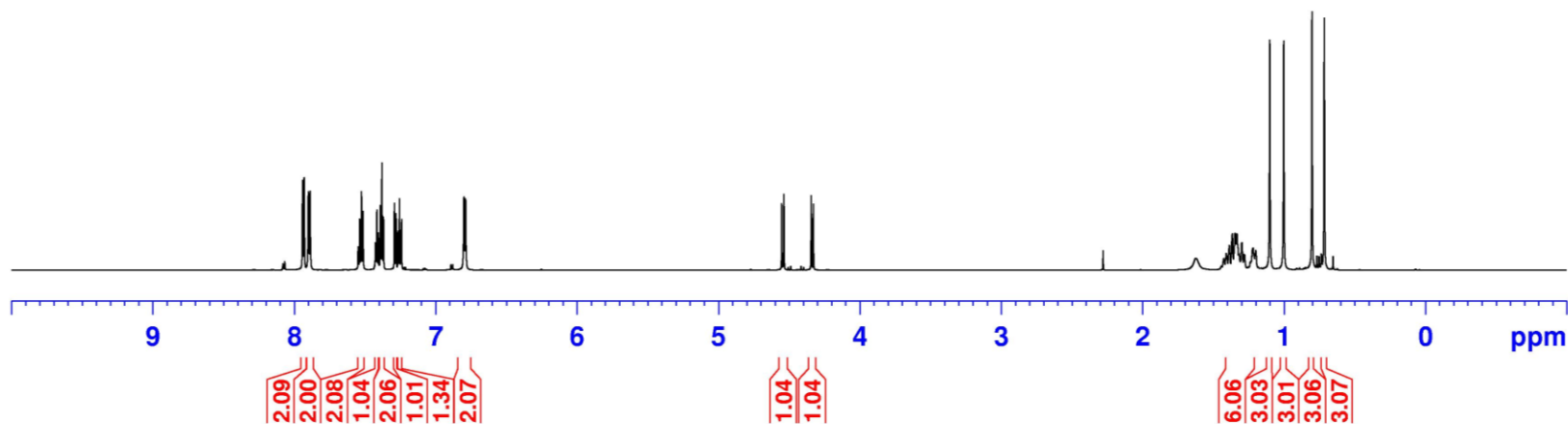
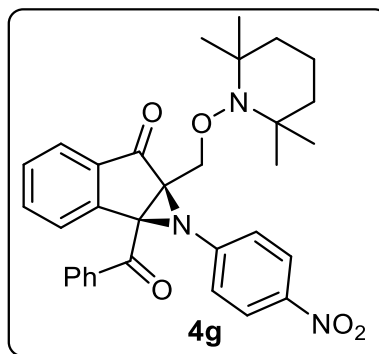
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.940  
7.929  
7.900  
7.887  
7.546  
7.536  
7.524  
7.512  
7.426  
7.415  
7.404  
7.390  
7.379  
7.368  
7.290  
7.279  
7.266  
7.255  
7.244  
7.240  
6.800  
6.787  
4.551  
4.536  
4.343  
4.328  
1.626  
1.428  
1.424  
1.415  
1.410  
1.406  
1.389  
1.368  
1.350  
1.347  
1.339  
1.335  
1.322  
1.302  
1.299  
1.284  
1.281  
1.225  
1.220  
1.216  
1.206  
1.202  
1.103  
1.004  
0.804  
0.718

CM-2-87

Current Data Parameters  
NAME CM-2-87-H.tid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438023 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.18  
190.77

151.37  
144.92  
143.23  
135.18  
134.77  
134.12  
132.42  
129.99  
129.83  
128.69  
127.49  
125.60  
124.77  
120.11

77.18  
77.00  
76.82  
70.90  
60.98  
60.19  
60.11  
59.32

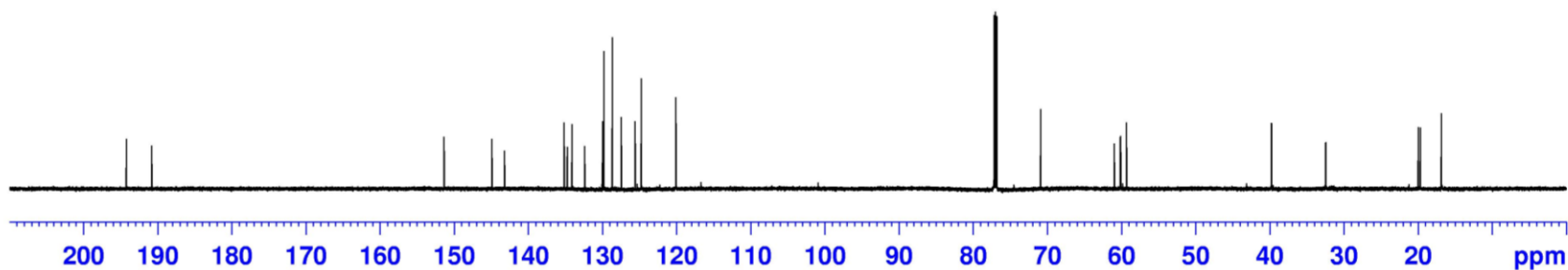
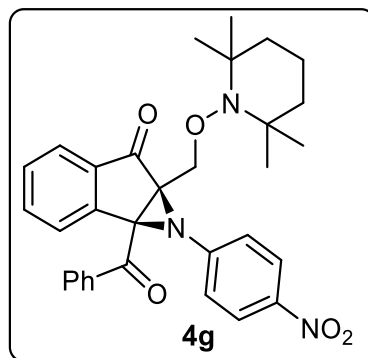
39.77  
39.76  
32.49  
32.43

19.98  
19.70  
16.85

CM-2-87

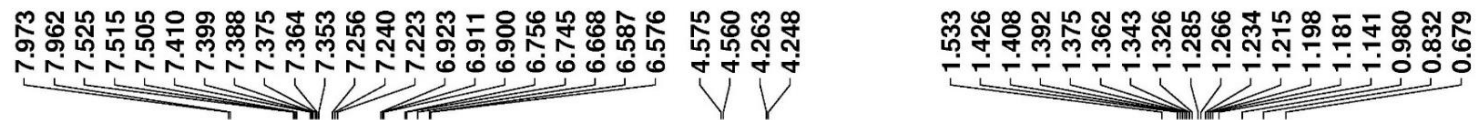
Current Data Parameters  
NAME CM-2-87-Cfid.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9514629 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





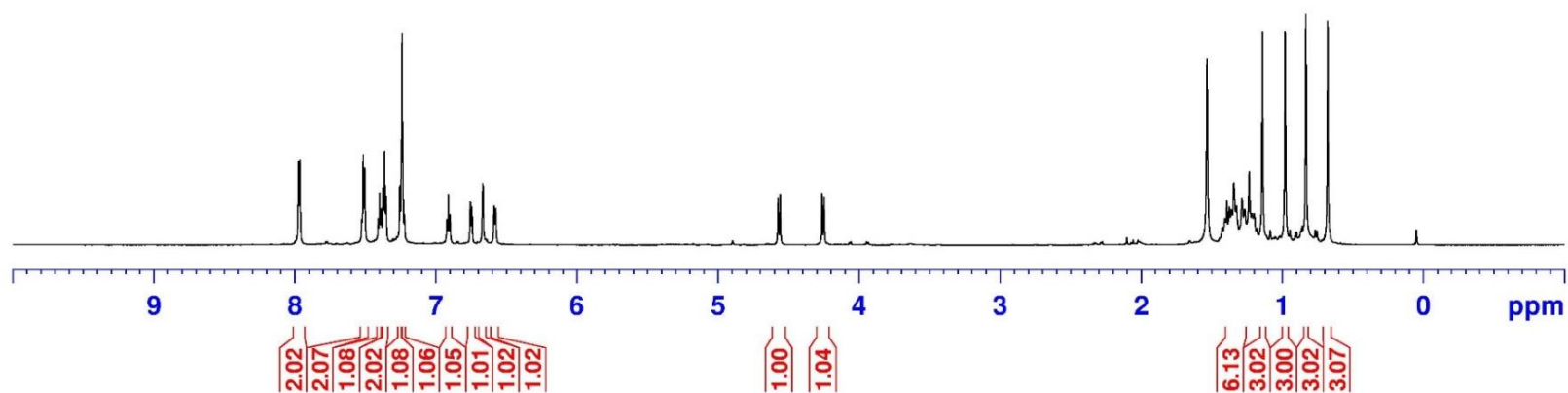
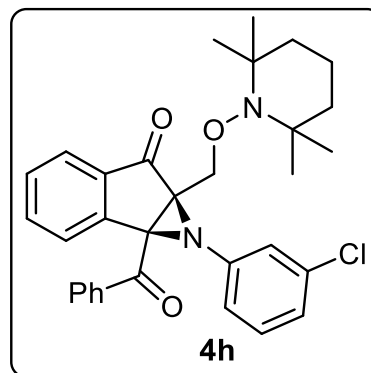
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



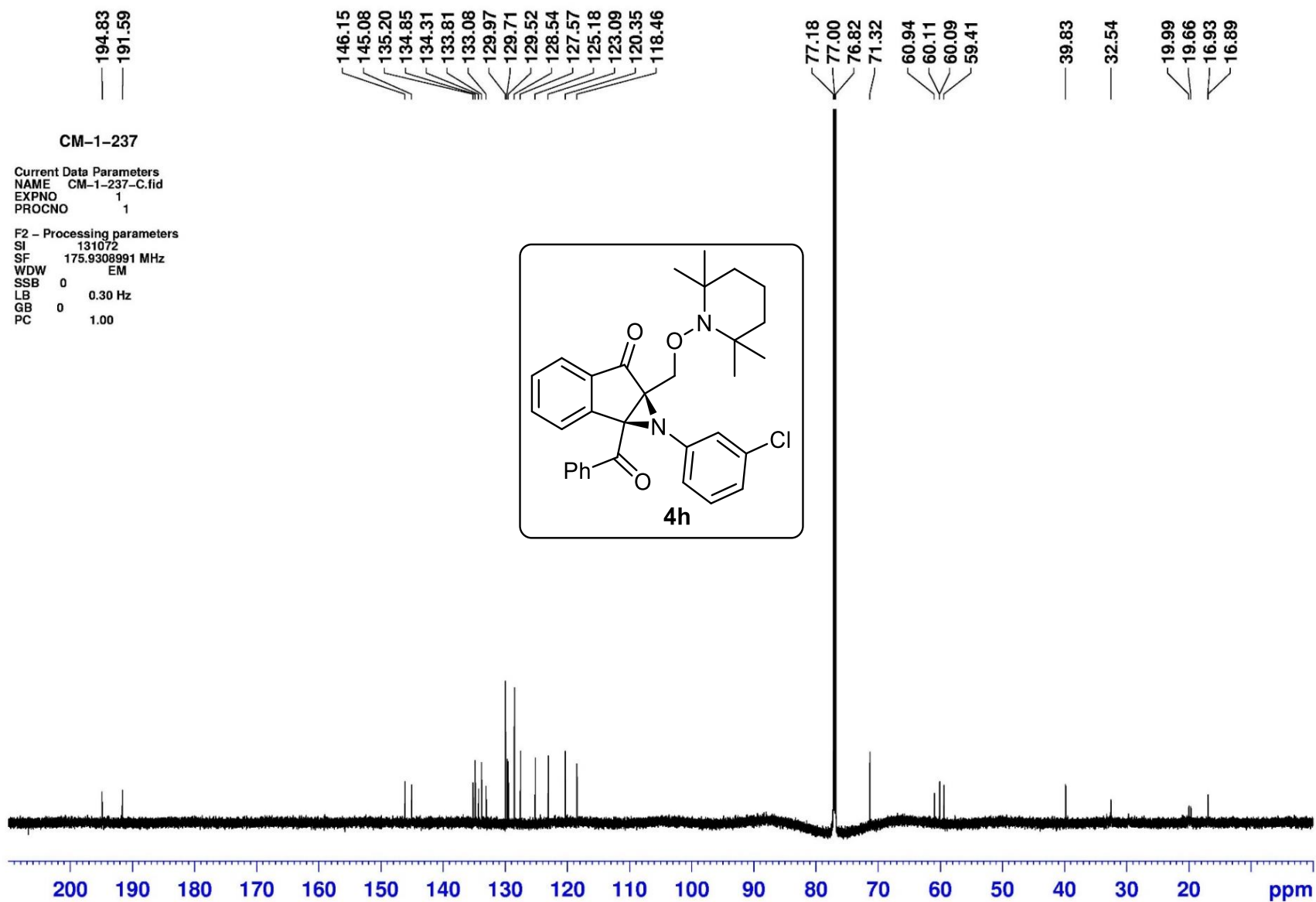
CM-1-237

Current Data Parameters  
NAME CM-1-237-H.fid  
EXPNO 1  
PROCNO 1

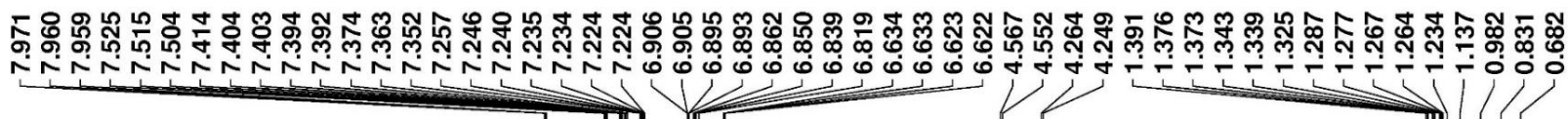
F2 - Processing parameters  
SI 65536  
SF 699.7438001 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)



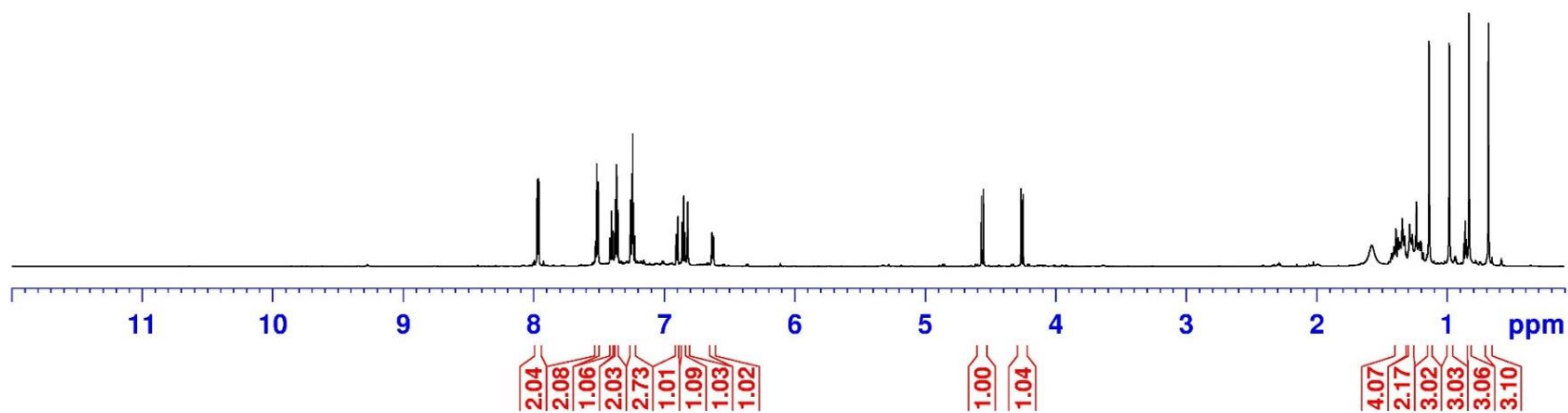
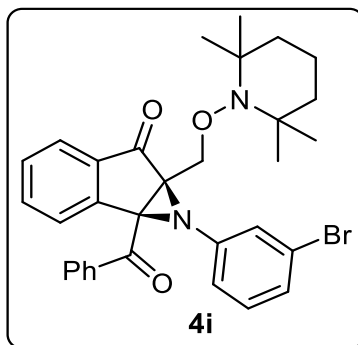
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-1-213-F

Current Data Parameters  
NAME CM-1-213-F-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7427525 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.80  
191.56

146.26  
145.04  
135.18  
134.84  
133.82  
133.05  
129.97  
129.96  
129.54  
128.53  
127.57  
125.97  
125.19  
123.24  
122.30  
118.90

77.18  
77.00  
76.82  
71.30  
60.94  
60.11  
60.09  
59.40

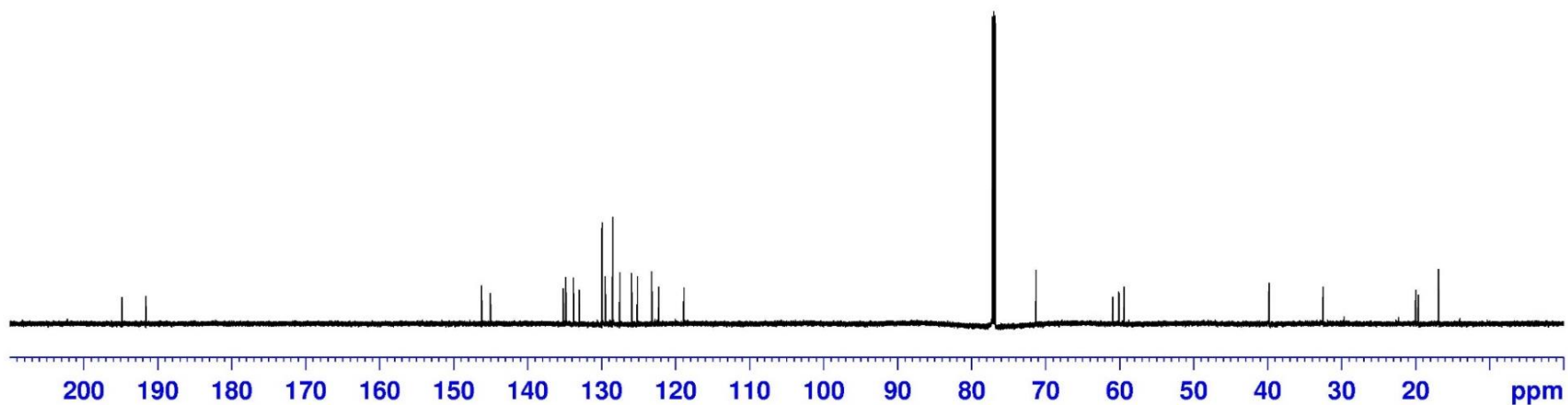
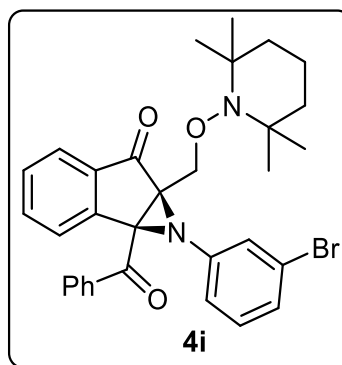
39.82  
39.80  
32.51

19.99  
19.64  
16.89

CM-1-213-F

Current Data Parameters  
NAME CM-1-213-F-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9318335 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



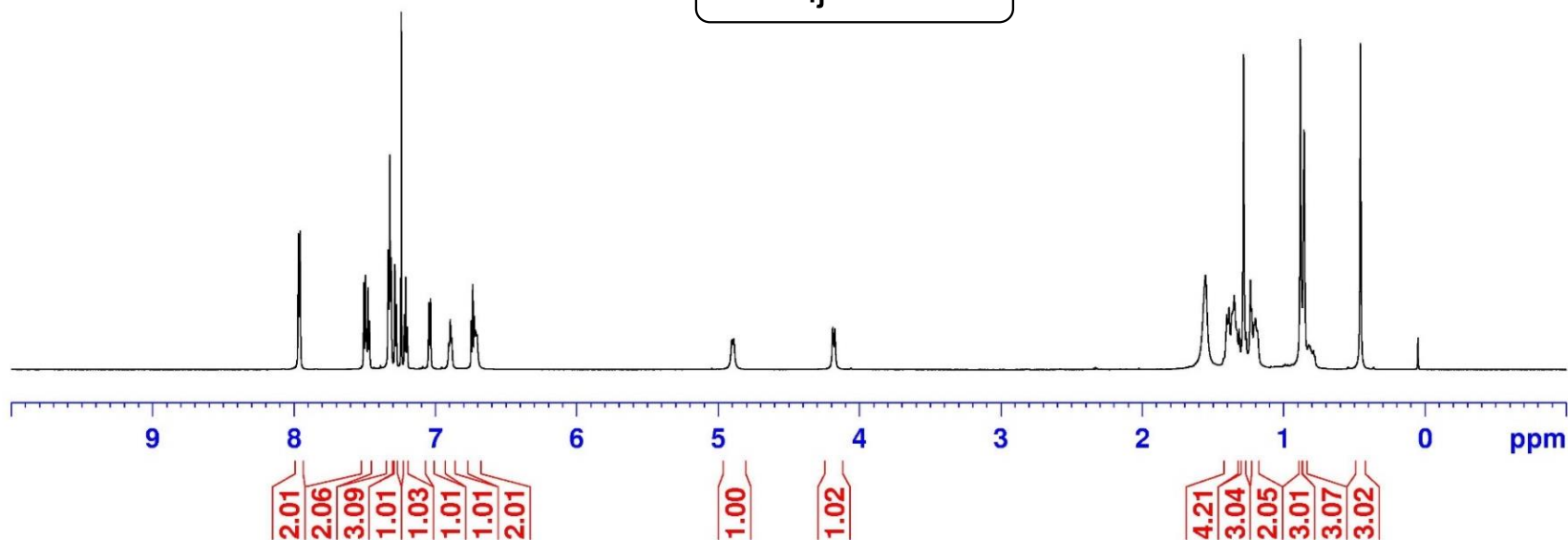
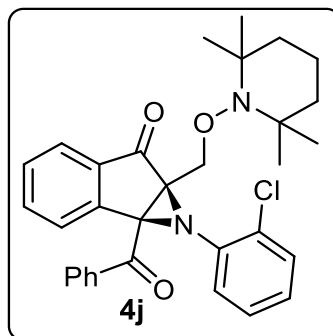
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.968  
7.957  
7.505  
7.494  
7.486  
7.475  
7.465  
7.333  
7.322  
7.311  
7.285  
7.275  
7.240  
7.219  
7.208  
7.197  
7.045  
7.034  
6.904  
6.894  
6.883  
6.745  
6.734  
6.723  
6.715  
6.705  
4.902  
4.888  
4.188  
4.173

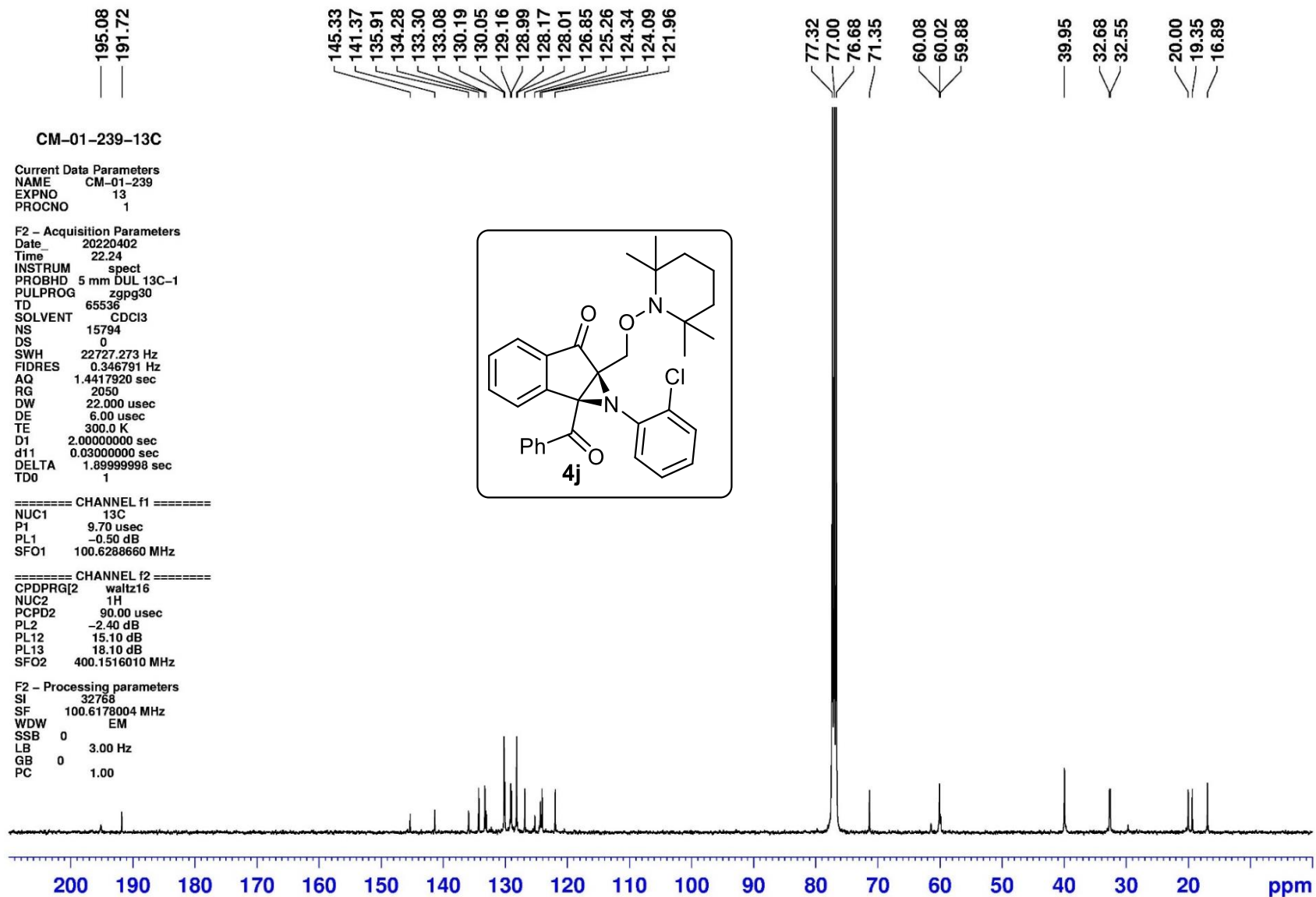
1.552  
1.402  
1.386  
1.366  
1.349  
1.312  
1.282  
1.264  
1.234  
1.225  
1.208  
1.198  
1.185  
0.880  
0.855  
0.456

Current Data Parameters  
NAME CM-1-239-F-H.fid  
EXPNO 1  
PROCNO 1

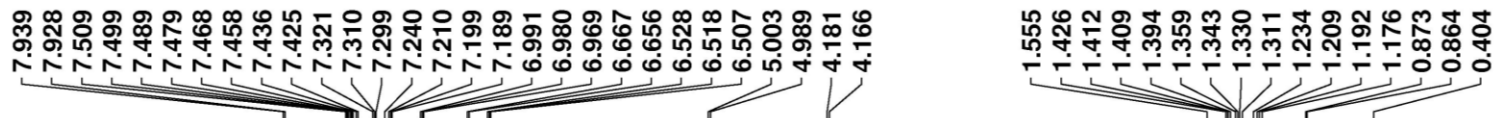
F2 - Processing parameters  
SI 65536  
SF 699.7434152 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 100 MHz)



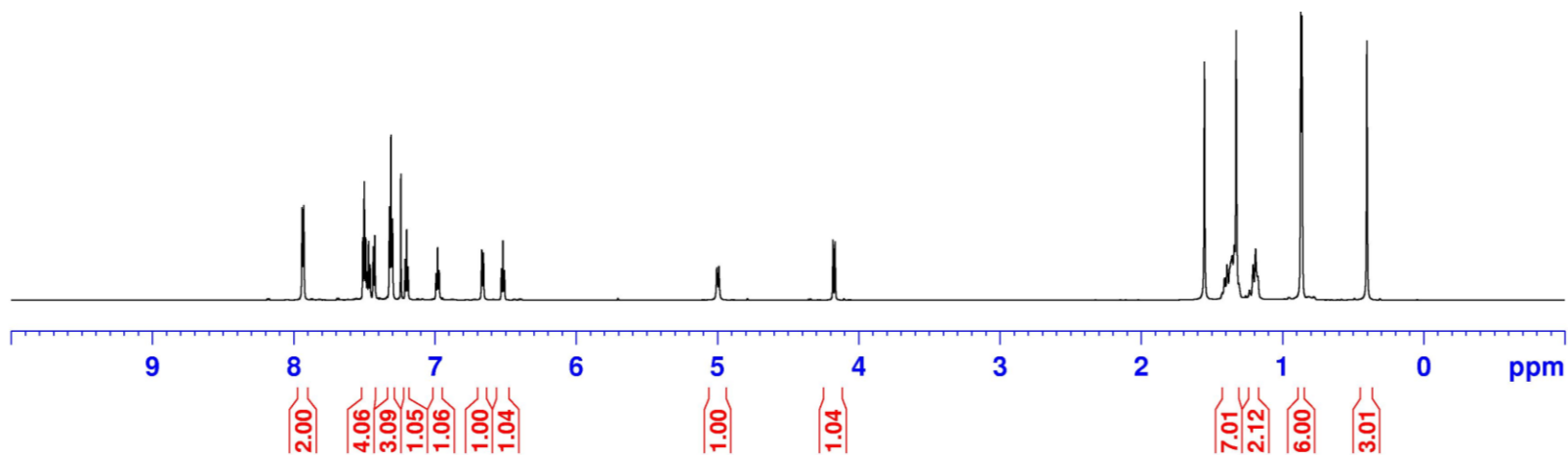
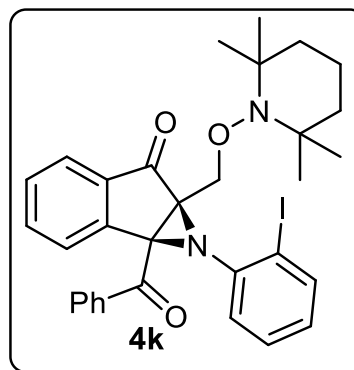
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-80

Current Data Parameters  
NAME CM-2-80-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7437992 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.22  
192.10

145.51  
145.00  
140.12  
136.37  
133.96  
133.18  
133.10  
130.20  
130.14  
129.10  
128.25  
128.05  
124.86  
124.29  
122.06

88.09  
77.18  
77.00  
76.82  
71.61  
60.60  
60.10  
60.01

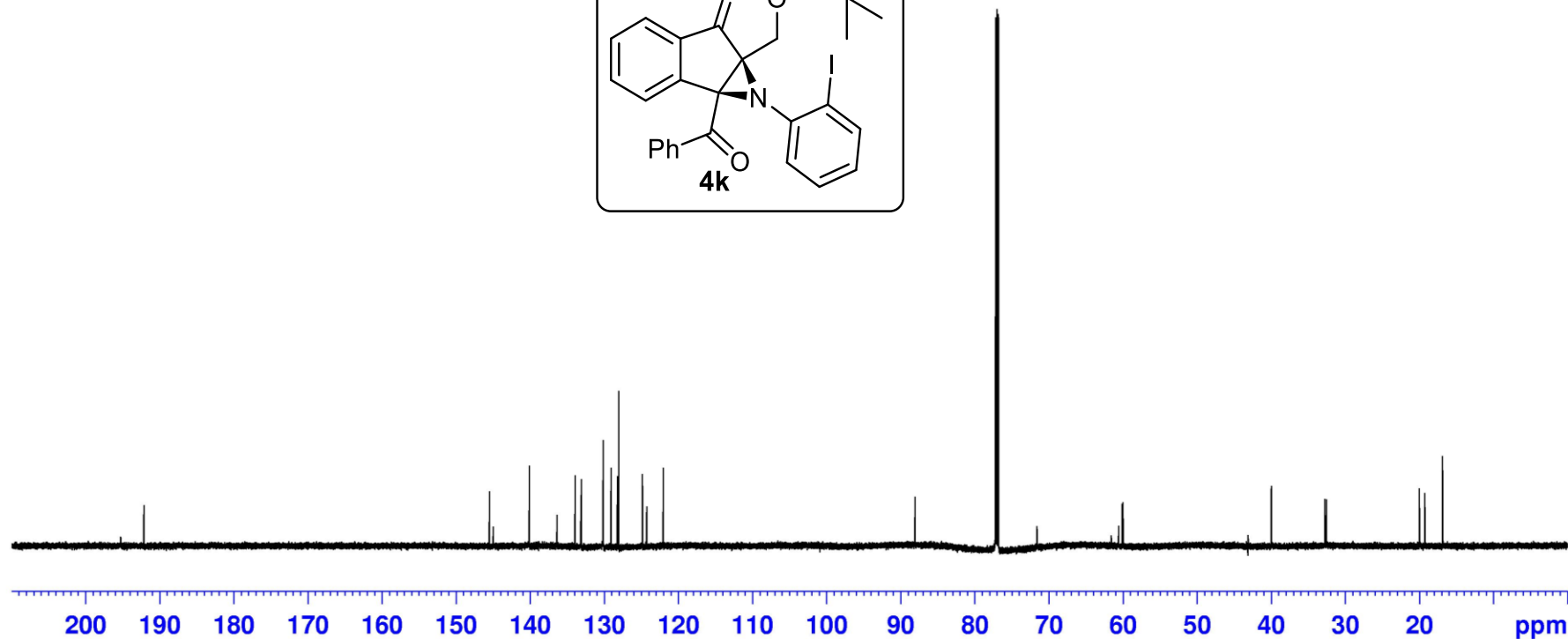
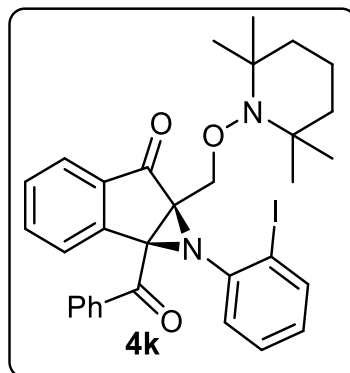
40.01  
39.98  
32.76  
32.56

20.01  
19.27  
16.88

CM-2-80

Current Data Parameters  
NAME CM-2-80-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9514602 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





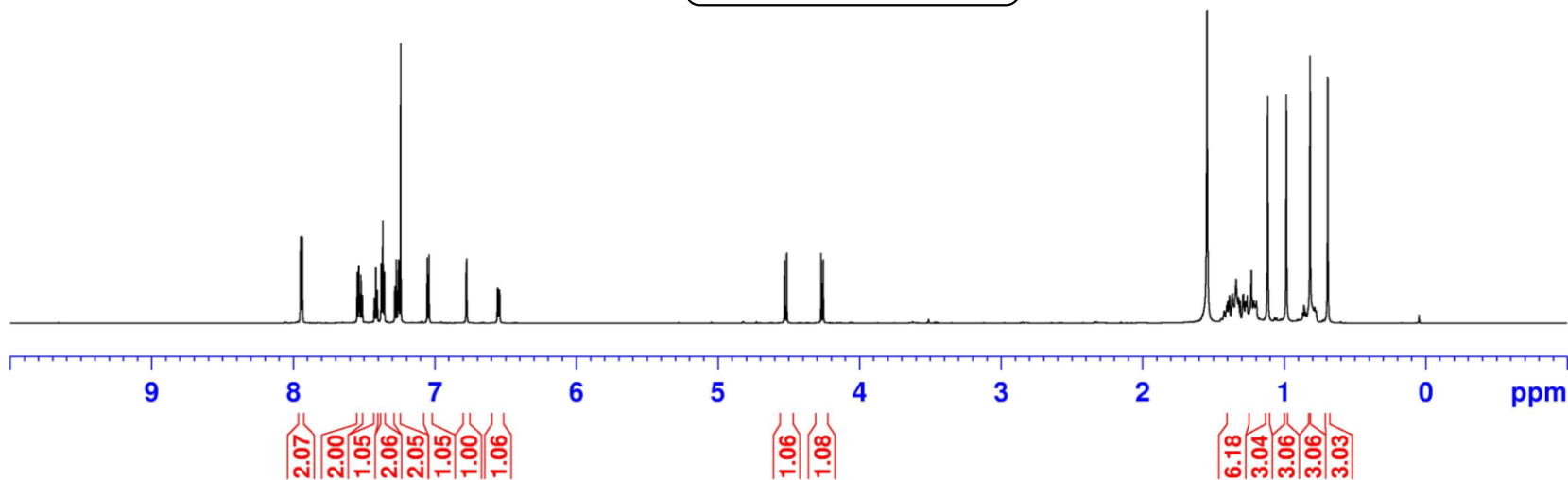
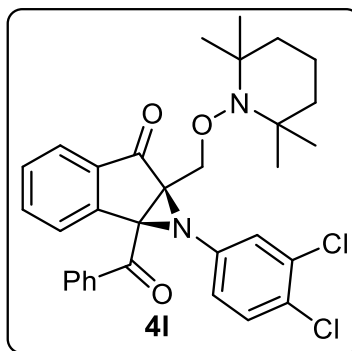
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.947  
7.936  
7.546  
7.535  
7.521  
7.511  
7.426  
7.415  
7.404  
7.377  
7.366  
7.355  
7.281  
7.271  
7.260  
7.254  
7.240  
7.052  
7.040  
6.777  
6.773  
6.556  
6.553  
6.544  
6.541  
4.528  
4.513  
4.269  
4.254  
1.544  
1.401  
1.388  
1.372  
1.368  
1.362  
1.342  
1.323  
1.312  
1.293  
1.290  
1.275  
1.271  
1.263  
1.233  
1.222  
1.217  
1.203  
1.199  
1.118  
0.987  
0.819  
0.694

CM-2-85

Current Data Parameters  
NAME CM-2-85-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438017 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

194.60  
191.27

144.85  
144.62  
135.02  
135.01  
133.94  
132.95  
132.48  
130.31  
129.90  
129.81  
128.60  
127.48  
126.40  
125.40  
121.90  
119.63

77.18  
77.00  
76.82  
71.17  
61.02  
60.15  
60.11  
59.38

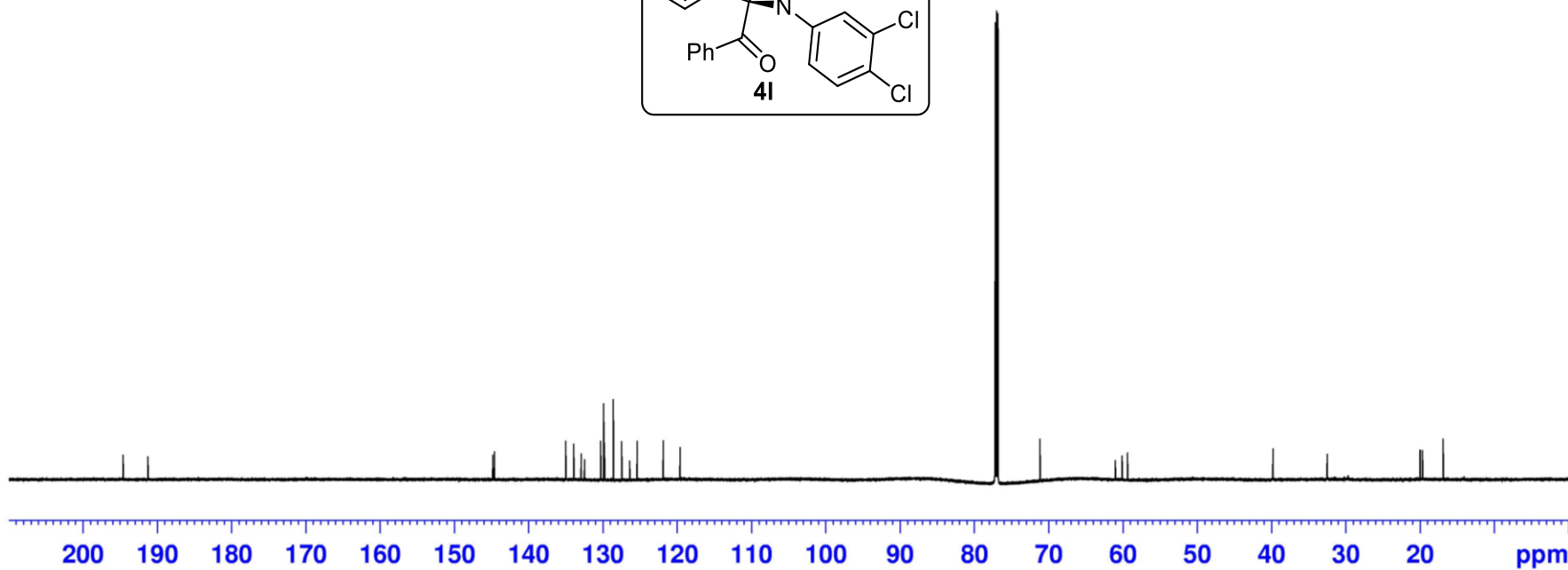
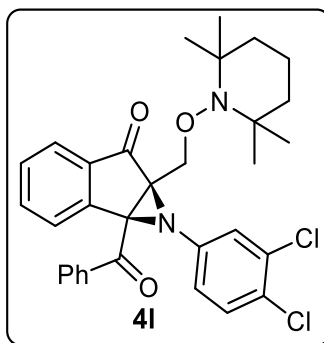
39.81  
39.80  
32.51  
32.48

20.00  
19.67  
16.89

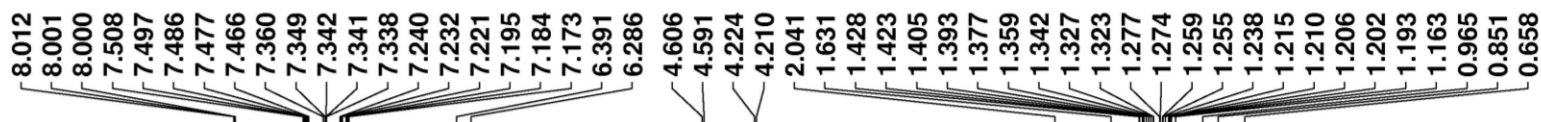
CM-2-85

Current Data Parameters  
NAME CM-2-85-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523391 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



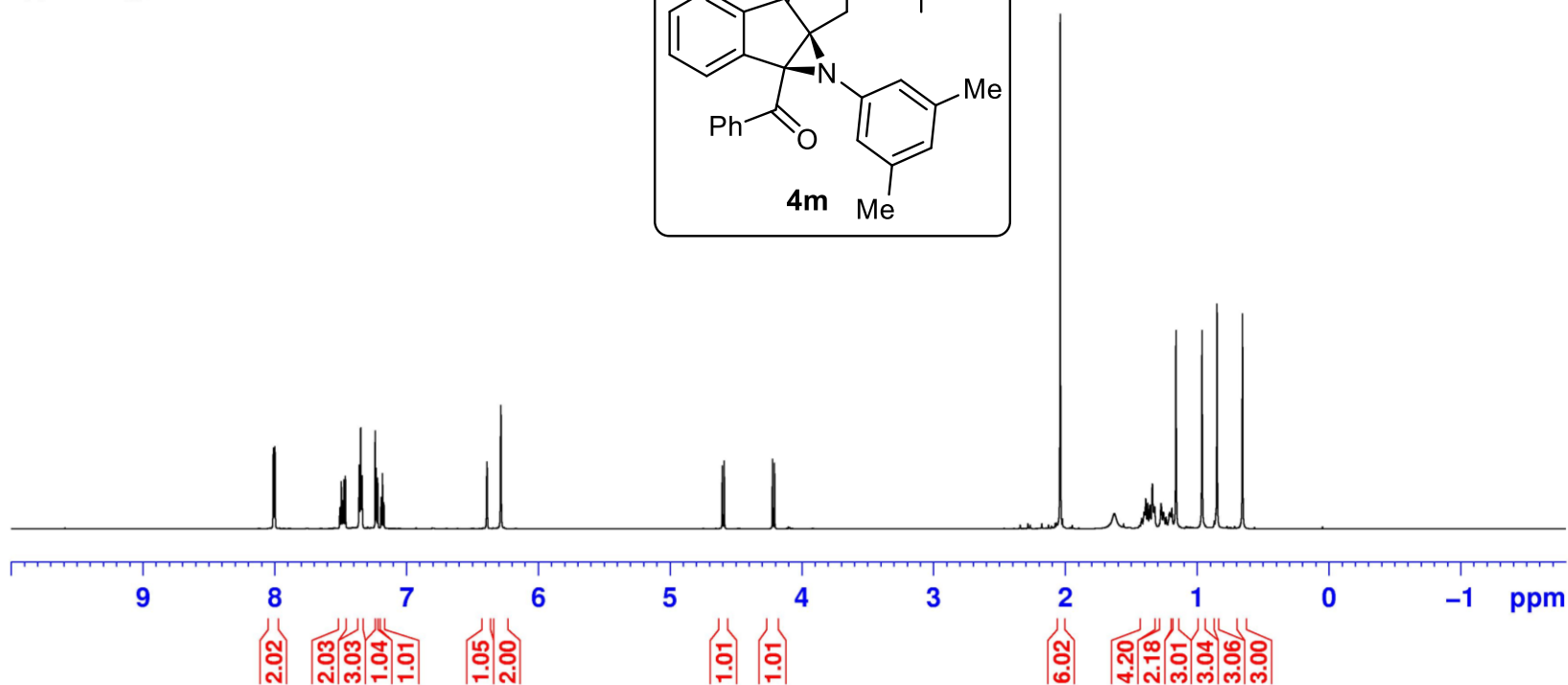
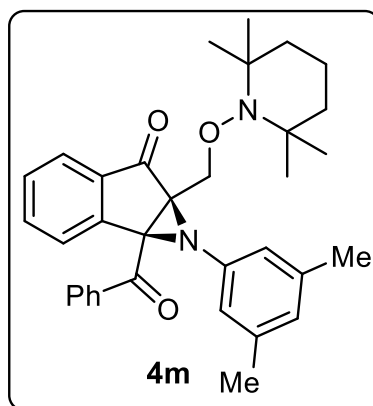
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-84

Current Data Parameters  
NAME CM-2-84-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441501 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.43  
192.35

145.47  
144.40  
138.19  
135.55  
134.28  
133.54  
133.42  
130.06  
129.05  
128.37  
127.51  
124.77  
124.62  
118.05

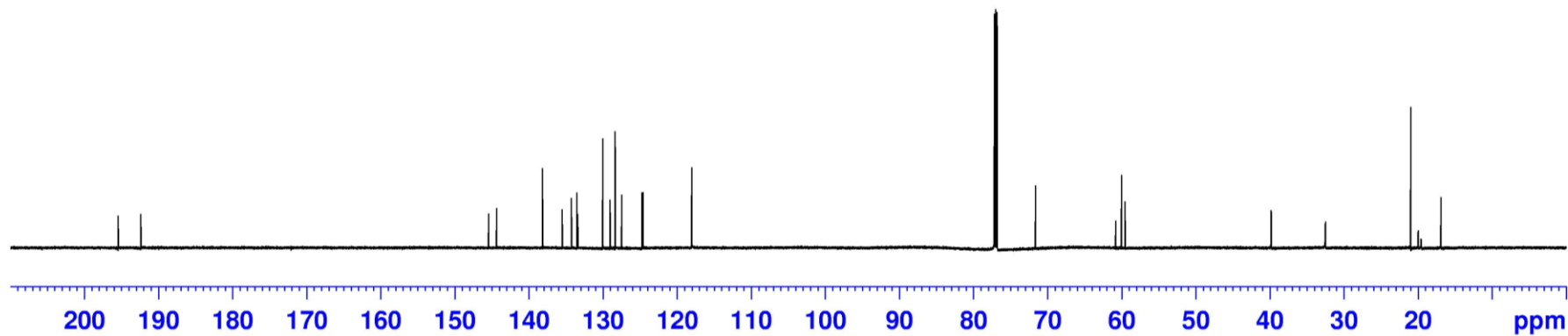
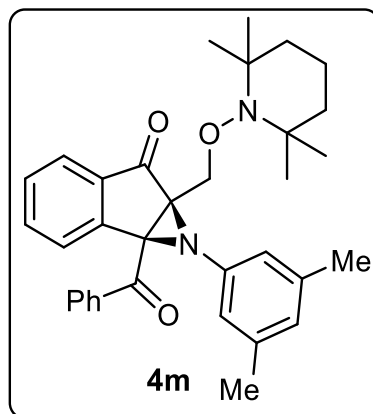
77.18  
77.00  
76.82  
71.65  
60.83  
60.04  
59.55

39.84  
39.81  
32.55  
32.51  
20.98  
19.99  
19.61  
19.57  
16.91

CM-2-84

Current Data Parameters  
NAME CM-2-84-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523423 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



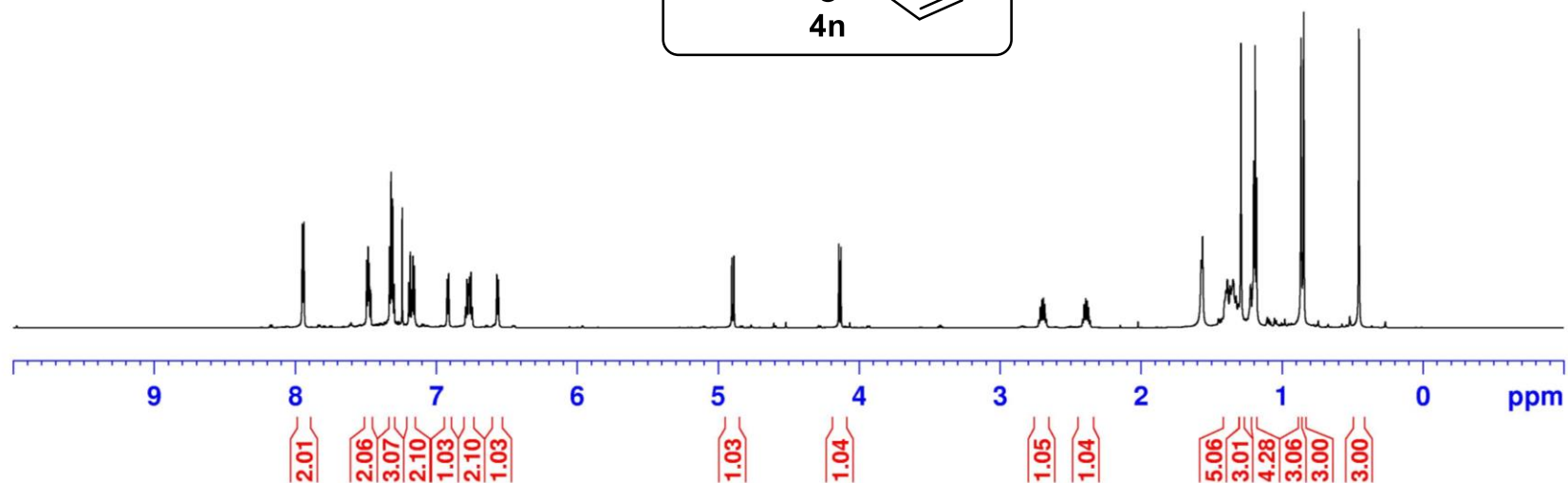
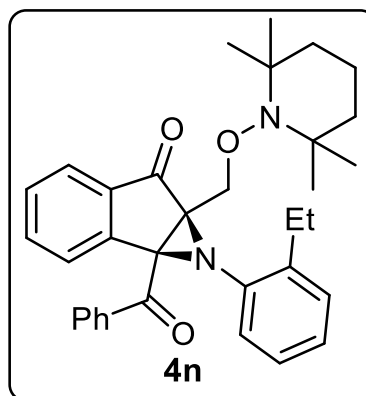
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.949  
7.938  
7.492  
7.482  
7.474  
7.463  
7.330  
7.319  
7.308  
7.297  
7.240  
7.197  
7.186  
7.175  
7.167  
7.157  
6.924  
6.913  
6.784  
6.782  
6.774  
6.771  
6.767  
6.765  
6.757  
6.755  
6.572  
6.561  
4.905  
4.890  
4.146  
4.131  
2.695  
2.395  
1.576  
1.566  
1.402  
1.397  
1.390  
1.370  
1.357  
1.349  
1.345  
1.331  
1.327  
1.293  
1.203  
1.193  
1.182  
0.867  
0.848  
0.456

CM-2-111

Current Data Parameters  
NAME CM-2-111-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438013 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.83  
192.13

145.54  
141.73  
135.74  
134.83  
134.31  
133.54  
133.38  
130.16  
129.00  
128.22  
128.12  
127.96  
125.62  
124.54  
123.26  
120.51

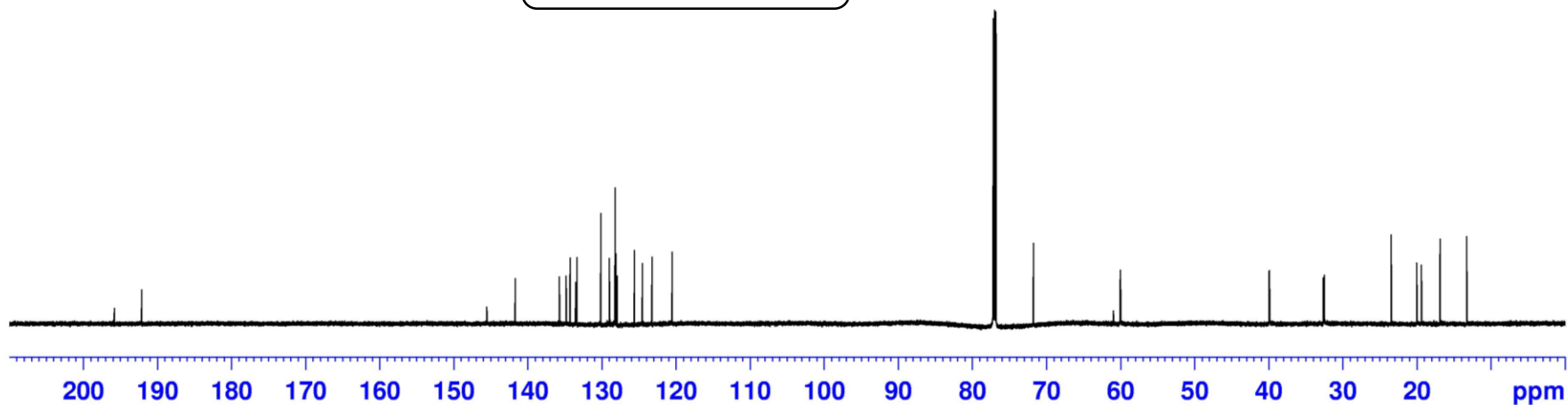
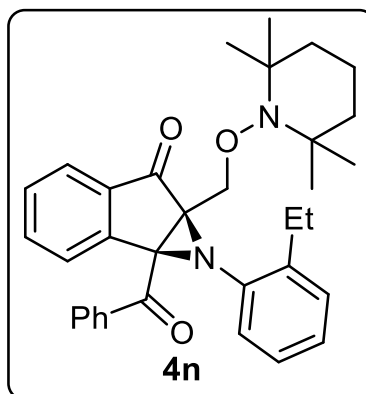
77.18  
77.00  
76.82  
71.77  
60.96  
60.08  
60.01

39.96  
39.90  
32.63  
32.50  
23.46  
20.02  
19.38  
16.88  
13.30

CM-2-111

Current Data Parameters  
NAME CM-2-111-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532214 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)

7.968 7.950 7.947 7.497 7.479 7.346 7.331 7.313 7.240 7.208 7.189 7.171 7.159 7.140 6.986 6.978 6.970 6.963 6.804 6.795 6.786 6.640 6.633 6.617 4.811 4.785 4.212 4.186 3.120 3.102 3.086 3.069 3.053 1.513 1.365 1.298 1.279 1.245 1.215 1.199 1.066 1.049 0.900 0.830 0.546 0.055

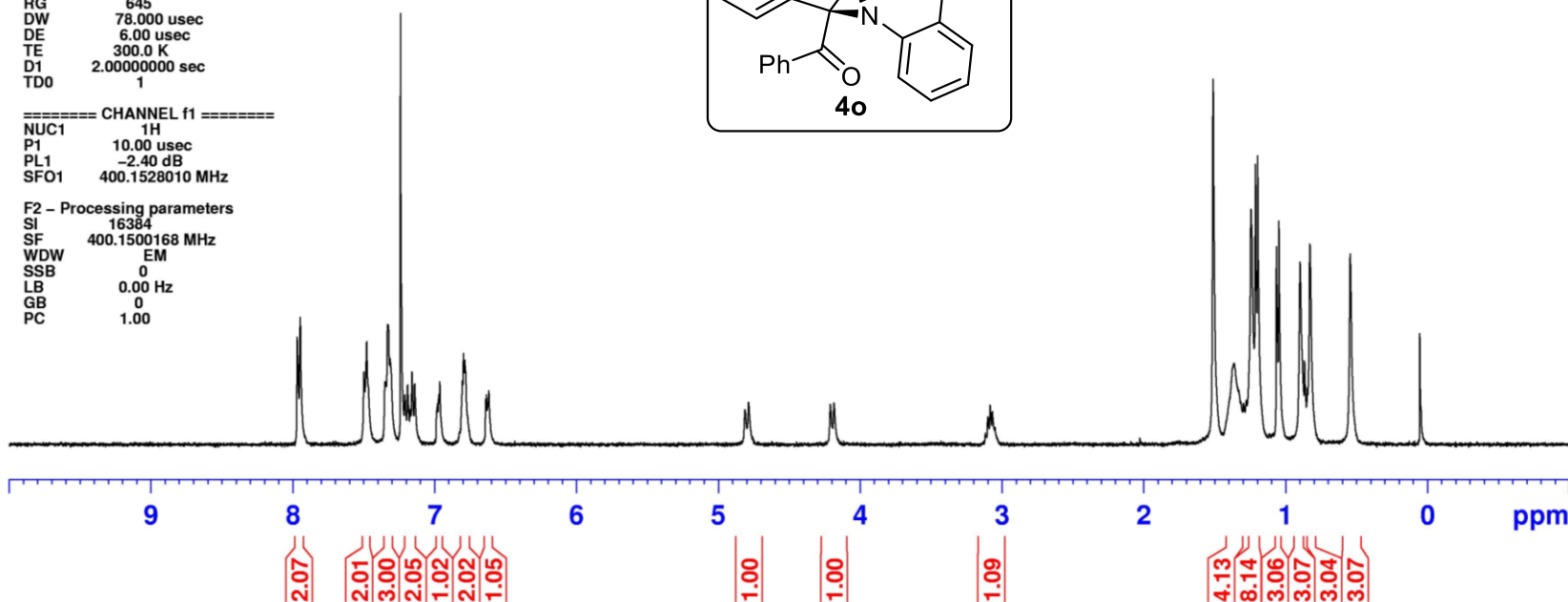
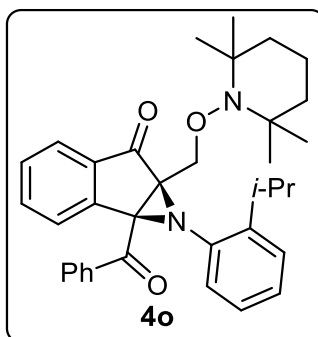
CM-02-120

Current Data Parameters  
NAME CM-02-120  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230413  
Time 16.34  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 13  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 645  
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 0.00 Hz  
GB 0  
PC 1.00



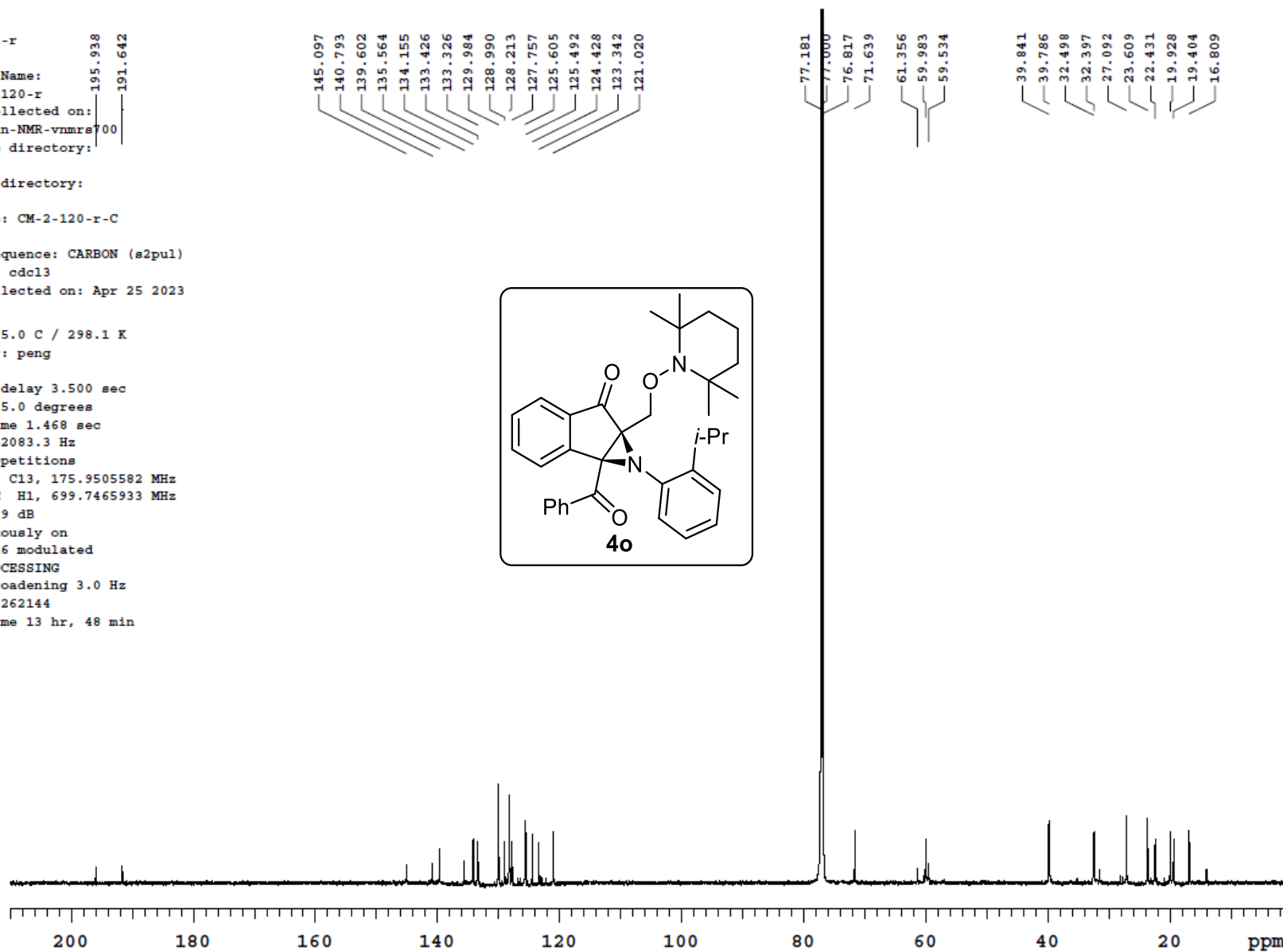
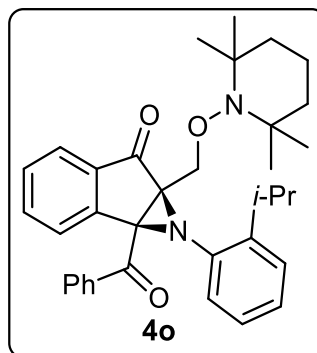
<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

CM-2-120-r  
Sample Name: CM-2-120-r  
Data Collected on: Varian-NMR-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: CM-2-120-r-C  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 25 2023  
Temp. 25.0 C / 298.1 K  
Operator: peng  
Relax. delay 3.500 sec  
Pulse 45.0 degrees  
Acq. time 1.468 sec  
Width 52083.3 Hz  
1220 repetitions  
OBSERVE C13, 175.9505582 MHz  
DECOUPLE H1, 699.7465933 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 3.0 Hz  
FT size 262144  
Total time 13 hr, 48 min

145.097  
140.793  
139.602  
135.564  
134.155  
133.426  
133.326  
129.984  
128.990  
128.213  
127.757  
125.605  
125.492  
124.428  
123.342  
121.020

77.181  
77.000  
76.817  
71.639  
61.356  
59.983  
59.534

39.841  
39.786  
32.498  
32.397  
27.092  
23.609  
22.431  
19.928  
19.404  
16.809





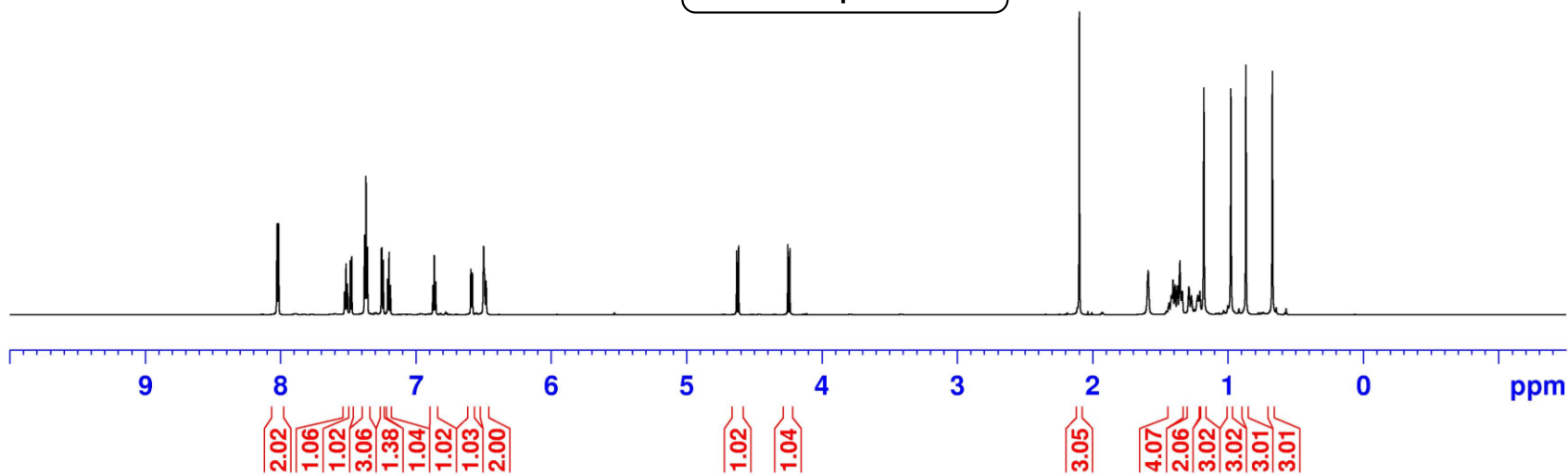
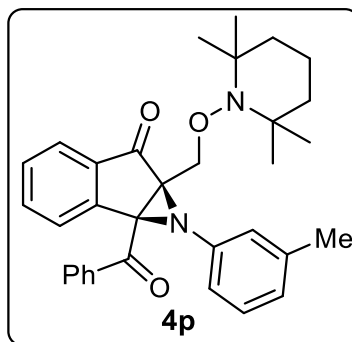
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

8.025  
8.014  
7.526  
7.515  
7.505  
7.484  
7.473  
7.379  
7.368  
7.357  
7.255  
7.251  
7.240  
7.208  
7.197  
7.186  
6.874  
6.863  
6.852  
6.593  
6.582  
6.499  
6.494  
6.481  
4.629  
4.614  
4.251  
4.236  
2.101  
1.592  
1.457  
1.452  
1.439  
1.421  
1.408  
1.393  
1.375  
1.357  
1.343  
1.339  
1.290  
1.275  
1.271  
1.252  
1.231  
1.226  
1.222  
1.209  
1.181  
0.981  
0.870  
0.674

CM-2-66

Current Data Parameters  
NAME CM-2-66-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7437894 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.38  
192.26

145.45  
144.50  
138.45  
135.50  
134.44  
133.60  
133.43  
130.05  
129.11  
128.43  
128.41  
127.56  
124.82  
123.66  
120.93  
117.28

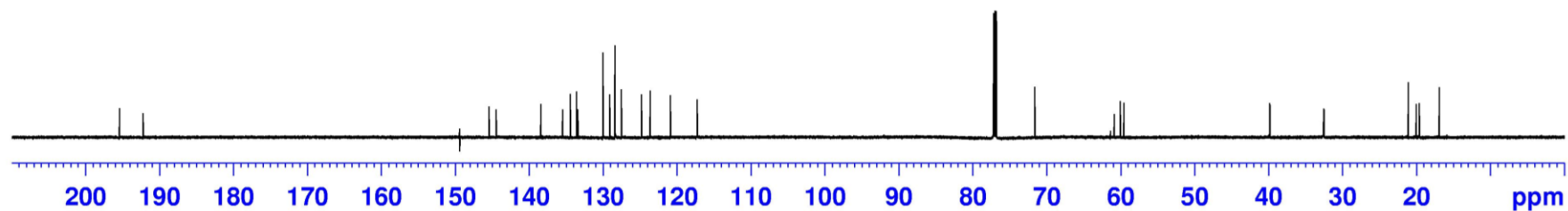
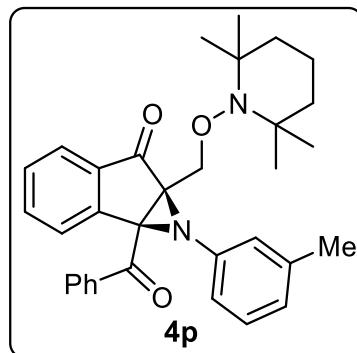
77.18  
77.00  
76.82  
71.63  
60.89  
60.07  
60.06  
59.57

39.85  
39.82  
32.56  
32.51  
21.10  
20.02  
19.61  
16.91

CM-2-64

Current Data Parameters  
NAME CM-2-66-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523405 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



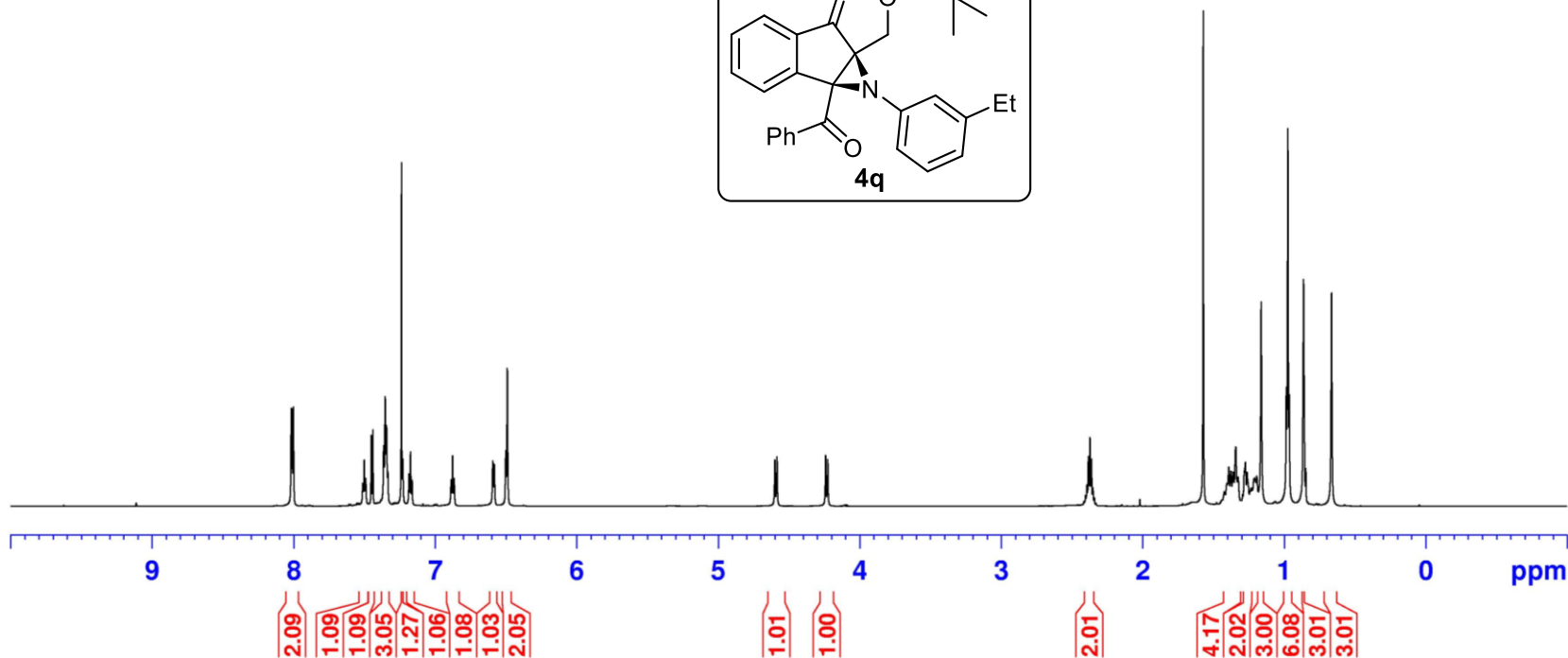
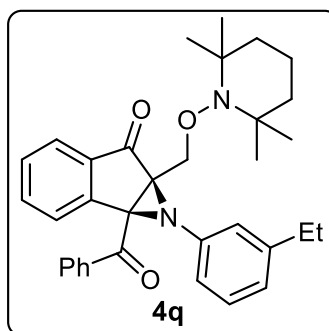
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

8.015  
8.005  
7.514  
7.503  
7.493  
7.454  
7.443  
7.366  
7.356  
7.346  
7.337  
7.240  
7.231  
7.187  
7.176  
7.165  
6.890  
6.879  
6.868  
6.595  
6.584  
6.503  
6.492  
4.602  
4.587  
4.243  
4.228  
2.396  
2.386  
2.375  
2.365  
1.574  
1.408  
1.395  
1.379  
1.363  
1.345  
1.330  
1.286  
1.276  
1.266  
1.237  
1.218  
1.212  
1.197  
1.165  
0.988  
0.977  
0.966  
0.866  
0.861  
0.668

CM-2-129

Current Data Parameters  
NAME CM-2-129-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441498 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.40  
192.32

145.48  
144.83  
144.59  
135.51  
134.44  
133.62  
133.48  
130.06  
129.09  
128.52  
128.42  
127.57  
124.81  
122.51  
119.82  
117.66

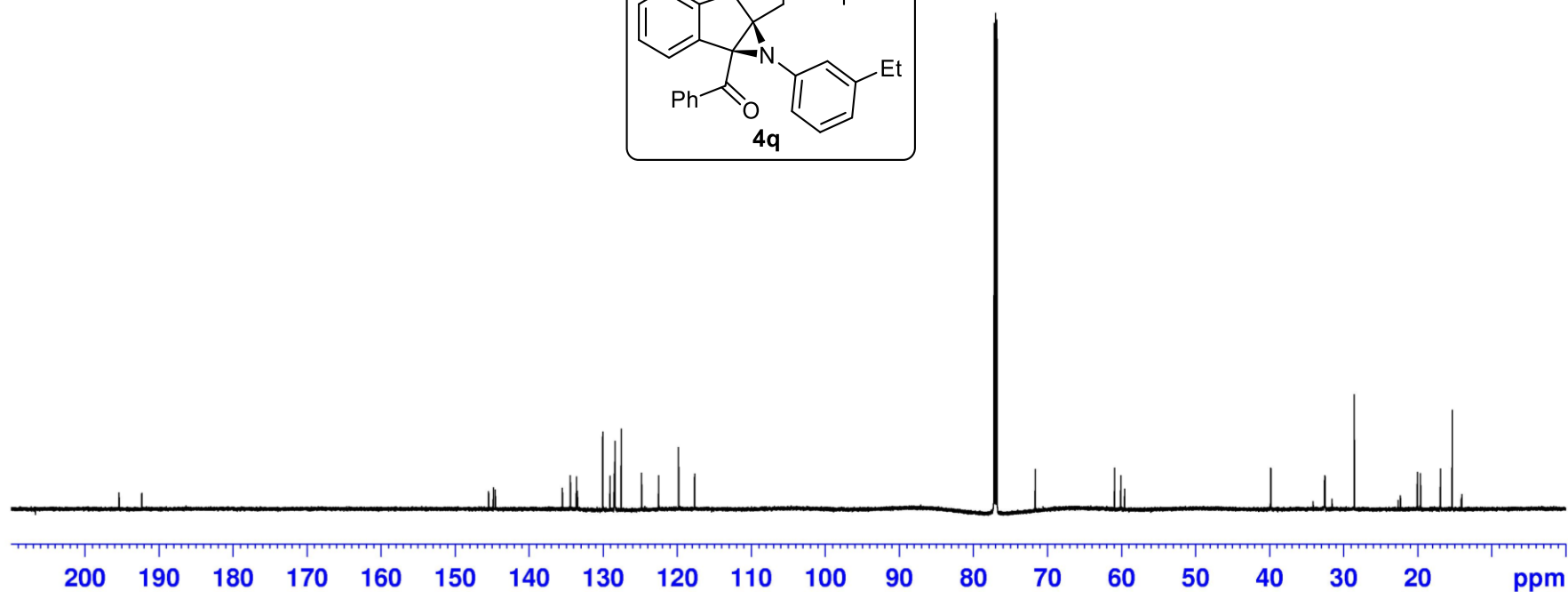
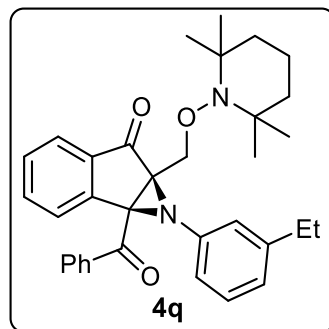
77.18  
77.00  
76.82  
71.64  
60.93  
60.08  
59.59

39.84  
39.82  
32.57  
28.57  
20.04  
19.62  
16.92  
15.32  
14.10  
14.05

CM-2-129

Current Data Parameters  
NAME CM-2-129-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532188 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



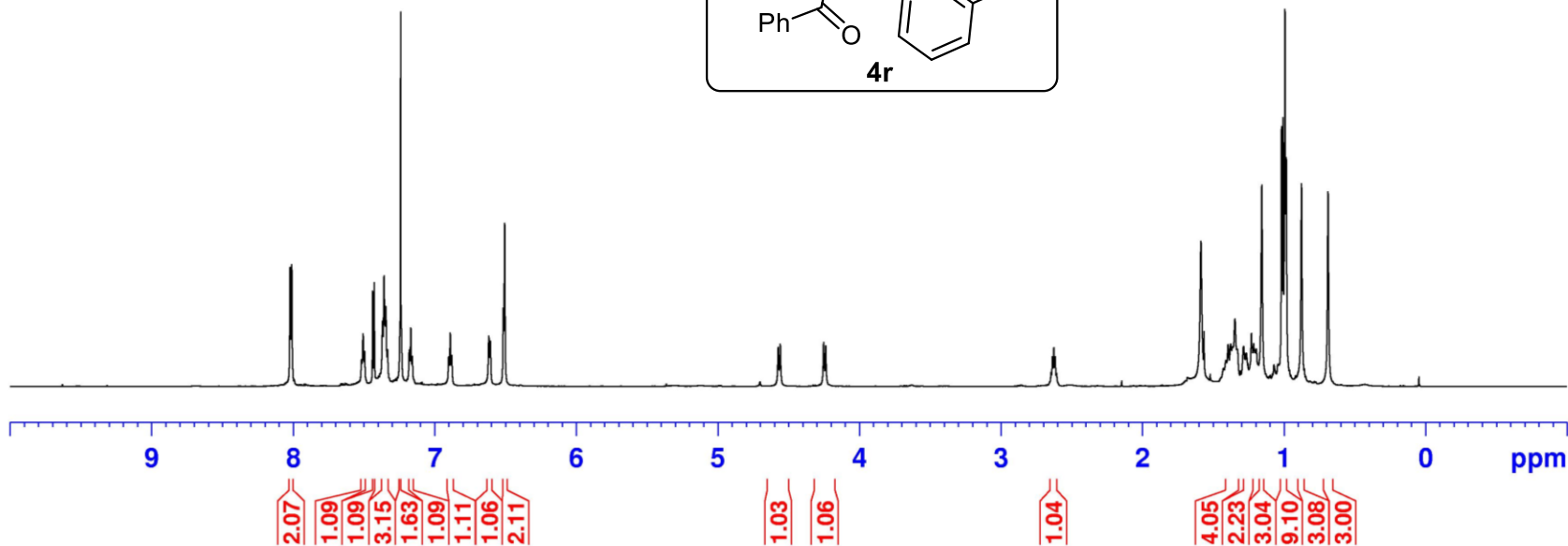
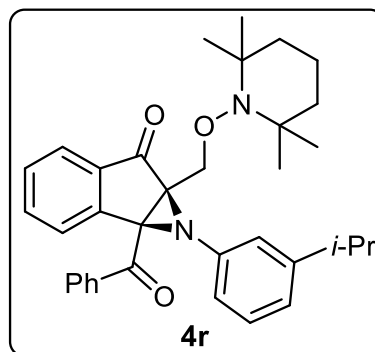
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

8.021  
8.010  
7.516  
7.505  
7.495  
7.437  
7.427  
7.369  
7.358  
7.345  
7.333  
7.240  
7.179  
7.168  
7.158  
6.901  
6.889  
6.878  
6.617  
6.607  
6.515  
6.505  
4.573  
4.558  
4.255  
4.240  
2.638  
2.628  
2.619  
1.589  
1.413  
1.410  
1.397  
1.379  
1.366  
1.349  
1.332  
1.288  
1.269  
1.263  
1.232  
1.227  
1.217  
1.198  
1.187  
1.159  
1.020  
1.010  
0.995  
0.986  
0.879  
0.691

CM-2-126

Current Data Parameters  
NAME CM-2-126-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441498 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.39  
192.33

149.33  
145.46  
144.58  
135.52  
134.40  
133.61  
133.51  
130.04  
129.04  
128.48  
128.41  
127.55  
124.77  
121.09  
118.40  
117.90

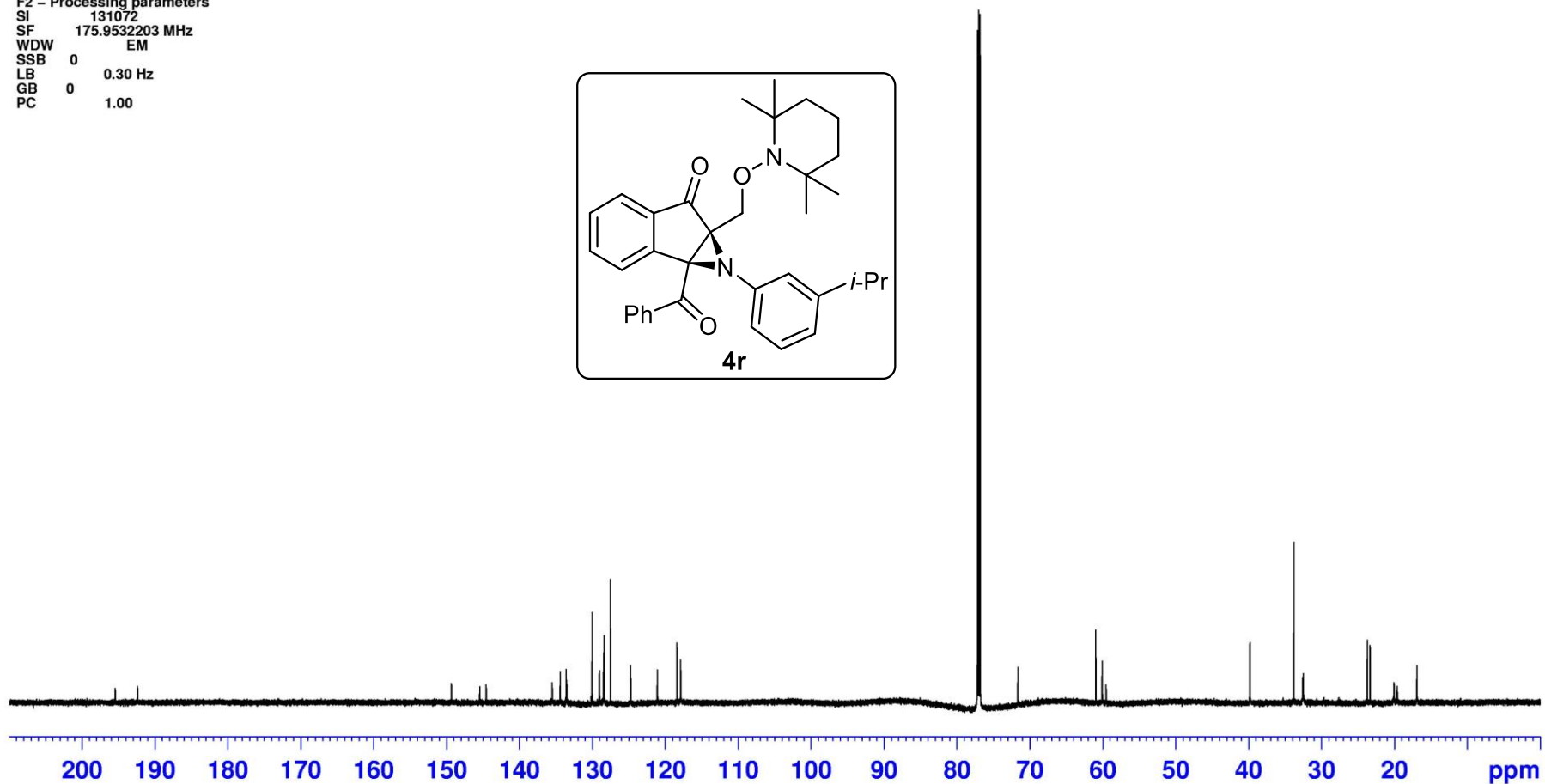
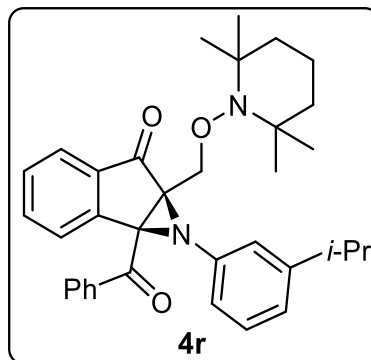
77.18  
77.00  
76.82  
71.64  
60.97  
60.08  
59.55

39.82  
33.81  
32.57  
32.50  
23.73  
23.34  
20.06  
19.64  
16.92

CM-2-126

Current Data Parameters  
NAME CM-2-126-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532203 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



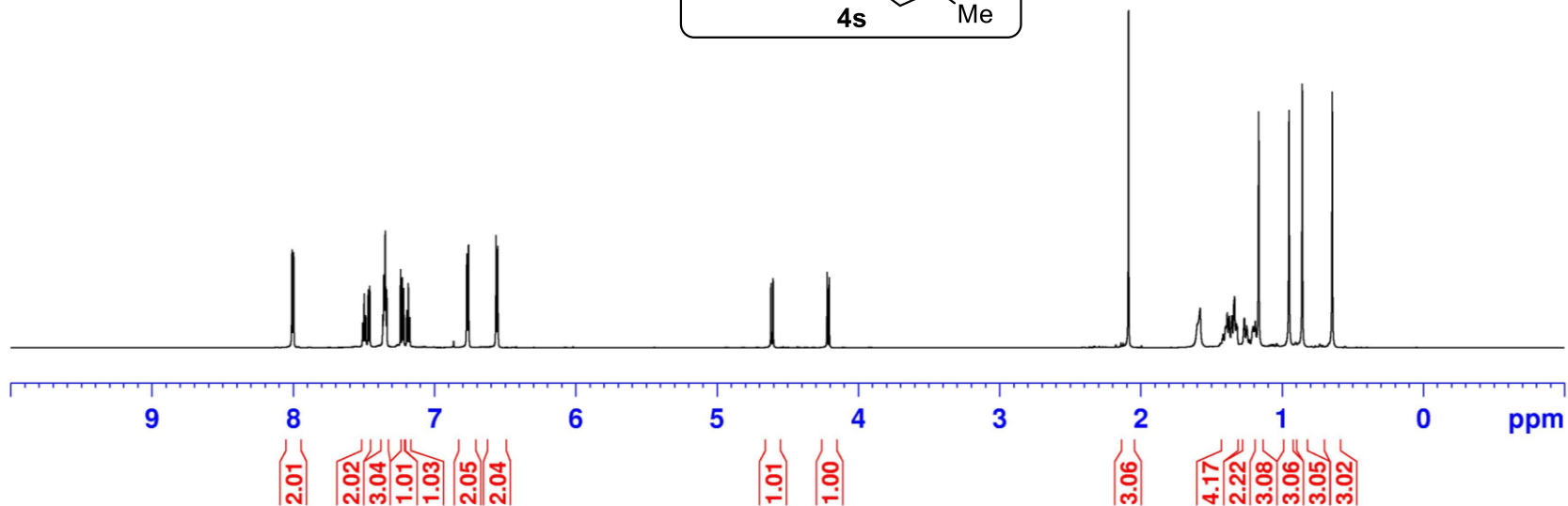
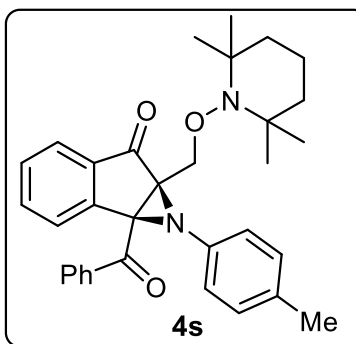
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

8.008  
7.997  
7.507  
7.496  
7.486  
7.468  
7.457  
7.365  
7.359  
7.354  
7.348  
7.337  
7.240  
7.228  
7.217  
7.195  
7.184  
7.174  
6.770  
6.758  
6.563  
6.551  
4.617  
4.602  
4.220  
4.205  
2.089  
1.582  
1.439  
1.421  
1.403  
1.398  
1.391  
1.376  
1.361  
1.356  
1.342  
1.339  
1.324  
1.319  
1.269  
1.253  
1.250  
1.233  
1.213  
1.208  
1.204  
1.191  
1.168  
0.953  
0.859  
0.647

CM-2-68

Current Data Parameters  
NAME CM-2-68-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7437996 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

195.49  
192.36

149.43  
145.47  
141.95  
135.55  
134.53  
133.60  
133.56  
132.13  
130.06  
129.20  
129.08  
128.38  
127.57  
124.78  
119.98

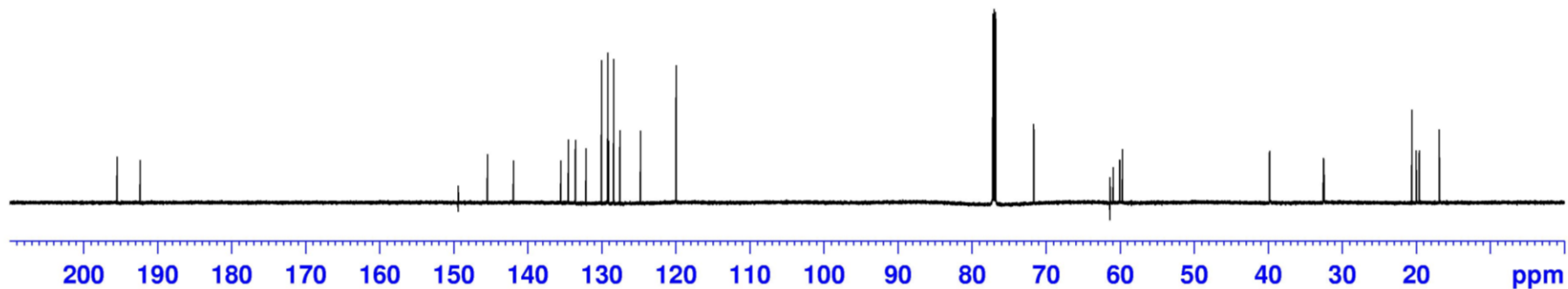
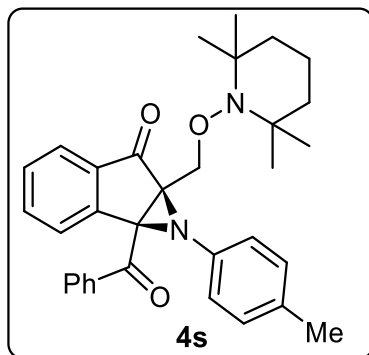
77.18  
77.00  
76.82  
71.66  
61.37  
60.94  
60.07  
60.04  
59.70

39.84  
39.81  
32.55  
32.48  
20.61  
20.03  
19.60  
16.91

CM-2-68

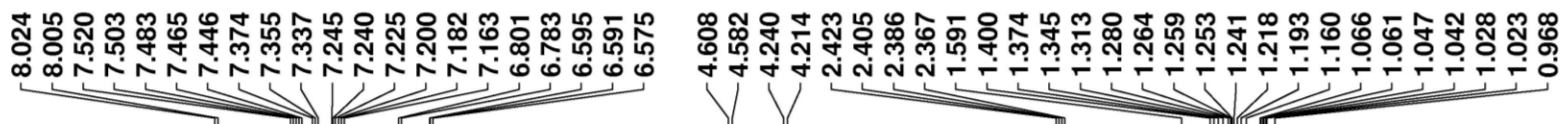
Current Data Parameters  
NAME CM-2-68-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9523410 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)



CM-02-121-1-hplc

Current Data Parameters

NAME CM-02-121  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters

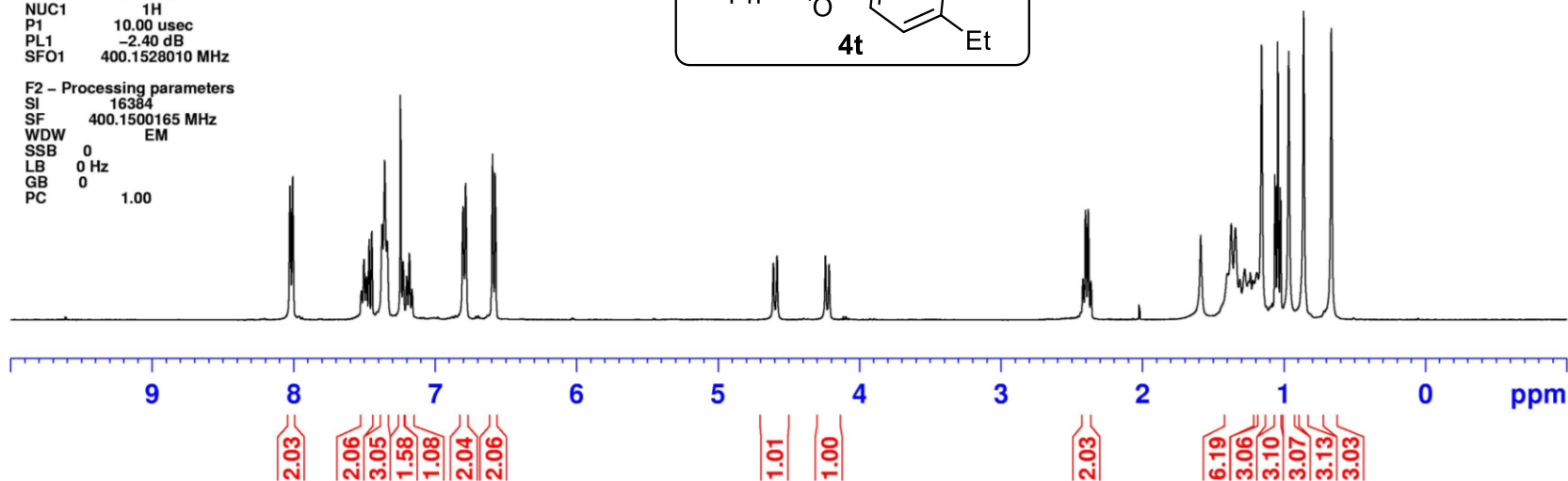
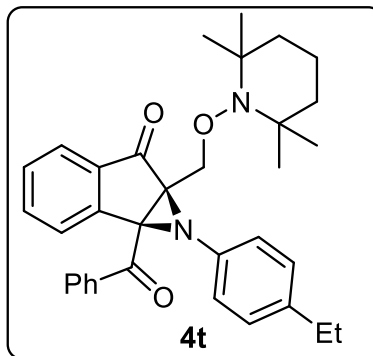
Date\_ 20230419  
Time 0.38  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 45  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559039 sec  
RG 322  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 16384  
SF 400.1500165 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 100 MHz)

195.53  
192.33

145.46  
142.13  
138.56  
135.60  
134.51  
133.61  
133.54  
130.03  
129.02  
128.38  
127.96  
127.52  
124.75  
120.00

77.31  
77.00  
76.68  
71.65  
60.90  
60.05  
59.64

39.82  
32.55  
32.49  
27.94  
20.03  
19.62  
16.90  
15.31

CM-02-121-1-hplc-c13

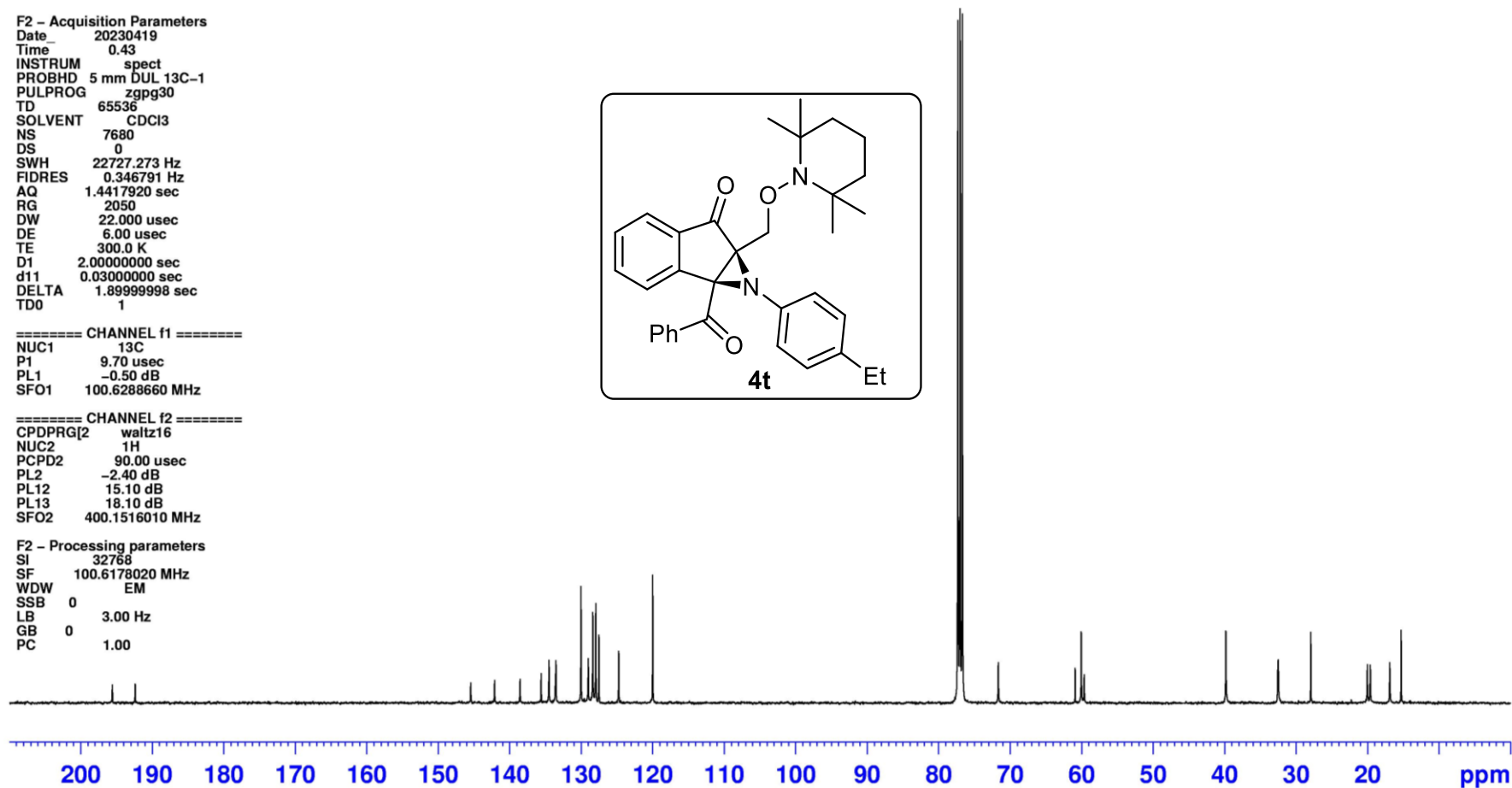
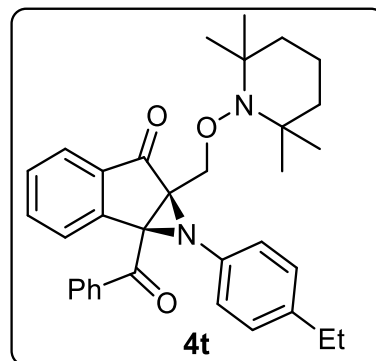
Current Data Parameters  
NAME CM-02-121  
EXPNO 9  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230419  
Time 0.43  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 7680  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4417920 sec  
RG 2050  
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 =====  
CPDPRG[2] 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 100.6178020 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



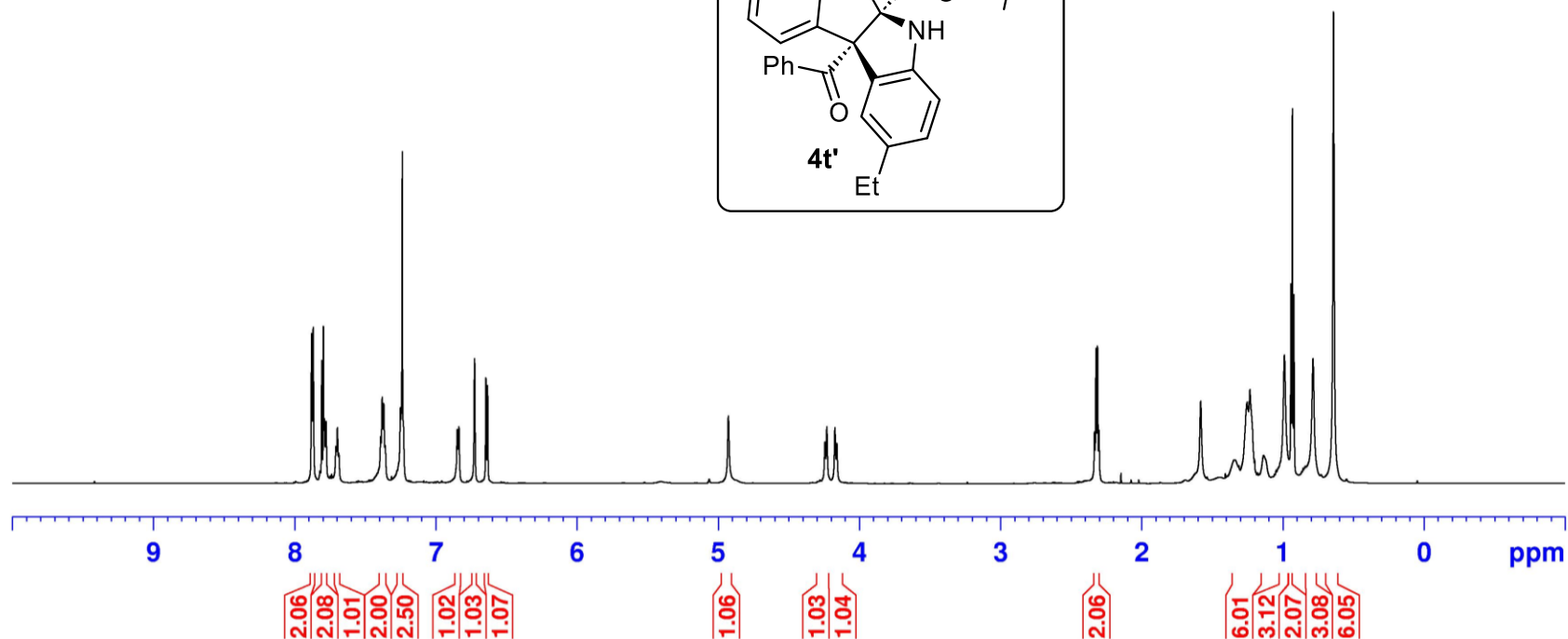
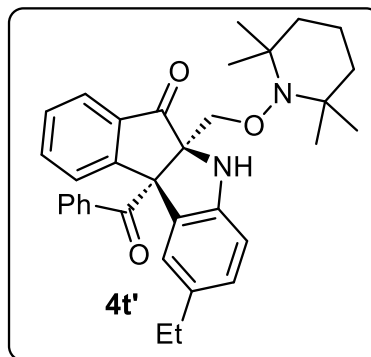
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-121-2

Current Data Parameters  
NAME CM-2-121-2-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7382002 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



S139

<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

207.17  
196.98

157.87  
145.77  
136.67  
136.48  
135.55  
135.51  
132.52  
132.12  
130.04  
128.59  
127.90  
127.85  
127.38  
124.29  
123.80  
111.13

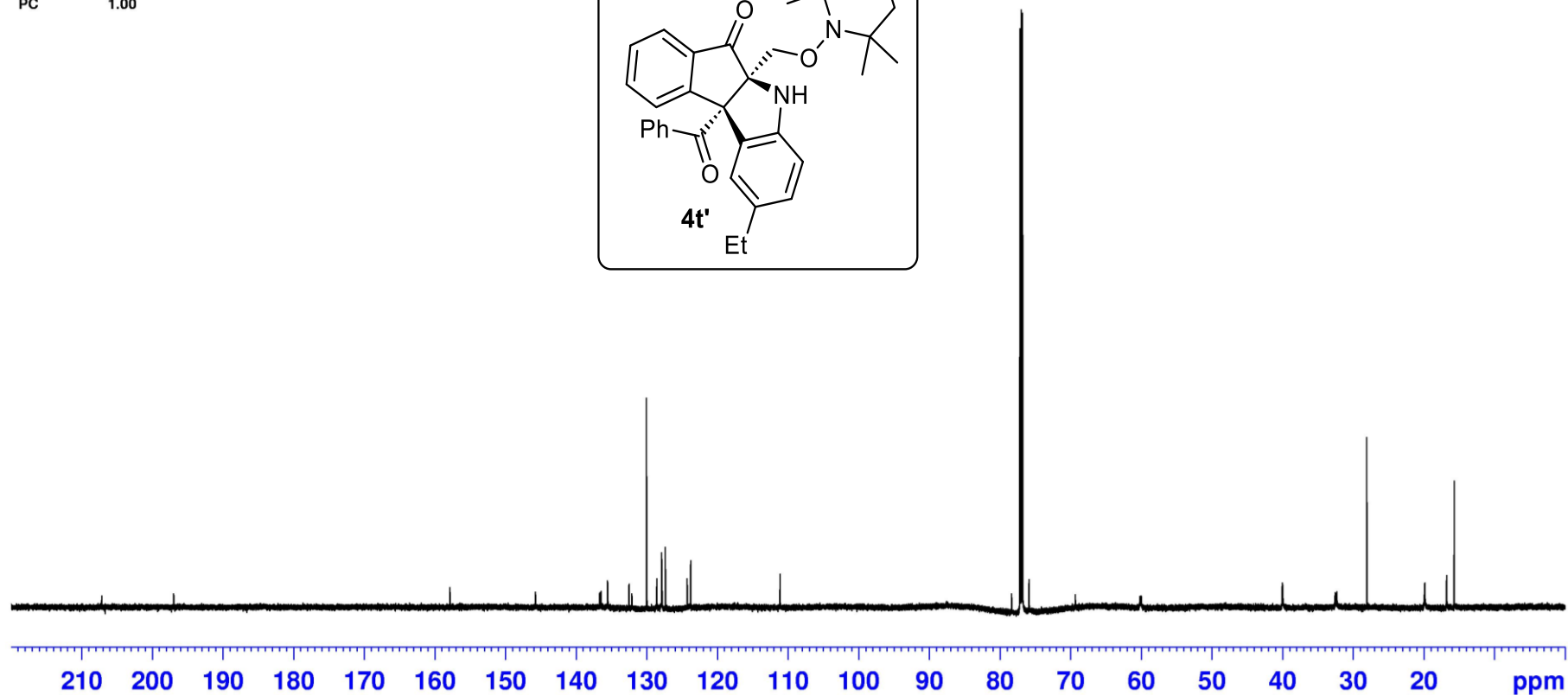
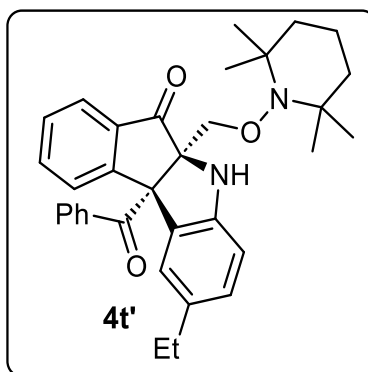
78.35  
77.18  
77.00  
76.82  
75.90  
69.34  
60.19  
60.01

40.04  
40.02  
40.00  
39.99  
32.57  
32.32  
28.09  
19.88  
16.79  
15.71

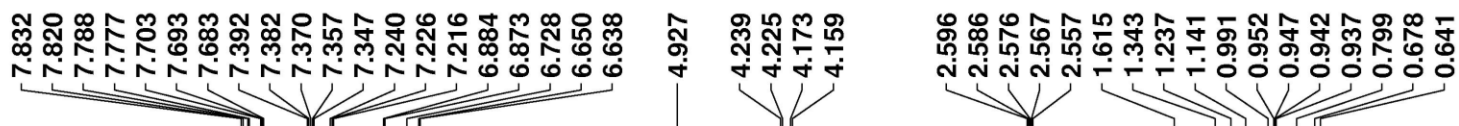
CM-2-1221-2

Current Data Parameters  
NAME CM-2-121-2-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9309003 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



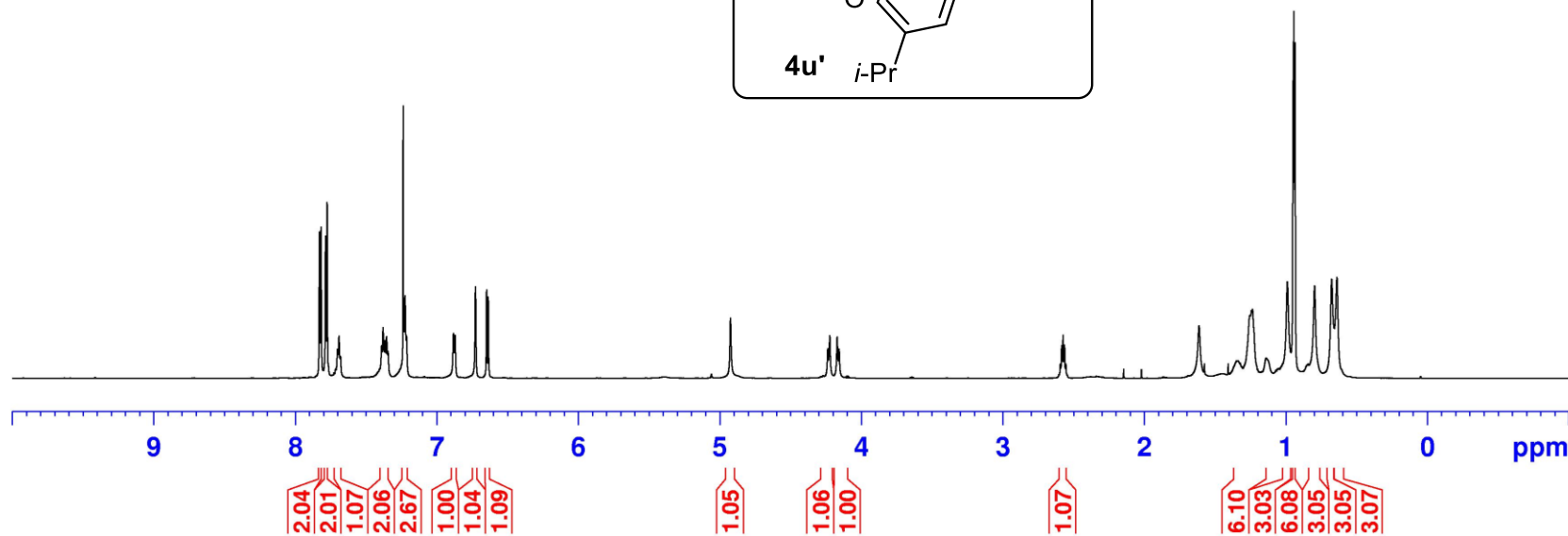
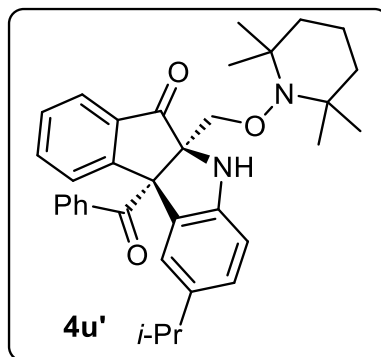
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-119

Current Data Parameters  
NAME CM-2-119-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438002 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

207.06  
197.49

157.95  
145.89  
141.21  
136.79  
135.58  
135.49  
132.39  
131.97  
129.94  
127.93  
127.81  
127.21  
126.98  
123.85  
123.05  
111.01

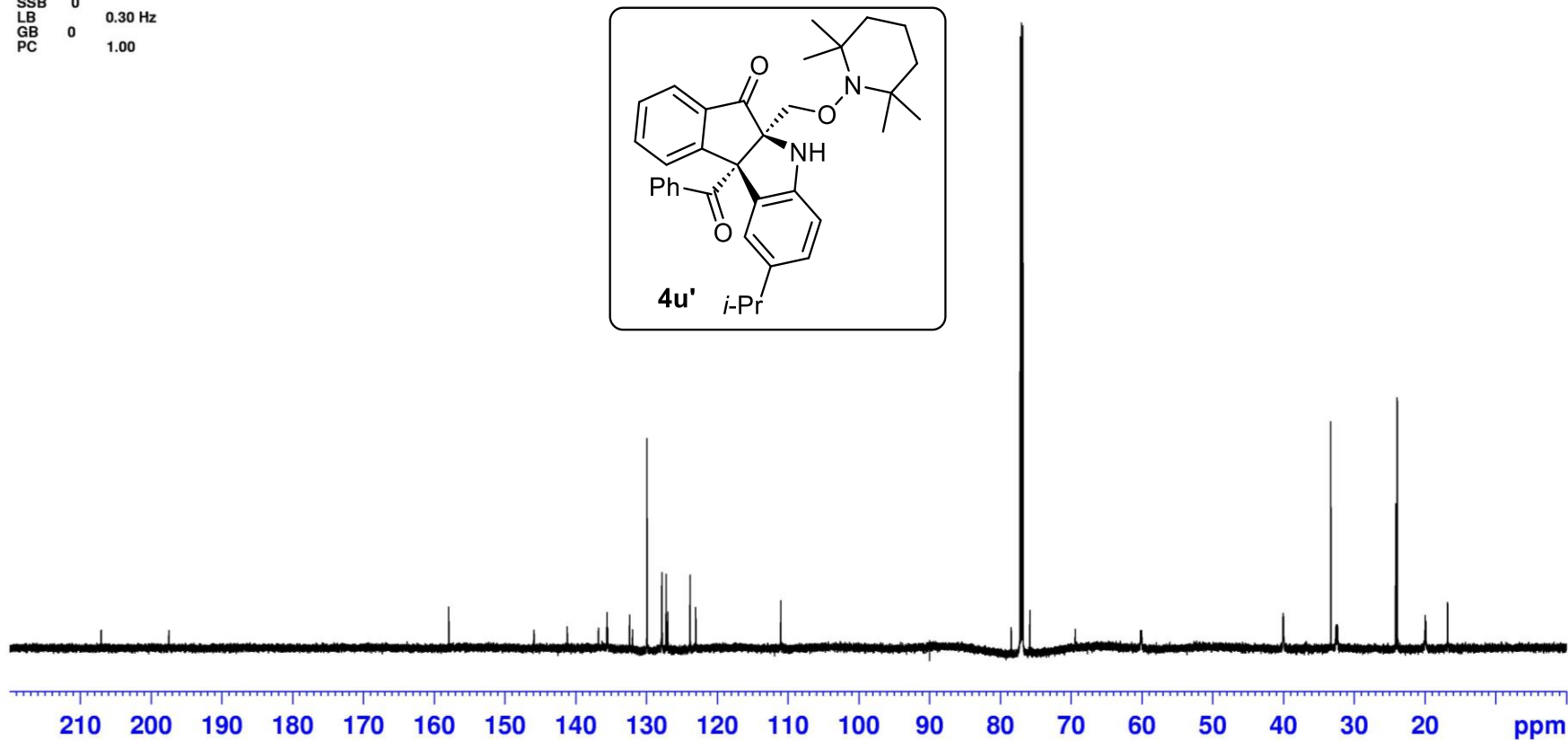
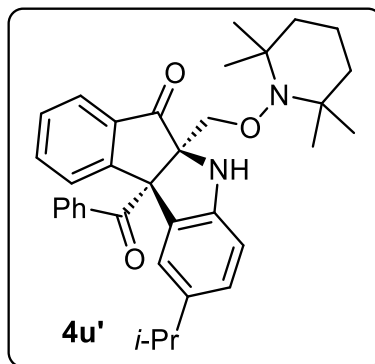
78.46  
77.18  
77.00  
76.82  
75.83  
69.41  
60.19  
60.03

40.04  
40.00  
33.32  
32.56  
32.37  
24.13  
23.92  
19.96  
19.88  
16.80

CM-2-119

Current Data Parameters  
NAME CM-2-119-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532206 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



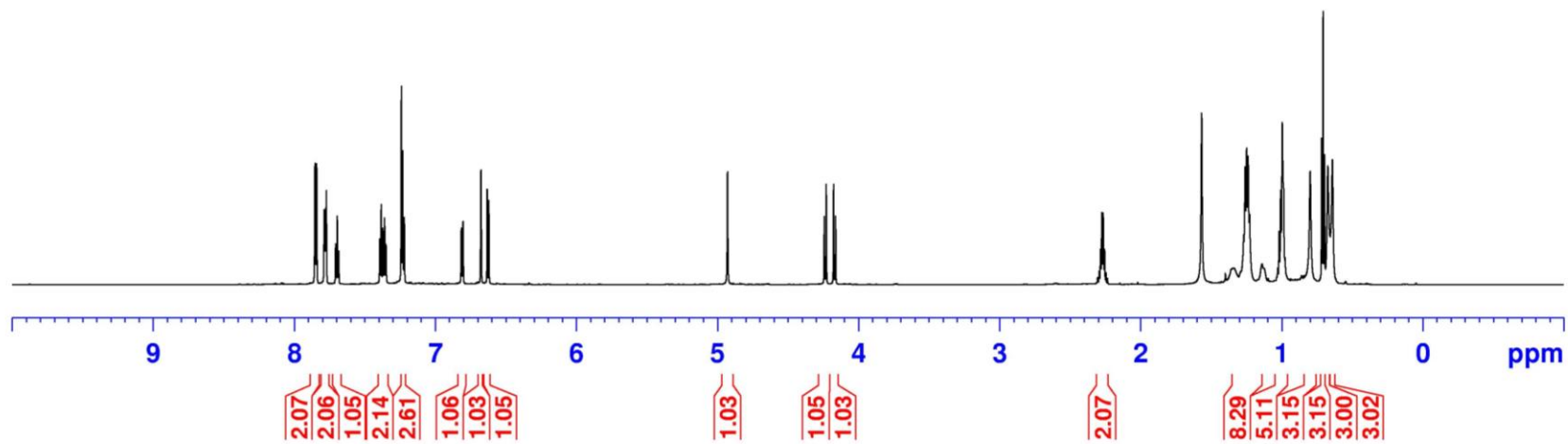
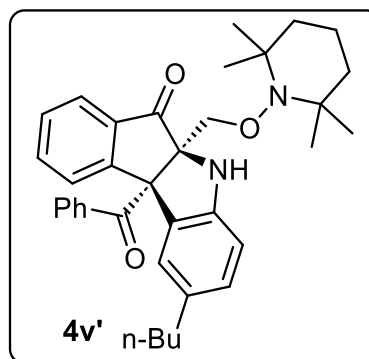
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

7.852  
7.841  
7.787  
7.783  
7.776  
7.772  
7.705  
7.695  
7.684  
7.393  
7.383  
7.372  
7.359  
7.349  
7.240  
7.230  
7.219  
6.817  
6.806  
6.678  
6.635  
6.623  
4.931  
4.245  
4.231  
4.179  
4.165  
2.287  
2.277  
2.268  
2.258  
1.570  
1.343  
1.273  
1.262  
1.252  
1.241  
1.230  
1.141  
1.130  
1.031  
1.021  
1.010  
0.999  
0.989  
0.979  
0.801  
0.720  
0.709  
0.699  
0.676  
0.643

CM-2-71

Current Data Parameters  
NAME CM-2-71-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7441498 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

207.11  
197.45

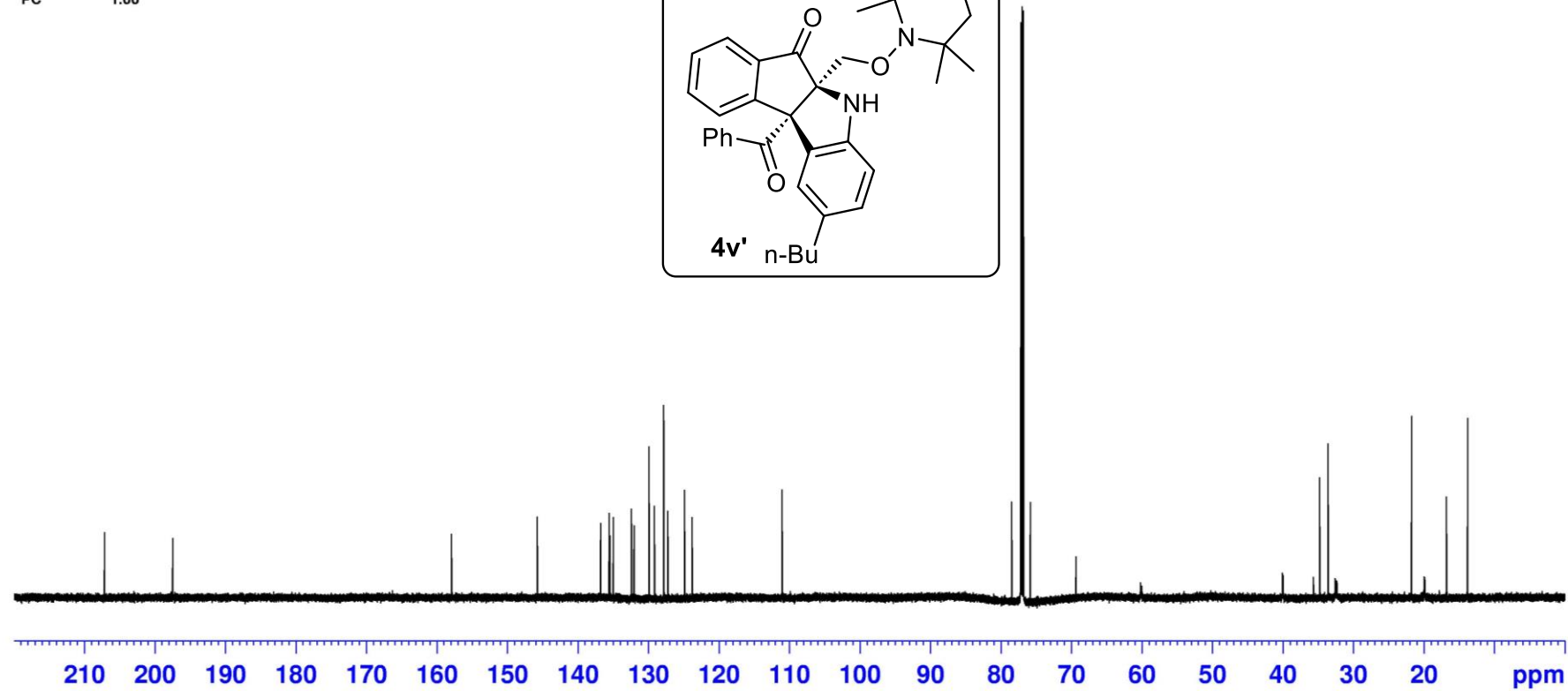
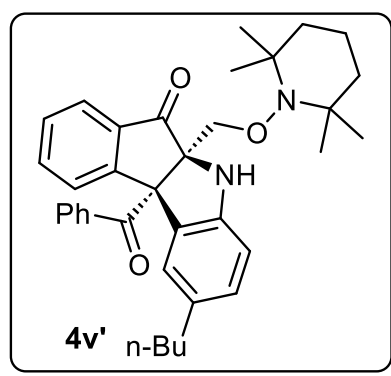
157.94  
145.76  
136.80  
135.58  
135.48  
134.99  
132.41  
132.05  
129.93  
129.17  
127.86  
127.84  
127.25  
124.89  
123.82  
111.06

78.47  
77.18  
77.00  
76.82  
75.84  
69.37  
60.20  
60.04

40.06  
40.01  
35.71  
34.80  
33.62  
32.58  
32.37  
21.76  
19.96  
19.90  
16.81  
13.79

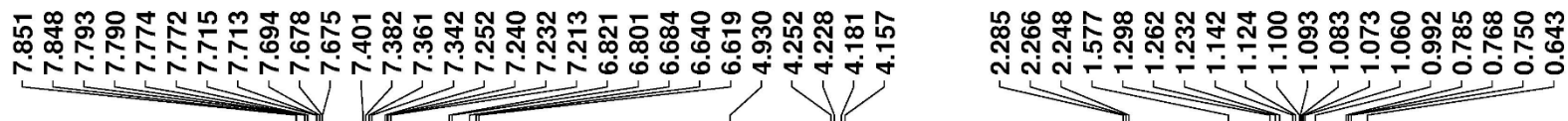
CM-2-71

Current Data Parameters  
NAME CM-2-71-C.fid  
EXPNO 1  
PROCNO 1  
  
F2 - Processing parameters  
SI 131072  
SF 175.9540983 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





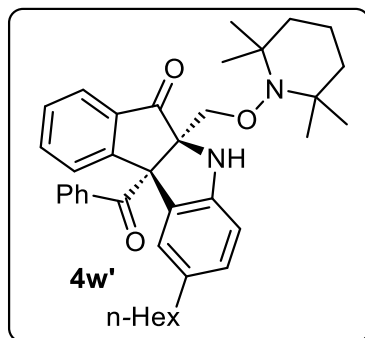
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)



CM-02-99

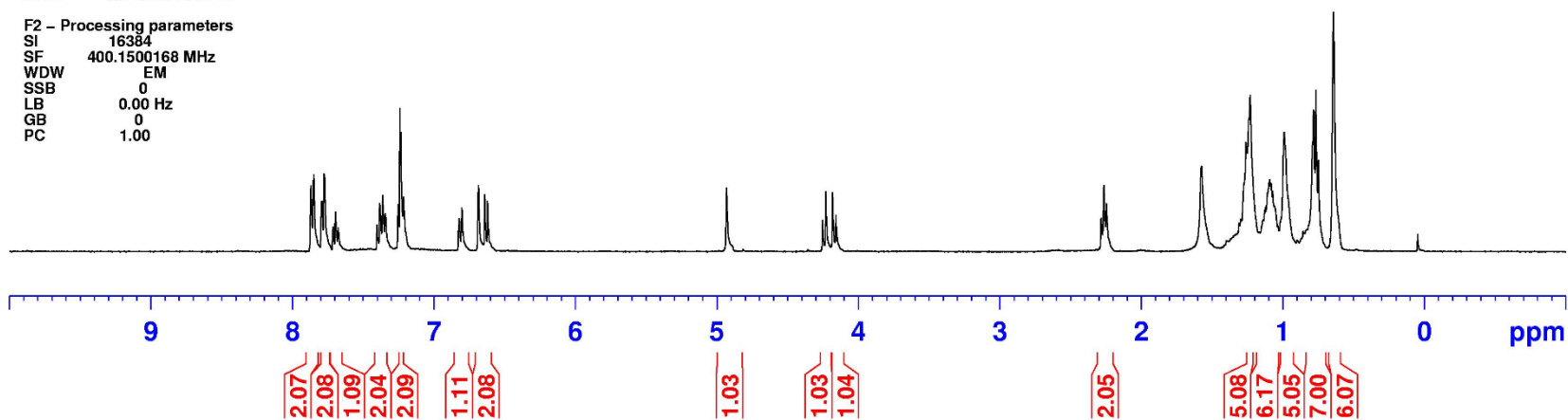
Current Data Parameters  
NAME CM-02-99  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date 20230223  
Time 23.18  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 51  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 456  
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 0.00 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

207.13  
197.23

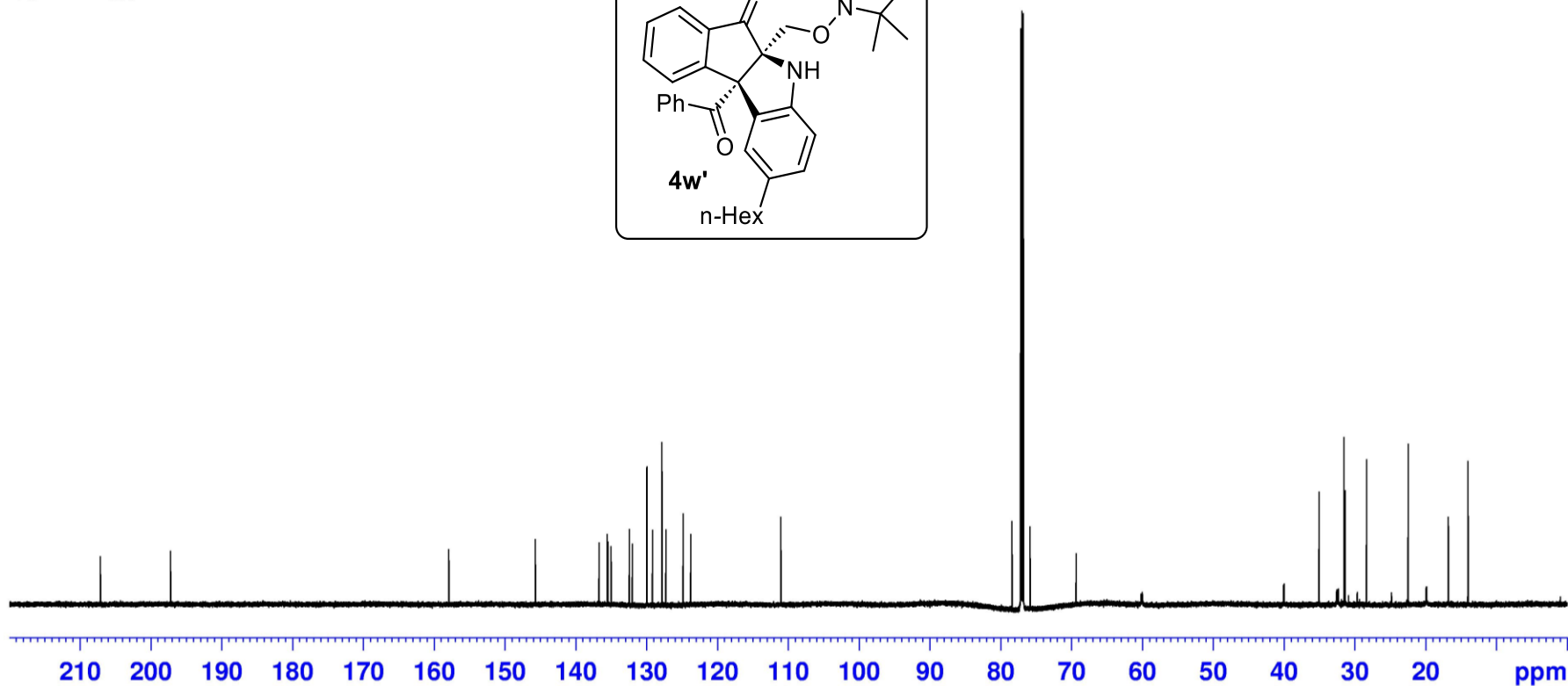
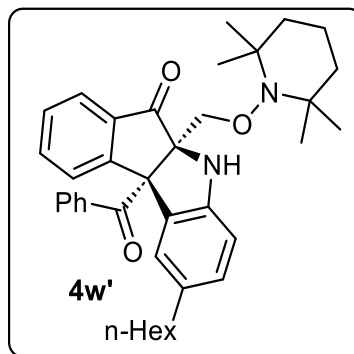
157.92  
145.73  
136.72  
135.55  
135.48  
135.02  
132.45  
132.04  
129.97  
129.18  
127.84  
127.83  
127.28  
124.85  
123.79  
111.06

78.41  
77.18  
77.00  
76.82  
75.87  
69.35  
60.19  
60.01  
40.06  
40.00  
35.07  
32.57  
32.34  
31.54  
31.39  
29.67  
28.35  
24.84  
22.48  
19.94  
19.87  
16.80  
14.01

CM-2-99

Current Data Parameters  
NAME CM-2-99-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532206 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)

7.885  
7.864  
7.801  
7.784  
7.768  
7.715  
7.712  
7.697  
7.677  
7.406  
7.394  
7.388  
7.376  
7.369  
7.361  
7.358  
7.263  
7.243  
7.239  
7.225  
7.034  
7.015  
6.995  
6.926  
6.907  
6.729  
6.710  
6.574  
6.556  
6.537  
5.040  
4.272  
4.247  
4.195  
4.171

1.568  
1.402  
1.351  
1.313  
1.263  
1.238  
1.150  
1.126  
0.999  
0.859  
0.802  
0.656

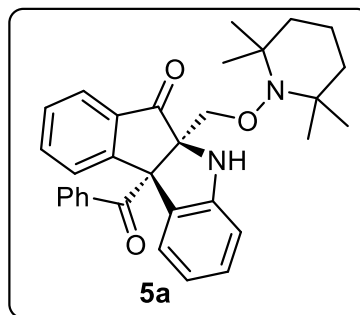
CM-02-06

Current Data Parameters

NAME CM-02-06  
EXPNO 9  
PROCNO 1

F2 - Acquisition Parameters

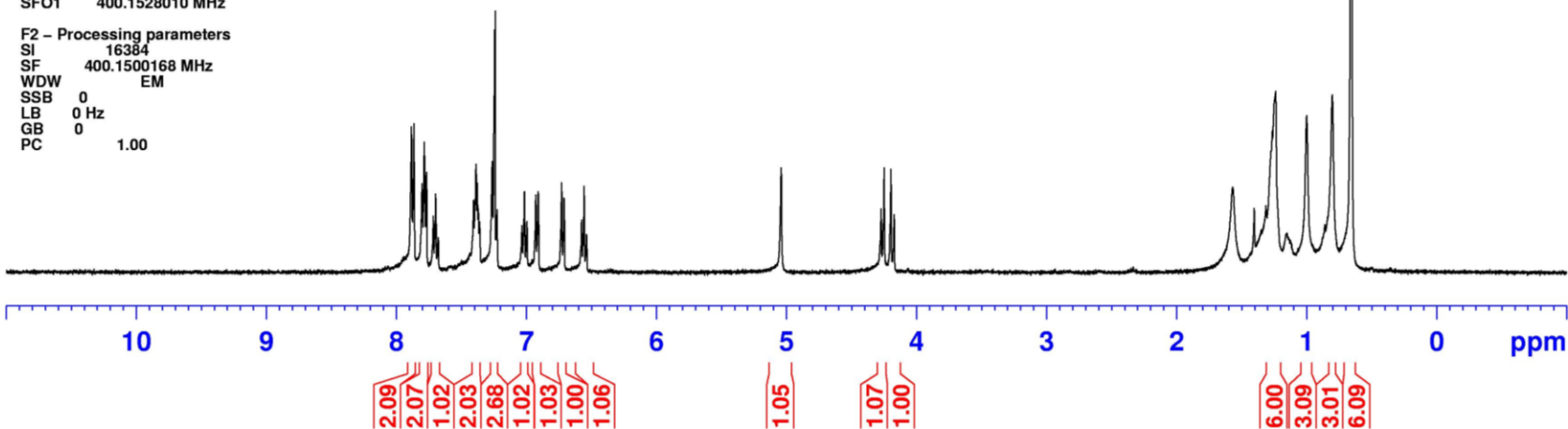
Date\_ 20220710  
Time\_ 2.53  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559039 sec  
RG 512  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
TD0 1



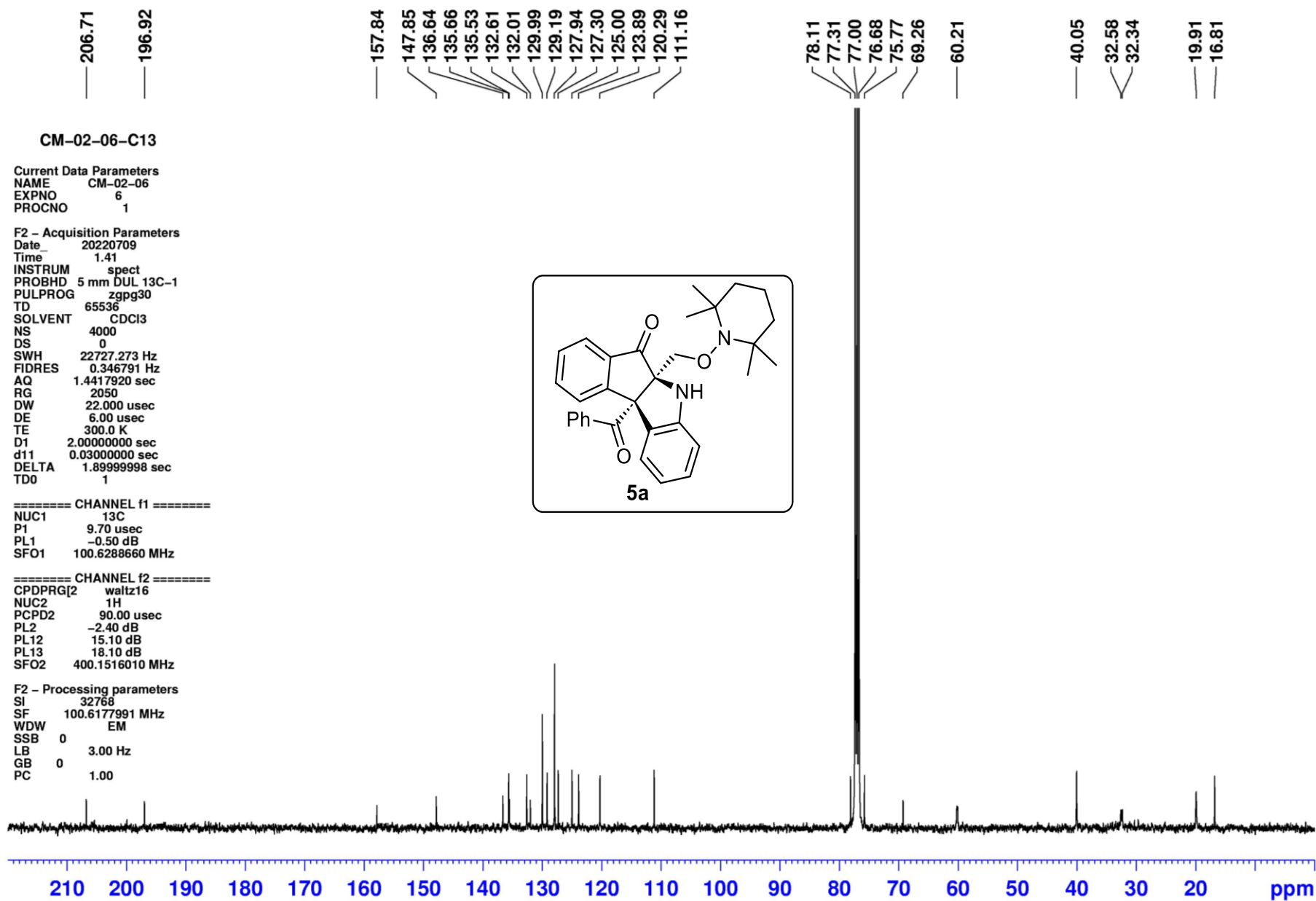
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters

SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 100 MHz)



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)

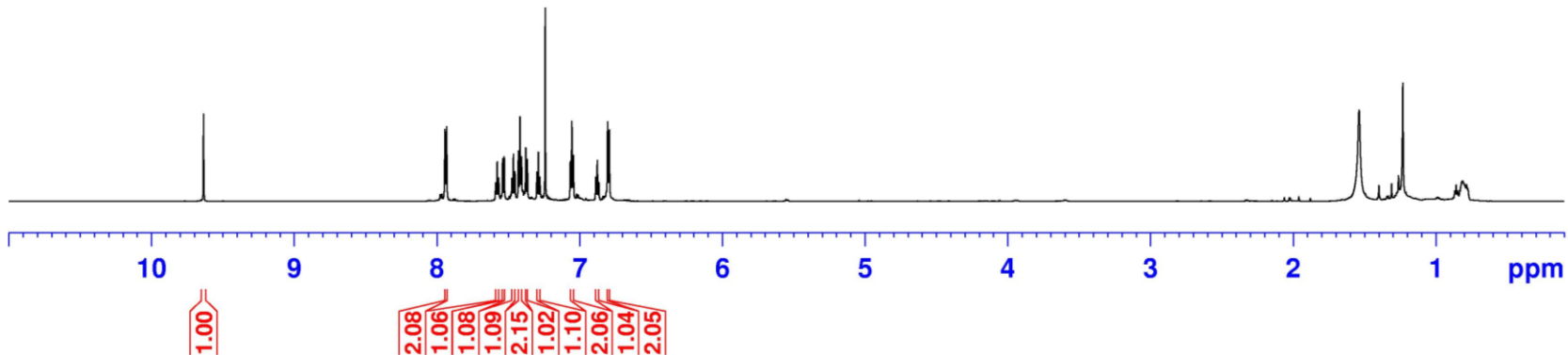
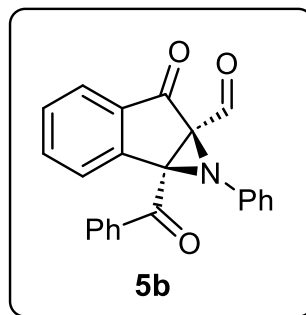
9.634  
7.943  
7.931  
7.587  
7.577  
7.566  
7.538  
7.527  
7.474  
7.463  
7.453  
7.428  
7.417  
7.406  
7.376  
7.365  
7.299  
7.288  
7.277  
7.240  
7.064  
7.054  
7.042  
6.885  
6.875  
6.864  
6.803  
6.791

1.541

CM-2-108

Current Data Parameters  
NAME CM-2-108-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7438013 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

193.08  
190.90  
190.22

143.17  
142.95  
135.38  
134.60  
134.44  
133.92  
130.35  
129.59  
129.06  
127.22  
125.39  
124.10  
120.23

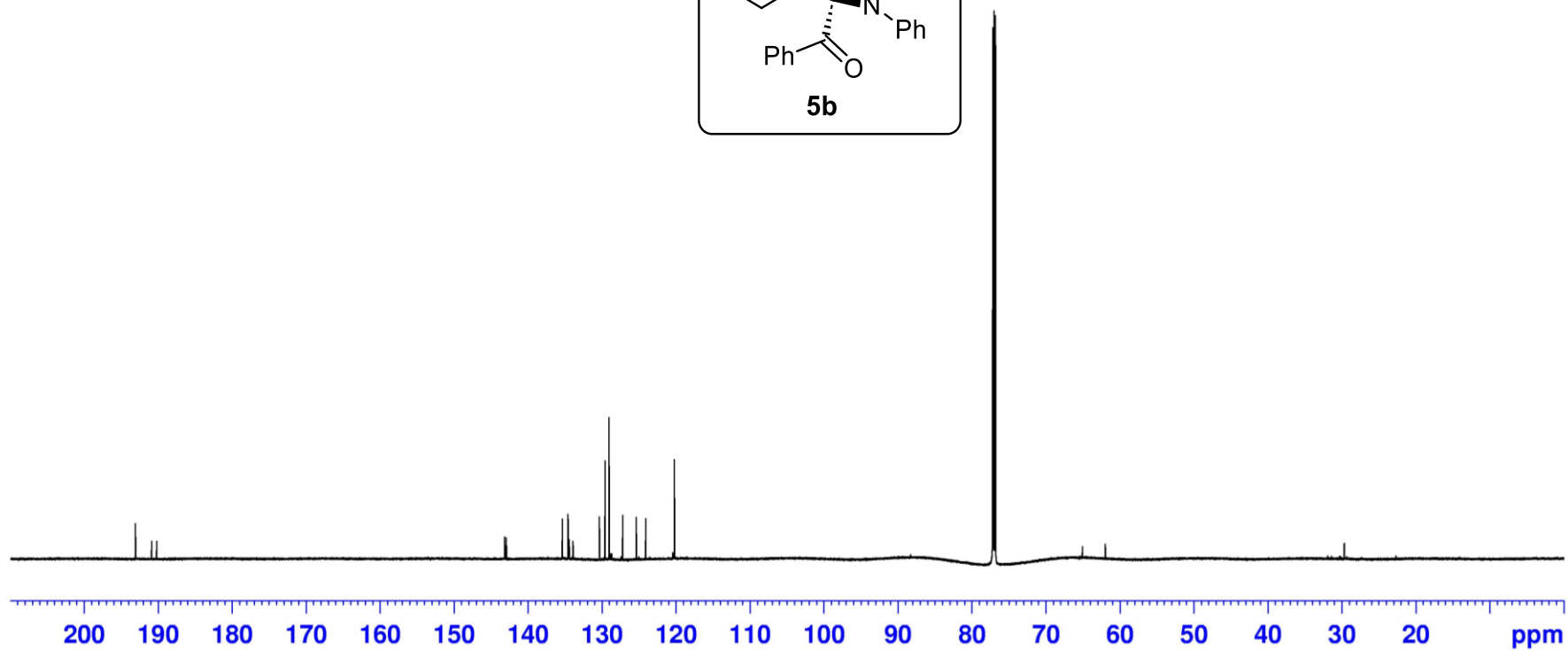
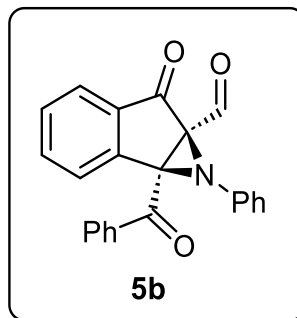
77.18  
77.00  
76.82

65.07  
61.98

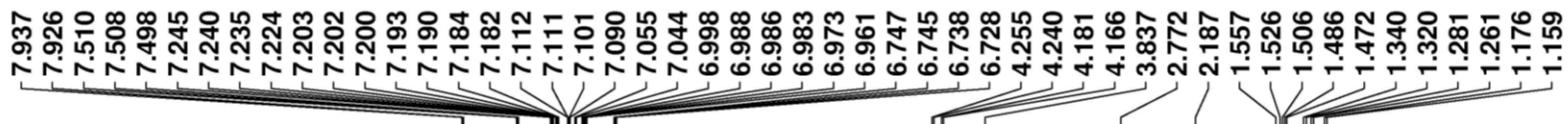
CM-2-108

Current Data Parameters  
NAME CM-2-108-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9317777 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



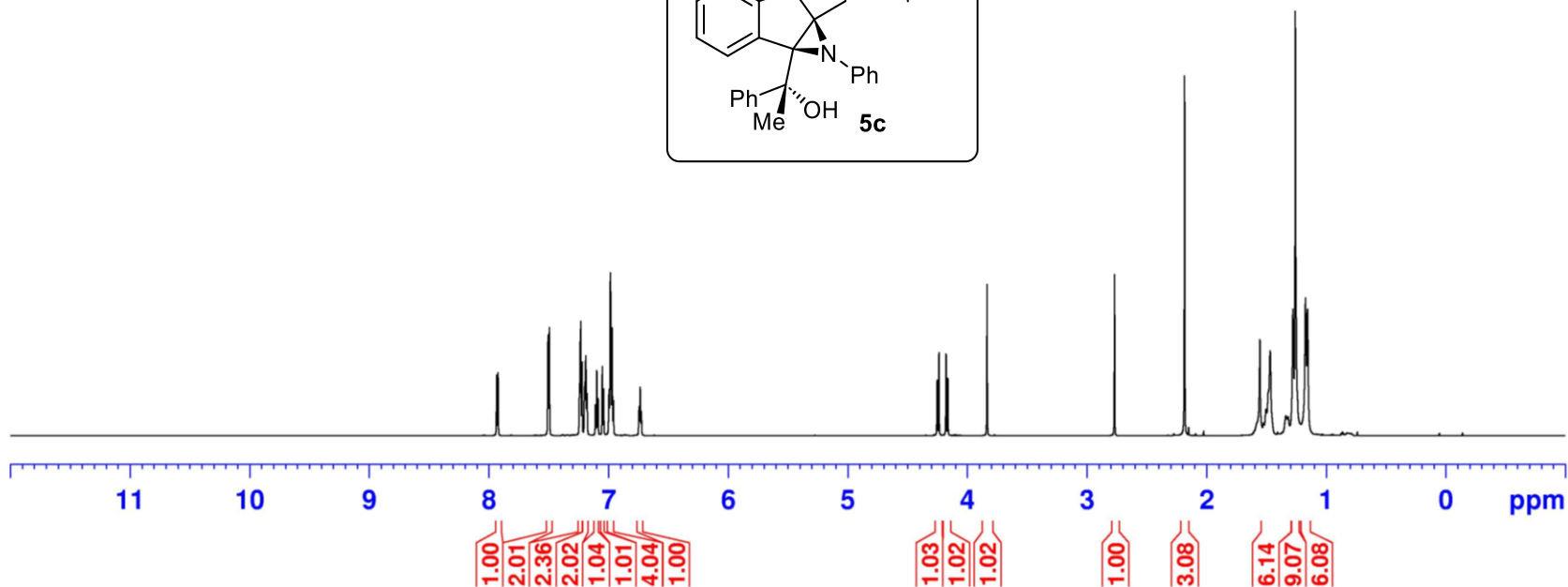
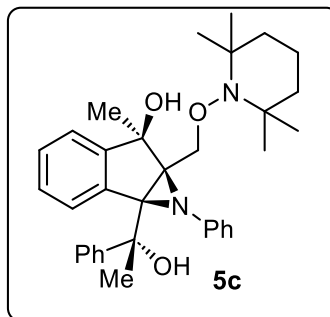
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-97

Current Data Parameters  
NAME CM-2-97-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7382206 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



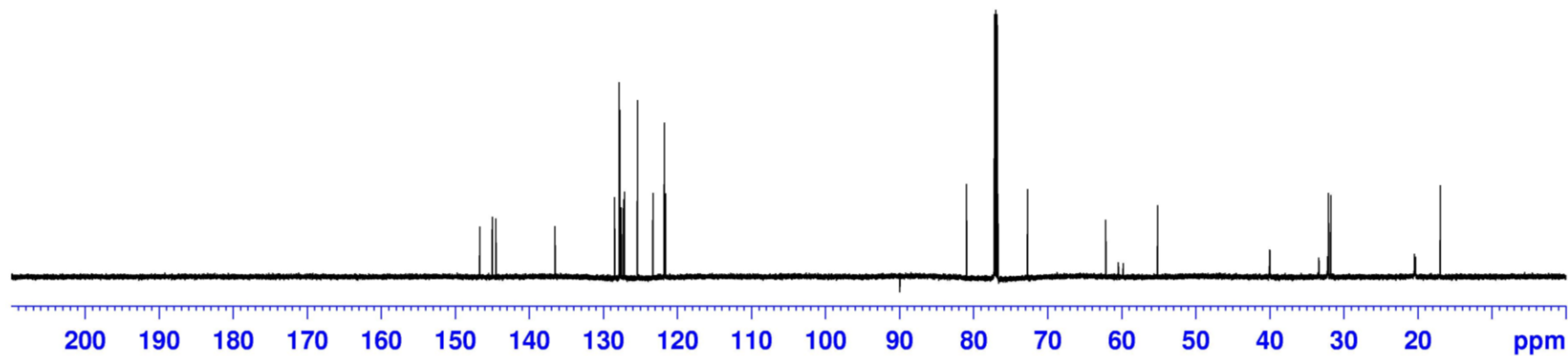
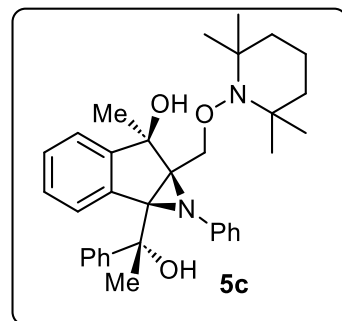
<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)



CM-2-97

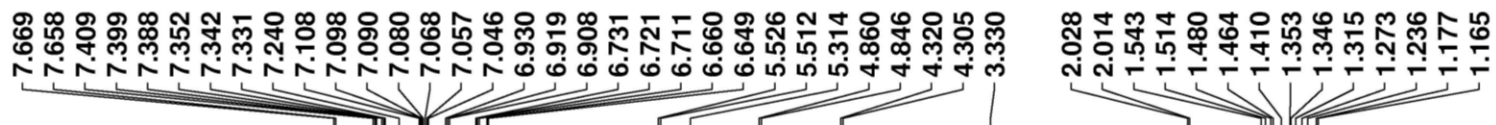
Current Data Parameters  
NAME CM-2-97-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9291831 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





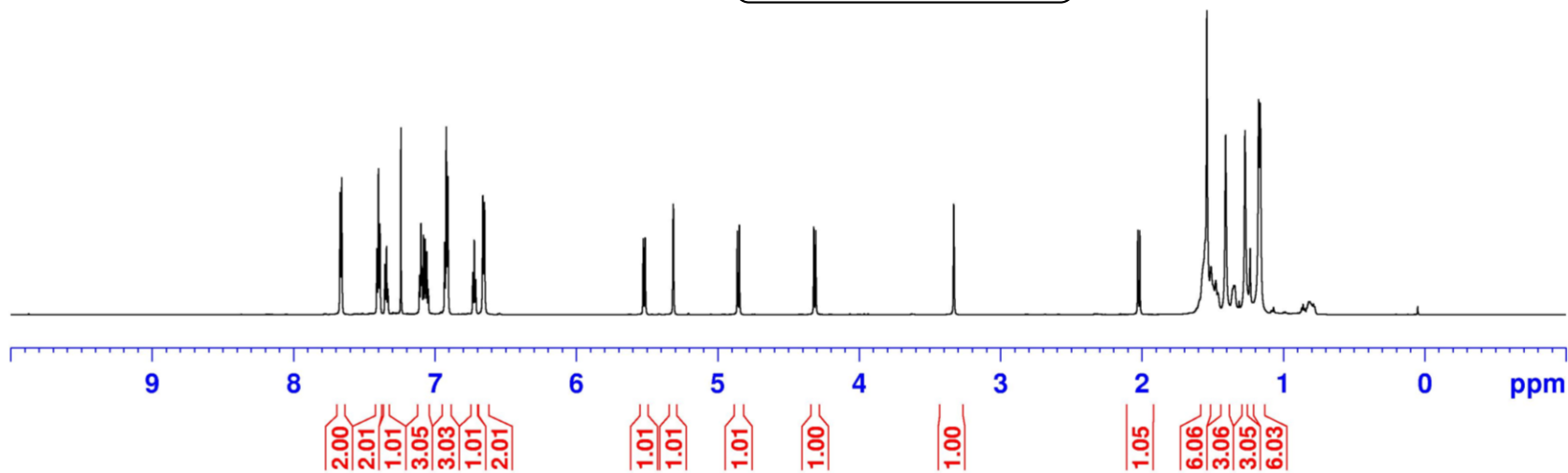
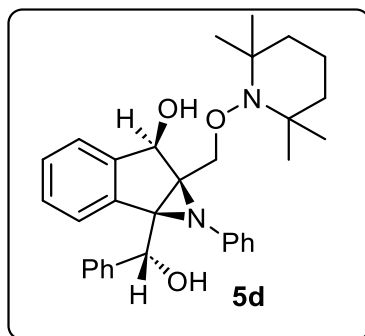
<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 700 MHz)



CM-2-89-2

Current Data Parameters  
NAME CM-2-89-2-H.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 699.7382206 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

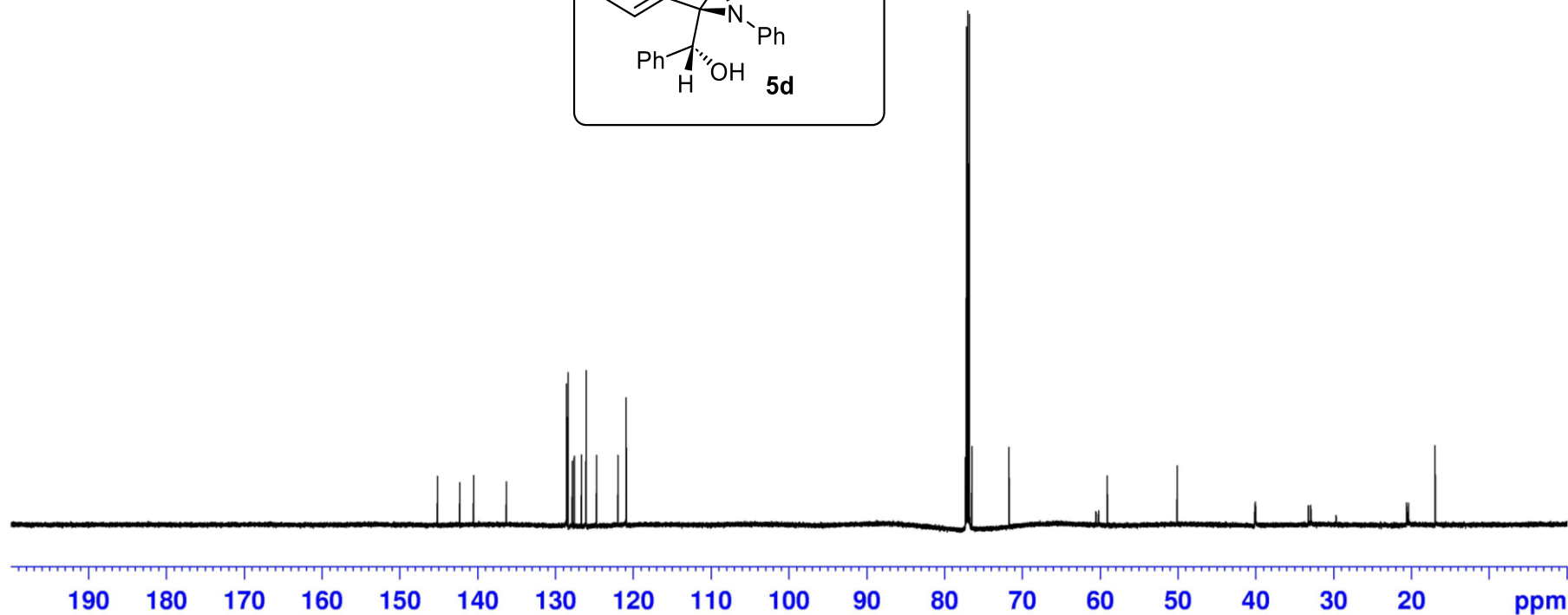
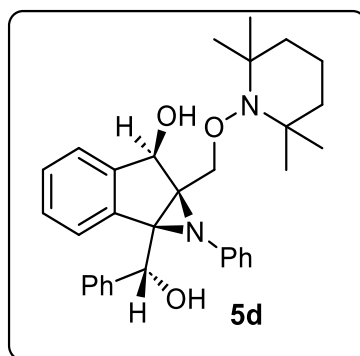
145.16  
142.32  
140.52  
136.33  
128.57  
128.42  
128.40  
127.85  
127.60  
126.66  
126.05  
124.72  
121.95  
120.92

77.32  
77.18  
77.00  
76.82  
76.49  
71.72  
60.54  
60.19  
59.10  
50.11  
40.12  
40.05  
33.23  
32.93  
20.62  
20.38  
16.96

CM-2-89-2

Current Data Parameters  
NAME CM-2-89-2-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532181 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 400 MHz)

7.542  
7.523  
7.408  
7.402  
7.396  
7.387  
7.290  
7.272  
7.252  
7.242  
7.240  
7.199  
7.182  
7.069  
7.056  
7.049  
7.037  
7.019  
7.011  
7.001  
6.999  
6.989  
6.969  
6.950  
6.907  
6.886  
6.751  
6.748  
6.732  
6.731  
6.715  
6.712  
5.523  
5.500  
5.107  
5.099  
4.706  
4.681  
4.413  
4.388  
2.839  
2.829  
2.144  
2.121  
1.551  
1.521  
1.490  
1.465  
1.419  
1.242  
1.216  
1.143

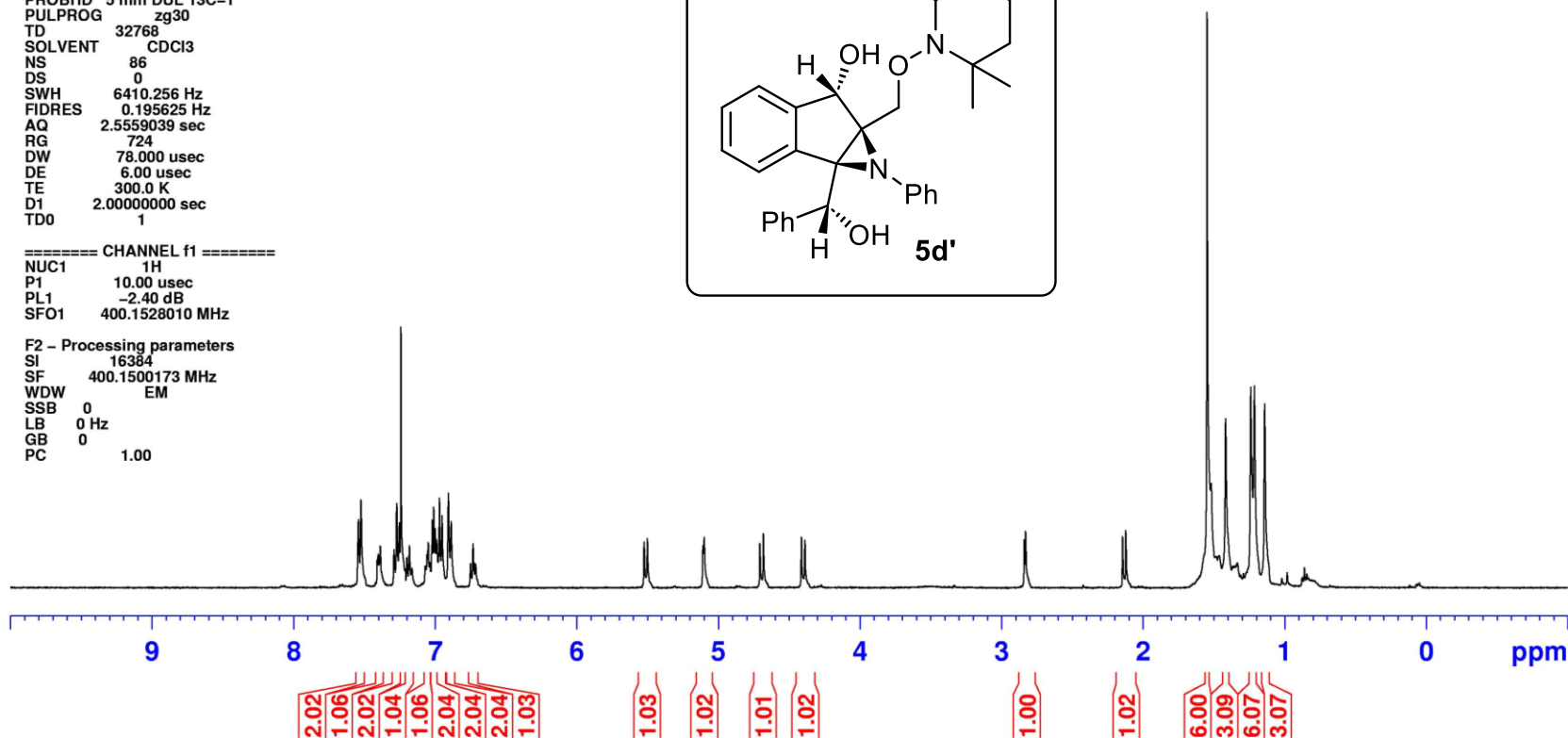
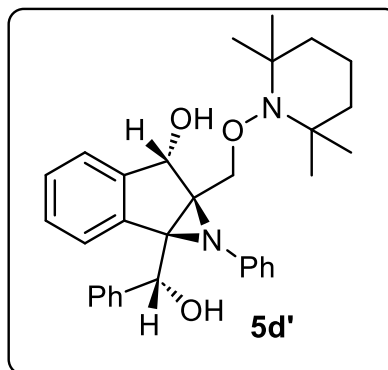
CM-02-89-1

Current Data Parameters  
NAME CM-02-89  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230203  
Time 9.44  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 86  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559039 sec  
RG 724  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 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 400.1500173 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



<sup>13</sup>C-NMR (CDCl<sub>3</sub>, 175 MHz)

145.75  
141.39  
139.86  
136.46  
128.56  
128.27  
128.13  
127.89  
127.46  
127.24  
126.19  
124.32  
121.83  
120.92

77.43  
77.18  
77.00  
76.82  
76.76  
73.87  
60.47  
60.24  
59.65  
52.69

39.94  
33.20  
32.88

20.54  
20.41  
17.02

CM-2-89-1

Current Data Parameters  
NAME CM-2-89-1-C.fid  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 131072  
SF 175.9532179 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

