

# Copper(I)-Catalyzed Asymmetric Intramolecular C-Arylation with Ureas as the Additives: Highly Enantioselective Formation of Spirooxindoles

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## Supporting Information

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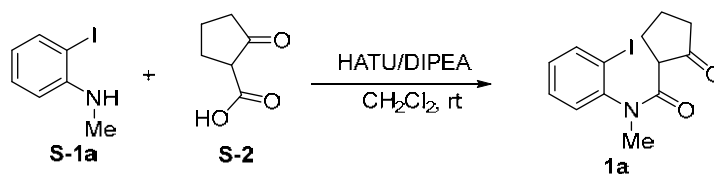
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## I. General Remarks

<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded on a Bruker AV-400 or 500 MHz spectrometer. Chemical shifts ( $\delta$ ) are given in relative to tetramethylsilane ( $\delta$  0.00 ppm) in CDCl<sub>3</sub>. Coupling constants, *J*, were reported in hertz unit (Hz). High resolution mass spectra (HRMS) were obtained on the Thermo Q Exactive Focus mass spectrometer with Orbitrap analyzer technology and the Agilent LC-UV-TOF or the SCIEX X500R QTOF mass spectrometer in ESI mode with TOF as the mass analyzer type. Chemical names were generated using Cambridge Soft. ChemDraw Ultra 10.0. Optical rotations were measured on a Perkin Elmer 341 polarimeter. Enantiomeric ratios were determined by chiral HPLC using a chiralpak AD-H (Amylose tris (3,5-dimethylphenylcarbamate) coated on 5 $\mu$ m silica-gel), chiralpak AS-H (Amylose tris-[(S)- $\alpha$ -methylbenzylcarbamate] coated on 5 $\mu$ m silica-gel) or chiralcel OD-H column (Cellulose tris (3,5-dimethylphenylcarbamate) coated on 5 $\mu$ m silica-gel) with hexane and *i*-PrOH as solvents. Commercially obtained reagents were used without further purification.

## II. Substrate Synthesis and Procedure for Asymmetric Coupling

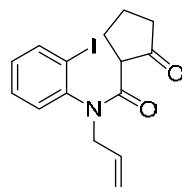
General procedure for the synthesis of compound **1a-1l**:



A mixture of 2-iodo-*N*-methylaniline (**S-1a**, 2.3 g, 10 mmol), 2-oxocyclopentane-1-carboxylic acid (**S-2**, 1.4 g, 11 mmol), HATU (4.6 g, 15 mmol), DIPEA (1.9 g, 2.6 mL, 15 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (50 mL) was stirred at room temperature for 12 hours. The solvent was removed in vacuum. The residue was purified by column chromatography (silica gel, petroleum ester/EtOAc) to give the corresponding product **1a** (2.4 g, 70% yield) as a white solid. m.p.: 95.6-96.4 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  8.00-7.97 & 7.93-7.91 (m, 1H), 7.62-7.59 (m, 1H), 7.47-7.43 (m, 1H), 7.22-7.20 & 7.12-7.07 (m, 1H), 3.22 & 3.21 (2s, 3H), 2.89-2.84 (m, 1H), 2.55-2.44 (m, 1H), 2.28-2.11 (m, 4H), 1.75-1.62 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  214.3, 169.4, 145.6, 139.7, 130.6, 130.0, 129.9, 99.7, 53.1, 38.3, 36.2, 28.2, 20.9; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd. for C<sub>13</sub>H<sub>15</sub>INO<sub>2</sub><sup>+</sup> 344.0142; Found 344.0142.

Substrates **1b-1l** were synthesized similarly to that of **1a**.

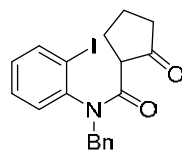
### *N*-allyl-*N*-(2-iodophenyl)-2-oxocyclopentane-1-carboxamide (**1b**)



2.6g, 72% yield, white solid. m.p.: 85.6-86.4 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  8.00 & 7.94 (2d, *J* = 8.0 Hz, 1H), 7.55-7.53 (m, 1H), 7.43-7.39 (m, 1H), 7.12-7.07 (m, 1H), 5.96-5.88 (m, 1H), 5.18-5.14 (m, 2H), 4.90-4.84 (m, 1H), 3.66-3.61 (m, 1H), 2.89-2.84 (m, 1H), 2.57-2.44 (m, 1H), 2.26-2.12 (m, 4H), 1.75-1.62 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  214.3, 213.4, 170.8, 169.2, 143.8, 143.5, 140.5, 139.6, 132.2, 132.0, 130.8, 130.0, 129.4,

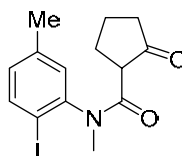
119.0, 118.3, 100.8, 53.3, 53.1, 51.5, 51.1, 38.7, 38.4, 29.3, 28.0, 21.1, 20.9; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{15}H_{17}INO_2^+$  370.0298; Found 370.0296.

***N*-benzyl-*N*-(2-iodophenyl)-2-oxocyclopentane-1-carboxamide (1c)**



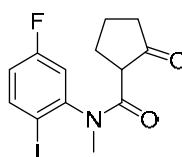
2.7g, 65% yield, white solid. m.p.: 91.1-92.0 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  8.00-7.97 & 7.93-7.91 (m, 1H), 7.30-7.13 (m, 7H), 7.05-7.03 (m, 1H), 5.70 (d,  $J$  = 14.4 Hz, 1H), 4.01 (d,  $J$  = 14.4 Hz, 1H), 2.90-2.85 (m, 1H), 2.55-2.44 (m, 1H), 2.29-2.16 (m, 3H), 1.75-1.63 (m, 2H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  214.1, 169.5, 143.5, 140.5, 139.6, 132.0, 130.0, 129.3, 129.2, 128.8, 128.3, 127.5, 127.4, 100.5, 53.2, 52.9, 51.8, 51.3, 38.4, 38.3, 29.4, 28.0, 21.1, 20.9; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{19}H_{19}INO_2^+$  420.0455; Found 420.0456.

***N*-(2-iodo-5-methylphenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1d)**



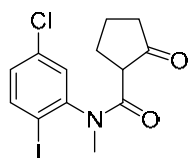
2.3g, 65% yield, white solid. m.p.: 87.5-88.4 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.82 & 7.76 (2d,  $J$  = 8.0 Hz, 1H), 7.41 & 7.02 (2s, 1H), 6.92-6.90 (m, 1H), 3.20 & 3.19 (2s, 3H), 2.91-2.86 (m, 1H), 2.54-2.43 (m, 1H), 2.35 (s, 3H), 2.26-2.08 (m, 4H), 1.75-1.63 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  214.4, 213.4, 171.0, 169.5, 145.4, 140.5, 140.1, 139.2, 113.2, 131.0, 129.7, 95.5, 95.2, 53.1, 52.8, 38.6, 38.4, 36.2, 33.9, 29.3, 28.2, 25.6, 24.9, 20.9, 20.8; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{14}H_{17}INO_2^+$  358.0298; Found 358.0299.

***N*-(5-fluoro-2-iodophenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1e)**



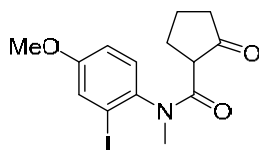
2.6g, 72% yield, white solid. m.p.: 91.3-91.6 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.90-7.79 (m, 1H), 7.36-7.33 (m, 1H), 6.90-6.83 (m, 1H), 3.20 (s, 3H), 2.83-2.79 (m, 1H), 2.50-2.42 (m, 1H), 2.06-2.08 (m, 4H), 1.69-1.62 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  214.0, 213.3, 170.7, 169.1, 163.3 (d,  $J$  = 250.1 Hz), 147.0 (d,  $J$  = 9.8 Hz), 141.5, 140.3 (d,  $J$  = 8.5 Hz), 118.4 (d,  $J$  = 22.5 Hz), 117.8 (d,  $J$  = 21.5 Hz), 116.7 (d,  $J$  = 22.0 Hz), 93.1, 93.0, 53.2, 52.8, 38.6, 38.3, 36.2, 36.0, 29.2, 28.0, 21.2, 20.9; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{13}H_{14}FINO_2^+$  362.0048; Found 362.0046.

***N*-(5-chloro-2-iodophenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1f)**



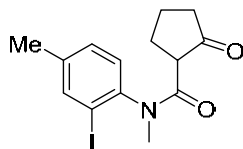
2.4g, 63% yield, white solid. m.p.: 133.3-133.7 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.86 & 7.79 (2d,  $J = 8.4$  Hz, 1H), 7.59 & 7.18 (2d,  $J = 2.0$  Hz, 1H), 7.07 (dd,  $J = 8.4$  Hz, 2.0 Hz, 1H), 3.16 (s, 3H), 2.83-2.79 (m, 1H), 2.47-2.43 (m, 1H), 2.22-2.13 (m, 4H), 1.70-1.62 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  214.0, 213.0, 169.1, 146.7, 141.3, 140.3, 135.8, 130.9, 130.5, 130.4, 129.3, 97.2, 53.2, 52.8, 38.6, 38.3, 36.2, 36.1, 29.2, 28.0, 21.2, 21.0; HRMS (ESI) m/z:  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{14}\text{ClINO}_2^+$  377.9752; Found 377.9751.

***N*-(2-iodo-4-methoxyphenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1g)**



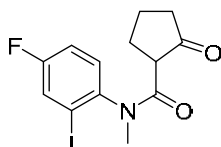
2.8g, 76% yield, white solid. m.p.: 119.2-200.1 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.50-7.46 (m, 1H), 7.41 & 7.09 (d,  $J = 2.8$  Hz, 1H), 6.97-6.92 (m, 1H), 3.84 & 3.83 (2s, 3H), 3.20 & 3.19 (2s, 3H), 2.95-2.90 (m, 1H), 2.54-2.44 (m, 1H), 2.31-2.09 (m, 4H), 1.76-1.63 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  214.6, 213.6, 169.9, 159.5, 138.5, 130.6, 129.0, 125.0, 124.6, 115.4, 115.2, 100.2, 99.9, 55.7, 53.1, 52.8, 38.7, 38.4, 36.4, 36.2, 29.2, 28.2, 21.2, 20.9; HRMS (ESI) m/z:  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{17}\text{INO}_3^+$  374.0248; Found 374.0250.

***N*-(2-iodo-4-methylphenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1h)**



2.5g, 70% yield, white solid. m.p.: 104.1-105.0 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.80 & 7.73 (s, 1H), 7.46 & 7.05 (d,  $J = 7.6$  Hz, 1H), 7.24-7.20 (m, 1H), 3.20 & 3.18 (2s, 3H), 2.92-2.87 (m, 1H), 2.53-2.43 (m, 1H), 2.36 & 2.35 (2s, 3H), 2.25-2.10 (m, 4H), 1.74-1.62 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  214.4, 213.4, 171.2, 169.6, 143.0, 140.9, 140.4, 140.0, 130.7, 130.3, 129.9, 128.4, 99.4, 53.1, 52.8, 38.6, 38.3, 36.2, 36.1, 29.2, 28.1, 21.0, 20.9, 20.5; HRMS (ESI) m/z:  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{17}\text{INO}_2^+$  358.0298; Found 358.0299.

***N*-(4-fluoro-2-iodophenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1i)**

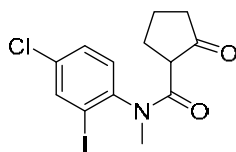


2.6g, 73% yield, white solid. m.p.: 97.4-98.3 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.68-7.55 (m, 2H), 7.17-7.12 (m, 1H), 3.18 & 3.17 (2s, 3H), 2.87-2.82 (m, 1H), 2.53-2.43 (m, 1H), 2.29-2.09 (m, 4H), 1.75-1.63 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  214.2, 169.3, 161.3 (d,  $J = 253.0$  Hz), 141.9 (d,  $J = 4.0$  Hz), 131.3 (d,  $J = 9.0$  Hz), 126.4 (d,  $J = 25.0$  Hz).



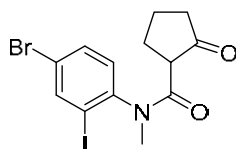
Hz), 116.9 (d,  $J = 21.0$  Hz), 99.6 (d,  $J = 9.0$  Hz), 53.0, 52.7, 38.5, 38.2, 36.3, 29.1, 28.0, 21.1, 20.8; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{13}H_{14}FINO_2^+$  362.0048; Found 362.0046.

***N*-(4-chloro-2-iodophenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1j)**



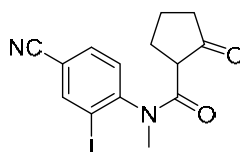
2.8g, 78% yield, white solid. m.p.: 123.2-124.1 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.97 & 7.90 (2d,  $J = 2.4$  Hz, 1H), 7.54 (d,  $J = 8.4$  Hz, 1H), 7.42 (dd,  $J = 8.4$  Hz, 2.4 Hz, 1H), 3.20 & 3.19 (s, 3H), 2.88-2.83 (m, 1H), 2.55-2.44 (m, 1H), 2.31-2.12 (m, 4H), 1.75-1.65 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  214.2, 213.1, 170.9, 169.2, 144.4, 144.3, 139.9, 138.9, 134.9, 131.2, 129.8, 130.2, 129.5, 100.4, 100.1, 53.1, 52.8, 38.5, 38.3, 36.2, 36.1, 29.1, 28.0, 20.9; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{13}H_{14}ClINO_2^+$  377.9752; Found 377.9751.

***N*-(4-bromo-2-iodophenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1k)**



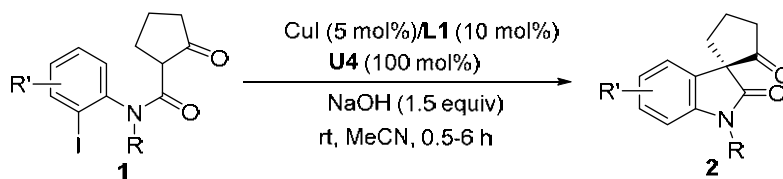
3.2g, 76% yield, white solid. m.p.: 115.6-116.6 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  8.12 & 8.06 (2d,  $J = 2.4$  Hz, 1H), 7.59-7.58 (dd,  $J = 8.4$  Hz, 2.4 Hz, 1H), 7.49 & 7.07 (2d,  $J = 8.4$  Hz, 1H), 3.20 & 3.19 (2s, 3H), 2.88-2.83 (m, 1H), 2.55-2.45 (m, 1H), 2.38-2.12 (m, 4H), 1.77-1.65 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  214.2, 213.1, 170.8, 169.1, 144.8, 142.7, 141.7, 140.2, 133.2, 132.8, 131.6, 129.9, 122.9, 110.8, 100.9, 100.6, 53.2, 52.8, 38.5, 38.3, 36.2, 36.0, 29.1, 28.0, 21.1, 20.9; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{13}H_{14}BrINO_2^+$  421.9247; Found 421.9246.

***N*-(4-cyano-2-iodophenyl)-*N*-methyl-2-oxocyclopentane-1-carboxamide (1l)**



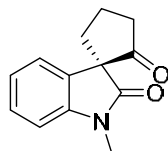
2.7g, 75% yield, white solid. m.p.: 85.6-86.4 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  8.26 & 8.25 (2s, 1H), 7.73 (s, 2H), 3.20 (s, 3H), 2.80-2.72 (m, 1H), 2.50-2.45 (m, 1H), 2.23-2.20 (m, 4H), 1.73-1.63 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  213.9, 212.7, 170.2, 168.6, 149.8, 143.9, 142.9, 133.6, 133.3, 131.4, 129.7, 116.2, 114.1, 100.5, 53.4, 53.0, 38.5, 38.3, 36.2, 29.0, 27.9, 21.1, 20.9; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{14}H_{14}IN_2O_2^+$  369.0094; Found 369.0091.

**Procedure for Asymmetric Coupling Reaction of 1a-1l**



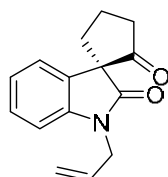
The reaction mixture of substrates **1** (0.2 mmol), CuI (0.01 mmol), (*S,S*)-L1 (0.02 mmol), NaOH (0.3 mmol) and 1,3-bis(trimethylsilyl)urea (**U4**, 0.2 mmol) in MeCN (2 mL) were stirred at room temperature for 0.5-6 hours. Then H<sub>2</sub>O (5.0 mL) and ethyl acetate (5.0 mL) were added into the mixture. The organic phase was separated and the aqueous phase was extracted with ethyl acetate (5.0 mL × 3). The combined organic phase was washed with H<sub>2</sub>O and brine, dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/10 to 1/3) to afford the desired products **2**.

#### (*S*)-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (**2a**)



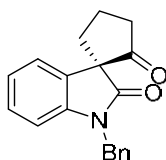
37.8 mg, 88% yield, white solid, m.p.: 156.5-157.4 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.31-7.27 (m, 1H), 7.10-7.02 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 3.20 (s, 3H), 2.71-2.59 (m, 2H), 2.57-2.46 (m, 2H), 2.39-2.27 (m, 1H), 2.20-2.16 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 212.8, 175.1, 144.3, 130.3, 128.7, 122.9, 122.4, 108.5, 62.9, 38.3, 34.1, 26.5, 20.2; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>14</sub>NO<sub>2</sub><sup>+</sup> 216.1019; Found 216.1017; HPLC (OJ-H, n-hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 11.6 min (major), 9.2 min (minor); [α]<sub>D</sub><sup>25</sup> -21.3 (*c* 1.0, CHCl<sub>3</sub>, 96.5% *ee*).

#### (*S*)-1'-allylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (**2b**)



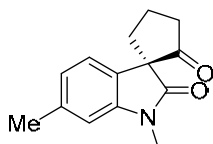
39.5 mg, 82% yield, white solid, m.p.: 176.3-177.2 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.27-7.24 (m, 1H), 7.10-7.02 (m, 2H), 6.83 (d, *J* = 7.6 Hz, 1H), 5.86-5.79 (m, 1H), 5.28-5.23 (m, 2H), 4.36-4.28 (m, 2H), 2.74-2.63 (m, 2H), 2.59-2.46 (m, 2H), 2.42-2.35 (m, 1H), 2.27-2.20 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 212.6, 174.9, 143.6, 130.8, 130.4, 128.6, 122.9, 122.5, 117.5, 109.3, 62.9, 42.4, 38.3, 34.1, 20.3; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>15</sub>H<sub>16</sub>NO<sub>2</sub><sup>+</sup> 242.1176; Found 242.1177; HPLC (IC-H, n-hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 17.6 min (major), 14.7 min (minor); [α]<sub>D</sub><sup>25</sup> -67.2 (*c* 1.0, CHCl<sub>3</sub>, 87% *ee*).

#### (*S*)-1'-benzylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (**2c**)



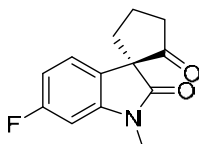
47.7 mg, 82% yield, white solid, m.p.: 184.9-185.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.34-7.25 (m, 5H), 7.15-7.13 (m, 1H), 7.12-7.09 (m, 1H), 7.03-6.99 (m, 1H), 6.70 (d,  $J = 8.0$  Hz, 1H), 5.00 (d,  $J = 16.0$  Hz, 1H), 4.82 (d,  $J = 16.0$  Hz, 1H), 2.79-2.64 (m, 2H), 2.60-2.46 (m, 2H), 2.44-2.39 (m, 1H), 2.30-2.23 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  212.6, 175.3, 143.4, 135.3, 130.4, 128.8, 128.6, 127.6, 127.0, 122.9, 122.5, 109.5, 63.0, 43.9, 38.3, 34.1, 20.3; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{19}\text{H}_{18}\text{NO}_2^+$  292.1332; Found 292.1335; HPLC (OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm)  $t_R = 19.8$  min (major), 17.8 min (minor);  $[\alpha]_D^{25} +57.2$  (c 1.0,  $\text{CHCl}_3$ , 85% *ee*).

**(S)-1',6'-dimethylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2d)**



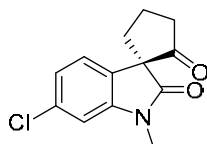
33.4 mg, 73% yield, white solid, m.p.: 176.8-177.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.96 (d,  $J = 7.6$  Hz, 1H), 6.86 (d,  $J = 7.6$  Hz, 1H), 6.68 (s, 1H), 3.19 (s, 3H), 2.69-2.59 (m, 2H), 2.56-2.45 (m, 2H), 2.38 (s, 3H), 2.35-2.30 (m, 1H), 2.24-2.19 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  213.1, 175.4, 144.4, 139.0, 127.4, 123.3, 122.1, 109.4, 62.7, 38.2, 34.1, 26.5, 21.8, 20.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{16}\text{NO}_2^+$  230.1176; Found 230.1183; HPLC (AS-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm)  $t_R = 9.6$  min (major), 8.5 min (minor);  $[\alpha]_D^{25} +17.6$  (c 1.0,  $\text{CHCl}_3$ , 88% *ee*).

**(S)-6'-fluoro-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2e)**



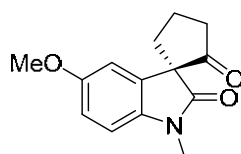
34.0 mg, 73% yield, white solid, m.p.: 189.4-190.3 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.00 (dd,  $J = 8.0$  Hz, 4.2 Hz, 1H), 6.75-6.70 (m, 1H), 6.60 (dd,  $J = 8.4$  Hz, 2.4 Hz, 1H), 3.18 (s, 3H), 2.69-2.59 (m, 2H), 2.56-2.45 (m, 2H), 2.37-2.30 (m, 1H), 2.26-2.19 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  212.5, 175.4, 163.4 (d,  $J = 246.2$  Hz), 146.0 (d,  $J = 1.6$  Hz), 125.6 (d,  $J = 2.9$  Hz), 123.5 (d,  $J = 9.8$  Hz), 108.9 (d,  $J = 22.5$  Hz), 97.4 (d,  $J = 27.6$  Hz), 62.5, 38.2, 34.1, 26.7, 20.1; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{FNO}_2^+$  234.0925; Found 234.0926; HPLC (AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm)  $t_R = 9.4$  min (major), 8.4 min (minor);  $[\alpha]_D^{25} -11.3$  (c 1.0,  $\text{CHCl}_3$ , 92.5% *ee*).

**(S)-6'-chloro-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2f)**



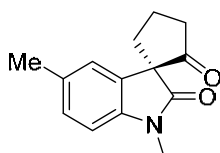
31.4 mg, 63% yield, white solid, m.p.: 165.7-166.5 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.03 (dd,  $J = 8.0$  Hz, 1.6 Hz, 1H), 6.99 (d,  $J = 8.0$  Hz, 1H), 6.85 (d,  $J = 1.6$  Hz, 3.19 (s, 3H), 2.70-2.59 (m, 2H), 2.56-2.46 (m, 2H), 2.37-2.30 (m, 1H), 2.25-2.17 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  212.2, 175.0, 145.6, 134.6, 128.6, 123.4, 122.7, 109.3, 62.6, 38.3, 34.1, 26.6, 20.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{ClNO}_2^+$  250.0629; Found 250.0632; HPLC(AS-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 11.7 min (major), 9.6 min(minor);  $[\alpha]_{\text{D}}^{25}$  -8.3 (*c* 1.0,  $\text{CHCl}_3$ , 93% *ee*).

**(S)-5'-methoxy-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2g)**



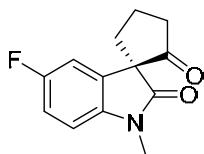
38.3 mg, 80% yield, white solid, m.p.: 158.6-159.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.82 (dd,  $J = 8.4$  Hz, 2.4 Hz, 1H), 6.77 (d,  $J = 8.4$  Hz, 1H), 6.72 (d,  $J = 2.4$  Hz, 1H), 3.77 (s, 3H), 3.18 (s, 3H), 2.70-2.63 (m, 2H), 2.59-2.49 (m, 2H), 2.40-2.33 (m, 1H), 2.20-2.17 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  212.8, 174.7, 156.2, 137.9, 131.5, 112.5, 110.4, 108.7, 63.2, 55.9, 38.3, 34.2, 26.6, 20.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{16}\text{NO}_3^+$  246.1125; Found 246.1134; HPLC(OD-H, hexane/*i*-PrOH = 80:20, flow rate=1.0 ml/min, I=254 nm) tR = 10.1 min (major), 12.2 min (minor);  $[\alpha]_{\text{D}}^{25}$  -24.6 (*c* 1.0,  $\text{CHCl}_3$ , 92% *ee*).

**(S)-1',5'-dimethylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2h)**



40.4 mg, 88% yield, white solid, m.p.: 168.5-169.3 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.10 (d,  $J = 8.0$  Hz, 1H), 6.90 (s, 1H), 6.74 (d,  $J = 8.0$  Hz, 1H), 3.18 (s, 3H), 2.70-2.60 (m, 2H), 2.57-2.46 (m, 2H), 2.38-2.34 (m, 1H), 2.32 (s, 3H), 2.25-2.16 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  213.1, 175.1, 142.0, 132.5, 130.4, 129.0, 123.3, 108.2, 63.0, 38.3, 34.2, 26.6, 21.1, 20.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{16}\text{NO}_2^+$  230.1176; Found 230.1183; HPLC(AS-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 8.3 min (major), 10.9 min (minor);  $[\alpha]_{\text{D}}^{25}$  -12.2 (*c* 1.0,  $\text{CHCl}_3$ , 97.5% *ee*).

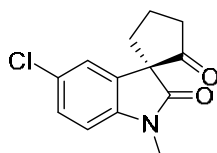
**(S)-5'-fluoro-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2i)**



40.1 mg, 86% yield, white solid, m.p.: 175.8-176.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

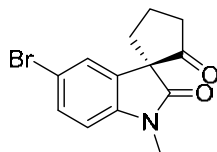
$\delta$  7.06-7.00 (m, 1H), 6.88-6.85 (m, 1H), 6.81-6.78 (m, 1H), 3.22 (s, 3H), 2.74-2.64 (m, 2H), 2.59-2.51 (m, 2H), 2.40-2.33 (m, 1H), 2.27-2.19 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  212.0, 174.7, 159.3 (d,  $J = 239.8$  Hz), 140.4 (d,  $J = 1.6$  Hz), 131.5 (d,  $J = 8.3$  Hz), 114.9 (d,  $J = 23.4$  Hz), 110.8 (d,  $J = 25.1$  Hz), 108.9 (d,  $J = 8.3$  Hz), 63.2, 38.2, 34.1, 26.6, 20.1; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{FNO}_2^+$  234.0925; Found 234.0926; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm) tR = 12.6 min (major), 10.5 min (minor);  $[\alpha]_{\text{D}}^{25}$  -21.4 (*c* 1.0,  $\text{CHCl}_3$ , 95% *ee*).

**(S)-5'-chloro-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2j)**



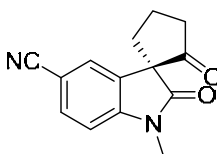
42.3 mg, 85% yield, white solid, m.p.: 184.7-185.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.25 (dd,  $J = 8.0$  Hz, 2.0 Hz, 1H), 7.05 (d,  $J = 2.0$  Hz, 1H), 6.75 (d,  $J = 8.0$  Hz, 1H), 3.16 (s, 3H), 2.70-2.61 (m, 2H), 2.58-2.46 (m, 2H), 2.39-2.32 (m, 1H), 2.26-2.16 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  211.9, 174.6, 143.0, 131.8, 128.6, 128.1, 123.1, 109.4, 63.0, 38.3, 34.0, 26.6, 20.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{ClNO}_2^+$  250.0629; Found 250.0631; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 12.0 min (major), 10.5 min (minor);  $[\alpha]_{\text{D}}^{25}$  -11.7 (*c* 1.0,  $\text{CHCl}_3$ , 93% *ee*).

**(S)-5'-bromo-1'-methylspiro[cyclopentane-1,3'-indoline]-2,2'-dione (2k)**



41.0 mg, 70% yield, white solid, m.p.: 139.7-140.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 (dd,  $J = 8.4$  Hz, 2.0 Hz, 1H), 7.21 (d,  $J = 2.0$  Hz, 1H), 6.75 (d,  $J = 8.4$  Hz, 1H), 3.20 (s, 3H), 2.73-2.63 (m, 2H), 2.59-2.47 (m, 2H), 2.40-2.33 (m, 1H), 2.28-2.17 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  211.8, 174.5, 143.4, 132.1, 131.5, 125.7, 115.3, 109.8, 62.8, 38.2, 34.0, 26.6, 20.1; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{BrNO}_2^+$  294.0124; Found 294.0131; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 14.0 min (major), 11.4 min (minor);  $[\alpha]_{\text{D}}^{25}$  +5.6 (*c* 1.0,  $\text{CHCl}_3$ , 92% *ee*).

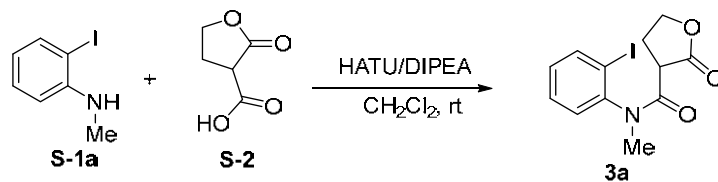
**(S)-1'-methyl-2,2'-dioxospiro[cyclopentane-1,3'-indoline]-5'-carbonitrile (2l)**



32.6 mg, 68% yield, white solid, m.p.: 164.8-165.5 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 (d,  $J = 8.0$  Hz, 1H), 7.32 (s, 1H), 6.91 (d,  $J = 8.0$  Hz, 1H), 3.22 (s, 3H), 2.71-2.62 (m, 2H), 2.59-2.48 (m, 2H), 2.40-2.33 (m, 1H), 2.25-2.19 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  211.1, 174.7, 148.3, 134.0, 131.2, 125.9, 118.9, 108.9, 106.0, 62.6, 38.2, 33.9, 26.8, 20.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}_2^+$  241.0972; Found 241.0972; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 30.4 min (major), 24.3 min (minor);  $[\alpha]_{\text{D}}^{25}$  +10.0 (*c*

1.0, CHCl<sub>3</sub>, 89% *ee*).

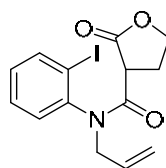
### General procedure for the synthesis of 3a-3q:



A mixture of 2-iodo-N-methylaniline (S-1a, 2.3 g, 10 mmol), 2-oxotetrahydrofuran-3-carboxylic acid (S-2, 1.4 g, 11 mmol), HATU (4.6 g, 15 mmol), DIPEA (1.9 g, 2.6 mL, 15 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (50 mL) was stirred at room temperature for 12 hours. The solvent was removed in vacuum. The residue was purified by column chromatography (silica gel, petroleum ester/EtOAc) to give the corresponding product 3a (2.5g, 72% yield) as a white solid. m.p.: 101.3-101.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 8.00 & 7.92 (2dd, *J* = 8.0, 1.2 Hz, 1H), 7.63 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.49-7.45 (m, 1H), 7.09-7.21 (m, 1H), 4.53-4.48 (m, 1H), 4.18-4.14 (m, 1H), 3.28-3.15 (m, 4H), 2.92-2.80 (m, 1H), 2.39-2.29 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 173.5, 167.4, 145.1, 140.9, 139.8, 130.7, 130.4, 130.3, 129.9, 128.8, 99.3, 67.6, 66.9, 44.5, 43.9, 36.6, 36.4, 28.1, 27.2; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>12</sub>INNaO<sub>3</sub><sup>+</sup> 367.9754; Found 367.9755.

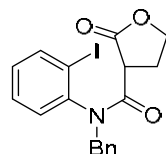
Substrates **3b-3r** were synthesized similarly to that of **3a**.

### *N*-allyl-*N*-(2-iodophenyl)-2-oxotetrahydrofuran-3-carboxamide (3b)



2.5g, 69% yield, yellow solid. m.p.: 116.2-117.0 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 8.02 & 7.93 (2dd, *J* = 7.6, 1.6 Hz, 1H), 7.55 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.45-7.41 (m, 1H), 7.13-7.09 (m, 1H), 5.94-5.83 (m, 1H), 5.17-5.07 (m, 2H), 4.86-4.80 (m, 1H), 4.53-4.48 (m, 1H), 4.18-4.14 (m, 1H), 3.70-3.64 (m, 1H), 3.26-3.11 (m, 1H), 2.93-2.82 (m, 1H), 2.45-2.19 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 173.4, 172.9, 168.3, 167.2, 143.3, 143.2, 140.9, 139.8, 132.1, 131.7, 130.5, 130.4, 129.8, 129.3, 119.5, 118.9, 100.8, 100.5, 67.6, 66.9, 51.9, 51.4, 44.8, 44.1, 28.2, 27.0; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>14</sub>H<sub>14</sub>INNaO<sub>3</sub><sup>+</sup> 393.9911; Found 393.9915.

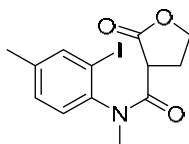
### *N*-benzyl-*N*-(2-iodophenyl)-2-oxotetrahydrofuran-3-carboxamide (3c)



3.2g, 78% yield, white solid. m.p.: 103.2-104.1 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 8.01 & 7.92 (2dd, *J* = 8.0, 1.6 Hz, 1H), 7.28-7.21 (m, 6H), 7.17-7.14 (m, 1H), 7.06-7.02 (m, 1H), 5.69 & 5.66 (2d, *J* = 14.4 Hz, 1H), 4.56-4.50 (m, 1H), 4.21-4.14 (m, 1H), 4.05 & 4.03 (2d, *J* = 14.4 Hz, 1H), 3.28-3.24 & 3.16-3.13 (m, 1H), 2.96-2.90 (m, 1H), 2.42-2.32 (m, 1H); <sup>13</sup>C NMR

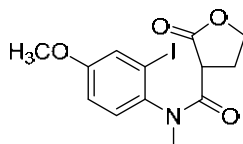
(100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  173.4, 172.9, 168.6, 167.7, 143.0, 142.9, 140.9, 139.8, 136.3, 135.9, 132.2, 130.8, 130.4, 129.6, 129.5, 129.1, 129.0, 128.6, 127.9, 127.7, 100.6, 100.3, 67.6, 66.8, 52.3, 51.8, 44.8, 44.0, 28.2, 27.1; HRMS (ESI)  $m/z$ : [M + Na]<sup>+</sup> Calcd for C<sub>18</sub>H<sub>16</sub>INNaO<sub>3</sub><sup>+</sup> 444.0067; Found 444.0074.

***N*-(2-iodo-4-methylphenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3d)**



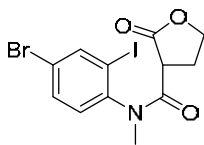
2.5g, 71% yield, yellow solid. m.p.: 108.5-108.8 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  7.82 & 7.74 (2s, 1H), 7.48 & 7.20 (2d,  $J$  = 8.0 Hz, 1H), 7.30 & 7.06 (2d,  $J$  = 8.0 Hz, 1H), 4.53-4.48 (m, 1H), 4.19-4.13 (m, 1H), 3.29 (t,  $J$  = 8.8 Hz, 1H), 3.22 (s, 3H), 2.88-2.83 (m, 1H), 2.35 (s, 3H), 2.37-2.29 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  173.5, 167.6, 142.5, 142.2, 140.9, 140.1, 131.1, 130.5, 130.0, 128.2, 99.1, 67.6, 66.8, 44.4, 43.8, 36.6, 36.4, 28.1, 27.2, 20.6; HRMS (ESI)  $m/z$ : [M + Na]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>14</sub>INNaO<sub>3</sub><sup>+</sup> 381.9911; Found 381.9917.

***N*-(2-iodo-4-methoxyphenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3e)**



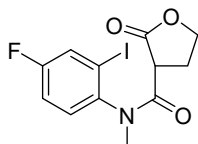
2.5g, 69% yield, white solid. m.p.: 95.4-95.7 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  7.48 & 7.45 (2d,  $J$  = 8.8 Hz, 1H), 7.39 & 7.07 (2d,  $J$  = 2.8 Hz, 1H), 6.95 & 6.90 (2dd,  $J$  = 8.8, 2.8 Hz, 1H), 4.51-4.45 (m, 1H), 4.18-4.12 (m, 1H), 3.81 & 3.80 (2s, 3H), 3.30 (t,  $J$  = 8.8 Hz, 1H), 3.19 (s, 3H), 2.86-2.81 (m, 1H), 2.37-2.26 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  173.6, 173.1, 169.1, 167.9, 159.8, 137.9, 130.6, 128.9, 125.2, 124.8, 115.7, 115.4, 100.0, 99.5, 67.6, 66.9, 55.8, 44.4, 43.7, 38.6, 36.8, 28.1, 27.2; HRMS (ESI)  $m/z$ : [M + Na]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>14</sub>INNaO<sub>4</sub><sup>+</sup> 397.9860; Found 397.9853.

***N*-(4-bromo-2-iodophenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3f)**



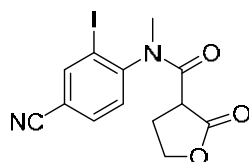
3.3g, 78% yield, white solid. m.p.: 134.2-134.8 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  8.14 & 8.06 (2d,  $J$  = 2.0 Hz, 1H), 7.61-7.57 (m, 1H), 7.50 & 7.06 (2d,  $J$  = 8.4 Hz, 1H), 4.53-4.48 (m, 1H), 4.22-4.15 (m, 1H), 3.24 (t,  $J$  = 8.8 Hz, 1H), 3.22 (s, 3H), 2.89-2.82 (m, 1H), 2.39-2.28 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers)  $\delta$  173.3, 167.1, 144.2, 143.0, 141.8, 133.5, 133.0, 131.7, 129.7, 123.4, 100.3, 67.6, 66.9, 44.4, 43.9, 36.6, 36.4, 28.0, 27.0; HRMS (ESI)  $m/z$ : [M + Na]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>11</sub>BrINNaO<sub>3</sub><sup>+</sup> 445.8859; Found 445.8865.

***N*-(4-fluoro-2-iodophenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3g)**



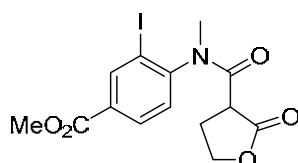
2.75g, 76% yield, yellow solid. m.p.: 125.3-126.1 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64-7.52 (m, 2H), 7.15-7.10 (m, 1H), 4.46-4.41 (m, 1H), 4.15-4.09 (m, 1H), 3.21 (t,  $J = 8.8$  Hz, 1H), 3.15 (s, 3H), 2.81-2.75 (m, 1H), 2.33-2.24 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.4, 172.9, 168.7, 167.5, 161.5 (d,  $J = 253.2$  Hz), 141.4, 131.5 (d,  $J = 8.8$  Hz), 129.7 (d,  $J = 8.9$  Hz), 127.6 (d,  $J = 24.4$  Hz), 126.7 (d,  $J = 24.6$  Hz), 117.3 (d,  $J = 22.0$  Hz), 116.9, 99.4, 99.3, 67.6, 67.0, 44.4, 43.8, 36.7, 36.5, 28.0, 27.0; HRMS (ESI)  $m/z$ :  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{12}\text{H}_{11}\text{FINaO}_3^+$  385.9660; Found 385.9655.

### ***N*-(4-cyano-2-iodophenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3h)**



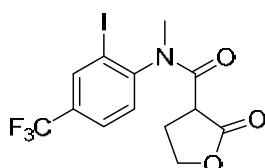
2.8g, 76% yield, white solid. m.p.: 96.7-97.5 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  8.30 & 8.22 (2s, 1H), 7.79 (s, 2H), 4.59-4.47 (m, 1H), 4.24-4.18 (m, 1H), 3.25 & 3.24 (2s, 3H), 3.16-3.13 (m, 1H), 2.99-2.83 (m, 1H), 2.38-2.30 (m, 1H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  173.0, 172.3, 167.7, 166.6, 149.1, 144.2, 143.0, 133.9, 133.4, 131.6, 129.4, 116.1, 114.5, 100.1, 67.7, 67.1, 44.5, 44.2, 36.6, 27.8, 26.8; HRMS (ESI)  $m/z$ :  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{13}\text{H}_{11}\text{IN}_2\text{NaO}_3^+$  392.9707; Found 392.9712.

### **Methyl 3-iodo-4-(*N*-methyl-2-oxotetrahydrofuran-3-carboxamido)benzoate (3i)**



3.1g, 78% yield, white solid. m.p.: 92.5-93.4 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  8.22 & 7.82 (2d,  $J = 2.4$  Hz, 1H), 8.10 & 8.02 (2d,  $J = 8.4$ , 1H), 7.75 & 7.73 (2dd,  $J = 8.4$  Hz, 2.4 Hz, 1H), 4.52-4.48 (m, 1H), 4.18-4.14 (m, 1H), 3.93 & 3.92 (2s, 3H), 3.24 (s, 3H), 3.22-3.19 & 3.15-3.11 (m, 1H), 2.89-2.85 (m, 1H), 2.36-2.30 (m, 1H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 172.7, 168.3, 167.2, 165.4, 145.6, 145.3, 141.2, 140.1, 132.7, 132.2, 131.3, 131.1, 130.8, 129.5, 106.4, 105.8, 67.6, 67.0, 52.7, 52.5, 44.5, 44.0, 36.7, 36.4, 28.0, 27.0; HRMS (ESI)  $m/z$ :  $[\text{M} + \text{Na}]^+$  Calcd for  $\text{C}_{14}\text{H}_{14}\text{INNaO}_5^+$  425.9809; Found 425.9813.

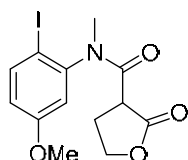
### ***N*-(2-Iodo-4-(trifluoromethyl)phenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3j)**





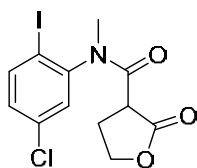
3g, 73% yield, white solid. m.p.: 93.4-94.2 °C. (PE/EA=3/1) <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.25 & 8.17 (2s, 1H), 7.78-7.60 (m, 2H), 4.55-4.49 (m, 1H), 4.25-4.15 (m, 1H), 3.25 & 3.24 (2s, 3H), 3.21-3.15 (m, 1H), 2.91-2.86 (m, 1H), 2.37-2.23 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 173.2, 172.7, 168.1, 166.9, 148.4, 148.3, 136.8, 136.7 (q, *J* = 3.7 Hz), 132.4 (q, *J* = 33.1 Hz), 131.1, 127.4 (q, *J* = 4.5 Hz), 122.4 (q, *J* = 272 Hz), 100.0, 99.7, 67.7, 67.0, 44.6, 44.1, 36.5, 36.3, 27.9, 26.9; HRMS (ESI) *m/z*: [M + Na]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>11</sub>F<sub>3</sub>INNaO<sub>3</sub><sup>+</sup> 435.9628; Found 435.9631.

***N*-(2-iodo-5-methoxyphenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3k)**



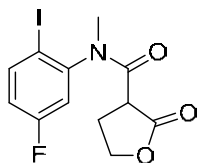
2.8g, 76% yield, white solid. m.p.: 132.4-133.3 °C. (PE/EA=3/1) <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.83 & 7.73 (2d, *J* = 9.0 Hz, 1H), 7.22 (d, *J* = 3.0 Hz, 1H), 6.72 (dd, *J* = 9.0, 3.0 Hz, 1H), 4.53-4.49 (m, 1H), 4.19-4.15 (m, 1H), 3.81 & 3.80 (2s, 3H), 3.29 (t, *J* = 9.0 Hz, 1H), 3.23 & 3.22 (2s, 3H), 2.89-2.85 (m, 1H), 2.40-2.30 (m, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 173.6, 172.9, 168.5, 167.3, 161.3, 161.0, 145.8, 141.0, 139.8, 117.8, 115.6, 115.4, 87.1, 86.9, 67.6, 66.9, 55.8, 55.7, 44.5, 43.8, 36.5, 36.3, 28.2, 27.1; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>14</sub>INNaO<sub>4</sub><sup>+</sup> 397.9860; Found 397.9854.

***N*-(5-chloro-2-iodophenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3l)**



2.8g, 74% yield, white solid. m.p.: 124.4-125.3 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.91 & 7.83 (2d, *J* = 8.4 Hz, 1H), 7.64 & 7.20 (2d, *J* = 2.4 Hz, 1H), 7.12 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.54-4.47 (m, 1H), 4.21-4.15 (m, 1H), 3.24 (t, *J* = 8.8 Hz, 1H), 3.21 (s, 3H), 2.89-2.84 (m, 1H), 2.38-2.27 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 173.3, 172.8, 168.4, 167.2, 146.2, 140.5, 136.2, 131.1, 130.9, 130.8, 129.1, 97.2, 96.9, 67.7, 67.1, 44.6, 44.1, 36.7, 36.5, 28.1, 27.1; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>11</sub>ClINNaO<sub>3</sub><sup>+</sup> 401.9364; Found 401.9372.

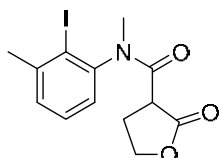
***N*-(5-fluoro-2-iodophenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3m)**



2.7g, 75% yield, white solid. m.p.: 97.5-98.3 °C. (PE/EA=3/1) <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.96-7.85 (m, 1H), 7.43-7.41 (m, 1H), 6.98-6.90 (m, 1H), 4.53-4.48 (m, 1H), 4.21-4.15 (m, 1H), 3.25 (t, *J* = 9.0 Hz, 1H), 3.22 & 3.21 (2s, 3H), 2.88-2.79 (m, 1H), 2.37-2.31 (m, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 173.3, 172.7, 168.3, 167.1, 163.5 (q, *J* = 251.0 Hz), 146.4 (q, *J* = 9.8 Hz), 141.7 (d, *J* = 8.4 Hz), 140.5 (q, *J* = 8.67 Hz), 118.6 (q, *J* = 22.7 Hz), 118.3 (q, *J* = 21.6 Hz), 92.7, 92.6, 67.6, 67.0,

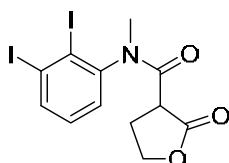
44.5, 44.0, 36.5, 36.3, 28.0, 27.0; HRMS (ESI)  $m/z$ :  $[M+Na]^+$  Calcd for  $C_{12}H_{11}FINNaO_3^+$  385.9660; Found 385.9656.

***N*-(2-iodo-3-methylphenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3n)**



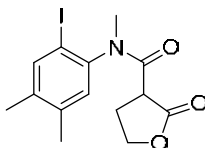
2.7g, 76% yield, white solid. m.p.: 116.4-117.3 °C. (PE/EA=3/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ , two rotamers)  $\delta$  7.40 (dd,  $J = 7.6$  Hz, 1.2 Hz, 1H), 7.35-7.30 (m, 1H), 7.25-7.23 & 7.00-6.98 (m, 1H), 4.52-4.41 (m, 1H), 4.18-4.12 (m, 1H), 3.26 (t,  $J = 8.8$  Hz, 1H), 3.22 (s, 3H), 2.84-2.78 (m, 1H), 2.54 & 2.52 (2s, 3H), 2.36-2.27 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ , two rotamers)  $\delta$  173.6, 173.1, 168.8, 167.6, 145.4, 145.3, 129.9, 129.8, 129.6, 129.2, 127.6, 125.7, 106.8, 106.4, 67.6, 66.8, 44.6, 43.8, 36.5, 36.3, 29.5, 29.3, 28.2, 27.3; HRMS (ESI)  $m/z$ :  $[M+Na]^+$  Calcd for  $C_{13}H_{14}INNaO_3^+$  381.9911; Found 381.9918.

***N*-(2,3-diiodophenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3o)**



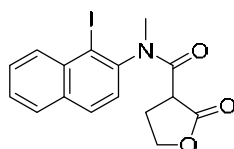
3.4g, 73% yield, white solid. m.p.: 108.5-108.4 °C. (PE/EA=3/1)  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  7.88 (d,  $J = 7.8$  Hz, 1H), 7.57 (d,  $J = 7.8$  Hz, 1H), 7.20 (t,  $J = 7.8$  Hz, 1H), 4.53-4.47 (m, 1H), 4.21-4.15 (m, 1H), 3.25 (t,  $J = 8.4$  Hz, 1H), 3.21 (s, 3H), 2.89-2.86 (m, 1H), 2.39-2.32 (m, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  173.3, 172.8, 168.3, 167.0, 146.3, 139.8, 131.4, 130.8, 129.7, 127.6, 115.0, 114.4, 111.0, 109.3, 67.7, 66.8, 44.7, 44.0, 36.5, 36.3, 28.1, 27.1; HRMS (ESI)  $m/z$ :  $[M+Na]^+$  Calcd for  $C_{12}H_{11}I_2NNaO_3^+$  493.8721; Found 493.8731.

***N*-(2-iodo-4,5-dimethylphenyl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3p)**



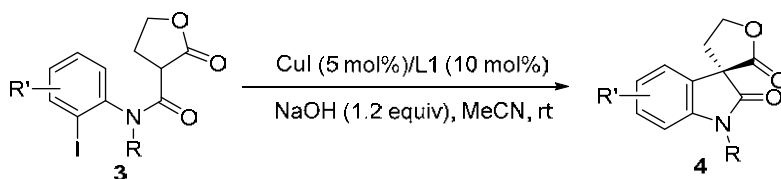
2.7g, 73% yield, white solid. m.p.: 112.6-113.5 °C. (PE/EA=3/1)  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  7.75 & 7.67 (2s, 1H), 7.39 & 6.98 (2s, 1H), 4.54-4.51 (m, 1H), 4.18-4.15 (m, 1H), 3.34-3.31 (m, 1H), 3.25 (s, 3H), 2.88-2.86 (m, 1H), 2.37-2.34 (m, 1H), 2.27 (s, 3H), 2.26 (s, 3H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  173.6, 173.0, 168.7, 167.7, 142.7, 141.2, 140.1, 139.8, 139.5, 131.2, 129.4, 94.9, 67.6, 66.8, 44.4, 43.8, 36.6, 35.9, 28.2, 27.3, 19.5, 19.4, 19.1, 19.0; HRMS (ESI)  $m/z$ :  $[M+Na]^+$  Calcd for  $C_{14}H_{16}INNaO_3^+$  396.0067; Found 396.0070.

***N*-(1-iodonaphthalen-2-yl)-*N*-methyl-2-oxotetrahydrofuran-3-carboxamide (3q)**



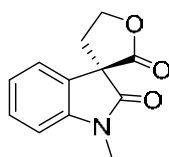
3.1g, 79% yield, white solid. m.p.: 117.8-118.4 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.54 & 8.46 (2s, 1H), 8.15 (s, 1H), 7.90-7.86 (m, 1H), 7.79-7.76 (m, 1H), 7.60-7.57 (m, 2H), 4.52-4.48 (m, 1H), 4.14-4.10 (m, 1H), 3.32 (s, 3H), 3.30 (t,  $J = 9.0$  Hz, 1H), 2.95-2.88 (m, 1H), 2.40-2.30 (m, 1H).  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  173.5, 167.7, 141.0, 140.6, 139.7, 134.3, 133.4, 129.4, 128.4, 128.1, 127.7, 127.3, 126.8, 126.4, 95.9, 67.5, 66.8, 44.7, 44.1, 37.3, 37.1, 28.2, 27.2; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{16}\text{H}_{14}\text{INNaO}_3^+$  417.9911; Found 417.9912.

### Procedure for asymmetric Ullmann-Hurtley coupling reactions of 3a-3q:



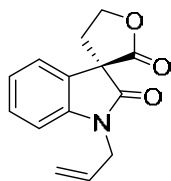
The reaction mixture of substrates **3** (0.2 mmol), CuI (0.01 mmol), (*S,S*)-L1 (0.02 mmol) and NaOH (0.3 mmol) in MeCN (2 mL) were stirred at room temperature for 3-10 hours. Then  $\text{H}_2\text{O}$  (5.0 mL) and ethyl acetate (5.0 mL) were added into the mixture. The organic phase was separated and the aqueous phase was extracted with ethyl acetate (5.0 mL  $\times$  3). The combined organic phase was washed with  $\text{H}_2\text{O}$  and brine, dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/10 to 1/3) to afford the desired products **4**. For **4d**, 1,3-bis(trimethylsilyl)urea (**U4**, 0.04 mmol, 0.2 equiv) was added as co-catalyst. For **4h**, 1,3-bis(trimethylsilyl)urea (**U4**, 0.2 mmol) or 1,3-diphenyl urea (**U3**, 0.2 mmol) was added as the catalyst.

### (*R*)-1'-methyl-4,5-dihydro-2*H*-spiro[furan-3,3'-indoline]-2,2'-dione (**4a**)



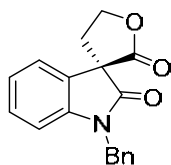
39.1 mg, 90% yield, white solid, m.p.: 189.6-190.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39-7.35 (m, 1H), 7.23 (dd,  $J = 7.6$  Hz, 0.8 Hz, 1H), 7.14-7.09 (m, 1H), 6.89 (d,  $J = 7.6$  Hz, 1H), 4.85-4.79 (m, 1H), 4.64-4.59 (m, 1H), 3.24 (s, 3H), 2.94-2.87 (m, 1H), 2.71-2.63 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.3, 173.0, 144.4, 129.8, 127.8, 123.5, 123.0, 108.9, 66.8, 55.6, 33.6, 26.8; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{12}\text{H}_{11}\text{NNaO}_3^+$  240.0631; Found 240.0632; HPLC(OJ-H, hexane/*i*-PrOH) = 60:40, flow rate=1.0 mL/min,  $I = 254$  nm),  $t_R = 16.8$  min (major), 14.2 min(minor);  $[\alpha]_D^{25} +27.0$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 98% ee).

### (*R*)-1'-allyl-4,5-dihydro-2*H*-spiro[furan-3,3'-indoline]-2,2'-dione (**4b**)



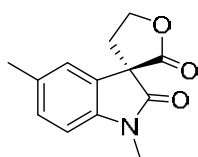
36.9 mg, 76% yield, white solid, m.p.: 175.7-176.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.34-7.30 (m, 1H), 7.23 (d,  $J = 7.2$  Hz, 1H), 7.12-7.08 (m, 1H), 6.88 (d,  $J = 8.0$  Hz, 1H), 5.88-5.77 (m, 1H), 5.26 (d,  $J = 15.2$  Hz, 1H), 5.23 (d,  $J = 9.6$  Hz, 1H), 4.84-4.78 (m, 1H), 4.64-4.58 (m, 1H), 4.40-4.25 (m, 2H), 2.94-2.88 (m, 1H), 2.72-2.65 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.2, 172.9, 143.6, 130.5, 129.7, 127.8, 123.4, 123.1, 117.9, 109.8, 66.8, 55.6, 42.6, 33.5; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{14}\text{H}_{13}\text{NNaO}_3^+$  266.0788; Found 266.0790; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm)  $t_R = 13.9$  min (major), 10.9 min (minor);  $[\alpha]_D^{25} +15.2$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 94% ee).

**(R)-1'-allyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4c)**



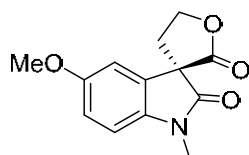
49.2 mg, 84% yield, white solid, m.p.: 178.6-179.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37-7.24 (m, 7H), 7.10 (t,  $J = 7.6$  Hz, 1H), 6.78 (d,  $J = 8.0$  Hz, 1H), 5.03 (d,  $J = 16.0$  Hz, 1H), 4.94-4.80 (m, 2H), 4.69-4.64 (m, 1H), 3.03-2.96 (m, 1H), 2.78-2.71 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.6, 172.9, 143.5, 135.0, 129.7, 129.0, 127.8, 127.1, 123.5, 123.1, 110.0, 66.8, 55.7, 44.1, 33.5; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{18}\text{H}_{15}\text{NNaO}_3^+$  316.0944; Found 316.0944; HPLC(OJ-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm),  $t_R = 41.4$  min (major), 34.3 min (minor);  $[\alpha]_D^{25} +15.8$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 99% ee).

**(R)-1',5'-dimethyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4d)**



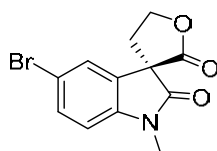
With 20 mol% U4 as the co-catalyst. 42.0 mg, 91% yield, white solid, m.p.: 198.7-199.5 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.10 (d,  $J = 7.6$  Hz, 1H), 6.92 (d,  $J = 7.6$  Hz, 1H), 6.72 (s, 1H), 4.81 (dd,  $J = 16.4$  Hz, 8.8 Hz, 1H), 4.62-4.57 (m, 1H), 3.23 (s, 3H), 2.88-2.85 (m, 1H), 2.67-2.62 (m, 1H), 2.40 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.6, 173.1, 144.4, 140.2, 124.8, 123.9, 122.7, 109.9, 66.8, 55.4, 33.5, 26.7, 21.9; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{NNaO}_3^+$  254.0788; Found 254.0788; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm)  $t_R = 14.4$  min (major), 11.6 min (minor);  $[\alpha]_D^{25} +18.0$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 98% ee).

**(R)-6'-Methoxy-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4e)**



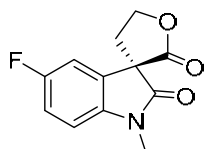
45.6 mg, 92% yield, white solid, m.p.: 138.7-149.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.88 (dd,  $J = 8.4, 2.4$  Hz, 1H), 6.83 (d,  $J = 2.4$  Hz, 1H), 6.79 (d,  $J = 8.4$  Hz, 1H), 4.81 (dd,  $J = 1$  Hz), 4.62-4.56 (m, 1H), 3.78 (s, 3H), 3.21 (s, 3H), 2.92-2.87 (m, 1H), 2.69-2.61 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 172.9, 156.6, 137.8, 128.8, 113.9, 110.6, 109.3, 66.8, 56.0, 55.9, 33.6, 26.8; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{NNaO}_4^+$  270.0737; Found 270.0739; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm) tR = 20.9 min (major), 19.4 min (minor);  $[\alpha]_{\text{D}}^{25} +16.0$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 99% ee).

**(R)-5'-Bromo-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4f)**



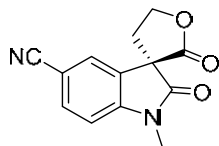
50.2 mg, 85% yield, white solid, m.p.: 157.8-158.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48 (dd,  $J = 8.0, 2.0$  Hz, 1H), 7.34 (d,  $J = 2.0$  Hz, 1H), 6.77 (d,  $J = 8.0$  Hz, 1H), 4.81 (dd,  $J = 16.4$  Hz, 7.6 Hz, 1H), 4.62-4.57 (m, 1H), 3.21 (s, 3H), 2.91-2.85 (m, 1H), 2.69-2.62 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.8, 172.2, 143.5, 132.6, 129.5, 126.4, 115.9, 110.4, 66.8, 55.6, 33.4, 26.9; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{12}\text{H}_{10}\text{BrNNaO}_3^+$  317.9736; Found 317.9736; HPLC(AS-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 31.8 min (major), 5.7 min (minor);  $[\alpha]_{\text{D}}^{25} +11.0$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 98% ee).

**(R)-5'-fluoro-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4g)**



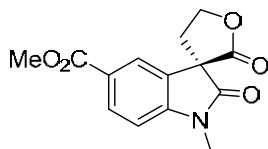
40.0 mg, 85% yield, white solid, m.p.: 178.8-179.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.09-7.04 (m, 1H), 6.98 (dd,  $J = 7.6, 2.4$  Hz, 1H), 6.83-6.80 (m, 1H), 4.82 (dd,  $J = 16.4$  Hz, 8.0 Hz, 1H), 4.62-4.57 (m, 1H), 3.22 (s, 3H), 2.92-2.86 (m, 1H), 2.70-2.62 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 172.4, 159.5 (d,  $J = 240.9$  Hz), 140.4 (d,  $J = 2.0$  Hz), 128.9 (d,  $J = 8.3$  Hz), 116.1 (d,  $J = 23.3$  Hz), 111.4 (d,  $J = 25.2$  Hz), 109.5 (d,  $J = 8.1$  Hz), 66.8, 56.0, 33.5, 26.9; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{12}\text{H}_{10}\text{FNNaO}_3^+$  258.0537; Found 258.0535; HPLC(OJ-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm) tR = 19.5 min (major), 17.1 min (minor);  $[\alpha]_{\text{D}}^{25} +25.0$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 97% ee).

**(R)-1'-Methyl-2,2'-dioxo-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-5'-carbonitrile (4h)**



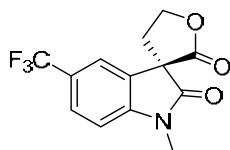
With 100 mol% **U3** as the co-catalyst, 44.0 mg, 91% yield, white solid, m.p.: 204.7-205.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (dd,  $J = 8.4, 1.2$  Hz, 1H), 7.50 (d,  $J = 1.2$  Hz, 1H), 6.98 (d,  $J = 8.4$  Hz, 1H), 4.82 (dd,  $J = 16.2$  Hz, 8.4 Hz, 1H), 4.66-4.63 (m, 1H), 3.27 (s, 3H), 2.92-2.88 (m, 1H), 2.74-2.70 (m, 1H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 171.6, 148.3, 135.0, 128.6, 126.6, 118.5, 109.4, 106.8, 66.9, 55.4, 33.3, 27.1; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{NaO}_3$  265.0584; Found, 265.0586; HPLC(OJ-H, hexane/*i*-PrOH = 50:50, flow rate=1.0 mL/min, I=254 nm), tR = 43.7 min (major), 30.1 min (minor);  $[\alpha]_{\text{D}}^{25} +14.7$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 94% ee).

**(R)-Methyl 1'-methyl-2,2'-dioxo-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-5'-carboxylate (4i)**



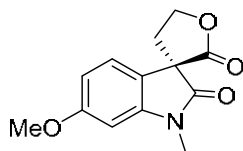
50.1 mg, 91% yield, white solid, m.p.: 123.6-124.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10 (dd,  $J = 8.0, 1.2$  Hz, 1H), 7.90 (d,  $J = 1.2$  Hz, 1H), 6.93 (d,  $J = 8.0$  Hz, 1H), 4.82 (dd,  $J = 16.4$  Hz, 8.0 Hz, 1H), 4.68-4.63 (m, 1H), 3.90 (s, 3H), 3.26 (s, 3H), 2.94-2.87 (m, 1H), 2.75-2.68 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.6, 172.3, 166.2, 148.4, 132.3, 127.8, 125.5, 124.4, 108.5, 66.8, 55.4, 52.2, 33.30, 27.0; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{14}\text{H}_{13}\text{NNaO}_5^+$  298.0686; Found 298.0685; HPLC(IC-H, hexane/*i*-PrOH = 50:50, flow rate=1.0 ml/min, I=254 nm) tR = 38.4 min (major), 58.9 min (minor);  $[\alpha]_{\text{D}}^{25} +25.0$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 97% ee).

**(R)-1'-methyl-5'-(trifluoromethyl)-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4j)**



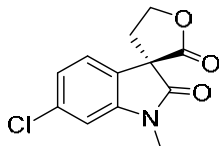
45.6 mg, 80% yield, white solid, m.p.: 165.7-166.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (d,  $J = 8.0$  Hz, 1H), 7.46 (s, 1H), 6.97 (d,  $J = 8.0$  Hz, 1H), 4.84 (dd,  $J = 16.8$  Hz, 8.0 Hz, 1H), 4.67-4.61 (m, 1H), 3.27 (s, 3H), 2.94-2.88 (m, 1H), 2.77-2.66 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.3, 172.0, 147.4, 128.2, 127.6 (q,  $J = 3.9$  Hz), 125.8 (q,  $J = 32.9$  Hz), 123.9 (q,  $J = 270.2$  Hz), 120.3 (q,  $J = 3.6$  Hz), 108.8, 66.8, 55.6, 33.3, 27.0; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calcd for  $\text{C}_{13}\text{H}_{10}\text{F}_3\text{NO}_3^+$  308.0505; Found 308.0504; HPLC(OJ-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm) tR = 21.9 min (major), 15.0 min (minor);  $[\alpha]_{\text{D}}^{25} +5.5$  ( $c = 1.0$ ,  $\text{CHCl}_3$ , 96% ee).

**(R)-6'-Methoxy-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4k)**



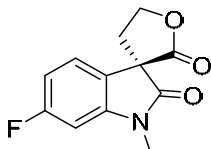
43.5 mg, 88% yield, white solid, m.p.: 156.7-157.6 °C; (PE/EA=5/1) <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.11 (d, *J* = 8.4 Hz, 1H), 6.60 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.46 (d, *J* = 1.8 Hz, 1H), 4.82-4.78 (m, 1H), 4.60-4.57 (m, 1H), 3.83 (s, 3H), 3.22 (s, 3H), 2.89-2.86 (m, 1H), 2.64-2.61 (m, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 173.9, 173.4, 161.3, 145.7, 123.8, 119.5, 107.2, 97.0, 66.7, 55.7, 55.2, 33.6, 26.8; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>13</sub>NNaO<sub>4</sub><sup>+</sup> (M + Na)<sup>+</sup> 270.0737; Found, 270.0732; HPLC(AD-H, hexane/*i*-PrOH = 90:10, flow rate=1.0 mL/min, I=254 nm), tR = 33.8 min (major), 29.0 min (minor); [α]<sub>D</sub><sup>25</sup> +18.0 (c = 1.0, CHCl<sub>3</sub>, 99% ee).

**(R)-6'-Chloro-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4l)**



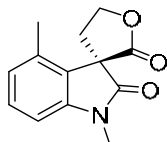
45.2 mg, 90% yield, white solid, m.p.: 146.7-147.8 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.14 (d, *J* = 8.0 Hz, 1H), 7.09 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.90 (d, *J* = 1.6 Hz, 1H), 4.81 (dd, *J* = 16.4 Hz, 8.0 Hz, 1H), 4.63-4.59 (m, 1H), 3.22 (s, 3H), 2.89-2.85 (m, 1H), 2.69-2.63 (m, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 173.3, 172.5, 145.6, 135.7, 125.9, 124.0, 123.3, 109.8, 66.8, 55.3, 33.4, 26.9; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>ClNNaO<sub>3</sub><sup>+</sup> 274.0241; Found 274.0239; HPLC(AD-H, hexane/*i*-PrOH = 80:20, flow rate=1.0 mL/min, I=254 nm), tR = 12.2 min (major), 10.9 min (minor); [α]<sub>D</sub><sup>25</sup> +4.3 (c = 1.0, CHCl<sub>3</sub>, 99% ee).

**(R)-6'-Fluoro-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4m)**



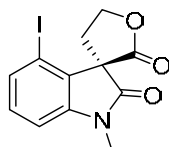
42.8 mg, 91% yield, white solid, m.p.: 210.8-211.7 °C; (PE/EA=5/1) <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.18-7.14 (m, 1H), 6.81-6.77 (m, 1H), 6.65-6.63 (m, 1H), 4.82 (dd, *J* = 16.8 Hz, 8.4 Hz, 1H), 4.62-4.59 (m, 1H), 3.22 (s, 3H), 2.89-2.86 (m, 1H), 2.68-2.63 (m, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 173.6, 172.7, 163.8 (d, *J* = 247.9 Hz), 146.1 (d, *J* = 11.8 Hz), 124.3 (d, *J* = 10.0 Hz), 123.0 (d, *J* = 3.0 Hz), 109.7 (d, *J* = 23.0 Hz), 98.0 (d, *J* = 27.0 Hz), 66.7, 55.2, 33.5, 26.9; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>FNNaO<sub>3</sub> 258.0537; Found 258.0533; HPLC(AD-H, hexane/*i*-PrOH = 90:10, flow rate=1.0 mL/min, I=254 nm), tR = 23.7 min (major), 20.9 min (minor); [α]<sub>D</sub><sup>25</sup> +11.5 (c = 1.0, CHCl<sub>3</sub>, 97% ee).

**(R)-1',4'-Dimethyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4n)**



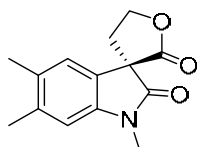
33.3 mg, 72% yield, white solid, m.p.: 209.7-210.3 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.26 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 4.90-4.83 (m, 1H), 4.66-4.60 (m, 1H), 3.21 (s, 3H), 2.91-2.87 (m, 1H), 2.73-2.70 (m, 1H), 2.27 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 173.6, 172.7, 144.8, 134.2, 129.6, 125.6, 125.2, 106.5, 66.6, 55.4, 31.3, 26.8, 18.1; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>13</sub>NNaO<sub>3</sub><sup>+</sup> 254.0788; Found 254.0782; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm) t<sub>R</sub> = 12.4 min (major), 8.3 min (minor); [α]<sub>D</sub><sup>25</sup> +16.8 (c = 1.0, CHCl<sub>3</sub>, 96% ee).

**(R)-4'-iodo-1'-methyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4o)**



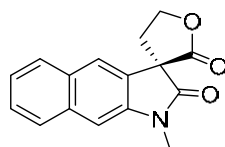
50.8 mg, 74% yield, white solid, m.p.: 195.7-196.4 °C; (PE/EA=5/1) <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.48 (d, *J* = 7.8 Hz, 1H), 7.08 (t, *J* = 7.8 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 4.82 (dd, *J* = 16.8 Hz, 8.4 Hz, 1H), 4.75-4.72 (m, 1H), 3.28-3.22 (m 1H), 3.20 (s, 3H), 2.63-2.59 (m 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 172.9, 171.1, 146.2, 133.3, 131.2, 129.5, 108.6, 91.3, 66.8, 58.6, 30.1, 26.8; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>10</sub>NNaO<sub>3</sub><sup>+</sup> 365.9598; Found, 365.9595; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 mL/min, I=254 nm), t<sub>R</sub> = 14.6 min (major), 9.9 min (minor); [α]<sub>D</sub><sup>25</sup> -12.3 (c = 1.0, CHCl<sub>3</sub>, 97% ee).

**(R)-1',5',6'-trimethyl-4,5-dihydro-2H-spiro[furan-3,3'-indoline]-2,2'-dione (4p)**



44.1 mg, 90% yield, white solid, m.p.: 187.7-188.5 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 6.99 (s, 1H), 6.68 (s, 1H), 4.80 (dd, *J* = 16.4 Hz, 8.4 Hz, 1H), 4.62-4.56 (m, 1H), 3.21 (s, 3H), 2.88-2.85 (m, 1H), 2.65-2.61 (m, 1H), 2.29 (s, 3H), 2.24 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 173.5, 173.4, 142.3, 138.3, 131.5, 125.0, 124.2, 110.4, 66.8, 55.5, 33.6, 26.7, 20.3, 19.5; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>14</sub>H<sub>15</sub>NNaO<sub>3</sub><sup>+</sup> 268.0944; Found 268.0938; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm) t<sub>R</sub> = 13.3 min (major), 9.7 min (minor); [α]<sub>D</sub><sup>25</sup> +26.4 (c = 1.0, CHCl<sub>3</sub>, 99% ee).

**(R)-1-methyl-4',5'-dihydro-2'H-spiro[benzo[f]indole-3,3'-furan]-2,2'(1H)-dione (4q)**



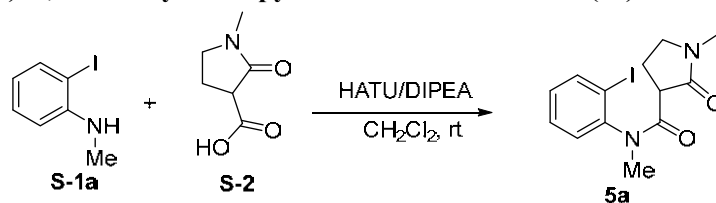
47.0 mg, 88% yield, white solid, m.p.: 143.7-144.4 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.80-7.74 (m, 2H), 7.68 (s, 1H), 7.52-7.48 (m, 1H), 7.43-7.39 (m, 1H), 7.16 (s, 1H), 4.86 (dd, *J* = 16.4 Hz, 7.6 Hz, 1H), 4.72-4.67 (m, 1H), 3.34 (s, 3H), 3.03-2.96 (m, 1H), 2.79-2.71 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 173.1, 172.9, 141.9, 134.3, 130.5, 128.5, 128.3, 127.4, 127.3, 124.9, 122.9, 104.8, 66.9, 55.2, 34.1, 27.0; HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calcd for C<sub>16</sub>H<sub>13</sub>NNaO<sub>3</sub><sup>+</sup>



290.0788; Found, 290.0785; HPLC(AS-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 mL/min, I=254 nm), tR = 22.9 min (major), 17.2 min (minor);  $[\alpha]_{\text{D}}^{25} +69.7$  (c = 1.0, CHCl<sub>3</sub>, 99% ee).

### General procedure for the synthesis of 5a-5m:

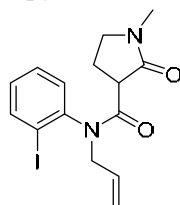
#### *N*-(2-iodophenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5a)



A mixture of 2-iodo-*N*-methylaniline (S-1a, 2.3 g, 10 mmol), 1-methyl-2-oxopyrrolidine-3-carboxylic acid (S-2, 1.6 g, 11 mmol), HATU (4.6 g, 15 mmol), DIPEA (1.9 g, 2.6 mL, 15 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (50 mL) was stirred at room temperature for 12 hours. The solvent was removed in vacuum. The residue was purified by column chromatography (silica gel, petroleum ester/EtOAc) to give the corresponding product 5a (2.6 g, 73% yield) as a white solid. m.p.: 100.8-101.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.99 & 7.91 (2dd, *J* = 8.0 Hz, 1.2 Hz, 1H), 7.73-7.71 (m, 1H), 7.49-7.45 & 7.42-7.40 (m, 1H), 7.19-7.16 & 7.11-7.07 (m, 1H), 3.55-3.48 (m, 1H), 3.28-3.17 (m, 5H), 2.82 & 2.80 (2s, 3H), 2.65-2.55 (m, 1H), 2.16-2.06 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.8, 170.6, 170.4, 170.0, 145.4, 140.5, 139.3, 130.9, 129.9, 129.8, 129.4, 128.8, 99.7, 99.3, 47.8, 47.6, 46.3, 45.7, 36.3, 36.1, 29.6, 23.5, 22.7; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>16</sub>IN<sub>2</sub>O<sub>2</sub><sup>+</sup> 359.0251; Found 359.0251.

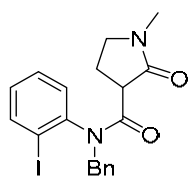
Substrates 5b-5m were synthesized similarly to that of 5a.

#### *N*-allyl-*N*-(2-iodophenyl)-1-methyl-2-oxopyrrolidine-3-carboxamide (5b)



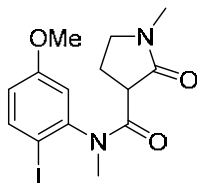
2.8 g, 73% yield, white solid. m.p.: 132.6-133.5 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.98 & 7.90 (2d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.44-7.35 (m, 1H), 7.09-7.04 (m, 1H), 5.95-5.85 (m, 1H), 5.18-5.07 (m, 2H), 4.87-4.81 (m, 1H), 3.68-3.62 (m, 1H), 3.52-3.46 (m, 1H), 3.26-3.14 (m, 2H), 2.81 & 2.78 (2s, 3H), 2.64-2.55 (m, 1H), 2.14-2.05 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.7, 169.9, 143.7, 140.6, 139.4, 132.5, 132.0, 130.6, 129.9, 129.8, 129.4, 128.9, 118.9, 118.3, 100.6, 51.6, 51.1, 47.9, 47.8, 46.7, 46.0, 29.7, 23.6, 22.6; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>15</sub>H<sub>18</sub>IN<sub>2</sub>O<sub>2</sub><sup>+</sup> 385.0407; Found 385.0406.

#### *N*-benzyl-*N*-(2-iodophenyl)-1-methyl-2-oxopyrrolidine-3-carboxamide (5c)



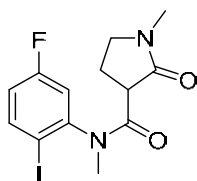
3.2g, 75% yield, white solid, m.p.: 145.5-146.4 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 8.01 & 7.91 (2dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.32-7.19 (m, 7H), 7.05-7.01 (m, 1H), 5.75 & 5.69 (2d, *J* = 14.4 Hz, 1H), 4.07 & 4.02 (d, *J* = 14.4 Hz, 1H), 3.55-3.50 (m, 1H), 3.29-3.19 (m, 2H), 2.86 & 2.82 (2s, 3H), 2.72-2.63 (m, 1H), 2.19-2.10 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.8, 170.4, 143.5, 139.4, 136.2, 132.6, 129.9, 129.3, 128.8, 128.4, 127.4, 100.4, 52.1, 48.0, 46.0, 29.8, 22.8; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>19</sub>H<sub>20</sub>IN<sub>2</sub>O<sub>2</sub><sup>+</sup> 435.0564; Found 435.0564.

***N*-(2-iodo-5-methoxyphenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5d)**



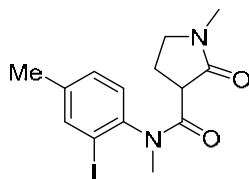
2.9g, 76% yield, white solid. m.p.: 137.6-138.5 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.80 & 7.69 (2d, *J* = 8.8 Hz, 1H), 7.30 (d, *J* = 3.2 Hz, 1H), 6.72-6.67 (m, 1H), 3.81 & 3.79 (2s, 3H), 3.52-3.47 (m, 1H), 3.26-3.18 (m, 5H), 2.81 & 2.78 (2s, 3H), 2.60-2.51 (m, 1H), 2.13-2.03 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.8, 170.1, 161.0, 146.3, 139.3, 117.3, 115.9, 86.9, 55.7, 55.6, 48.0, 45.8, 36.2, 36.1, 29.8, 23.7, 22.9; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>14</sub>H<sub>18</sub>IN<sub>2</sub>O<sub>3</sub><sup>+</sup> 389.0357; Found 389.0360.

***N*-(5-fluoro-2-iodophenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5e)**



2.6g, 73% yield, white solid. m.p.: 127.5-128.4 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.92-7.88 & 7.83-7.80 (m, 1H), 7.49-7.46 (m, 1H), 6.94-6.83 (m, 1H), 3.50-3.44 (m, 1H), 3.26-3.13 (m, 5H), 2.77 & 2.80 (2s, 3H), 2.61-2.52 (m, 1H), 2.12-2.04 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.4, 169.7, 163.2 (d, *J* = 251.0 Hz), 146.8 (d, *J* = 10.0 Hz), 141.4, 140.0 (d, *J* = 9.0 Hz), 118.8 (d, *J* = 23.0 Hz), 117.7 (d, *J* = 13.0 Hz), 117.5 (d, *J* = 11.0 Hz), 116.5 (d, *J* = 22.0 Hz), 92.7 (d, *J* = 4.0 Hz), 47.9, 47.6, 46.4, 45.8, 36.2, 36.0, 29.7, 23.5, 22.6; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>15</sub>FIN<sub>2</sub>O<sub>2</sub><sup>+</sup> 377.0157; Found 377.0155.

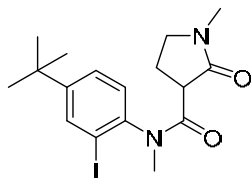
***N*-benzyl-*N*-(2-iodo-4-methylphenyl)-1-methyl-2-oxopyrrolidine-3-carboxamide (5f)**



2.9g, 79% yield, white solid. m.p.: 147.8-148.6 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.80 & 7.71 (2s, 1H), 7.56 & 7.03 (2d, *J* = 8.0 Hz, 1H), 7.26-7.23 & 7.20-7.17 (m, 1H), 3.52-3.46 (m, 1H), 3.26-3.20 (m, 5H), 2.82 & 2.79 (2s, 3H), 2.62-2.53 (m, 1H), 2.34 (s, 3H), 2.13-

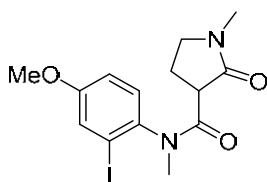
2.05 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  170.9, 170.3, 143.0, 141.0, 140.4, 139.7, 130.7, 130.4, 130.2, 128.3, 99.2, 48.0, 47.7, 46.4, 45.7, 36.4, 36.2, 29.7, 23.6, 22.8, 20.5; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{18}\text{IN}_2\text{O}_2^+$  ( $\text{M} + \text{H}$ ) $^+$  373.0407; Found 373.0407.

***N*-(4-(*tert*-butyl)-2-iodophenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5g)**



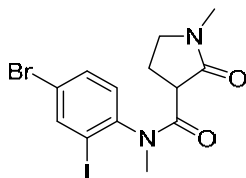
3.3g, 73% yield, white solid, m.p.: 123.6-123.3 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.94 & 7.85 (2d,  $J = 2.0$  Hz, 1H), 7.60-7.58 & 7.06 (2d,  $J = 8.4$  Hz, 1H), 7.45 & 7.438 (2dd,  $J = 8.4$  Hz, 2.0 Hz, 1H), 3.53-3.47 (m, 1H), 3.27-3.20 (m, 5H), 2.82 & 2.80 (2s, 3H), 2.62-2.53 (m, 1H), 2.16-2.08 (m, 1H), 1.31 & 1.28 (2s, 9H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  170.9, 170.3, 153.4, 142.8, 137.8, 136.4, 130.1, 128.1, 127.3, 126.6, 99.3, 48.0, 47.8, 46.4, 45.7, 36.4, 36.3, 34.6, 33.9, 31.1, 29.7, 23.6, 22.9; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{17}\text{H}_{24}\text{IN}_2\text{O}_2^+$  415.0877; Found 415.0876.

***N*-(2-iodo-4-methoxyphenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5h)**



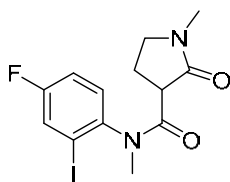
2.9g, 76% yield, white solid, m.p.: 139.3-139.2 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  7.58 (d,  $J = 8.8$  Hz, 1H), 7.46 & 7.38 (2d,  $J = 2.8$  Hz, 1H), 6.98-6.89 (m, 1H), 3.81 & 3.80 (2s, 1H), 3.52-3.46 (m, 1H), 3.26-3.19 (m, 5H), 2.80 & 2.79 (2s, 3H), 2.61-2.52 (m, 1H), 2.14-2.04 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  170.9, 170.5, 159.4, 138.4, 131.0, 128.9, 125.0, 124.5, 115.4, 115.1, 99.6, 55.7, 48.0, 47.7, 46.3, 45.7, 36.6, 36.4, 29.7, 23.6, 22.8; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{18}\text{IN}_2\text{O}_3^+$  389.0357; Found 389.0357.

***N*-(4-bromo-2-iodophenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5i)**



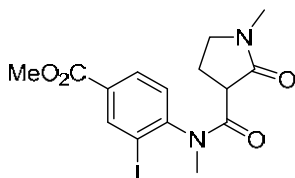
3.3g, 76% yield, white solid. m.p.: 127.7-128.3 °C. (PE/EA=3/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  8.13 & 8.04 (2d,  $J = 2.0$  Hz, 1H), 7.62-7.57 & 7.03-7.00 (m, 2H), 3.53-3.43 (m, 1H), 3.29-3.16 (m, 5H), 2.83 & 2.80 (2s, 3H), 2.63-2.54 (m, 1H), 2.14-2.06 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , two rotamers)  $\delta$  171.8, 170.6, 169.9, 169.7, 144.7, 142.8, 141.4, 133.2, 132.1, 129.9, 122.8, 100.3, 48.0, 47.6, 46.3, 45.9, 36.4, 30.2, 29.8, 22.7, 20.9; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{15}\text{BrIN}_2\text{O}_2^+$  436.9356; Found 436.9357.

***N*-(4-fluoro-2-iodophenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5j)**



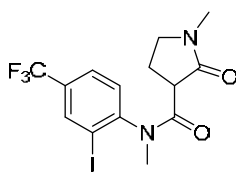
2.7g, 73% yield, white solid. m.p.: 119.5-120.3 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.71-7.68 (m, 1H), 7.61-7.58 (m, 1H), 7.19-7.14 (m, 1H), 3.52-3.47 (m, 1H), 3.28-3.15 (m, 5H), 2.82 & 2.79 (2s, 1H), 2.63-2.54 (m, 1H), 2.13-2.05 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.6, 170.1, 161.3 (d, *J* = 252.0 Hz), 141.8 (d, *J* = 4.0 Hz), 131.9 (d, *J* = 10.9 Hz), 126.1 (d, *J* = 24.0 Hz), 116.9 (d, *J* = 22.0 Hz), 99.4 (d, *J* = 9.0 Hz), 47.9, 47.8, 46.0, 45.7, 36.5, 29.7, 23.5, 22.7; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>15</sub>FIN<sub>2</sub>O<sub>2</sub><sup>+</sup> 377.0157; Found 377.0159.

**Methyl 4-(*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamido)-3-iodobenzoate (5k)**



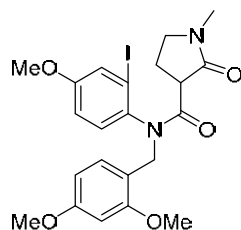
3.2g, 78% yield, white solid. m.p.: 116.8-117.6 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 8.27 & 7.79 (2d, *J* = 2.0 Hz, 1H), 8.07 & 7.98 (d, *J* = 8.4 Hz, 1H), 7.73-7.70 (m, 1H), 3.92 & 3.90 (2s, 3H), 3.55-3.47 (m, 1H), 3.25-3.13 (m, 4H), 3.19-3.11 (m, 1H), 2.81 & 2.78 (2s, 3H), 2.61-2.53 (m, 1H), 2.13-2.04 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.7, 170.4, 170.3, 170.0, 165.5, 165.4, 146.0, 145.8, 141.0, 139.7, 132.3, 131.7, 131.6, 130.3, 130.6, 129.5, 106.6, 106.0, 52.5, 52.2, 48.0, 47.7, 46.4, 45.9, 36.4, 36.2, 29.8, 23.5, 22.7; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>15</sub>H<sub>18</sub>IN<sub>2</sub>O<sub>4</sub><sup>+</sup> (M + H)<sup>+</sup> 417.0306; Found 417.0305.

***N*-(2-iodo-4-(trifluoromethyl)phenyl)-*N*,1-dimethyl-2-oxopyrrolidine-3-carboxamide (5l)**



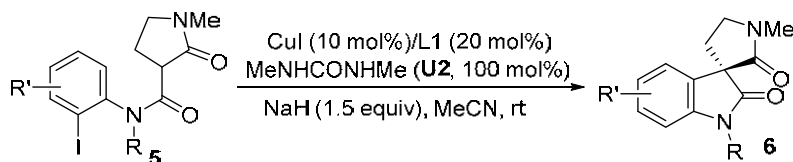
3.2g, 76% yield, white solid. m.p.: 109.7-110.6 °C. (PE/EA=3/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 8.15 (d, *J* = 2.4 Hz, 1H), 7.88-7.86 (m, 1H), 7.74-7.72 (m, 1H), 3.55-3.48 (m, 1H), 3.30-3.24 (m, 4H), 3.14-3.10 (m, 1H), 2.84 & 2.80 (2s, 3H), 2.66-2.57 (m, 1H), 2.15-2.07 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.5, 169.6, 148.8, 136.4 (q, *J* = 4.0 Hz), 131.9 (q, *J* = 33.0 Hz), 131.4, 129.3 (q, *J* = 15.0 Hz), 127.1 (q, *J* = 4.0 Hz), 122.4 (q, *J* = 272.0 Hz), 100.2, 99.8, 48.0, 47.8, 46.6, 46.1, 38.7, 38.3, 29.8, 23.4, 22.6; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>IN<sub>2</sub>O<sub>2</sub><sup>+</sup> 427.0125; Found 427.0125.

***N*-(2,4-dimethoxybenzyl)-*N*-(2-iodo-4-methoxyphenyl)-1-methyl-2-oxopyrrolidine-3-carboxamide (5m)**



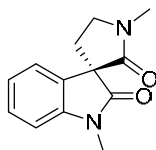
3.9g, 75% yield, white solid. m.p.: 117.8-118.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, two rotamers) δ 7.43-7.35 (m, 2H), 7.23-7.18 (m, 1H), 6.76-6.65 (m, 1H), 6.47-6.44 (m, 1H), 6.37-6.30 (m, 1H), 5.42 & 5.36 (d, *J* = 14.4 Hz, 1H), 4.30 & 4.28 (d, *J* = 14.4 Hz, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 3.58 (s, 3H), 3.54-3.48 (m, 1H), 3.27-3.21 (m, 1H), 2.84 & 2.80 (2s, 3H), 2.68-2.59 (m, 1H), 2.15-2.06 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, two rotamers) δ 170.9, 170.5, 160.2, 159.1, 158.4, 136.8, 132.3, 132.1, 131.0, 130.5, 124.3, 124.1, 116.9, 114.2, 114.0, 104.0, 100.7, 98.0, 97.9, 55.5, 55.2, 55.0, 48.0, 47.7, 46.6, 46.3, 45.9, 33.5, 29.7, 23.7, 22.8; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>22</sub>H<sub>26</sub>IN<sub>2</sub>O<sub>5</sub><sup>+</sup> 525.0881; Found 525.0881.

#### Procedure for Asymmetric Ullmann-Hurtley Coupling Reaction of 5a-5m:



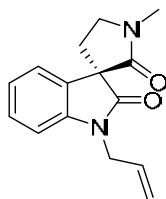
The reaction mixture of substrates **5** (0.2 mmol), CuI (0.02 mmol), (*S,S*)-L1 (0.04 mmol), NaH (0.3 mmol) and 1,3-dimethyl urea (**U2**, 0.2 mmol) in MeCN (2 mL) were stirred at room temperature for 3-12 hours. Then H<sub>2</sub>O (5.0 mL) and ethyl acetate (5.0 mL) were added into the mixture. The organic phase was separated and the aqueous phase was extracted with ethyl acetate (5.0 mL × 3). The combined organic phase was washed with H<sub>2</sub>O and brine, dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/10 to 1/3) to afford the desired products **6**.

#### (*S*)-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (**6a**)



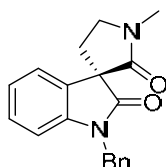
42.8 mg, 93%, white solid, m.p.: 85.6-86.4 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.33-7.29 (m, 1H), 7.14 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.09-7.05 (m, 1H), 6.82 (dd, *J* = 8.0 Hz, 1.2 Hz, 1H), 3.79-3.72 (m, 1H), 3.60-3.54 (m, 1H), 3.19 (s, 3H), 2.95 (s, 3H), 2.65-2.62 (m, 1H), 2.40-2.33 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 175.6, 170.4, 144.4, 129.8, 128.9, 122.9, 122.7, 108.4, 57.7, 47.1, 30.4, 29.4, 26.4; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup> 231.1128; Found 231.1129; HPLC(OD-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) t<sub>R</sub> = 10.5 min (major), 14.9 min (minor); [α]<sub>D</sub><sup>25</sup> -14.1 (*c* 1.0, CHCl<sub>3</sub>, 97% *ee*).

#### (*S*)-1-allyl-1'-methylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (**6b**)



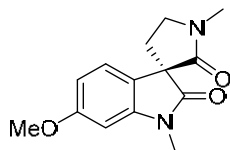
48.1 mg, 94%, white solid, m.p.: 178.6-179.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.31-7.27 (m, 1H), 7.19-7.17 (m, 1H), 7.09-7.06 (m, 1H), 6.86 (d,  $J = 8.0$  Hz, 1H), 5.91-5.81 (m, 1H), 5.30 (d,  $J = 17.2$  Hz, 1H), 5.23 (d,  $J = 10.8$  Hz, 1H), 4.42-4.30 (m, 2H), 3.85-3.78 (m, 1H), 3.64-3.58 (m, 1H), 3.00 (s, 3H), 2.75-2.69 (m, 1H), 2.47-2.40 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  175.5, 170.5, 143.7, 130.8, 130.0, 128.9, 123.0, 122.9, 117.6, 109.4, 57.8, 47.2, 42.5, 30.5, 29.4; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2^+$  257.1285; Found 257.1285; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm)  $t_R = 7.3$  min (major), 12.7 min (minor);  $[\alpha]_D^{25} -22.1$  ( $c$  1.0,  $\text{CHCl}_3$ , 98% *ee*).

**(S)-1-benzyl-1'-methylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6c)**



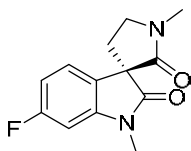
56.9 mg, 93%, white solid, m.p.: 187.6-188.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.38-7.32 (m, 4H), 7.28-7.24 (m, 1H), 7.20 (d,  $J = 7.6$  Hz, 2H), 7.05 (t,  $J = 7.6$  Hz, 1H), 6.70 (d,  $J = 8.0$  Hz, 1H), 5.04 (d,  $J = 16.0$  Hz, 1H), 4.87 (d,  $J = 16.0$  Hz, 1H), 3.88-3.82 (m, 1H), 3.67-3.62 (m, 1H), 3.03 (s, 3H), 2.81-2.75 (m, 1H), 2.50-2.43 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  175.9, 170.5, 143.5, 135.3, 130.0, 128.9, 128.8, 127.5, 127.0, 123.0, 122.8, 109.5, 57.8, 47.2, 43.9, 30.5, 29.4; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}_2^+$  307.1441; Found 307.1440; HPLC(AD-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm)  $t_R = 11.6$  min (major), 6.6 min (minor);  $[\alpha]_D^{25} -4.8$  ( $c$  1.0,  $\text{CHCl}_3$ , 99% *ee*).

**(S)-6-methoxy-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6d)**



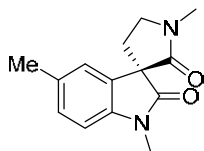
36.4 mg, 70%, white solid, m.p.: 169.6-170.5 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.04 (d,  $J = 8.0$  Hz, 1H), 6.55 (dd,  $J = 8.0$  Hz, 2.4 Hz, 1H), 6.43 (d,  $J = 2.4$  Hz, 1H), 3.81 (s, 3H), 3.80-3.76 (m, 1H), 3.60-3.54 (m, 1H), 3.18 (s, 3H), 2.96 (s, 3H), 2.69-2.62 (m, 1H), 2.39-2.30 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  176.3, 170.7, 160.8, 145.7, 123.4, 121.8, 106.8, 96.6, 57.3, 55.61, 47.1, 30.5, 29.5, 26.5; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_3^+$  261.1234; Found 261.1233; HPLC(OJ-H, hexane/*i*-PrOH = 60:40, flow rate=1.0 ml/min, I=254 nm)  $t_R = 9.0$  min (major), 10.9 min (minor);  $[\alpha]_D^{25} -22.7$  ( $c$  1.0,  $\text{CHCl}_3$ , 99% *ee*).

**(S)-6-fluoro-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6e)**



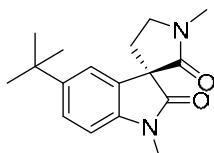
43.2 mg, 87%, white solid, m.p.: 187.7-188.6 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.10 (dd,  $J = 8.0$  Hz, 5.2 Hz, 1H), 6.79-6.74 (m, 1H), 6.62 (dd,  $J = 8.8$  Hz, 2.0 Hz, 1H), 3.85-3.78 (m, 1H), 3.62-3.56 (m, 1H), 3.22 (s, 3H), 3.00 (s, 3H), 2.71-2.65 (m, 1H), 2.42-2.35 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  176.0, 170.2, 163.5 (d,  $J = 244.0$  Hz), 146.1 (d,  $J = 11.0$  Hz), 125.1 (d,  $J = 2.0$  Hz), 123.9 (d,  $J = 9.0$  Hz), 109.0 (d,  $J = 23.0$  Hz), 97.46 (d,  $J = 28.0$  Hz), 57.3, 47.1, 30.6, 29.4, 26.7; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{13}\text{H}_{14}\text{FN}_2\text{O}_2^+$  249.1034; Found 249.1034; HPLC(AD-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 7.8 min (major), 6.3 min (minor);  $[\alpha]_{\text{D}}^{25} -7.7$  (*c* 1.0,  $\text{CHCl}_3$ , 98.5% *ee*).

**(S)-1,1',5-trimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6f)**



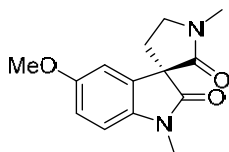
39.0 mg, 80%, white solid, m.p.: 206.1-206.4 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.12 (d,  $J = 7.6$  Hz, 1H), 6.99 (s, 1H), 6.76 (d,  $J = 8.0$  Hz, 1H), 3.84-3.78 (m, 1H), 3.63-3.57 (m, 1H), 3.22 (s, 3H), 3.00 (s, 3H), 2.72-2.65 (m, 1H), 2.43-2.34 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  175.6, 170.7, 142.1, 132.6, 129.9, 129.2, 123.6, 108.2, 57.8, 47.2, 30.5, 29.5, 26.6, 21.1; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{14}\text{H}_{16}\text{N}_2\text{NaO}_2^+$  267.1104; Found 267.1104; HPLC(OJ-H, hexane/*i*-PrOH = 80/20, flow rate=1.0 ml/min, I=254 nm) tR = 12.2 min (major), 14.4 min (minor);  $[\alpha]_{\text{D}}^{25} +11.0$  (*c* 1.0,  $\text{CHCl}_3$ , 98.5% *ee*).

**(S)-5-(tert-butyl)-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6g)**



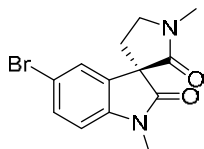
49.2 mg, 86%, white solid, m.p.: 158.2-158.7 °C; (PE/EA=5/1)  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.34 (dd,  $J = 8.4$  Hz, 2.0 Hz, 1H), 7.16 (d,  $J = 2.0$  Hz, 1H), 6.79 (d,  $J = 8.0$  Hz, 1H), 3.84-3.78 (m, 1H), 3.61-3.56 (m, 1H), 3.20 (s, 3H), 3.00 (s, 3H), 2.69-2.63 (m, 1H), 2.44-2.37 (m, 1H), 1.30 (s, 9H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  175.9, 170.7, 146.3, 142.1, 129.5, 125.8, 119.8, 108.0, 58.1, 47.2, 34.6, 31.6, 30.6, 29.7, 26.6; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{17}\text{H}_{23}\text{N}_2\text{O}_2^+$  287.1754; Found 287.1755; HPLC(AS-H, hexane/*i*-PrOH = 80/20, flow rate=1.0 ml/min, I=254 nm) tR = 7.6 min (major), 6.2 min (minor);  $[\alpha]_{\text{D}}^{25} +15.2$  (*c* 1.0,  $\text{CHCl}_3$ , 98% *ee*).

**(S)-5-methoxy-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6h)**



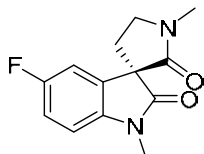
47.8 mg, 92%, white solid, m.p.: 178.2-178.6 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 6.84 (dd, *J* = 8.4 Hz, 2.8 Hz, 1H), 6.79-6.76 (m, 2H), 3.83-3.77 (m, 4H), 3.62-3.56 (m, 1H), 3.21 (s, 3H), 2.99 (s, 3H), 2.72-2.66 (m, 1H), 2.42-2.35 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 175.3, 170.4, 156.3, 138.0, 131.0, 113.1, 110.5, 108.8, 58.1, 55.8, 47.1, 30.5, 29.5, 26.6; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>14</sub>H<sub>17</sub>N<sub>2</sub>O<sub>3</sub><sup>+</sup> 261.1234; Found 261.1234; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 10.5 min (major), 12.8 min (minor); [α]<sub>D</sub><sup>25</sup> +11.2 (*c* 1.0, CHCl<sub>3</sub>, 96% *ee*).

**(S)-5-bromo-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6i)**



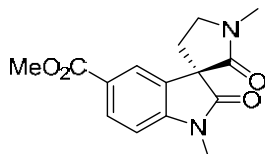
49.9 mg, 81%, white solid, m.p.: 203.4-203.7 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.45 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H), 7.28 (d, *J* = 2.0 Hz, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 3.83-3.77 (m, 1H), 3.63-3.57 (m, 1H), 3.22 (s, 3H), 3.00 (s, 3H), 2.73-2.66 (m, 1H), 2.43-2.36 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 175.2, 169.8, 143.6, 131.9, 131.8, 126.2, 115.6, 109.9, 57.8, 47.1, 30.6, 29.3, 26.7; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>14</sub>BrN<sub>2</sub>O<sub>2</sub><sup>+</sup> 309.0233; Found 309.0234; HPLC(AS-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 15.6 min (major), 12.4 min (minor); [α]<sub>D</sub><sup>25</sup> -26.4 (*c* 1.0, CHCl<sub>3</sub>, 97% *ee*).

**(S)-5-fluoro-1,1'-dimethylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6j)**



36.2 mg, 73%, white solid, m.p.: 205.6-206.4 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.06-7.01 (m, 1H), 6.93 (dd, *J* = 8.0 Hz, 2.8 Hz, 1H), 6.81-6.78 (m, 1H), 3.85-3.79 (m, 1H), 3.62-3.56 (m, 1H), 3.23 (s, 3H), 3.00 (s, 3H), 2.73-2.67 (m, 1H), 2.43-2.36 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 175.4, 169.9, 159.4 (d, *J* = 249.9 Hz), 140.5 (d, *J* = 2.0 Hz), 131.2 (d, *J* = 8.2 Hz), 115.2 (d, *J* = 23.3 Hz), 111.2 (d, *J* = 24.9 Hz), 109.0 (d, *J* = 8.1 Hz), 58.1, 47.1, 30.6, 29.4, 26.7; HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>2</sub><sup>+</sup> 249.1034; Found 249.1034; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm) tR = 9.2 min (major), 10.4 min (minor); [α]<sub>D</sub><sup>25</sup> -3.8 (*c* 1.0, CHCl<sub>3</sub>, 95% *ee*).

**Methyl (S)-1,1'-dimethyl-2,2'-dioxospiro[indoline-3,3'-pyrrolidine]-5-carboxylate (6k)**

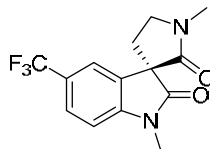


49.1 mg, 85%, white solid, m.p.: 169.6-170.4 °C; (PE/EA=5/1) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.79 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.50 (d, *J* = 1.2 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 3.93 (s, 3H), 3.83-3.78 (m, 1H), 3.62-3.56 (m, 1H), 3.26 (s, 3H), 2.98 (s, 3H), 2.69-2.64 (m, 1H), 2.44-2.36 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 175.4, 169.7, 166.5, 144.9, 134.9, 131.1, 124.9, 122.7, 109.1, 57.9,



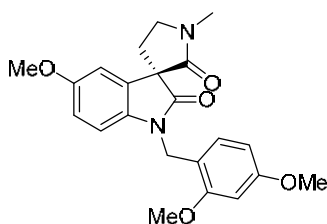
52.4, 47.2, 30.6, 29.4, 26.8; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{15}H_{17}N_2O_4^+$  289.1183; Found 289.1183; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm)  $t_R$  = 18.3 min (major), 23.2 min (minor);  $[a]_D^{25}$  -2.0 (*c* 1.0,  $CHCl_3$ , 98% *ee*).

**(S)-1,1'-dimethyl-5-(trifluoromethyl)spiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6l)**



45.3 mg, 76%, white solid, m.p.: 178.9-179.6 °C; (PE/EA=5/1)  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.60 (d,  $J$  = 7.2 Hz, 1H), 7.40 (s, 1H), 6.94 (d,  $J$  = 8.4 Hz, 1H), 3.85-3.79 (m, 1H), 3.66-3.60 (m, 1H), 3.26 (s, 3H), 3.00 (s, 3H), 2.74-2.67 (m, 1H), 2.47-2.40 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  175.6, 169.5, 147.5, 130.4, 126.8 (q,  $J$  = 4.0 Hz), 125.2 (q,  $J$  = 26.8 Hz), 124.2 (q,  $J$  = 270.0 Hz), 120.0 (q,  $J$  = 3.7 Hz), 108.4, 57.7, 47.1, 30.6, 29.2, 26.8; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{14}H_{14}F_3N_2O_2^+$  299.1002; Found 299.1002; HPLC(OJ-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm)  $t_R$  = 7.7 min (major), 6.5 min (minor);  $[a]_D^{25}$  -13.8 (*c* 1.0,  $CHCl_3$ , 98% *ee*).

**(S)-1-(2,4-dimethoxybenzyl)-5-methoxy-1'-methylspiro[indoline-3,3'-pyrrolidine]-2,2'-dione (6m)**



The reaction mixture of **5m** (1.05 g, 2 mmol), CuI (38 mg, 0.2 mmol), L1 (96 mg, 0.4 mmol), U2 (176mg, 0.2 mmol), NaH (120 mg, 60%, 3 mmol) in MeCN (10 mL) were stirred at room temperature for 8 hours. Then  $H_2O$  (5.0 mL) and ethyl acetate (15.0 mL) were added into the mixture. The organic phase was separated and the aqueous phase was extracted with ethyl acetate (15.0 mL  $\times$  3). The combined organic phase was washed with  $H_2O$  and brine, dried over  $Na_2SO_4$ . The solvent was removed under reduced pressure. The residue was purified by flash chromatography (ethyl acetate/petroleum ether = 1/1) to afford the desired product **6m** as a white solid (673 mg, 85% yield), m.p.: 189.8-190.5 °C; (PE/EA=3/1)  $^1H$  NMR (600 MHz,  $CDCl_3$ ):  $\delta$  7.14 (d,  $J$  = 8.4 Hz, 1H), 6.78 (d,  $J$  = 2.4 Hz, 1H), 6.73-6.68 (m, 2H), 6.46-6.41 (m, 2H), 4.92 (d,  $J$  = 16.2 Hz, 1H), 4.78 (d,  $J$  = 16.2 Hz, 1H), 3.87-3.80 (m, 4H), 3.76 (s, 3H), 3.75 (s, 3H), 3.64-3.59 (m, 1H), 3.00 (s, 3H), 2.76-2.72 (m, 1H), 2.45-2.40 (m, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ ):  $\delta$  175.5, 170.5, 160.1, 157.8, 156.0, 137.2, 131.0, 128.8, 115.6, 113.0, 110.2, 109.9, 104.2, 98.3, 58.2, 55.7, 55.3, 55.2, 47.1, 38.2, 30.4, 29.4; HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calcd for  $C_{22}H_{25}N_2O_5^+$  397.1758; Found 397.1744; HPLC(AS-H, hexane/*i*-PrOH = 70:30, flow rate=1.0 ml/min, I=254 nm)  $t_R$  = 12.3 min (major), 10.7 min (minor);  $[a]_D^{25}$  -24.5 (*c* 1.0,  $CHCl_3$ , 95% *ee*).

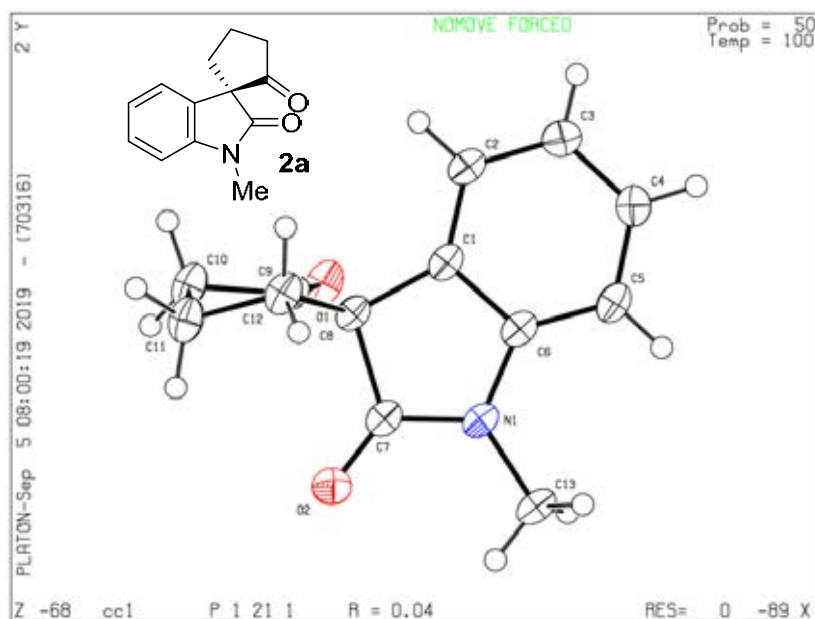
### III. X-ray crystallographic data

Compounds **2a**, **4e** and **6a** were collected at 100 K on a Rigaku Oxford Diffraction Supernova

Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu K $\alpha$  radiation. The data were collected and processed using CrysAlisPro22.

Chiral **2a** was completely dissolved in dichloromethane (0.3 mL) and Hexanes (1.0 mL) was added slowly at room temperature. The solvents diffused slowly, the single crystal was obtained after three days. The single crystals of chiral **4e** and **6a** were prepared in the same conditions of **2a**. The absolute configuration of **2a** was determined as *S* through X-ray experiments (CCDC number: 2044520). The absolute configuration of **4e** was determined as *R* (CCDC number: 2044521). The absolute configuration of **6a** was determined as *S* (CCDC number: 2044522). These details can be obtained free of charge via [www.ccdc.com.ac.uk/data\\_request/cif](http://www.ccdc.com.ac.uk/data_request/cif) from the Cambridge Crystallographic Data Centre.

Thermal Ellipsoid Plot for **2a** (30% probability level)

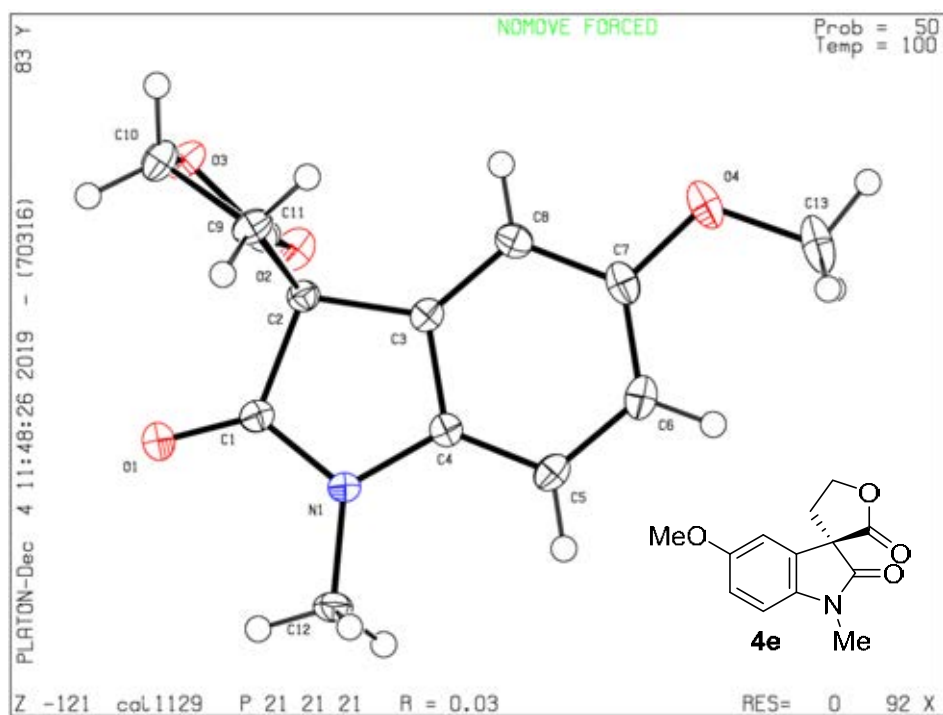


### Crystal Data for **2a**

Identification code	cc1
Empirical formula	C <sub>13</sub> H <sub>13</sub> NO <sub>2</sub>
Formula weight	215.24
Temperature/K	99.9(2)
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	8.8556(3)

b/Å	6.92143(19)
c/Å	9.4280(3)
$\alpha$ /°	90
$\beta$ /°	111.887(4)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	536.22(3)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.333
$\mu/\text{mm}^{-1}$	0.730
F(000)	228.0
Crystal size/mm <sup>3</sup>	0.13 × 0.12 × 0.11
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54184)
2 $\theta$ range for data collection/°	10.112 to 146.702
Index ranges	-10 ≤ h ≤ 9, -8 ≤ k ≤ 8, -11 ≤ l ≤ 11
Reflections collected	7302
Independent reflections	2055 [R <sub>int</sub> = 0.0465, R <sub>sigma</sub> = 0.0261]
Data/restraints/parameters	2055/1/146
Goodness-of-fit on F <sup>2</sup>	1.054
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0399, wR <sub>2</sub> = 0.1079
Final R indexes [all data]	R <sub>1</sub> = 0.0404, wR <sub>2</sub> = 0.1086
Largest diff. peak/hole / e Å <sup>-3</sup>	0.27/-0.24
Flack parameter	0.05(17)

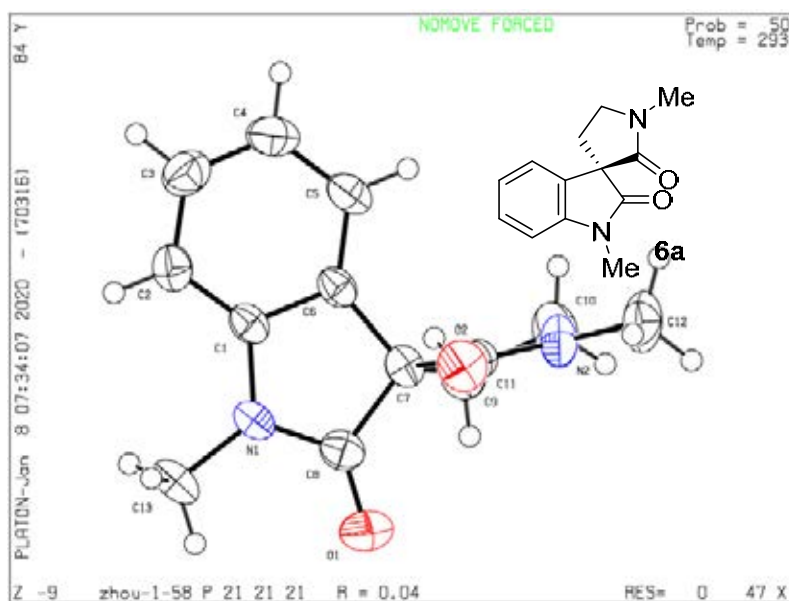
Thermal Ellipsoid Plot for 4e (30% probability level)



### Crystal Data for 4e

Identification code	cai1129
Empirical formula	C <sub>13</sub> H <sub>13</sub> NO <sub>4</sub>
Formula weight	247.24
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	6.94293(12)
b/Å	9.02763(16)
c/Å	18.0531(3)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	1131.54(4)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.451
μ/mm <sup>-1</sup>	0.907
F(000)	520.0
Crystal size/mm <sup>3</sup>	0.12 × 0.11 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	10.958 to 147.094
Index ranges	-5 ≤ h ≤ 8, -11 ≤ k ≤ 11, -22 ≤ l ≤ 21
Reflections collected	4173
Independent reflections	2201 [R <sub>int</sub> = 0.0159, R <sub>sigma</sub> = 0.0198]
Data/restraints/parameters	2201/0/165
Goodness-of-fit on F <sup>2</sup>	1.050
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0311, wR <sub>2</sub> = 0.0822
Final R indexes [all data]	R <sub>1</sub> = 0.0315, wR <sub>2</sub> = 0.0824
Largest diff. peak/hole / e Å <sup>-3</sup>	0.18/-0.24
Flack/Hoof parameter	-0.04(8)/0.01(8)

### Thermal Ellipsoid Plot for 6a (30% probability level)



### Crystal Data for 6a

Identification code	ZHOU-1-58
Empirical formula	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Formula weight	230.26
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	6.9560(2)
b/Å	8.4636(3)
c/Å	19.6496(6)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	1156.83(6)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.322
μ/mm <sup>-1</sup>	0.737
F(000)	488.0
Crystal size/mm <sup>3</sup>	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	9 to 147.322
Index ranges	-8 ≤ h ≤ 8, -10 ≤ k ≤ 10, -24 ≤ l ≤ 23
Reflections collected	10363
Independent reflections	2300 [R <sub>int</sub> = 0.0387, R <sub>sigma</sub> = 0.0214]

Data/restraints/parameters 2300/0/156  
 Goodness-of-fit on  $F^2$  1.055  
 Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0366$ ,  $wR_2 = 0.0984$   
 Final R indexes [all data]  $R_1 = 0.0374$ ,  $wR_2 = 0.0993$   
 Largest diff. peak/hole /  $e \text{ \AA}^{-3}$  0.17/-0.18  
 Flack/Hooft parameter 0.04(11)/0.03(10)

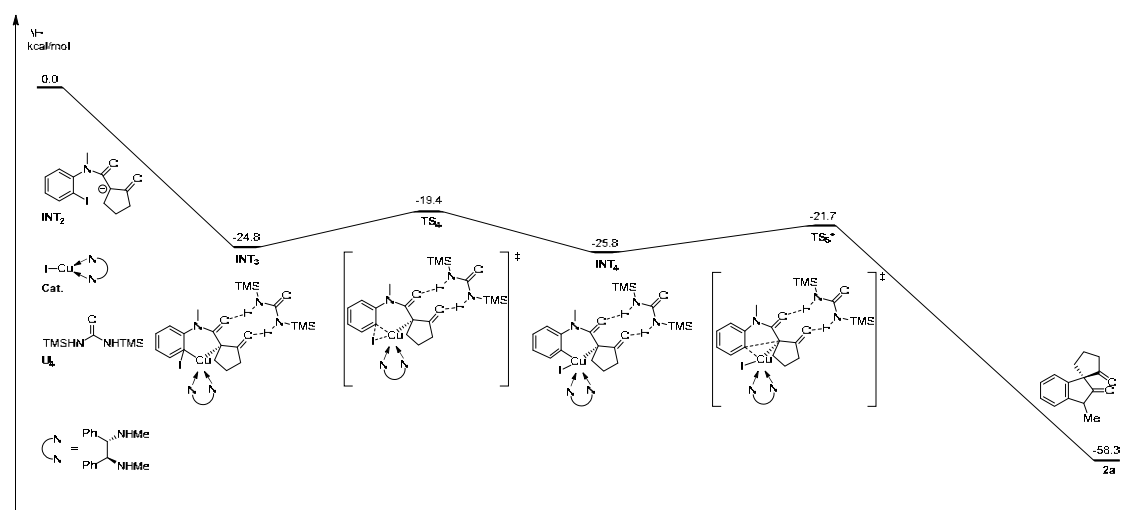
## IV. Computational Results

### 1. Computational methods

All the density functional theory (DFT) computations were performed using B3LYP functional<sup>1,2</sup> with the Gaussian 16 program package.<sup>3</sup> The geometry optimization and frequency calculations were conducted with the SMD solvation model<sup>4</sup> in acetonitrile, B3LYP functional with Grimme's D3(BJ) dispersion,<sup>5-6</sup> and a mixed basis set, in which the basis set 6-31G(d)<sup>7-8</sup> for H, C, N, O, Si and the Lan12dz with effective core potential (ECP)<sup>9</sup> was used for I ( $\xi(d) = 0.289$ ) and Cu ( $\xi(f) = 3.525$ )<sup>10-11</sup>. Single point energies were calculated with larger basis sets, def2-TZVP<sup>12</sup> with ECP<sup>13</sup> was used for Cu, I and 6-311+G\*\*<sup>14-15</sup> was used for H, C, N, O, Si. Some structures shown in figures were generated with the CYLview<sup>16</sup>. Moreover, the reduced density gradient (RDG) of TS4-S-1 and TS4-R-7 were calculated by using Multiwfn program<sup>17</sup> to examine the non-covalent interactions (NCI). The NCI isosurfaces were plotted by using VMD program<sup>18</sup> at 0.40 isovalue. Because it has been reported that the entropy contribution might be wrongly estimated in H-bonded systems and association/dissociation processes<sup>19-20</sup>, our discussion in the following will be primarily based on enthalpy energies.

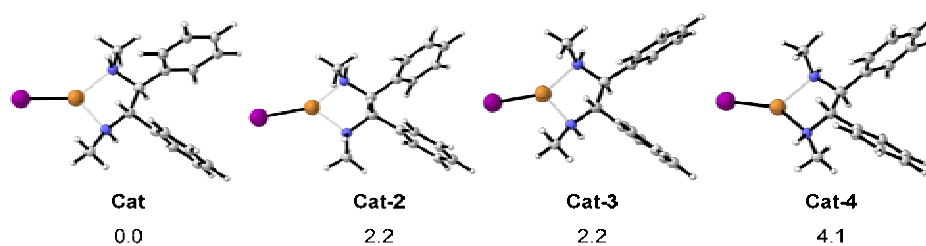
### 2. Computational results

#### 2.1 Reaction energy profile

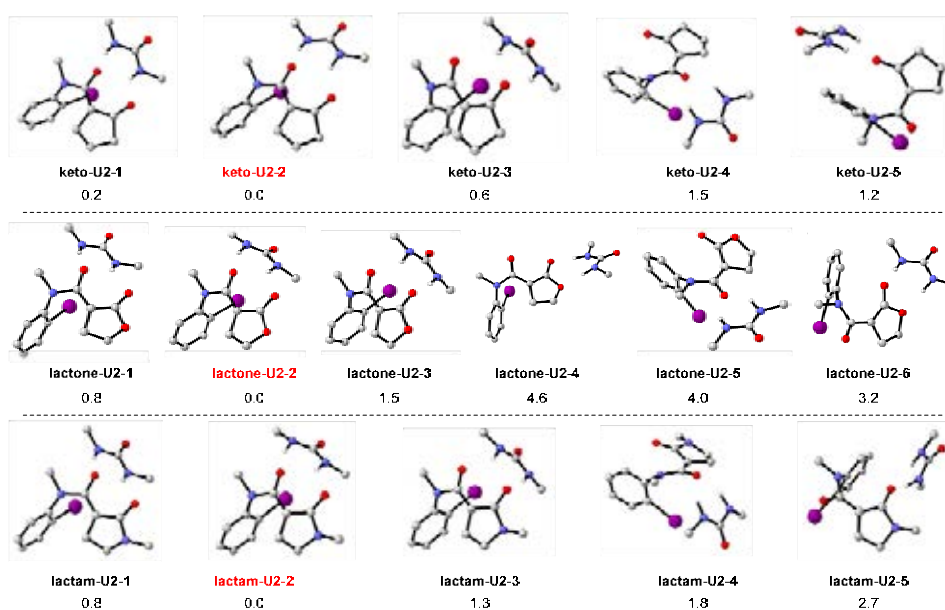


**Figure S1.** Potential energy surface of  $\beta$ -ketoamide. Enthalpies are given in kcal/mol. “\*” represents that the TS5 was optimized in the gas phase.

## 2.2 The binding energy of urea complexes

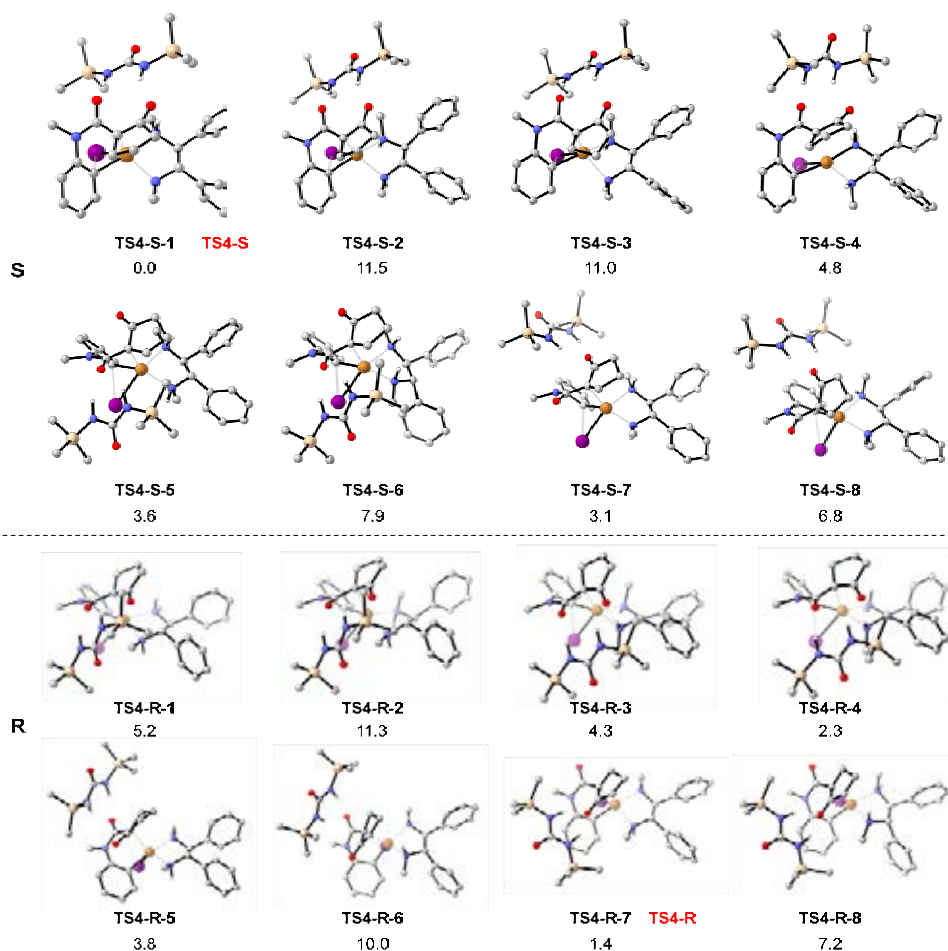


**Figure S2.** Optimized structures of four different coordinative modes of CuI and ligand L1. Enthalpies relative to the Cat are given in kcal/mol.

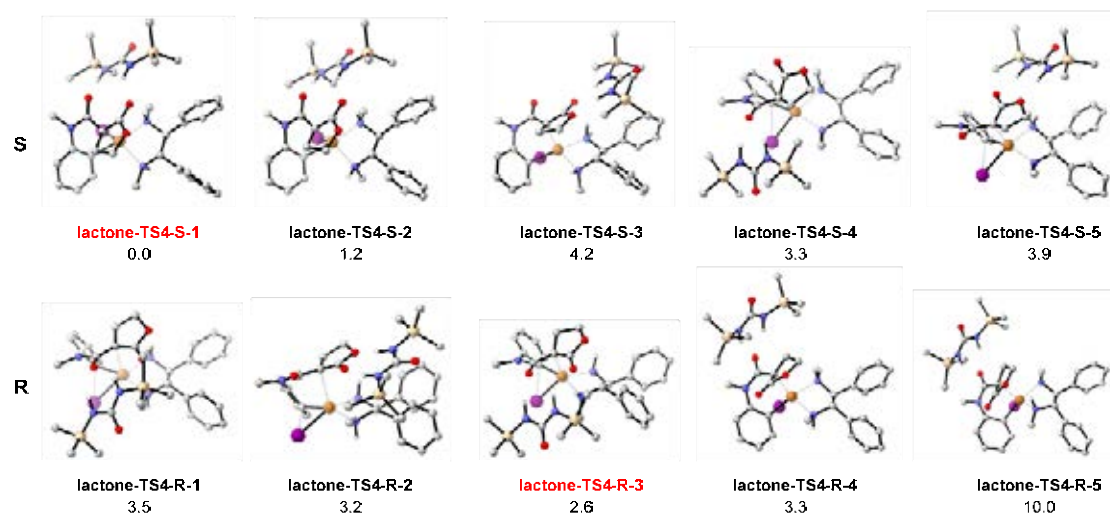


**Figure S3.** Optimized structures of different binding modes of  $\beta$ -ketoamide,  $\beta$ -lactone amide,  $\beta$ -lactam amide and urea U2. Enthalpies are given in kcal/mol. Some H atoms are hidden for simplicity.

## 2.3 Conformation search of TS4 for different substrates

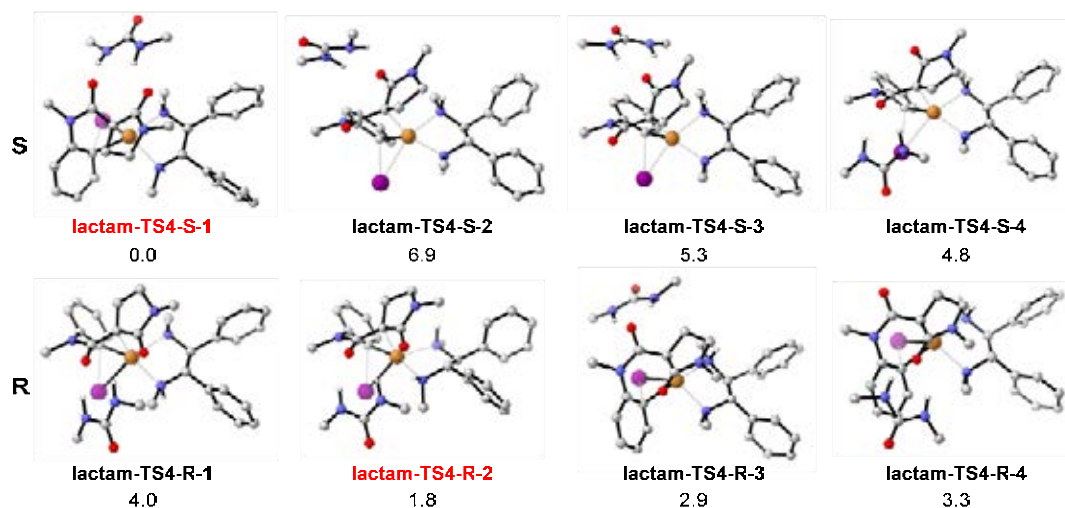


**Figure S4.** Conformation search of transition state TS4 of  $\beta$ -ketoamide. Enthalpies relative to TS4-S-1 are given in kcal/mol. Some H atoms are hidden for simplicity.



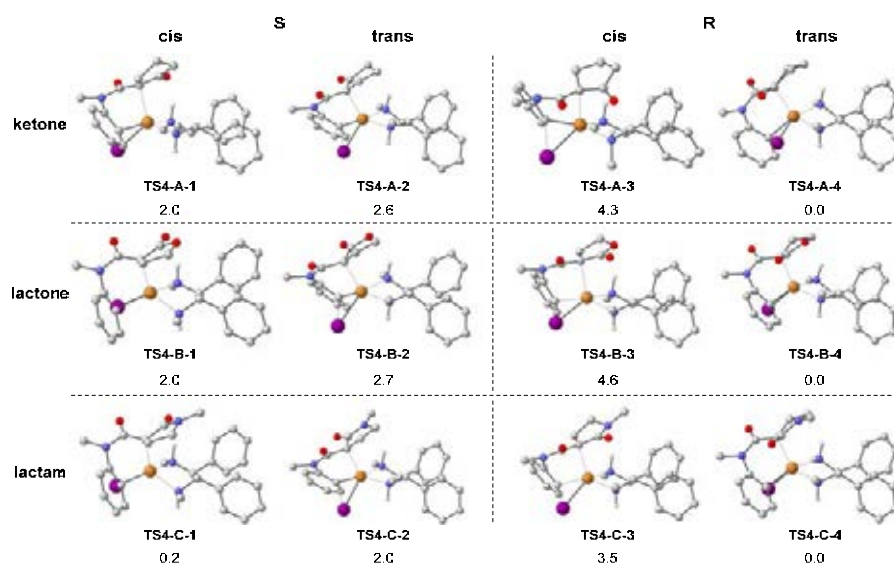
**Figure S5.** Conformation search of transition state TS4 of  $\beta$ -lactone amide. Enthalpies relative to lactone-TS4-S-1 are given in kcal/mol. Some H atoms are hidden for simplicity.





**Figure S6.** Conformation search of transition state TS4 of  $\beta$ -lactam amide. Enthalpies relative to lactam-TS4-S-1 are given in kcal/mol. Some H atoms are hidden for simplicity.

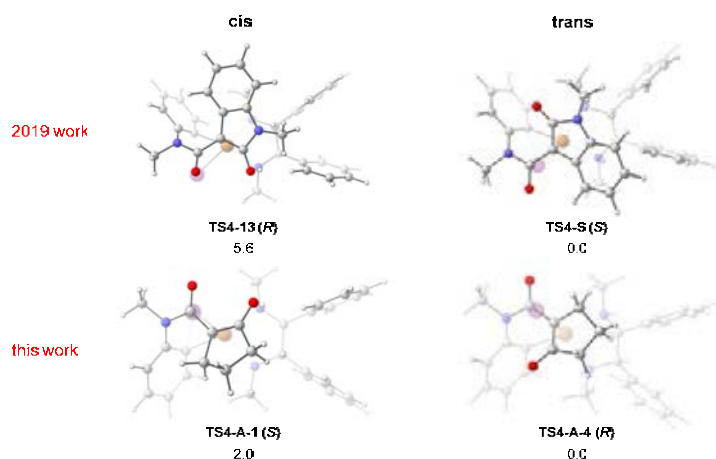
#### 2.4 The model without urea



**Figure S7.** Transition state TS4 without ureas in this work. Enthalpies relative to TS4-A-4, TS4-B-4, and TS4-C-4 are given in kcal/mol. Some H atoms are hidden for simplicity.

We used the previous model of TS4 (Figure S7).<sup>21</sup> It reveals that TS4-A-4, *R*-trans conformation, was favored by 2.0 kcal/mol compared to *S*-cis conformation TS4-A-1. A similar tendency was also observed in lactone and lactam substrates. This result is not consistent with the experimental observation that *S*-product was the major product.

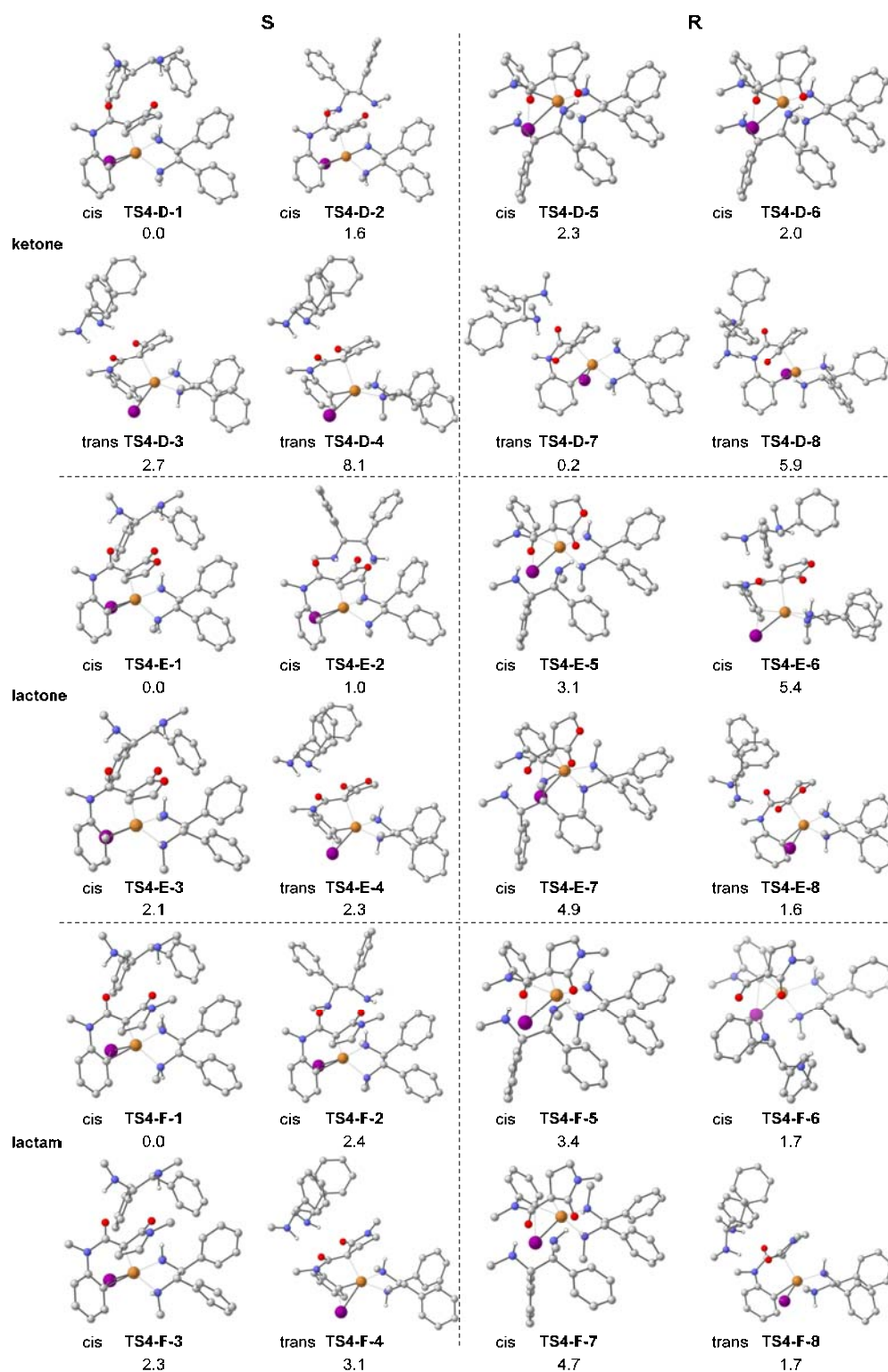
#### 2.5 Comparison with the previous work.



**Figure S8.** Comparison between cis and trans conformations of **TS4** in previous work and in this work. Enthalpies are given in kcal/mol.

It should be noted that *S*-product was experimentally observed as the major product in this work and previous work. However, the ligand used in this work was (*S,S*) conformer and in previous work was (*R,R*) conformer. We compared the critical TSs of two substrates. The barrier for transformation from trans to cis conformer in this work is much lower than that of substrate of previous work (2.0 vs. 5.6, see Figure S8). The difference implies that previous substrates contain an additional phenyl group and show less flexibility. As a consequence, the substrates in this work would be more likely to be locked into a cis conformation by additive, like ureas.

## 2.5 Background reaction



**Figure S9.** Conformation search of transition state TS4 that forms hydrogen bond with ligand in this work. Enthalpies are given in kcal/mol. Some H atoms are hidden for simplicity.

Given the fact that the result of model without urea (Figure S7) is not consistent with the experimental observation that *S*-product was the major product. We investigated the possible background reaction. Considering the ligand is excessive and can serve as a hydrogen bond donor,

we explored the model that ligand stabilizes the cis conformation (Figure S9). In ketone substrate, the **TS4-D-1** and **TS4-D-7** were the lowest enthalpic conformers leading to *S* and *R* products, respectively. **TS4-D-1** was preferred with a difference of 0.2 kcal/mol. In lactone and lactam substrates, *S*-cis conformation was also preferred, and the enthalpy difference was 1.6 kcal/mol and 1.7 kcal/mol, respectively. This distinction of enthalpy is consistent with the experimental observations that lactone and lactam substrates showed higher enantioselectivity than ketone substrates in the background reaction. Further, with the addition of ureas, the enthalpy difference was 1.4 kcal/mol in ketone substrates (Figure S4), 2.6 kcal/mol in lactone substrates (Figure S5) and 1.8 kcal/mol in lactam substrates (Figure S6). The calculations are generally in line with experimental observations, that the addition of ureas can largely improve the enantioselectivity of ketone substrates, but is not beneficial to lactone or lactam substrates. On this basis, we believe that ureas could stabilize two carbonyl groups on the same side and thus improve the enantioselectivity.

**Table S1.** Energies of optimized structures (units of H is Hartree).

	<i>H</i>		<i>H</i>		<i>H</i>
U4	-1042.625684	lactone-TS4-R-1	-4456.594011	TS4-A-4	-3377.996705
U2	-303.879484	lactone-TS4-R-2	-4456.594596	TS4-B-1	-3413.948795
I	-297.986618	lactone-TS4-R-3	-4456.595531	TS4-B-2	-3413.947653
INT2	-1006.322458	lactone-TS4-R-4	-4456.594329	TS4-B-3	-3413.944621
INT3	-4420.653920	lactone-TS4-R-5	-4456.583733	TS4-B-4	-3413.951916
TS4-1	-4420.645308	lactam-TS4-S-1	-3737.259378	TS4-C-1	-3433.359296
INT4	-4420.655533	lactam-TS4-S-2	-3737.248372	TS4-C-2	-3433.356467
TS5	-4420.649008	lactam-TS4-S-3	-3737.250925	TS4-C-3	-3433.354068
2a	-708.428805	lactam-TS4-S-4	-3737.251703	TS4-C-4	-3433.359614
Cat	-2669.652874	lactam-TS4-R-1	-3737.253053	TS4-D-1	-4109.146464
Cat-2	-2669.649318	lactam-TS4-R-2	-3737.256547	TS4-D-2	-4109.143907
Cat-3	-2669.649405	lactam-TS4-R-3	-3737.254756	TS4-D-3	-4109.142143
Cat-4	-2669.646331	lactam-TS4-R-4	-3737.254111	TS4-D-4	-4109.133513
TS4-S-1	-4420.645308	keto-U2-1	-1310.220384	TS4-D-5	-4109.142862
TS4-S-2	-4420.626996	keto-U2-2	-1310.220723	TS4-D-6	-4109.143254
TS4-S-3	-4420.627840	keto-U2-3	-1310.219699	TS4-D-7	-4109.146154
TS4-S-4	-4420.637630	keto-U2-4	-1310.218294	TS4-D-8	-4109.136993
TS4-S-5	-4420.639595	keto-U2-5	-1310.218808	TS4-E-1	-4145.101983
TS4-S-6	-4420.632745	lactone-U2-1	-1346.173762	TS4-E-2	-4145.100318
TS4-S-7	-4420.640333	lactone-U2-2	-1346.174963	TS4-E-3	-4145.098688
TS4-S-8	-4420.634480	lactone-U2-3	-1346.172506	TS4-E-4	-4145.098248
TS4-R-1	-4420.637079	lactone-U2-4	-1346.167581	TS4-E-5	-4145.097075
TS4-R-2	-4420.627257	lactone-U2-5	-1346.168664	TS4-E-6	-4145.093344
TS4-R-3	-4420.638423	lactone-U2-6	-1346.169875	TS4-E-7	-4145.094206
TS4-R-4	-4420.641711	lactam-U2-1	-1365.579229	TS4-E-8	-4145.099424
TS4-R-5	-4420.639236	lactam-U2-2	-1365.580428	TS4-F-1	-4164.513607
TS4-R-6	-4420.629440	lactam-U2-3	-1365.578433	TS4-F-2	-4164.509704
TS4-R-7	-4420.643088	lactam-U2-4	-1365.577539	TS4-F-3	-4164.509940
TS4-R-8	-4420.633844	lactam-U2-5	-1365.576186	TS4-F-4	-4164.508597
lactone-TS4-S-1	-4456.599633	TS4-S	-3585.797495	TS4-F-5	-4164.508214
lactone-TS4-S-2	-4456.597781	TS4-13	-3585.788650	TS4-F-6	-4164.510838
lactone-TS4-S-3	-4456.592988	TS4-A-1	-3377.993449	TS4-F-7	-4164.506051
lactone-TS4-S-4	-4456.594337	TS4-A-2	-3377.992499	TS4-F-8	-4164.510865
lactone-TS4-S-5	-4456.593461	TS4-A-3	-3377.989782		

### Cartesian Coordinates

Cat.log			
I	4.377997	0.027011	0.126981
Cu	1.837099	-0.112895	-0.153562
N	0.288945	1.375357	-0.229427
C	-0.925342	0.673153	0.254601
C	-1.012392	-0.707723	-0.451001
N	0.216553	-1.485096	-0.143938
H	0.142379	-1.833861	0.813168
C	0.411873	-2.639668	-1.040275
H	1.297801	-3.188788	-0.711419
H	-0.451456	-3.319385	-1.052377
H	0.586893	-2.272797	-2.055887
C	-2.288781	-1.453753	-0.096562
C	-2.538530	-1.852276	1.225659
C	-3.236819	-1.753459	-1.081835
C	-3.711788	-2.533011	1.553732
H	-1.815366	-1.624681	2.005690
C	-4.414225	-2.433545	-0.756613
H	-3.054052	-1.446511	-2.108830
C	-4.654862	-2.824920	0.562493
H	-3.891883	-2.832713	2.582887
H	-5.140357	-2.657361	-1.533805
H	-5.569224	-3.353903	0.818035
H	-0.997402	-0.526295	-1.531392
C	-2.201235	1.481885	0.080202
C	-2.618621	1.894174	-1.194408
C	-2.982417	1.824927	1.189938
C	-3.794326	2.629240	-1.353897
H	-2.024460	1.635577	-2.068325
C	-4.161209	2.559934	1.034112
H	-2.667217	1.508990	2.181519
C	-4.570575	2.963620	-0.238935
H	-4.106718	2.939040	-2.347827
H	-4.756340	2.817131	1.906577
H	-5.486778	3.534828	-0.363220
H	-0.766371	0.490960	1.323459
H	0.138479	1.648802	-1.201894
C	0.622322	2.580048	0.549697
H	0.866824	2.281208	1.573438
H	1.505534	3.046698	0.105795
H	-0.196898	3.311866	0.579824

I	-4.381926	0.086408	-0.057049
Cu	-1.833914	-0.154747	-0.180408
N	-0.311688	1.370495	-0.145520
C	0.962059	0.652126	-0.440585
C	0.988227	-0.706663	0.310156
N	-0.202776	-1.497944	-0.103567
H	-0.041020	-1.838847	-1.053286
C	-0.459300	-2.661532	0.766006
H	-1.312055	-3.213716	0.363255
H	0.405390	-3.335173	0.841418
H	-0.718016	-2.303744	1.766707
C	2.292436	-1.458740	0.094940
C	2.721967	-1.796829	-1.197551
C	3.078623	-1.843033	1.188045
C	3.914740	-2.495535	-1.390527
H	2.123385	-1.510793	-2.059419
C	4.274072	-2.542308	0.998835
H	2.754138	-1.586576	2.193662
C	4.696307	-2.868985	-0.292020
H	4.235920	-2.746425	-2.398166
H	4.872780	-2.830580	1.859028
H	5.626231	-3.410916	-0.442769
H	0.866507	-0.522286	1.381291
C	2.204621	1.500739	-0.221281
C	2.779073	1.674177	1.047798
C	2.778319	2.167347	-1.312704
C	3.897165	2.493288	1.218135
H	2.355372	1.164181	1.907579
C	3.897835	2.986483	-1.146827
H	2.345845	2.037838	-2.302502
C	4.461106	3.151866	0.121290
H	4.329414	2.614429	2.208074
H	4.331266	3.489969	-2.007152
H	5.333463	3.786347	0.254077
H	0.898425	0.419302	-1.508980
C	-0.411898	2.056608	1.155967
H	-0.323164	1.327445	1.965386
H	0.347563	2.835817	1.297540
H	-1.405543	2.508417	1.216538
H	-0.451172	2.061433	-0.881301

### Cat-3.log

Cat-2.log	I	-4.374726	0.002620	0.179106
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Cu	-1.827443	-0.247461	0.024596	C	-0.987539	-0.697322	-0.330782
N	-0.332273	1.300081	-0.099182	C	-0.957397	0.626160	0.478068
C	0.956365	0.632000	-0.414352	N	0.336659	1.329212	0.235686
C	1.007867	-0.721275	0.344298	C	-2.176244	1.508896	0.253601
N	-0.172009	-1.561773	-0.027400	C	-2.744294	1.698414	-1.015779
C	2.335837	-1.450851	0.215429	C	-2.729555	2.195226	1.343480
C	3.029402	-1.540647	-1.001680	C	-3.838301	2.549281	-1.187394
C	2.876092	-2.086259	1.342288	H	-2.336139	1.176778	-1.876244
C	4.231041	-2.247150	-1.087072	C	-3.824340	3.046643	1.176373
H	2.635652	-1.051474	-1.887227	H	-2.300775	2.054864	2.333503
C	4.078039	-2.793573	1.261110	C	-4.383184	3.225726	-0.091950
H	2.351849	-2.019974	2.293184	H	-4.266389	2.681543	-2.177742
C	4.760037	-2.875503	0.044134	H	-4.242436	3.564451	2.035791
H	4.755732	-2.303059	-2.037341	H	-5.236883	3.884868	-0.225835
H	4.483257	-3.274195	2.147822	H	-0.928077	0.369580	1.540246
H	5.697406	-3.421529	-0.022138	C	-2.305104	-1.451911	-0.237044
H	0.849388	-0.496811	1.404287	C	-3.024590	-1.570020	0.962224
C	2.155299	1.515682	-0.105246	C	-2.804203	-2.088076	-1.382556
C	2.452005	1.884527	1.216235	C	-4.212362	-2.303231	1.011306
C	2.963953	2.005399	-1.138114	H	-2.663066	-1.083401	1.862991
C	3.537059	2.716217	1.496536	C	-3.991903	-2.821783	-1.337714
H	1.833689	1.518864	2.032928	H	-2.258733	-2.000745	-2.319849
C	4.051629	2.838990	-0.861301	C	-4.700844	-2.930826	-0.138329
H	2.742602	1.727289	-2.165683	H	-4.757740	-2.381143	1.948294
C	4.342291	3.195271	0.457676	H	-4.364910	-3.302100	-2.238625
H	3.755736	2.988885	2.525761	H	-5.627358	-3.497653	-0.100043
H	4.669131	3.208904	-1.675749	H	-0.823937	-0.449816	-1.383105
H	5.187959	3.841929	0.676360	H	0.499461	1.953871	1.023518
H	0.938356	0.433789	-1.489655	C	0.449350	2.116158	-1.006869
H	-0.260561	1.698172	0.838861	H	1.456884	2.539056	-1.041518
C	-0.677853	2.382715	-1.035496	H	0.329292	1.459113	-1.872125
H	-0.842165	1.952567	-2.028018	H	-0.285701	2.927857	-1.076273
H	-1.610023	2.845570	-0.700864	C	0.138160	-2.251847	1.321209
H	0.102957	3.153027	-1.107649	H	-0.716600	-2.935227	1.395270
H	-0.254443	-2.292681	0.678498	H	1.064462	-2.822087	1.427485
C	-0.134084	-2.210097	-1.353704	H	0.086647	-1.532117	2.141779
H	-1.054208	-2.788972	-1.466713	H	0.307697	-2.231336	-0.707849
H	-0.114160	-1.448092	-2.136732				
H	0.728243	-2.875501	-1.484184				
				<b>U2.log</b>			
				N	-1.159573	-0.643236	0.000027
				H	-1.124265	-1.653082	0.000013
				C	0.000000	0.087741	0.000053
				O	-0.000000	1.326669	0.000115
				N	1.159573	-0.643236	-0.000279
<b>Cat-4.log</b>							
I	4.386308	0.043623	-0.075846				
Cu	1.841472	-0.218849	0.088414				
N	0.197825	-1.536450	0.029904				





H	-4.277819	-1.905077	2.566167	C	-2.965900	-2.645943	1.186749
H	-3.867823	-2.973238	1.213179	H	-1.960858	-3.050112	1.343898
<b>keto-U2-2.log</b>				H	-3.541323	-2.781617	2.116771
C	0.119881	0.851671	1.289750	H	-3.458903	-3.229184	0.403221
C	2.256628	-0.388298	0.920080	<b>keto-U2-3.log</b>			
C	4.693155	-0.472276	0.778765	C	0.411262	1.091393	1.519328
O	-1.044369	0.675799	1.735186	C	2.379489	-0.200842	0.634687
N	1.107018	-0.077809	1.702150	C	4.640770	-0.277039	-0.287819
C	2.194252	-0.946203	-0.371307	O	-0.479807	1.039550	2.391408
H	5.661313	-0.289658	1.236507	N	1.529859	0.235555	1.691903
C	0.705270	-1.120119	2.647256	C	1.946278	-0.996392	-0.444015
C	3.360847	-1.226103	-1.092324	H	5.687792	0.003717	-0.216005
H	1.594273	-1.502106	3.157706	C	1.546513	-0.613007	2.883535
H	0.201901	-1.960329	2.146071	C	2.838512	-1.394778	-1.446936
H	0.017589	-0.697310	3.380773	H	2.577202	-0.910326	3.098007
H	3.294141	-1.641433	-2.092400	H	0.940501	-1.521348	2.750054
C	0.498967	1.950818	0.459635	H	1.143913	-0.055440	3.730058
C	3.527023	-0.176884	1.480144	H	2.485216	-1.994871	-2.279048
H	3.574284	0.246386	2.479464	C	0.391228	1.998251	0.396675
I	0.328406	-1.430752	-1.265928	C	3.743214	0.131372	0.695190
C	1.658419	3.918949	-0.292889	H	4.077756	0.738858	1.531378
H	2.480018	4.297639	-0.912592	I	-0.070137	-1.645066	-0.591637
H	1.551269	4.594565	0.566223	C	1.055808	3.715810	-1.154048
C	1.905551	2.478546	0.214502	H	1.554378	3.914314	-2.110261
H	2.455991	1.908615	-0.552759	H	1.238438	4.577593	-0.498512
H	2.537725	2.465908	1.111189	C	1.570147	2.428443	-0.467471
C	-0.445983	2.715667	-0.275889	H	1.836360	1.684691	-1.236182
O	-1.687928	2.588889	-0.415628	H	2.488072	2.612019	0.104945
C	4.610020	-0.987372	-0.517481	C	-0.794002	2.602667	-0.064686
H	5.510722	-1.210886	-1.082418	O	-1.998245	2.481741	0.319456
C	0.319263	3.820115	-1.032293	C	4.184392	-1.034692	-1.369578
H	-0.258823	4.751342	-1.058945	H	4.869482	-1.352116	-2.150781
H	0.461723	3.497009	-2.075612	C	-0.454358	3.483611	-1.278110
C	-3.935297	-0.597628	0.255675	H	-1.058727	4.398529	-1.284151
O	-4.983424	-1.178461	-0.075160	H	-0.702372	2.926330	-2.195866
N	-2.853217	-1.261173	0.781744	C	-3.349187	-0.557962	0.021718
H	-2.111311	-0.692266	1.200507	O	-3.573570	-1.757814	-0.214597
N	-3.765769	0.757626	0.119470	N	-3.023803	-0.090238	1.273174
H	-2.828216	1.173781	0.176352	H	-2.475348	0.776036	1.297979
C	-4.726065	1.515636	-0.657995	N	-3.447549	0.419827	-0.944726
H	-4.802443	1.171035	-1.701103	H	-2.997512	1.309469	-0.706649
H	-5.728520	1.455505	-0.218622	C	-3.444173	0.029761	-2.342615
H	-4.402740	2.559210	-0.663021	H	-2.483893	-0.402995	-2.664702

H	-4.224973	-0.713147	-2.528447	C	3.317733	-2.251424	1.333182
H	-3.648271	0.913211	-2.955247	H	2.831428	-2.798411	0.509945
C	-2.754493	-1.053126	2.324981	H	4.384289	-2.490422	1.315652
H	-2.483290	-0.504525	3.228459	H	2.893453	-2.606407	2.277585
H	-3.643863	-1.660735	2.525082	C	4.086472	2.141221	-0.690175
H	-1.928598	-1.735403	2.079070	H	3.406256	2.941679	-0.994902
<b>keto-U2-4.log</b>				H	4.911349	2.588948	-0.114476
C	-2.150171	2.380504	0.338745	H	4.514859	1.683840	-1.587322
C	-0.227455	0.948850	1.256066	<b>keto-U2-5.log</b>			
C	-1.987589	-0.731199	0.805076	C	-0.313010	2.045437	-0.347049
C	-4.301151	-1.462251	0.541210	C	1.342595	1.268912	1.466186
O	0.967121	1.011361	1.675915	C	0.200687	-0.842863	0.792981
N	-0.995506	-0.158333	1.654454	C	-1.714758	-2.147891	0.017951
C	-1.705423	-1.279743	-0.460310	O	2.225189	1.702747	2.232328
H	-5.309188	-1.531709	0.940845	N	0.729102	0.038539	1.778963
C	-0.409478	-1.085712	2.623346	C	0.958485	-1.398319	-0.255334
C	-2.708761	-1.883147	-1.227868	H	-2.760678	-2.419495	0.126934
H	-1.211384	-1.651898	3.106094	C	1.105114	-0.593852	3.043496
H	0.283318	-1.796726	2.149248	C	0.381935	-2.280382	-1.177173
H	0.139936	-0.522314	3.379186	H	0.328423	-1.306525	3.335044
H	-2.473209	-2.294954	-2.203595	H	2.062374	-1.130362	2.966834
C	-0.796796	1.943274	0.413296	H	1.203453	0.171040	3.815482
C	-3.302206	-0.838435	1.283878	H	0.979807	-2.689301	-1.984908
H	-3.518871	-0.400035	2.250846	C	0.941253	1.972413	0.269601
I	0.268914	-1.272312	-1.256623	C	-1.137304	-1.248697	0.909605
C	-0.856380	3.545133	-1.371558	H	-1.719739	-0.822295	1.717055
H	-0.958263	2.899526	-2.253966	I	3.038128	-0.989317	-0.465743
H	-0.507673	4.525500	-1.717814	C	1.287880	3.214477	-1.751423
C	0.109896	2.877541	-0.366075	H	1.656286	2.446415	-2.444009
H	0.930698	2.351351	-0.871425	H	1.548587	4.192613	-2.172874
H	0.585634	3.642284	0.273866	C	1.900638	2.969380	-0.353188
O	-3.172842	1.996043	0.947236	H	2.931145	2.592462	-0.408876
C	-4.007084	-1.976384	-0.724178	H	1.952937	3.914218	0.216031
H	-4.779553	-2.454008	-1.320868	O	-1.423533	1.512221	-0.034118
C	-2.192718	3.594742	-0.618845	C	-0.956021	-2.654798	-1.040010
H	-2.277214	4.509951	-0.012065	H	-1.395164	-3.344561	-1.755538
H	-3.079956	3.555322	-1.262513	C	-0.220653	3.020687	-1.532378
C	3.859970	-0.087012	0.320168	H	-0.716069	3.963393	-1.251529
O	4.890391	-0.510968	-0.225065	H	-0.757378	2.628359	-2.405665
N	3.340772	1.157373	0.065363	C	-4.321948	-0.033801	-0.131255
H	2.514134	1.444413	0.589316	O	-5.200870	-0.908766	-0.131029
N	3.139172	-0.815896	1.241866	N	-3.936961	0.636516	1.014013
H	2.225969	-0.432652	1.495160	H	-3.012412	1.066007	0.970326

N	-3.680980	0.395218	-1.270576	H	-2.417539	1.126547	0.126865
H	-2.791589	0.880613	-1.103241	C	-3.956039	1.461050	-1.277457
C	-3.795091	-0.387129	-2.486577	H	-4.234141	0.883871	-2.166760
H	-3.261897	-1.348535	-2.428978	H	-4.884855	1.850881	-0.833044
H	-4.846867	-0.596505	-2.700212	H	-3.331775	2.304583	-1.578903
H	-3.376366	0.188900	-3.317559	C	-3.467916	-2.242668	1.858520
C	-4.359873	0.118291	2.302581	H	-2.653592	-2.691091	2.435785
H	-4.029851	0.809692	3.083392	H	-4.265906	-1.947909	2.558521
H	-5.450478	0.043935	2.339788	H	-3.880304	-3.003838	1.188516
H	-3.949300	-0.879018	2.524547	O	0.620915	3.885671	-0.588756

**lactone-U2-1.log**

C	0.179087	0.828337	1.360421
C	2.131451	-0.650311	0.877994
C	4.535314	-1.048974	0.711743
O	-1.001198	0.780316	1.807666
N	1.033372	-0.251835	1.692572
C	1.998479	-1.089212	-0.453717
H	5.518056	-1.033970	1.174517
C	0.501198	-1.297262	2.567487
C	3.119215	-1.467260	-1.202365
H	1.333997	-1.826876	3.039366
H	-0.109002	-2.026791	2.014835
H	-0.121448	-0.841779	3.338646
H	3.000227	-1.788574	-2.231812
C	0.696674	1.915994	0.611351
C	3.417527	-0.654775	1.442713
H	3.518362	-0.320856	2.471583
I	0.090365	-1.225161	-1.377329
C	1.982619	3.728138	-0.150906
H	2.642123	4.029520	-0.970587
H	2.156444	4.397428	0.704480
C	2.130639	2.254050	0.258257
H	2.529433	1.661884	-0.580218
H	2.838835	2.144784	1.087008
C	-0.156291	2.882142	0.004055
O	-1.382345	2.972995	-0.117496
C	4.387125	-1.446805	-0.619545
H	5.251073	-1.745508	-1.206672
C	-3.721729	-0.499499	0.161506
O	-4.806888	-0.962286	-0.228374
N	-2.937859	-1.131129	1.097024
H	-2.159822	-0.592757	1.490135
N	-3.185153	0.654788	-0.353667

**lactone-U2-2.log**

C	0.238192	0.973528	1.393356
C	2.058791	-0.648900	0.823547
C	4.422377	-1.162950	0.484506
O	-0.879528	1.038954	1.978506
N	1.051796	-0.145910	1.695251
C	1.791870	-1.183806	-0.451333
H	5.442298	-1.154821	0.858398
C	0.568649	-1.100966	2.692461
C	2.827239	-1.666582	-1.260764
H	1.424088	-1.610010	3.147061
H	-0.092971	-1.859452	2.250029
H	0.013164	-0.566076	3.463420
H	2.605805	-2.061380	-2.246808
C	0.728931	1.978633	0.519060
C	3.388947	-0.666837	1.274954
H	3.593008	-0.260283	2.261516
I	-0.194441	-1.311466	-1.191389
C	2.030030	3.643444	-0.513715
H	2.584363	3.847325	-1.435076
H	2.379153	4.335687	0.266534
C	2.121936	2.183459	-0.041929
H	2.356786	1.519623	-0.888579
H	2.928002	2.059548	0.689082
C	-0.123008	2.988855	-0.013252
O	-1.342933	3.182088	0.035699
C	4.141817	-1.655102	-0.792928
H	4.938597	-2.035210	-1.426180
C	-3.419675	-0.412352	0.194287
O	-4.061217	-1.182679	-0.538174
N	-2.973436	-0.773105	1.449315
H	-2.177076	-0.226977	1.796972
N	-3.139926	0.883116	-0.166263

H	-2.416765	1.401864	0.335270	H	-2.911124	1.323833	-0.612890
C	-3.352601	1.292943	-1.541108	C	-3.317735	0.149022	-2.336387
H	-2.775170	0.686663	-2.256213	H	-2.374021	-0.315634	-2.661523
H	-4.409980	1.214119	-1.816911	H	-4.133649	-0.532315	-2.594861
H	-3.031821	2.332585	-1.630190	H	-3.452549	1.083193	-2.889623
C	-2.994529	-2.178976	1.810472	C	-2.809598	-1.253731	2.268842
H	-2.702440	-2.276265	2.860390	H	-2.651480	-0.783204	3.241957
H	-4.003137	-2.584858	1.689787	H	-3.682684	-1.910502	2.328581
H	-2.311405	-2.791373	1.201122	H	-1.932050	-1.875638	2.040210
O	0.635930	3.896879	-0.762255	O	-0.455554	3.603097	-1.080132

**lactone-U2-3.log**

C	0.313238	1.085613	1.463650
C	2.337188	-0.180305	0.680785
C	4.637677	-0.216004	-0.140940
O	-0.633348	1.005784	2.281654
N	1.431518	0.241853	1.696397
C	1.967454	-0.988677	-0.412121
H	5.674924	0.085527	-0.025037
C	1.387323	-0.623306	2.874955
C	2.910308	-1.374643	-1.372663
H	2.408819	-0.896003	3.156935
H	0.817755	-1.546161	2.689338
H	0.912455	-0.088391	3.698044
H	2.605678	-1.984631	-2.216744
C	0.356397	2.005945	0.370855
C	3.690009	0.178814	0.800020
H	3.975247	0.795780	1.647498
I	-0.029474	-1.673185	-0.640142
C	0.979377	3.692933	-1.147847
H	1.264054	3.832767	-2.195158
H	1.301360	4.575014	-0.575253
C	1.518516	2.396425	-0.522516
H	1.740306	1.653648	-1.304351
H	2.457186	2.582299	0.010303
C	-0.793510	2.708649	-0.060502
O	-1.996882	2.656773	0.257301
C	4.244132	-0.987370	-1.237618
H	4.969189	-1.294501	-1.986180
C	-3.308293	-0.589459	-0.012246
O	-3.550291	-1.765539	-0.331625
N	-3.035496	-0.207680	1.285714
H	-2.418770	0.600850	1.399515
N	-3.338139	0.444188	-0.916170

**lactone-U2-4.log**

C	0.798318	0.282587	1.734888
C	2.846367	0.950655	0.446754
C	4.155318	2.583080	-0.816984
O	0.447209	-0.462988	2.668003
N	2.179576	0.631201	1.662545
C	2.957280	0.068639	-0.645703
H	4.622850	3.562164	-0.872331
C	3.046710	0.130799	2.728520
C	3.620330	0.449399	-1.818272
H	3.956569	0.737451	2.764180
H	3.332642	-0.920265	2.573093
H	2.523921	0.203875	3.683364
H	3.681246	-0.238454	-2.655150
C	-0.090493	0.868969	0.771851
C	3.473822	2.203357	0.336309
H	3.394052	2.882509	1.180524
I	2.157843	-1.900545	-0.559201
C	-1.275633	2.397674	-0.573556
H	-1.392325	2.725595	-1.610532
H	-1.672219	3.176457	0.093198
C	0.160863	2.013243	-0.193542
H	0.726699	1.718247	-1.090759
H	0.689780	2.865592	0.246968
C	-1.399877	0.386086	0.568974
O	-2.050167	-0.573029	1.011363
C	4.218668	1.707262	-1.903942
H	4.735405	1.993240	-2.815849
C	-5.515723	-0.184074	-0.293289
O	-6.715130	-0.387116	-0.534191
N	-4.591216	-1.192937	-0.187535
H	-3.683988	-0.971808	0.240469
N	-4.998254	1.081442	-0.103952

H	-3.986422	1.179052	-0.186321	H	2.797076	-1.015580	0.686421
C	-5.791384	2.238316	-0.477463	C	4.101616	-2.643431	1.161787
H	-5.930668	2.334894	-1.565795	H	4.284829	-3.266812	0.272598
H	-6.781900	2.176718	-0.018095	H	5.000310	-2.680197	1.785178
H	-5.290598	3.140087	-0.112329	H	3.269320	-3.080335	1.721385
C	-5.037535	-2.571179	-0.117698	C	5.118579	1.852714	-0.496998
H	-4.162135	-3.224700	-0.178650	H	4.561463	2.597553	-1.073154
H	-5.578366	-2.802954	0.813261	H	5.528768	2.345435	0.398562
H	-5.704093	-2.799654	-0.955240	H	5.961761	1.501894	-1.099963
O	-2.054290	1.198636	-0.392034	O	-1.448042	3.784538	-0.325576

**lactone-U2-5.log**

C	-1.305435	2.668971	0.518569
C	0.295741	0.669353	0.572721
C	-1.870753	-0.367614	1.195820
C	-4.116615	-0.354004	2.153810
O	1.487958	0.313748	0.337347
N	-0.474788	-0.165491	1.405249
C	-2.416562	-0.899849	0.012159
H	-4.770409	-0.142360	2.995435
C	0.217702	-1.271576	2.069642
C	-3.792966	-1.122165	-0.114447
H	-0.400092	-1.629346	2.898018
H	0.409930	-2.111902	1.386573
H	1.174136	-0.921625	2.462958
H	-4.195466	-1.525552	-1.037662
C	-0.254485	1.846841	0.019885
C	-2.750829	-0.106864	2.257808
H	-2.329848	0.314525	3.163875
I	-1.183496	-1.463622	-1.629939
C	-0.625819	3.595621	-1.493076
H	-1.251557	3.194835	-2.304037
H	-0.240478	4.573128	-1.800083
C	0.458335	2.587362	-1.086150
H	0.755977	1.948213	-1.926636
H	1.370991	3.103217	-0.741390
O	-2.024697	2.615054	1.516436
C	-4.642749	-0.851378	0.958798
H	-5.708777	-1.035797	0.857263
C	4.731197	-0.421709	0.334166
O	5.942715	-0.691179	0.347146
N	4.233278	0.750414	-0.182813
H	3.239168	0.937546	-0.047551
N	3.773365	-1.271463	0.834589

**lactone-U2-6.log**

C	0.933903	-1.197035	0.675144
C	-1.510756	-1.474636	1.397178
C	-1.263118	0.990711	1.081663
C	-0.035553	3.103149	1.114705
O	-2.367294	-2.331740	1.695539
N	-1.718854	-0.140378	1.818141
C	-1.644673	1.275089	-0.243318
H	0.588420	3.810863	1.653244
C	-2.878211	0.110654	2.674797
C	-1.200274	2.432782	-0.893661
H	-2.731377	1.052495	3.211343
H	-3.812309	0.178030	2.097436
H	-2.979639	-0.703812	3.393763
H	-1.497740	2.628357	-1.918501
C	-0.335180	-1.795420	0.643075
C	-0.454163	1.932248	1.738798
H	-0.150600	1.707759	2.755622
I	-2.972654	0.004475	-1.318638
C	1.037020	-2.875524	-0.927643
H	0.812615	-2.439984	-1.911123
H	1.651623	-3.769402	-1.067317
C	-0.244254	-3.101311	-0.113209
H	-1.105767	-3.292582	-0.764901
H	-0.146520	-3.976616	0.550101
O	1.433690	-0.244393	1.300394
C	-0.399364	3.349832	-0.212248
H	-0.068155	4.252289	-0.718647
C	4.670068	0.479685	-0.313933
O	5.728108	1.027276	-0.657970
N	3.486015	1.158699	-0.161116
H	2.732479	0.691177	0.356454
N	4.586638	-0.872749	-0.050461

H	3.654654	-1.283589	-0.059940	H	2.440116	0.923323	-0.227515
C	5.675896	-1.743171	-0.455000	C	3.977597	1.330469	1.151194
H	5.770794	-1.838655	-1.548023	H	4.248889	0.823428	2.084341
H	6.624663	-1.359247	-0.069948	H	4.911998	1.667374	0.675687
H	5.503646	-2.738736	-0.035005	H	3.367944	2.206492	1.382258
C	3.480193	2.608784	-0.175739	C	3.431894	-2.597291	-1.687081
H	2.453389	2.955923	-0.318159	H	2.614524	-3.058731	-2.249619
H	3.868849	3.051597	0.755244	H	4.254897	-2.383144	-2.387337
H	4.095993	2.974369	-1.002013	H	3.802428	-3.322282	-0.954612
O	1.807977	-1.917570	-0.170638	N	-0.572736	3.692995	0.362064
<b>lactam-U2-1.log</b>				C	-0.017726	5.012551	0.559473
C	-0.186206	0.532052	-1.437893	H	1.032270	4.912045	0.844486
C	-2.170920	-0.867477	-0.839461	H	-0.071975	5.631964	-0.354454
C	-4.578395	-1.214744	-0.599163	H	-0.557911	5.538494	1.355993
O	0.987258	0.404243	-1.892843	<b>lactam-U2-2.log</b>			
N	-1.087519	-0.537697	-1.701668	C	0.227083	0.643955	1.493581
C	-2.018574	-1.226436	0.514299	C	2.059026	-0.922404	0.794516
H	-5.570197	-1.211898	-1.042611	C	4.419597	-1.427698	0.409803
C	-0.598379	-1.642283	-2.527043	O	-0.894120	0.636608	2.080495
C	-3.129444	-1.535932	1.308169	N	1.060810	-0.488660	1.710896
H	-1.453156	-2.187248	-2.938584	C	1.789851	-1.340261	-0.523387
H	0.021297	-2.347269	-1.952545	H	5.439050	-1.462830	0.783614
H	0.004902	-1.245082	-3.344626	C	0.585929	-1.520686	2.632138
H	-2.993339	-1.794999	2.352984	C	2.821900	-1.757107	-1.373193
C	-0.658494	1.679726	-0.761750	H	1.444282	-2.066199	3.036445
C	-3.470081	-0.886000	-1.375183	H	-0.081884	-2.241623	2.137850
H	-3.587851	-0.614500	-2.420546	H	0.038158	-1.049867	3.449080
I	-0.093964	-1.352810	1.405782	H	2.597320	-2.060140	-2.390529
C	-1.942274	3.578901	-0.124104	C	0.707529	1.721639	0.714057
H	-2.659775	3.943852	0.620576	C	3.390131	-0.993968	1.240555
H	-2.077050	4.178485	-1.043869	H	3.597693	-0.678363	2.259214
C	-2.085540	2.073469	-0.423552	I	-0.196668	-1.396744	-1.273859
H	-2.480740	1.558204	0.466676	C	2.057530	3.475267	-0.166422
H	-2.802491	1.896146	-1.232220	H	2.698256	3.745058	-1.014542
C	0.222273	2.682869	-0.234357	H	2.366713	4.091982	0.698333
O	1.470402	2.753771	-0.203902	C	2.108094	1.974692	0.182683
C	-4.409168	-1.529808	0.751777	H	2.341500	1.394030	-0.724135
H	-5.265167	-1.775656	1.374030	H	2.905675	1.764391	0.902603
C	3.713216	-0.728861	-0.133907	C	-0.142377	2.789056	0.267683
O	4.792333	-1.176459	0.290560	O	-1.370769	2.980526	0.404292
N	2.925662	-1.414276	-1.024844	C	4.136269	-1.800134	-0.907101
H	2.138953	-0.907023	-1.444421	H	4.930048	-2.129046	-1.571980
N	3.189291	0.465733	0.297370	C	-3.426436	-0.611484	0.176963

O	-4.069095	-1.299639	-0.632848	O	-2.338861	1.990687	0.754100
N	-2.984167	-1.103179	1.388781	C	4.406509	-0.236492	-1.386062
H	-2.184178	-0.597691	1.788442	H	5.144689	-0.310479	-2.179833
N	-3.141062	0.712436	-0.046339	C	-3.098701	-1.323588	0.007093
H	-2.419189	1.178175	0.508889	O	-3.155660	-2.459976	-0.492220
C	-3.358302	1.268000	-1.367896	N	-2.810954	-1.105833	1.339390
H	-2.798577	0.730321	-2.148829	H	-2.330289	-0.229030	1.561336
H	-4.419164	1.238473	-1.641359	N	-3.363378	-0.183477	-0.712469
H	-3.017586	2.304843	-1.348202	H	-3.068679	0.699062	-0.280621
C	-3.003733	-2.540037	1.594658	C	-3.365988	-0.244332	-2.161894
H	-2.707783	-2.750957	2.626770	H	-2.375304	-0.480374	-2.580838
H	-4.012575	-2.931669	1.434263	H	-4.067482	-1.008027	-2.510842
H	-2.322819	-3.082276	0.919839	H	-3.683300	0.727508	-2.551762
N	0.650924	3.699423	-0.474512	C	-2.350470	-2.237553	2.125921
C	0.193479	5.057861	-0.657297	H	-2.179613	-1.896836	3.149453
H	-0.889366	5.046761	-0.802517	H	-3.108189	-3.027297	2.134774
H	0.420833	5.698894	0.214115	H	-1.414248	-2.671515	1.746047
H	0.669937	5.504903	-1.538196	N	-1.009437	3.313376	-0.610791
<b>lactam-U2-3.log</b>				C	-2.039467	4.309925	-0.798032
C	0.272430	0.720056	1.642565	H	-3.015616	3.830913	-0.692356
C	2.461301	-0.036824	0.654018	H	-1.971812	5.128604	-0.058367
C	4.714505	0.408718	-0.185302	H	-1.962392	4.751868	-1.798702
O	-0.603193	0.336991	2.456752	<b>lactam-U2-4.log</b>			
N	1.543615	0.080301	1.735959	C	-2.569984	1.520842	0.626996
C	2.183325	-0.713914	-0.550231	C	-0.277584	0.672748	1.442668
H	5.697528	0.845276	-0.032094	C	-1.423012	-1.426447	0.753545
C	1.706545	-0.926260	2.784665	C	-3.350030	-2.883416	0.383378
C	3.141926	-0.797254	-1.567777	O	0.864141	1.041331	1.869136
H	2.772609	-1.057199	2.993711	N	-0.659382	-0.667037	1.685120
H	1.285942	-1.900560	2.493186	C	-1.033439	-1.664871	-0.578644
H	1.196841	-0.593143	3.689413	H	-4.248267	-3.357372	0.769820
H	2.905134	-1.309986	-2.494300	C	0.182461	-1.468711	2.573816
C	0.099976	1.776169	0.702141	C	-1.809816	-2.462939	-1.428929
C	3.748947	0.504403	0.813101	H	-0.416503	-2.274532	3.009239
H	3.965733	1.021614	1.743665	H	1.035178	-1.919181	2.045170
I	0.309511	-1.659573	-0.874849	H	0.568613	-0.836487	3.374694
C	0.382568	3.746713	-0.606040	H	-1.497730	-2.624605	-2.455449
H	0.691239	4.105160	-1.595231	C	-1.138852	1.545985	0.750404
H	0.524881	4.575332	0.112872	C	-2.591069	-2.060402	1.208821
C	1.141015	2.485365	-0.149404	H	-2.896863	-1.868448	2.231564
H	1.448299	1.903369	-1.032754	I	0.788147	-0.895426	-1.367907
H	2.058637	2.748234	0.387099	C	-1.796769	3.323902	-0.679190
C	-1.180408	2.303650	0.366817	H	-1.666381	2.939946	-1.708443







N	-2.081093	3.116259	-0.107939	H	-4.679090	-2.037133	2.696531
H	-2.239678	2.318047	0.514986	H	-4.846611	-2.140072	0.923214
C	0.798403	-1.139518	3.442457	H	-4.565078	-0.566462	1.701450
H	1.277870	-0.564410	4.241653	H	0.501183	-4.351614	-0.134085
H	1.596365	-1.534898	2.800566	C	-0.600752	-1.170726	2.191135
Si	-3.161646	3.428154	-1.480487	C	-3.082141	-4.234842	1.341311
Si	1.480520	4.294799	1.315753	H	-4.064856	-4.212049	1.800412
C	-4.628124	2.270010	-1.253323	I	-0.331118	-2.188170	-2.625788
H	-5.123644	2.427339	-0.287742	Cu	-0.068579	-1.493887	0.108469
H	-5.370904	2.445040	-2.043022	N	0.728476	0.358569	-0.373175
H	-4.320415	1.221488	-1.311661	C	2.173594	0.303764	-0.725111
C	-3.767853	5.212039	-1.479347	C	2.912164	-0.688950	0.204652
H	-4.299101	5.443536	-0.546764	N	2.251632	-2.009211	0.140083
H	-2.925982	5.904924	-1.570264	H	2.341430	-2.380894	-0.806488
H	-4.461782	5.390378	-2.311827	C	2.822142	-2.975895	1.089299
C	-2.264621	3.020443	-3.089870	H	2.279152	-3.920316	1.013236
H	-2.037783	1.947715	-3.145826	H	3.890062	-3.168101	0.915344
H	-2.869463	3.282154	-3.968207	H	2.702757	-2.591712	2.105912
H	-1.318982	3.571240	-3.151053	C	4.399450	-0.728037	-0.123669
C	1.150265	6.095443	1.769379	C	4.844059	-1.207100	-1.364920
H	2.089182	6.630357	1.966482	C	5.345224	-0.282377	0.806771
H	0.626336	6.607005	0.955252	C	6.206088	-1.233761	-1.669200
H	0.529395	6.167109	2.671938	H	4.122787	-1.558642	-2.099553
C	2.568788	4.211072	-0.221915	C	6.709851	-0.305830	0.505048
H	3.505369	4.764877	-0.075279	H	5.008896	0.090959	1.771128
H	2.828016	3.177782	-0.473639	C	7.143779	-0.781256	-0.734813
H	2.039899	4.649751	-1.075078	H	6.535939	-1.605532	-2.635862
C	2.300242	3.413660	2.766586	H	7.431221	0.045827	1.238163
H	3.351677	3.714671	2.857909	H	8.204161	-0.801034	-0.972221
H	1.797357	3.663425	3.710085	H	2.795042	-0.340945	1.236728
H	2.248861	2.327573	2.647330	C	2.811418	1.685430	-0.689181
C	-3.280887	-5.113870	-0.163985	C	2.887815	2.405035	0.513592
H	-3.207186	-6.133540	-0.531433	C	3.321583	2.264051	-1.856368
				C	3.468470	3.673474	0.546874
				H	2.481918	1.980659	1.427531
<b>INT4.log</b>				C	3.902762	3.535512	-1.826342
C	-2.046123	-0.794473	2.002392	H	3.265777	1.714216	-2.792622
C	-2.363121	-3.038845	1.158256	C	3.978816	4.242981	-0.624317
C	-2.508957	-5.456516	0.992524	H	3.513357	4.219955	1.485184
O	-2.478402	0.347616	2.222611	H	4.293365	3.971456	-2.742117
N	-2.888291	-1.804531	1.593505	H	4.427575	5.232418	-0.599885
C	-1.084759	-3.094810	0.589463	H	2.222029	-0.090105	-1.744997
H	-3.074269	-6.372274	1.141258	H	0.627659	0.855042	0.516903
C	-4.334349	-1.629544	1.738754	C	-0.061468	1.135819	-1.354908
C	-0.490706	-4.318052	0.301158				

H	0.117909	0.751745	-2.358258	H	-0.467884	4.219675	3.545780
H	-1.115539	1.018393	-1.113315	H	0.795811	3.488527	2.546018
H	0.202754	2.196958	-1.323267	C	-1.208719	-5.506415	0.484050
C	0.304279	-1.656526	4.423439	H	-0.761391	-6.455393	0.200714
H	0.911705	-2.347816	5.014875				
H	-0.502311	-1.276305	5.061907	<b>2a.log</b>			
C	-0.283376	-2.333359	3.169642	C	-0.308287	1.566642	-0.262491
H	0.464583	-2.996470	2.730908	C	1.525232	0.205857	-0.040999
H	-1.163035	-2.937502	3.398606	C	3.058817	-1.620454	0.094064
C	0.262799	-0.026696	2.676380	O	-0.988319	2.576971	-0.381108
O	0.269694	1.125521	2.250667	N	1.057542	1.526989	-0.092151
N	-1.841068	3.126529	0.908720	C	0.447777	-0.688803	-0.162587
H	-1.630568	2.301364	1.467765	H	4.074817	-1.993102	0.193114
C	-2.715409	2.969566	-0.142461	C	1.904513	2.702365	-0.027613
O	-2.920285	3.888427	-0.957405	C	0.678502	-2.057168	-0.150600
N	-3.338525	1.747442	-0.278725	H	2.458613	2.720457	0.916941
H	-3.174673	1.074504	0.468347	H	1.263282	3.582759	-0.091210
C	1.103723	-0.485589	3.848446	H	2.617530	2.707731	-0.859547
H	1.295578	0.347622	4.529598	H	-0.146948	-2.757933	-0.234852
H	2.070216	-0.828064	3.450530	C	-0.826896	0.118146	-0.265060
Si	-4.199641	1.294891	-1.769167	C	2.838258	-0.234694	0.086225
Si	-0.915287	4.634026	1.121461	H	3.662037	0.466478	0.174265
C	-4.635713	-0.524157	-1.549794	C	-1.712556	-0.115571	1.000380
H	-5.424298	-0.669162	-0.803580	O	-1.384649	0.180075	2.128839
H	-4.997065	-0.938141	-2.500352	C	-2.779500	-1.231699	-0.870204
H	-3.759458	-1.110664	-1.245995	H	-2.332212	-2.232067	-0.868654
C	-5.758251	2.331378	-1.972612	H	-3.698454	-1.277286	-1.461623
H	-6.427670	2.212228	-1.110922	C	-1.778978	-0.201741	-1.435841
H	-5.502564	3.393169	-2.058927	H	-1.241840	-0.559919	-2.317970
H	-6.313614	2.037388	-2.873171	H	-2.306576	0.721765	-1.703549
C	-3.062208	1.500015	-3.257995	C	1.998255	-2.522657	-0.024542
H	-2.303484	0.708724	-3.286981	H	2.192677	-3.591369	-0.016588
H	-3.634718	1.449324	-4.193689	C	-3.020951	-0.759522	0.568921
H	-2.552123	2.468573	-3.222593	H	-3.779379	0.037094	0.596996
C	-2.103041	6.068959	1.407516	H	-3.327717	-1.534099	1.277975
H	-1.556765	7.012516	1.539127				
H	-2.779440	6.180547	0.553404	<b>TS4-R-1.log</b>			
H	-2.712434	5.906200	2.305850	C	1.569716	-1.247274	1.806950
C	0.155585	4.974796	-0.390892	C	1.378568	-3.570933	1.035566
H	0.696774	5.924385	-0.283187	C	0.607135	-5.873396	1.192933
H	0.899446	4.186295	-0.543974	O	2.332366	-0.257848	1.852809
H	-0.471990	5.035521	-1.286504	N	2.146078	-2.494217	1.544730
C	0.150480	4.365424	2.650424	C	0.514925	-3.386939	-0.064413
H	0.785343	5.244329	2.824076	H	0.655095	-6.841875	1.682210

C	3.605665	-2.575091	1.459398	C	0.177044	1.377552	-0.948867
C	-0.295902	-4.428389	-0.525021	H	1.112226	0.969777	-1.335142
H	4.054130	-2.013685	2.281298	H	-0.066329	2.295705	-1.498307
H	3.906979	-3.621961	1.531621	H	0.300696	1.594574	0.110090
H	3.975568	-2.163245	0.513499	H	-0.937801	0.091530	-2.078425
H	-0.919588	-4.279416	-1.398490	C	-0.484465	0.046948	2.468750
C	0.130907	-1.210537	2.091445	C	-1.887763	-1.729644	3.381878
C	1.410831	-4.825947	1.651498	H	-2.191565	-2.147590	4.347069
H	2.051443	-4.961261	2.518585	H	-2.692989	-1.963514	2.675533
I	1.473984	-2.112102	-1.920211	C	-0.554238	-2.336086	2.883670
Cu	-0.384598	-1.495655	-0.139376	H	0.071391	-2.639919	3.736918
N	-0.866963	0.346382	-1.091074	H	-0.741655	-3.241379	2.301536
C	-2.208903	0.750679	-0.615870	O	-0.170232	1.208463	2.156467
C	-3.164710	-0.450344	-0.835065	C	-1.646780	-0.219056	3.429096
N	-2.625422	-1.639189	-0.127431	H	-2.517473	0.396973	3.179973
H	-2.771756	-1.501336	0.871977	H	-1.304964	0.101709	4.424239
C	-3.296396	-2.889038	-0.514565	N	3.617852	1.445187	-0.114042
H	-3.075927	-3.103213	-1.564964	H	3.373355	0.642894	0.469249
H	-2.902077	-3.703921	0.096599	C	3.086715	2.658767	0.274917
H	-4.386531	-2.841200	-0.387015	O	3.269172	3.687090	-0.404241
C	-4.594297	-0.114323	-0.439651	N	2.365855	2.670107	1.446540
C	-4.912138	0.192218	0.891934	H	2.070528	1.753544	1.793247
C	-5.614122	-0.095467	-1.398068	Si	4.574994	1.261941	-1.594115
C	-6.220582	0.513399	1.255326	Si	1.529381	4.099837	2.082709
H	-4.131874	0.186788	1.648910	C	6.006727	2.486831	-1.613451
C	-6.925848	0.227954	-1.038562	H	6.665308	2.332841	-0.748585
H	-5.377381	-0.328701	-2.433400	H	6.613292	2.367402	-2.521172
C	-7.232453	0.533636	0.289541	H	5.632986	3.514591	-1.575316
H	-6.449680	0.751730	2.290769	C	5.261454	-0.493119	-1.539245
H	-7.705782	0.239551	-1.795598	H	5.843816	-0.665108	-0.625184
H	-8.251317	0.785724	0.571520	H	4.467135	-1.246309	-1.584306
H	-3.144401	-0.695326	-1.903694	H	5.929042	-0.663312	-2.394533
C	-2.733911	2.016576	-1.273855	C	3.485705	1.492223	-3.116734
C	-2.829323	2.117741	-2.669281	H	2.955522	2.450452	-3.067427
C	-3.128997	3.105600	-0.488324	H	4.080488	1.479633	-4.039847
C	-3.311112	3.284793	-3.264981	H	2.737429	0.692377	-3.187505
H	-2.524584	1.281727	-3.295162	C	-0.040796	4.458537	1.101480
C	-3.612634	4.275386	-1.080734	H	-0.722903	3.607965	1.199290
H	-3.057991	3.034650	0.593842	H	-0.553503	5.356679	1.471631
C	-3.704803	4.367812	-2.471627	H	0.171620	4.607437	0.035995
H	-3.379475	3.349745	-4.347854	C	1.085179	3.670042	3.863560
H	-3.912693	5.112701	-0.456008	H	0.435525	2.788739	3.884213
H	-4.078384	5.276766	-2.935759	H	1.981650	3.455820	4.459936
H	-2.110209	0.929608	0.458758	H	0.555328	4.502821	4.345115

C	2.686519	5.588234	2.068344	C	-2.852249	3.310376	-0.341801
H	2.948130	5.874860	1.045734	C	-2.820374	3.863917	-3.074758
H	2.214925	6.447057	2.565108	H	-2.220706	1.811311	-3.327778
H	3.618560	5.364804	2.603914	C	-3.178349	4.590718	-0.797220
C	-0.265895	-5.668068	0.122507	H	-2.859859	3.094637	0.723486
H	-0.900816	-6.473571	-0.236130	C	-3.163547	4.870607	-2.165923
<b>TS4-R-2.log</b>							
C	1.367853	-1.331492	1.871485	H	-3.413659	5.866124	-2.523132
C	0.930623	-3.637120	1.149798	H	-2.103753	0.942857	0.358022
C	-0.089620	-5.841408	1.296361	C	0.300207	1.380438	-0.988112
O	2.238546	-0.438470	1.933584	H	1.215796	0.890300	-1.324714
N	1.797619	-2.645668	1.673657	H	0.160952	2.307467	-1.557563
C	0.135492	-3.375391	0.015010	H	0.394348	1.604311	0.072331
H	-0.167498	-6.801745	1.797633	H	-0.864221	0.183765	-2.161347
C	3.239437	-2.903885	1.654918	C	-0.531297	0.230303	2.412718
C	-0.755671	-4.334001	-0.475557	C	-2.229881	-1.324348	3.168993
H	3.721074	-2.349944	2.462543	H	-2.744862	-1.709002	4.055452
H	3.411372	-3.972398	1.798309	H	-2.918671	-1.405479	2.323127
H	3.688774	-2.595979	0.703800	C	-0.940862	-2.107449	2.849289
H	-1.318032	-4.134185	-1.380910	H	-0.432386	-2.406105	3.779814
C	-0.074100	-1.108562	2.061526	H	-1.171859	-3.028025	2.309862
C	0.799505	-4.877968	1.781108	O	-0.043549	1.333277	2.121733
H	1.383334	-5.068370	2.677507	C	-1.766665	0.124460	3.308512
I	1.324484	-2.256485	-1.842135	H	-2.513247	0.883572	3.052057
Cu	-0.532979	-1.401715	-0.126429	H	-1.428067	0.337153	4.333930
N	-0.815037	0.434429	-1.171413	N	3.751205	1.042154	-0.071362
C	-2.145240	0.911290	-0.733182	H	3.404887	0.303225	0.542921
C	-3.194595	-0.146191	-1.176648	C	3.352831	2.327061	0.238443
N	-2.699863	-1.535037	-0.852030	O	3.675588	3.289769	-0.483336
C	-4.573632	0.177895	-0.631242	N	2.602561	2.484895	1.380379
C	-4.781637	0.475431	0.724028	H	2.186135	1.631658	1.761471
C	-5.675959	0.184344	-1.495487	Si	4.749265	0.684084	-1.492160
C	-6.059569	0.767934	1.202336	Si	1.931023	4.038330	1.917297
H	-3.943273	0.474329	1.411772	C	6.313618	1.735264	-1.488543
C	-6.957353	0.478942	-1.021495	H	6.906299	1.551219	-0.582865
H	-5.527869	-0.039210	-2.549379	H	6.945588	1.498638	-2.355080
C	-7.152848	0.771399	0.330407	H	6.063802	2.800127	-1.518862
H	-6.200298	0.995077	2.255900	C	5.233657	-1.130687	-1.330236
H	-7.799534	0.482006	-1.708561	H	5.750469	-1.320253	-0.380855
H	-8.147689	1.002482	0.701978	H	4.366016	-1.796839	-1.385321
H	-3.255714	-0.084551	-2.269077	H	5.918985	-1.410041	-2.141709
C	-2.509604	2.295813	-1.243509	C	3.764806	0.969953	-3.075020
C	-2.496001	2.586074	-2.615516	H	3.369732	1.992239	-3.098790

H	4.389201	0.825403	-3.966793	N	-1.811799	-2.289569	-0.483030
H	2.917095	0.275910	-3.140675	C	-4.113026	-1.454956	-1.076507
C	0.437438	4.530998	0.876329	C	-5.013856	-1.370103	-0.004344
H	-0.349409	3.778898	0.992317	C	-4.585967	-1.908414	-2.315547
H	0.032035	5.502672	1.189593	C	-6.353391	-1.727530	-0.169870
H	0.689530	4.599861	-0.188669	H	-4.671203	-1.017016	0.963569
C	1.400477	3.766080	3.705385	C	-5.925020	-2.268617	-2.485343
H	0.653324	2.967336	3.758075	H	-3.897562	-1.974894	-3.155624
H	2.253242	3.486839	4.337857	C	-6.813839	-2.178259	-1.410833
H	0.960378	4.681170	4.123828	H	-7.038317	-1.651992	0.670751
C	3.259119	5.375028	1.856688	H	-6.273318	-2.613658	-3.455469
H	3.576574	5.569546	0.828271	H	-7.857359	-2.453514	-1.539433
H	2.882238	6.310451	2.292241	H	-2.257350	-0.885412	-1.927994
H	4.145096	5.073779	2.430879	C	-3.223105	1.277322	-0.150634
C	-0.883476	-5.562463	0.182096	C	-3.658215	1.746155	-1.399270
H	-1.579800	-6.303290	-0.201092	C	-3.622072	1.968633	1.001895
H	-2.437739	-1.956264	-1.741922	C	-4.473966	2.876232	-1.490090
C	-3.660297	-2.457314	-0.221467	H	-3.367464	1.221515	-2.304651
H	-3.161844	-3.419130	-0.082448	C	-4.438320	3.098741	0.915575
H	-3.957125	-2.085694	0.758450	H	-3.292128	1.613034	1.975057
H	-4.566393	-2.609582	-0.822940	C	-4.867856	3.555467	-0.333227
				H	-4.803460	3.224812	-2.465447
				H	-4.737861	3.619108	1.821484
				H	-5.503960	4.433670	-0.405329
				H	-2.397915	-0.283553	1.029440
				C	0.044986	-0.069730	2.782580
				C	-0.738450	-2.140255	3.780439
				H	-0.833707	-2.640786	4.749539
				H	-1.515533	-2.543729	3.125185
				C	0.644045	-2.376547	3.135692
				H	1.422792	-2.468458	3.908726
				H	0.649778	-3.312765	2.574891
				O	0.001252	1.137501	2.460195
				C	-0.875849	-0.618328	3.869384
				H	-1.897274	-0.240039	3.749859
				H	-0.499436	-0.232968	4.828609
				N	2.778625	2.387676	-0.289073
				H	2.761216	1.635119	0.404341
				C	1.890682	3.425950	-0.124521
				O	1.876783	4.391343	-0.914173
				N	1.015638	3.357444	0.933673
				H	0.975584	2.489031	1.474626
				Si	3.888141	2.327596	-1.672794
				Si	-0.182393	4.642015	1.215622
<b>TS4-R-3.log</b>							
C	2.239958	-0.789346	1.776089				
C	2.483705	-3.093660	0.954125				
C	2.311643	-5.506975	1.199155				
O	2.712559	0.362580	1.781211				
N	3.042145	-1.852743	1.341271				
C	1.437382	-3.135150	0.004673				
H	2.664713	-6.426667	1.656477				
C	4.485960	-1.677967	1.192919				
C	0.819189	-4.350217	-0.316058				
H	4.725870	-0.635945	1.397552				
H	5.030545	-2.318977	1.896205				
H	4.799830	-1.924493	0.173922				
H	0.040645	-4.379654	-1.069669				
C	0.891638	-1.126055	2.276224				
C	2.915554	-4.291879	1.531781				
H	3.704561	-4.258548	2.277804				
I	1.769423	-1.736799	-1.934245				
Cu	0.133994	-1.464245	0.191874				
N	-0.866055	0.401151	-0.158383				
C	-2.311789	0.070990	-0.003176				
C	-2.636733	-1.124893	-0.931660				







C	7.421989	-0.199715	2.646474	C	-3.494310	4.588092	0.762878
H	7.763961	-1.537415	0.986109	H	-4.139467	4.316606	1.605834
H	6.777403	1.170580	4.184621	H	-2.487577	4.202799	0.969193
H	8.424976	-0.311852	3.049655	H	-3.433855	5.683386	0.715216
H	2.860844	0.922400	1.690329	C	-5.835562	4.650721	-1.262827
C	4.253408	2.156029	-0.423625	H	-5.744962	5.740795	-1.358670
C	3.861402	3.281039	0.317376	H	-6.226879	4.260562	-2.211045
C	5.421762	2.225540	-1.190655	H	-6.572382	4.438346	-0.479775
C	4.625922	4.448467	0.293973	C	-4.843459	-2.611117	1.313643
H	2.956634	3.245703	0.920254	H	-5.162707	-3.342531	2.067650
C	6.191362	3.392193	-1.214379	H	-5.194869	-2.962036	0.335469
H	5.733526	1.358284	-1.767682	H	-3.747834	-2.583395	1.308911
C	5.795473	4.506881	-0.471339	C	-4.726569	-0.316586	3.356162
H	4.310965	5.311496	0.874813	H	-3.666423	-0.596461	3.384540
H	7.097356	3.428921	-1.813703	H	-4.807028	0.771492	3.460939
H	6.391839	5.415265	-0.488026	H	-5.224562	-0.779338	4.218583
H	3.865464	0.149180	-1.076362	C	-7.364427	-0.825070	1.788743
H	1.598603	1.757578	-0.189298	H	-7.802605	-1.201516	0.855396
C	1.896082	1.566765	-2.189104	H	-7.758638	-1.431815	2.614634
H	2.386881	0.866540	-2.869044	H	-7.703862	0.207388	1.928734
H	0.836051	1.614577	-2.450707	C	0.885531	-4.845394	0.601103
H	2.346617	2.559076	-2.314457	H	1.618811	-5.563417	0.958004
C	-1.008320	1.417439	0.300361				
H	-0.480499	1.864093	-0.547476				
H	-2.022654	1.833324	0.284749	<b>TS4-R-6.log</b>			
C	-0.355782	1.728314	1.661318	C	-1.280294	-0.716766	1.585184
H	0.734243	1.634041	1.596961	C	-1.768530	-0.619080	-0.919457
H	-0.580750	2.740832	2.013280	C	-0.582592	-2.781513	-0.701569
O	-1.572820	-1.658892	2.081374	C	0.125864	-4.883621	0.304980
C	-0.909051	0.628629	2.572012	O	-2.470935	0.070417	-1.700233
H	-0.261246	0.345190	3.408198	N	-1.610460	-1.964132	-1.233249
H	-1.878286	0.925540	2.998190	C	0.761321	-2.363490	-0.692667
C	-5.035946	1.479181	0.309064	H	-0.132832	-5.867319	0.686633
O	-5.755657	2.106745	1.105582	C	-2.377365	-2.472522	-2.375714
N	-4.881894	0.112205	0.393129	C	1.775222	-3.192519	-0.199520
H	-4.276006	-0.302060	-0.308423	H	-2.014512	-2.041260	-3.316218
N	-4.344165	2.104594	-0.705534	H	-3.434894	-2.220497	-2.265768
H	-3.666561	1.512623	-1.193082	H	-2.271682	-3.556860	-2.419267
Si	-5.483298	-0.891908	1.729952	H	2.806599	-2.869094	-0.242454
Si	-4.177866	3.866397	-0.838251	C	-1.174501	-0.059147	0.292255
C	-2.938803	4.083854	-2.242365	C	-0.877392	-4.049452	-0.186852
H	-2.728920	5.145775	-2.423497	H	-1.915361	-4.364643	-0.157109
H	-1.987044	3.590998	-2.004677	I	1.500546	-1.167395	-2.691649
H	-3.314652	3.652953	-3.179200	Cu	1.000977	-0.354893	-0.208491
				N	1.896689	1.653286	-0.212692

C	3.320114	1.360894	0.084256	N	-4.951113	-0.395286	0.118180
C	3.464504	0.527058	1.398777	H	-4.248924	-0.622327	-0.579648
N	2.240408	-0.301284	1.620607	N	-4.670633	1.778612	-0.696188
C	4.729945	-0.309316	1.341918	H	-3.879766	1.361124	-1.193633
C	4.956801	-1.208147	0.287805	Si	-5.461023	-1.638688	1.280379
C	5.689337	-0.204312	2.355009	Si	-4.771383	3.547688	-0.591157
C	6.109594	-1.993440	0.256881	C	-3.520143	4.136704	-1.872149
H	4.226839	-1.294572	-0.512185	H	-3.467516	5.232698	-1.897318
C	6.851115	-0.981812	2.322461	H	-2.515508	3.759598	-1.639994
H	5.526475	0.491871	3.174062	H	-3.783828	3.791389	-2.879994
C	7.062272	-1.881420	1.275353	C	-4.278347	4.136396	1.130408
H	6.265916	-2.689095	-0.563445	H	-4.897284	3.644382	1.889080
H	7.587849	-0.883833	3.115468	H	-3.228446	3.897741	1.342813
H	7.962961	-2.489020	1.249694	H	-4.405730	5.222011	1.234518
H	3.559513	1.224182	2.240543	C	-6.511302	4.127460	-1.014530
C	4.222726	2.583818	0.138317	H	-6.589361	5.221310	-0.959819
C	3.923143	3.661027	0.985542	H	-6.795946	3.819425	-2.028694
C	5.379129	2.642768	-0.647989	H	-7.236959	3.698339	-0.314245
C	4.760800	4.776136	1.039887	C	-4.541327	-3.177614	0.710365
H	3.028283	3.628850	1.603652	H	-4.805186	-4.045563	1.328821
C	6.224889	3.754366	-0.590256	H	-4.759588	-3.431323	-0.334482
H	5.619458	1.810987	-1.306063	H	-3.464963	-3.000040	0.816401
C	5.916230	4.825018	0.252315	C	-4.889376	-1.172143	3.013400
H	4.513804	5.605862	1.697138	H	-3.803286	-1.305802	3.086142
H	7.120307	3.784103	-1.205708	H	-5.132345	-0.126876	3.236467
H	6.569588	5.692447	0.295577	H	-5.362484	-1.802361	3.778126
H	3.641862	0.735031	-0.751885	C	-7.330372	-1.856222	1.212927
H	1.487892	2.195263	0.548311	H	-7.657338	-2.164926	0.211617
C	1.722244	2.409159	-1.465314	H	-7.667366	-2.618911	1.927378
H	2.203701	1.861374	-2.279325	H	-7.832039	-0.912839	1.456221
H	0.655668	2.487858	-1.688035	C	1.452755	-4.447375	0.320894
H	2.155351	3.415429	-1.411863	H	2.243882	-5.084675	0.706431
C	-1.362245	1.440816	0.526788	C	2.388487	-1.443718	2.537632
H	-0.832919	2.069411	-0.194550	H	1.392313	-1.862318	2.703466
H	-2.423051	1.704227	0.449621	H	3.014197	-2.214439	2.086827
C	-0.882098	1.671149	1.975197	H	2.826777	-1.153484	3.502882
H	0.194980	1.871136	2.000677	H	1.568536	0.320835	2.068440
H	-1.372844	2.533274	2.439533				
O	-1.492790	-1.910615	1.852434				
C	-1.191246	0.349034	2.689131	<b>TS4-R-7.log</b>			
H	-0.459473	0.061736	3.453538	C	0.916811	-0.202646	1.733281
H	-2.173637	0.378533	3.179657	C	1.097758	-2.609590	0.883017
C	-5.310579	0.933271	0.184439	C	1.708736	-1.306611	-1.138625
O	-6.161048	1.341759	0.994453	C	2.632254	0.403363	-2.610374
				O	1.052345	-3.760276	1.345213

N	1.921204	-2.366068	-0.223227	H	-8.582614	-0.203215	0.180437
C	0.427956	-0.965321	-1.607151	H	-8.697432	0.139638	2.643804
H	3.501309	0.931799	-2.990330	H	-4.051651	-0.402609	-0.902317
C	2.719574	-3.502119	-0.699675	H	-2.884441	-1.139531	1.668192
C	0.249658	0.015348	-2.590703	C	-3.631337	-2.627661	0.507977
H	2.091083	-4.241196	-1.213373	H	-3.824224	-2.806413	-0.552355
H	3.208662	-3.990270	0.144218	H	-2.918342	-3.376582	0.860691
H	3.479717	-3.141200	-1.393633	H	-4.570960	-2.727850	1.064559
H	-0.740420	0.206723	-2.989812	C	-0.498292	-1.866482	2.724450
C	0.353542	-1.505247	1.508049	H	-1.365090	-2.491201	2.482544
C	2.800082	-0.589949	-1.648338	H	0.100369	-2.440322	3.447602
H	3.786668	-0.806275	-1.254305	C	-0.892440	-0.499829	3.325844
I	-1.044867	-2.940679	-2.092041	H	-1.784563	-0.103689	2.828421
Cu	-1.100999	-1.038446	-0.221852	H	-1.113846	-0.557815	4.396408
N	-3.029587	-1.292131	0.670838	O	1.831784	0.375556	1.104283
C	-3.892636	-0.193777	0.161426	C	0.299799	0.403437	2.995292
C	-3.113053	1.139912	0.281399	H	0.057512	1.463581	2.868930
N	-1.834269	1.012051	-0.454817	H	1.074423	0.342868	3.774683
H	-2.043004	1.044496	-1.453589	C	4.896590	1.555847	0.509314
C	-0.872657	2.086830	-0.153433	O	6.038034	1.948986	0.207992
H	0.073024	1.857113	-0.644182	N	4.666454	0.316444	1.063984
H	-1.228681	3.071286	-0.483302	H	3.678610	0.075698	1.175092
H	-0.701628	2.116795	0.923772	N	3.777457	2.335622	0.307562
C	-3.943798	2.329595	-0.172789	H	2.893092	1.910454	0.590490
C	-4.381674	2.427489	-1.502434	Si	5.881535	-0.935476	1.352737
C	-4.283320	3.345706	0.727663	Si	3.789343	3.928144	-0.464273
C	-5.146554	3.517721	-1.919562	C	1.963548	4.386441	-0.579830
H	-4.128937	1.645870	-2.215829	H	1.838025	5.413433	-0.946500
C	-5.050280	4.438548	0.313365	H	1.438084	3.718895	-1.273360
H	-3.949234	3.277184	1.760062	H	1.467335	4.318079	0.396785
C	-5.484258	4.526889	-1.011456	C	4.552976	3.830296	-2.183952
H	-5.481429	3.578786	-2.951764	H	5.531264	3.339433	-2.133775
H	-5.306111	5.219314	1.024880	H	3.916035	3.255543	-2.867287
H	-6.080844	5.375376	-1.335875	H	4.692703	4.830311	-2.615394
H	-2.848912	1.275835	1.335111	C	4.734132	5.166436	0.596204
C	-5.240592	-0.113908	0.860405	H	4.761892	6.157196	0.123621
C	-5.314424	0.077259	2.248472	H	4.270919	5.277655	1.585042
C	-6.428268	-0.216150	0.127390	H	5.767352	4.830992	0.743717
C	-6.551784	0.166490	2.887770	C	6.535716	-1.617797	-0.279143
H	-4.400946	0.160123	2.833561	H	7.350249	-2.335413	-0.113031
C	-7.669189	-0.123755	0.764089	H	5.744469	-2.133806	-0.837743
H	-6.380177	-0.363430	-0.948874	H	6.922972	-0.808948	-0.910637
C	-7.733902	0.067961	2.146275	C	7.296226	-0.256174	2.391673
H	-6.593803	0.316442	3.963446	H	7.783246	0.576173	1.872364

H	6.931574	0.115252	3.357964	H	-3.473821	1.565558	1.827939
H	8.050069	-1.029335	2.590438	C	-5.303867	-0.108727	1.071368
C	4.916222	-2.259372	2.287161	C	-5.554321	-0.173973	2.449835
H	3.969935	-2.483620	1.779626	C	-6.386201	0.003372	0.190867
H	5.485996	-3.194121	2.363829	C	-6.861877	-0.132164	2.936557
H	4.675829	-1.928739	3.305809	H	-4.723208	-0.262521	3.146230
C	1.352568	0.719766	-3.076968	C	-7.696449	0.053820	0.675137
H	1.209257	1.487562	-3.832224	H	-6.199385	0.057440	-0.878999
<b>TS4-R-8.log</b>				C	-7.937441	-0.015710	2.049486
C	1.045206	-0.558200	1.778977	H	-7.041928	-0.188571	4.006983
C	1.113955	-2.705750	0.381155	H	-8.526357	0.143476	-0.021012
C	1.465236	-0.950666	-1.345012	H	-8.955488	0.019091	2.428281
C	2.239159	1.078288	-2.451171	H	-3.924935	-0.271007	-0.547668
O	1.125260	-3.934264	0.563092	H	-2.878901	-1.155464	2.019514
N	1.765295	-2.200970	-0.751327	C	-3.654185	-2.571285	0.775679
C	0.144923	-0.507816	-1.542459	H	-3.873499	-2.669563	-0.290335
H	3.066549	1.686682	-2.803181	H	-2.937005	-3.347037	1.053737
C	2.446268	-3.190099	-1.596503	H	-4.581062	-2.713407	1.343988
C	-0.131373	0.695024	-2.201373	C	-0.216033	-2.455116	2.539428
H	1.722038	-3.839420	-2.104551	H	-1.127560	-2.995374	2.263968
H	3.104280	-3.814740	-0.990271	H	0.452763	-3.194385	3.003843
H	3.040065	-2.668169	-2.347485	C	-0.502316	-1.292669	3.519822
H	-1.156891	0.988752	-2.382179	H	-1.502215	-0.879326	3.347600
C	0.480857	-1.799031	1.349436	H	-0.476132	-1.617977	4.564789
C	2.502067	-0.126178	-1.801883	O	1.872254	0.179175	1.188320
H	3.524532	-0.434651	-1.612684	C	0.565790	-0.236892	3.195976
I	-1.432690	-2.303009	-2.264019	H	0.225936	0.802842	3.280429
Cu	-1.181921	-0.899889	-0.037205	H	1.444262	-0.331375	3.850240
N	-3.043989	-1.252354	1.017797	C	4.994156	1.196413	0.551743
C	-3.881371	-0.126206	0.534741	O	6.139239	1.563422	0.232969
C	-3.183520	1.240763	0.821278	N	4.689129	-0.119114	0.827803
N	-1.697328	1.062857	0.810654	H	3.693164	-0.301302	0.974162
C	-3.658086	2.297687	-0.158980	N	3.942289	2.081269	0.652428
C	-3.599599	2.089873	-1.545713	H	3.050491	1.665862	0.924867
C	-4.148813	3.519320	0.317030	Si	5.801358	-1.490036	0.719327
C	-4.011636	3.084396	-2.433700	Si	4.021751	3.808561	0.278889
H	-3.231780	1.145350	-1.935367	C	2.229819	4.375906	0.440600
C	-4.570037	4.515364	-0.568660	H	2.139197	5.455315	0.263289
H	-4.202085	3.691334	1.389240	H	1.592697	3.862369	-0.290492
C	-4.499325	4.301661	-1.947065	H	1.830271	4.168069	1.441420
H	-3.955168	2.907219	-3.504487	C	4.652294	4.089817	-1.474054
H	-4.951993	5.455852	-0.180437	H	5.576475	3.523989	-1.636174
H	-4.824682	5.074990	-2.637793	H	3.916361	3.764938	-2.219311
				H	4.865055	5.152035	-1.653189

C	5.131626	4.701237	1.513088	C	2.216329	0.389744	-0.979766
H	5.184466	5.776531	1.296924	C	2.952701	-0.726160	-0.199691
H	4.761314	4.581647	2.539367	N	2.225393	-2.010695	-0.343280
H	6.150244	4.297392	1.473505	H	2.292586	-2.319826	-1.315167
C	6.222188	-1.863937	-1.080636	C	2.773116	-3.069382	0.521851
H	6.954101	-2.679147	-1.157346	H	2.160900	-3.966989	0.414516
H	5.329477	-2.162320	-1.643976	H	3.815371	-3.313539	0.278619
H	6.650748	-0.980733	-1.570182	H	2.723879	-2.736300	1.561184
C	7.372631	-1.143894	1.696254	C	4.416491	-0.813239	-0.605929
H	7.883362	-0.261036	1.298039	C	4.777942	-1.175067	-1.912199
H	7.144684	-0.954502	2.753090	C	5.426867	-0.534280	0.321897
H	8.063196	-1.996303	1.648701	C	6.121680	-1.251958	-2.282245
C	4.835654	-2.913018	1.493834	H	4.005686	-1.395612	-2.645896
H	3.828221	-3.000901	1.070784	C	6.773394	-0.607758	-0.045541
H	5.348346	-3.870755	1.336558	H	5.155445	-0.252760	1.336481
H	4.727794	-2.766804	2.576468	C	7.124240	-0.966851	-1.349281
C	0.920488	1.503506	-2.635971	H	6.386593	-1.531956	-3.298553
H	0.702780	2.442688	-3.137053	H	7.545838	-0.386960	0.686564
C	-0.890302	2.273510	0.576410	H	8.170479	-1.025614	-1.637512
H	0.154880	1.999081	0.731855	H	2.900507	-0.475664	0.862088
H	-1.011314	2.613934	-0.452134	C	2.921492	1.725514	-0.795907
H	-1.160336	3.094857	1.254442	C	3.050860	2.282739	0.486162
H	-1.462445	0.756193	1.753293	C	3.457420	2.413670	-1.889796
				C	3.715885	3.495652	0.668581
				H	2.612631	1.775755	1.341609
				C	4.119070	3.632621	-1.710328
				H	3.361684	1.989499	-2.886439
				C	4.254485	4.174003	-0.429825
				H	3.805357	3.914730	1.667133
				H	4.528601	4.155841	-2.570545
				H	4.770123	5.120130	-0.288083
				H	2.226331	0.120295	-2.041801
				H	0.701695	0.883941	0.346635
				C	-0.031396	1.209271	-1.527998
				H	-0.023792	0.709343	-2.500734
				H	-1.056780	1.233664	-1.160484
				H	0.333402	2.235954	-1.653169
				C	1.072250	-1.921220	4.006125
				H	1.901454	-2.607672	4.208865
				H	0.555100	-1.739813	4.956226
				C	0.066675	-2.498958	2.978207
				H	0.558391	-3.215981	2.311311
				H	-0.735109	-3.047434	3.483389
				C	0.351942	-0.137786	2.534483
<b>TS4-S-1.log</b>							
C	-1.864823	-1.142772	1.832405				
C	-1.819598	-3.452023	0.973317				
C	-1.234267	-5.811732	1.088044				
O	-2.509911	-0.075936	1.875773				
N	-2.525593	-2.330254	1.474069				
C	-0.936736	-3.320059	-0.120865				
H	-1.362484	-6.782274	1.558567				
C	-3.985502	-2.382187	1.434812				
C	-0.205163	-4.414430	-0.596628				
H	-4.360831	-3.173025	2.094425				
H	-4.342774	-2.572073	0.417113				
H	-4.369614	-1.419851	1.770807				
H	0.442592	-4.294300	-1.458370				
C	-0.462635	-1.269892	2.225681				
C	-1.955710	-4.713911	1.562480				
H	-2.613032	-4.819481	2.420744				
I	-1.773336	-1.920406	-1.915780				
Cu	0.099227	-1.512928	-0.121032				
N	0.789203	0.440262	-0.577550				

O	0.244217	1.059394	2.160857	N	-2.091865	-2.616319	1.528552
N	-1.465700	3.143436	1.056387	C	-0.335328	-3.405510	0.016940
H	-1.181869	2.255360	1.481695	H	-0.350614	-6.875541	1.720442
C	-2.478465	3.128750	0.125399	C	-3.516810	-2.917745	1.649319
O	-2.717181	4.125490	-0.585885	C	0.544866	-4.391951	-0.429689
N	-3.216779	1.974885	-0.001350	H	-3.708800	-3.594618	2.490702
H	-2.988466	1.197925	0.625459	H	-3.887480	-3.381442	0.729989
C	1.524745	-0.582171	3.412106	H	-4.047772	-1.981994	1.816621
H	1.751109	0.191093	4.154271	H	1.188655	-4.195259	-1.280138
H	2.418455	-0.695009	2.784675	C	-0.171964	-1.208030	2.070986
Si	-4.439142	1.787679	-1.273136	C	-1.213913	-4.904397	1.682366
Si	-0.454270	4.591810	1.267509	H	-1.875402	-5.093830	2.522673
C	-5.241535	0.116350	-0.942454	I	-1.423914	-2.229875	-1.905291
H	-5.725455	0.091498	0.041803	Cu	0.446080	-1.489948	-0.118209
H	-6.010832	-0.093138	-1.697456	C	1.461249	-1.482747	3.880885
H	-4.506551	-0.693836	-0.980942	H	2.400460	-2.000727	4.103401
C	-5.742351	3.144577	-1.170656	H	0.925744	-1.350827	4.829023
H	-6.236147	3.140851	-0.190079	C	0.570397	-2.280157	2.894920
H	-5.284984	4.128148	-1.315612	H	1.177233	-2.943655	2.270282
H	-6.517583	3.002336	-1.935610	H	-0.124952	-2.924928	3.441674
C	-3.598892	1.796775	-2.961579	C	0.405017	0.085373	2.371976
H	-2.932335	0.931519	-3.069334	O	0.012854	1.223764	2.055303
H	-4.331740	1.762711	-3.778587	N	-2.174868	2.914920	1.073126
H	-2.997618	2.705558	-3.081086	H	-1.701466	2.105064	1.484167
C	-1.532317	6.076236	1.705821	C	-3.127758	2.673834	0.108712
H	-0.915130	6.967370	1.883690	O	-3.563755	3.591362	-0.614911
H	-2.235808	6.297699	0.897130	N	-3.583514	1.382884	-0.024850
H	-2.111701	5.885182	2.618590	H	-3.198924	0.684843	0.617501
C	0.521293	4.952132	-0.306018	C	1.665514	-0.114668	3.221833
H	1.139575	5.852805	-0.194801	H	1.773609	0.717986	3.924559
H	1.185765	4.121837	-0.565730	H	2.550477	-0.107454	2.574209
H	-0.171064	5.111520	-1.140287	Si	-4.747786	0.910394	-1.275383
C	0.690987	4.213949	2.715489	Si	-1.444932	4.527708	1.244574
H	1.485980	4.967641	2.784234	C	-5.179448	-0.881805	-0.886976
H	0.134364	4.230504	3.662038	H	-5.695443	-0.966616	0.077528
H	1.144621	3.224114	2.616715	H	-5.846116	-1.290367	-1.657934
C	-0.340485	-5.658670	0.024524	H	-4.285327	-1.512375	-0.850782
H	0.231572	-6.506013	-0.343177	C	-6.306668	1.965409	-1.188168
				H	-6.782353	1.879252	-0.202454
<b>TS4-S-2.log</b>				H	-6.068765	3.020034	-1.357856
C	-1.612804	-1.329968	1.817486	H	-7.039152	1.645904	-1.941632
C	-1.229788	-3.641878	1.079721	C	-3.945534	1.050612	-2.976189
C	-0.336549	-5.900492	1.241960	H	-3.094684	0.362407	-3.063613
O	-2.421736	-0.386692	1.905825	H	-4.655854	0.813311	-3.779252

H	-3.575745	2.069713	-3.139877	H	2.692816	4.409688	1.485299
C	-2.775729	5.795288	1.665947	H	3.942616	4.834036	-2.612809
H	-2.337502	6.792912	1.804596	H	3.636345	5.814580	-0.343561
H	-3.519562	5.852805	0.864767	H	2.704517	0.403502	-2.305912
H	-3.295643	5.527206	2.594957	C	-0.088832	1.384423	-1.109157
C	-0.557902	5.031570	-0.342493	H	0.044356	2.186836	-1.845143
H	-0.102196	6.026110	-0.245116	H	-1.084742	0.951138	-1.228983
H	0.237985	4.324601	-0.597559	H	-0.018924	1.786425	-0.104501
H	-1.270596	5.060239	-1.174240	H	0.691890	-0.127216	-2.187008
C	-0.228555	4.387439	2.677160				
H	0.385406	5.294531	2.750111				
H	-0.758687	4.267312	3.631373	<b>TS4-S-3.log</b>			
H	0.427920	3.521212	2.552401	C	-1.521134	-1.215930	1.903396
C	0.558347	-5.641100	0.202688	C	-1.281816	-3.563205	1.231296
H	1.243513	-6.409559	-0.144431	C	-0.452549	-5.831170	1.529596
N	0.884914	0.289643	-1.277951	O	-2.286693	-0.243156	2.041453
C	2.346987	0.635772	-1.297200	N	-2.076157	-2.476727	1.655818
C	3.124620	-0.282082	-0.317333	C	-0.421024	-3.422493	0.122940
N	2.644836	-1.679326	-0.428757	H	-0.480192	-6.770457	2.074323
H	2.776348	-2.007716	-1.387231	C	-3.497884	-2.713730	1.903574
C	3.345513	-2.595405	0.486756	C	0.424162	-4.464499	-0.264142
H	2.869284	-3.576891	0.440706	H	-3.654088	-3.258894	2.843092
H	4.411063	-2.701811	0.246598	H	-3.927932	-3.292708	1.081796
H	3.253533	-2.212293	1.506183	H	-3.999830	-1.749936	1.965858
C	4.624709	-0.121851	-0.513530	H	1.041233	-4.358982	-1.147447
C	5.247877	-0.580530	-1.683234	C	-0.054550	-1.132205	2.044459
C	5.404975	0.499587	0.468731	C	-1.290741	-4.782086	1.917888
C	6.622011	-0.416851	-1.867756	H	-1.934776	-4.890613	2.785562
H	4.656650	-1.071334	-2.453361	I	-1.459386	-2.334634	-1.831582
C	6.780010	0.669283	0.285959	Cu	0.423518	-1.506094	-0.108891
H	4.929372	0.858924	1.378008	C	2.101218	-1.516856	3.109426
C	7.392337	0.211352	-0.883560	H	2.761526	-1.738619	2.263651
H	7.091445	-0.778279	-2.779093	H	2.590319	-1.894165	4.013452
H	7.371278	1.156328	1.057124	C	0.726795	-2.172346	2.868939
H	8.461822	0.340504	-1.027585	H	0.842770	-3.142530	2.383318
H	2.870624	0.025040	0.697524	H	0.218330	-2.358314	3.828202
C	2.671737	2.094309	-1.020260	C	0.532143	0.168530	2.328081
C	2.498365	2.657812	0.254501	O	0.118584	1.303144	2.034813
C	3.192024	2.895703	-2.044005	N	-2.137177	2.946734	1.097648
C	2.843464	3.988504	0.495084	H	-1.657069	2.145665	1.517571
H	2.061671	2.069386	1.055179	C	-3.103130	2.683855	0.152166
C	3.538068	4.229129	-1.805465	O	-3.544755	3.582735	-0.591036
H	3.335485	2.469802	-3.034225	N	-3.565997	1.391429	0.058876
C	3.367555	4.778679	-0.532921	H	-3.173845	0.712882	0.716956
				C	1.804433	-0.017522	3.160252

H	1.555229	0.304896	4.182131	H	8.460052	0.114533	-0.266911
H	2.618316	0.627225	2.811478	H	2.705252	-0.077644	0.611821
Si	-4.721524	0.887406	-1.187838	C	2.631220	2.084025	-1.078619
Si	-1.397303	4.560265	1.213174	C	2.529521	2.634139	0.208406
C	-5.151771	-0.896892	-0.762502	C	3.071714	2.905483	-2.125008
H	-5.690484	-0.959994	0.191116	C	2.871988	3.967287	0.441186
H	-5.797409	-1.329281	-1.538382	H	2.144329	2.036890	1.026236
H	-4.255591	-1.521248	-0.689259	C	3.412436	4.241592	-1.895746
C	-6.284012	1.939172	-1.134765	H	3.156178	2.492853	-3.127664
H	-6.764365	1.876784	-0.149546	C	3.318379	4.775699	-0.608522
H	-6.048658	2.989832	-1.330537	H	2.777741	4.376151	1.443512
H	-7.011615	1.597751	-1.883366	H	3.753660	4.860609	-2.721455
C	-3.909404	0.993245	-2.886574	H	3.584236	5.813488	-0.425368
H	-3.062195	0.299078	-2.958820	H	2.644257	0.420073	-2.380350
H	-4.617595	0.746257	-3.688619	C	-0.129346	1.366647	-1.149966
H	-3.533520	2.007438	-3.065782	H	-0.017046	2.163094	-1.896460
C	-2.718057	5.846021	1.611095	H	-1.127107	0.930379	-1.241577
H	-3.235940	5.602118	2.547891	H	-0.035416	1.780043	-0.151060
H	-2.272159	6.843234	1.726290	H	0.637577	-0.155761	-2.228396
H	-3.464949	5.891586	0.812042	C	2.922006	-2.316838	-1.914442
C	-0.527285	5.011200	-0.398961	H	3.978163	-2.202828	-2.190673
H	-0.073228	6.009518	-0.341278	H	2.691641	-3.383234	-1.875552
H	0.267067	4.297158	-0.637916	H	2.301193	-1.864914	-2.692884
H	-1.249533	5.009263	-1.222989	H	3.026657	-2.295841	0.121185
C	-0.167442	4.457822	2.637356				
H	0.447758	5.366045	2.680030				
H	-0.689214	4.364451	3.599211	<b>TS4-S-4.log</b>			
H	0.487252	3.588057	2.529087	C	-1.547268	-1.660338	-0.128168
C	0.425287	-5.664045	0.457536	C	-0.364996	-3.770538	0.329133
H	1.083891	-6.471433	0.149308	C	0.565716	-5.490470	1.783722
N	0.842318	0.273440	-1.327397	O	-2.231783	-1.086569	-1.010874
C	2.304981	0.627040	-1.362343	N	-1.493428	-3.062572	-0.158598
C	3.053505	-0.318677	-0.393682	C	0.944078	-3.480079	-0.111938
N	2.600053	-1.724143	-0.606738	H	0.409279	-6.274069	2.519379
C	4.566788	-0.162816	-0.402554	C	-2.408952	-3.767226	-1.057165
C	5.312639	0.033038	-1.575270	C	2.042785	-4.204646	0.367481
C	5.252604	-0.253601	0.818494	H	-2.474850	-4.812234	-0.745462
C	6.705950	0.130578	-1.525862	H	-2.070086	-3.728768	-2.100072
H	4.810710	0.121296	-2.533667	H	-3.398679	-3.310419	-0.995733
C	6.644381	-0.156737	0.871428	H	3.027484	-4.021395	-0.044542
H	4.685498	-0.397286	1.735444	C	-0.910302	-0.996714	0.990233
C	7.376729	0.035249	-0.303729	C	-0.527221	-4.780645	1.286182
H	7.266126	0.285261	-2.444461	H	-1.530579	-4.985424	1.648902
H	7.155032	-0.225030	1.828587	I	1.112494	-3.025408	-2.503729
				Cu	1.309053	-1.448234	-0.444150



N	1.442203	0.514256	-1.211753	O	-5.126763	2.581319	0.049451
C	2.629974	1.182634	-0.621233	N	-3.301879	1.972674	-1.214488
C	2.745019	0.730202	0.854635	H	-2.550249	1.281284	-1.184972
N	2.834717	-0.762470	0.921257	C	-0.658398	0.788192	2.595937
C	3.828904	1.432714	1.655738	H	-1.304612	1.635597	2.852053
C	5.092724	1.728571	1.122926	H	0.376655	1.119986	2.757891
C	3.570839	1.762425	2.993696	Si	-2.751709	3.626335	-1.556872
C	6.070689	2.342631	1.908471	Si	-5.254128	-0.088102	1.610980
H	5.315431	1.484505	0.088801	C	-4.064265	4.558655	-2.535250
C	4.546468	2.375978	3.782835	H	-4.998740	4.613792	-1.965769
H	2.594227	1.539826	3.417810	H	-3.737532	5.583230	-2.757958
C	5.800810	2.668876	3.240775	H	-4.277643	4.059676	-3.489377
H	7.043026	2.567768	1.478028	C	-2.338002	4.531399	0.043845
H	4.325063	2.629240	4.816405	H	-3.235943	4.659345	0.659327
H	6.561400	3.149793	3.850234	H	-1.616712	3.934496	0.614212
H	1.788583	0.959878	1.325108	H	-1.904829	5.522395	-0.143526
C	2.575125	2.698290	-0.756814	C	-1.192824	3.371563	-2.584139
C	1.553965	3.437995	-0.139917	H	-0.721940	4.325999	-2.851058
C	3.532283	3.375584	-1.521982	H	-0.467995	2.789594	-2.007360
C	1.500766	4.825758	-0.281680	H	-1.406780	2.828588	-3.513759
H	0.778546	2.925043	0.421834	C	-7.106152	-0.072668	1.265189
C	3.480884	4.765216	-1.665143	H	-7.679038	-0.382319	2.149437
H	4.325094	2.810724	-2.006699	H	-7.435207	0.934128	0.982717
C	2.464902	5.494948	-1.042698	H	-7.361336	-0.754192	0.443505
H	0.700011	5.382438	0.197975	C	-4.857092	1.029015	3.076031
H	4.231894	5.274529	-2.263618	H	-5.403497	0.725361	3.978585
H	2.421418	6.575381	-1.152996	H	-3.784353	1.006652	3.305798
H	3.496983	0.815325	-1.178375	H	-5.128261	2.065204	2.843513
H	0.583065	0.926973	-0.814453	C	-4.644600	-1.847789	1.913118
C	1.380331	0.633828	-2.675906	H	-5.116499	-2.283993	2.802914
H	2.200512	0.064985	-3.124474	H	-4.874412	-2.500134	1.060693
H	0.435015	0.206799	-3.018702	H	-3.559043	-1.867014	2.065100
H	1.443497	1.676966	-3.010186	C	1.856237	-5.190674	1.337535
C	-0.974063	-0.502382	3.361370	H	2.714128	-5.740301	1.714656
H	-0.408747	-0.604764	4.294272	C	4.143426	-1.347938	0.578037
H	-2.040583	-0.523872	3.616058	H	4.095916	-2.420879	0.766342
C	-0.675973	-1.641185	2.356388	H	4.349872	-1.191073	-0.483881
H	0.359387	-1.997809	2.471244	H	4.965635	-0.927591	1.168254
H	-1.323931	-2.503015	2.538995	H	2.595356	-1.040179	1.873175
C	-0.851381	0.419441	1.120966				
O	-0.888756	1.312518	0.232065	<b>TS4-S-5.log</b>			
N	-4.335553	0.430181	0.193499	C	-0.523031	-1.838165	2.801262
H	-3.605582	-0.187057	-0.178572	C	1.755096	-1.486292	1.685198
C	-4.305580	1.714129	-0.299836	C	0.869204	-3.419464	0.430853

C	-0.212333	-5.495332	-0.256694	C	-4.876604	4.107534	-2.701117
O	2.781966	-0.785723	1.867049	H	-4.248548	2.881161	-4.364055
N	1.902983	-2.750586	1.111454	H	-5.352118	5.111935	-0.850785
C	-0.009283	-2.737136	-0.430677	H	-5.373919	4.844530	-3.326115
H	-0.280248	-6.576965	-0.178662	H	-2.963908	1.494268	0.831986
C	3.220457	-3.392463	1.131624	C	-0.663584	2.220984	-0.181777
C	-0.937745	-3.409571	-1.223727	H	0.387479	2.011532	-0.394527
H	3.266458	-4.179244	1.894823	H	-0.980712	3.101809	-0.754077
H	3.437280	-3.833883	0.155321	H	-0.774742	2.435996	0.882856
H	3.969899	-2.636834	1.358641	H	-1.367896	0.875784	-1.525566
H	-1.548624	-2.853195	-1.926130	C	-1.034722	0.516246	3.237565
C	0.447693	-1.013115	2.098092	H	-1.704332	0.833342	2.431190
C	0.735694	-4.813294	0.508871	H	-1.117581	1.254307	4.042176
H	1.373140	-5.363500	1.193719	C	0.398300	0.390393	2.688098
I	1.149150	-0.931329	-1.864551	H	0.640286	1.167300	1.961955
Cu	-0.672798	-0.894491	0.067814	H	1.131073	0.488959	3.504048
N	-1.456106	1.024071	-0.517764	O	-0.659368	-3.069828	2.803769
C	-2.901082	1.165902	-0.210174	C	4.079298	1.822214	0.073488
C	-3.583801	-0.224131	-0.301989	O	4.582687	2.749729	-0.588619
N	-2.846894	-1.160858	0.576547	N	3.252380	2.074779	1.148737
H	-2.855143	-0.778506	1.521138	H	2.905444	1.254019	1.646220
C	-3.407939	-2.518184	0.639237	N	4.320869	0.504074	-0.230321
H	-3.441278	-2.943173	-0.366310	H	3.854117	-0.184648	0.363672
H	-2.746177	-3.126870	1.259211	C	-1.380176	-0.911153	3.683815
H	-4.422281	-2.532267	1.058686	H	-1.064424	-1.086206	4.722616
C	-5.067746	-0.113166	0.015732	H	-2.443841	-1.173084	3.630630
C	-5.498204	0.236221	1.304379	Si	2.978030	3.725828	1.746872
C	-6.025549	-0.337832	-0.979332	Si	5.331650	-0.007265	-1.594845
C	-6.858957	0.361754	1.588625	C	1.889466	3.551572	3.276551
H	-4.767713	0.412583	2.090640	H	2.293041	2.815335	3.982612
C	-7.388943	-0.209034	-0.699450	H	1.832847	4.515209	3.800224
H	-5.700716	-0.607691	-1.981378	H	0.866313	3.252593	3.022772
C	-7.809207	0.141642	0.585803	C	2.103758	4.762332	0.439197
H	-7.177825	0.633478	2.591581	H	2.665857	4.734296	-0.500591
H	-8.120114	-0.383723	-1.484492	H	1.091034	4.389251	0.243631
H	-8.868675	0.241418	0.806540	H	2.019145	5.809730	0.758147
H	-3.466495	-0.601426	-1.324437	C	4.621985	4.516327	2.221208
C	-3.591116	2.199317	-1.085782	H	4.481167	5.548708	2.567791
C	-3.605913	2.057773	-2.481379	H	5.111212	3.955368	3.028132
C	-4.223257	3.307936	-0.511361	H	5.298692	4.531588	1.360106
C	-4.243485	3.004848	-3.284268	C	5.256183	-1.889740	-1.553161
H	-3.120932	1.201492	-2.945211	H	4.224223	-2.243278	-1.665536
C	-4.864861	4.257004	-1.312268	H	5.849471	-2.318811	-2.371163
H	-4.216856	3.425020	0.569551	H	5.651122	-2.288829	-0.610874

C	7.101119	0.594135	-1.352766	H	4.537612	-1.208601	2.366670
H	7.122591	1.686763	-1.272059	C	7.093893	-1.279984	-0.549842
H	7.538774	0.177848	-0.436241	H	5.474485	-0.554593	-1.777879
H	7.741296	0.299977	-2.195038	C	7.489162	-1.670435	0.731914
C	4.638701	0.649070	-3.219142	H	6.864904	-1.940752	2.781825
H	5.284553	0.378090	-4.064892	H	7.806276	-1.299245	-1.370582
H	3.638030	0.243364	-3.415322	H	8.510659	-1.993688	0.914220
H	4.560835	1.741193	-3.182401	H	3.368856	0.063246	-0.991755
C	-1.060147	-4.799469	-1.118996	C	2.602476	-2.376113	-1.330025
H	-1.790116	-5.323039	-1.729922	C	2.244726	-1.745521	-2.531940
<b>TS4-S-6.log</b>				C	3.107406	-3.680144	-1.374730
C	0.652440	2.191314	2.809337	C	2.382451	-2.410148	-3.750384
C	-1.523914	1.953788	1.465420	H	1.841650	-0.736836	-2.508393
C	-0.240094	3.587083	0.130397	C	3.256736	-4.345458	-2.595653
C	1.277716	5.382573	-0.503043	H	3.390908	-4.175859	-0.449575
O	-2.650695	1.397183	1.530890	C	2.893013	-3.712627	-3.786085
N	-1.435953	3.152226	0.754568	H	2.093280	-1.911612	-4.671931
C	0.583245	2.696666	-0.581541	H	3.655511	-5.356299	-2.613672
H	1.538362	6.436749	-0.468736	H	3.006077	-4.228558	-4.735908
C	-2.694954	3.712646	0.248978	H	2.821851	-2.331403	0.784983
C	1.722469	3.134330	-1.263209	C	0.723755	-0.080760	3.735460
H	-2.525279	4.742307	-0.069237	H	1.425820	-0.700072	3.163562
H	-3.075950	3.136080	-0.602007	H	0.555443	-0.600669	4.684377
H	-3.447076	3.701737	1.039721	C	-0.588048	0.125612	2.944518
H	2.303638	2.429518	-1.847886	H	-0.838008	-0.739842	2.324721
C	-0.366751	1.402802	2.143645	H	-1.432557	0.252877	3.637472
C	0.137530	4.934417	0.164786	O	0.978513	3.375152	2.635078
H	-0.466528	5.626728	0.743884	C	-3.903097	-1.508085	0.234417
I	-0.690030	1.057207	-1.981447	O	-4.298603	-2.579806	-0.263444
Cu	0.797437	0.825782	0.177186	N	-3.387790	-1.457151	1.511346
N	1.062203	-1.268122	0.341524	H	-3.067117	-0.539194	1.825664
C	2.475293	-1.653970	-0.002924	N	-3.968958	-0.324656	-0.464422
C	3.412664	-0.398243	-0.000629	H	-3.588112	0.498552	0.005684
N	2.892089	0.633458	0.919629	C	1.292538	1.333480	3.914337
H	2.788348	0.238328	1.853992	H	0.988357	1.772654	4.874830
C	3.727873	1.838986	1.022249	H	2.386743	1.391948	3.871702
H	3.900001	2.240945	0.021229	Si	-3.402592	-2.879271	2.576576
H	3.182992	2.582880	1.607952	Si	-4.718384	-0.225685	-2.071500
H	4.700403	1.637637	1.489411	C	-2.826879	-2.277361	4.268673
C	4.847869	-0.829697	0.262971	H	-3.361603	-1.372157	4.582380
C	5.252117	-1.227131	1.546196	H	-3.023816	-3.053938	5.019868
C	5.780720	-0.859028	-0.779755	H	-1.752947	-2.062588	4.289841
C	6.564197	-1.640665	1.781307	C	-2.224460	-4.202727	1.933330
				H	-2.434097	-4.426208	0.881376

H	-1.180831	-3.874693	2.011861	I	1.111220	-3.168084	-1.751419
H	-2.327532	-5.133420	2.507162	Cu	1.108703	-1.040663	-0.144343
C	-5.154936	-3.558278	2.714421	N	3.164602	-1.292263	0.439179
H	-5.184303	-4.445612	3.360646	C	3.824646	0.000607	0.754737
H	-5.833659	-2.809195	3.142796	C	3.181867	1.125314	-0.097545
H	-5.535924	-3.835450	1.726352	N	1.717628	1.087510	0.120324
C	-4.698630	1.604042	-2.522763	H	1.551831	1.180912	1.122189
H	-3.677982	1.983207	-2.647333	C	0.965629	2.160901	-0.550421
H	-5.231975	1.764651	-3.469208	H	1.173233	2.136603	-1.621701
H	-5.196696	2.210437	-1.755739	H	-0.097384	1.976673	-0.388904
C	-6.497908	-0.841024	-1.988154	H	1.229974	3.153964	-0.165797
H	-6.527121	-1.871231	-1.618095	C	3.819722	2.470108	0.218004
H	-7.099056	-0.219325	-1.312021	C	3.665235	3.055845	1.483431
H	-6.972462	-0.815277	-2.978106	C	4.582607	3.136196	-0.747379
C	-3.737514	-1.234273	-3.325103	C	4.266034	4.281080	1.776241
H	-4.227295	-1.233088	-4.307950	H	3.072495	2.552896	2.244480
H	-2.723781	-0.833744	-3.452914	C	5.188973	4.361515	-0.456416
H	-3.651332	-2.272811	-2.986314	H	4.707404	2.688312	-1.730308
C	2.085090	4.482306	-1.203886	C	5.032193	4.937061	0.806751
H	2.974317	4.823640	-1.726702	H	4.137945	4.723346	2.760801
C	-0.000813	-2.142015	-0.193032	H	5.780551	4.865170	-1.216528
H	-0.937918	-1.857689	0.290496	H	5.501521	5.890293	1.035262
H	-0.109931	-1.988997	-1.266877	H	3.343145	0.896548	-1.157139
H	0.199662	-3.202958	-0.000000	C	5.334674	-0.045059	0.581840
H	1.005134	-1.347418	1.354754	C	5.903609	-0.336714	-0.667070
				C	6.180378	0.214222	1.666463
				C	7.289848	-0.364961	-0.826547
<b>TS4-S-7.log</b>				H	5.262491	-0.537239	-1.522742
C	-0.926075	-0.061809	1.643704	C	7.569095	0.189322	1.509570
C	-1.402238	-2.424579	0.783942	H	5.747583	0.443298	2.637189
C	-1.629418	-1.109394	-1.304989	C	8.127261	-0.099998	0.262150
C	-2.124725	0.541308	-3.033972	H	7.716483	-0.589768	-1.800578
O	-1.565155	-3.563709	1.251648	H	8.212223	0.395025	2.361230
N	-2.091487	-2.077183	-0.383783	H	9.206635	-0.119589	0.137211
C	-0.268642	-0.921026	-1.595269	H	3.599348	0.212774	1.804908
H	-2.864546	1.117396	-3.581606	C	3.506995	-2.373115	1.381256
C	-3.026273	-3.087255	-0.898118	H	2.972243	-3.276220	1.076464
C	0.167170	-0.085268	-2.622326	H	4.584532	-2.578891	1.399126
H	-3.676303	-2.635432	-1.646989	H	3.186244	-2.090456	2.385824
H	-2.487270	-3.927721	-1.354315	H	3.489613	-1.585487	-0.485408
H	-3.638275	-3.471043	-0.081810	C	0.787019	-0.608688	3.281533
H	1.223953	-0.024892	-2.858658	H	1.738881	-0.393804	2.784815
C	-0.563437	-1.436350	1.462799	H	0.980873	-0.670714	4.357269
C	-2.544259	-0.324574	-2.024134	C	0.188118	-1.907041	2.702568
H	-3.595552	-0.393141	-1.767060				

H	0.947656	-2.663659	2.485389	C	-1.772597	-1.445021	-1.077550
H	-0.512736	-2.362173	3.419506	C	-2.608605	0.334924	-2.523019
O	-1.720303	0.642176	0.977404	O	-1.219546	-4.161281	1.127970
C	-4.930257	1.334181	0.227270	N	-2.032255	-2.586900	-0.287935
O	-6.121931	1.648142	0.059580	C	-0.471221	-1.012046	-1.376669
N	-4.553531	0.161800	0.846459	H	-3.455583	0.861809	-2.951229
H	-3.543204	0.014017	0.900879	C	-2.839849	-3.656510	-0.889683
N	-3.894849	2.135356	-0.202034	C	-0.228688	0.023436	-2.282152
H	-2.961958	1.798878	0.029012	H	-3.554792	-3.223779	-1.589150
C	-0.243113	0.466609	2.909501	H	-2.206426	-4.375002	-1.425286
H	-1.028688	0.547414	3.675636	H	-3.383250	-4.189741	-0.108232
H	0.161855	1.475824	2.768025	H	0.789552	0.267408	-2.566094
Si	-5.632735	-0.939963	1.715492	C	-0.513915	-1.951797	1.578281
Si	-4.070545	3.666864	-1.068640	C	-2.833957	-0.726777	-1.649920
C	-4.472875	-2.019070	2.737864	H	-3.848100	-1.001419	-1.383692
H	-3.846191	-1.398270	3.392070	I	1.156754	-2.987408	-1.919093
H	-5.049342	-2.697623	3.380617	Cu	0.976150	-1.133550	0.049706
H	-3.803710	-2.632407	2.124503	N	3.101734	-1.327488	0.556131
C	-6.638447	-1.978618	0.506560	C	3.702976	0.011021	0.804058
H	-7.266178	-1.340092	-0.127120	C	3.025929	1.008431	-0.166882
H	-5.982768	-2.564331	-0.149785	N	1.555114	1.006154	0.073232
H	-7.297814	-2.678975	1.036437	C	3.622157	2.406364	-0.177279
C	-6.777149	0.032251	2.852704	C	4.055012	3.053560	0.989597
H	-7.468912	-0.635085	3.383497	C	3.681455	3.101332	-1.393241
H	-6.201945	0.586933	3.605429	C	4.540608	4.362143	0.937978
H	-7.364661	0.754970	2.277199	H	4.016137	2.535960	1.943085
C	-5.057385	3.423788	-2.654081	C	4.164790	4.410472	-1.448554
H	-6.045007	3.008841	-2.423430	H	3.347236	2.608570	-2.304048
H	-5.200310	4.375446	-3.182781	C	4.597143	5.044777	-0.280654
H	-4.550617	2.731252	-3.337554	H	4.875065	4.848074	1.850867
C	-2.287562	4.158260	-1.441803	H	4.207663	4.931442	-2.401501
H	-1.707910	4.280538	-0.517694	H	4.976943	6.062298	-0.319647
H	-1.789976	3.394237	-2.052242	H	3.135711	0.593416	-1.175216
H	-2.243403	5.107972	-1.990196	C	5.217309	0.003331	0.661542
C	-4.911748	4.954035	0.020999	C	5.819926	-0.280393	-0.573162
H	-5.031005	5.909418	-0.507015	C	6.034726	0.253939	1.769984
H	-5.906854	4.606985	0.323260	C	7.210065	-0.302076	-0.696713
H	-4.329453	5.143209	0.931973	H	5.202468	-0.484576	-1.444995
C	-0.767997	0.667674	-3.338978	C	7.427057	0.234606	1.649821
H	-0.432143	1.328972	-4.132684	H	5.575965	0.469139	2.732100
				C	8.018485	-0.042181	0.414846
<b>TS4-S-8.log</b>				H	7.662648	-0.520098	-1.660569
C	-1.098584	-0.698644	1.986673	H	8.046894	0.433868	2.520126
C	-1.244106	-2.965343	0.802376	H	9.100816	-0.057750	0.317922

H	3.449100	0.272955	1.834975	H	-1.114335	1.533886	-3.535219
C	0.708495	-1.209461	3.515846	H	1.111415	1.423773	-0.743351
H	1.566231	-0.734463	3.024324	C	1.089673	1.752471	1.253722
H	0.978787	-1.403672	4.559042	H	1.353960	2.814911	1.210748
C	0.313410	-2.483041	2.746370	H	0.005137	1.655289	1.299204
H	1.169862	-3.082791	2.432326	H	1.520265	1.320906	2.157614
H	-0.308726	-3.132309	3.381869	H	3.396733	-1.619374	-0.379129
O	-1.976228	-0.014364	1.416442	C	3.565842	-2.367248	1.490590
C	-4.594065	1.819332	0.334699	H	3.086412	-3.311193	1.220039
O	-5.587633	2.460399	-0.055183	H	4.654648	-2.497306	1.456739
N	-4.699984	0.544758	0.840651	H	3.277896	-2.097936	2.508608
H	-3.814628	0.091679	1.074397				
N	-3.321228	2.346167	0.275632				
H	-2.578358	1.733203	0.610432	<b>TS5.log</b>			
C	-0.527915	-0.319122	3.356680	C	-1.640734	-2.451780	1.005707
H	-1.298197	-0.595044	4.093798	C	-0.093789	-4.069678	0.206996
H	-0.356020	0.755643	3.456578	C	1.395431	-5.966146	0.146863
Si	-6.191814	-0.405610	0.882926	O	-2.744641	-1.917151	1.084722
Si	-2.933857	3.891514	-0.502155	N	-1.363588	-3.470542	0.125703
C	-5.621239	-2.056552	1.593051	C	0.951744	-3.278156	0.695320
H	-5.264478	-1.945449	2.625143	H	1.576058	-7.009712	-0.092900
H	-6.433687	-2.794184	1.597095	C	-2.384128	-3.961411	-0.790762
H	-4.795667	-2.468736	0.998629	C	2.173811	-3.848309	1.027545
C	-6.879576	-0.629104	-0.857787	H	-2.926580	-4.817392	-0.371446
H	-7.010668	0.346548	-1.339769	H	-1.902870	-4.252561	-1.727184
H	-6.201899	-1.226734	-1.480834	H	-3.092865	-3.157680	-0.980707
H	-7.853647	-1.135646	-0.841067	H	2.973228	-3.240777	1.430811
C	-7.473903	0.415001	1.991233	C	-0.474278	-2.072493	1.889345
H	-8.400232	-0.173179	2.031709	C	0.135259	-5.413769	-0.095376
H	-7.098410	0.523269	3.016826	H	-0.668422	-6.029681	-0.486276
H	-7.720450	1.414256	1.614529	Cu	0.959579	-1.355524	0.332375
C	-3.559881	3.923892	-2.279307	N	0.486076	0.643896	-0.013988
H	-4.606307	3.601674	-2.314663	C	1.705832	1.379547	-0.435223
H	-3.498745	4.937042	-2.698398	C	2.868768	1.075350	0.546256
H	-2.971972	3.258176	-2.921724	N	3.019812	-0.382332	0.789019
C	-1.050816	3.976008	-0.467325	H	3.440279	-0.802986	-0.041946
H	-0.668412	4.047559	0.557213	C	3.892027	-0.644334	1.944178
H	-0.607307	3.087965	-0.935407	H	4.094110	-1.715352	2.014667
H	-0.694239	4.856325	-1.017887	H	4.852006	-0.113491	1.882516
C	-3.681931	5.320409	0.472193	H	3.382259	-0.332088	2.861360
H	-3.437402	6.286631	0.011216	C	4.154941	1.726709	0.058770
H	-4.773570	5.228634	0.510182	C	4.739156	1.304150	-1.144586
H	-3.307907	5.335345	1.503987	C	4.770320	2.746844	0.790178
C	-1.303784	0.719672	-2.841703	C	5.916375	1.894523	-1.603063
				H	4.269423	0.515888	-1.730851



I	1.708987	-2.025779	-1.874062	C	-0.665665	-2.355906	2.744683
Cu	-0.321737	-1.499547	-0.333305	H	-0.064039	-2.938589	3.449573
N	-0.869645	0.338379	-1.224578	H	-1.065933	-3.062409	2.008852
C	-2.211067	0.717641	-0.721141	O	-0.379649	1.190429	2.079821
C	-3.125825	-0.531940	-0.785875	N	3.565947	1.521780	-0.015374
N	-2.499264	-1.634340	-0.008461	H	3.331984	0.709152	0.558714
H	-2.579976	-1.395649	0.980066	C	2.975175	2.712934	0.356449
C	-3.152415	-2.934436	-0.225157	O	3.140327	3.750183	-0.313592
H	-3.019583	-3.229619	-1.270183	N	2.214786	2.691992	1.502210
H	-2.670566	-3.682022	0.408046	H	1.965219	1.762127	1.849528
H	-4.226502	-2.907661	0.001287	Si	4.628036	1.389378	-1.427081
C	-4.538554	-0.212427	-0.322382	Si	1.317217	4.088556	2.125788
C	-4.777136	0.199404	0.998548	C	5.995589	2.683995	-1.352410
C	-5.619072	-0.315897	-1.205624	H	6.586221	2.576871	-0.433108
C	-6.072233	0.502574	1.421564	H	6.680989	2.579384	-2.204169
H	-3.949234	0.287265	1.698907	H	5.572469	3.693017	-1.366396
C	-6.916554	-0.010008	-0.784431	C	5.399249	-0.327995	-1.319680
H	-5.441625	-0.631465	-2.230984	H	5.920912	-0.469673	-0.364578
C	-7.146224	0.400389	0.530874	H	4.652738	-1.123307	-1.420436
H	-6.242975	0.822314	2.446369	H	6.136481	-0.460791	-2.122770
H	-7.744954	-0.093761	-1.483169	C	3.638221	1.571645	-3.022271
H	-8.153905	0.638801	0.860968	H	3.066102	2.506786	-3.011913
H	-3.158884	-0.870514	-1.827758	H	4.296228	1.585696	-3.901450
C	-2.819233	1.901753	-1.455509	H	2.930912	0.741329	-3.144232
C	-3.008742	1.868893	-2.844678	C	-0.222624	4.420950	1.089563
C	-3.203297	3.046867	-0.747695	H	-0.878173	3.546116	1.142102
C	-3.569910	2.959972	-3.510840	H	-0.778885	5.293568	1.457797
H	-2.721114	0.985288	-3.410408	H	0.027573	4.600670	0.037116
C	-3.766206	4.140656	-1.410863	C	0.822321	3.619979	3.883457
H	-3.062443	3.079614	0.329074	H	0.195906	2.721928	3.873207
C	-3.950464	4.100077	-2.795067	H	1.703861	3.421619	4.507027
H	-3.712353	2.920214	-4.587678	H	0.254727	4.431756	4.357792
H	-4.056848	5.022732	-0.846139	C	2.434430	5.606520	2.176043
H	-4.386847	4.949635	-3.313729	H	2.741297	5.902492	1.168678
H	-2.071442	0.991072	0.327636	H	1.915941	6.451739	2.648784
C	0.149386	1.394558	-1.069065	H	3.342751	5.405169	2.759074
H	1.088979	1.029298	-1.485918	O	-1.842623	-0.281615	2.938354
H	-0.134475	2.321679	-1.582733	C	-0.196462	-5.614759	-0.013154
H	0.284342	1.587427	-0.006170	H	-0.803208	-6.419373	-0.419113
H	-0.948574	0.108842	-2.217751				
C	-0.612079	0.011811	2.345260	<b>lactone-TS4-R-2.log</b>			
C	-1.805827	-1.622497	3.476654	C	-2.631665	1.449937	-1.973307
H	-1.621030	-1.549844	4.554976	C	-4.554752	0.019232	-1.381658
H	-2.788844	-2.073740	3.316982	C	-6.019353	-1.926523	-1.501145



O	-2.247642	2.625292	-2.039320	H	2.687486	-0.340314	5.524704
N	-4.016760	1.185404	-1.980316	H	5.177352	-0.380011	2.010277
C	-4.169656	-0.402508	-0.092275	H	4.952733	-0.296986	4.493902
H	-6.742384	-2.514886	-2.058799	H	0.865352	-0.404707	0.312181
C	-4.921254	2.315282	-2.196007	C	-0.120368	1.764975	1.553616
C	-4.713423	-1.546568	0.496771	H	-0.962040	2.384829	1.871515
H	-4.513914	2.959535	-2.976947	H	0.748712	1.988397	2.183785
H	-5.897276	1.939828	-2.511704	H	0.110135	1.985833	0.512185
H	-5.049844	2.912945	-1.283665	H	-0.859336	0.173100	2.598921
H	-4.432447	-1.817479	1.508286	C	-0.344927	0.406313	-1.922839
C	-1.765120	0.275180	-1.936869	C	-0.728727	-1.596316	-3.025313
C	-5.477867	-0.773546	-2.075086	H	-0.553446	-1.500412	-4.102523
H	-5.753512	-0.479628	-3.084200	H	-0.557872	-2.636220	-2.733902
I	-3.950490	1.456942	1.555302	C	-2.112503	-1.055440	-2.607376
Cu	-2.205107	-0.133141	0.450640	H	-2.756923	-0.923514	-3.483077
N	-0.526016	0.349918	1.648997	H	-2.625941	-1.759343	-1.943028
C	0.556386	-0.613383	1.340238	O	0.419833	1.318694	-1.589449
C	-0.049907	-2.039293	1.396318	N	2.946512	2.373606	-0.608990
N	-1.189771	-2.118362	0.445623	H	1.977598	2.201173	-0.869414
H	-0.799125	-2.120862	-0.495614	C	3.856356	1.450810	-1.069432
C	-1.988214	-3.342749	0.609669	O	5.070820	1.537740	-0.811782
H	-2.469226	-3.326538	1.591902	N	3.351519	0.411835	-1.822656
H	-2.765924	-3.362113	-0.155755	H	2.342276	0.409877	-1.965667
H	-1.379690	-4.253028	0.528958	Si	3.379967	3.787597	0.369499
C	0.995858	-3.113932	1.145309	Si	4.380695	-0.850595	-2.528608
C	1.645300	-3.192144	-0.096041	C	4.677690	4.819759	-0.524026
C	1.324994	-4.039761	2.141159	H	4.294542	5.187855	-1.484614
C	2.600634	-4.180482	-0.336169	H	4.974296	5.690639	0.075359
H	1.413132	-2.468771	-0.873503	H	5.570020	4.217336	-0.724273
C	2.288149	-5.025956	1.906608	C	1.773484	4.761855	0.531398
H	0.829016	-3.984302	3.107197	H	1.314306	4.935592	-0.450343
C	2.927024	-5.100036	0.666640	H	1.039081	4.245337	1.159879
H	3.096086	-4.225485	-1.302012	H	1.966076	5.742624	0.985654
H	2.535449	-5.735896	2.691578	C	4.009341	3.262318	2.065677
H	3.674380	-5.866991	0.481606	H	4.895594	2.625288	1.972123
H	-0.471930	-2.178125	2.398510	H	4.282655	4.138307	2.669267
C	1.776891	-0.496084	2.241027	H	3.245603	2.699169	2.615645
C	1.657080	-0.451972	3.636779	C	3.204360	-1.964415	-3.492801
C	3.054912	-0.468477	1.670749	H	2.684993	-1.400070	-4.277467
C	2.795212	-0.377665	4.443753	H	3.765338	-2.773198	-3.979428
H	0.673859	-0.475365	4.101311	H	2.441356	-2.419058	-2.854059
C	4.195134	-0.402831	2.474268	C	5.633493	-0.078376	-3.706059
H	3.154339	-0.504630	0.591435	H	5.132676	0.434376	-4.537419
C	4.068305	-0.354590	3.864931	H	6.249461	0.656245	-3.175877

H	6.298997	-0.840312	-4.133380	C	-6.991259	-1.842153	-0.646076
C	5.280931	-1.798993	-1.172482	H	-6.584624	-1.974618	1.470840
H	4.583112	-2.222637	-0.442216	H	-7.076366	-1.648539	-2.793973
H	5.869983	-2.624907	-1.593381	H	-8.053632	-2.044398	-0.538234
H	5.965004	-1.128395	-0.640744	H	-2.529457	-0.857776	-2.123337
O	0.251157	-0.780254	-2.342295	C	-3.171419	1.386415	-0.353884
C	-5.626709	-2.324644	-0.221538	C	-3.619797	1.871648	-1.591375
H	-6.039622	-3.221379	0.232028	C	-3.541645	2.070369	0.812393
<b>lactone-TS4-R-3.log</b>				C	-4.414335	3.018621	-1.658355
C	1.822093	-0.785645	1.997938	H	-3.355873	1.348654	-2.505834
C	2.328013	-3.037518	1.174572	C	-4.337479	3.216356	0.749095
C	2.249797	-5.464585	1.334275	H	-3.192695	1.699526	1.772221
O	2.224219	0.387636	2.142385	C	-4.775664	3.694382	-0.488764
N	2.743352	-1.785566	1.685333	H	-4.753872	3.382515	-2.624644
C	1.493721	-3.105683	0.037439	H	-4.612487	3.733982	1.664379
H	2.555231	-6.376810	1.838506	H	-5.394785	4.586003	-0.542754
C	4.178312	-1.548789	1.833552	H	-2.345327	-0.163194	0.819268
C	1.049281	-4.340932	-0.440924	C	-0.544547	-0.187052	2.541350
H	4.332925	-0.488397	2.026595	C	-1.490574	-2.205084	3.133209
H	4.588366	-2.129640	2.668913	H	-1.848888	-2.586989	4.092071
H	4.704368	-1.828058	0.916559	H	-2.126115	-2.603156	2.333377
H	0.472216	-4.387375	-1.354931	C	-0.008668	-2.481045	2.864637
C	0.421369	-1.197051	2.150056	H	0.544787	-2.621692	3.803943
C	2.696385	-4.227726	1.808610	H	0.102083	-3.394925	2.278921
H	3.312477	-4.173781	2.701650	O	-0.558688	1.034552	2.388137
I	2.069092	-1.601886	-1.801178	N	2.875374	2.091409	-0.106361
Cu	0.095542	-1.487565	-0.054232	H	2.796666	1.379995	0.624868
N	-0.840553	0.412600	-0.454920	C	1.976891	3.131734	-0.057169
C	-2.290572	0.155407	-0.223245	O	2.035253	4.068525	-0.878764
C	-2.751236	-1.050368	-1.069928	N	1.011197	3.112551	0.923617
N	-1.936786	-2.234436	-0.679874	H	0.946406	2.291999	1.528287
H	-2.310279	-2.585896	0.202739	Si	4.243702	2.133947	-1.239550
C	-2.026425	-3.319283	-1.671829	Si	-0.069937	4.512230	1.139343
H	-1.420725	-3.058687	-2.545446	C	5.242110	3.717455	-1.012390
H	-1.635716	-4.237389	-1.230595	H	5.637040	3.789308	0.009510
H	-3.058764	-3.505178	-1.998020	H	6.095624	3.746243	-1.702972
C	-4.241978	-1.314640	-0.922334	H	4.616267	4.596205	-1.196905
C	-4.801358	-1.543636	0.344989	C	5.325470	0.657612	-0.793671
C	-5.075939	-1.357872	-2.045631	H	5.693769	0.728286	0.237120
C	-6.165216	-1.804203	0.482646	H	4.787855	-0.290151	-0.899173
H	-4.170622	-1.512645	1.230918	H	6.200580	0.622647	-1.456301
C	-6.443003	-1.619152	-1.911119	C	3.620051	1.999705	-3.012780
H	-4.652114	-1.180970	-3.031255	H	2.895215	2.796246	-3.214705
				H	4.442681	2.093288	-3.734201

H	3.125700	1.035924	-3.187999	C	3.240927	0.326099	1.058609
C	-1.177606	4.719947	-0.369785	N	2.591114	-1.007396	1.029132
H	-1.780023	3.823821	-0.545906	H	3.231967	-1.659541	0.575922
H	-1.864222	5.567724	-0.246729	C	2.271096	-1.522558	2.371822
H	-0.562944	4.899590	-1.258433	H	1.846053	-2.523167	2.267793
C	-1.082148	4.167190	2.689336	H	3.153015	-1.570771	3.024654
H	-1.548672	3.180030	2.657209	H	1.519508	-0.873829	2.828165
H	-0.448780	4.206923	3.585443	C	4.682311	0.266087	1.536005
H	-1.867176	4.926430	2.803509	C	5.643223	-0.456745	0.812507
C	0.951426	6.074973	1.412765	C	5.072303	0.924765	2.707527
H	1.595927	6.272898	0.550491	C	6.966430	-0.515931	1.251861
H	0.299476	6.945716	1.565701	H	5.357504	-0.971116	-0.102632
H	1.589773	5.977259	2.300664	C	6.397128	0.867844	3.150437
O	-1.637465	-0.767930	3.142319	H	4.334391	1.489034	3.272621
C	1.408078	-5.519915	0.223012	C	7.347605	0.147706	2.423078
H	1.058438	-6.474676	-0.160159	H	7.700796	-1.076688	0.679493
C	-0.470258	1.052862	-1.726309	H	6.684022	1.385077	4.062326
H	-0.719072	0.398226	-2.565420	H	8.378223	0.102339	2.764857
H	-0.959848	2.022496	-1.868644	H	2.662855	0.933833	1.762885
H	0.610893	1.202142	-1.722467	C	3.815515	2.327526	-0.394529
H	-0.522856	1.011494	0.310366	C	3.392274	3.392501	0.414850
<b>lactone-TS4-R-4.log</b>				C	4.907048	2.520096	-1.248757
C	-1.189685	-1.084608	1.768203	C	4.050868	4.622238	0.372446
C	-1.933728	-1.091554	-0.673843	H	2.546505	3.260710	1.085947
C	-0.878820	-3.303801	-0.394540	C	5.570899	3.749475	-1.291837
C	-0.200564	-5.366394	0.704452	H	5.241929	1.700232	-1.879562
O	-2.629760	-0.391773	-1.450785	C	5.144575	4.803823	-0.480680
N	-1.904215	-2.459701	-0.893918	H	3.712957	5.437594	1.006789
C	0.479565	-2.966217	-0.535786	H	6.418234	3.882195	-1.959484
H	-0.475378	-6.301223	1.184604	H	5.658834	5.760683	-0.512486
C	-2.788390	-2.984477	-1.939977	H	3.552099	0.311301	-1.080233
C	1.487261	-3.822296	-0.079417	H	1.217564	1.673620	0.017076
H	-2.457726	-2.661878	-2.934454	C	1.388173	1.614878	-2.005893
H	-3.809425	-2.629808	-1.781097	H	1.907207	1.012206	-2.754790
H	-2.776913	-4.074041	-1.897897	H	0.313996	1.551368	-2.196742
H	2.528724	-3.576597	-0.253674	H	1.714016	2.657908	-2.100002
C	-1.176787	-0.502696	0.427717	C	-1.325691	0.995530	0.655882
C	-1.198019	-4.506152	0.244618	H	-0.872243	1.628246	-0.110280
H	-2.246118	-4.745790	0.397420	H	-2.380621	1.277244	0.718422
I	1.072183	-2.001148	-2.725902	C	-0.667591	1.155726	2.025188
Cu	0.860823	-0.907273	-0.298083	H	0.418147	1.295744	1.959182
N	1.661888	1.062634	-0.667951	H	-1.093799	1.956930	2.633615
C	3.107322	0.983478	-0.338085	O	-1.424954	-2.215102	2.170512
				C	-4.919858	1.732977	0.039735

O	-5.600617	2.491798	0.750302	C	-2.235170	-2.899189	-2.214008
N	-4.931887	0.364087	0.203836	C	2.009464	-3.284605	-0.154318
H	-4.287365	-0.136170	-0.407964	H	-1.898504	-2.475489	-3.167758
N	-4.088872	2.211363	-0.955629	H	-3.302575	-2.695705	-2.101741
H	-3.465924	1.506801	-1.353329	H	-2.076046	-3.978025	-2.229403
Si	-5.451767	-0.452553	1.692541	H	3.015142	-2.895682	-0.246735
Si	-3.559461	3.906467	-1.017887	C	-1.149518	-0.366815	0.392223
C	-2.206471	3.904148	-2.330299	C	-0.577645	-4.316523	-0.005628
H	-1.787034	4.909678	-2.463668	H	-1.593651	-4.690274	0.082596
H	-1.383490	3.236651	-2.043226	I	1.502749	-1.340648	-2.676811
H	-2.587348	3.568832	-3.303397	Cu	1.024591	-0.497068	-0.219711
C	-2.848787	4.429725	0.648679	N	1.592591	1.594240	-0.240896
H	-3.570531	4.228327	1.448198	C	3.039330	1.546214	0.082487
H	-1.927730	3.878086	0.875076	C	3.312047	0.691106	1.370276
H	-2.611924	5.501768	0.663713	N	2.179058	-0.249414	1.621345
C	-4.991097	5.023836	-1.509322	C	4.635786	-0.037394	1.230416
H	-4.673811	6.073701	-1.561085	C	4.863156	-0.910328	0.154839
H	-5.393457	4.744260	-2.491335	C	5.645601	0.137855	2.182149
H	-5.802588	4.947970	-0.776806	C	6.069461	-1.601240	0.041615
C	-4.907784	-2.238711	1.435407	H	4.088301	-1.050798	-0.593979
H	-5.289574	-2.878059	2.242414	C	6.860866	-0.544919	2.066575
H	-5.289668	-2.639748	0.487572	H	5.480486	0.813093	3.018133
H	-3.814620	-2.326548	1.433265	C	7.074148	-1.419054	0.998688
C	-4.572284	0.315216	3.172274	H	6.226687	-2.278719	-0.793662
H	-3.487975	0.157209	3.115221	H	7.637165	-0.393999	2.812088
H	-4.757536	1.395352	3.201043	H	8.016497	-1.952894	0.908961
H	-4.926315	-0.115996	4.118077	H	3.387431	1.369286	2.228733
C	-7.319389	-0.327167	1.892654	C	3.702621	2.909013	0.205524
H	-7.840866	-0.796281	1.048448	C	3.209338	3.866864	1.104465
H	-7.653778	-0.823980	2.813004	C	4.826745	3.221531	-0.567124
H	-7.629613	0.722987	1.939960	C	3.825718	5.113097	1.223362
O	-0.915514	-0.096481	2.702982	H	2.338141	3.636161	1.714444
C	1.144126	-5.016958	0.559692	C	5.451993	4.466208	-0.444799
H	1.930772	-5.678582	0.911992	H	5.215291	2.484234	-1.265818
				C	4.951565	5.415515	0.449293
<b>lactone-TS4-R-5.log</b>				H	3.430741	5.846942	1.921139
C	-1.069494	-1.009148	1.692835	H	6.325768	4.693583	-1.049955
C	-1.731444	-0.993358	-0.785914	H	5.433664	6.384935	0.543814
C	-0.385728	-3.055492	-0.579745	H	3.483141	1.026293	-0.769640
C	0.497418	-5.062474	0.476533	H	1.089517	2.071359	0.507097
O	-2.477417	-0.354712	-1.571786	C	1.310386	2.294004	-1.505884
N	-1.489872	-2.327062	-1.087741	H	1.855895	1.798107	-2.313071
C	0.924830	-2.545257	-0.639580	H	0.240654	2.220794	-1.717756
H	0.321625	-6.044673	0.906086	H	1.602037	3.351010	-1.475459





H	4.431762	-0.357813	-2.607470	H	-4.605956	-0.732646	-0.749182
C	6.543981	-1.506328	0.435651	C	-5.734532	3.132876	-1.014248
H	4.684533	-1.509420	1.527566	H	-6.169874	3.171977	-0.007134
C	7.162945	-1.269592	-0.795095	H	-5.258431	4.097555	-1.215154
H	6.867857	-0.668300	-2.846842	H	-6.556978	2.992961	-1.728648
H	7.134228	-1.818507	1.293379	C	-3.743898	1.673650	-2.886347
H	8.236754	-1.399675	-0.901217	H	-3.107836	0.788603	-3.013925
H	2.705256	-0.649009	0.742851	H	-4.528257	1.639697	-3.654108
C	2.954216	1.708536	-0.789222	H	-3.129115	2.563099	-3.066491
C	3.164847	2.158110	0.524210	C	-1.474771	6.069031	1.559930
C	3.403863	2.500194	-1.853436	H	-0.862561	6.971730	1.689792
C	3.818041	3.368497	0.762163	H	-2.183342	6.244737	0.744543
H	2.800582	1.574217	1.363993	H	-2.048821	5.920512	2.483972
C	4.056687	3.713569	-1.617004	C	0.604923	4.855838	-0.382902
H	3.245674	2.160366	-2.874162	H	1.230751	5.754472	-0.305288
C	4.268317	4.149565	-0.307065	H	1.262515	4.006445	-0.593544
H	3.969668	3.704253	1.784497	H	-0.073831	4.982648	-1.233752
H	4.397413	4.315637	-2.455339	C	0.746509	4.262085	2.662065
H	4.775181	5.092455	-0.119331	H	1.468195	5.083914	2.758826
H	2.261222	0.207665	-2.136795	H	0.171673	4.212818	3.596359
H	0.698024	0.958672	0.198723	H	1.293492	3.321937	2.557968
C	-0.023710	1.174528	-1.690398	O	1.751261	-0.463448	3.000796
H	-0.021647	0.612414	-2.628624	C	-0.586223	-5.658220	0.306558
H	-1.049631	1.230488	-1.325624	H	-0.086662	-6.555129	-0.049395
H	0.349652	2.189028	-1.879808	H	2.457325	-2.771580	-0.009143
C	1.791316	-1.906364	3.098393	C	2.282432	-2.548569	-2.030669
H	2.488012	-2.274803	2.336539	H	1.787962	-3.518669	-2.099515
H	2.179082	-2.164858	4.086554	H	1.787247	-1.866742	-2.725980
C	0.361353	-2.395774	2.841984	H	3.329975	-2.670515	-2.332728
H	0.382321	-3.333410	2.284125				
H	-0.169512	-2.586298	3.785130				
C	0.581132	-0.070551	2.394473	<b>lactone-TS4-S-3.log</b>			
O	0.437511	1.133291	2.162109	C	2.498687	-2.235326	1.191723
N	-1.402604	3.116500	1.026863	C	4.420593	-0.758156	1.586405
H	-1.149375	2.252768	1.511056	C	5.740471	0.874698	2.821992
C	-2.422785	3.070784	0.105260	O	2.134161	-3.314257	0.712363
O	-2.651224	4.032831	-0.654805	N	3.853670	-2.052361	1.494463
N	-3.181540	1.924103	0.044694	C	4.176515	0.220773	0.601927
H	-2.956875	1.183350	0.714153	H	6.348618	1.120340	3.687749
Si	-4.479240	1.733973	-1.151092	C	4.754240	-3.188333	1.291759
Si	-0.389855	4.570508	1.192078	C	4.726894	1.500077	0.716185
C	-5.313805	0.101711	-0.718687	H	5.691225	-2.998898	1.819362
H	-5.759832	0.134593	0.283138	H	4.970450	-3.344263	0.226741
H	-6.118207	-0.115002	-1.434089	H	4.293738	-4.094779	1.688738
				H	4.597505	2.215180	-0.085118

C	1.604317	-1.106662	1.523082	C	0.192021	-1.278605	1.315738
C	5.198755	-0.406253	2.695649	O	-0.444340	-1.963963	0.506882
H	5.352626	-1.150066	3.472662	N	-3.568752	-0.677935	1.757017
I	4.266022	-0.578868	-1.740874	H	-2.558793	-0.723091	1.880628
Cu	2.232278	0.167245	-0.224351	C	-4.133533	-1.565697	0.863883
N	0.523395	-0.074394	-1.550428	O	-5.359872	-1.571559	0.644416
C	-0.135202	1.242711	-1.754444	N	-3.270290	-2.418212	0.223455
C	-0.026694	2.022920	-0.423400	H	-2.271504	-2.270021	0.396685
N	1.417339	2.234702	-0.101702	Si	-3.730454	-3.650459	-0.964029
C	-0.858818	3.292578	-0.347455	Si	-4.453751	0.622369	2.579270
C	-1.011776	4.174630	-1.427686	C	-4.723451	-5.015734	-0.125711
C	-1.480906	3.607835	0.868436	H	-5.639482	-4.608975	0.319445
C	-1.772517	5.338583	-1.292699	H	-5.014339	-5.793775	-0.843925
H	-0.548753	3.947300	-2.383067	H	-4.144217	-5.494825	0.673944
C	-2.246433	4.767800	1.006857	C	-4.723638	-2.929233	-2.392119
H	-1.368818	2.931255	1.711461	H	-5.629998	-2.436849	-2.024163
C	-2.394489	5.637877	-0.076808	H	-4.141096	-2.190401	-2.954051
H	-1.884173	6.008952	-2.140951	H	-5.023585	-3.724436	-3.088018
H	-2.731128	4.984832	1.955191	C	-2.071749	-4.296444	-1.585899
H	-2.992689	6.539695	0.023137	H	-1.455806	-4.684607	-0.765404
H	-0.387287	1.355088	0.363805	H	-2.213764	-5.106626	-2.312705
C	-1.566731	1.110974	-2.247431	H	-1.502435	-3.498710	-2.080071
C	-2.565524	0.584411	-1.416429	C	-5.907167	-0.073473	3.551724
C	-1.907197	1.507585	-3.546312	H	-6.453486	0.725472	4.070394
C	-3.881616	0.473879	-1.869016	H	-6.602270	-0.589939	2.881681
H	-2.318782	0.259584	-0.410755	H	-5.566394	-0.793151	4.307158
C	-3.222721	1.394838	-4.005456	C	-5.043618	1.916577	1.342851
H	-1.138358	1.915601	-4.198394	H	-5.532483	2.752614	1.861179
C	-4.213759	0.881336	-3.165341	H	-4.206814	2.325396	0.764409
H	-4.641534	0.057794	-1.215008	H	-5.766315	1.490170	0.637818
H	-3.470958	1.708750	-5.016093	C	-3.172443	1.363187	3.747461
H	-5.237956	0.792533	-3.517943	H	-3.583224	2.234683	4.273302
H	0.445337	1.761829	-2.522147	H	-2.857308	0.633530	4.504090
H	-0.091453	-0.664023	-0.981360	H	-2.278570	1.692244	3.206499
C	0.771987	-0.800346	-2.805351	O	-0.532366	-0.463105	2.162796
H	1.494839	-0.246952	-3.411327	C	5.490481	1.834428	1.839272
H	1.199473	-1.776184	-2.562499	H	5.909399	2.833671	1.920556
H	-0.147055	-0.944301	-3.388747	H	1.469410	2.529382	0.872920
C	0.367401	0.343709	2.962595	C	2.116904	3.234538	-0.928262
H	0.341365	1.363411	2.564398	H	3.080745	3.448636	-0.466074
H	-0.012446	0.352363	3.986064	H	2.297843	2.830892	-1.927737
C	1.754237	-0.295557	2.813349	H	1.566142	4.178546	-1.017120
H	2.524246	0.477915	2.775514				
H	1.984635	-0.945895	3.668588				

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C	-0.635731	-1.763486	2.716551	H	-3.149538	1.188562	-2.997001
C	1.701557	-1.421853	1.744086	C	-4.908480	4.195327	-1.290781
C	0.902036	-3.398062	0.493141	H	-4.207665	3.352157	0.566914
C	-0.128897	-5.514054	-0.146652	C	-4.947025	4.061826	-2.680797
O	2.703861	-0.698013	1.962181	H	-4.333801	2.865974	-4.371168
N	1.895573	-2.690339	1.199068	H	-5.400151	5.036413	-0.809007
C	0.060822	-2.764481	-0.440007	H	-5.469650	4.797547	-3.286326
H	-0.193556	-6.591229	-0.020320	H	-2.911408	1.445994	0.778648
C	3.222616	-3.307360	1.287377	C	-0.647149	2.186582	-0.316431
C	-0.822034	-3.481543	-1.244513	H	0.402390	1.972625	-0.531171
H	3.253566	-4.070077	2.075196	H	-0.970099	3.052151	-0.907889
H	3.481138	-3.773064	0.332999	H	-0.750713	2.428945	0.742943
H	3.951026	-2.532450	1.517892	H	-1.382465	0.819664	-1.622545
H	-1.406201	-2.963952	-1.997309	C	-1.173870	0.458457	3.165450
C	0.366490	-0.949242	2.051607	H	-1.846609	0.902723	2.425330
C	0.773146	-4.786804	0.633500	H	-1.312707	0.973300	4.119356
H	1.378373	-5.296514	1.376554	C	0.272534	0.433628	2.670834
I	1.239860	-0.975744	-1.889669	H	0.477799	1.242676	1.971446
Cu	-0.632278	-0.911091	-0.029450	H	0.979736	0.539361	3.505314
N	-1.442985	0.981490	-0.614467	O	-0.794075	-2.974004	2.800847
C	-2.878475	1.121298	-0.265277	C	4.027800	1.868613	0.114669
C	-3.565607	-0.266446	-0.343141	O	4.543512	2.783239	-0.555685
N	-2.802955	-1.223056	0.489308	N	3.151081	2.141229	1.144750
H	-2.799943	-0.892189	1.455222	H	2.799823	1.331694	1.657179
C	-3.351827	-2.587230	0.493116	N	4.304364	0.546086	-0.135673
H	-3.380177	-2.970027	-0.529561	H	3.829984	-0.131393	0.464504
H	-2.688670	-3.216195	1.089488	Si	2.843887	3.805467	1.688873
H	-4.366902	-2.626378	0.909579	Si	5.379380	0.013599	-1.442832
C	-5.035229	-0.153496	0.037343	C	1.705530	3.659319	3.185275
C	-5.408115	0.149357	1.355324	H	2.087582	2.938005	3.918311
C	-6.035669	-0.327385	-0.925527	H	1.630793	4.632932	3.687738
C	-6.754365	0.280174	1.700035	H	0.690833	3.353960	2.905578
H	-4.644448	0.284082	2.118041	C	2.006635	4.800499	0.325970
C	-7.384577	-0.193438	-0.584720	H	2.600883	4.755161	-0.593143
H	-5.755684	-0.560539	-1.949946	H	1.004499	4.413538	0.104756
C	-7.747466	0.111262	0.729464	H	1.902179	5.854573	0.615787
H	-7.028407	0.515301	2.725232	C	4.464954	4.621023	2.197672
H	-8.149483	-0.328833	-1.345010	H	4.305882	5.662206	2.508087
H	-8.795637	0.214701	0.997381	H	4.928734	4.087446	3.037489
H	-3.491367	-0.628850	-1.374943	H	5.171037	4.615161	1.360389
C	-3.596617	2.156764	-1.115850	C	5.332687	-1.867921	-1.353118
C	-3.638497	2.030956	-2.512449	H	5.962164	-2.307036	-2.138128
C	-4.234445	3.248011	-0.515025	H	5.699938	-2.236110	-0.387402
C	-4.308139	2.976904	-3.290294	H	4.311434	-2.241881	-1.493217

C	7.127833	0.650468	-1.145300	C	3.680721	2.828858	1.234162
H	7.131718	1.745469	-1.103529	H	2.463085	1.698797	-0.133185
H	7.530803	0.273554	-0.196427	C	2.528310	3.849681	3.097092
H	7.807722	0.335848	-1.948178	H	0.401917	3.504385	3.183356
C	4.747308	0.615031	-3.112633	C	3.712194	3.603869	2.397781
H	5.450060	0.360072	-3.917018	H	4.599064	2.625885	0.692388
H	3.777433	0.163926	-3.357409	H	2.542660	4.447842	4.004515
H	4.622239	1.703266	-3.097884	H	4.654671	4.007547	2.758239
O	-1.551571	-0.928542	3.351849	H	-0.784883	2.088911	1.783799
C	-0.935796	-4.867134	-1.082428	C	-0.634511	4.228568	-0.037939
H	-1.629750	-5.425795	-1.704138	C	-1.507753	4.775767	0.913949
<b>lactone-TS4-S-5.log</b>				C	0.199469	5.086428	-0.763733
C	-0.168756	-1.775123	-1.455815	C	-1.542757	6.153292	1.135607
C	-2.590069	-2.350688	-1.984786	H	-2.158066	4.123968	1.493120
C	-2.526408	-2.804410	0.458935	C	0.169341	6.466080	-0.541857
C	-1.993803	-3.527072	2.732106	H	0.881451	4.669585	-1.500901
O	-3.280368	-2.470811	-3.007533	C	-0.702064	7.002893	0.408843
N	-2.875852	-3.139674	-0.860666	H	-2.222462	6.563174	1.878062
C	-2.592215	-1.488592	0.954763	H	0.825021	7.118980	-1.112007
H	-1.748051	-4.335936	3.414194	H	-0.727337	8.075213	0.583553
C	-3.726004	-4.319830	-1.044353	H	0.115702	2.526158	-1.089812
C	-2.439201	-1.196997	2.308269	C	-2.383373	2.616193	-1.955306
H	-3.135635	-5.244234	-1.047313	H	-3.319343	2.096772	-2.176600
H	-4.466052	-4.376200	-0.240552	H	-2.560731	3.698653	-1.956236
H	-4.237425	-4.222657	-2.000914	H	-1.652045	2.382027	-2.731229
H	-2.568916	-0.178446	2.657554	H	-2.569633	2.427709	0.052168
C	-1.472332	-1.411028	-1.938777	C	0.140819	-0.000850	-2.940541
C	-2.190708	-3.810997	1.379530	H	0.106510	0.959634	-2.420005
H	-2.078493	-4.829177	1.020579	H	0.756801	0.095940	-3.835791
I	-4.608719	-0.080231	0.058174	C	-1.255309	-0.569955	-3.187274
Cu	-1.987703	0.049367	-0.185383	H	-1.998403	0.219025	-3.322604
N	-1.885206	2.140035	-0.651950	H	-1.274269	-1.197055	-4.089225
C	-0.574244	2.726886	-0.264004	O	0.234429	-2.619824	-0.654025
C	-0.044748	1.975622	0.982883	C	3.983197	-1.539366	-0.168010
N	0.002055	0.529462	0.671399	O	5.145192	-1.486884	0.276783
H	0.611757	0.384106	-0.135567	N	2.998941	-2.261985	0.464956
C	0.511525	-0.298251	1.776410	H	2.079904	-2.322573	0.017454
H	-0.062181	-0.083532	2.679920	N	3.625521	-0.870382	-1.318546
H	0.372940	-1.343133	1.506100	H	2.651517	-0.947423	-1.608010
H	1.571095	-0.109848	1.978660	Si	3.288235	-3.168761	1.963706
C	1.279744	2.545945	1.467781	Si	4.796336	-0.135883	-2.430712
C	2.471676	2.308176	0.767968	C	1.627712	-3.960584	2.375392
C	1.322072	3.317167	2.635380	H	1.188706	-4.450345	1.498128
				H	1.747316	-4.719196	3.160051

H	0.906633	-3.219801	2.737642	N	-0.776621	0.820176	-0.982783
C	3.820532	-1.995009	3.337976	C	-2.097445	0.447790	-0.423579
H	4.706218	-1.427808	3.031165	C	-2.369426	-1.036798	-0.775999
H	3.022817	-1.279103	3.573312	N	-1.275177	-1.868101	-0.219535
H	4.064633	-2.541929	4.258337	H	-1.363671	-1.854455	0.799050
C	4.595455	-4.496239	1.678946	C	-1.316505	-3.261411	-0.683313
H	4.813049	-5.047518	2.603360	H	-1.174656	-3.281612	-1.768335
H	4.261068	-5.221995	0.926206	H	-0.495626	-3.814068	-0.221765
H	5.526450	-4.042654	1.321682	H	-2.265081	-3.762020	-0.444638
C	3.739409	0.429532	-3.885940	C	-3.750273	-1.483101	-0.320031
H	4.361312	0.898891	-4.659167	C	-4.084683	-1.470101	1.042081
H	3.208404	-0.411210	-4.349469	C	-4.705374	-1.917343	-1.245996
H	2.992991	1.167963	-3.567123	C	-5.348750	-1.878865	1.468292
C	6.065315	-1.418636	-2.970469	H	-3.352023	-1.133630	1.768928
H	6.590503	-1.821824	-2.097408	C	-5.973596	-2.327239	-0.823225
H	5.583406	-2.255574	-3.491941	H	-4.456069	-1.929715	-2.304412
H	6.810884	-0.983022	-3.648512	C	-6.298719	-2.308691	0.535302
C	5.650057	1.344020	-1.639700	H	-5.593196	-1.859296	2.527330
H	6.481863	1.699254	-2.262346	H	-6.704648	-2.661603	-1.554863
H	4.949955	2.178088	-1.510202	H	-7.284017	-2.626682	0.865926
H	6.051199	1.073194	-0.656924	H	-2.309330	-1.138640	-1.866016
O	0.787408	-0.956531	-2.060346	C	-3.223672	1.358761	-0.884148
C	-2.117255	-2.220788	3.205755	C	-3.542046	1.478179	-2.244999
H	-1.983840	-1.991056	4.258974	C	-3.957704	2.099347	0.049374
				C	-4.578444	2.315292	-2.661239
				H	-2.978291	0.912308	-2.983472
<b>lactam-TS4-R-1.log</b>				C	-4.997634	2.937371	-0.363183
C	2.440203	-0.091935	1.622989	H	-3.713062	2.015885	1.105675
C	3.179523	-2.011327	0.288241	C	-5.311417	3.046394	-1.720123
C	3.393060	-4.388823	-0.191895	H	-4.815742	2.396203	-3.718919
O	2.712966	1.093688	1.922696	H	-5.559062	3.504886	0.374535
N	3.473744	-0.886735	1.100967	H	-6.119292	3.697280	-2.044005
C	2.271539	-1.909734	-0.787731	H	-1.996501	0.534018	0.662424
H	3.842005	-5.349842	0.041978	C	-0.346996	2.185626	-0.632095
C	4.816537	-0.310498	1.026231	H	0.632829	2.363929	-1.079339
C	1.924904	-3.028349	-1.550596	H	-1.048860	2.950088	-0.988778
H	5.038707	0.218792	1.954560	H	-0.255217	2.238827	0.451243
H	5.541155	-1.116336	0.889314	H	-0.824899	0.745339	-2.001357
H	4.910076	0.396673	0.191447	C	0.042574	0.006221	2.412767
H	1.251767	-2.918682	-2.393461	C	-0.180240	-2.199393	3.210584
C	1.151847	-0.727139	1.808910	H	0.153729	-2.254558	4.259206
C	3.727613	-3.264781	0.571144	H	-0.869808	-3.033030	3.035825
H	4.399490	-3.355021	1.420354	C	1.020167	-2.196992	2.236152
I	2.507930	0.090140	-2.151866	H	1.920513	-2.562382	2.738894
Cu	0.628943	-0.677606	-0.421581				



N	0.870166	3.543673	0.781534	C	-2.306576	-0.901592	-0.534181
H	1.015963	2.782562	1.443504	C	-2.706336	0.494142	0.003557
C	-0.408397	4.225114	0.790605	N	-1.660119	1.468810	-0.382561
H	-0.907893	4.170541	-0.184090	H	-1.722968	1.624168	-1.389970
H	-1.041533	3.739839	1.534516	C	-1.805711	2.764210	0.301692
H	-0.304848	5.287511	1.050783	H	-0.984941	3.416171	0.000629
C	4.086973	3.422185	-0.951739	H	-2.762023	3.254199	0.074688
H	4.984195	2.901738	-0.605090	H	-1.737214	2.600380	1.377718
H	3.794233	2.995193	-1.922635	C	-4.101810	0.900968	-0.441897
H	4.334614	4.477307	-1.110694	C	-4.396614	1.070354	-1.802917
N	-0.892670	-0.604380	3.265760	C	-5.114177	1.113440	0.500865
C	-2.199767	-0.227610	3.754846	C	-5.679083	1.440279	-2.210926
H	-2.209932	0.847445	3.943999	H	-3.621569	0.906914	-2.548618
H	-2.996147	-0.464950	3.033565	C	-6.400180	1.482552	0.095992
H	-2.411459	-0.759531	4.689100	H	-4.893522	0.984143	1.557837
C	2.753362	-4.266286	-0.676115	C	-6.685916	1.646153	-1.261571
H	2.584883	-5.195264	-1.214155	H	-5.894201	1.564920	-3.269043
H	-0.553690	1.548442	0.320108	H	-7.175717	1.642500	0.840572
C	-0.688207	1.690496	-1.720660	H	-7.684980	1.932797	-1.579179
H	-1.465377	2.458129	-1.812746	H	-2.688300	0.447580	1.097705
H	0.287133	2.177314	-1.754520	C	-3.372300	-1.946294	-0.243064
H	-0.759885	1.009737	-2.573181	C	-3.700263	-2.280098	1.079677
				C	-4.044646	-2.588746	-1.288834
				C	-4.682674	-3.234177	1.348684
				H	-3.190032	-1.789073	1.905732
				C	-5.030822	-3.543195	-1.023106
				H	-3.796860	-2.335890	-2.316911
				C	-5.352448	-3.868264	0.296822
				H	-4.927726	-3.480841	2.378507
				H	-5.544469	-4.032386	-1.846640
				H	-6.118376	-4.610344	0.505995
				H	-2.171641	-0.820667	-1.618787
				H	-1.087027	-1.400149	1.026051
				C	-0.414860	-2.492012	-0.548514
				H	-0.318254	-2.371249	-1.630616
				H	0.581152	-2.647015	-0.129318
				H	-1.043135	-3.367908	-0.343000
				C	0.819837	-0.600361	2.728717
				H	0.652183	-1.524500	2.169286
				H	1.563406	-0.831833	3.504558
				C	-0.469391	-0.072917	3.379715
				H	-1.366860	-0.313447	2.785103
				H	-0.632615	-0.466806	4.389835
				O	0.986211	2.977590	2.328347
<b>lactam-TS4-R-3.log</b>							
C	0.707802	1.783486	2.499431				
C	2.684859	0.529390	1.465085				
C	2.491852	2.446657	-0.074281				
C	2.060204	4.687240	-0.925364				
O	3.420620	-0.449917	1.750395				
N	3.254942	1.574341	0.744057				
C	1.505897	1.957264	-0.950816				
H	2.282667	5.750354	-0.906051				
C	4.687946	1.476613	0.441283				
C	0.831819	2.812247	-1.830221				
H	4.878689	0.762971	-0.371271				
H	5.229245	1.146236	1.328871				
H	5.057530	2.458247	0.140484				
H	0.120803	2.404960	-2.540413				
C	1.289158	0.575518	1.870630				
C	2.736462	3.823528	-0.062442				
H	3.458588	4.211503	0.649802				
I	2.026238	-0.178081	-2.061034				
Cu	0.295255	0.480981	-0.108672				
N	-0.977304	-1.256179	0.023232				

C	3.655049	-3.428206	0.102215	C	-2.326105	0.946399	-0.141838
O	3.705609	-4.491390	-0.532336	N	-0.989751	0.864981	-0.773837
N	4.520143	-2.381995	-0.120257	H	-1.116132	0.699556	-1.773682
H	4.295662	-1.498733	0.335597	C	-0.197188	2.092747	-0.600459
N	2.727525	-3.193108	1.091642	H	0.772879	1.950386	-1.075363
H	2.814120	-2.327330	1.620530	H	-0.685799	2.975659	-1.033303
N	-0.250288	1.361003	3.410923	H	-0.038708	2.261942	0.465701
C	-1.187229	2.251744	4.049761	C	-3.236845	1.972690	-0.796961
H	-0.849544	3.278307	3.890086	C	-3.610641	1.841047	-2.142890
H	-2.201227	2.141089	3.634619	C	-3.712297	3.068234	-0.067445
H	-1.239620	2.053306	5.128250	C	-4.447092	2.783408	-2.742996
C	5.303873	-2.334076	-1.339171	H	-3.250107	0.995233	-2.724628
H	6.039364	-1.529008	-1.252856	C	-4.551028	4.013695	-0.664831
H	5.834042	-3.280014	-1.481318	H	-3.426336	3.177779	0.975966
H	4.691117	-2.148182	-2.234717	C	-4.921381	3.872826	-2.004352
C	1.949335	-4.278836	1.653464	H	-4.731116	2.666829	-3.785666
H	1.100802	-3.860404	2.202296	H	-4.912385	4.858550	-0.084253
H	1.567420	-4.915207	0.850793	H	-5.573755	4.605981	-2.471288
H	2.531560	-4.910541	2.341640	H	-2.150392	1.244595	0.897817
C	1.098164	4.184029	-1.804477	C	-4.367520	-0.446530	0.445953
H	0.570318	4.844040	-2.487539	C	-4.594833	-0.034095	1.768043
				C	-5.459421	-0.837023	-0.337243
				C	-5.888095	-0.010248	2.291898
				H	-3.758638	0.275714	2.391381
				C	-6.756481	-0.812629	0.183752
				H	-5.292632	-1.157341	-1.362840
				C	-6.974042	-0.398624	1.499963
				H	-6.049247	0.314238	3.316680
				H	-7.593990	-1.117883	-0.438181
				H	-7.981349	-0.378567	1.907431
				H	-2.995119	-0.835044	-1.156825
				H	-2.066558	-1.105889	1.592175
				C	-2.448363	-2.793275	0.534647
				H	-2.423481	-3.116450	-0.509035
				H	-1.725586	-3.390184	1.096836
				H	-3.454387	-2.965086	0.938186
				C	0.160430	-1.256048	3.028727
				H	-0.633658	-1.976480	2.813760
				H	0.720486	-1.650952	3.887722
				C	-0.387662	0.142655	3.358534
				H	-1.311549	0.373743	2.803156
				H	-0.597783	0.287092	4.424205
				O	2.454791	1.018796	1.445483
				C	4.545227	3.249913	0.087262
<b>lactam-TS4-R-4.log</b>							
C	1.516419	0.407698	2.002024				
C	2.078177	-2.064299	1.594662				
C	2.907322	-1.017965	-0.495125				
C	3.865626	0.646609	-1.996051				
O	2.063703	-3.128227	2.235715				
N	3.055281	-1.898851	0.604414				
C	1.711036	-0.947710	-1.234570				
H	4.703721	1.281247	-2.268098				
C	4.039595	-2.976691	0.469764				
C	1.602270	-0.120190	-2.358815				
H	3.598085	-3.868264	0.004908				
H	4.419897	-3.254493	1.454515				
H	4.868305	-2.629695	-0.149834				
H	0.691528	-0.126427	-2.947183				
C	1.107635	-0.993281	1.855856				
C	3.968801	-0.196321	-0.889419				
H	4.874187	-0.206890	-0.291778				
I	0.572989	-3.075737	-1.623754				
Cu	-0.013963	-0.968339	-0.027882				
N	-2.047636	-1.378481	0.610876				
C	-2.958337	-0.467009	-0.125482				

O	5.329497	3.875914	-0.638957	H	1.224217	-2.034148	-1.698908
N	3.178715	3.431602	0.051076	C	1.236437	-3.277737	-0.085550
H	2.622724	2.681833	0.462459	H	0.369136	-3.851731	-0.417450
N	4.972972	2.355310	1.044528	H	2.150840	-3.821681	-0.355309
H	4.274637	1.695037	1.379179	H	1.193135	-3.186233	1.001363
N	0.687637	1.017328	2.919567	C	3.662936	-1.604753	-0.464597
C	0.640466	2.443357	3.139386	C	4.072741	-2.030505	-1.736860
H	1.520950	2.899067	2.680880	C	4.565524	-1.696984	0.600699
H	-0.262793	2.890358	2.696967	C	5.360288	-2.530264	-1.938699
H	0.638997	2.666375	4.213622	H	3.383225	-1.969261	-2.575860
C	2.588280	4.177863	-1.044591	C	5.857150	-2.192820	0.402185
H	2.576865	3.613683	-1.989420	H	4.255313	-1.373225	1.591306
H	1.558252	4.438472	-0.784792	C	6.258381	-2.610543	-0.869002
H	3.153604	5.098865	-1.206715	H	5.663813	-2.855374	-2.930517
C	6.353398	1.907180	1.024031	H	6.546545	-2.254572	1.240351
H	6.521657	1.256943	1.887112	H	7.261547	-2.998016	-1.026167
H	6.612197	1.349669	0.111021	H	2.121814	-0.868421	0.827693
H	7.030529	2.763460	1.094135	C	3.223854	1.295162	-0.655958
C	2.676184	0.694742	-2.727388	C	3.301449	1.917362	0.599366
H	2.582828	1.343382	-3.593962	C	4.216971	1.563940	-1.605936
				C	4.354811	2.784954	0.895854
				H	2.531063	1.735883	1.343405
<b>lactam-TS4-S-1.log</b>				C	5.274027	2.428771	-1.309666
C	-2.355353	0.178880	1.678206	H	4.166554	1.085506	-2.580898
C	-3.176209	-1.904758	0.673602	C	5.346834	3.041348	-0.055927
C	-3.445994	-4.322770	0.596255	H	4.400201	3.260313	1.872555
O	-2.595146	1.396995	1.830344	H	6.036984	2.624791	-2.058718
N	-3.415517	-0.658676	1.311665	H	6.167078	3.715475	0.176657
C	-2.349164	-1.986317	-0.469356	H	2.117037	0.109561	-2.049593
H	-3.882288	-5.226175	1.012276	H	0.741302	1.303303	0.245632
C	-4.751739	-0.071109	1.200197	C	0.344391	1.894748	-1.663622
C	-2.076146	-3.221479	-1.068525	H	0.273257	1.439173	-2.656192
H	-5.491651	-0.874545	1.196192	H	-0.641083	2.269323	-1.387732
H	-4.860967	0.517765	0.280042	H	1.053500	2.732558	-1.708424
H	-4.935276	0.583698	2.054033	C	0.419287	-1.742776	3.335193
H	-1.470870	-3.260756	-1.967682	H	1.170956	-2.344393	2.804346
C	-1.055707	-0.449305	1.896961	H	0.386430	-2.099679	4.371396
C	-3.708822	-3.086043	1.194777	C	-0.958654	-1.792910	2.639752
H	-4.315939	-3.025432	2.093851	H	-1.027712	-2.666341	1.987155
I	-2.586016	-0.223480	-2.054468	H	-1.757963	-1.888157	3.386577
Cu	-0.634248	-0.736200	-0.287464	C	0.031136	0.389750	2.410070
N	0.750805	0.874018	-0.686725	O	0.317985	1.576679	2.118865
C	2.094788	0.324968	-0.974754	N	-0.896361	3.871491	0.917427
C	2.270152	-1.034254	-0.245054	H	-0.900959	2.919738	1.286509
N	1.175240	-1.935279	-0.683347				

C	-1.797045	4.225654	-0.057790	H	-1.085070	1.642971	0.301379
O	-1.704709	5.278329	-0.707861	C	-0.941251	1.268922	2.291030
N	-2.798870	3.306545	-0.270483	H	-1.181744	0.456706	2.980845
H	-2.910869	2.564509	0.421923	H	0.134152	1.454823	2.327363
C	0.373785	4.566033	1.009339	H	-1.479666	2.170603	2.612257
H	1.032830	4.370014	0.149470	C	-3.695536	1.549648	1.178846
H	0.215034	5.646855	1.070418	C	-3.613573	2.854376	0.670060
H	0.884089	4.227022	1.913658	C	-4.709963	1.243838	2.092959
C	-3.939163	3.639572	-1.099617	C	-4.529397	3.830469	1.066111
H	-3.601108	4.081150	-2.041508	H	-2.828844	3.110774	-0.038228
H	-4.490678	2.720984	-1.321526	C	-5.631405	2.217390	2.489115
H	-4.628653	4.352432	-0.620937	H	-4.781852	0.234799	2.491775
N	0.795245	-0.339284	3.286769	C	-5.543300	3.513978	1.976536
C	2.083836	0.095804	3.773836	H	-4.452298	4.837615	0.664630
H	2.136142	1.184436	3.714809	H	-6.414730	1.962660	3.198334
H	2.211832	-0.214730	4.817257	H	-6.256679	4.273612	2.285003
H	2.907295	-0.332738	3.182834	H	-2.867039	-0.421505	1.335287
C	-2.611269	-4.392319	-0.520405	C	-4.357711	-0.262960	-1.050381
H	-2.393005	-5.348201	-0.988797	C	-4.927036	-1.404094	-0.465171
				C	-5.142735	0.521905	-1.902857
				C	-6.253914	-1.749517	-0.726205
				H	-4.334034	-2.023895	0.204183
				C	-6.472761	0.180688	-2.164302
				H	-4.710812	1.409122	-2.359417
				C	-7.031885	-0.956276	-1.576160
				H	-6.681981	-2.635094	-0.263799
				H	-7.069200	0.802105	-2.827246
				H	-8.065712	-1.223970	-1.777741
				H	-2.665667	1.012232	-1.345861
				C	-1.887851	-1.138577	-2.613999
				H	-1.127543	-1.895189	-2.824422
				H	-2.851082	-1.468918	-3.023433
				H	-1.602404	-0.203333	-3.101342
				H	-2.232716	-1.804525	-0.727519
				C	0.345648	2.081641	-2.079768
				H	-0.719138	1.842184	-1.931921
				H	0.411799	2.869477	-2.837992
				C	1.162537	0.827219	-2.424180
				H	0.584389	0.099399	-2.996224
				H	2.038089	1.100892	-3.030097
				O	2.225622	1.692817	0.901784
				C	5.437575	2.232109	-0.560643
				O	6.569008	2.245020	-1.061657
				N	4.335745	2.759594	-1.208442
<b>lactam-TS4-S-2.log</b>							
C	1.654439	1.514386	-0.197422				
C	2.733022	-0.629280	-1.080772				
C	2.491942	-1.195854	1.312741				
C	2.365014	-1.055969	3.744565				
O	3.248800	-1.003434	-2.145129				
N	3.244360	-1.134212	0.118787				
C	1.128307	-1.537798	1.311680				
H	2.862004	-0.862841	4.691189				
C	4.422530	-1.999425	0.002588				
C	0.397568	-1.679168	2.491662				
H	4.162883	-2.962479	-0.455692				
H	5.176782	-1.513929	-0.619214				
H	4.837763	-2.180072	0.994163				
H	-0.637404	-2.000659	2.451971				
C	1.616336	0.323831	-1.054364				
C	3.085786	-0.935338	2.553611				
H	4.123342	-0.617847	2.574246				
I	0.489928	-3.434575	-0.271149				
Cu	-0.049892	-0.725996	-0.131911				
N	-1.941012	-0.923511	-1.156979				
C	-2.915972	0.122465	-0.757949				
C	-2.704622	0.482173	0.735757				
N	-1.288895	0.860839	0.922545				



H	3.539469	2.986098	-0.626399	C	0.259528	1.976991	-1.084361
N	5.161558	1.696872	0.673266	H	0.363160	1.686563	-2.132700
H	4.183974	1.493709	0.887627	H	-0.797768	1.957103	-0.822437
C	6.185948	0.960751	1.389359	H	0.650839	2.995754	-0.962648
H	6.330175	-0.059788	1.007335	C	3.189269	2.113171	-0.457138
H	7.139223	1.489349	1.307934	C	3.236406	2.825467	0.751235
H	5.909098	0.900234	2.445959	C	3.889335	2.611184	-1.561349
C	4.516508	3.577592	-2.394552	C	3.969201	4.008842	0.851693
H	3.533373	3.777749	-2.829768	H	2.699999	2.452841	1.620771
H	5.011107	4.537975	-2.185218	C	4.627700	3.794568	-1.463701
H	5.122005	3.038064	-3.127437	H	3.860094	2.066115	-2.501733
N	0.950358	2.521569	-0.829228	C	4.669096	4.496930	-0.256959
C	0.604470	3.777175	-0.204218	H	3.995591	4.548837	1.794659
H	-0.470683	3.835038	0.025135	H	5.167279	4.167116	-2.330606
H	1.169150	3.865877	0.726241	H	5.240705	5.418000	-0.179438
H	0.857219	4.617975	-0.861960	H	2.427182	0.459362	-1.592742
C	1.017754	-1.416851	3.718914	C	4.446882	-0.515071	0.066653
H	0.449916	-1.521622	4.639226	C	4.850709	-1.026910	-1.175491
				C	5.423136	-0.217968	1.024763
				C	6.203186	-1.233016	-1.452780
				H	4.106739	-1.260778	-1.933882
				C	6.778380	-0.420668	0.749795
				H	5.119077	0.181742	1.989177
				C	7.171884	-0.928447	-0.490664
				H	6.501684	-1.627441	-2.420604
				H	7.523845	-0.182959	1.504199
				H	8.225010	-1.086565	-0.707597
				H	2.888578	0.085335	1.398540
				C	2.506977	-2.505672	1.292751
				H	1.813735	-3.346319	1.206331
				H	3.534944	-2.869025	1.168272
				H	2.409592	-2.067826	2.289201
				H	2.276849	-1.910686	-0.637437
				C	0.331563	0.486128	3.289686
				H	1.307589	0.532761	2.783575
				H	0.485509	0.783552	4.333006
				C	-0.323225	-0.898015	3.137299
				H	0.419062	-1.692972	3.041183
				H	-0.934370	-1.130499	4.020808
				O	-2.373709	1.290992	1.144532
				C	-4.622467	3.157695	-0.486299
				O	-5.428937	3.614822	-1.307363
				N	-3.273861	3.439939	-0.516603
				H	-2.683059	2.824079	0.040439
<b>lactam-TS4-S-3.log</b>							
C	-1.501397	0.699707	1.819684				
C	-2.278089	-1.734863	1.763032				
C	-2.874607	-0.989627	-0.517726				
C	-3.548544	0.393655	-2.409440				
O	-2.405987	-2.673477	2.565533				
N	-3.184750	-1.638947	0.698840				
C	-1.607746	-1.101926	-1.114959				
H	-4.314337	0.991192	-2.895170				
C	-4.278901	-2.614539	0.681958				
C	-1.313344	-0.519010	-2.347466				
H	-3.923827	-3.609172	0.380556				
H	-4.716274	-2.692301	1.678609				
H	-5.046161	-2.286207	-0.020707				
H	-0.340894	-0.674641	-2.801385				
C	-1.215909	-0.732847	1.906473				
C	-3.832290	-0.220180	-1.187564				
H	-4.801084	-0.082547	-0.720738				
I	-0.590508	-3.421815	-0.992284				
Cu	0.030180	-1.037816	0.093822				
N	2.142607	-1.492863	0.286127				
C	2.976146	-0.268935	0.366648				
C	2.385248	0.823960	-0.559881				
N	0.954196	0.998147	-0.236447				
H	0.885479	1.322618	0.727190				

N	-5.010597	2.369963	0.577453	H	-1.903329	-2.643888	-1.725954
H	-4.282805	1.789460	0.989079	H	-1.136534	-3.333320	-0.277220
C	-6.368113	1.856559	0.615058	H	-2.912039	-3.128015	-0.342904
H	-7.087283	2.681262	0.626979	C	-4.174356	-0.742064	-0.222179
H	-6.610701	1.215649	-0.245813	C	-4.586249	-0.993620	1.095477
H	-6.492569	1.271684	1.530588	C	-5.109702	-0.861954	-1.255726
C	-2.686715	4.024077	-1.708437	C	-5.905728	-1.354524	1.371793
H	-1.689550	4.402321	-1.465014	H	-3.873399	-0.905196	1.911725
H	-2.591963	3.303163	-2.534539	C	-6.433220	-1.220675	-0.982841
H	-3.305211	4.856779	-2.052246	H	-4.800416	-0.668595	-2.280139
N	-0.624080	1.374456	2.640170	C	-6.834797	-1.467973	0.332003
C	-0.480510	2.812186	2.659649	H	-6.209249	-1.545275	2.397946
H	0.443889	3.135910	2.157887	H	-7.147721	-1.308087	-1.797298
H	-1.334522	3.255536	2.142820	H	-7.862741	-1.748028	0.546582
H	-0.454852	3.179657	3.692713	H	-2.611153	-0.247356	-1.604509
C	-2.285715	0.257865	-2.988264	C	-3.365092	2.102117	-0.271917
H	-2.055452	0.727113	-3.940704	C	-3.465627	2.504841	-1.612103
				C	-4.186862	2.715127	0.681036
				C	-4.371375	3.497340	-1.989721
<b>lactam-TS4-S-4.log</b>				H	-2.837575	2.037146	-2.367330
C	0.531526	-2.321548	1.934173	C	-5.096783	3.707760	0.306253
C	2.672038	-1.032402	1.339350	H	-4.117558	2.407440	1.721650
C	2.373532	-2.425792	-0.671492	C	-5.191624	4.101076	-1.030813
C	1.806593	-4.268297	-2.161496	H	-4.439908	3.796991	-3.032248
O	3.471313	-0.229907	1.886590	H	-5.728954	4.172497	1.058427
N	3.178968	-1.887441	0.362624	H	-5.898282	4.872467	-1.325182
C	1.412646	-1.647982	-1.340053	H	-2.450424	0.877700	1.224203
H	1.968174	-5.296578	-2.472663	C	-0.480288	2.502171	0.634910
C	4.623491	-1.832879	0.106697	H	0.583569	2.631606	0.426140
C	0.685496	-2.144800	-2.422186	H	-1.016896	3.430188	0.400091
H	4.887789	-0.964853	-0.512099	H	-0.605845	2.285302	1.697903
H	5.159436	-1.762263	1.053685	H	-0.903535	1.604074	-1.137070
H	4.932577	-2.741463	-0.412360	C	-0.524300	-0.653375	3.251239
H	-0.008035	-1.499112	-2.949295	H	-1.335797	-0.129733	2.720890
C	1.268752	-1.065252	1.704973	H	-0.717410	-0.558498	4.326138
C	2.539205	-3.750065	-1.091118	C	0.855354	-0.121030	2.831602
H	3.239161	-4.380021	-0.549923	H	0.812433	0.927350	2.533446
I	2.102639	0.747504	-1.818284	H	1.562130	-0.190413	3.671370
Cu	0.289378	-0.390157	-0.205828	O	0.704727	-3.446674	1.441860
N	-0.973557	1.354630	-0.147768	C	4.002907	3.007121	0.913204
C	-2.387917	1.011954	0.139645	O	4.150893	4.167499	0.504149
C	-2.734485	-0.347162	-0.519905	N	3.004245	2.652329	1.789380
N	-1.741676	-1.350064	-0.077676	H	3.001238	1.697613	2.141124
H	-1.797360	-1.427006	0.937376	N	4.824793	1.968042	0.539336
C	-1.946193	-2.694692	-0.635325				

H	4.515366	1.031366	0.795620	C	-2.44434200	-2.65774600	-0.12984400
C	5.672750	2.098249	-0.629774	H	-3.07578500	-4.45183400	-1.13570500
H	5.107459	2.069289	-1.574305	H	-5.95035800	0.43775700	-0.35965500
H	6.216982	3.045534	-0.588783	H	-5.19349400	1.11838200	1.10607500
H	6.395593	1.277044	-0.636467	H	-5.45523500	2.15222500	-0.31164900
C	2.266285	3.667877	2.513961	H	-1.71900900	-3.16413800	0.49801300
H	1.440973	3.187638	3.045389	C	-1.55868400	1.48376700	-0.99741200
H	2.888127	4.203895	3.246618	C	-4.38595800	-1.34747200	-1.63490700
H	1.851767	4.405898	1.820664	H	-5.10667500	-0.81880900	-2.25073400
N	-0.469469	-2.052657	2.858006	I	-2.44141600	-0.65648600	2.44865400
C	-1.517887	-2.985993	3.193649	Cu	-0.92528600	-0.20612800	0.35137700
H	-2.491674	-2.667803	2.790304	N	0.83077500	0.65667200	1.21155100
H	-1.259903	-3.957932	2.767051	C	1.97037900	-0.27589900	1.04834000
H	-1.618499	-3.084370	4.282365	C	1.89294700	-0.88876200	-0.37313300
C	0.870370	-3.472575	-2.823233	N	0.59191400	-1.58480300	-0.51791300
H	0.300257	-3.863448	-3.661514	H	0.58227500	-2.38286800	0.11898500

**TS4-S.log**

C	-0.50235600	2.48863700	-0.86993500	H	1.08570200	-2.84263000	-2.18451300
C	0.40835700	2.30178000	-1.94381200	H	0.39908700	-1.24512700	-2.57511300
C	-0.23865200	3.49399300	0.06596100	C	3.09395900	-1.76487700	-0.68356200
C	1.56098200	3.06943000	-2.08604900	C	3.31344800	-2.95600100	0.02092000
C	0.92001400	4.27345300	-0.06940300	C	4.00611300	-1.39047500	-1.67450500
H	-0.94633000	3.67083400	0.86677900	C	4.42172300	-3.75480600	-0.25871700
C	1.80885200	4.06710800	-1.12969400	H	2.61933000	-3.26397700	0.80104600
H	2.23689800	2.91396800	-2.92229200	C	5.11876900	-2.18510700	-1.95660600
H	1.12197600	5.05662200	0.65609500	H	3.84765900	-0.46356900	-2.22051000
H	2.69872200	4.68428000	-1.22030500	C	5.32895200	-3.36994200	-1.24949800
C	-1.33561100	0.82948000	-2.30352000	H	4.57935200	-4.67497200	0.29738500
O	-2.01581100	0.03599600	-2.95055000	H	5.81955000	-1.87856400	-2.72832500
N	-0.06768000	1.28532000	-2.75966400	H	6.19348600	-3.99066200	-1.46773700
C	0.45275700	0.96729800	-4.06926000	H	1.86376600	-0.05789500	-1.08772900
H	0.50703100	1.86346000	-4.70067500	C	3.32213100	0.36421400	1.31660200
H	1.45676900	0.52713000	-4.00269000	C	3.71556900	1.50574700	0.60599000
H	-0.23037600	0.24656000	-4.52368000	C	4.19555700	-0.18125900	2.26199300
C	-2.88415700	1.73699100	-0.39606100	C	4.96090100	2.08791800	0.83887000
C	-3.62777600	-0.60188400	-0.72273500	H	3.05230000	1.95045300	-0.13044200
C	-4.19891800	-2.71871500	-1.78426800	C	5.44508200	0.39723600	2.49367000
O	-3.13599600	2.77893500	0.21257000	H	3.89947300	-1.06940300	2.81529900
N	-3.88910300	0.77292100	-0.53304200	C	5.83074900	1.53453400	1.78212700
C	-2.62873200	-1.27703200	-0.00196500	H	5.24947500	2.97594500	0.28281400
C	-3.22133700	-3.37964000	-1.03653200	H	6.11384300	-0.03901700	3.23071100
H	-4.81097700	-3.27050800	-2.49177300	H	6.80137100	1.98838500	1.96274000
C	-5.20212300	1.14125400	0.00947100	H	1.81134800	-1.08468300	1.77371500

H	0.97183900	1.46006200	0.59571100	N	0.805869	-1.778765	0.309409
C	0.69363300	1.18456900	2.58060600	C	2.021197	-1.328609	-0.404637
H	0.46799800	0.36053000	3.26184700	C	1.899344	0.187923	-0.726122
H	-0.14819400	1.87901700	2.59474500	N	0.646732	0.409688	-1.495002
H	1.60418100	1.69729300	2.91269700	H	0.699344	-0.132212	-2.359075
<b>TS4-13.log</b>				C	0.411536	1.825539	-1.847623
C	-2.551191	0.131602	1.932321	H	-0.591098	1.916755	-2.268707
C	-3.553201	0.673519	-0.293699	H	1.153395	2.201310	-2.562792
C	-4.250252	1.939468	-2.262238	H	0.455009	2.428644	-0.941686
O	-2.749558	-0.549147	2.930454	C	3.134538	0.734356	-1.419642
N	-3.656710	0.417744	1.088384	C	3.482460	0.313330	-2.710290
C	-2.665639	-0.045946	-1.119571	C	3.945430	1.674454	-0.777789
H	-4.880623	2.708956	-2.698171	C	4.623366	0.810393	-3.339308
C	-4.957125	-0.025542	1.609279	H	2.862704	-0.414902	-3.230707
C	-2.566957	0.228682	-2.491045	C	5.091171	2.172508	-1.400943
H	-5.024542	-1.119378	1.604657	H	3.674337	2.019103	0.216816
H	-5.075126	0.318690	2.637898	C	5.434300	1.740326	-2.682816
H	-5.753234	0.387910	0.987958	H	4.880754	0.472241	-4.339502
H	-1.913132	-0.376904	-3.109998	H	5.712639	2.899943	-0.885907
C	-4.344527	1.662431	-0.899445	H	6.324634	2.127492	-3.170485
H	-5.020961	2.236532	-0.272104	H	1.762516	0.715917	0.221862
I	-2.673114	-2.440649	-0.720036	C	3.320578	-1.648530	0.326160
Cu	-0.870850	-0.572540	-0.258987	C	3.419706	-1.503512	1.716412
C	-3.340246	1.240475	-3.059127	C	4.450734	-2.057592	-0.392294
H	-3.255597	1.452615	-4.121142	C	4.630881	-1.746243	2.367249
C	-1.240130	0.740530	1.598595	H	2.550133	-1.221506	2.302705
C	-0.061584	0.329896	2.379672	C	5.662014	-2.297060	0.256685
O	0.250517	-0.762361	2.887999	H	4.386757	-2.172267	-1.470958
C	-1.021902	2.159930	1.270847	C	5.756794	-2.138162	1.640802
C	-1.779112	3.168288	0.668106	H	4.689396	-1.632893	3.446552
C	0.277222	2.509472	1.731012	H	6.529105	-2.610509	-0.318519
C	-1.220477	4.435185	0.455200	H	6.698346	-2.326450	2.149605
H	-2.794954	2.982622	0.355694	H	2.026917	-1.860448	-1.366440
C	0.849083	3.759357	1.519989	H	0.836913	-1.493807	1.297847
C	0.084459	4.728970	0.858155	C	0.663462	-3.245125	0.306127
H	-1.819495	5.200838	-0.030872	H	0.435785	-3.592434	-0.706250
H	1.854322	3.979255	1.868078	H	-0.170286	-3.511049	0.957880
H	0.504833	5.714258	0.677101	H	1.575611	-3.739099	0.664491
N	0.830361	1.415600	2.383705	<b>TS4-A-1.log</b>			
C	2.071544	1.430009	3.124691	C	2.603121	-1.555431	1.243561
H	2.138783	2.344667	3.724174	C	3.639674	0.545097	0.459995
H	2.073121	0.562332	3.786505	C	4.365585	2.855560	0.720092
H	2.947097	1.372090	2.464656	O	2.603035	-2.783569	1.087537

N	3.737780	-0.822708	0.819211	H	-6.380641	-1.901117	-1.948332
C	2.638113	0.994358	-0.428885	H	-6.697638	-3.174236	0.168276
H	5.048706	3.573971	1.164014	H	-2.048213	-0.144143	-1.766267
C	4.901000	-1.576676	0.354583	H	-0.870390	-1.796734	0.370087
C	2.491997	2.355554	-0.726216	C	-0.685065	-2.354305	-1.572740
H	5.778529	-0.925725	0.369873	H	-0.540091	-1.884582	-2.550200
H	4.760635	-1.956605	-0.666283	H	0.206578	-2.939962	-1.335980
H	5.072256	-2.426268	1.018459	H	-1.552392	-3.026423	-1.627484
H	1.734284	2.673232	-1.434585	C	0.947660	0.334232	4.017908
C	1.557403	-0.778056	1.927525	H	0.667517	1.317293	4.412451
C	4.495872	1.498233	1.022918	H	1.446443	-0.214103	4.826817
H	5.249839	1.160907	1.728923	C	1.904177	0.436816	2.803550
I	2.306822	-0.395213	-2.354665	H	1.759112	1.386800	2.275619
Cu	0.820322	-0.037693	-0.155314	H	2.949357	0.423932	3.130276
N	-0.849568	-1.320047	-0.542129	C	0.332040	-1.364528	2.398946
C	-2.066878	-0.503677	-0.730485	O	-0.283001	-2.383006	2.001610
C	-2.010870	0.736400	0.200522	C	3.345801	3.288417	-0.132331
N	-0.751118	1.483909	-0.034021	H	3.227146	4.343986	-0.361006
H	-0.781606	1.894430	-0.969022	C	-0.245504	-0.483423	3.514226
C	-0.539933	2.565137	0.943205	H	-0.723118	-1.108240	4.276982
H	0.418607	3.045456	0.736283	H	-1.030033	0.156046	3.087449
H	-1.335135	3.321712	0.913505				
H	-0.502246	2.133078	1.945924	<b>TS4-A-2.log</b>			
C	-3.258025	1.594452	0.054689	C	1.859299	-2.098826	1.579687
C	-3.526656	2.265612	-1.147216	C	3.479721	-0.118135	1.496404
C	-4.166306	1.713389	1.112769	C	3.386431	-0.790371	-0.888614
C	-4.682485	3.035500	-1.288231	C	3.288595	-2.025886	-2.991102
H	-2.833928	2.182089	-1.981765	O	4.084793	0.578861	2.325160
C	-5.326339	2.480762	0.974456	N	4.089317	-0.396422	0.261123
H	-3.966661	1.193618	2.046722	C	2.149321	-0.215546	-1.233200
C	-5.587574	3.143909	-0.227124	H	3.748045	-2.736256	-3.672967
H	-4.878814	3.547909	-2.226545	C	5.527734	-0.162603	0.123196
H	-6.023086	2.560777	1.804896	C	1.507119	-0.496863	-2.437803
H	-6.488647	3.741467	-0.337351	H	6.096554	-1.099677	0.174115
H	-1.955329	0.368759	1.229243	H	5.737545	0.324378	-0.834014
C	-3.354096	-1.283757	-0.498345	H	5.844321	0.488131	0.937337
C	-3.536869	-2.009359	0.689289	H	0.586448	0.017013	-2.691771
C	-4.387003	-1.257338	-1.442545	C	2.163159	-0.690879	1.796028
C	-4.734267	-2.687214	0.925974	C	3.933317	-1.713687	-1.792279
H	-2.737725	-2.053017	1.426718	H	4.868816	-2.202005	-1.537540
C	-5.587273	-1.933200	-1.205882	I	2.024174	2.320451	-0.832932
H	-4.253606	-0.695219	-2.363546	Cu	0.801374	0.123284	0.235121
C	-5.765110	-2.648141	-0.018776	N	-0.976569	1.286727	0.761062
H	-4.863709	-3.245103	1.849989	C	-2.225822	0.492694	0.657151

C	-2.060344	-0.594856	-0.437266	H	1.566224	-1.658112	-4.251600
N	-0.845684	-1.379022	-0.129200	C	0.811082	-2.526733	2.622569
H	-0.946671	-1.758016	0.812155	H	1.329786	-3.172403	3.346007
C	-0.593458	-2.505167	-1.040678	H	0.018549	-3.133680	2.168551
H	-0.540533	-2.134399	-2.066377				
H	0.370405	-2.945080	-0.775299				
H	-1.377189	-3.272177	-0.987557	<b>TS4-A-3.log</b>			
C	-3.326097	-1.432136	-0.558738	C	-2.438123	-1.285353	1.657311
C	-3.724090	-2.280350	0.485347	C	-3.579179	0.678033	0.691107
C	-4.119783	-1.359117	-1.708902	C	-4.309683	2.999096	0.561803
C	-4.893926	-3.034607	0.381677	O	-2.492621	-2.519565	1.721447
H	-3.116031	-2.353292	1.384324	N	-3.619392	-0.582576	1.332556
C	-5.293656	-2.110464	-1.815449	C	-2.741641	0.907176	-0.423539
H	-3.819352	-0.704462	-2.523495	H	-4.924806	3.806211	0.949230
C	-5.684244	-2.950181	-0.769572	C	-4.856201	-1.357104	1.218753
H	-5.189390	-3.687443	1.198975	C	-2.709191	2.161546	-1.046313
H	-5.899599	-2.040802	-2.715142	H	-4.910538	-2.076394	2.037794
H	-6.595554	-3.536819	-0.850163	H	-5.710330	-0.678752	1.278905
H	-1.872379	-0.096039	-1.395445	H	-4.907328	-1.907130	0.269488
C	-3.458261	1.349793	0.412422	H	-2.117666	2.299708	-1.942821
C	-3.546333	2.168912	-0.723530	C	-1.256876	-0.466096	1.982349
C	-4.532636	1.320246	1.308967	C	-4.349398	1.743296	1.171997
C	-4.687002	2.938577	-0.957461	H	-4.964984	1.576273	2.051698
H	-2.724432	2.201231	-1.436051	I	-2.635636	-0.875887	-2.043030
C	-5.677825	2.087139	1.076046	Cu	-0.847079	-0.015079	-0.247129
H	-4.474261	0.685749	2.189960	N	0.825544	-1.318038	-0.501653
C	-5.757892	2.898321	-0.058384	C	2.017411	-0.539020	-0.070290
H	-4.741944	3.566098	-1.843207	C	2.051764	0.824139	-0.794948
H	-6.504562	2.050709	1.780752	N	0.782238	1.541245	-0.489327
H	-6.647380	3.495047	-0.242381	H	0.839463	1.872880	0.474211
H	-2.343912	-0.022731	1.616182	C	0.575476	2.713190	-1.354706
C	-0.918205	2.123738	1.971891	H	0.339219	2.375735	-2.368787
H	0.019883	2.684769	1.958526	H	-0.267332	3.290735	-0.971175
H	-1.758526	2.827676	2.033619	H	1.457033	3.367221	-1.398307
H	-0.933670	1.479771	2.854117	C	3.275891	1.645698	-0.415174
H	-0.941310	1.915053	-0.044029	C	3.545357	1.949754	0.928734
C	0.337291	-1.225456	3.284251	C	4.138390	2.137359	-1.402415
H	-0.519757	-0.817799	2.737014	C	4.658868	2.716728	1.274527
H	0.030741	-1.355854	4.327520	H	2.883305	1.585964	1.711212
C	1.541779	-0.276122	3.127903	C	5.254663	2.905894	-1.059804
H	1.253952	0.778976	3.160437	H	3.936638	1.910075	-2.446449
H	2.261428	-0.430923	3.946958	C	5.519320	3.195581	0.280803
O	2.352331	-2.896461	0.768405	H	4.856625	2.939175	2.319923
C	2.069106	-1.430432	-3.315900	H	5.914569	3.277078	-1.839664
				H	6.387431	3.791187	0.550535

H	2.057767	0.662776	-1.877055	H	4.920580	-1.526408	-1.355804
C	3.299797	-1.355174	-0.134401	H	5.725180	-1.748908	0.210986
C	4.150641	-1.361901	-1.248354	H	1.047592	2.587210	-1.384385
C	3.602577	-2.190831	0.951438	C	2.013862	-1.113762	1.674642
C	5.288952	-2.172390	-1.268955	C	4.408784	1.858682	0.388989
H	3.929640	-0.732265	-2.104615	H	5.341705	1.643673	0.901787
C	4.739218	-3.001652	0.932995	I	1.731773	-0.408101	-2.419128
H	2.920307	-2.218326	1.798474	Cu	0.782476	-0.187138	0.101485
C	5.589633	-2.991176	-0.176928	N	-0.970977	-1.459158	-0.060442
H	5.940517	-2.162819	-2.139028	C	-2.113319	-0.572588	-0.392980
H	4.961562	-3.639917	1.784514	C	-2.086168	0.640960	0.570281
H	6.477235	-3.618357	-0.192496	N	-0.779370	1.328444	0.441110
H	1.828749	-0.318715	0.981389	H	-0.788607	1.855941	-0.432690
C	-0.053331	-1.117094	2.452750	C	-0.505969	2.263438	1.544287
C	0.036288	1.186009	3.214323	H	0.476679	2.713238	1.386700
H	0.037827	1.820195	4.107050	H	-1.260177	3.058294	1.621379
H	0.595153	1.721198	2.436921	H	-0.486342	1.704078	2.482376
C	-1.390482	0.879045	2.710664	C	-3.270888	1.568402	0.348628
H	-2.087202	0.797148	3.560500	C	-3.446621	2.218269	-0.882706
H	-1.764032	1.691510	2.082043	C	-4.206880	1.784922	1.366281
O	0.409698	-2.239256	2.161501	C	-4.536633	3.064498	-1.090599
C	-3.474302	3.214170	-0.537124	H	-2.731668	2.057253	-1.686708
H	-3.436706	4.185513	-1.022573	C	-5.300966	2.630754	1.161131
C	0.667311	-0.189825	3.439651	H	-4.080188	1.282836	2.322460
H	1.754452	-0.224551	3.306272	C	-5.468899	3.272160	-0.068338
H	0.452167	-0.564205	4.451808	H	-4.661375	3.558280	-2.050820
H	0.654879	-2.018184	0.229827	H	-6.019672	2.787438	1.961312
C	0.925080	-1.981672	-1.808912	H	-6.318953	3.929554	-0.230668
H	1.778567	-2.667979	-1.871374	H	-2.129263	0.252892	1.593520
H	0.004859	-2.546141	-1.974527	C	-3.457772	-1.282867	-0.358735
H	1.012207	-1.235962	-2.604262	C	-3.906327	-1.905805	0.815639
<b>TS4-A-4.log</b>				C	-4.271466	-1.320170	-1.496657
C	2.095067	-0.067679	2.690637	C	-5.145262	-2.547553	0.850256
C	3.167470	-1.521320	0.859070	H	-3.287132	-1.886829	1.710065
C	3.581421	0.782446	0.044939	C	-5.513922	-1.959793	-1.465038
C	4.042056	3.174867	0.113113	H	-3.931299	-0.840398	-2.411208
O	3.449132	-2.716771	0.671916	C	-5.954382	-2.574828	-0.290695
N	3.998217	-0.547681	0.292111	H	-5.480778	-3.024233	1.767642
C	2.346125	1.068837	-0.566333	H	-6.134517	-1.978101	-2.357215
H	4.711117	3.988237	0.379680	H	-6.919616	-3.073492	-0.263389
C	5.188108	-1.031363	-0.413062	H	-1.928299	-0.205871	-1.408965
C	1.969618	2.388489	-0.850166	H	-1.114206	-1.818430	0.882747
H	5.842517	-0.186198	-0.632462	C	-0.844936	-2.613796	-0.966553
				H	-0.748192	-2.254188	-1.993613

H	0.062483	-3.165443	-0.708018	C	-3.616899	2.094903	-1.403162
H	-1.709619	-3.286299	-0.906747	C	-4.039087	1.837222	0.958397
C	1.181438	-2.250830	2.270473	C	-4.797065	2.828055	-1.536292
H	0.657770	-2.855035	1.523508	H	-2.997007	1.912285	-2.278152
H	1.829317	-2.947408	2.826191	C	-5.223106	2.568901	0.828832
C	0.224539	-1.534050	3.244526	H	-3.743704	1.448055	1.929916
H	-0.627755	-1.113478	2.697036	C	-5.605690	3.065583	-0.419601
H	-0.173997	-2.200510	4.017081	H	-5.087312	3.211950	-2.510944
O	2.871120	0.892459	2.774796	H	-5.843754	2.751188	1.702356
C	2.810352	3.443921	-0.490517	H	-6.525735	3.634729	-0.523354
H	2.511813	4.464689	-0.713466	H	-1.800199	0.536039	1.049159
C	1.077363	-0.389836	3.799703	C	-3.328699	-1.324073	-0.427909
H	0.517454	0.500443	4.105065	C	-3.502365	-1.848150	0.862898
H	1.659840	-0.719601	4.672915	C	-4.349983	-1.491249	-1.370471
<b>TS4-B-1.log</b>				C	-4.678853	-2.520074	1.199540
C	2.538439	-1.282953	1.595468	H	-2.712601	-1.743649	1.603415
C	3.554621	0.746455	0.622501	C	-5.528785	-2.163209	-1.034468
C	4.161872	3.104448	0.520521	H	-4.223629	-1.085773	-2.371437
O	2.643911	-2.513876	1.657357	C	-5.696986	-2.677902	0.253220
N	3.673047	-0.524858	1.238431	H	-4.801505	-2.920406	2.202788
C	2.684149	0.955881	-0.470252	H	-6.312198	-2.284483	-1.778222
H	4.743419	3.934894	0.910318	H	-6.612511	-3.200546	0.517870
C	4.941436	-1.238050	1.082153	H	-2.089107	-0.318100	-1.856413
C	2.563668	2.218082	-1.064295	H	-0.869357	-1.820122	0.341936
H	5.764615	-0.522068	1.138378	C	-0.662940	-2.428320	-1.580818
H	4.996307	-1.766248	0.120827	H	-0.484734	-1.981439	-2.563412
H	5.046123	-1.969665	1.885152	H	0.210507	-3.027511	-1.311990
H	1.919148	2.346290	-1.927195	H	-1.543110	-3.083090	-1.641270
C	1.334736	-0.506182	1.922076	C	0.073010	0.869866	3.437842
C	4.275592	1.842537	1.109726	H	-0.573353	1.666917	3.059143
H	4.916389	1.693984	1.974606	H	0.177404	0.996812	4.519921
I	2.590015	-0.811934	-2.103421	C	1.429847	0.804369	2.707065
Cu	0.850995	-0.049690	-0.246829	H	1.573366	1.687227	2.078381
N	-0.830498	-1.366545	-0.577323	H	2.260817	0.785881	3.424133
C	-2.059157	-0.566952	-0.789122	C	0.148234	-1.194541	2.375783
C	-1.954287	0.769880	-0.010289	O	-0.601929	-0.383299	3.201021
N	-0.731622	1.483404	-0.457460	O	-0.314762	-2.306117	2.104720
H	-0.799990	1.643271	-1.464417	C	3.292369	3.296975	-0.555441
C	-0.540435	2.785316	0.200915	H	3.191042	4.275198	-1.017353
H	0.409937	3.211103	-0.124868	<b>TS4-B-2.log</b>			
H	-1.346964	3.494552	-0.024598	C	1.624074	-2.051082	1.591488
H	-0.499992	2.637542	1.281434	C	3.376654	-0.207447	1.613050
C	-3.228004	1.588348	-0.154327	C	3.394087	-0.880160	-0.776332



C	3.357295	-2.135498	-2.870300	C	-5.794203	2.896270	-0.101090
O	3.970409	0.448377	2.481429	H	-4.878664	3.470518	-1.970761
N	4.042622	-0.527865	0.419107	H	-6.437029	2.146304	1.817939
C	2.230336	-0.222657	-1.216143	H	-6.693414	3.483791	-0.266482
H	3.810285	-2.888990	-3.508747	H	-2.292929	0.059566	1.530424
C	5.502480	-0.418494	0.386697	C	-0.910285	2.253205	1.756256
C	1.660743	-0.470411	-2.463610	H	0.036348	2.798483	1.720046
H	5.983862	-1.397313	0.507502	H	-1.740794	2.970175	1.782482
H	5.822232	0.015838	-0.564996	H	-0.938491	1.649893	2.666476
H	5.812574	0.231280	1.204050	H	-0.966540	1.947640	-0.250180
H	0.798941	0.102693	-2.787364	C	0.145493	-1.200681	3.170921
C	1.998445	-0.663166	1.810163	H	-0.733856	-0.743183	2.705292
C	3.932096	-1.856734	-1.627971	H	-0.123435	-1.546456	4.172264
H	4.805254	-2.411625	-1.299137	O	0.523860	-2.360461	2.388343
I	2.180639	2.312216	-0.793919	C	1.351230	-0.261552	3.127761
Cu	0.797215	0.216268	0.139150	H	1.052284	0.788191	3.177909
N	-0.979243	1.359411	0.586262	H	2.031738	-0.449584	3.970242
C	-2.216228	0.541185	0.550664	O	2.087995	-2.925500	0.870440
C	-2.067727	-0.578658	-0.510009	C	2.216433	-1.452666	-3.291684
N	-0.822249	-1.328927	-0.241976	H	1.769321	-1.653571	-4.261157
H	-0.879060	-1.744371	0.689125				
C	-0.568482	-2.419054	-1.196049				
H	-0.520790	-2.010975	-2.208146	<b>TS4-B-3.log</b>			
H	0.395083	-2.867538	-0.948580	C	-2.558634	0.191741	2.037788
H	-1.349914	-3.190183	-1.167393	C	-3.613289	0.880248	-0.080317
C	-3.318127	-1.447027	-0.545174	C	-4.252844	2.478476	-1.804426
C	-3.657813	-2.251596	0.552698	O	-2.615116	-0.625070	2.966336
C	-4.156682	-1.443927	-1.665465	N	-3.711067	0.399221	1.248212
C	-4.815322	-3.031266	0.530818	C	-2.689287	0.324895	-0.991542
H	-3.016200	-2.268474	1.431214	H	-4.872009	3.314981	-2.115591
C	-5.318107	-2.221309	-1.690144	C	-4.943997	-0.277843	1.647418
H	-3.901327	-0.823069	-2.520860	C	-2.544475	0.835289	-2.284707
C	-5.650966	-3.016741	-0.591047	H	-5.054188	-0.220478	2.731790
H	-5.066519	-3.648631	1.389440	H	-5.794491	0.217087	1.172719
H	-5.959885	-2.205571	-2.567300	H	-4.941851	-1.336256	1.353797
H	-6.553118	-3.622553	-0.607449	H	-1.851993	0.367102	-2.975237
H	-1.936514	-0.107612	-1.491235	C	-1.400708	1.019282	1.694868
C	-3.468887	1.373207	0.322979	C	-4.386167	1.963299	-0.511318
C	-3.620590	2.132567	-0.847107	H	-5.075795	2.418599	0.194283
C	-4.492659	1.390287	1.277102	I	-2.548891	-2.111492	-0.945737
C	-4.774074	2.889429	-1.058224	Cu	-0.856028	-0.205706	-0.176708
H	-2.837655	2.127874	-1.602339	N	0.832411	-1.489745	0.094383
C	-5.650393	2.145135	1.067846	C	2.047689	-0.655431	0.240643
H	-4.383863	0.803605	2.186046	C	2.059577	0.396543	-0.897896
				N	0.795848	1.172275	-0.862211

H	0.839386	1.788826	-0.051322	H	-3.196061	2.334278	-3.685847
C	0.594534	1.999804	-2.060318				
H	0.483037	1.346545	-2.931094				
H	-0.326803	2.573836	-1.941859	<b>TS4-B-4.log</b>			
H	1.428412	2.691315	-2.243827	C	1.905053	0.361997	2.666349
C	3.297897	1.277840	-0.827716	C	3.170146	-1.285843	1.180742
C	3.512399	2.116609	0.277815	C	3.533814	0.872017	0.021186
C	4.240839	1.265722	-1.861583	C	3.863646	3.265306	-0.301710
C	4.649305	2.923685	0.343232	O	3.514847	-2.477766	1.214967
H	2.790882	2.136557	1.092195	N	3.996568	-0.369206	0.523271
C	5.381354	2.071682	-1.796934	C	2.336696	0.973019	-0.712098
H	4.083288	0.616298	-2.719384	H	4.467108	4.153309	-0.136029
C	5.588227	2.903225	-0.693819	C	5.258694	-0.889665	-0.010221
H	4.804558	3.566845	1.205694	C	1.918525	2.194087	-1.254822
H	6.104657	2.049796	-2.608089	H	5.894393	-0.053540	-0.305872
H	6.473783	3.531135	-0.641167	H	5.088246	-1.532418	-0.883836
H	2.062092	-0.143992	-1.851397	H	5.770851	-1.477040	0.754577
C	3.338923	-1.459387	0.266407	H	1.026780	2.234568	-1.870468
C	3.684927	-2.302413	-0.799915	C	1.926340	-0.821893	1.811146
C	4.208561	-1.361034	1.358896	C	4.274830	2.041729	0.227433
C	4.877738	-3.027197	-0.774887	H	5.174830	1.979248	0.832148
H	3.021491	-2.392390	-1.657317	I	1.925935	-0.860927	-2.293786
C	5.405133	-2.082816	1.386466	Cu	0.766161	-0.187538	0.047460
H	3.946821	-0.711638	2.190757	N	-0.981706	-1.469544	0.055064
C	5.743200	-2.917810	0.318652	C	-2.129774	-0.634332	-0.378005
H	5.133061	-3.675526	-1.609154	C	-2.094807	0.688113	0.428926
H	6.069805	-1.994043	2.241924	N	-0.789722	1.354580	0.209086
H	6.672288	-3.481386	0.337742	H	-0.809717	1.801934	-0.707890
H	1.940064	-0.134912	1.196133	C	-0.487987	2.379246	1.223553
C	0.648847	-2.474924	1.177425	H	0.479656	2.827054	0.988840
H	-0.245906	-3.062156	0.956320	H	-1.252486	3.167012	1.265945
H	1.506628	-3.153009	1.272884	H	-0.415454	1.894727	2.200050
H	0.497929	-1.929853	2.110420	C	-3.279884	1.586923	0.114592
H	0.889657	-1.993828	-0.793151	C	-3.473480	2.085139	-1.182969
C	-0.176439	0.924724	2.456821	C	-4.195099	1.934136	1.114879
O	0.552764	2.109687	2.311169	C	-4.562119	2.908907	-1.472627
C	-0.310618	3.157489	1.821921	H	-2.773685	1.823249	-1.973698
H	-0.575906	3.802144	2.668235	C	-5.286968	2.758902	0.828298
H	0.257583	3.749857	1.098643	H	-4.054228	1.551221	2.122789
C	-1.545093	2.465832	1.211319	C	-5.473570	3.247803	-0.466764
H	-2.467150	2.934607	1.570991	H	-4.701127	3.284120	-2.483203
H	-1.547088	2.562981	0.120258	H	-5.988636	3.018572	1.616718
O	0.335358	0.028459	3.118568	H	-6.322062	3.888244	-0.692647
C	-3.315025	1.933193	-2.683134	H	-2.128023	0.422544	1.491145
				C	-3.472714	-1.334097	-0.237799

C	-3.900981	-1.813121	1.009524	I	2.694505	0.025660	-2.272266
C	-4.308518	-1.498458	-1.347987	Cu	0.887300	0.088786	-0.270460
C	-5.140985	-2.439778	1.142053	N	-0.778162	-1.004362	-1.136677
H	-3.265530	-1.693156	1.884263	C	-1.998660	-0.172647	-1.092165
C	-5.552482	-2.122766	-1.218452	C	-1.910279	0.804604	0.113900
H	-3.984565	-1.129416	-2.318084	N	-0.685208	1.627056	-0.039995
C	-5.972228	-2.594592	0.027580	H	-0.733993	2.123997	-0.930887
H	-5.460275	-2.804139	2.115040	C	-0.496715	2.611842	1.035569
H	-6.190772	-2.240652	-2.090278	H	0.449124	3.132776	0.876377
H	-6.938661	-3.080768	0.131237	H	-1.308395	3.349175	1.084854
H	-1.955818	-0.399283	-1.434022	H	-0.443530	2.087078	1.991642
H	-1.126505	-1.712658	1.034377	C	-3.187741	1.615474	0.266827
C	-0.849872	-2.726181	-0.701609	C	-3.539389	2.591197	-0.677188
H	-0.723007	-2.494458	-1.761809	C	-4.048834	1.376951	1.343996
H	0.044021	-3.250311	-0.353783	C	-4.730990	3.307141	-0.548878
H	-1.724173	-3.377980	-0.581819	H	-2.881227	2.791807	-1.519551
C	1.135365	-1.876996	2.575136	C	-5.245106	2.087776	1.473449
H	0.600003	-2.593031	1.944908	H	-3.782882	0.623018	2.081275
H	1.794541	-2.460713	3.233609	C	-5.589904	3.055030	0.526186
C	0.184221	-1.003078	3.396310	H	-4.990810	4.059796	-1.288797
H	-0.742337	-0.775798	2.854394	H	-5.904442	1.886913	2.313989
H	-0.074528	-1.417662	4.374363	H	-6.518865	3.610467	0.624661
O	0.891923	0.235941	3.608713	H	-1.763448	0.205216	1.019672
O	2.603080	1.365200	2.697252	C	-3.289250	-0.981397	-1.060527
C	2.674093	3.347413	-1.030304	C	-3.452798	-2.033355	-0.146899
H	2.343391	4.293526	-1.450089	C	-4.351822	-0.656009	-1.912880
				C	-4.658527	-2.735117	-0.082565
				H	-2.633781	-2.314996	0.509412
<b>TS4-C-1.log</b>				C	-5.559880	-1.355259	-1.848623
C	2.548901	-1.746417	0.974069	H	-4.235939	0.158845	-2.623132
C	3.622080	0.471910	0.810576	C	-5.718124	-2.396075	-0.929695
C	4.226344	2.697309	1.599840	H	-4.770137	-3.546885	0.632020
O	2.642205	-2.922911	0.600004	H	-6.374781	-1.087600	-2.516417
N	3.708133	-0.937937	0.926743	H	-6.656773	-2.941543	-0.877091
C	2.787564	1.073665	-0.158840	H	-1.995418	0.441956	-2.000780
H	4.794054	3.321514	2.283865	H	-0.822328	-1.741955	-0.422681
C	4.964941	-1.574169	0.532603	C	-0.579283	-1.657278	-2.437200
C	2.677591	2.467857	-0.245340	H	-0.384061	-0.901359	-3.204370
H	5.799422	-0.940804	0.843100	H	0.294094	-2.311059	-2.370426
H	5.023050	-1.728160	-0.553548	H	-1.450664	-2.254319	-2.741406
H	5.049363	-2.545480	1.023176	C	0.126098	-0.333676	3.481344
H	2.060629	2.911438	-1.019373	H	-0.535531	0.517270	3.258727
C	1.345226	-1.104511	1.525727	H	0.220085	-0.397808	4.572072
C	4.326596	1.305141	1.684976	C	1.485785	-0.204703	2.767238
H	4.940690	0.842388	2.452842				

H	1.702137	0.841357	2.537643	C	4.898481	-2.899552	0.121572
H	2.292726	-0.560604	3.423090	H	3.098875	-2.375317	-0.932816
C	0.158425	-1.940830	1.755313	C	5.343215	-1.659324	2.147529
O	-0.329383	-2.841406	1.036760	H	3.878936	-0.164863	2.672189
C	3.384387	3.277734	0.649127	C	5.713838	-2.644862	1.229442
H	3.290634	4.358038	0.578774	H	5.178439	-3.666083	-0.596428
N	-0.444915	-1.553804	2.936949	H	5.969167	-1.455512	3.012501
C	-1.788696	-1.946368	3.293849	H	6.629366	-3.211975	1.375582
H	-2.534304	-1.207921	2.958687	H	1.909603	0.271851	1.510239
H	-2.012816	-2.907656	2.827691	C	3.442943	1.418456	-0.550221
H	-1.871516	-2.046717	4.382328	C	3.578103	2.387417	0.455552
<b>TS4-C-2.log</b>				C	4.469034	1.273687	-1.490856
C	-1.699573	-2.302750	-1.160773	C	4.717084	3.191579	0.518970
C	-3.359773	-0.364503	-1.495441	H	2.791987	2.512085	1.197314
C	-3.410642	-0.606489	0.963690	C	5.612157	2.075969	-1.429445
C	-3.327250	-1.554470	3.209137	H	4.373262	0.524080	-2.272686
O	-3.915141	0.207333	-2.448057	C	5.739254	3.036848	-0.423551
N	-4.057702	-0.464045	-0.284469	H	4.808937	3.936366	1.305276
C	-2.239966	0.107985	1.274858	H	6.400346	1.950152	-2.167258
H	-3.762238	-2.210333	3.958152	H	6.626817	3.662046	-0.373658
C	-5.431584	0.047449	-0.280508	H	2.288807	-0.118094	-1.489197
C	-1.635859	0.030409	2.530377	C	0.880670	1.988373	-2.111731
H	-5.934118	-0.273103	0.633215	H	-0.078139	2.509254	-2.179160
H	-5.450140	1.144357	-0.329553	H	1.695373	2.709458	-2.258560
H	-5.973797	-0.343998	-1.143329	H	0.931523	1.236994	-2.903565
H	-0.763955	0.636623	2.750092	H	0.918913	2.035851	-0.081723
C	-2.011334	-0.929690	-1.607185	C	-0.206712	-1.795114	-2.928247
C	-3.925759	-1.455093	1.950413	H	0.717077	-1.322546	-2.554923
H	-4.796435	-2.058053	1.708757	H	0.021592	-2.253505	-3.897388
I	-2.177913	2.507983	0.482892	C	-1.364566	-0.787594	-2.983888
Cu	-0.816495	0.204312	-0.183797	H	-1.020451	0.223845	-3.209815
N	0.953488	1.313554	-0.804374	H	-2.077569	-1.071580	-3.771852
C	2.204326	0.538544	-0.616767	O	-2.192751	-2.971553	-0.239341
C	2.072216	-0.368224	0.634991	C	-2.174658	-0.823668	3.499491
N	0.854348	-1.189943	0.487340	H	-1.703514	-0.889781	4.476304
H	0.936479	-1.731574	-0.372134	N	-0.693025	-2.791008	-1.985932
C	0.609523	-2.128397	1.591015	C	0.047973	-3.996208	-1.700942
H	0.545570	-1.571679	2.528911	H	-0.492716	-4.558268	-0.936175
H	-0.347291	-2.621949	1.407709	H	0.146258	-4.614543	-2.602229
H	1.400776	-2.884295	1.687507	H	1.061957	-3.777707	-1.328851
C	3.344866	-1.176582	0.849232	<b>TS4-C-3.log</b>			
C	3.723595	-2.169720	-0.066594	C	-2.634929	0.499898	1.902787
C	4.163962	-0.933229	1.957481	C	-3.668978	0.758322	-0.325128

C	-4.263542	2.019438	-2.324898	C	5.683799	-2.929617	0.751810
O	-2.707711	-0.134084	2.965163	H	4.999964	-4.052761	-0.961140
N	-3.783745	0.540132	1.069680	H	6.085328	-1.640599	2.435893
C	-2.737258	0.035571	-1.104233	H	6.608874	-3.490898	0.853819
H	-4.870075	2.788523	-2.794593	H	1.933517	0.038126	1.159724
C	-5.009600	-0.078593	1.569833	C	0.607490	-2.227276	1.660443
C	-2.559190	0.308975	-2.464388	H	-0.301072	-2.830842	1.583585
H	-5.146428	0.183297	2.620729	H	1.456045	-2.887511	1.884034
H	-5.860268	0.293513	0.993410	H	0.480807	-1.492239	2.457102
H	-4.979833	-1.173956	1.487755	H	0.815100	-2.180110	-0.370099
H	-1.857885	-0.279775	-3.045092	C	-0.258219	1.355615	2.212045
C	-1.483868	1.260077	1.423412	C	-0.507966	3.477678	1.219916
C	-4.423699	1.747953	-0.961963	H	-0.870617	4.180920	1.988393
H	-5.118857	2.330276	-0.363115	H	-0.015220	4.065311	0.436844
I	-2.552550	-2.295492	-0.610052	C	-1.655005	2.596282	0.679861
Cu	-0.888351	-0.248468	-0.131739	H	-2.623238	3.063762	0.882725
N	0.782081	-1.498547	0.390783	H	-1.579192	2.494803	-0.408204
C	2.008949	-0.671600	0.330266	O	0.233509	0.590525	3.055684
C	1.994353	0.124371	-1.002765	C	-3.311351	1.321942	-3.069777
N	0.766111	0.950315	-1.060016	H	-3.167638	1.536311	-4.125232
H	0.840052	1.673381	-0.338810	N	0.424077	2.524316	1.813064
C	0.562637	1.593431	-2.364843	C	1.490438	3.042520	2.645550
H	0.435547	0.820807	-3.129748	H	1.100254	3.582555	3.524602
H	-0.351288	2.190039	-2.328346	H	2.108944	2.213762	2.995922
H	1.401389	2.240352	-2.657616	H	2.109752	3.735758	2.066455
C	3.270028	0.932588	-1.189818				
C	3.588706	1.970311	-0.301599				
C	4.143425	0.658021	-2.248279	<b>TS4-C-4.log</b>			
C	4.758347	2.713325	-0.465564	C	-1.674130	1.497074	-2.149272
H	2.919375	2.193851	0.523393	C	-3.142615	-0.532587	-1.615586
C	5.317188	1.399212	-2.415501	C	-3.489037	0.845204	0.415359
H	3.905462	-0.144806	-2.942151	C	-3.719348	2.784043	1.876296
C	5.628121	2.428841	-1.523945	O	-3.558842	-1.541325	-2.210126
H	4.992130	3.512273	0.233531	N	-3.976191	0.059793	-0.656747
H	5.985549	1.172562	-3.242245	C	-2.369747	0.451927	1.173736
H	6.539947	3.006231	-1.652083	H	-4.252792	3.692985	2.140132
H	1.916665	-0.601804	-1.821032	C	-5.312691	-0.522675	-0.503819
C	3.291442	-1.475002	0.483155	C	-1.949475	1.190764	2.286247
C	3.592384	-2.522705	-0.399837	H	-5.933963	0.152620	0.086912
C	4.199496	-1.170979	1.504025	H	-5.271799	-1.498026	-0.000474
C	4.779350	-3.245266	-0.267713	H	-5.769006	-0.662377	-1.485616
H	2.898066	-2.773955	-1.198696	H	-1.122089	0.834630	2.889853
C	5.390209	-1.890751	1.638567	C	-1.822433	0.047598	-1.890551
H	3.973528	-0.361041	2.193595	C	-4.135942	2.032799	0.776442
				H	-4.966871	2.370321	0.163894



C	4.090750	5.389191	0.953033	H	-4.015568	2.889771	2.547773
H	2.795084	3.990124	1.961618	H	-5.188564	1.967938	3.506458
C	4.793126	5.678117	-0.219581	C	-4.462522	1.352279	0.410503
H	5.288605	5.000959	-2.209259	C	-3.292242	1.883315	-0.151177
H	4.123587	6.078282	1.793018	C	-5.696150	1.856368	-0.021291
H	5.374249	6.593196	-0.297505	C	-3.355548	2.877979	-1.129311
H	2.041201	1.979174	1.093139	H	-2.327293	1.524763	0.192078
C	0.427855	3.308500	-0.703551	C	-5.766931	2.847926	-1.004507
C	-0.256978	3.508824	0.505505	H	-6.612365	1.464337	0.415475
C	0.348891	4.291217	-1.697092	C	-4.593966	3.361103	-1.564487
C	-0.991623	4.675837	0.718056	H	-2.436879	3.285432	-1.541406
H	-0.239779	2.738461	1.272360	H	-6.735771	3.221789	-1.327178
C	-0.388821	5.460477	-1.486509	H	-4.642094	4.136437	-2.325042
H	0.877748	4.144974	-2.635826	H	-5.416777	0.067187	1.816125
C	-1.056885	5.657908	-0.275545	C	-4.164186	-1.479913	-0.370989
H	-1.521567	4.814033	1.657034	C	-5.506095	-1.450880	-0.780455
H	-0.439221	6.214860	-2.267488	C	-3.217866	-2.038271	-1.246016
H	-1.630216	6.566071	-0.109119	C	-5.886955	-1.937031	-2.034674
H	1.685239	2.067294	-1.924526	H	-6.260943	-1.034261	-0.120130
H	-0.086461	0.827450	0.063291	C	-3.592309	-2.522432	-2.502032
C	-0.412518	0.599317	-1.935644	H	-2.184011	-2.111289	-0.919534
H	0.177342	0.411082	-2.837390	C	-4.930336	-2.468439	-2.904713
H	-1.036701	-0.274322	-1.742298	H	-6.932069	-1.897769	-2.332833
H	-1.060914	1.465829	-2.109437	H	-2.838323	-2.940102	-3.165622
C	1.831293	-0.611209	4.027206	H	-5.225757	-2.839532	-3.882970
H	2.767563	-0.251941	4.468085	H	-2.634021	-0.778126	0.921156
H	1.249090	-1.082501	4.828607	C	-4.998165	-2.818751	2.143862
C	2.066693	-1.640494	2.893664	H	-5.817088	-2.146372	2.427989
H	3.035600	-1.471959	2.409264	H	-5.316338	-3.351157	1.229954
H	2.094225	-2.661382	3.289078	H	-4.892146	-3.561603	2.943559
C	0.236520	-0.197457	2.249200	H	-2.971930	-2.696747	1.836002
O	-0.767012	0.351027	1.715617				
C	0.996551	0.500454	3.381091				
H	0.289505	0.991729	4.058675	<b>TS4-D-2.log</b>			
H	1.628820	1.289488	2.951893	C	-0.657291	-1.999507	1.180801
C	5.143081	-3.204626	0.088488	C	0.962506	-3.837413	0.964438
H	6.198091	-3.078909	-0.138679	C	2.751717	-5.268440	1.787279
N	-3.752720	-2.072814	2.026494	O	-1.757844	-1.586284	0.764050
C	-3.698741	-1.008758	1.006263	N	-0.375270	-3.370528	1.040375
C	-4.385712	0.293472	1.510618	C	1.880513	-3.266083	0.056952
N	-3.669777	0.754152	2.712044	H	3.081495	-6.056778	2.457681
H	-2.670560	0.795518	2.503959	C	-1.449096	-4.239812	0.558210
C	-4.125678	2.034303	3.238335	C	3.218403	-3.680426	0.023766
H	-3.565070	2.267808	4.151550	H	-1.169757	-5.280184	0.738880
				H	-1.634531	-4.102124	-0.514656

H	-2.371886	-4.016344	1.098024	H	0.268266	1.675343	-2.732836
H	3.896009	-3.250004	-0.705806	C	1.223286	-0.656578	4.104158
C	0.318205	-1.195720	1.906252	H	2.161175	-0.664183	4.670334
C	1.421565	-4.843342	1.821254	H	0.405720	-0.796050	4.822010
H	0.724412	-5.269444	2.537236	C	1.165519	-1.782877	3.041165
I	0.962811	-2.882162	-2.136532	H	2.173336	-2.061309	2.710395
Cu	1.641707	-1.210889	-0.225855	H	0.719249	-2.690284	3.461188
N	1.117570	0.671283	-1.048002	C	0.189424	0.216830	2.087799
C	2.294691	1.575316	-1.011933	O	-0.423315	1.068654	1.394908
C	3.175414	1.254446	0.218005	C	0.995943	0.642208	3.321910
N	3.531061	-0.186824	0.197786	H	0.448102	1.413944	3.874151
H	4.110060	-0.368722	-0.624512	H	1.942233	1.096198	2.998494
C	4.275126	-0.612797	1.394659	C	3.658074	-4.667999	0.908680
H	4.425087	-1.693977	1.351321	H	4.697807	-4.982393	0.887078
H	5.250400	-0.116783	1.482211	N	-2.073742	2.150466	-0.928612
H	3.682356	-0.378890	2.281627	C	-3.101240	1.321453	-0.267084
C	4.378727	2.180537	0.296607	C	-3.852871	0.407859	-1.280079
C	5.384124	2.139447	-0.680518	N	-2.893035	-0.566583	-1.830091
C	4.492221	3.100178	1.345721	H	-2.470514	-1.079542	-1.053963
C	6.478047	3.003894	-0.610072	C	-3.454534	-1.500894	-2.797752
H	5.311421	1.432539	-1.504264	H	-2.661229	-2.176669	-3.138716
C	5.583926	3.969861	1.417381	H	-4.286783	-2.119340	-2.417193
H	3.716137	3.138453	2.106437	H	-3.828481	-0.952354	-3.672396
C	6.580532	3.923179	0.439377	C	-5.074483	-0.261029	-0.646866
H	7.249004	2.962479	-1.375238	C	-4.939790	-1.085580	0.482415
H	5.655866	4.680302	2.236906	C	-6.347203	-0.104273	-1.209945
H	7.431095	4.597649	0.492814	C	-6.054689	-1.712718	1.042074
H	2.565489	1.399918	1.111222	H	-3.956540	-1.240438	0.916451
C	1.897668	3.044010	-1.058680	C	-7.466364	-0.731919	-0.653242
C	1.080606	3.593329	-0.056967	H	-6.465049	0.523375	-2.090992
C	2.324606	3.864375	-2.108820	C	-7.324039	-1.536719	0.479437
C	0.695837	4.934039	-0.114638	H	-5.933157	-2.342204	1.920717
H	0.726777	2.966327	0.757758	H	-8.445393	-0.593044	-1.105749
C	1.944042	5.208914	-2.165317	H	-8.190611	-2.025567	0.917528
H	2.960009	3.448473	-2.887072	H	-4.213391	1.015191	-2.121146
C	1.126758	5.747305	-1.168720	C	-4.001471	2.154760	0.641562
H	0.057484	5.343820	0.664049	C	-5.154325	2.814716	0.188746
H	2.282897	5.831605	-2.989347	C	-3.606621	2.347390	1.975044
H	0.826117	6.790837	-1.212319	C	-5.901052	3.626922	1.047030
H	2.886045	1.341372	-1.904923	H	-5.478780	2.685031	-0.839595
H	0.419171	0.976950	-0.356567	C	-4.349864	3.157302	2.837247
C	0.490692	0.660790	-2.380150	H	-2.696356	1.864648	2.324792
H	1.166935	0.176414	-3.091384	C	-5.504268	3.798310	2.376555
H	-0.443850	0.102100	-2.329738	H	-6.794212	4.124625	0.676605



H	-4.030378	3.285811	3.868896	H	-6.478381	0.537232	1.631923
H	-6.087438	4.426184	3.045580	C	-6.396901	3.886704	2.242326
H	-2.525603	0.651654	0.376203	H	-4.718209	5.174454	1.810296
C	-2.517258	3.315721	-1.682284	H	-7.887011	2.357052	2.556805
H	-3.134652	3.004811	-2.533447	H	-7.011802	4.686567	2.646321
H	-3.100664	4.053870	-1.104400	H	-4.467229	-0.252596	0.754993
H	-1.635039	3.827509	-2.083230	C	-5.097849	1.068958	-1.650196
H	-1.411476	2.432125	-0.211724	C	-6.016465	0.009259	-1.684564
<b>TS4-D-3.log</b>				C	-5.424346	2.269173	-2.291887
C	0.673936	0.654174	1.096895	C	-7.237875	0.150402	-2.345243
C	1.502624	-1.332458	-0.289678	H	-5.780409	-0.929219	-1.187520
C	0.407557	-2.462855	1.615857	C	-6.647348	2.414585	-2.952680
C	-0.317036	-3.089118	3.856424	H	-4.717979	3.095480	-2.268702
O	2.269841	-1.482427	-1.265171	C	-7.557017	1.354820	-2.981322
N	1.432964	-2.344451	0.657869	H	-7.941709	-0.677658	-2.361714
C	-0.944506	-2.318075	1.273393	H	-6.886304	3.353095	-3.446095
H	-0.058790	-3.384326	4.869622	H	-8.508319	1.465071	-3.495083
C	2.397678	-3.446709	0.557017	H	-3.198444	1.846033	-1.057179
C	-1.973464	-2.614373	2.163686	C	-2.454122	0.089343	-2.847931
H	2.021824	-4.300344	1.122697	H	-1.836726	-0.755358	-3.164074
H	2.511503	-3.733923	-0.490638	H	-3.282610	0.216807	-3.556272
H	3.376502	-3.150859	0.946205	H	-1.845730	0.996271	-2.851747
H	-3.005954	-2.561993	1.836009	H	-3.495171	-1.019328	-1.504003
C	0.707491	-0.109584	-0.132766	C	0.038832	2.131767	-0.749225
C	0.700767	-2.822676	2.938649	H	-1.039907	2.037498	-0.911920
H	1.743098	-2.884306	3.237715	H	0.364528	3.050863	-1.247506
I	-1.483302	-3.378311	-1.065827	C	0.750089	0.875997	-1.296544
Cu	-1.478752	-0.891056	-0.034550	H	0.282342	0.491316	-2.207843
N	-2.927101	-0.169502	-1.476383	H	1.794058	1.108446	-1.557130
C	-3.769454	0.921313	-0.926246	O	0.928967	0.291825	2.261632
C	-3.958078	0.705318	0.597790	C	0.352370	2.117833	0.754860
N	-2.616865	0.574336	1.210373	H	1.250881	2.701291	0.989749
H	-2.089384	1.415231	0.980058	H	-0.443338	2.514323	1.397594
C	-2.617700	0.445841	2.675567	C	-1.656329	-2.985008	3.475683
H	-3.221801	-0.416202	2.965179	H	-2.455286	-3.207216	4.177568
H	-1.587980	0.282565	3.000386	N	3.970462	-0.294569	1.861318
H	-3.021999	1.337579	3.171282	C	4.420820	0.451421	0.681398
C	-4.806111	1.819402	1.193723	C	5.558493	-0.274868	-0.100173
C	-4.319456	3.133840	1.250760	N	5.221947	-1.688685	-0.283667
C	-6.093426	1.553262	1.673212	H	4.288310	-1.762269	-0.688466
C	-5.108119	4.160641	1.772249	C	6.182963	-2.440583	-1.081609
H	-3.319174	3.357912	0.886947	H	5.858663	-3.486215	-1.139238
C	-6.887704	2.579757	2.191883	H	6.322528	-2.070533	-2.112607
				H	7.165245	-2.419754	-0.591222

C	5.818858	0.482280	-1.405391	H	-3.031730	-3.031807	1.385784
C	4.852547	0.486538	-2.424948	C	0.655084	-0.195881	-0.094576
C	7.014381	1.179989	-1.612192	C	0.611576	-3.241124	2.683087
C	5.076063	1.184844	-3.613215	H	1.637171	-3.293958	3.036872
H	3.922311	-0.059045	-2.282865	I	-1.251957	-3.445723	-1.496216
C	7.241551	1.881369	-2.800715	Cu	-1.553914	-1.090965	-0.196487
H	7.771036	1.182392	-0.830561	N	-2.764123	0.093060	-1.574239
C	6.271171	1.887211	-3.805714	C	-3.579315	1.102652	-0.816565
H	4.316284	1.181413	-4.391432	C	-3.962708	0.544764	0.573887
H	8.175694	2.420048	-2.940847	N	-2.692661	0.178326	1.247756
H	6.444186	2.430800	-4.731116	H	-2.090289	1.001258	1.228859
H	6.481549	-0.237214	0.493428	C	-2.830381	-0.220324	2.656406
C	4.787014	1.916185	0.926414	H	-3.510103	-1.071180	2.733155
C	5.930996	2.296511	1.648379	H	-1.845104	-0.515938	3.020273
C	3.970613	2.930171	0.404434	H	-3.219604	0.594307	3.279623
C	6.225893	3.644863	1.867928	C	-4.789231	1.546505	1.368154
H	6.609233	1.538207	2.026884	C	-4.268153	2.810173	1.685557
C	4.262285	4.280055	0.616895	C	-6.071534	1.213250	1.818263
H	3.106899	2.655454	-0.194563	C	-5.021156	3.724048	2.424279
C	5.389768	4.642932	1.358437	H	-3.265880	3.081273	1.361531
H	7.115306	3.915498	2.431818	C	-6.829617	2.126520	2.556477
H	3.613830	5.045173	0.196920	H	-6.480610	0.233386	1.584465
H	5.621880	5.691233	1.527868	C	-6.306863	3.385921	2.859711
H	3.552447	0.450260	0.015657	H	-4.604396	4.699490	2.661422
C	4.851209	-0.387715	3.014353	H	-7.825351	1.852225	2.895098
H	5.806949	-0.839864	2.723707	H	-6.893448	4.098026	3.434100
H	5.073345	0.569874	3.516624	H	-4.533662	-0.382658	0.458478
H	4.385824	-1.048821	3.755548	C	-4.738771	1.680521	-1.611331
H	3.045902	0.031225	2.137221	C	-6.011108	1.090698	-1.632060
				C	-4.518959	2.832433	-2.378589
				C	-7.038711	1.643572	-2.398451
				H	-6.203358	0.196520	-1.047216
				C	-5.543785	3.387348	-3.148923
				H	-3.536793	3.300392	-2.367606
				C	-6.808691	2.793908	-3.159326
				H	-8.019864	1.176000	-2.400148
				H	-5.355409	4.283967	-3.733674
				H	-7.610167	3.225097	-3.753331
				H	-2.889130	1.927755	-0.629064
				C	0.044129	2.126182	-0.484947
				H	-1.024885	2.139096	-0.707126
				H	0.459776	3.070357	-0.852537
				C	0.703491	0.898704	-1.155430
				H	0.201141	0.618414	-2.089307
<b>TS4-D-4.log</b>							
C	0.563724	0.429076	1.207244				
C	1.495676	-1.370551	-0.336217				
C	0.374206	-2.722267	1.401528				
C	-0.438220	-3.685126	3.489187				
O	2.294049	-1.411286	-1.297351				
N	1.445262	-2.456967	0.526766				
C	-0.963673	-2.587578	1.000989				
H	-0.219825	-4.102822	4.468165				
C	2.461498	-3.502719	0.352565				
C	-2.018400	-3.071555	1.770703				
H	2.137825	-4.405143	0.872053				
H	2.579251	-3.724966	-0.710843				
H	3.428414	-3.179553	0.749485				

H	1.746995	1.118740	-1.423015	H	2.945794	-0.109969	2.169769
O	0.764412	-0.061462	2.334633	C	-3.548524	-0.801449	-2.450448
C	0.262955	1.924269	1.021723	H	-4.147229	-0.247593	-3.180633
H	1.140580	2.468420	1.390869	H	-2.854885	-1.453935	-2.979870
H	-0.577995	2.245229	1.649850	H	-4.209968	-1.421277	-1.839890
C	-1.756685	-3.608012	3.036554	H	-2.120330	0.616280	-2.167633
H	-2.578982	-3.973578	3.645269				
N	3.877166	-0.376971	1.858331	<b>TS4-D-5.log</b>			
C	4.303566	0.503160	0.764936	C	0.612413	-2.085109	1.601147
C	5.492655	-0.081322	-0.058896	C	-0.773845	-3.973808	0.840542
N	5.259641	-1.497810	-0.344424	C	-2.564113	-5.613417	1.033992
H	4.325363	-1.612615	-0.738136	O	1.758664	-1.607140	1.537180
C	6.258014	-2.115890	-1.207947	N	0.456813	-3.447214	1.307630
H	6.013205	-3.176898	-1.335466	C	-1.470943	-3.376558	-0.233520
H	6.349204	-1.665647	-2.212020	H	-2.981234	-6.485365	1.529414
H	7.245759	-2.054233	-0.732029	C	1.675821	-4.218105	1.049077
C	5.696093	0.789182	-1.302854	C	-2.684648	-3.911747	-0.680729
C	4.749739	0.768876	-2.340595	H	2.402912	-4.037986	1.844069
C	6.812301	1.623960	-1.429610	H	1.423446	-5.280142	1.027626
C	4.914192	1.574893	-3.468900	H	2.133526	-3.939353	0.091897
H	3.879660	0.121678	-2.257045	H	-3.164428	-3.493006	-1.556054
C	6.978853	2.435235	-2.556656	C	-0.572781	-1.338269	2.033311
H	7.552792	1.647295	-0.633087	C	-1.344257	-5.087715	1.466147
C	6.028773	2.413803	-3.580759	H	-0.823987	-5.523212	2.314800
H	4.170684	1.549860	-4.262279	I	-0.066293	-2.666317	-2.098773
H	7.850696	3.080390	-2.634613	Cu	-1.365245	-1.286537	-0.256063
H	6.155880	3.041608	-4.459101	N	-0.778798	0.728886	-0.566894
H	6.410232	-0.018588	0.541365	C	-1.936440	1.552251	-0.121785
C	4.587044	1.956714	1.147542	C	-3.231190	1.042538	-0.793582
C	5.685802	2.327507	1.941248	N	-3.414433	-0.387015	-0.416494
C	3.745485	2.973579	0.672572	H	-3.735782	-0.413399	0.551880
C	5.910949	3.665661	2.275817	C	-4.426224	-1.060823	-1.246732
H	6.385118	1.571885	2.284556	H	-4.016729	-1.226520	-2.248110
C	3.967862	4.313638	0.999950	H	-4.666249	-2.026349	-0.798586
H	2.917771	2.711621	0.019564	H	-5.352602	-0.477645	-1.335546
C	5.050065	4.664620	1.811285	C	-4.442910	1.885737	-0.425651
H	6.766790	3.928660	2.892762	C	-4.806601	2.062611	0.918512
H	3.301379	5.081191	0.614044	C	-5.231217	2.475858	-1.420403
H	5.228526	5.705350	2.069288	C	-5.928043	2.820723	1.257557
H	3.447304	0.517423	0.084309	H	-4.209007	1.608613	1.706243
C	4.763572	-0.573109	2.994056	C	-6.355383	3.236045	-1.084624
H	5.728457	-0.966777	2.653746	H	-4.958078	2.343944	-2.464600
H	4.962049	0.328366	3.599191	C	-6.705889	3.411724	0.256064
H	4.316838	-1.323387	3.657871	H	-6.194030	2.952305	2.303192



H	-0.823987	-5.523212	2.314800	C	-1.522281	0.370003	3.468703
I	-0.066293	-2.666317	-2.098773	H	-1.939395	1.371203	3.313644
Cu	-1.365245	-1.286537	-0.256063	H	-1.034453	0.369114	4.455073
N	-0.778798	0.728886	-0.566894	C	-3.244320	-5.013924	-0.028689
C	-1.936440	1.552251	-0.121785	H	-4.190879	-5.417119	-0.378028
C	-3.231190	1.042538	-0.793582	C	-0.222628	1.036827	-1.892477
N	-3.414433	-0.387015	-0.416494	H	0.660021	0.411382	-2.041830
H	-3.735782	-0.413399	0.551880	H	-0.950190	0.794205	-2.671910
C	-4.426224	-1.060823	-1.246732	H	0.071830	2.087605	-1.992101
H	-4.016729	-1.226520	-2.248110	H	-0.047999	0.844612	0.144649
H	-4.666249	-2.026349	-0.798586	N	3.403117	1.482699	2.724577
H	-5.352602	-0.477645	-1.335546	C	3.503776	1.200233	1.281207
C	-4.442910	1.885737	-0.425651	C	4.697406	0.265063	0.939510
C	-4.806601	2.062611	0.918512	N	4.656599	-0.912920	1.813056
C	-5.231217	2.475858	-1.420403	H	3.716457	-1.306154	1.791101
C	-5.928043	2.820723	1.257557	C	5.640855	-1.939264	1.495502
H	-4.209007	1.608613	1.706243	H	5.557432	-2.753569	2.225486
C	-6.355383	3.236045	-1.084624	H	5.548976	-2.380300	0.486553
H	-4.958078	2.343944	-2.464600	H	6.653315	-1.520881	1.576220
C	-6.705889	3.411724	0.256064	C	4.679989	-0.062448	-0.556933
H	-6.194030	2.952305	2.303192	C	3.617303	-0.788390	-1.121308
H	-6.955371	3.688407	-1.869978	C	5.733683	0.334091	-1.389617
H	-7.578679	4.003005	0.520128	C	3.607619	-1.087948	-2.485649
H	-3.104862	1.058389	-1.880272	H	2.803916	-1.129697	-0.485501
C	-1.700807	3.050769	-0.235317	C	5.726694	0.037075	-2.756136
C	-1.984235	3.778248	-1.400358	H	6.566866	0.888673	-0.963585
C	-1.153941	3.726964	0.864934	C	4.659415	-0.673248	-3.310316
C	-1.746858	5.154196	-1.455548	H	2.777057	-1.649719	-2.905534
H	-2.402920	3.273911	-2.266167	H	6.554308	0.358557	-3.384054
C	-0.918100	5.102383	0.813598	H	4.648372	-0.907628	-4.371825
H	-0.888860	3.158604	1.752865	H	5.644106	0.782205	1.147067
C	-1.219987	5.822038	-0.345990	C	3.471784	2.462741	0.417236
H	-1.977752	5.704192	-2.364262	C	4.617494	3.209515	0.097887
H	-0.495203	5.609970	1.676699	C	2.231895	2.936890	-0.035292
H	-1.039929	6.893060	-0.387882	C	4.525633	4.377583	-0.664964
H	-2.035314	1.323650	0.940998	H	5.593660	2.873554	0.434351
C	-0.446255	0.042212	2.429358	C	2.132303	4.098612	-0.804284
C	-2.533195	-0.772858	3.348726	H	1.334123	2.392597	0.234022
H	-3.067368	-0.985910	4.280525	C	3.283371	4.823652	-1.125799
H	-3.284760	-0.516093	2.592141	H	5.427524	4.936793	-0.902684
C	-1.699567	-1.975316	2.856032	H	1.157786	4.434428	-1.147213
H	-1.290381	-2.536836	3.711292	H	3.213413	5.727774	-1.725488
H	-2.323297	-2.675337	2.295196	H	2.594332	0.633741	1.068449
O	0.364314	0.912659	2.037771	C	4.388426	2.393446	3.291100

H	5.389705	1.951736	3.217040	H	9.192368	-1.636241	2.111625
H	4.432603	3.391855	2.821082	H	3.819900	0.681494	1.753237
H	4.169206	2.534542	4.356038	C	5.143688	1.939566	-0.389375
H	2.458251	1.822243	2.892871	C	5.051124	3.014115	0.507730
<b>TS4-D-7.log</b>				C	6.208534	1.905935	-1.296782
C	-0.577756	-0.242856	1.851767	C	6.006182	4.032026	0.496731
C	-1.319420	0.155738	-0.563308	H	4.231041	3.057458	1.220872
C	-0.849907	-2.271368	-0.520962	C	7.168388	2.921871	-1.308540
C	-0.697051	-4.529906	0.375610	H	6.287181	1.076526	-1.995497
O	-1.840212	1.078784	-1.227560	C	7.069704	3.987775	-0.410976
N	-1.635086	-1.156535	-0.908344	H	5.922453	4.857973	1.198331
C	0.544551	-2.282196	-0.707419	H	7.989654	2.880641	-2.019415
H	-1.190767	-5.402745	0.793415	H	7.814093	4.779641	-0.418507
C	-2.618186	-1.350911	-1.980237	H	4.317036	0.134084	-1.198901
C	1.309983	-3.405514	-0.366983	H	2.488098	1.934106	0.191411
H	-2.283211	-0.876052	-2.909230	C	2.529969	2.029425	-1.838390
H	-3.584518	-0.924613	-1.702524	H	2.846228	1.394476	-2.669242
H	-2.740903	-2.421033	-2.151797	H	1.466803	2.251253	-1.960066
H	2.373814	-3.420196	-0.575167	H	3.102885	2.964421	-1.870469
C	-0.426284	0.427641	0.566679	C	-0.140336	1.898699	0.877815
C	-1.449847	-3.406124	0.035985	H	0.396911	2.425994	0.084605
H	-2.519634	-3.385429	0.219445	H	-1.085703	2.439338	1.031809
I	1.302183	-1.312852	-2.812136	C	0.637489	1.840014	2.207881
Cu	1.440080	-0.428839	-0.261772	H	1.689571	1.591290	2.022531
N	2.720664	1.300365	-0.572603	H	0.610860	2.787189	2.757263
C	4.110930	0.823676	-0.372417	O	-1.137605	-1.317346	2.119535
C	4.164275	0.019424	0.951381	C	-0.034215	0.681774	2.951903
N	3.186608	-1.093000	0.879666	H	0.610782	0.140982	3.652430
H	3.586027	-1.824312	0.290370	H	-0.909152	1.032708	3.515827
C	2.876746	-1.676515	2.194840	C	0.688822	-4.523017	0.194822
H	2.153874	-2.484137	2.057767	H	1.287233	-5.391421	0.456782
H	3.767352	-2.071137	2.702262	N	-3.484261	0.833388	2.365031
H	2.424732	-0.906072	2.823727	C	-4.358244	0.684041	1.187391
C	5.572953	-0.449854	1.279406	C	-4.876922	2.052004	0.660014
C	6.244585	-1.341934	0.429266	N	-3.732692	2.949143	0.462174
C	6.223166	0.003607	2.432748	H	-3.040133	2.485281	-0.127875
C	7.539872	-1.767782	0.726966	C	-4.075429	4.255128	-0.088293
H	5.757087	-1.700912	-0.474832	H	-3.162718	4.855001	-0.180434
C	7.521179	-0.419753	2.733202	H	-4.565624	4.228591	-1.077199
H	5.711474	0.697164	3.095587	H	-4.753297	4.778115	0.599222
C	8.182977	-1.306394	1.880553	C	-5.733842	1.837511	-0.591409
H	8.048815	-2.456259	0.057381	C	-5.139343	1.453534	-1.803818
H	8.012573	-0.057053	3.632257	C	-7.120742	2.028009	-0.557901
				C	-5.918593	1.240442	-2.943312

H	-4.061969	1.321439	-1.852829	I	-1.966683	3.894703	-0.622997
C	-7.904464	1.816482	-1.696450	Cu	-1.700414	1.315581	-0.002110
H	-7.593295	2.338133	0.371116	N	-3.067591	0.299865	-1.250391
C	-7.305499	1.417004	-2.893947	C	-3.901131	-0.597318	-0.395659
H	-5.441339	0.937824	-3.872525	C	-2.930461	-1.361036	0.534440
H	-8.980316	1.966567	-1.647594	N	-2.225744	-0.373955	1.406861
H	-7.911117	1.250719	-3.781266	C	-3.550949	-2.523432	1.293133
H	-5.520347	2.513393	1.420197	C	-4.845387	-2.468115	1.831055
C	-5.455163	-0.356745	1.394057	C	-2.787097	-3.680153	1.498179
C	-6.657692	-0.084934	2.066174	C	-5.363574	-3.545740	2.551407
C	-5.222735	-1.669214	0.955192	H	-5.453698	-1.580693	1.685635
C	-7.597240	-1.095713	2.289168	C	-3.301055	-4.760115	2.220357
H	-6.871700	0.923664	2.405979	H	-1.782195	-3.735158	1.085315
C	-6.159347	-2.682100	1.172459	C	-4.593221	-4.696017	2.748173
H	-4.293607	-1.893064	0.436317	H	-6.369894	-3.487234	2.957926
C	-7.352678	-2.397841	1.843094	H	-2.695211	-5.650789	2.365534
H	-8.523591	-0.863734	2.809128	H	-4.998385	-5.535589	3.306859
H	-5.958792	-3.689784	0.816506	H	-2.149884	-1.774220	-0.104066
H	-8.086202	-3.181760	2.013376	C	-4.791569	-1.511742	-1.220867
H	-3.704090	0.293208	0.403170	C	-4.245221	-2.548053	-1.992461
C	-4.091536	1.337843	3.590051	C	-6.176930	-1.310786	-1.244668
H	-4.416720	2.375042	3.449208	C	-5.068863	-3.368440	-2.764716
H	-4.957462	0.759481	3.955572	H	-3.172870	-2.722365	-1.984693
H	-3.331458	1.334796	4.379590	C	-7.004979	-2.130730	-2.016312
H	-3.039201	-0.065224	2.540215	H	-6.609348	-0.508665	-0.651215
<b>TS4-D-8.log</b>				C	-6.452406	-3.163011	-2.778216
C	0.706778	-0.328686	0.056100	H	-4.630959	-4.170355	-3.353381
C	1.101120	1.909153	-1.119872	H	-8.078583	-1.961554	-2.021704
C	0.655036	2.668237	1.206189	H	-7.093416	-3.803127	-3.378572
C	0.646710	3.028956	3.620228	H	-4.532114	0.063346	0.207127
O	1.523890	2.274057	-2.234386	H	-2.499196	-0.293039	-1.856758
N	1.362056	2.711919	-0.008098	C	-3.866372	1.180577	-2.123653
C	-0.744195	2.553053	1.265166	H	-4.469933	1.847319	-1.502856
H	1.204813	3.204811	4.535882	H	-3.184947	1.786943	-2.723358
C	2.336447	3.801731	-0.153024	H	-4.526189	0.610581	-2.787830
C	-1.445910	2.768774	2.450981	C	0.162968	-0.120126	-2.287540
H	2.420603	4.044904	-1.211215	H	-0.669652	0.294343	-2.871385
H	3.319343	3.494323	0.215734	H	1.049613	-0.029781	-2.927878
H	1.987617	4.679580	0.397306	C	-0.076280	-1.599433	-1.895103
H	-2.529410	2.783278	2.436887	H	-1.144900	-1.831807	-1.870445
C	0.404011	0.625178	-0.976447	H	0.369713	-2.285549	-2.622720
C	1.335652	2.874279	2.417705	O	1.119645	-0.140137	1.224360
H	2.420179	2.904027	2.400130	C	0.537012	-1.748883	-0.496049
				H	-0.044627	-2.372987	0.192598





H	1.039957	4.114363	-2.632711	H	-2.140776	3.442712	-1.449062
C	-0.677339	5.728542	-0.174696	H	-6.441850	3.498918	-1.604479
H	-1.074052	4.913447	1.785005	H	-4.245440	4.346656	-2.425108
H	-0.137524	6.253219	-2.197909	H	-5.489110	0.359485	1.678809
H	-1.194452	6.664590	0.019140	C	-4.061564	-1.275997	-0.358249
H	1.759674	2.008959	-1.975438	C	-5.341383	-1.208726	-0.929001
H	-0.093257	0.904582	-0.007731	C	-3.041626	-1.904228	-1.092030
C	-0.379782	0.668486	-2.008821	C	-5.588691	-1.729736	-2.202892
H	0.217742	0.389285	-2.881307	H	-6.151032	-0.735983	-0.381008
H	-1.102534	-0.125174	-1.815546	C	-3.282123	-2.423323	-2.366260
H	-0.921871	1.595508	-2.229108	H	-2.056229	-1.999292	-0.644137
C	2.214026	-0.006895	3.483947	C	-4.558929	-2.334572	-2.929801
H	3.087338	0.585011	3.196914	H	-6.587300	-1.661133	-2.627936
H	2.189772	-0.081027	4.575240	H	-2.470243	-2.894218	-2.916407
C	2.164478	-1.382536	2.786876	H	-4.750832	-2.734198	-3.922477
H	3.095250	-1.578865	2.248339	H	-2.665767	-0.595027	1.081131
H	2.043390	-2.189350	3.520091	C	-5.233771	-2.515756	2.074324
C	0.283387	-0.021112	2.199275	H	-6.046265	-1.806323	2.273709
O	-0.767186	0.485509	1.783449	H	-5.483300	-3.042832	1.136305
O	1.040416	0.727058	3.066303	H	-5.238192	-3.255129	2.884146
C	4.838175	-3.589235	-0.081769	H	-3.187072	-2.492536	1.976758
H	5.862740	-3.581398	-0.443212				
C	4.510797	0.311557	0.426292				
H	4.903433	-0.676502	0.182285	<b>TS4-E-2.log</b>			
H	5.290247	1.061307	0.241592	C	0.980109	-2.482115	1.200341
H	4.256235	0.330063	1.487338	C	3.389526	-2.820461	0.862686
H	3.555849	0.582844	-1.353702	C	5.766806	-2.753843	1.386991
N	-3.949777	-1.827324	2.077261	O	-0.144856	-2.935631	0.946241
C	-3.740899	-0.785736	1.052317	N	2.090483	-3.333274	1.108154
C	-4.429739	0.548762	1.458876	C	3.613939	-1.852538	-0.138956
N	-3.808548	1.017653	2.710101	H	6.599958	-3.110936	1.985401
H	-2.798128	1.063269	2.575032	C	1.843385	-4.742158	0.795337
C	-4.302934	2.303340	3.188987	C	4.899132	-1.364085	-0.393008
H	-3.810048	2.547236	4.137507	H	2.722601	-5.329918	1.067699
H	-4.144849	3.150605	2.498252	H	1.635232	-4.887675	-0.272713
H	-5.381968	2.234996	3.379804	H	0.983260	-5.093974	1.367225
C	-4.379292	1.588370	0.339122	H	5.055673	-0.660533	-1.203485
C	-3.150479	2.080618	-0.125129	C	1.259413	-1.113547	1.656254
C	-5.556787	2.120302	-0.202383	C	4.480449	-3.245027	1.628357
C	-3.102058	3.066409	-1.112977	H	4.304020	-3.959877	2.427451
H	-2.227959	1.699815	0.300902	I	2.370917	-2.248404	-2.230609
C	-5.515039	3.102380	-1.196697	Cu	2.143119	-0.396702	-0.331774
H	-6.517798	1.758825	0.157657	N	0.594001	0.884238	-1.094742
C	-4.284651	3.578212	-1.657070	C	0.951755	2.317591	-0.883671
				C	2.002967	2.461077	0.240350

N	3.151106	1.574253	-0.080324	H	6.970752	-1.415681	0.188513
H	3.502000	1.819195	-1.008295	N	-2.937560	0.954894	-1.489644
C	4.263553	1.686449	0.875907	C	-3.584330	0.083062	-0.490327
H	5.037008	0.965568	0.606881	C	-3.502812	-1.422939	-0.868162
H	4.703799	2.691287	0.894263	N	-2.118889	-1.799414	-1.181761
H	3.903230	1.446651	1.877794	H	-1.526845	-1.633481	-0.366540
C	2.381733	3.920088	0.442502	C	-1.971916	-3.186672	-1.608643
C	3.030074	4.642431	-0.569896	H	-0.913062	-3.390215	-1.796242
C	2.081679	4.565124	1.647988	H	-2.332380	-3.933837	-0.880986
C	3.366468	5.983966	-0.380639	H	-2.523788	-3.343290	-2.545528
H	3.276606	4.153688	-1.509857	C	-4.130329	-2.267474	0.245429
C	2.413672	5.909121	1.839860	C	-3.497470	-2.376022	1.494542
H	1.579714	4.010726	2.437326	C	-5.327770	-2.963528	0.038639
C	3.057107	6.622271	0.825186	C	-4.063551	-3.146529	2.512342
H	3.868985	6.531717	-1.173678	H	-2.547248	-1.875228	1.656856
H	2.172047	6.396641	2.780826	C	-5.897548	-3.735811	1.055832
H	3.317971	7.667043	0.972047	H	-5.822905	-2.895606	-0.927414
H	1.579945	2.077772	1.171540	C	-5.268002	-3.826516	2.299708
C	-0.291679	3.163107	-0.659409	H	-3.561209	-3.220709	3.474285
C	-1.012597	3.081397	0.543108	H	-6.828957	-4.267157	0.874742
C	-0.782890	3.978897	-1.686157	H	-5.706613	-4.426137	3.093473
C	-2.200845	3.795386	0.706126	H	-4.089698	-1.595569	-1.779430
H	-0.666035	2.436055	1.343238	C	-5.000326	0.546009	-0.151091
C	-1.977292	4.689451	-1.527381	C	-6.122602	0.228193	-0.933945
H	-0.229315	4.054350	-2.618808	C	-5.183524	1.396715	0.950303
C	-2.691323	4.597937	-0.330375	C	-7.383634	0.746362	-0.625264
H	-2.749978	3.718494	1.640754	H	-6.018055	-0.439402	-1.783621
H	-2.347104	5.311341	-2.338430	C	-6.441196	1.917160	1.263854
H	-3.622086	5.144499	-0.204042	H	-4.325178	1.651498	1.568335
H	1.436019	2.647854	-1.809454	C	-7.548638	1.593514	0.474289
H	-0.211709	0.655870	-0.503221	H	-8.238982	0.484183	-1.243370
C	0.207941	0.631999	-2.495101	H	-6.557174	2.569620	2.125957
H	1.099882	0.672513	-3.127080	H	-8.530259	1.993449	0.715424
H	-0.236830	-0.361093	-2.561223	H	-2.980117	0.204526	0.411218
H	-0.525444	1.364530	-2.849959	C	-3.514486	0.987591	-2.826965
C	1.697728	0.432454	3.442656	H	-3.386874	0.014538	-3.314893
H	2.323003	1.307292	3.242716	H	-4.586257	1.248750	-2.867700
H	1.560655	0.344025	4.523998	H	-2.969477	1.729839	-3.420838
C	2.248888	-0.853295	2.793509	H	-2.915435	1.898146	-1.109361
H	3.279673	-0.708922	2.459663	O	0.400897	0.683393	2.853618
H	2.258870	-1.682263	3.513011				
C	0.141288	-0.225872	1.851794				
O	-0.935081	-0.128826	1.258100				
C	5.975041	-1.803384	0.385729				
				<b>TS4-E-3.log</b>			
				C	0.202266	-2.366458	1.620304
				C	2.215741	-3.575332	0.903004

C	4.515668	-4.351322	1.097297	H	-0.122321	0.894475	-0.068153
O	-1.037543	-2.391251	1.645734	C	-0.390054	0.617405	-2.068651
N	0.883715	-3.563002	1.385445	H	0.222257	0.339660	-2.931361
C	2.601204	-2.787809	-0.201075	H	-1.092785	-0.192419	-1.868044
H	5.254112	-4.963258	1.607098	H	-0.955249	1.525605	-2.309118
C	0.082608	-4.781343	1.248367	C	2.431198	0.188621	3.248256
C	3.918165	-2.807989	-0.667620	H	3.214083	0.734685	2.711768
H	0.744760	-5.647830	1.295072	H	2.629936	0.258657	4.320741
H	-0.460864	-4.797684	0.295220	C	2.283927	-1.255211	2.741643
H	-0.643763	-4.838500	2.061622	H	3.185167	-1.562799	2.205154
H	4.178119	-2.267152	-1.568337	H	2.148286	-1.957042	3.575339
C	1.028638	-1.177235	1.869549	C	0.373401	0.069355	2.188418
C	3.193223	-4.341407	1.547567	O	-0.706963	0.547245	1.822359
H	2.903317	-4.915868	2.423179	O	1.173031	0.853693	2.987659
I	0.986110	-2.762555	-2.079770	C	4.882155	-3.572383	-0.001801
Cu	1.659804	-0.917468	-0.304936	H	5.904810	-3.578245	-0.368713
N	0.477474	0.800085	-0.893395	N	-3.895491	-1.844888	2.172831
C	1.332960	2.013226	-1.009102	C	-3.697879	-0.820455	1.128037
C	2.527302	1.874166	-0.037007	C	-4.408917	0.510588	1.507601
N	3.267965	0.612156	-0.335893	N	-3.775458	1.026322	2.734109
C	3.419211	3.104426	0.040156	H	-2.769035	1.091609	2.579516
C	3.811419	3.832280	-1.094308	C	-4.290438	2.312484	3.189692
C	3.890840	3.515979	1.294857	H	-3.785158	2.591826	4.121760
C	4.658460	4.936456	-0.975249	H	-4.164901	3.144933	2.474717
H	3.449517	3.543922	-2.076359	H	-5.363767	2.224551	3.403157
C	4.738290	4.619526	1.418122	C	-4.399057	1.518159	0.358824
H	3.581375	2.970469	2.183272	C	-3.188391	2.014549	-0.146267
C	5.125654	5.333528	0.281044	C	-5.596114	2.011809	-0.175691
H	4.949049	5.489340	-1.864808	C	-3.176707	2.963692	-1.170236
H	5.088331	4.924784	2.400865	H	-2.251164	1.663741	0.274042
H	5.782268	6.194704	0.372777	C	-5.591286	2.958148	-1.204856
H	2.108262	1.717167	0.957991	H	-6.543171	1.646213	0.215792
C	0.557615	3.301429	-0.770967	C	-4.378546	3.436557	-1.707378
C	-0.027787	3.568482	0.477136	H	-2.229255	3.343295	-1.539319
C	0.419458	4.244613	-1.797080	H	-6.532704	3.325057	-1.606837
C	-0.726306	4.757583	0.691205	H	-4.367536	4.177230	-2.503156
H	0.041609	2.837914	1.278411	H	-5.460057	0.305300	1.751348
C	-0.277835	5.437502	-1.583387	C	-4.001714	-1.345165	-0.273933
H	0.868481	4.046622	-2.767333	C	-5.279860	-1.316448	-0.851716
C	-0.850707	5.698071	-0.336287	C	-2.965457	-1.967150	-0.989808
H	-1.179990	4.946656	1.660744	C	-5.510127	-1.869149	-2.115393
H	-0.373798	6.158943	-2.390710	H	-6.101693	-0.849050	-0.317408
H	-1.395589	6.623103	-0.167277	C	-3.189060	-2.518289	-2.253651
H	1.710267	2.021261	-2.035114	H	-1.980094	-2.030988	-0.536451

C	-4.464630	-2.468047	-2.824603	H	-2.669596	1.556103	3.091953
H	-6.507817	-1.829982	-2.546301	C	-4.486251	2.057934	1.161205
H	-2.364527	-2.983441	-2.789644	C	-3.896726	3.323679	1.023784
H	-4.643309	-2.892804	-3.809292	C	-5.739366	1.958941	1.775775
H	-2.626054	-0.611263	1.157788	C	-4.551253	4.465818	1.487648
C	-5.164271	-2.561612	2.169708	H	-2.921037	3.419900	0.552819
H	-5.994491	-1.865660	2.341474	C	-6.399291	3.101000	2.238550
H	-5.389294	-3.115816	1.241314	H	-6.203520	0.981790	1.886103
H	-5.163594	-3.281703	2.996729	C	-5.806808	4.357955	2.095117
H	-3.118439	-2.496058	2.092486	H	-4.082135	5.439778	1.374491
C	4.085537	0.618045	-1.560575	H	-7.373142	3.007209	2.712108
H	4.672151	-0.300449	-1.586135	H	-6.316802	5.247374	2.455610
H	3.436503	0.634777	-2.440080	H	-4.354459	-0.070780	0.933750
H	4.778387	1.466531	-1.610520	C	-5.069868	1.021388	-1.546268
H	3.876782	0.421518	0.459466	C	-6.061539	0.041989	-1.387199
				C	-5.362702	2.165628	-2.297235
				C	-7.320729	0.206506	-1.966511
				H	-5.851932	-0.851320	-0.802642
				C	-6.623462	2.334845	-2.876383
				H	-4.600307	2.930673	-2.422672
				C	-7.605868	1.355378	-2.711959
				H	-8.080359	-0.559379	-1.833601
				H	-6.836083	3.229903	-3.455165
				H	-8.586843	1.484307	-3.161545
				H	-3.081925	1.709597	-1.186371
				C	-2.607936	-0.265741	-2.823314
				H	-2.049811	-1.166712	-3.090674
				H	-3.484164	-0.174974	-3.477306
				H	-1.968628	0.607411	-2.970708
				H	-3.605281	-1.155584	-1.294603
				C	0.073073	1.902713	-1.037991
				H	-1.011316	1.918378	-1.180594
				H	0.496329	2.827084	-1.437932
				C	0.700550	0.627419	-1.598912
				H	0.150123	0.243438	-2.460596
				H	1.732720	0.812121	-1.923549
				O	1.026898	0.404038	1.944883
				O	0.344933	1.874830	0.386727
				C	-1.310604	-2.711514	3.690090
				H	-2.038501	-2.830963	4.487752
				N	3.993048	-0.485808	1.700049
				C	4.339158	0.404898	0.582571
				C	5.462135	-0.170271	-0.334960
				N	5.219219	-1.589111	-0.601993
<b>TS4-E-4.log</b>							
C	0.721810	0.589567	0.769526				
C	1.501411	-1.496967	-0.479623				
C	0.562121	-2.455919	1.591634				
C	0.057665	-2.802934	3.948871				
O	2.219208	-1.701906	-1.481015				
N	1.491272	-2.441410	0.532201				
C	-0.815478	-2.326427	1.364363				
H	0.411340	-2.984098	4.960009				
C	2.466639	-3.535202	0.457743				
C	-1.753100	-2.491025	2.380184				
H	3.462441	-3.193680	0.756263				
H	2.143150	-4.341715	1.117364				
H	2.515117	-3.907315	-0.567830				
H	-2.812388	-2.454930	2.151716				
C	0.672000	-0.288235	-0.383108				
C	0.982784	-2.667309	2.911071				
H	2.048984	-2.713273	3.113462				
I	-1.617421	-3.590231	-0.764101				
Cu	-1.453935	-1.026622	-0.047825				
N	-2.980124	-0.352765	-1.399343				
C	-3.699852	0.850263	-0.909861				
C	-3.780556	0.814670	0.636851				
N	-2.416555	0.627888	1.177250				
H	-1.831622	1.403742	0.862293				
C	-2.351893	0.604278	2.646493				
H	-2.999596	-0.188370	3.027593				
H	-1.321693	0.392297	2.937133				

H	4.263750	-1.720235	-0.934009	C	-2.661156	-3.926982	-0.674939
C	6.165763	-2.204125	-1.524231	H	2.424024	-4.028721	1.870069
H	5.920521	-3.267215	-1.631393	H	1.474320	-5.273863	1.023505
H	6.189575	-1.758013	-2.533899	H	2.179793	-3.911742	0.114889
H	7.181092	-2.133780	-1.111862	H	-3.145071	-3.508291	-1.547914
C	5.561609	0.705387	-1.588550	C	-0.631484	-1.376319	1.947958
C	4.578344	0.621024	-2.587398	C	-1.316449	-5.106230	1.467577
C	6.617041	1.608508	-1.763097	H	-0.795509	-5.539444	2.317032
C	4.642068	1.434053	-3.721144	I	-0.062684	-2.659153	-2.099580
H	3.760142	-0.085971	-2.472800	Cu	-1.327777	-1.284340	-0.226277
C	6.683601	2.426210	-2.895630	N	-0.748112	0.748063	-0.562077
H	7.388537	1.679842	-1.000032	C	-1.912373	1.564864	-0.117350
C	5.694169	2.342838	-3.878737	C	-3.202533	1.053011	-0.795603
H	3.870252	1.357217	-4.483507	N	-3.377850	-0.382794	-0.441067
H	7.509067	3.124658	-3.010250	H	-3.708157	-0.424164	0.523585
H	5.743660	2.975952	-4.761059	C	-4.379158	-1.050007	-1.289339
H	6.424775	-0.108296	0.188287	H	-3.957092	-1.208889	-2.286625
C	4.631784	1.845924	1.006976	H	-4.625067	-2.018692	-0.851366
C	5.860520	2.232621	1.568989	H	-5.304765	-0.466495	-1.385616
C	3.630114	2.819590	0.878037	C	-4.418054	1.883758	-0.410762
C	6.078489	3.548396	1.986298	C	-4.773679	2.042504	0.938150
H	6.661978	1.507378	1.671645	C	-5.218200	2.478299	-1.393223
C	3.844495	4.137141	1.290746	C	-5.899477	2.786366	1.293449
H	2.668689	2.543272	0.454820	H	-4.164719	1.587421	1.716313
C	5.071751	4.508005	1.847033	C	-6.347205	3.223948	-1.040864
H	7.038704	3.824322	2.415428	H	-4.951172	2.360897	-2.440706
H	3.053281	4.873966	1.173637	C	-6.690069	3.380930	0.304050
H	5.243149	5.532825	2.166511	H	-6.158935	2.904153	2.342376
H	3.435072	0.433330	-0.034925	H	-6.956877	3.679710	-1.816743
C	4.973097	-0.651237	2.762628	H	-7.566414	3.961023	0.580852
H	5.888524	-1.100910	2.359940	H	-3.079465	1.086966	-1.882090
H	5.258490	0.276452	3.288452	C	-1.690277	3.065548	-0.226548
H	4.565572	-1.344331	3.508114	C	-1.941355	3.787316	-1.402712
H	3.093755	-0.187434	2.074192	C	-1.200684	3.751936	0.894014
<b>TS4-E-5.log</b>				C	-1.723592	5.166695	-1.450860
C	0.602210	-2.103225	1.621784	H	-2.319947	3.275700	-2.282656
C	-0.746231	-3.996885	0.836907	C	-0.983812	5.130793	0.849451
C	-2.540213	-5.629928	1.040650	H	-0.976349	3.190667	1.797659
O	1.738366	-1.600124	1.623391	C	-1.250066	5.843752	-0.322912
N	0.478740	-3.458558	1.309468	H	-1.928975	5.712363	-2.368261
C	-1.443290	-3.398039	-0.236029	H	-0.606121	5.646645	1.728440
H	-2.958378	-6.499557	1.539149	H	-1.085063	6.917360	-0.359781
C	1.712055	-4.209067	1.061594	H	-2.014718	1.336360	0.944707
				C	-0.516135	0.000761	2.389642



H	6.278603	2.171605	0.097936	C	-4.509669	-0.088927	1.893727
C	5.489345	4.336423	-2.409553	C	-6.718375	0.391479	1.052264
H	3.549435	4.473731	-3.347986	C	-4.912446	0.304265	3.171427
H	7.294631	3.960432	-1.287515	H	-3.492454	-0.435615	1.727762
H	5.930238	5.122791	-3.016477	C	-7.125054	0.786757	2.330860
H	4.463068	0.880842	0.759322	H	-7.425621	0.425926	0.226326
C	2.462431	2.930122	1.426614	C	-6.221481	0.745799	3.395409
C	3.591080	3.379216	2.126645	H	-4.203443	0.266344	3.995272
C	1.295380	3.708044	1.455234	H	-8.146188	1.123188	2.493770
C	3.556599	4.586647	2.829051	H	-6.533275	1.052064	4.390777
H	4.504232	2.791831	2.120664	H	-5.835501	-0.420077	-1.242739
C	1.258301	4.914490	2.157201	C	-4.313848	1.940326	-1.134952
H	0.411920	3.349689	0.931619	C	-5.548583	2.340218	-1.671892
C	2.391669	5.359060	2.844652	C	-3.431522	2.935200	-0.682617
H	4.441340	4.923795	3.363049	C	-5.888351	3.693668	-1.757540
H	0.347119	5.507266	2.165018	H	-6.258563	1.594137	-2.015660
H	2.367597	6.299834	3.388415	C	-3.769392	4.288171	-0.765051
H	1.682586	1.714233	-0.118733	H	-2.475015	2.636559	-0.259444
C	-0.450626	0.535662	-0.490827	C	-5.000198	4.673487	-1.305115
C	0.275645	0.585071	-2.693790	H	-6.850645	3.981546	-2.174115
H	-0.271816	0.871099	-3.595834	H	-3.073478	5.041227	-0.402431
H	1.325640	0.869740	-2.823999	H	-5.266806	5.725487	-1.368690
C	0.113322	-0.896897	-2.321285	H	-3.048428	0.425453	-0.353906
H	-0.748512	-1.336852	-2.838225	C	-4.125696	-0.064770	-3.512509
H	1.001165	-1.464338	-2.612648	H	-4.846293	-0.874685	-3.354957
O	-0.810816	1.070613	0.560366	H	-4.688740	0.853726	-3.750013
O	-0.255766	1.352539	-1.589749	H	-3.521823	-0.323045	-4.389968
C	3.127028	-4.295372	-2.230681	H	-2.494823	0.695944	-2.564523
H	4.086622	-4.589336	-2.646987				
C	2.570748	0.292073	2.814710				
H	3.611354	-0.002872	2.656626	<b>TS4-E-7.log</b>			
H	2.545923	1.192606	3.439487	C	0.629909	-2.242959	1.462629
H	2.064393	-0.519396	3.340953	C	-0.932886	-3.974117	0.696739
H	0.909020	0.680950	1.679830	C	-2.875458	-5.405378	1.012730
N	-3.241175	0.035677	-2.355370	O	1.793941	-1.820715	1.361857
C	-3.857445	0.482608	-1.086498	N	0.370585	-3.567922	1.087300
C	-4.961542	-0.481455	-0.582067	C	-1.648142	-3.257400	-0.289830
N	-4.477059	-1.864373	-0.649644	H	-3.343015	-6.247271	1.514771
H	-3.593127	-1.927113	-0.143347	C	1.511367	-4.394190	0.687371
C	-5.416669	-2.852287	-0.131104	C	-2.970020	-3.603624	-0.602431
H	-4.985057	-3.853389	-0.246679	H	2.308372	-4.307983	1.429529
H	-5.689631	-2.721505	0.930893	H	1.186255	-5.435051	0.629359
H	-6.346497	-2.819377	-0.714241	H	1.911154	-4.089181	-0.287750
C	-5.408830	-0.042435	0.815377	H	-3.499227	-3.065481	-1.381162
				C	-0.499363	-1.469014	1.991759

C	-1.563687	-5.045833	1.333928	H	-0.757081	0.936764	-2.481655
H	-1.019638	-5.574847	2.111472	H	0.219227	2.238921	-1.754616
I	-0.405897	-2.522582	-2.156508	H	0.818950	0.565176	-1.773106
Cu	-1.333410	-1.145349	-0.057832	H	0.017231	0.978662	0.367711
N	-0.686375	0.872292	-0.367842	N	3.718155	0.931203	2.661182
C	-1.876475	1.673947	0.033922	C	3.673389	0.881363	1.189356
C	-3.100818	1.174466	-0.771974	C	4.750687	-0.068080	0.591921
N	-3.315112	-0.271278	-0.440880	N	4.732618	-1.346645	1.310066
C	-4.360773	2.010628	-0.616624	H	3.771578	-1.680834	1.366407
C	-4.715434	2.622336	0.594957	C	5.596382	-2.373262	0.742116
C	-5.232162	2.129579	-1.707932	H	5.540855	-3.274167	1.365044
C	-5.908712	3.338430	0.708698	H	5.355505	-2.666616	-0.295583
H	-4.056759	2.546748	1.454720	H	6.638630	-2.026285	0.747251
C	-6.428314	2.842742	-1.597942	C	4.536440	-0.188152	-0.920619
H	-4.966997	1.660828	-2.653404	C	3.377537	-0.792881	-1.435825
C	-6.769775	3.451100	-0.386975	C	5.498434	0.285159	-1.821551
H	-6.164835	3.810002	1.653958	C	3.185040	-0.899092	-2.815297
H	-7.088736	2.926956	-2.457166	H	2.630512	-1.189306	-0.752242
H	-7.697377	4.010400	-0.297853	C	5.308365	0.182064	-3.203148
H	-2.830558	1.179438	-1.831056	H	6.404597	0.747145	-1.436272
C	-1.617124	3.171087	-0.010254	C	4.146481	-0.408221	-3.705531
C	-1.840391	3.949881	-1.154468	H	2.280489	-1.366343	-3.195974
C	-1.087216	3.788896	1.132315	H	6.067206	0.561182	-3.883490
C	-1.558014	5.318494	-1.149571	H	3.992240	-0.490950	-4.778459
H	-2.248922	3.492342	-2.050686	H	5.749093	0.363637	0.742785
C	-0.807420	5.156806	1.141842	C	3.684334	2.268108	0.540633
H	-0.883532	3.184429	2.013214	C	4.865028	2.966236	0.237876
C	-1.047160	5.927808	0.000229	C	2.461198	2.908145	0.287574
H	-1.742601	5.908863	-2.043395	C	4.822483	4.247256	-0.320682
H	-0.400518	5.618787	2.037558	H	5.830097	2.505714	0.425927
H	-0.833409	6.993399	0.004987	C	2.410616	4.184256	-0.278184
H	-2.043513	1.403216	1.081190	H	1.538508	2.401742	0.549221
C	-0.245770	-0.140845	2.520250	C	3.594868	4.859134	-0.588377
C	-2.038749	-0.936435	3.757975	H	5.750916	4.765039	-0.549874
H	-2.029219	-1.144338	4.831821	H	1.448424	4.648693	-0.473978
H	-3.045777	-0.616242	3.476481	H	3.561517	5.851570	-1.030933
C	-1.540500	-2.119273	2.907830	H	2.703598	0.425077	0.977772
H	-1.089205	-2.895356	3.539488	C	4.844712	1.628935	3.265371
H	-2.373670	-2.584378	2.375547	H	5.776347	1.096840	3.037178
O	0.569599	0.729692	2.200802	H	4.975078	2.678395	2.946870
O	-1.141598	0.168604	3.513808	H	4.720930	1.623096	4.354653
C	-3.587130	-4.665056	0.065730	H	2.836310	1.333754	2.971528
H	-4.612786	-4.925370	-0.181134	H	-3.711603	-0.723748	-1.262740
C	-0.073426	1.185695	-1.665594	C	-4.192348	-0.550431	0.709222



H	-5.235284	-0.258079	0.536273	H	3.110584	1.934609	0.773866
H	-4.150331	-1.622723	0.915850	C	4.947643	1.612039	-1.335936
H	-3.822254	-0.014357	1.584468	C	4.611334	2.968572	-1.460244
<b>TS4-E-8.log</b>				C	6.191824	1.177800	-1.806423
C	-0.968133	0.501089	0.823657	C	5.504415	3.871462	-2.038805
C	-1.293164	-1.013354	-1.231268	H	3.647776	3.322341	-1.099569
C	-0.731241	-2.597294	0.579123	C	7.089791	2.079735	-2.384757
C	-0.847331	-3.476991	2.841350	H	6.460299	0.128064	-1.714906
O	-1.769659	-0.844362	-2.371311	C	6.748347	3.429209	-2.501836
N	-1.373996	-2.264354	-0.638015	H	5.231582	4.919954	-2.126309
C	0.659792	-2.463988	0.724580	H	8.053155	1.727173	-2.743989
H	-1.439997	-3.875866	3.659800	H	7.444608	4.132337	-2.951177
C	-2.076138	-3.353159	-1.322179	H	4.408235	-0.374629	-0.727378
C	1.295955	-2.839326	1.913714	H	2.255990	1.466183	-1.422853
H	-2.117110	-3.125911	-2.387626	C	2.821574	0.120163	-2.831973
H	-3.097922	-3.461946	-0.945977	H	3.321161	-0.850623	-2.868356
H	-1.524176	-4.284938	-1.170351	H	1.823495	0.011466	-3.264511
H	2.375678	-2.784745	1.994130	H	3.399242	0.838669	-3.426424
C	-0.612474	0.094920	-0.529131	C	-0.505069	1.401723	-1.309360
C	-1.472725	-3.099932	1.652498	H	0.207736	1.378012	-2.137663
H	-2.552980	-3.145791	1.551196	H	-1.478306	1.693146	-1.725458
I	1.964439	-3.117698	-1.230575	C	-0.087969	2.373516	-0.206382
Cu	1.394457	-0.710095	-0.210014	H	0.998186	2.394055	-0.057098
N	2.682043	0.539910	-1.426852	H	-0.448214	3.395725	-0.344304
C	3.974347	0.631149	-0.701705	O	-1.472145	-0.101475	1.767592
C	3.675439	0.996423	0.774273	O	-0.691031	1.848467	0.996393
N	2.773462	-0.026714	1.356802	C	0.535196	-3.328205	2.979604
H	3.333975	-0.847904	1.587528	H	1.034644	-3.618497	3.900070
C	2.091933	0.437048	2.577279	N	-4.685970	-1.399874	-1.241006
H	1.484744	-0.381264	2.969726	C	-4.638357	-0.088024	-0.569210
H	2.795525	0.768844	3.352981	C	-5.172257	-0.176796	0.886635
H	1.427356	1.264271	2.315786	N	-4.331779	-1.128957	1.630922
C	4.944005	1.195817	1.587776	H	-3.363178	-0.803206	1.617744
C	5.872888	0.153502	1.731010	C	-4.741942	-1.347175	3.013265
C	5.201902	2.421308	2.212895	H	-4.062112	-2.073314	3.473955
C	7.036896	0.337351	2.478480	H	-4.748198	-0.441744	3.645448
H	5.688909	-0.805350	1.251141	H	-5.754756	-1.770381	3.038527
C	6.366745	2.608753	2.962965	C	-5.256631	1.195521	1.557577
H	4.488441	3.234829	2.105967	C	-4.147069	2.053763	1.602220
C	7.287840	1.567236	3.096460	C	-6.433642	1.598809	2.201956
H	7.749919	-0.477154	2.576367	C	-4.220164	3.284713	2.256092
H	6.552284	3.566671	3.441930	H	-3.217231	1.765055	1.127005
H	8.195310	1.711077	3.676914	C	-6.512182	2.829656	2.861095
				H	-7.301165	0.942263	2.181898

C	-5.403993	3.679790	2.888566	C	2.579559	1.815558	-0.145488
H	-3.348661	3.935027	2.272882	N	3.278152	0.547082	-0.464010
H	-7.437054	3.121539	3.352738	H	3.550439	0.562756	-1.448463
H	-5.460069	4.638080	3.398653	C	4.481823	0.317175	0.348713
H	-6.187514	-0.594073	0.870239	H	4.900434	-0.657455	0.091648
C	-5.257157	1.017213	-1.423847	H	5.249454	1.087408	0.199214
C	-6.593794	1.426474	-1.314242	H	4.201819	0.304339	1.403800
C	-4.469198	1.581332	-2.439741	C	3.465862	3.048515	-0.226414
C	-7.119358	2.393923	-2.176441	C	4.171127	3.350503	-1.400412
H	-7.230412	0.998392	-0.546052	C	3.574671	3.912614	0.868961
C	-4.988821	2.548618	-3.302103	C	4.963971	4.496833	-1.477534
H	-3.444416	1.235753	-2.560065	H	4.101240	2.687268	-2.259552
C	-6.317988	2.963594	-3.169403	C	4.363732	5.063816	0.794196
H	-8.156862	2.701703	-2.070701	H	3.032753	3.683346	1.783719
H	-4.357298	2.979131	-4.075608	C	5.060195	5.359404	-0.380356
H	-6.725811	3.719418	-3.835799	H	5.505092	4.718429	-2.393860
H	-3.571083	0.142594	-0.488330	H	4.435113	5.726665	1.652743
C	-5.987261	-1.842379	-1.729416	H	5.675551	6.253181	-0.441182
H	-6.676784	-1.988266	-0.889680	H	2.214036	1.712834	0.882299
H	-6.474744	-1.156164	-2.443042	C	0.616672	3.259718	-0.876940
H	-5.861576	-2.811793	-2.224803	C	-0.033404	3.524323	0.337667
H	-4.012238	-1.376788	-2.003940	C	0.587032	4.231479	-1.884254
				C	-0.687746	4.738980	0.544211
				H	-0.051651	2.766528	1.113668
				C	-0.070559	5.449027	-1.681336
				H	1.088164	4.037316	-2.829507
				C	-0.706557	5.707561	-0.464451
				H	-1.191799	4.924231	1.489422
				H	-0.085396	6.192885	-2.473854
				H	-1.219188	6.652626	-0.305542
				H	1.732177	1.914974	-2.113422
				H	-0.093089	0.856316	-0.079404
				C	-0.424630	0.572996	-2.072917
				H	0.157190	0.276485	-2.951066
				H	-1.130781	-0.226028	-1.841610
				H	-0.987566	1.483190	-2.311934
				C	2.233812	-0.081510	3.469374
				H	3.041848	0.546701	3.066593
				H	2.403033	-0.180067	4.548157
				C	2.144566	-1.442390	2.748086
				H	3.089311	-1.678644	2.252625
				H	1.956409	-2.244375	3.474070
				C	0.262276	-0.053332	2.178363
				O	-0.766776	0.469789	1.683585
<b>TS4-F-1.log</b>							
C	0.143181	-2.467697	1.472296				
C	2.181783	-3.659484	0.768349				
C	4.497543	-4.384815	0.975402				
O	-1.097958	-2.510596	1.443209				
N	0.844661	-3.663427	1.240324				
C	2.557115	-2.872835	-0.343243				
H	5.245661	-4.980256	1.490646				
C	0.056687	-4.885174	1.068150				
C	3.882980	-2.849169	-0.791659				
H	0.721744	-5.748445	1.138189				
H	-0.453225	-4.905316	0.096287				
H	-0.698845	-4.948895	1.853954				
H	4.143047	-2.269258	-1.670609				
C	0.954804	-1.284970	1.782177				
C	3.171768	-4.400046	1.420517				
H	2.890924	-4.975601	2.298411				
I	0.981229	-2.792483	-2.140595				
Cu	1.656685	-0.952129	-0.307774				
N	0.477293	0.759149	-0.926992				
C	1.352239	1.943890	-1.085155				

N	0.950500	0.548621	3.204204	H	-3.135980	-2.471144	2.006520
C	0.694900	1.897524	3.654771				
H	-0.338921	2.162561	3.424815				
H	0.847928	1.961700	4.738104	<b>TS4-F-2.log</b>			
H	1.364943	2.623103	3.168274	C	-0.655264	-2.005816	1.231115
C	4.856630	-3.594004	-0.117675	C	0.901761	-3.893303	1.034136
H	5.884794	-3.568988	-0.468238	C	2.700519	-5.313165	1.854748
N	-3.895367	-1.802402	2.110555	O	-1.787733	-1.591731	0.914466
C	-3.719867	-0.797453	1.043267	N	-0.418666	-3.386103	1.149891
C	-4.379116	0.556974	1.435470	C	1.785359	-3.381935	0.057914
N	-3.690183	1.058680	2.636735	H	3.046494	-6.071955	2.550555
H	-2.684195	1.053848	2.462230	C	-1.534782	-4.248944	0.760961
C	-4.116154	2.379406	3.081457	C	3.111911	-3.822949	-0.008508
H	-3.575433	2.641273	3.999003	H	-1.276232	-5.285241	0.989399
H	-3.955374	3.193592	2.352126	H	-1.759030	-4.165142	-0.310543
H	-5.188326	2.362102	3.318416	H	-2.428420	-3.969275	1.322486
C	-4.376152	1.557178	0.279412	H	3.765752	-3.446059	-0.787509
C	-3.168231	2.036727	-0.248091	C	0.443925	-1.172840	1.725408
C	-5.575716	2.065889	-0.235409	C	1.379451	-4.857772	1.924149
C	-3.161647	2.986513	-1.271993	H	0.707856	-5.227330	2.694181
H	-2.229886	1.673257	0.157714	I	0.834867	-2.986913	-2.088465
C	-5.576283	3.009976	-1.266594	Cu	1.585582	-1.260869	-0.173150
H	-6.520799	1.715073	0.173966	N	1.101145	0.622440	-1.141541
C	-4.366307	3.473572	-1.789697	C	2.279790	1.522053	-1.116030
H	-2.215235	3.356312	-1.655439	C	3.218023	1.153836	0.061575
H	-6.519682	3.388001	-1.653409	N	3.573970	-0.281692	-0.065161
H	-4.359967	4.214019	-2.585738	H	4.017224	-0.427557	-0.973613
H	-5.428713	0.385425	1.711855	C	4.488878	-0.761034	0.980947
C	-4.097728	-1.328380	-0.338016	H	4.662435	-1.829362	0.835554
C	-5.397481	-1.269185	-0.862739	H	5.453830	-0.237241	0.976261
C	-3.108671	-1.982024	-1.091981	H	4.020013	-0.617465	1.956553
C	-5.694274	-1.821299	-2.112739	C	4.417566	2.088852	0.106972
H	-6.184241	-0.778316	-0.297645	C	5.365685	2.091064	-0.927237
C	-3.398638	-2.532131	-2.342818	C	4.579373	2.982276	1.171885
H	-2.108766	-2.072834	-0.676286	C	6.447656	2.972493	-0.897894
C	-4.694863	-2.450077	-2.861370	H	5.256764	1.403388	-1.763182
H	-6.707676	-1.758244	-2.502182	C	5.659556	3.868717	1.203575
H	-2.610606	-3.022306	-2.910556	H	3.850507	2.987212	1.978596
H	-4.925280	-2.873652	-3.835762	C	6.596172	3.867353	0.167138
H	-2.643002	-0.615418	1.024388	H	7.173279	2.963678	-1.707229
C	-5.179527	-2.487338	2.172937	H	5.768070	4.558412	2.036720
H	-5.984166	-1.769460	2.374670	H	7.436879	4.555856	0.188439
H	-5.460612	-3.044302	1.261381	H	2.659328	1.248794	0.998993
H	-5.159515	-3.199880	3.006319	C	1.887734	2.992392	-1.120506
				C	1.090965	3.521427	-0.092924

C	2.291394	3.834651	-2.163083	C	-7.500007	-0.740399	-0.575660
C	0.702687	4.862047	-0.114774	H	-6.489366	0.404639	-2.096714
H	0.751421	2.876192	0.711418	C	-7.362143	-1.473626	0.605187
C	1.907556	5.179361	-2.184867	H	-5.974177	-2.206479	2.087475
H	2.911033	3.435983	-2.962724	H	-8.479795	-0.616281	-1.030791
C	1.110518	5.696879	-1.161007	H	-8.232801	-1.921642	1.077516
H	0.079716	5.254117	0.685304	H	-4.226259	0.842602	-2.180541
H	2.227646	5.818531	-3.003790	C	-4.020591	2.203974	0.470684
H	0.807275	6.740431	-1.178186	C	-5.141744	2.859525	-0.061245
H	2.840972	1.314152	-2.034662	C	-3.657421	2.479769	1.798514
H	0.389254	0.958480	-0.483675	C	-5.886837	3.751747	0.715207
C	0.503843	0.561777	-2.484586	H	-5.443442	2.662919	-1.085957
H	1.193891	0.048287	-3.161667	C	-4.399000	3.369965	2.578988
H	-0.430967	0.003492	-2.434254	H	-2.774497	1.994043	2.208685
H	0.290494	1.561911	-2.884515	C	-5.520552	4.008171	2.039800
C	1.723167	-0.377637	3.642315	H	-6.755473	4.244883	0.285173
H	2.764608	-0.100459	3.422473	H	-4.104457	3.562928	3.608025
H	1.632229	-0.460869	4.732091	H	-6.102621	4.698740	2.644939
C	1.300378	-1.667054	2.906651	H	-2.571281	0.658318	0.358310
H	2.180190	-2.241034	2.606278	C	-2.469729	3.125113	-1.931849
H	0.713734	-2.310124	3.575662	H	-3.056872	2.739863	-2.774109
C	0.166180	0.247906	1.982536	H	-3.067262	3.917266	-1.447516
O	-0.515830	1.053461	1.312058	H	-1.568060	3.592138	-2.344333
N	0.825018	0.639962	3.125813	H	-1.417410	2.373220	-0.353039
C	0.980014	2.021925	3.515574				
H	0.178323	2.609712	3.064817				
H	0.922170	2.112539	4.606555	<b>TS4-F-3.log</b>			
H	1.948072	2.430966	3.188061	C	0.179044	-2.389892	1.560441
C	3.573074	-4.775904	0.906792	C	2.175882	-3.640754	0.848967
H	4.604572	-5.113046	0.851069	C	4.485634	-4.385878	1.058725
N	-2.065124	2.032587	-1.057626	O	-1.062829	-2.414938	1.589386
C	-3.121565	1.282958	-0.348872	N	0.849520	-3.604564	1.345918
C	-3.873416	0.301092	-1.292780	C	2.544842	-2.901859	-0.296120
N	-2.915604	-0.716638	-1.757304	H	5.233098	-4.969237	1.588553
H	-2.498344	-1.169126	-0.941427	C	0.036195	-4.816460	1.233486
C	-3.475476	-1.721949	-2.652012	C	3.863202	-2.920181	-0.763571
H	-2.682286	-2.423065	-2.937470	H	0.689093	-5.688828	1.305005
H	-4.310232	-2.307752	-2.227667	H	-0.505153	-4.853427	0.279168
H	-3.845530	-1.240850	-3.567025	H	-0.694634	-4.846703	2.044218
C	-5.101660	-0.306618	-0.612534	H	4.114064	-2.406970	-1.683546
C	-4.971711	-1.058268	0.567145	C	1.016124	-1.204475	1.776153
C	-6.375426	-0.166063	-1.177281	C	3.164716	-4.369723	1.516624
C	-6.092066	-1.632232	1.171280	H	2.886785	-4.907454	2.419069
H	-3.988231	-1.201398	1.004576	I	0.948060	-2.868483	-2.096959
				Cu	1.638919	-0.971822	-0.338100

N	0.466658	0.735287	-0.987499	H	1.140700	2.165544	4.577570
C	1.333760	1.930666	-1.150088	H	1.464685	2.794077	2.944404
C	2.513116	1.821678	-0.151436	C	4.838782	-3.644619	-0.070140
N	3.258479	0.552096	-0.395511	H	5.860802	-3.650839	-0.439085
C	3.414791	3.046028	-0.092410	N	-3.852620	-1.720390	2.258238
C	3.800991	3.762430	-1.235828	C	-3.686238	-0.762316	1.147120
C	3.917008	3.453123	1.152099	C	-4.344842	0.606247	1.487045
C	4.663186	4.856825	-1.134721	N	-3.633805	1.167040	2.648515
H	3.422709	3.472856	-2.211100	H	-2.631334	1.157813	2.455916
C	4.779356	4.546889	1.257725	C	-4.057785	2.504449	3.042056
H	3.625410	2.907687	2.046238	H	-3.502888	2.807708	3.938151
C	5.154547	5.253936	0.112241	H	-3.912635	3.286522	2.275189
H	4.947475	5.401515	-2.031360	H	-5.125692	2.493622	3.297872
H	5.151461	4.849126	2.233296	C	-4.371318	1.550128	0.285482
H	5.822424	6.107806	0.190020	C	-3.176671	2.004505	-0.291482
H	2.074383	1.692334	0.840447	C	-5.583319	2.032841	-0.224932
C	0.569798	3.237657	-0.987902	C	-3.194923	2.906422	-1.357339
C	-0.067721	3.543812	0.223499	H	-2.228876	1.660340	0.109503
C	0.489395	4.155966	-2.042056	C	-5.608962	2.929141	-1.297628
C	-0.751530	4.749460	0.383247	H	-6.518003	1.700118	0.221764
H	-0.055048	2.823143	1.034120	C	-4.411892	3.369317	-1.868389
C	-0.197068	5.364232	-1.886289	H	-2.258531	3.259555	-1.778502
H	0.975908	3.927851	-2.987303	H	-6.561483	3.288739	-1.679638
C	-0.815086	5.666797	-0.670195	H	-4.424714	4.073364	-2.696701
H	-1.244439	4.966588	1.327560	H	-5.387497	0.443265	1.792925
H	-0.248374	6.066467	-2.714433	C	-4.072506	-1.350076	-0.208471
H	-1.349387	6.605119	-0.546810	C	-5.380963	-1.333857	-0.714819
H	1.728787	1.885843	-2.169068	C	-3.081415	-2.008194	-0.955608
H	-0.113085	0.846643	-0.148289	C	-5.684923	-1.934072	-1.940658
C	-0.419335	0.521644	-2.141114	H	-6.168415	-0.837864	-0.154924
H	0.177206	0.216408	-3.006176	C	-3.378740	-2.606418	-2.182473
H	-1.120077	-0.281193	-1.905524	H	-2.073518	-2.063665	-0.553561
H	-0.988366	1.421855	-2.402204	C	-4.684053	-2.568214	-2.682966
C	2.440537	0.102575	3.242199	H	-6.704894	-1.903948	-2.316649
H	3.188165	0.678803	2.674764	H	-2.589081	-3.099267	-2.745628
H	2.747908	0.106515	4.294010	H	-4.920166	-3.029522	-3.638692
C	2.265868	-1.315566	2.668053	H	-2.609855	-0.579873	1.112653
H	3.168176	-1.626154	2.136059	C	-5.137083	-2.399558	2.363860
H	2.107160	-2.037878	3.480663	H	-5.939218	-1.671483	2.536740
C	0.353384	0.050047	2.154366	H	-5.426053	-2.999857	1.482894
O	-0.710983	0.548004	1.713353	H	-5.111312	-3.070371	3.231087
N	1.125911	0.706399	3.085402	H	-3.095646	-2.394638	2.174678
C	0.877395	2.063051	3.518656	H	3.846725	0.385785	0.420312
H	-0.183685	2.287932	3.392703	C	4.106017	0.517444	-1.598512

H	4.700302	-0.396675	-1.569954	H	-4.407728	-0.141083	0.859818
H	3.478997	0.490024	-2.493927	C	-5.097110	0.911106	-1.652628
H	4.792085	1.370542	-1.669465	C	-6.078613	-0.078963	-1.496081
<b>TS4-F-4.log</b>				C	-5.390403	2.037082	-2.430565
C	0.698557	0.612538	0.827780	C	-7.327657	0.057064	-2.104058
C	1.486868	-1.504381	-0.378810	H	-5.868445	-0.958834	-0.891650
C	0.478397	-2.460400	1.660977	C	-6.640977	2.177910	-3.038851
C	-0.136340	-2.737031	4.000194	H	-4.636021	2.810288	-2.554849
O	2.242040	-1.717841	-1.352663	C	-7.613176	1.187971	-2.876471
N	1.457117	-2.439463	0.647009	H	-8.079261	-0.717003	-1.972723
C	-0.890097	-2.394786	1.352859	H	-6.853734	3.059142	-3.638465
H	0.169643	-2.870360	5.034124	H	-8.586184	1.294779	-3.348624
C	2.442300	-3.526230	0.631390	H	-3.124391	1.631883	-1.261667
C	-1.873636	-2.537415	2.330928	C	-2.602668	-0.362890	-2.862951
H	2.573694	-3.879085	-0.393596	H	-2.024229	-1.258219	-3.105647
H	3.412203	-3.190564	1.011866	H	-3.470101	-0.300313	-3.532573
H	2.072529	-4.346270	1.249442	H	-1.975288	0.517718	-3.019662
H	-2.920982	-2.539986	2.050223	H	-3.598304	-1.242370	-1.326718
C	0.630346	-0.312893	-0.318996	C	0.081465	1.907045	-1.057392
C	0.836619	-2.610452	3.004622	H	-1.005379	1.946574	-1.227217
H	1.892194	-2.609052	3.260116	H	0.526564	2.791545	-1.527464
I	-1.552960	-3.658431	-0.731077	C	0.684342	0.584141	-1.556681
Cu	-1.437558	-1.027057	-0.058265	H	0.145393	0.183153	-2.417820
N	-2.989934	-0.428528	-1.442608	H	1.725991	0.743707	-1.868632
C	-3.737993	0.768400	-0.986338	O	0.986761	0.391271	2.019927
C	-3.850178	0.754035	0.559831	N	0.382877	1.879128	0.366032
N	-2.491844	0.611673	1.122200	C	0.213830	3.028088	1.222748
H	-1.924130	1.387270	0.782577	H	-0.837881	3.346328	1.278818
C	-2.432710	0.625519	2.590212	H	0.556477	2.759961	2.224321
H	-3.055802	-0.180309	2.985390	H	0.806572	3.875177	0.856256
H	-1.397058	0.451090	2.888609	C	-1.491009	-2.691059	3.669337
H	-2.781258	1.575380	3.017530	H	-2.255115	-2.797347	4.434492
C	-4.596463	1.986226	1.053444	N	3.949715	-0.304757	1.838344
C	-4.050971	3.267315	0.879289	C	4.337157	0.419303	0.620484
C	-5.840080	1.861944	1.682256	C	5.488882	-0.279968	-0.163750
C	-4.738660	4.398683	1.320822	N	5.199904	-1.708767	-0.310061
H	-3.085272	3.383064	0.392844	H	4.271401	-1.827421	-0.716212
C	-6.533645	2.992974	2.122999	C	6.187827	-2.448533	-1.086175
H	-6.270656	0.873061	1.821003	H	5.899225	-3.505688	-1.116930
C	-5.984475	4.264799	1.943240	H	6.318012	-2.101259	-2.126290
H	-4.303401	5.384505	1.178572	H	7.167266	-2.381717	-0.594216
H	-7.499931	2.879009	2.607555	C	5.705539	0.453257	-1.490554
H	-6.520814	5.145676	2.286072	C	4.738642	0.376307	-2.506475
				C	6.863417	1.204528	-1.723499

C	4.922385	1.049919	-3.715794	I	0.013489	-2.666237	-2.153134
H	3.840897	-0.217061	-2.347683	Cu	-1.252871	-1.355592	-0.191202
C	7.050965	1.880963	-2.933084	N	-0.729226	0.705264	-0.566233
H	7.621757	1.267649	-0.946259	C	-1.934104	1.485186	-0.179292
C	6.078863	1.807101	-3.933884	C	-3.190049	0.882899	-0.854442
H	4.162274	0.982895	-4.490791	N	-3.327499	-0.527133	-0.399122
H	7.956474	2.461247	-3.093564	H	-3.628096	-0.506827	0.576822
H	6.221403	2.330786	-4.875804	C	-4.336436	-1.273885	-1.167594
H	6.418869	-0.199983	0.414122	H	-3.955041	-1.456207	-2.177220
C	4.625792	1.906725	0.830450	H	-4.513129	-2.233840	-0.679181
C	5.813781	2.368670	1.421879	H	-5.292139	-0.737898	-1.243456
C	3.670868	2.856184	0.439384	C	-4.442262	1.700761	-0.573222
C	6.030792	3.734064	1.625767	C	-4.856679	1.939627	0.746285
H	6.584476	1.661440	1.712905	C	-5.215086	2.209209	-1.623670
C	3.884776	4.222913	0.636078	C	-6.011121	2.679013	1.006938
H	2.749099	2.516420	-0.023737	H	-4.273843	1.548093	1.576835
C	5.066897	4.667958	1.234052	C	-6.372743	2.949913	-1.366941
H	6.957882	4.068826	2.084870	H	-4.904089	2.027962	-2.649811
H	3.131109	4.938261	0.315860	C	-6.773063	3.188374	-0.050100
H	5.238819	5.730161	1.388437	H	-6.314830	2.859912	2.034842
H	3.455670	0.356786	-0.025805	H	-6.960194	3.337809	-2.195158
C	4.864387	-0.284069	2.969018	H	-7.671774	3.764871	0.152767
H	5.825684	-0.729467	2.685405	H	-3.030076	0.841054	-1.936300
H	5.071856	0.716087	3.388091	C	-1.791695	2.989176	-0.360002
H	4.441161	-0.898728	3.772319	C	-2.013917	3.625711	-1.590388
H	3.016632	0.001350	2.113213	C	-1.420105	3.771376	0.742089
				C	-1.883970	5.011478	-1.709462
				H	-2.302356	3.039984	-2.458037
<b>TS4-F-5.log</b>				C	-1.294397	5.157948	0.628762
C	0.764650	-2.153636	1.513544	H	-1.224558	3.284195	1.692784
C	-0.515624	-4.099424	0.740004	C	-1.531268	5.783595	-0.598084
C	-2.245798	-5.797686	0.968064	H	-2.065042	5.488713	-2.669131
O	1.882763	-1.608745	1.489662	H	-1.011198	5.747122	1.497123
N	0.695015	-3.514802	1.190974	H	-1.437332	6.862463	-0.689979
C	-1.256795	-3.514696	-0.311784	H	-2.042634	1.299729	0.892369
H	-2.620517	-6.687207	1.466072	C	-0.402548	-0.106646	2.398066
C	1.951507	-4.209054	0.902676	C	-2.334584	-1.032064	3.363663
C	-2.469592	-4.078958	-0.722161	H	-2.683426	-1.236514	4.381866
H	2.685254	-3.982727	1.679257	H	-3.218265	-0.784008	2.751495
H	1.763714	-5.284680	0.888418	C	-1.537257	-2.193768	2.750654
H	2.369056	-3.906243	-0.066011	H	-1.058805	-2.784414	3.545679
H	-2.993046	-3.666212	-1.575106	H	-2.199539	-2.866625	2.202827
C	-0.487139	-1.483457	1.881146	O	0.364800	0.823222	2.066664
C	-1.030253	-5.235112	1.370340	N	-1.391174	0.073929	3.346936
H	-0.473991	-5.657767	2.202602				

C	-1.788531	1.381475	3.816637	C	4.337208	2.484471	3.279187
H	-0.932473	2.055609	3.751363	H	5.356891	2.093429	3.175806
H	-2.613740	1.798361	3.218367	H	4.324073	3.495125	2.834040
H	-2.119287	1.318609	4.859504	H	4.132203	2.588281	4.351212
C	-2.974933	-5.206067	-0.064379	H	2.428931	1.827751	2.903160
H	-3.919344	-5.633450	-0.390464				
H	-0.031130	0.853977	0.169426				
C	-0.135416	1.002017	-1.875686	<b>TS4-F-6.log</b>			
H	0.135047	2.057907	-1.990549	C	-1.417713	-2.454290	1.172233
H	0.769369	0.399266	-1.980521	C	-3.810055	-2.585003	0.621737
H	-0.825445	0.722067	-2.676691	C	-6.174433	-2.245814	1.097563
N	3.385970	1.541372	2.707643	O	-0.316615	-3.000332	0.980602
C	3.472904	1.302543	1.255846	N	-2.575629	-3.214813	0.923018
C	4.700494	0.430637	0.867435	C	-3.886981	-1.574798	-0.364170
N	4.734575	-0.767260	1.714178	H	-7.060579	-2.517877	1.663706
H	3.813949	-1.204938	1.700996	C	-2.397181	-4.608963	0.516020
C	5.758811	-1.737874	1.351110	C	-5.094762	-0.911259	-0.609353
H	5.730013	-2.571424	2.063438	H	-1.674355	-5.093778	1.175190
H	5.664911	-2.160119	0.334409	H	-3.356548	-5.125386	0.594542
H	6.751928	-1.273689	1.420077	H	-2.032230	-4.689810	-0.516346
C	4.665768	0.133764	-0.635346	H	-5.154147	-0.179776	-1.406142
C	3.621294	-0.622455	-1.194022	C	-1.620716	-1.086653	1.667700
C	5.688001	0.584880	-1.479507	C	-4.964534	-2.904180	1.340926
C	3.596595	-0.896493	-2.563587	H	-4.893122	-3.658147	2.120303
H	2.835013	-1.008032	-0.549589	I	-2.649497	-1.942793	-2.358371
C	5.666052	0.313289	-2.851191	Cu	-2.157373	-0.261012	-0.299222
H	6.507903	1.162568	-1.058442	N	-0.369144	0.734185	-0.924611
C	4.615723	-0.426370	-3.399367	C	-0.399460	2.033327	-0.203533
H	2.779903	-1.481448	-2.978936	C	-1.720123	2.775948	-0.523031
H	6.468845	0.677534	-3.487928	N	-2.853572	1.906724	-0.108311
H	4.593038	-0.641009	-4.464866	H	-2.920815	1.948620	0.909079
H	5.627260	0.985638	1.066722	C	-4.139565	2.356339	-0.661844
C	3.371049	2.587571	0.430443	H	-4.152618	2.168386	-1.740231
C	4.482288	3.373579	0.085054	H	-4.943988	1.783065	-0.196904
C	2.100917	3.041353	0.045074	H	-4.324954	3.425886	-0.488872
C	4.329336	4.556351	-0.644650	C	-1.776292	4.152843	0.121923
H	5.479760	3.057605	0.374928	C	-1.713800	4.288392	1.516886
C	1.940591	4.216197	-0.692976	C	-1.904899	5.306373	-0.660779
H	1.227951	2.469812	0.340218	C	-1.765117	5.548504	2.114225
C	3.058431	4.977919	-1.045639	H	-1.624601	3.403007	2.140418
H	5.206097	5.145061	-0.904179	C	-1.956848	6.571079	-0.066906
H	0.945547	4.532068	-0.991470	H	-1.957823	5.213449	-1.742839
H	2.939947	5.891884	-1.622356	C	-1.884409	6.695777	1.322662
H	2.585409	0.702145	1.042522	H	-1.710553	5.634894	3.196395
				H	-2.055767	7.456275	-0.689917



H	-1.923481	7.677832	1.786493	C	5.358479	0.666478	0.500546
H	-1.811483	2.899118	-1.605636	C	6.509975	-0.694505	-1.117383
C	0.861620	2.859664	-0.401523	C	6.581238	1.043422	1.058225
C	1.062037	3.687215	-1.516726	H	4.437241	1.060837	0.917828
C	1.887490	2.753994	0.549746	C	7.738590	-0.322015	-0.562670
C	2.260130	4.387451	-1.678630	H	6.485798	-1.372462	-1.967870
H	0.279162	3.791747	-2.261521	C	7.778270	0.548546	0.529131
C	3.081821	3.464171	0.396646	H	6.600371	1.723322	1.906716
H	1.747708	2.094055	1.401981	H	8.662216	-0.710930	-0.984399
C	3.274249	4.279150	-0.722162	H	8.731040	0.841012	0.963007
H	2.399646	5.020609	-2.551034	H	4.173244	-1.330581	-2.010951
H	3.862321	3.377234	1.147315	C	3.624982	-2.374526	0.582394
H	4.204395	4.827111	-0.846723	C	4.414440	-3.359481	-0.031204
H	-0.443685	1.764549	0.853529	C	3.330108	-2.514848	1.948342
C	-0.439255	-0.357563	2.169058	C	4.900525	-4.448051	0.700267
C	-2.270000	0.493998	3.386085	H	4.666952	-3.275036	-1.084005
H	-2.547876	0.513412	4.446329	C	3.815887	-3.598360	2.682675
H	-2.679406	1.407059	2.923020	H	2.694252	-1.771023	2.422020
C	-2.755086	-0.772705	2.659833	C	4.606220	-4.570584	2.060607
H	-2.888308	-1.592614	3.380290	H	5.513505	-5.197944	0.205881
H	-3.726521	-0.594662	2.194652	H	3.579727	-3.683592	3.740895
O	0.738237	-0.373552	1.765605	H	4.988310	-5.414099	2.630155
N	-0.828609	0.444786	3.226458	H	2.810213	-0.417266	0.563152
C	0.031225	1.454052	3.799356	C	1.625024	-2.524284	-1.773254
H	1.070242	1.147942	3.661361	H	2.082579	-2.141069	-2.693309
H	-0.107657	2.439468	3.330303	H	2.119746	-3.479366	-1.523002
H	-0.175338	1.552933	4.871325	H	0.573064	-2.740466	-1.987646
C	-6.232069	-1.231261	0.140687	H	1.093412	-1.813513	0.064230
H	-7.164314	-0.708566	-0.056030				
H	0.397310	0.153548	-0.557168				
C	-0.188062	0.807326	-2.382406	<b>TS4-F-7.log</b>			
H	0.730282	1.331364	-2.668416	C	0.758094	-2.284638	1.411601
H	-0.128416	-0.213447	-2.763010	C	-0.761096	-4.054082	0.633960
H	-1.047202	1.294406	-2.851158	C	-2.658152	-5.546006	0.956103
N	1.678747	-1.518516	-0.720835	O	1.916730	-1.841870	1.321472
C	3.009535	-1.197775	-0.176138	N	0.532622	-3.612900	1.016808
C	3.965444	-0.587071	-1.231663	C	-1.504654	-3.352390	-0.343313
N	3.299900	0.538375	-1.901936	H	-3.095822	-6.405147	1.455974
H	2.980200	1.202822	-1.199545	C	1.692506	-4.405119	0.605542
C	4.121037	1.231931	-2.888904	C	-2.818648	-3.736251	-0.645549
H	3.524136	2.022394	-3.356332	H	2.491731	-4.301677	1.343102
H	5.039932	1.692178	-2.486928	H	1.396140	-5.454469	0.543077
H	4.421906	0.525425	-3.673042	H	2.079819	-4.085094	-0.370209
C	5.304570	-0.211872	-0.592560	H	-3.371335	-3.210830	-1.416623
				C	-0.392958	-1.537832	1.933336

C	-1.354872	-5.147945	1.268662	H	-1.406460	1.227152	5.218374
H	-0.788894	-5.664826	2.038800	C	-3.398578	-4.820492	0.020367
I	-0.309607	-2.546185	-2.186247	H	-4.417953	-5.109371	-0.221132
Cu	-1.262307	-1.198191	-0.052864	H	-0.004978	0.966421	0.377891
N	-0.675068	0.844180	-0.388515	C	-0.019313	1.153955	-1.664261
C	-1.905305	1.607597	-0.048683	H	0.268619	2.208506	-1.752392
C	-3.086838	1.029942	-0.869402	H	0.881820	0.541261	-1.736119
N	-3.255477	-0.411281	-0.500273	H	-0.670233	0.892864	-2.503601
C	-4.380215	1.823697	-0.778786	N	3.738287	1.003873	2.604048
C	-4.805600	2.436757	0.409454	C	3.672479	0.966533	1.132273
C	-5.208472	1.902958	-1.906648	C	4.785540	0.076688	0.510022
C	-6.025578	3.113489	0.465132	N	4.835696	-1.208388	1.215704
H	-4.181543	2.392500	1.296796	H	3.890793	-1.583870	1.287479
C	-6.430779	2.577520	-1.855221	C	5.731098	-2.191880	0.621167
H	-4.888341	1.434363	-2.835019	H	5.729469	-3.098742	1.237934
C	-6.843227	3.186000	-0.666732	H	5.481125	-2.488558	-0.413424
H	-6.336896	3.585536	1.393450	H	6.757005	-1.799492	0.606685
H	-7.056274	2.631277	-2.742539	C	4.556855	-0.043966	-0.999994
H	-7.791638	3.714961	-0.623054	C	3.425344	-0.708904	-1.501411
H	-2.783197	1.012124	-1.919304	C	5.480755	0.481118	-1.912156
C	-1.727204	3.113882	-0.153062	C	3.220514	-0.822487	-2.878577
C	-1.867147	3.807881	-1.364311	H	2.710564	-1.146953	-0.808466
C	-1.376395	3.835565	0.996651	C	5.277824	0.371185	-3.291382
C	-1.670007	5.189703	-1.420343	H	6.367107	0.988339	-1.537908
H	-2.143060	3.270900	-2.267148	C	4.142287	-0.278999	-3.780000
C	-1.184464	5.218122	0.946279	H	2.337389	-1.336615	-3.248898
H	-1.256424	3.306483	1.938462	H	6.006491	0.791085	-3.980730
C	-1.332514	5.900714	-0.264579	H	3.978342	-0.367762	-4.851023
H	-1.786123	5.711764	-2.366651	H	5.765174	0.552574	0.652095
H	-0.919534	5.760247	1.850373	C	3.600989	2.361439	0.503257
H	-1.185138	6.976606	-0.307993	C	4.737268	3.106753	0.149077
H	-2.088205	1.369984	1.004521	C	2.343478	2.961670	0.330046
C	-0.151287	-0.205080	2.508100	C	4.619191	4.393529	-0.385553
C	-1.969406	-1.085793	3.722513	H	5.727134	2.680136	0.278543
H	-2.107900	-1.359021	4.775160	C	2.217464	4.243462	-0.210468
H	-2.943802	-0.749450	3.338071	H	1.456358	2.419662	0.638447
C	-1.390561	-2.234661	2.875174	C	3.358115	4.964567	-0.575931
H	-0.879077	-2.962378	3.520504	H	5.515133	4.947342	-0.656164
H	-2.190421	-2.771379	2.361115	H	1.230148	4.676230	-0.344863
O	0.628879	0.696681	2.127955	H	3.265232	5.961361	-0.999969
N	-0.990031	-0.019411	3.587902	H	2.722903	0.464771	0.932847
C	-1.264537	1.290241	4.133340	C	4.826587	1.769269	3.195392
H	-0.418156	1.945074	3.918343	H	5.787256	1.302341	2.945403
H	-2.174981	1.728207	3.692951	H	4.882455	2.827686	2.884360

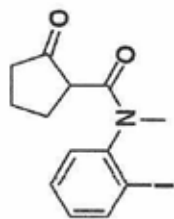
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H	-3.619058	-0.900273	-1.316252	H	-5.481740	-4.719488	2.837324
C	-4.145085	-0.691052	0.640023	H	-7.298819	-3.302010	3.779635
H	-5.194409	-0.441415	0.440279	H	-2.740384	-1.870945	0.383855
H	-4.068507	-1.755459	0.876479	C	-4.933662	-1.495468	-1.363003
H	-3.811257	-0.120319	1.508133	C	-4.405425	-2.698315	-1.856194
<b>TS4-F-8.log</b>				C	-6.296116	-1.231784	-1.542775
C	0.912999	-0.438148	0.275097	C	-5.224859	-3.617554	-2.512719
C	1.152814	1.607946	-1.233926	H	-3.348827	-2.920876	-1.721833
C	0.657285	2.686768	0.940574	C	-7.120466	-2.151354	-2.197827
C	0.659788	3.098127	3.341355	H	-6.714360	-0.302823	-1.162798
O	1.576895	1.790423	-2.393677	C	-6.586654	-3.346866	-2.684634
N	1.356314	2.606756	-0.282671	H	-4.802122	-4.545957	-2.887915
C	-0.748510	2.608049	0.987236	H	-8.176898	-1.931621	-2.328566
H	1.218767	3.292287	4.252608	H	-7.225149	-4.063084	-3.195014
C	2.262628	3.714095	-0.604968	H	-4.630571	0.387004	-0.379014
C	-1.442961	2.794642	2.188046	H	-2.386324	-0.829605	-1.788882
H	2.241829	3.882112	-1.682262	C	-3.348455	0.721498	-2.675668
H	3.289438	3.477222	-0.308616	H	-3.920112	1.600831	-2.368093
H	1.924357	4.616054	-0.089249	H	-2.461997	1.060724	-3.217448
H	-2.527382	2.786754	2.191241	H	-3.969160	0.108106	-3.341295
C	0.448802	0.371573	-0.865595	C	0.278566	-0.619810	-2.019902
C	1.343371	2.924559	2.136497	H	-0.531896	-0.368223	-2.710498
H	2.427900	2.950393	2.107460	H	1.198596	-0.666586	-2.616683
I	-1.918235	3.629423	-0.877908	C	0.045246	-1.961914	-1.308625
Cu	-1.523521	1.045725	-0.185813	H	-1.024087	-2.173501	-1.141224
N	-2.913887	-0.015121	-1.477605	H	0.467000	-2.816108	-1.851368
C	-4.040045	-0.498114	-0.641840	O	1.436079	-0.077901	1.348638
C	-3.455818	-1.089933	0.664836	C	-0.734361	3.018787	3.372573
N	-2.669648	-0.040777	1.353259	H	-1.278860	3.159107	4.302446
H	-3.318973	0.652764	1.727524	N	4.452159	1.350272	-1.373100
C	-1.860446	-0.570463	2.463353	C	4.430209	0.065487	-0.658644
H	-1.304422	0.251104	2.916884	C	5.121393	0.186253	0.736159
H	-2.471495	-1.061432	3.232594	N	4.340959	1.129994	1.550263
H	-1.146073	-1.291943	2.064190	H	3.368982	0.816012	1.581277
C	-4.531922	-1.708508	1.543026	C	4.847885	1.319238	2.904725
C	-5.556826	-0.916519	2.081958	H	4.209904	2.038909	3.430485
C	-4.516179	-3.078924	1.826473	H	4.894656	0.399733	3.514100
C	-6.547648	-1.486314	2.883023	H	5.862670	1.736554	2.864221
H	-5.584913	0.150200	1.870683	C	5.297325	-1.188072	1.382867
C	-5.507479	-3.653331	2.627355	C	4.175835	-1.919621	1.802241
H	-3.724706	-3.699558	1.412988	C	6.567939	-1.744505	1.571437
				C	4.322204	-3.185420	2.372205

H	3.186987	-1.485007	1.687364
C	6.720293	-3.011111	2.144998
H	7.446856	-1.185290	1.257813
C	5.596092	-3.739289	2.543009
H	3.439928	-3.740125	2.683398
H	7.715836	-3.427232	2.279965
H	5.710712	-4.724988	2.986979
H	6.121832	0.618014	0.599987
C	4.907941	-1.127849	-1.481213
C	6.261549	-1.340928	-1.788796
C	3.965391	-2.043773	-1.970593
C	6.655930	-2.425646	-2.575719
H	7.014729	-0.665336	-1.394631
C	4.354191	-3.132374	-2.755919
H	2.917497	-1.909777	-1.714491
C	5.703194	-3.324661	-3.065837
H	7.709482	-2.572726	-2.800966
H	3.604557	-3.831508	-3.118813
H	6.011143	-4.169894	-3.676095
H	3.373959	-0.115121	-0.440376
C	5.671363	1.745866	-2.062422
H	6.508097	1.803878	-1.356175
H	5.981792	1.081559	-2.887275
H	5.522349	2.749025	-2.479445
H	3.654802	1.399075	-2.003384
N	0.720686	-1.774402	-0.036604
C	0.800596	-2.850680	0.923138
H	1.133975	-2.446657	1.880617
H	-0.181905	-3.326318	1.060985
H	1.510197	-3.620484	0.593561

## V. References

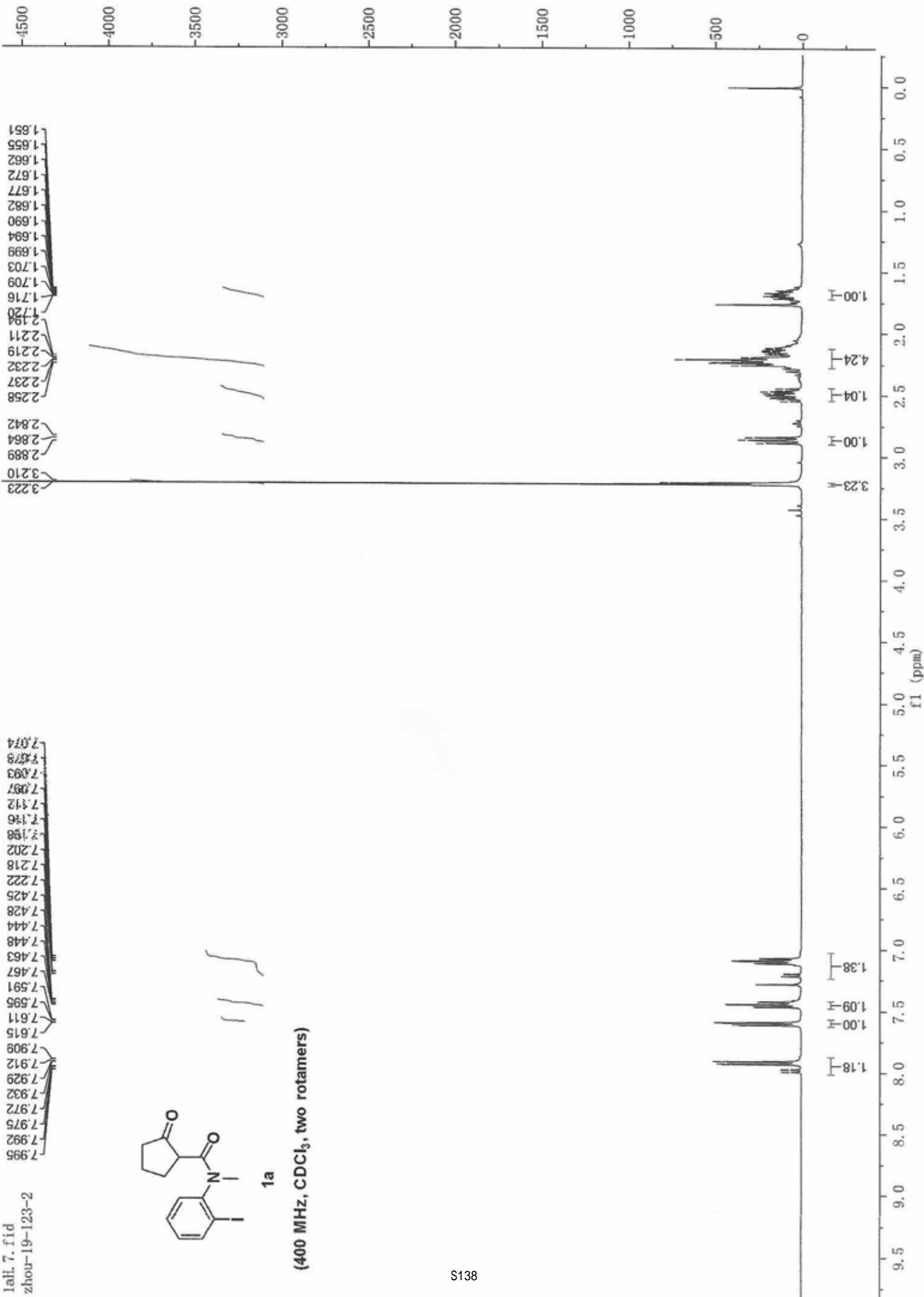
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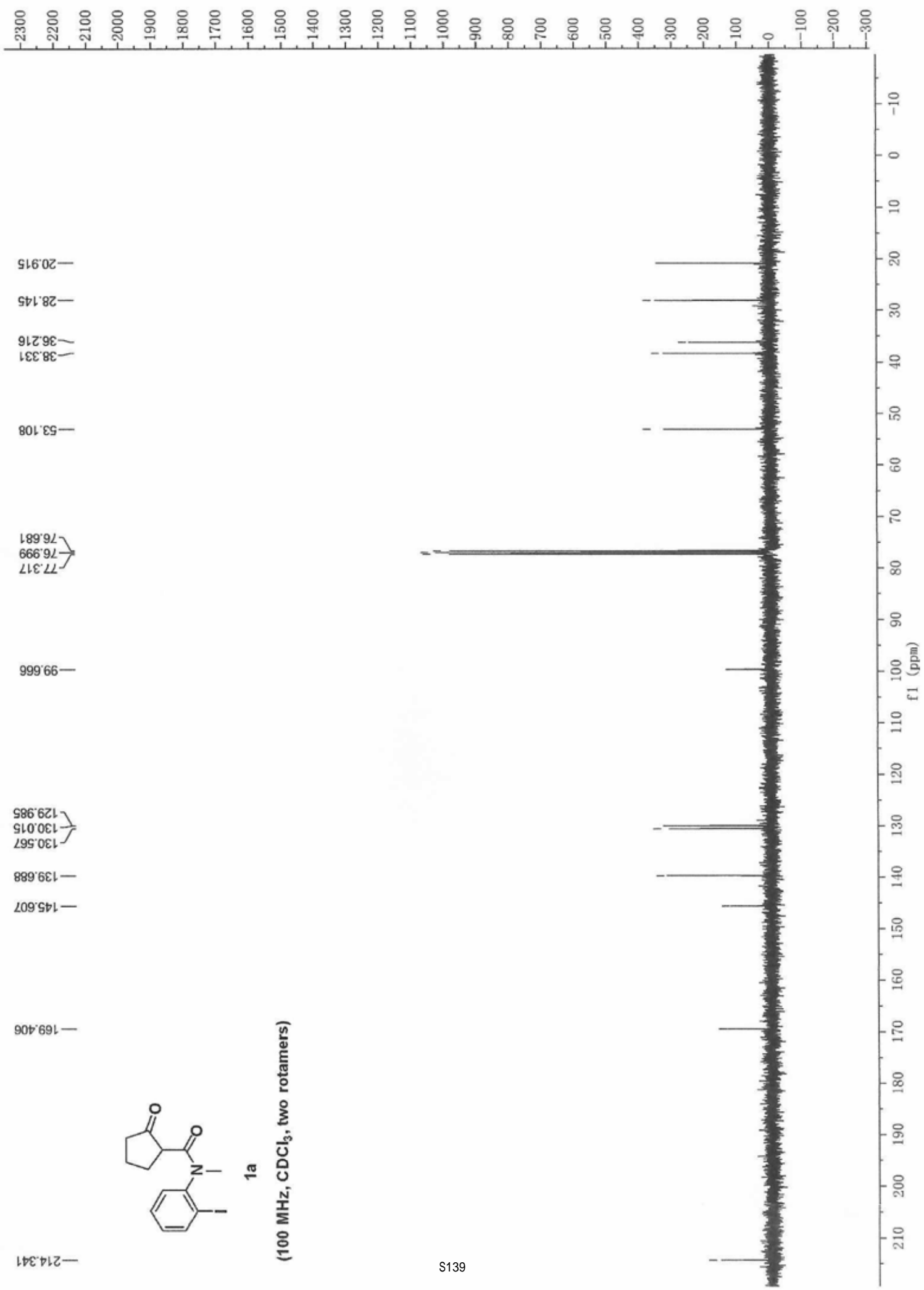
## VI. NMR and HPLC Spectra

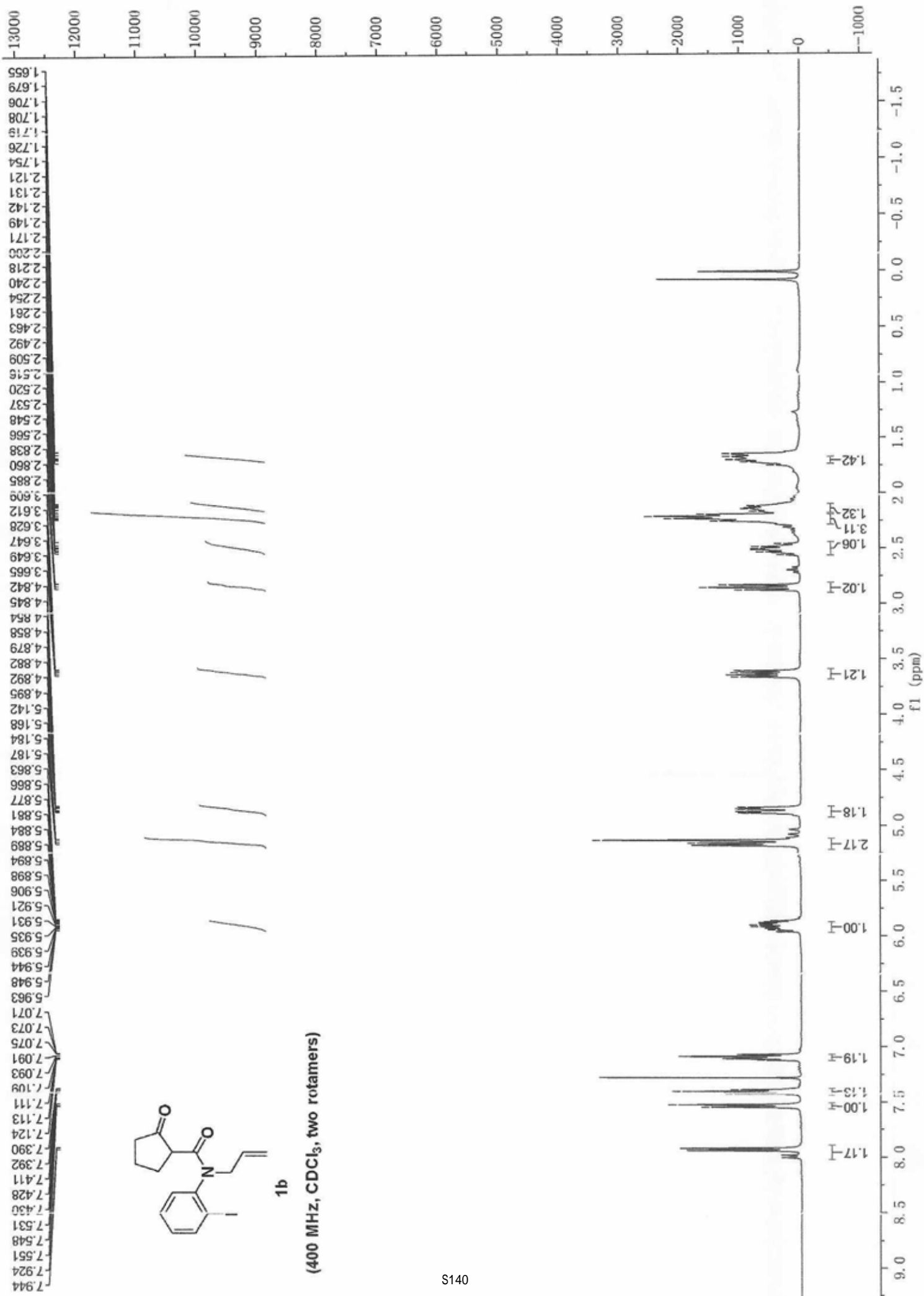


1a

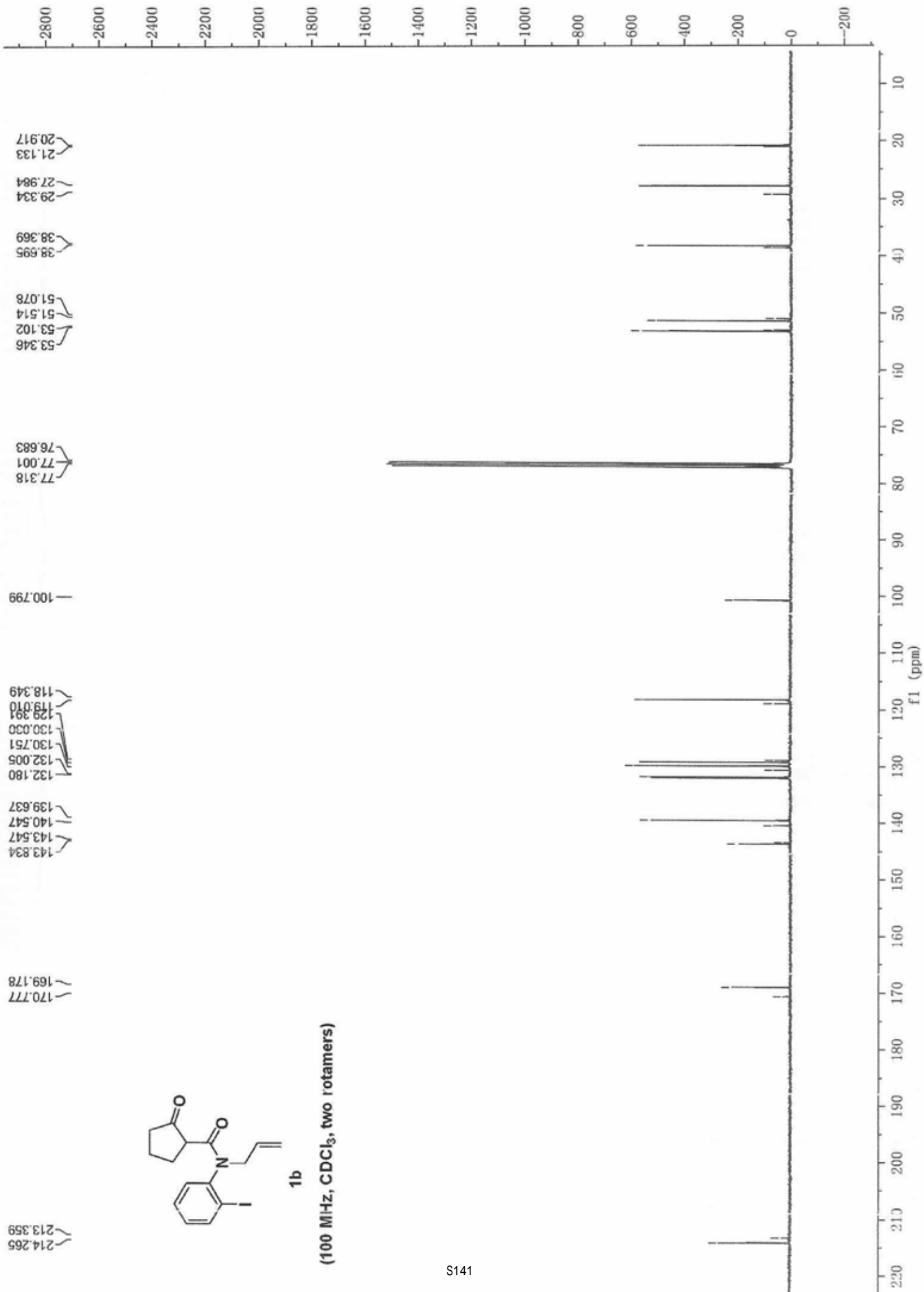
(400 MHz, CDCl<sub>3</sub>, two rotamers)

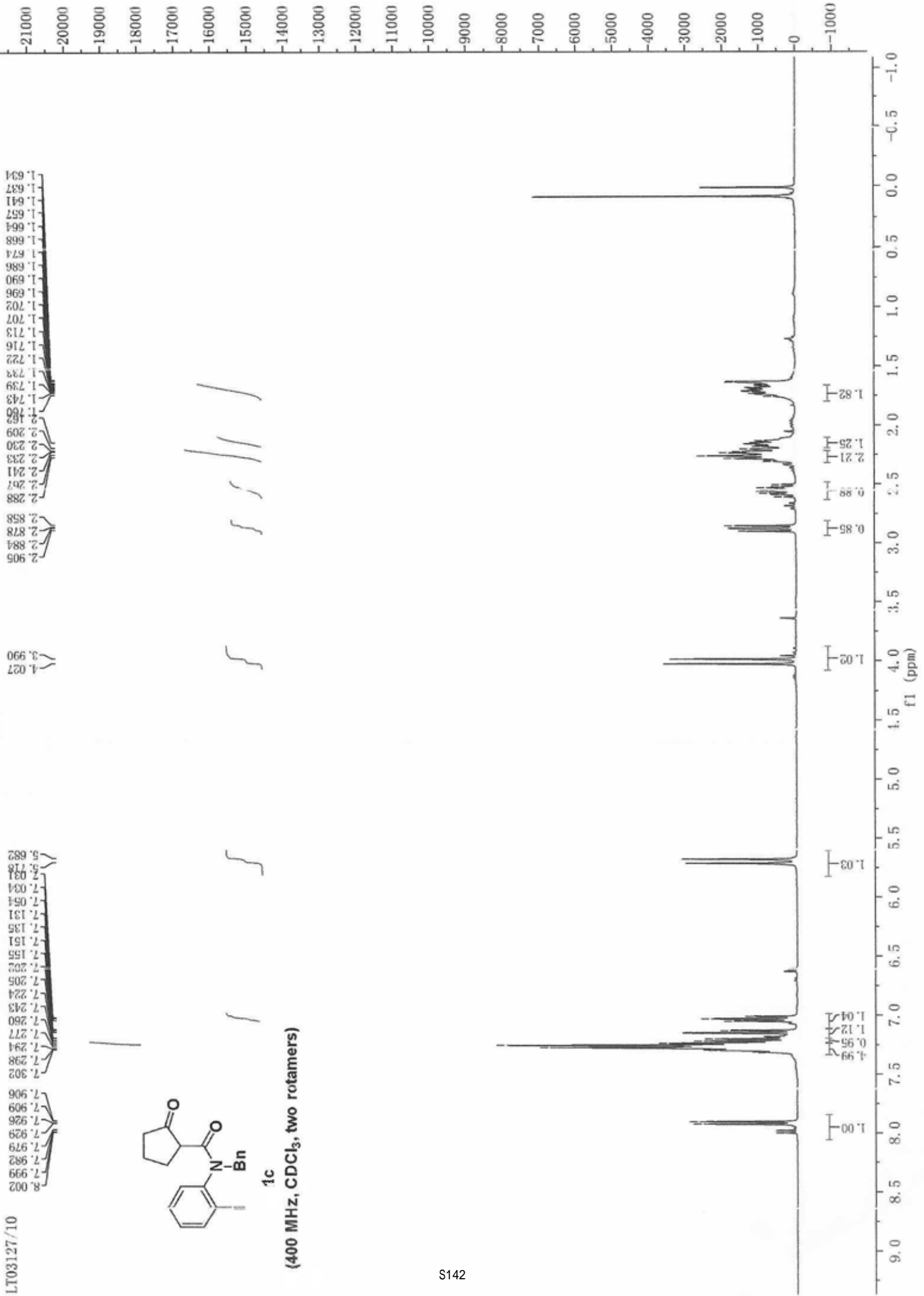


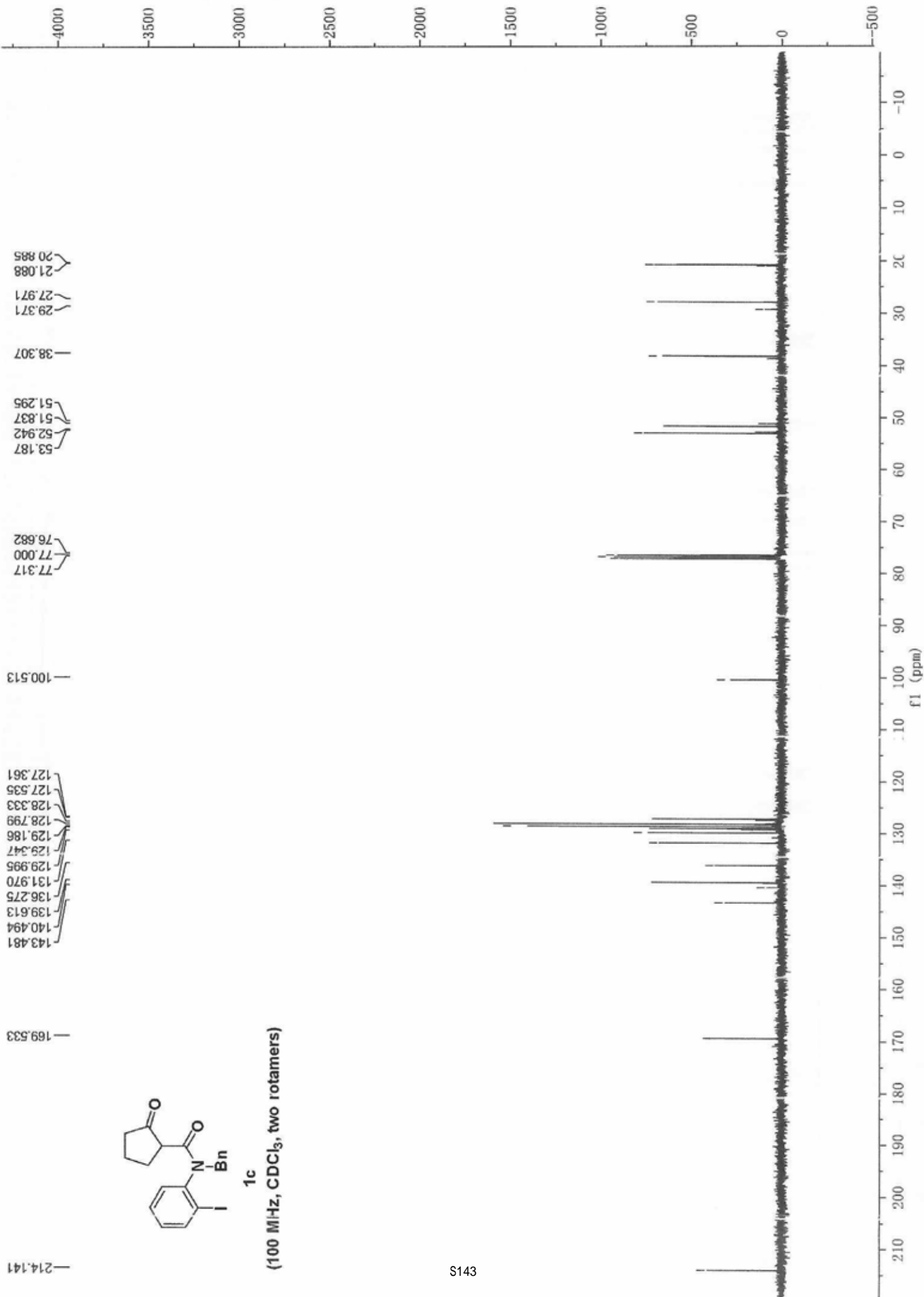


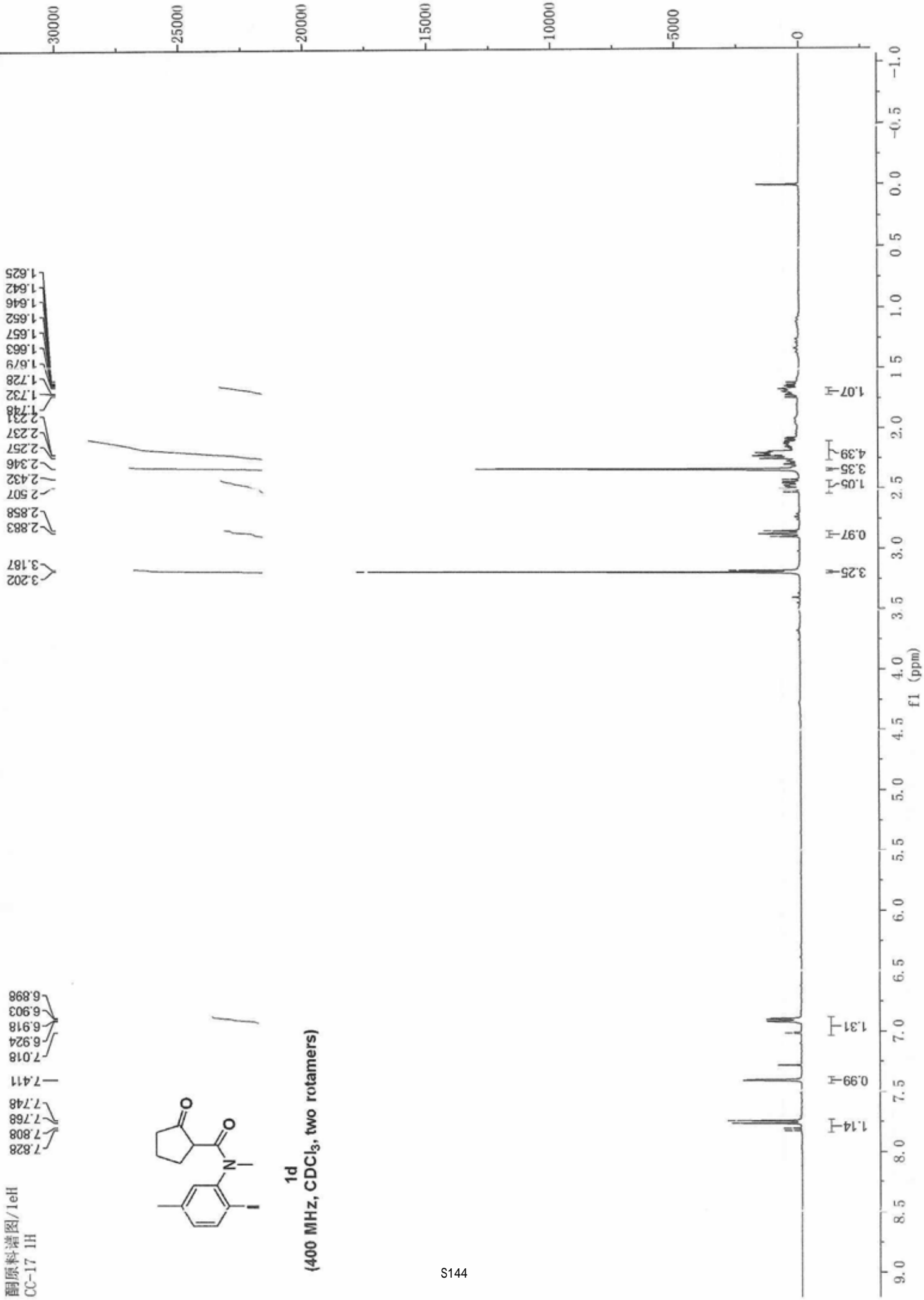


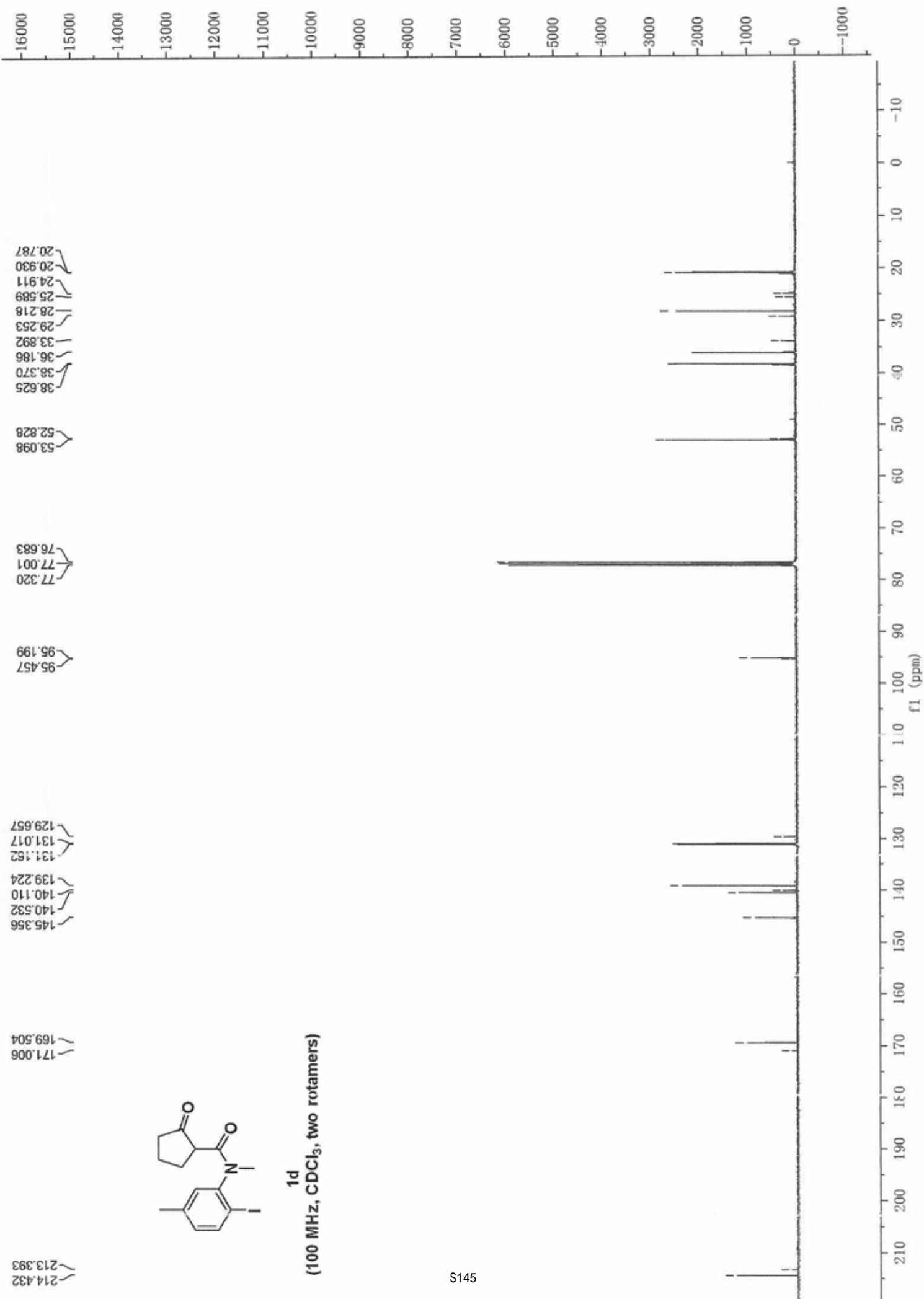






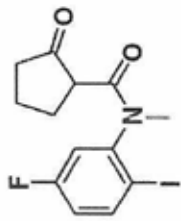




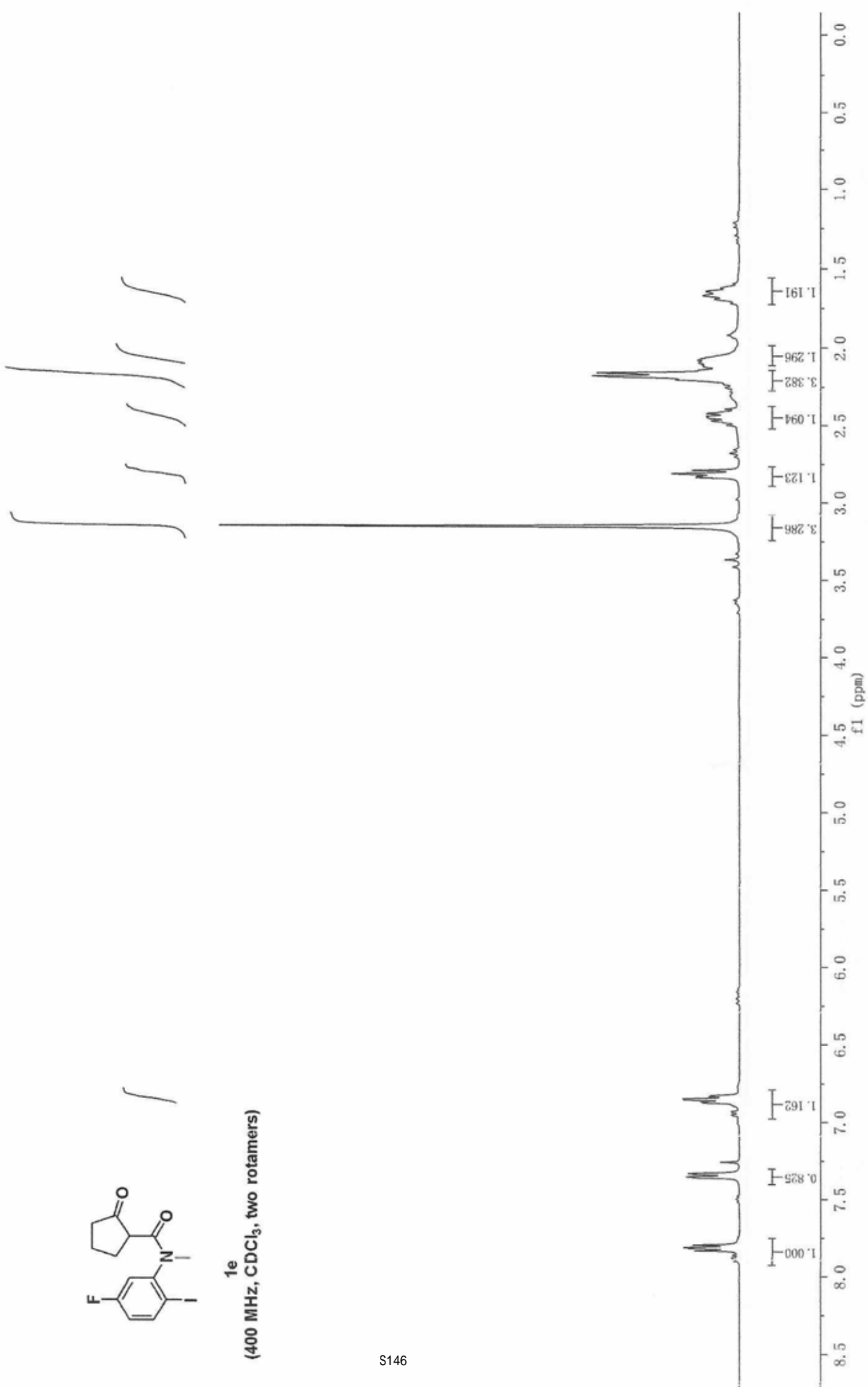


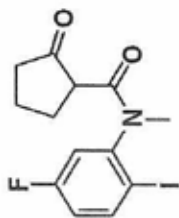
- 7.901
- 7.885
- 7.880
- 7.864
- 7.835
- 7.820
- 7.814
- 7.798
- 7.361
- 7.356
- 7.339
- 7.331
- 6.960
- 6.951
- 6.939
- 6.932
- 6.877
- 6.871
- 6.857
- 6.851
- 6.837
- 6.830

- 2.838
- 2.829
- 2.814
- 2.791
- 2.451
- 2.442
- 2.424
- 2.207
- 2.183
- 2.163
- 2.146
- 2.079
- 1.671
- 1.644
- 1.623



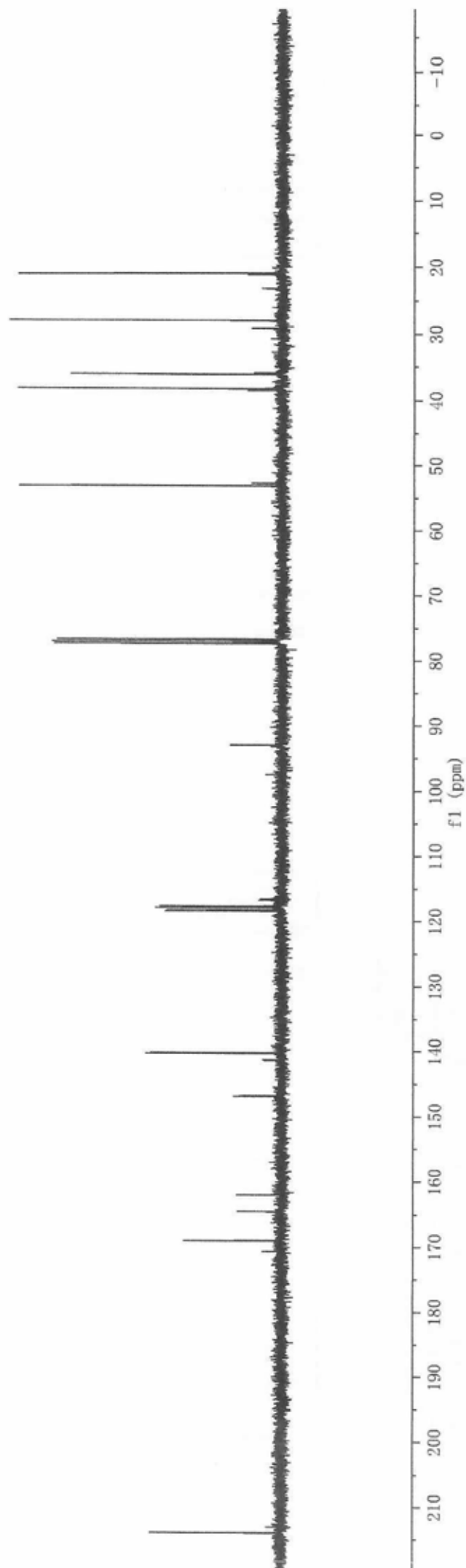
**1e**  
(400 MHz, CDCl<sub>3</sub>, two rotamers)





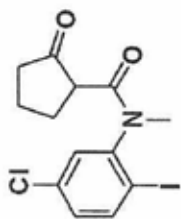
1e  
(100 MHz, CDCl<sub>3</sub>, two rotamers)

214.042	213.271
170.247	169.094
162.091	164.592
147.004	146.906
141.553	140.387
140.302	118.522
118.297	117.951
117.736	116.844
116.624	93.067
93.029	53.209
52.840	38.601
38.310	36.156
35.967	29.211
27.984	21.157
20.935	



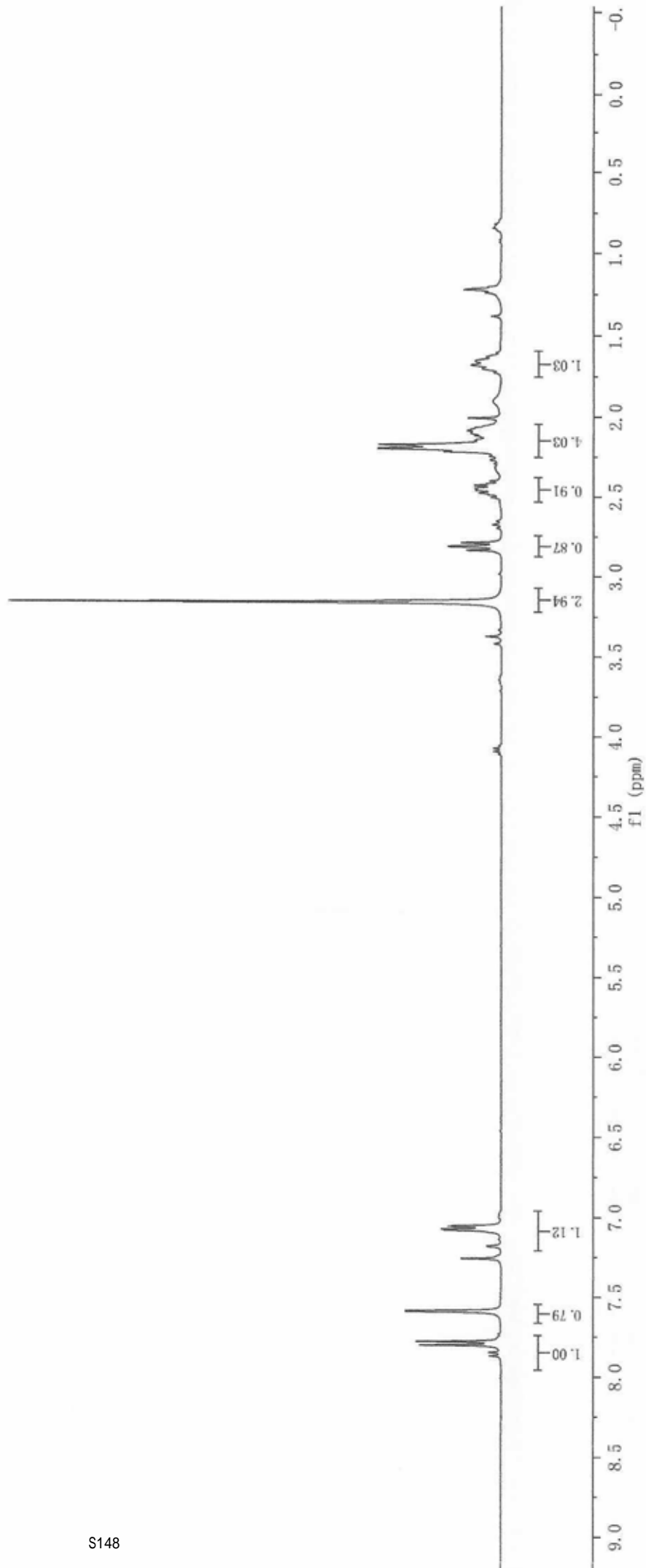
7.869  
7.848  
7.802  
7.780  
7.593  
7.588  
7.184  
7.179  
7.081  
7.075  
7.060  
7.054

3.161  
2.835  
2.811  
2.788  
2.461  
2.447  
2.429  
2.221  
2.199  
2.185  
2.177  
1.703  
1.681  
1.656  
1.634



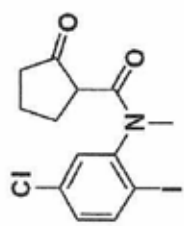
1f

(400 MHz, CDCl<sub>3</sub>, two rotamers)





213.981  
213.003



1f

(100 MHz, CDCl<sub>3</sub>, two rotamers)

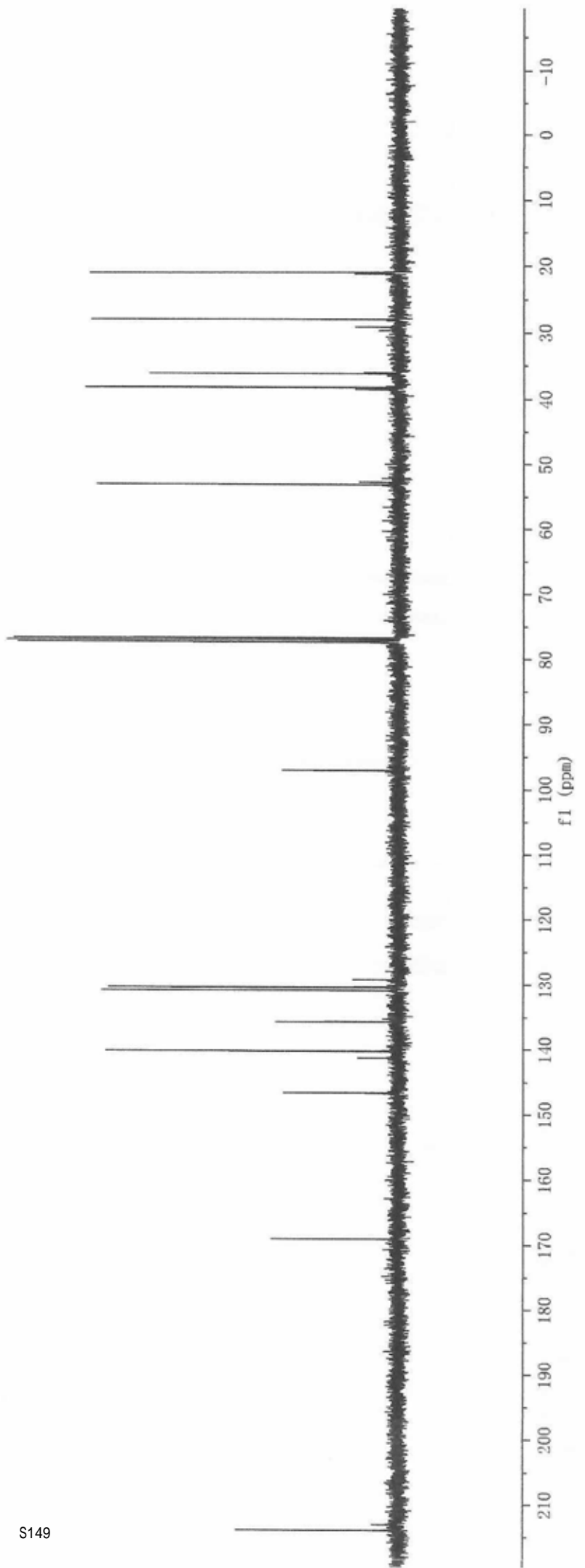
146.705

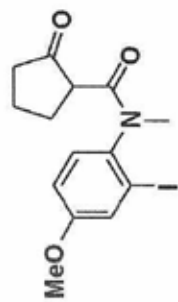
141.322  
140.311  
135.784  
130.931  
130.455  
130.378  
129.292

97.205

53.198  
52.837

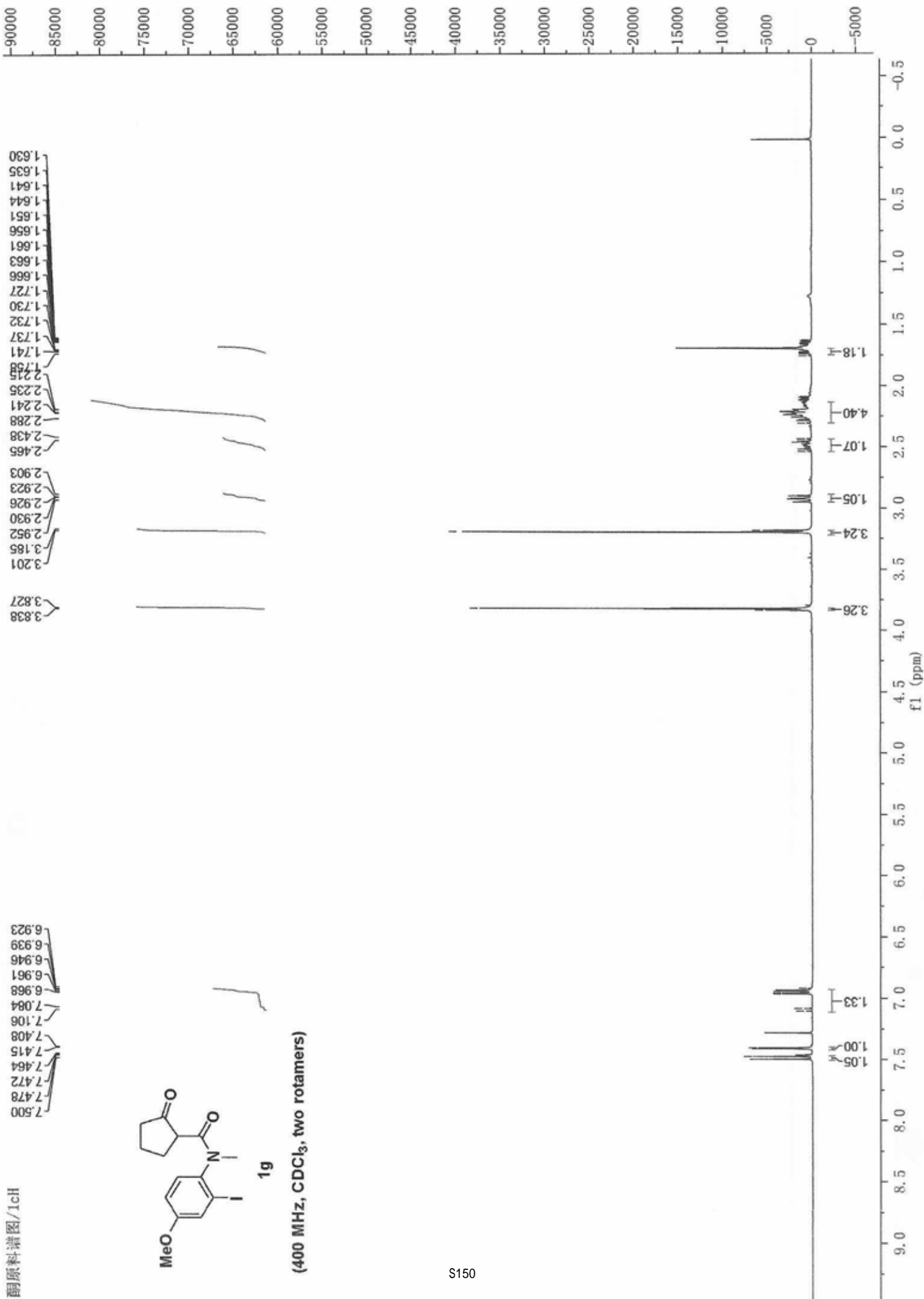
38.633  
38.337  
36.246  
36.059  
29.199  
28.036  
21.178  
20.955

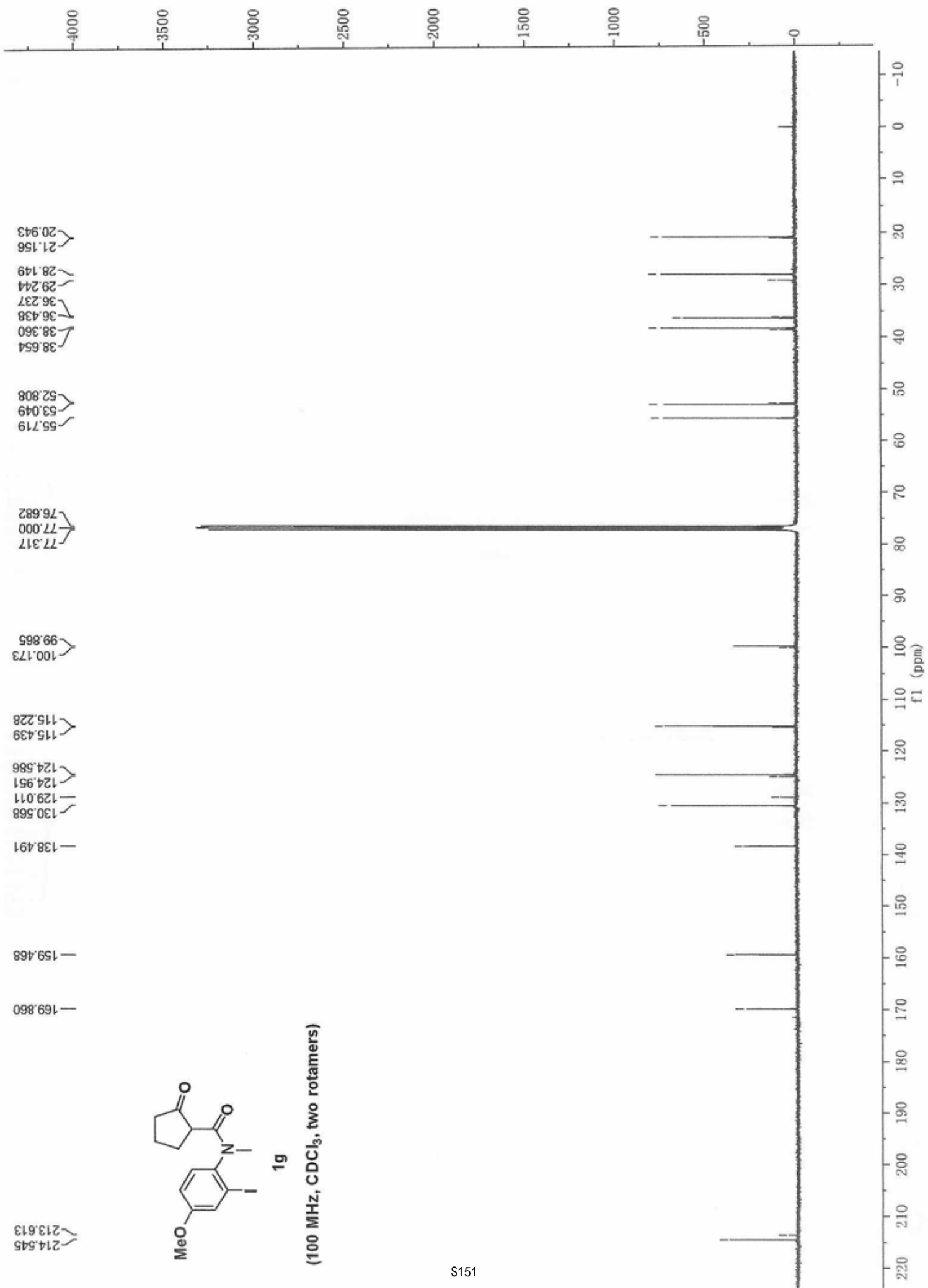


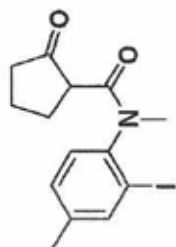


1g

(400 MHz, CDCl<sub>3</sub>, two rotamers)

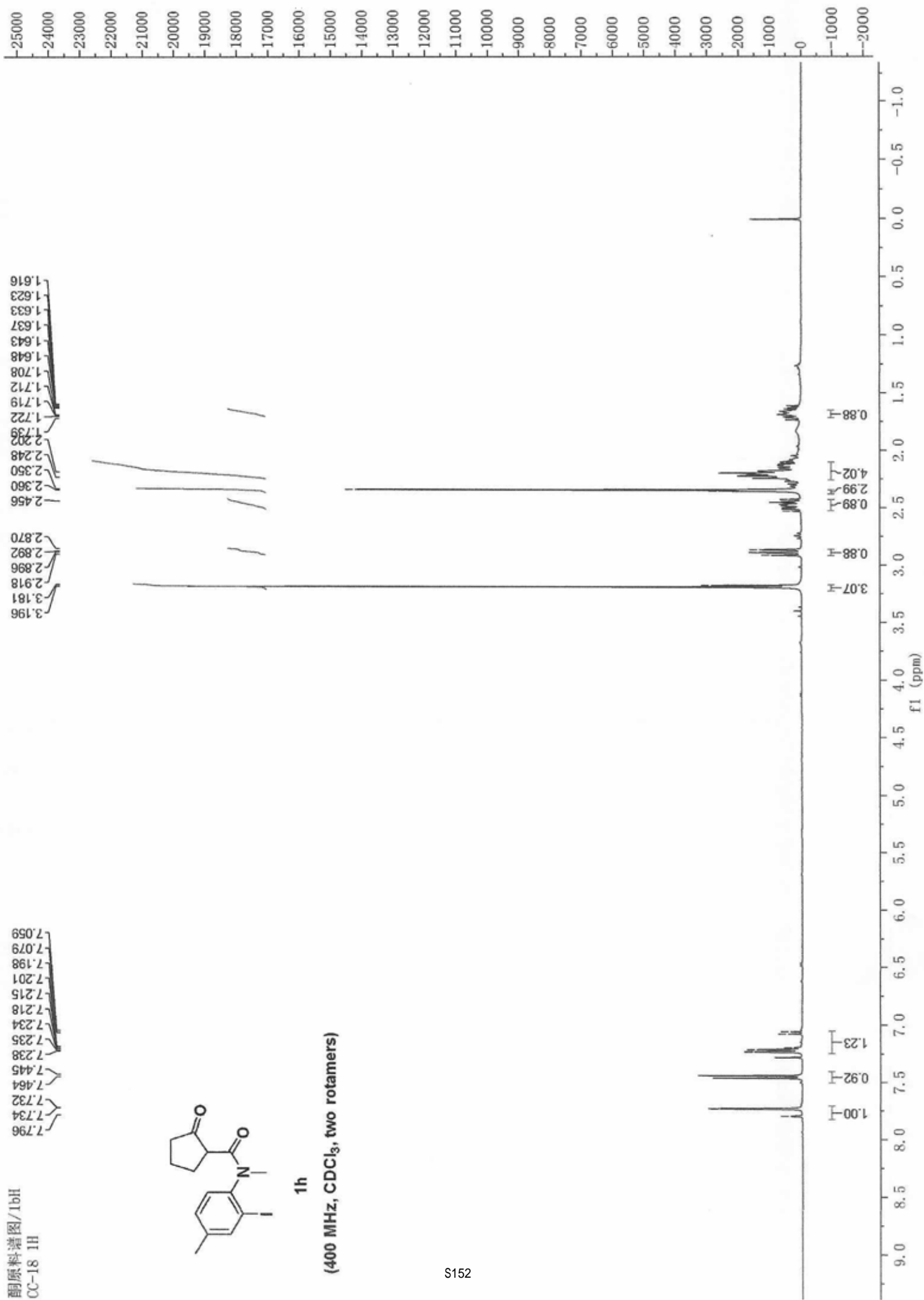


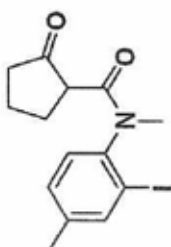
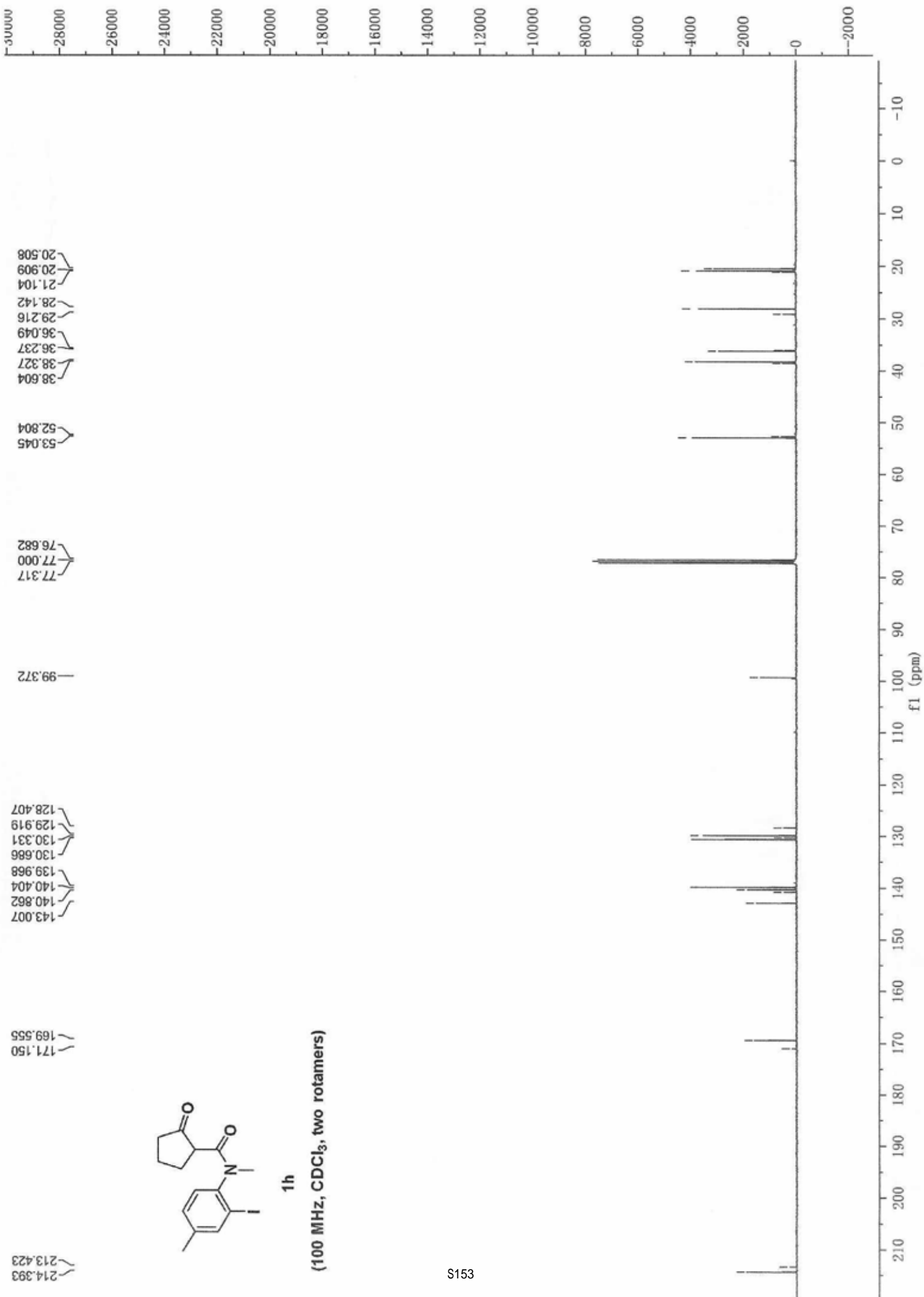




1h

(400 MHz, CDCl<sub>3</sub>, two rotamers)

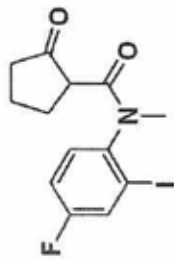




1h

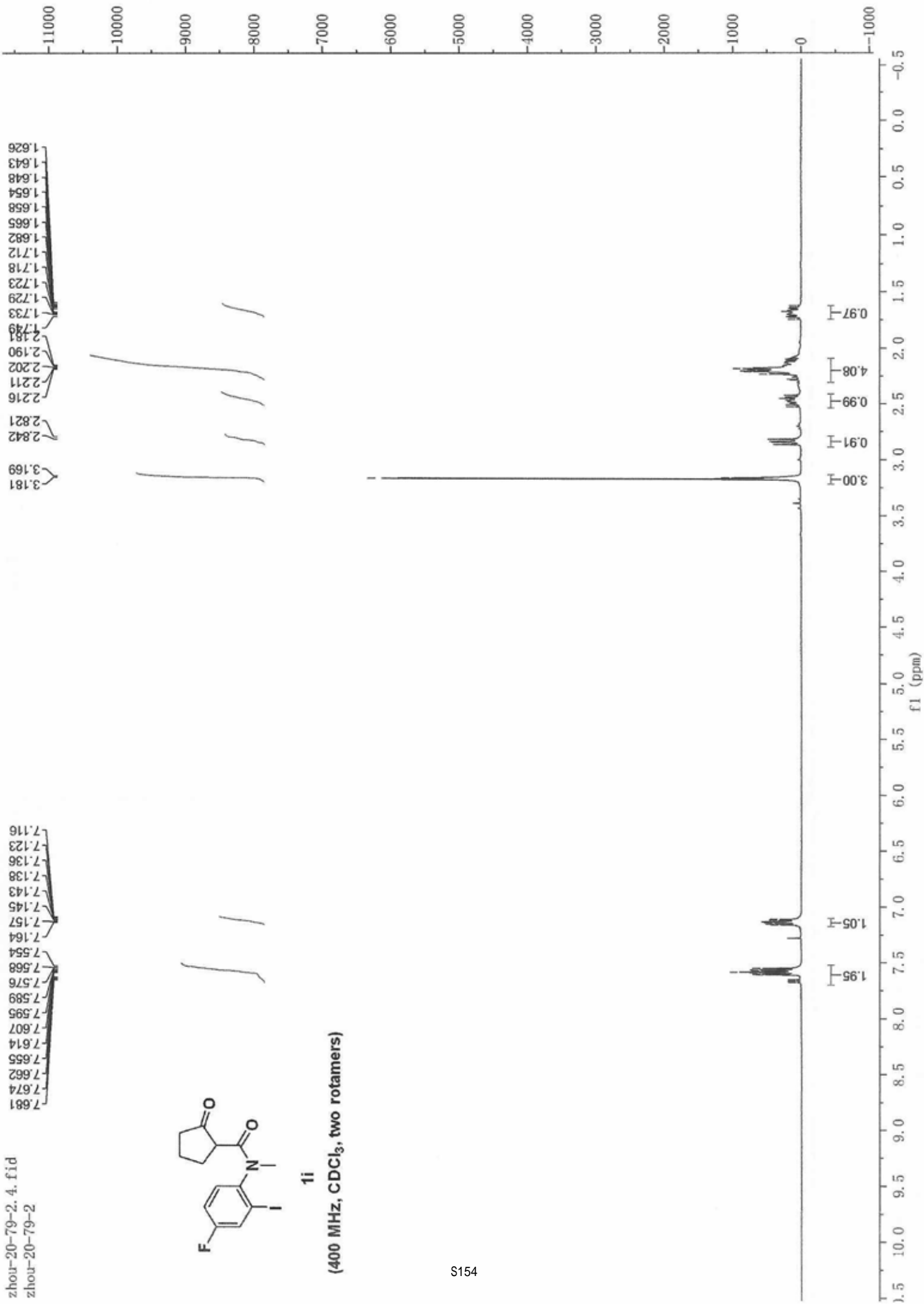
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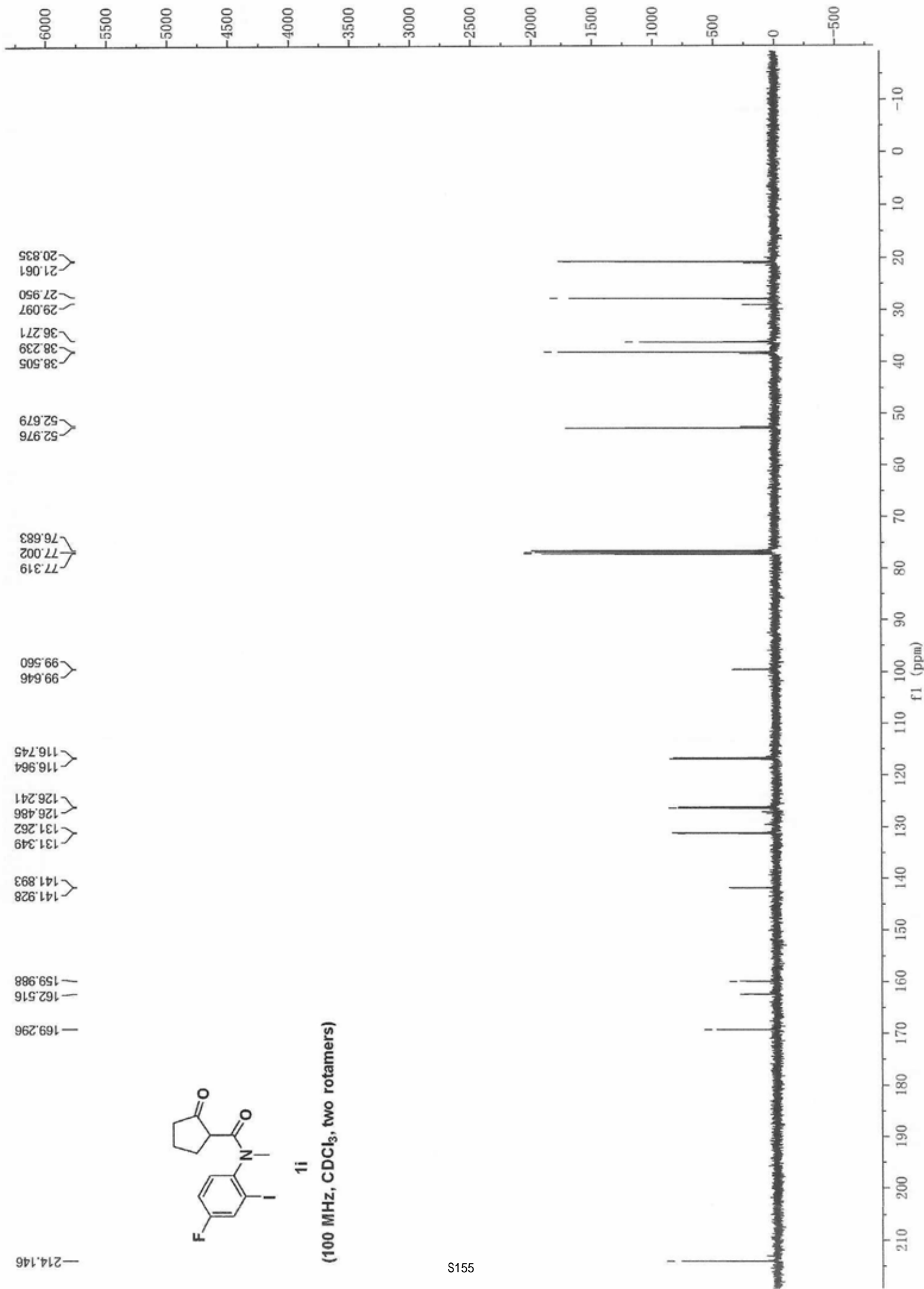
zhou-20-79-2, 4. fid  
zhou-20-79-2



1i

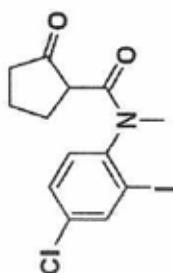
(400 MHz, CDCl<sub>3</sub>, two rotamers)





OYVF-420.10.fid

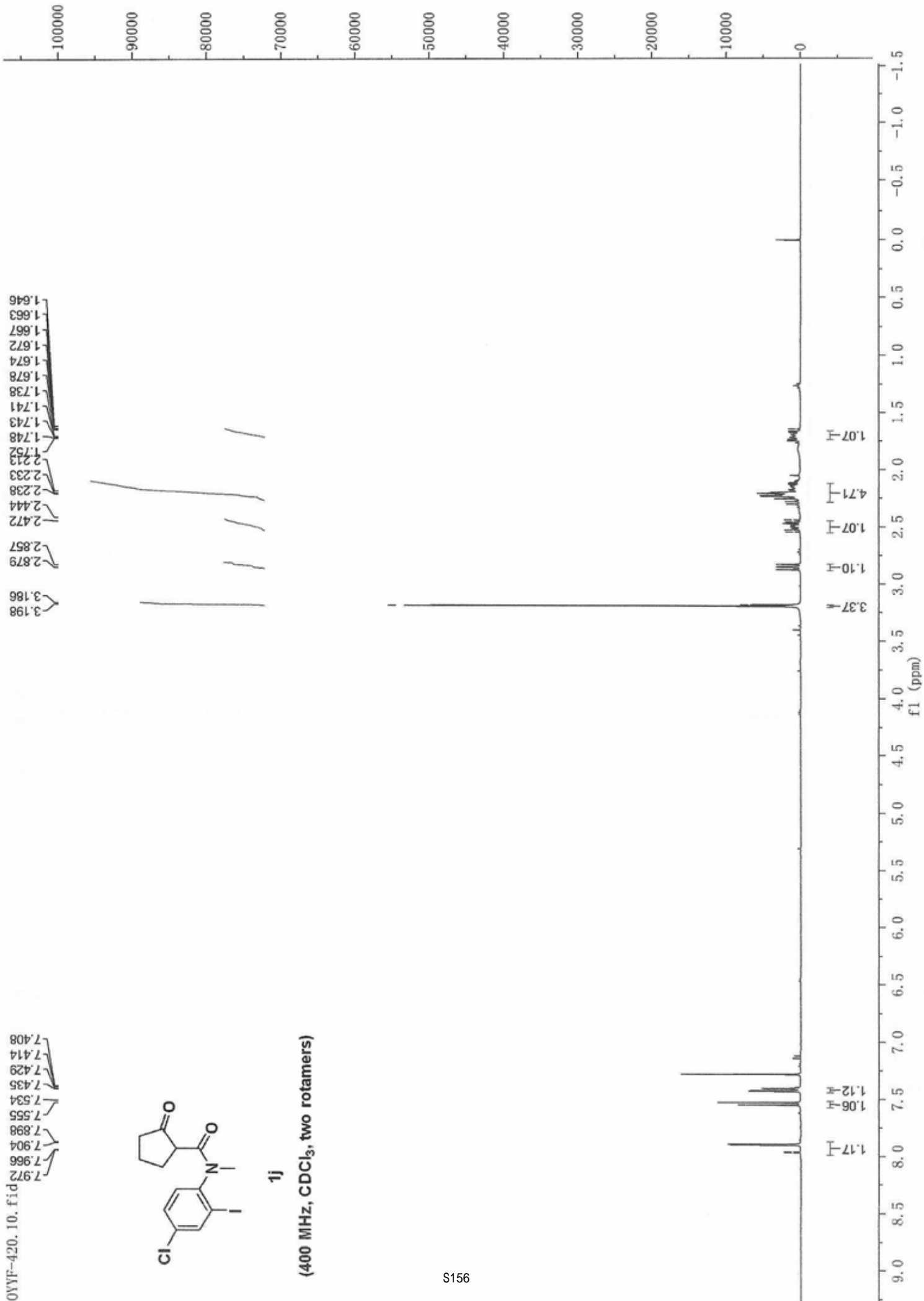
7.972  
7.966  
7.904  
7.898  
7.555  
7.534  
7.435  
7.429  
7.414  
7.408



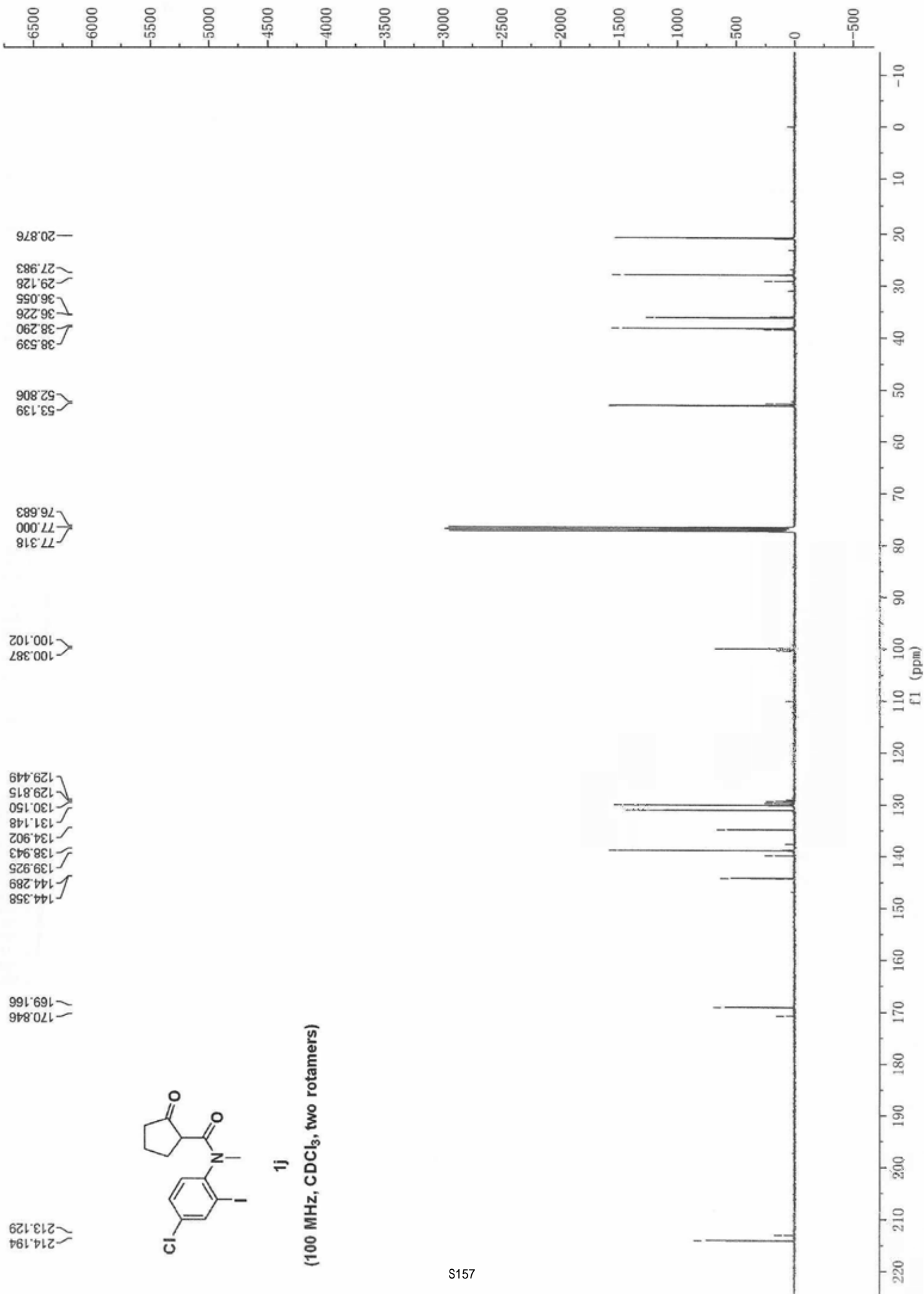
1j

(400 MHz, CDCl<sub>3</sub>, two rotamers)

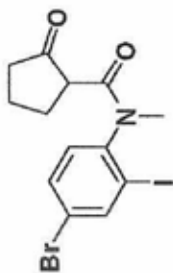
3.196  
2.879  
2.857  
2.472  
2.444  
2.238  
2.213  
1.752  
1.748  
1.743  
1.741  
1.738  
1.678  
1.674  
1.672  
1.667  
1.663  
1.646





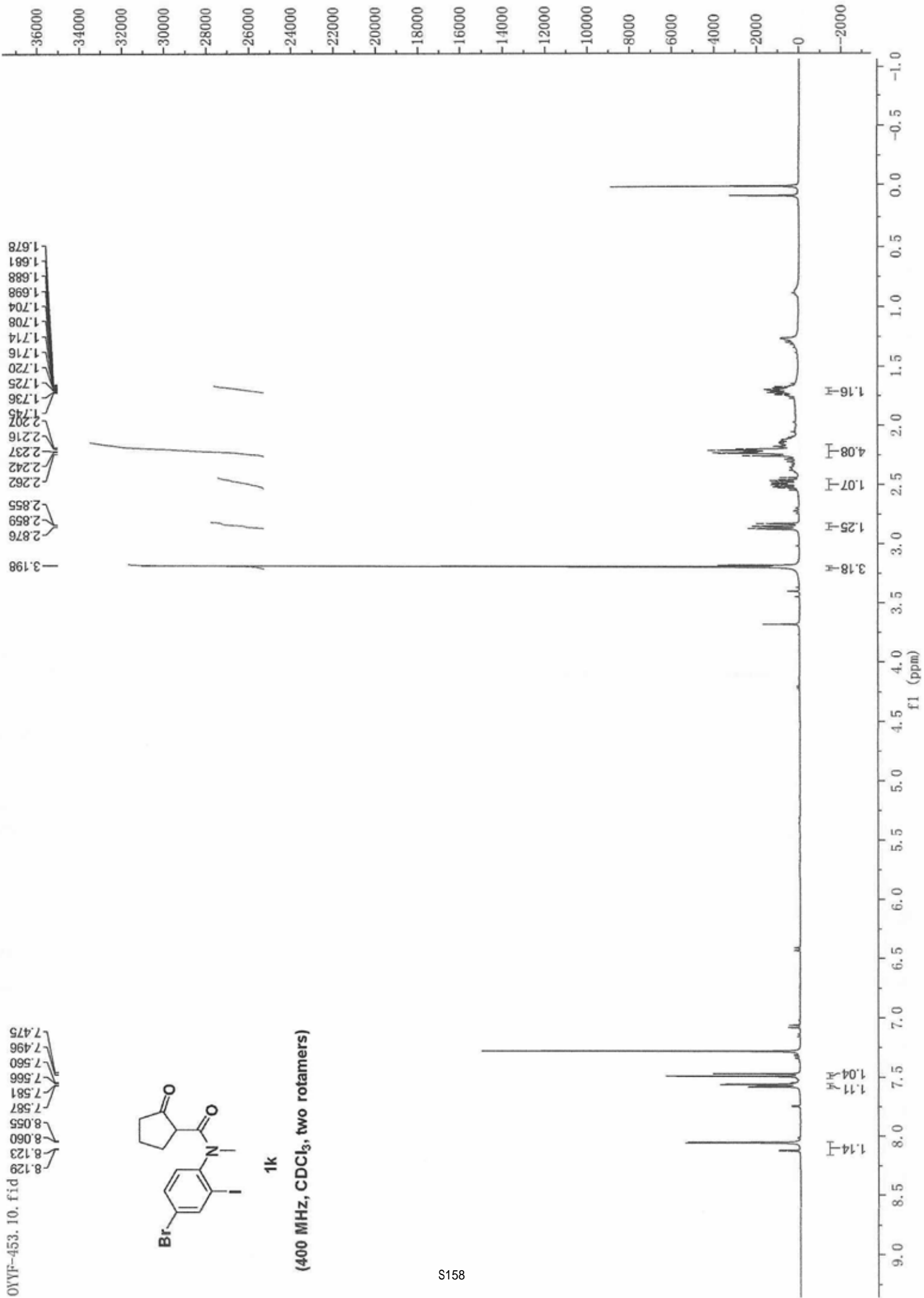


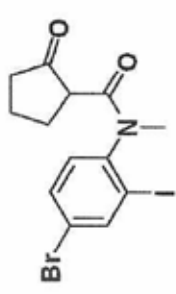
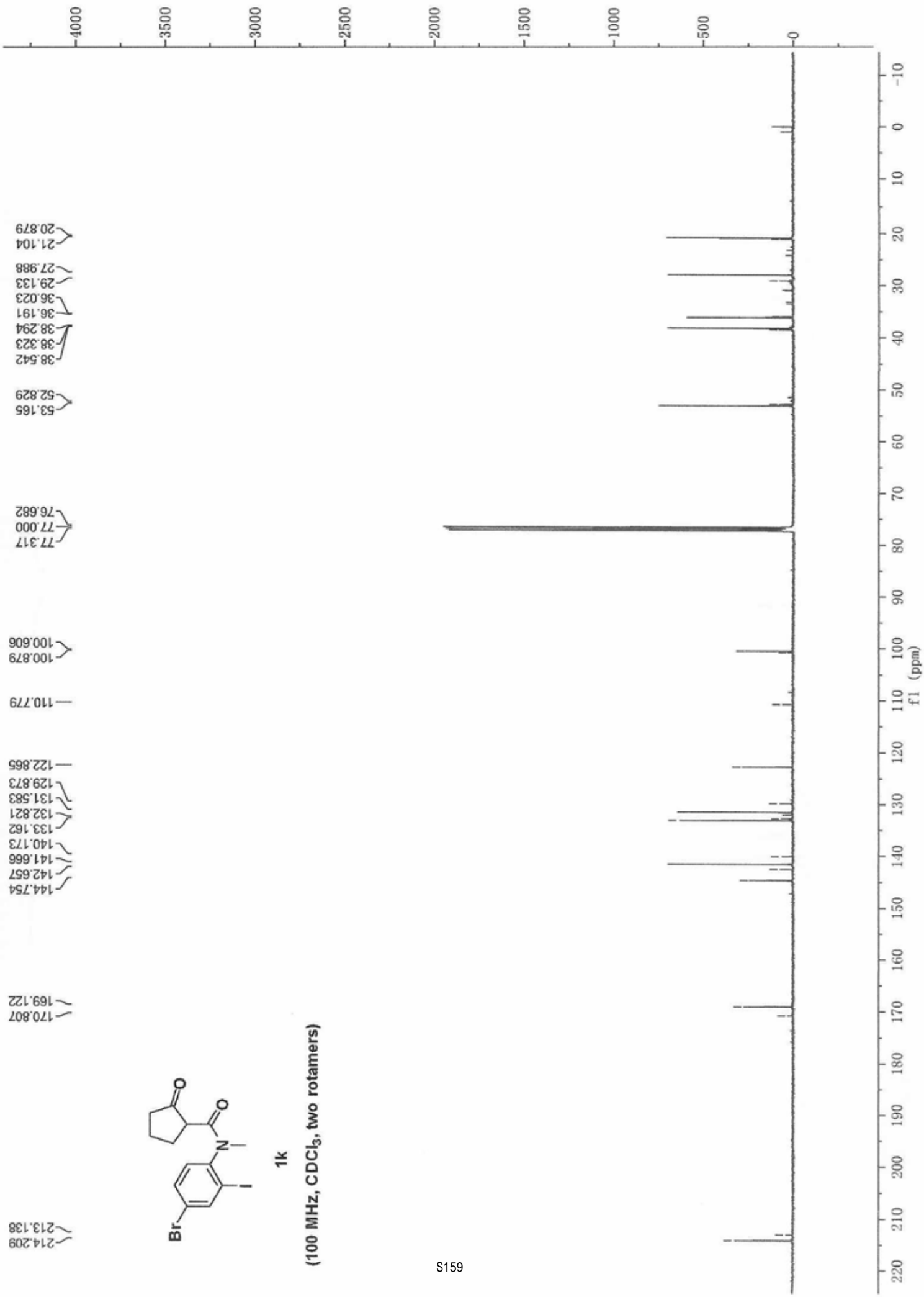
OYVF-453.10. fid  
8.129  
8.123  
8.060  
8.055  
7.587  
7.581  
7.566  
7.560  
7.496  
7.475



1k

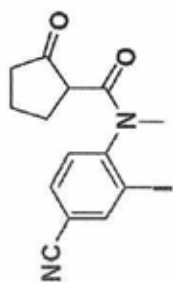
(400 MHz, CDCl<sub>3</sub>, two rotamers)





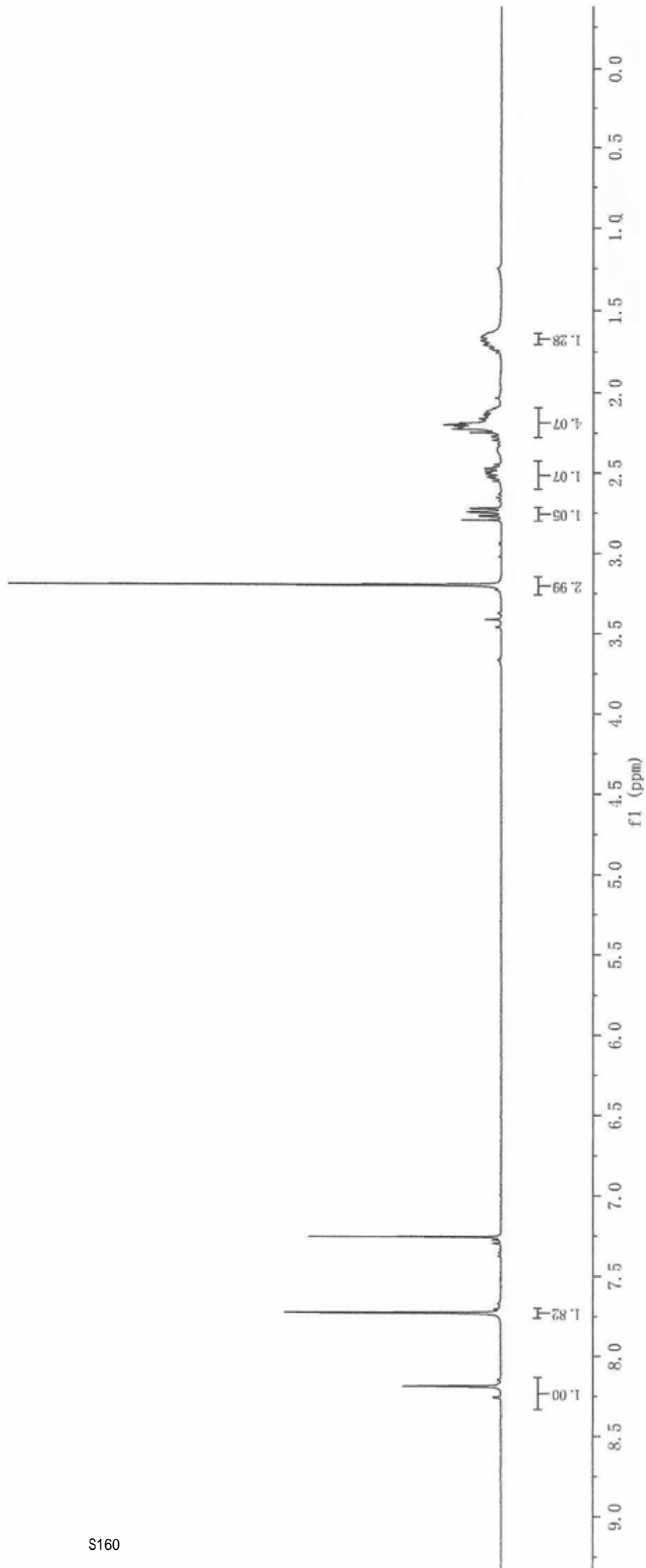
1k  
 (100 MHz, CDCl<sub>3</sub>, two rotamers)

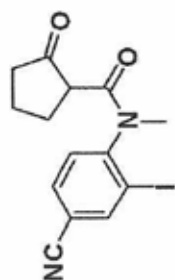
8.263  
8.258  
7.732



**11**  
(400 MHz, CDCl<sub>3</sub>, two rotamers)

3.202  
2.796  
2.770  
2.748  
2.745  
2.723  
2.509  
2.493  
2.477  
2.229  
2.224  
2.211  
2.203  
1.731  
1.709  
1.705  
1.699  
1.693  
1.683  
1.673  
1.661  
1.654  
1.635

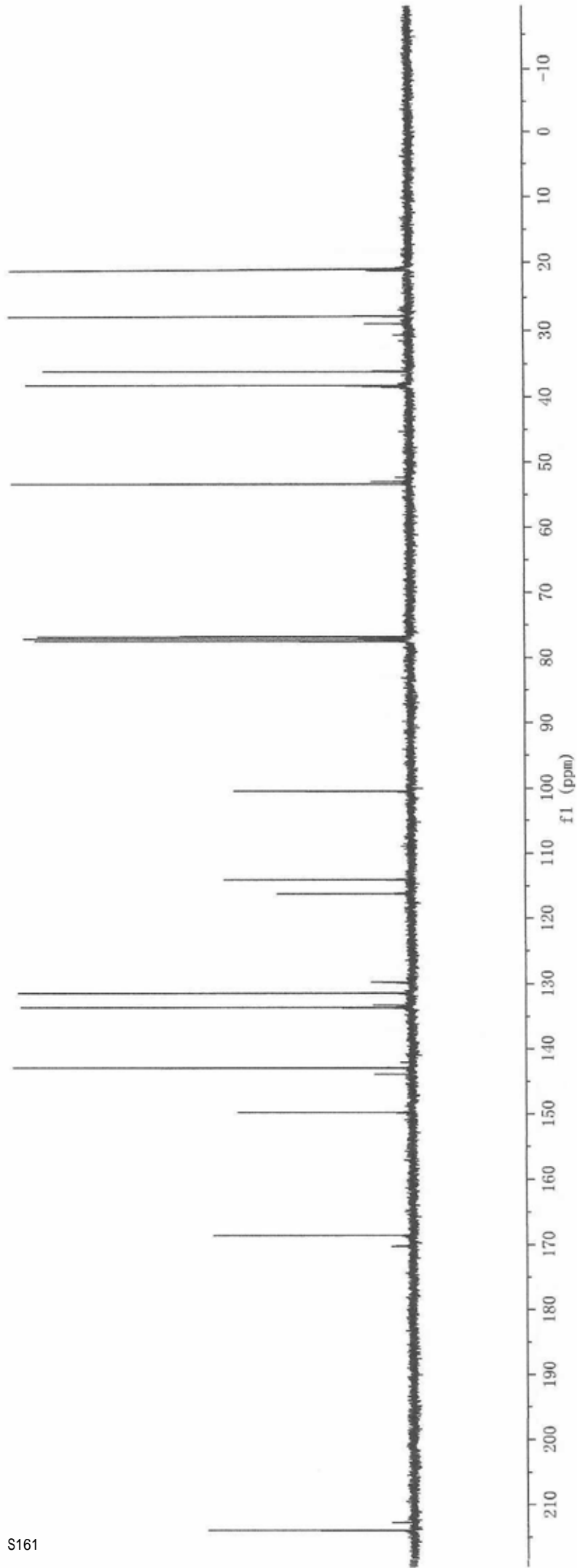




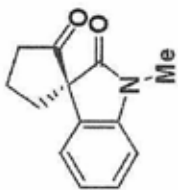
11

(100 MHz, CDCl<sub>3</sub>, two rotamers)

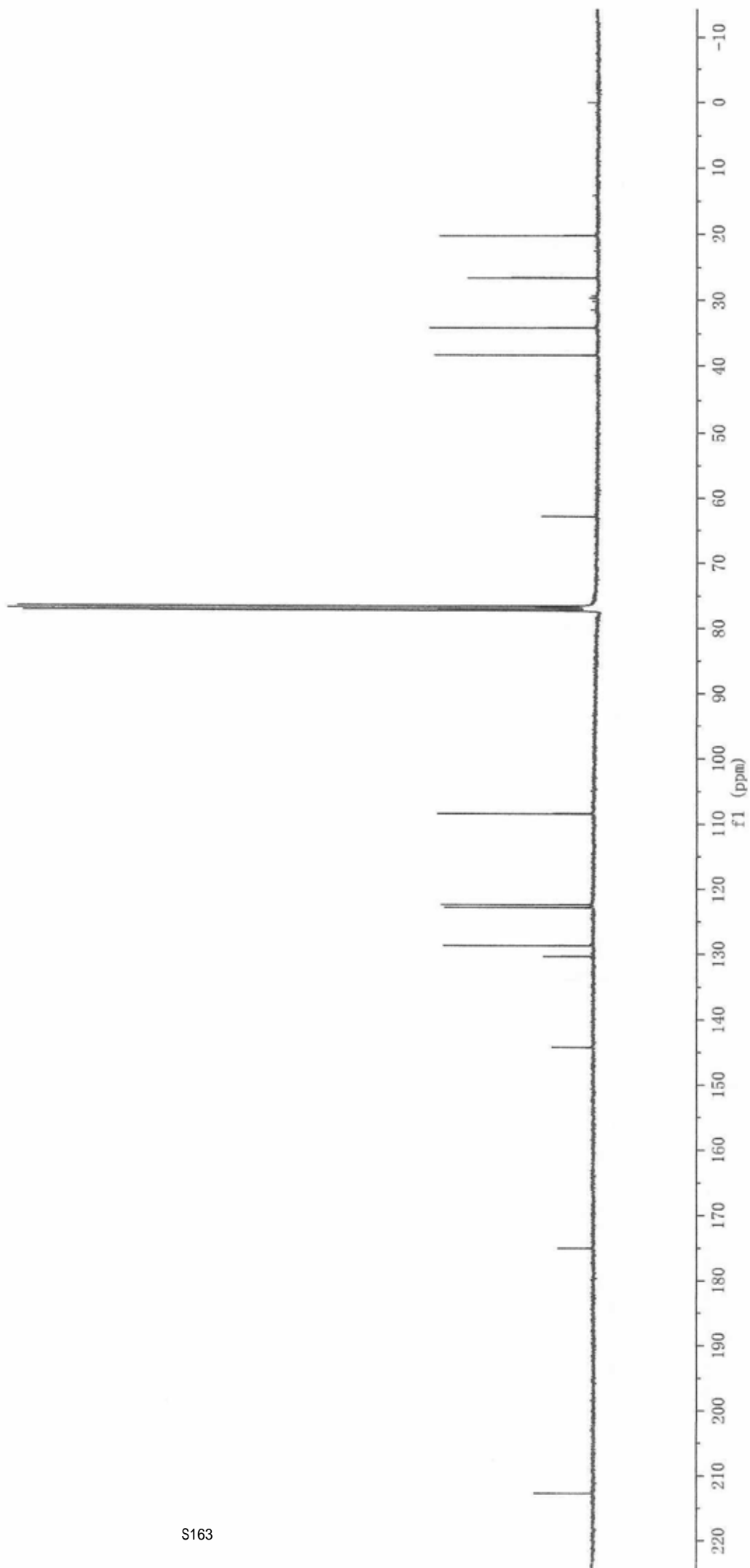
- 213.928
- 212.741
- 170.239
- 168.571
- 149.767
- 143.924
- 142.903
- 133.643
- 133.327
- 131.147
- 129.734
- 116.236
- 114.057
- 100.475
- 53.391
- 52.973
- 38.505
- 38.318
- 36.198
- 29.012
- 27.905
- 21.108
- 20.884



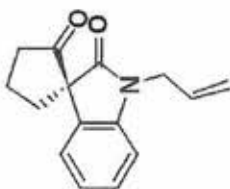




2a

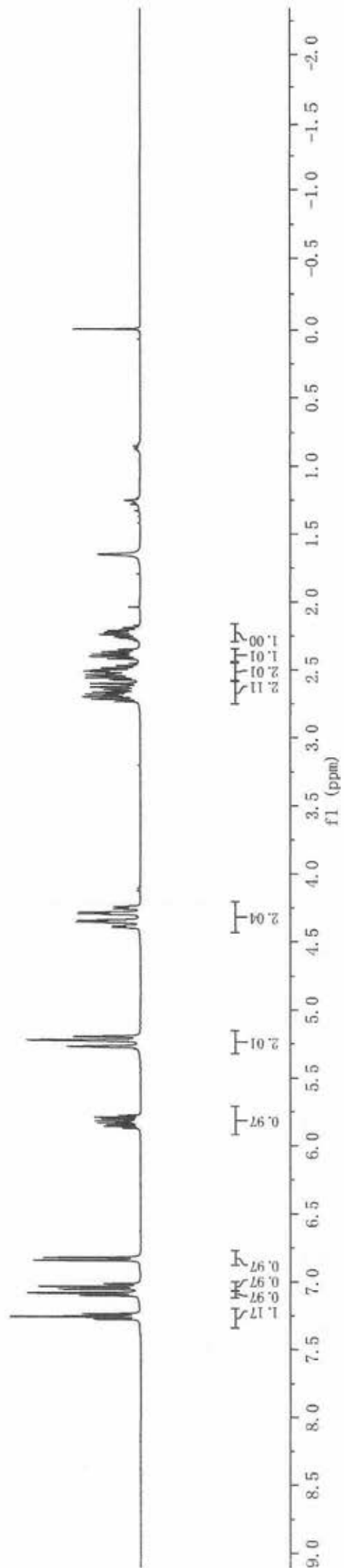
(100 MHz, CDCl<sub>3</sub>)

7.281  
7.278  
7.260  
7.243  
7.239  
7.107  
7.105  
7.089  
7.086  
7.058  
7.056  
7.039  
7.037  
7.021  
7.018  
6.844  
6.825  
6.825  
5.863  
5.850  
5.837  
5.833  
5.820  
5.807  
5.794  
5.275  
5.272  
5.231  
5.229  
5.227  
5.225  
5.225  
5.215  
5.215  
5.208

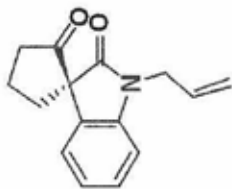


**2b**

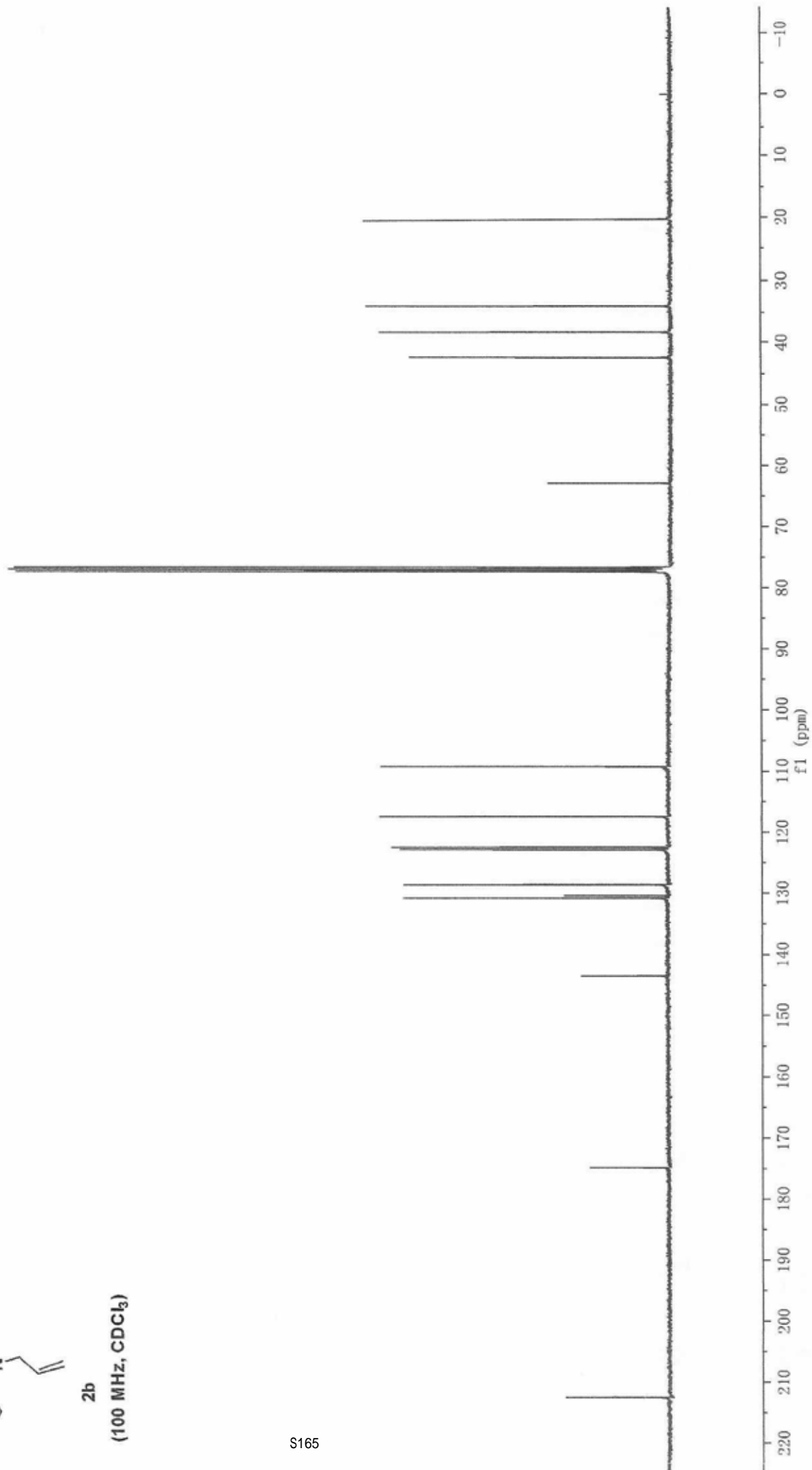
(400 MHz, CDCl<sub>3</sub>)

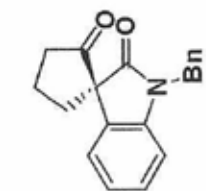




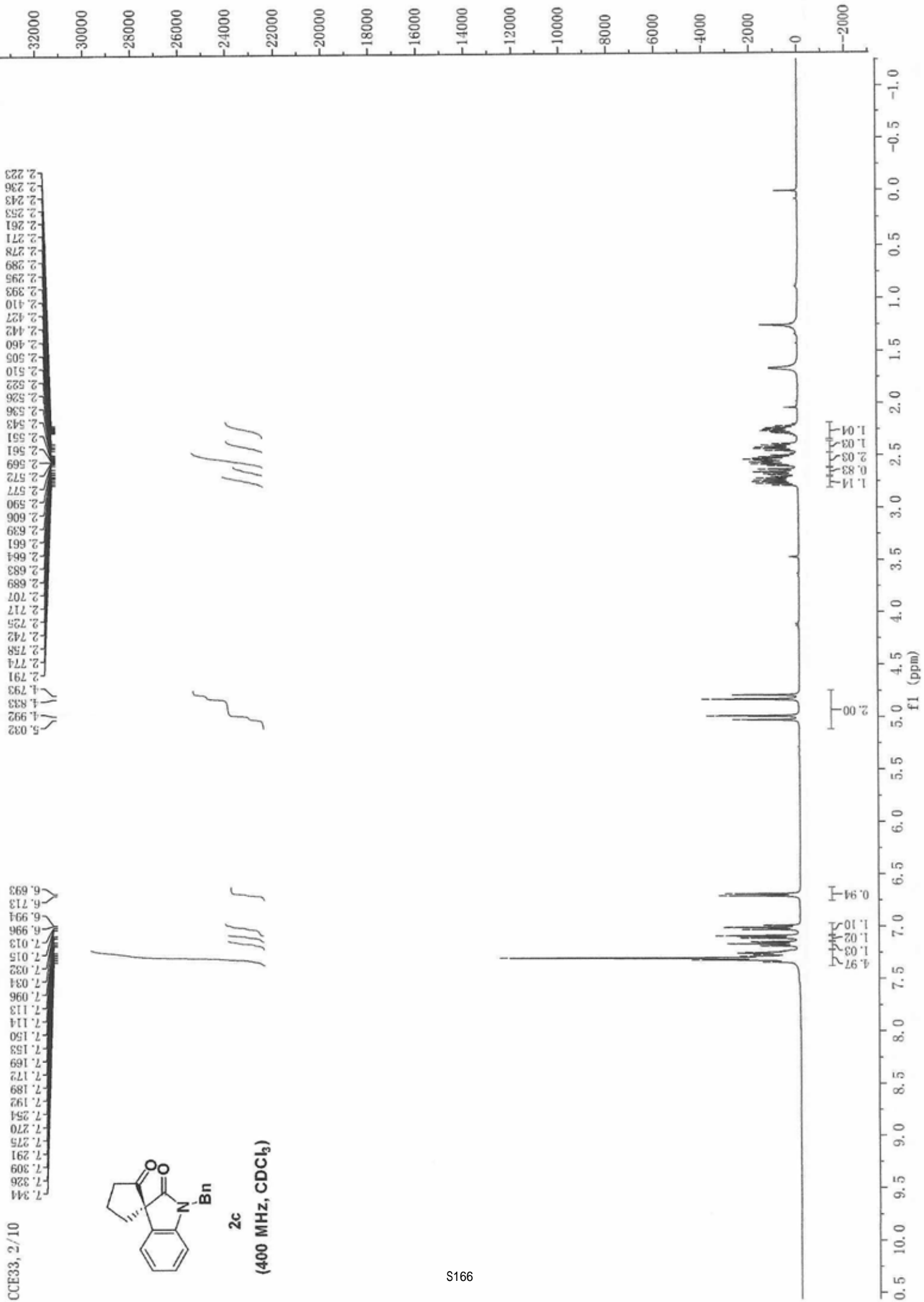
**2b****(100 MHz, CDCl<sub>3</sub>)**

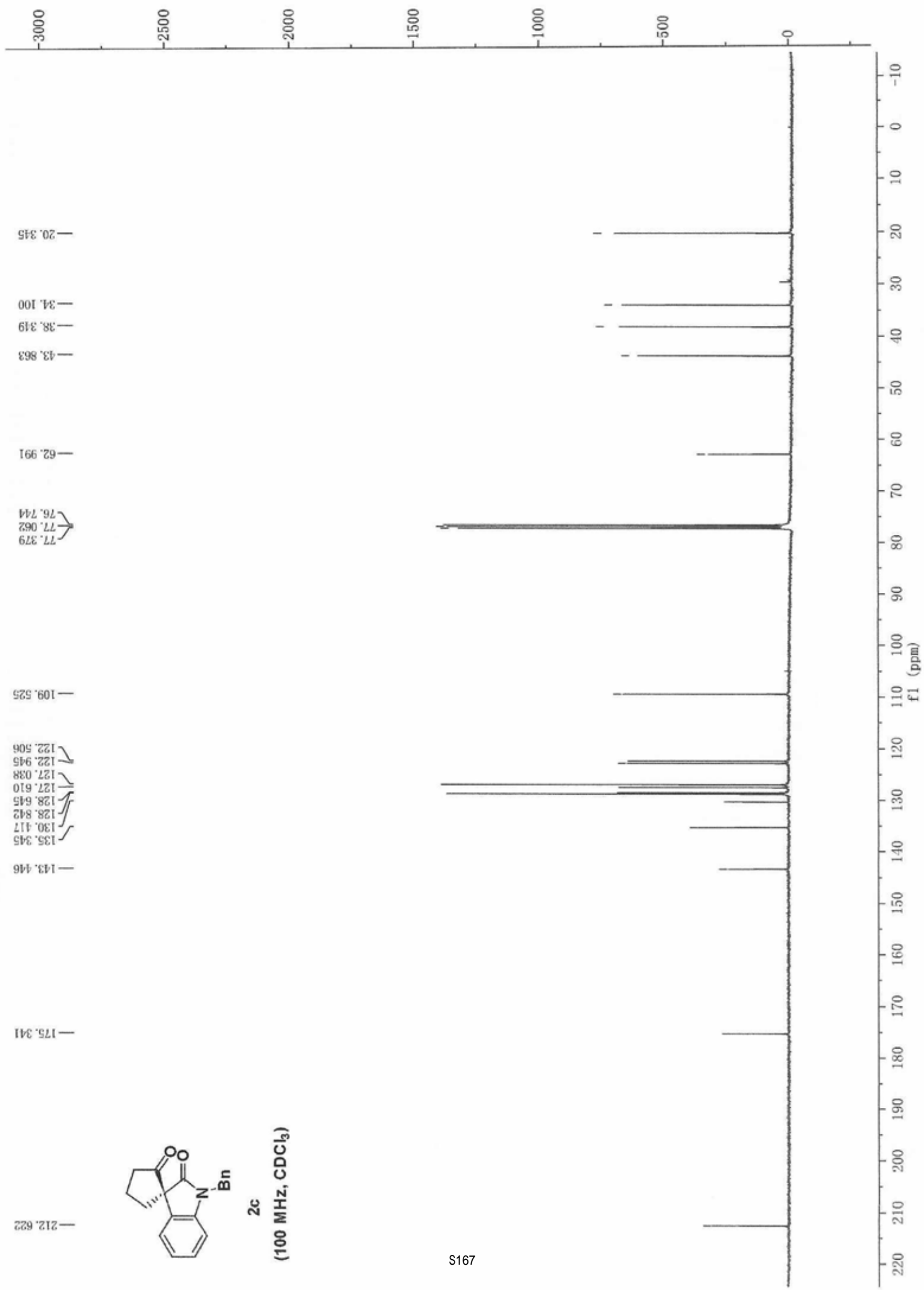
212.575 —  
174.887 —  
143.550 —  
130.803 —  
130.392 —  
128.614 —  
122.858 —  
122.515 —  
117.491 —  
109.314 —  
77.370 —  
77.254 —  
77.052 —  
76.734 —  
62.925 —  
42.410 —  
38.322 —  
34.084 —  
20.283 —

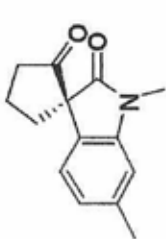




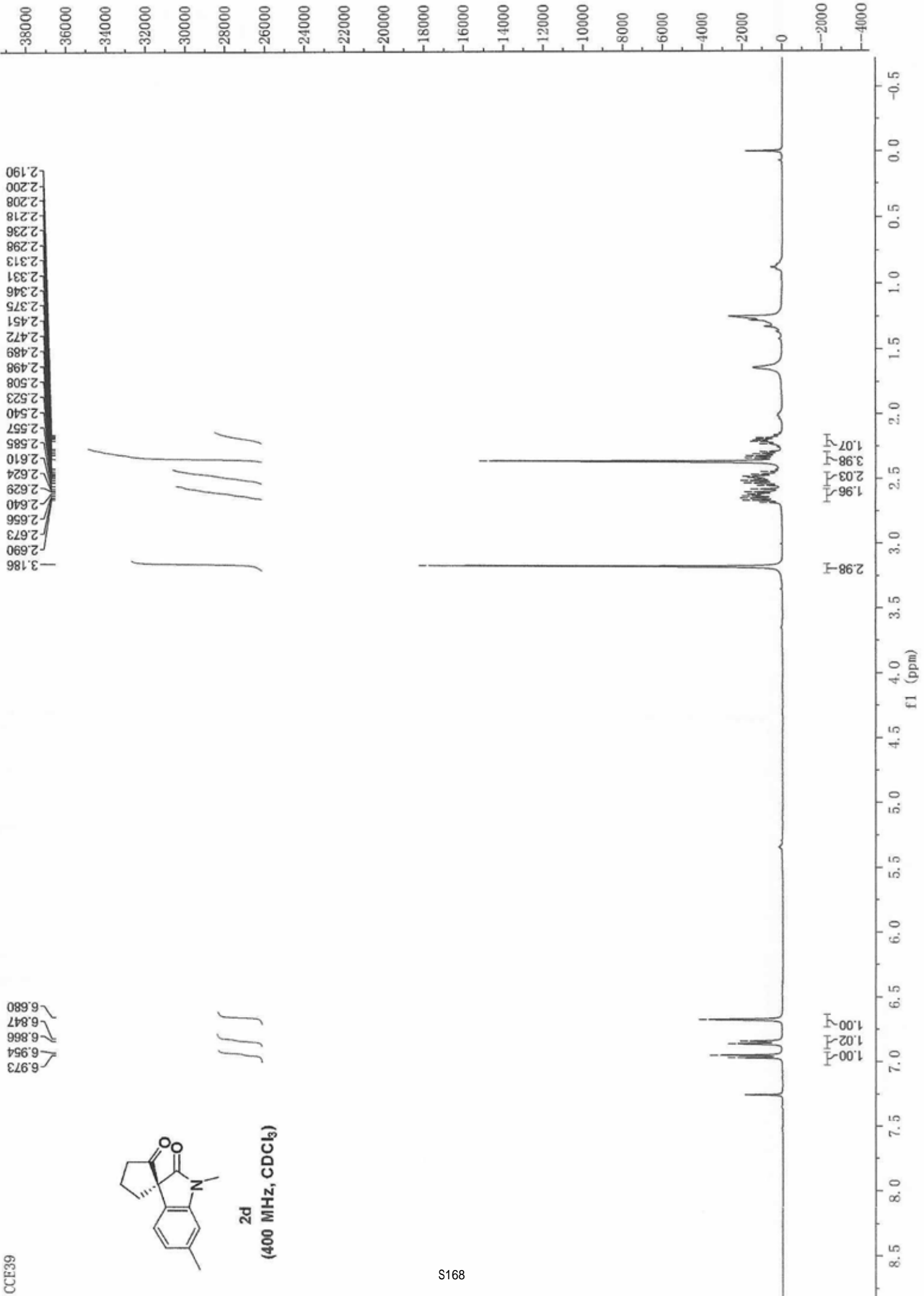
**2c**  
(400 MHz, CDCl<sub>3</sub>)

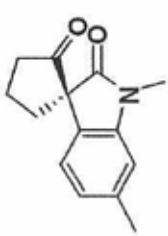
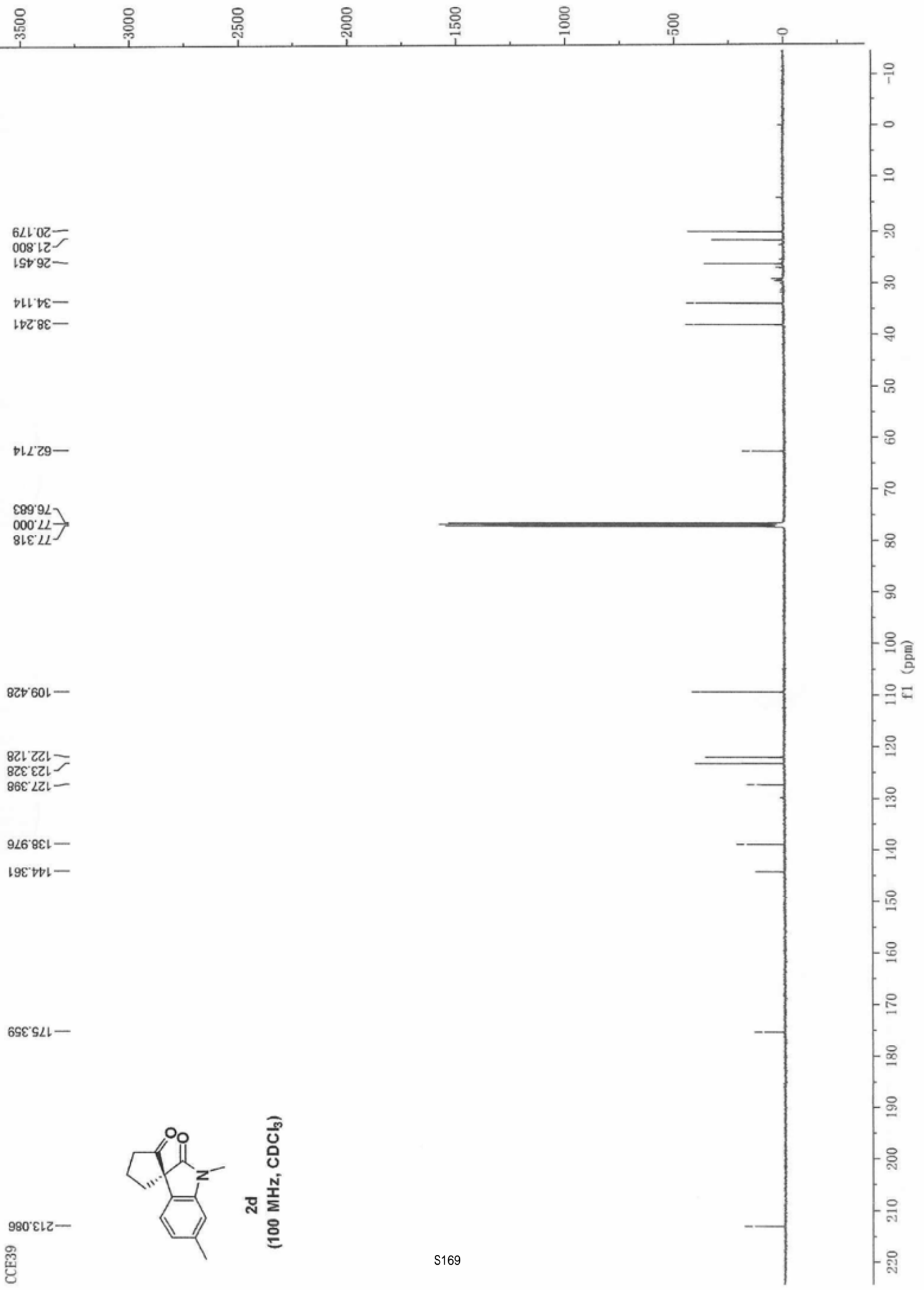






2d  
(400 MHz, CDCl<sub>3</sub>)

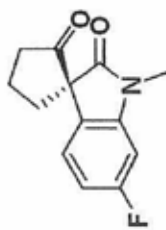




**2d**  
(100 MHz, CDCl<sub>3</sub>)

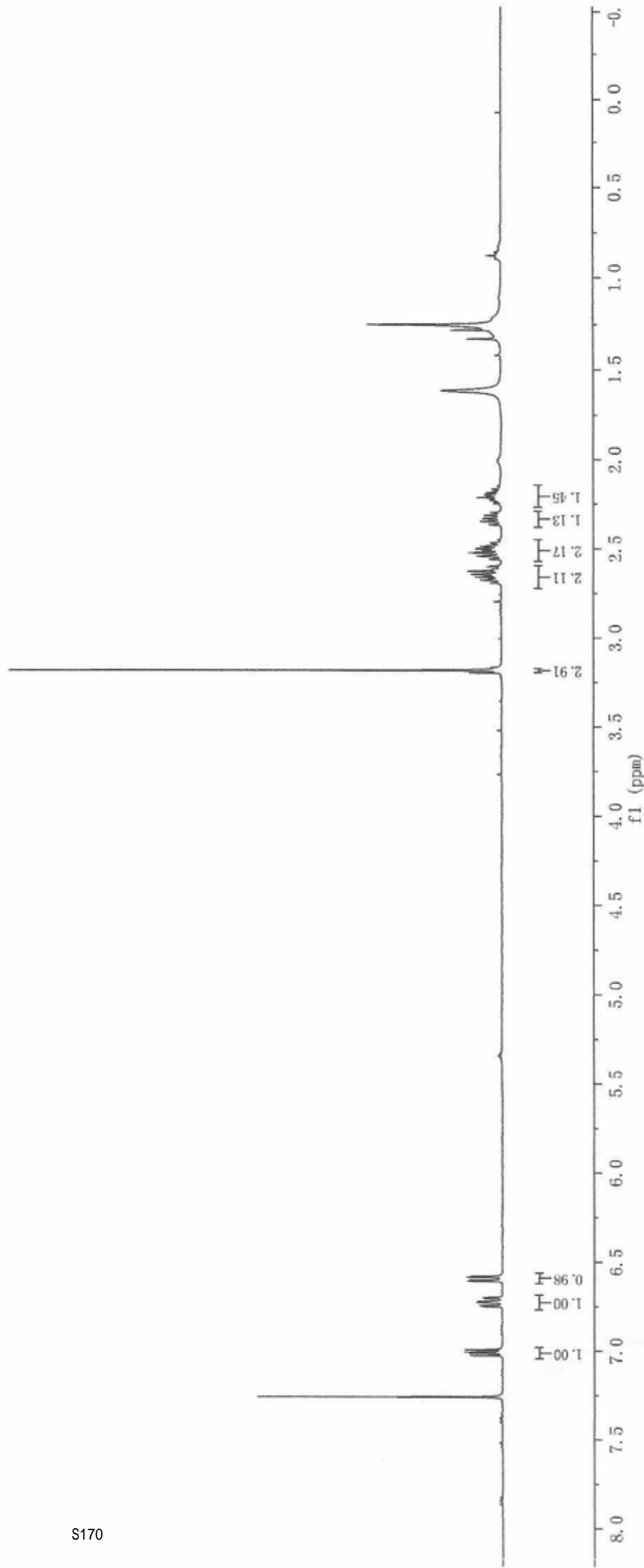
CCCE39

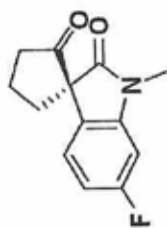
7.026  
7.013  
7.006  
6.993  
6.750  
6.741  
6.729  
6.726  
6.724  
6.721  
6.706  
6.700  
6.608  
6.602  
6.586  
6.581



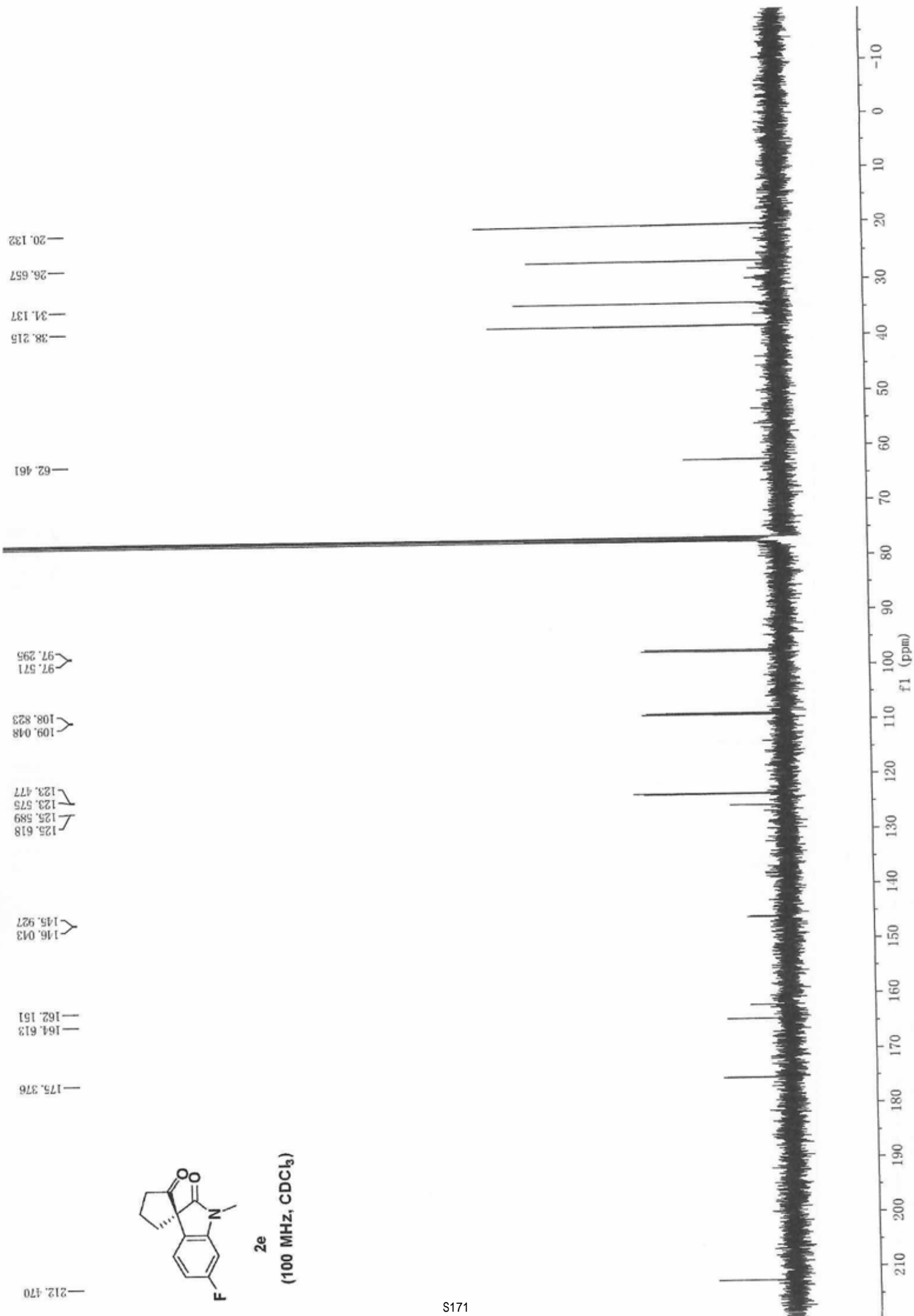
**2e**  
(400 MHz, CDCl<sub>3</sub>)

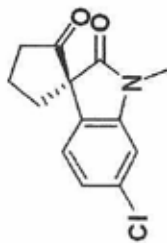
3.183  
2.694  
2.676  
2.670  
2.660  
2.653  
2.645  
2.628  
2.624  
2.619  
2.602  
2.560  
2.556  
2.541  
2.529  
2.523  
2.512  
2.507  
2.502  
2.500  
2.488  
2.484  
2.475  
2.472  
2.466  
2.365  
2.362  
2.348  
2.331  
2.321  
2.315  
2.303  
2.296





2e  
(100 MHz, CDCl<sub>3</sub>)

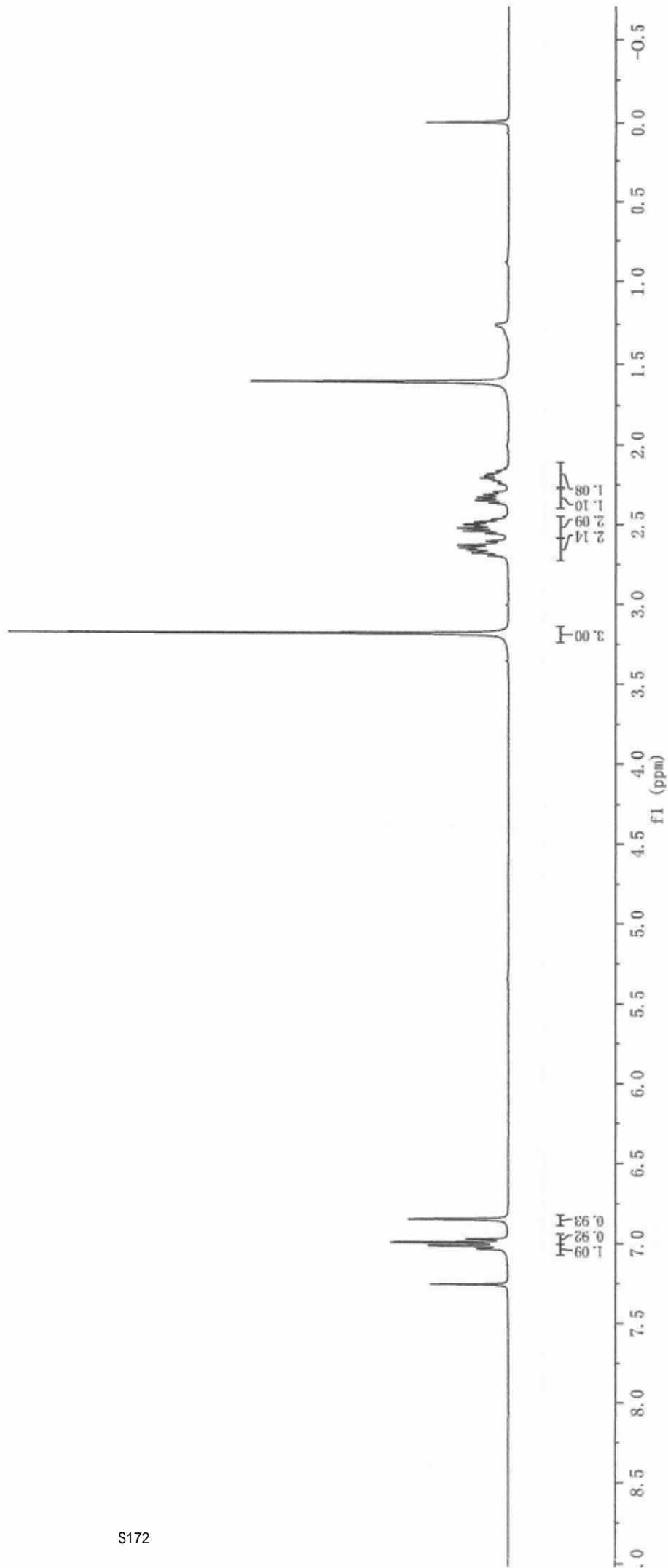




**2f**  
(400 MHz, CDCl<sub>3</sub>)

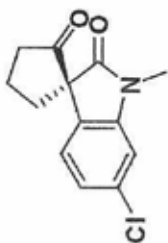
3.185  
2.696  
2.680  
2.663  
2.657  
2.648  
2.632  
2.614  
2.606  
2.561  
2.543  
2.526  
2.514  
2.503  
2.490  
2.474  
2.469  
2.368  
2.350  
2.317  
2.317  
2.305  
2.300  
2.247  
2.239  
2.227  
2.218  
2.212  
2.201  
2.195  
2.185  
2.177  
2.166

7.039  
7.035  
7.019  
7.015  
6.996  
6.976  
6.853  
6.849

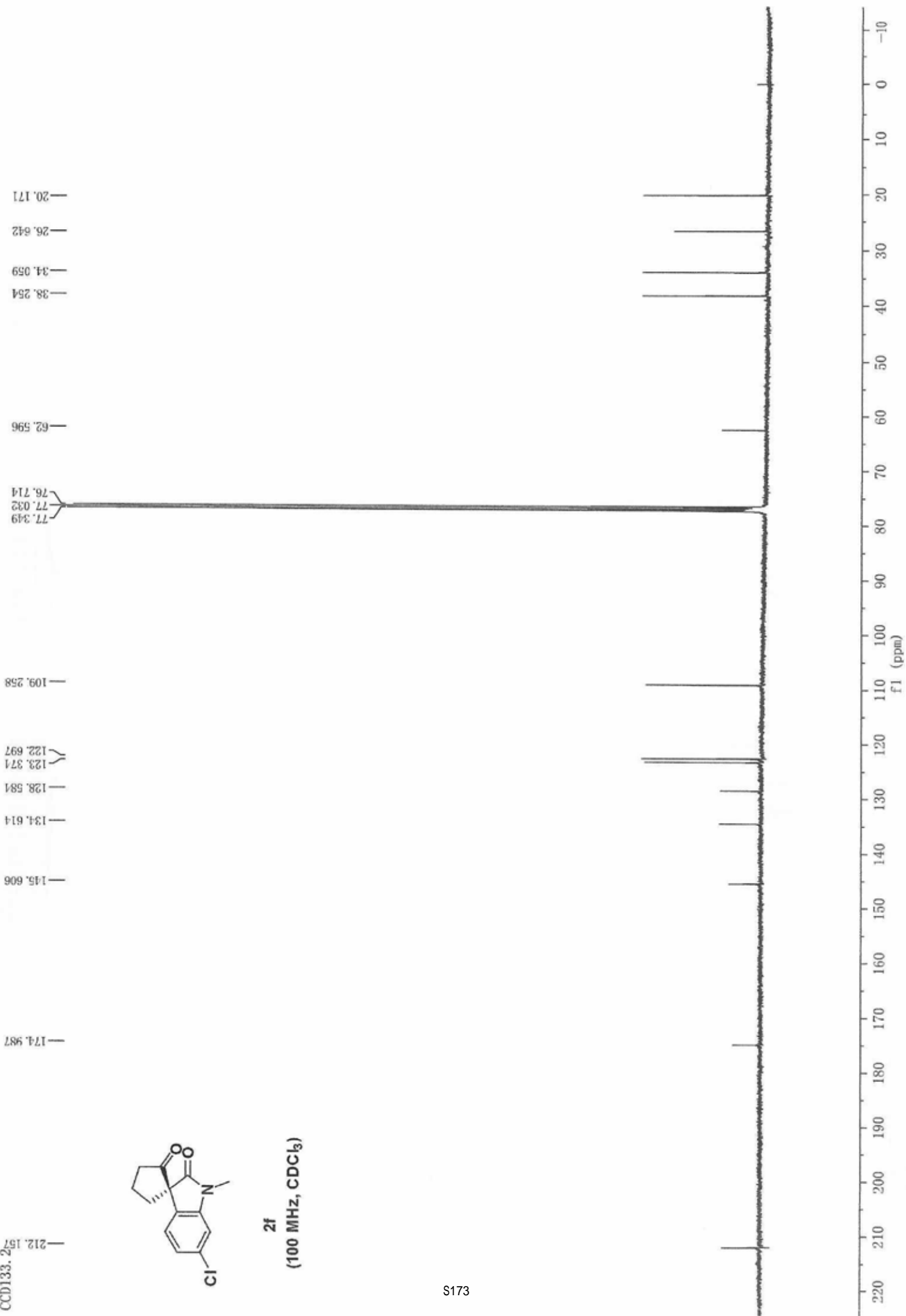




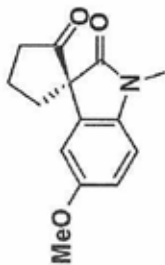
CCD133.2



**2f**  
(100 MHz, CDCl<sub>3</sub>)

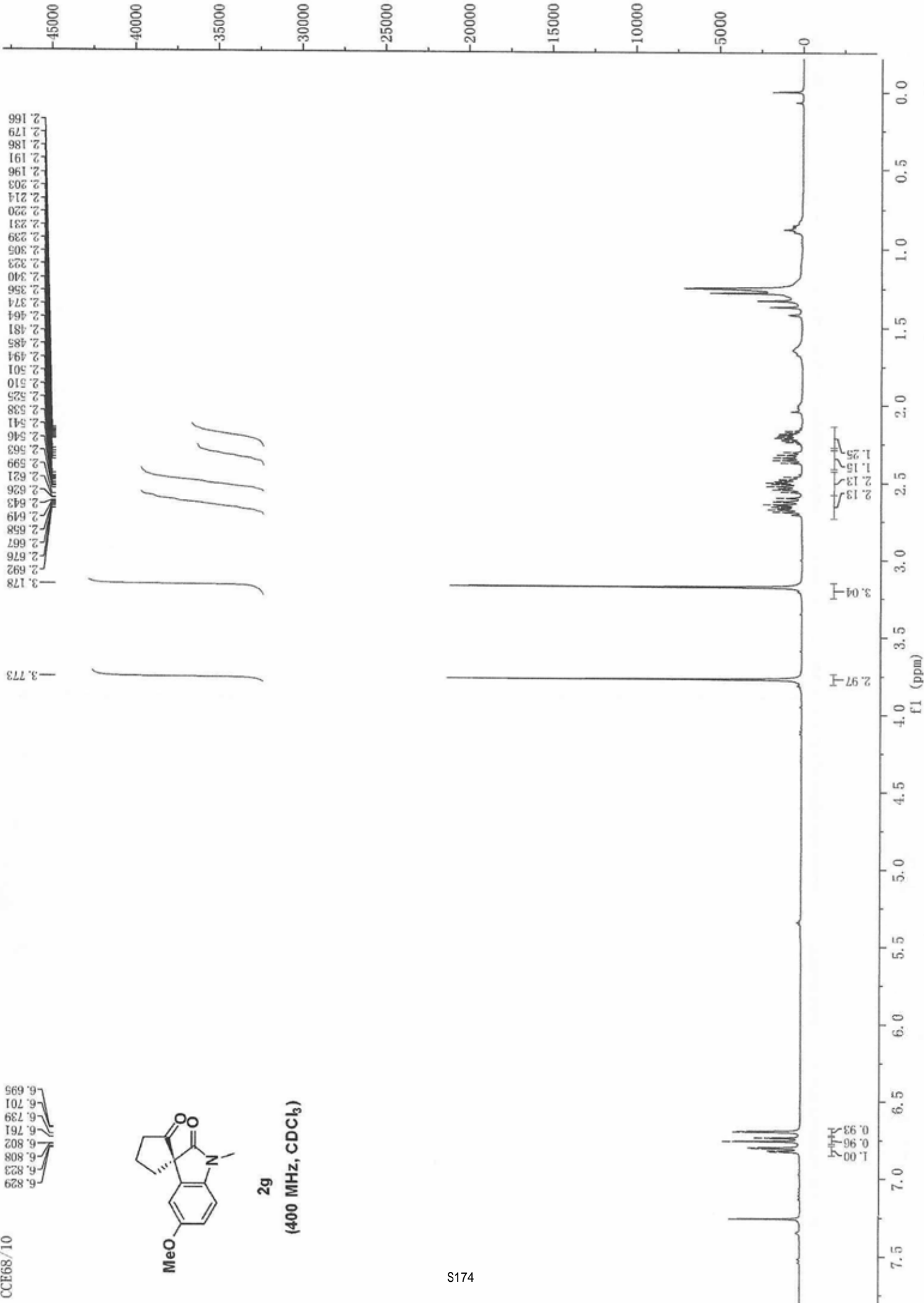
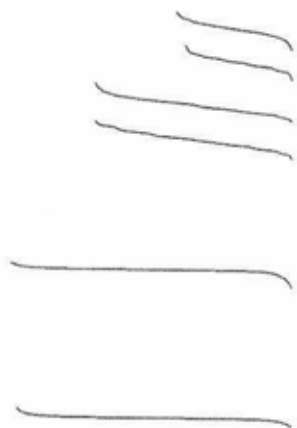


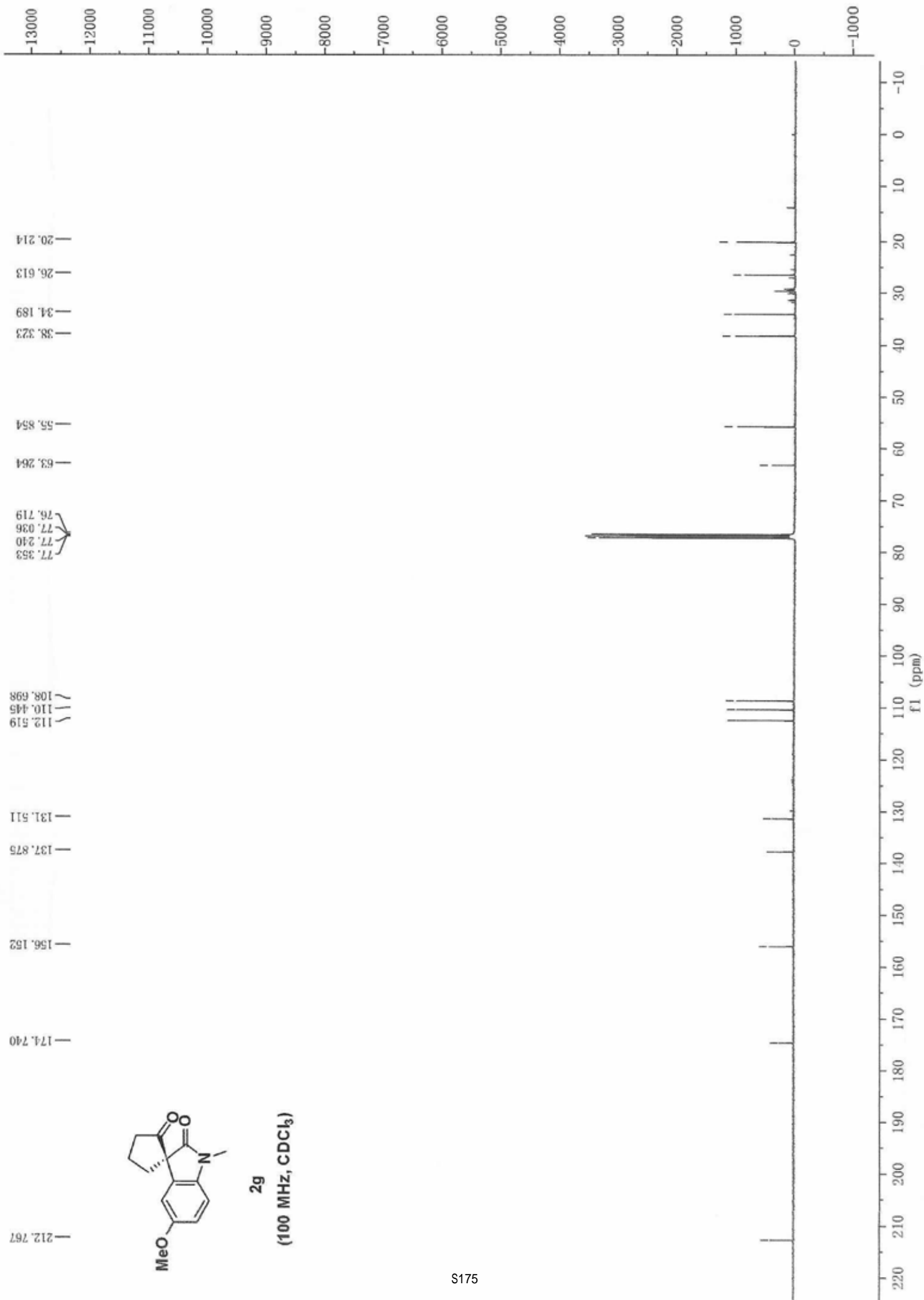
6.829  
6.823  
6.808  
6.802  
6.761  
6.739  
6.701  
6.695

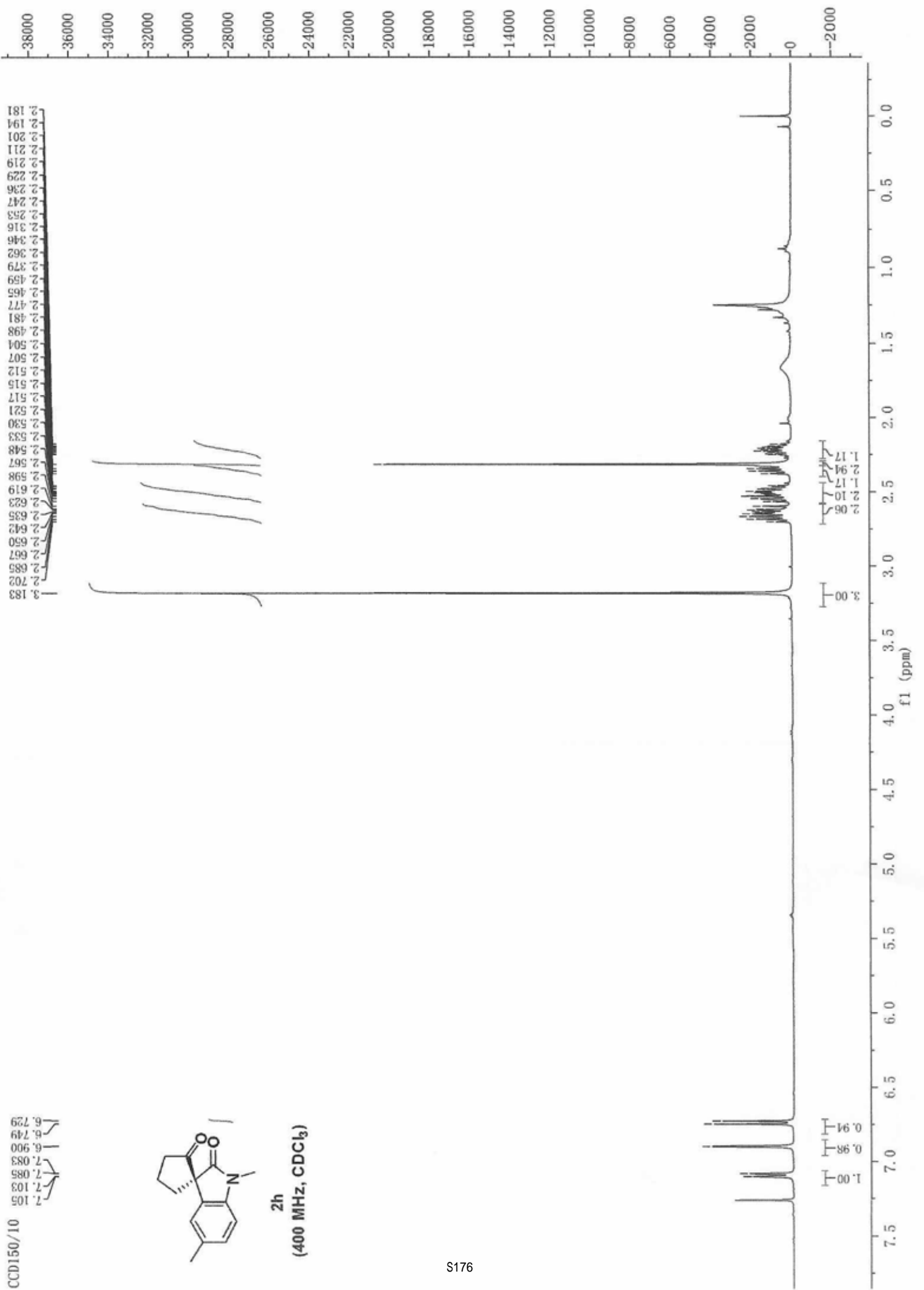


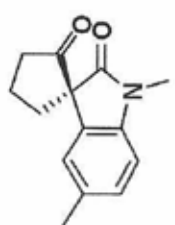
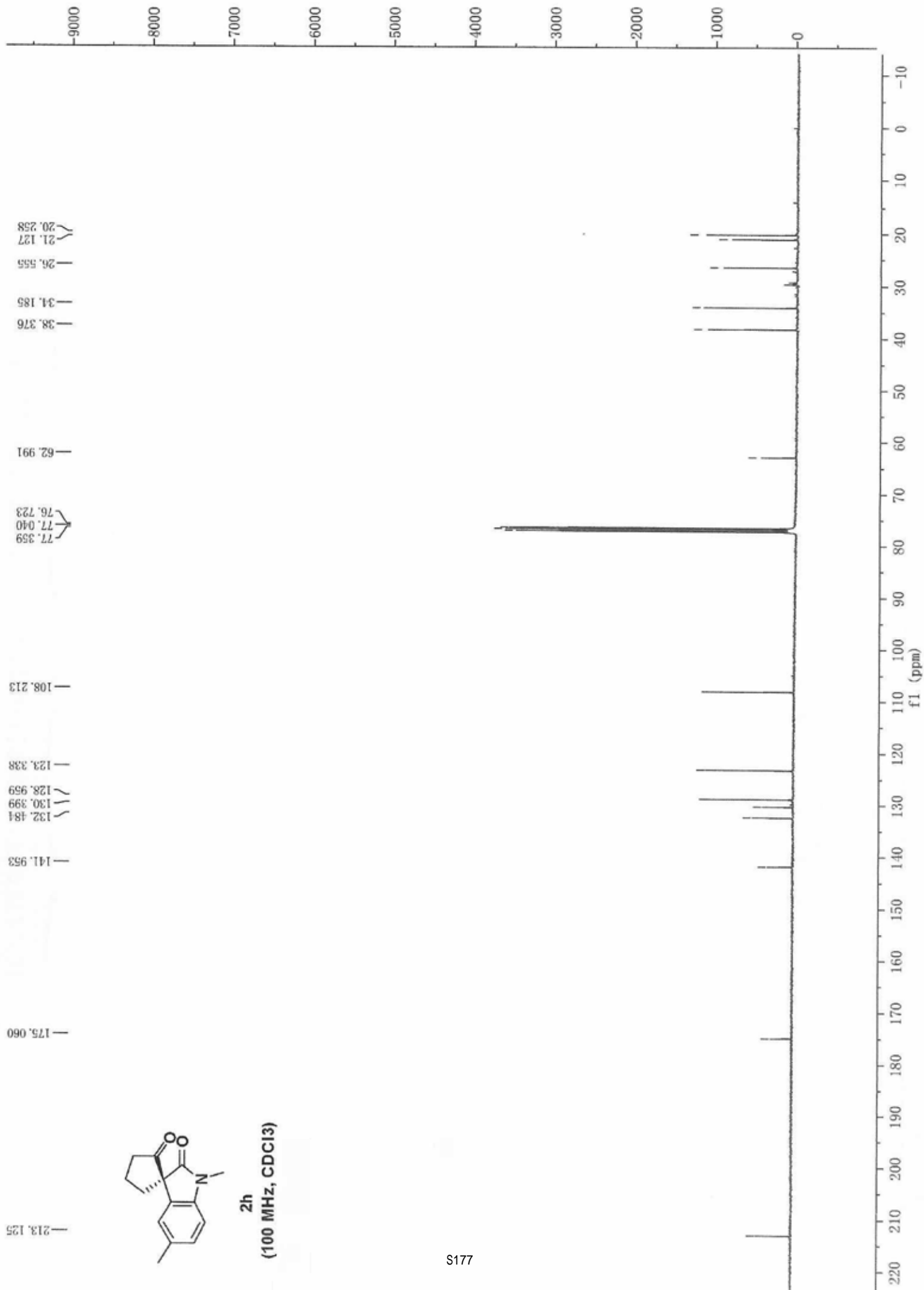
2g  
(400 MHz, CDCl<sub>3</sub>)

3.178  
2.692  
2.676  
2.667  
2.658  
2.649  
2.643  
2.626  
2.621  
2.599  
2.563  
2.546  
2.541  
2.538  
2.525  
2.510  
2.501  
2.494  
2.485  
2.481  
2.464  
2.374  
2.356  
2.340  
2.323  
2.305  
2.239  
2.231  
2.220  
2.214  
2.203  
2.196  
2.191  
2.186  
2.179  
2.166



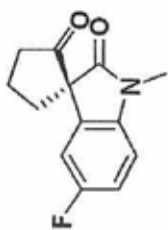




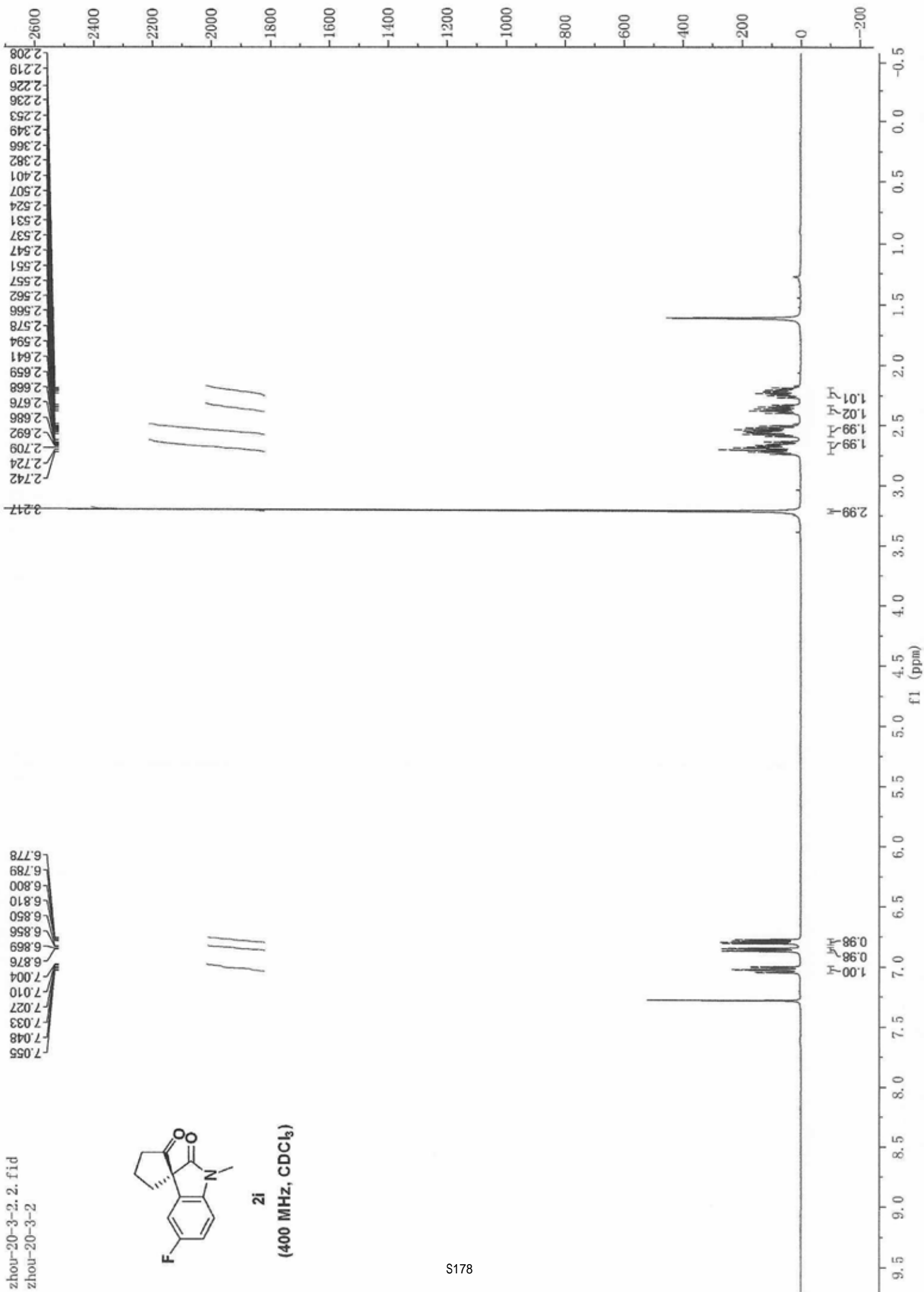


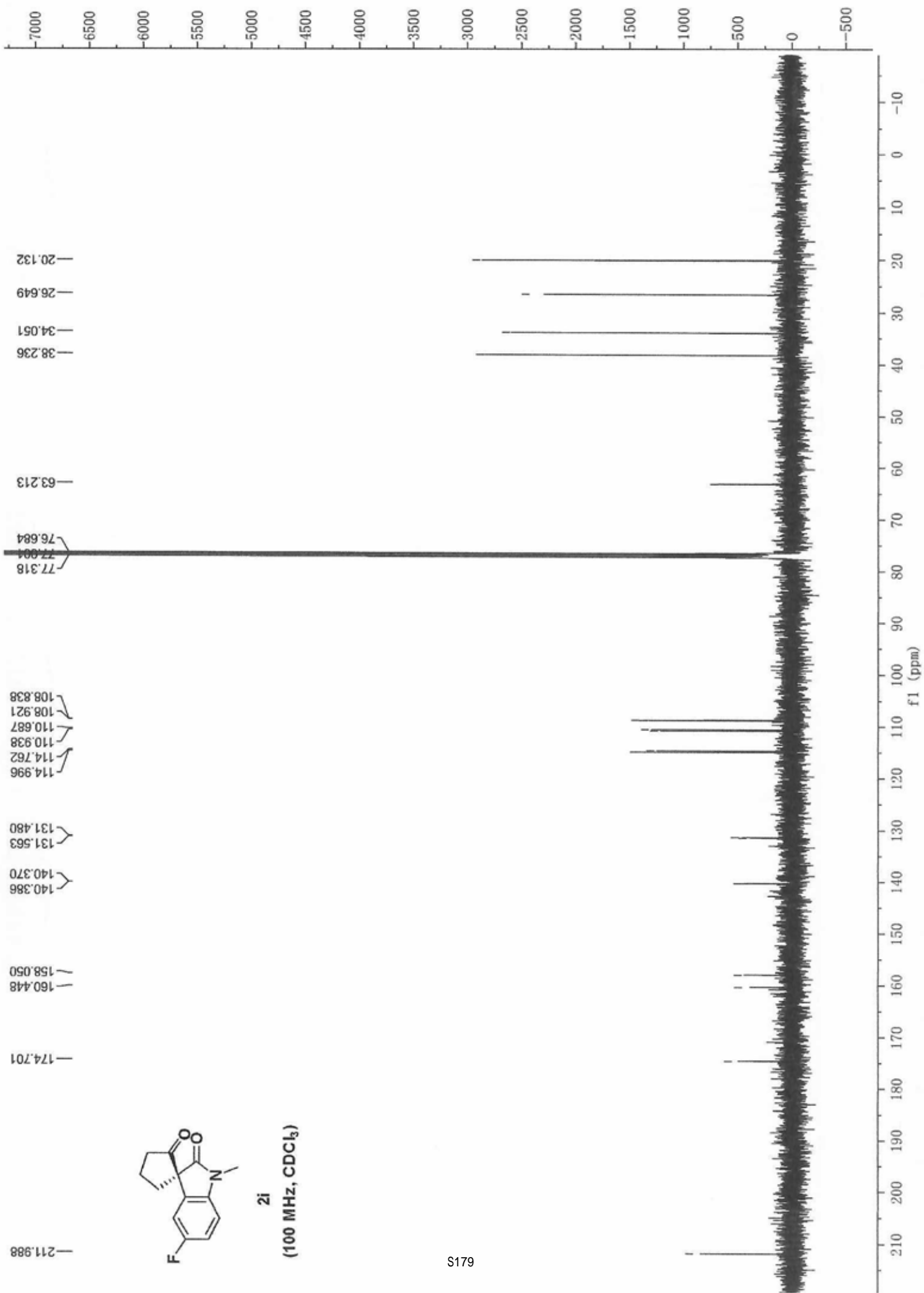
2h  
(100 MHz, CDCl<sub>3</sub>)

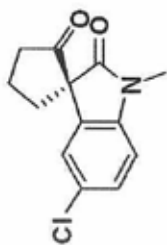
zhou-20-3-2.2.fid  
zhou-20-3-2



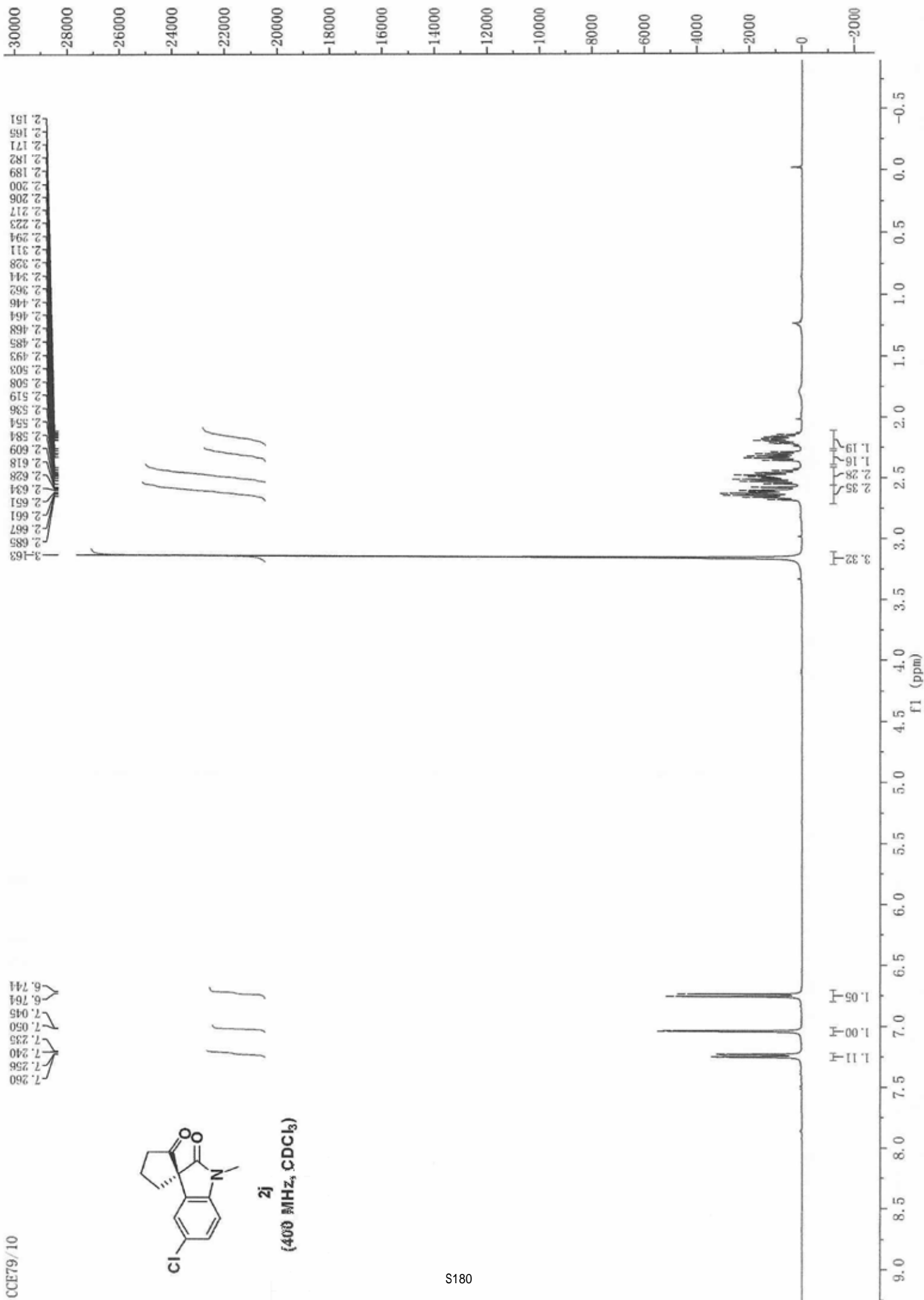
2i  
(400 MHz, CDCl<sub>3</sub>)



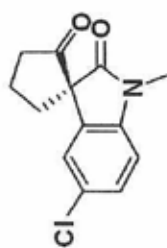
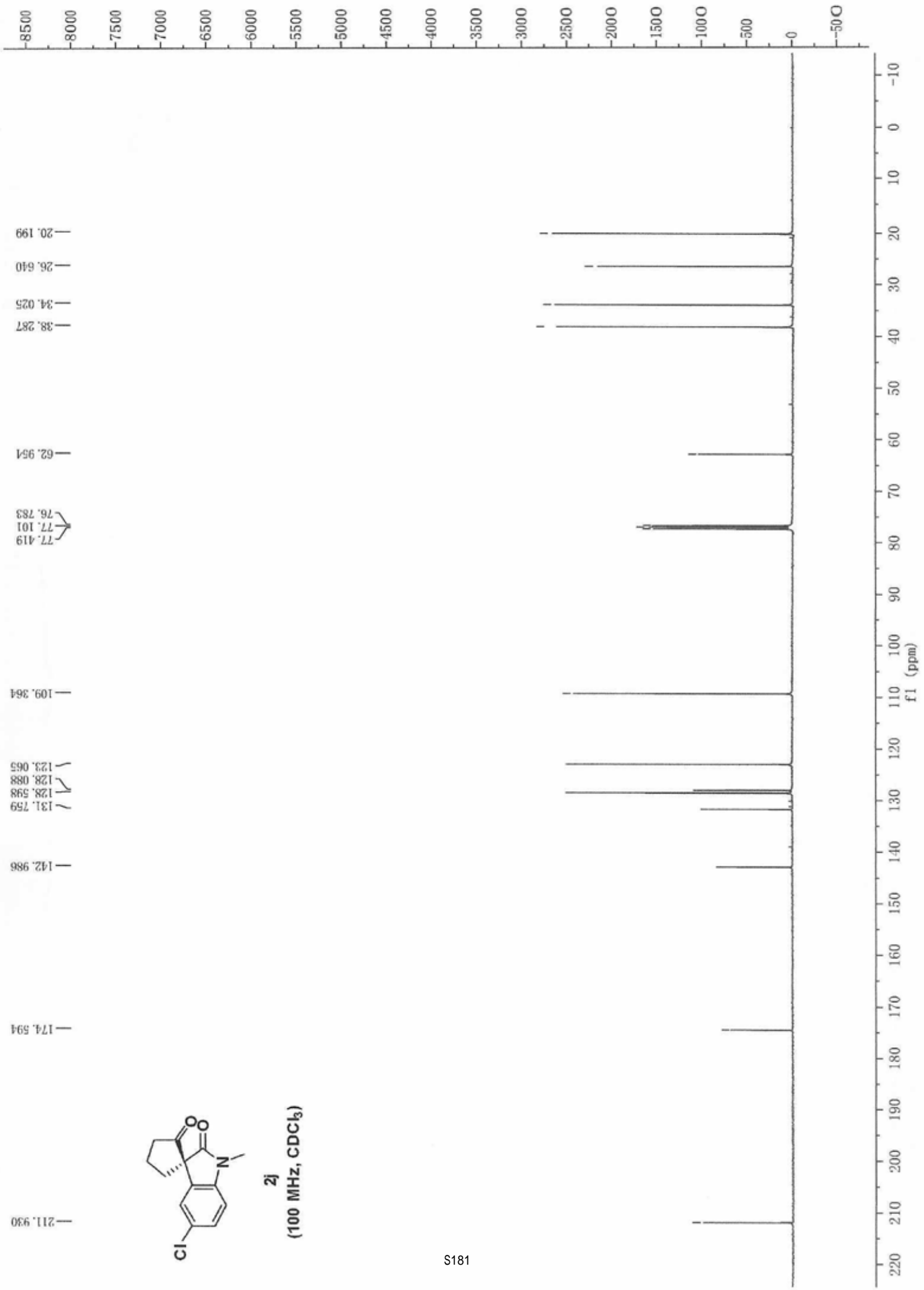




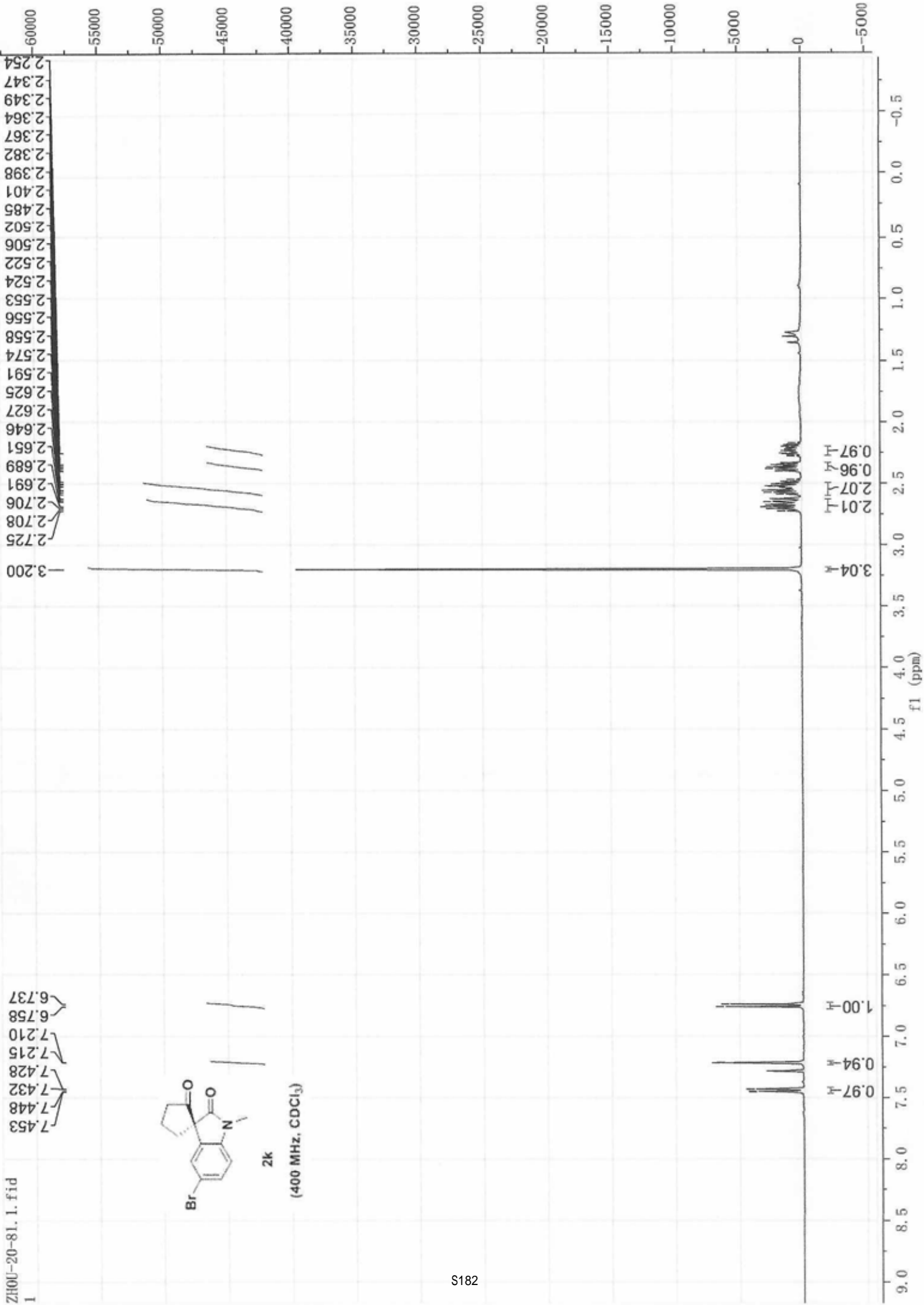
**2j**  
(400 MHz, CDCl<sub>3</sub>)

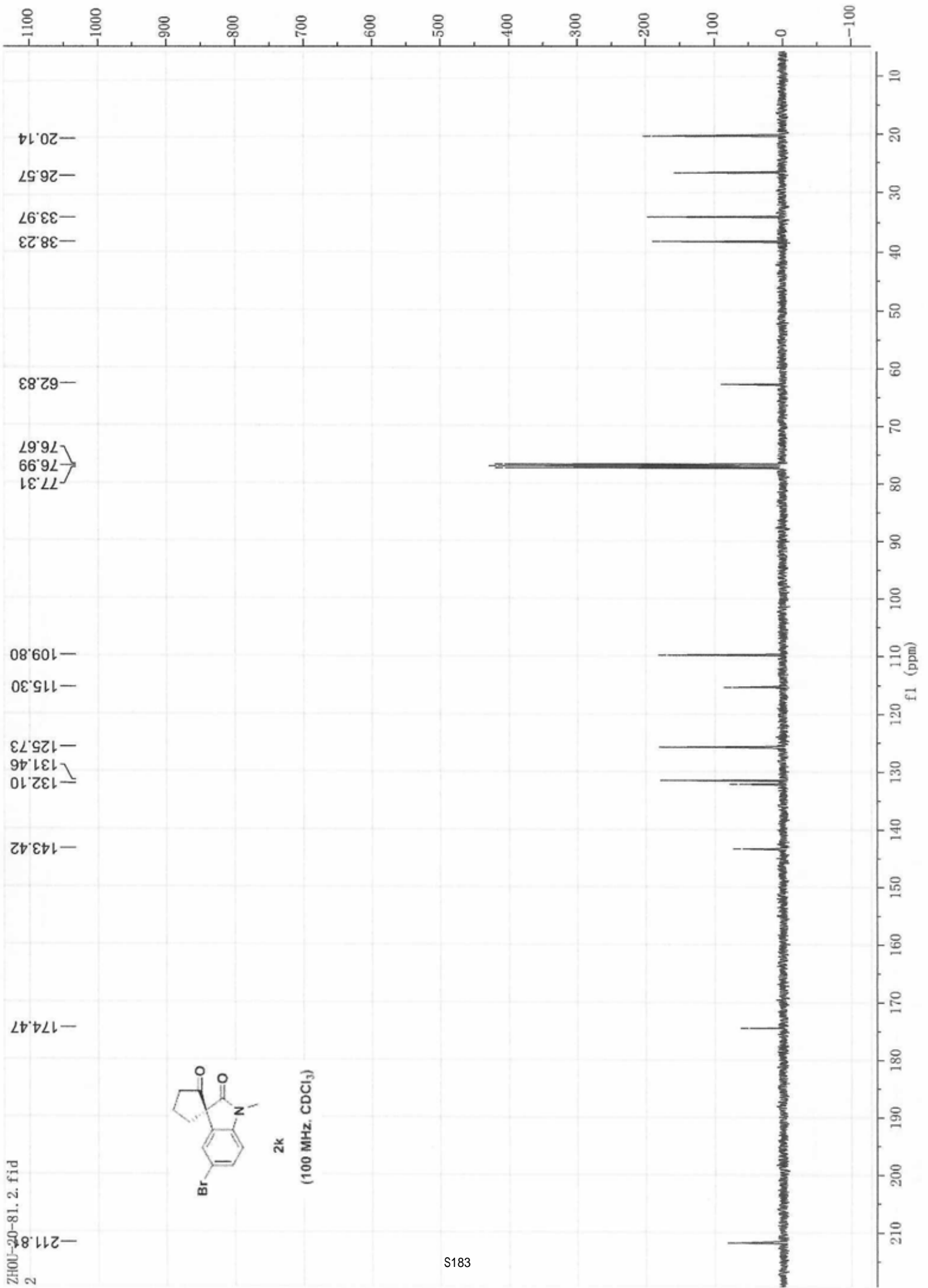






**2j**  
(100 MHz, CDCl<sub>3</sub>)

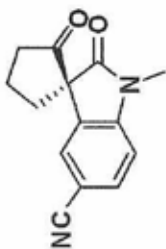




MHWF042  
MHWF042

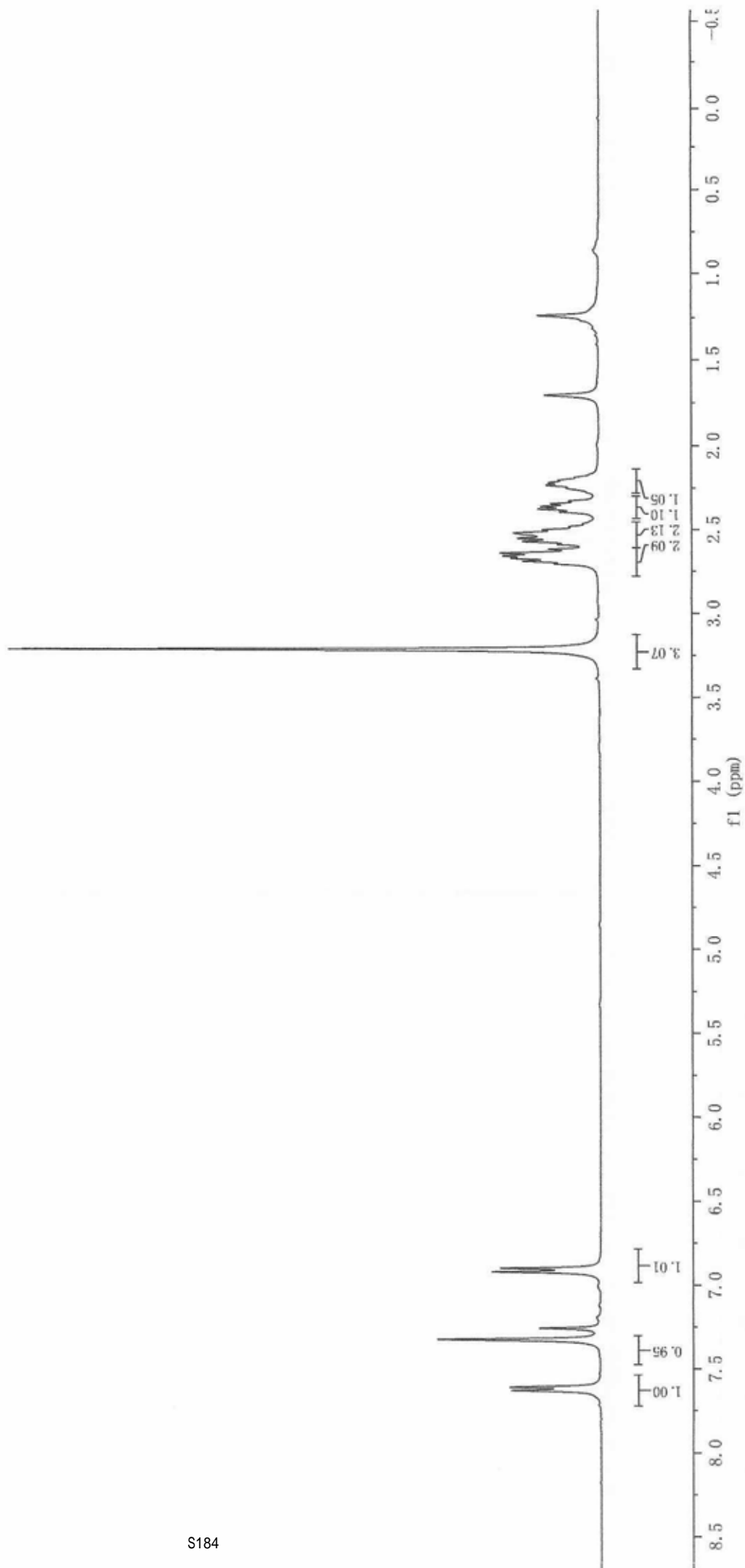
7.632  
7.612  
7.328  
6.922  
6.902

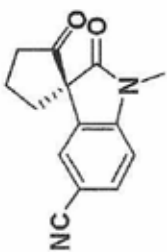
3.216  
2.707  
2.690  
2.672  
2.660  
2.643  
2.620  
2.589  
2.572  
2.555  
2.522  
2.504  
2.485  
2.398  
2.380  
2.364  
2.347  
2.332  
2.253  
2.237  
2.224  
2.208  
2.190



21

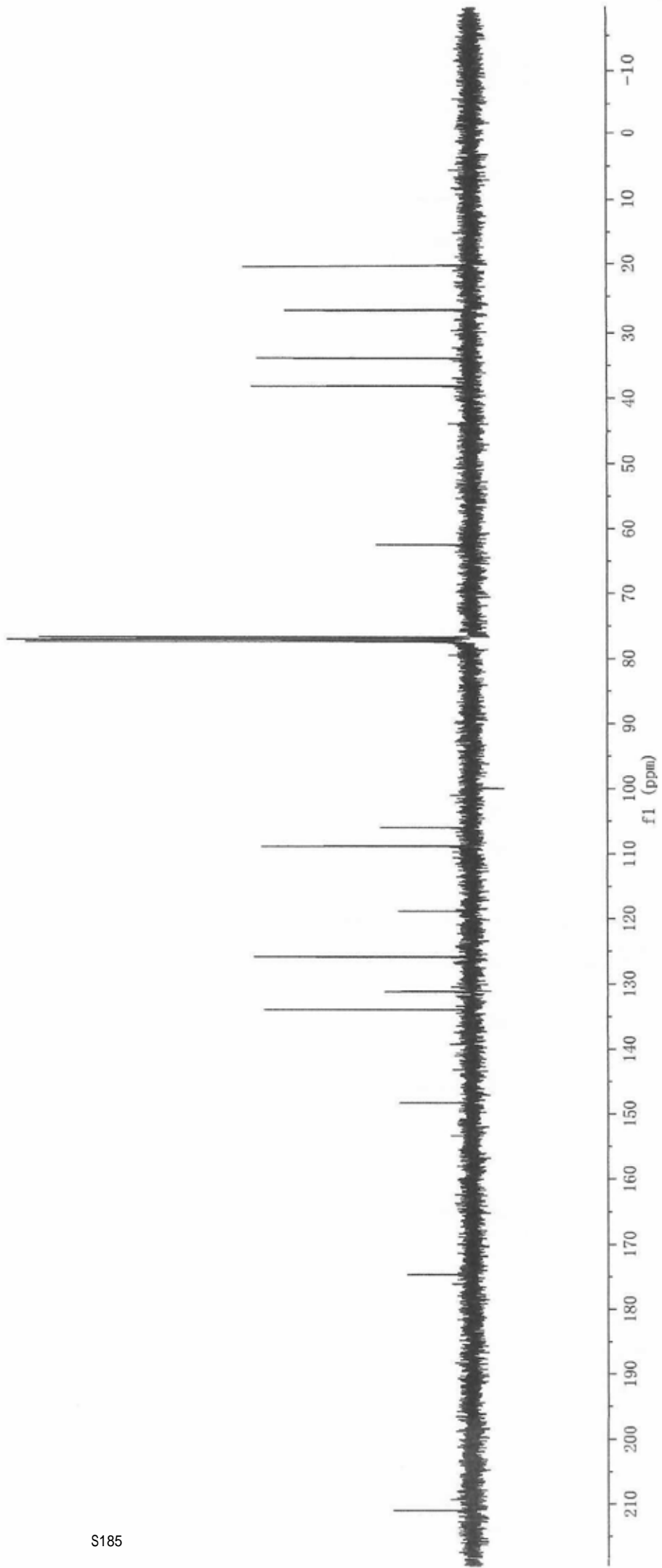
(400 MHz, CDCl<sub>3</sub>)

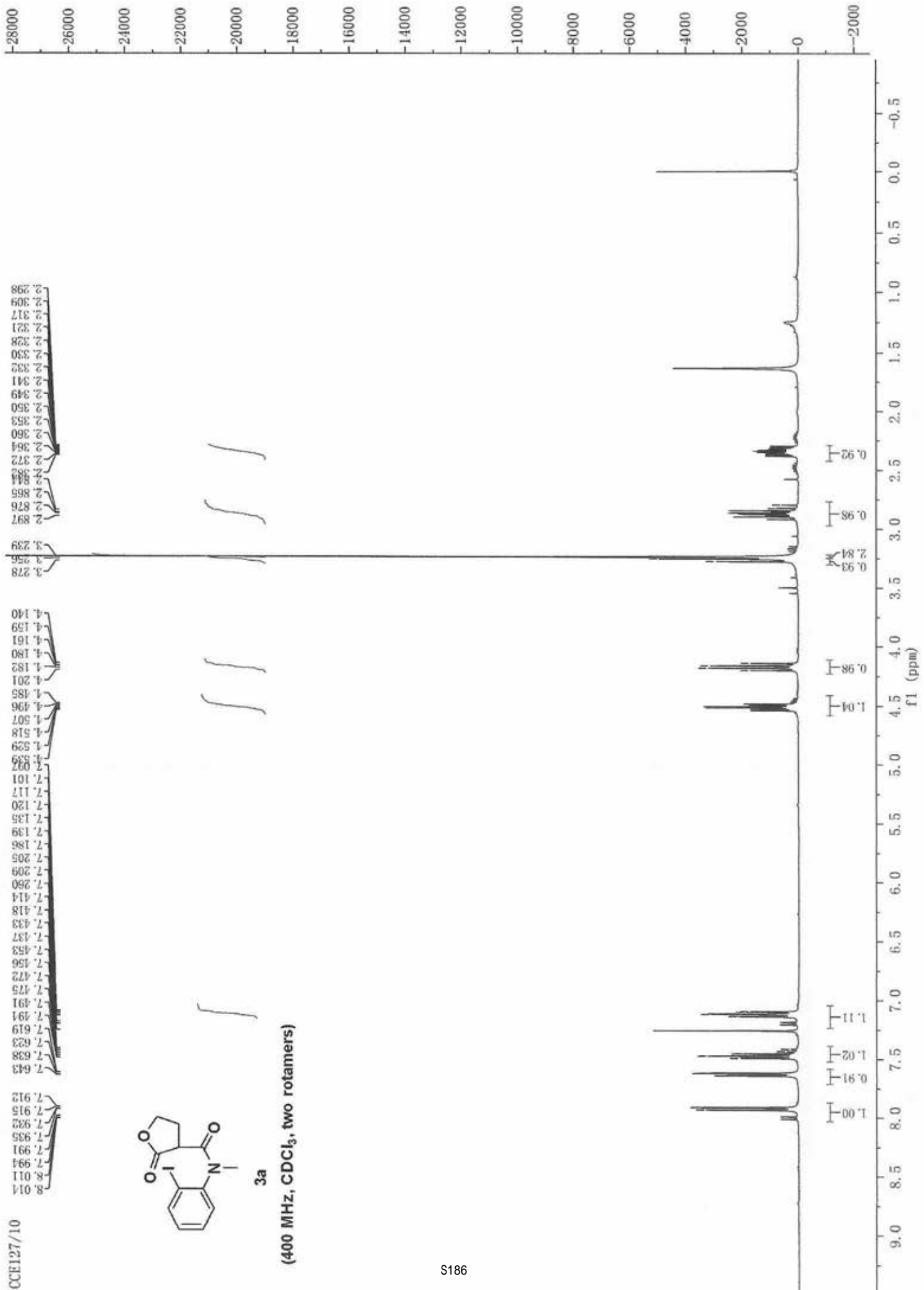


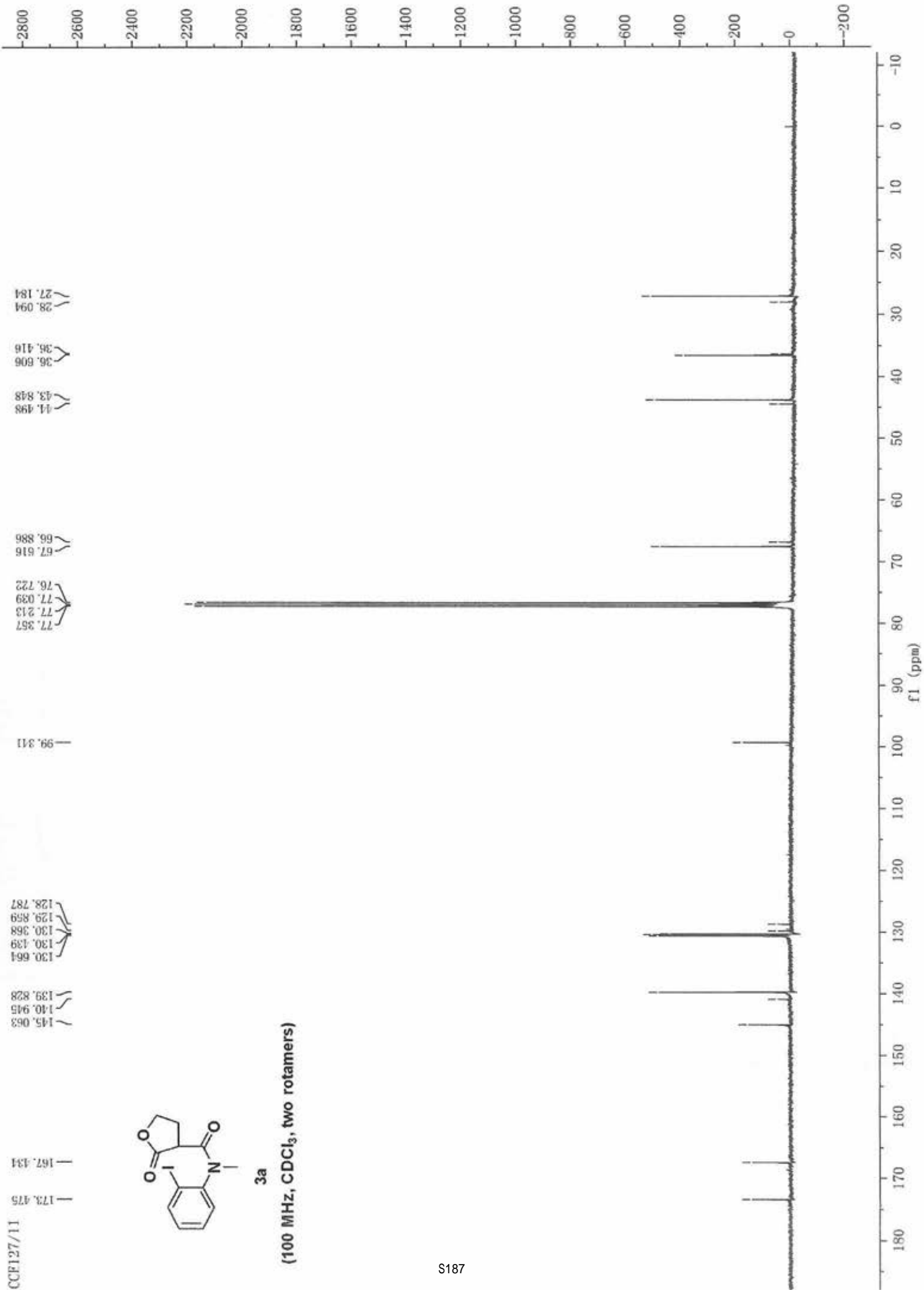


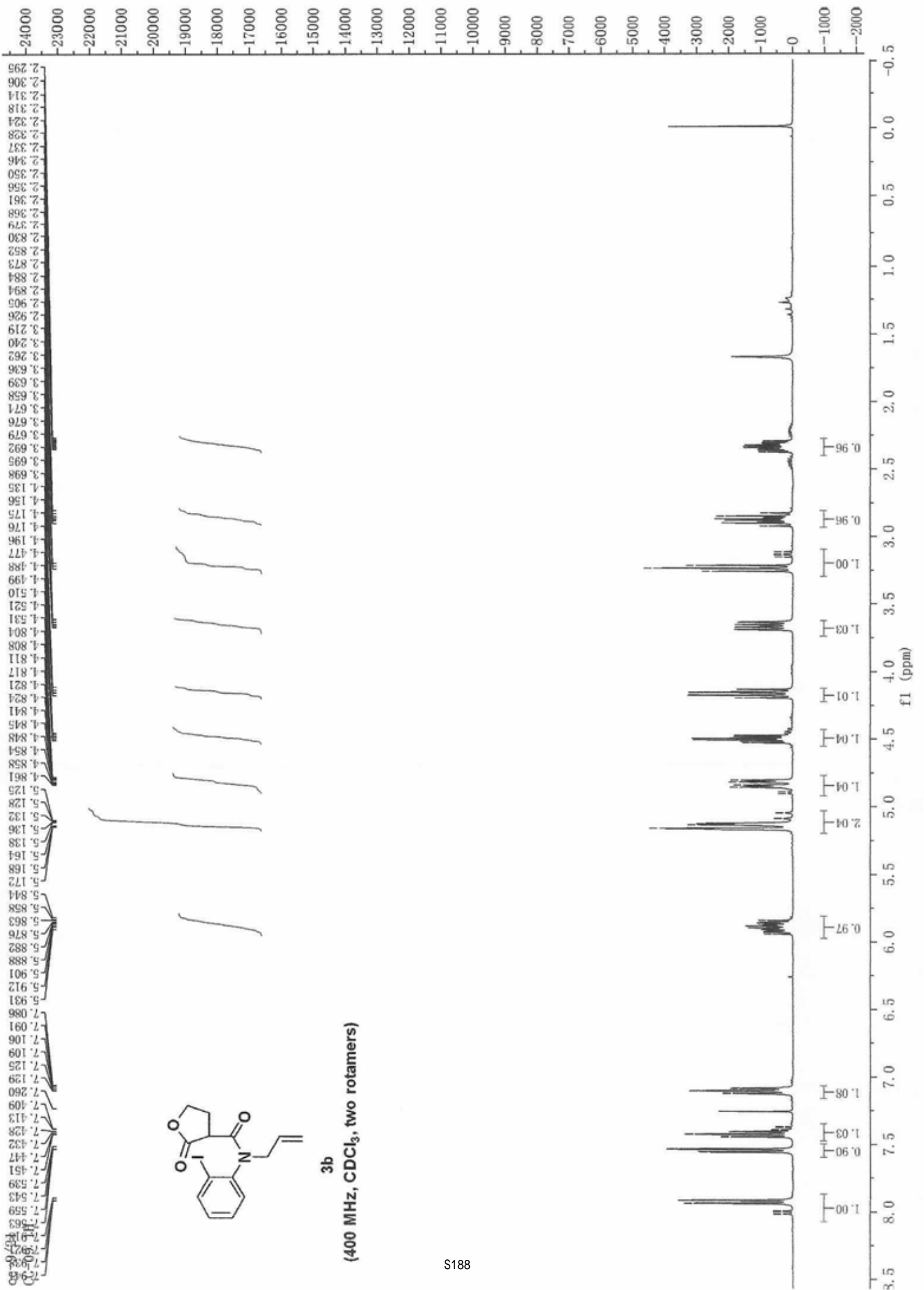
**21**  
(100 MHz, CDCl<sub>3</sub>)

- 211.070
- 174.709
- 148.311
- 134.003
- 131.192
- 125.922
- 118.873
- 108.884
- 106.020
- 77.408
- 77.090
- 76.771
- 62.550
- 38.226
- 33.923
- 26.783
- 20.161

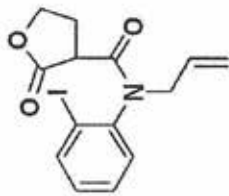




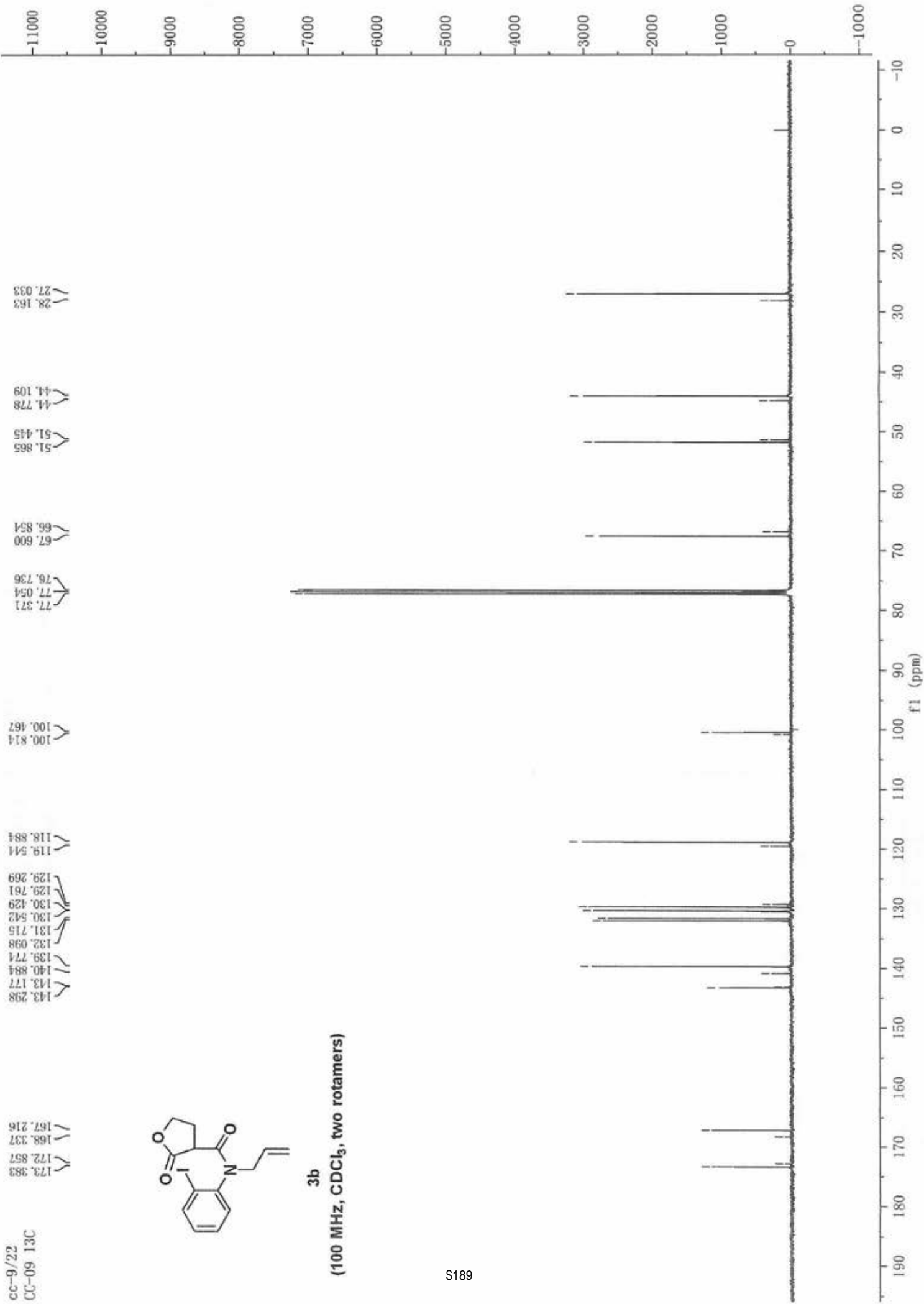






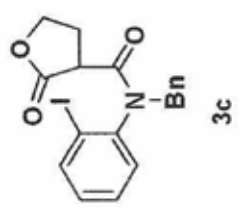


**3b**  
(100 MHz, CDCl<sub>3</sub>, two rotamers)

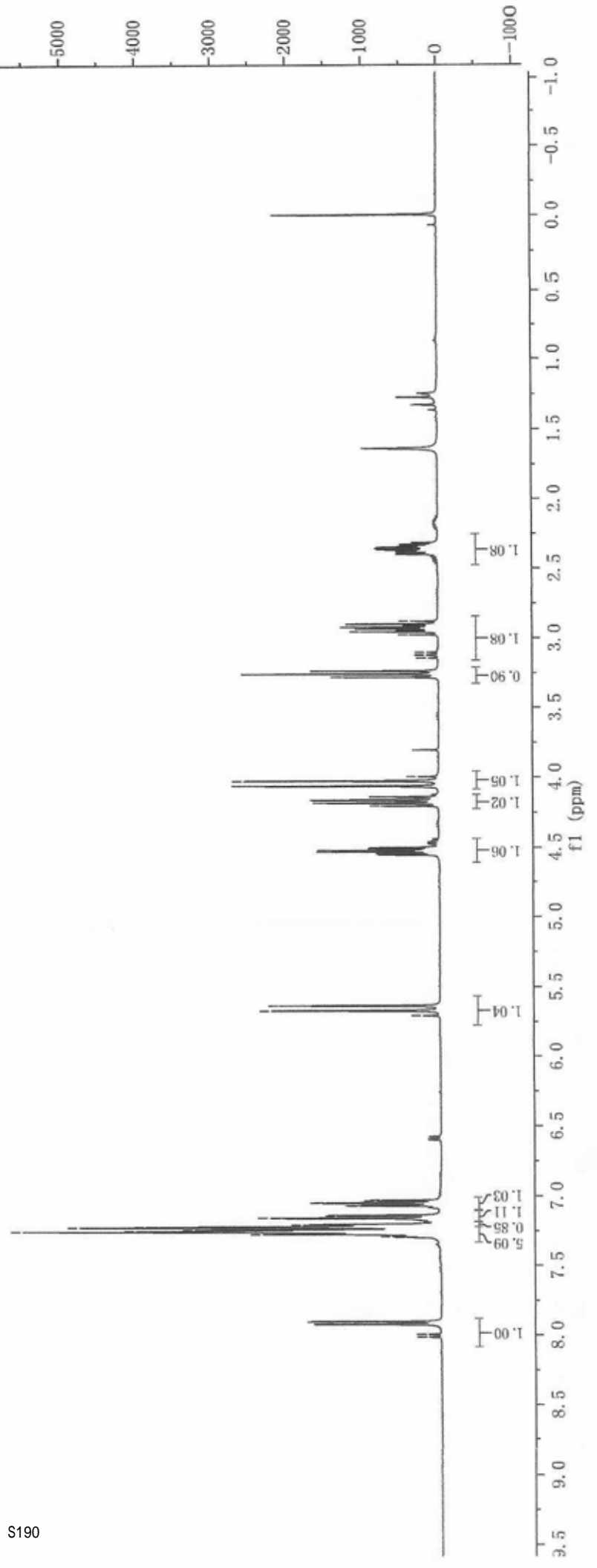


cc-13/29  
CC-13 IH

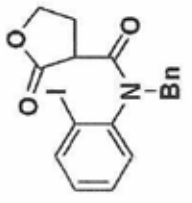
8.018  
7.998  
7.995  
7.927  
7.923  
7.907  
7.904  
7.279  
7.275  
7.271  
7.260  
7.255  
7.248  
7.245  
7.230  
7.226  
7.210  
7.207  
7.163  
7.159  
7.051  
5.709  
5.675  
5.639  
4.556  
4.546  
4.535  
4.524  
4.513  
4.503  
4.205  
4.184  
4.166  
4.144  
4.067  
4.031  
3.284  
3.262  
3.240  
2.958  
2.947  
2.936  
2.926  
2.903  
2.893  
2.381  
2.380  
2.374  
2.370  
2.361  
2.352  
2.348  
2.342  
2.338  
2.330



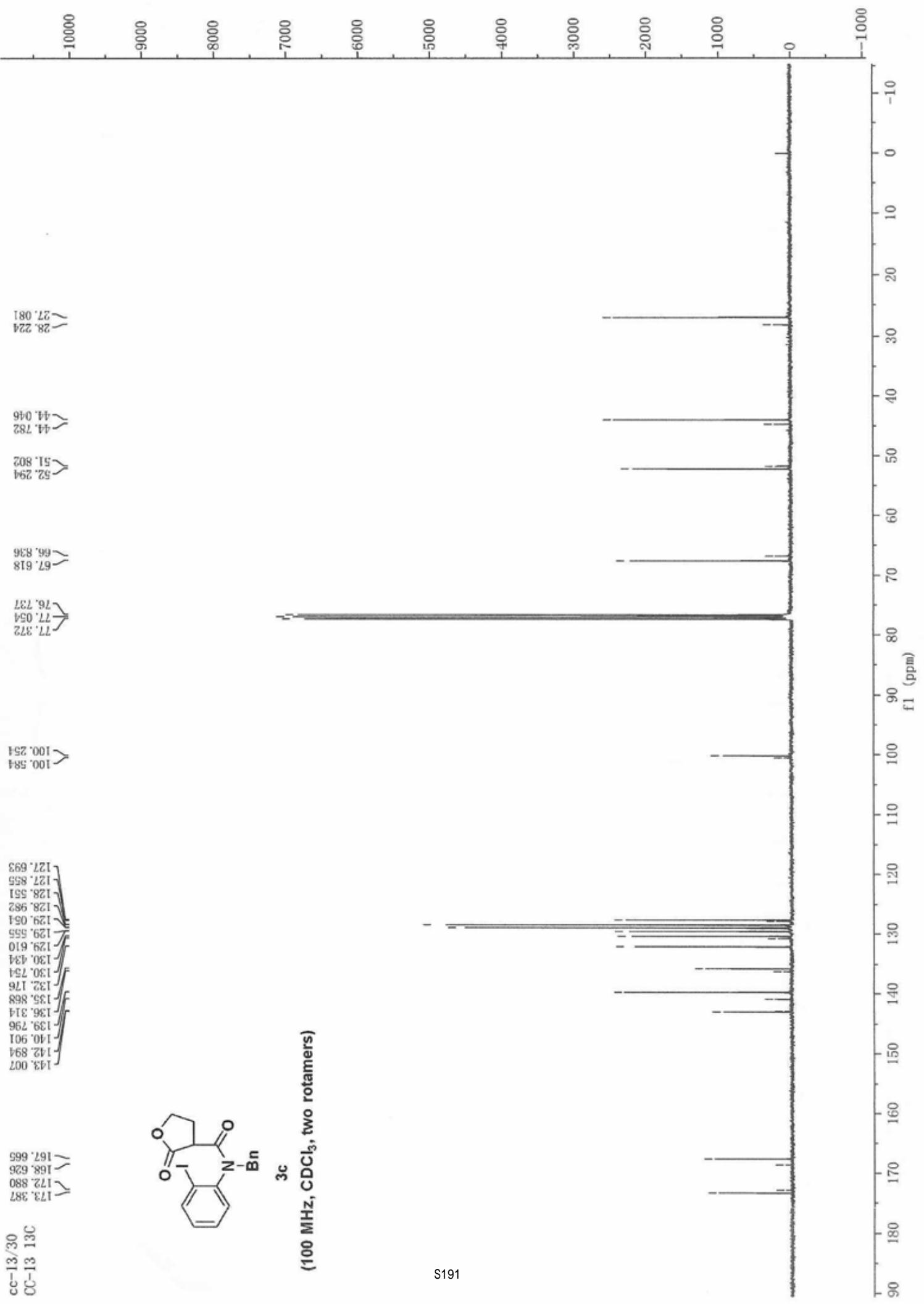
(400 MHz, CDCl<sub>3</sub>, two rotamers)



cc-13/30  
CC-13 13C



**3c**  
(100 MHz, CDCl<sub>3</sub>, two rotamers)

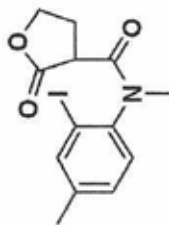


cc-2/4  
CC-02 1H

7.816  
7.739  
7.736  
7.493  
7.474  
7.267  
7.264  
7.247  
7.244  
7.222  
7.202  
7.199  
7.066  
7.046

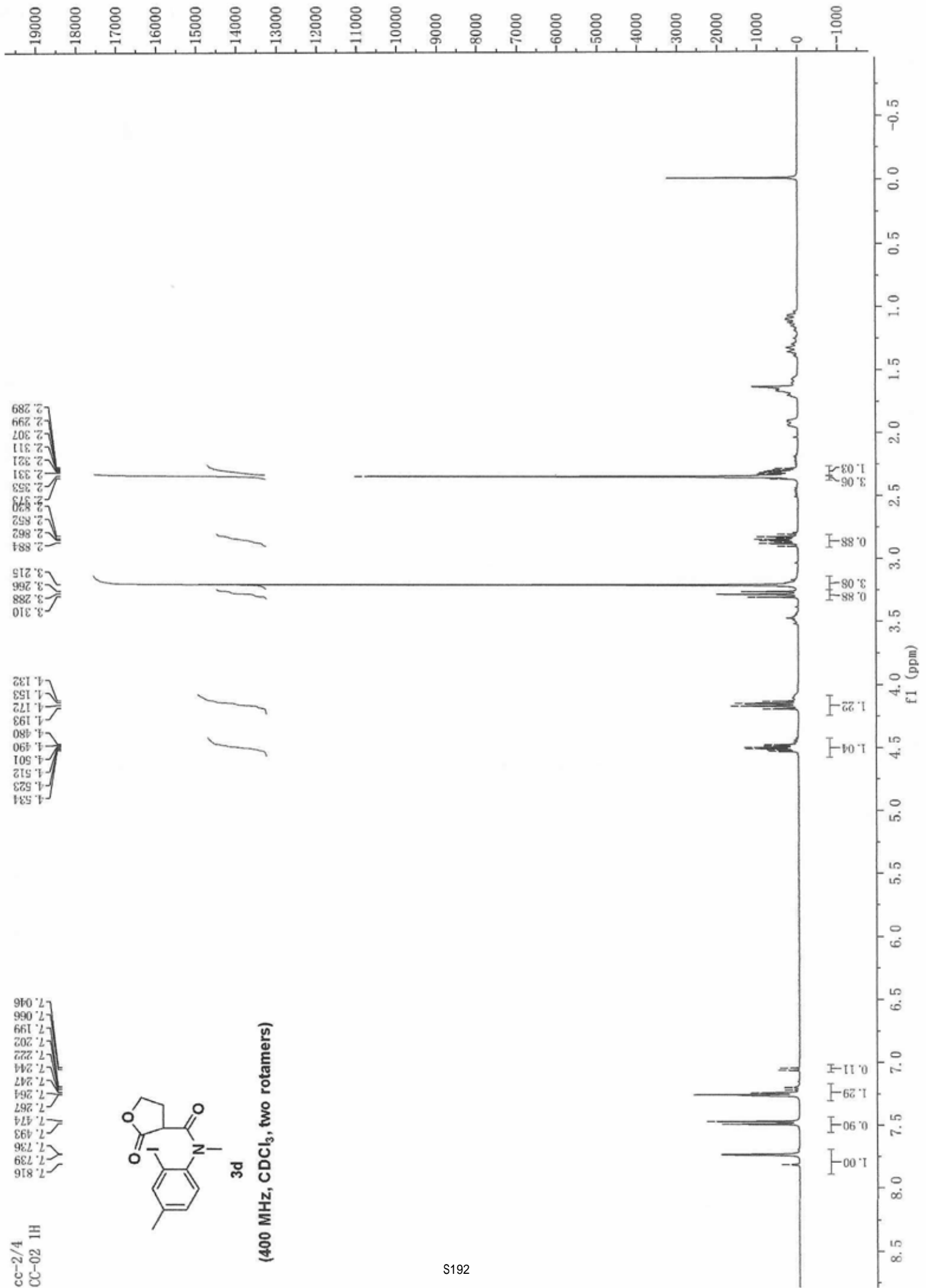
4.534  
4.523  
4.512  
4.501  
4.490  
4.480  
4.193  
4.172  
4.153  
4.132

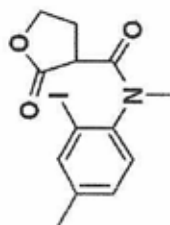
3.310  
3.288  
3.266  
3.215  
2.884  
2.862  
2.852  
2.840  
2.819  
2.353  
2.331  
2.321  
2.311  
2.307  
2.299  
2.289



3d

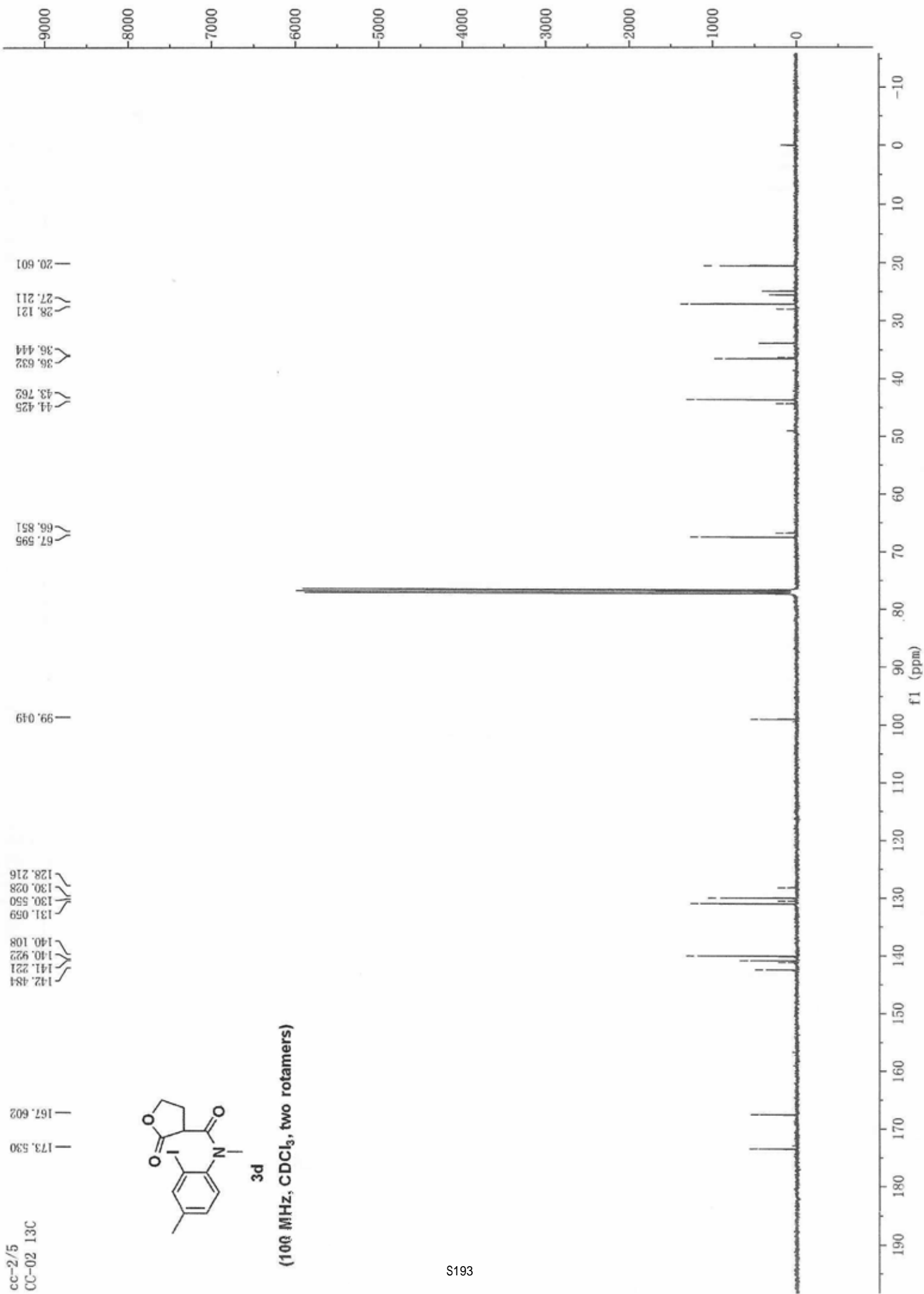
(400 MHz, CDCl<sub>3</sub>, two rotamers)





3d

(100 MHz, CDCl<sub>3</sub>, two rotamers)



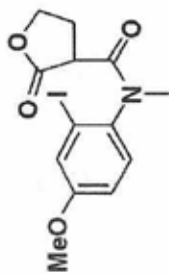
cc-3/6  
CC-02 1H

7.496  
7.474  
7.457  
7.450  
7.392  
7.385  
7.083  
7.061  
6.967  
6.960  
6.945  
6.938  
6.925  
6.911  
6.904

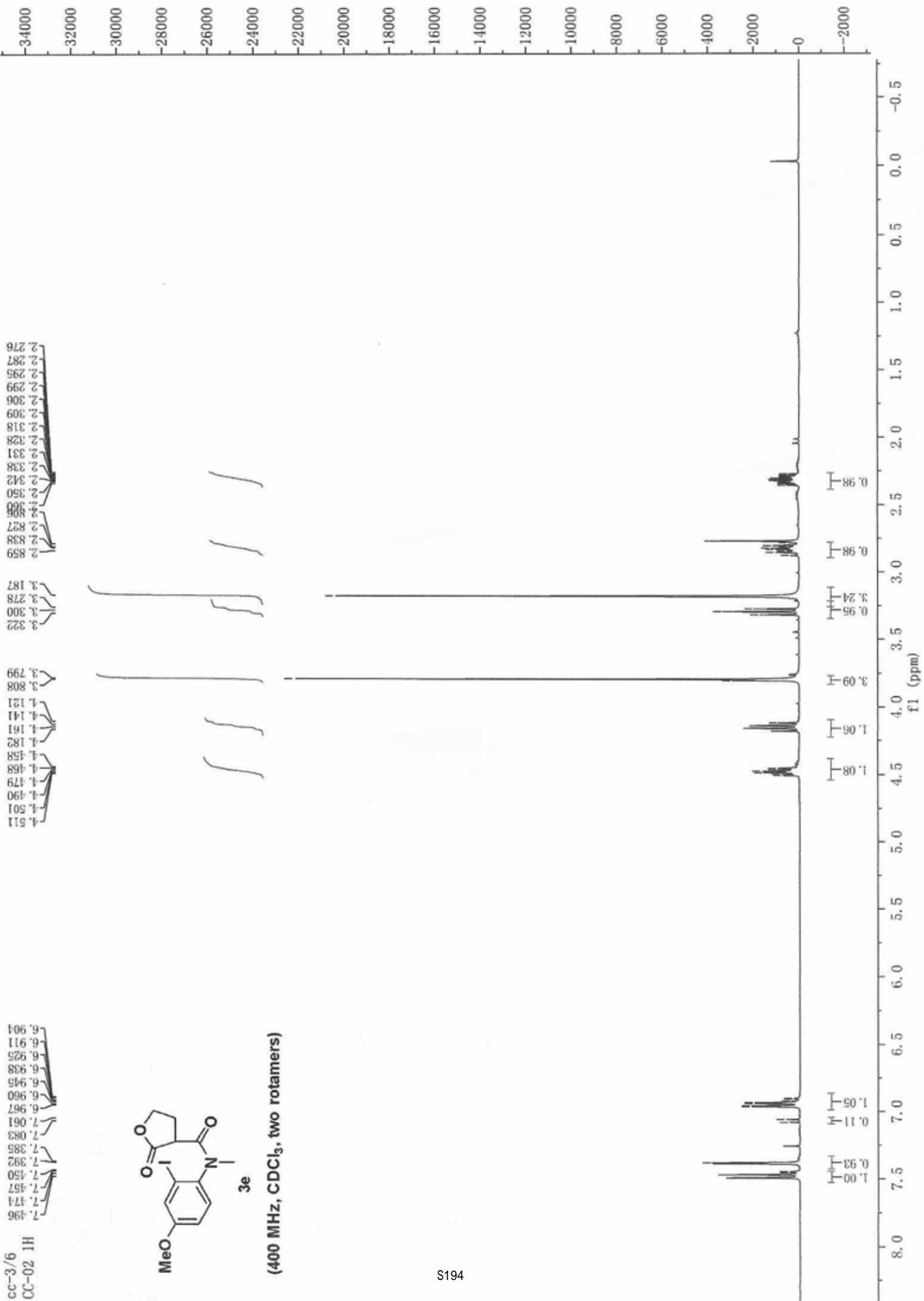
4.511  
4.501  
4.490  
4.479  
4.468  
4.458  
4.182  
4.161  
4.141  
4.121  
3.808  
3.799

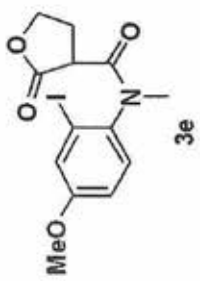
3.322  
3.300  
3.278  
3.187

2.859  
2.838  
2.827  
2.806  
2.806  
2.350  
2.342  
2.338  
2.331  
2.328  
2.318  
2.309  
2.306  
2.299  
2.295  
2.287  
2.276

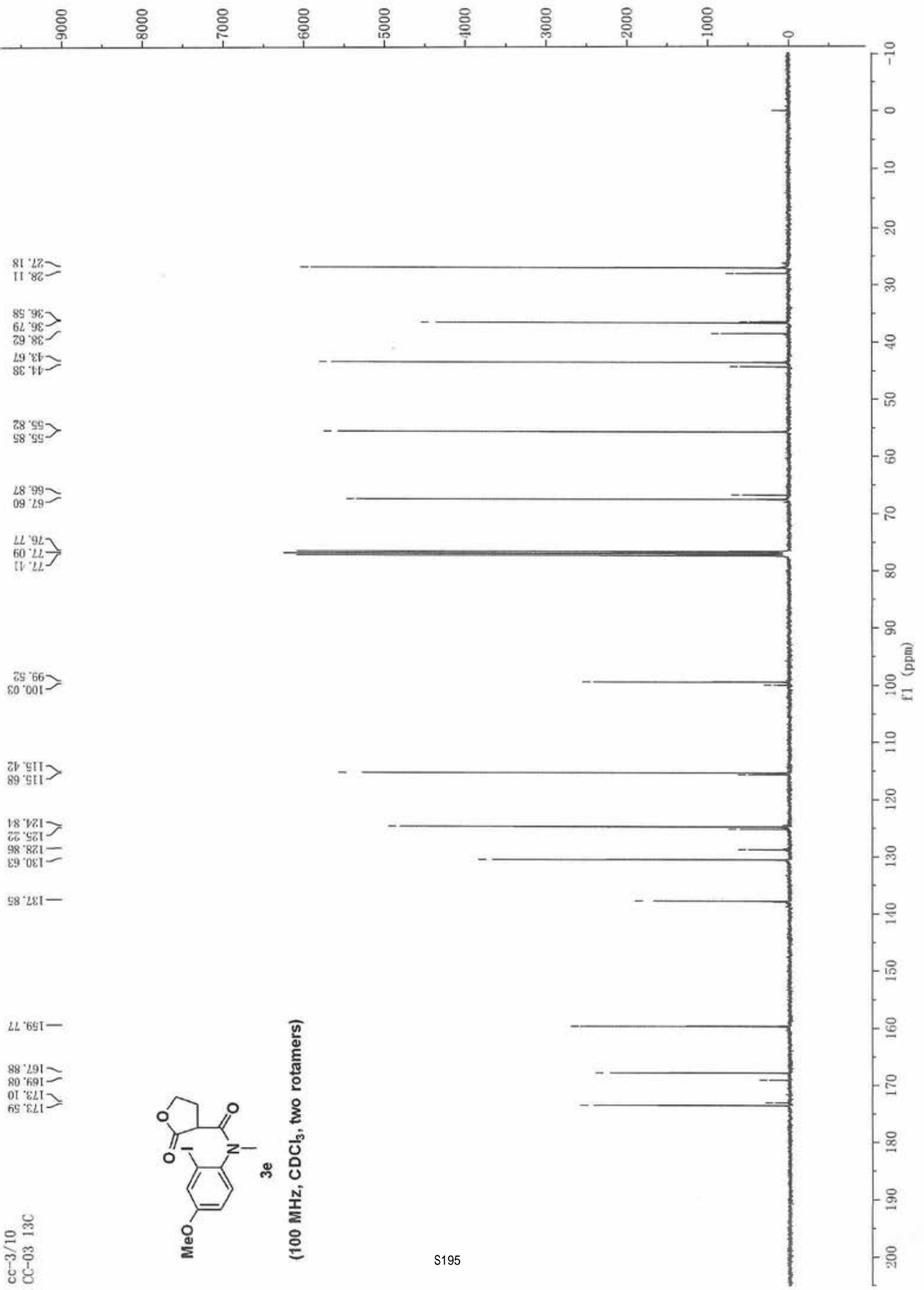


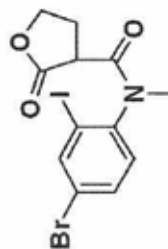
(400 MHz, CDCl<sub>3</sub>, two rotamers)





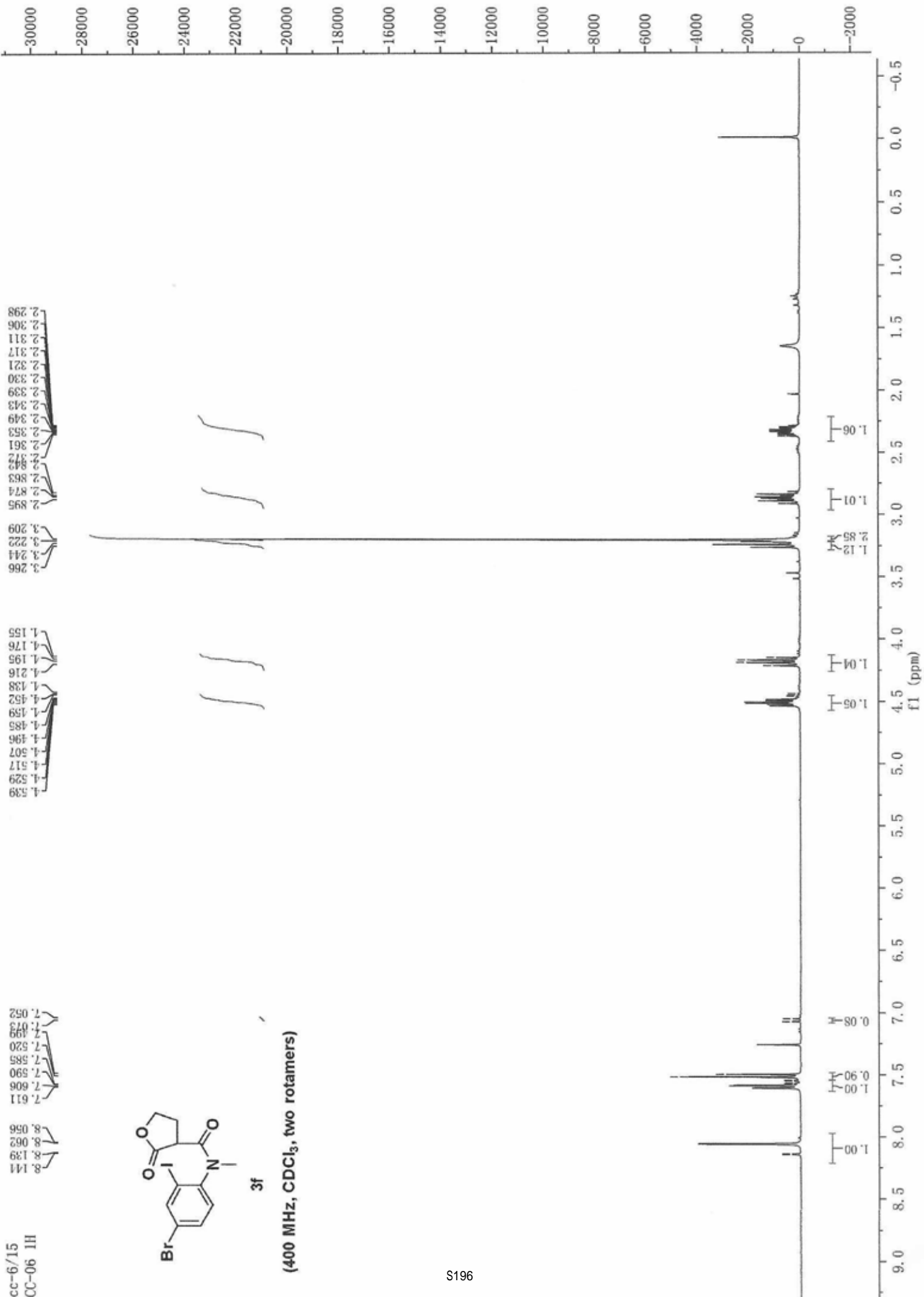
(100 MHz, CDCl<sub>3</sub>, two rotamers)



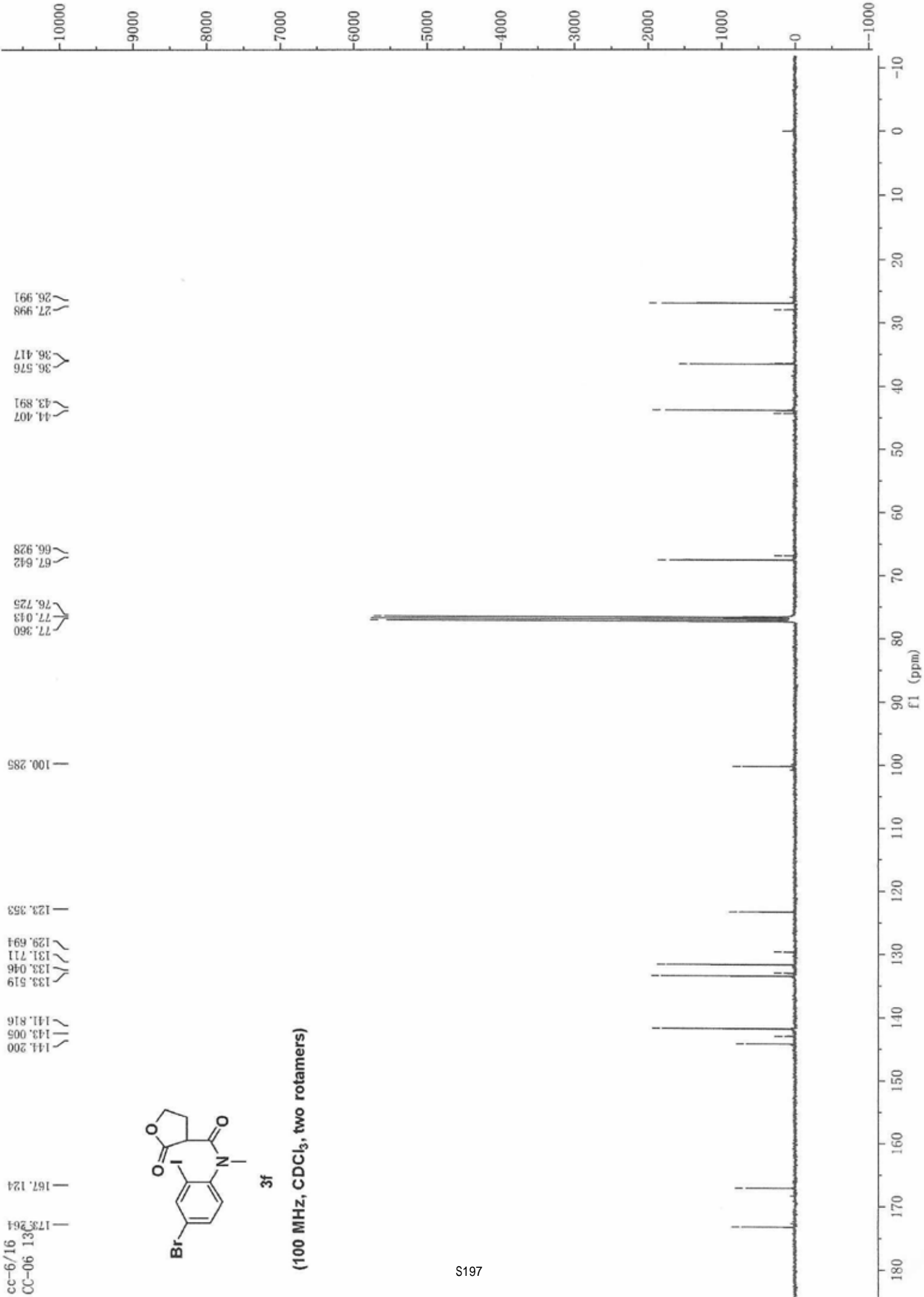


3f

(400 MHz, CDCl<sub>3</sub>, two rotamers)





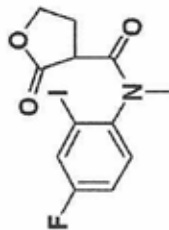


1  
mhwf1

7.647  
7.640  
7.628  
7.621  
7.581  
7.574  
7.563  
7.555  
7.550  
7.541  
7.528  
7.154  
7.147  
7.133  
7.127  
7.113  
7.105

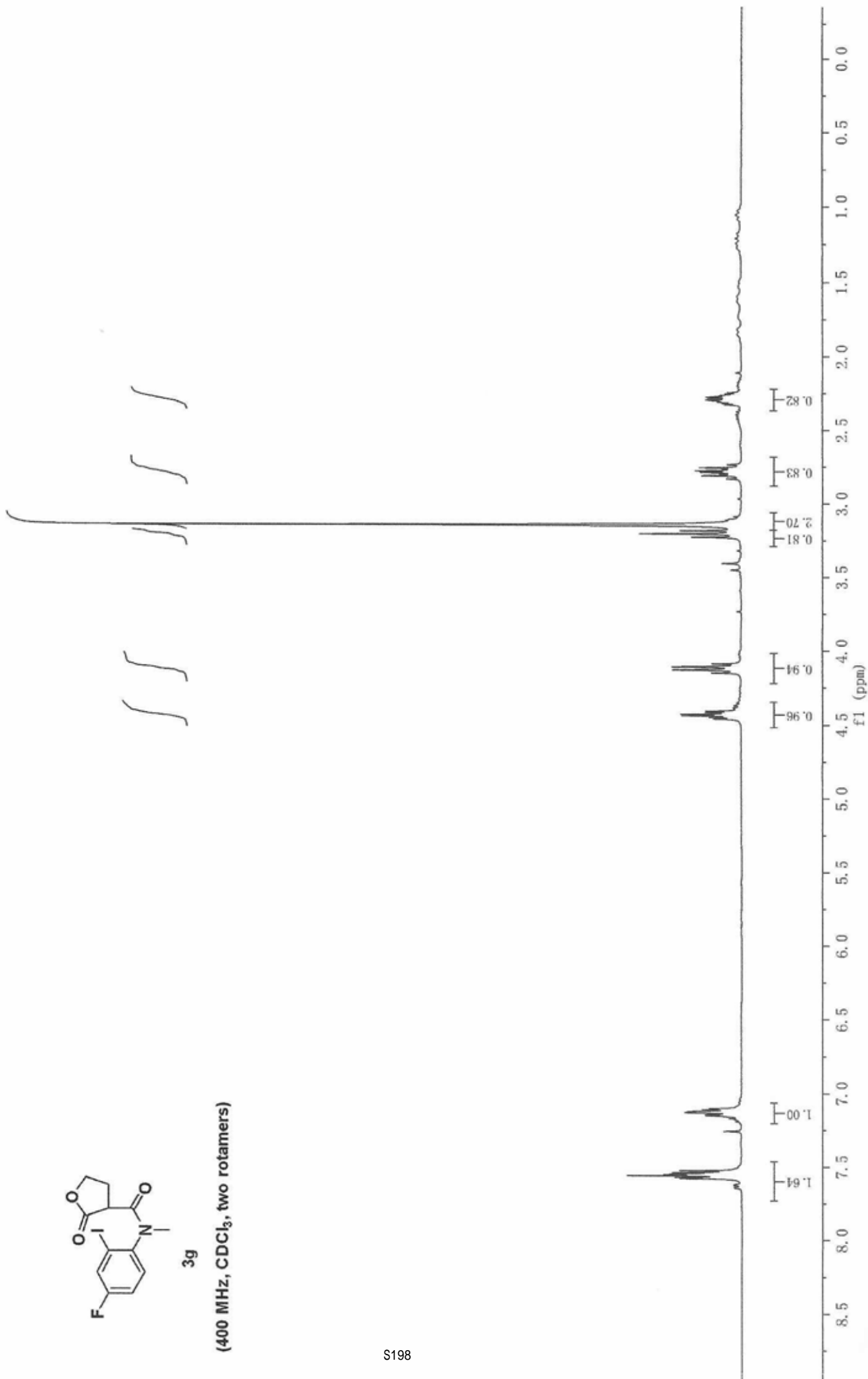
4.461  
4.451  
4.140  
4.429  
4.418  
4.408  
4.151  
4.130  
4.111  
4.090

3.229  
3.207  
3.185  
3.147  
2.811  
2.800  
2.789  
2.779  
2.557  
2.530  
2.320  
2.311  
2.307  
2.298  
2.288  
2.279  
2.269  
2.265  
2.257  
2.247

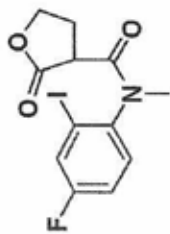


3g

(400 MHz, CDCl<sub>3</sub>, two rotamers)

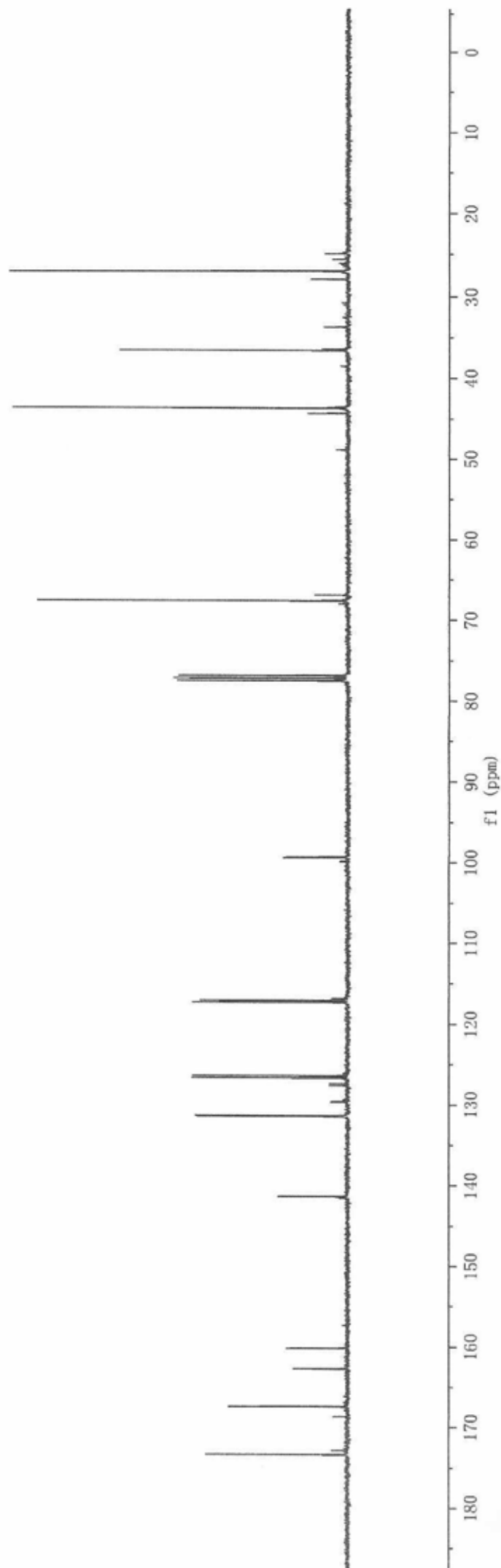


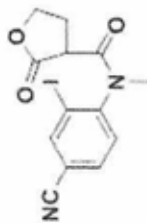
- 173.403
- 172.927
- 168.714
- 167.478
- 162.769
- 160.237
- 141.404
- 141.368
- 131.489
- 131.401
- 129.721
- 129.632
- 127.689
- 127.445
- 126.710
- 126.464
- 117.367
- 117.147
- 116.882
- 99.421
- 99.335
- 67.612
- 66.954
- 44.423
- 43.762
- 36.669
- 27.991
- 27.032



3g

(100 MHz, CDCl<sub>3</sub>, two rotamers)

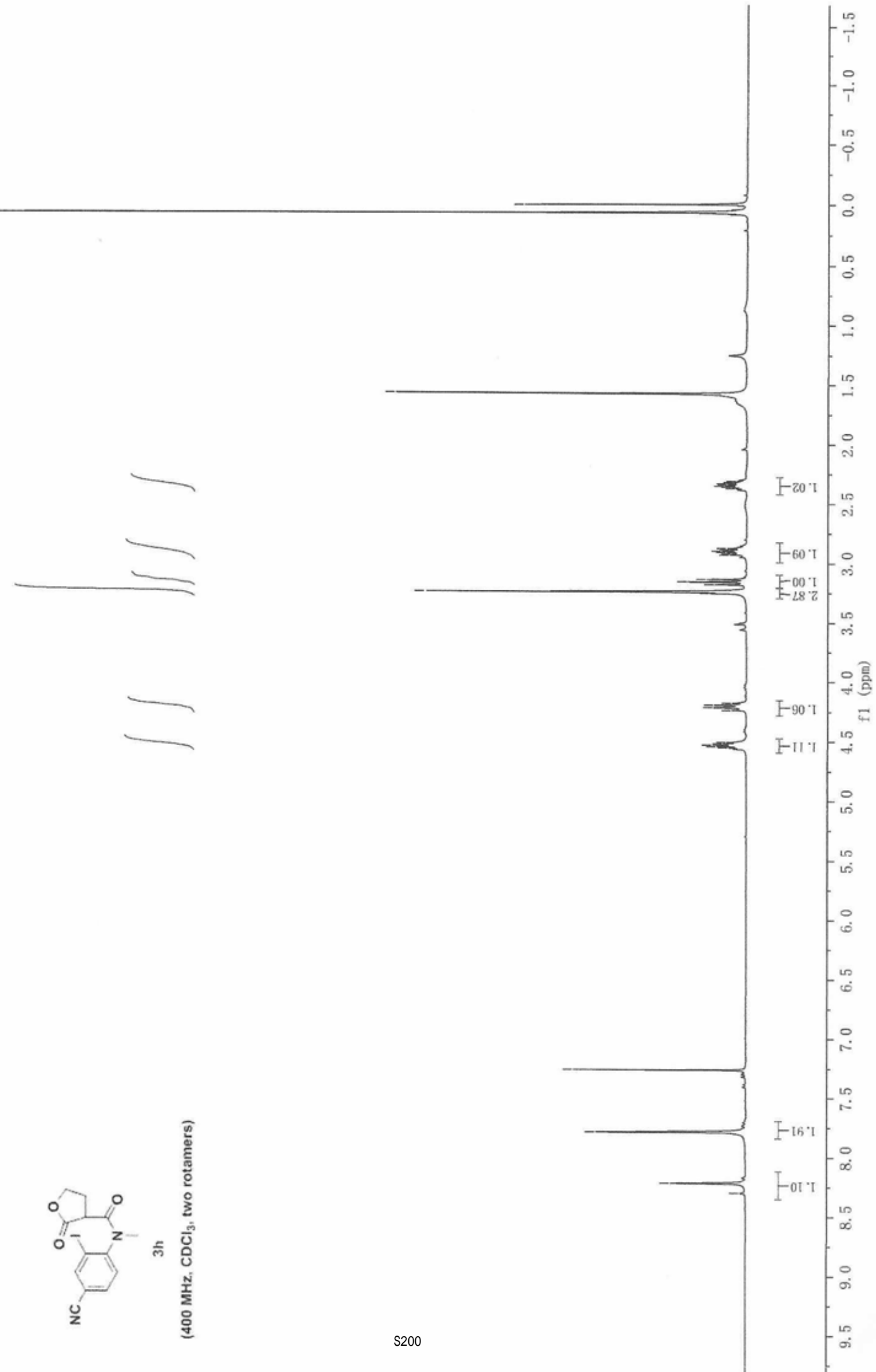


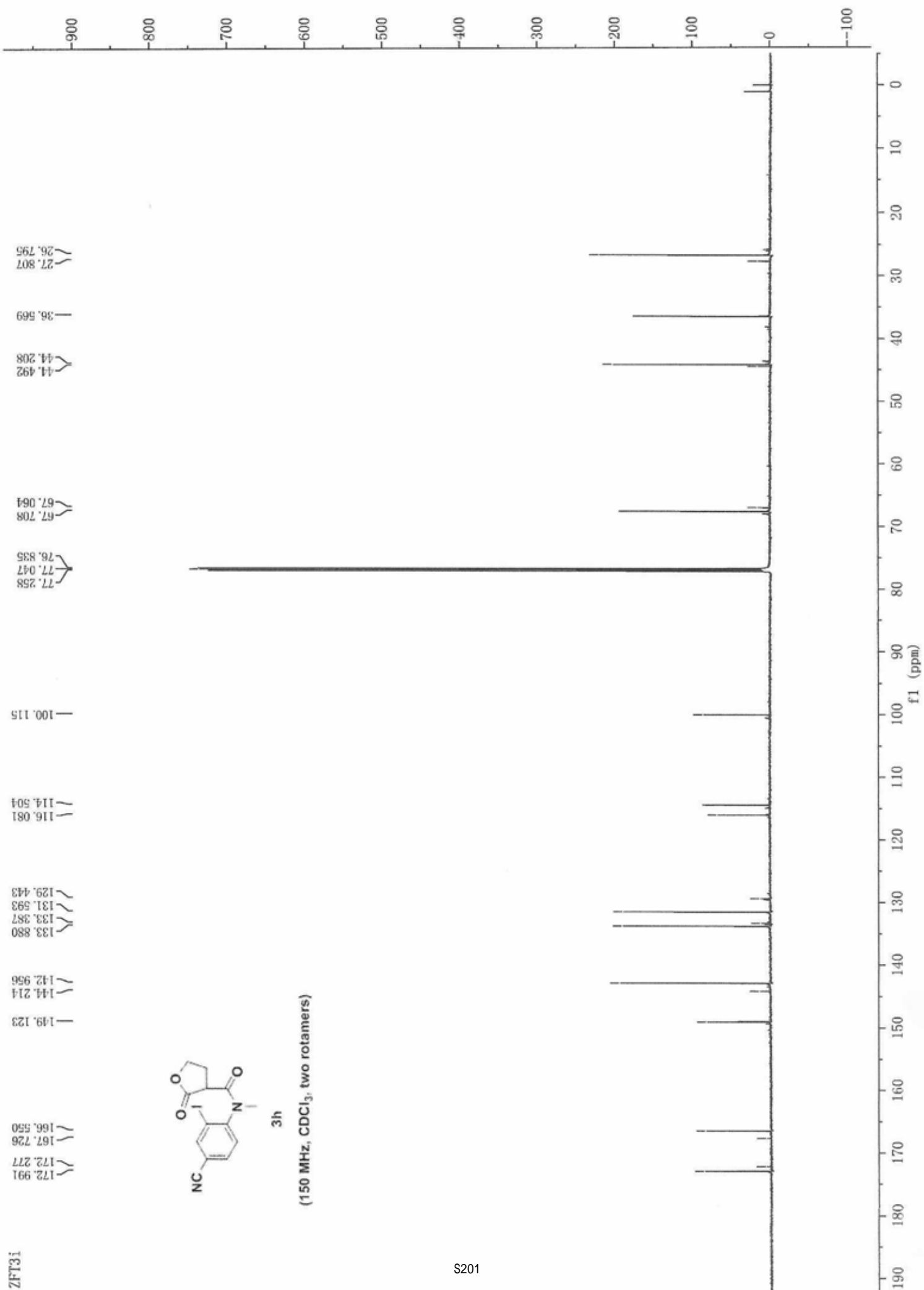


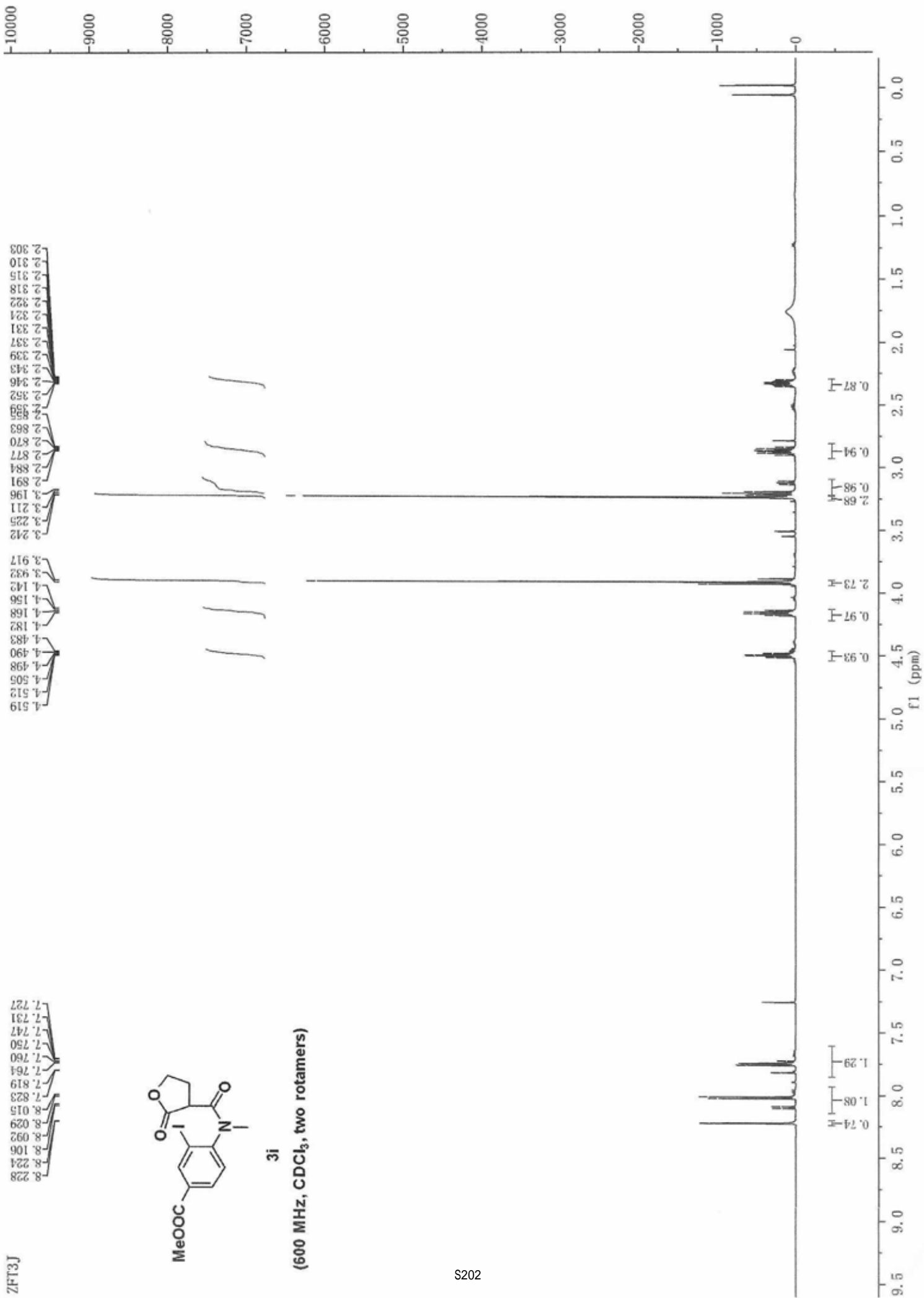
3h

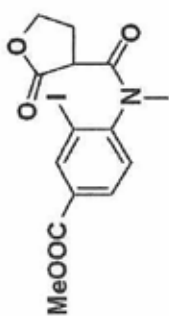
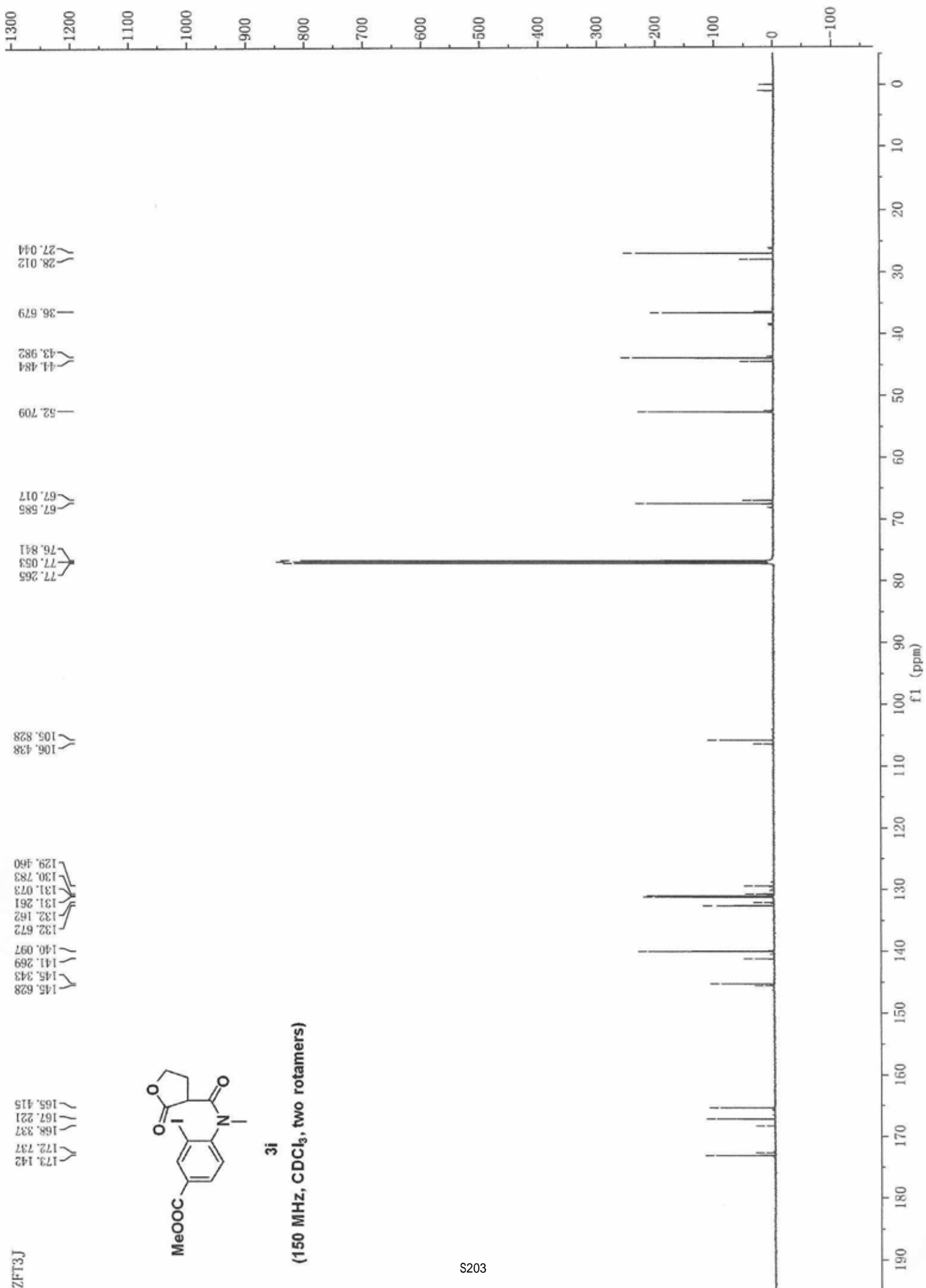
(400 MHz, CDCl<sub>3</sub>, two rotamers)

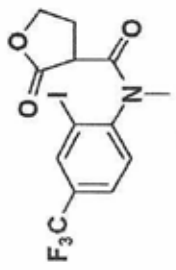
4.550  
4.539  
4.528  
4.517  
4.506  
4.236  
4.215  
4.195  
4.175  
3.255  
3.243  
3.180  
3.159  
3.137  
2.930  
2.919  
2.909  
2.898  
2.877  
2.373  
2.362  
2.351  
2.342  
2.332  
2.322  
2.319  
2.310  
1.574  
0.067  
-0.003





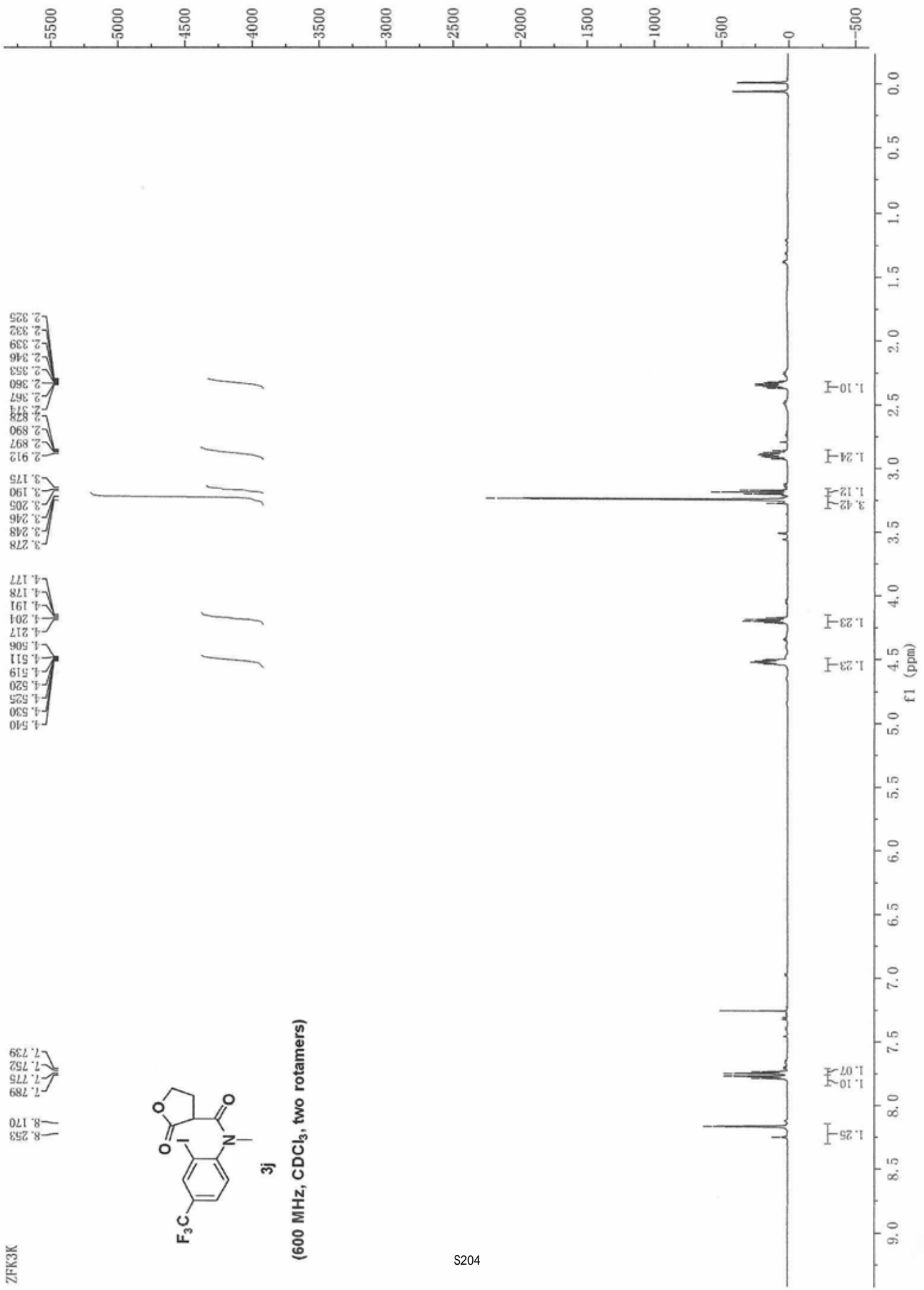


**3i****(150 MHz, CDCl<sub>3</sub>, two rotamers)**



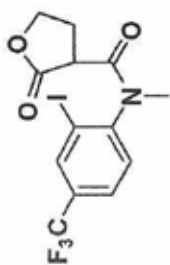
3j

(600 MHz, CDCl<sub>3</sub>, two rotamers)



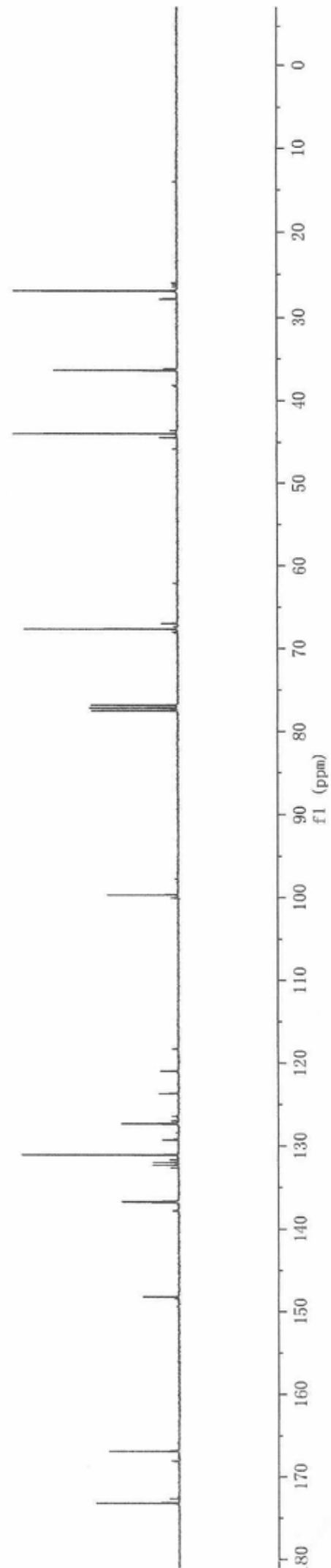


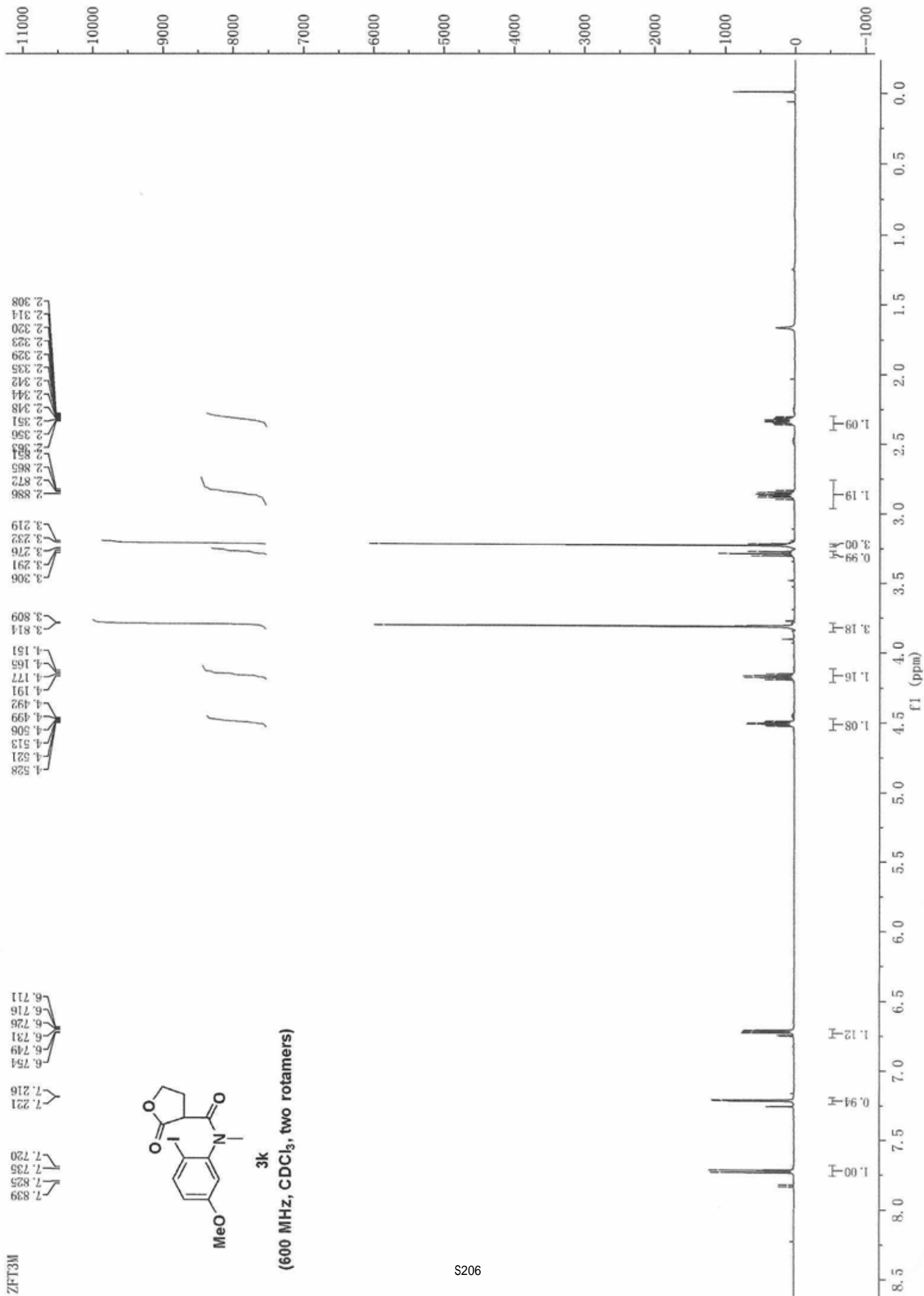
173.208  
 172.654  
 168.142  
 166.932  
 148.274  
 136.811  
 136.775  
 136.738  
 136.701  
 132.715  
 132.384  
 132.052  
 131.721  
 131.141  
 129.353  
 127.445  
 127.411  
 127.375  
 127.340  
 100.080  
 99.723  
 67.645  
 66.979  
 44.550  
 44.050  
 36.451  
 36.277  
 27.889  
 26.931

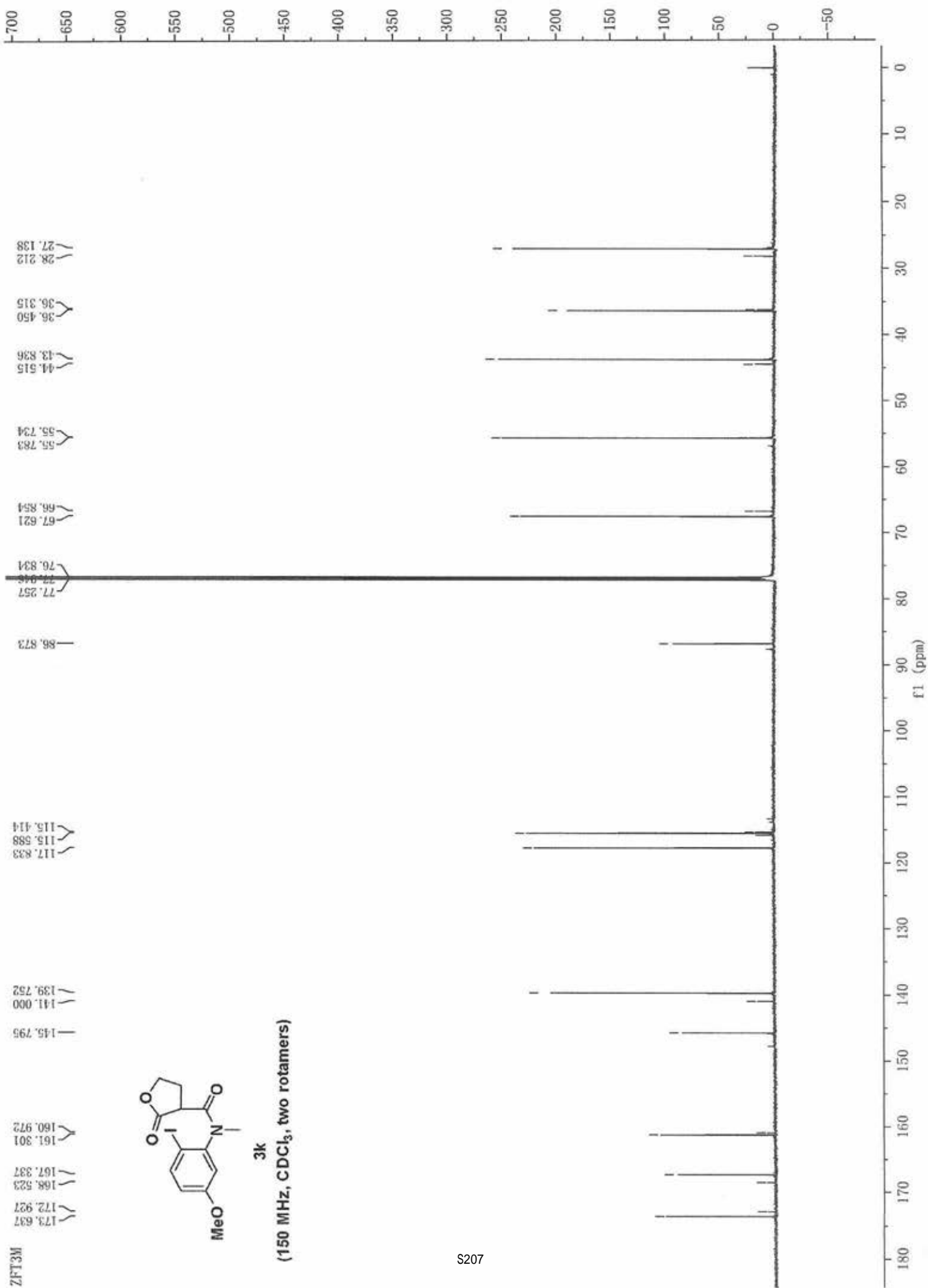


3j

(100 MHz, CDCl<sub>3</sub>, two rotamers)

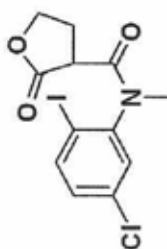








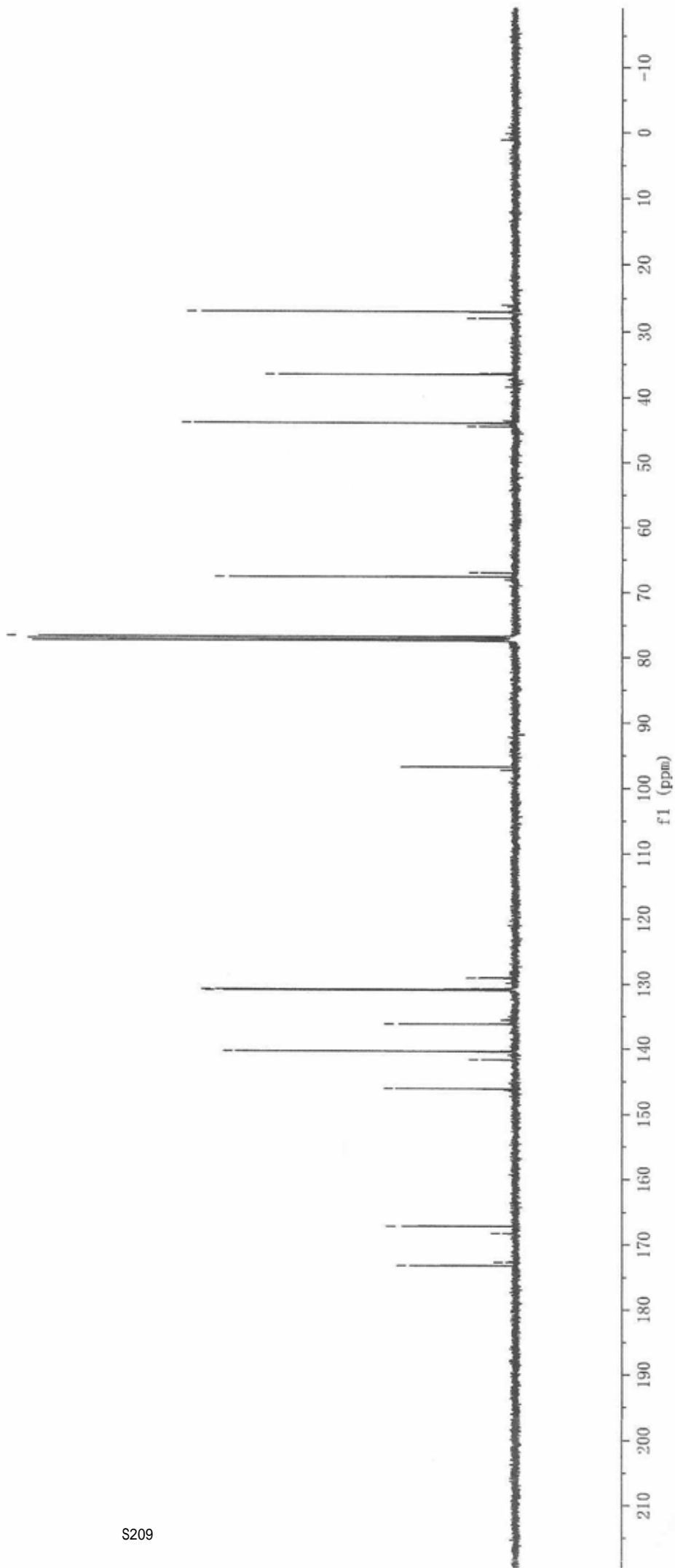
zft202007064Cl. 12. fid  
zft202007064Cl 13C

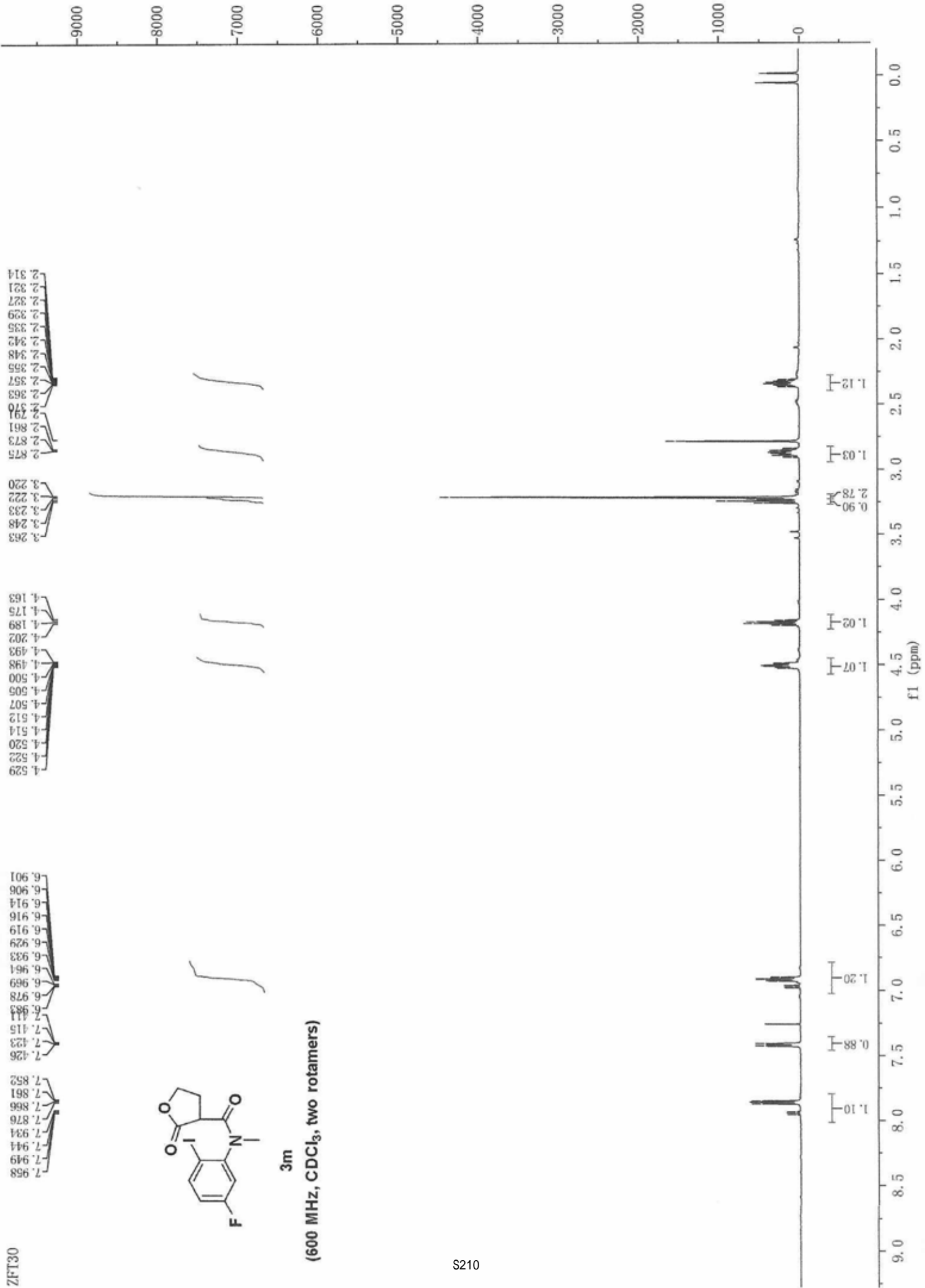


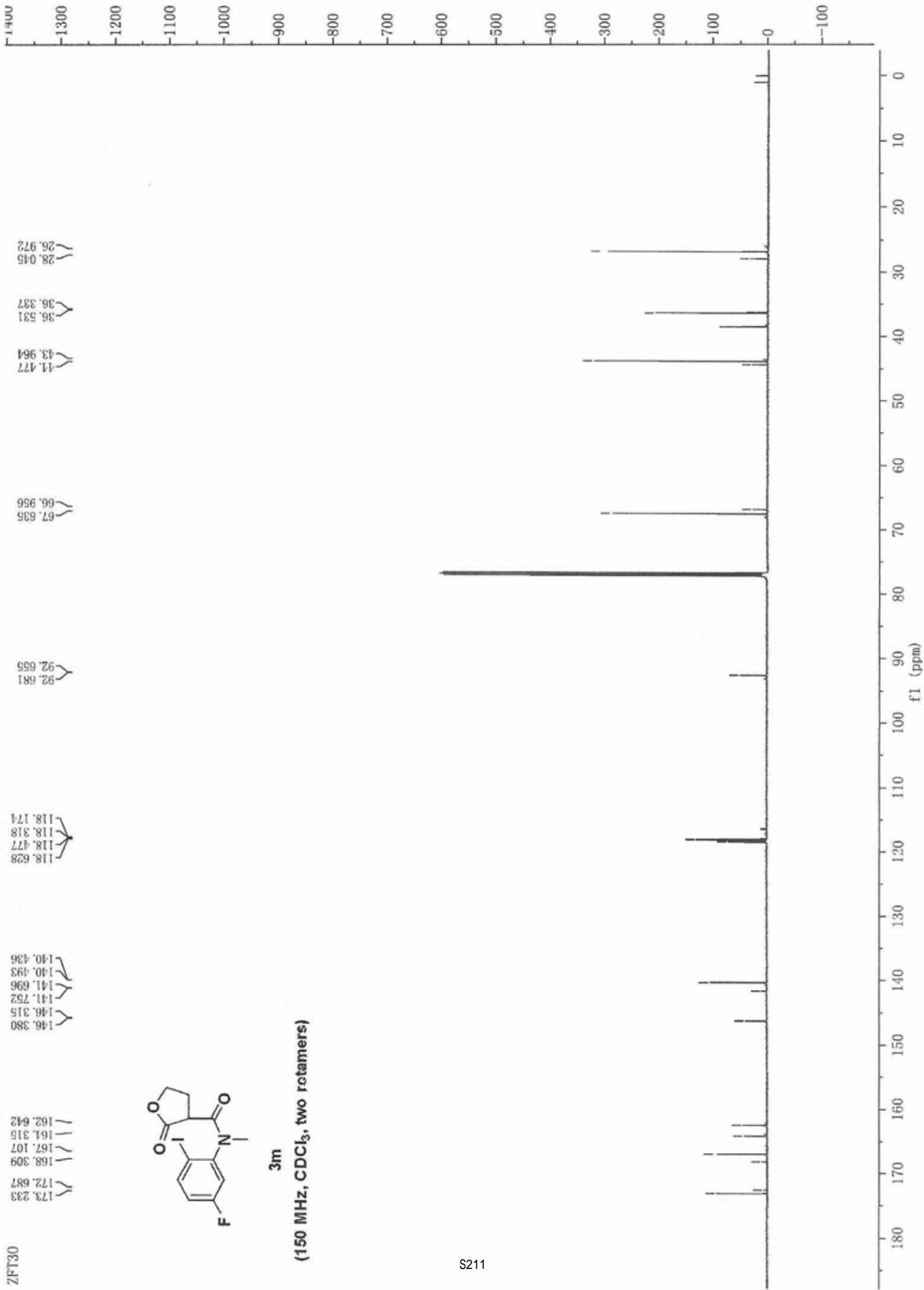
3I

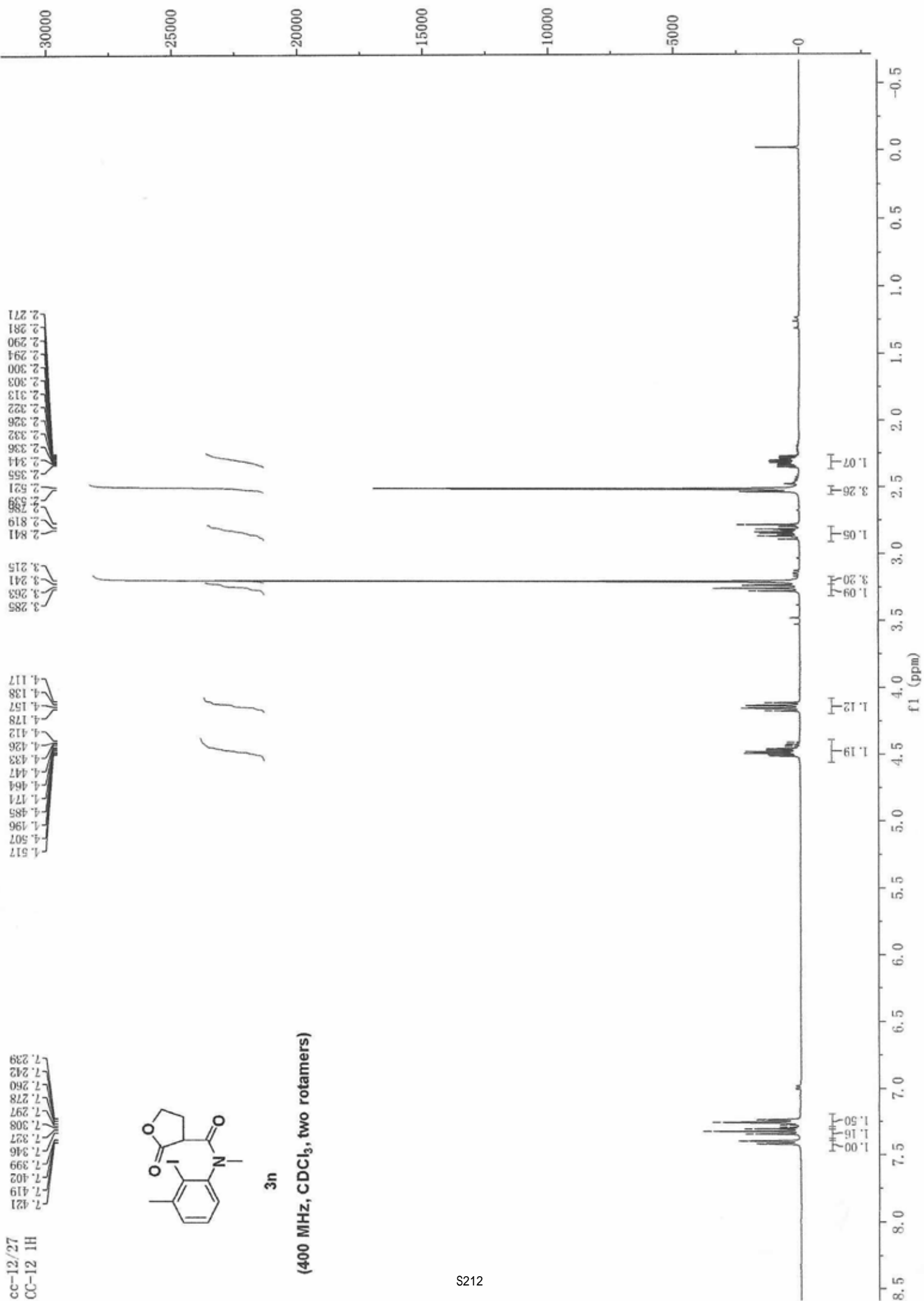
(101 MHz, CDCl<sub>3</sub>, two rotamers)

173.271  
172.756  
168.365  
167.223  
146.169  
141.698  
140.486  
136.237  
131.051  
130.916  
130.792  
129.145  
96.872  
77.477  
77.160  
76.840  
67.686  
67.066  
44.551  
44.063  
36.677  
36.500  
28.109  
27.094

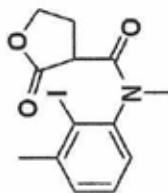








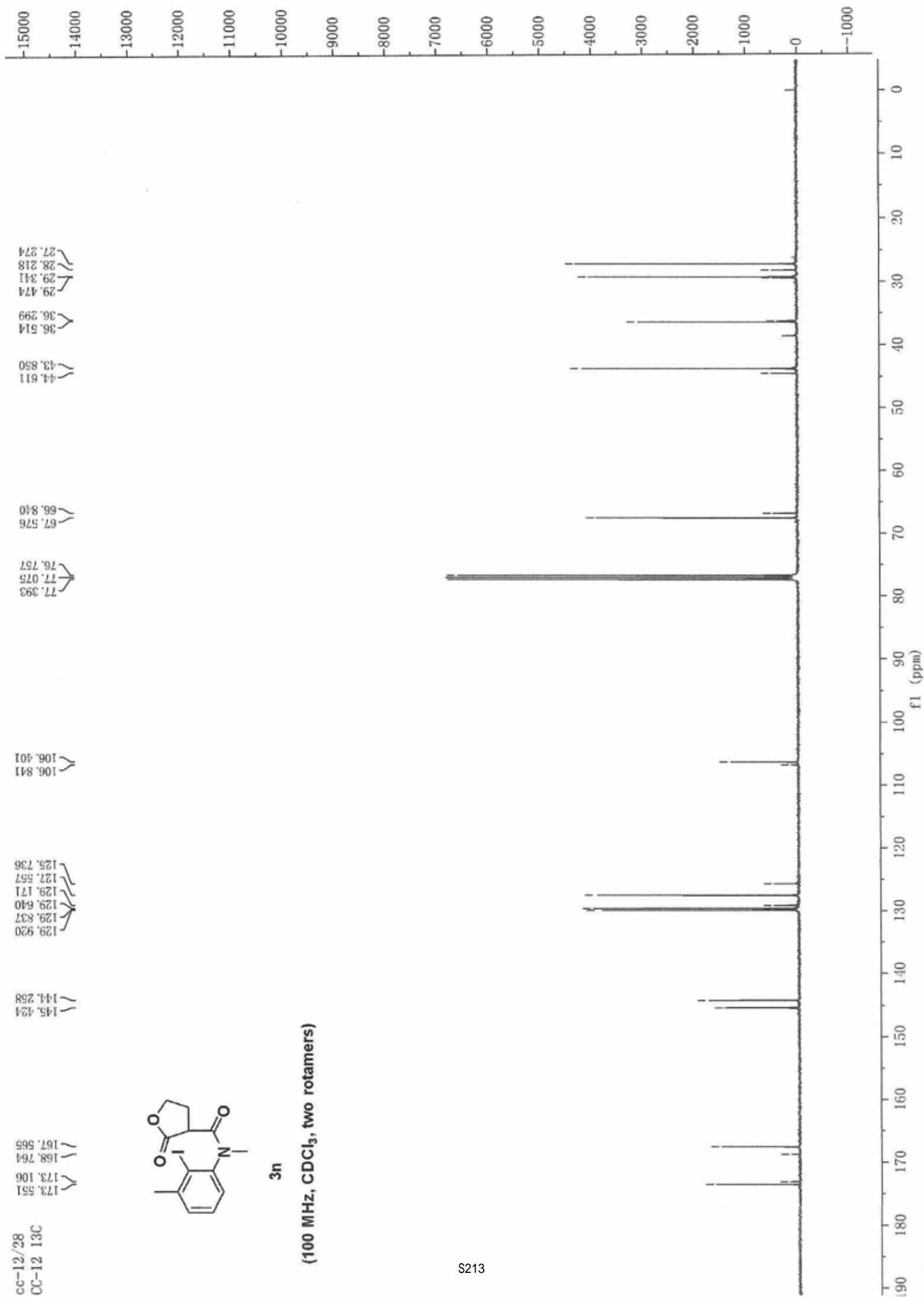


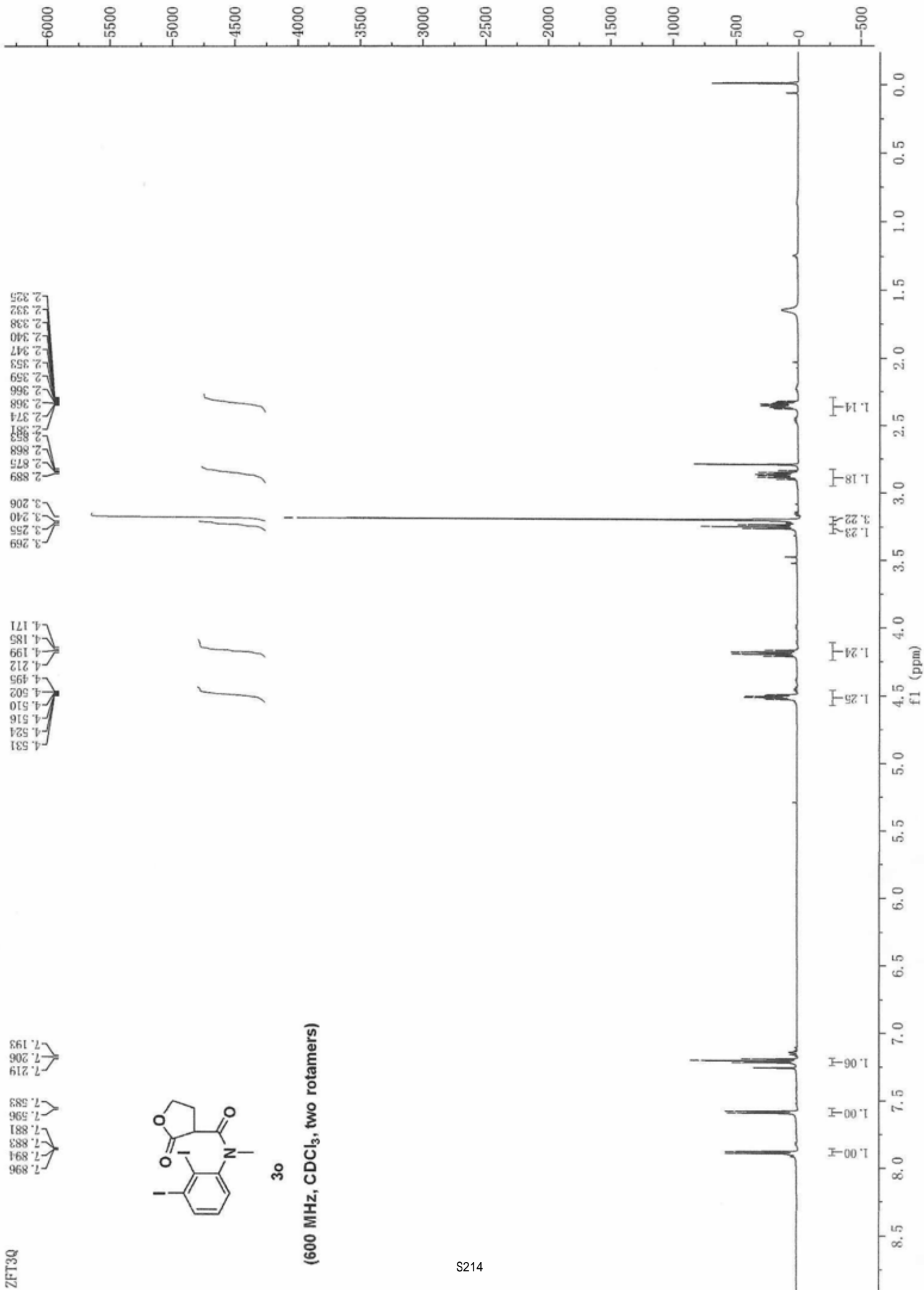


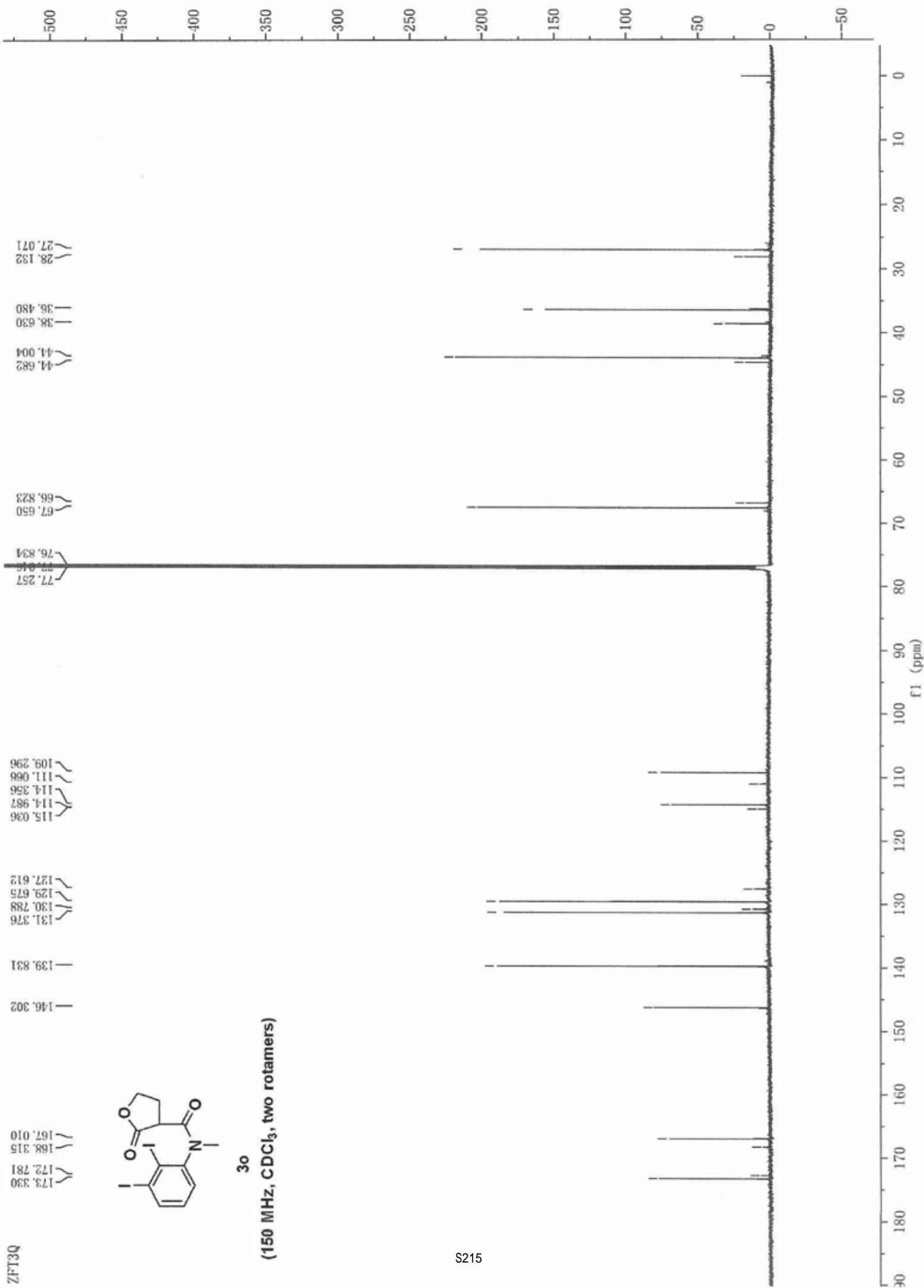
3n

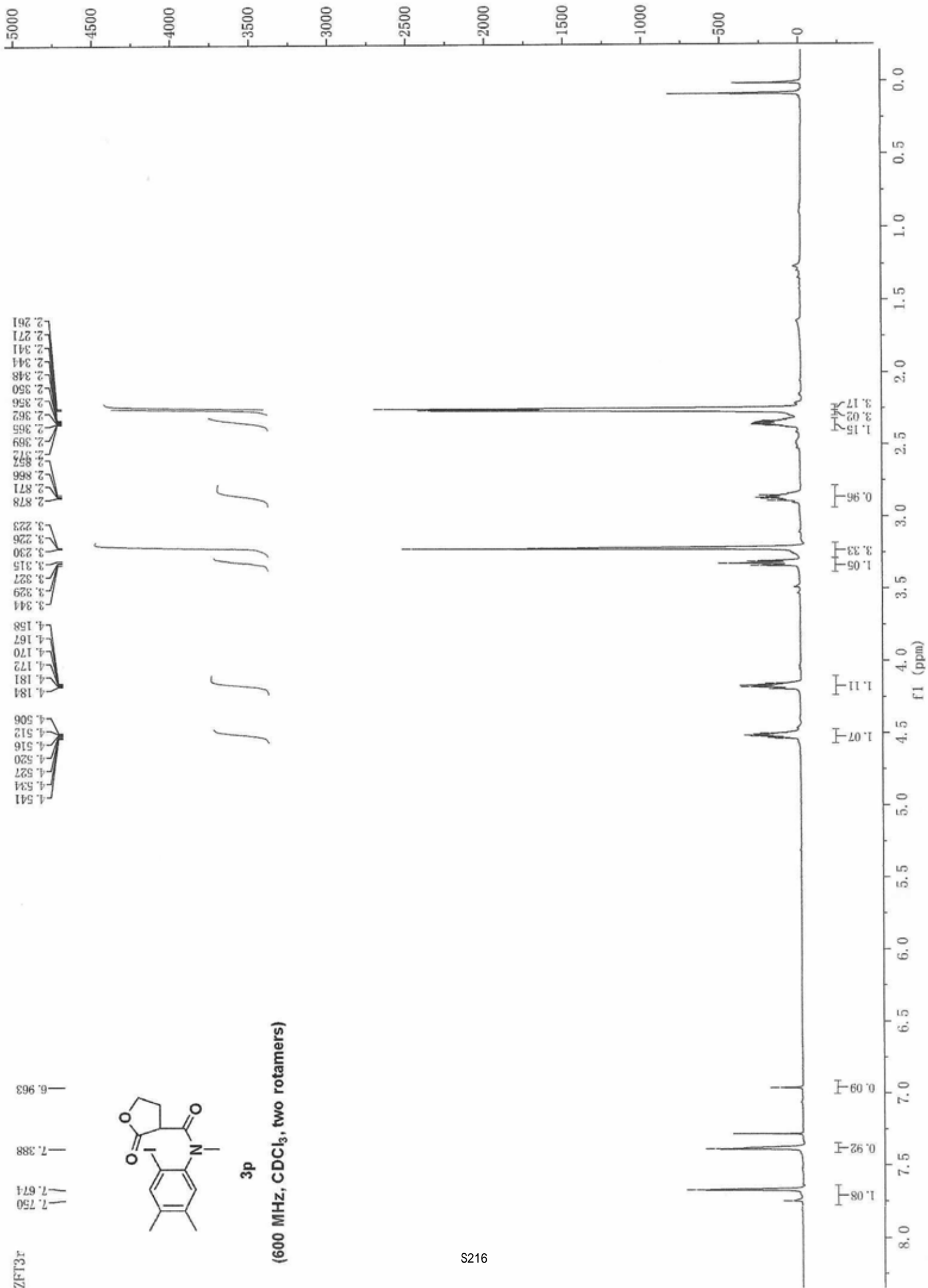
(100 MHz, CDCl<sub>3</sub>, two rotamers)

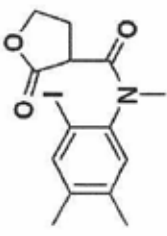
- 173.551
- 173.106
- 168.764
- 167.565
- 145.424
- 144.258
- 129.920
- 129.837
- 129.640
- 129.171
- 127.557
- 125.736
- 106.841
- 106.401
- 77.393
- 77.075
- 76.757
- 67.576
- 66.840
- 44.611
- 43.850
- 36.514
- 36.299
- 29.474
- 29.341
- 28.218
- 27.274





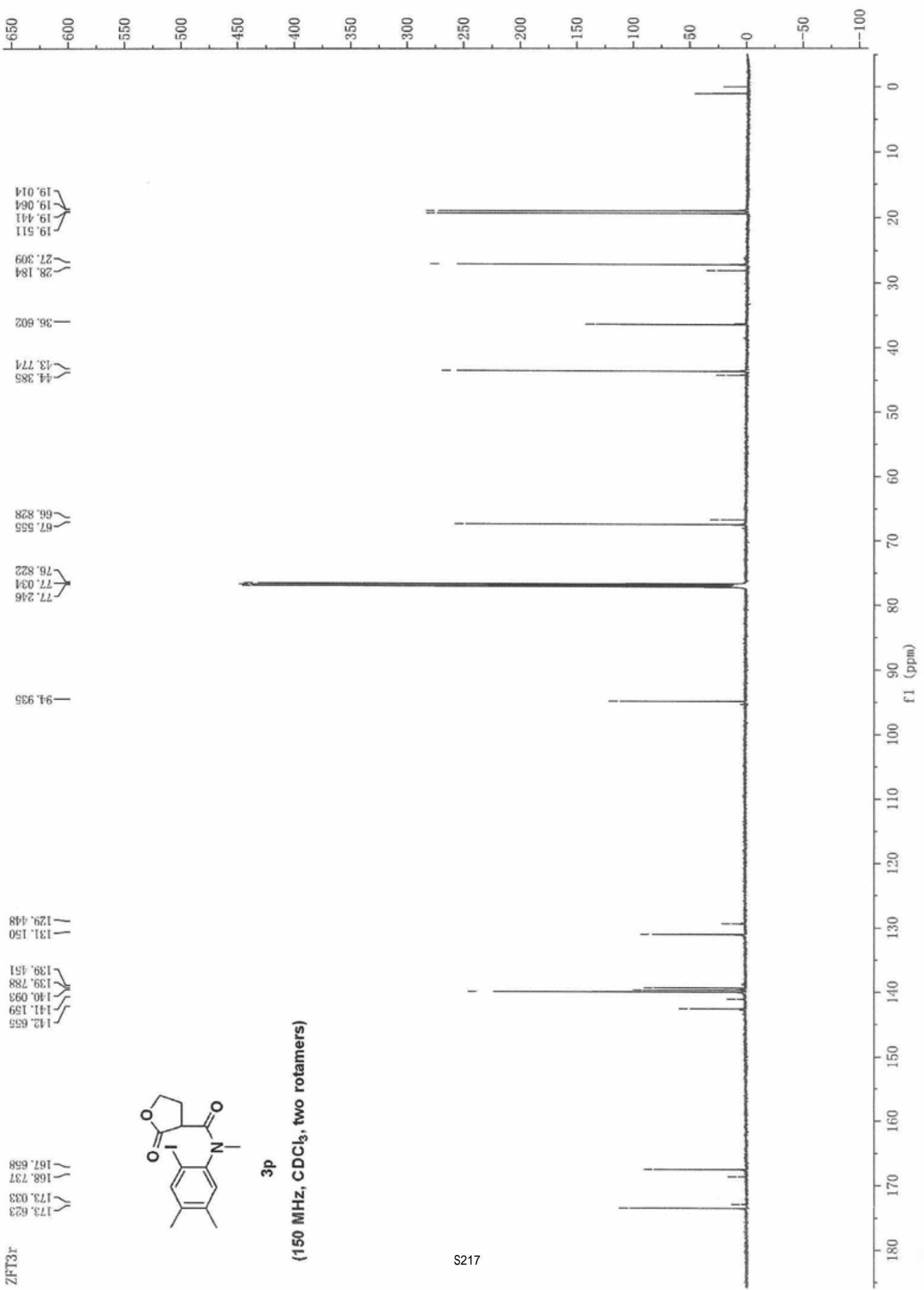


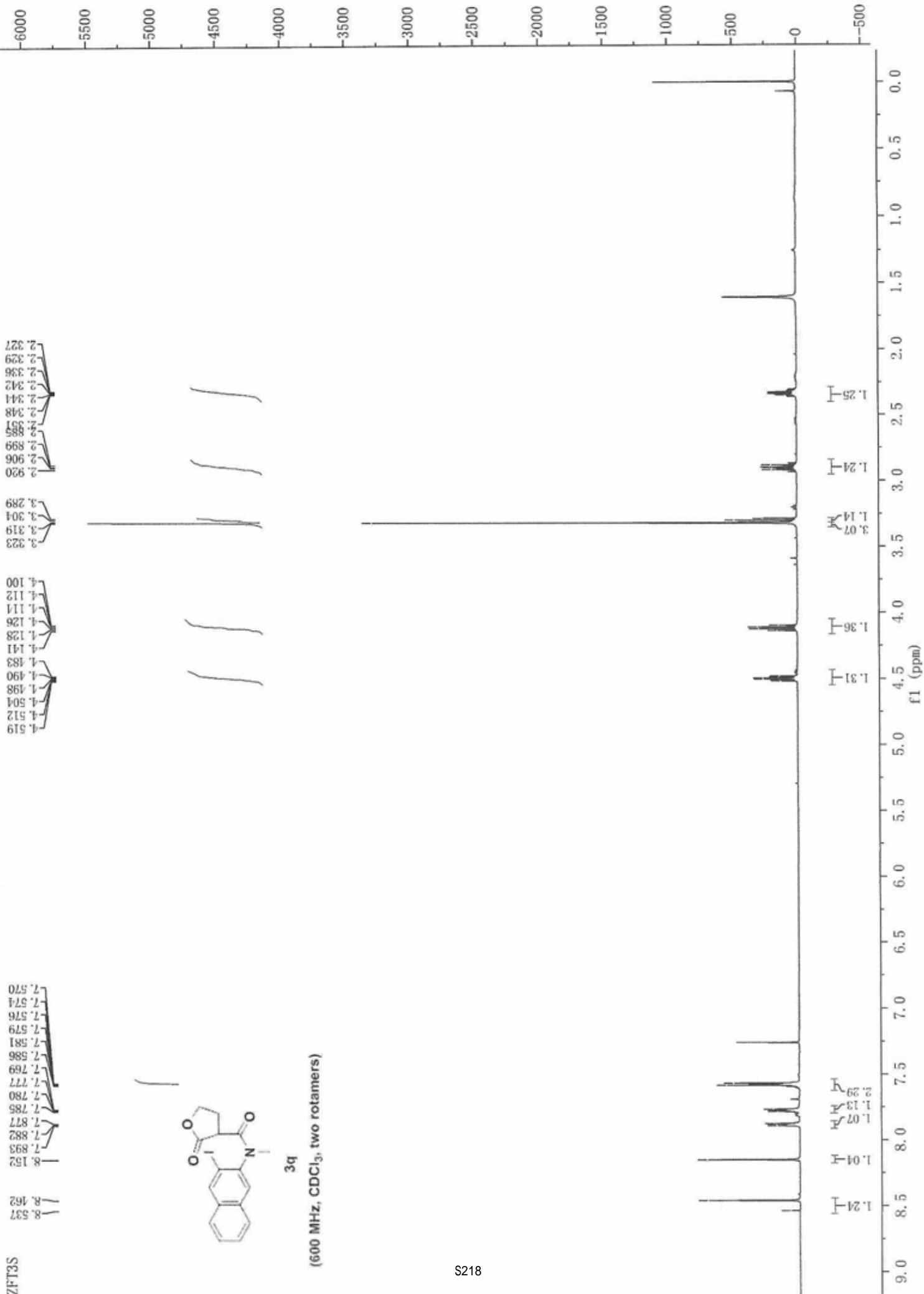


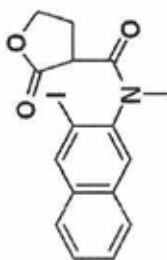


3p

(150 MHz, CDCl<sub>3</sub>, two rotamers)

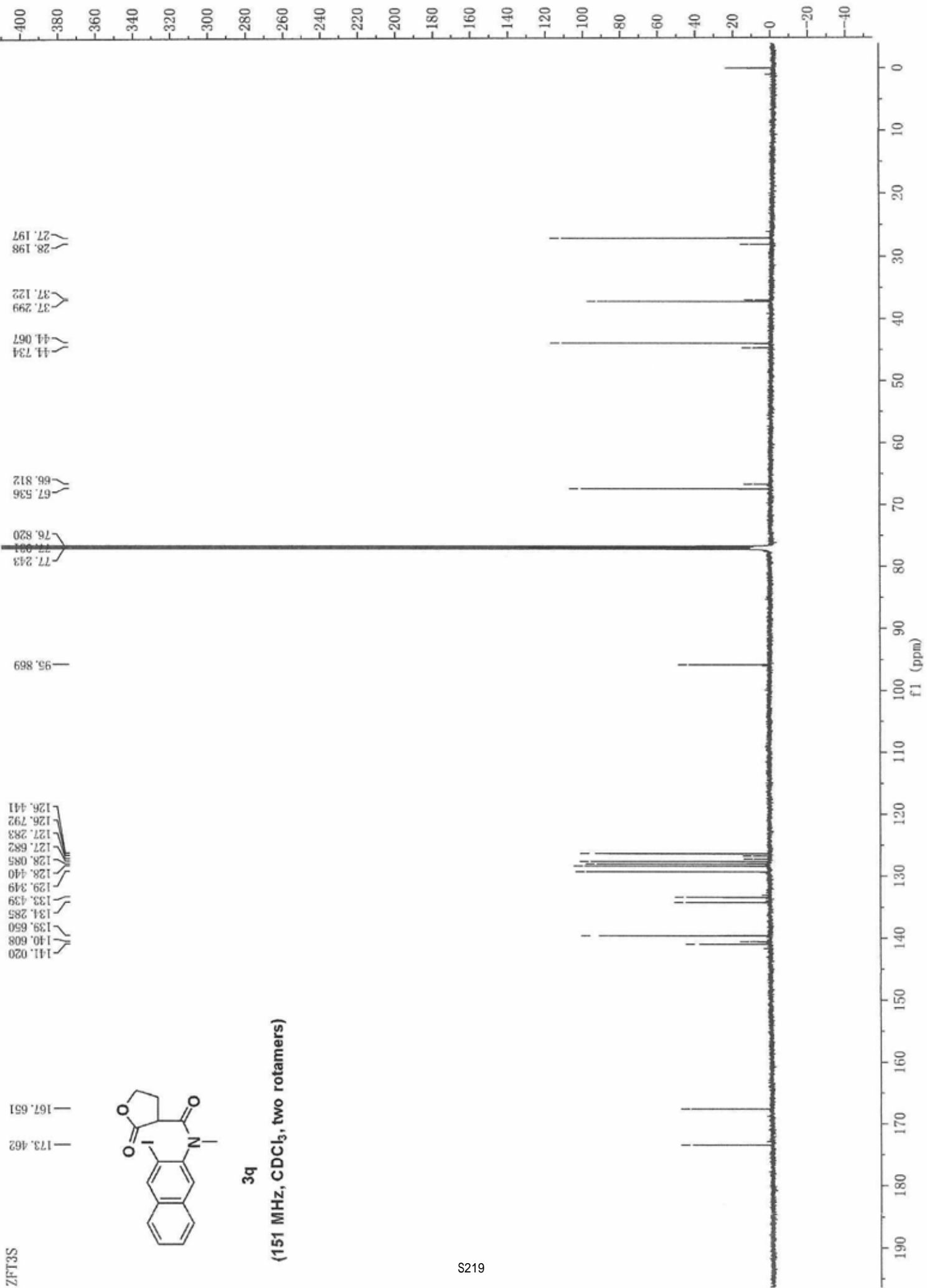


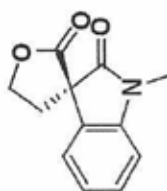




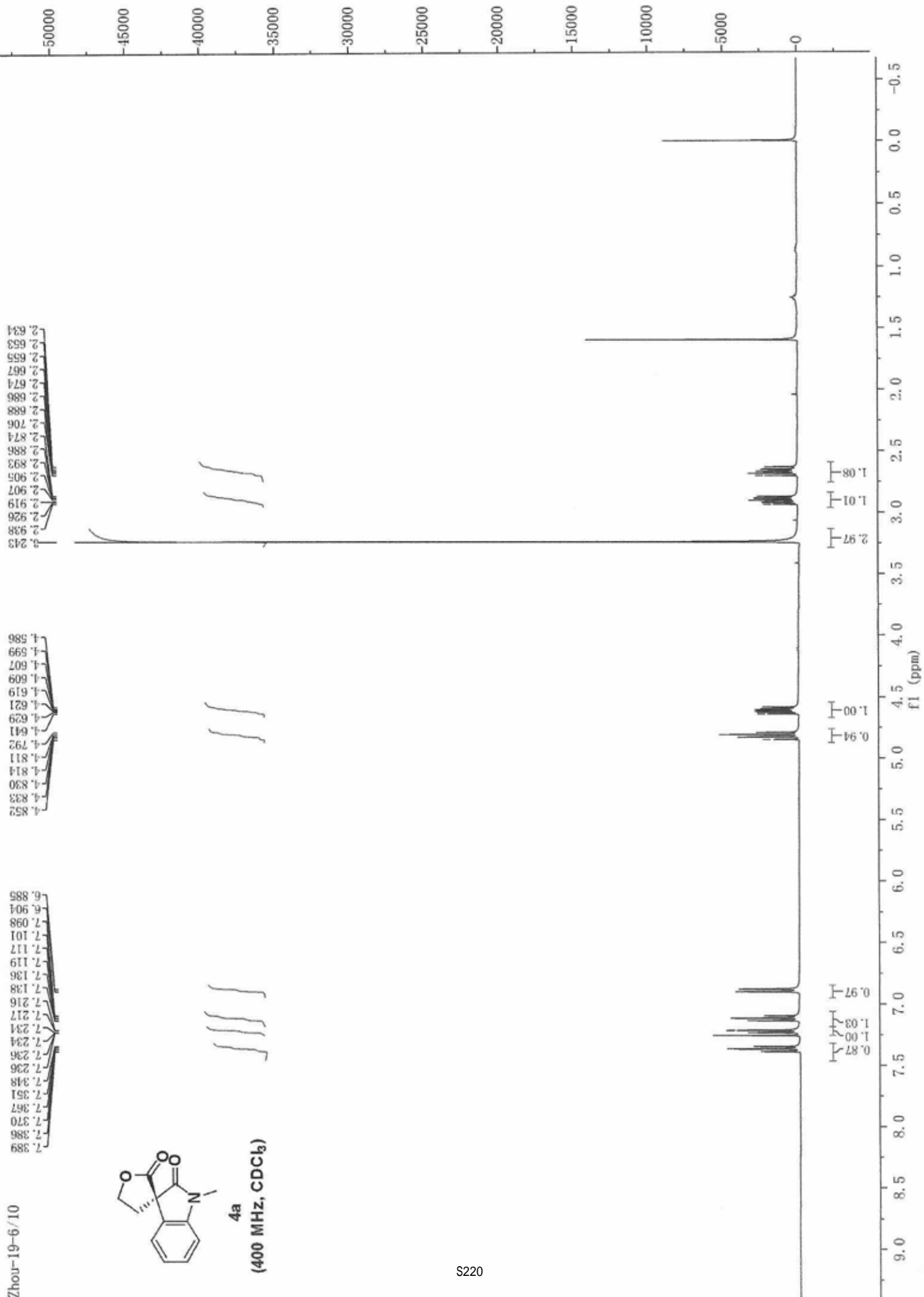
3q

(151 MHz, CDCl<sub>3</sub>, two rotamers)

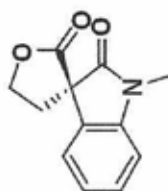




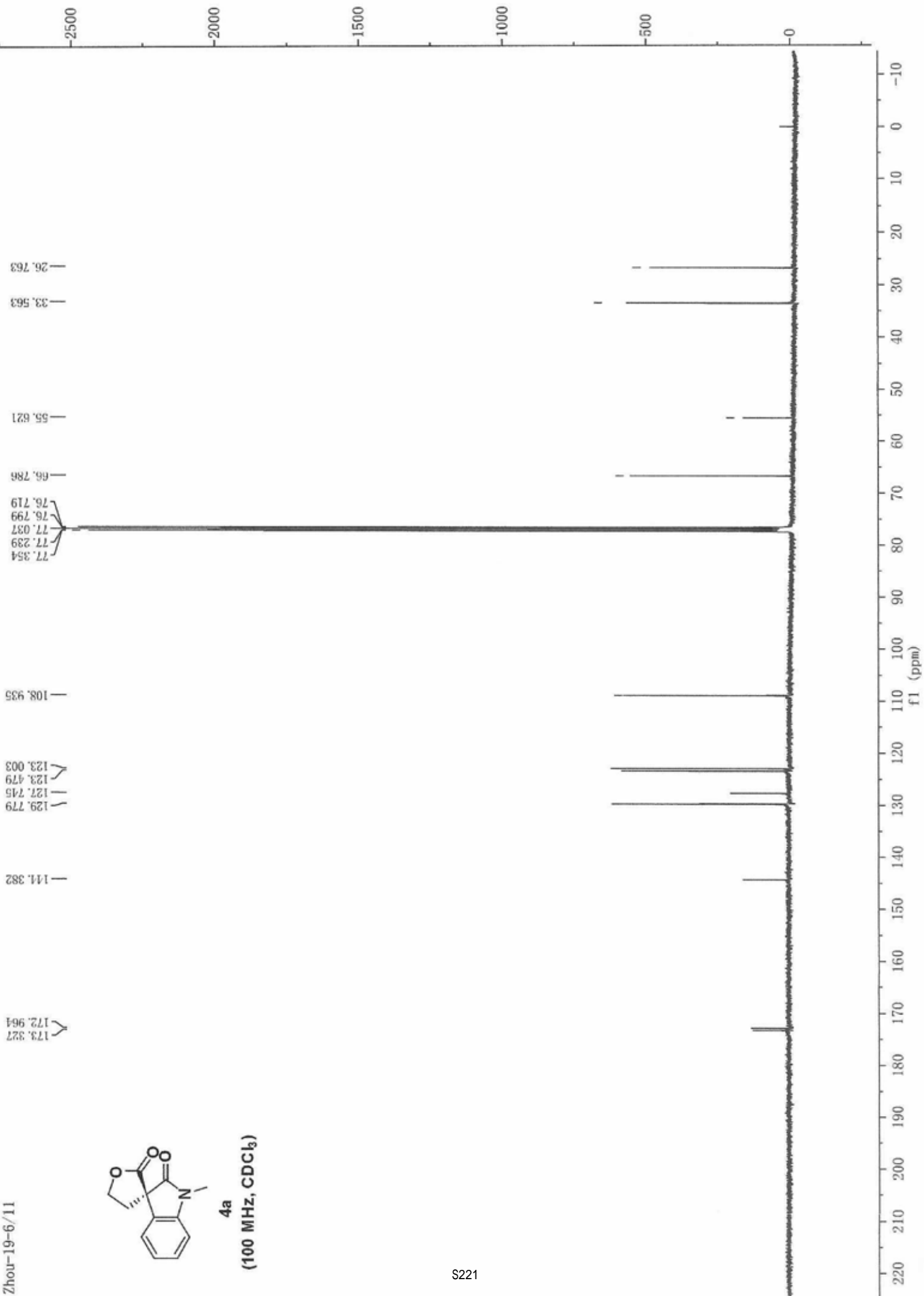
**4a**  
(400 MHz, CDCl<sub>3</sub>)

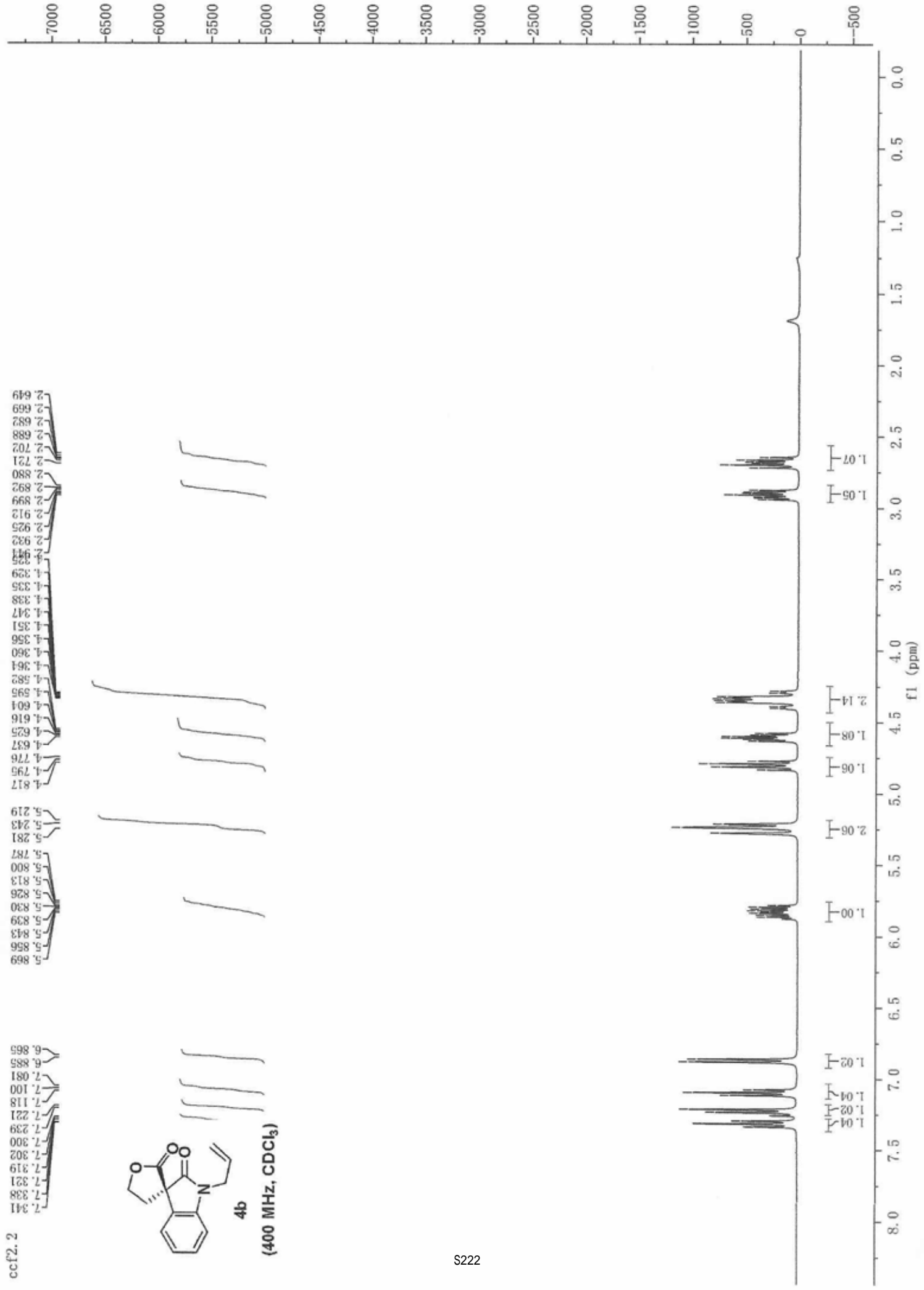


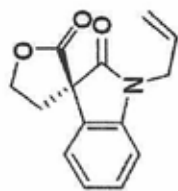
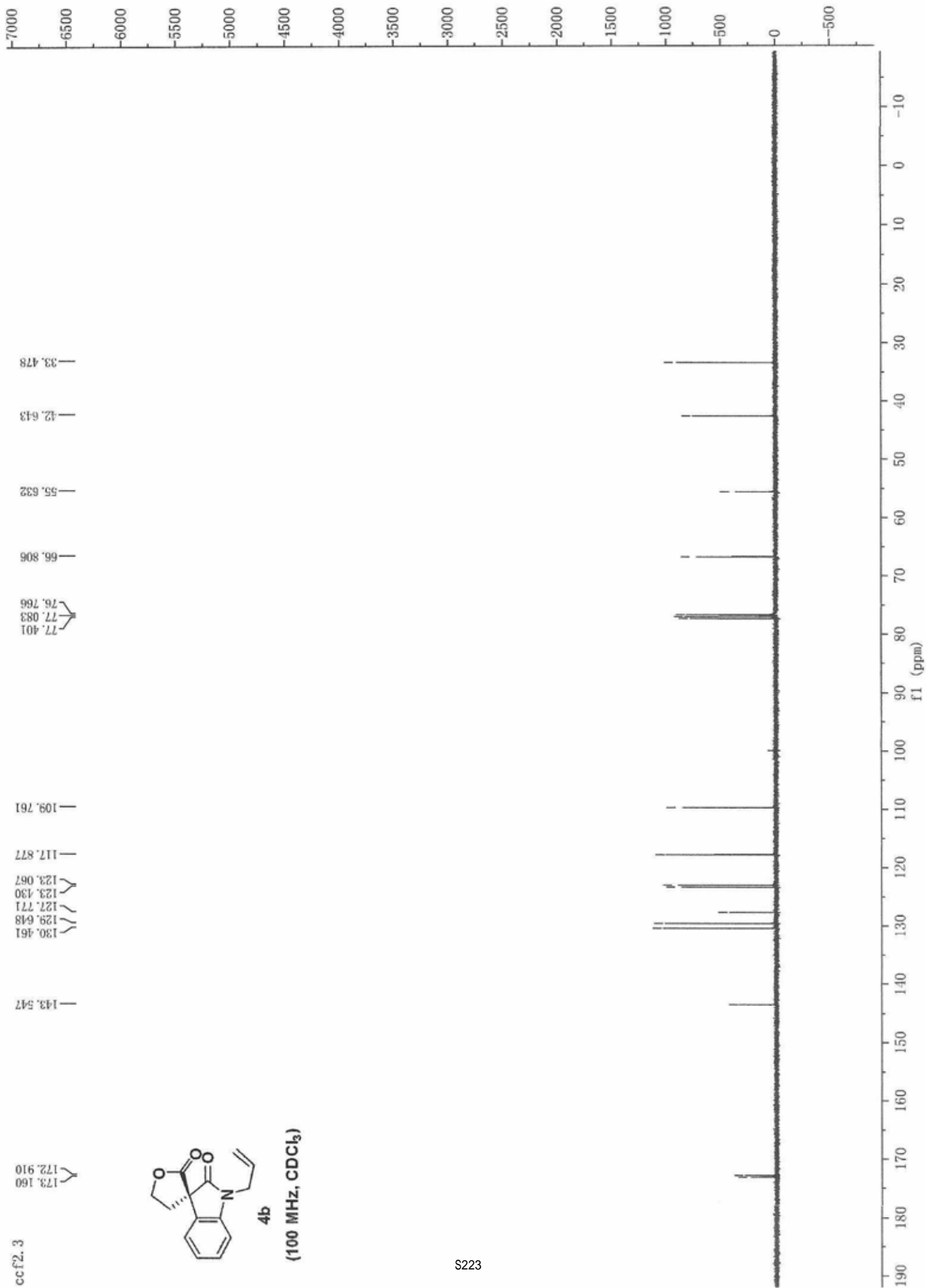




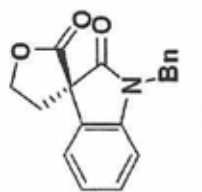
**4a**  
(100 MHz, CDCl<sub>3</sub>)



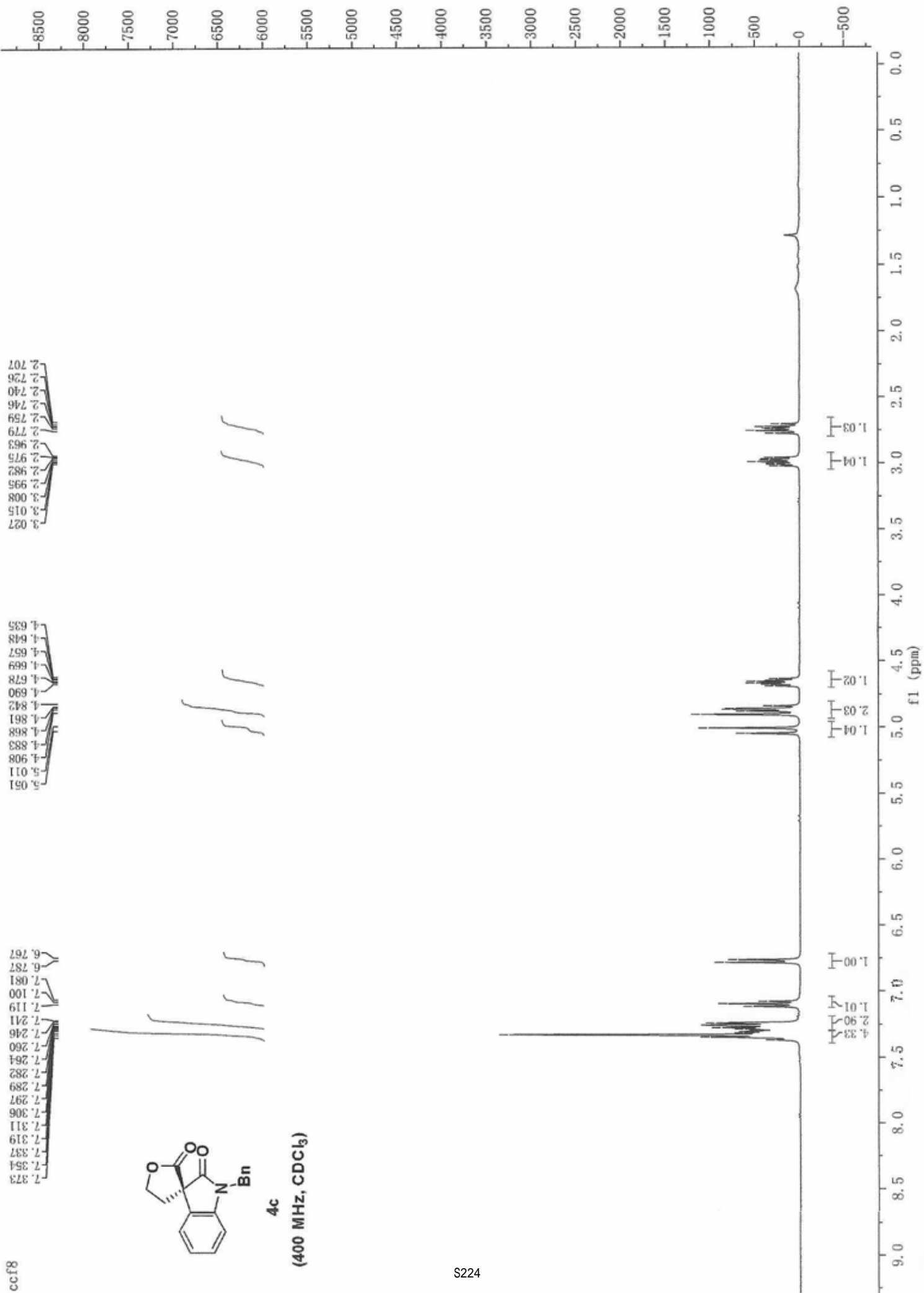




(100 MHz, CDCl<sub>3</sub>)



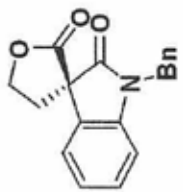
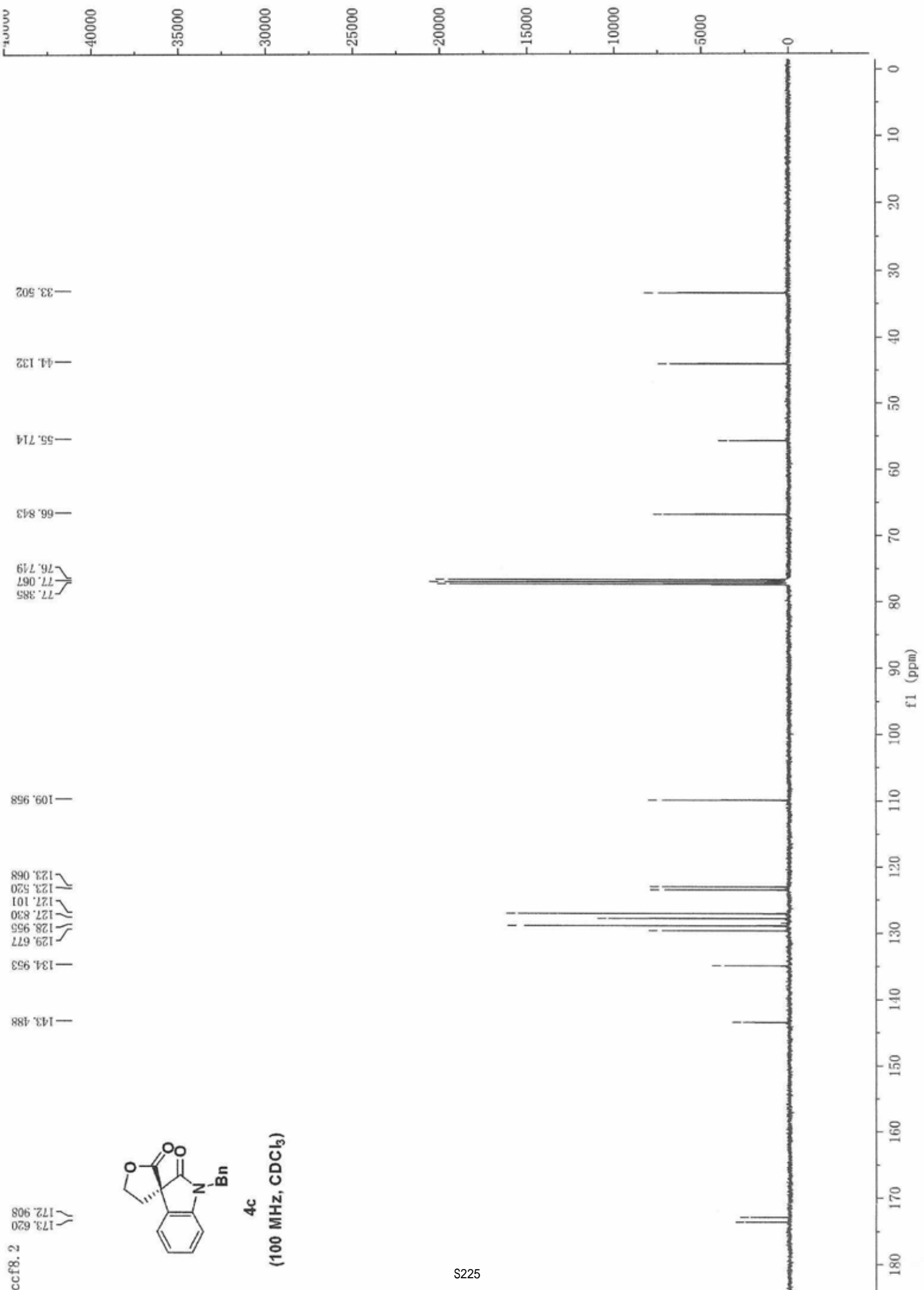
**4c**  
(400 MHz, CDCl<sub>3</sub>)



3.027  
3.015  
3.008  
2.995  
2.982  
2.975  
2.963  
2.799  
2.779  
2.759  
2.746  
2.740  
2.726  
2.707

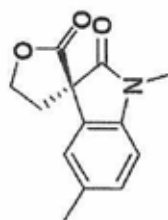
5.051  
5.011  
4.908  
4.883  
4.868  
4.861  
4.842  
4.690  
4.678  
4.669  
4.657  
4.648  
4.635

7.373  
7.354  
7.337  
7.319  
7.311  
7.306  
7.297  
7.289  
7.282  
7.264  
7.260  
7.246  
7.241  
7.119  
7.100  
7.081  
6.787  
6.767



**4c**  
(100 MHz, CDCl<sub>3</sub>)

ccf8. 2  
173.620  
172.908



**4d**  
(400 MHz, CDCl<sub>3</sub>)

3.225  
2.881  
2.871  
2.861  
2.852  
2.673  
2.653  
2.633  
2.624  
2.397

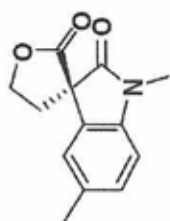
4.837  
4.818  
4.815  
4.796  
4.777  
4.624  
4.611  
4.603  
4.590  
4.581  
4.569

7.108  
7.089  
6.933  
6.914  
6.716

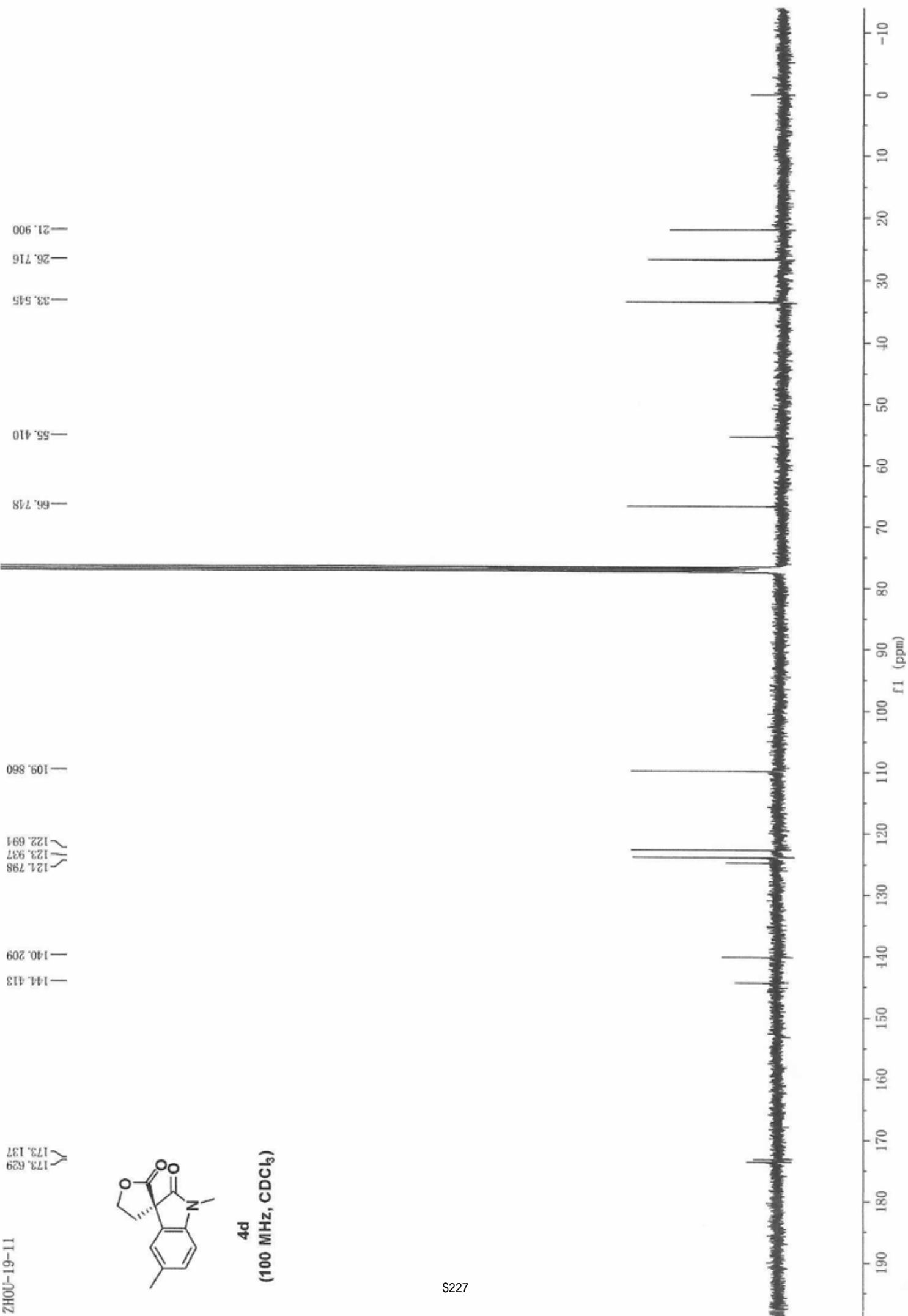
1.00  
1.01  
1.03  
3.12  
1.05  
1.12  
3.13  
1.06  
1.06  
1.00  
1.01  
1.03

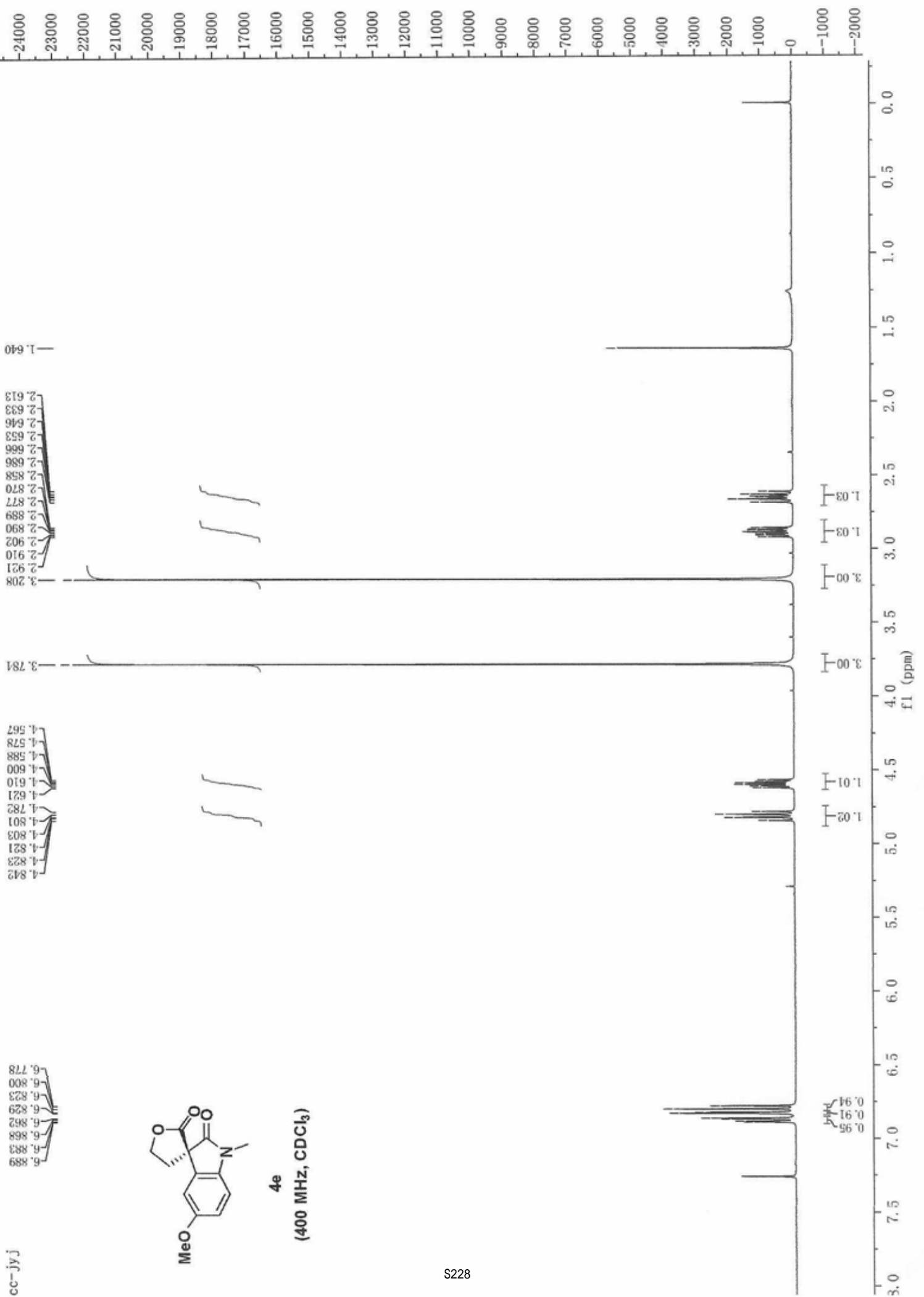
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

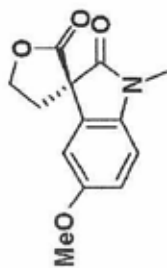


**4d**  
(100 MHz, CDCl<sub>3</sub>)

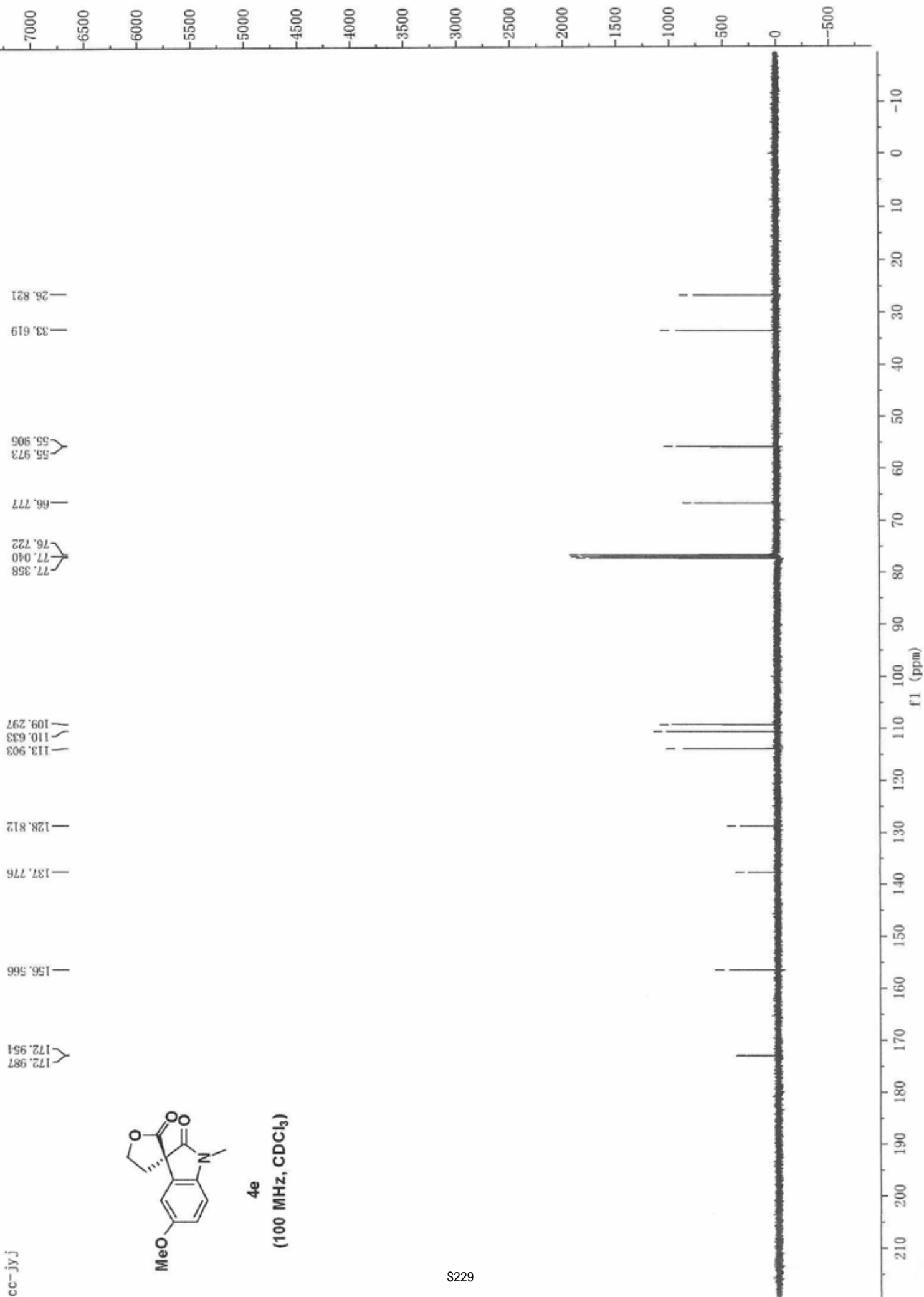


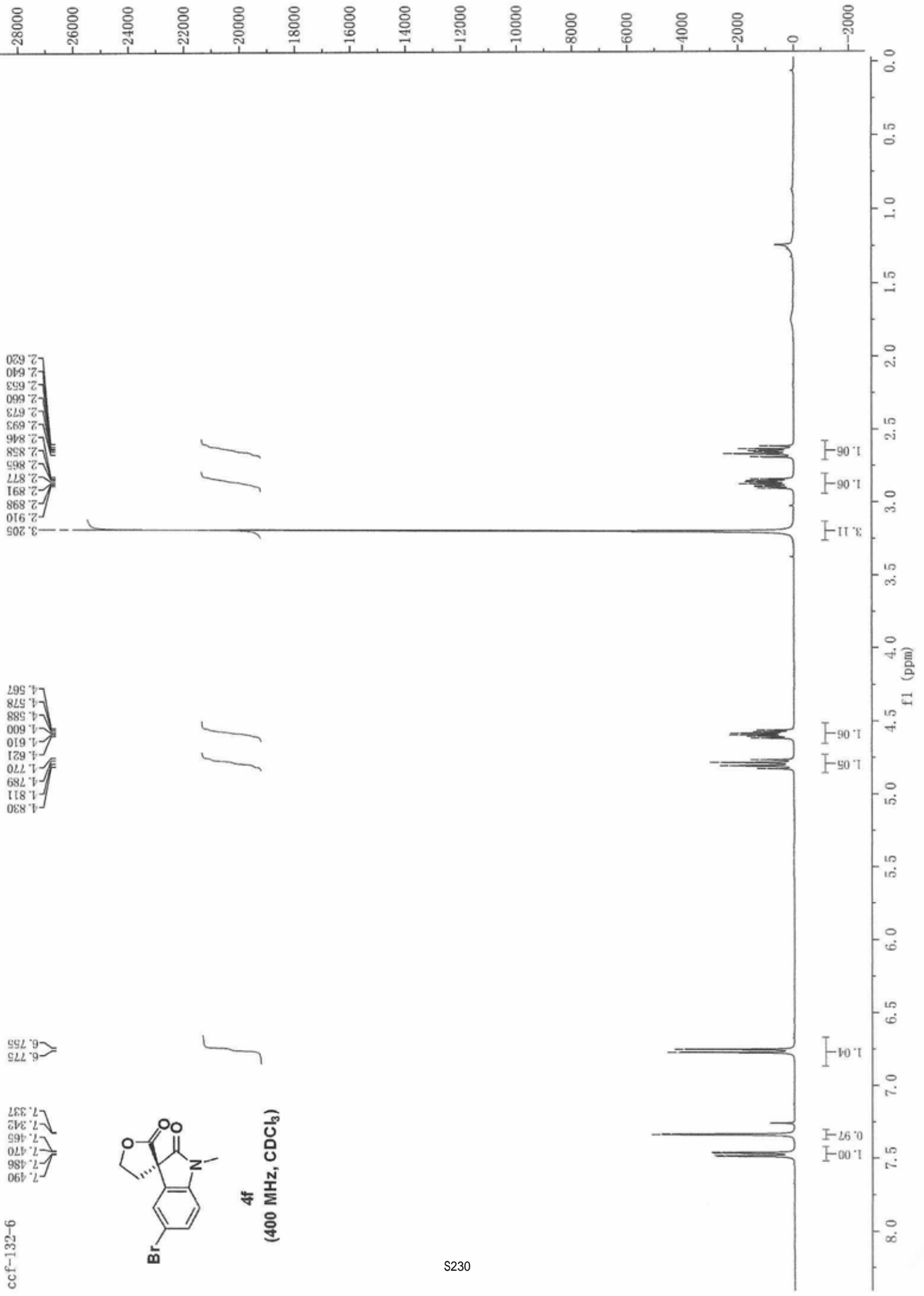


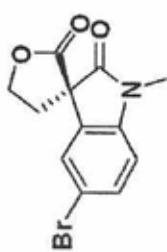




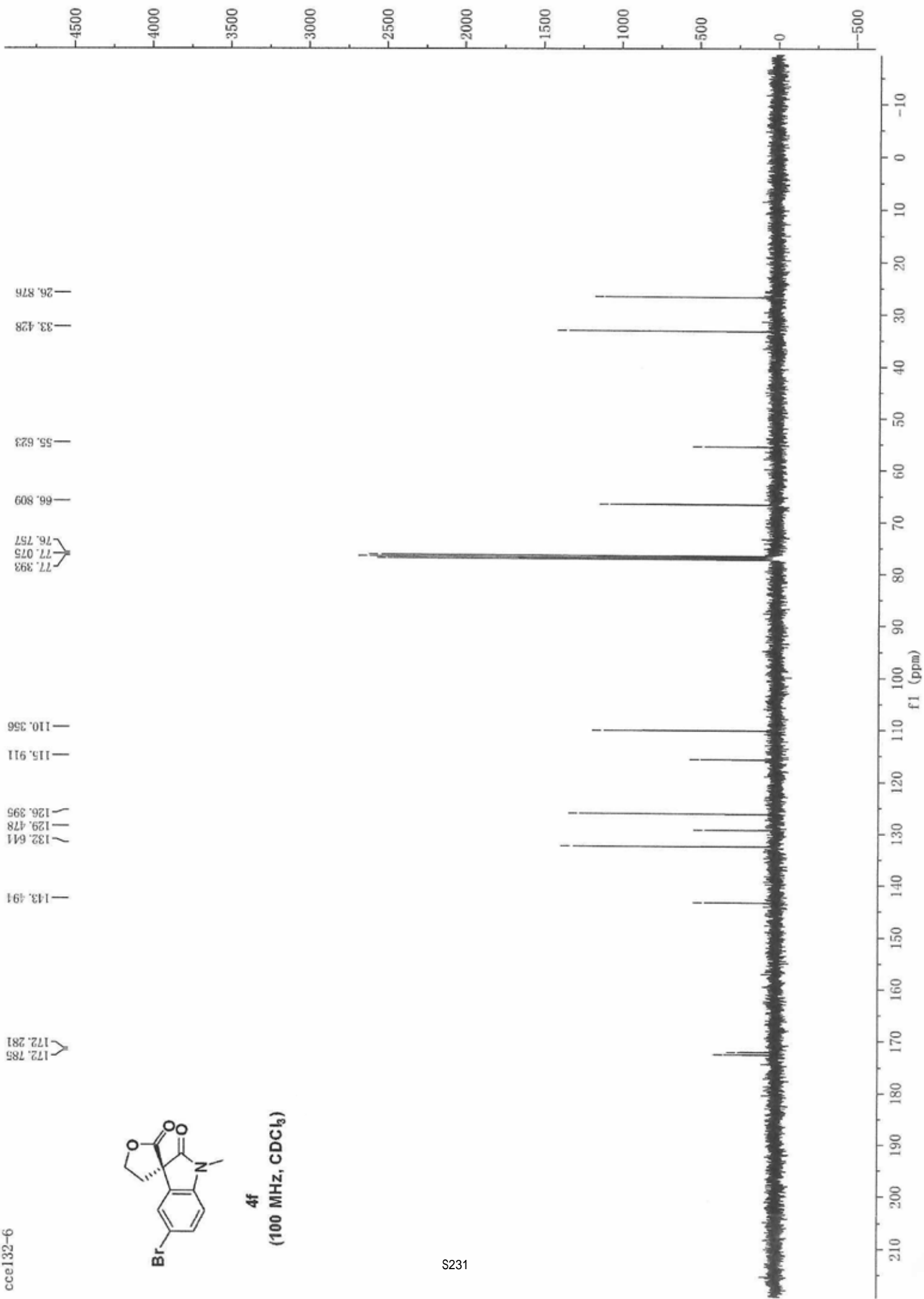
4e  
(100 MHz, CDCl<sub>3</sub>)

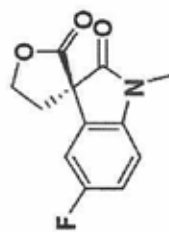




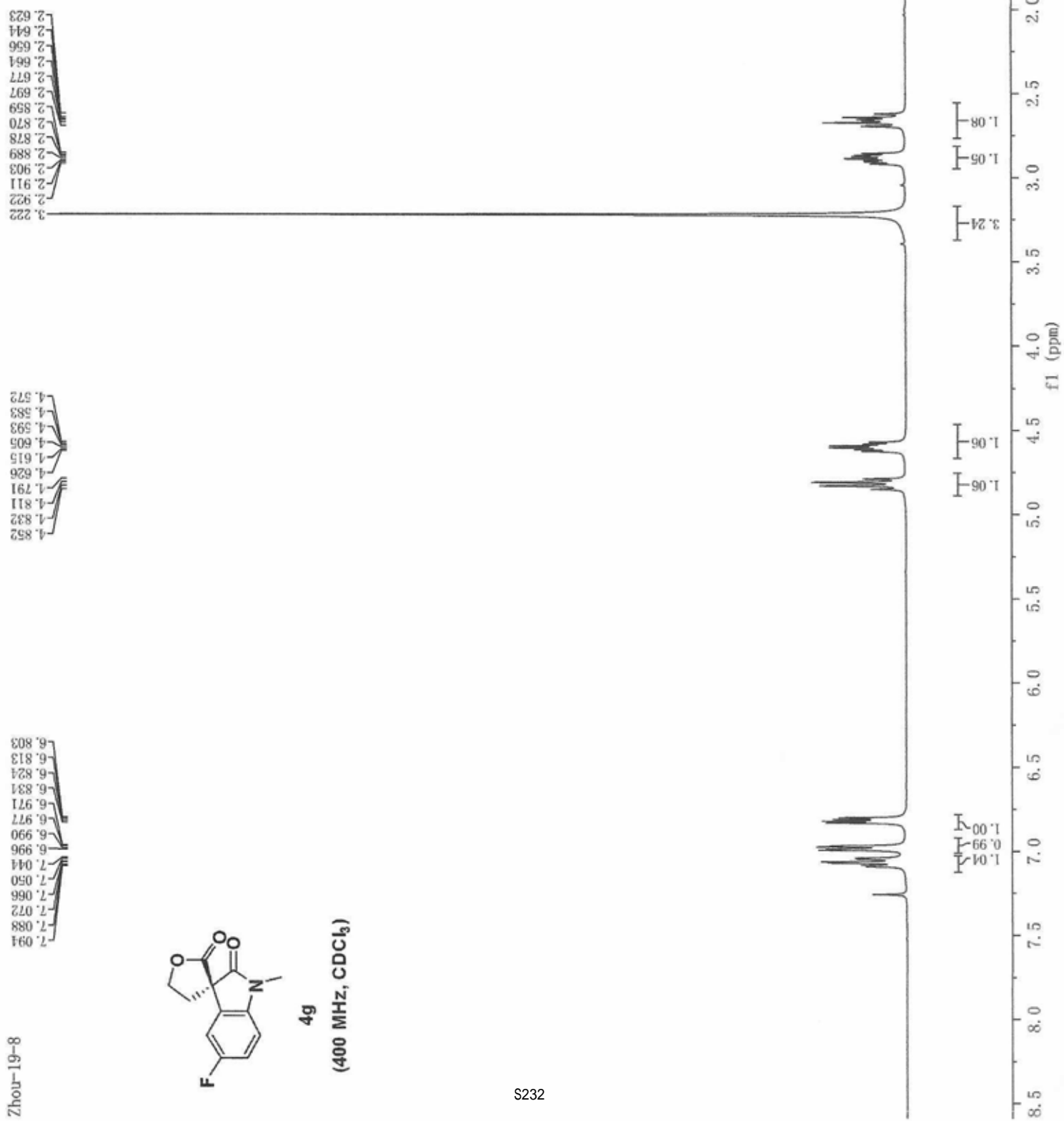


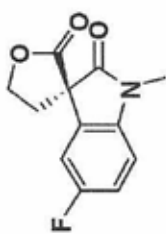
**4f**  
(100 MHz, CDCl<sub>3</sub>)



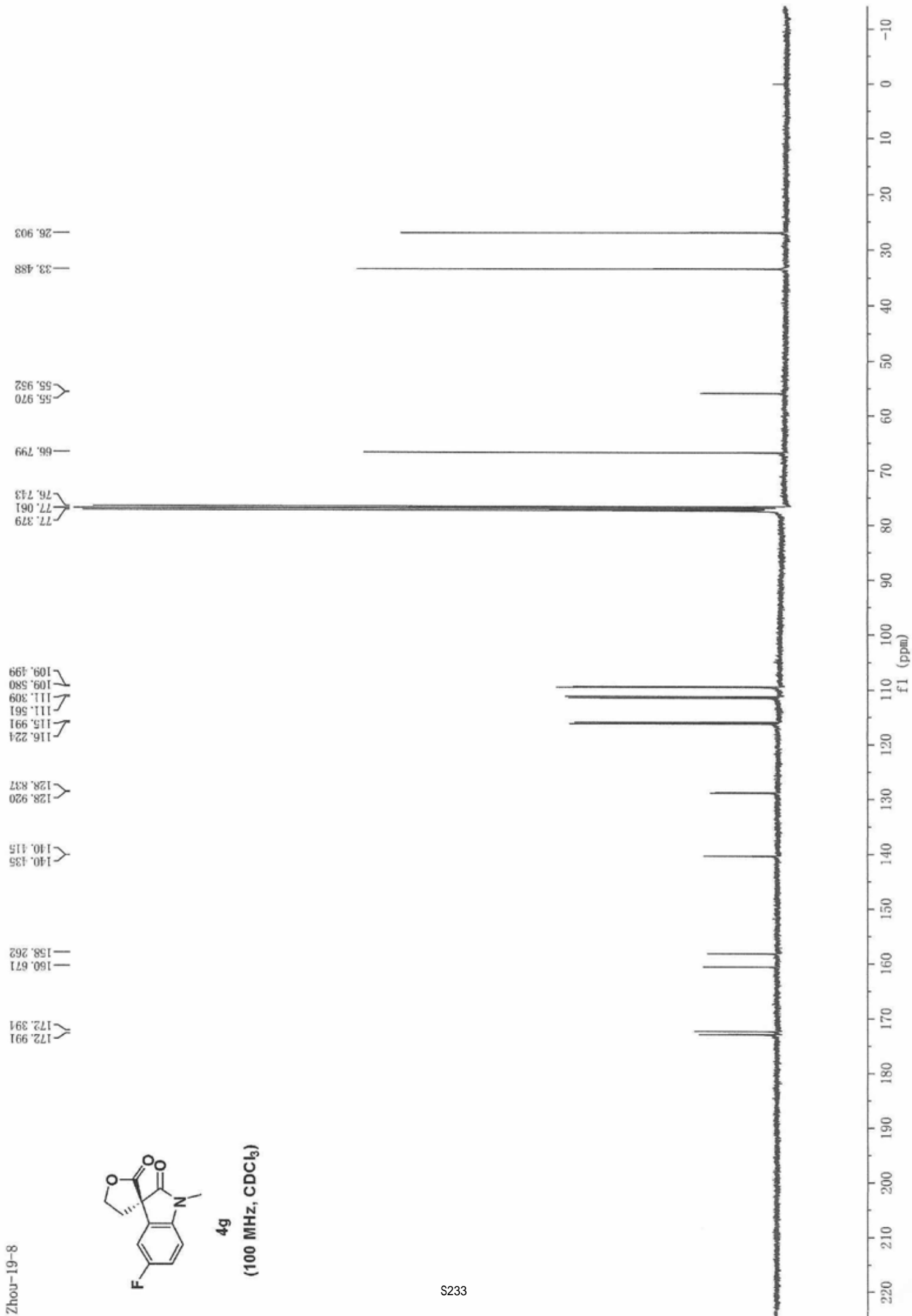


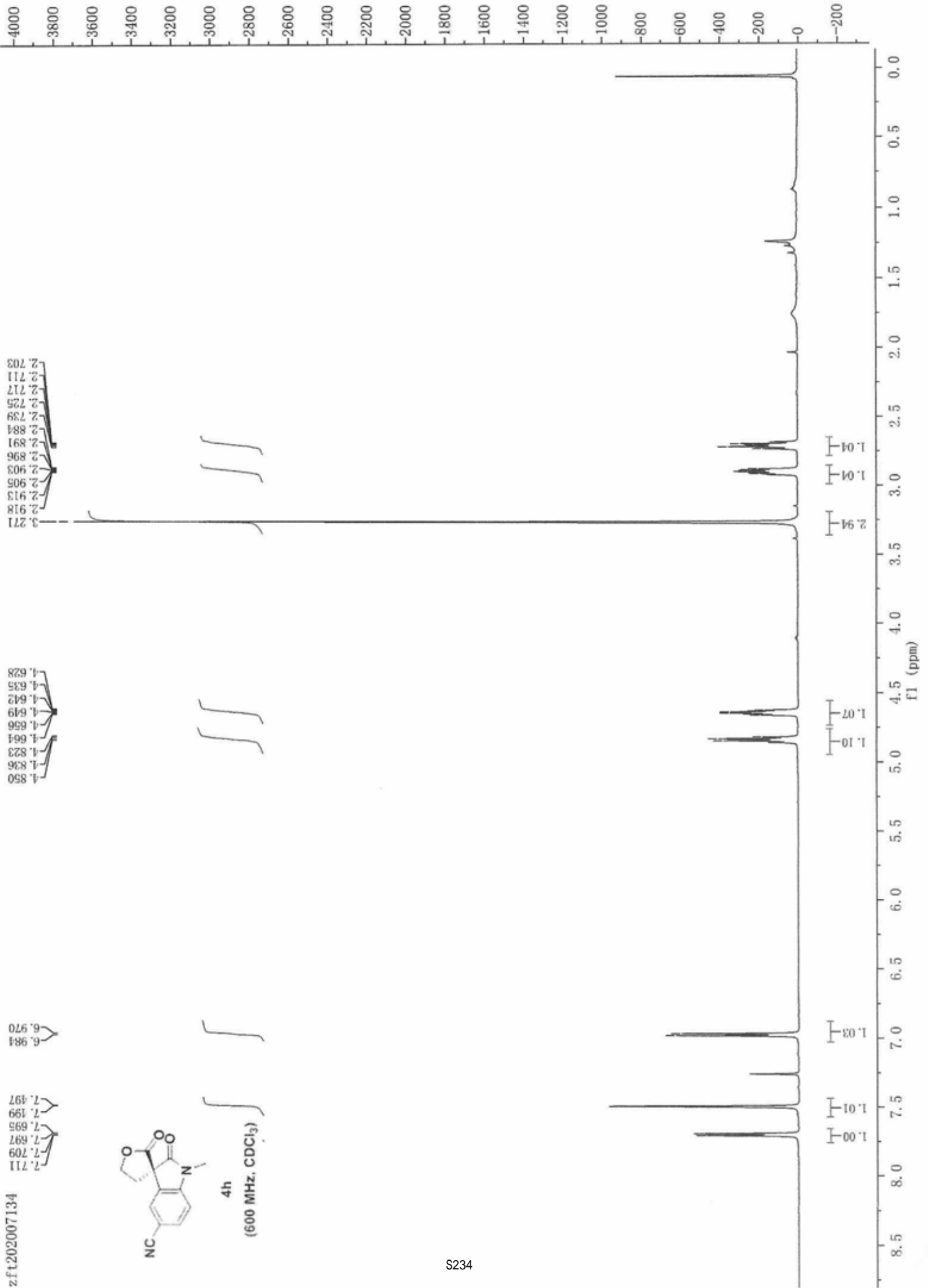
4g

(400 MHz, CDCl<sub>3</sub>)

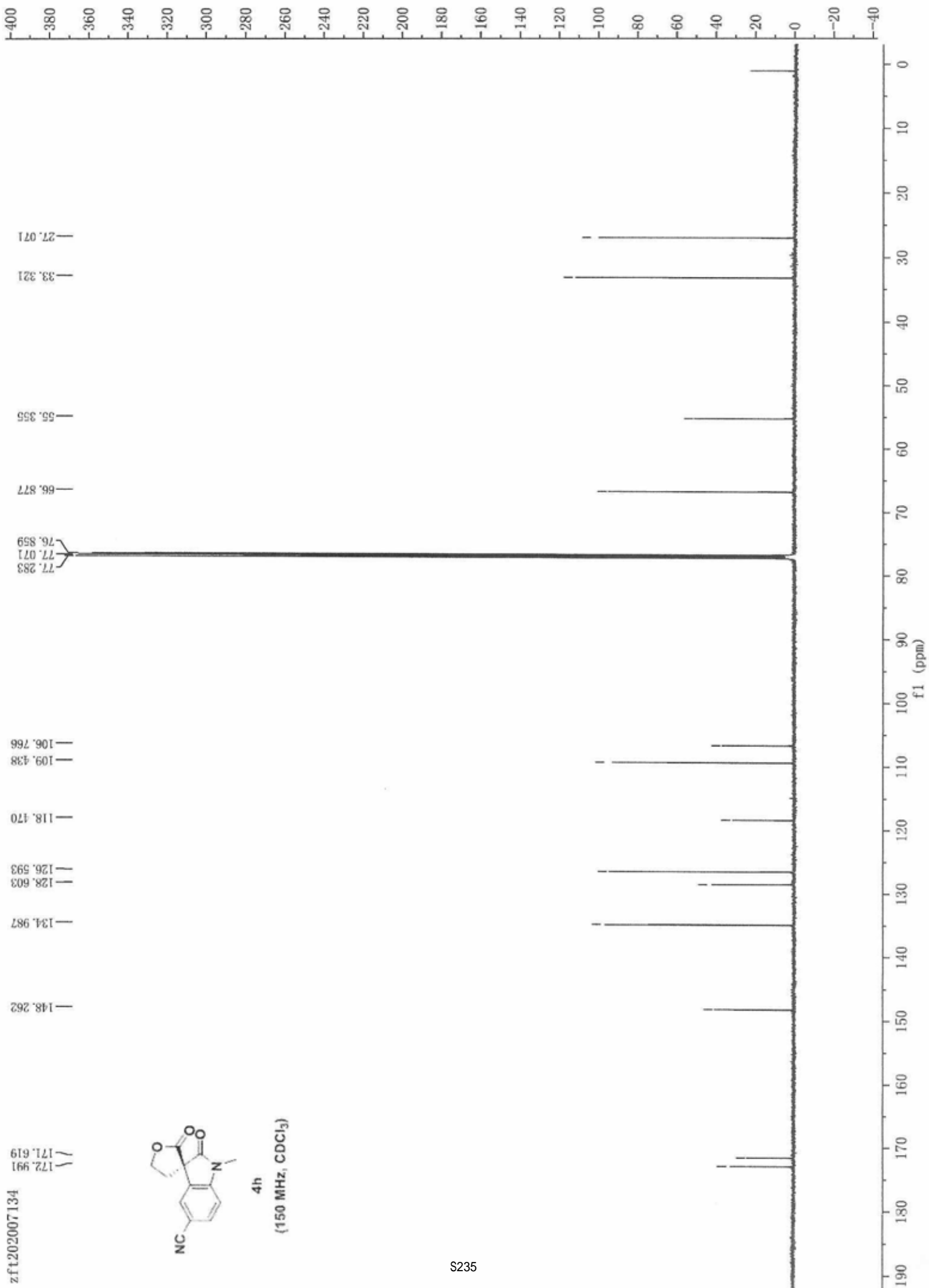


4g  
(100 MHz, CDCl<sub>3</sub>)



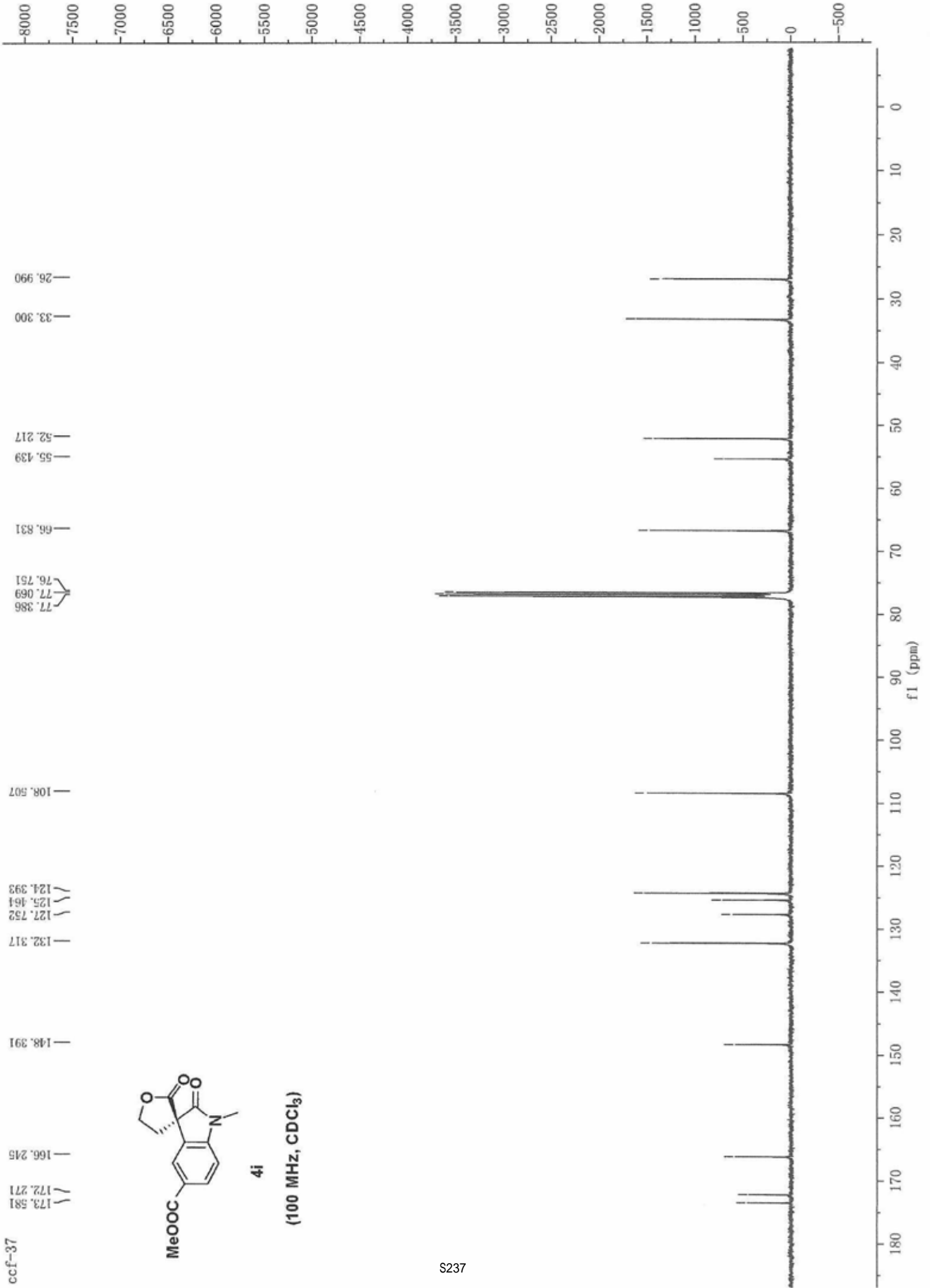


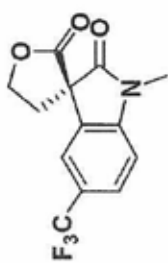
zft202007134





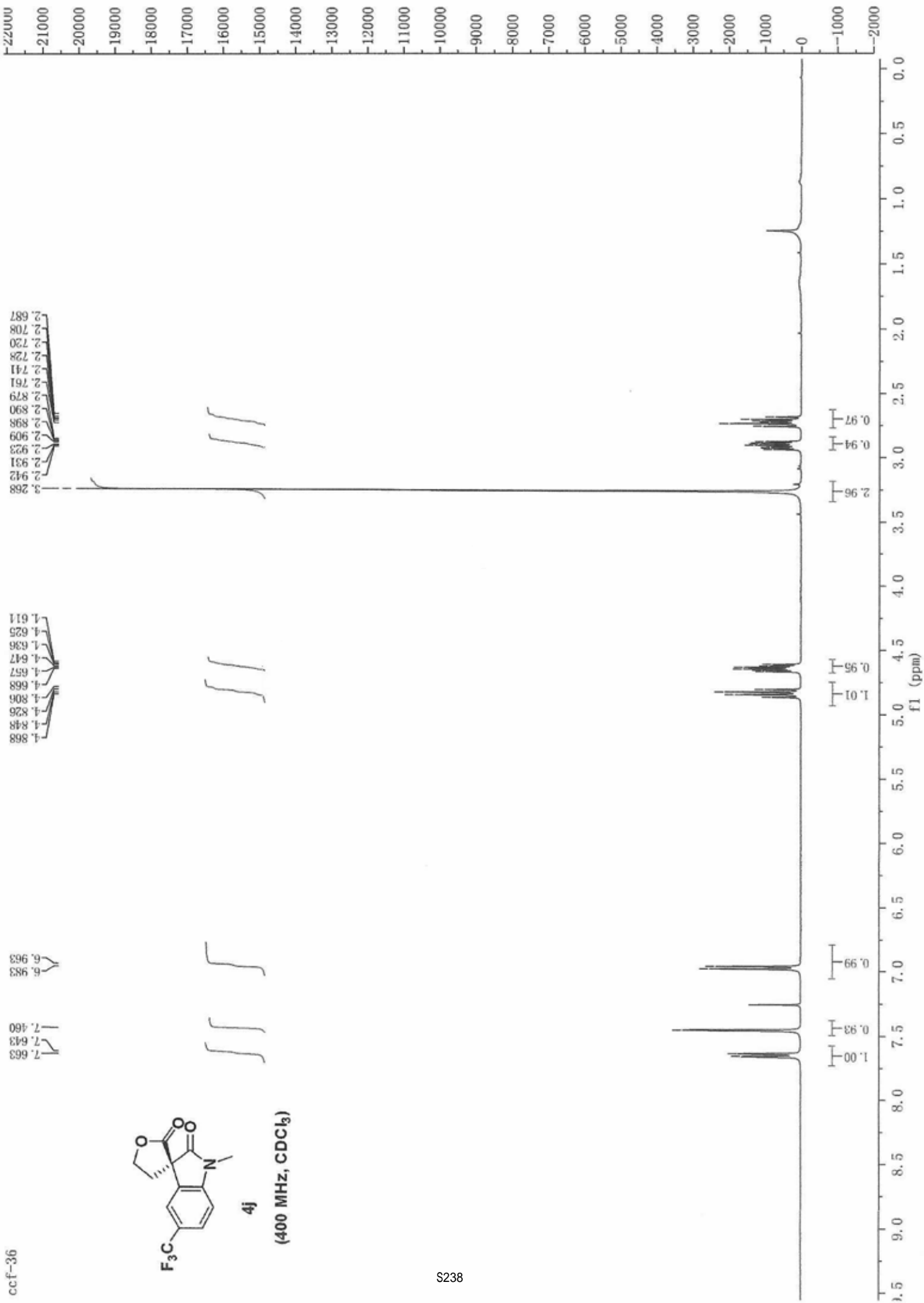


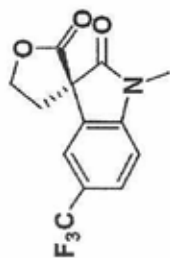




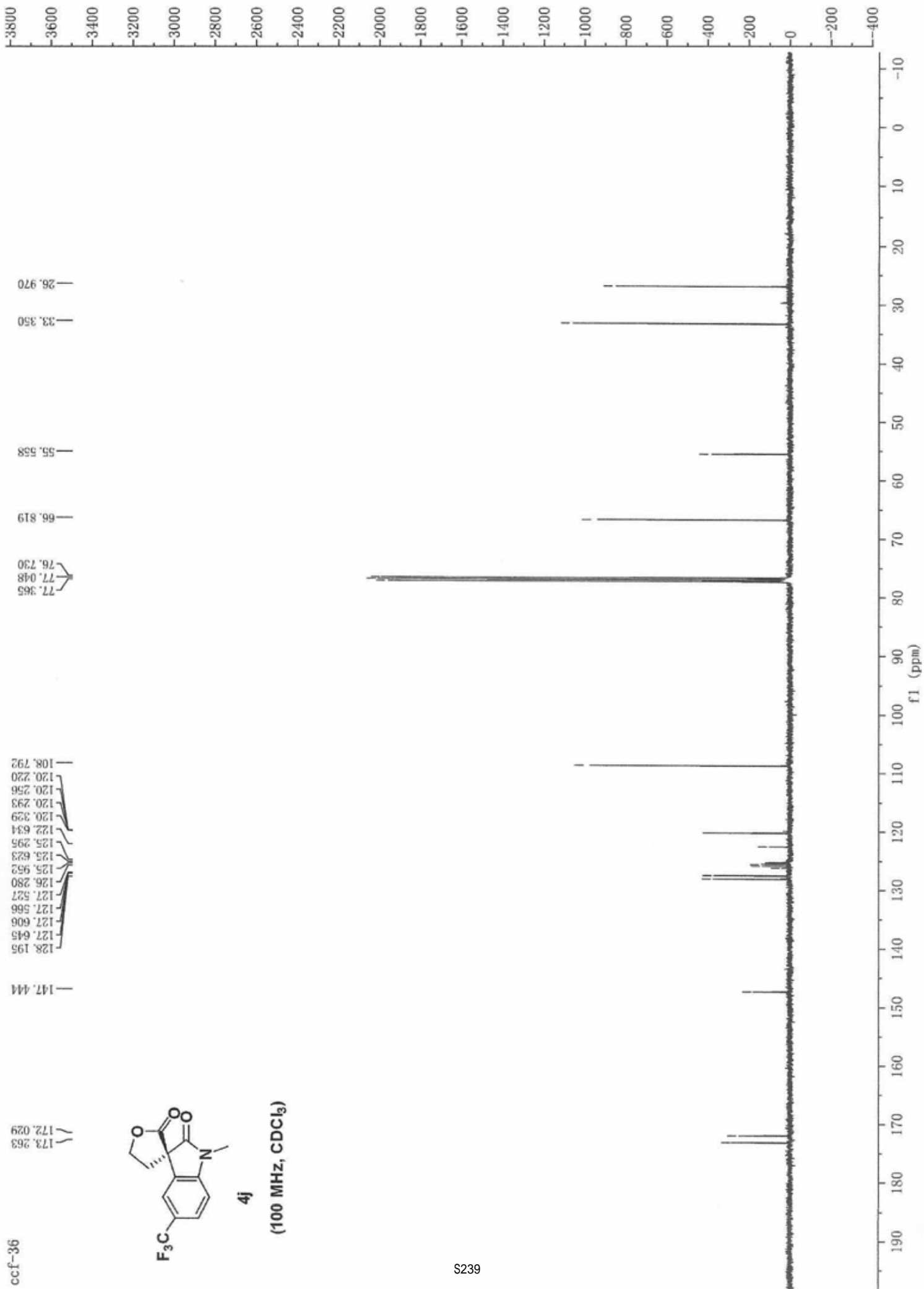
4j

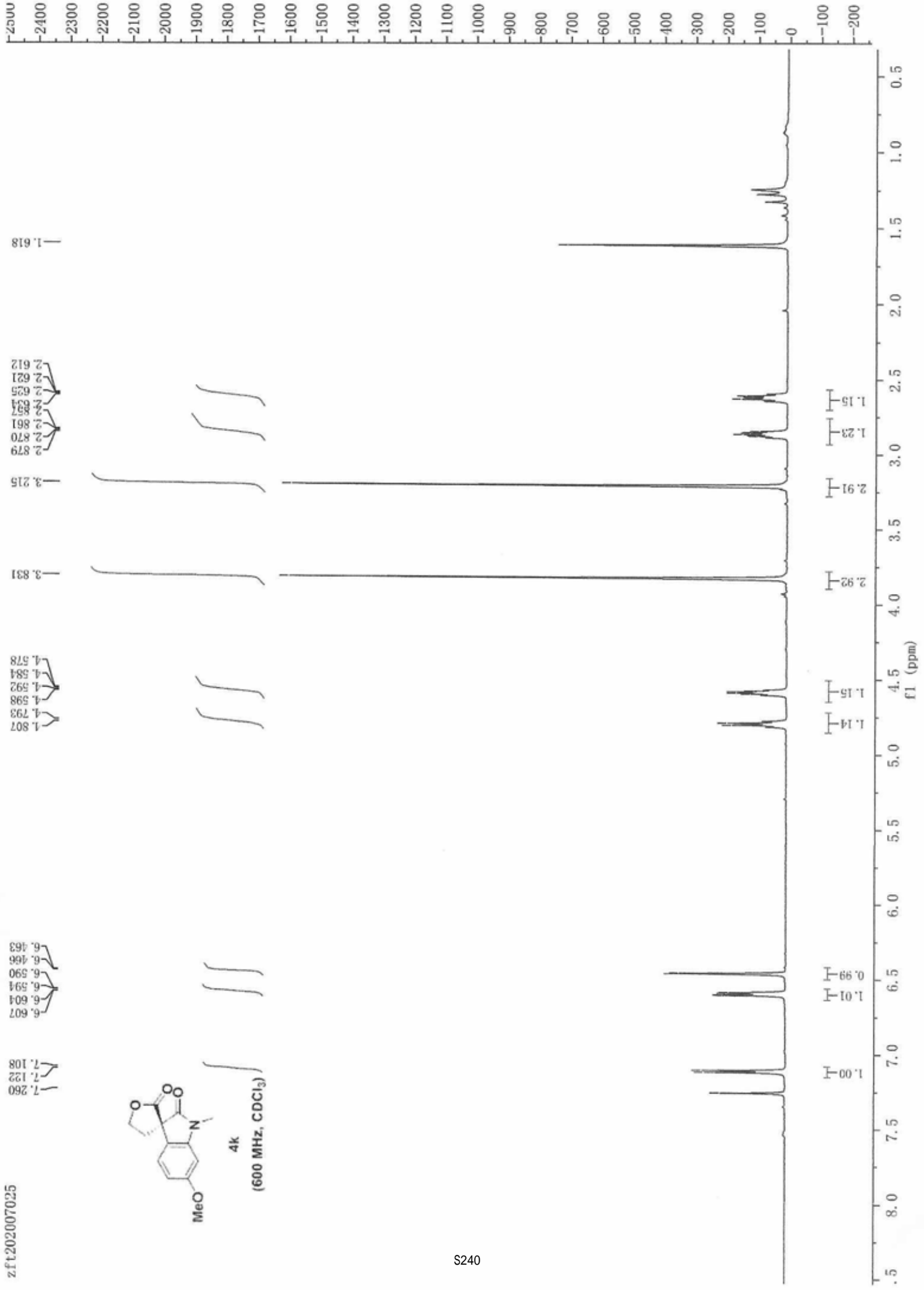
(400 MHz, CDCl<sub>3</sub>)

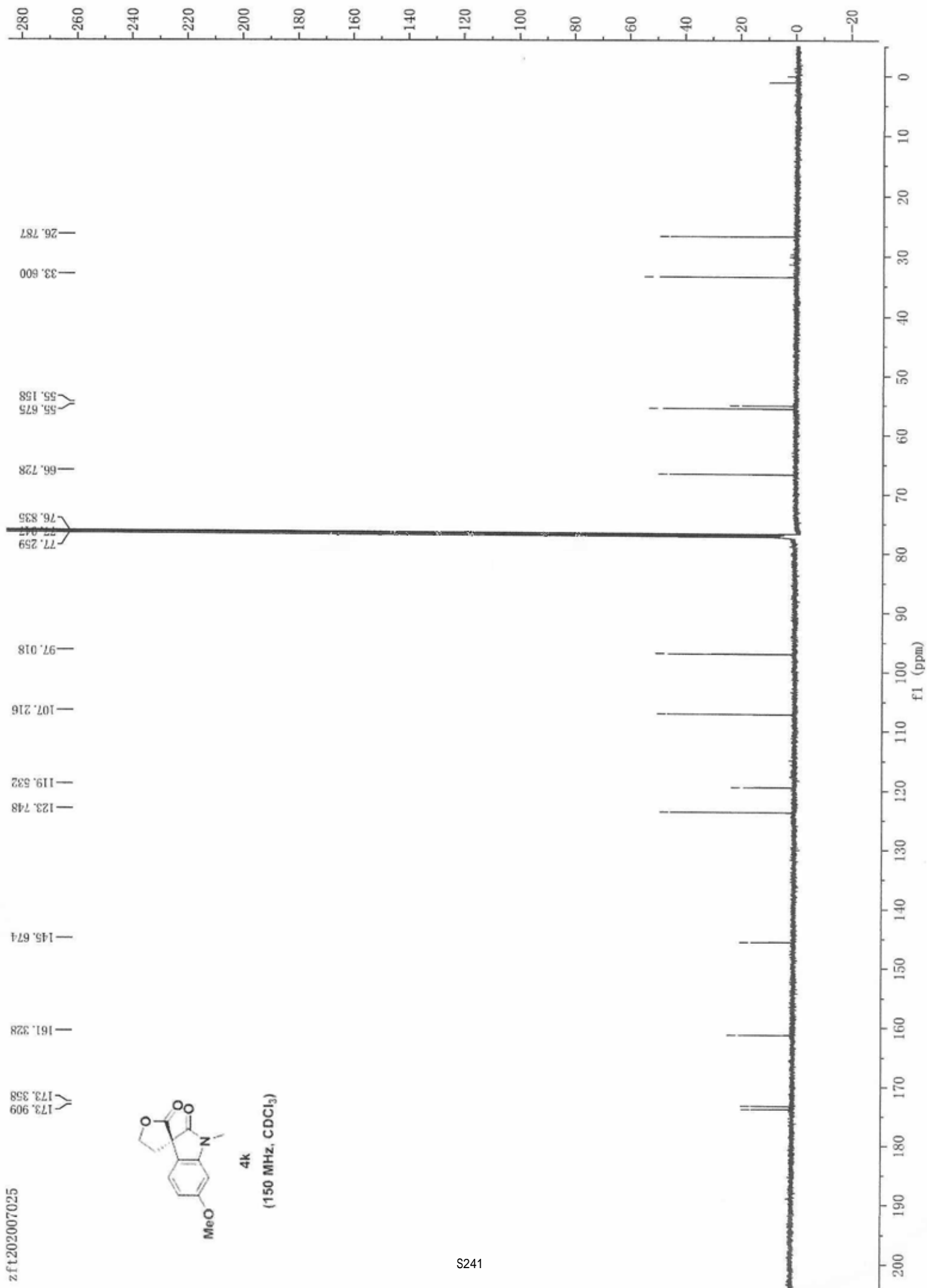




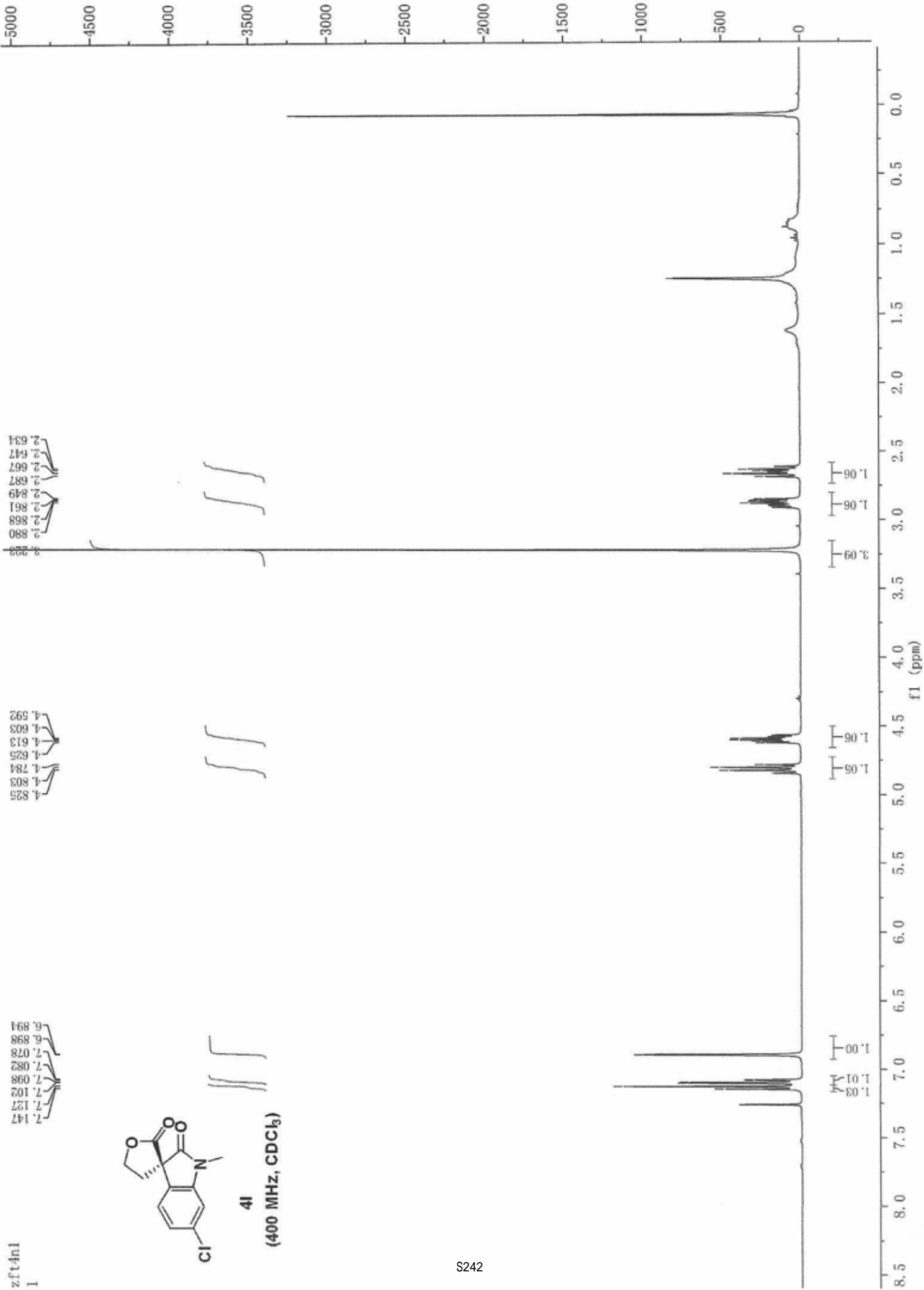
4j

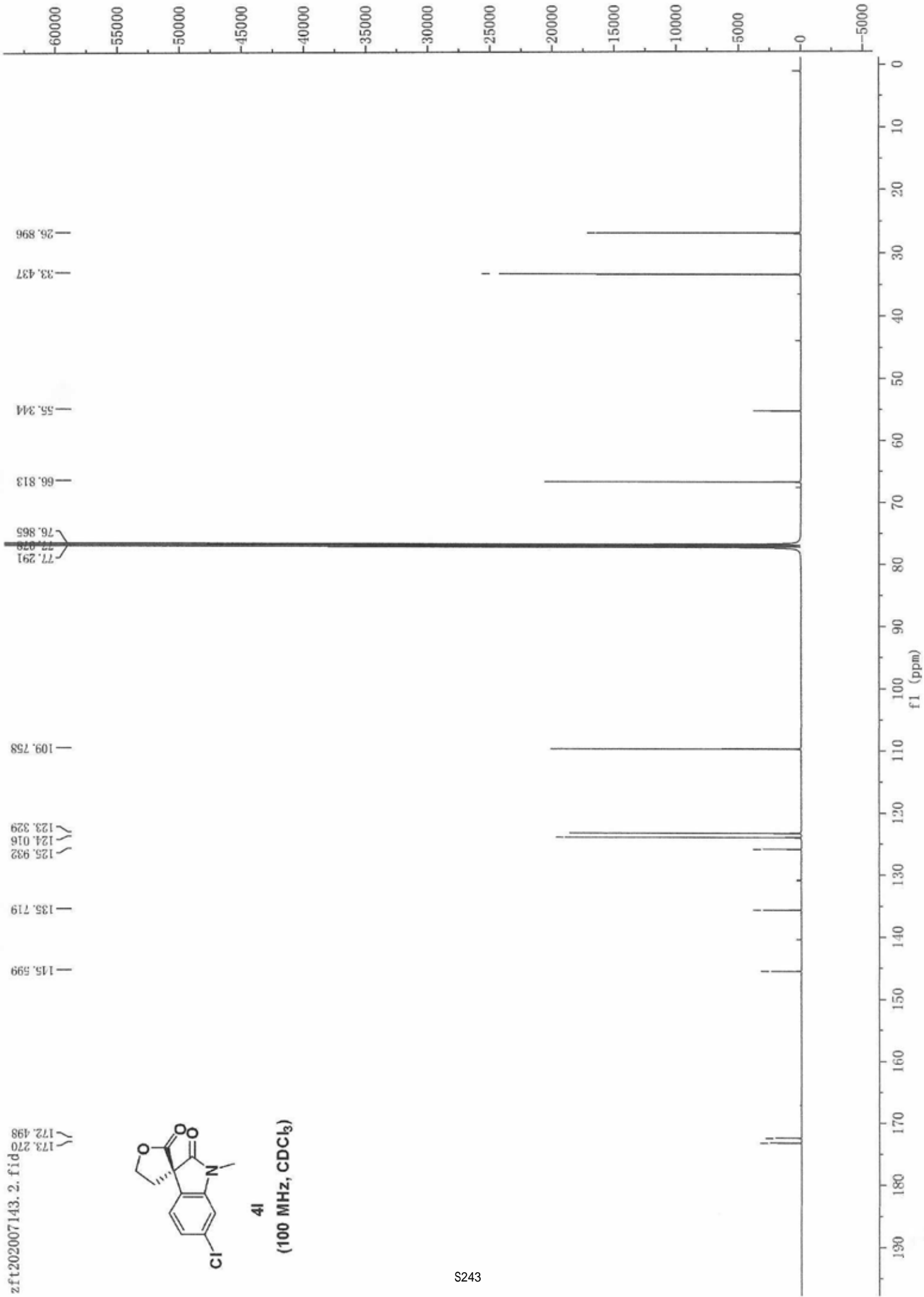
(100 MHz,  $CDCl_3$ )

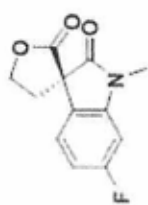




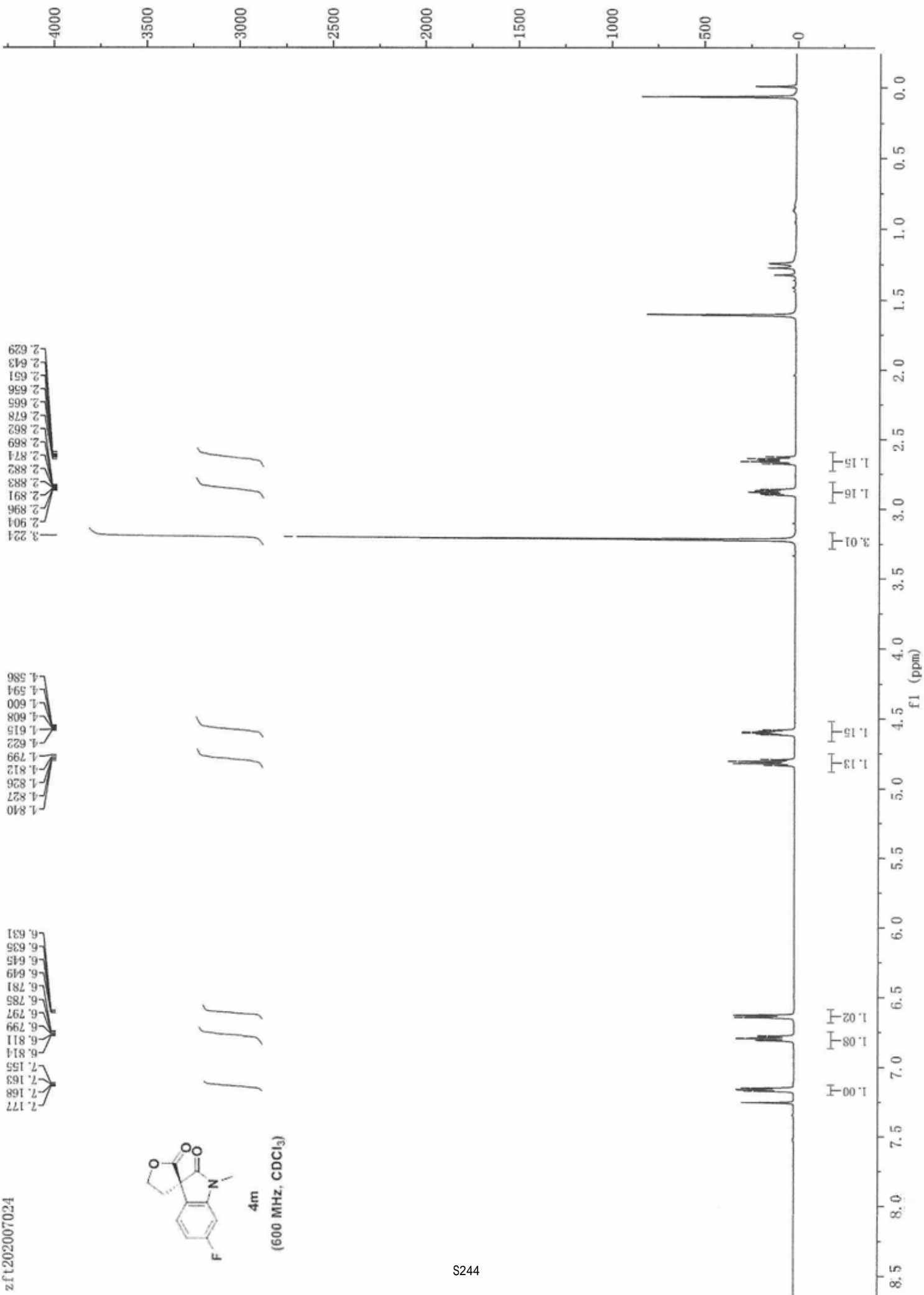
zft202007025



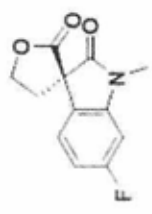
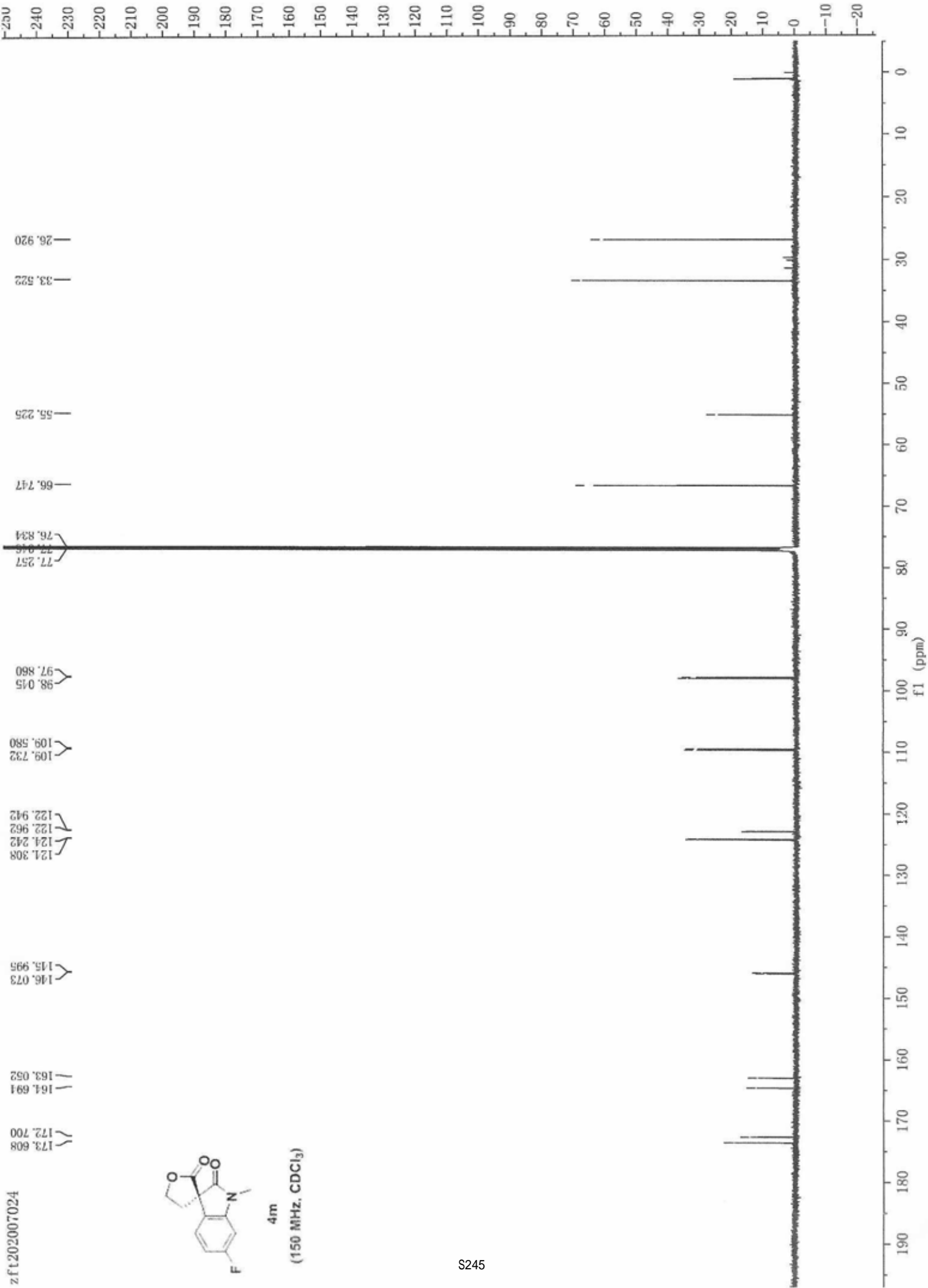




4m  
(600 MHz, CDCl<sub>3</sub>)

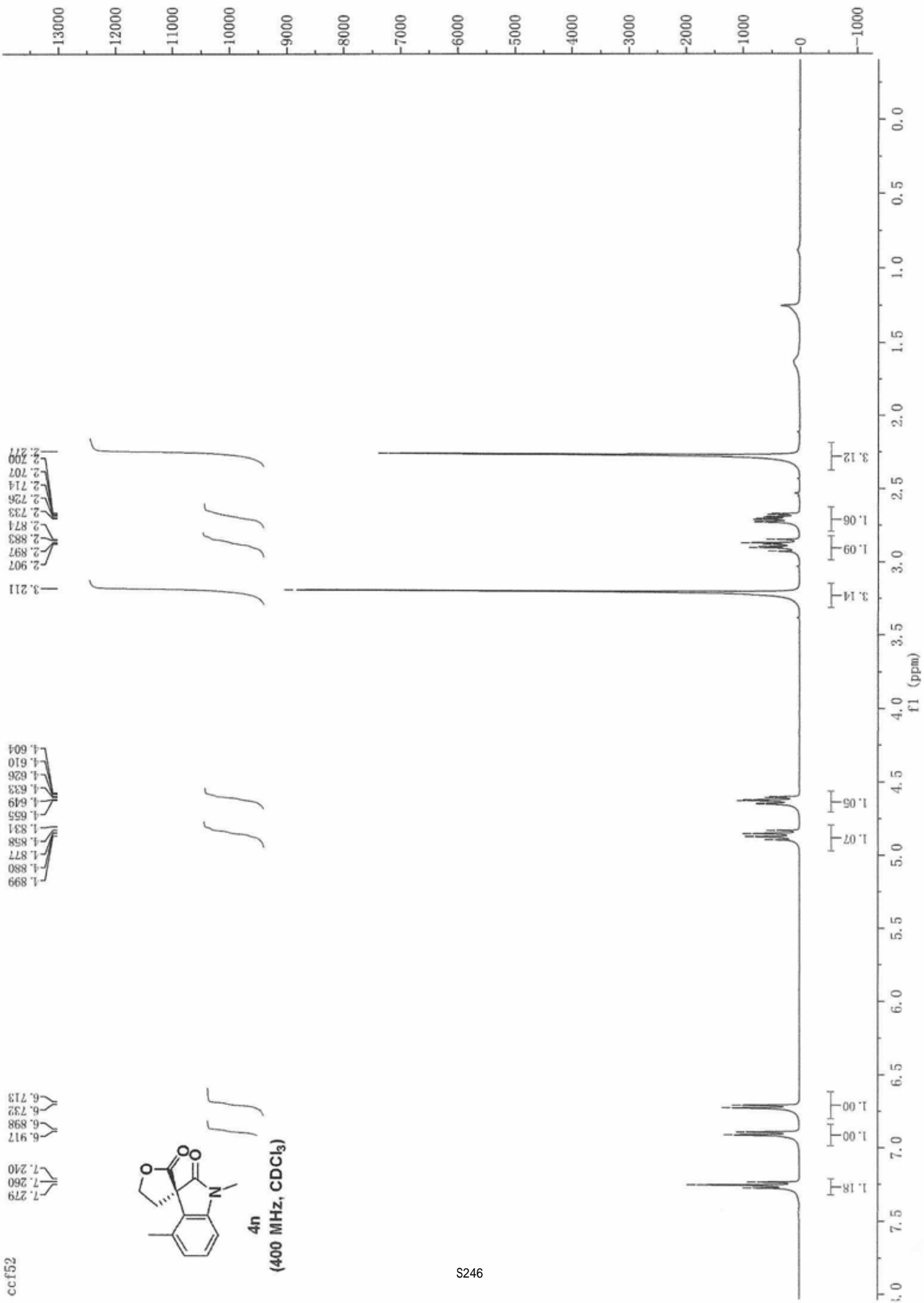




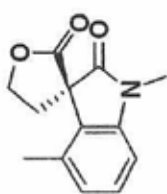


4m  
(150 MHz, CDCl<sub>3</sub>)

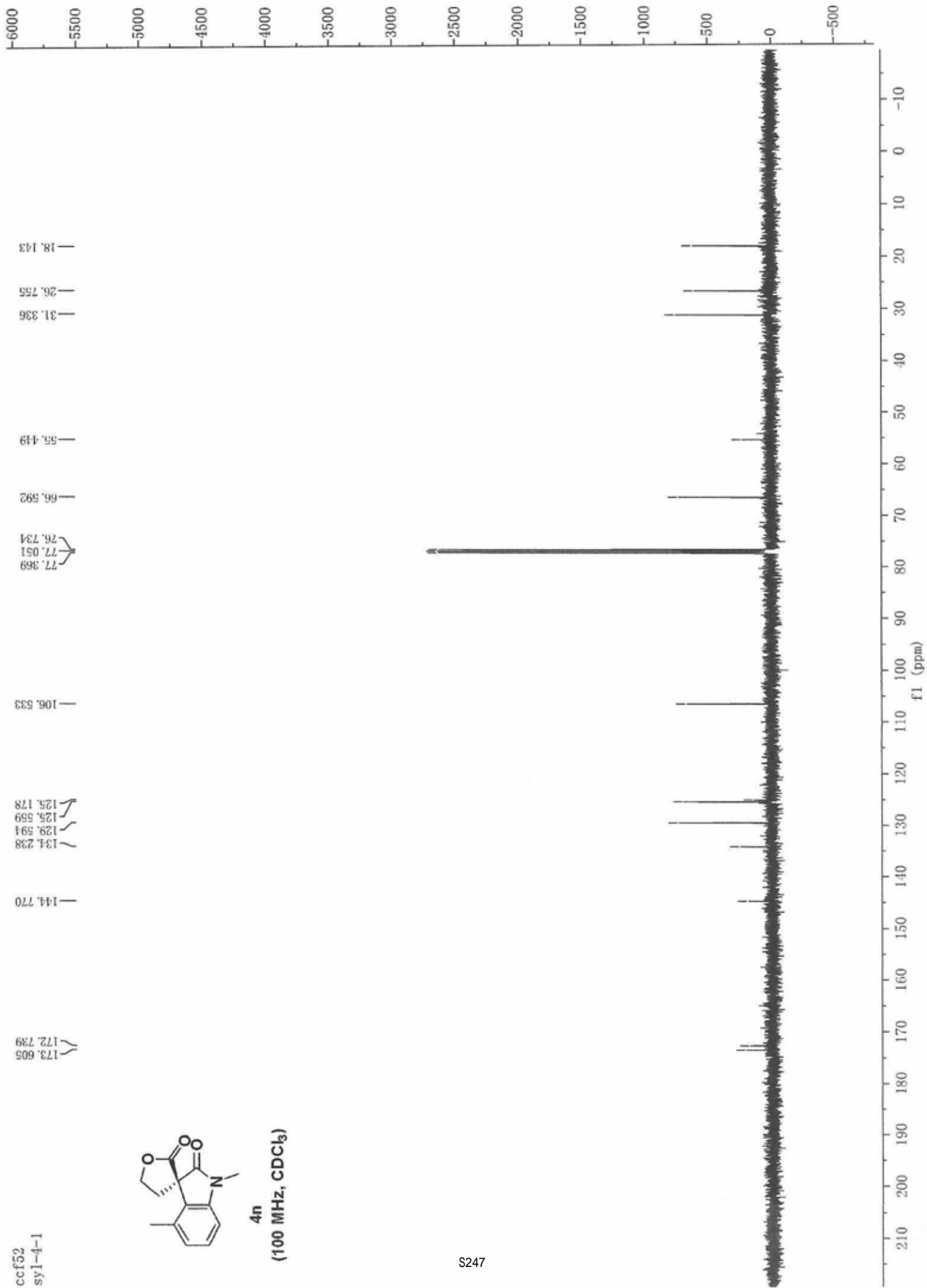
zft202007024

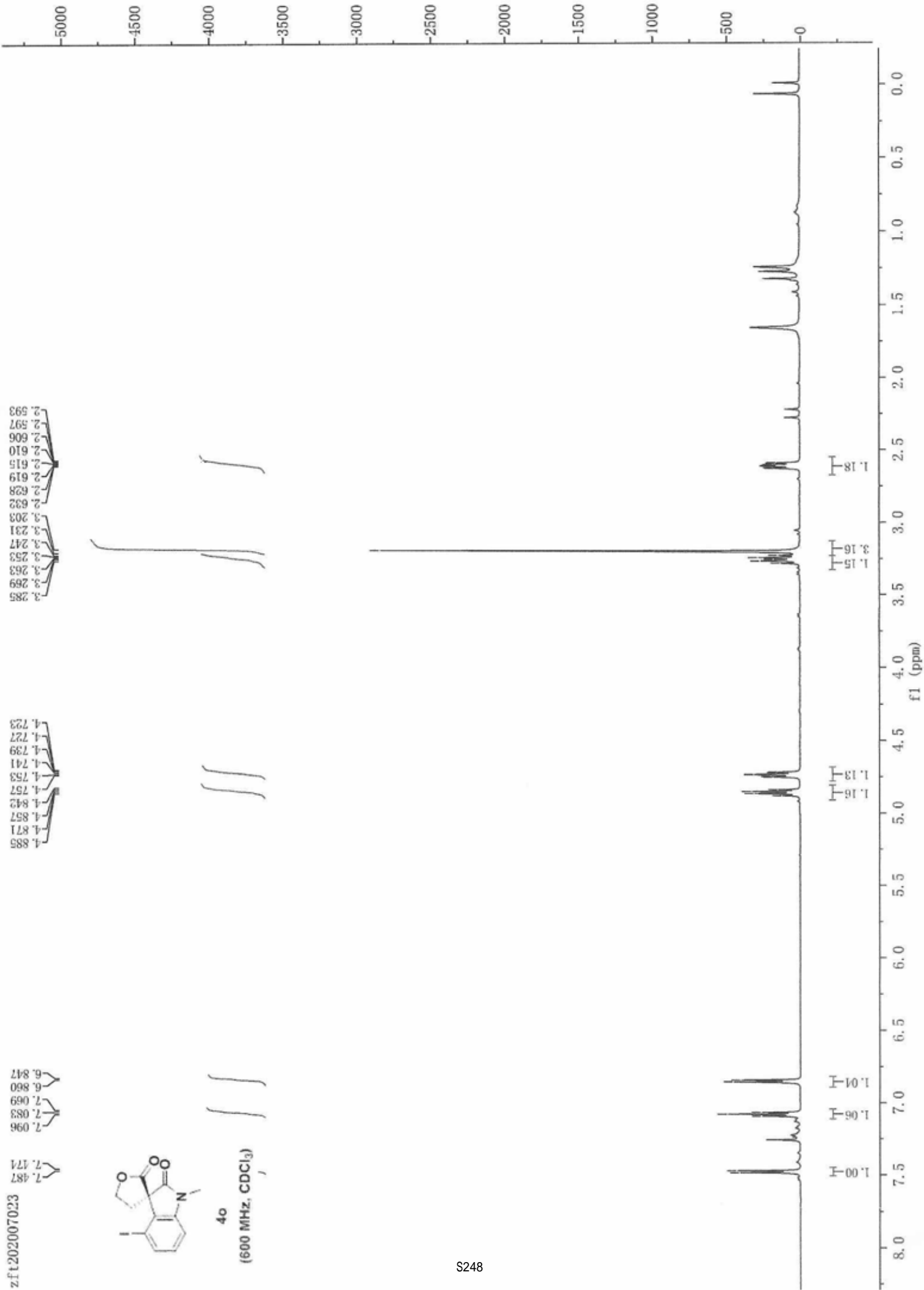


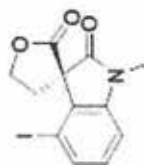
ccf52  
syl-4-1



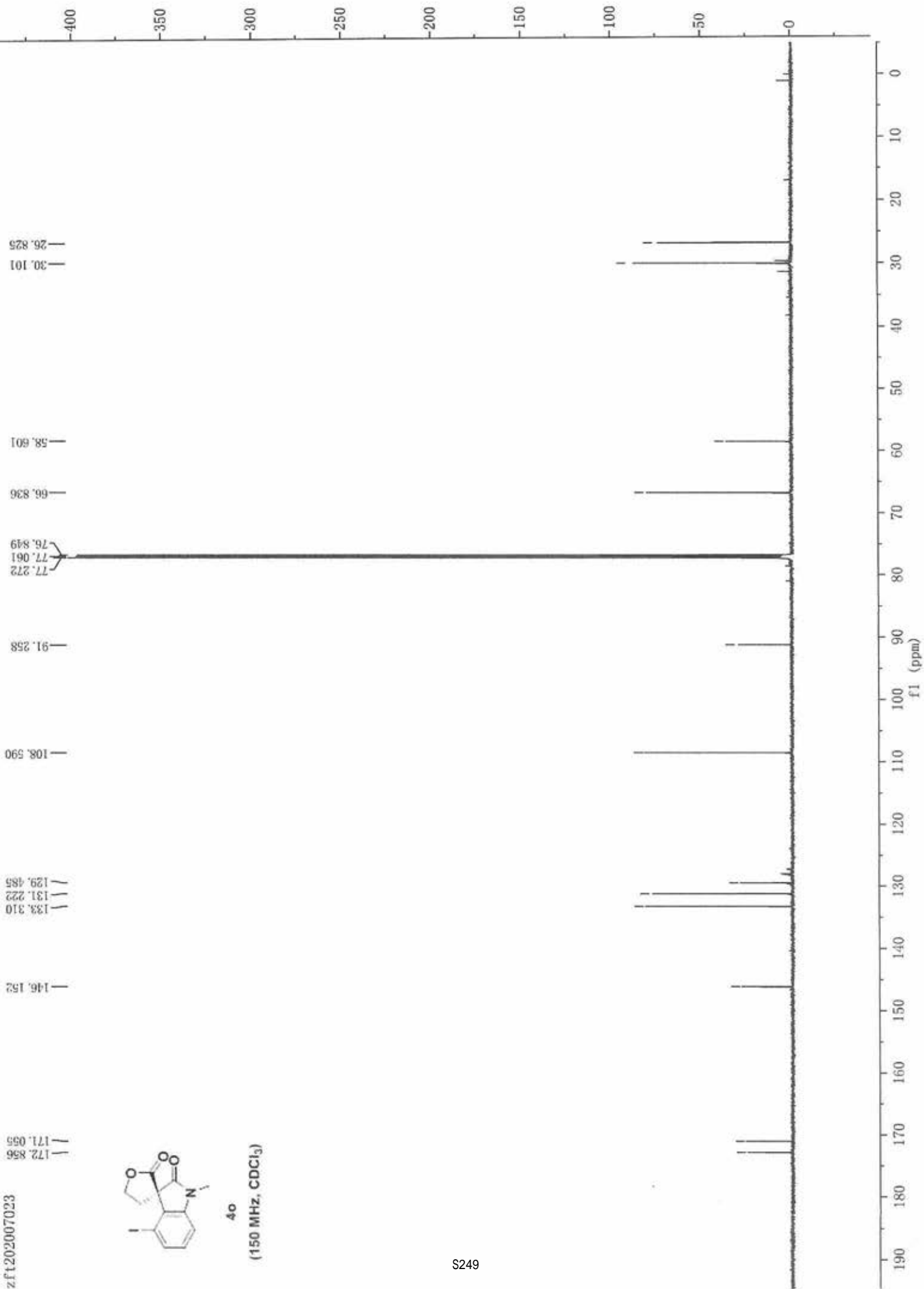
**4n**  
(100 MHz, CDCl<sub>3</sub>)

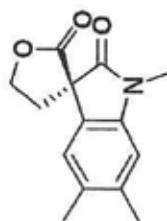




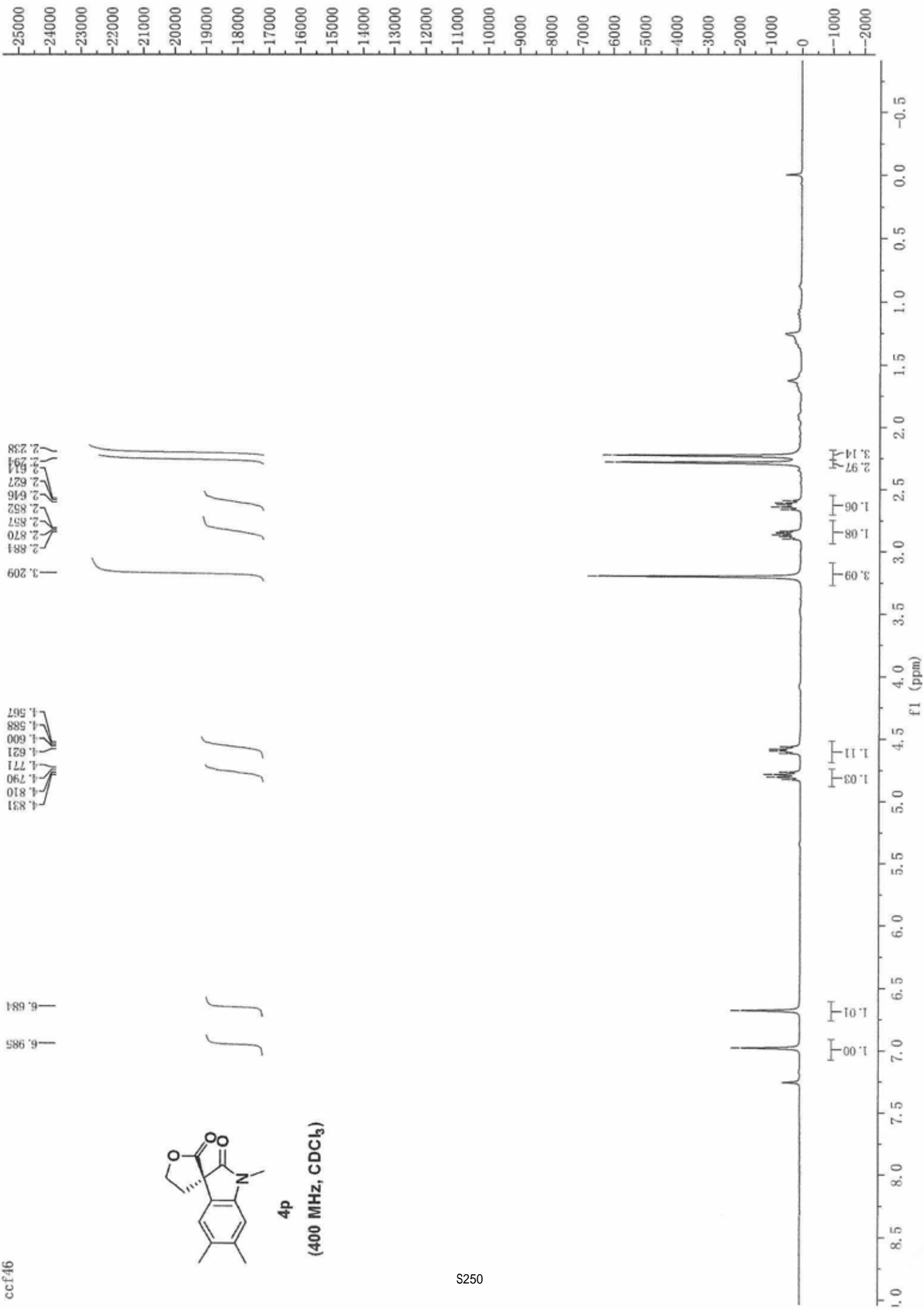


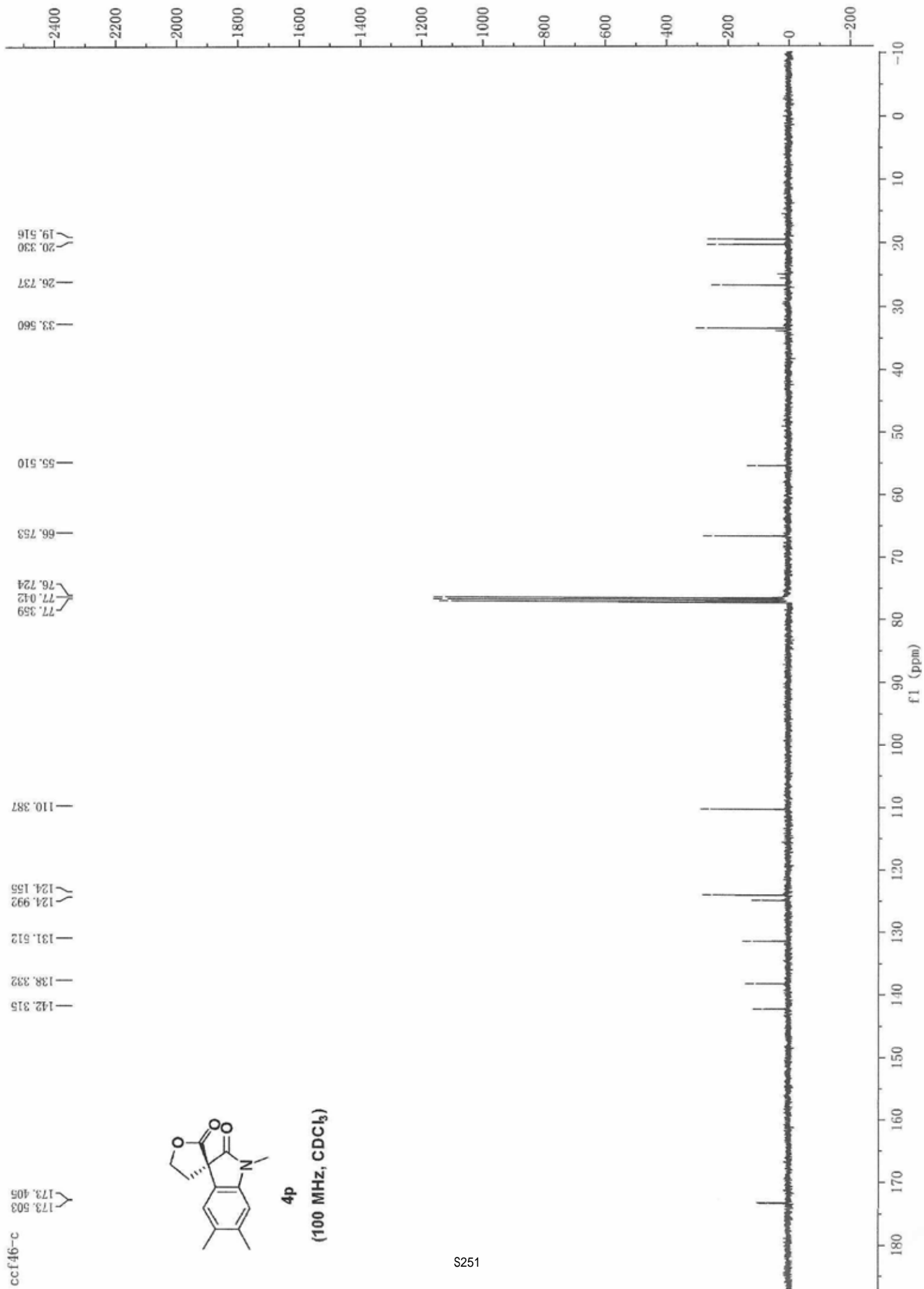
4o

(150 MHz, CDCl<sub>3</sub>)

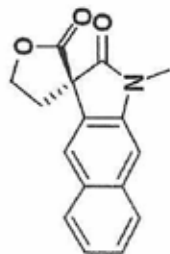


4p

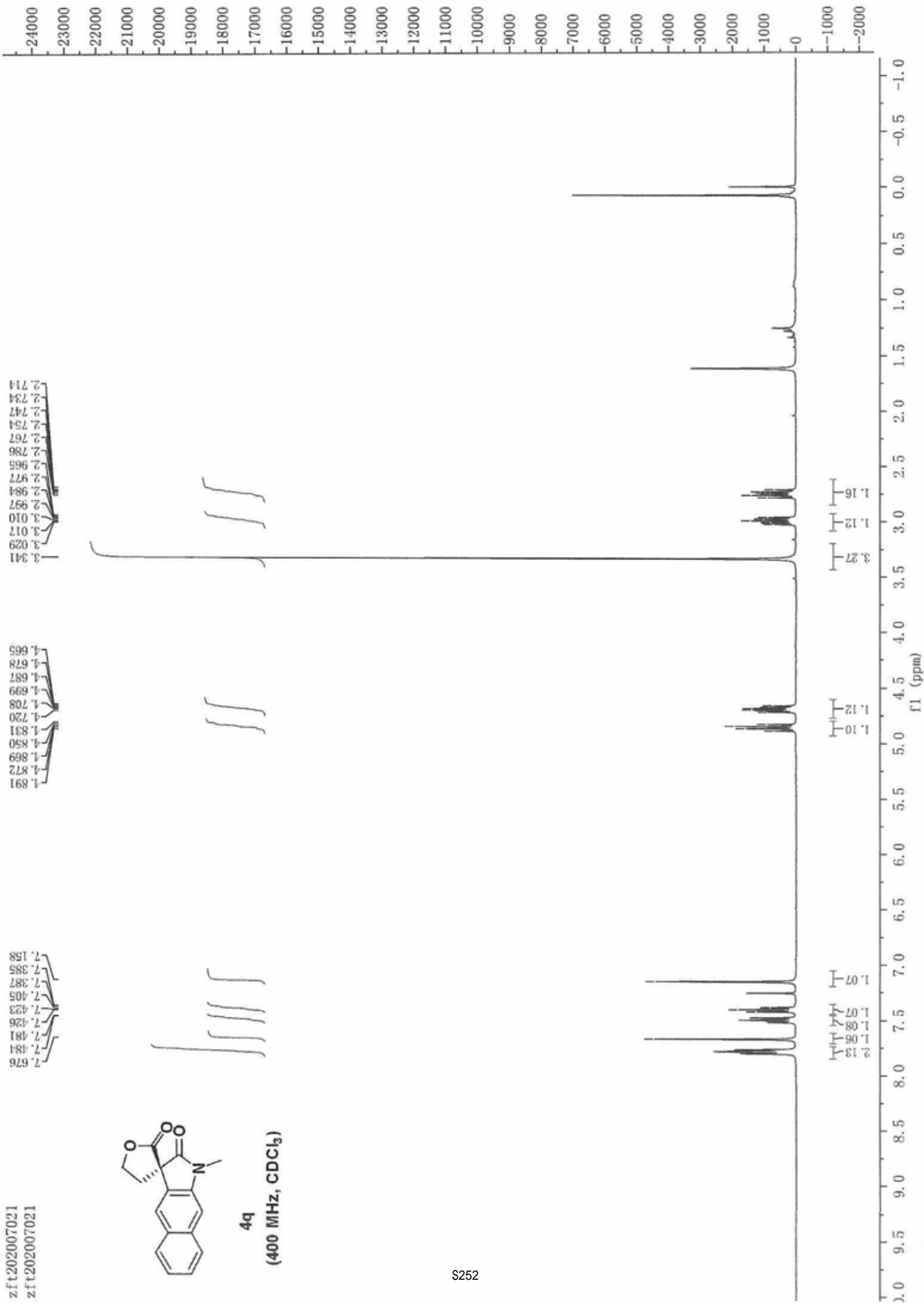
(400 MHz, CDCl<sub>3</sub>)



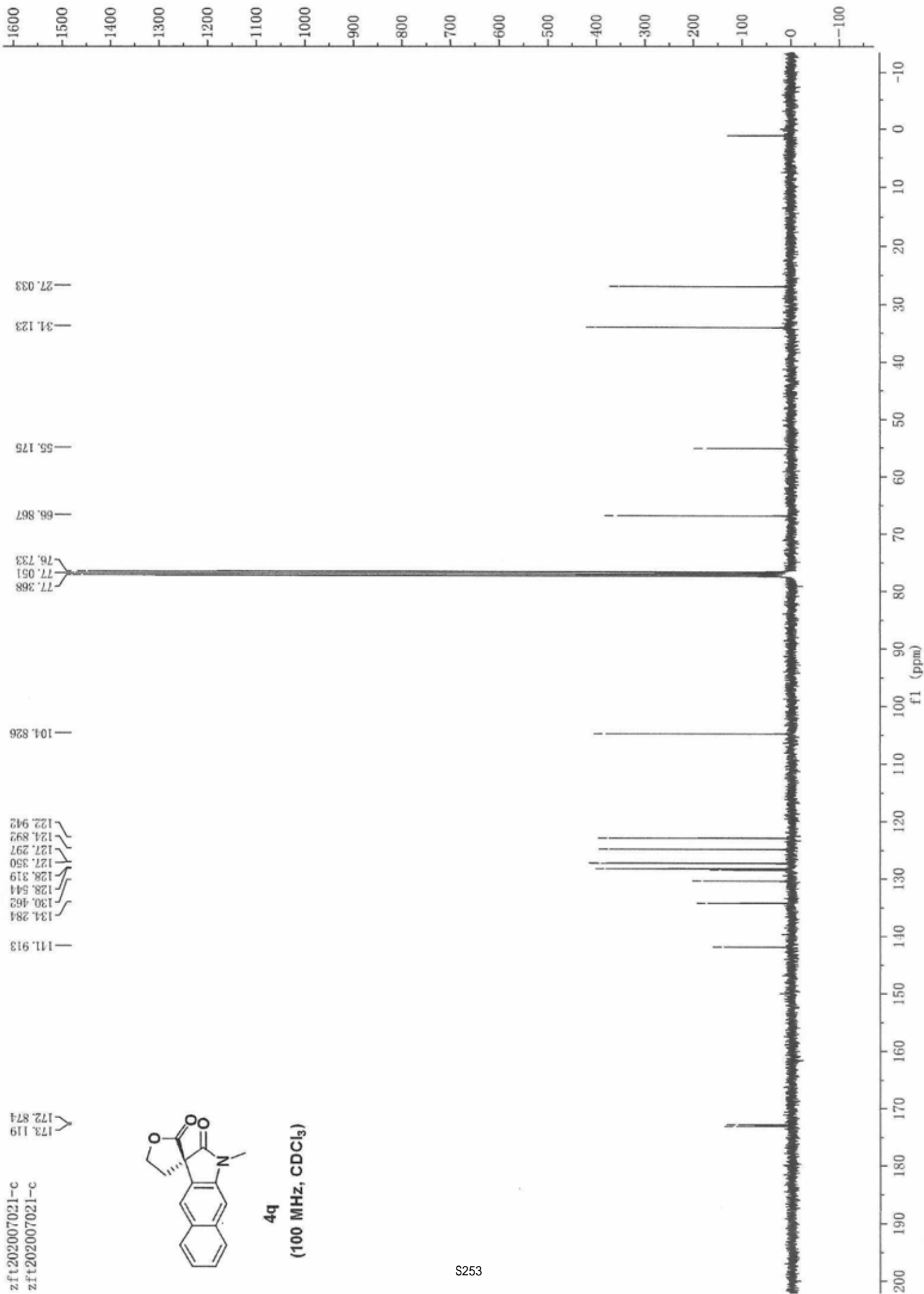
zft202007021  
zft202007021

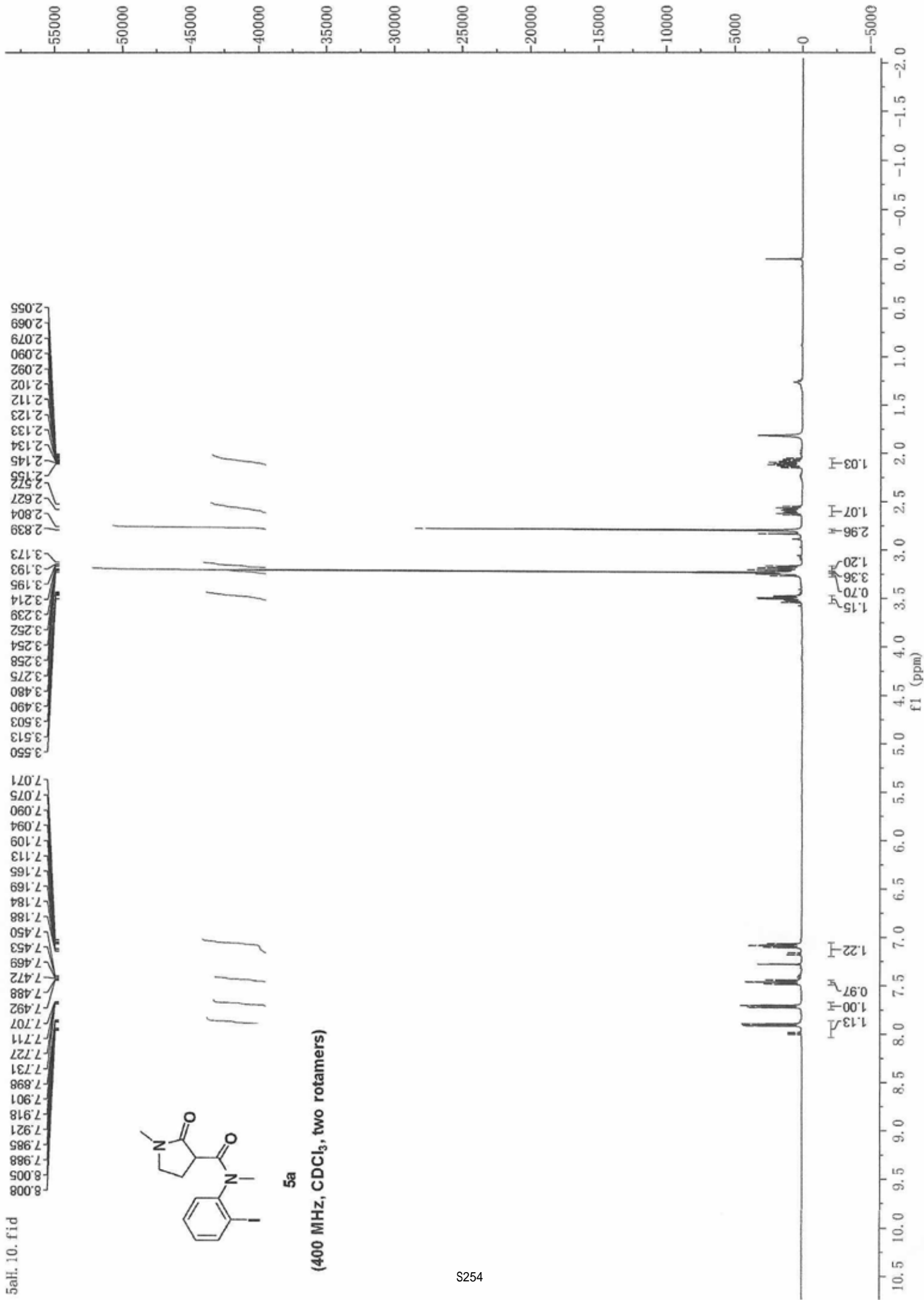


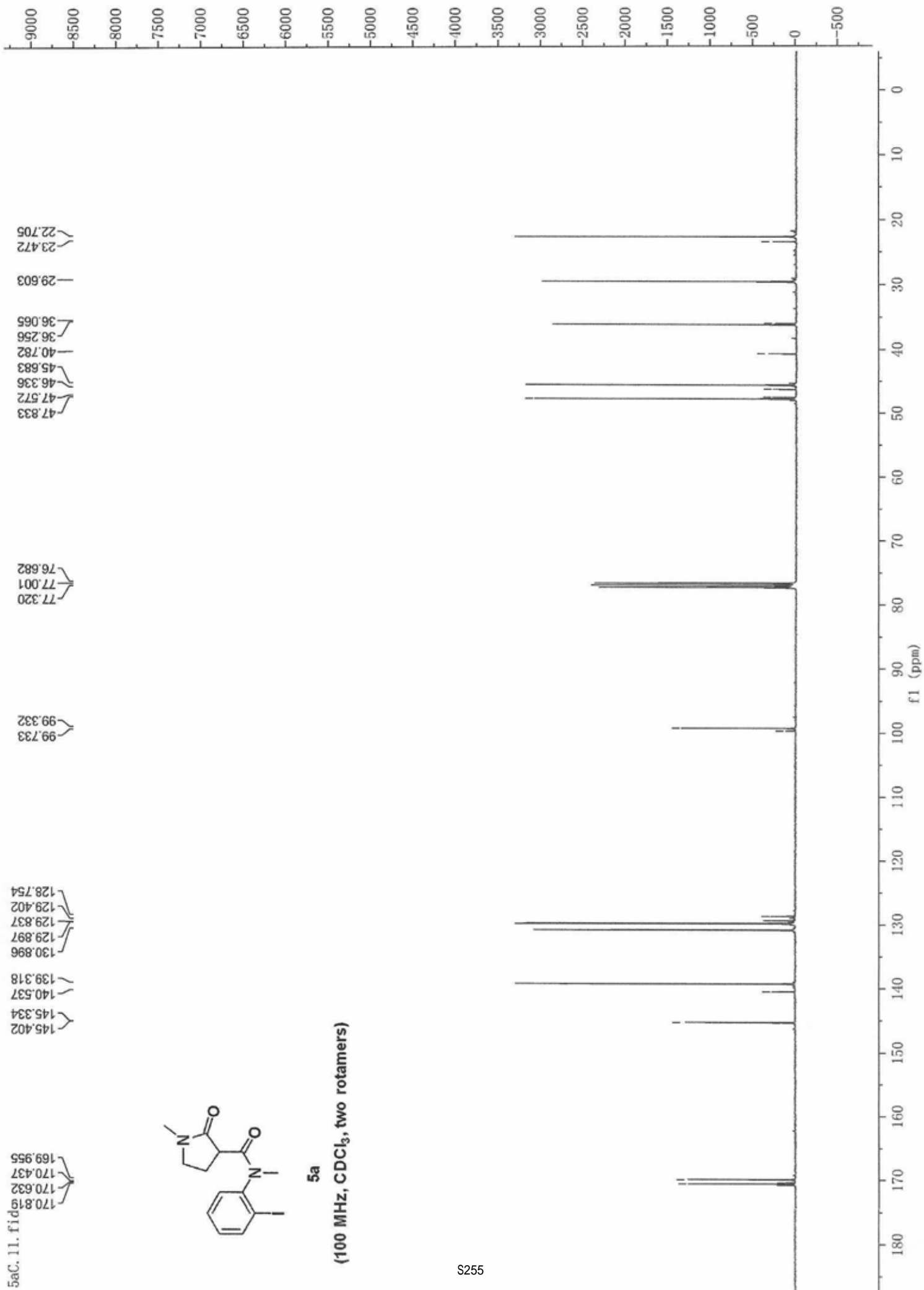
4q  
(400 MHz, CDCl<sub>3</sub>)

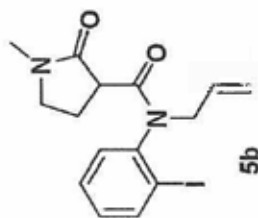




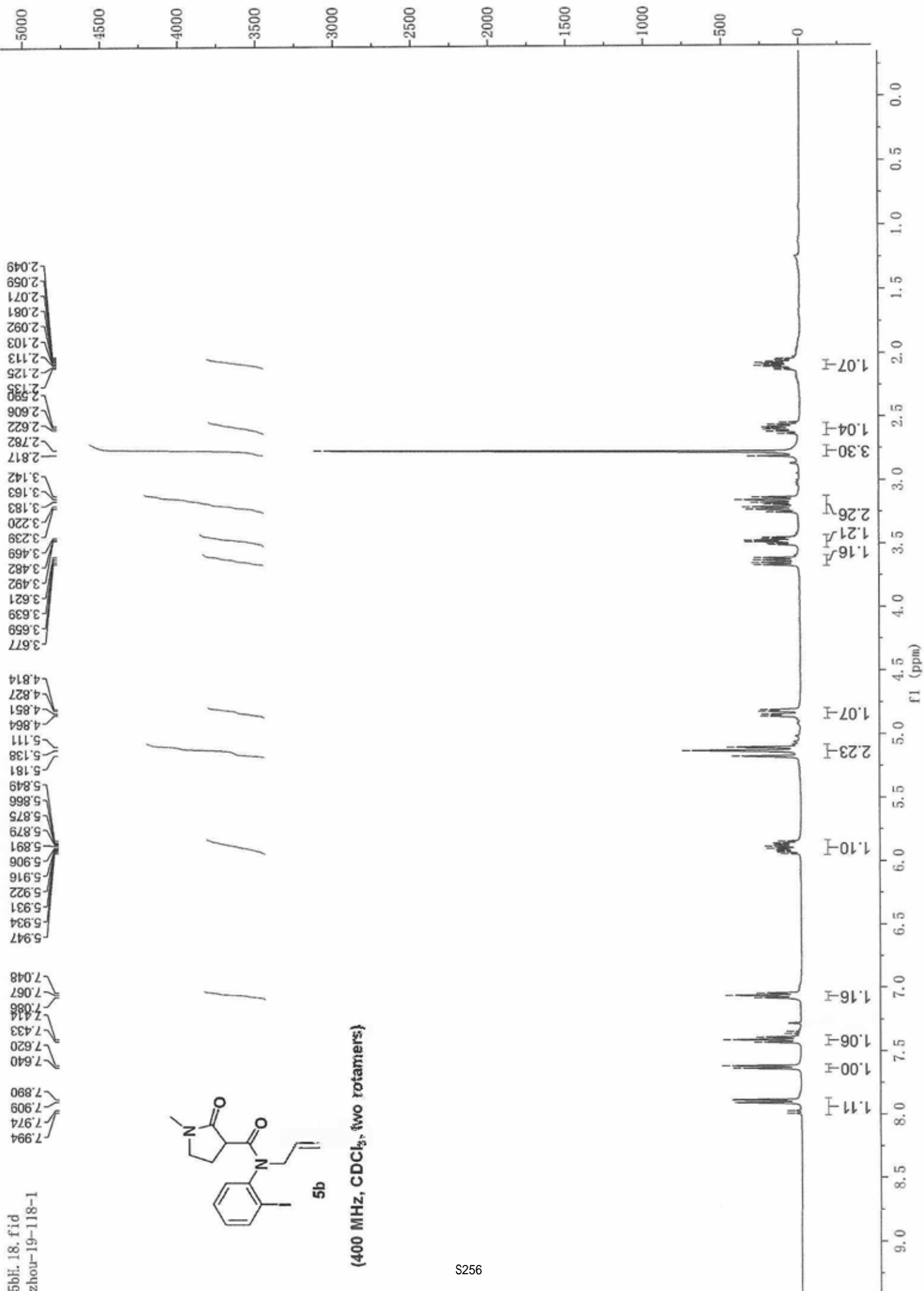




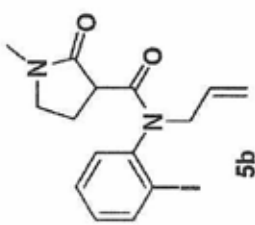




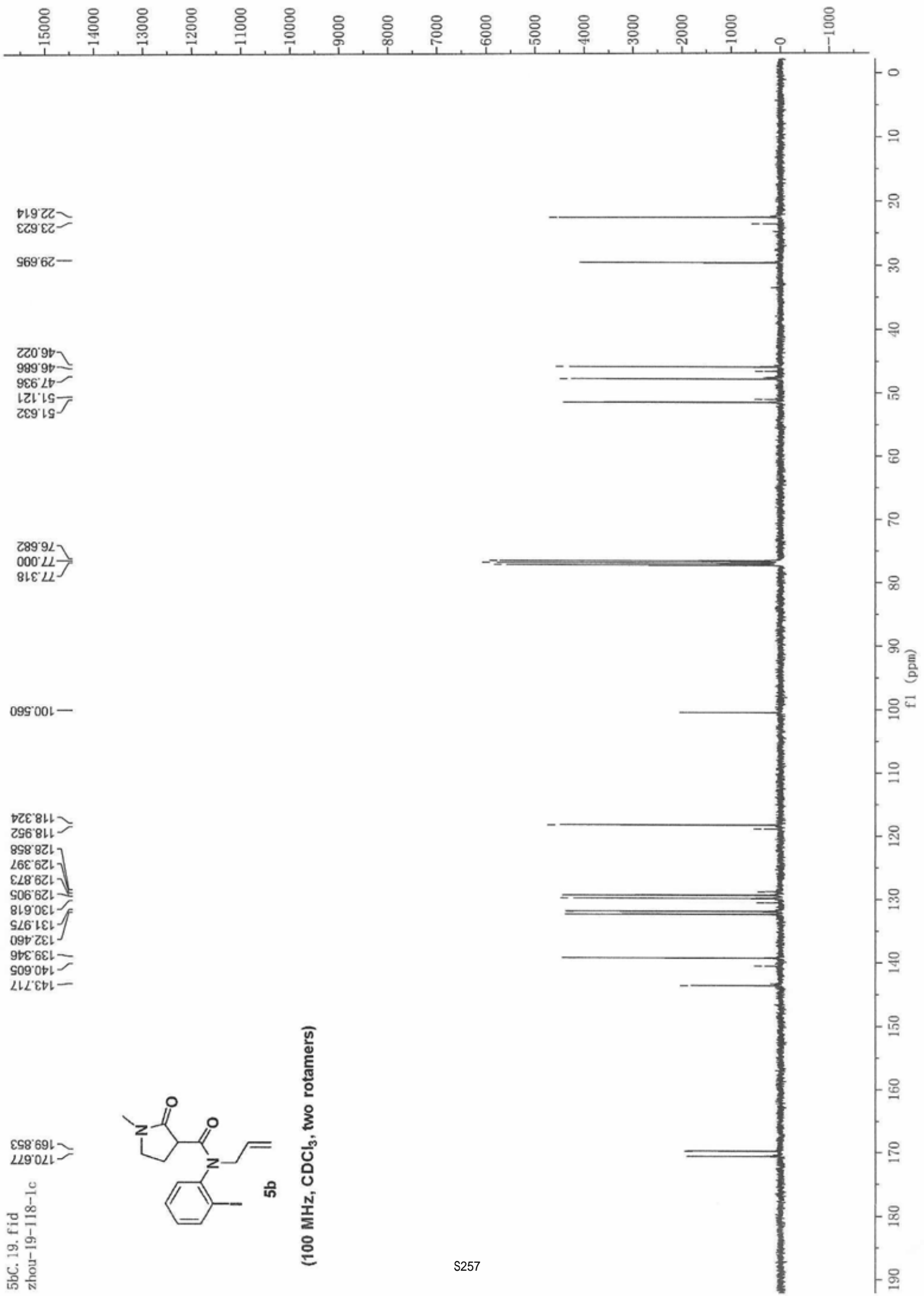
(400 MHz, CDCl<sub>3</sub>, two rotamers)



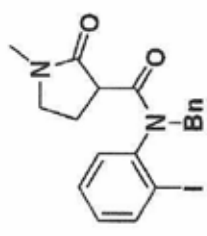
5bC. 19. fid  
zhou-19-118-1c



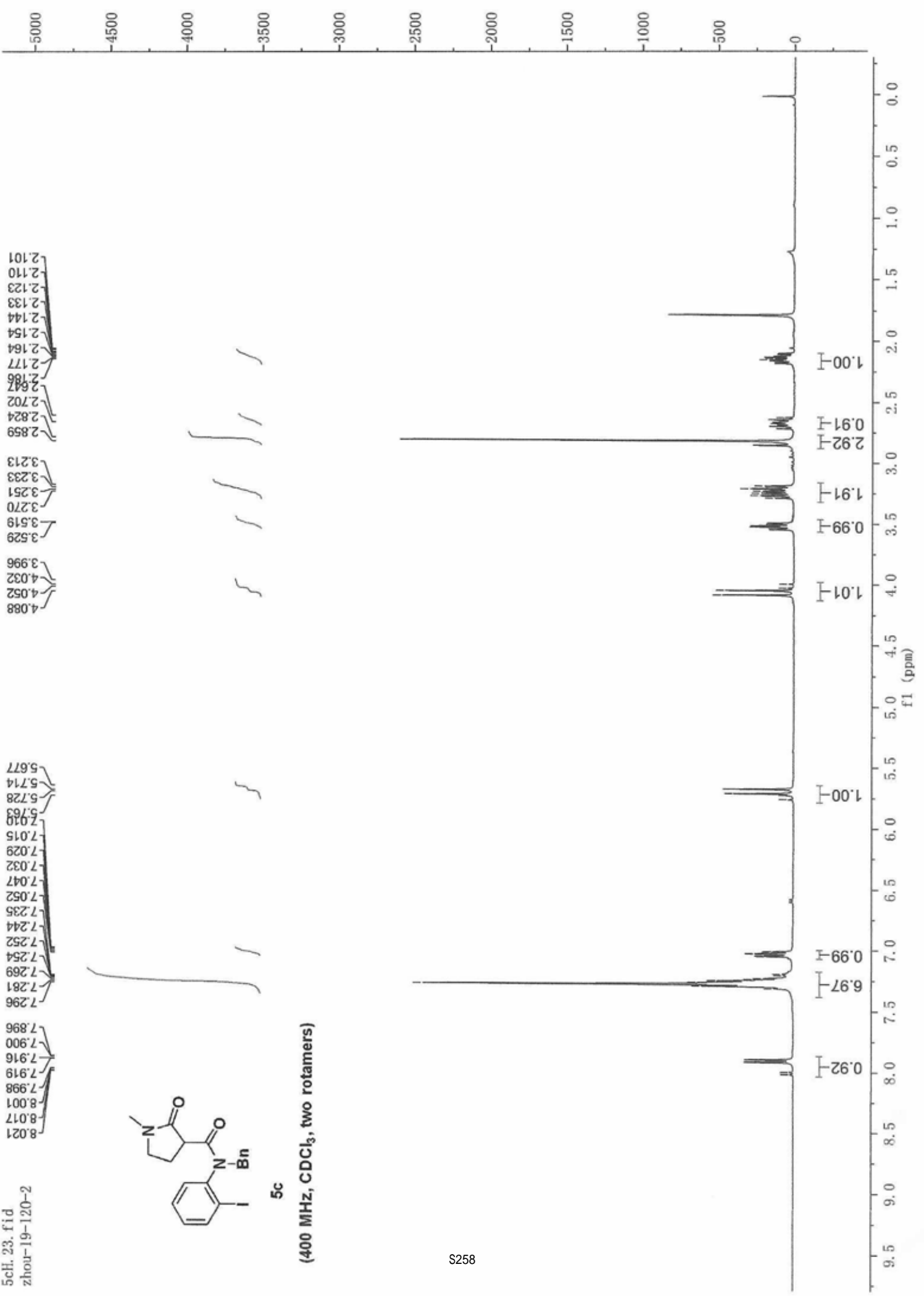
(100 MHz, CDCl<sub>3</sub>, two rotamers)

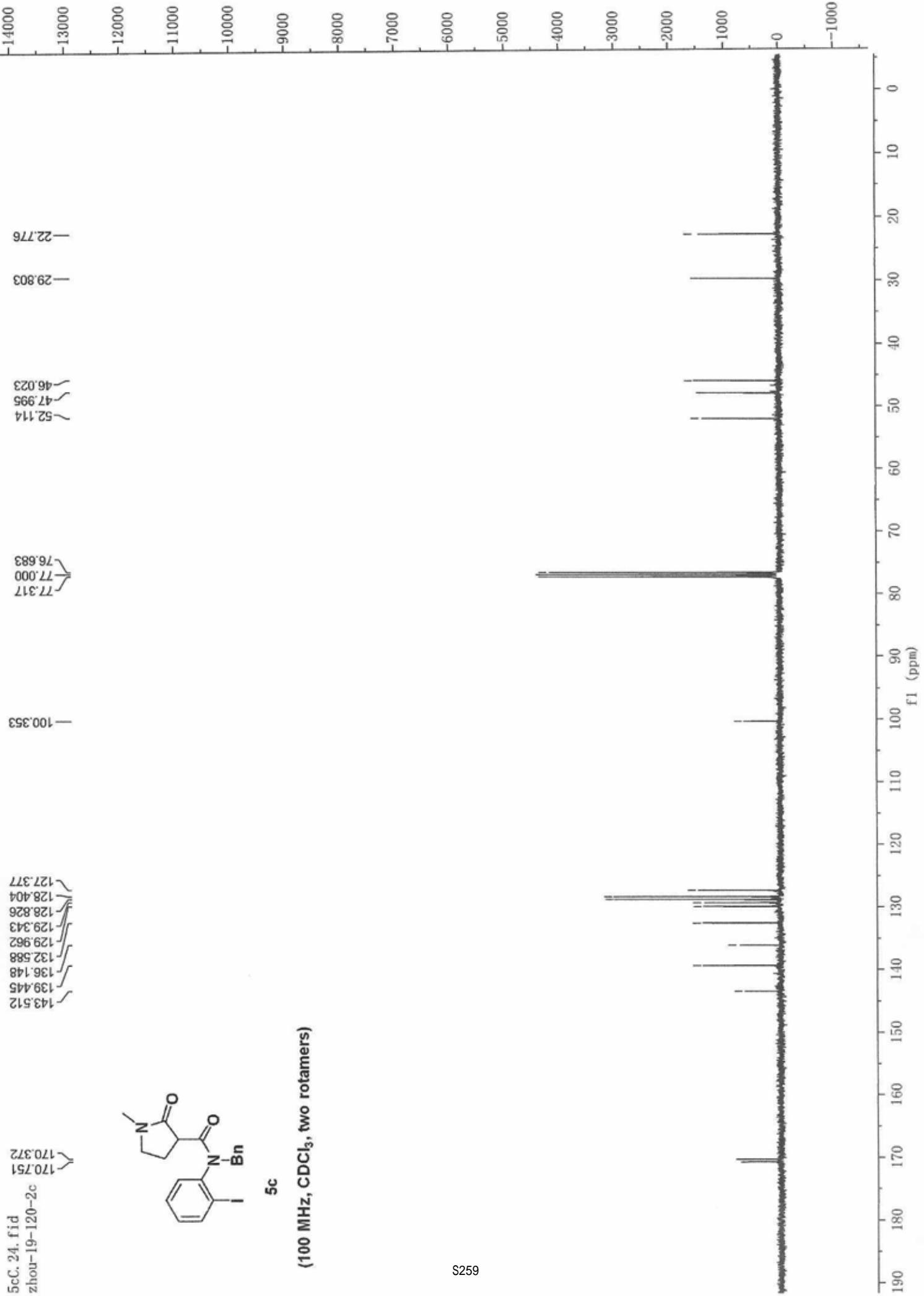


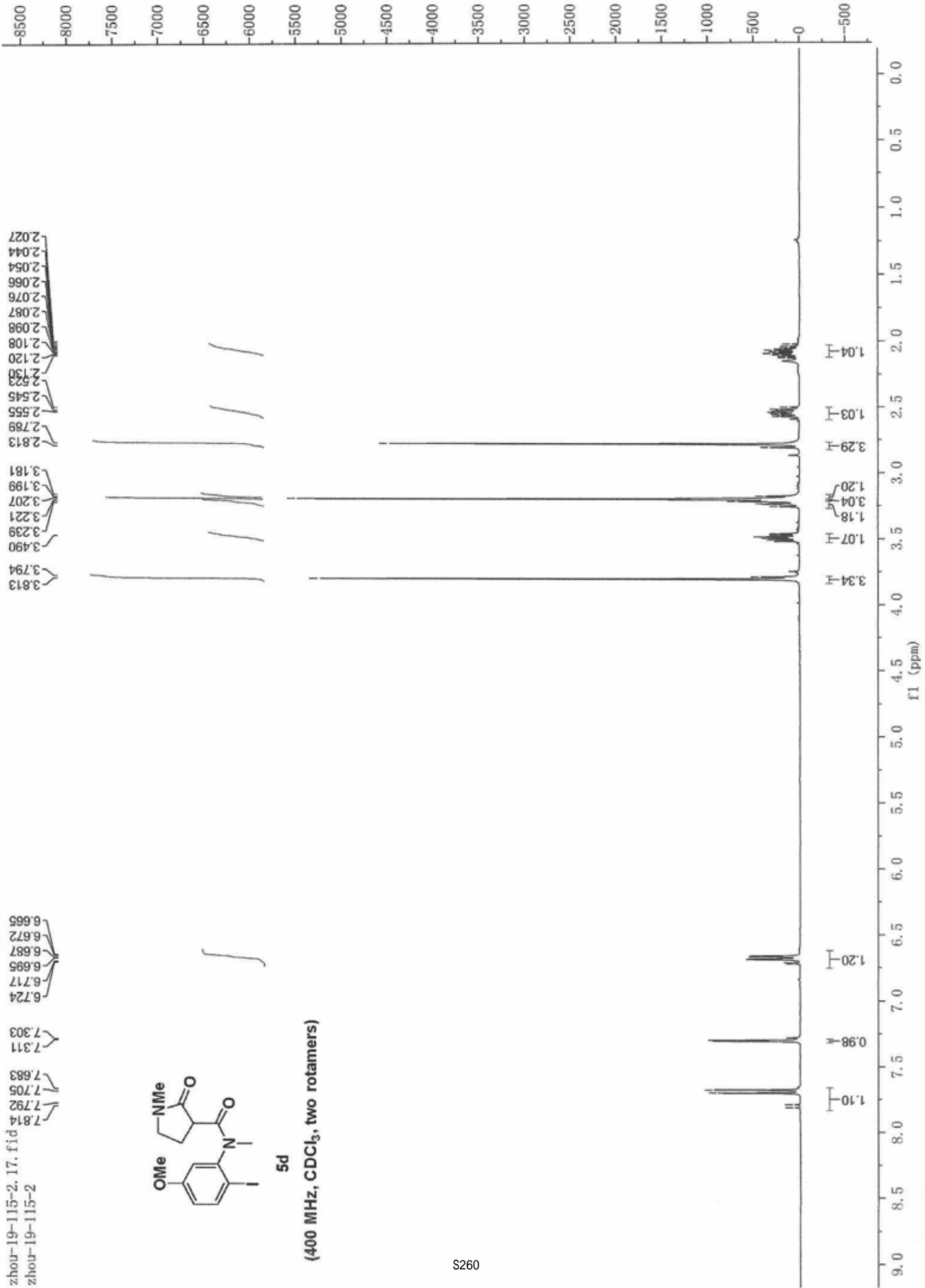
5cH. 23. fid  
zhou-19-120-2



5c  
(400 MHz, CDCl<sub>3</sub>, two rotamers)

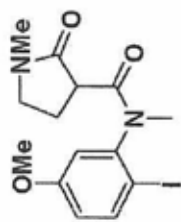






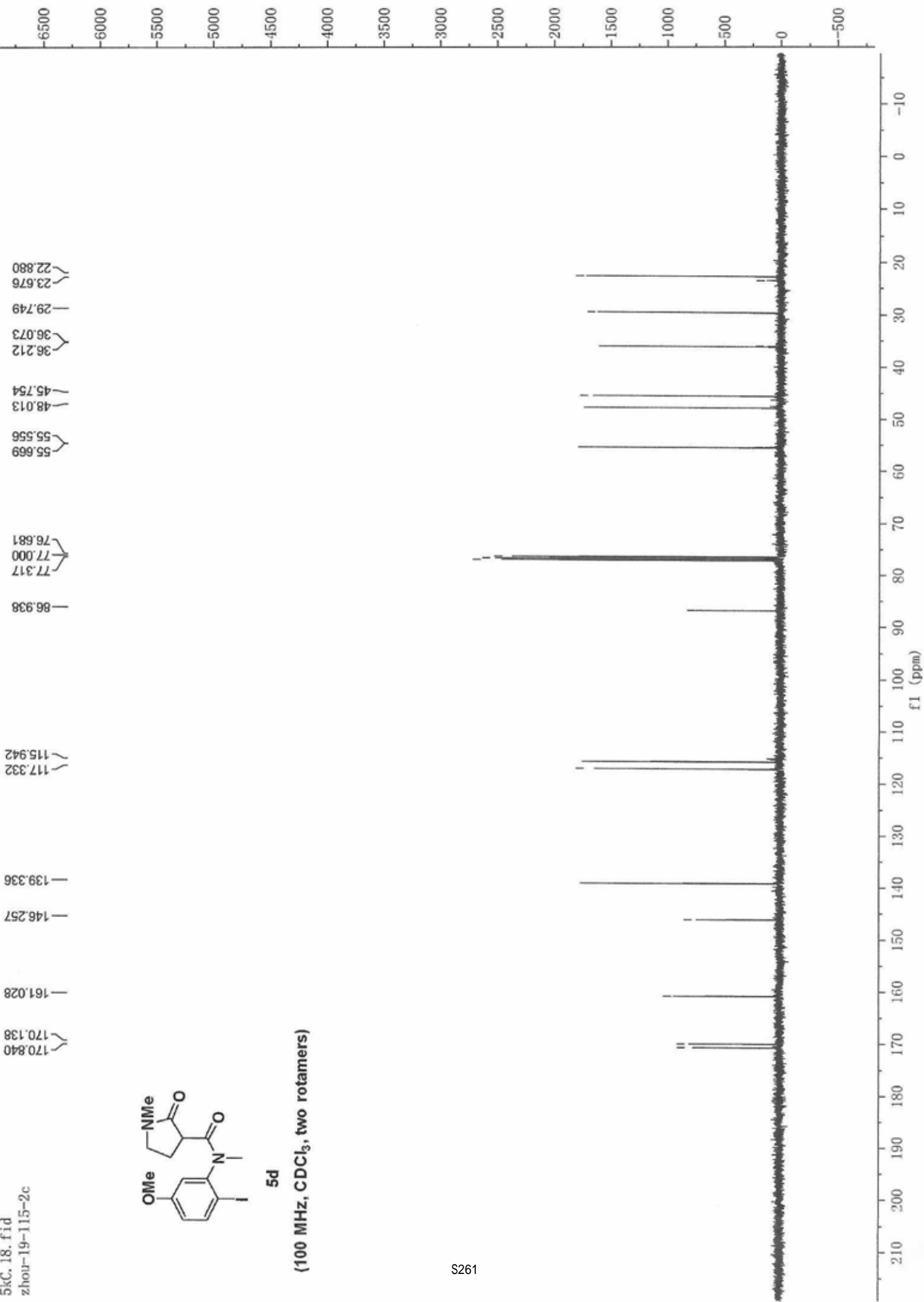
zhou-19-115-2.17. fid  
zhou-19-115-2

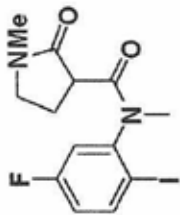




5d

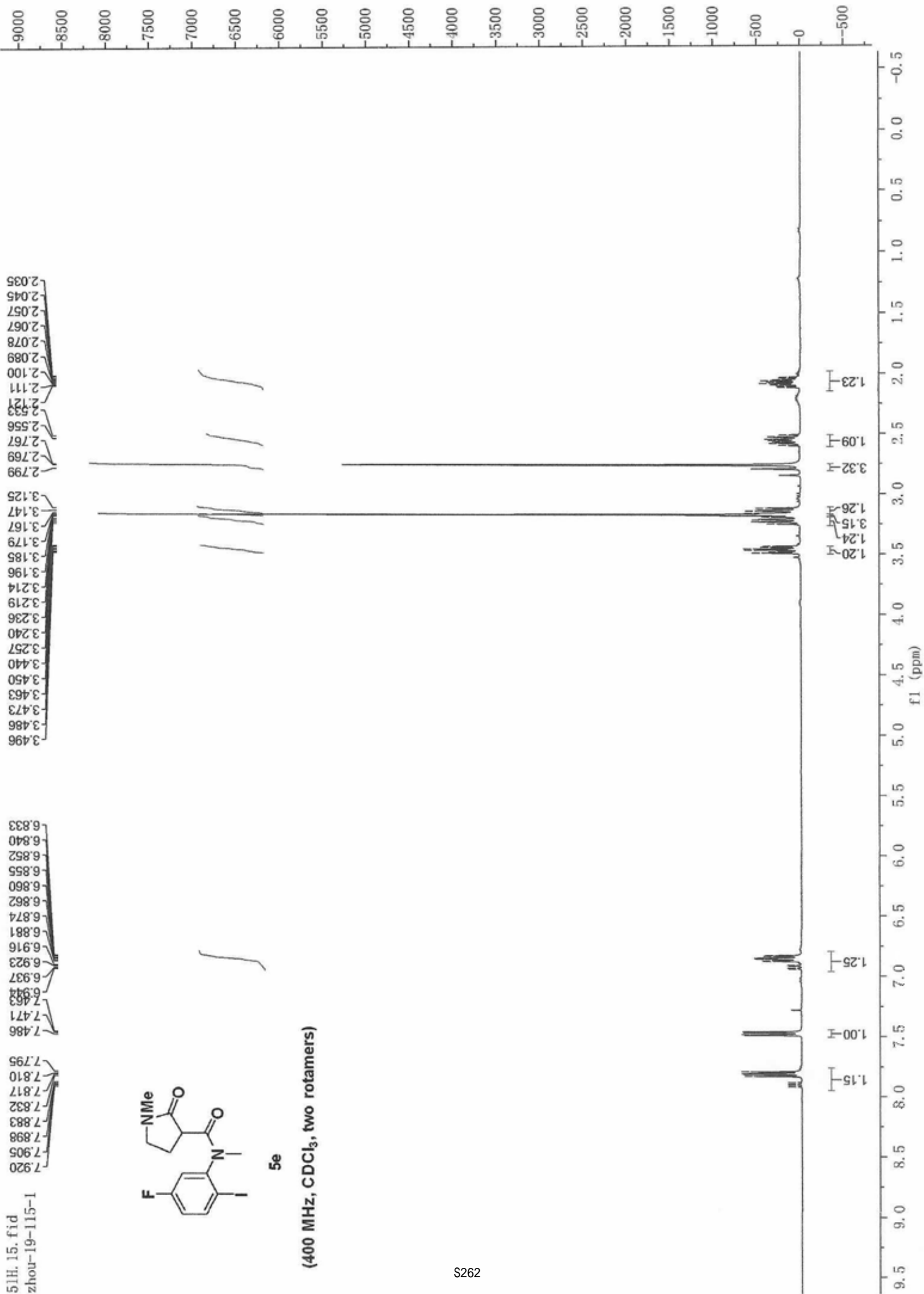
(100 MHz, CDCl<sub>3</sub>, two rotamers)

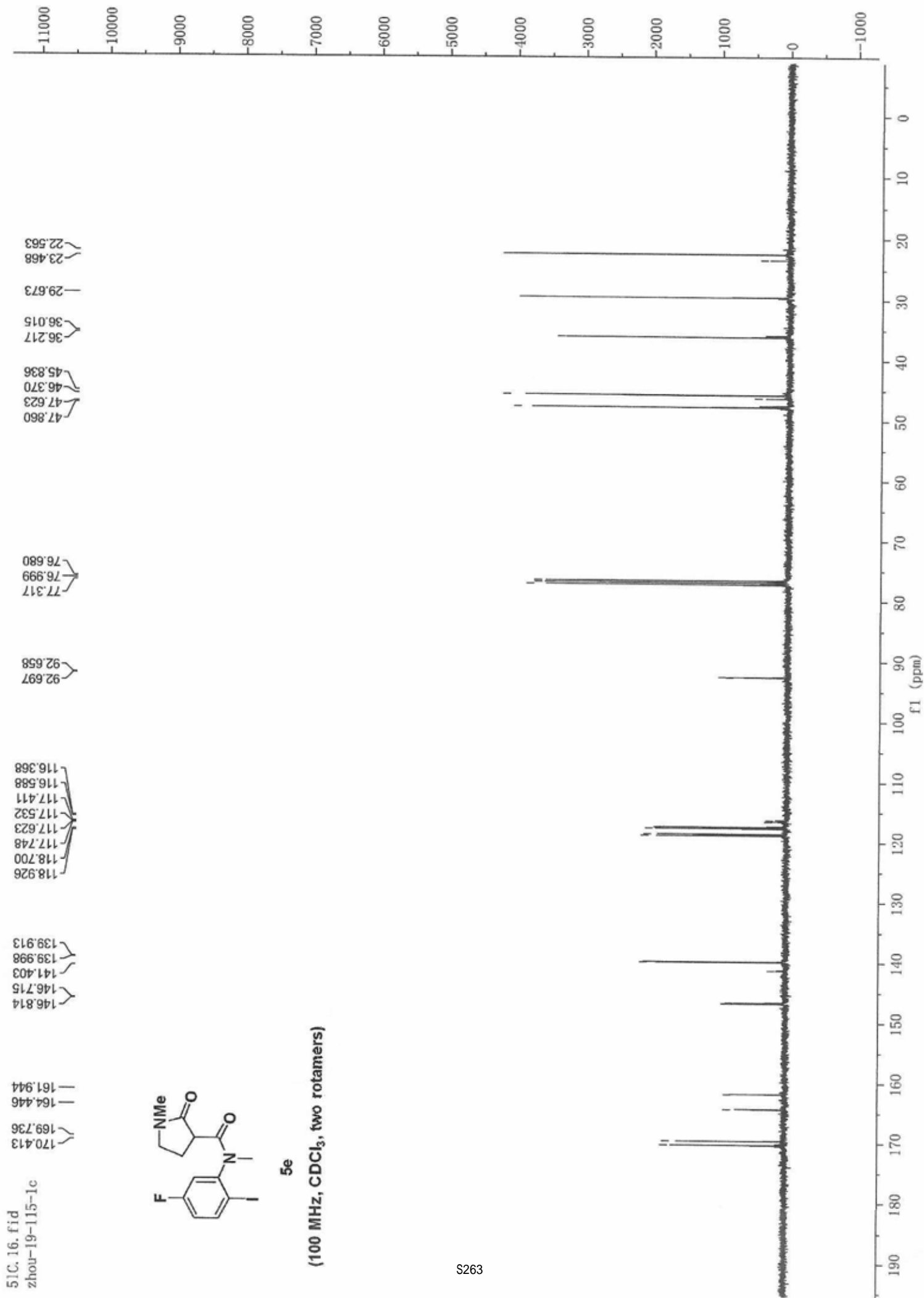




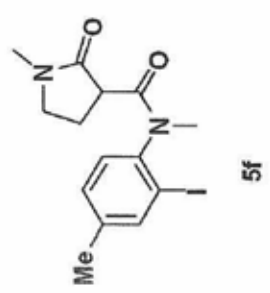
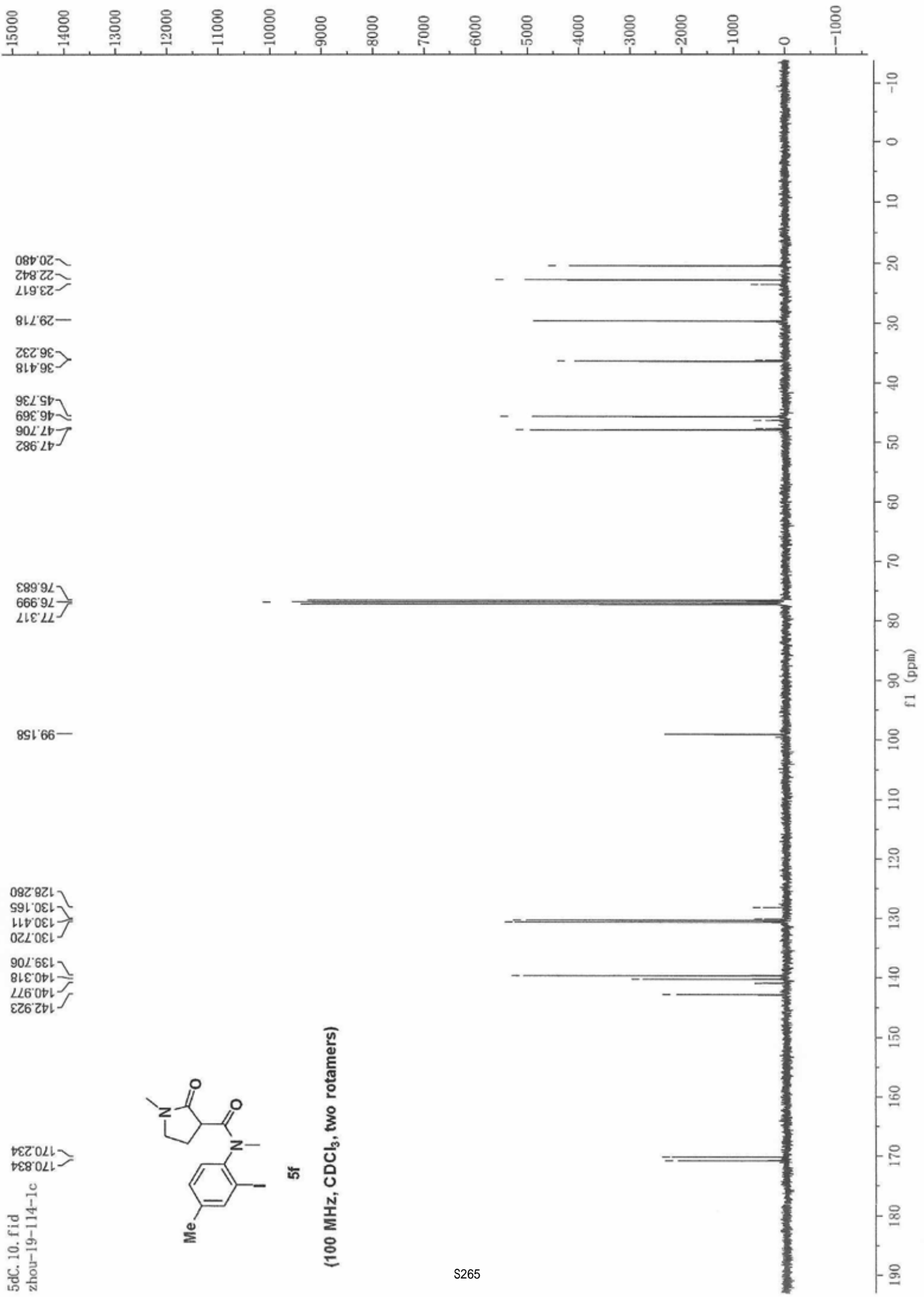
5e

(400 MHz, CDCl<sub>3</sub>, two rotamers)



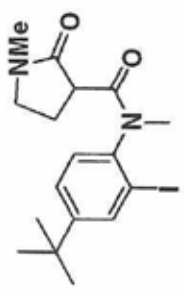






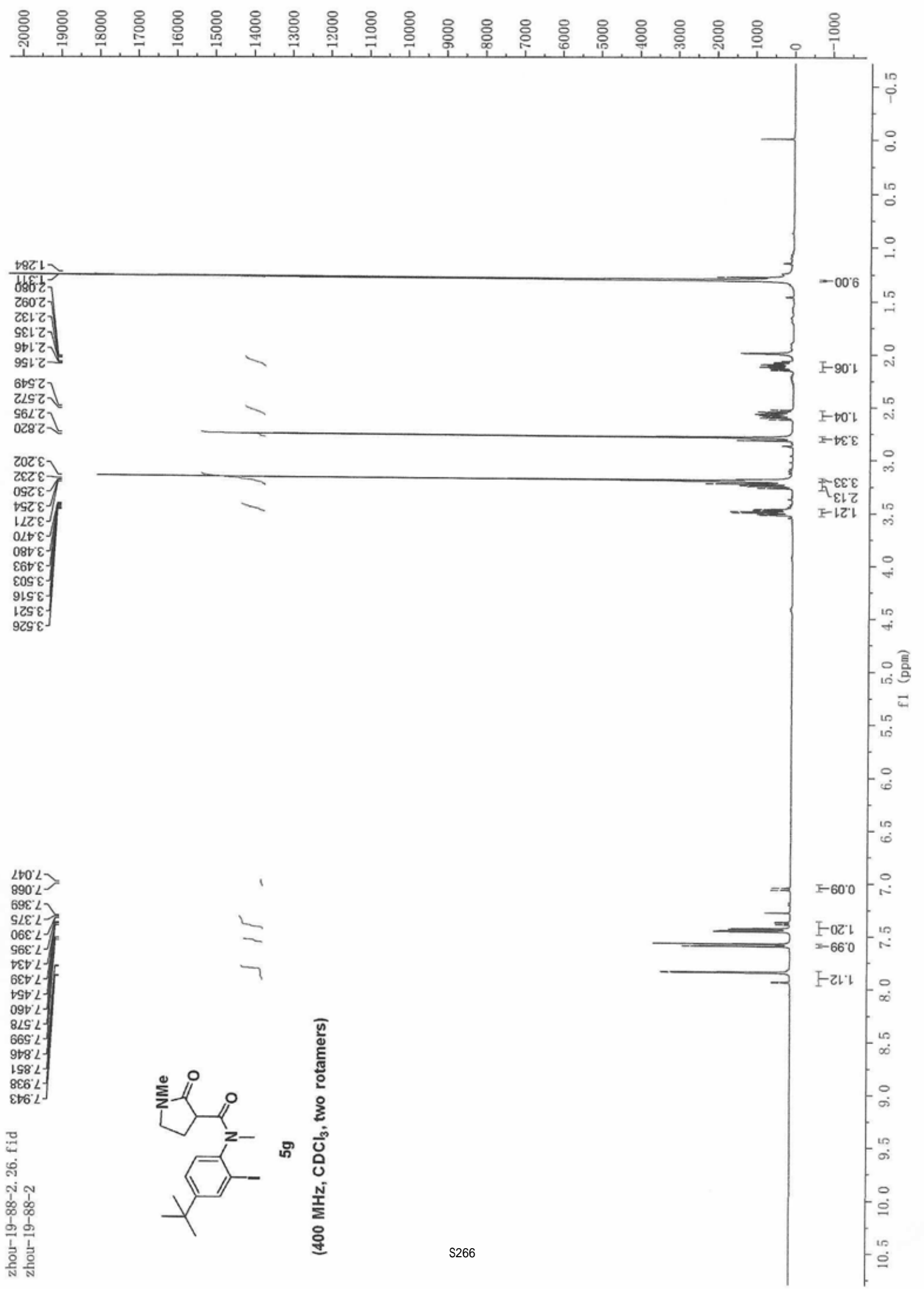
(100 MHz, CDCl<sub>3</sub>, two rotamers)

zhou-19-88-2.26.fid  
zhou-19-88-2

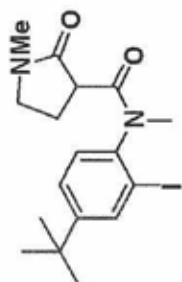


5g

(400 MHz, CDCl<sub>3</sub>, two rotamers)

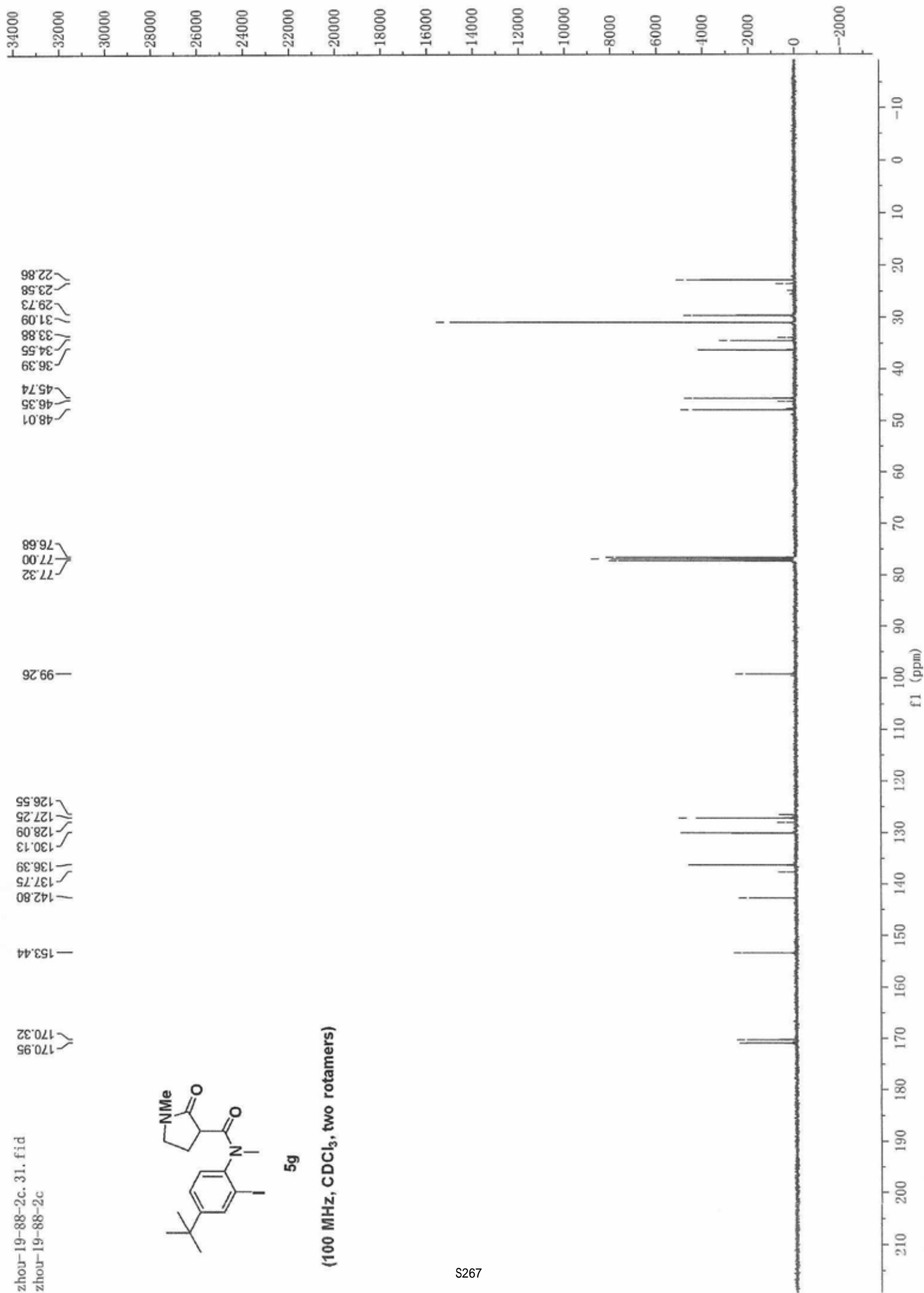


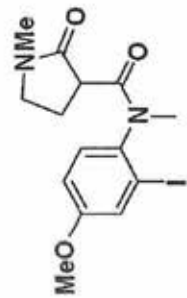
zhou-19-88-2c, 31. fid  
zhou-19-88-2c



5g

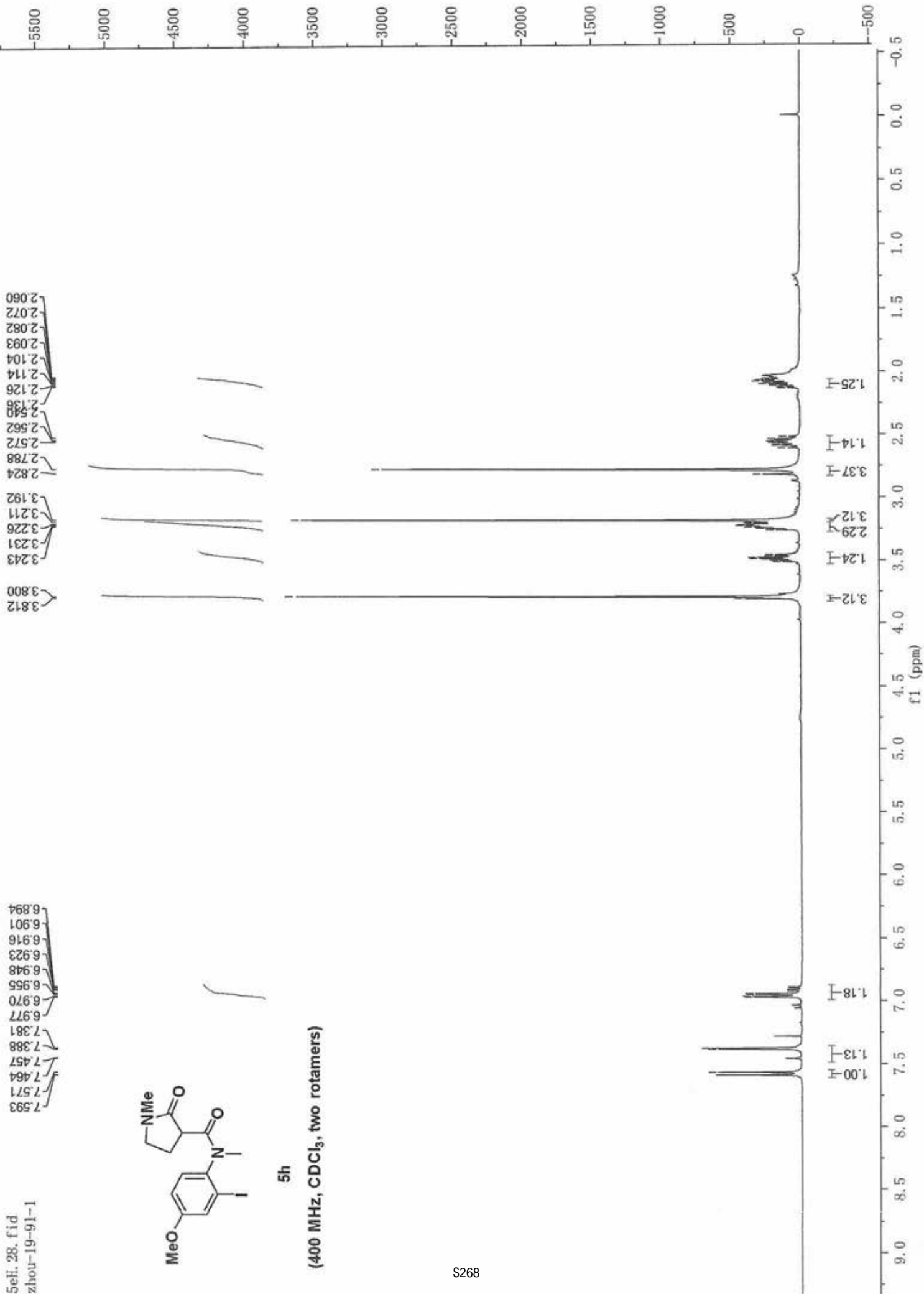
(100 MHz, CDCl<sub>3</sub>, two rotamers)



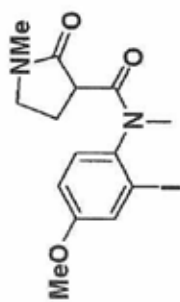


5h

(400 MHz, CDCl<sub>3</sub>, two rotamers)

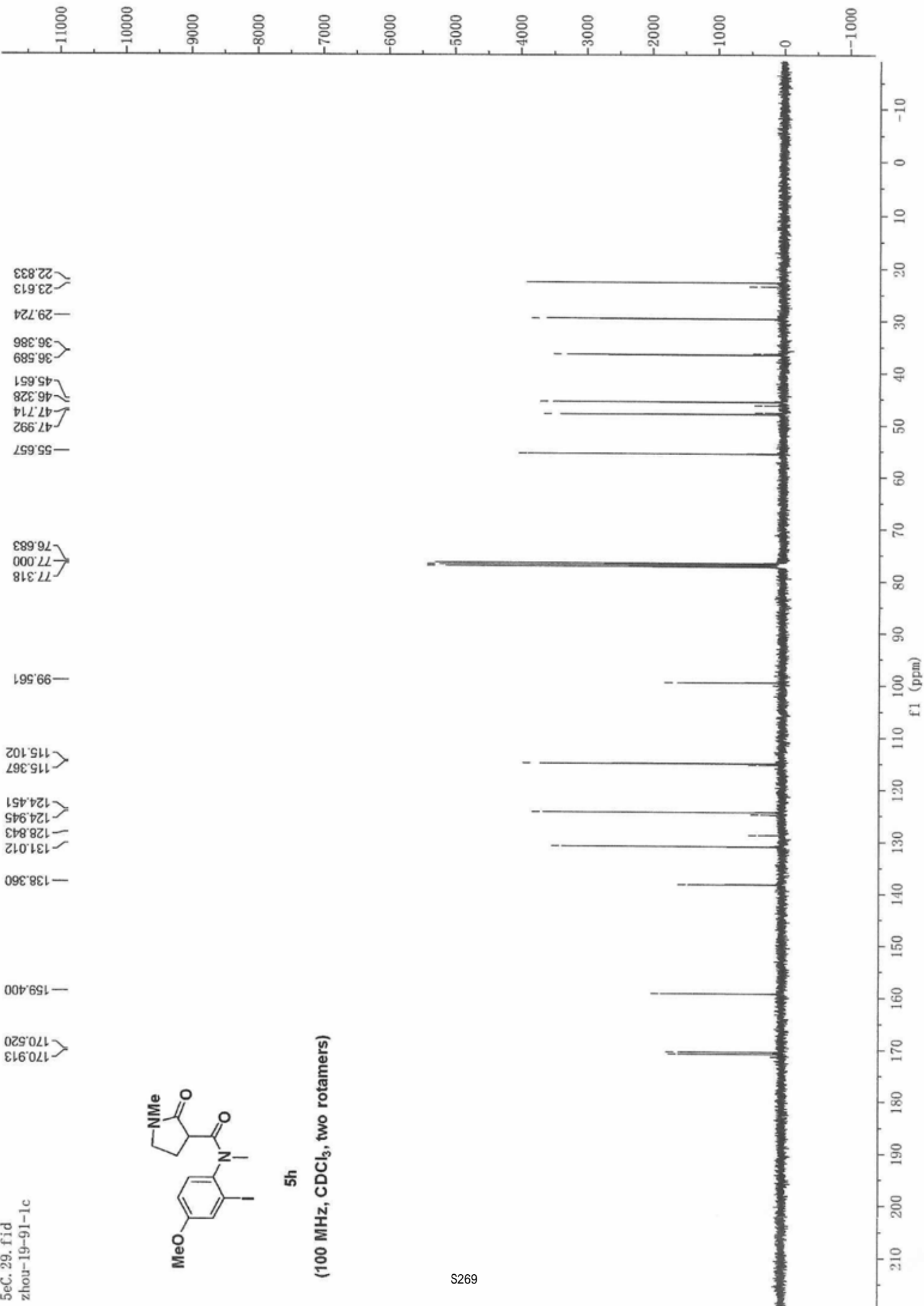






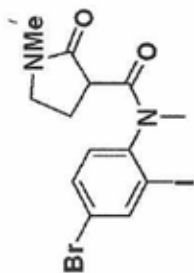
5h

(100 MHz, CDCl<sub>3</sub>, two rotamers)



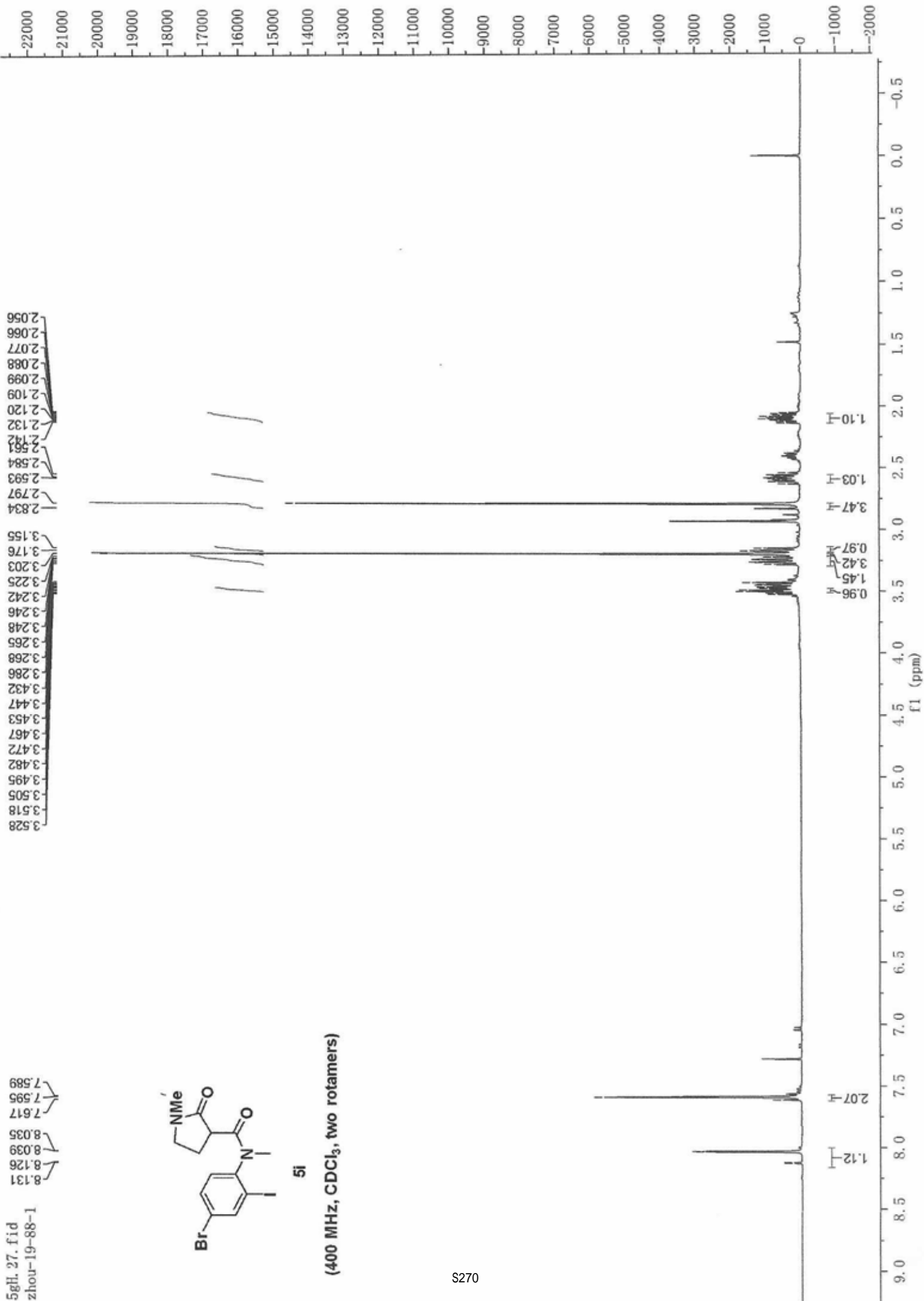
5gH. 27. fid  
zhou-19-88-1

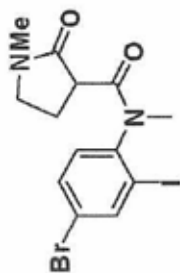
8.131  
8.126  
8.039  
8.035  
7.617  
7.595  
7.589



5i

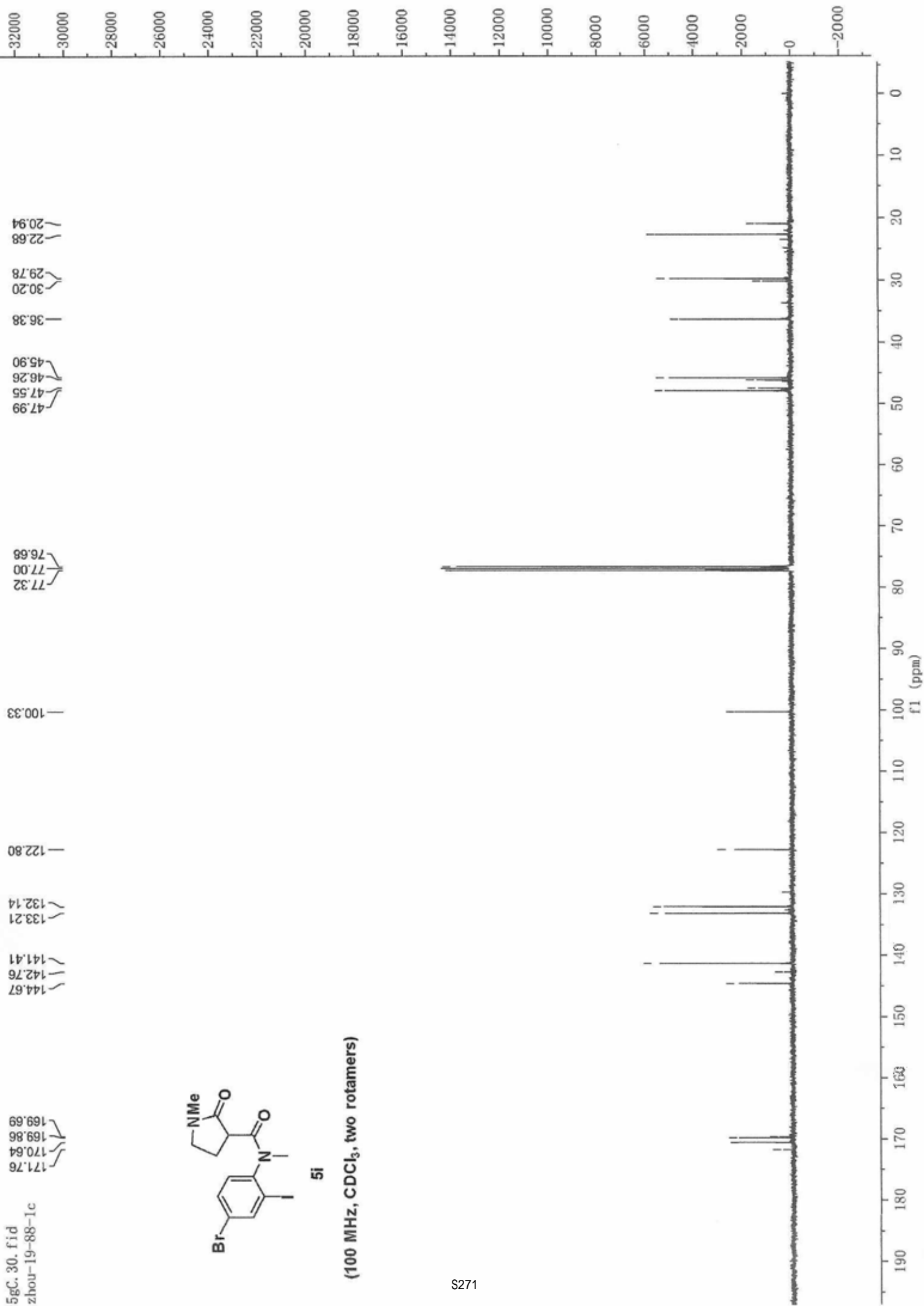
(400 MHz, CDCl<sub>3</sub>, two rotamers)

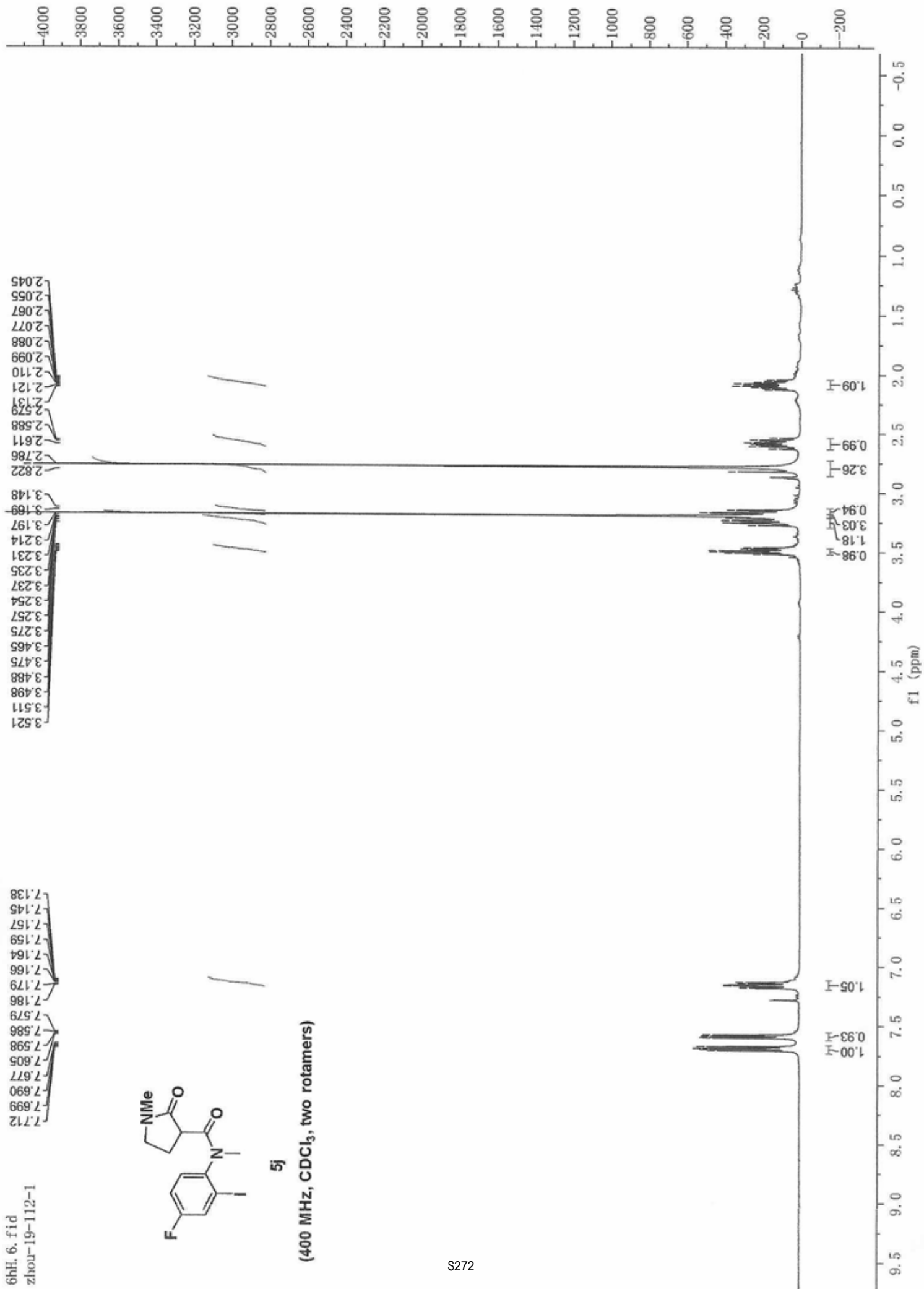


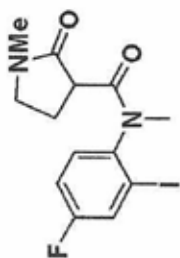


5i

(100 MHz, CDCl<sub>3</sub>, two rotamers)

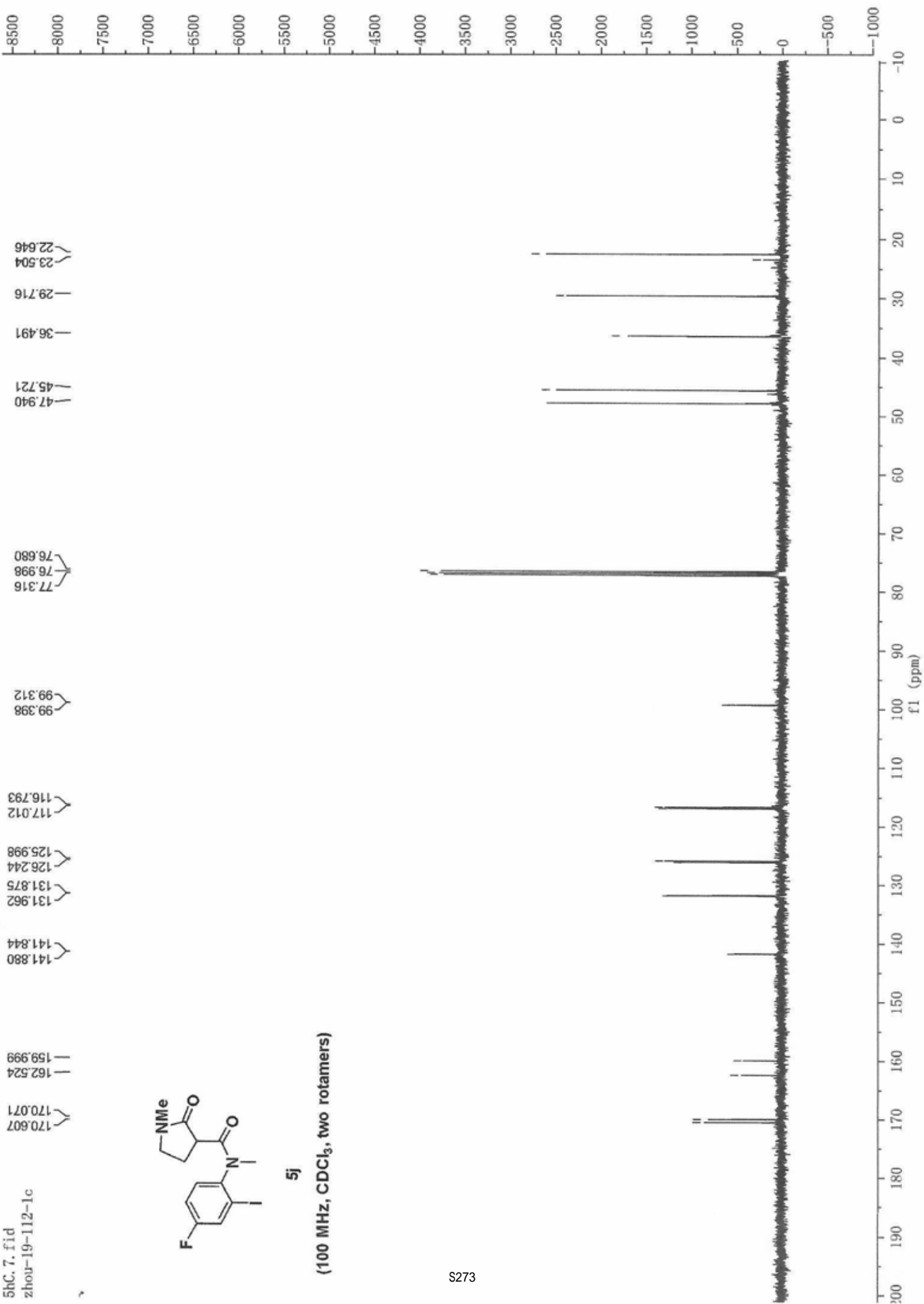


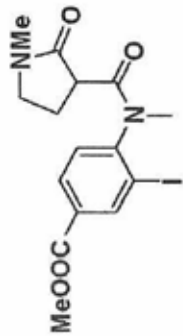




5j

(100 MHz, CDCl<sub>3</sub>, two rotamers)



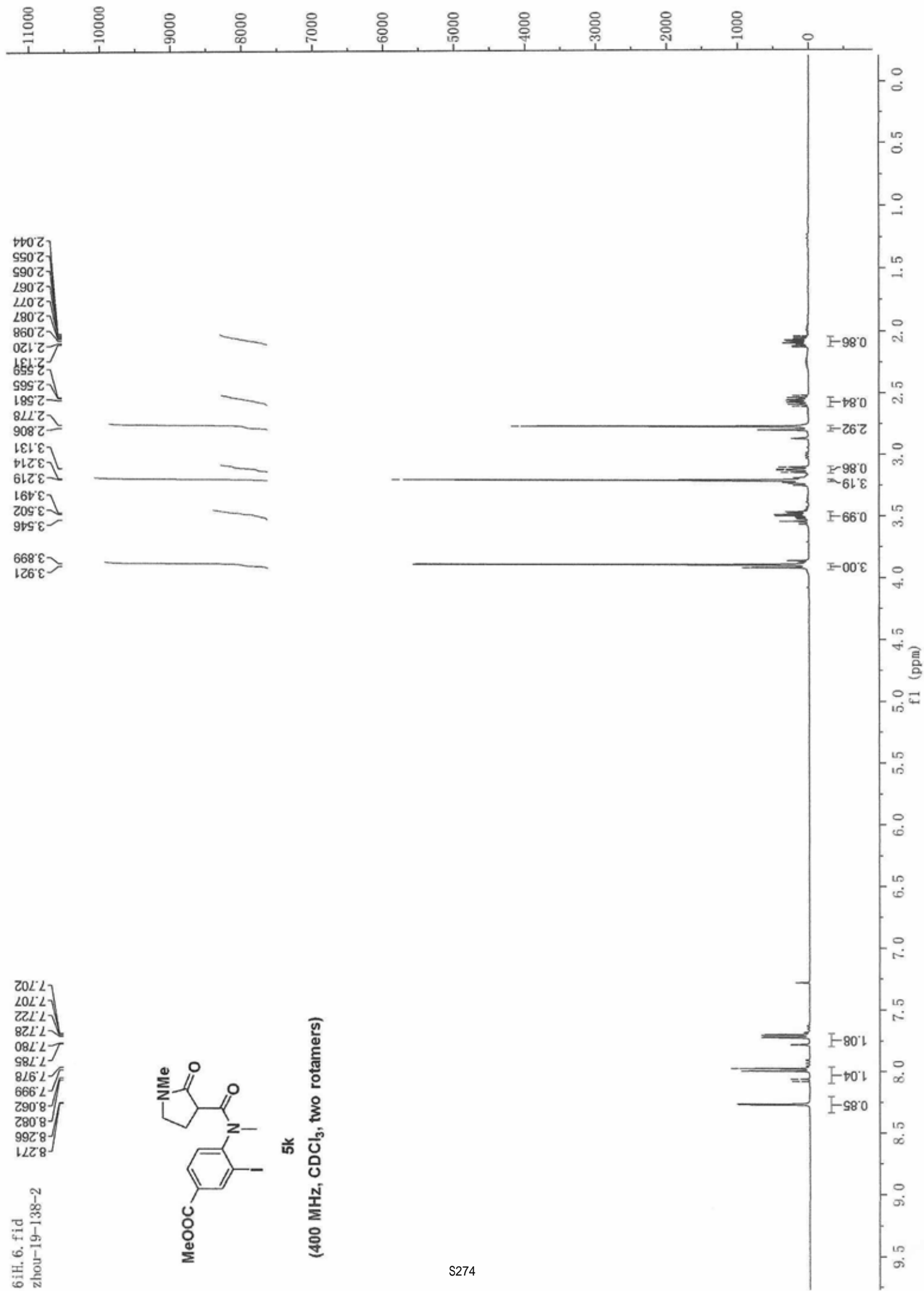


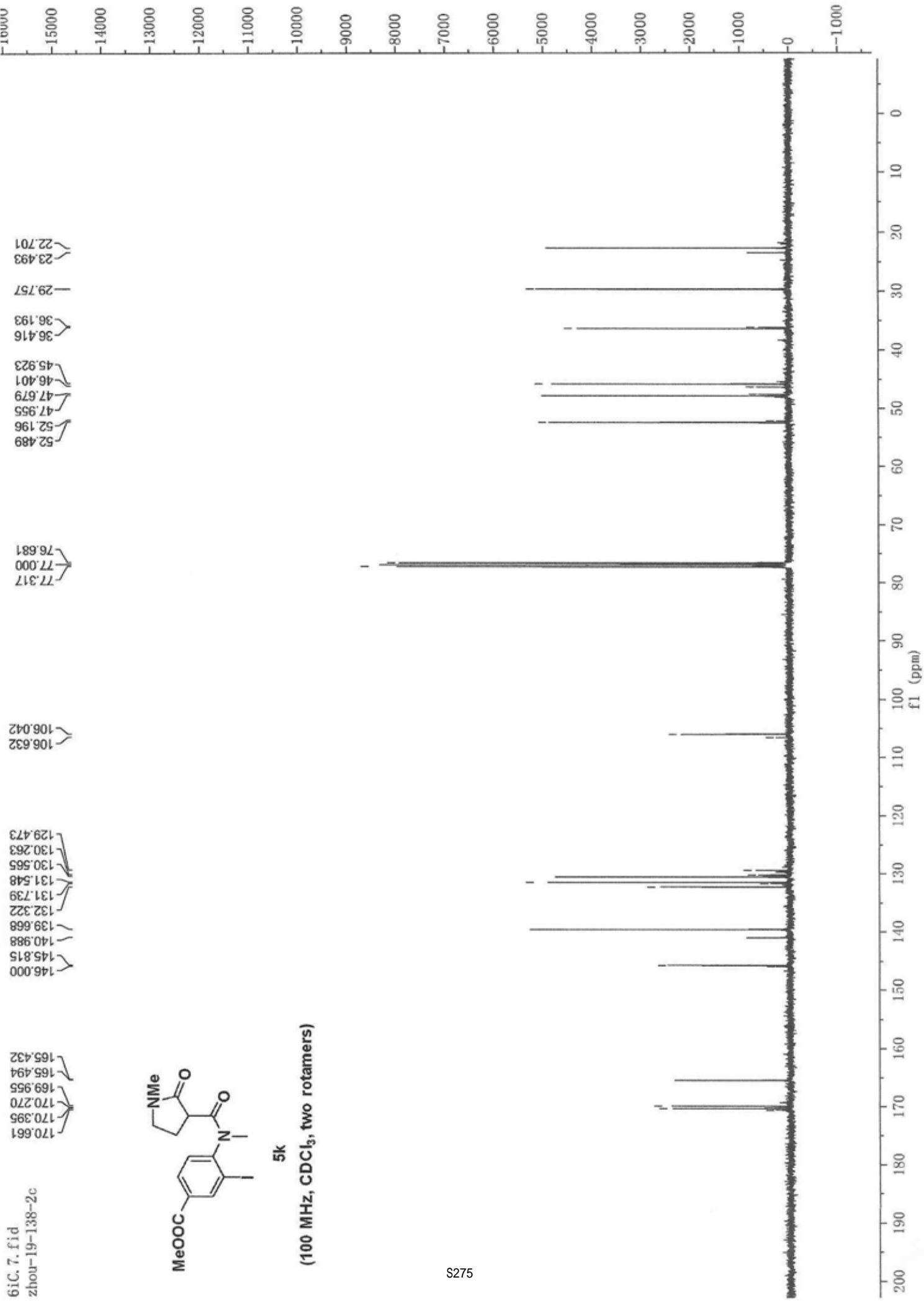
5k

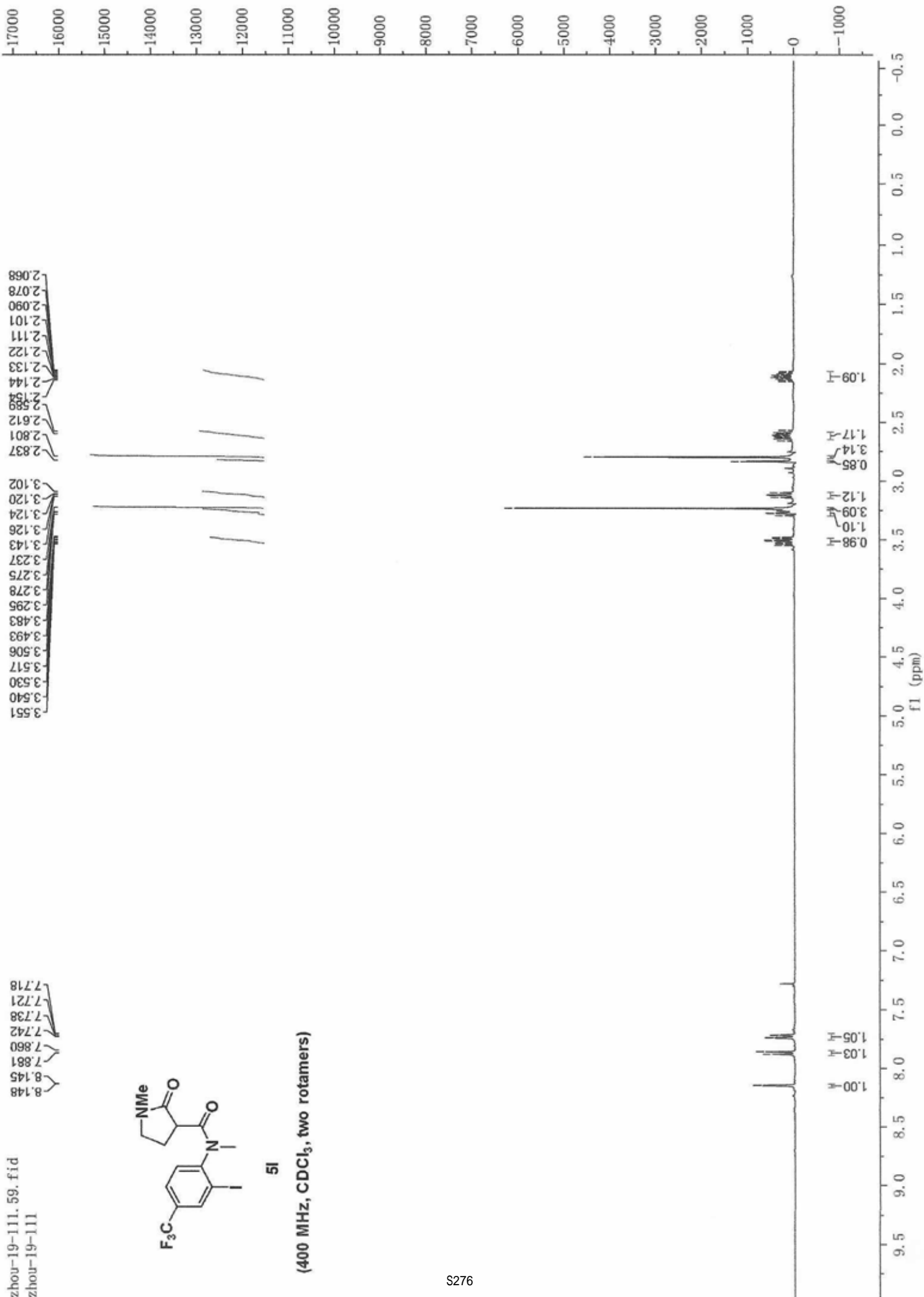
(400 MHz, CDCl<sub>3</sub>, two rotamers)

3.921  
3.899  
3.546  
3.502  
3.491  
3.219  
3.214  
3.131  
2.806  
2.778  
2.581  
2.565  
2.559  
2.120  
2.098  
2.087  
2.077  
2.067  
2.065  
2.055  
2.044

8.271  
8.266  
8.082  
8.062  
7.999  
7.978  
7.785  
7.780  
7.728  
7.722  
7.707  
7.702

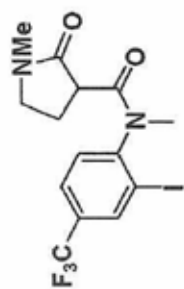






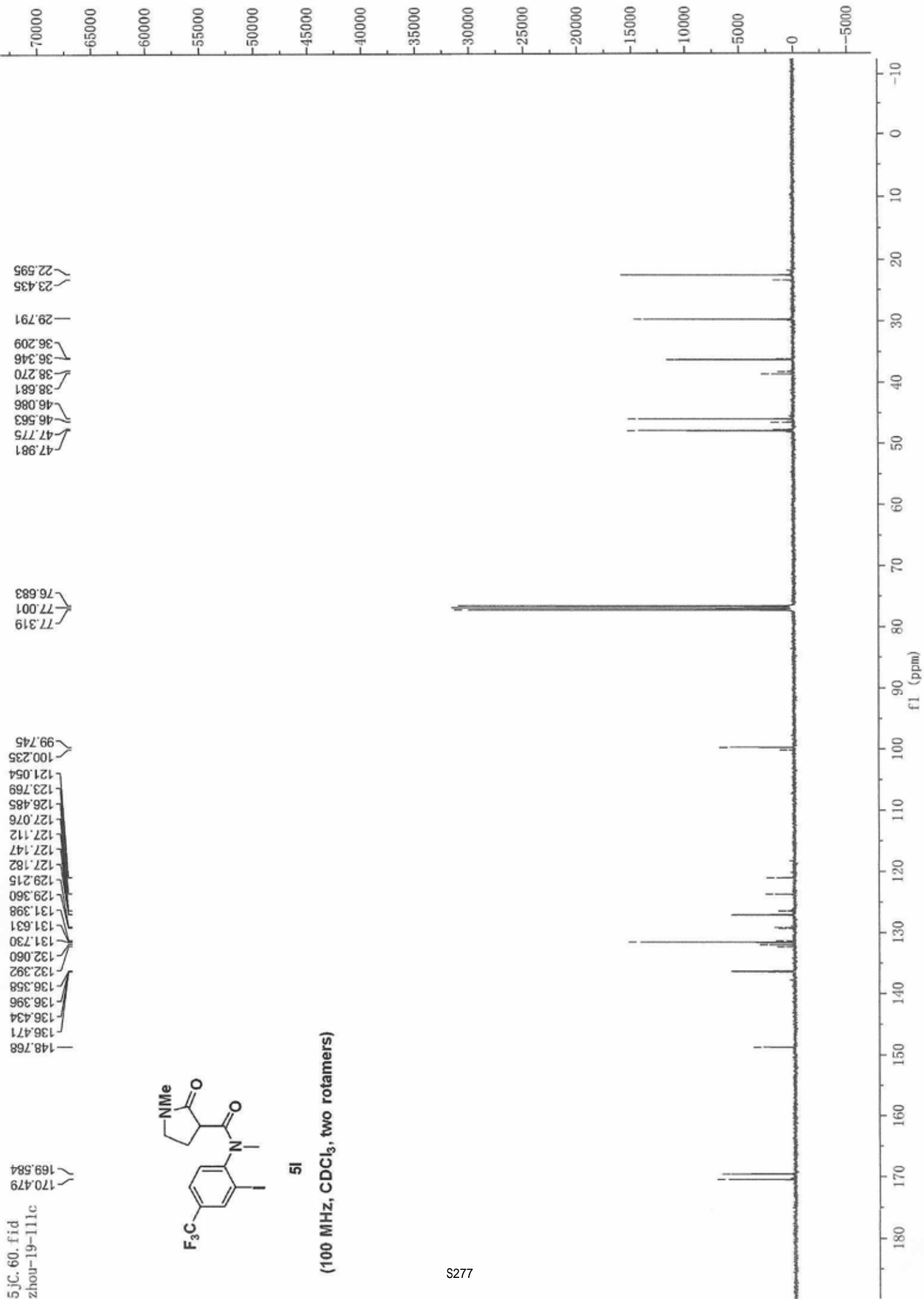
zhou-19-111.59.fid  
zhou-19-111

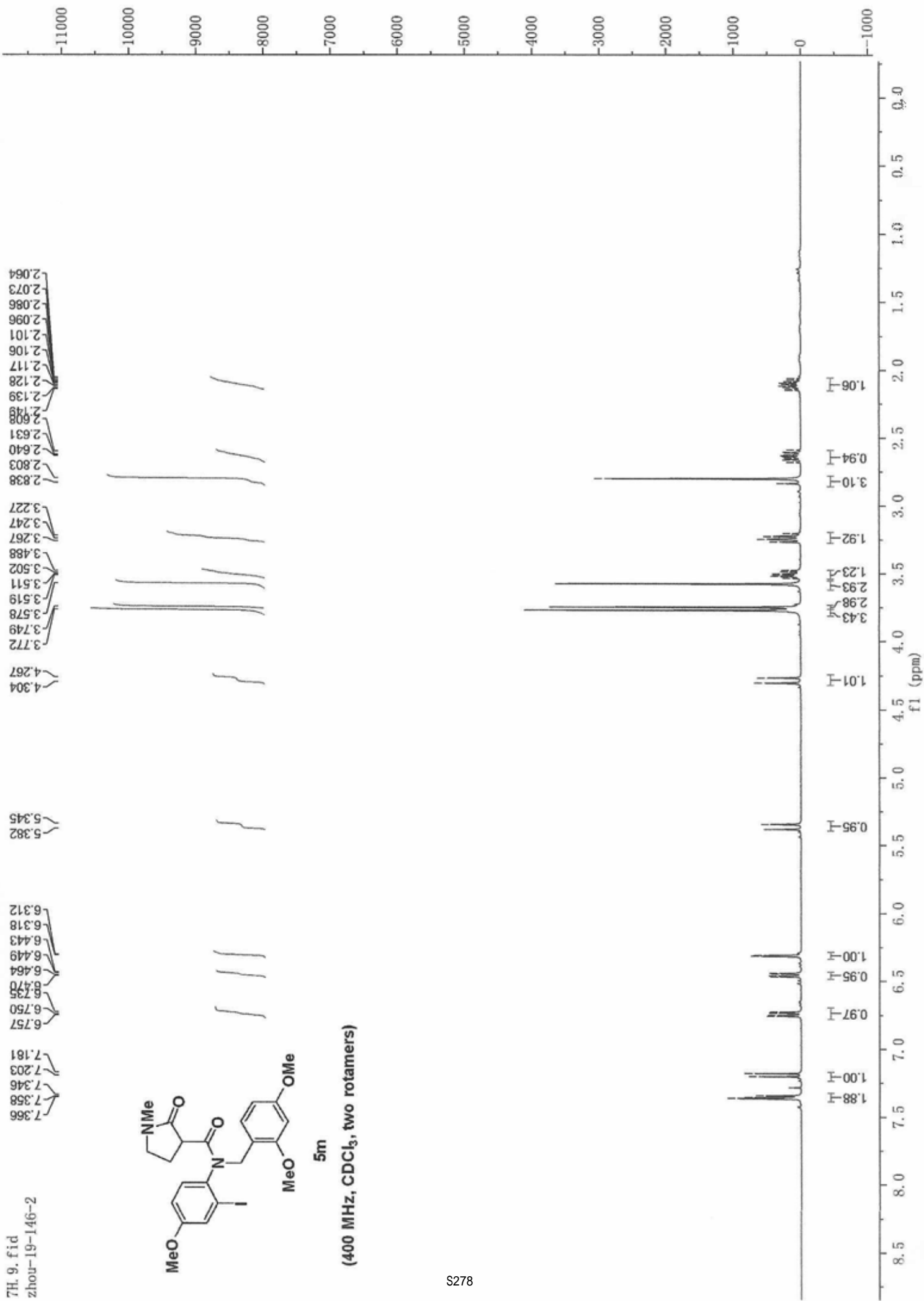


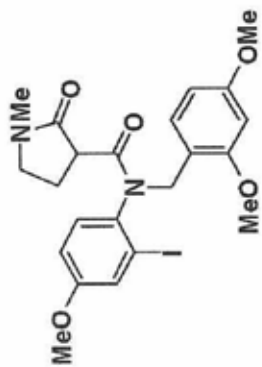


5i

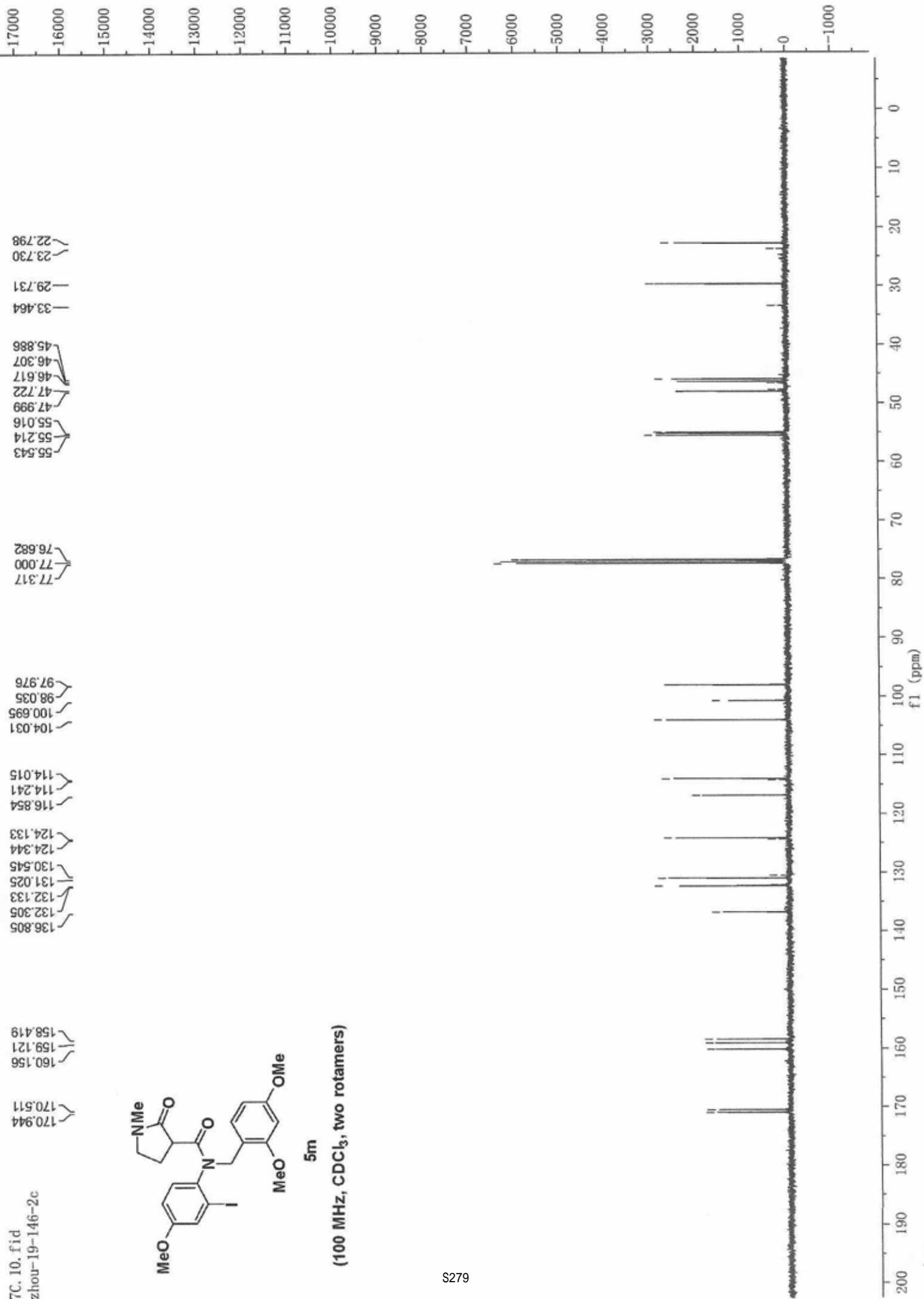
(100 MHz, CDCl<sub>3</sub>, two rotamers)

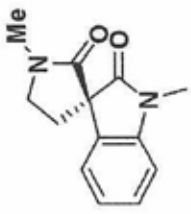




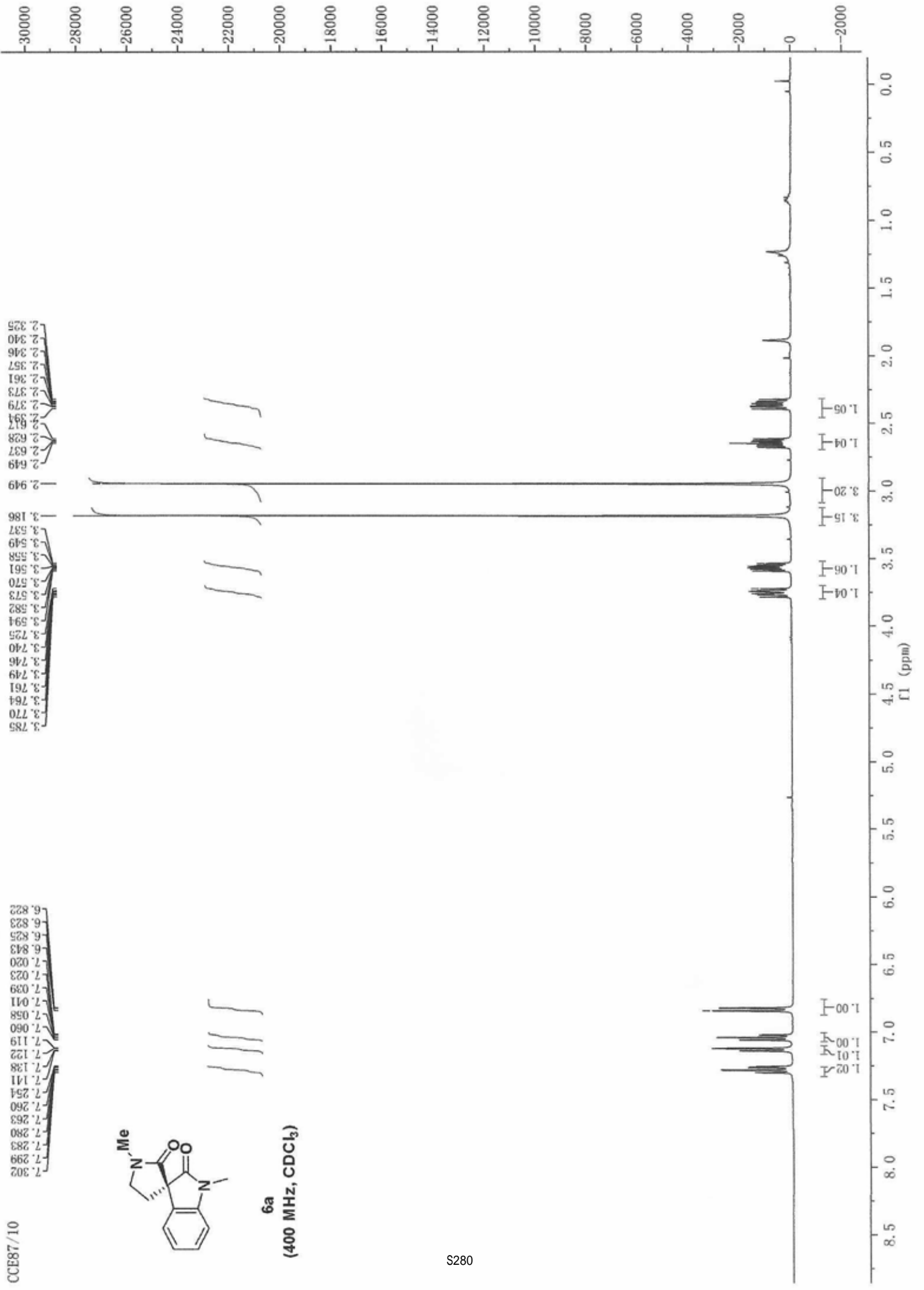


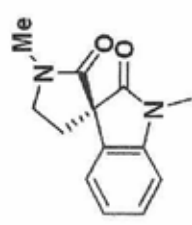
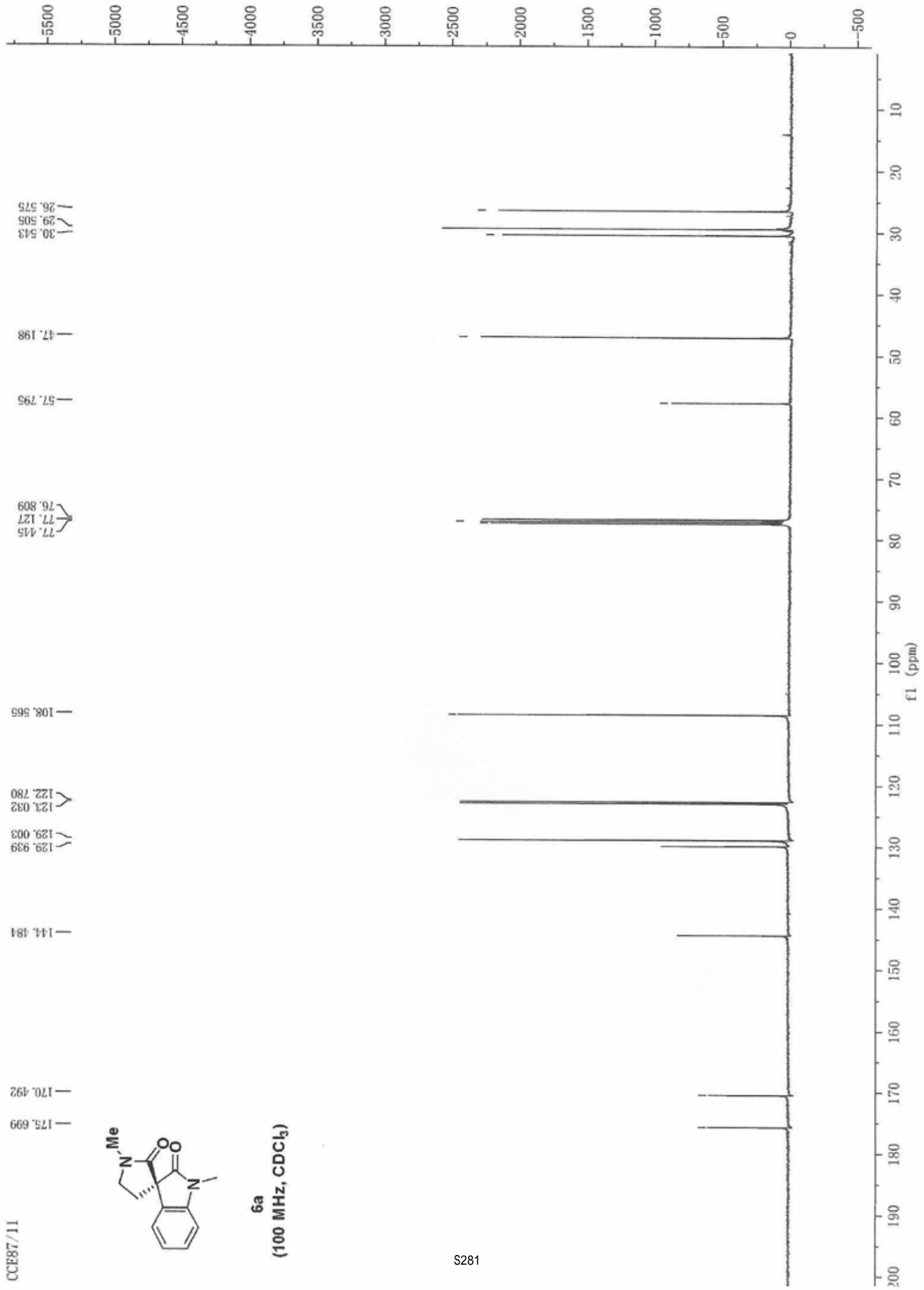
5m  
(100 MHz, CDCl<sub>3</sub>, two rotamers)





6a  
(400 MHz, CDCl<sub>3</sub>)

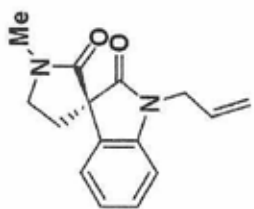




**6a**  
(100 MHz, CDCl<sub>3</sub>)

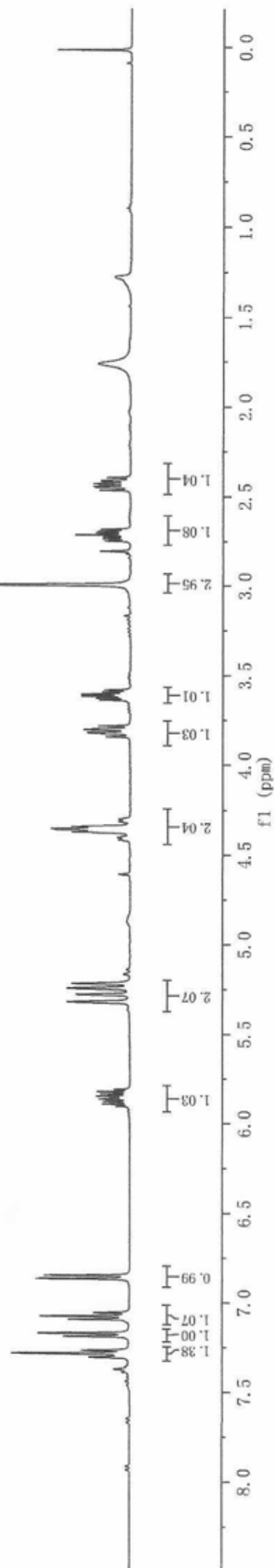
zhou-19-122-2  
zhou-19-122-2

7.306  
7.285  
7.267  
7.189  
7.172  
7.091  
7.076  
7.057  
6.868  
6.848  
5.905  
5.893  
5.880  
5.867  
5.863  
5.851  
5.850  
5.837  
5.824  
5.812  
5.823  
5.280  
5.246  
5.219  
4.416  
4.403  
4.375  
4.370  
4.366  
4.361  
4.356  
4.347  
4.343  
4.314  
4.302  
3.829  
3.822  
3.806  
3.801  
3.785  
3.641  
3.630  
3.619  
3.607  
3.596  
2.740  
2.730  
2.718  
2.707  
2.697  
2.686  
2.688  
2.452  
2.446  
2.435  
2.431  
2.419  
2.413  
2.398

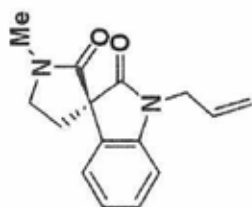


6b

(400 MHz, CDCl<sub>3</sub>)



zhou-19-122-2c  
zhou-19-122-2c



6b

(100 MHz, CDCl<sub>3</sub>)

175.511  
170.459  
143.703  
130.779  
129.950  
128.894  
123.007  
122.864  
117.571  
109.364  
77.371  
77.053  
76.735  
57.804  
47.224  
42.479  
30.553  
29.379

f1 (ppm)

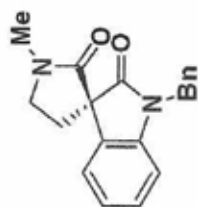
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

zhou-19-NBn  
zhou-19-NBn

7.324  
7.313  
7.242  
7.231  
7.189  
7.170  
7.152  
7.045  
7.027  
7.007  
6.701  
6.681

5.032  
4.993  
4.861  
4.822

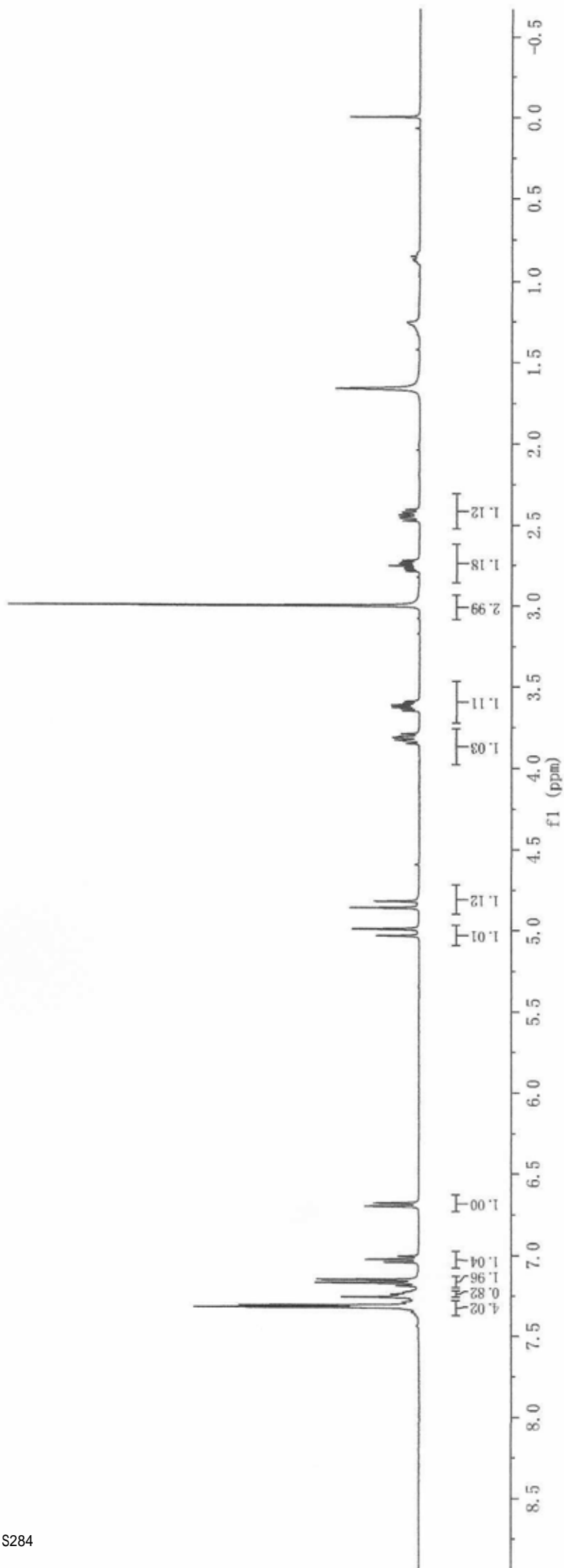
3.852  
3.836  
3.829  
3.813  
3.807  
3.792  
3.648  
3.637  
3.626  
3.614  
3.603  
3.592  
3.002  
2.755  
2.743  
2.734  
2.718  
2.463  
2.457  
2.442  
2.430  
2.424  
2.409



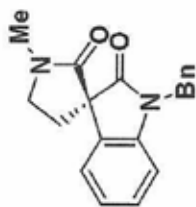
6c

(400 MHz, CDCl<sub>3</sub>)

S284







6c

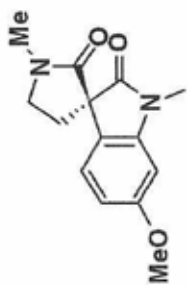
(100 MHz, CDCl<sub>3</sub>)

175.941  
170.502  
143.575  
135.316  
130.000  
128.917  
128.847  
127.573  
127.076  
123.090  
122.837  
109.583  
57.883  
47.283  
43.932  
30.585  
29.392

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

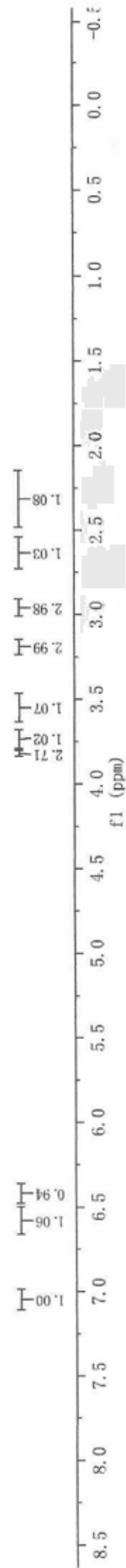
zhou-19-1-OMeH  
zhou-19-1-OMeH



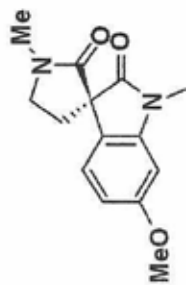
6d  
(400 MHz, CDCl<sub>3</sub>)

3.807  
3.792  
3.776  
3.771  
3.768  
3.755  
3.752  
3.747  
3.731  
3.573  
3.562  
3.551  
3.540  
3.528  
3.517  
3.181  
2.988  
2.631  
2.620  
2.610  
2.588  
2.584  
2.362  
2.346  
2.335  
2.330  
2.319  
2.311  
2.298

7.042  
7.032  
6.563  
6.558  
6.543  
6.537  
6.435  
6.429

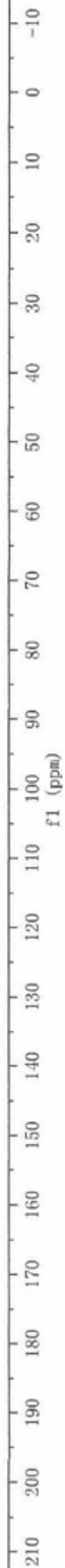


zhou-19-I-OMeC  
zhou-19-I-OMeC



6d  
(100 MHz, CDCl<sub>3</sub>)

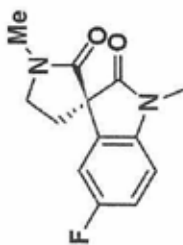
176.312  
170.800  
160.850  
145.803  
123.468  
121.812  
106.902  
96.647  
77.380  
77.063  
76.745  
57.314  
55.614  
47.125  
30.562  
29.602  
26.585



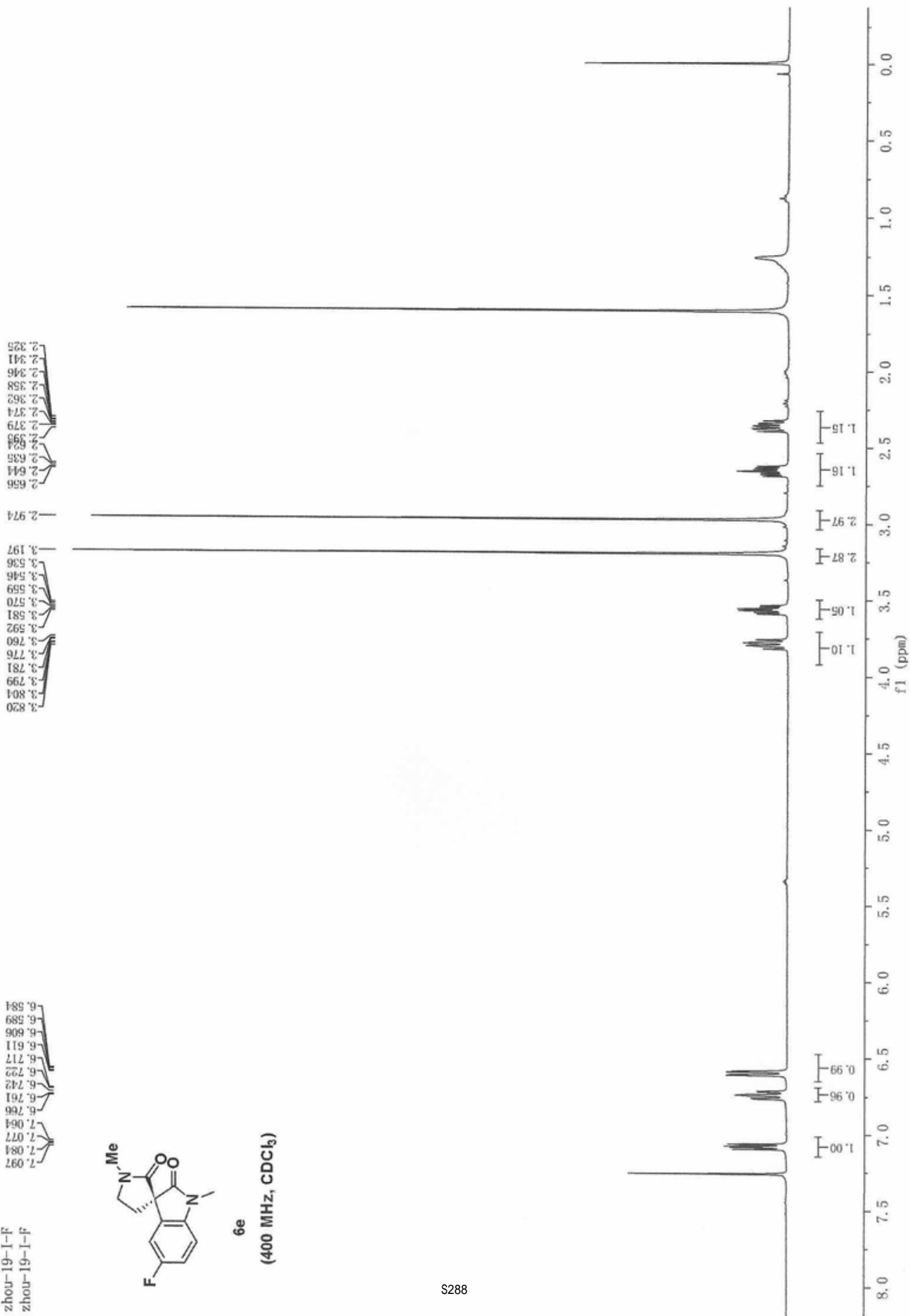
zhou-19-I-F  
zhou-19-I-F

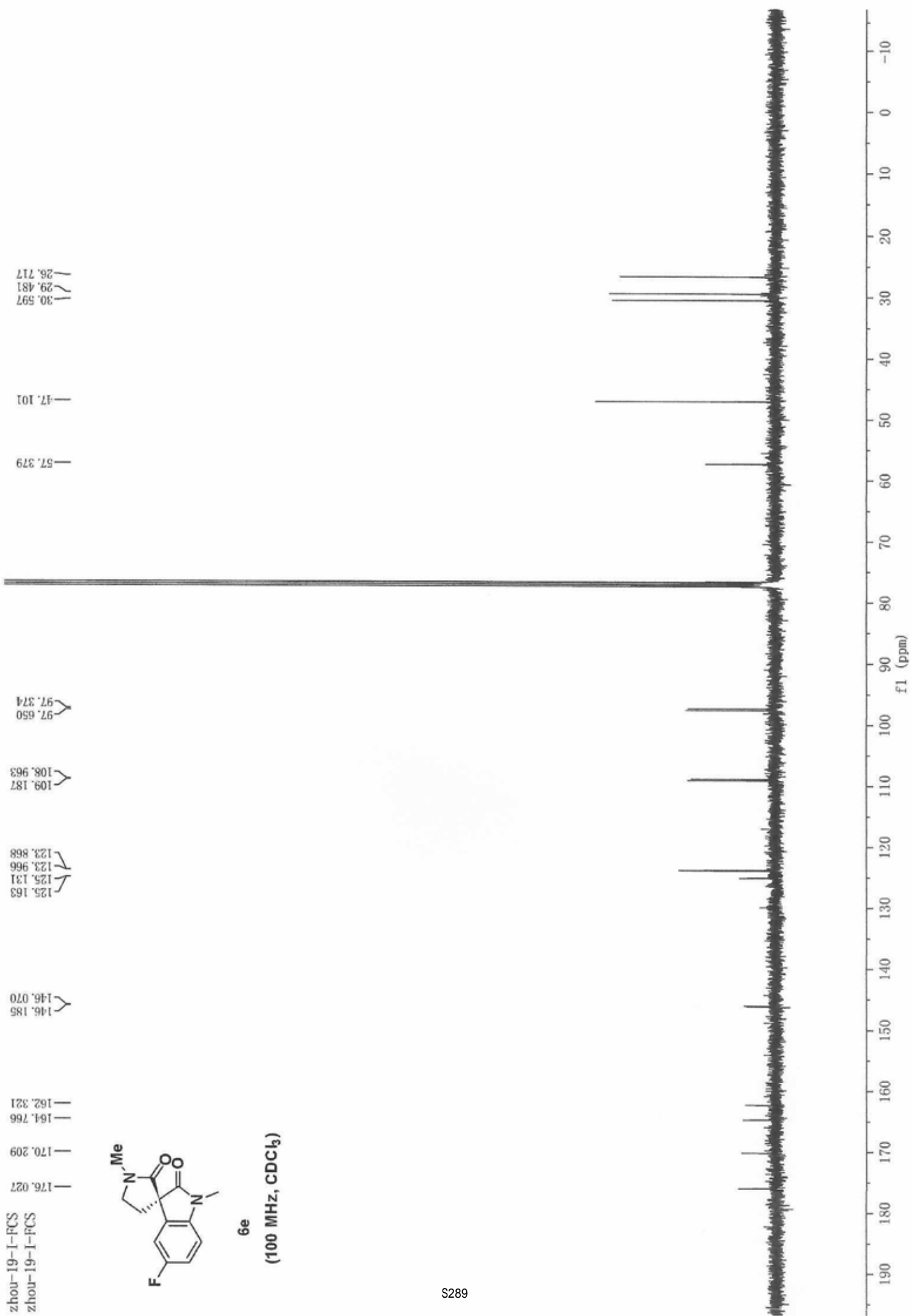
7.097  
7.084  
7.077  
7.064  
7.066  
7.061  
7.042  
7.022  
7.017  
7.011  
7.006  
7.006  
6.989  
6.984

3.820  
3.804  
3.799  
3.781  
3.776  
3.760  
3.592  
3.581  
3.570  
3.559  
3.546  
3.536  
3.197  
2.974  
2.656  
2.644  
2.635  
2.599  
2.594  
2.379  
2.374  
2.362  
2.358  
2.346  
2.341  
2.325



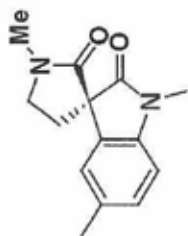
6e  
(400 MHz, CDCl<sub>3</sub>)





zhou-19-1119-3  
zhou-19-1119-3

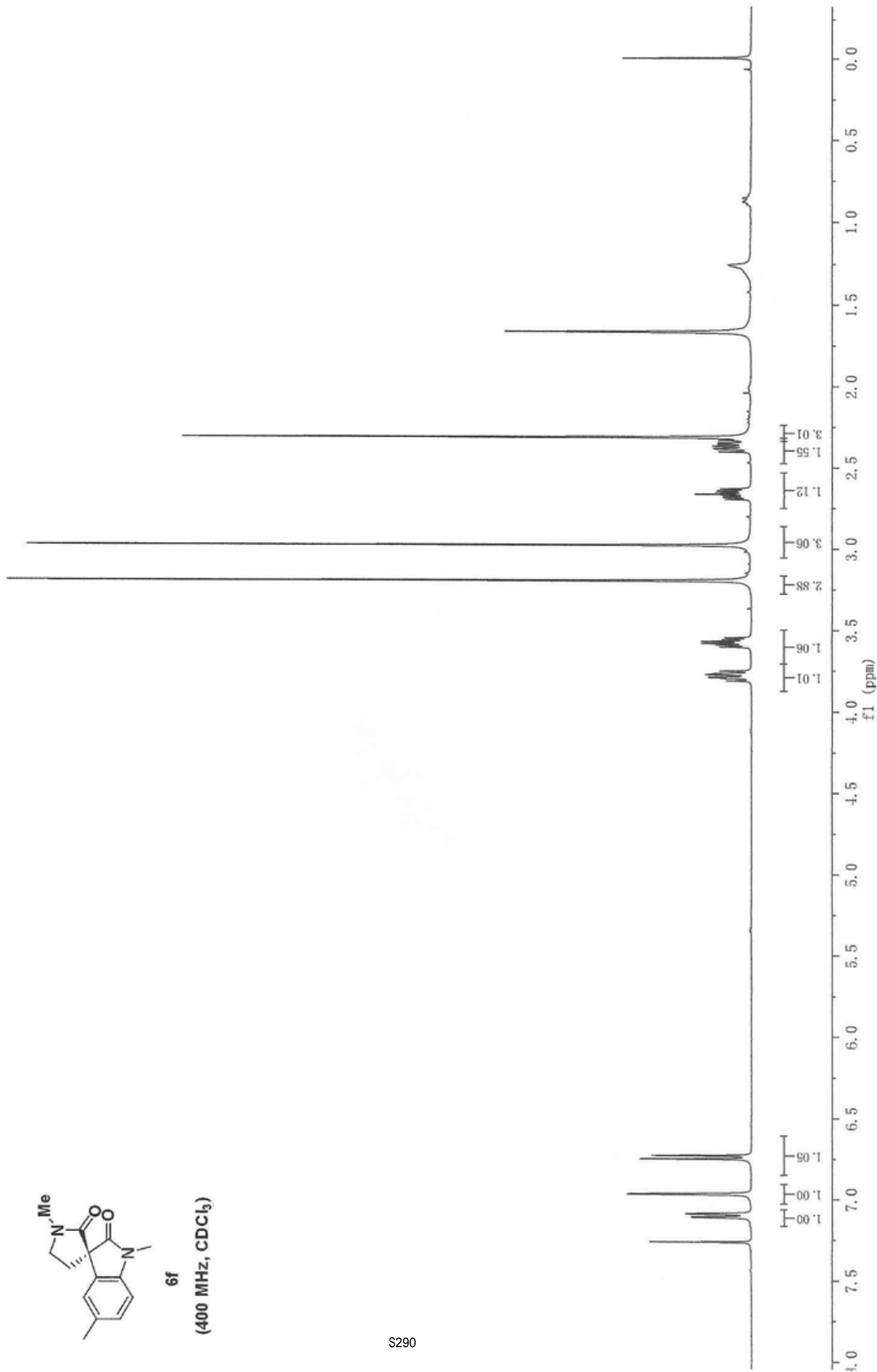
7.108  
7.088  
6.965  
6.749  
6.729



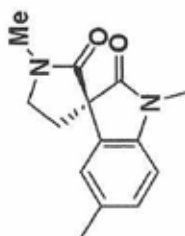
6f

(400 MHz, CDCl<sub>3</sub>)

3.812  
3.796  
3.789  
3.773  
3.768  
3.752  
3.604  
3.592  
3.582  
3.570  
3.559  
3.547  
3.195  
2.977  
2.664  
2.652  
2.643  
2.631  
2.603  
2.387  
2.381  
2.370  
2.366  
2.354  
2.349  
2.333  
2.314

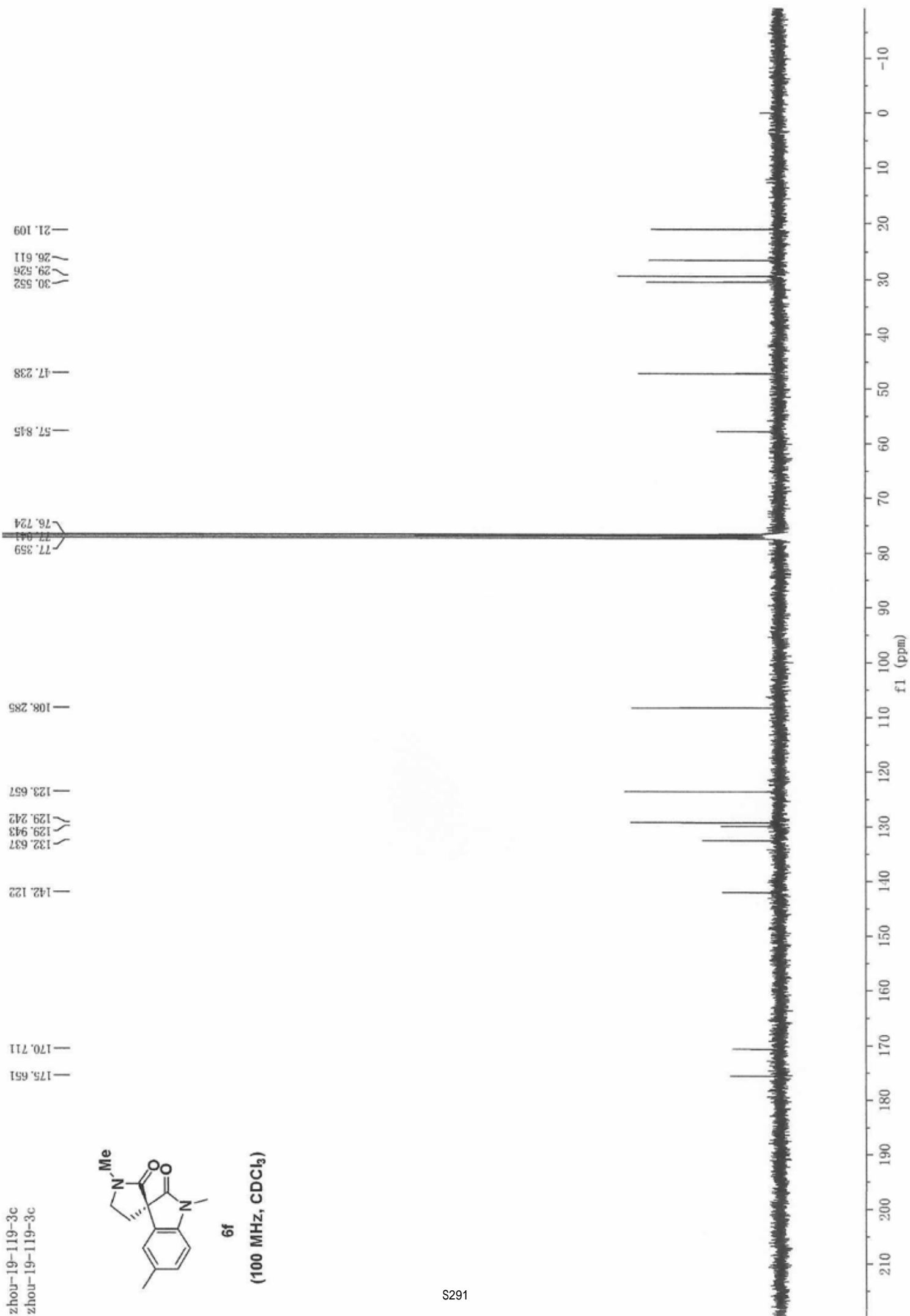


zhou-19-119-3c  
zhou-19-119-3c



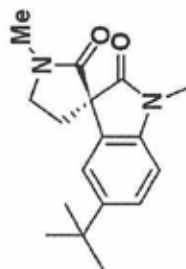
6f

(100 MHz, CDCl<sub>3</sub>)



zhou-19-107-2  
zhou-19-107-2

7.346  
7.341  
7.325  
7.321  
7.163  
7.158  
6.795  
6.775



**6g**  
(400 MHz, CDCl<sub>3</sub>)

3.838  
3.817  
3.798  
3.777  
3.610  
3.600  
3.588  
3.578  
3.565  
3.555  
2.685  
2.675  
2.664  
2.653  
2.642  
2.631  
2.621  
2.439  
2.422  
2.417  
2.406  
2.400  
2.389  
2.384  
2.367

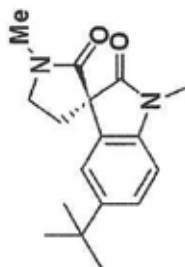
1.298

0.96  
1.04  
2.79  
3.00  
1.03  
9.06

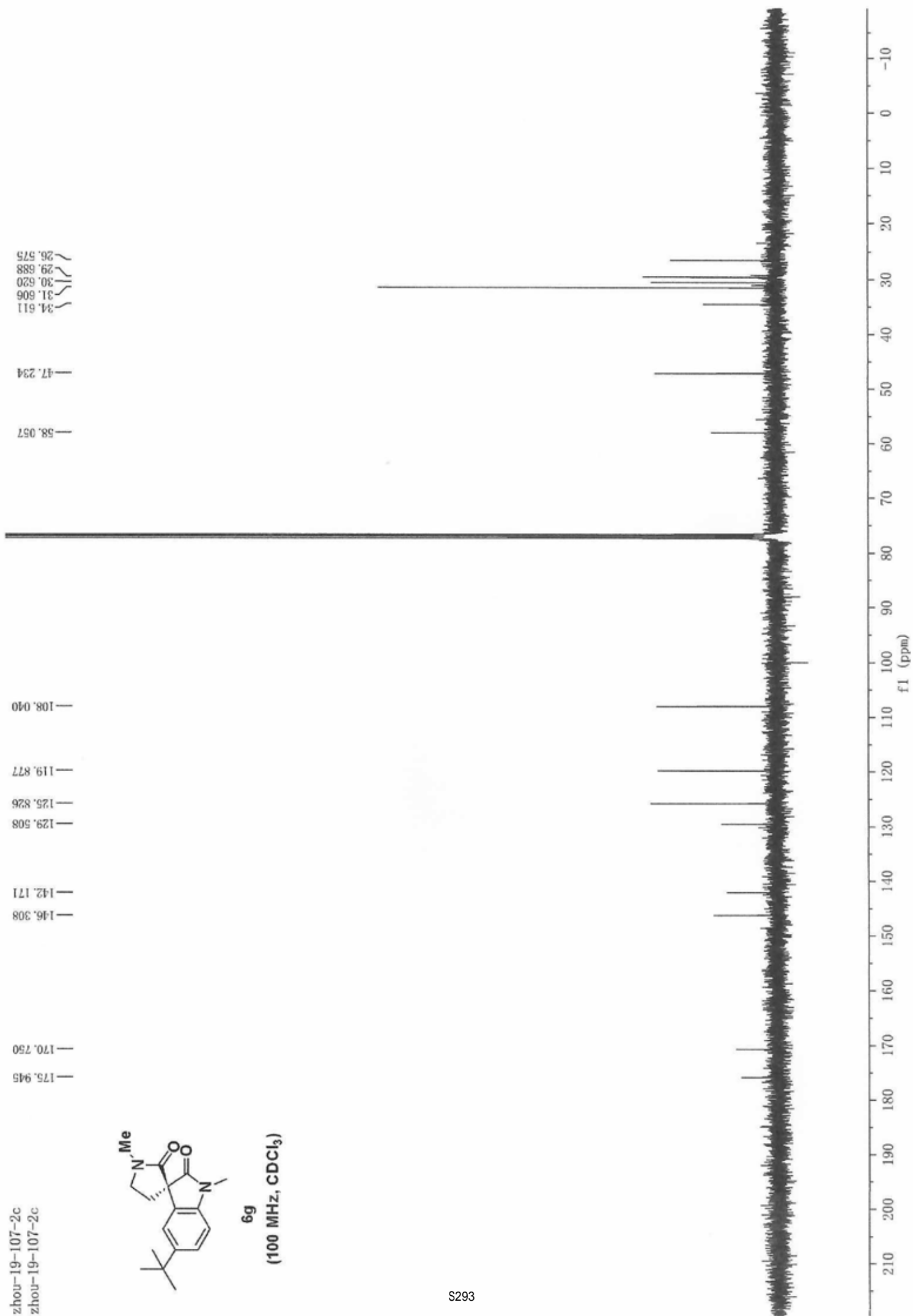
f1 (ppm)



zhou-19-107-2c  
zhou-19-107-2c



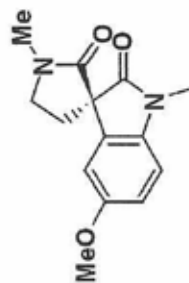
**6g**  
(100 MHz, CDCl<sub>3</sub>)



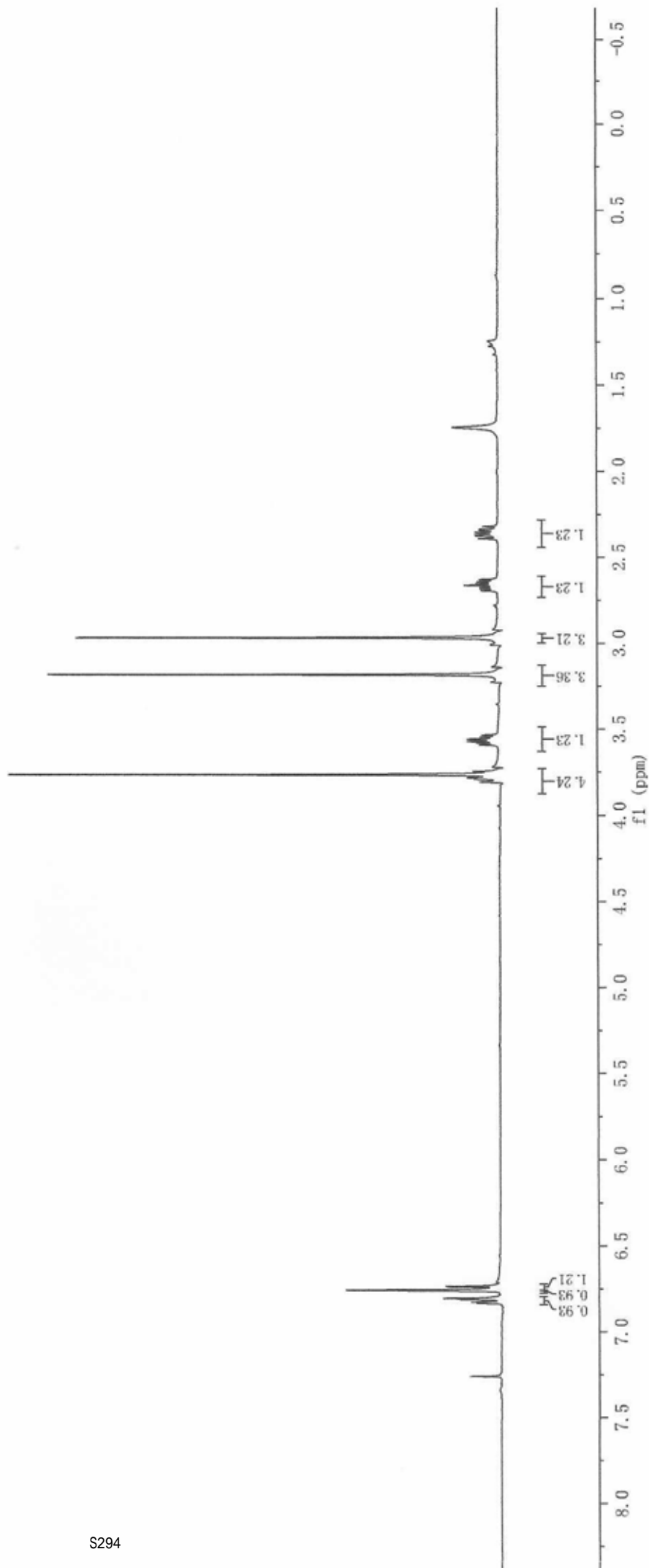
zhou-19-110-3  
zhou-19-110-3

6.834  
6.827  
6.813  
6.808  
6.761  
6.757  
6.737

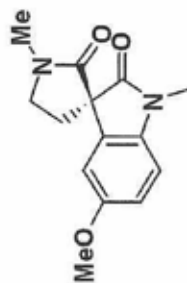
3.807  
3.791  
3.786  
3.767  
3.747  
3.693  
3.582  
3.571  
3.560  
3.548  
3.537  
3.185  
2.969  
2.665  
2.654  
2.644  
2.993  
2.377  
2.372  
2.360  
2.356  
2.345  
2.339  
2.323



6h  
(400 MHz, CDCl<sub>3</sub>)

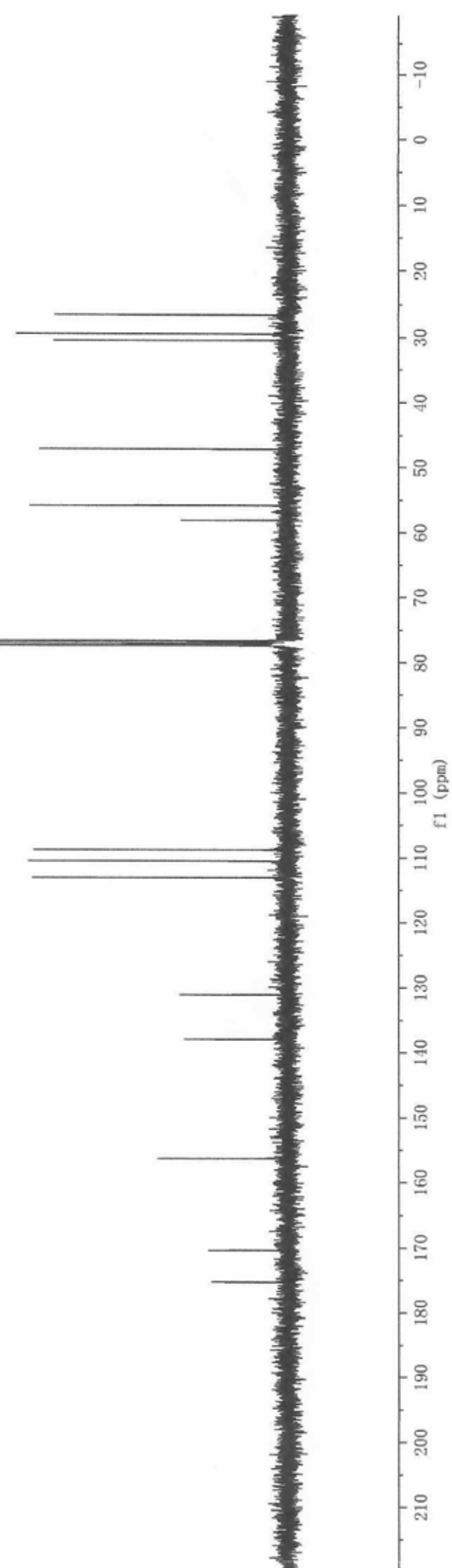


zhou-19-110-3c  
zhou-19-110-3c



6h  
(100 MHz, CDCl<sub>3</sub>)

175.373  
170.487  
156.347  
138.014  
131.082  
113.129  
110.534  
108.853  
77.378  
77.060  
76.743  
58.170  
55.878  
47.206  
30.559  
29.553  
26.667

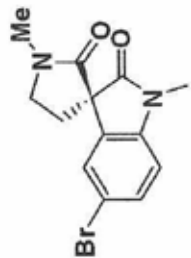


zhou-19-109-2s  
zhou-19-109-2s

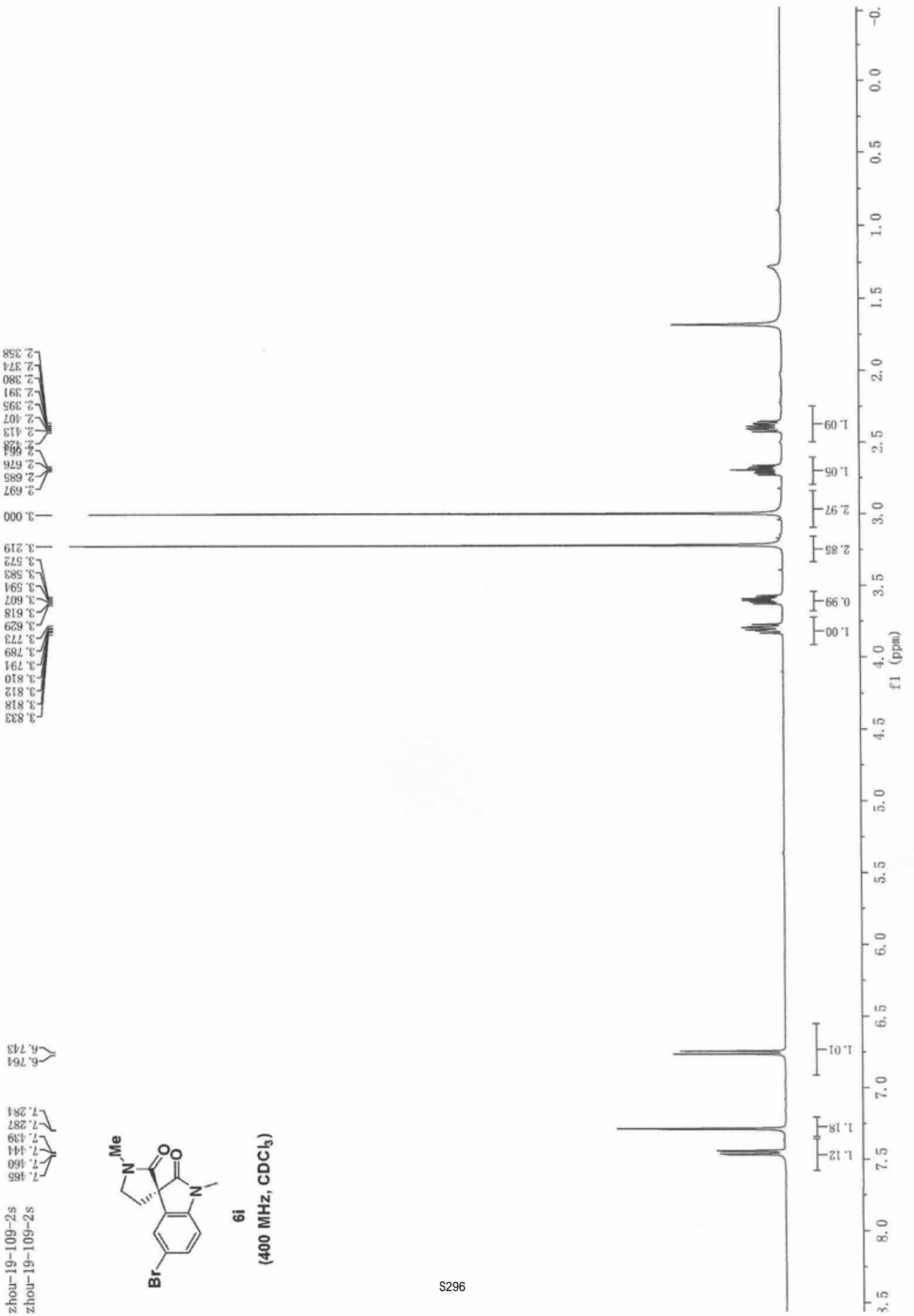
7.465  
7.460  
7.444  
7.439  
7.287  
7.284

6.764  
6.743

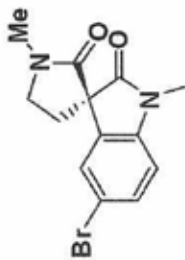
3.833  
3.818  
3.812  
3.810  
3.791  
3.789  
3.773  
3.629  
3.618  
3.607  
3.594  
3.572  
3.572  
3.583  
3.219  
3.000  
2.697  
2.685  
2.676  
2.668  
2.428  
2.413  
2.407  
2.395  
2.391  
2.380  
2.374  
2.358



**6i**  
(400 MHz, CDCl<sub>3</sub>)

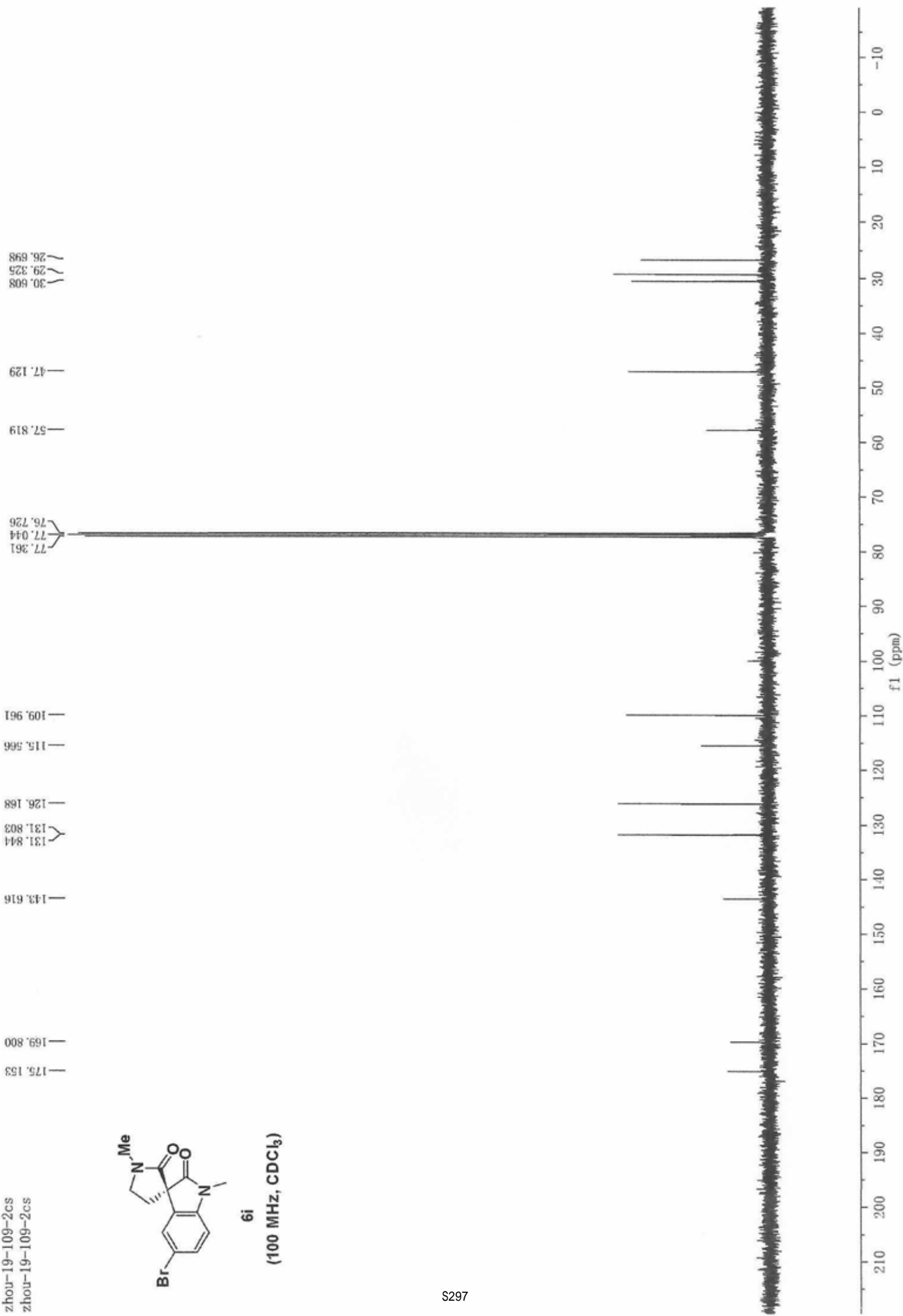


zhou-19-109-2cs  
zhou-19-109-2cs



6i

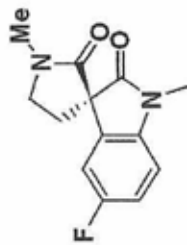
(100 MHz, CDCl<sub>3</sub>)



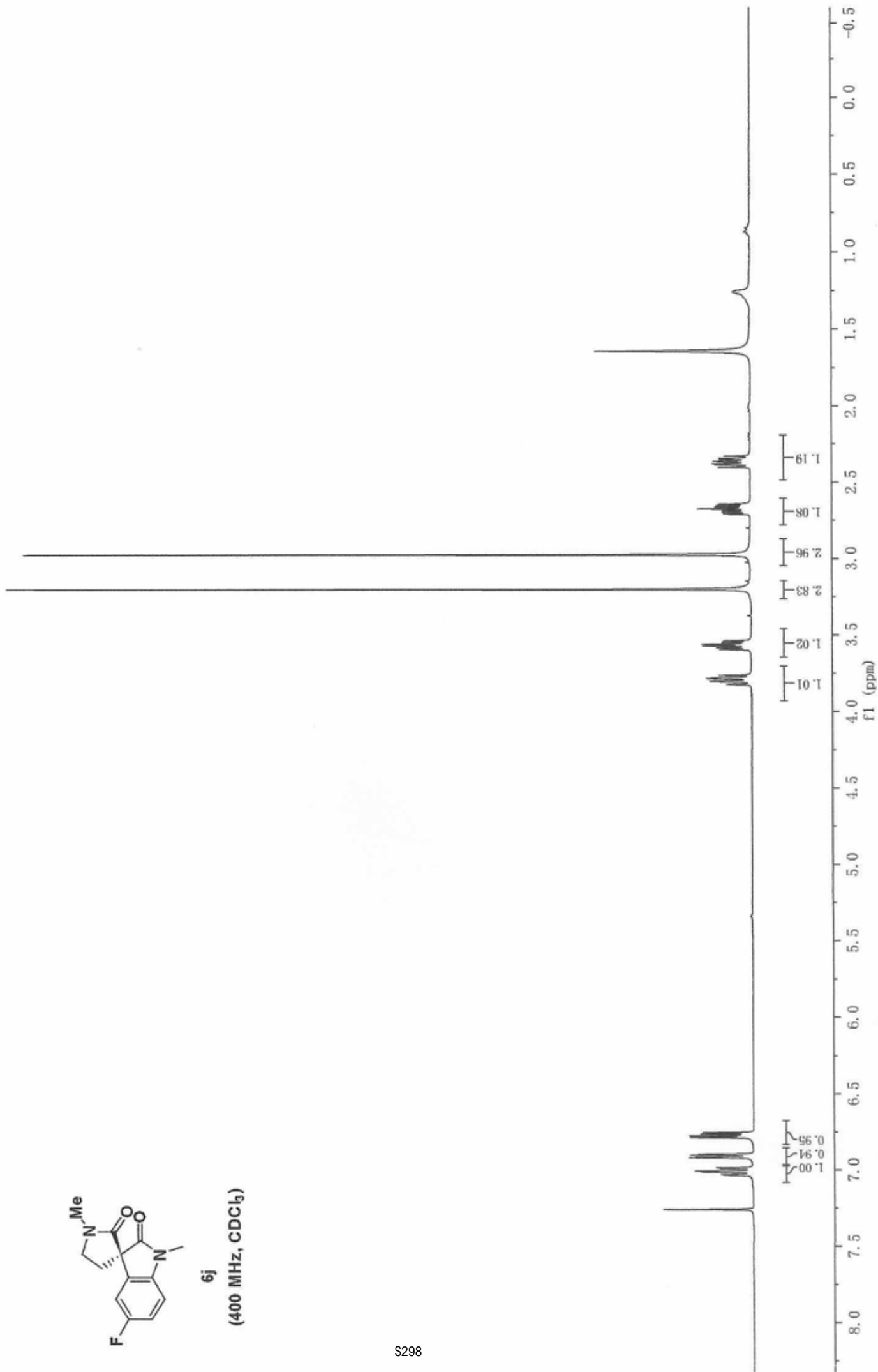
zhou-19-116-1  
zhou-19-116-1

7.035  
7.029  
7.013  
7.007  
6.991  
6.985  
6.921  
6.914  
6.901  
6.895  
6.787  
6.777  
6.766  
6.756

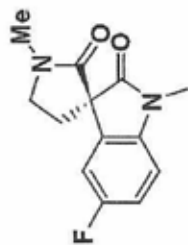
3.827  
3.811  
3.806  
3.803  
3.787  
3.782  
3.766  
3.597  
3.586  
3.574  
3.563  
3.551  
3.540  
3.203  
2.977  
2.678  
2.666  
2.656  
2.646  
2.402  
2.386  
2.381  
2.369  
2.365  
2.353  
2.348  
2.331



6j  
(400 MHz, CDCl<sub>3</sub>)



zhou-19-116-1c  
zhou-19-116-1c



6j  
(100 MHz, CDCl<sub>3</sub>)

30.595  
29.412  
28.732

47.126

58.136

115.349  
115.116  
111.303  
111.054  
109.075  
108.994

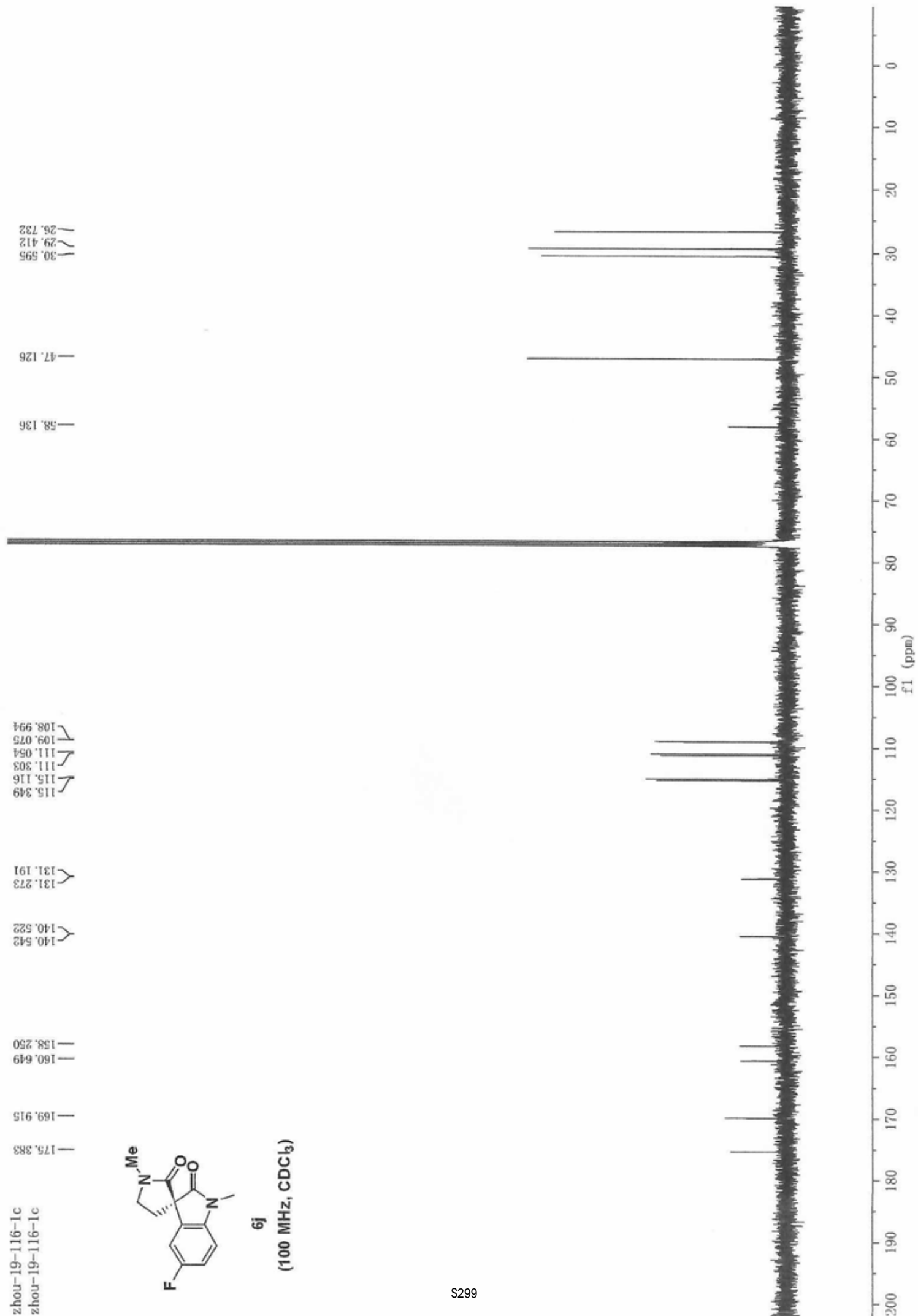
131.273  
131.191

140.542  
140.522

158.250  
160.649

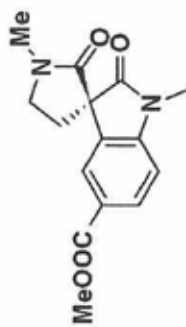
169.915

175.383



zhou-19-140-2  
zhou-19-140-2

7.803  
7.800  
7.784  
7.781  
7.498  
7.495  
7.223  
7.203



6k  
(400 MHz, CDCl<sub>3</sub>)

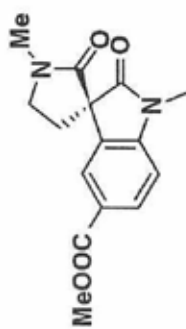
3.926  
3.833  
3.818  
3.813  
3.810  
3.794  
3.789  
3.773  
3.621  
3.610  
3.598  
3.587  
3.576  
3.565  
3.257  
2.976  
2.686  
2.675  
2.665  
2.654  
2.648  
2.422  
2.417  
2.405  
2.401  
2.389  
2.384  
2.368

3.23  
1.11  
1.14  
3.17  
3.17  
1.05  
1.10

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0



zhou-19-140-2c  
zhou-19-140-2c

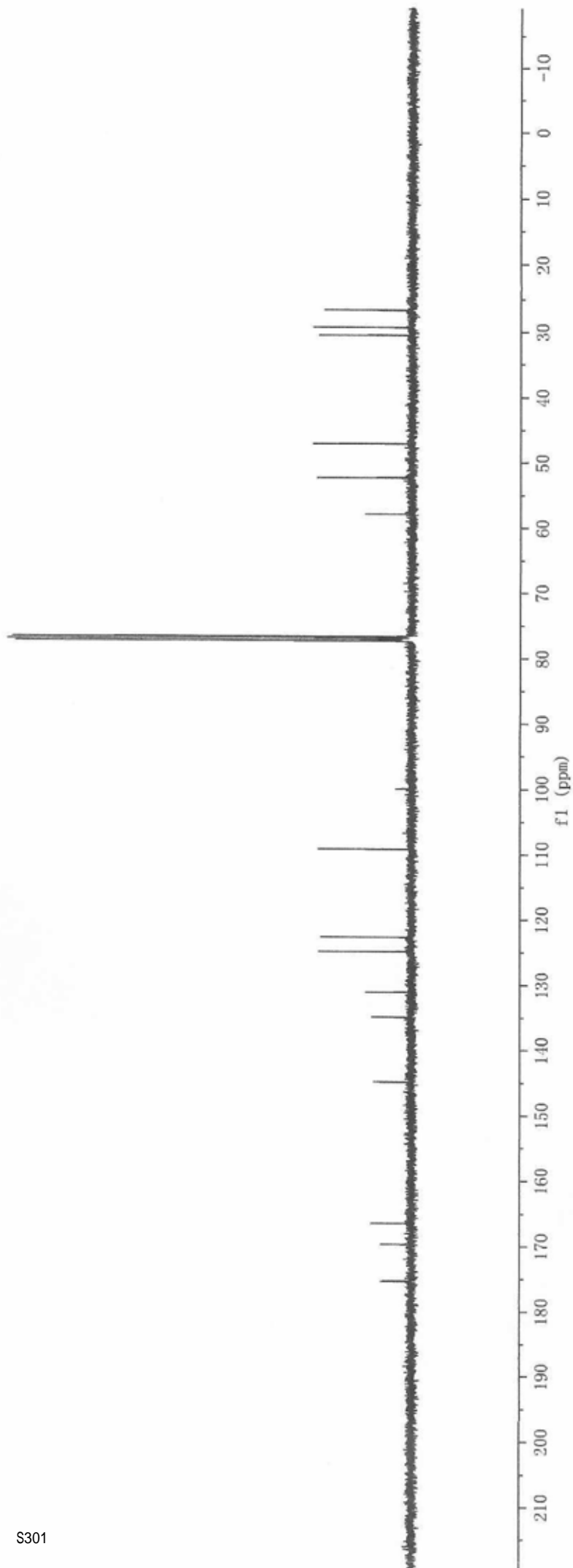


6k  
(100 MHz, CDCl<sub>3</sub>)

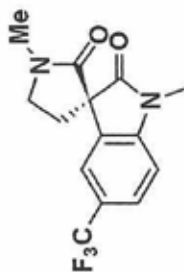
— 57.944  
— 52.377  
— 47.167  
— 30.606  
— 29.368  
— 26.778

— 175.378  
— 169.730  
— 166.517  
— 144.905  
— 134.916  
— 131.084  
— 121.917  
— 122.695  
— 109.168

S301

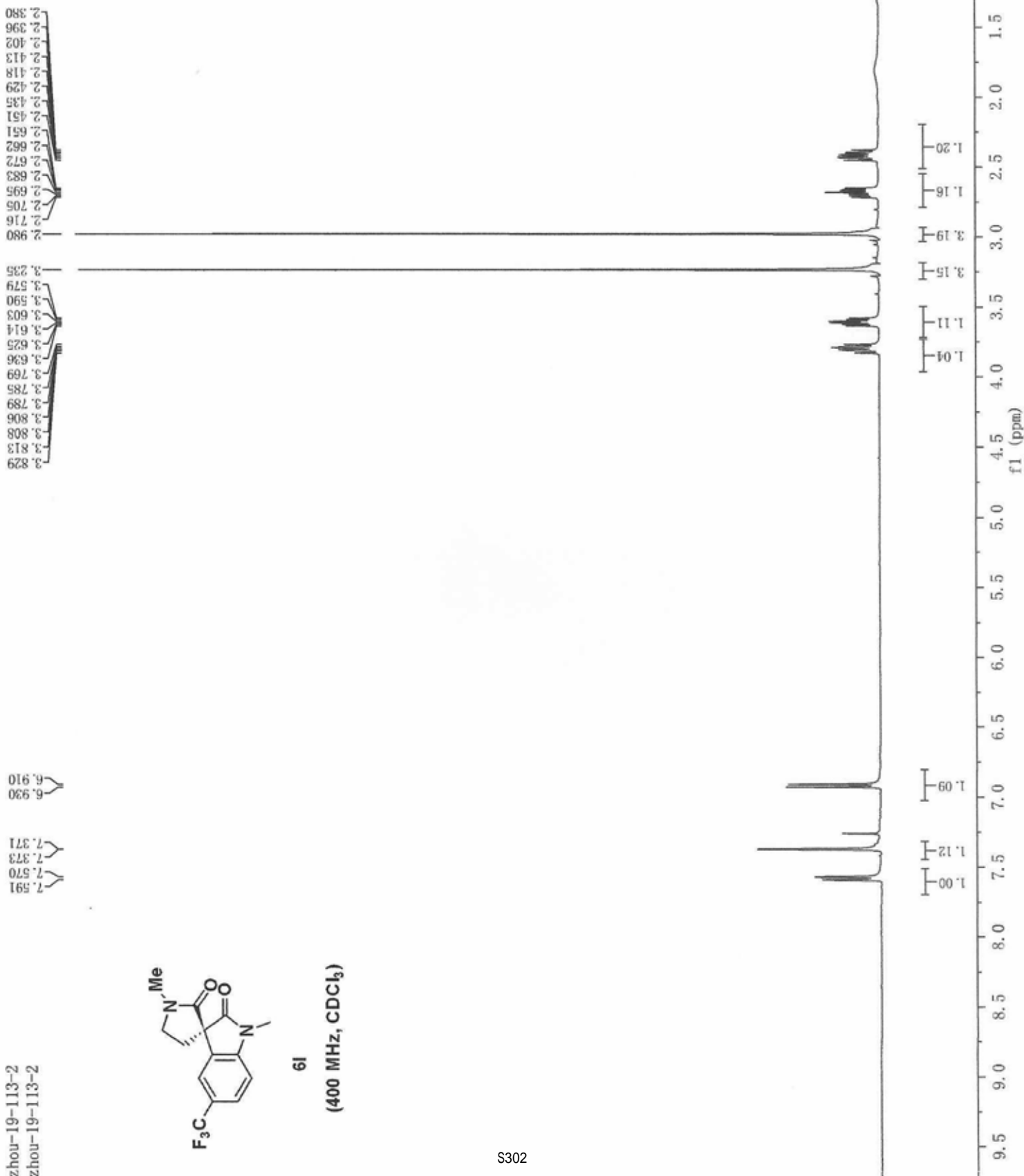


zhou-19-113-2  
zhou-19-113-2



6I

(400 MHz, CDCl<sub>3</sub>)



zhou-19-113-2c  
zhou-19-113-2c

169.584  
175.677

147.565  
147.556

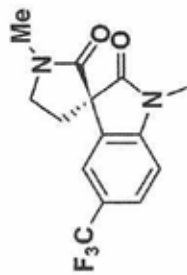
130.412  
126.876  
126.837  
126.797  
125.741  
125.573  
125.415  
125.089  
124.763  
122.873  
120.003  
119.966

108.362

57.715

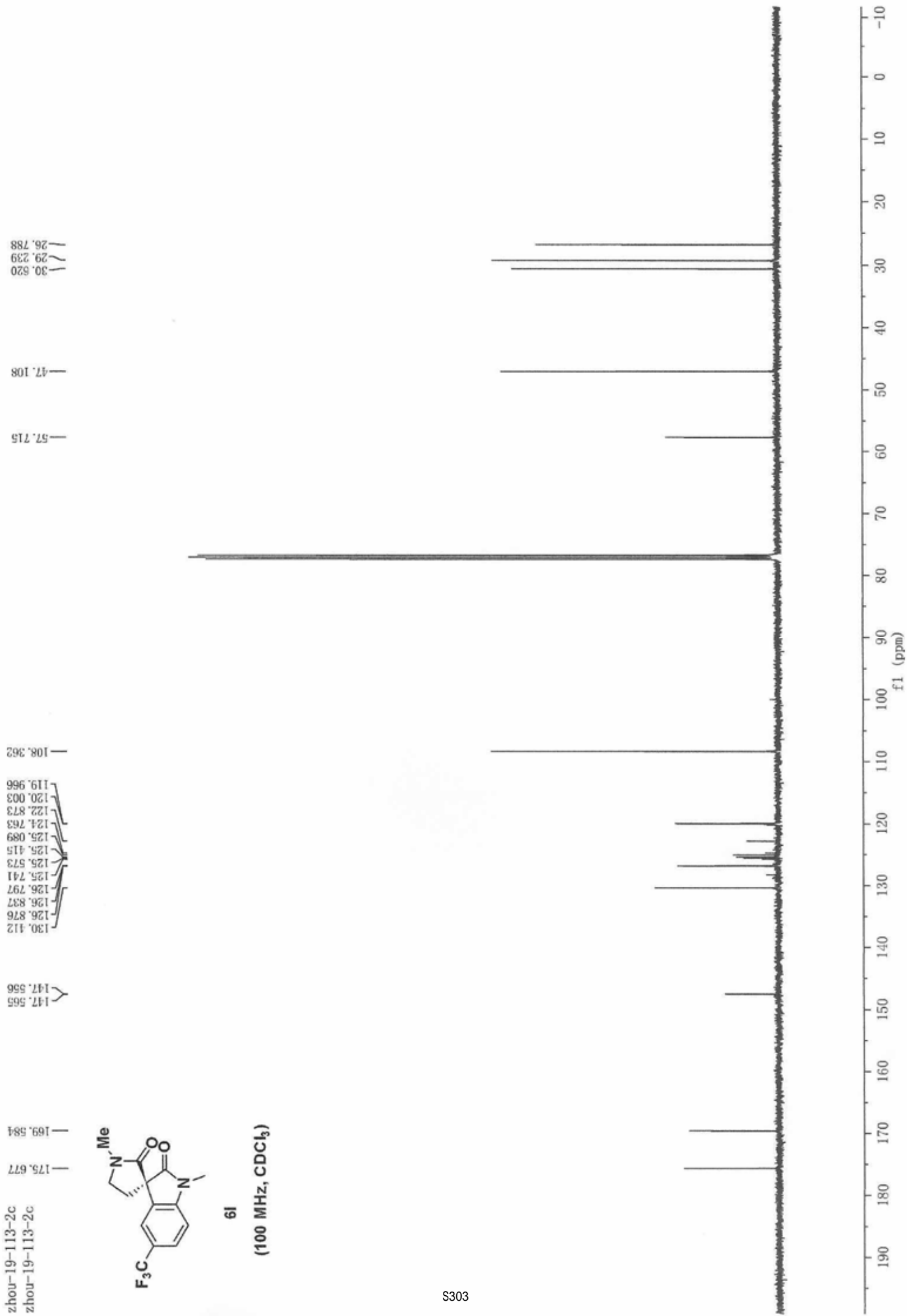
47.108

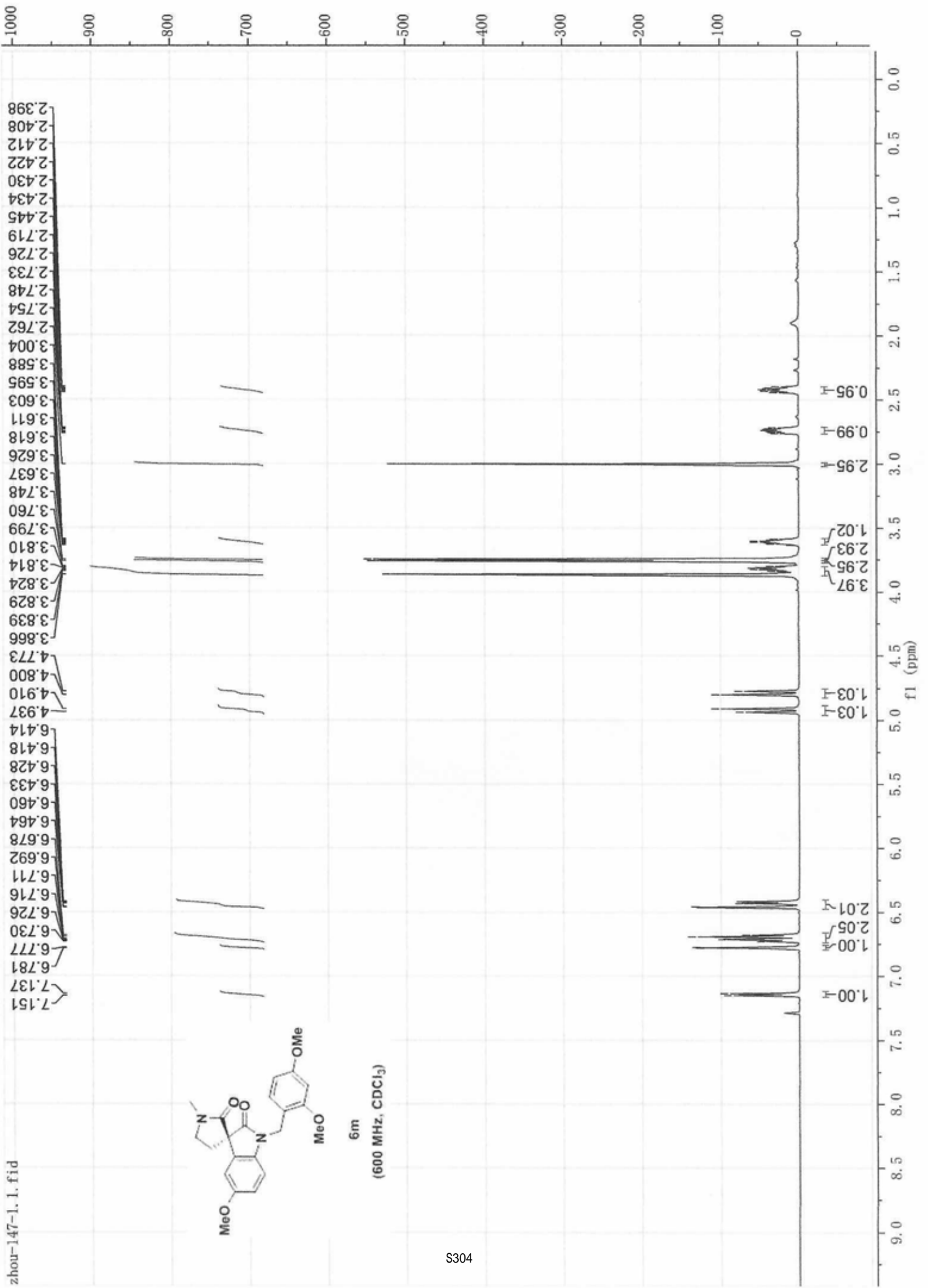
30.520  
29.239  
26.788



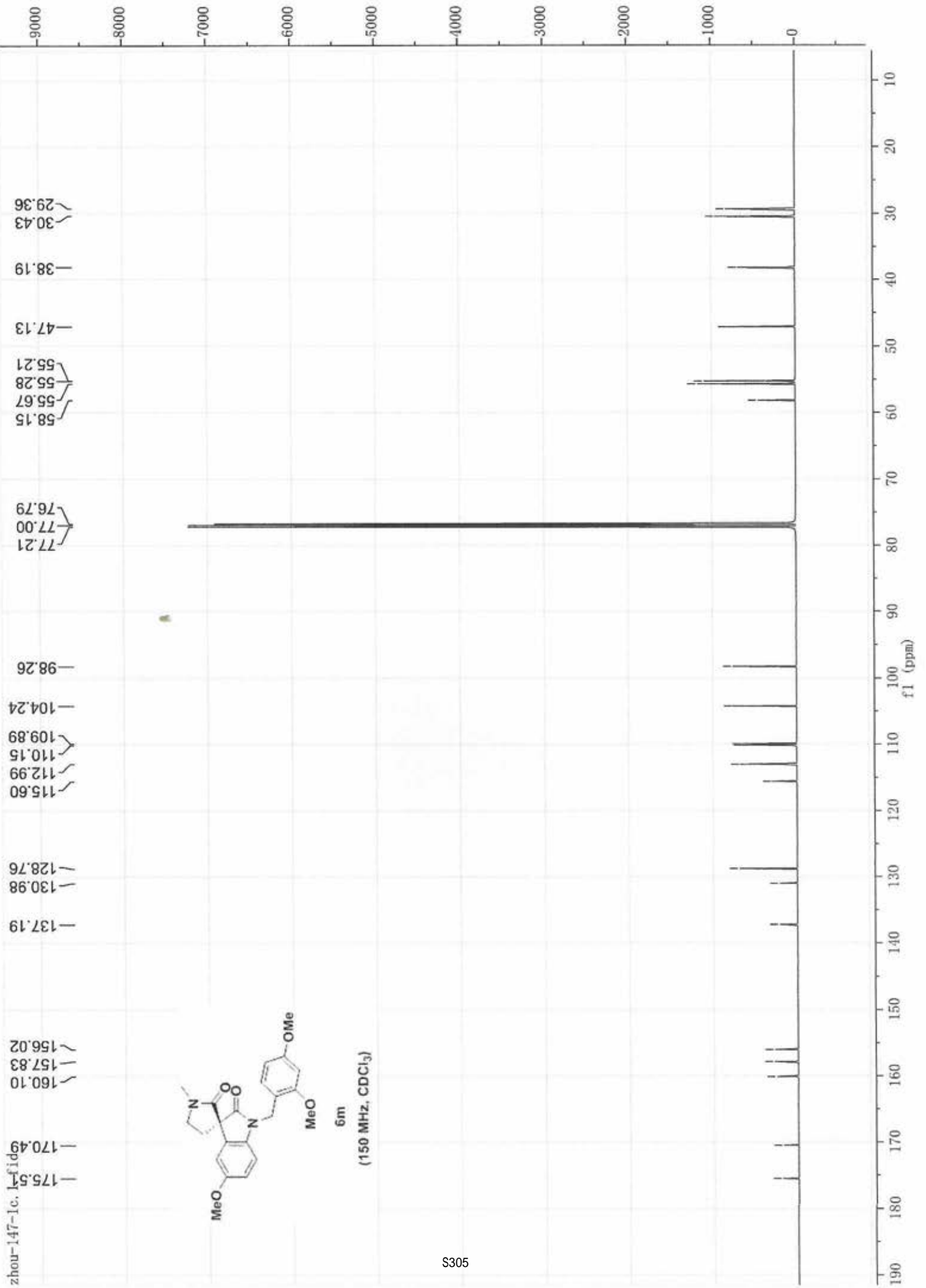
6I

(100 MHz, CDCl<sub>3</sub>)





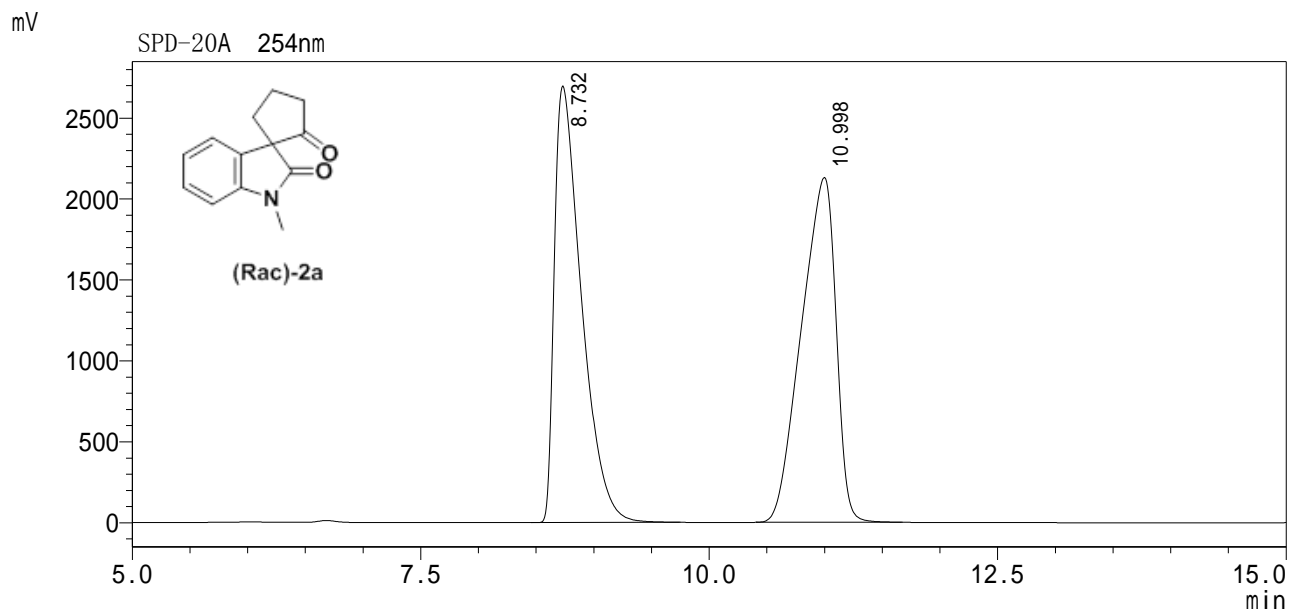
zhou-147-1.1.fid




**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : dzj  
 Data name : CCD51-2.2-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/5/21 21:12:18  
 Pro. Data : 2019/5/21 21:45:09  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

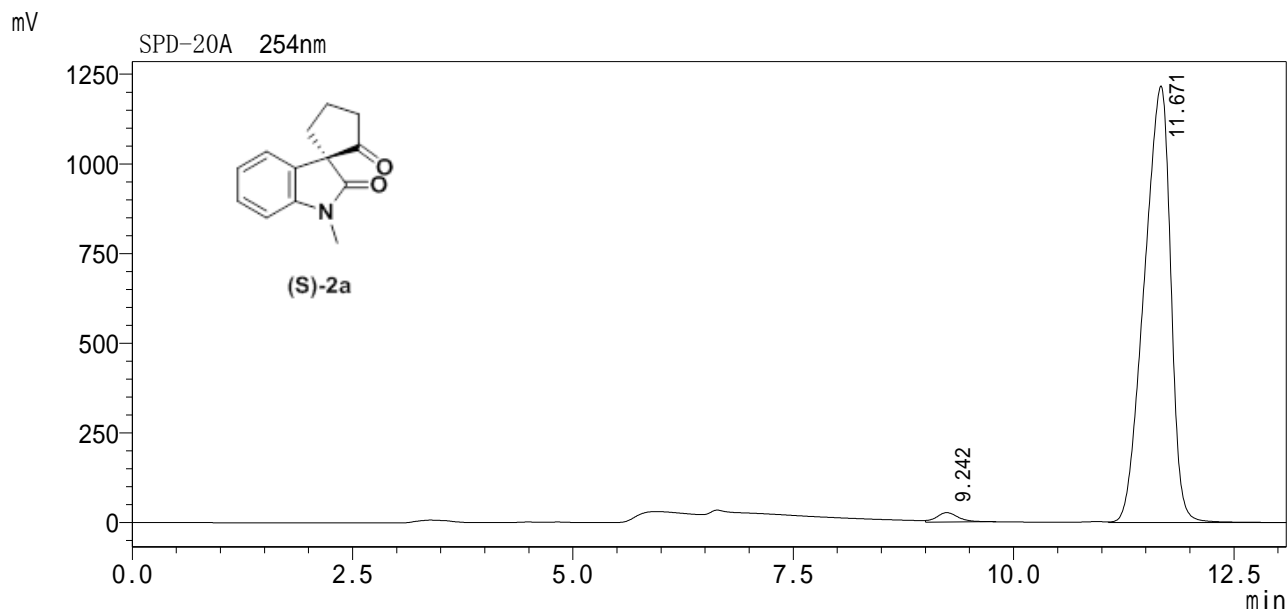
Entry	RT [min]	Area	Height	Area%		
1	8.732	43962873	2696836	49.952		M
2	10.998	44046679	2129536	50.048		M
Sum		88009552	4826372			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD126jn100%TMS  
 Data name : MHWD126jn100%TMS-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/16 18:00:42  
 Pro. Data : 2021/1/8 22:34:00

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

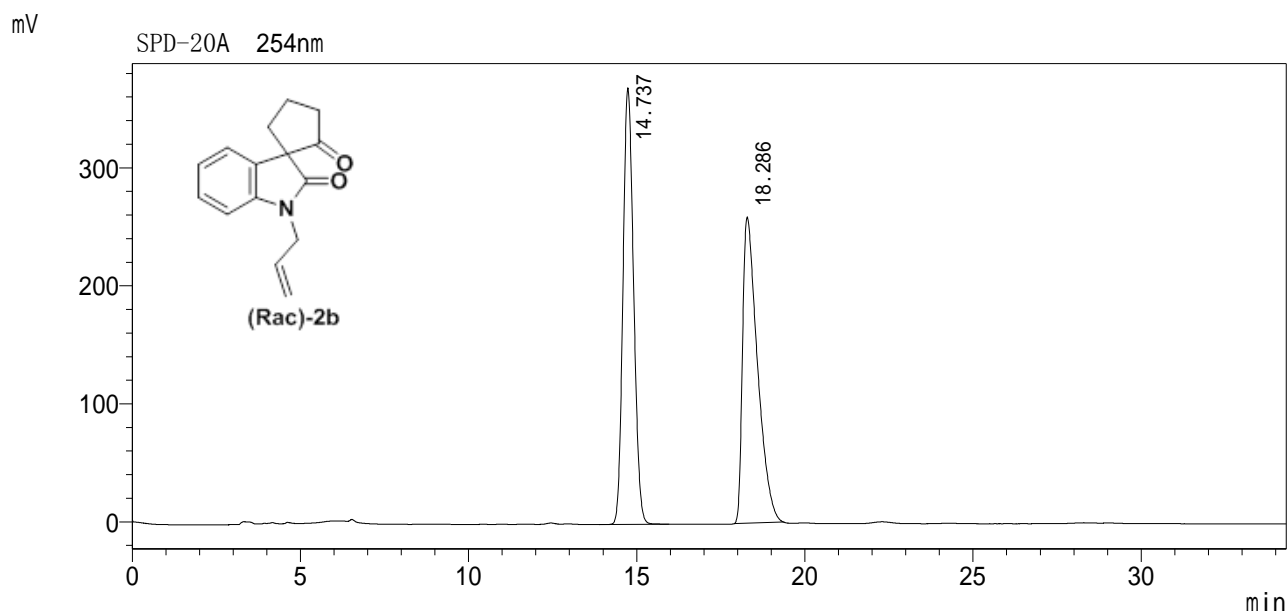
Entry	RT[min]	Area	Height	Area%		
1	9.242	449828	26229	1.742		M
2	11.671	25366761	1216835	98.258		
Sum		25816589	1243064			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE75RAC-IC-H-30%.lcd  
 Acq. method : IC-H-30%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/9/12 14:34:19  
 Pro. Data : 2019/9/12 21:00:01

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	14.737	8083400	369712	50.305		M
2	18.286	7985391	259424	49.695		M
Sum		16068791	629136			

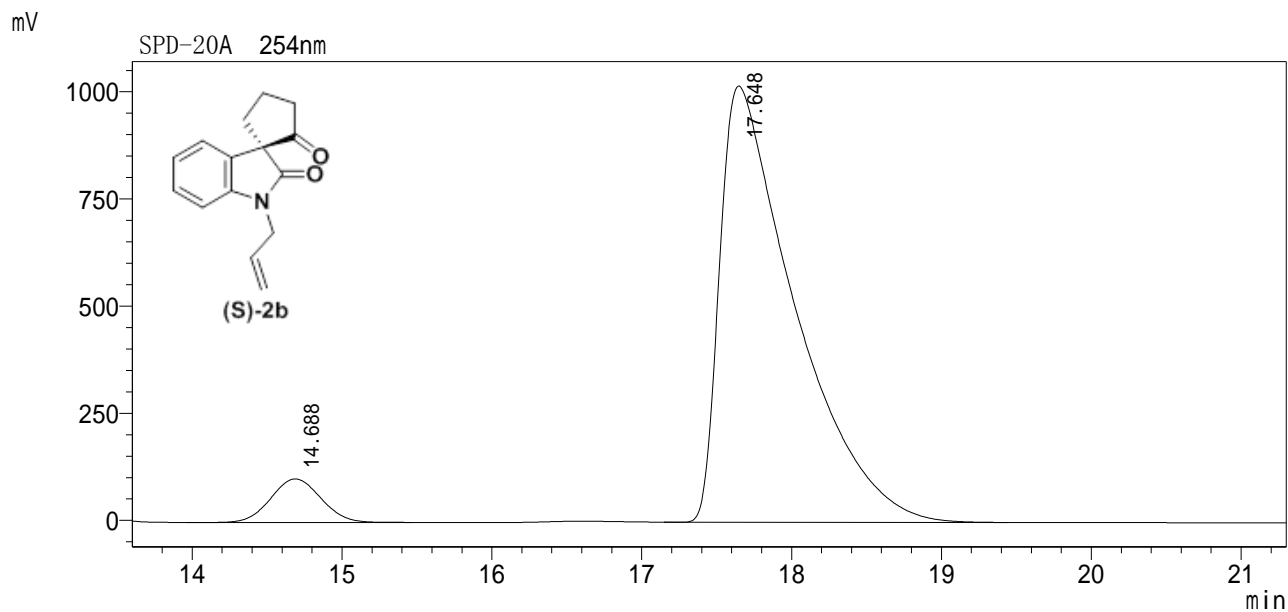



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD129BJN  
 Data name : MHWD129BJN-IC-H-30%.lcd  
 Acq. method : IC-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/17 19:50:17  
 Pro. Data : 2021/1/17 21:07:07

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

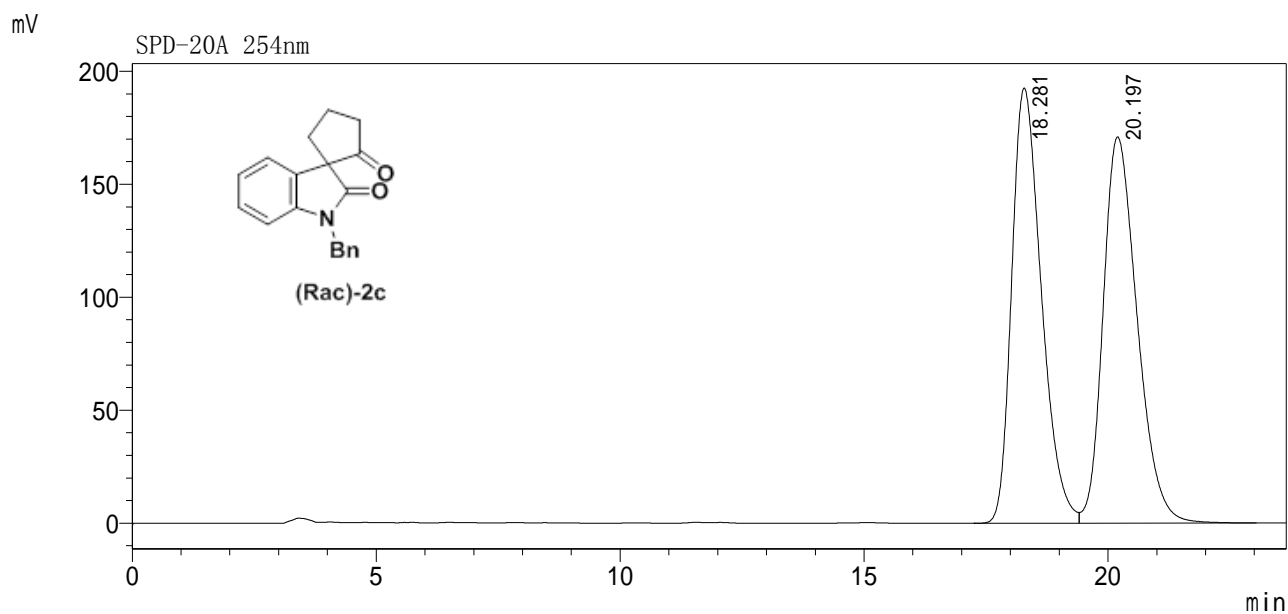
Entry	RT[min]	Area	Height	Area%			
1	14.688	2360639	101555	6.256		M	
2	17.648	35372315	1017912	93.744		M	
Sum		37732954	1119467				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE46RAC-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/8/28 16:48:00  
 Pro. Data : 2019/8/28 19:02:22

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



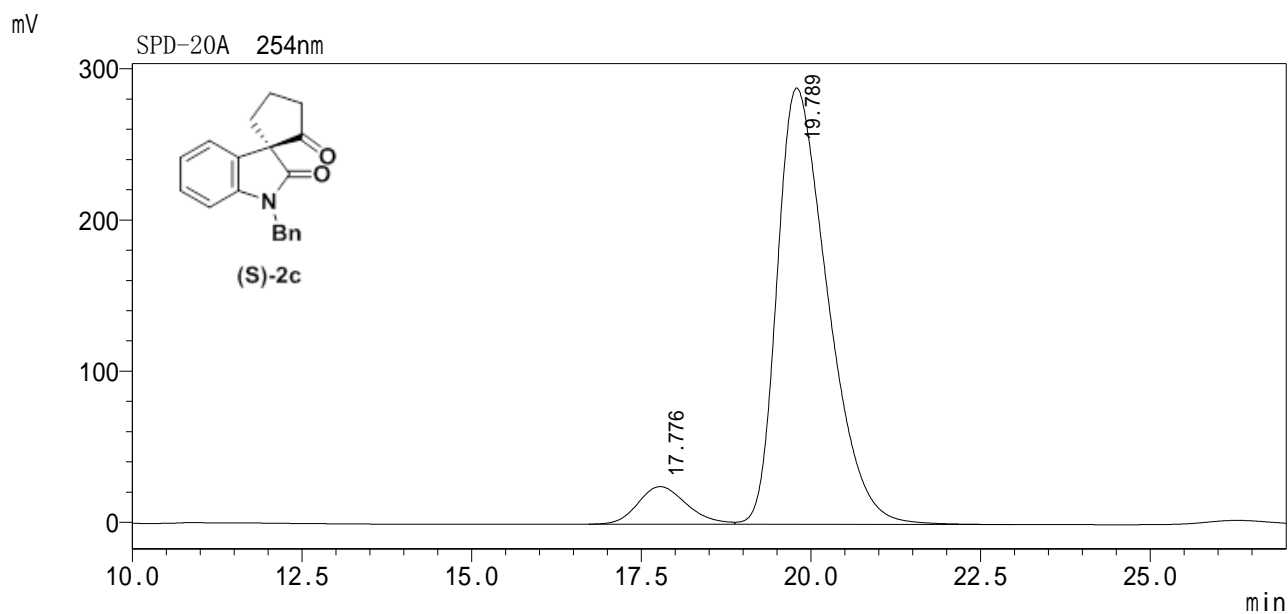
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	18.281	8151288	192629	49.519	V	
2	20.197	8309775	171013	50.481	V	
Sum		16461063	363642			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD149jn100%TMS-4  
 Data name : MHWD149jn100%TMS-4-OJ-H-30%.lcd  
 : OJ-H-30%.lcm  
 Location : 1-1 Sample Type : unknown  
 : 1  $\mu$ L  
 Ana. Data : 2021/1/1 13:40:33 Analyst : System Administrator  
 Pro. Data : 2021/1/1 15:23:50 Processor : System Administrator



SPD-20A

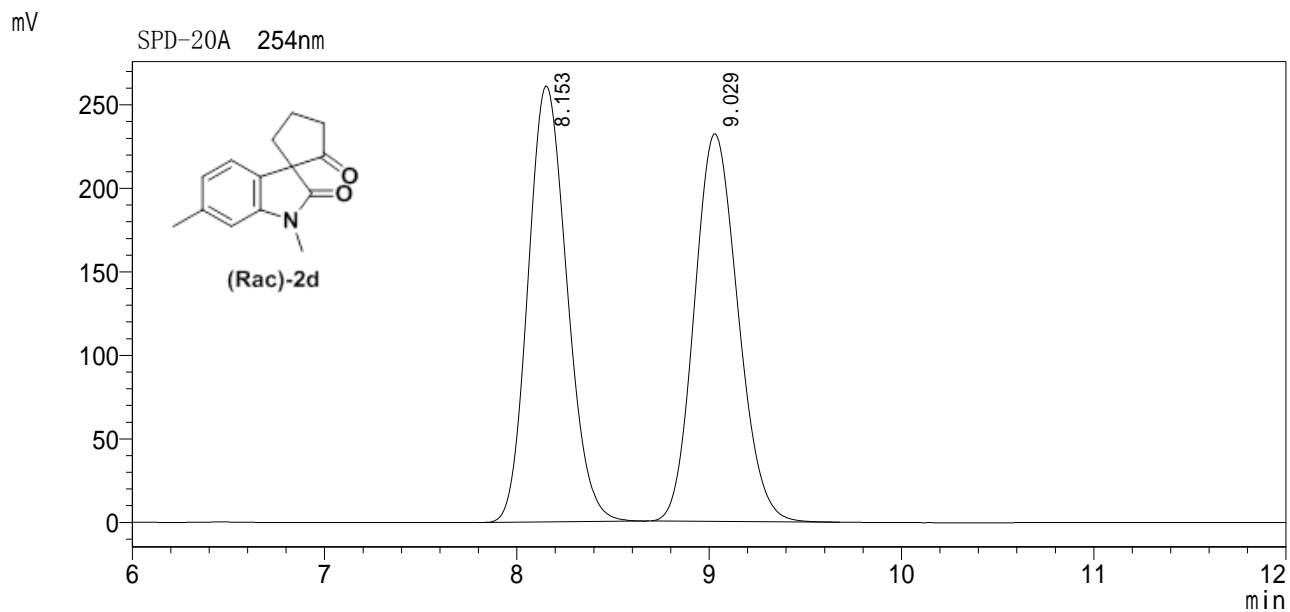
Entry	RT[min]	Area	Height	Area%		
1	17.776	1247792	24883	7.711		M
2	19.789	14934751	288555	92.289		V M
Sum		16182542	313438			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE66RAC-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/9/7 15:59:34  
 Pro. Data : 2020/6/6 20:36:26

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

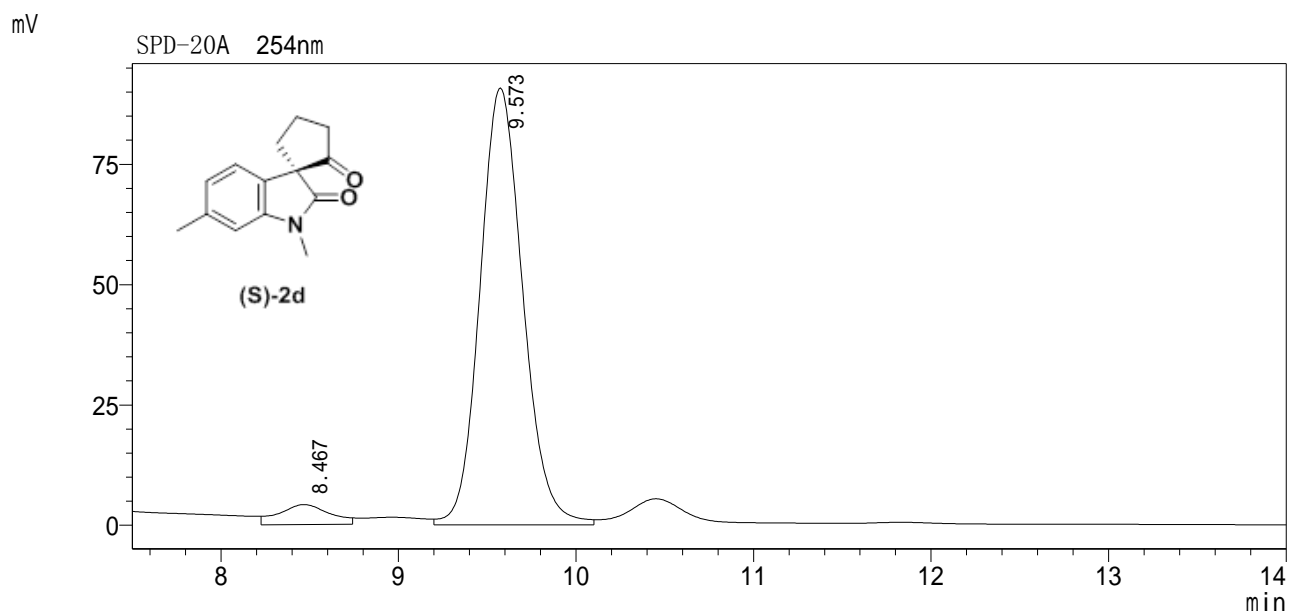
Entry	RT [min]	Area	Height	Area%		
1	8.153	3678188	261038	50.140		M
2	9.029	3657613	231909	49.860		M
Sum		7335801	492946			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD1474  
 Data name : MHWD1474-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/30 18:14:56  
 Pro. Data : 2020/12/30 19:29:53

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

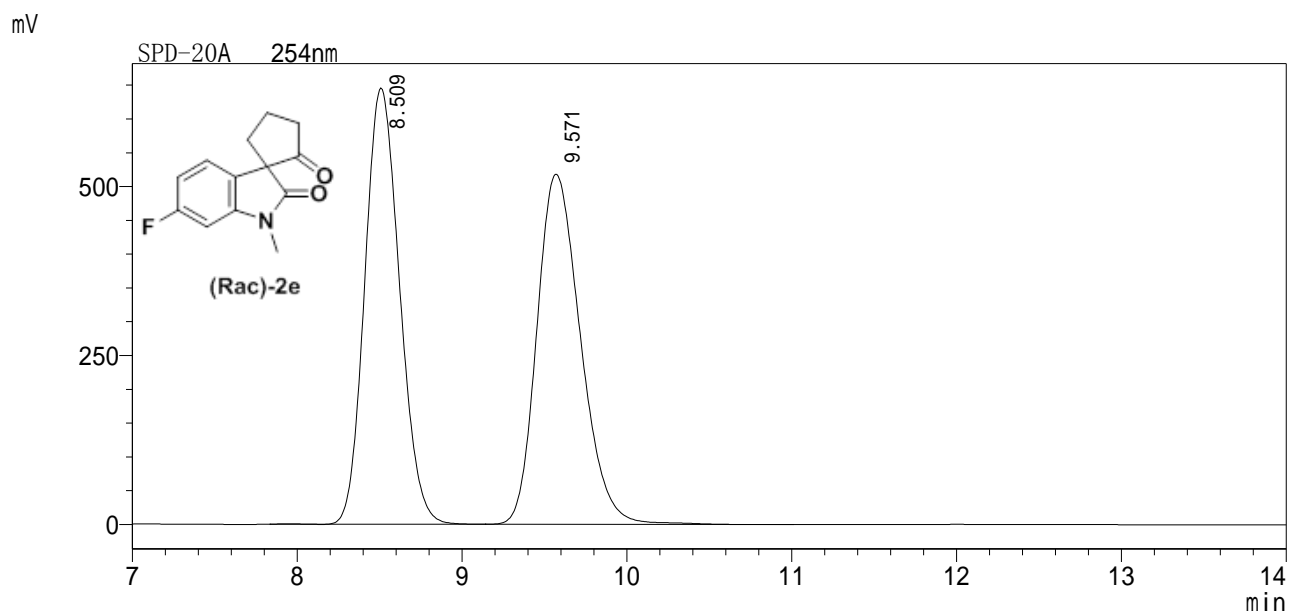
Entry	RT[min]	Area	Height	Area%		
1	8.467	83620	4172	5.199		M
2	9.573	1524690	90784	94.801		M
Sum		1608310	94956			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD146rac  
 Data name : MHWD146rac-AS-H-40%.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/2 11:09:17  
 Pro. Data : 2021/1/2 11:30:24

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



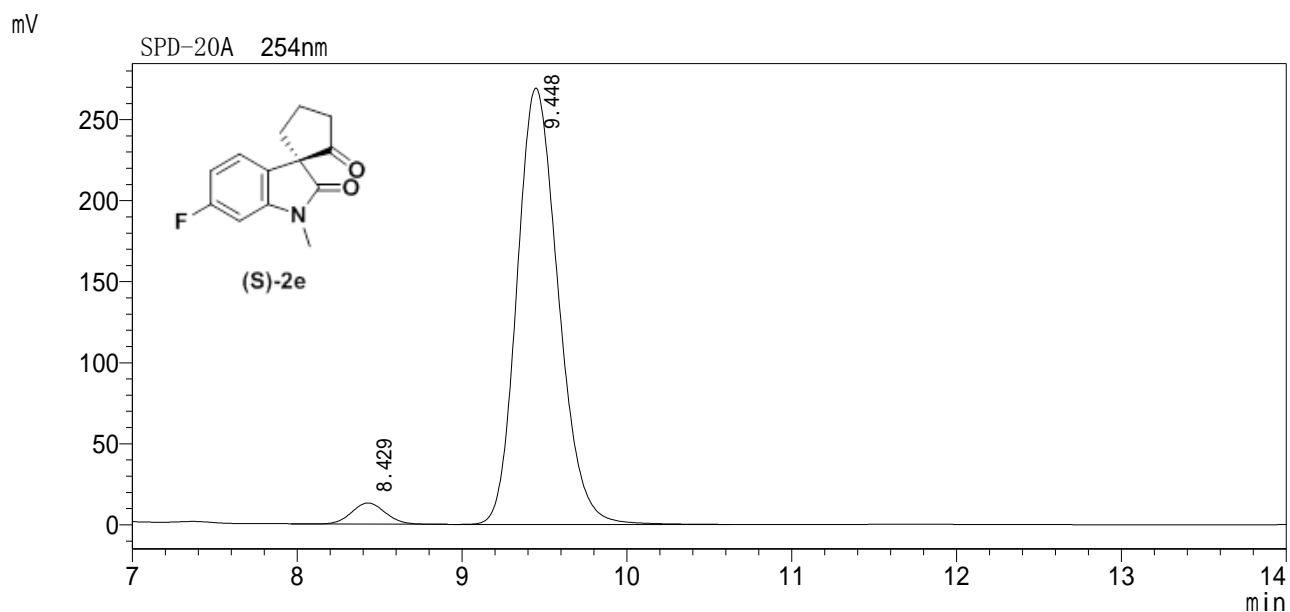
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	8.509	9472739	645457	49.856		M
2	9.571	9527392	518074	50.144		V M
Sum		19000131	1163531			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD151-2  
 Data name : MHWD151-2-AS-H-40%.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/3 15:33:55  
 Pro. Data : 2021/1/3 15:54:54  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

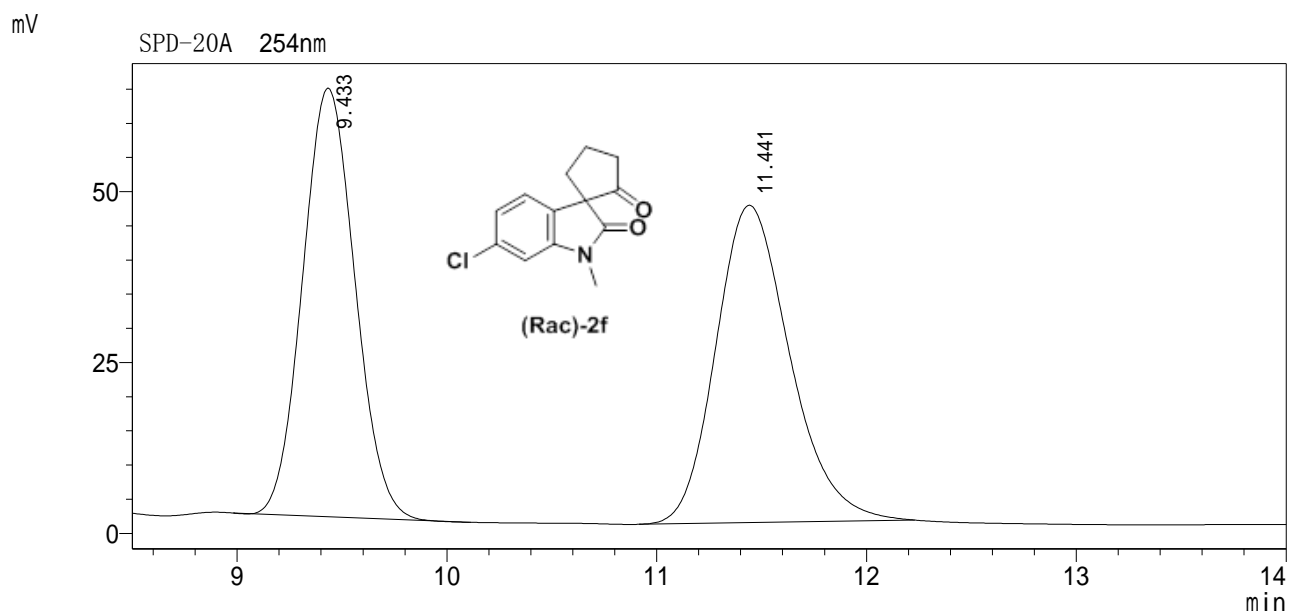
Entry	RT [min]	Area	Height	Area%		
1	8.429	184720	13036	3.800		M
2	9.448	4676815	269276	96.200		M
Sum		4861535	282312			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWCL  
 Data name : MHWCL-AS-H-30%.lcd  
 Acq. method : AS-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/30 20:12:56  
 Pro. Data : 2021/1/30 20:29:01

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

Entry	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.433	1088360	62728	48.876		M	
2	11.441	1138409	46438	51.124		M	
		2226769	109166				

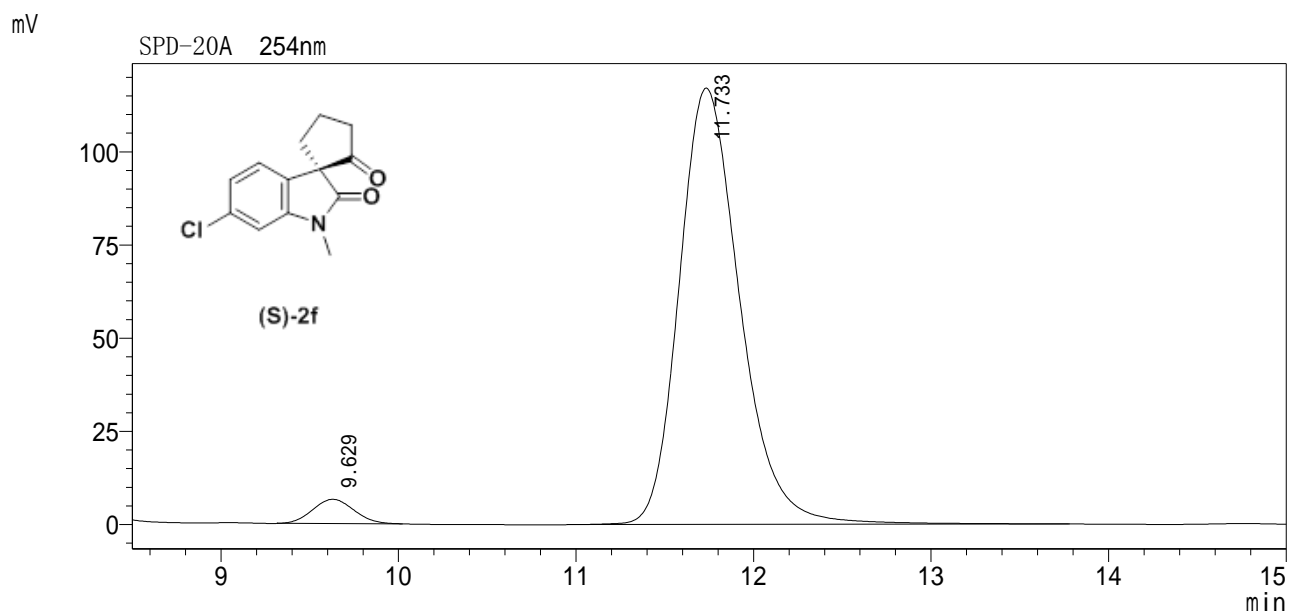



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF006jn100%TMS-1  
 Data name : MHWF006jn100%TMS-1-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/7 21:13:36  
 Pro. Data : 2021/1/7 21:28:48

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



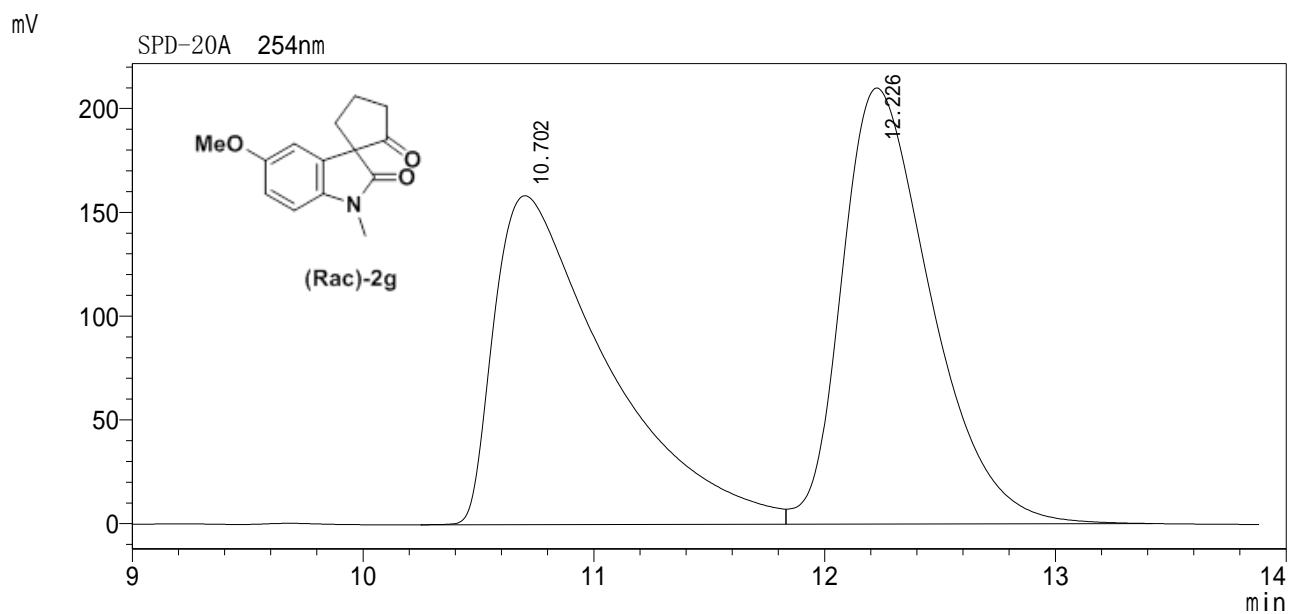
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	9.629	105728	6526	3.657		M
2	11.733	2785350	117088	96.343		M
Sum		2891077	123613			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE69RAC-OD-H-20%.lcd  
 Acq. method : OD-H-20%-40min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/9/10 12:34:27  
 Pro. Data : 2019/9/10 14:09:38  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

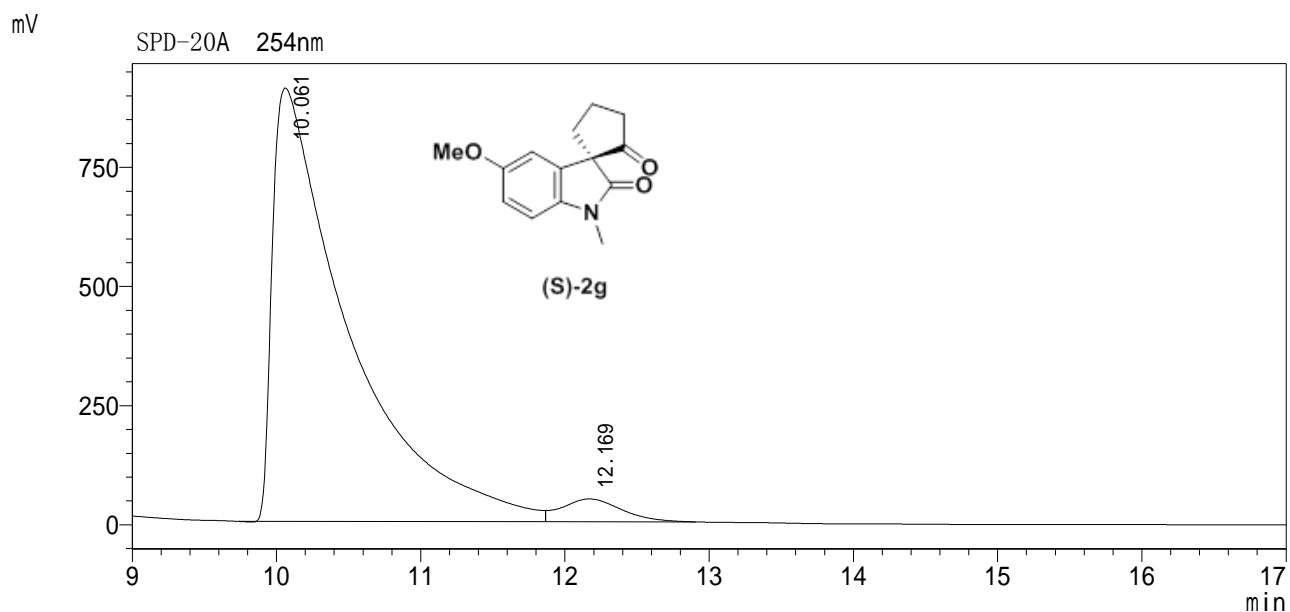
Entry	RT[min]	Area	Height	Area%		
1	10.702	5434115	158438	49.097		M
2	12.226	5633919	210042	50.903		V M
Sum		11068033	368480			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD134jn100%TMS-2  
 Data name : MHWD134jn100%TMS-2-OD-H-20%.lcd  
 Acq. method : OD-H-20%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/1 14:50:59  
 Pro. Data : 2021/1/1 15:21:55

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

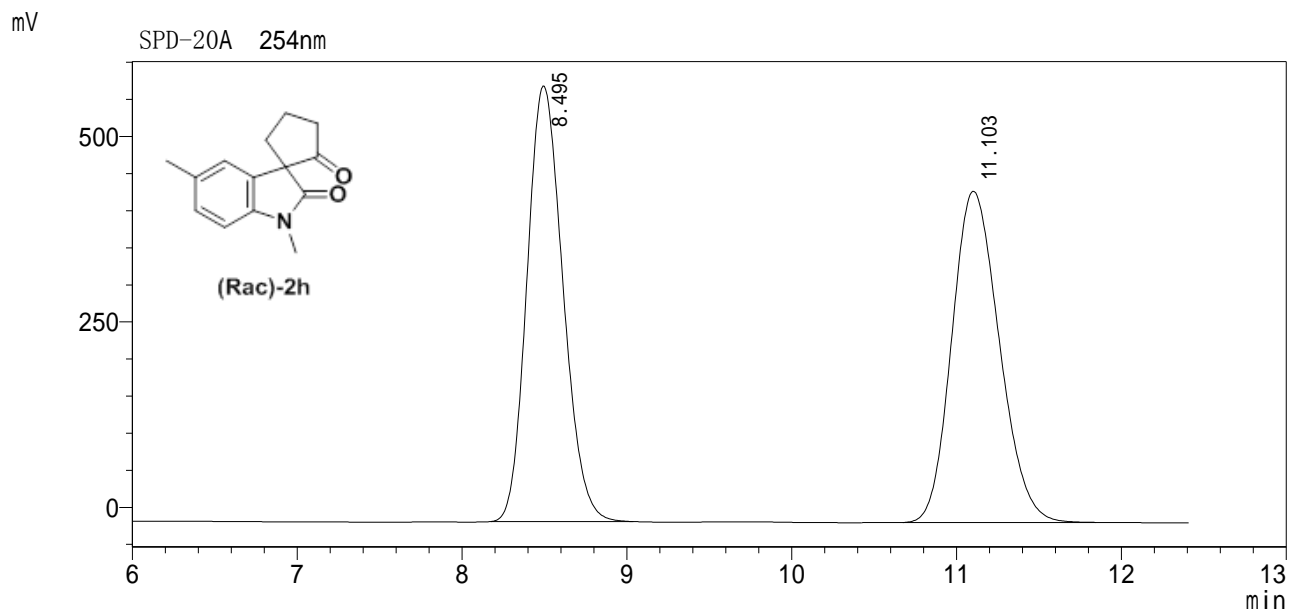
Entry	RT[min]	Area	Height	Area%		
1	10.061	33260541	909584	95.990		M
2	12.169	1389293	47993	4.010		V M
Sum		34649834	957577			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhwb1422  
 Data name : CCD76RAC-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/6/9 11:37:23  
 Pro. Data : 2019/6/9 12:19:20

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

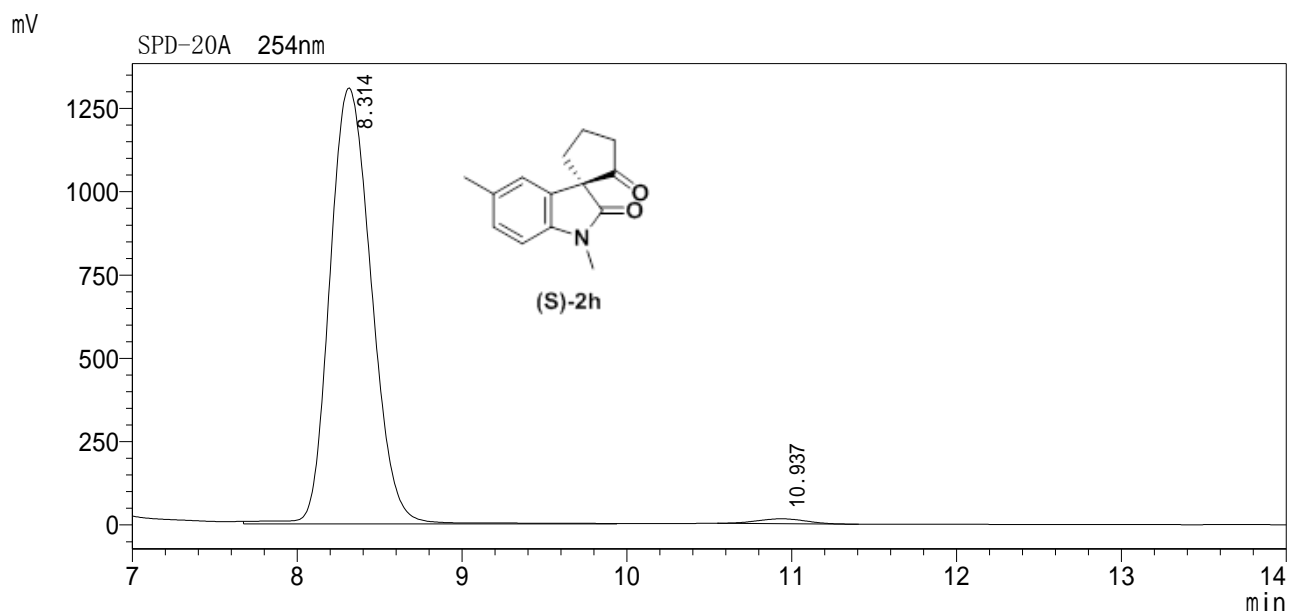
Entry	RT[min]	Area	Height	Area%		
1	8.495	8902444	587226	49.922		M
2	11.103	8930270	446627	50.078		M
Sum		17832714	1033853			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD131jn100%TMS-1  
 Data name : MHWD131jn100%TMS-1-AS-H-30%.lcd  
 Acq. method : AS-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/22 20:45:47  
 Pro. Data : 2021/1/22 21:01:29

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



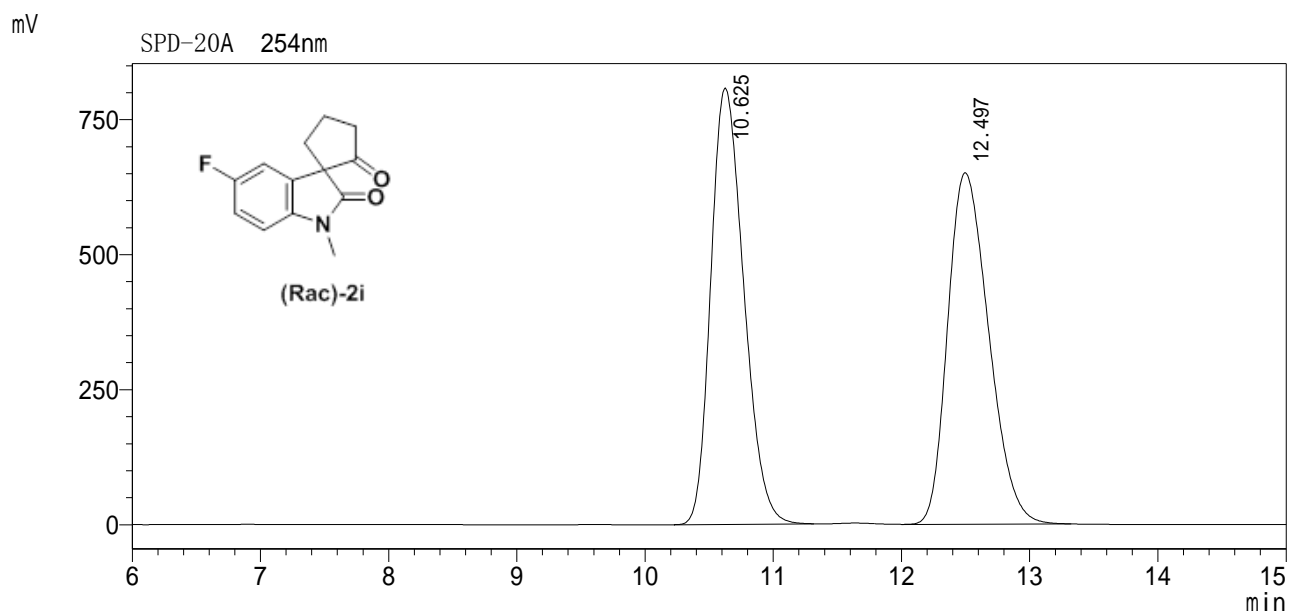
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	8.314	22991168	1307785	98.703		M
2	10.937	302039	14654	1.297		M
Sum		23293207	1322439			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202006061-AS-30% F  
 Data name : ZFT202006061-AS-30% F.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/6 19:45:42  
 Pro. Data : 2020/6/6 20:08:14  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



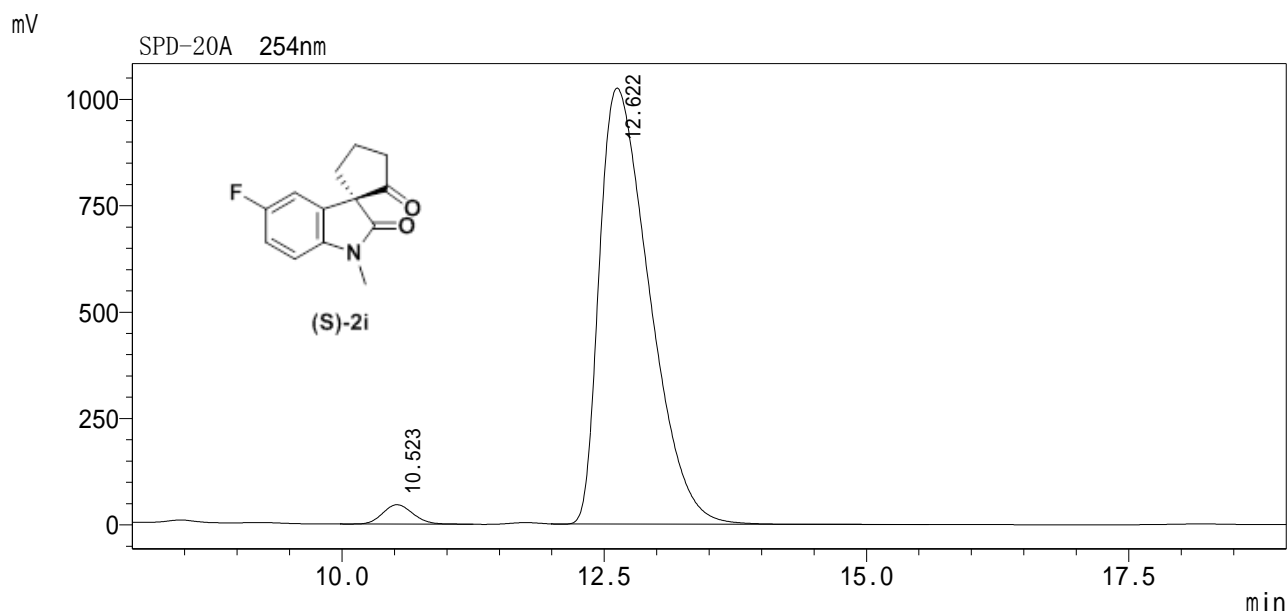
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.625	14433409	808018	49.951		M
2	12.497	14461591	650902	50.049		M
Sum		28895000	1458919			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD133jn100%TMS  
 Data name : MHWD133jn100%TMS-AS-H-40%.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/22 13:20:33  
 Pro. Data : 2020/12/26 22:25:37  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



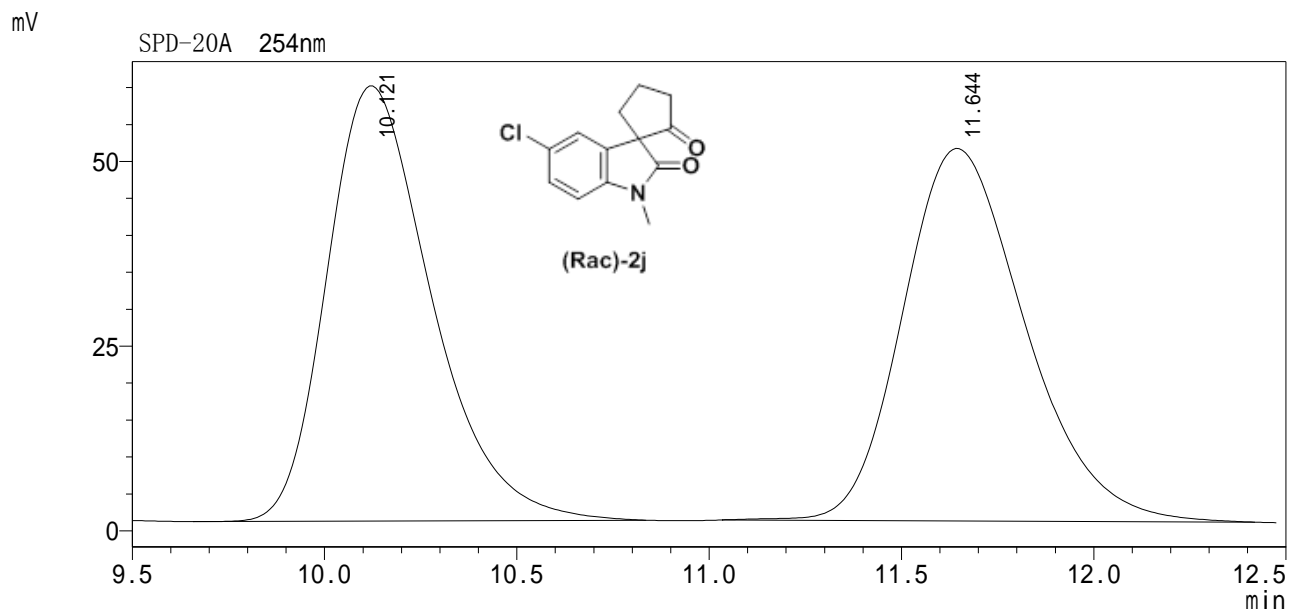
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.523	923793	45767	2.655		M
2	12.622	33865870	1024841	97.345		M
Sum		34789663	1070609			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE54.2-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/9/4 11:32:55  
 Pro. Data : 2020/6/20 20:38:54  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

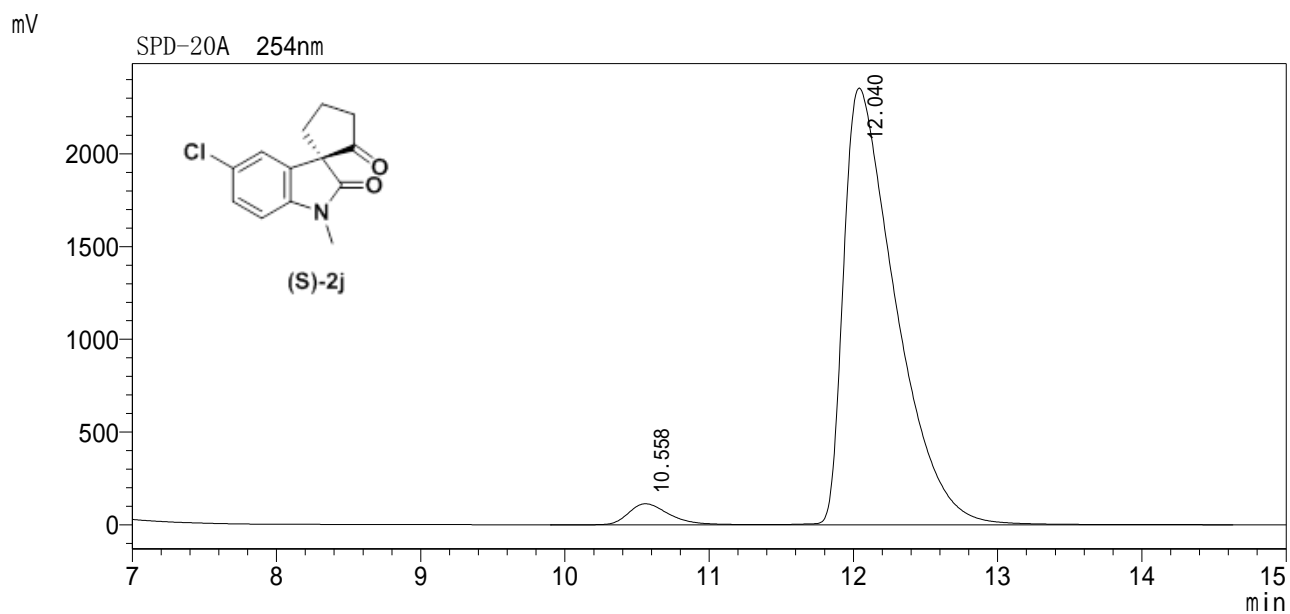
Entry	RT[min]	Area	Height	Area%		
1	10.121	1111596	58870	49.919		M
2	11.644	1115197	50410	50.081		M
Sum		2226793	109280			




**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD130jn100%TMS  
 Data name : MHWD130jn100%TMS-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/21 12:09:50  
 Pro. Data : 2020/12/26 16:13:58  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

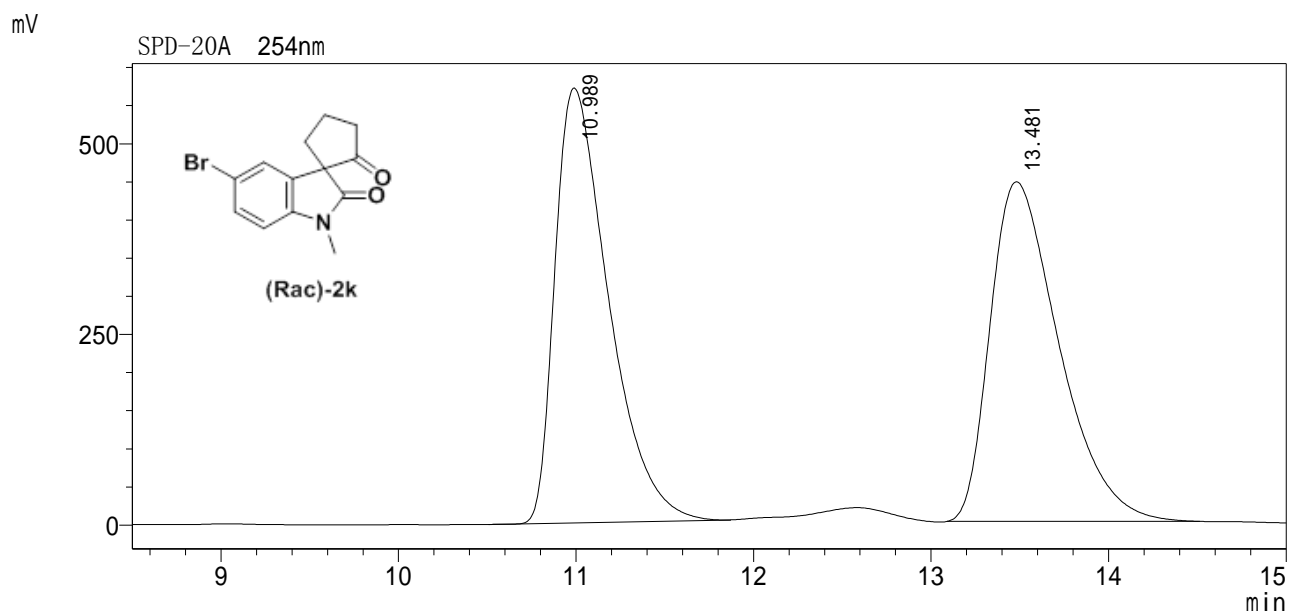
Entry	RT[min]	Area	Height	Area%		
1	10.558	2201540	113169	3.597		M
2	12.040	58996532	2354548	96.403		V M
Sum		61198072	2467717			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE70RAC-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/9/10 13:53:32  
 Pro. Data : 2019/9/10 14:09:36

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



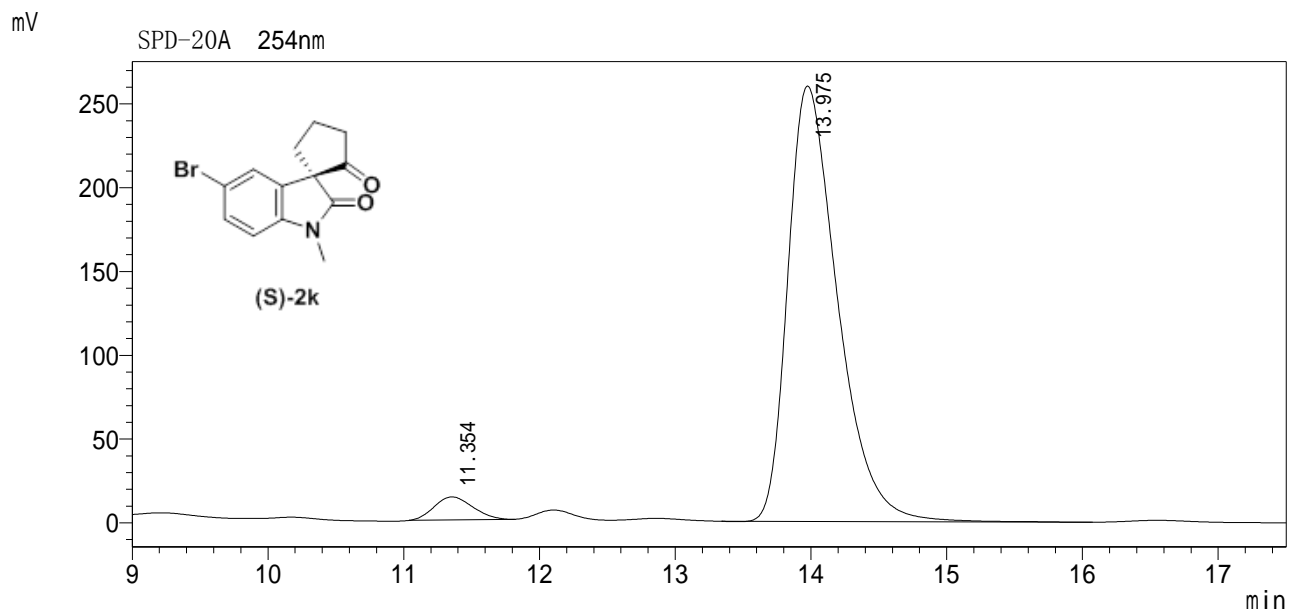
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.989	11974671	570156	49.925		M
2	13.481	12010543	445342	50.075		M
Sum		23985214	1015498			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD148jn100%TMS  
 Data name : MHWD148jn100%TMS-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/30 22:21:06  
 Pro. Data : 2020/12/30 22:47:51  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



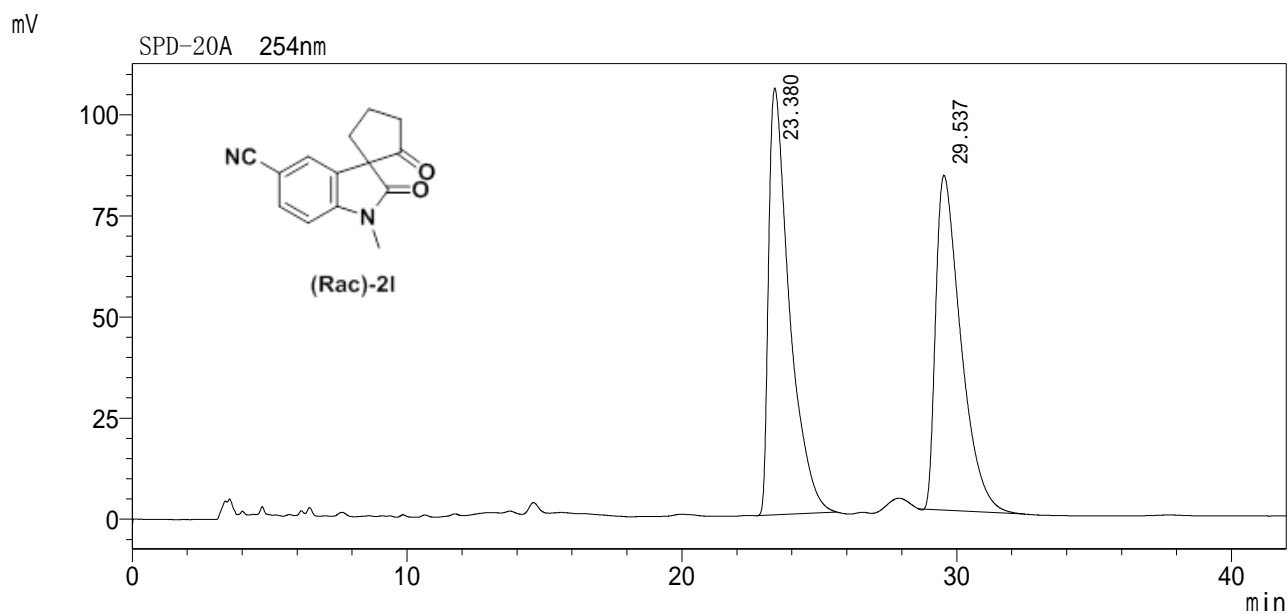
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	11.354	271431	13793	3.939		M
2	13.975	6619822	259940	96.061		M
Sum		6891253	273733			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw  
 Data name : CCE123-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/10/16 20:42:33  
 Pro. Data : 2020/6/6 21:01:45  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



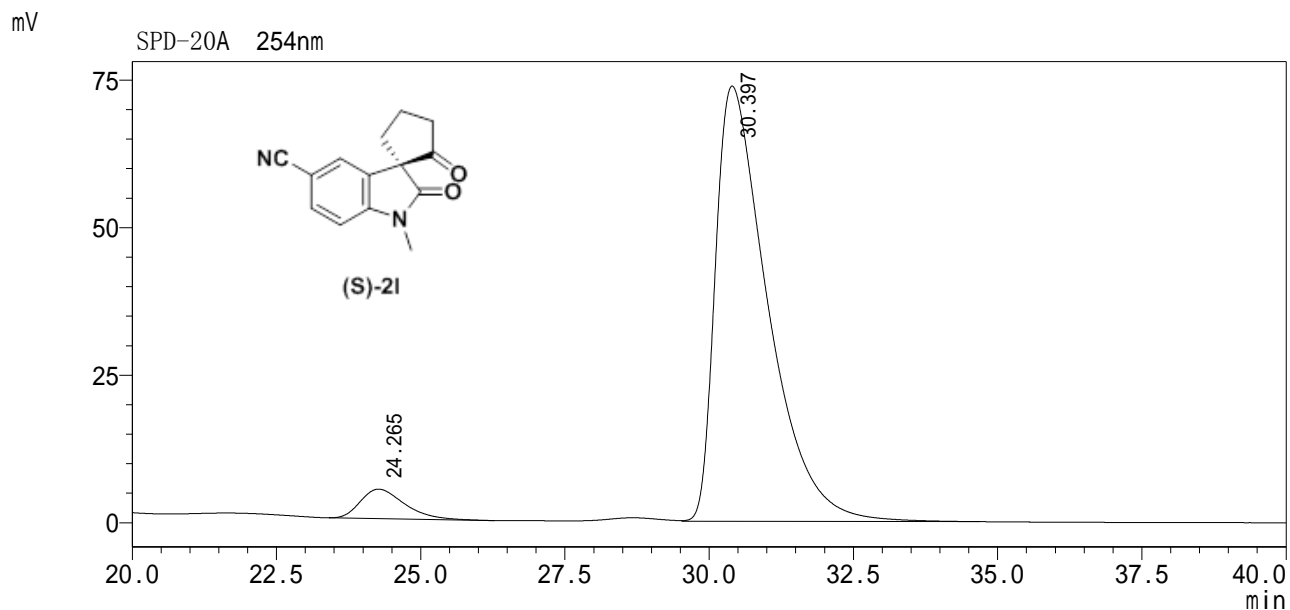
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	23.380	5574989	105555	51.399		M
2	29.537	5271428	82774	48.601		M
Sum		10846417	188329			

**SHIMADZU**  
**LabSolutions HPLC Report**

<Sample information>

Sample name : MHWF026-2  
 Data name : MHWF026-2-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/21 22:04:35  
 Pro. Data : 2021/1/21 22:47:07  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

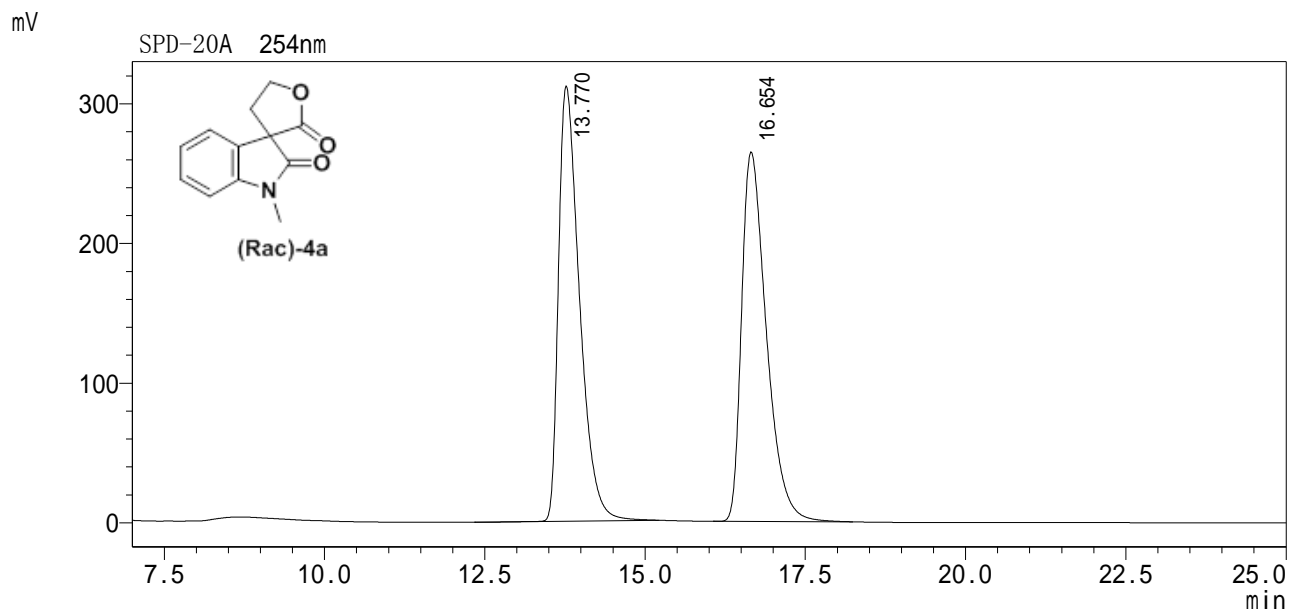
Entry	RT[min]	Area	Height	Area%			
1	24.265	266857	5001	5.424			
2	30.397	4653466	73738	94.576			
Sum		4920323	78739				


**SHIMADZU**  
**LabSolutions** HPLC Report

## &lt;Sample information&gt;

Sample name : zft cce121- 6291 rac oj 40%  
 Data name : zft cce121- 6291 rac oj 40%.lcd  
 Acq. method : OD-H-40.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/30 11:16:56  
 Pro. Data : 2020/11/30 19:40:55

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

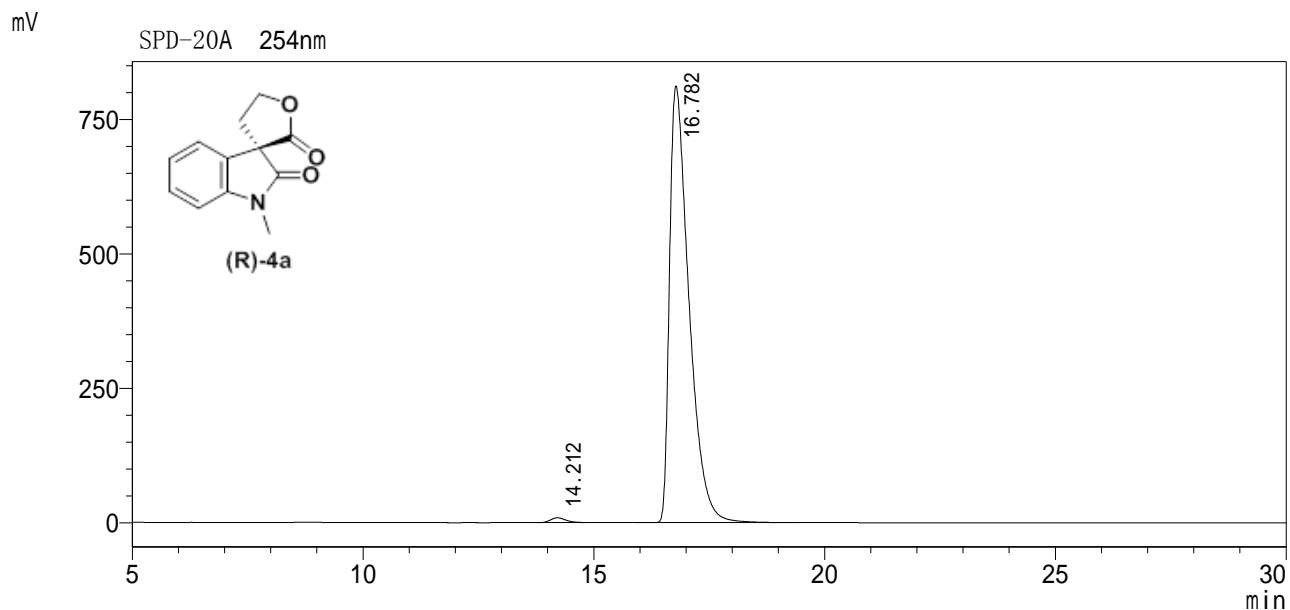
Entry	RT[min]	Area	Height	Area%		
1	13.770	7108318	311667	50.068		M
2	16.654	7088999	264573	49.932		M
Sum		14197317	576241			


**SHIMADZU**  
**LabSolutions** HPLC Report

## &lt;Sample information&gt;

Sample name : zft202006291 repeat oj 40%  
 Data name : zft202006291 repeat oj40%.lcd  
 Acq. method : OJ-H-20%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/29 9:46:45  
 Pro. Data : 2020/6/29 10:24:35

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



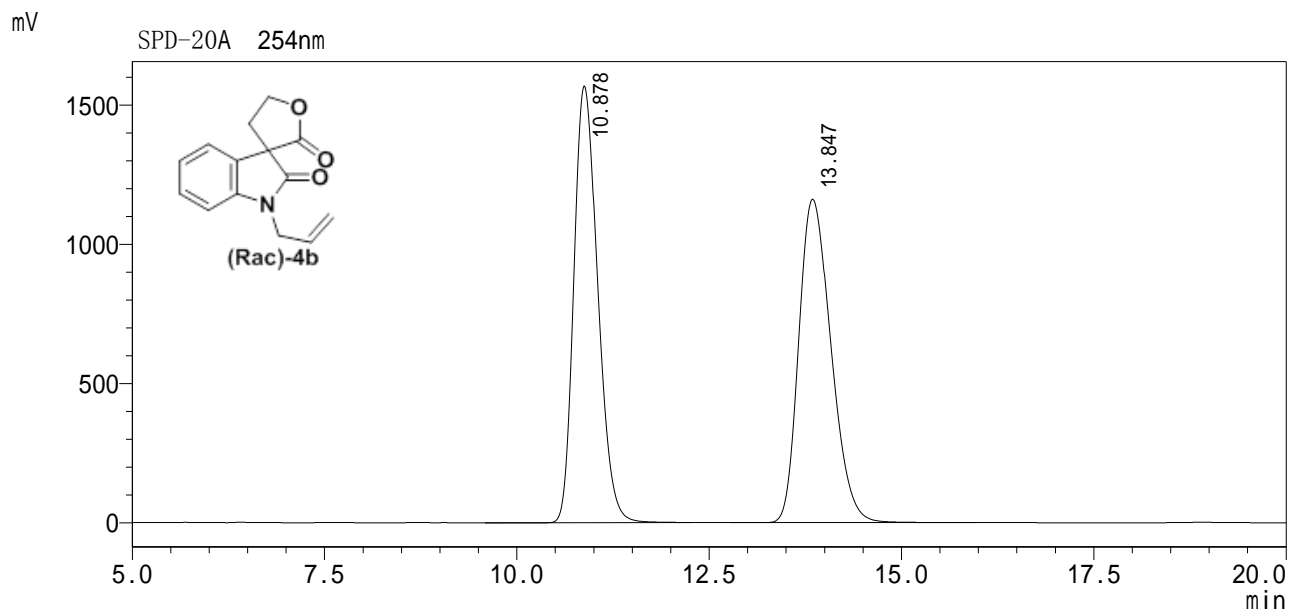
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	14.212	199044	8887	0.831		M
2	16.782	23752083	812314	99.169		M
Sum		23951127	821201			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7173 RAC 40%AS  
 : zft7173 RAC 40%AS  
 Data name : zft7173 RAC AS40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/3 0:22:58 Analyst : System Administrator  
 Pro. Data : 2020/12/3 0:43:45 Processor : System Administrator



SPD-20A

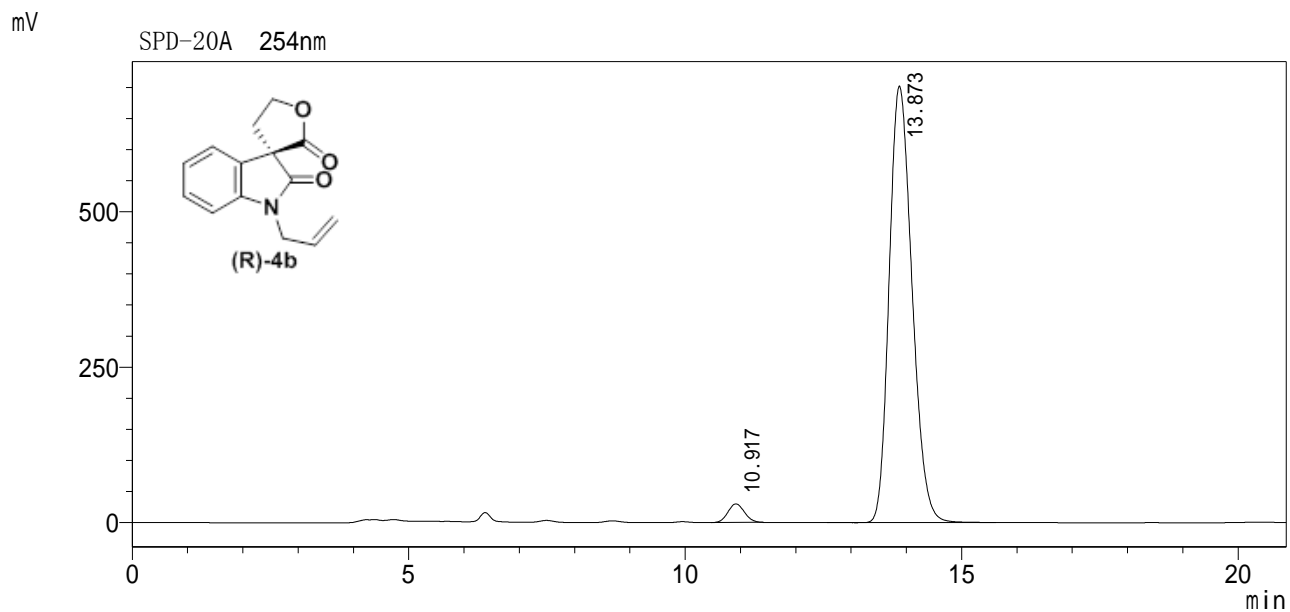
Entry	RT[min]	Area	Height	Area%			
1	10.878	33569118	1567930	49.943		M	
2	13.847	33645357	1161381	50.057		M	
Sum		67214475	2729311				




**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7173 40%AS  
 : zft7173 40%AS  
 Data name : zft7173 AS40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/3 0:45:00 Analyst : System Administrator  
 Pro. Data : 2020/12/3 1:05:53 Processor : System Administrator



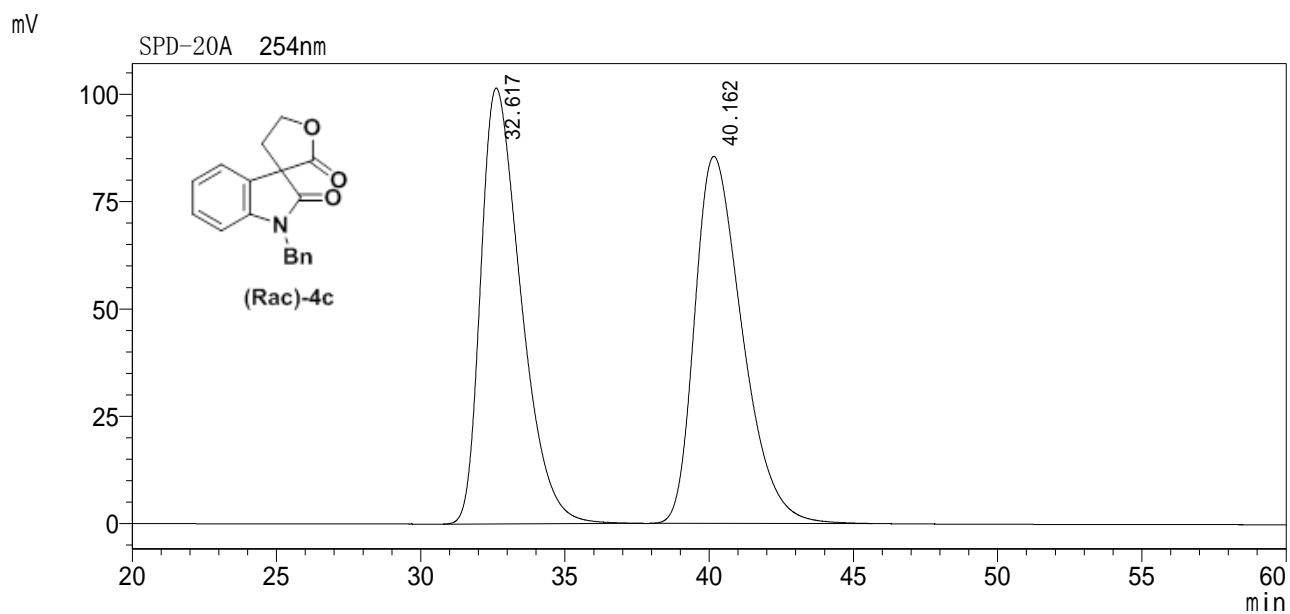
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	10.917	622738	29976	2.997		M	
2	13.873	20155011	702144	97.003		M	
Sum		20777749	732120				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7132 RAC40%OJ  
 : zft71732RAC40%OJ  
 Data name : zft7132 RAC40%OJ.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/3 2:54:51 Analyst : System Administrator  
 Pro. Data : 2020/12/3 7:26:57 Processor : System Administrator



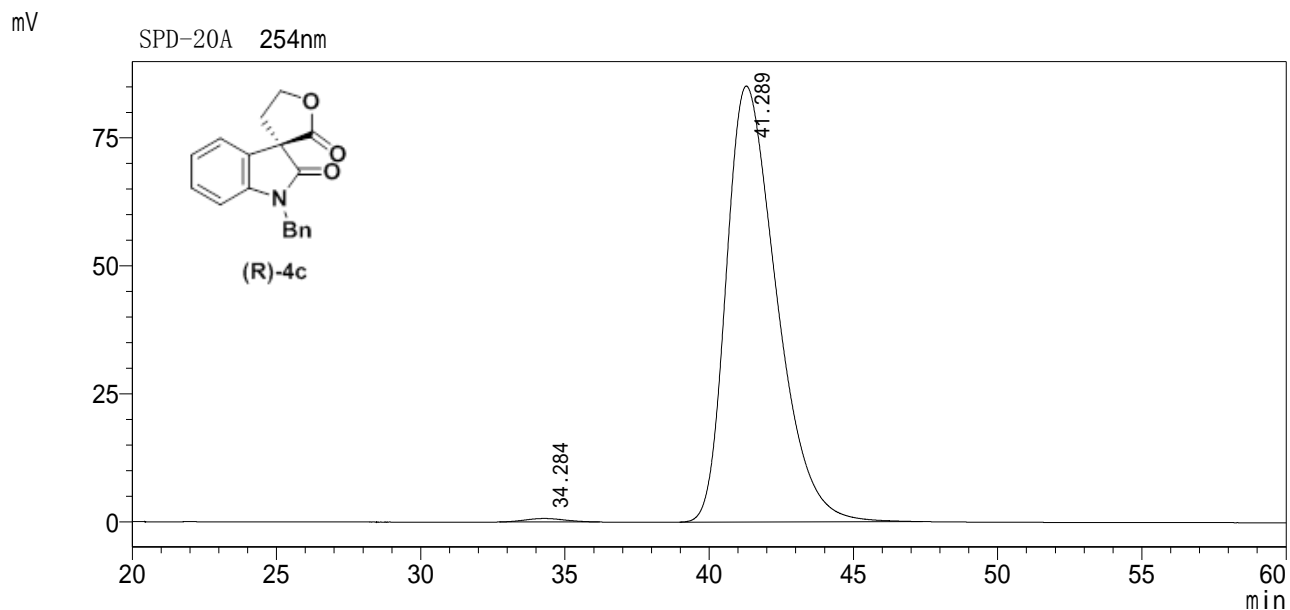
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	32.617	9837198	101533	50.096			
2	40.162	9799668	85512	49.904			
Sum		19636865	187045				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7132 40%OJ  
               : zft7173240%OJ  
 Data name   : zft7132 OJ40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
               :  
 Location    : 1-1                                 Sample Type : unknown  
               : 1 uL  
 Ana. Data   : 2020/12/3 6:19:16                 Analyst      : System Administrator  
 Pro. Data   : 2020/12/3 7:27:20                 Processor    : System Administrator



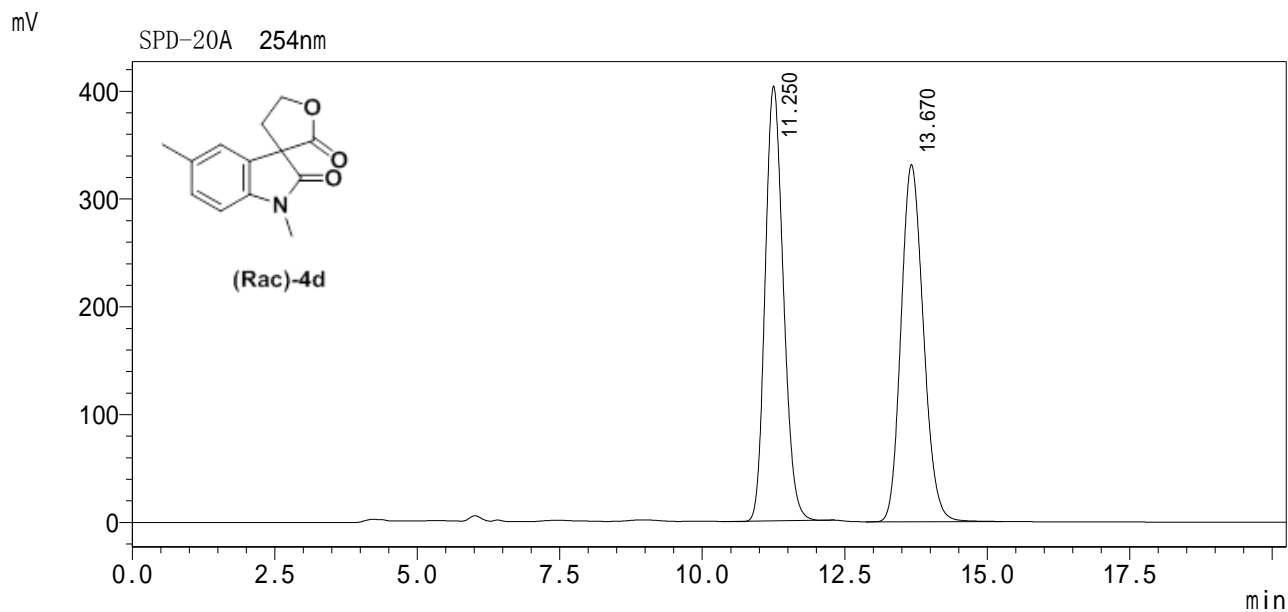
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	34.284	66184	689	0.637			
2	41.289	10321027	85159	99.363			
Sum		10387210	85848				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7161 40%AS  
 : zft7161 40%AS  
 Data name : zft7161 RAC AS40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/3 1:09:00 Analyst : System Administrator  
 Pro. Data : 2020/12/3 1:29:15 Processor : System Administrator



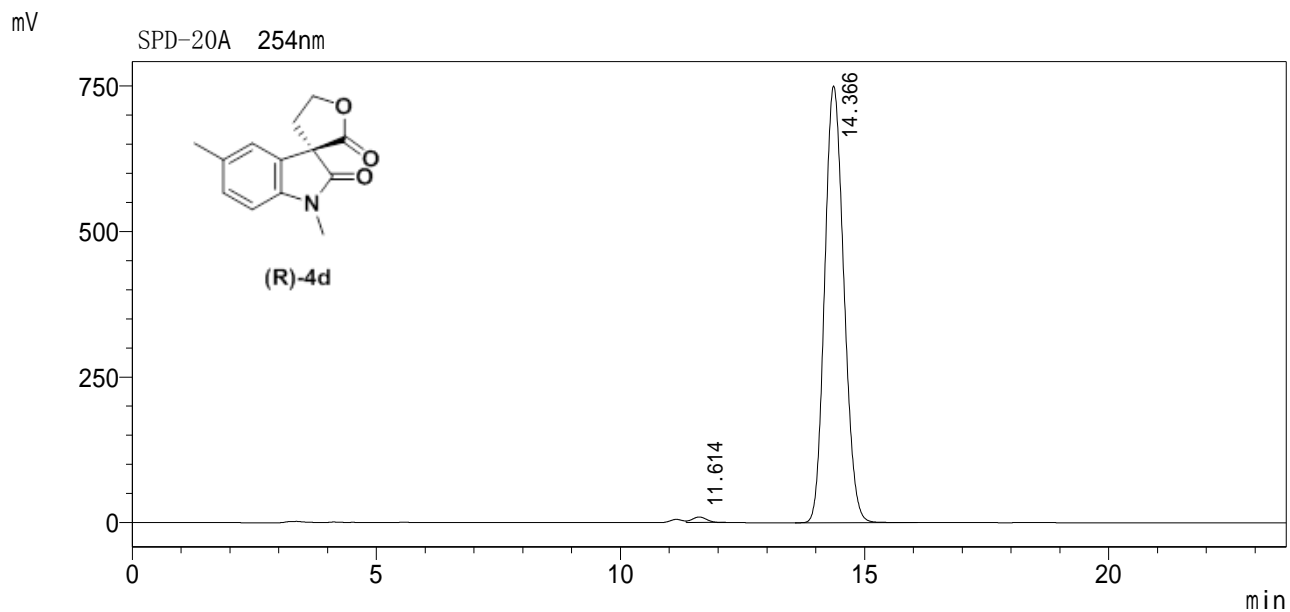
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	11.250	8939849	403411	49.728		M
2	13.670	9037646	331369	50.272		M
Sum		17977495	734780			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHW136JNCHIRAL  
 Data name : MHW136JNCHIRA-AS-H-40%.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/15 20:08:20  
 Pro. Data : 2021/1/15 21:18:47  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



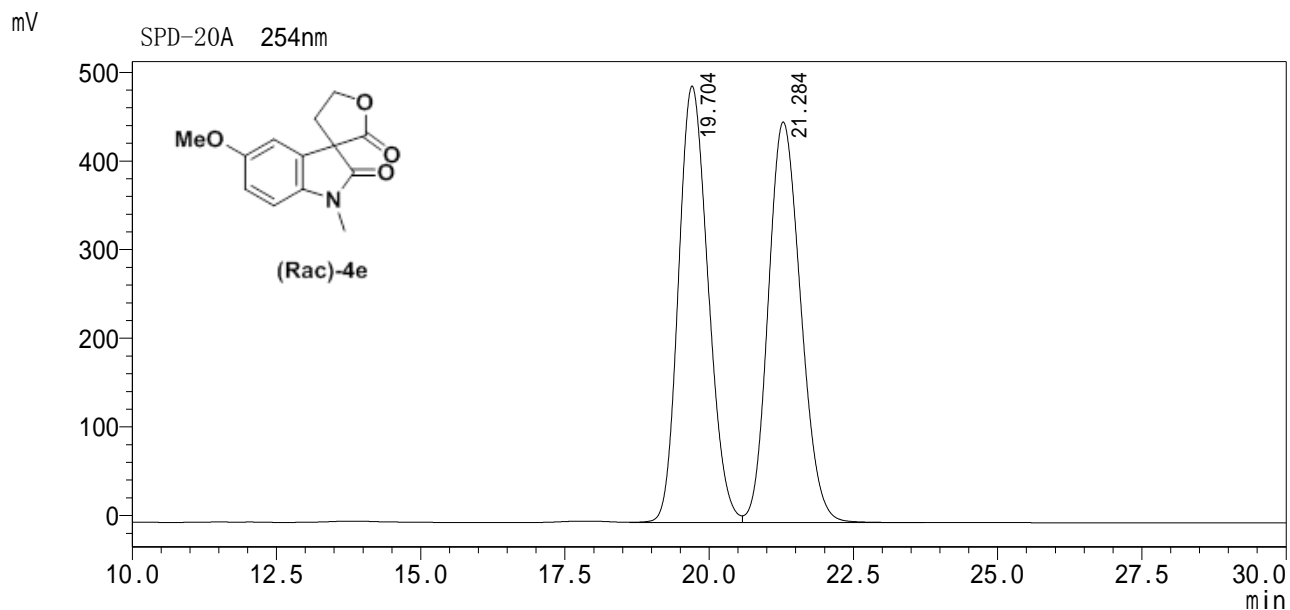
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	11.614	188472	9392	0.911		M
2	14.366	20497688	749875	99.089		
Sum		20686160	759267			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft 202006301 rac as 40%  
 Data name : zft 202006301 rac as 40%.lcd  
 Acq. method : OD-H-40.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/30 11:48:31  
 Pro. Data : 2020/6/30 12:32:12  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



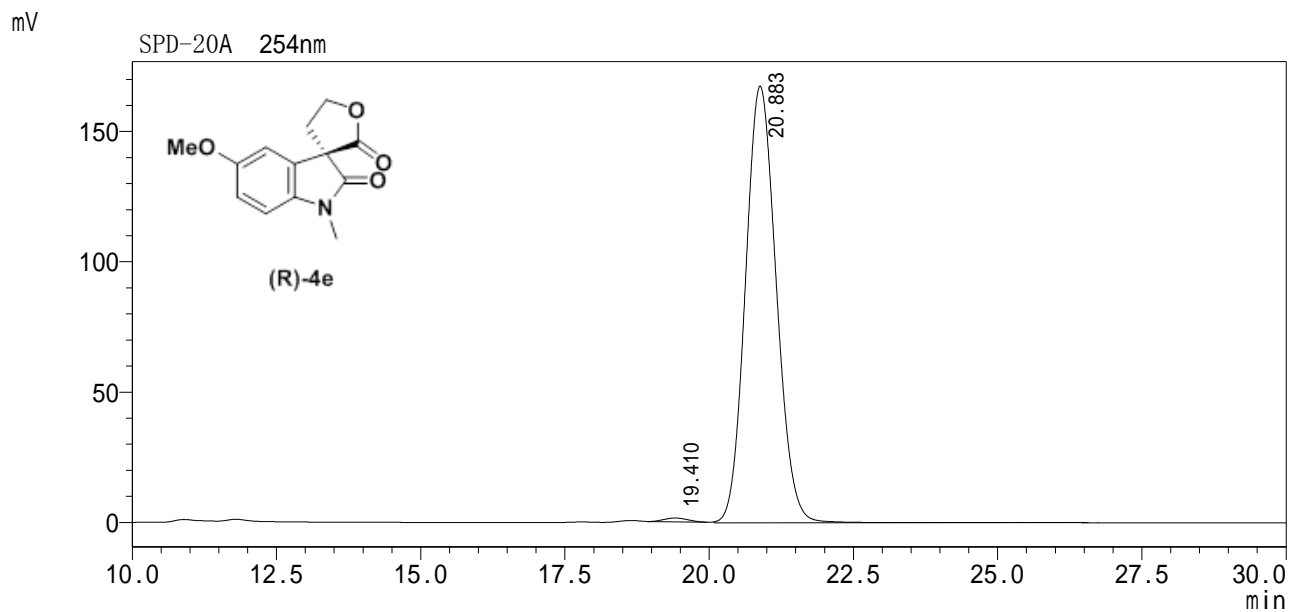
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	19.704	17581670	492501	49.868		
2	21.284	17674561	452149	50.132	V	
Sum		35256231	944650			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft 202006301 as 40%  
 Data name : zft 202006301 as 40%.lcd  
 Acq. method : OD-H-40.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/30 12:34:22  
 Pro. Data : 2020/6/30 14:14:57  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

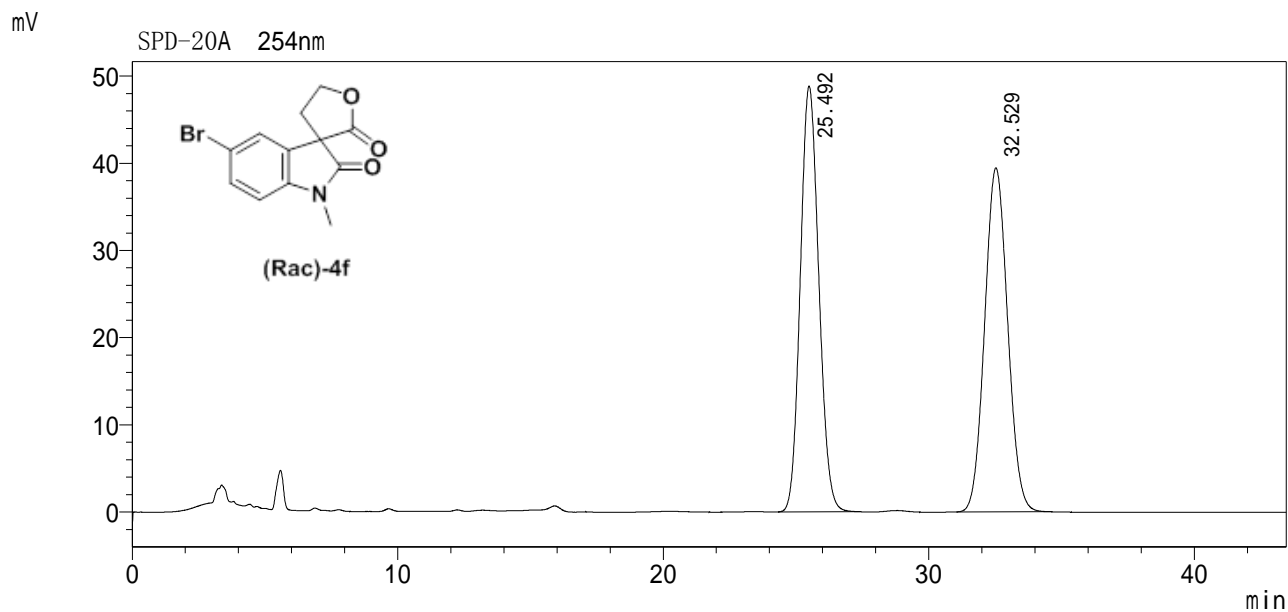
Entry	RT[min]	Area	Height	Area%		
1	19.410	41371	1446	0.660	M	
2	20.883	6226921	167607	99.340	M	
Sum		6268292	169053			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD124rac  
 Data name : MHWD124rac-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/8 16:19:23  
 Pro. Data : 2021/1/8 22:34:20

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	25.492	2363322	48824	49.896			
2	32.529	2373182	39444	50.104			
Sum		4736505	88268				

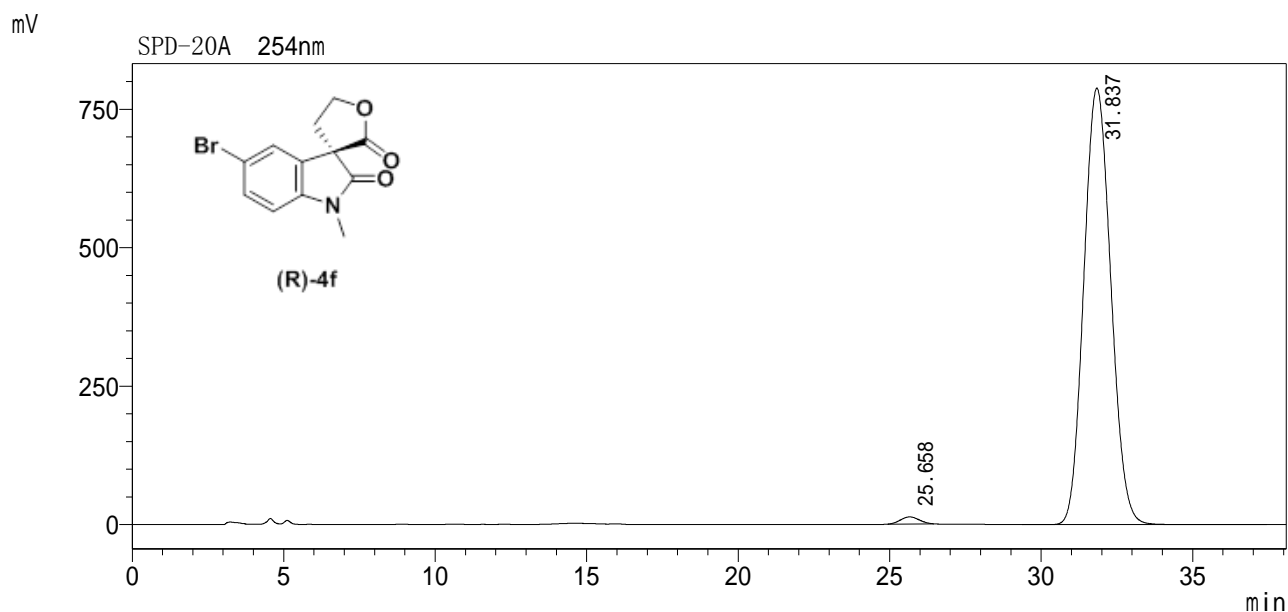



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD124jn20%TMS  
 Data name : MHWD124jn20%TMS-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/16 15:48:56  
 Pro. Data : 2020/12/24 23:59:21

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



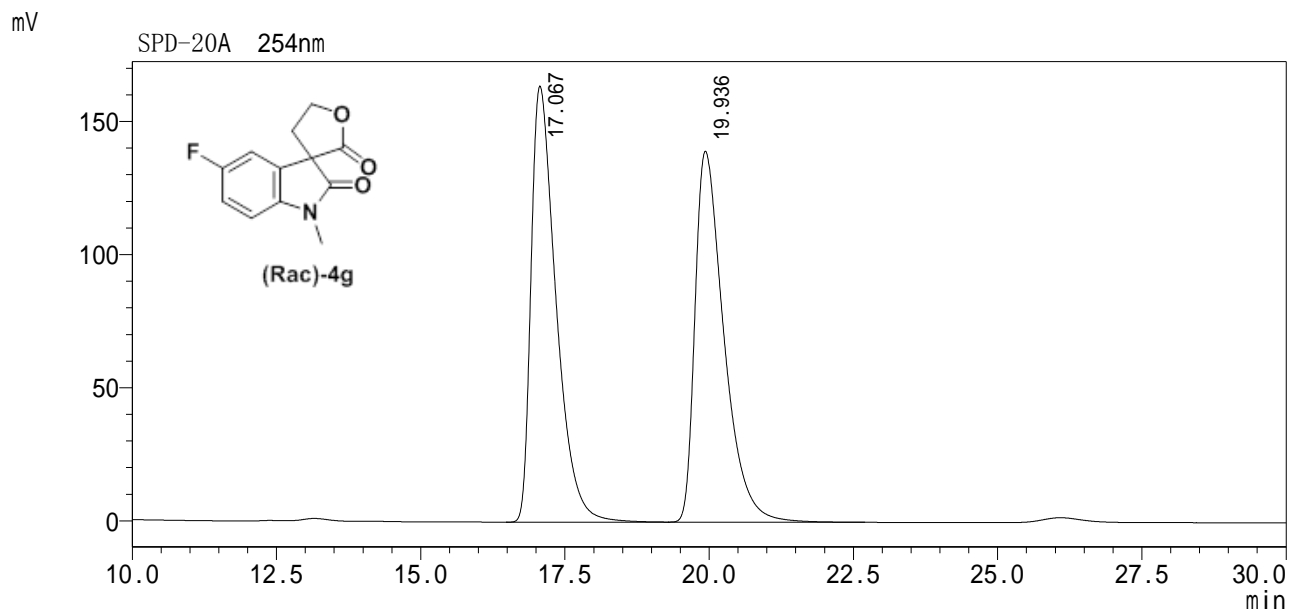
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	25.658	541119	12764	1.097		M
2	31.837	48784640	788187	98.903		M
Sum		49325759	800951			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft202006302oj 40%  
 Data name : zft202006302racoj40%.lcd  
 Acq. method : OD-H-40.lcm  
 Location : 1-1  
 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/6/30 10:06:56  
 Analyst : System Administrator  
 Pro. Data : 2020/6/30 10:42:33  
 Processor : System Administrator



SPD-20A

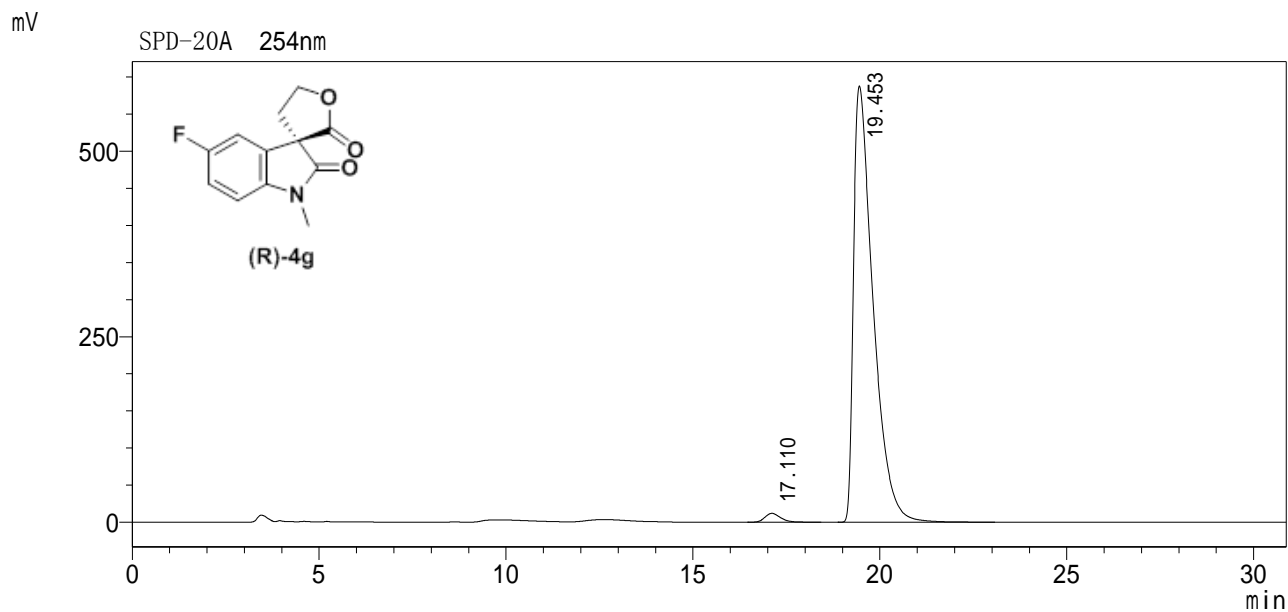
Entry	RT[min]	Area	Height	Area%		
1	17.067	4950947	163821	50.540		
2	19.936	4845153	139398	49.460	V	
Sum		9796100	303219			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft202006302-1oj 40%  
 Data name : zft202006302-1oj40%.lcd  
 Acq. method : OD-H-40.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/30 10:44:10  
 Pro. Data : 2020/7/5 17:50:57

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

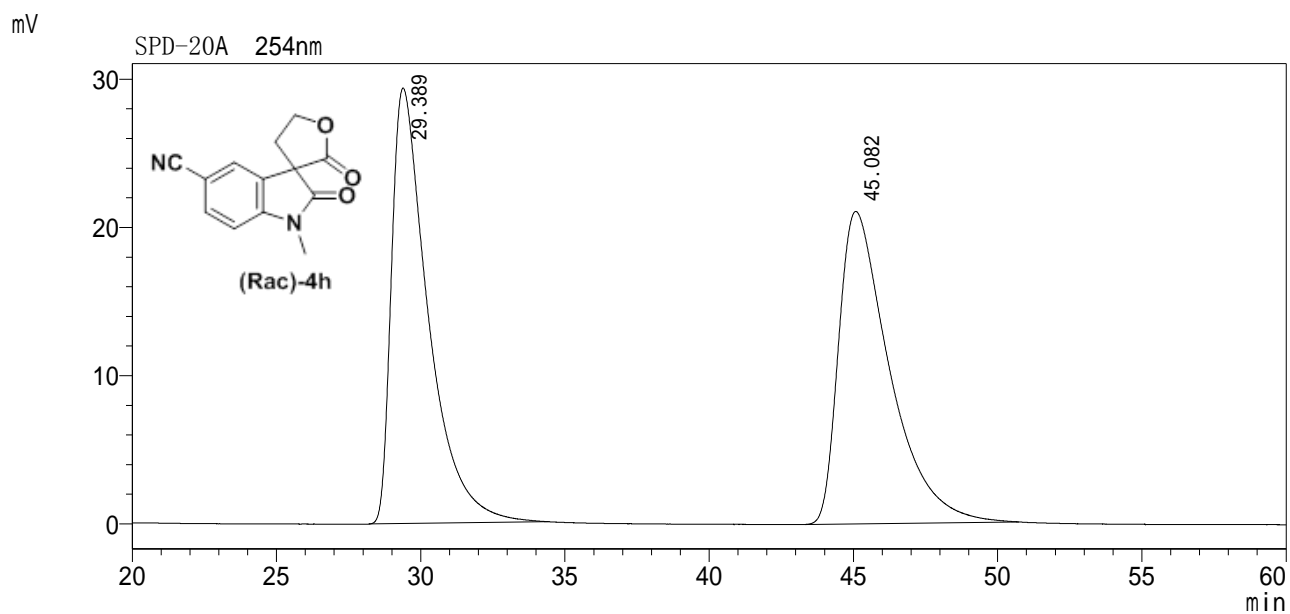
Entry	RT[min]	Area	Height	Area%			
1	17.110	347445	11969	1.599			
2	19.453	21376076	587943	98.401			
Sum		21723521	599912				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF014cRAC  
 Data name : MHWF014cRAC-OJ-H-50%.lcd  
 Acq. method : OJ-H-50%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/18 11:05:51  
 Pro. Data : 2021/1/18 12:45:52

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



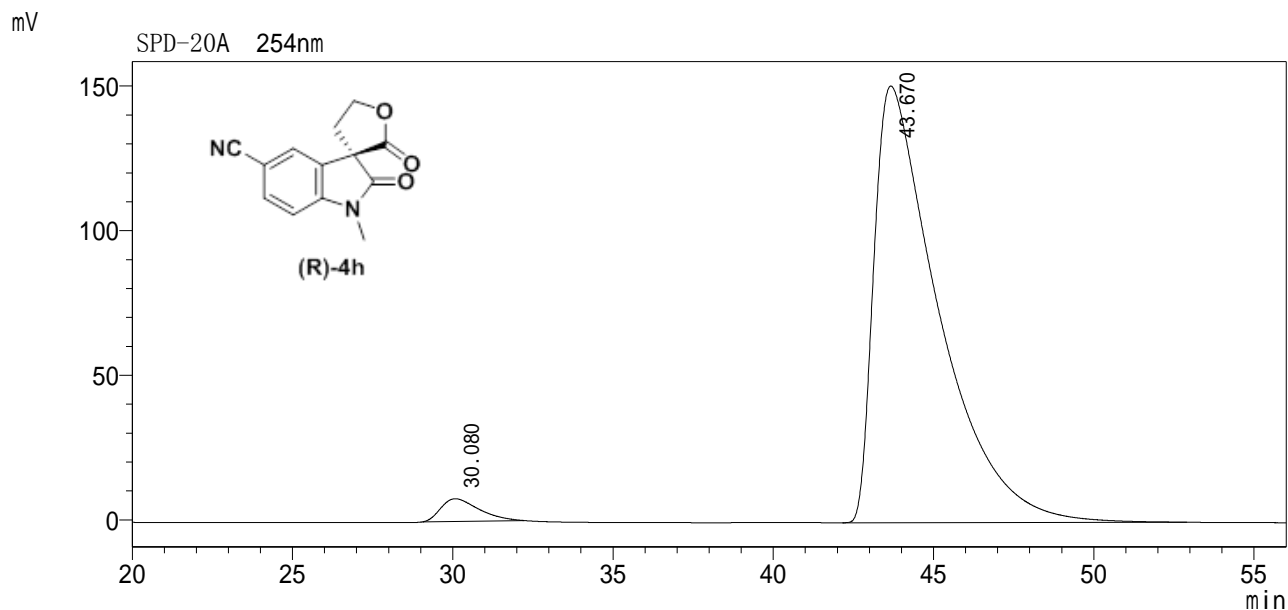
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	29.389	2594330	29381	50.080			
2	45.082	2586025	21073	49.920			
Sum		5180355	50454				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF014c  
 Data name : MHWF014c-OJ-H-50%.lcd  
 Acq. method : OJ-H-50%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Date : 2021/1/18 10:06:01  
 Pro. Date : 2021/1/18 11:02:57  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



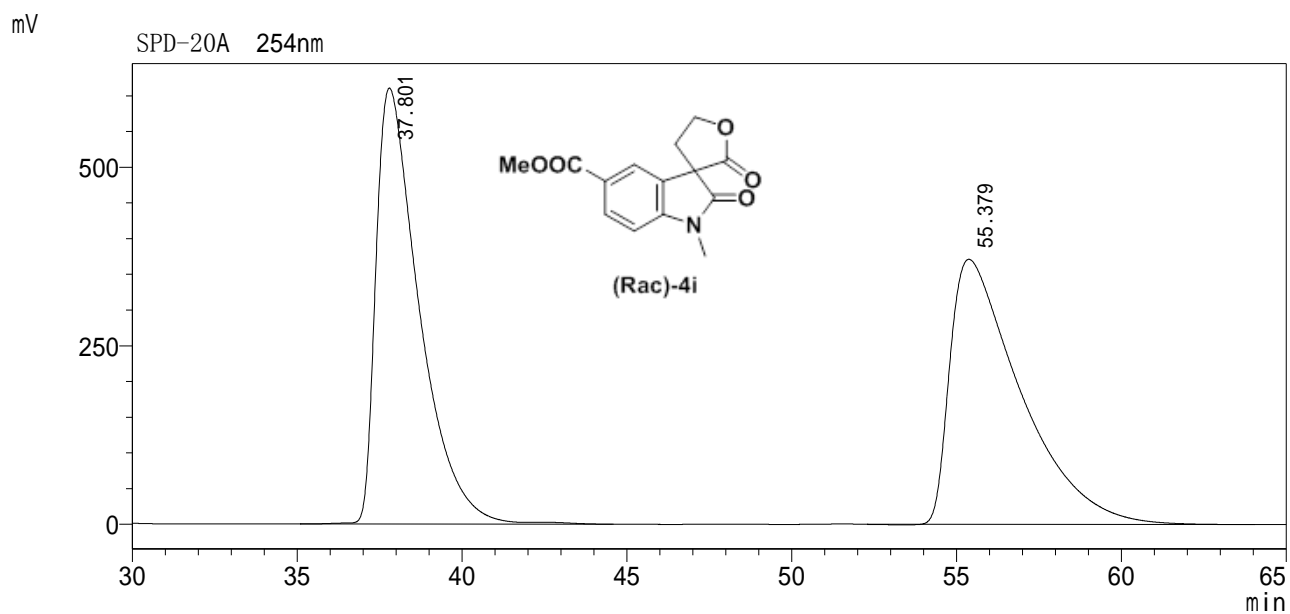
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	30.080	642623	7827	2.948		M
2	43.670	21154411	150996	97.052		S
Sum		21797033	158823			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD139RAC  
 Data name : MHWD139RAC-IC-H-50%.lcd  
 Acq. method : IC-H-50%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/25 19:23:12  
 Pro. Data : 2021/1/15 21:18:24  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

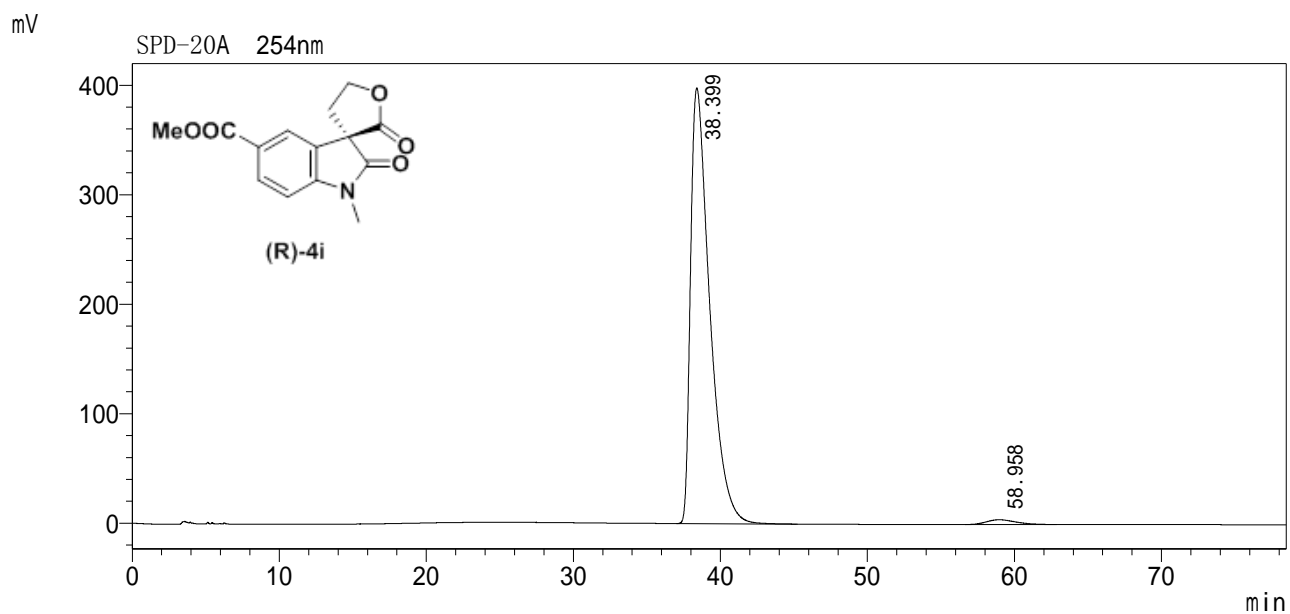
Entry	RT[min]	Area	Height	Area%			
1	37.801	55788561	610663	50.195		M	
2	55.379	55354731	371320	49.805		M	
Sum		111143292	981984				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD139CHIRAL  
 Data name : MHWD139CHIRAL-IC-H-50%.lcd  
 Acq. method : IC-H-50%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/25 20:34:08  
 Pro. Data : 2020/12/25 23:27:11

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



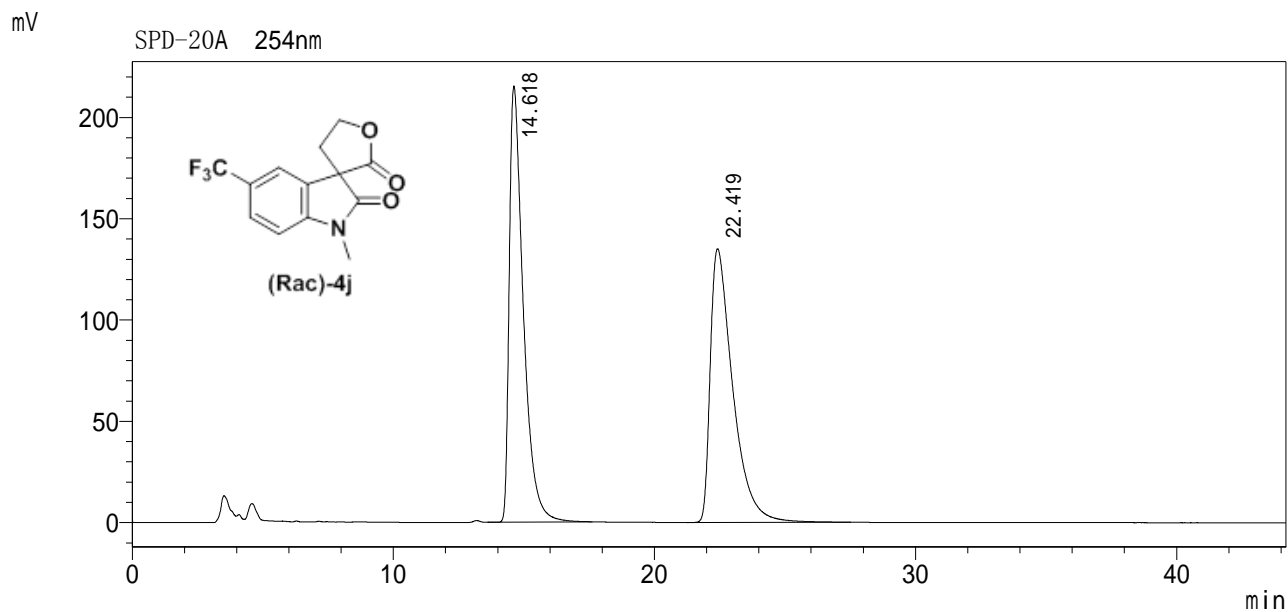
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	38.399	36038267	397869	98.341		
2	58.958	608143	4377	1.659	S	
Sum		36646410	402246			


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**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft1124rac oj 40%  
 : zft1124rac oj 40%  
 Data name : zft1124rac oj 40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/2 18:28:15 Analyst : System Administrator  
 Pro. Data : 2020/12/2 19:12:27 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	14.618	8054896	215309	49.930		M
2	22.419	8077385	135096	50.070		M
Sum		16132282	350405			



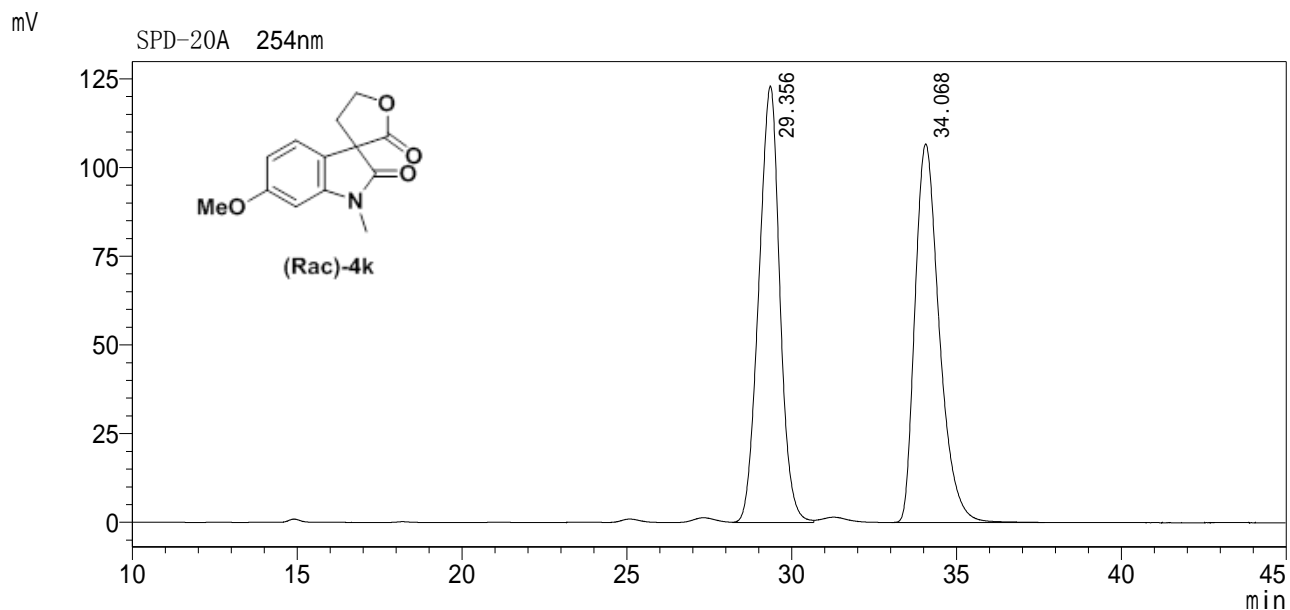



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202007025 AD RAC 10%  
 Data name : ZFT202007025 AD RAC 10%.lcd  
 Acq. method : OD-H-80%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/11 14:17:01  
 Pro. Data : 2020/7/11 22:03:22

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



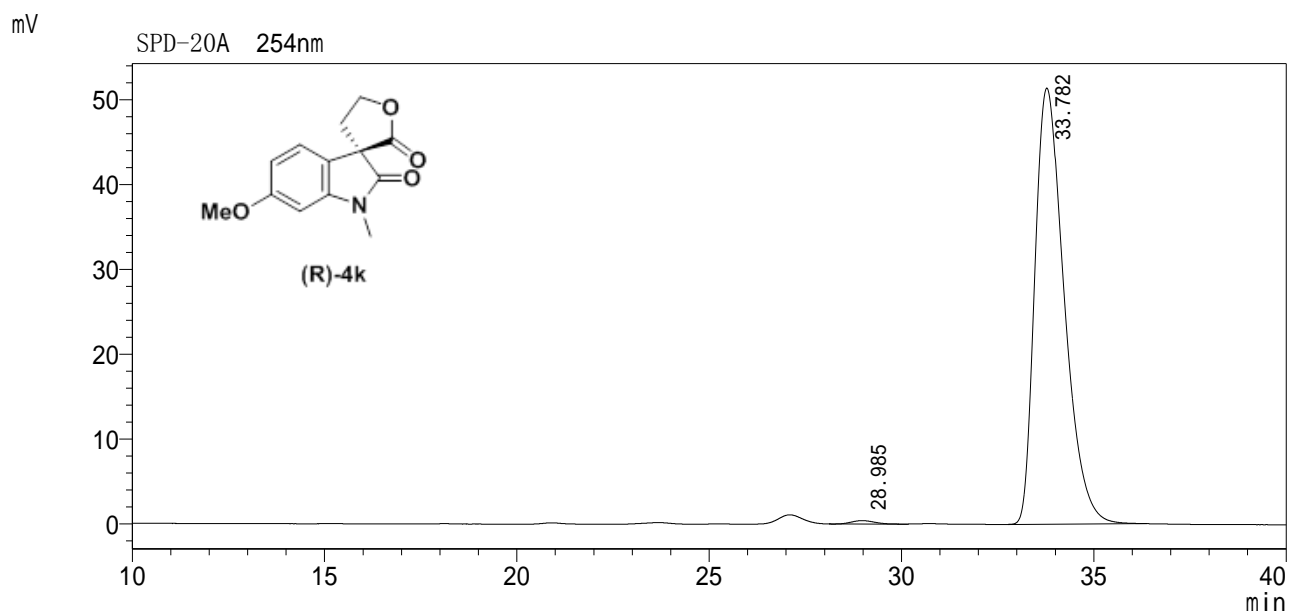
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	29.356	5452322	123018	49.946			
2	34.068	5464034	106723	50.054			
Sum		10916355	229741				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202007112 AD OMe 10%  
 Data name : ZFT202007112 AD OMe 10%.lcd  
 Acq. method : OD-H-80%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/11 16:41:24  
 Pro. Data : 2020/7/11 22:03:23  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



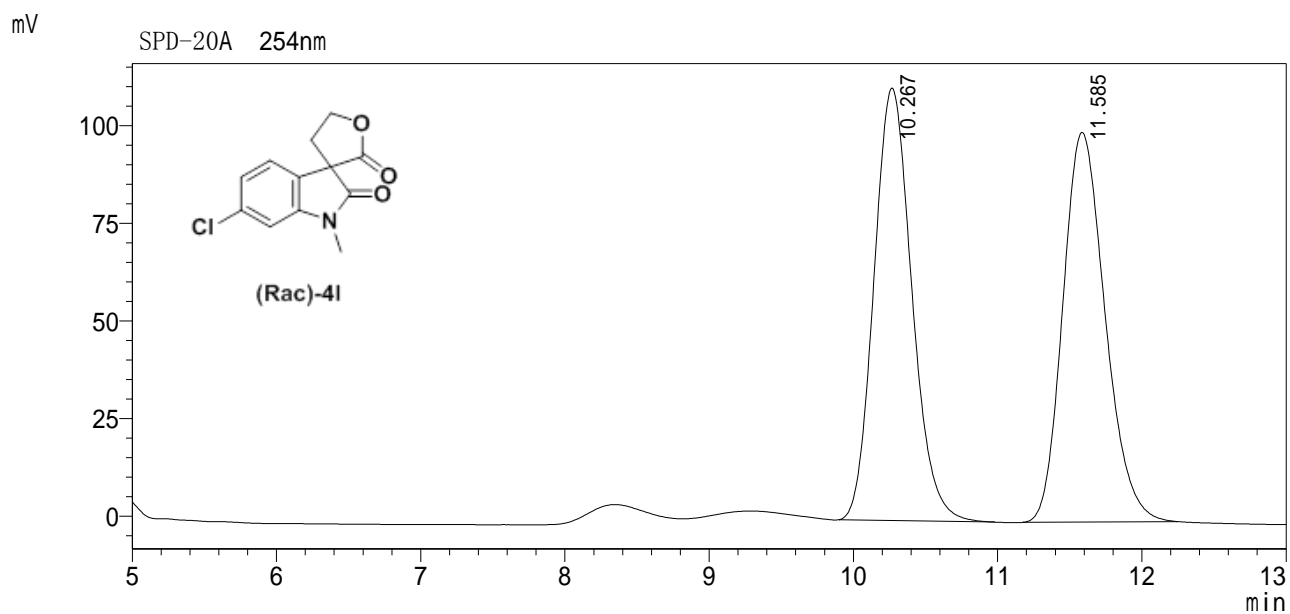
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	28.985	16625	405	0.611		M
2	33.782	2703158	51416	99.389		
Sum		2719783	51821			


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**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT-7143 RAC AD 20%  
 Data name : ZFT-7143 RAC AS 20%.lcd  
 Acq. method : OJ-H-40%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/14 21:29:51  
 Pro. Data : 2020/7/28 22:33:39  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

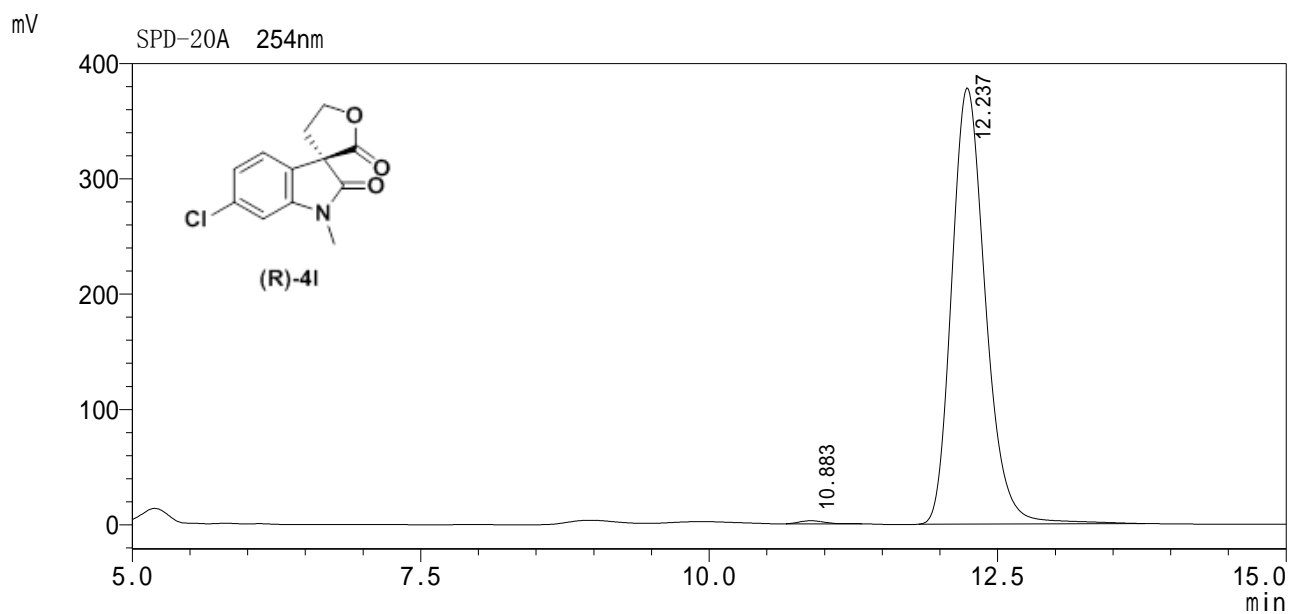
Entry	RT[min]	Area	Height	Area%		
1	10.267	2023330	110769	49.905	M	
2	11.585	2031020	99825	50.095	M	
Sum		4054350	210594			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT-7142 AD 20%  
 Data name : ZFT202007142 AD 20%.lcd  
 Acq. method : OJ-H-40%-60min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/14 21:44:48  
 Pro. Data : 2020/7/14 22:03:38

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



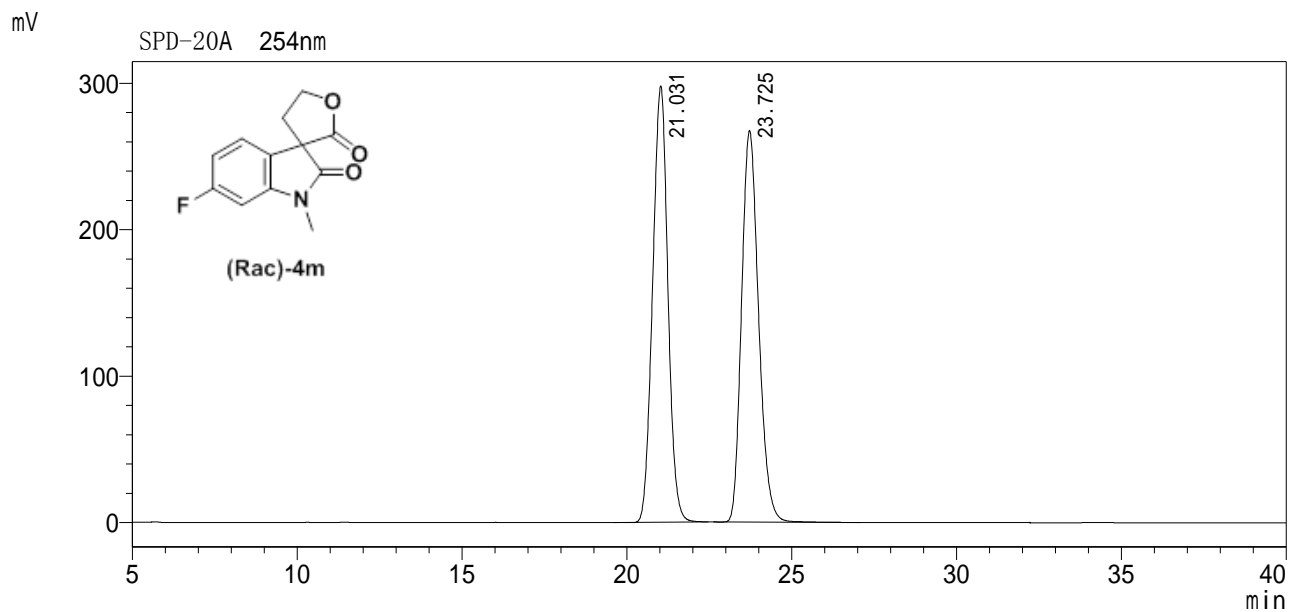
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.883	38041	2618	0.492	M	
2	12.237	7699491	378118	99.508	M	
Sum		7737532	380736			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202007024 AD RAC 10%  
 Data name : ZFT202007024 AD RAC 10%.lcd  
 Acq. method : OD-H-80%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/11 15:03:36  
 Pro. Data : 2020/7/11 16:36:59  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



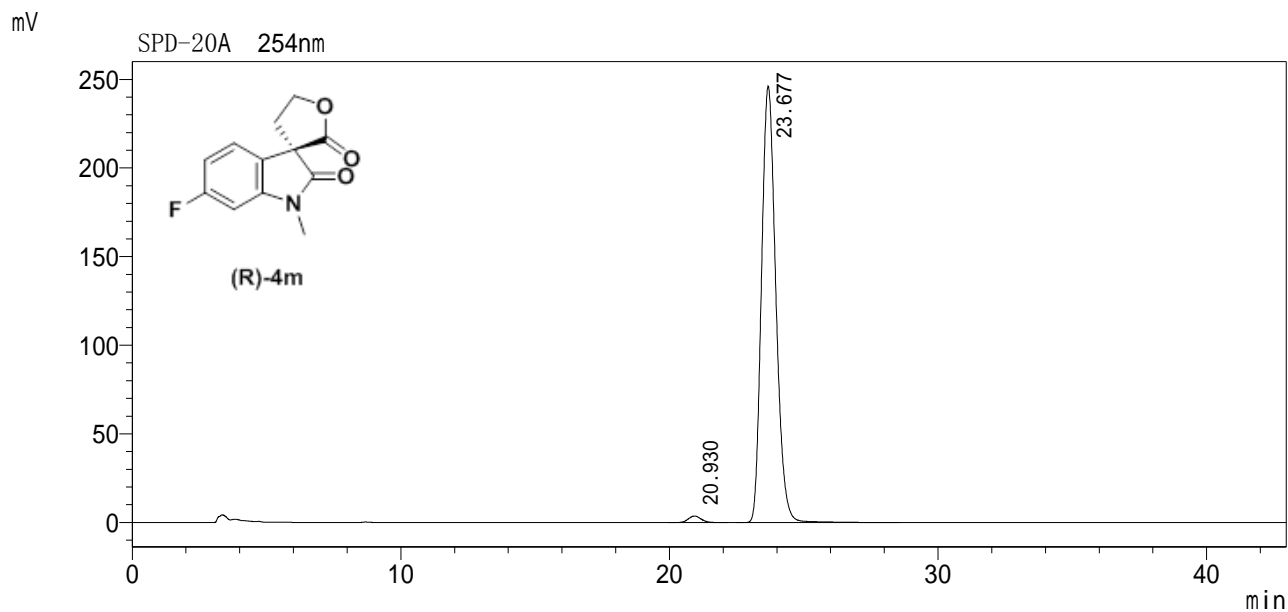
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	21.031	9555999	297933	49.892		M	
2	23.725	9597359	267421	50.108		M	
Sum		19153358	565354				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202007111 AD F 10%  
 Data name : ZFT202007111 AD F 10%.lcd  
 Acq. method : OD-H-80%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/11 17:36:51  
 Pro. Data : 2020/7/11 20:08:23  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



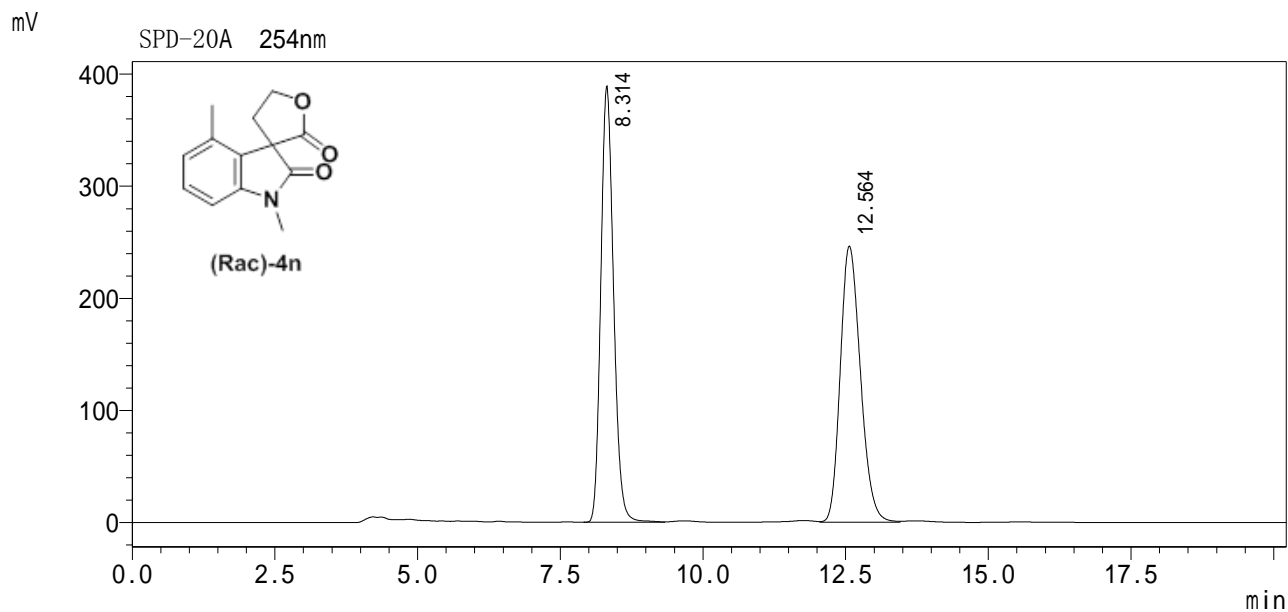
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	20.930	120879	3683	1.304		M
2	23.677	9146794	246302	98.696		M
Sum		9267674	249985			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7172 RAC 40%AS  
               : zft7172-RAC40%AS  
 Data name   : zft7172 RAC AS40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
               :  
 Location    : 1-1                                 Sample Type : unknown  
               : 1 uL  
 Ana. Data   : 2020/12/3 1:56:19                 Analyst      : System Administrator  
 Pro. Data   : 2020/12/3 2:16:33                 Processor    : System Administrator



SPD-20A

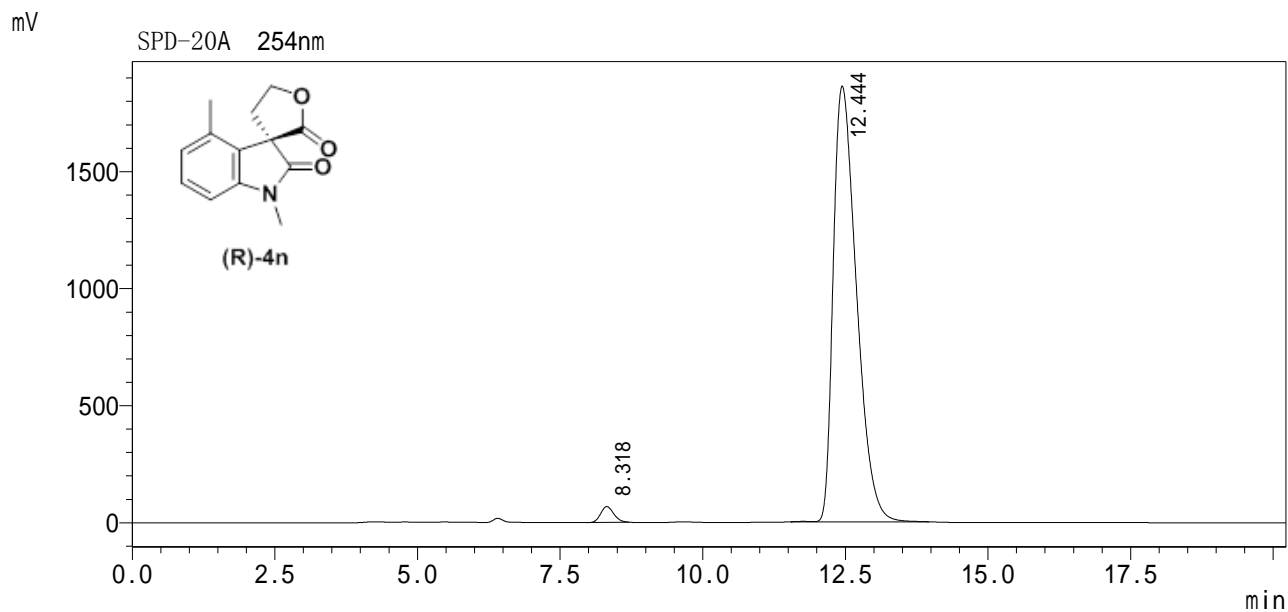
Entry	RT[min]	Area	Height	Area%			
1	8.314	6061222	389132	49.979			
2	12.564	6066303	246462	50.021			
Sum		12127525	635595				




**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Data name : zft7172 40%AS  
 : zft717240%AS  
 Data name : zft7172 AS40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/3 2:18:53 Analyst : System Administrator  
 Pro. Data : 2020/12/3 2:39:08 Processor : System Administrator



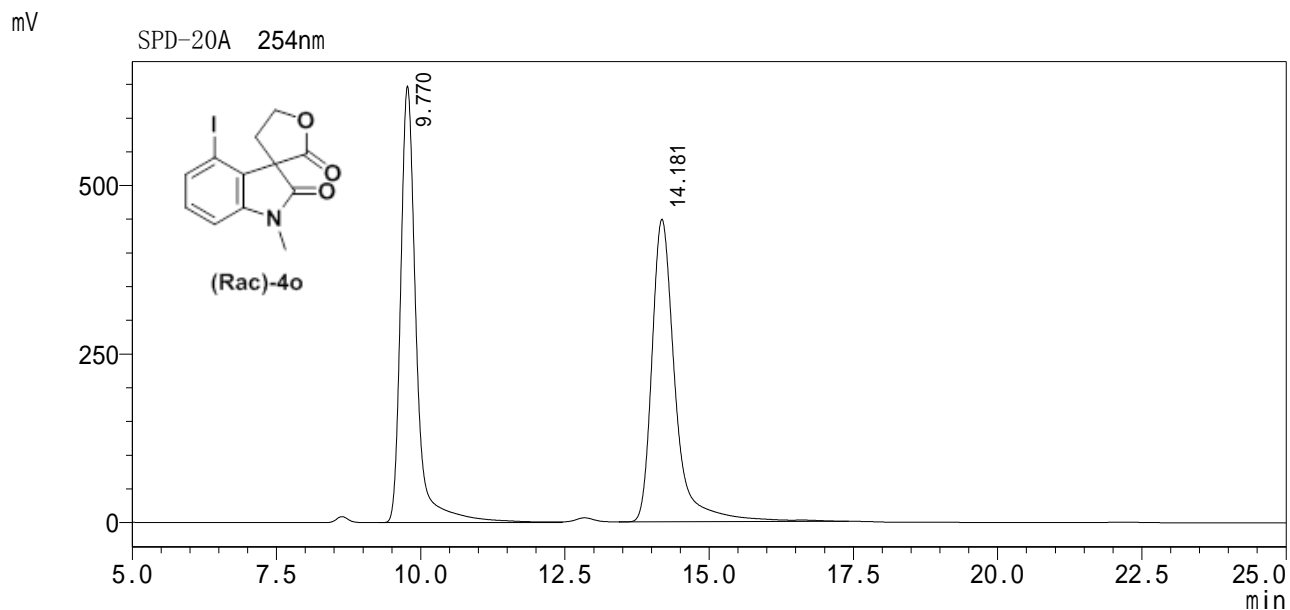
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	8.318	1067321	67366	1.987		M	
2	12.444	52655388	1861890	98.013		M	
Sum		53722710	1929257				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202007021rac Nath 40% AS  
 Data name : ZFT202007021 rac diiodo 40% AS.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/6 13:34:55  
 Pro. Data : 2020/7/6 14:08:01  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



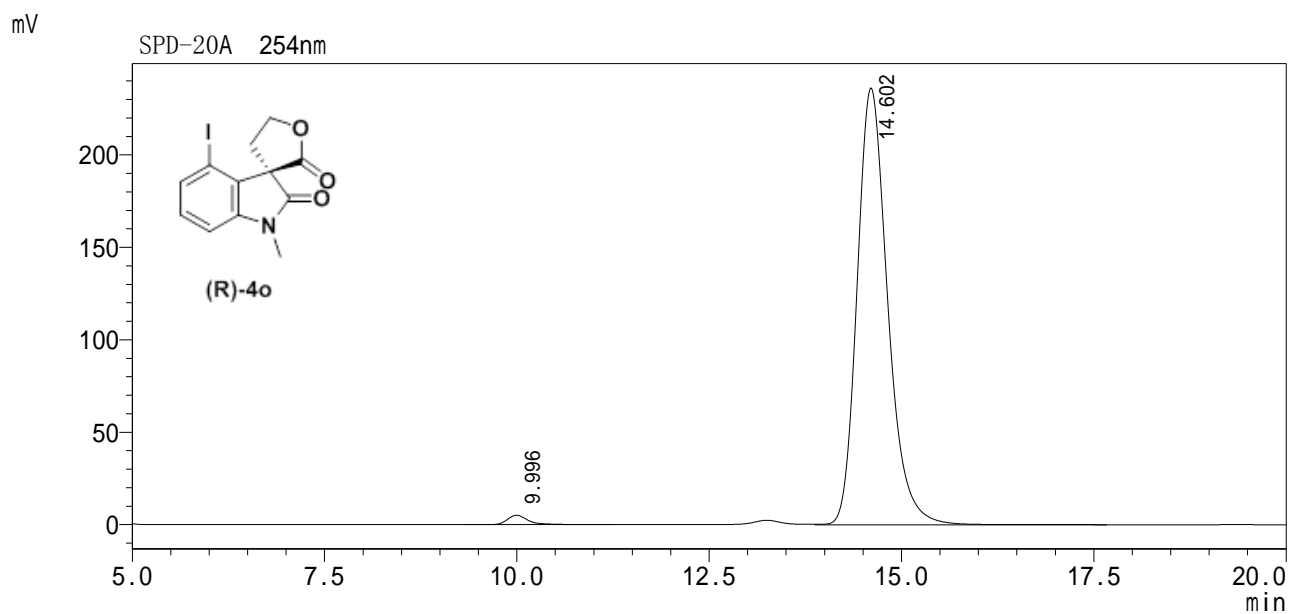
SPD-20A

Entry	RT[min]	Area	Height	Area		
1	9.770	12196311	647500	49.213		M
2	14.181	12586409	448638	50.787		M
Sum		24782720	1096137			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT2020070902 As 40% idio chiral  
 Data name : ZFT2020070901 As 40% idio chiral.lcd  
 Acq. method : OJ-H-40%.lcm  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/7/9 20:52:26 Analyst : System Administrator  
 Pro. Data : 2020/7/10 21:57:07 Processor : System Administrator



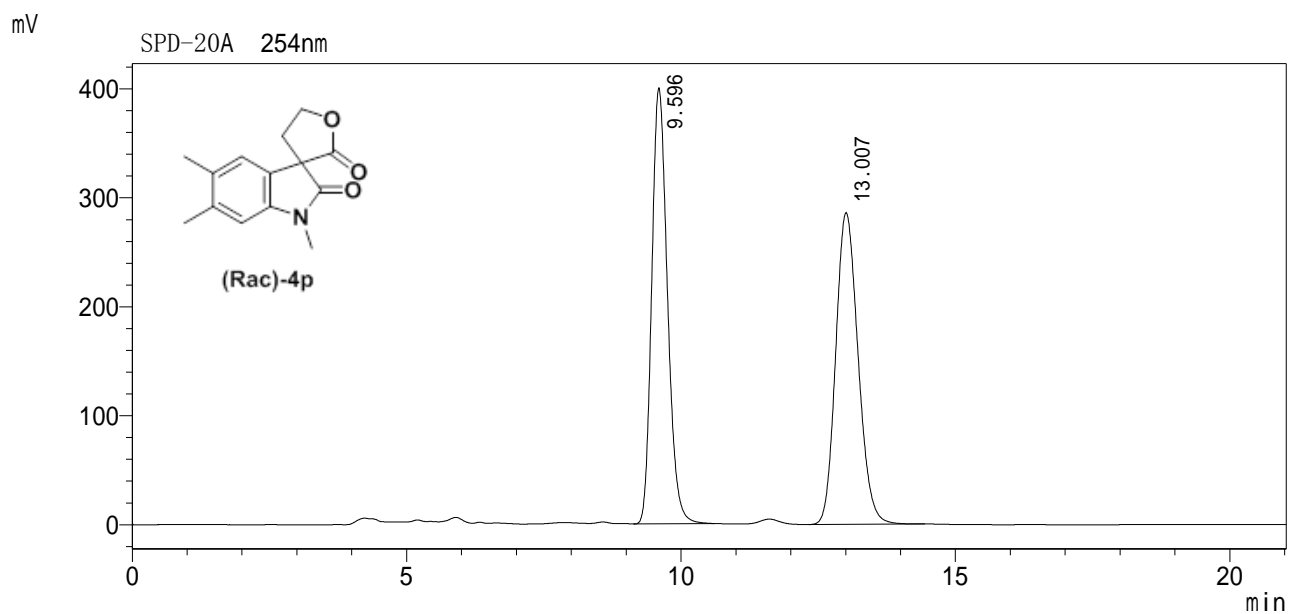
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	9.996	97017	5081	1.466		M
2	14.602	6521230	236239	98.534		M
Sum		6618247	241319			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7141 RAC40%  
               : zft7141 RAC40%  
 Data name   : zft7141 RAC40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
               :  
 Location    : 1-1                               Sample Type : unknown  
               : 1 uL  
 Ana. Data   : 2020/12/2 22:43:19           Analyst      : System Administrator  
 Pro. Data   : 2020/12/2 23:04:21           Processor    : System Administrator



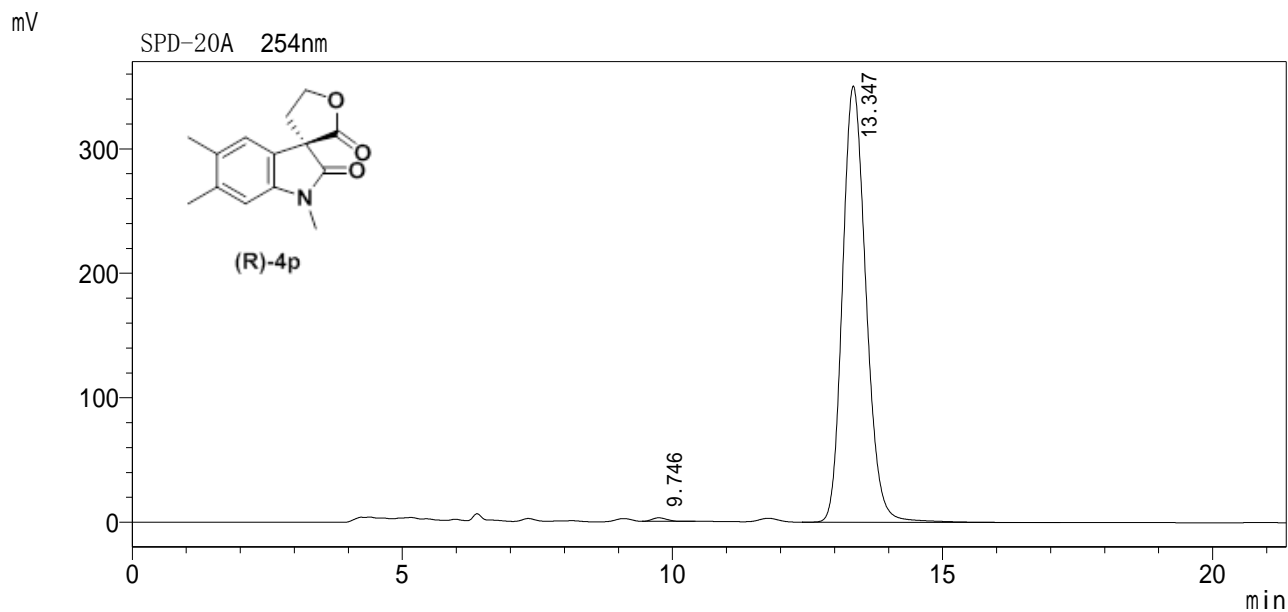
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	9.596	7957354	399993	49.566		M
2	13.007	8096777	286124	50.434		M
Sum		16054131	686117			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zft7141 40%AS  
 : zft7141 40%AS  
 Data name : zft7141 AS40%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/12/2 23:05:38 Analyst : System Administrator  
 Pro. Data : 2020/12/2 23:26:59 Processor : System Administrator



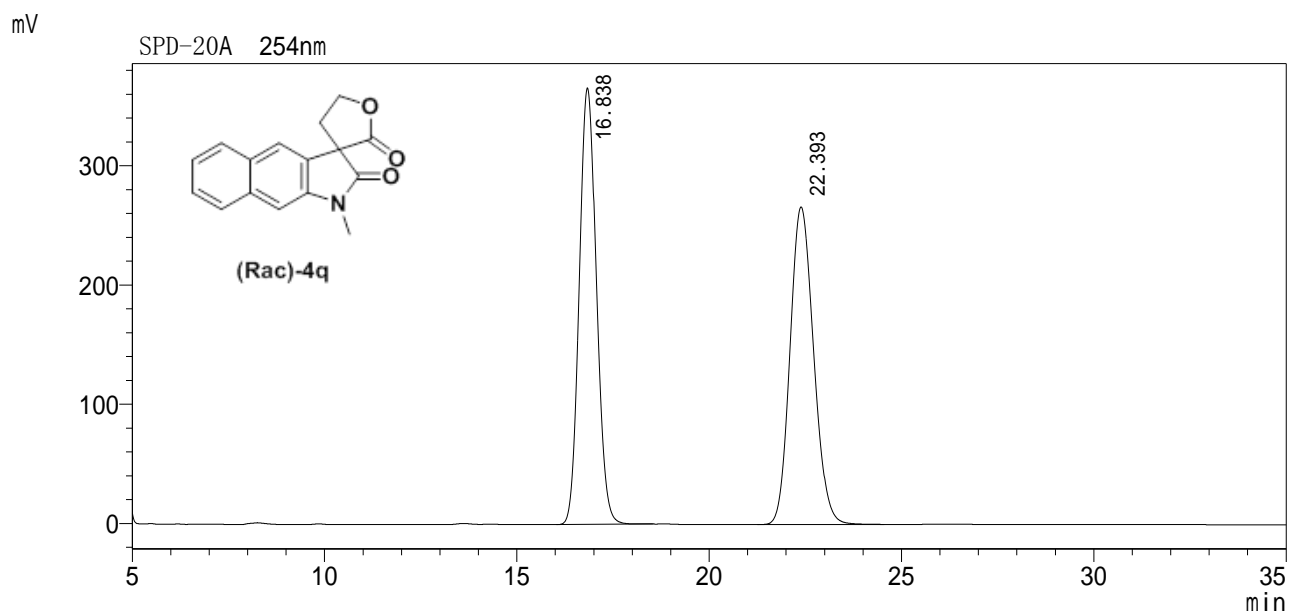
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	9.746	54185	2862	0.509		M
2	13.347	10583970	350438	99.491		M
Sum		10638155	353301			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT202007023 rac Nath 40% OJ  
 Data name : ZFT2020070223 rac Nath 40% AS.lcd  
 Acq. method : AS-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/6 12:47:52  
 Pro. Data : 2020/7/6 13:33:27  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



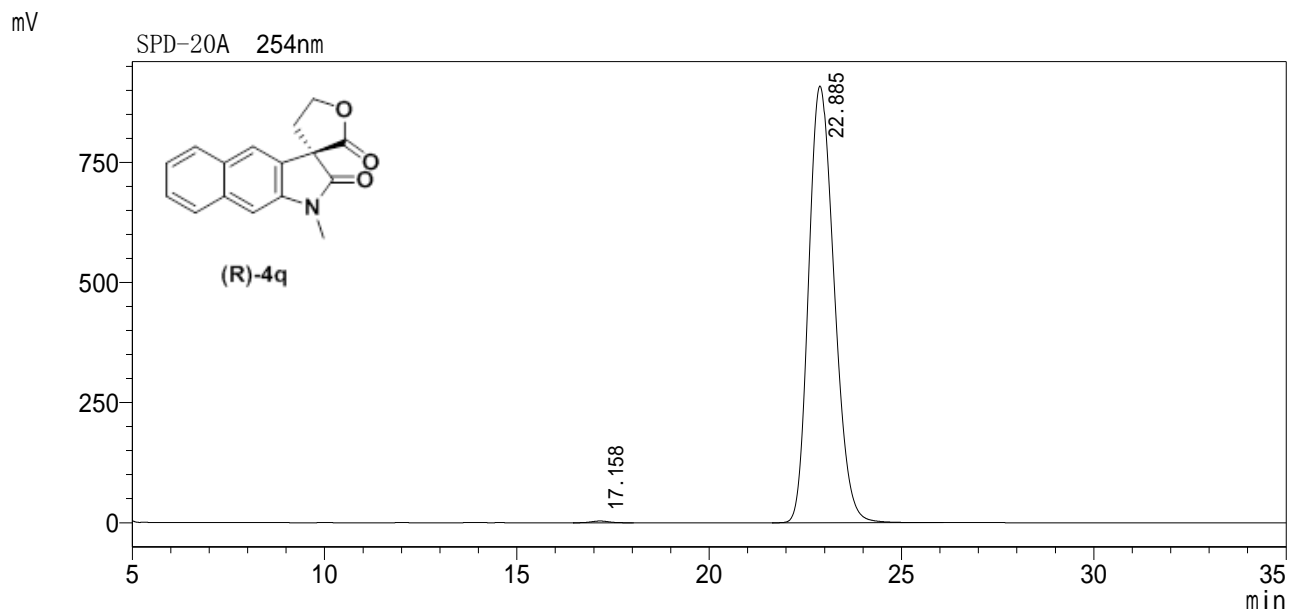
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	16.838	11261033	366101	49.813		M
2	22.393	11345573	266400	50.187		M
Sum		22606606	632501			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : ZFT2020070903 As 60% nath chiral  
 Data name : ZFT2020070903 As 40% nath chiral.lcd  
 Acq. method : OJ-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/9 20:10:49  
 Pro. Data : 2020/7/9 21:31:36  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



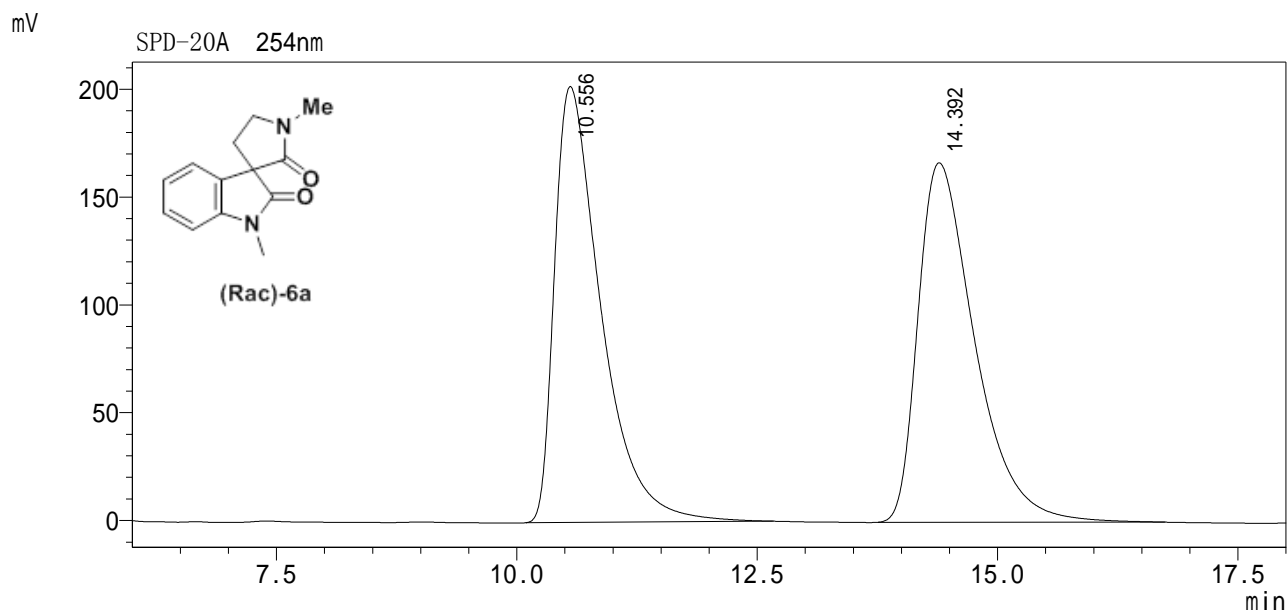
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	17.158	111122	3622	0.266			
2	22.885	41623530	909092	99.734			
Sum		41734652	912713				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : mhw\CC\  
 Data name : ZW-1-54rac-ODH30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2019/12/27 9:41:45  
 Pro. Data : 2020/6/6 21:55:24  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.556	6777925	202179	49.778		M
2	14.392	6838429	166713	50.222		M
Sum		13616354	368892			

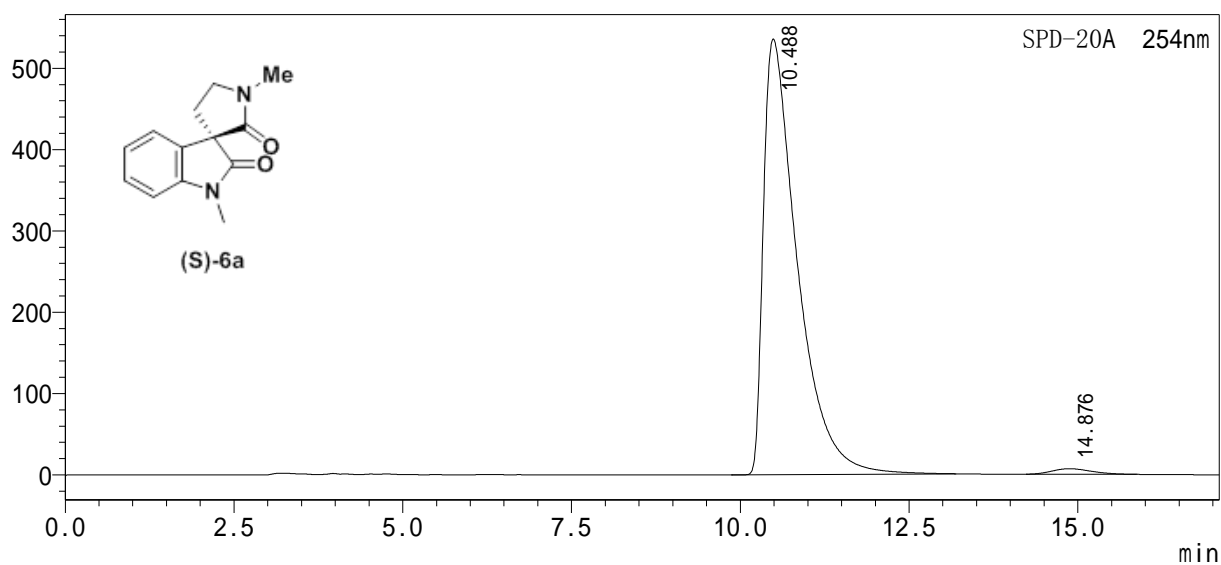



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD116jn100%  
 Data name : MHWD116jn100%-OD-H-30%.lcd  
 Acq. method : OD-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/12/11 20:27:32  
 Pro. Data : 2020/12/11 22:18:58  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator

mV



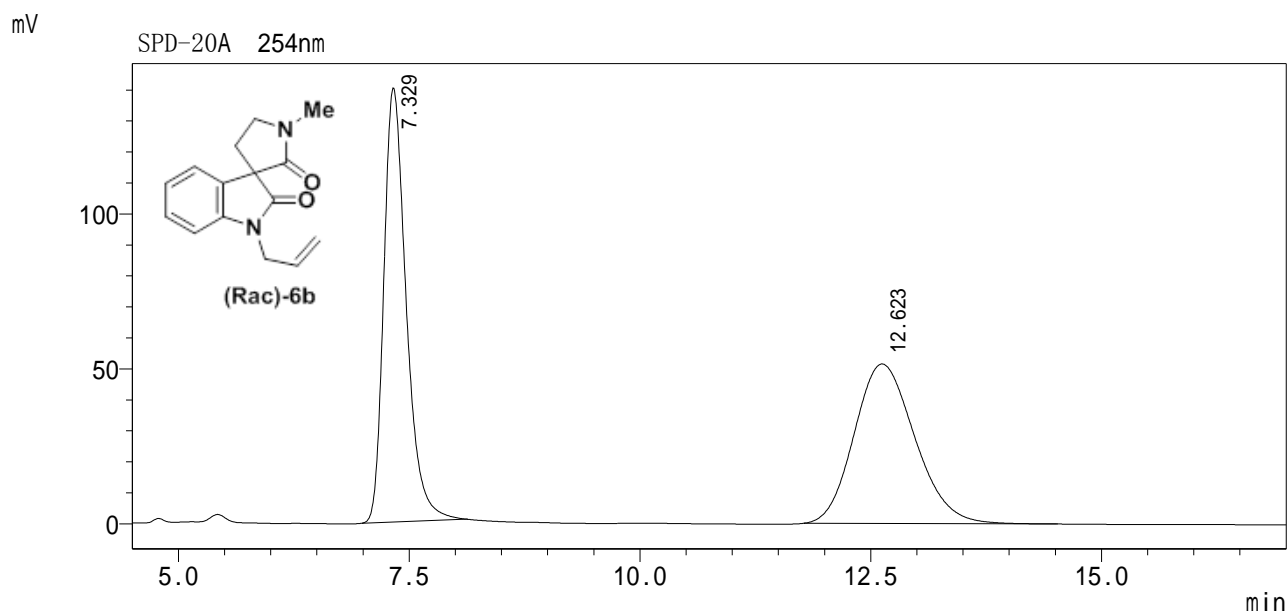
SPD-20A 254nm

Entry	RT[min]	Area	Height	Area%		
1	10.488	18721511	535727	98.535		M
2	14.876	278295	6864	1.465		M
Sum		18999807	542591			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Data name : zw-19-122-1-ojh-703010  
 Data name : zw-19-122-1-ojh-703010.lcd  
 Acq. method : OJ-H-50%.lcm  
 Location : 1-1  
 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/6/17 14:26:40  
 Analyst : System Administrator  
 Pro. Data : 2020/6/17 14:51:59  
 Processor : System Administrator



SPD-20A

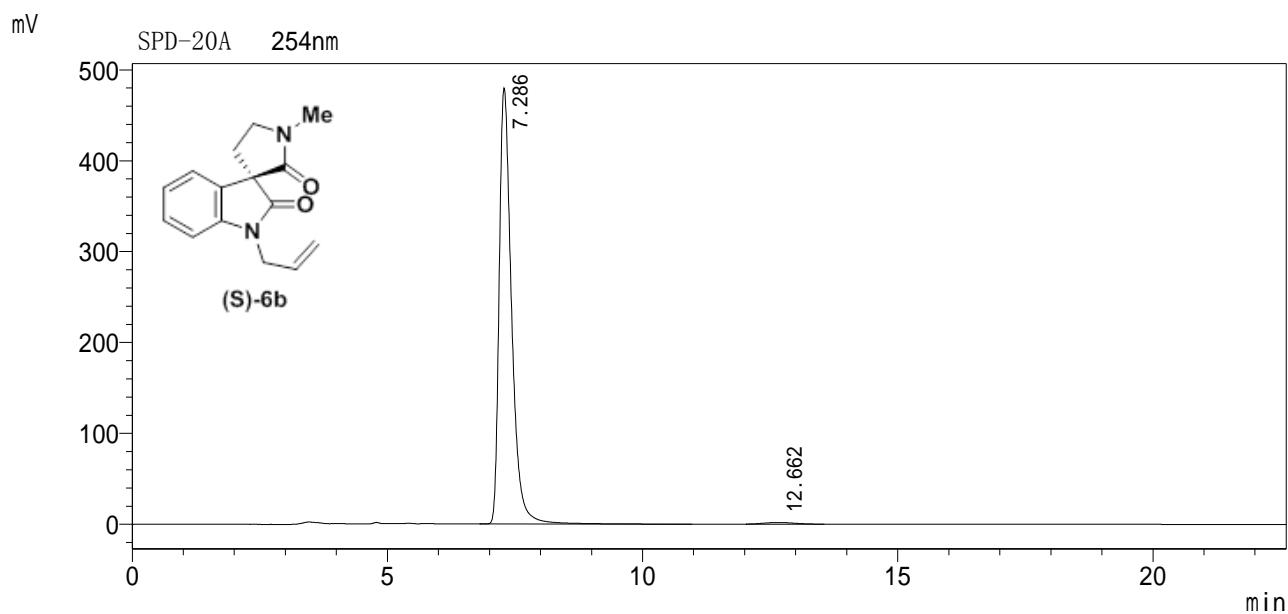
Entry	RT[min]	Area	Height	Area%		
1	7.329	2364720	140058	50.089		M
2	12.623	2356353	51500	49.911		M
Sum		4721073	191559			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-122-2-ojh-703010  
 Data name : zw-19-122-2-ojh-703010.lcd  
 Acq. name : OJ-H-50%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/17 14:54:03  
 Pro. Data : 2021/1/9 20:12:29

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



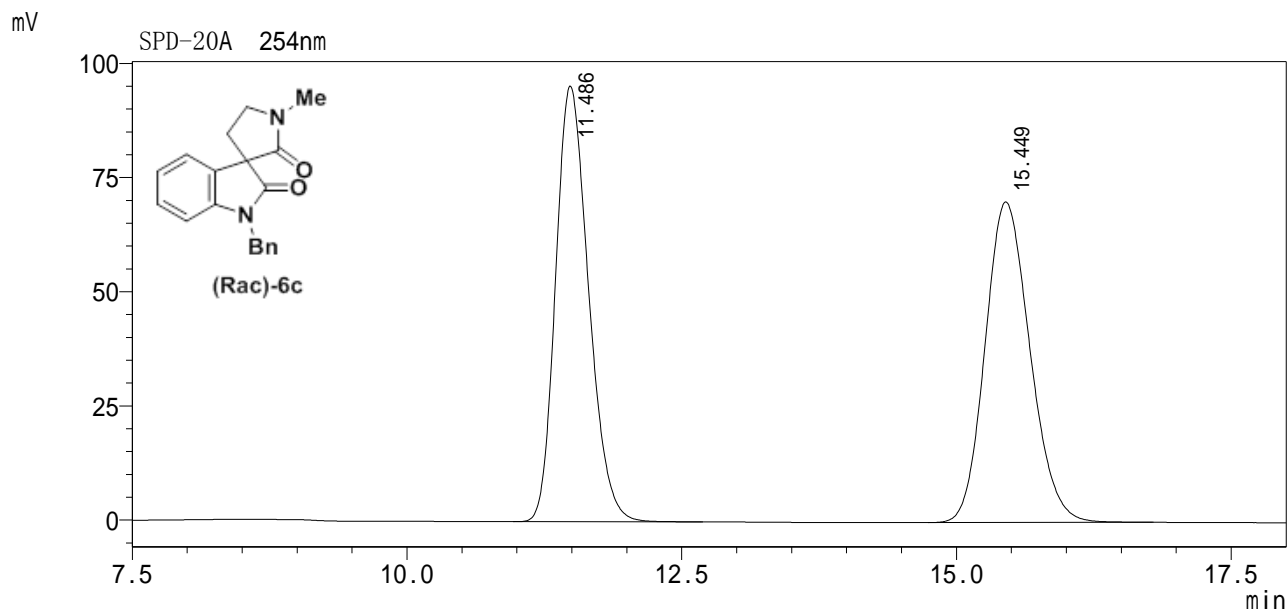
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	7.286	8116918	479640	99.055		M
2	12.662	77405	1823	0.945		M
Sum		8194323	481463			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-NBnrac-adh-604010  
 Data name : zw-19-NBnrac-adh-604010.lcd  
 Acq. method : OD-H-40.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/18 16:44:24  
 Pro. Data : 2020/6/18 17:03:30  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



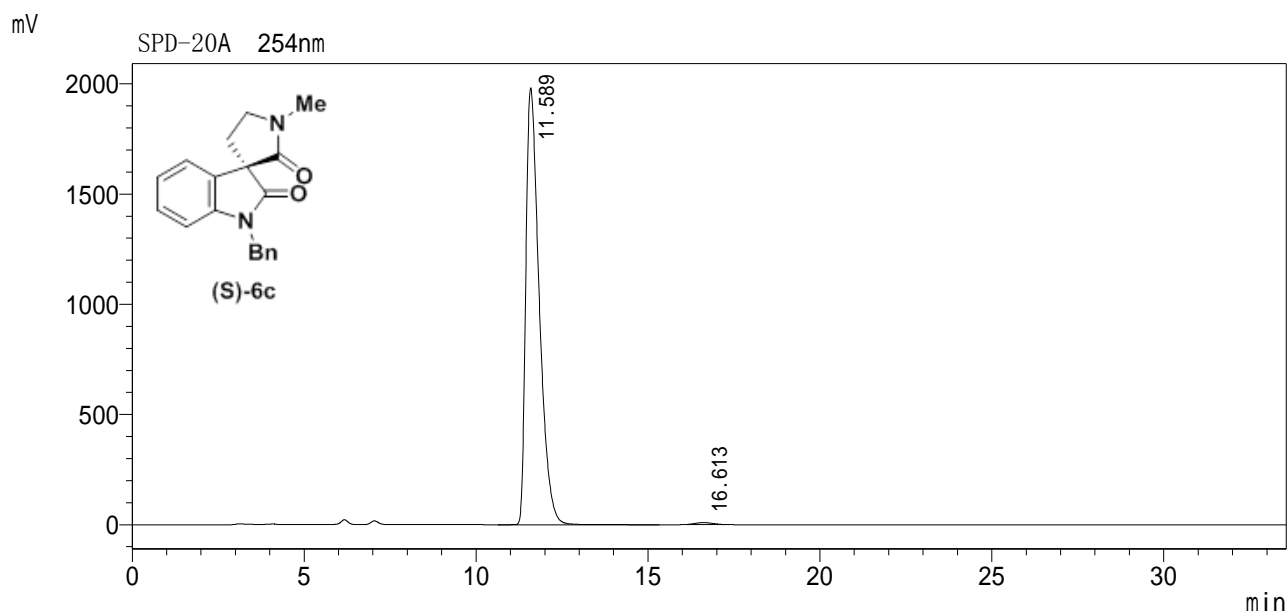
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	11.486	1987774	95403	49.980			
2	15.449	1989367	70181	50.020			
Sum		3977141	165584				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF007jn100%CH3-1  
 Data name : MHWF007jn100%CH3-1-AD-H-40%.lcd  
 Acq. method : AD-H-40%.lcm  
 Location : 1-1  
 Sample Type : unknown  
 : 1  $\mu$ L  
 Ana. Data : 2021/1/8 15:13:36 Analyst : System Administrator  
 Pro. Data : 2021/1/8 15:54:09 Processor : System Administrator



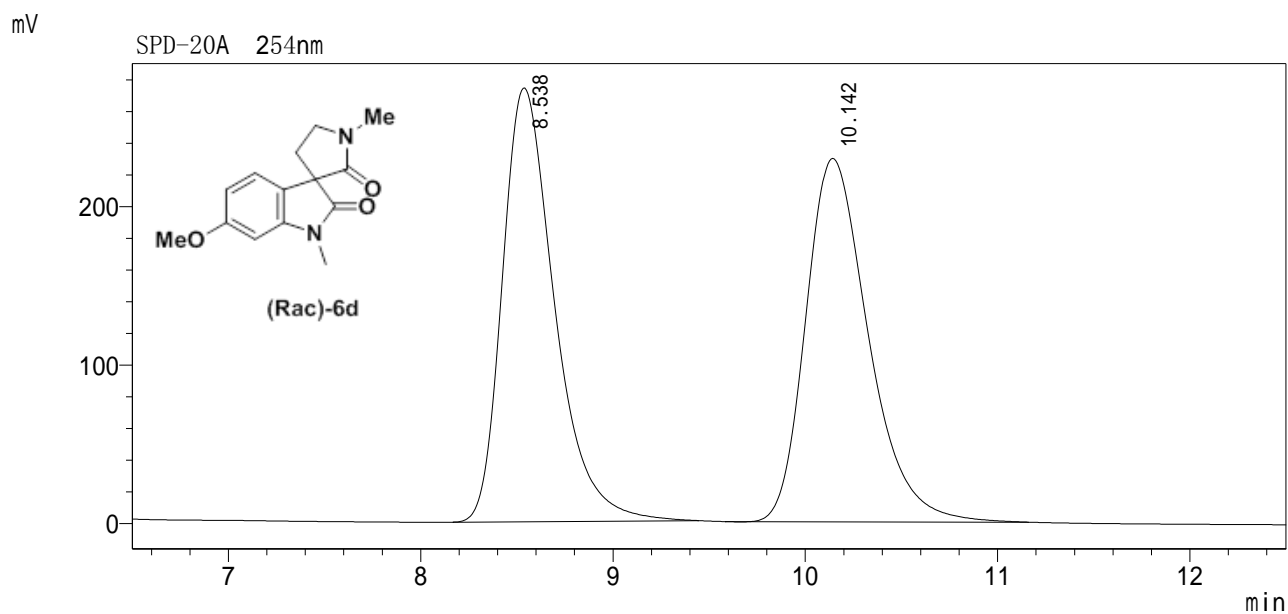
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	11.589	53714615	1981085	99.474		M
2	16.613	283802	8510	0.526		M
Sum		53998416	1989595			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-10Me-rac-604010ojh230  
 Data name : zw-19-10Me-rac-604010ojh230.lcd  
 Acq. method : OJ-H-40%.lcm  
 Location : 1-1  
 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/6/27 15:15:43  
 Analyst : System Administrator  
 Pro. Data : 2020/6/27 15:29:48  
 Processor : System Administrator



SPD-20A

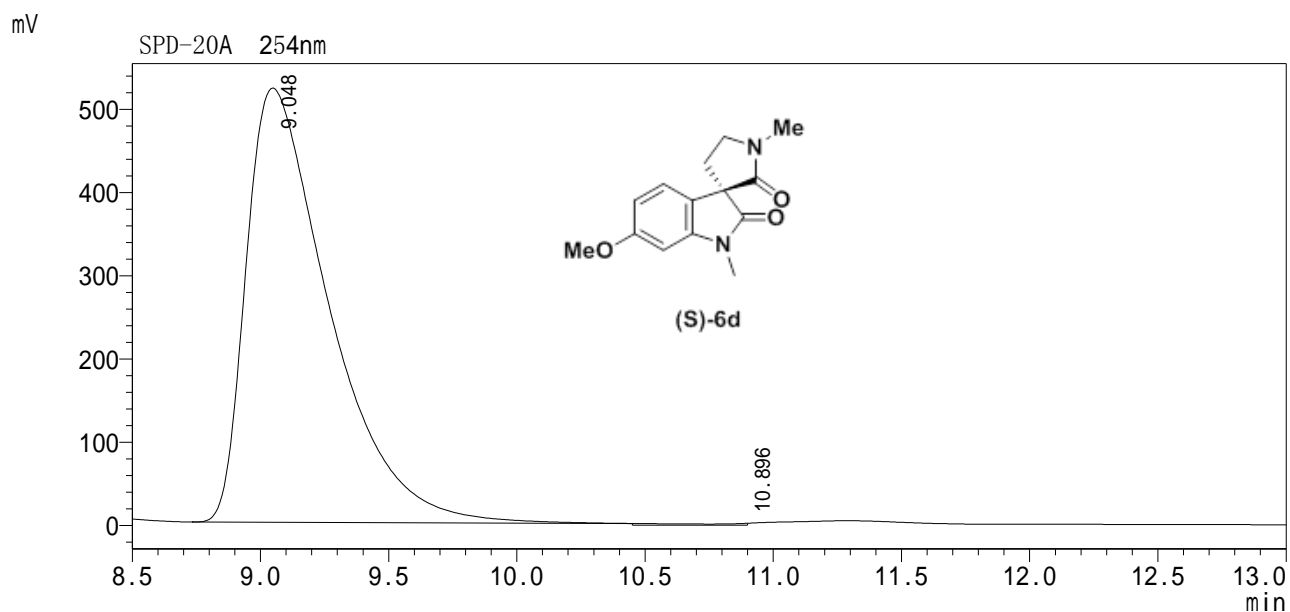
Entry	RT[min]	Area	Height	Area%			
1	8.538	5163324	273756	49.967		M	
2	10.142	5170236	229388	50.033		M	
Sum		10333559	503143				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD154jn100%TMS  
 Data name : MHWD154jn100%TMS-OJ-H-40%.lcd  
 Acq. METHOD : OJ-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/4 22:26:13  
 Pro. Data : 2021/1/4 23:04:32

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



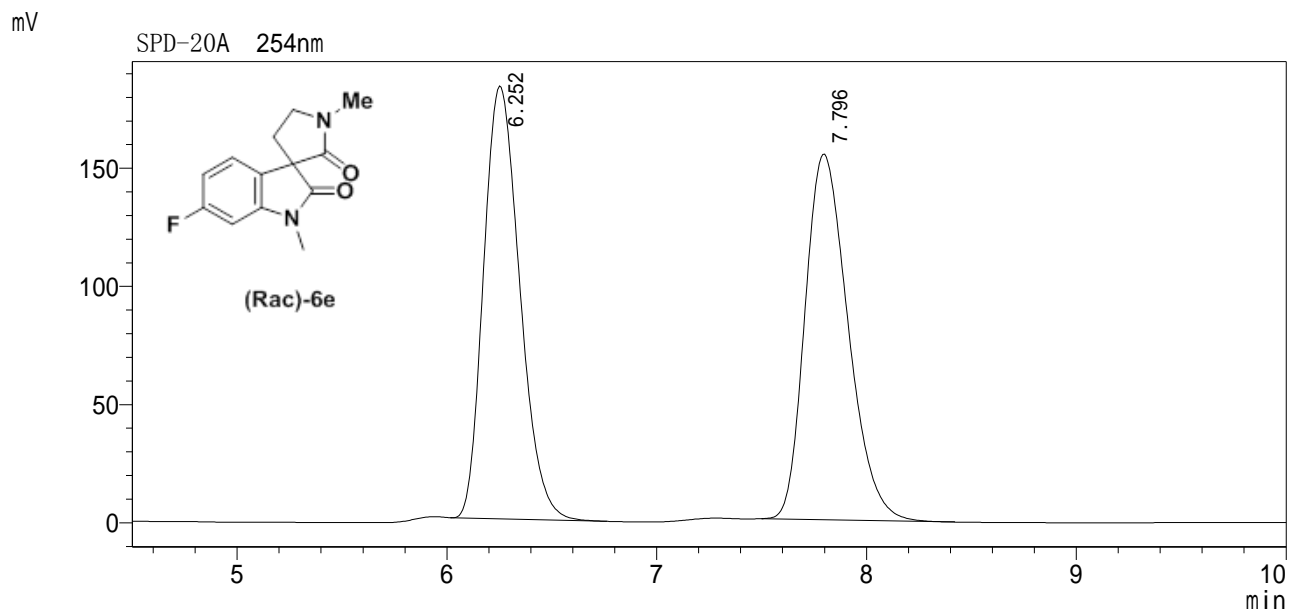
SPD-20A

Entr	RT[min]	Area	Height	Area%			
1	9.048	11758813	522194	99.594		M	
2	10.896	47972	2348	0.406		M	
Sum		11806785	524542				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-l-Frac-adh-703010  
 Data name : zw-19-l-Frac-adh-703010.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/22 14:14:22  
 Pro. Data : 2020/6/22 14:25:27  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

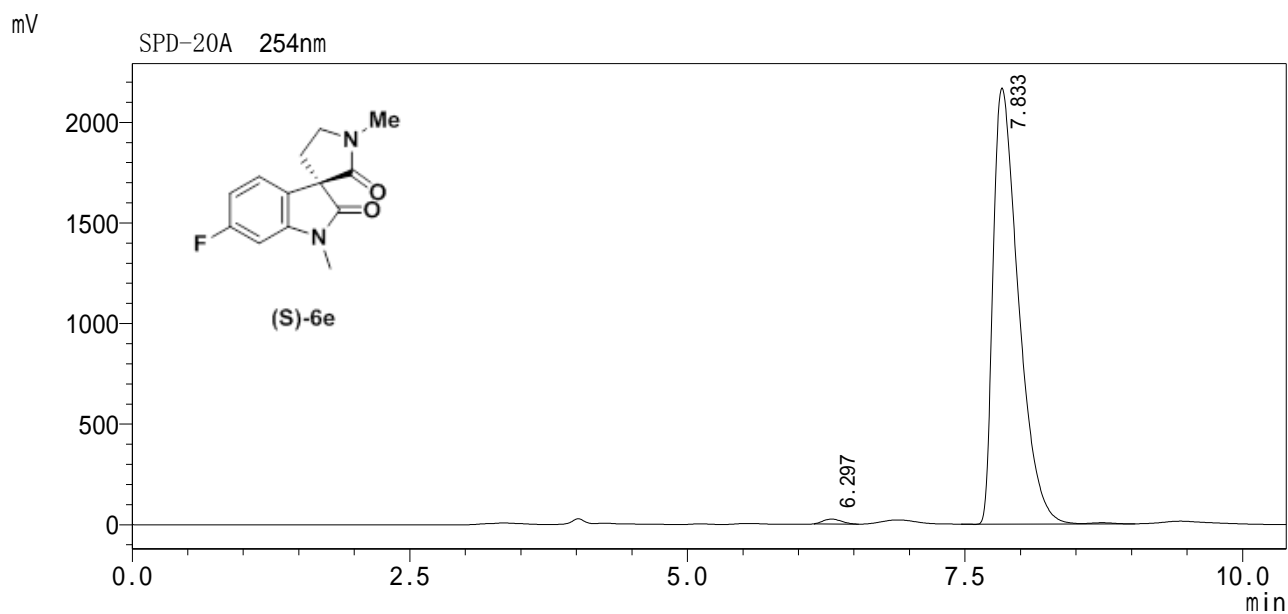
Entry	RT[min]	Area	Height	Area%		
1	6.252	2197392	183170	49.903		M
2	7.796	2205902	154619	50.097		M
Sum		4403294	337790			




**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWD155jn100%TMS  
 Data name : MHWD155jn100%TMS-AD-H-30%.lcd  
 Acq. method : AD-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/4 19:04:28  
 Pro. Data : 2021/1/4 23:04:42  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

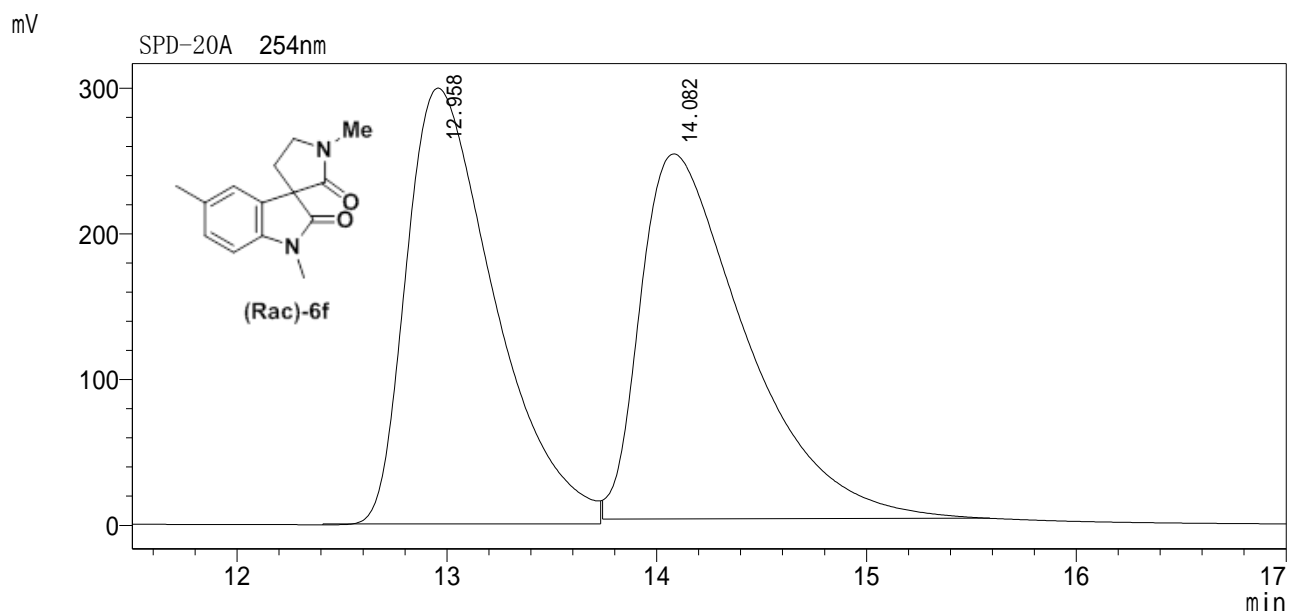
Entry	RT[min]	Area	Height	Area%		
1	6.297	272814	24028	0.784		M
2	7.833	34543012	2167969	99.216		M
Sum		34815826	2191997			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-119-1-ojh802008  
 Data name : zw-19-119-1-ojh802008.lcd  
 Acq. method : OJ-H-40%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/16 14:29:55  
 Pro. Data : 2020/6/16 14:49:23

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



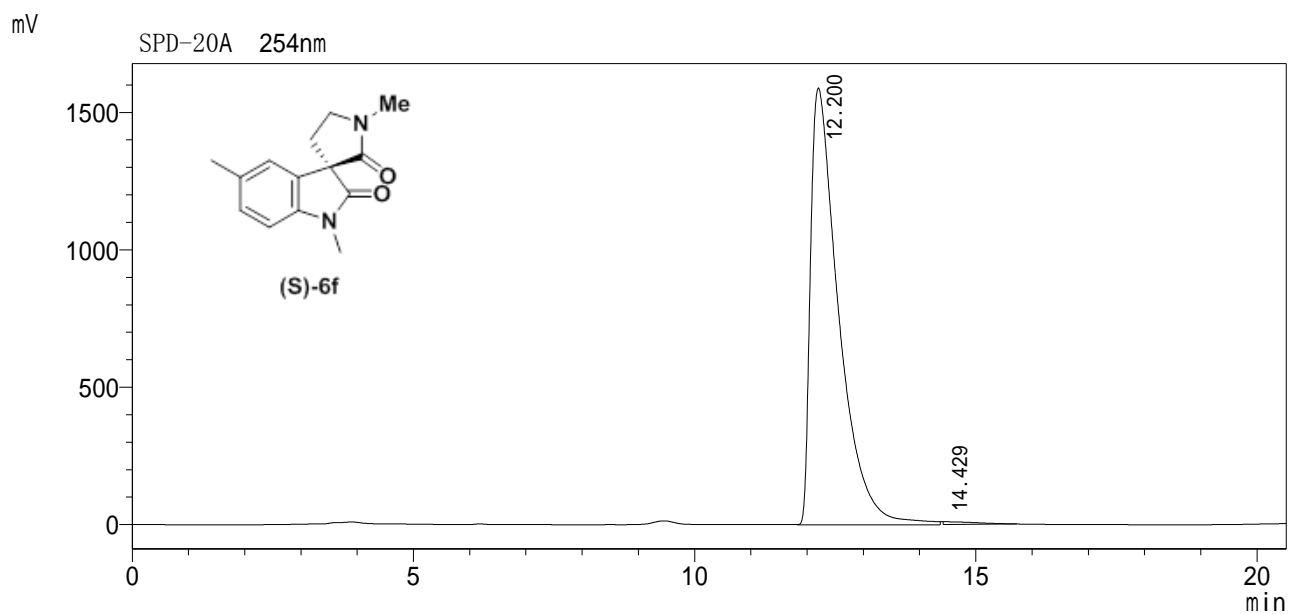
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	12.958	8744390	299104	49.872		M	
2	14.082	8789208	250604	50.128		M	
Sum		17533598	549708				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF011-2  
 Data name : MHWF011-2-OJ-H-20%.lcd  
 Acq. method : OJ-H-20%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/10 19:17:59  
 Pro. Data : 2021/1/10 19:44:16  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



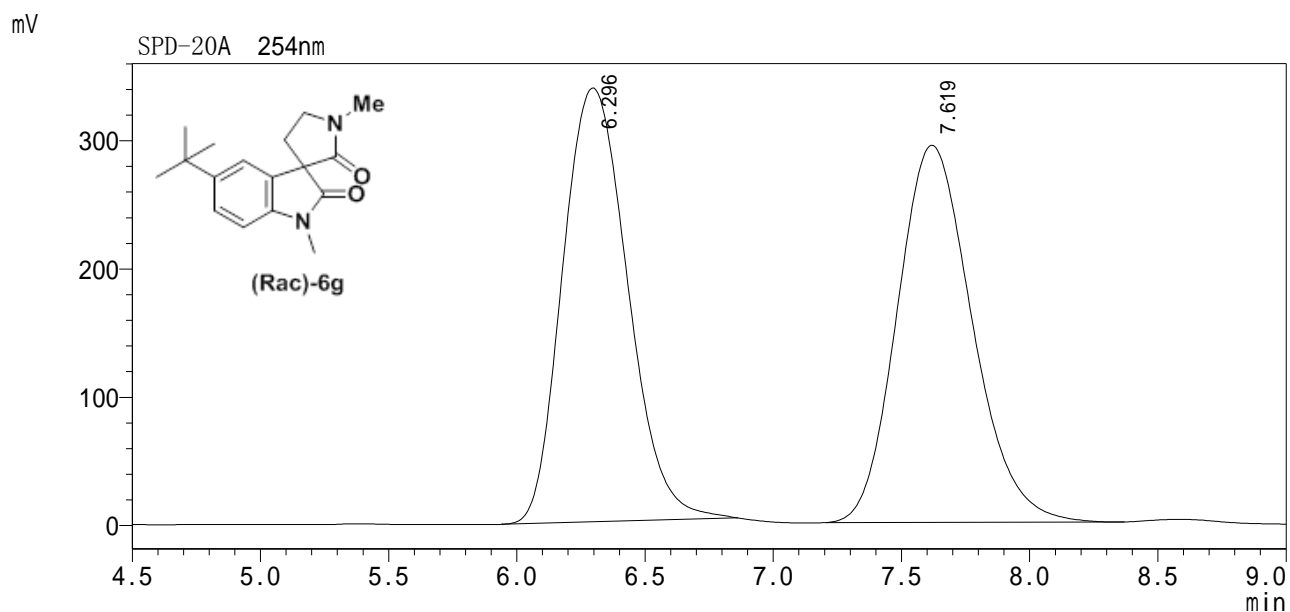
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	12.200	55330483	1589269	99.250		M
2	14.429	418297	10595	0.750		M
Sum		55748780	1599864			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-107-1-ash-802010  
 Data name : zw-19-107-1-ash-802010.lcd  
 Acq. method : AS-H-60%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/6 16:26:21  
 Pro. Data : 2020/6/6 16:38:21  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



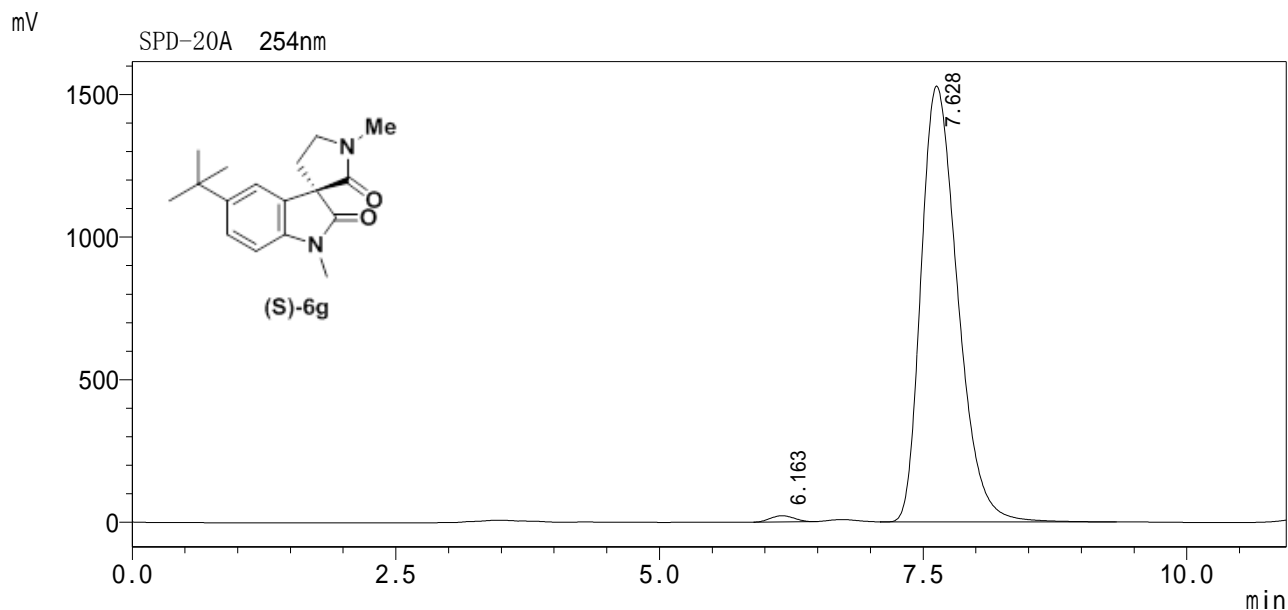
SPD-20A

Entry	RT[min]	Area	Height	Area%			
1	6.296	5972383	338212	50.000		M	
2	7.619	5972489	294138	50.000		M	
Sum		11944872	632350				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF002-1  
 Data Name : MHWF002-1-AS-H-20%.lcd  
 Acq. Method : AS-H-20%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/6 17:01:32  
 Pro. Data : 2021/1/6 17:15:36  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



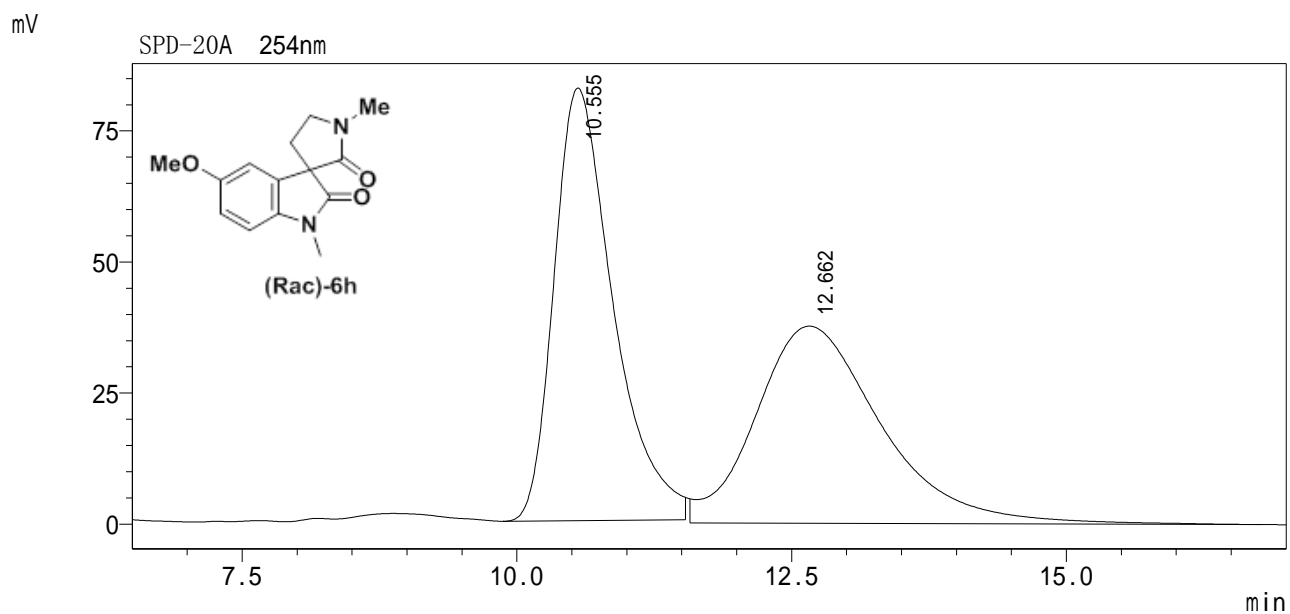
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	6.163	338184	21617	0.908		M
2	7.628	36890263	1528275	99.092		M
Sum		37228447	1549892			


**SHIMADZU**  
**LabSolutions** HPLC Report

## &lt;Sample information&gt;

Sample name : zw-19-110-11-ojh-703010  
 Data name : zw-19-110-11-ojh-703010.lcd  
 Acq. method : AS-H-60%.lcm  
 Location : 1-1  
 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/6/9 11:35:42 Analyst : System Administrator  
 Pro. Data : 2020/6/9 12:13:03 Processor : System Administrator



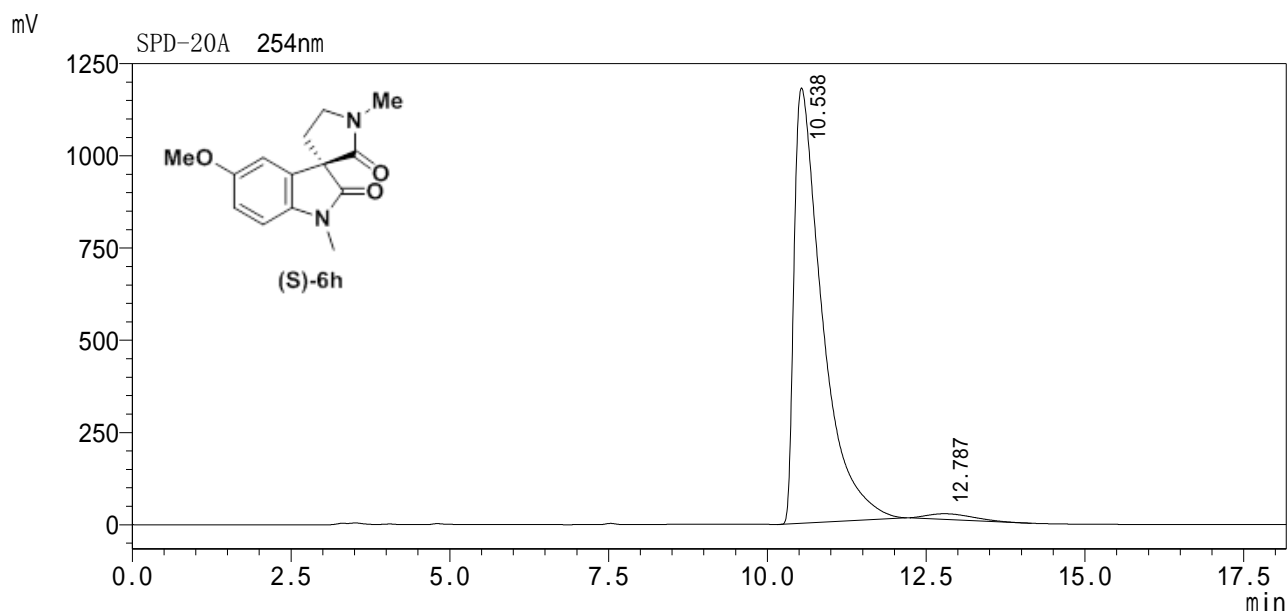
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.555	3082599	82516	50.695		M
2	12.662	2998110	37630	49.305		M
Sum		6080709	120146			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF015jn100%CH3-1  
 Data name : MHWF015jn100%CH3-1-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/14 16:27:39  
 Pro. Data : 2021/1/14 17:07:40  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.538	36454406	1179624	97.962		M
2	12.787	758448	15047	2.038		M
Sum		37212854	1194671			

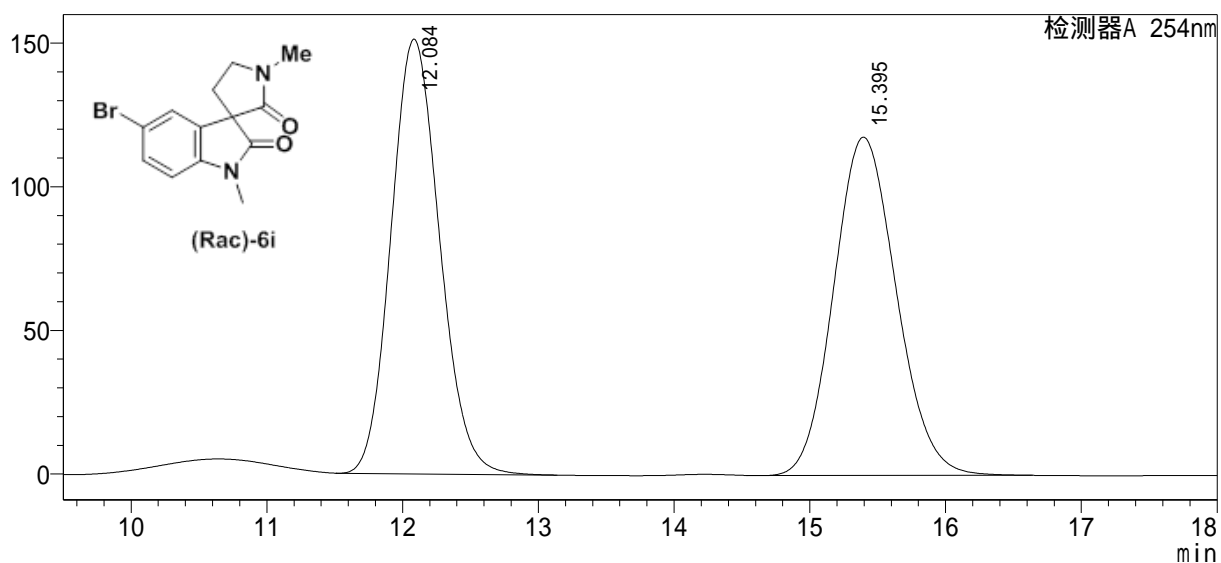

**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-109-11-ash-703010  
 Data name : zw-19-109-11-ash-703010.lcd  
 Acq. method : AS-H-60%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/8 14:14:24  
 Pro. Data : 2020/6/8 14:33:30  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator

## &lt;色谱图&gt;

mV



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	12.084	3765937	151382	49.948		M
2	15.395	3773711	117770	50.052		M
Sum		7539648	269151			

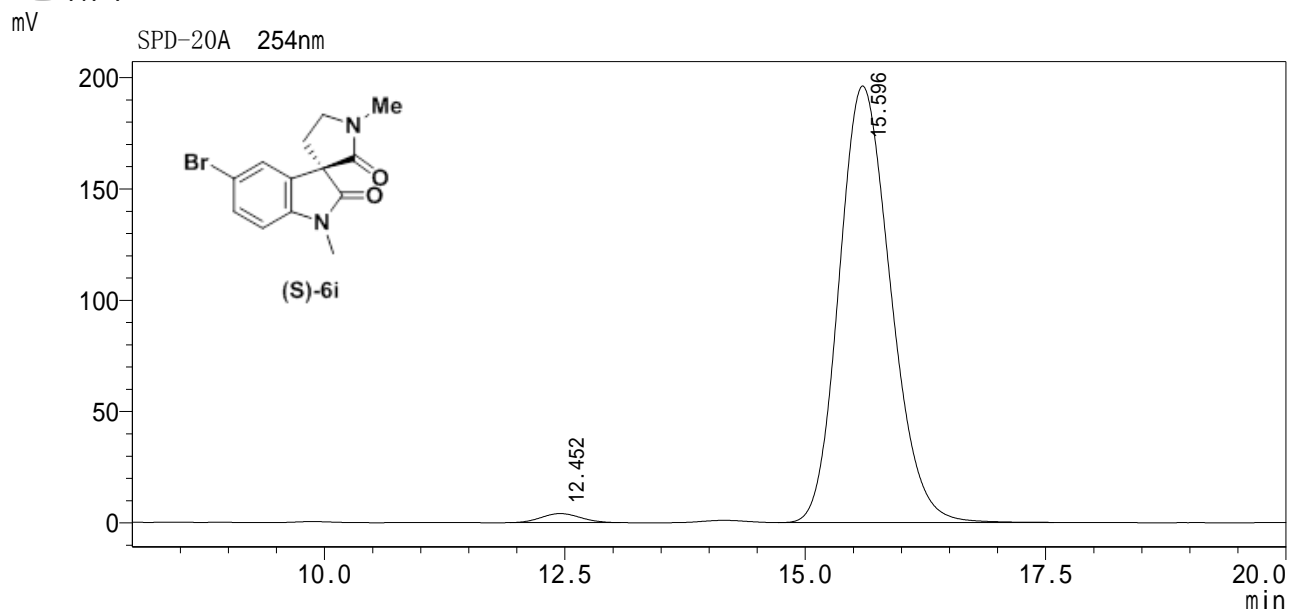



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF016-1  
 Data name : MHWF016-1-AS-H-30%.lcd  
 Acq. method : AS-H-30%-100min.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/14 15:29:33  
 Pro. Data : 2021/1/14 15:52:16  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator

## &lt;色谱图&gt;



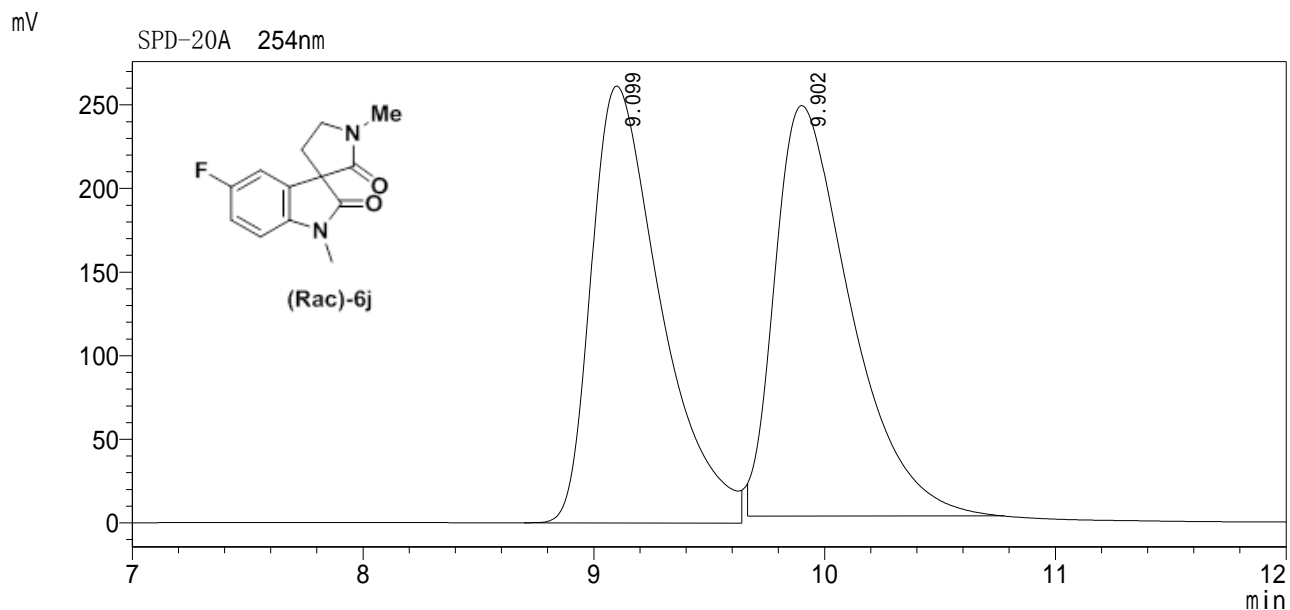
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	12.452	115536	4064	1.559		M
2	15.596	7296987	196093	98.441		
Sum		7412522	200156			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-116-1-ojh-703010.lcd  
 Data name : zw-19-116-1-ojh-703010.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/12 19:17:12  
 Pro. Data : 2020/6/12 19:31:15  
 Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

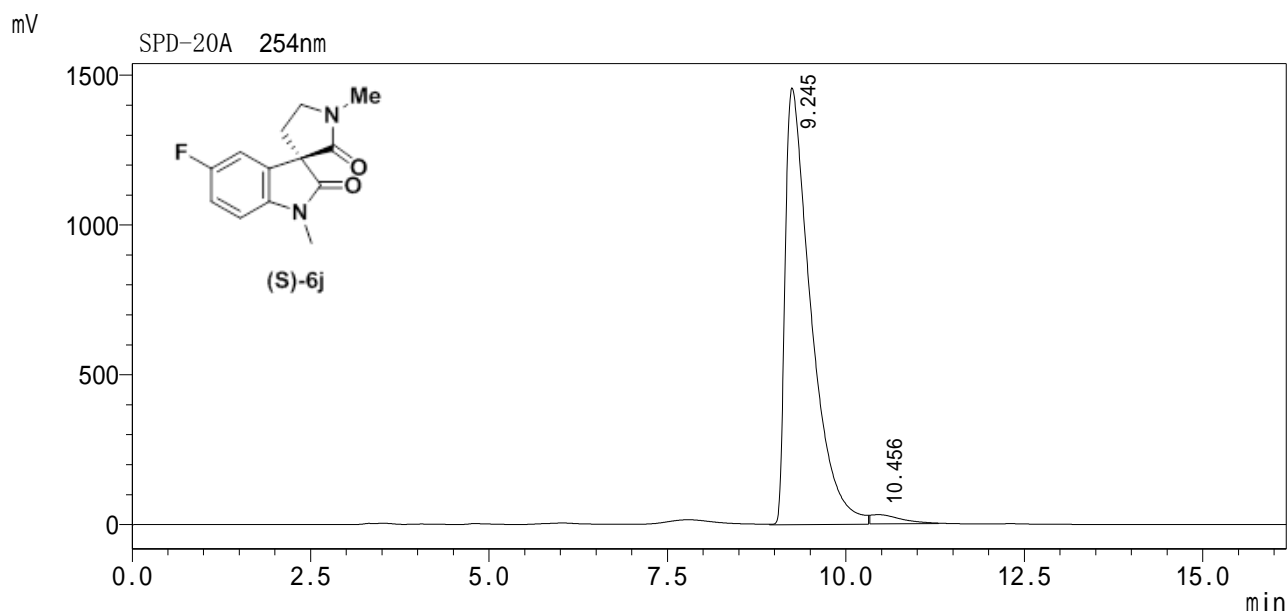
Entry	RT [min]	Area	Height	Area%	Area%		
1	9.099	5442681	261269	49.279		M	
2	9.902	5601948	245550	50.721		M	
Sum		11044629	506820				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF017jn100%ch3  
 Data name : MHWF017jn100%ch3-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2021/1/15 14:47:50  
 Pro. Data : 2021/1/15 15:16:00

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



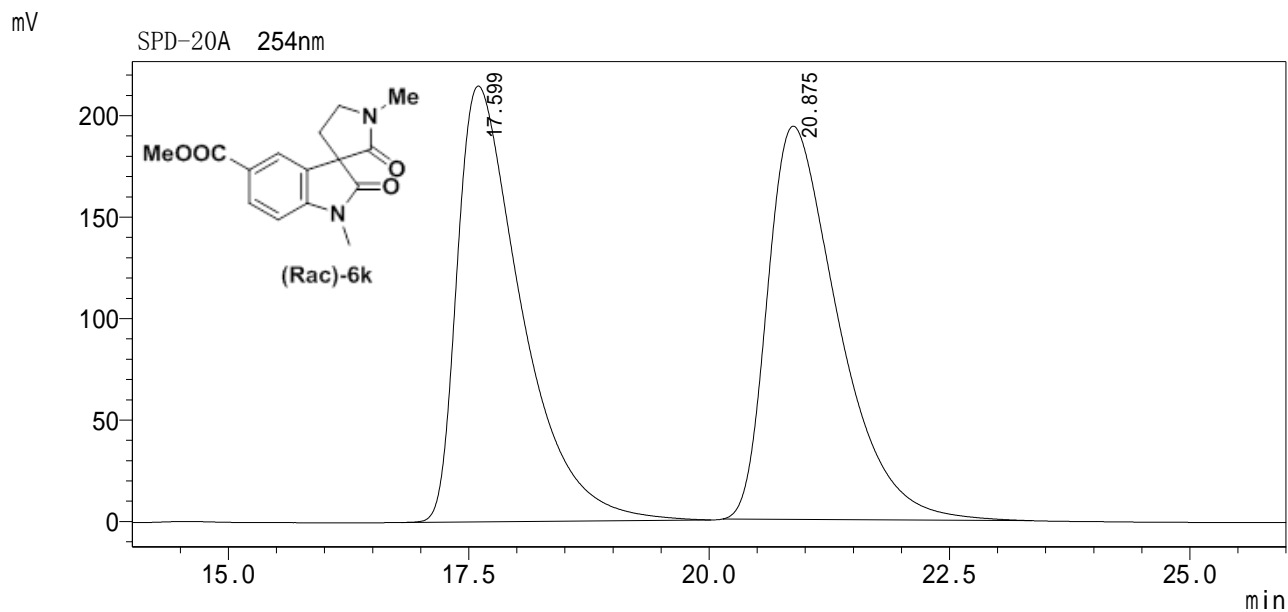
SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	9.245	36519634	1457293	97.650		M
2	10.456	878967	30149	2.350		M
Sum		37398602	1487442			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-140-1-OJH703010  
 Data name : zw-19-140-1-OJH703010.lcd  
 Acq. method : OJ-H-40%.lcm  
 Location : 1-1  
 Sample Type : unknown  
 : 1 uL  
 Ana. Data : 2020/7/9 15:54:19  
 Analyst : System Administrator  
 Pro. Data : 2020/7/9 16:20:59  
 Processor : System Administrator



SPD-20A

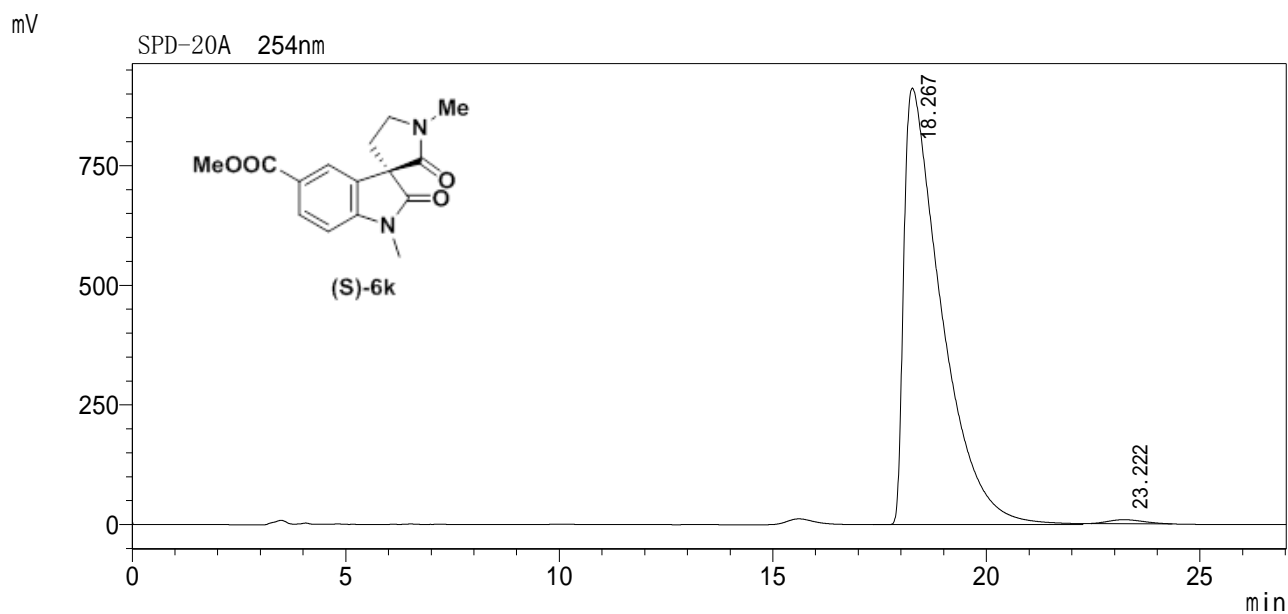
Entry	RT[min]	Area	Height	Area%			
1	17.599	9948133	214800	50.104		M	
2	20.875	9906798	193833	49.896		M	
Sum		19854932	408633				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : MHWF001  
 Data name : MHWF001-OJ-H-30%.lcd  
 Acq. Method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1  $\mu$ L  
 Ana. Data : 2021/1/6 15:52:11  
 Pro. Data : 2021/1/6 16:53:11

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

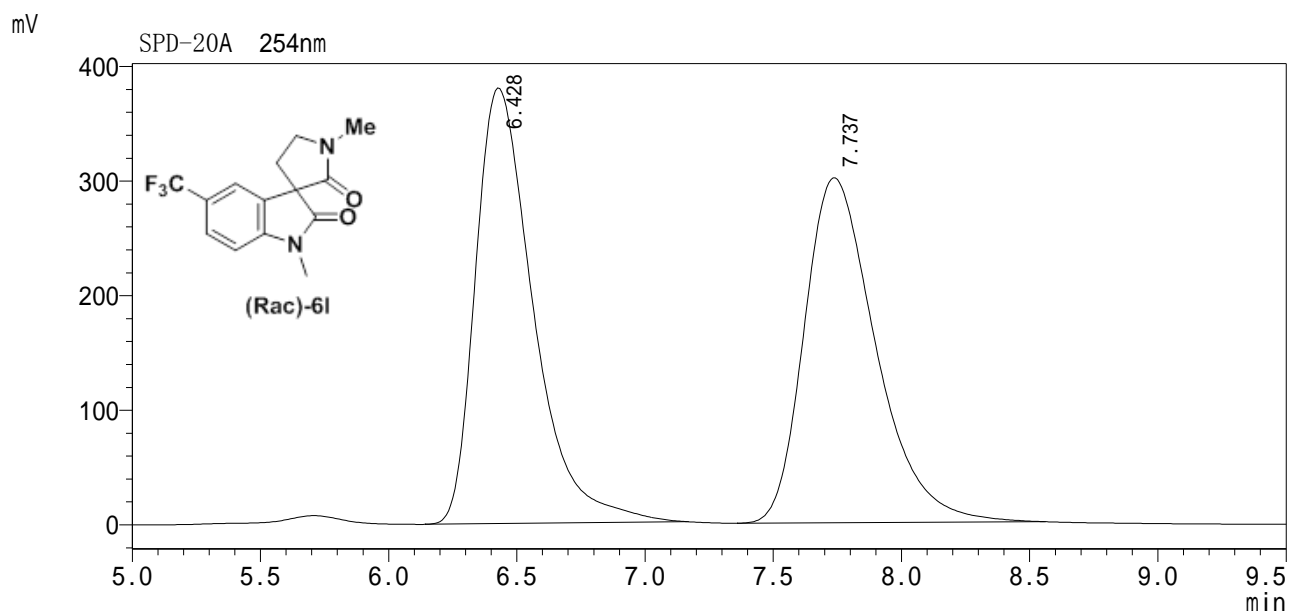
Entry	RT[min]	Area	Height	Area%			
1	18.267	55748171	912326	99.180		M	
2	23.222	461177	8273	0.820		M	
Sum		56209348	920599				


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-113-1-ojh-703010  
 Data name : zw-19-113-1-ojh-703010.lcd  
 Acq. method : OJ-H-30%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/6/10 10:00:55  
 Pro. Data : 2020/6/11 9:41:00

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



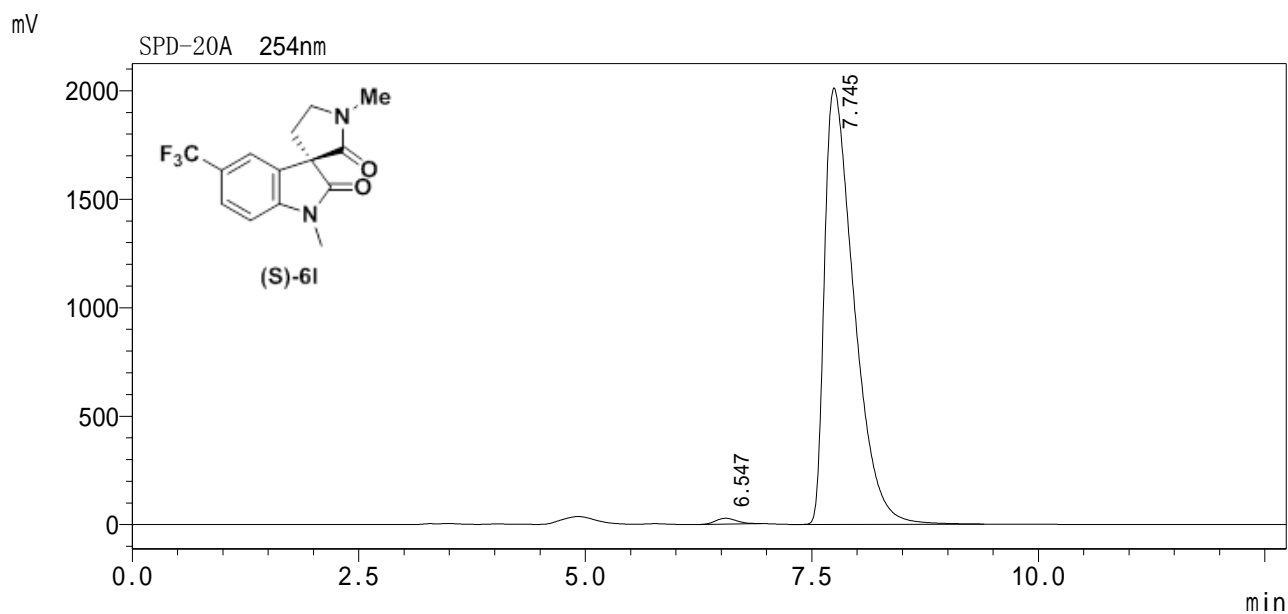
SPD-20A

Entry	RT [min]	Area	Height	Area%		
1	6.428	5964259	380172	50.540		M
2	7.737	5836891	301044	49.460		M
Sum		11801150	681215			


**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Data name : MHWF019jn100%CH3  
 :  
 Data name : MHWF019jn100%CH3-OJ-H-30%.lcd  
 Acq. method : OJ-H-30%.lcm  
 :  
 Location : 1-1 Sample Type : unknown  
 : 1  $\mu$ L  
 Ana. Data : 2021/1/16 15:37:55 Analyst : System Administrator  
 Pro. Data : 2021/1/16 21:57:11 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	6.547	428118	26678	0.934		M
2	7.745	45404688	2011179	99.066		M
Sum		45832806	2037857			



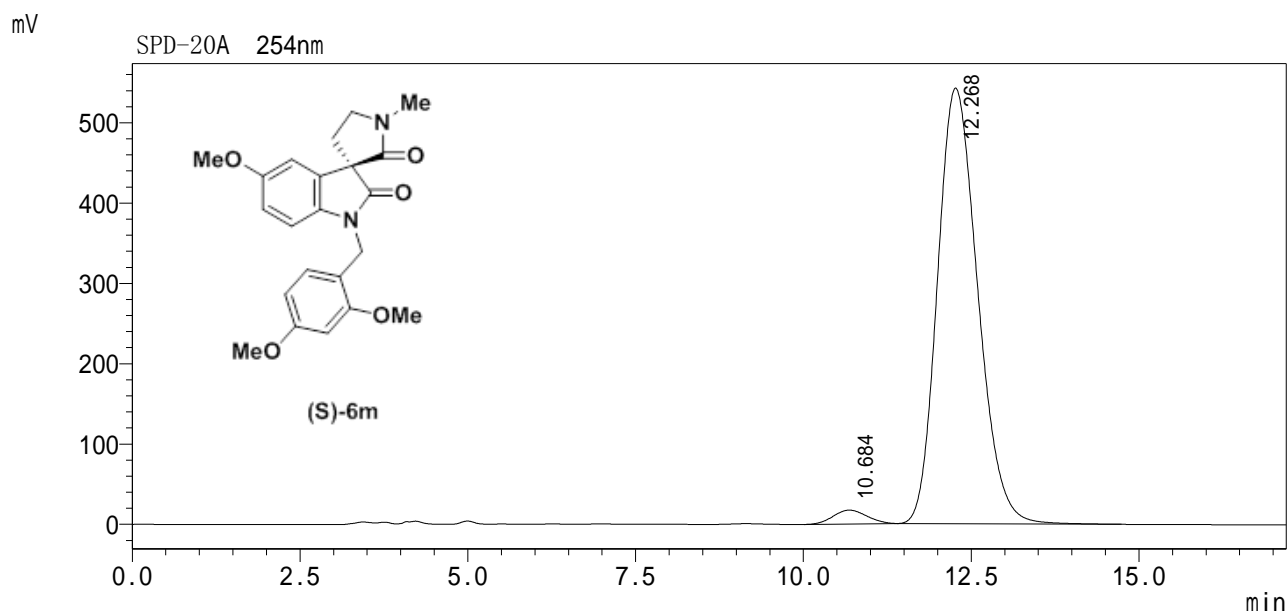



**SHIMADZU**  
**LabSolutions HPLC Report**

## &lt;Sample information&gt;

Sample name : zw-19-147-2-ash703010  
 Data name : zw-19-147-2-ash703010.lcd  
 Acq. method : OD-H-80%.lcm  
 Location : 1-1  
 : 1 uL  
 Ana. Data : 2020/7/17 15:27:34  
 Pro. Data : 2020/11/25 10:40:01

Sample Type : unknown  
 Analyst : System Administrator  
 Processor : System Administrator



SPD-20A

Entry	RT[min]	Area	Height	Area%		
1	10.684	599755	17257	2.585		M
2	12.268	22603051	542503	97.415		M
Sum		23202805	559759			